



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:57 PM EDT

PDB ID : 1VF5 / pdb_00001vf5
Title : Crystal Structure of Cytochrome b6f Complex from M.laminosus
Authors : Kurisu, G.; Zhang, H.; Smith, J.L.; Cramer, W.A.
Deposited on : 2004-04-08
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

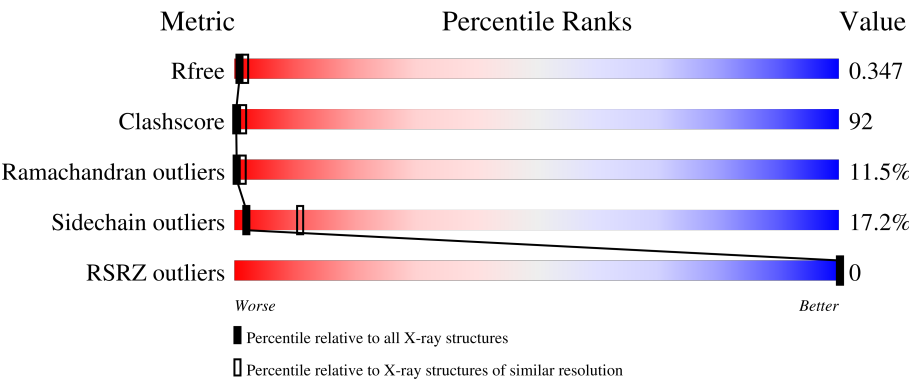
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



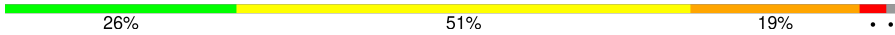
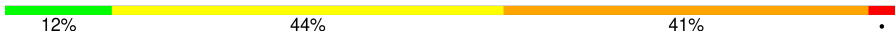
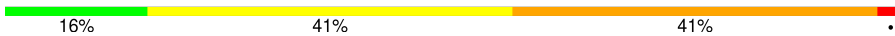
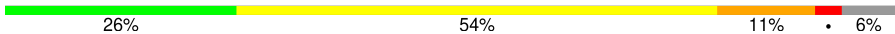
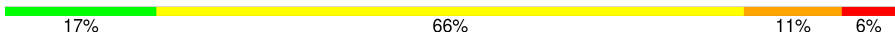
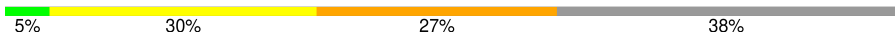
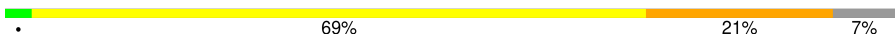
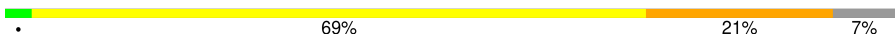
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	32%43%13%6%6%
1	N	215	31%45%14%6%
2	B	160	16%39%21%10%14%
2	O	160	12%41%25%8%14%
3	C	289	25%53%18%..

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Mol	Chain	Length	Quality of chain
3	P	289	
4	D	179	
4	Q	179	
5	E	32	
5	R	32	
6	F	35	
6	S	35	
7	G	37	
7	T	37	
8	H	29	
8	U	29	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	HEC	A	303	X	-	-	-
10	HEC	C	301	X	-	-	-
10	HEC	N	303	X	-	-	-
10	HEC	P	301	X	-	-	-
12	PL9	Q	1305	-	-	X	-
13	OPC	D	306	-	-	X	-
13	OPC	Q	1307	-	-	X	-
14	CLA	B	201	X	-	-	-
14	CLA	O	1201	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 15091 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			
1	N	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			

- Molecule 2 is a protein called SUBUNIT IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1075	727	165	178	5			
2	O	138	Total	C	N	O	S	0	0	0
			1075	727	165	178	5			

- Molecule 3 is a protein called CYTOCHROME F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			
3	P	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			

- Molecule 4 is a protein called RIESKE IRON-SULFUR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			
4	Q	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			

- Molecule 5 is a protein called PROTEIN PET L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			
5	R	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			

- Molecule 6 is a protein called PROTEIN PET M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			251	170	36	43	2			
6	S	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			

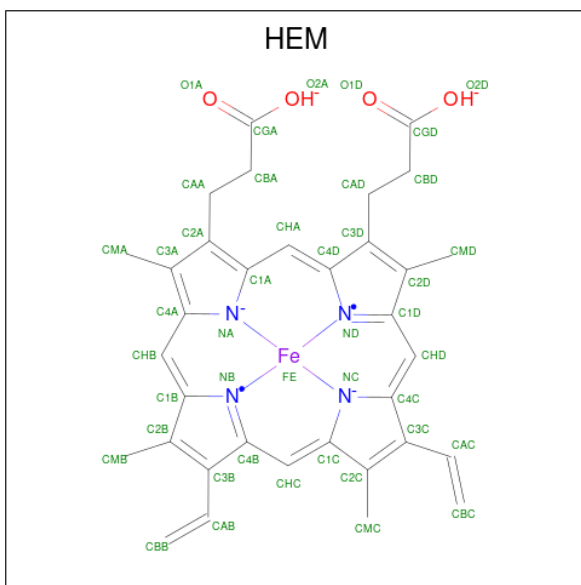
- Molecule 7 is a protein called PROTEIN PET G.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	23	Total	C	N	O	0	0	0
			184	126	29	29			
7	T	27	Total	C	N	O	0	0	0
			216	146	34	36			

- Molecule 8 is a protein called PROTEIN PET N.

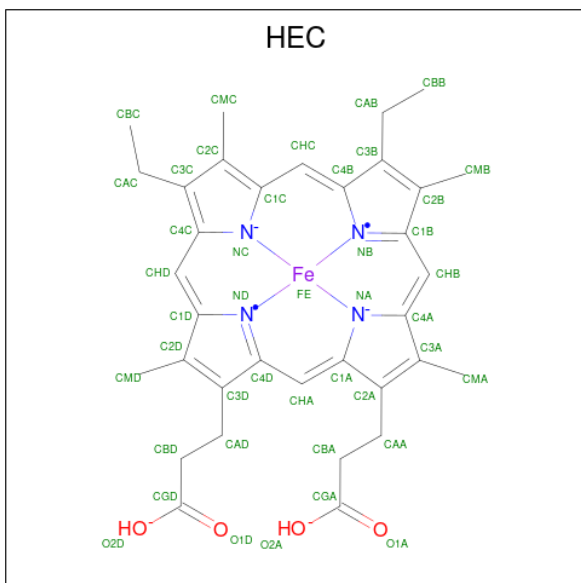
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			
8	U	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



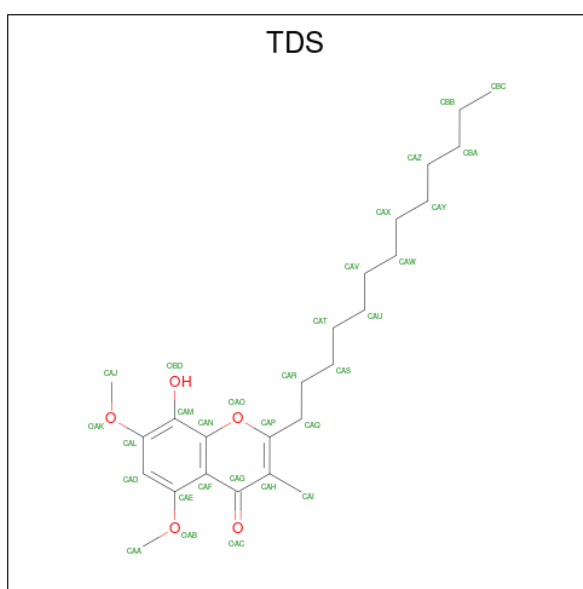
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 10 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



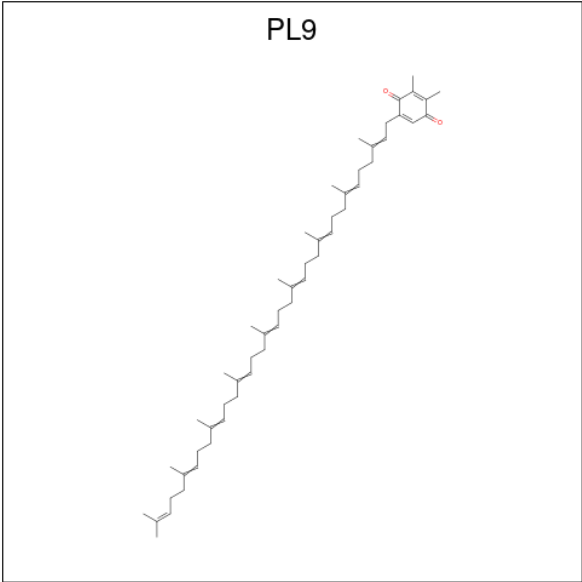
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	N	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 11 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (CCD ID: TDS) (formula: C₂₅H₃₈O₅).



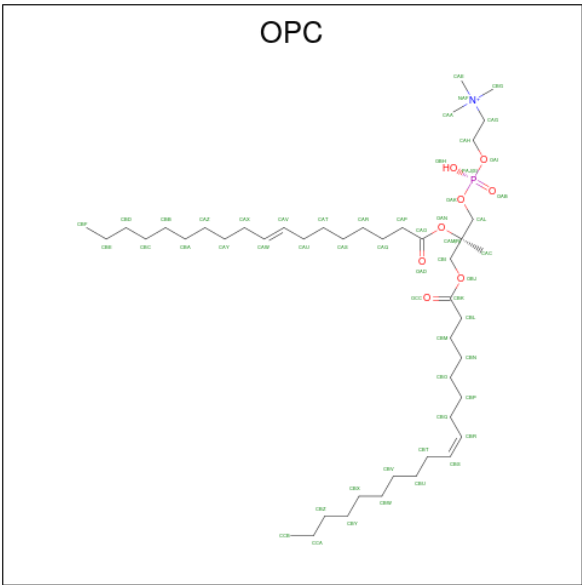
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			30	25	5		
11	N	1	Total	C	O	0	0
			30	25	5		

- Molecule 12 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			55	53	2		
12	Q	1	Total	C	O	0	0
			55	53	2		

- Molecule 13 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: C₄₅H₈₇NO₈P).



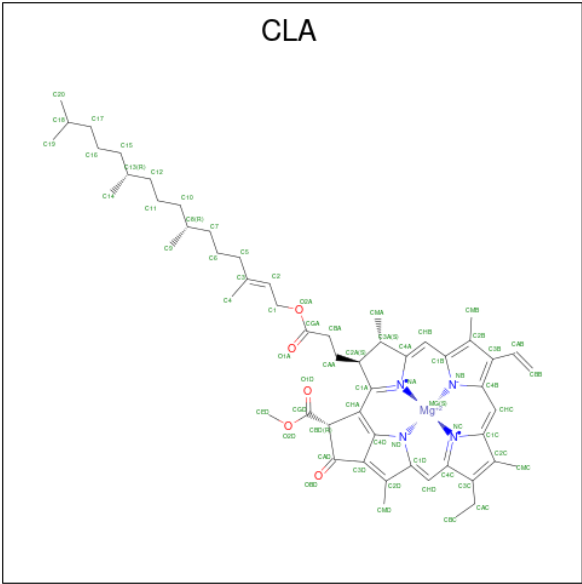
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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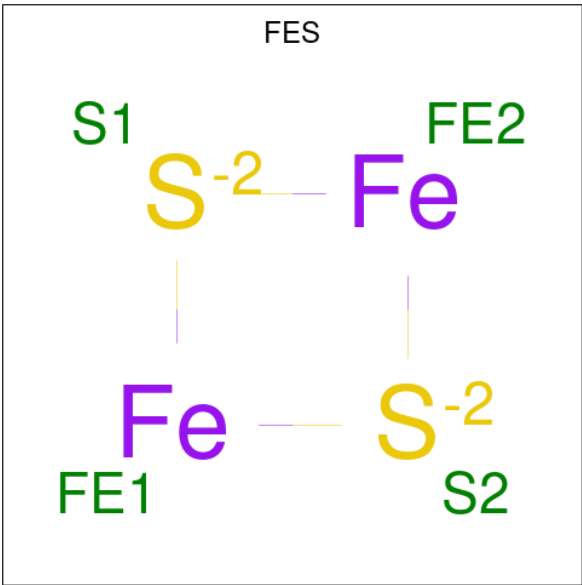
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	D	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
13	N	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
13	Q	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



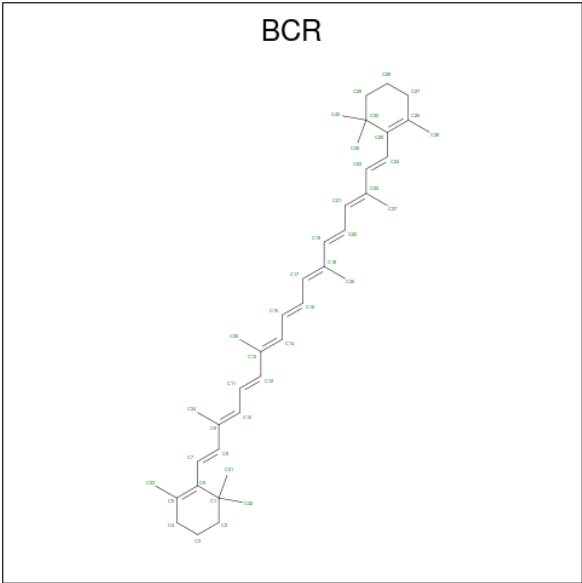
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
14	O	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	Fe	S	0	0
			4	2	2		
15	Q	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	E	1	Total	C	0	0
			40	40		
16	R	1	Total	C	0	0
			40	40		

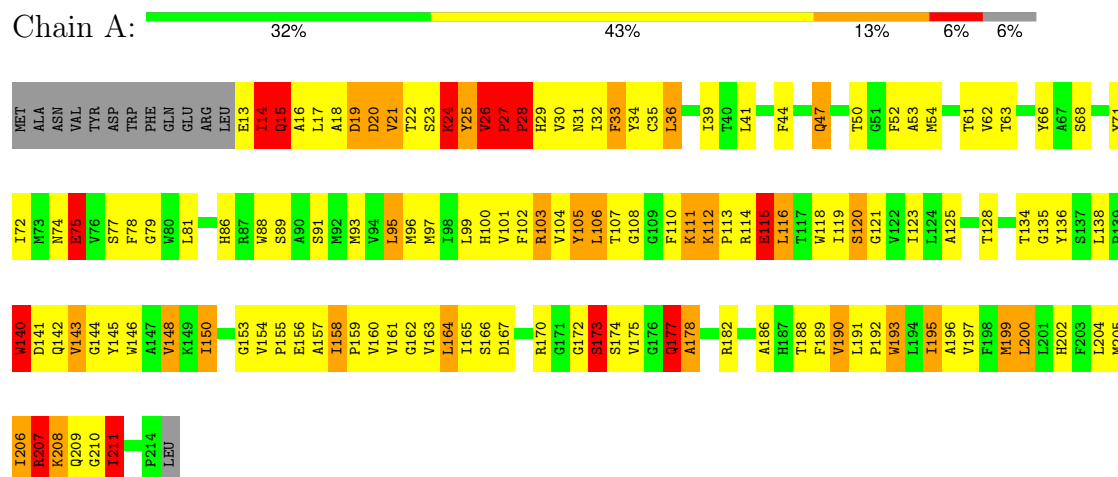
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	O	0	0
			1	1		
17	N	1	Total	O	0	0
			1	1		

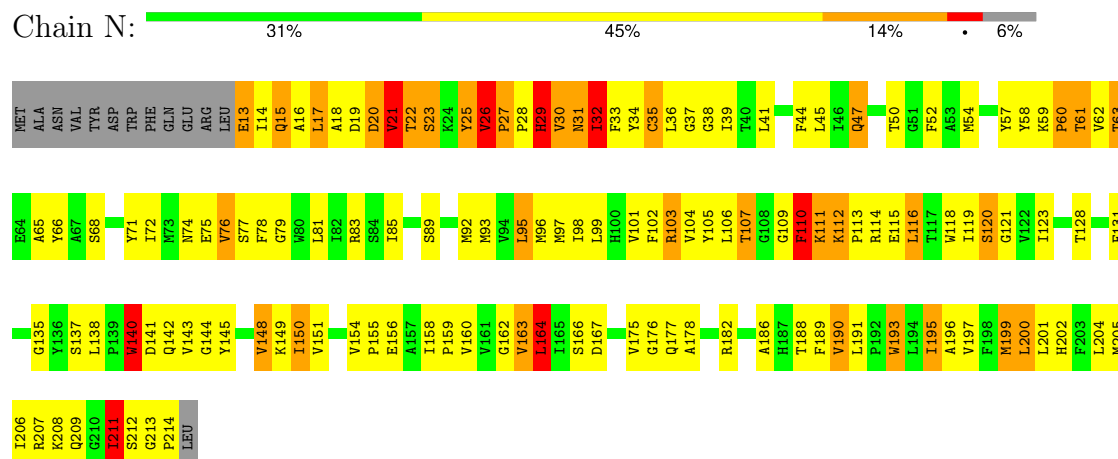
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

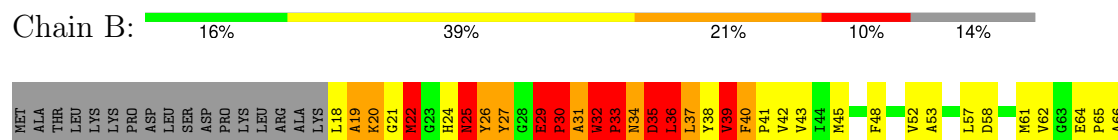
• Molecule 1: CYTOCHROME B6

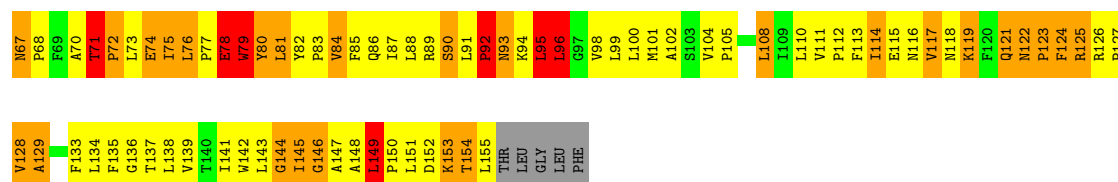


• Molecule 1: CYTOCHROME B6

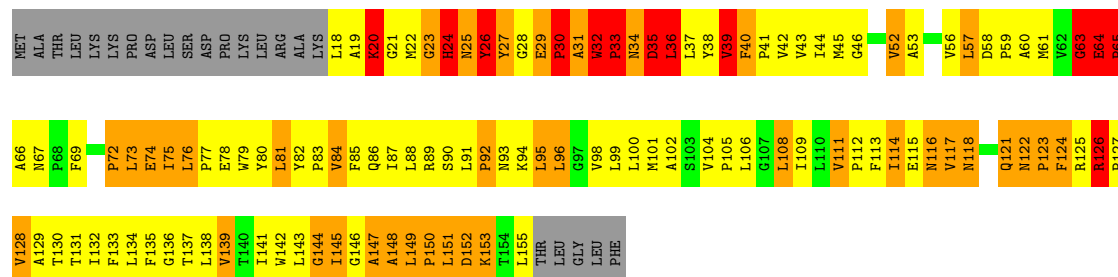


• Molecule 2: SUBUNIT IV

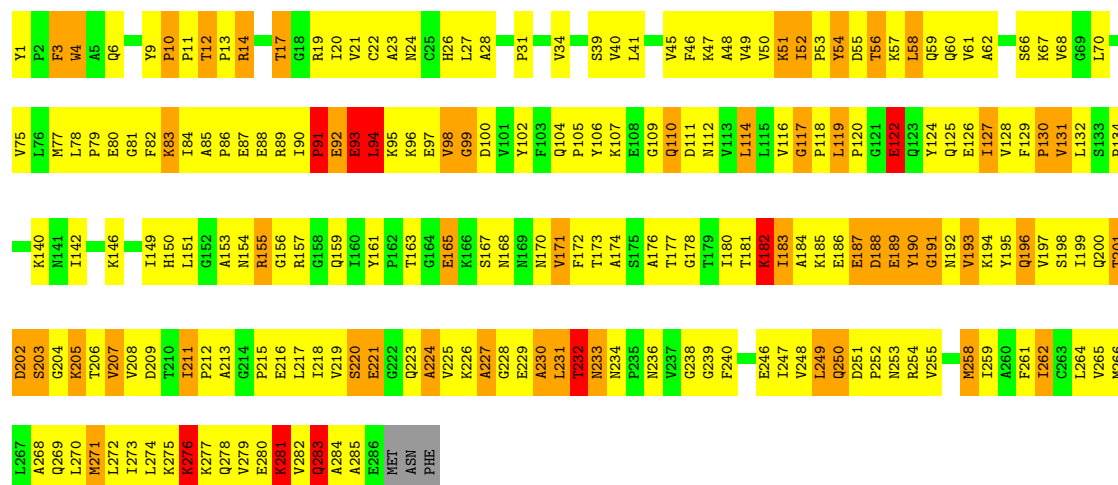




• Molecule 2: SUBUNIT IV

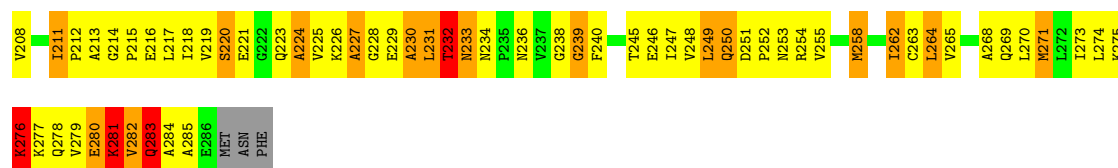


• Molecule 3: CYTOCHROME F



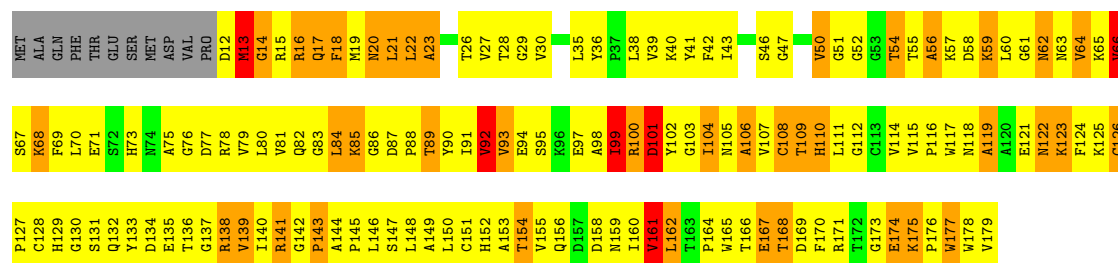
• Molecule 3: CYTOCHROME F





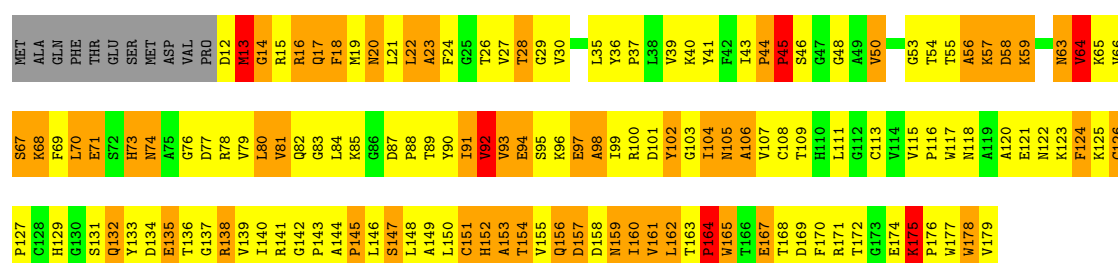
• Molecule 4: RIESKE IRON-SULFUR PROTEIN

Chain D: 11% 57% 22% 6%



• Molecule 4: RIESKE IRON-SULFUR PROTEIN

Chain Q: 14% 47% 29% 6%



• Molecule 5: PROTEIN PET L

Chain E: 12% 44% 41%



• Molecule 5: PROTEIN PET L

Chain R: 16% 41% 41%

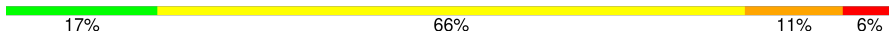


• Molecule 6: PROTEIN PET M

Chain F: 26% 54% 11% 6%

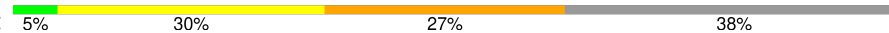


- Molecule 6: PROTEIN PET M

Chain S:  17% 66% 11% 6%



- Molecule 7: PROTEIN PET G

Chain G:  5% 30% 27% 38%

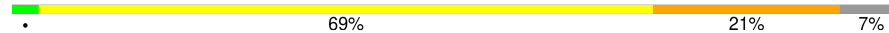


- Molecule 7: PROTEIN PET G

Chain T:  8% 30% 32% 27%



- Molecule 8: PROTEIN PET N

Chain H:  69% 21% 7%



- Molecule 8: PROTEIN PET N

Chain U:  69% 21% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	157.54Å 157.54Å 360.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 – 3.00 48.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.16-3.00) 99.8 (48.16-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.258 , 0.346 0.259 , 0.347	Depositor DCC
R_{free} test set	2788 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 141.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15091	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, HEC, TDS, OPC, CLA, FES, BCR, PL9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	0/1641	1.28	20/2239 (0.9%)
1	N	0.75	0/1641	1.23	24/2239 (1.1%)
2	B	0.67	0/1110	1.49	28/1526 (1.8%)
2	O	0.77	1/1110 (0.1%)	1.52	30/1526 (2.0%)
3	C	0.54	0/2248	1.13	22/3061 (0.7%)
3	P	0.55	0/2248	1.10	22/3061 (0.7%)
4	D	0.63	0/1312	1.30	25/1786 (1.4%)
4	Q	0.65	0/1312	1.23	21/1786 (1.2%)
5	E	0.78	0/253	1.20	3/340 (0.9%)
5	R	0.79	0/253	1.22	4/340 (1.2%)
6	F	0.64	0/255	1.02	3/343 (0.9%)
6	S	0.59	0/274	0.98	2/366 (0.5%)
7	G	0.71	0/188	1.42	3/253 (1.2%)
7	T	0.71	0/221	1.45	6/299 (2.0%)
8	H	0.76	0/220	1.59	6/301 (2.0%)
8	U	0.71	0/220	1.51	5/301 (1.7%)
All	All	0.66	1/14506 (0.0%)	1.26	224/19767 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	145	ILE	CA-CB	5.46	1.59	1.55

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	LEU	N-CA-C	-17.90	91.85	114.04
2	O	36	LEU	N-CA-C	-17.40	92.47	114.04
1	A	26	VAL	CA-C-N	15.65	136.50	120.38
1	A	26	VAL	C-N-CA	15.65	136.50	120.38
8	H	5	VAL	N-CA-C	-13.87	97.49	110.53
8	U	5	VAL	N-CA-C	-13.47	97.86	110.53
2	B	144	GLY	N-CA-C	-10.63	98.42	112.14
7	G	28	GLN	N-CA-C	-10.40	99.94	111.07
1	N	15	GLN	N-CA-C	-10.39	99.95	111.28
4	Q	44	PRO	CA-C-N	10.29	132.71	119.84
4	Q	44	PRO	C-N-CA	10.29	132.71	119.84
2	B	125	ARG	N-CA-C	-10.11	101.06	113.50
2	B	64	GLU	CA-C-N	10.06	130.68	119.92
2	B	64	GLU	C-N-CA	10.06	130.68	119.92
2	O	126	ARG	CA-C-N	10.01	130.16	119.05
2	O	126	ARG	C-N-CA	10.01	130.16	119.05
7	T	28	GLN	N-CA-C	-9.92	100.42	111.14
4	D	54	THR	N-CA-C	9.70	125.52	110.20
8	H	28	GLY	N-CA-C	-9.66	102.66	115.32
1	N	29	HIS	N-CA-C	9.59	125.59	111.02
1	A	27	PRO	N-CA-C	9.56	122.36	110.70
3	C	125	GLN	N-CA-C	-9.50	101.71	113.20
3	P	52	ILE	CA-C-N	9.32	129.26	120.03
3	P	52	ILE	C-N-CA	9.32	129.26	120.03
2	O	64	GLU	N-CA-C	9.08	129.88	109.81
3	P	125	GLN	N-CA-C	-8.88	102.46	113.20
3	C	52	ILE	CA-C-N	8.78	128.72	120.03
3	C	52	ILE	C-N-CA	8.78	128.72	120.03
4	Q	43	ILE	CA-C-N	8.74	129.38	120.38
4	Q	43	ILE	C-N-CA	8.74	129.38	120.38
8	H	4	ASP	N-CA-C	-8.71	100.66	112.94
1	A	27	PRO	CA-C-N	8.65	130.66	119.84
1	A	27	PRO	C-N-CA	8.65	130.66	119.84
4	D	21	LEU	N-CA-C	-8.54	103.39	113.21
1	A	199	MET	N-CA-C	-8.52	101.50	112.23
1	N	120	SER	N-CA-C	-8.43	102.01	111.71
1	N	207	ARG	N-CA-C	-8.40	100.36	110.44
1	A	178	ALA	N-CA-C	-8.39	102.09	111.82
3	P	10	PRO	N-CA-C	8.27	120.79	110.70
3	C	10	PRO	N-CA-C	8.13	120.61	110.70
1	N	20	ASP	N-CA-C	8.12	128.08	110.80
1	N	140	TRP	N-CA-C	8.11	122.33	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	18	ALA	N-CA-C	-8.07	98.33	109.71
1	N	199	MET	N-CA-C	-8.07	102.06	112.23
2	O	63	GLY	N-CA-C	8.06	132.29	113.18
8	U	4	ASP	N-CA-C	-7.87	101.29	113.02
4	D	112	GLY	N-CA-C	7.86	125.13	114.92
4	D	167	GLU	N-CA-C	7.83	121.95	110.59
1	A	164	LEU	N-CA-C	-7.80	102.85	111.36
2	B	67	ASN	CA-C-N	7.74	127.38	119.56
2	B	67	ASN	C-N-CA	7.74	127.38	119.56
2	O	31	ALA	N-CA-C	7.71	122.35	108.48
4	Q	68	LYS	N-CA-C	-7.69	103.74	113.43
1	A	120	SER	N-CA-C	-7.63	101.98	111.75
2	B	71	THR	CA-C-N	7.61	129.35	119.84
2	B	71	THR	C-N-CA	7.61	129.35	119.84
4	D	17	GLN	N-CA-C	-7.61	102.86	113.20
1	A	207	ARG	N-CA-C	-7.49	94.84	110.80
4	Q	17	GLN	N-CA-C	-7.48	103.02	113.20
2	O	69	PHE	N-CA-C	-7.48	104.16	113.28
1	A	208	LYS	N-CA-C	7.42	121.01	109.52
8	U	28	GLY	N-CA-C	-7.39	103.98	115.73
4	Q	154	THR	CB-CA-C	-7.29	105.90	116.54
5	R	16	PHE	N-CA-C	-7.28	102.38	111.11
1	A	33	PHE	N-CA-C	-7.26	104.55	113.19
2	O	64	GLU	CA-C-N	7.23	128.87	119.84
2	O	64	GLU	C-N-CA	7.23	128.87	119.84
2	O	117	VAL	N-CA-C	-7.21	94.34	109.34
5	E	22	ILE	N-CA-C	7.20	117.30	110.53
2	B	37	LEU	N-CA-C	-7.20	103.41	113.20
4	Q	80	LEU	N-CA-C	7.11	120.32	108.73
2	B	35	ASP	N-CA-C	7.09	125.89	110.80
1	A	31	ASN	N-CA-C	7.08	125.89	110.80
4	D	161	VAL	N-CA-C	7.08	118.54	107.28
1	N	23	SER	N-CA-C	-7.08	104.64	113.28
2	O	35	ASP	N-CA-C	7.06	125.84	110.80
2	B	117	VAL	N-CA-C	-6.89	106.42	113.10
4	Q	135	GLU	N-CA-C	-6.86	105.32	113.21
3	C	168	ASN	N-CA-C	-6.80	104.72	113.16
1	N	61	THR	N-CA-C	-6.78	99.91	110.42
4	D	46	SER	N-CA-C	6.78	125.23	110.80
3	P	190	TYR	CB-CA-C	-6.76	108.76	116.54
2	O	40	PHE	N-CA-C	-6.75	103.57	112.75
2	O	24	HIS	N-CA-C	6.64	119.39	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	20	LYS	N-CA-C	6.64	124.94	110.80
4	D	162	LEU	N-CA-C	-6.60	100.44	110.14
1	A	177	GLN	N-CA-C	-6.56	105.31	113.38
1	N	76	VAL	N-CA-C	6.54	118.45	108.71
1	N	26	VAL	N-CA-C	6.53	122.99	108.88
4	D	66	VAL	N-CA-C	6.52	122.91	109.34
5	R	22	ILE	N-CA-C	6.51	117.14	110.82
8	H	13	VAL	N-CA-C	6.51	116.67	110.42
5	E	16	PHE	N-CA-C	-6.49	100.73	111.37
2	B	40	PHE	N-CA-C	-6.39	104.06	112.75
8	U	13	VAL	N-CA-C	6.39	116.56	110.42
7	T	24	ALA	N-CA-C	-6.36	103.27	111.02
1	N	107	THR	N-CA-C	-6.34	105.19	114.39
7	G	16	ALA	N-CA-C	-6.33	105.27	112.87
4	Q	156	GLN	N-CA-C	-6.32	102.99	112.54
2	B	111	VAL	CB-CA-C	-6.32	107.70	113.70
1	N	21	VAL	N-CA-C	6.31	122.47	109.34
8	H	9	VAL	N-CA-C	-6.26	104.41	110.42
2	O	111	VAL	CB-CA-C	-6.25	107.76	113.70
1	N	74	ASN	N-CA-C	6.23	119.27	111.24
5	E	23	ILE	N-CA-C	-6.21	103.84	110.36
1	A	18	ALA	N-CA-C	6.21	120.41	112.34
2	O	19	ALA	N-CA-C	6.20	120.74	107.67
5	R	23	ILE	N-CA-C	-6.18	104.49	110.42
2	O	144	GLY	N-CA-C	-6.17	98.55	113.18
1	N	176	GLY	N-CA-C	6.16	118.90	110.58
3	P	281	LYS	N-CA-C	6.16	117.99	111.28
4	Q	152	HIS	N-CA-C	6.14	114.65	108.75
4	Q	154	THR	N-CA-C	6.11	117.32	108.34
7	T	34	GLU	N-CA-C	6.10	118.11	107.49
4	D	83	GLY	N-CA-C	6.08	122.18	112.58
1	N	31	ASN	N-CA-C	6.07	123.72	110.80
4	D	59	LYS	N-CA-C	-6.02	105.79	113.01
7	T	16	ALA	N-CA-C	-6.00	105.67	112.87
4	Q	44	PRO	N-CA-C	5.99	118.00	110.70
4	Q	18	PHE	N-CA-C	-5.97	105.64	113.17
3	C	186	GLU	N-CA-C	-5.96	101.63	110.46
3	C	281	LYS	N-CA-C	5.96	117.78	111.28
3	P	12	THR	CA-C-N	5.96	126.47	120.04
3	P	12	THR	C-N-CA	5.96	126.47	120.04
2	O	29	GLU	CA-C-N	5.88	127.19	119.84
2	O	29	GLU	C-N-CA	5.88	127.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	12	THR	CA-C-N	5.87	126.38	120.04
3	C	12	THR	C-N-CA	5.87	126.38	120.04
3	P	168	ASN	N-CA-C	-5.84	105.81	113.17
3	C	207	VAL	N-CA-C	5.83	118.15	109.17
3	C	201	THR	N-CA-C	-5.83	104.78	112.24
2	O	139	VAL	N-CA-C	-5.82	104.83	110.42
2	O	81	LEU	N-CA-C	-5.82	105.49	112.59
4	D	104	ILE	N-CA-C	5.79	117.09	109.21
4	D	119	ALA	N-CA-C	-5.79	105.48	112.54
4	D	123	LYS	N-CA-C	-5.76	101.13	109.31
4	D	84	LEU	N-CA-C	5.75	118.66	110.10
2	O	39	VAL	N-CA-C	-5.71	97.47	109.34
3	C	283	GLN	N-CA-C	-5.71	105.81	112.89
4	D	71	GLU	N-CA-C	5.70	120.36	113.41
2	B	96	LEU	N-CA-C	-5.69	105.07	111.28
1	A	206	ILE	N-CA-C	5.69	116.06	107.75
3	P	283	GLN	N-CA-C	-5.69	105.83	112.89
3	P	190	TYR	N-CA-C	5.67	116.93	108.31
7	T	22	PHE	N-CA-C	-5.67	106.06	112.87
3	C	190	TYR	N-CA-C	5.67	116.39	108.00
8	U	9	VAL	N-CA-C	-5.64	104.87	110.62
4	Q	126	CYS	CA-C-N	5.60	126.84	119.84
4	Q	126	CYS	C-N-CA	5.60	126.84	119.84
1	A	150	ILE	N-CA-C	5.59	116.36	110.72
2	O	116	ASN	N-CA-C	5.59	118.35	108.24
4	D	92	VAL	N-CA-C	5.58	118.16	108.90
4	D	168	THR	N-CA-C	5.51	117.80	110.53
3	C	190	TYR	CB-CA-C	-5.50	108.63	116.34
3	C	171	VAL	N-CA-C	5.48	117.21	108.87
3	P	9	TYR	CA-C-N	5.48	126.03	120.38
3	P	9	TYR	C-N-CA	5.48	126.03	120.38
4	D	18	PHE	N-CA-C	-5.48	106.27	113.17
1	N	27	PRO	CA-C-N	5.47	126.68	119.84
1	N	27	PRO	C-N-CA	5.47	126.68	119.84
3	C	182	LYS	N-CA-C	5.46	116.58	108.60
3	C	93	GLU	N-CA-C	-5.45	105.42	111.36
4	Q	165	TRP	N-CA-C	5.45	117.61	108.73
3	C	78	LEU	CA-C-N	-5.44	114.64	120.03
3	C	78	LEU	C-N-CA	-5.44	114.64	120.03
2	B	29	GLU	CA-C-N	5.42	126.62	119.84
2	B	29	GLU	C-N-CA	5.42	126.62	119.84
3	P	239	GLY	N-CA-C	5.42	119.44	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	186	GLU	N-CA-C	-5.41	102.46	110.46
1	N	60	PRO	N-CA-C	5.40	123.20	113.70
7	G	22	PHE	N-CA-C	-5.39	106.40	112.87
4	D	89	THR	N-CA-C	5.39	117.51	108.73
2	B	31	ALA	N-CA-C	5.38	117.14	108.32
4	D	64	VAL	N-CA-C	5.37	115.69	108.17
1	A	158	ILE	CA-C-N	5.37	125.53	119.90
1	A	158	ILE	C-N-CA	5.37	125.53	119.90
4	Q	45	PRO	N-CA-C	5.36	123.52	112.47
2	B	122	ASN	CA-C-N	5.35	126.53	119.84
2	B	122	ASN	C-N-CA	5.35	126.53	119.84
3	P	207	VAL	N-CA-C	5.35	117.42	109.17
2	B	95	LEU	N-CA-C	-5.34	106.14	113.30
3	P	249	LEU	N-CA-C	-5.31	99.10	108.23
2	B	80	TYR	N-CA-C	-5.30	106.50	112.87
2	B	39	VAL	N-CA-C	-5.29	98.33	109.34
3	C	209	ASP	N-CA-C	5.29	115.37	108.07
4	D	23	ALA	N-CA-C	-5.29	105.21	110.97
3	P	182	LYS	N-CA-C	5.27	116.30	108.60
2	B	33	PRO	N-CA-C	5.26	123.31	112.47
4	D	108	CYS	N-CA-C	-5.25	99.20	108.23
3	P	133	SER	CA-C-N	5.23	126.38	119.84
3	P	133	SER	C-N-CA	5.23	126.38	119.84
6	F	5	MET	N-CA-C	-5.23	107.03	113.41
1	N	211	ILE	N-CA-C	5.22	120.21	109.34
2	O	26	TYR	N-CA-C	5.22	121.93	110.80
1	N	35	CYS	N-CA-C	-5.20	107.60	114.31
4	D	173	GLY	N-CA-C	5.20	120.88	114.69
2	B	119	LYS	N-CA-C	-5.19	105.69	112.23
1	N	32	ILE	N-CA-C	5.18	120.11	109.34
4	Q	23	ALA	N-CA-C	-5.17	105.30	111.03
3	C	122	GLU	N-CA-C	-5.16	106.76	113.16
4	D	122	ASN	N-CA-C	-5.15	102.99	113.29
3	P	201	THR	N-CA-C	-5.15	105.10	111.90
2	B	122	ASN	N-CA-C	5.15	115.52	109.60
3	P	27	LEU	N-CA-C	5.14	119.31	113.19
2	O	33	PRO	N-CA-C	5.13	123.04	112.47
2	O	113	PHE	N-CA-C	-5.13	107.15	113.41
2	B	129	ALA	N-CA-C	-5.11	99.91	110.80
4	Q	92	VAL	N-CA-C	5.11	119.96	109.34
4	Q	28	THR	N-CA-C	-5.10	105.23	111.75
2	O	122	ASN	CA-C-N	-5.09	113.48	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	122	ASN	C-N-CA	-5.09	113.48	119.84
2	O	23	GLY	CA-C-N	5.08	128.43	120.75
2	O	23	GLY	C-N-CA	5.08	128.43	120.75
6	F	11	LEU	N-CA-C	5.08	116.81	111.28
2	B	30	PRO	N-CA-C	5.07	122.92	112.47
6	S	7	TYR	N-CA-C	-5.07	106.25	112.90
1	A	115	GLU	N-CA-C	-5.07	107.77	114.31
6	F	7	TYR	N-CA-C	-5.06	106.27	112.90
8	H	16	THR	N-CA-C	-5.05	106.22	112.38
6	S	11	LEU	N-CA-C	5.04	116.77	111.28
7	T	18	LEU	N-CA-C	-5.03	104.75	111.24
1	N	164	LEU	N-CA-C	-5.03	105.08	111.11
5	R	9	ILE	CB-CA-C	-5.01	106.65	111.06
3	C	249	LEU	N-CA-C	-5.01	99.61	108.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	105	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1593	0	1623	256	0
1	N	1593	0	1623	238	0
2	B	1075	0	1117	264	0
2	O	1075	0	1117	301	0
3	C	2200	0	2216	369	0
3	P	2200	0	2216	345	0
4	D	1280	0	1263	332	0
4	Q	1280	0	1263	395	0
5	E	248	0	284	77	0
5	R	248	0	284	114	0
6	F	251	0	266	41	0
6	S	270	0	285	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	184	0	190	108	0
7	T	216	0	220	70	0
8	H	214	0	221	45	0
8	U	214	0	221	49	0
9	A	86	0	60	15	0
9	N	86	0	60	14	0
10	A	43	0	31	4	0
10	C	43	0	29	0	0
10	N	43	0	31	4	0
10	P	43	0	29	1	0
11	A	30	0	37	13	0
11	N	30	0	37	12	0
12	A	55	0	80	19	0
12	Q	55	0	80	22	0
13	B	54	0	83	14	0
13	D	54	0	83	24	0
13	N	54	0	83	10	0
13	Q	54	0	83	30	0
14	B	65	0	70	8	0
14	O	65	0	70	19	0
15	D	4	0	0	1	0
15	Q	4	0	0	1	0
16	E	40	0	56	7	0
16	R	40	0	56	7	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
All	All	15091	0	15467	2802	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 92.

All (2802) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:38:TYR:HB3	3:P:276:LYS:HG2	1.22	1.20
1:A:14:ILE:HA	1:A:17:LEU:HB2	1.26	1.18
1:N:214:PRO:HB3	5:R:29:ILE:HG22	1.19	1.17
4:D:166:THR:HA	4:D:179:VAL:HG13	1.22	1.17
2:B:71:THR:HB	2:B:72:PRO:HD3	1.28	1.15
12:A:305:PL9:H462	12:A:305:PL9:H412	1.18	1.13
2:B:20:LYS:HG3	2:B:21:GLY:H	1.05	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:1305:PL9:H212	12:Q:1305:PL9:H262	1.24	1.12
13:D:306:OPC:HAP2	13:D:306:OPC:HBI1	1.31	1.12
5:E:7:PHE:HA	5:E:10:VAL:HG12	1.29	1.11
4:Q:169:ASP:HB2	4:Q:176:PRO:HA	1.32	1.11
13:Q:1307:OPC:HBE1	13:Q:1307:OPC:HBU2	1.11	1.11
4:Q:94:GLU:HB3	4:Q:100:ARG:HD3	1.18	1.10
4:D:136:THR:HB	4:D:138:ARG:HD2	1.25	1.10
4:Q:168:THR:HA	4:Q:176:PRO:HD3	1.19	1.10
4:D:124:PHE:HB2	4:D:133:TYR:HB2	1.32	1.09
2:B:126:ARG:HE	2:B:128:VAL:HG23	0.99	1.08
3:C:255:VAL:HG11	7:G:14:VAL:HG12	1.36	1.08
5:E:5:ALA:HB1	6:F:9:ALA:HB2	1.35	1.08
2:O:118:ASN:HD22	2:O:121:GLN:NE2	1.51	1.08
3:C:273:ILE:HD13	7:G:30:LYS:HD3	1.20	1.07
2:O:132:ILE:HG22	14:O:1201:CLA:HBB2	1.35	1.07
4:Q:156:GLN:HB2	4:Q:161:VAL:HG21	1.37	1.07
3:C:172:PHE:H	3:C:231:LEU:HG	1.17	1.07
5:R:7:PHE:HA	5:R:10:VAL:HG12	1.34	1.06
4:D:66:VAL:HG22	4:D:160:ILE:HG13	1.07	1.06
1:N:27:PRO:HG3	2:O:33:PRO:HG3	1.34	1.06
4:Q:76:GLY:H	4:Q:93:VAL:HG13	1.12	1.06
2:O:64:GLU:HG3	2:O:65:PRO:HD3	1.37	1.05
7:T:25:ALA:HB1	7:T:29:TYR:CZ	1.89	1.05
1:A:209:GLN:HG2	1:A:210:GLY:H	1.19	1.05
12:A:305:PL9:H203	13:D:306:OPC:HBE2	1.37	1.05
5:E:16:PHE:HB3	16:E:101:BCR:H363	1.36	1.05
13:N:1306:OPC:HAP2	13:N:1306:OPC:HBI1	1.39	1.05
5:R:5:ALA:HB1	6:S:9:ALA:HB2	1.30	1.05
3:C:281:LYS:HA	3:C:284:ALA:HB3	1.34	1.04
4:D:70:LEU:HD12	4:D:160:ILE:HD11	1.34	1.04
1:N:29:HIS:O	1:N:30:VAL:HG13	1.56	1.04
4:Q:56:ALA:HA	4:Q:81:VAL:HG13	1.36	1.03
3:P:281:LYS:HA	3:P:284:ALA:HB3	1.37	1.03
3:C:278:GLN:HE21	7:G:30:LYS:HE2	1.20	1.03
4:D:155:VAL:HG22	4:D:160:ILE:HG12	1.39	1.03
3:C:93:GLU:HA	3:C:97:GLU:HB2	1.38	1.02
1:A:207:ARG:HB2	1:A:207:ARG:HH11	1.21	1.02
4:D:51:GLY:HA2	4:D:164:PRO:HG2	1.35	1.02
2:B:18:LEU:HD13	2:B:31:ALA:HB2	1.42	1.01
7:G:25:ALA:HB1	7:G:29:TYR:CZ	1.95	1.01
4:Q:155:VAL:HG12	4:Q:157:ASP:H	1.21	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:PHE:O	3:C:231:LEU:HB3	1.60	1.01
5:R:16:PHE:HB3	16:R:1101:BCR:H363	1.38	1.01
2:O:124:PHE:CZ	5:R:26:ILE:HB	1.95	1.01
4:Q:116:PRO:HD2	4:Q:126:CYS:HA	1.41	1.00
3:C:28:ALA:HB2	3:C:236:ASN:HD21	1.24	1.00
3:C:271:MET:HG3	4:D:22:LEU:HD21	1.37	1.00
3:C:262:ILE:HG13	7:G:21:LEU:HG	1.38	1.00
7:G:26:TYR:HA	7:G:29:TYR:CD1	1.97	1.00
5:R:9:ILE:HG21	6:S:9:ALA:O	1.62	1.00
4:D:123:LYS:HB3	4:D:133:TYR:O	1.62	0.99
3:P:94:LEU:HD22	3:P:94:LEU:H	1.28	0.99
2:B:20:LYS:HG3	2:B:21:GLY:N	1.70	0.99
4:D:116:PRO:HG3	4:D:127:PRO:HD3	1.40	0.99
2:B:31:ALA:O	2:B:32:TRP:HB2	1.59	0.98
1:N:61:THR:HG22	1:N:63:THR:H	1.26	0.98
4:Q:57:LYS:HG3	4:Q:82:GLN:HE21	1.27	0.98
7:T:23:TYR:HA	7:T:26:TYR:CG	1.98	0.98
3:P:28:ALA:HB2	3:P:236:ASN:HD21	1.29	0.98
1:A:29:HIS:NE2	1:A:30:VAL:HG22	1.79	0.97
2:B:149:LEU:CD1	2:B:150:PRO:HD2	1.94	0.97
3:P:202:ASP:HA	3:P:206:THR:HB	1.43	0.97
4:D:51:GLY:HA2	4:D:164:PRO:CG	1.95	0.97
3:C:202:ASP:HA	3:C:206:THR:HB	1.45	0.97
3:C:218:ILE:H	3:C:232:THR:HB	1.28	0.97
3:P:146:LYS:HD3	3:P:246:GLU:HG3	1.46	0.97
2:B:61:MET:HB2	3:C:146:LYS:HD2	1.47	0.97
1:A:207:ARG:HB2	1:A:207:ARG:NH1	1.79	0.96
3:C:185:LYS:HG2	3:C:195:TYR:HB3	1.43	0.96
3:P:93:GLU:HA	3:P:97:GLU:HB2	1.43	0.96
4:D:57:LYS:HD2	4:D:82:GLN:HE21	1.27	0.96
5:E:9:ILE:HG21	6:F:9:ALA:O	1.64	0.95
2:B:126:ARG:NE	2:B:128:VAL:HG23	1.82	0.95
3:P:185:LYS:HG2	3:P:195:TYR:HB3	1.47	0.95
1:N:112:LYS:HB2	1:N:113:PRO:HD3	1.49	0.95
4:Q:123:LYS:HD3	4:Q:140:ILE:HD12	1.45	0.94
7:G:23:TYR:HA	7:G:26:TYR:CG	2.02	0.94
3:P:275:LYS:HB2	4:Q:19:MET:HE2	1.50	0.94
13:D:306:OPC:HBL1	13:D:306:OPC:HAR2	1.46	0.94
1:N:66:TYR:HB2	2:O:65:PRO:HG2	1.49	0.94
1:N:154:VAL:HG21	11:N:1304:TDS:HAY2	1.50	0.94
4:Q:74:ASN:H	4:Q:93:VAL:HG11	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:126:ARG:HH11	2:O:126:ARG:HG2	1.33	0.94
5:R:1:MET:HE3	5:R:1:MET:H1	1.33	0.94
4:D:166:THR:HA	4:D:179:VAL:CG1	1.98	0.93
1:N:95:LEU:HD11	5:R:10:VAL:HG11	1.50	0.93
2:O:118:ASN:HD22	2:O:121:GLN:HE22	1.17	0.93
1:A:161:VAL:O	1:A:165:ILE:HG12	1.68	0.92
2:O:126:ARG:NH1	2:O:128:VAL:HG23	1.83	0.92
3:P:168:ASN:HA	3:P:172:PHE:CZ	2.04	0.92
3:P:172:PHE:H	3:P:231:LEU:HG	1.33	0.92
4:Q:73:HIS:CD2	4:Q:77:ASP:HB2	2.05	0.92
3:C:94:LEU:HD22	3:C:94:LEU:H	1.34	0.91
3:C:146:LYS:HD3	3:C:246:GLU:HG3	1.50	0.91
1:N:142:GLN:HG2	2:O:64:GLU:HG2	1.51	0.91
3:P:218:ILE:H	3:P:232:THR:HB	1.34	0.91
3:C:60:GLN:HE22	3:C:157:ARG:HG3	1.35	0.91
8:U:4:ASP:O	8:U:8:TRP:HB2	1.70	0.91
1:A:209:GLN:CG	1:A:210:GLY:H	1.79	0.90
2:B:22:MET:HE2	2:B:22:MET:HA	1.53	0.90
3:P:172:PHE:O	3:P:231:LEU:HB3	1.71	0.90
1:A:170:ARG:HD3	1:A:174:SER:O	1.68	0.90
2:O:124:PHE:HZ	5:R:26:ILE:HB	1.36	0.90
1:A:114:ARG:HH12	1:A:209:GLN:H	1.06	0.90
2:O:31:ALA:O	2:O:32:TRP:HB2	1.70	0.90
1:A:211:ILE:H	1:A:211:ILE:HD12	1.37	0.90
2:B:57:LEU:HD21	3:C:258:MET:HE2	1.51	0.90
4:D:99:ILE:HB	4:D:153:ALA:HB1	1.53	0.90
4:D:81:VAL:HG12	4:D:82:GLN:H	1.36	0.90
7:T:26:TYR:HA	7:T:29:TYR:CD1	2.06	0.90
1:A:24:LYS:HD3	1:A:24:LYS:H	1.35	0.89
4:Q:76:GLY:N	4:Q:93:VAL:HG13	1.86	0.89
2:O:80:TYR:HB3	14:O:1201:CLA:HED1	1.52	0.89
1:A:190:VAL:HG11	11:A:304:TDS:HAA3	1.54	0.89
4:Q:82:GLN:N	4:Q:89:THR:OG1	2.05	0.89
4:D:66:VAL:CG2	4:D:160:ILE:HG13	2.00	0.89
2:O:105:PRO:HG3	14:O:1201:CLA:H112	1.54	0.89
12:A:305:PL9:H412	12:A:305:PL9:C46	2.01	0.89
4:Q:57:LYS:HG3	4:Q:82:GLN:NE2	1.88	0.89
4:Q:91:ILE:HD12	4:Q:160:ILE:HD12	1.54	0.88
1:N:213:GLY:O	5:R:30:LYS:HD2	1.73	0.88
3:P:83:LYS:HB2	3:P:111:ASP:HB3	1.56	0.88
3:P:275:LYS:CE	4:Q:20:ASN:HB3	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:146:LEU:HD13	4:Q:177:TRP:HB2	1.56	0.88
3:C:280:GLU:HG2	3:C:281:LYS:HZ3	1.39	0.87
3:P:231:LEU:HD13	3:P:232:THR:H	1.37	0.87
3:C:226:LYS:NZ	3:C:230:ALA:HB3	1.88	0.87
3:C:278:GLN:NE2	7:G:30:LYS:HE2	1.90	0.87
3:P:60:GLN:HE22	3:P:157:ARG:HG3	1.40	0.87
4:Q:78:ARG:HH22	4:Q:100:ARG:NH2	1.71	0.87
4:Q:156:GLN:HB2	4:Q:161:VAL:CG2	2.04	0.87
2:O:79:TRP:CZ2	5:R:1:MET:HB2	2.09	0.87
4:D:102:TYR:HB2	4:D:150:LEU:HG	1.56	0.87
7:T:21:LEU:O	7:T:21:LEU:HD22	1.75	0.87
8:H:4:ASP:O	8:H:8:TRP:HB2	1.74	0.87
1:N:110:PHE:H	1:N:110:PHE:HD2	1.20	0.87
3:P:226:LYS:NZ	3:P:230:ALA:HB3	1.90	0.87
3:C:255:VAL:CG1	7:G:14:VAL:HG12	2.04	0.86
3:P:275:LYS:HE3	4:Q:20:ASN:HB3	1.55	0.86
4:Q:77:ASP:H	4:Q:93:VAL:HG12	1.40	0.86
4:D:117:TRP:HA	4:D:124:PHE:HD1	1.41	0.86
2:O:126:ARG:HG2	2:O:126:ARG:NH1	1.89	0.86
1:N:103:ARG:HE	1:N:107:THR:HG21	1.39	0.86
2:O:64:GLU:HG3	2:O:65:PRO:CD	2.05	0.86
4:Q:73:HIS:CG	4:Q:77:ASP:HB2	2.10	0.86
4:Q:163:THR:OG1	4:Q:164:PRO:HD2	1.73	0.86
1:A:159:PRO:O	1:A:161:VAL:N	2.08	0.86
2:B:38:TYR:HB3	3:C:276:LYS:HG2	1.58	0.86
2:B:149:LEU:HD22	4:Q:129:HIS:HA	1.57	0.86
4:Q:22:LEU:HD23	4:Q:23:ALA:N	1.91	0.86
13:N:1306:OPC:HBF2	13:N:1306:OPC:HBY1	1.56	0.85
1:A:211:ILE:HG22	5:E:26:ILE:HG12	1.59	0.85
4:Q:133:TYR:HA	4:Q:139:VAL:HA	1.57	0.85
4:D:22:LEU:HD23	4:D:23:ALA:N	1.92	0.85
4:D:142:GLY:HA2	4:D:144:ALA:H	1.42	0.85
1:A:158:ILE:HG23	1:A:159:PRO:HD2	1.59	0.85
1:A:170:ARG:HD2	1:A:172:GLY:O	1.76	0.85
10:N:303:HEC:HBC2	2:O:44:ILE:HD11	1.58	0.85
2:B:149:LEU:CD2	4:Q:129:HIS:HA	2.06	0.85
3:C:280:GLU:HG2	3:C:281:LYS:NZ	1.91	0.85
1:A:14:ILE:HD13	1:A:15:GLN:N	1.92	0.85
4:Q:138:ARG:HE	4:Q:171:ARG:HD3	1.43	0.84
5:E:7:PHE:HA	5:E:10:VAL:CG1	2.07	0.84
2:O:149:LEU:O	2:O:151:LEU:N	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ILE:HA	1:A:17:LEU:CB	2.07	0.84
1:A:206:ILE:C	1:A:207:ARG:HD3	2.03	0.84
3:P:280:GLU:HG2	3:P:281:LYS:HZ3	1.43	0.84
2:O:38:TYR:CB	3:P:276:LYS:HG2	2.07	0.84
2:B:98:VAL:HA	2:B:101:MET:HE2	1.59	0.84
1:N:155:PRO:HG2	1:N:166:SER:OG	1.78	0.84
4:Q:105:ASN:HB3	4:Q:149:ALA:HB3	1.58	0.84
1:A:142:GLN:HE21	2:B:66:ALA:HA	1.42	0.83
2:B:149:LEU:HD12	2:B:150:PRO:HD2	1.58	0.83
4:Q:73:HIS:HB3	4:Q:93:VAL:HG11	1.57	0.83
1:A:209:GLN:HG2	1:A:210:GLY:N	1.87	0.83
3:C:83:LYS:HB2	3:C:111:ASP:HB3	1.58	0.83
4:D:142:GLY:HA2	4:D:144:ALA:N	1.94	0.83
4:Q:64:VAL:HG12	4:Q:91:ILE:CG1	2.08	0.83
4:Q:150:LEU:H	4:Q:178:TRP:HZ2	1.25	0.83
3:P:184:ALA:HB2	3:P:198:SER:OG	1.79	0.83
3:C:26:HIS:CG	3:C:154:ASN:HD21	1.97	0.83
3:C:218:ILE:N	3:C:232:THR:HB	1.94	0.83
2:O:79:TRP:HZ2	5:R:1:MET:H3	1.27	0.83
2:O:122:ASN:HD21	5:R:30:LYS:HD3	1.44	0.83
3:C:255:VAL:HG11	7:G:14:VAL:CG1	2.08	0.82
4:D:165:TRP:HD1	4:D:179:VAL:HA	1.44	0.82
4:Q:176:PRO:HG2	4:Q:179:VAL:HB	1.58	0.82
2:O:67:ASN:ND2	3:P:16:PRO:HB3	1.94	0.82
4:Q:78:ARG:HH22	4:Q:100:ARG:HH22	1.26	0.82
12:Q:1305:PL9:H302	13:Q:1307:OPC:HBC1	1.60	0.82
1:A:14:ILE:HD13	1:A:15:GLN:H	1.45	0.82
3:P:275:LYS:NZ	4:Q:20:ASN:HD22	1.77	0.82
13:B:307:OPC:HAP1	13:B:307:OPC:HBI2	1.59	0.82
4:D:154:THR:O	4:D:160:ILE:HG23	1.78	0.82
4:Q:94:GLU:CB	4:Q:100:ARG:HD3	2.05	0.82
3:P:168:ASN:HA	3:P:172:PHE:HZ	1.39	0.82
2:B:137:THR:O	2:B:141:ILE:HG12	1.80	0.82
7:G:27:GLN:O	7:G:31:ARG:NH1	2.13	0.82
1:A:44:PHE:HD1	9:A:301:HEM:HBB1	1.45	0.81
1:A:62:VAL:HG12	1:A:140:TRP:CZ2	2.16	0.81
13:D:306:OPC:HBI1	13:D:306:OPC:CAP	2.08	0.81
2:O:126:ARG:CZ	2:O:128:VAL:HG23	2.10	0.81
2:O:95:LEU:N	2:O:95:LEU:HD23	1.96	0.81
4:Q:100:ARG:HD2	4:Q:102:TYR:OH	1.80	0.81
3:C:171:VAL:CG1	3:C:234:ASN:HB2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:1307:OPC:HBX2	13:Q:1307:OPC:HBF2	1.63	0.81
3:P:26:HIS:CG	3:P:154:ASN:HD21	1.98	0.81
3:P:231:LEU:O	3:P:232:THR:HG23	1.80	0.81
3:C:183:ILE:HD12	3:C:183:ILE:O	1.81	0.81
1:A:112:LYS:HA	1:A:115:GLU:OE1	1.80	0.81
3:C:93:GLU:HA	3:C:97:GLU:CB	2.11	0.81
3:P:90:ILE:HG23	3:P:95:LYS:HB2	1.62	0.81
3:P:217:LEU:HA	3:P:232:THR:HB	1.63	0.81
4:Q:155:VAL:HA	4:Q:161:VAL:H	1.43	0.81
1:A:14:ILE:CA	1:A:17:LEU:HB2	2.11	0.80
1:N:214:PRO:HB3	5:R:29:ILE:CG2	2.09	0.80
2:O:121:GLN:HB2	2:O:125:ARG:HD2	1.63	0.80
13:Q:1307:OPC:OBJ	13:Q:1307:OPC:HAP1	1.80	0.80
12:Q:1305:PL9:H412	12:Q:1305:PL9:H462	1.61	0.80
3:P:161:TYR:HE1	3:P:167:SER:HA	1.47	0.80
4:D:116:PRO:HG3	4:D:127:PRO:CD	2.11	0.80
3:P:183:ILE:HD12	3:P:183:ILE:O	1.80	0.80
12:Q:1305:PL9:H212	12:Q:1305:PL9:C26	2.10	0.80
7:T:11:LEU:HD22	7:T:11:LEU:H	1.44	0.80
3:C:184:ALA:HB2	3:C:198:SER:OG	1.81	0.80
3:C:269:GLN:HE22	7:G:24:ALA:CB	1.94	0.80
3:C:90:ILE:HG23	3:C:95:LYS:HB2	1.64	0.80
3:P:280:GLU:HG2	3:P:281:LYS:NZ	1.96	0.80
1:A:155:PRO:HG2	1:A:166:SER:OG	1.81	0.80
4:D:123:LYS:HA	4:D:134:ASP:C	2.07	0.80
13:N:1306:OPC:HBO1	13:N:1306:OPC:HAT1	1.64	0.80
7:G:30:LYS:HB3	7:G:31:ARG:NH2	1.95	0.80
4:D:138:ARG:HB3	4:D:138:ARG:NH1	1.97	0.80
7:G:30:LYS:O	7:G:31:ARG:NH2	2.15	0.80
4:D:58:ASP:HB2	4:D:62:ASN:O	1.82	0.79
4:Q:139:VAL:HG21	4:Q:144:ALA:HB3	1.64	0.79
3:C:199:ILE:O	3:C:208:VAL:HG12	1.81	0.79
3:C:231:LEU:O	3:C:232:THR:HG23	1.82	0.79
4:Q:67:SER:C	4:Q:68:LYS:HD2	2.07	0.79
3:C:91:PRO:HB2	3:C:94:LEU:HB2	1.65	0.79
3:C:161:TYR:HE1	3:C:167:SER:HA	1.48	0.79
7:T:23:TYR:HA	7:T:26:TYR:CD1	2.18	0.79
2:O:122:ASN:HD21	5:R:30:LYS:CD	1.94	0.79
4:D:134:ASP:CG	4:D:135:GLU:H	1.90	0.79
1:A:114:ARG:HH12	1:A:209:GLN:N	1.81	0.79
7:G:11:LEU:HD22	7:G:11:LEU:H	1.44	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:VAL:HA	4:D:100:ARG:HB2	1.64	0.79
4:D:156:GLN:OE1	4:D:161:VAL:HG21	1.83	0.79
2:O:122:ASN:ND2	5:R:30:LYS:HD3	1.98	0.79
12:A:305:PL9:H101	13:D:306:OPC:HBF2	1.65	0.79
3:C:102:TYR:H	3:C:118:PRO:HG3	1.46	0.79
4:D:70:LEU:HD12	4:D:160:ILE:CD1	2.13	0.78
13:D:306:OPC:HAP2	13:D:306:OPC:CBI	2.07	0.78
2:O:57:LEU:HD22	7:T:14:VAL:CG2	2.13	0.78
2:B:18:LEU:HD13	2:B:31:ALA:CB	2.14	0.78
5:E:20:VAL:HG12	5:E:21:GLY:N	1.99	0.78
3:P:219:VAL:HG11	3:P:223:GLN:HE21	1.48	0.78
4:Q:20:ASN:C	4:Q:22:LEU:H	1.89	0.78
12:Q:1305:PL9:H321	13:Q:1307:OPC:HBW2	1.66	0.78
4:D:64:VAL:HG11	4:D:81:VAL:HG13	1.66	0.78
1:N:71:TYR:HA	1:N:75:GLU:OE1	1.84	0.78
7:T:23:TYR:HA	7:T:26:TYR:CD2	2.17	0.78
1:A:29:HIS:CD2	1:A:30:VAL:HG13	2.19	0.78
2:B:71:THR:HB	2:B:72:PRO:CD	2.11	0.78
1:N:195:ILE:O	1:N:199:MET:HG3	1.84	0.78
4:Q:155:VAL:C	4:Q:161:VAL:HG22	2.09	0.78
2:O:112:PRO:O	2:O:116:ASN:HB2	1.84	0.78
1:N:114:ARG:HH21	1:N:209:GLN:N	1.82	0.77
2:O:149:LEU:HB3	2:O:150:PRO:HD2	1.66	0.77
3:P:134:PRO:HB3	3:P:142:ILE:HD13	1.65	0.77
1:A:28:PRO:HD2	2:B:31:ALA:O	1.85	0.77
3:P:188:ASP:CB	3:P:193:VAL:HA	2.15	0.77
4:Q:154:THR:O	4:Q:160:ILE:HA	1.83	0.77
1:A:112:LYS:H	1:A:113:PRO:HD2	1.50	0.77
1:A:39:ILE:HD11	16:E:101:BCR:H312	1.65	0.77
3:P:255:VAL:HG11	7:T:14:VAL:HG12	1.66	0.77
4:Q:169:ASP:HB2	4:Q:176:PRO:CA	2.12	0.77
13:Q:1307:OPC:HAL2	13:Q:1307:OPC:CAP	2.15	0.77
8:H:19:ILE:O	8:H:23:VAL:HG22	1.84	0.77
4:Q:155:VAL:HG12	4:Q:157:ASP:N	1.98	0.77
7:G:21:LEU:O	7:G:21:LEU:HD22	1.84	0.77
3:C:231:LEU:HD13	3:C:232:THR:H	1.49	0.77
1:N:116:LEU:H	1:N:116:LEU:HD12	1.50	0.77
2:O:57:LEU:HD21	3:P:258:MET:HE2	1.67	0.77
2:O:149:LEU:HB3	2:O:150:PRO:CD	2.14	0.77
3:C:92:GLU:O	3:C:96:LYS:HB3	1.85	0.77
3:P:102:TYR:H	3:P:118:PRO:HG3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:176:PRO:CG	4:Q:179:VAL:HB	2.14	0.77
5:R:23:ILE:O	5:R:27:LYS:HB2	1.85	0.77
3:C:259:ILE:HA	7:G:17:THR:HG21	1.65	0.77
2:B:34:ASN:HD21	13:B:307:OPC:CBK	1.97	0.77
2:O:38:TYR:CD1	3:P:276:LYS:HD3	2.20	0.77
1:A:47:GLN:HE22	1:A:89:SER:CB	1.97	0.76
4:D:16:ARG:C	4:D:18:PHE:H	1.94	0.76
4:D:20:ASN:C	4:D:22:LEU:H	1.91	0.76
13:Q:1307:OPC:HBU2	13:Q:1307:OPC:CBE	2.05	0.76
8:U:19:ILE:O	8:U:23:VAL:HG22	1.85	0.76
2:B:95:LEU:N	2:B:95:LEU:HD23	2.00	0.76
3:C:28:ALA:HB2	3:C:236:ASN:ND2	1.98	0.76
3:C:188:ASP:CB	3:C:193:VAL:HA	2.14	0.76
3:C:281:LYS:CA	3:C:284:ALA:HB3	2.16	0.76
4:D:57:LYS:HB2	4:D:82:GLN:HG2	1.66	0.76
7:G:25:ALA:HB1	7:G:29:TYR:CE2	2.21	0.76
1:N:29:HIS:ND1	1:N:29:HIS:N	2.31	0.76
3:P:199:ILE:O	3:P:208:VAL:HG12	1.85	0.76
2:B:112:PRO:O	2:B:116:ASN:HB2	1.85	0.76
2:O:53:ALA:O	2:O:57:LEU:HG	1.84	0.76
4:Q:150:LEU:HB2	4:Q:178:TRP:HH2	1.51	0.76
5:R:7:PHE:HA	5:R:10:VAL:CG1	2.12	0.76
1:A:158:ILE:HB	1:A:162:GLY:HA3	1.66	0.76
13:D:306:OPC:HBW2	13:D:306:OPC:HCA2	1.67	0.76
3:P:271:MET:HG3	4:Q:22:LEU:HD21	1.67	0.76
2:O:79:TRP:CZ3	5:R:4:GLY:CA	2.69	0.76
2:B:151:LEU:HD12	2:B:153:LYS:HD3	1.67	0.76
3:C:269:GLN:HE22	7:G:24:ALA:HB1	1.50	0.76
4:Q:175:LYS:HB2	4:Q:179:VAL:HG11	1.66	0.76
5:E:23:ILE:O	5:E:27:LYS:HB2	1.86	0.76
3:C:181:THR:O	3:C:221:GLU:HB3	1.86	0.76
3:P:218:ILE:N	3:P:232:THR:HB	1.99	0.76
4:Q:64:VAL:HG12	4:Q:91:ILE:HG12	1.64	0.76
2:B:151:LEU:HA	2:B:153:LYS:HD3	1.67	0.75
1:N:141:ASP:HA	2:O:65:PRO:HD3	1.68	0.75
1:N:142:GLN:HG2	2:O:64:GLU:CG	2.15	0.75
3:P:231:LEU:HD11	3:P:233:ASN:O	1.85	0.75
2:B:151:LEU:C	2:B:153:LYS:H	1.93	0.75
3:C:218:ILE:H	3:C:232:THR:CB	1.99	0.75
4:D:117:TRP:HA	4:D:124:PHE:CD1	2.21	0.75
2:O:57:LEU:HD22	7:T:14:VAL:HG23	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:O	1:A:199:MET:HG3	1.87	0.75
3:C:226:LYS:HZ2	3:C:230:ALA:HB3	1.49	0.75
4:Q:64:VAL:HB	4:Q:81:VAL:HG22	1.67	0.75
1:A:158:ILE:HB	1:A:162:GLY:CA	2.16	0.75
4:D:84:LEU:HD22	4:D:87:ASP:HB2	1.67	0.75
2:O:79:TRP:HZ2	5:R:1:MET:HB2	1.48	0.75
2:O:122:ASN:HD22	2:O:125:ARG:CZ	1.99	0.75
3:P:91:PRO:HB2	3:P:94:LEU:HB2	1.66	0.75
2:B:122:ASN:ND2	2:B:124:PHE:HB3	2.00	0.75
4:Q:151:CYS:HB3	4:Q:162:LEU:HD23	1.69	0.75
7:T:25:ALA:CB	7:T:29:TYR:CZ	2.69	0.75
13:D:306:OPC:HAR2	13:D:306:OPC:CBL	2.17	0.75
7:G:23:TYR:HA	7:G:26:TYR:CD2	2.20	0.75
2:O:122:ASN:OD1	5:R:30:LYS:HD3	1.87	0.75
2:O:146:GLY:N	2:O:149:LEU:HD12	2.02	0.75
2:O:146:GLY:H	2:O:149:LEU:HD12	1.49	0.75
1:A:24:LYS:H	1:A:24:LYS:CD	2.00	0.75
3:C:39:SER:HB3	3:C:248:VAL:HB	1.66	0.75
4:Q:156:GLN:O	4:Q:157:ASP:HB3	1.86	0.75
2:B:145:ILE:O	2:B:146:GLY:C	2.29	0.75
3:C:219:VAL:H	3:C:232:THR:HG22	1.52	0.75
4:D:81:VAL:HG21	4:D:91:ILE:HD11	1.68	0.75
4:Q:152:HIS:C	4:Q:162:LEU:HG	2.12	0.75
4:Q:159:ASN:O	4:Q:161:VAL:HG13	1.85	0.75
5:E:16:PHE:HB3	16:E:101:BCR:C36	2.17	0.74
3:P:188:ASP:HB2	3:P:193:VAL:HA	1.69	0.74
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.52	0.74
2:B:122:ASN:HD22	2:B:124:PHE:HD2	1.35	0.74
2:O:117:VAL:HG13	2:O:118:ASN:OD1	1.87	0.74
4:D:65:LYS:HB3	4:D:68:LYS:HD3	1.68	0.74
3:P:245:THR:HB	6:S:1:MET:HE2	1.68	0.74
4:Q:87:ASP:HB3	4:Q:88:PRO:HD2	1.67	0.74
4:Q:150:LEU:HD11	4:Q:171:ARG:HH21	1.53	0.74
4:Q:92:VAL:CG2	4:Q:100:ARG:HB2	2.17	0.74
3:P:52:ILE:HG12	3:P:153:ALA:HB1	1.69	0.74
4:Q:132:GLN:HE22	4:Q:141:ARG:HD3	1.53	0.74
12:A:305:PL9:H252	13:D:306:OPC:HBN1	1.68	0.74
3:P:229:GLU:HG3	3:P:230:ALA:H	1.53	0.74
11:A:304:TDS:HBC1	2:B:85:PHE:HA	1.70	0.73
2:B:127:PRO:C	2:B:129:ALA:H	1.94	0.73
3:C:182:LYS:HG2	3:C:198:SER:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:47:GLN:HE22	1:N:89:SER:HB3	1.53	0.73
3:C:172:PHE:C	3:C:231:LEU:HB3	2.13	0.73
2:O:76:LEU:HD12	5:R:1:MET:SD	2.28	0.73
1:A:29:HIS:CD2	1:A:30:VAL:HG22	2.21	0.73
7:G:25:ALA:CB	7:G:29:TYR:CZ	2.70	0.73
2:O:79:TRP:CH2	5:R:4:GLY:HA3	2.24	0.73
2:O:137:THR:O	2:O:141:ILE:HG12	1.89	0.73
3:P:28:ALA:HB2	3:P:236:ASN:ND2	2.03	0.73
1:A:146:TRP:CE3	2:B:71:THR:HG23	2.24	0.73
2:B:79:TRP:HA	2:B:82:TYR:CE2	2.24	0.73
2:B:133:PHE:O	2:B:137:THR:HG23	1.89	0.73
4:D:78:ARG:HE	4:D:92:VAL:CG1	2.02	0.73
1:A:154:VAL:CG1	2:B:101:MET:HE1	2.17	0.73
11:A:304:TDS:HBB2	2:B:88:LEU:HD22	1.70	0.73
2:B:144:GLY:O	2:B:145:ILE:HB	1.87	0.73
3:P:93:GLU:HA	3:P:97:GLU:CB	2.19	0.73
8:U:23:VAL:HA	8:U:26:ARG:HD2	1.71	0.73
4:D:133:TYR:HA	4:D:139:VAL:HA	1.71	0.73
4:D:138:ARG:HH21	4:D:171:ARG:CZ	2.02	0.73
4:Q:73:HIS:HB3	4:Q:93:VAL:CG1	2.18	0.73
12:A:305:PL9:H512	12:A:305:PL9:H401	1.71	0.73
3:C:188:ASP:HB2	3:C:193:VAL:HA	1.68	0.73
2:B:149:LEU:HD13	2:B:150:PRO:HD2	1.69	0.72
2:O:127:PRO:C	2:O:129:ALA:H	1.95	0.72
5:R:23:ILE:HG23	5:R:24:PHE:CD2	2.23	0.72
2:O:32:TRP:H	2:O:33:PRO:HD3	1.53	0.72
2:O:122:ASN:HD21	5:R:30:LYS:CG	2.01	0.72
6:S:1:MET:HE3	6:S:4:GLU:OE2	1.88	0.72
4:D:165:TRP:CD1	4:D:179:VAL:HA	2.24	0.72
7:T:25:ALA:HB1	7:T:29:TYR:OH	1.89	0.72
2:B:118:ASN:HB3	2:B:121:GLN:O	1.89	0.72
3:C:229:GLU:HG3	3:C:230:ALA:H	1.54	0.72
4:Q:76:GLY:HA2	4:Q:93:VAL:O	1.88	0.72
2:B:32:TRP:HH2	3:C:277:LYS:HD2	1.55	0.72
1:A:116:LEU:H	1:A:116:LEU:HD12	1.53	0.72
3:C:171:VAL:HG13	3:C:234:ASN:HB2	1.71	0.72
3:C:217:LEU:HA	3:C:232:THR:HB	1.72	0.72
3:P:211:ILE:HD11	3:P:231:LEU:HB2	1.71	0.72
4:Q:134:ASP:CG	4:Q:138:ARG:HB2	2.15	0.72
13:Q:1307:OPC:HBX2	13:Q:1307:OPC:CBF	2.19	0.72
13:Q:1307:OPC:HBG3	13:Q:1307:OPC:HAQ1	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:66:VAL:HG21	4:D:155:VAL:HG13	1.71	0.72
2:O:79:TRP:CZ3	5:R:4:GLY:HA3	2.25	0.72
4:Q:91:ILE:HG23	4:Q:160:ILE:HD12	1.71	0.72
4:Q:131:SER:OG	4:Q:144:ALA:HB2	1.89	0.72
4:Q:178:TRP:N	4:Q:178:TRP:HE3	1.88	0.72
6:S:6:LEU:O	6:S:10:LEU:HG	1.88	0.72
5:E:23:ILE:HG23	5:E:24:PHE:CD2	2.25	0.72
1:N:200:LEU:O	1:N:204:LEU:HG	1.89	0.72
4:Q:103:GLY:O	4:Q:150:LEU:HA	1.89	0.72
1:A:17:LEU:HD23	1:A:17:LEU:O	1.88	0.72
1:A:114:ARG:NH1	1:A:209:GLN:H	1.85	0.72
1:A:135:GLY:O	9:A:301:HEM:HAA1	1.90	0.72
2:O:133:PHE:O	2:O:137:THR:HG23	1.90	0.72
3:P:275:LYS:HZ3	3:P:276:LYS:NZ	1.88	0.72
13:D:306:OPC:HAP2	13:D:306:OPC:HBL1	1.71	0.71
2:O:20:LYS:HD3	2:O:21:GLY:H	1.53	0.71
4:Q:16:ARG:C	4:Q:18:PHE:H	1.98	0.71
3:C:278:GLN:NE2	6:F:30:GLN:OE1	2.23	0.71
3:P:219:VAL:H	3:P:232:THR:HG22	1.55	0.71
4:Q:66:VAL:HG22	4:Q:160:ILE:CG1	2.20	0.71
4:Q:137:GLY:O	4:Q:147:SER:HB3	1.90	0.71
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.54	0.71
6:F:6:LEU:O	6:F:10:LEU:HG	1.90	0.71
8:H:11:LEU:HB3	8:H:15:PHE:CZ	2.24	0.71
3:P:218:ILE:H	3:P:232:THR:CB	2.03	0.71
4:Q:77:ASP:C	4:Q:78:ARG:HD3	2.15	0.71
4:Q:105:ASN:HB3	4:Q:149:ALA:CB	2.20	0.71
1:N:29:HIS:HE2	1:N:209:GLN:HG3	1.56	0.71
1:N:66:TYR:CB	2:O:65:PRO:HG2	2.20	0.71
4:Q:64:VAL:HB	4:Q:81:VAL:CG2	2.20	0.71
2:O:98:VAL:HA	2:O:101:MET:HE2	1.73	0.71
2:O:106:LEU:HD21	14:O:1201:CLA:H151	1.72	0.71
3:P:185:LYS:HE2	3:P:195:TYR:HB3	1.71	0.71
2:O:84:VAL:O	2:O:88:LEU:HD13	1.90	0.71
2:O:142:TRP:O	2:O:145:ILE:HG12	1.91	0.71
7:T:14:VAL:O	7:T:17:THR:HB	1.91	0.71
2:B:18:LEU:HD22	2:B:30:PRO:O	1.90	0.71
4:D:57:LYS:CB	4:D:82:GLN:HG2	2.21	0.71
2:B:118:ASN:HB3	2:B:121:GLN:HE21	1.55	0.71
3:P:92:GLU:O	3:P:96:LYS:HB3	1.91	0.71
1:N:212:SER:OG	5:R:26:ILE:HG12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:149:LEU:C	2:O:151:LEU:H	1.98	0.71
2:B:126:ARG:HE	2:B:128:VAL:CG2	1.93	0.71
4:Q:117:TRP:HE1	4:Q:135:GLU:HA	1.55	0.71
3:C:218:ILE:HG13	3:C:219:VAL:H	1.56	0.70
4:Q:145:PRO:HG2	4:Q:146:LEU:H	1.55	0.70
1:A:211:ILE:HD11	2:B:122:ASN:OD1	1.91	0.70
4:D:15:ARG:NH2	4:D:17:GLN:HG2	2.05	0.70
4:D:115:VAL:HG21	4:D:148:LEU:HD21	1.73	0.70
6:F:5:MET:HA	6:F:8:ALA:HB3	1.73	0.70
4:Q:56:ALA:O	4:Q:63:ASN:HA	1.91	0.70
7:T:11:LEU:O	7:T:14:VAL:HG22	1.90	0.70
3:C:226:LYS:HG2	3:C:229:GLU:HB3	1.73	0.70
4:D:108:CYS:C	4:D:110:HIS:H	1.99	0.70
2:O:132:ILE:CG2	14:O:1201:CLA:HBB2	2.18	0.70
3:P:3:PHE:HZ	3:P:119:LEU:HD11	1.56	0.70
3:C:219:VAL:HG11	3:C:223:GLN:HE21	1.54	0.70
4:D:147:SER:HB2	4:D:177:TRP:HH2	1.56	0.70
3:P:172:PHE:CZ	3:P:212:PRO:HG3	2.25	0.70
4:Q:64:VAL:HA	4:Q:69:PHE:CD1	2.26	0.70
4:Q:149:ALA:C	4:Q:150:LEU:HD22	2.17	0.70
12:Q:1305:PL9:H412	12:Q:1305:PL9:C46	2.21	0.70
5:R:1:MET:HE3	5:R:1:MET:N	2.04	0.70
1:A:111:LYS:HG2	1:A:112:LYS:N	2.06	0.70
1:N:189:PHE:O	1:N:193:TRP:HE3	1.74	0.70
1:A:29:HIS:HD2	1:A:30:VAL:HG13	1.56	0.70
1:A:189:PHE:O	1:A:193:TRP:HE3	1.75	0.70
1:N:209:GLN:NE2	2:O:28:GLY:H	1.90	0.70
4:Q:93:VAL:CA	4:Q:100:ARG:HG3	2.21	0.70
2:B:144:GLY:O	2:B:145:ILE:CB	2.39	0.70
2:O:79:TRP:CZ3	5:R:4:GLY:HA2	2.26	0.70
12:Q:1305:PL9:H462	12:Q:1305:PL9:C41	2.21	0.70
6:S:5:MET:HA	6:S:8:ALA:HB3	1.73	0.70
1:A:207:ARG:HH11	1:A:207:ARG:CB	2.00	0.70
4:D:115:VAL:HG11	4:D:148:LEU:HD11	1.74	0.70
2:O:79:TRP:CE3	5:R:4:GLY:HA2	2.26	0.70
3:C:232:THR:O	3:C:233:ASN:HB2	1.91	0.70
3:P:39:SER:HB3	3:P:248:VAL:HB	1.72	0.70
3:P:275:LYS:HZ1	4:Q:20:ASN:HD22	1.38	0.70
7:T:28:GLN:O	7:T:31:ARG:N	2.24	0.70
2:B:20:LYS:NZ	2:B:21:GLY:O	2.23	0.69
4:D:168:THR:HA	4:D:176:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:21:VAL:HG12	1:N:22:THR:H	1.55	0.69
1:N:34:TYR:OH	1:N:211:ILE:HG22	1.92	0.69
3:P:70:LEU:HD23	3:P:70:LEU:H	1.57	0.69
4:Q:168:THR:HG23	4:Q:174:GLU:C	2.17	0.69
7:G:23:TYR:HA	7:G:26:TYR:CD1	2.26	0.69
2:B:26:TYR:HD2	2:B:26:TYR:N	1.90	0.69
3:C:171:VAL:HB	3:C:231:LEU:HD12	1.75	0.69
4:D:66:VAL:HG23	4:D:158:ASP:C	2.17	0.69
5:E:7:PHE:CA	5:E:10:VAL:HG12	2.17	0.69
2:O:117:VAL:O	2:O:118:ASN:HB2	1.92	0.69
1:A:26:VAL:HB	2:B:29:GLU:CB	2.22	0.69
4:D:57:LYS:HD2	4:D:82:GLN:NE2	2.04	0.69
2:O:122:ASN:ND2	5:R:26:ILE:HG22	2.08	0.69
3:P:182:LYS:HG2	3:P:198:SER:HB2	1.74	0.69
1:A:206:ILE:O	1:A:207:ARG:HD3	1.93	0.69
2:B:26:TYR:N	2:B:26:TYR:CD2	2.61	0.69
4:D:57:LYS:CD	4:D:82:GLN:HE21	2.04	0.69
4:D:78:ARG:HE	4:D:92:VAL:HG11	1.58	0.69
6:F:1:MET:HE3	6:F:4:GLU:OE2	1.92	0.69
11:N:1304:TDS:HBB2	2:O:81:LEU:HD13	1.73	0.69
3:P:14:ARG:HG2	3:P:77:MET:HE1	1.72	0.69
3:P:119:LEU:N	3:P:119:LEU:HD12	2.07	0.69
4:Q:69:PHE:O	4:Q:91:ILE:HG21	1.92	0.69
4:Q:138:ARG:HE	4:Q:171:ARG:CD	2.05	0.69
4:Q:68:LYS:HD2	4:Q:68:LYS:N	2.08	0.69
2:B:22:MET:HA	2:B:22:MET:CE	2.23	0.69
3:C:119:LEU:N	3:C:119:LEU:HD12	2.08	0.69
3:C:172:PHE:CZ	3:C:212:PRO:HG3	2.28	0.69
4:D:132:GLN:HB2	4:D:140:ILE:HB	1.75	0.69
1:N:111:LYS:HB2	1:N:114:ARG:HH11	1.58	0.69
2:O:122:ASN:HD22	2:O:125:ARG:NH2	1.90	0.69
2:O:122:ASN:CG	5:R:30:LYS:HD3	2.17	0.69
4:Q:165:TRP:HZ2	4:Q:176:PRO:HB3	1.54	0.69
6:S:25:LEU:HD23	6:S:25:LEU:O	1.92	0.69
4:Q:123:LYS:HE3	4:Q:125:LYS:NZ	2.08	0.69
5:R:18:ILE:O	5:R:22:ILE:HB	1.91	0.69
4:D:123:LYS:HA	4:D:134:ASP:O	1.91	0.69
7:G:11:LEU:HA	7:G:14:VAL:CG1	2.22	0.69
1:N:102:PHE:HB3	5:R:18:ILE:HD11	1.75	0.69
2:O:132:ILE:HG22	14:O:1201:CLA:CBB	2.19	0.69
3:P:178:GLY:HA2	3:P:225:VAL:HG13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:65:LYS:HE2	4:Q:158:ASP:O	1.90	0.69
2:B:18:LEU:HB3	2:B:30:PRO:O	1.93	0.68
7:G:14:VAL:CG2	7:G:15:PHE:N	2.56	0.68
1:N:110:PHE:HD2	1:N:110:PHE:N	1.90	0.68
2:O:74:GLU:HG2	2:O:75:ILE:N	2.08	0.68
13:Q:1307:OPC:HAT1	13:Q:1307:OPC:HAX2	1.76	0.68
2:B:26:TYR:C	2:B:27:TYR:CD1	2.72	0.68
3:C:277:LYS:HE3	7:G:31:ARG:HG3	1.74	0.68
4:D:103:GLY:O	4:D:151:CYS:HB2	1.92	0.68
4:D:154:THR:HG23	4:D:161:VAL:O	1.94	0.68
3:C:60:GLN:NE2	3:C:157:ARG:HG3	2.08	0.68
2:O:18:LEU:HD13	2:O:31:ALA:CB	2.23	0.68
2:O:52:VAL:O	2:O:56:VAL:HG23	1.93	0.68
4:Q:109:THR:O	4:Q:145:PRO:HG3	1.93	0.68
2:B:32:TRP:HZ3	2:B:36:LEU:HA	1.59	0.68
3:C:134:PRO:HB3	3:C:142:ILE:HD13	1.75	0.68
1:N:110:PHE:N	1:N:110:PHE:CD2	2.61	0.68
2:O:22:MET:C	2:O:24:HIS:N	2.50	0.68
3:P:161:TYR:HE1	3:P:167:SER:CA	2.07	0.68
3:C:180:ILE:HD11	3:C:182:LYS:O	1.93	0.68
3:C:258:MET:O	3:C:262:ILE:HD13	1.93	0.68
4:Q:24:PHE:CE1	12:Q:1305:PL9:H202	2.28	0.68
4:Q:102:TYR:CE1	4:Q:136:THR:HG23	2.28	0.68
5:R:20:VAL:HG12	5:R:21:GLY:N	2.06	0.68
2:B:57:LEU:CD2	3:C:258:MET:HE2	2.24	0.68
4:D:126:CYS:HB3	15:D:200:FES:S1	2.34	0.68
3:P:226:LYS:HZ2	3:P:230:ALA:HB3	1.57	0.68
7:T:25:ALA:HB1	7:T:29:TYR:CE2	2.27	0.68
1:A:62:VAL:CG1	1:A:177:GLN:HB3	2.24	0.68
3:P:60:GLN:NE2	3:P:157:ARG:HG3	2.09	0.68
3:P:185:LYS:HD3	3:P:195:TYR:HD2	1.58	0.68
4:Q:92:VAL:HG23	4:Q:100:ARG:HB2	1.75	0.68
2:B:42:VAL:HG12	7:G:28:GLN:HE22	1.59	0.68
2:O:32:TRP:H	2:O:33:PRO:CD	2.06	0.68
4:Q:93:VAL:HA	4:Q:100:ARG:HG3	1.74	0.68
1:A:142:GLN:NE2	2:B:67:ASN:H	1.92	0.68
13:B:307:OPC:HBI2	13:B:307:OPC:CAP	2.24	0.68
3:C:52:ILE:HG12	3:C:153:ALA:HB1	1.75	0.68
3:P:181:THR:O	3:P:221:GLU:HB3	1.92	0.68
4:D:156:GLN:HB2	4:D:161:VAL:HG22	1.75	0.67
3:P:232:THR:O	3:P:233:ASN:HB2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:LEU:O	7:G:14:VAL:HG22	1.94	0.67
2:O:114:ILE:C	2:O:116:ASN:H	2.02	0.67
4:D:117:TRP:CZ3	4:D:119:ALA:HA	2.30	0.67
6:F:26:LEU:CD2	8:H:17:TRP:HE1	2.07	0.67
1:N:149:LYS:HA	1:N:175:VAL:HG21	1.76	0.67
1:N:188:THR:HG22	9:N:301:HEM:HBC2	1.75	0.67
2:O:89:ARG:HH12	2:O:148:ALA:H	1.43	0.67
4:Q:115:VAL:HG11	4:Q:124:PHE:HB3	1.76	0.67
7:T:14:VAL:CG2	7:T:15:PHE:N	2.56	0.67
8:U:11:LEU:HB3	8:U:15:PHE:CZ	2.29	0.67
3:C:1:TYR:HD2	3:C:119:LEU:HD21	1.59	0.67
3:C:81:GLY:C	3:C:134:PRO:HG3	2.19	0.67
3:C:226:LYS:HE3	3:C:229:GLU:C	2.19	0.67
1:N:137:SER:O	1:N:140:TRP:HD1	1.78	0.67
2:O:146:GLY:C	2:O:149:LEU:HG	2.19	0.67
3:C:269:GLN:OE1	7:G:24:ALA:HA	1.93	0.67
3:P:275:LYS:HE2	4:Q:17:GLN:HB2	1.76	0.67
4:Q:150:LEU:HB2	4:Q:178:TRP:CH2	2.29	0.67
12:A:305:PL9:H111	13:D:306:OPC:HB2	1.75	0.67
3:C:126:GLU:OE1	3:C:126:GLU:HA	1.92	0.67
2:O:79:TRP:HZ2	5:R:1:MET:CB	2.07	0.67
1:A:114:ARG:CZ	1:A:208:LYS:HG3	2.24	0.67
2:B:153:LYS:O	2:B:154:THR:O	2.12	0.67
4:Q:81:VAL:HG12	4:Q:82:GLN:HG3	1.76	0.67
1:N:110:PHE:HD1	2:O:112:PRO:HB3	1.60	0.67
2:O:126:ARG:HH11	2:O:126:ARG:CG	2.04	0.67
4:Q:138:ARG:NE	4:Q:171:ARG:HD3	2.10	0.67
4:D:94:GLU:OE2	4:D:98:ALA:HB3	1.95	0.67
5:E:11:PHE:CD1	5:E:11:PHE:C	2.72	0.66
3:P:226:LYS:HZ1	3:P:230:ALA:HB3	1.60	0.66
3:P:275:LYS:HZ3	3:P:276:LYS:HZ1	1.42	0.66
5:R:26:ILE:HA	5:R:29:ILE:HG13	1.77	0.66
2:B:38:TYR:OH	13:B:307:OPC:HAU2	1.94	0.66
3:C:211:ILE:HD11	3:C:231:LEU:HB2	1.76	0.66
3:C:226:LYS:HE3	3:C:229:GLU:HB3	1.77	0.66
7:G:9:LEU:N	7:G:9:LEU:HD23	2.10	0.66
3:P:171:VAL:HG13	3:P:234:ASN:HD22	1.61	0.66
9:N:301:HEM:HHA	9:N:301:HEM:HBD1	1.75	0.66
4:Q:108:CYS:HB2	4:Q:113:CYS:O	1.95	0.66
8:U:4:ASP:O	8:U:8:TRP:CB	2.43	0.66
5:R:11:PHE:CD1	5:R:11:PHE:C	2.73	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:MET:HE2	1:A:128:THR:HG23	1.77	0.66
4:D:167:GLU:C	4:D:176:PRO:HG3	2.21	0.66
3:P:271:MET:HB3	4:Q:23:ALA:HA	1.77	0.66
4:Q:115:VAL:HG13	4:Q:126:CYS:HB2	1.78	0.66
6:S:34:LYS:HE2	6:S:35:GLU:H	1.60	0.66
1:A:14:ILE:HG23	1:A:15:GLN:H	1.60	0.66
1:A:26:VAL:CG2	2:B:29:GLU:HG3	2.25	0.66
1:A:101:VAL:HG11	14:B:201:CLA:HMA1	1.78	0.66
2:B:77:PRO:HG3	2:B:85:PHE:HB2	1.76	0.66
4:D:66:VAL:HG12	4:D:67:SER:N	2.11	0.66
2:O:18:LEU:HB2	2:O:31:ALA:HB2	1.77	0.66
2:O:114:ILE:O	2:O:116:ASN:N	2.28	0.66
3:P:81:GLY:C	3:P:134:PRO:HG3	2.20	0.66
4:Q:65:LYS:HD3	4:Q:68:LYS:HG2	1.78	0.66
12:A:305:PL9:H203	13:D:306:OPC:CBE	2.20	0.66
3:C:161:TYR:HE1	3:C:167:SER:CA	2.09	0.66
4:Q:150:LEU:N	4:Q:178:TRP:CZ2	2.63	0.66
1:A:158:ILE:CG2	1:A:159:PRO:HD2	2.25	0.66
3:C:28:ALA:O	3:C:239:GLY:HA3	1.94	0.66
3:C:70:LEU:HD23	3:C:70:LEU:H	1.61	0.66
4:D:105:ASN:O	4:D:107:VAL:N	2.29	0.66
4:Q:150:LEU:N	4:Q:178:TRP:HZ2	1.94	0.66
3:C:14:ARG:HG2	3:C:77:MET:HE1	1.77	0.66
3:P:1:TYR:HD2	3:P:119:LEU:HD21	1.59	0.66
3:P:120:PRO:HB2	3:P:124:TYR:HB2	1.77	0.66
4:Q:66:VAL:HG22	4:Q:160:ILE:HG13	1.76	0.66
4:D:73:HIS:NE2	4:D:91:ILE:HG22	2.11	0.65
3:P:180:ILE:HD11	3:P:182:LYS:O	1.96	0.65
3:P:226:LYS:HE3	3:P:229:GLU:C	2.20	0.65
1:A:211:ILE:H	1:A:211:ILE:CD1	2.08	0.65
2:B:21:GLY:O	2:B:22:MET:HB2	1.97	0.65
3:C:177:THR:HA	3:C:227:ALA:HA	1.78	0.65
4:Q:104:ILE:HA	4:Q:150:LEU:HD13	1.78	0.65
2:B:80:TYR:HB2	14:B:201:CLA:HED1	1.77	0.65
3:C:120:PRO:HB2	3:C:124:TYR:HB2	1.79	0.65
4:D:124:PHE:O	4:D:133:TYR:N	2.29	0.65
14:O:1201:CLA:HHC	14:O:1201:CLA:HBB1	1.76	0.65
4:Q:78:ARG:HH12	4:Q:100:ARG:HH21	1.43	0.65
12:Q:1305:PL9:H262	12:Q:1305:PL9:C21	2.12	0.65
1:A:209:GLN:CG	1:A:210:GLY:N	2.53	0.65
2:B:118:ASN:HD21	2:B:126:ARG:HD2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:27:PRO:HG3	2:O:33:PRO:CG	2.18	0.65
1:N:114:ARG:HH21	1:N:209:GLN:H	1.41	0.65
3:P:188:ASP:HB3	3:P:192:ASN:O	1.95	0.65
6:S:20:TRP:O	6:S:24:VAL:HG23	1.96	0.65
1:A:27:PRO:HG3	2:B:33:PRO:CD	2.27	0.65
1:A:106:LEU:HD12	5:E:18:ILE:CD1	2.27	0.65
4:D:155:VAL:HA	4:D:160:ILE:HA	1.79	0.65
6:F:25:LEU:HD23	6:F:25:LEU:O	1.96	0.65
3:P:90:ILE:CG2	3:P:95:LYS:HB2	2.26	0.65
3:P:218:ILE:HG13	3:P:219:VAL:H	1.60	0.65
1:A:26:VAL:HB	2:B:29:GLU:HG3	1.79	0.65
2:B:76:LEU:H	2:B:76:LEU:HD22	1.62	0.65
3:C:188:ASP:HB3	3:C:192:ASN:O	1.97	0.65
3:C:281:LYS:HA	3:C:284:ALA:CB	2.19	0.65
3:C:172:PHE:N	3:C:231:LEU:HG	2.02	0.65
4:D:134:ASP:HB3	4:D:138:ARG:CG	2.27	0.65
5:E:5:ALA:CB	6:F:5:MET:HB2	2.27	0.65
2:O:74:GLU:HG2	2:O:75:ILE:H	1.61	0.65
3:P:277:LYS:HE3	7:T:31:ARG:O	1.96	0.65
6:S:26:LEU:CD2	8:U:17:TRP:HE1	2.09	0.65
1:A:36:LEU:HD23	1:A:100:HIS:HA	1.79	0.65
11:A:304:TDS:CBB	2:B:88:LEU:HD22	2.26	0.65
3:C:231:LEU:HD11	3:C:233:ASN:O	1.96	0.65
3:P:120:PRO:HB3	3:P:124:TYR:CD1	2.32	0.65
3:P:275:LYS:C	3:P:275:LYS:HD3	2.21	0.65
12:Q:1305:PL9:H302	13:Q:1307:OPC:CBC	2.27	0.65
1:A:157:ALA:HB3	2:B:98:VAL:HG21	1.79	0.65
1:A:177:GLN:HB2	1:N:59:LYS:HZ3	1.60	0.65
4:D:51:GLY:C	4:D:85:LYS:HZ1	2.04	0.65
8:H:19:ILE:O	8:H:23:VAL:HG13	1.97	0.65
1:N:103:ARG:HH11	1:N:103:ARG:HG3	1.61	0.65
2:O:146:GLY:O	2:O:149:LEU:HG	1.97	0.65
3:P:226:LYS:HG2	3:P:229:GLU:HB3	1.79	0.65
5:R:16:PHE:HB3	16:R:1101:BCR:C36	2.20	0.65
1:A:204:LEU:C	1:A:206:ILE:H	2.04	0.64
4:D:65:LYS:HZ2	4:D:158:ASP:HB3	1.61	0.64
4:D:81:VAL:HG12	4:D:82:GLN:N	2.11	0.64
5:E:1:MET:N	5:E:1:MET:HE3	2.11	0.64
2:O:122:ASN:CG	5:R:26:ILE:HG21	2.21	0.64
3:P:118:PRO:C	3:P:120:PRO:HD3	2.22	0.64
3:P:185:LYS:HE2	3:P:195:TYR:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:14:VAL:O	7:G:17:THR:HB	1.95	0.64
1:N:47:GLN:HE22	1:N:89:SER:CB	2.11	0.64
2:O:32:TRP:HZ3	2:O:36:LEU:HA	1.62	0.64
3:P:281:LYS:CA	3:P:284:ALA:HB3	2.21	0.64
4:Q:14:GLY:O	4:Q:16:ARG:HG2	1.96	0.64
7:T:26:TYR:HD1	7:T:26:TYR:H	1.44	0.64
4:D:14:GLY:O	4:D:16:ARG:HG2	1.96	0.64
1:A:24:LYS:HD3	1:A:24:LYS:N	2.11	0.64
1:A:156:GLU:HA	1:A:162:GLY:O	1.97	0.64
2:O:27:TYR:O	2:O:27:TYR:HD2	1.80	0.64
2:O:126:ARG:HH12	2:O:128:VAL:C	2.06	0.64
3:P:177:THR:HA	3:P:227:ALA:HA	1.78	0.64
3:P:178:GLY:C	3:P:225:VAL:HA	2.23	0.64
4:Q:76:GLY:H	4:Q:93:VAL:CG1	2.01	0.64
4:Q:125:LYS:HD3	4:Q:132:GLN:HG2	1.80	0.64
3:C:273:ILE:HD13	7:G:30:LYS:CD	2.14	0.64
3:C:273:ILE:CD1	7:G:30:LYS:HD3	2.12	0.64
4:D:73:HIS:HE2	4:D:91:ILE:HG22	1.62	0.64
3:P:54:TYR:HD2	3:P:70:LEU:HD13	1.63	0.64
2:B:26:TYR:HD2	2:B:26:TYR:H	1.45	0.64
3:P:283:GLN:C	3:P:285:ALA:H	2.04	0.64
4:Q:115:VAL:HG22	4:Q:126:CYS:HB2	1.79	0.64
4:Q:153:ALA:N	4:Q:162:LEU:HG	2.12	0.64
1:A:136:TYR:CD1	2:B:78:GLU:HG2	2.33	0.64
3:C:218:ILE:HG12	3:C:232:THR:HA	1.80	0.64
4:D:66:VAL:HB	4:D:158:ASP:HA	1.80	0.64
4:Q:133:TYR:HA	4:Q:139:VAL:CA	2.27	0.64
1:A:142:GLN:NE2	2:B:67:ASN:N	2.45	0.64
3:C:216:GLU:O	3:C:233:ASN:HB2	1.96	0.64
4:D:121:GLU:OE2	4:D:125:LYS:HG3	1.98	0.64
6:F:22:LEU:O	6:F:26:LEU:HD23	1.98	0.64
6:F:27:LEU:O	6:F:30:GLN:HG3	1.96	0.64
8:H:4:ASP:O	8:H:8:TRP:CB	2.45	0.64
3:P:79:PRO:HG2	3:P:82:PHE:CE1	2.33	0.64
3:P:107:LYS:HD3	3:P:110:GLN:NE2	2.12	0.64
3:P:126:GLU:OE1	3:P:126:GLU:HA	1.96	0.64
3:C:107:LYS:HD3	3:C:110:GLN:NE2	2.13	0.64
4:D:105:ASN:O	4:D:107:VAL:HG23	1.98	0.64
1:N:28:PRO:HG2	2:O:32:TRP:HB2	1.80	0.64
1:N:31:ASN:HB3	1:N:34:TYR:CG	2.32	0.64
1:N:111:LYS:CB	1:N:114:ARG:HH11	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:64:VAL:HG12	4:Q:91:ILE:HG13	1.78	0.64
2:B:91:LEU:HD22	2:B:96:LEU:HD13	1.80	0.64
3:C:57:LYS:O	3:C:58:LEU:HB2	1.98	0.64
4:D:136:THR:CB	4:D:138:ARG:HD2	2.16	0.64
1:N:81:LEU:C	1:N:81:LEU:HD13	2.23	0.64
1:N:204:LEU:C	1:N:206:ILE:H	2.05	0.64
3:P:218:ILE:HG12	3:P:232:THR:HA	1.79	0.64
4:Q:15:ARG:NH2	4:Q:17:GLN:HG2	2.12	0.64
4:Q:94:GLU:HG2	4:Q:95:SER:H	1.62	0.64
4:Q:133:TYR:HB3	4:Q:137:GLY:C	2.23	0.64
2:O:24:HIS:O	2:O:25:ASN:ND2	2.31	0.63
3:P:57:LYS:O	3:P:58:LEU:HB2	1.97	0.63
3:P:231:LEU:CD1	3:P:232:THR:H	2.11	0.63
4:Q:134:ASP:HB2	4:Q:138:ARG:HB2	1.80	0.63
1:A:146:TRP:HB2	2:B:75:ILE:HD11	1.79	0.63
2:B:122:ASN:ND2	2:B:124:PHE:HD2	1.96	0.63
4:D:166:THR:C	4:D:179:VAL:HG22	2.23	0.63
8:H:10:ALA:O	8:H:14:VAL:HG23	1.97	0.63
1:A:27:PRO:HG3	2:B:33:PRO:HD3	1.80	0.63
3:C:185:LYS:HD3	3:C:195:TYR:HD2	1.64	0.63
3:C:234:ASN:OD1	3:C:236:ASN:HB3	1.97	0.63
2:O:20:LYS:CG	2:O:21:GLY:N	2.61	0.63
3:P:171:VAL:CG1	3:P:234:ASN:HB2	2.27	0.63
4:Q:176:PRO:HB2	4:Q:178:TRP:CZ3	2.33	0.63
2:B:122:ASN:HD21	2:B:124:PHE:HB3	1.60	0.63
3:C:270:LEU:HA	7:G:27:GLN:OE1	1.98	0.63
4:D:66:VAL:HG22	4:D:160:ILE:CG1	2.03	0.63
4:D:132:GLN:N	4:D:144:ALA:HB2	2.13	0.63
3:P:265:VAL:O	3:P:269:GLN:HG3	1.98	0.63
7:T:21:LEU:C	7:T:23:TYR:H	2.05	0.63
3:C:218:ILE:HG13	3:C:232:THR:HG22	1.81	0.63
3:P:38:GLN:OE1	7:T:15:PHE:HE1	1.80	0.63
6:S:27:LEU:O	6:S:30:GLN:HG3	1.99	0.63
8:U:19:ILE:O	8:U:23:VAL:HG13	1.99	0.63
3:C:89:ARG:O	3:C:91:PRO:HD3	1.98	0.63
6:F:26:LEU:HD21	8:H:17:TRP:HE1	1.62	0.63
8:H:23:VAL:HA	8:H:26:ARG:HD2	1.81	0.63
2:O:124:PHE:CE2	5:R:26:ILE:HB	2.33	0.63
4:Q:138:ARG:NH2	4:Q:147:SER:OG	2.31	0.63
4:D:134:ASP:OD1	4:D:135:GLU:N	2.32	0.63
4:D:150:LEU:CD1	4:D:171:ARG:HD3	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:THR:CA	4:D:179:VAL:HG13	2.13	0.63
1:N:93:MET:HE2	1:N:128:THR:HG23	1.81	0.63
4:Q:24:PHE:CD1	12:Q:1305:PL9:H202	2.34	0.63
4:Q:64:VAL:HG21	4:Q:80:LEU:C	2.23	0.63
4:Q:121:GLU:OE1	4:Q:125:LYS:HE3	1.99	0.63
1:A:177:GLN:HB2	1:N:59:LYS:NZ	2.13	0.63
3:C:262:ILE:HG21	7:G:17:THR:CG2	2.29	0.63
7:G:25:ALA:HB1	7:G:29:TYR:OH	1.99	0.63
2:O:67:ASN:HD21	3:P:16:PRO:HB3	1.63	0.63
4:Q:165:TRP:CZ2	4:Q:176:PRO:HB3	2.33	0.63
6:F:26:LEU:HB3	7:G:30:LYS:HE3	1.81	0.62
1:N:113:PRO:C	1:N:115:GLU:OE1	2.42	0.62
2:O:22:MET:HE3	2:O:23:GLY:N	2.14	0.62
5:R:3:LEU:HA	5:R:6:VAL:CG2	2.29	0.62
12:A:305:PL9:H462	12:A:305:PL9:C41	2.12	0.62
8:H:6:LEU:C	8:H:8:TRP:H	2.05	0.62
1:N:13:GLU:OE1	1:N:14:ILE:HG22	1.98	0.62
2:O:117:VAL:O	2:O:118:ASN:CB	2.47	0.62
4:Q:168:THR:HA	4:Q:176:PRO:CD	2.13	0.62
7:T:26:TYR:CD1	7:T:26:TYR:N	2.65	0.62
1:A:26:VAL:HG21	2:B:29:GLU:HG3	1.81	0.62
1:A:62:VAL:HG13	1:A:177:GLN:HB3	1.79	0.62
4:Q:155:VAL:HG12	4:Q:156:GLN:N	2.14	0.62
5:R:3:LEU:HA	5:R:6:VAL:HG23	1.81	0.62
3:C:93:GLU:CA	3:C:97:GLU:HB2	2.23	0.62
3:C:271:MET:CG	4:D:22:LEU:HD21	2.23	0.62
1:N:27:PRO:O	2:O:29:GLU:HB3	1.99	0.62
1:N:45:LEU:HB3	12:Q:1305:PL9:H502	1.81	0.62
2:O:118:ASN:HD22	2:O:121:GLN:CD	2.06	0.62
2:O:122:ASN:CG	5:R:26:ILE:CG2	2.72	0.62
3:P:94:LEU:H	3:P:94:LEU:CD2	2.06	0.62
4:Q:116:PRO:CD	4:Q:126:CYS:HA	2.24	0.62
4:D:51:GLY:CA	4:D:164:PRO:HG2	2.21	0.62
3:P:83:LYS:HB2	3:P:111:ASP:CB	2.29	0.62
13:B:307:OPC:HBC1	13:B:307:OPC:HBU2	1.80	0.62
4:D:117:TRP:HD1	4:D:124:PHE:CE1	2.17	0.62
5:E:23:ILE:HG23	5:E:24:PHE:N	2.14	0.62
3:P:10:PRO:HG2	3:P:11:PRO:HD3	1.80	0.62
13:Q:1307:OPC:HBF1	13:Q:1307:OPC:HBZ2	1.80	0.62
1:A:26:VAL:CB	2:B:29:GLU:HG3	2.29	0.62
2:B:32:TRP:CE3	2:B:36:LEU:HG	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:PRO:HG2	3:C:11:PRO:HD3	1.82	0.62
2:O:22:MET:HE3	2:O:23:GLY:H	1.65	0.62
3:P:89:ARG:O	3:P:91:PRO:HD3	2.00	0.62
4:Q:19:MET:O	4:Q:22:LEU:HB3	1.99	0.62
3:C:185:LYS:HE2	3:C:195:TYR:HB3	1.81	0.62
8:H:6:LEU:C	8:H:8:TRP:N	2.56	0.62
2:O:57:LEU:HD21	3:P:258:MET:CE	2.28	0.62
5:R:5:ALA:CB	6:S:5:MET:HB2	2.30	0.62
2:B:149:LEU:HB2	2:B:150:PRO:CD	2.29	0.62
3:C:218:ILE:HG13	3:C:219:VAL:N	2.14	0.62
4:D:121:GLU:OE1	4:D:125:LYS:HE3	2.00	0.62
5:E:27:LYS:O	5:E:31:LEU:HD22	1.99	0.62
2:O:20:LYS:CD	2:O:21:GLY:H	2.13	0.62
13:Q:1307:OPC:HAP1	13:Q:1307:OPC:HAL2	1.82	0.62
2:B:57:LEU:HD21	3:C:258:MET:CE	2.25	0.62
2:B:114:ILE:C	2:B:116:ASN:H	2.07	0.62
4:D:90:TYR:CE2	4:D:106:ALA:HB2	2.34	0.62
7:G:26:TYR:CD1	7:G:26:TYR:N	2.67	0.62
1:N:21:VAL:HG12	1:N:22:THR:N	2.15	0.62
1:N:21:VAL:O	1:N:23:SER:N	2.32	0.62
2:O:122:ASN:HD21	5:R:30:LYS:HG3	1.64	0.62
3:P:111:ASP:O	3:P:114:LEU:HD21	2.00	0.62
4:Q:134:ASP:CB	4:Q:138:ARG:HB2	2.30	0.62
7:T:9:LEU:HD23	7:T:9:LEU:N	2.15	0.62
7:T:28:GLN:O	7:T:30:LYS:N	2.33	0.62
1:A:13:GLU:C	1:A:17:LEU:HD12	2.25	0.61
2:B:18:LEU:O	2:B:19:ALA:HB3	1.99	0.61
3:C:275:LYS:C	3:C:275:LYS:HD3	2.25	0.61
3:P:275:LYS:CD	4:Q:20:ASN:HB3	2.30	0.61
5:R:23:ILE:HG23	5:R:24:PHE:N	2.14	0.61
4:D:73:HIS:ND1	4:D:77:ASP:HB3	2.15	0.61
4:D:121:GLU:HB3	4:D:123:LYS:HG3	1.80	0.61
3:P:172:PHE:C	3:P:231:LEU:HB3	2.25	0.61
4:D:111:LEU:HB3	4:D:129:HIS:CE1	2.36	0.61
13:N:1306:OPC:HAP2	13:N:1306:OPC:CBI	2.23	0.61
2:O:20:LYS:CG	2:O:21:GLY:H	2.13	0.61
2:O:144:GLY:O	2:O:145:ILE:HD13	2.00	0.61
3:P:188:ASP:HB3	3:P:193:VAL:HA	1.82	0.61
1:A:30:VAL:HG21	5:E:26:ILE:HD11	1.82	0.61
4:D:136:THR:HG22	4:D:150:LEU:HD11	1.83	0.61
3:P:117:GLY:O	3:P:119:LEU:HG	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:O	1:A:16:ALA:HB3	2.00	0.61
1:A:116:LEU:HD12	1:A:116:LEU:N	2.14	0.61
3:C:171:VAL:HB	3:C:231:LEU:CD1	2.30	0.61
3:C:226:LYS:HG2	3:C:229:GLU:CB	2.30	0.61
3:C:269:GLN:CD	7:G:24:ALA:HA	2.26	0.61
3:C:275:LYS:HB2	4:D:19:MET:HE2	1.82	0.61
1:A:105:TYR:HD2	1:A:106:LEU:HD23	1.65	0.61
11:N:1304:TDS:HAU1	14:O:1201:CLA:H91	1.81	0.61
2:O:134:LEU:O	2:O:138:LEU:HD13	2.01	0.61
4:Q:66:VAL:C	4:Q:68:LYS:H	2.09	0.61
7:T:26:TYR:HD1	7:T:26:TYR:N	1.97	0.61
3:C:188:ASP:HB3	3:C:193:VAL:HA	1.81	0.61
3:P:231:LEU:HD13	3:P:232:THR:N	2.14	0.61
5:R:21:GLY:O	5:R:25:ALA:HB2	2.00	0.61
1:N:109:GLY:C	1:N:111:LYS:H	2.08	0.61
1:N:158:ILE:O	1:N:162:GLY:HA3	2.01	0.61
9:N:301:HEM:HBD1	9:N:301:HEM:CHA	2.31	0.61
4:D:65:LYS:HD3	4:D:68:LYS:NZ	2.16	0.61
13:N:1306:OPC:HAT1	13:N:1306:OPC:HBQ2	1.82	0.61
4:Q:104:ILE:CD1	4:Q:136:THR:HA	2.30	0.61
1:N:98:ILE:HD11	14:O:1201:CLA:HED3	1.81	0.61
1:N:196:ALA:O	1:N:200:LEU:HB2	2.00	0.61
2:O:124:PHE:HZ	5:R:26:ILE:CB	2.10	0.61
3:P:226:LYS:HE3	3:P:229:GLU:HB3	1.81	0.61
1:A:200:LEU:O	1:A:204:LEU:HG	2.00	0.60
2:B:75:ILE:O	2:B:76:LEU:O	2.18	0.60
5:E:18:ILE:O	5:E:22:ILE:HB	2.01	0.60
1:N:116:LEU:HD12	1:N:116:LEU:N	2.14	0.60
3:P:91:PRO:HD2	3:P:95:LYS:CG	2.31	0.60
4:Q:65:LYS:HB2	4:Q:68:LYS:HB2	1.82	0.60
4:Q:172:THR:HB	4:Q:174:GLU:OE2	2.01	0.60
2:B:112:PRO:O	2:B:116:ASN:CB	2.49	0.60
3:C:171:VAL:HG12	3:C:233:ASN:O	2.01	0.60
1:N:214:PRO:CB	5:R:29:ILE:HG22	2.13	0.60
2:O:118:ASN:ND2	2:O:121:GLN:HE22	1.95	0.60
3:C:86:PRO:HG2	3:C:89:ARG:HG3	1.83	0.60
1:N:110:PHE:HE1	2:O:111:VAL:HG12	1.67	0.60
2:O:75:ILE:O	2:O:77:PRO:HD2	2.01	0.60
4:Q:56:ALA:CA	4:Q:81:VAL:HG13	2.21	0.60
4:Q:58:ASP:OD1	4:Q:64:VAL:HG22	2.01	0.60
4:D:42:PHE:CD1	13:D:306:OPC:HAG2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:136:THR:HB	4:D:138:ARG:CD	2.17	0.60
4:D:168:THR:CA	4:D:176:PRO:HD3	2.31	0.60
1:N:37:GLY:HA3	9:N:302:HEM:HBA1	1.82	0.60
3:C:83:LYS:HB2	3:C:111:ASP:CB	2.30	0.60
3:C:90:ILE:CG2	3:C:95:LYS:HB2	2.32	0.60
3:C:275:LYS:CE	4:D:17:GLN:HB2	2.32	0.60
3:P:45:VAL:HG22	3:P:85:ALA:HB2	1.83	0.60
5:R:5:ALA:HA	5:R:8:TYR:HB2	1.84	0.60
2:B:155:LEU:C	2:B:155:LEU:HD23	2.25	0.60
3:C:180:ILE:O	3:C:221:GLU:HA	2.02	0.60
3:C:188:ASP:O	3:C:189:GLU:HB2	2.01	0.60
4:D:19:MET:O	4:D:22:LEU:HB3	2.01	0.60
4:D:123:LYS:HD2	4:D:140:ILE:HD11	1.83	0.60
2:O:106:LEU:HD11	14:O:1201:CLA:H171	1.84	0.60
4:Q:81:VAL:HB	4:Q:89:THR:OG1	2.01	0.60
1:A:175:VAL:O	1:A:175:VAL:HG12	2.01	0.60
12:A:305:PL9:H252	13:D:306:OPC:CBN	2.31	0.60
3:C:262:ILE:HG21	7:G:17:THR:HG23	1.82	0.60
1:N:28:PRO:HG2	2:O:32:TRP:CB	2.31	0.60
2:O:141:ILE:HD11	5:R:11:PHE:CZ	2.36	0.60
3:C:218:ILE:HG12	3:C:232:THR:CA	2.31	0.60
6:F:11:LEU:O	6:F:15:LEU:HD23	2.02	0.60
3:P:180:ILE:O	3:P:221:GLU:HA	2.02	0.60
3:P:218:ILE:HG13	3:P:219:VAL:N	2.17	0.60
16:R:1101:BCR:H362	6:S:17:PHE:HZ	1.67	0.60
3:C:116:VAL:O	3:C:116:VAL:HG12	2.00	0.60
4:D:100:ARG:O	4:D:153:ALA:HB2	2.02	0.60
4:D:101:ASP:HA	4:D:153:ALA:HB2	1.82	0.60
4:Q:129:HIS:HB2	15:Q:1200:FES:S1	2.42	0.60
2:B:38:TYR:OH	13:B:307:OPC:HAS2	2.01	0.59
2:B:42:VAL:HG23	3:C:272:LEU:HD13	1.82	0.59
2:B:124:PHE:HE1	5:E:23:ILE:HG13	1.67	0.59
3:C:55:ASP:OD1	3:C:57:LYS:HG3	2.02	0.59
4:D:13:MET:SD	4:D:13:MET:N	2.75	0.59
4:D:66:VAL:HG11	4:D:155:VAL:HG11	1.83	0.59
4:D:137:GLY:CA	4:D:148:LEU:HB2	2.32	0.59
1:N:191:LEU:HD21	11:N:1304:TDS:OBD	2.02	0.59
2:B:70:ALA:HB1	3:C:17:THR:HA	1.83	0.59
5:E:1:MET:HE3	5:E:1:MET:H3	1.65	0.59
7:G:26:TYR:CA	7:G:29:TYR:CD1	2.82	0.59
2:O:146:GLY:O	2:O:149:LEU:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:HD13	1:A:96:MET:CE	2.32	0.59
4:D:121:GLU:O	4:D:122:ASN:HB2	2.03	0.59
13:D:306:OPC:HAY2	13:D:306:OPC:HBC2	1.83	0.59
1:N:39:ILE:HD11	16:R:1101:BCR:H312	1.83	0.59
3:P:217:LEU:CA	3:P:232:THR:HB	2.32	0.59
4:Q:66:VAL:O	4:Q:70:LEU:HB2	2.02	0.59
4:Q:96:LYS:O	4:Q:97:GLU:HB2	2.01	0.59
12:A:305:PL9:H111	13:D:306:OPC:CBF	2.32	0.59
2:B:34:ASN:ND2	13:B:307:OPC:CBK	2.64	0.59
3:C:45:VAL:HG22	3:C:85:ALA:HB2	1.84	0.59
3:C:266:MET:HE3	7:G:23:TYR:CB	2.32	0.59
4:D:138:ARG:NE	4:D:171:ARG:HD2	2.18	0.59
7:G:11:LEU:HA	7:G:14:VAL:HG11	1.84	0.59
3:P:194:LYS:HE3	3:P:212:PRO:HB3	1.83	0.59
4:D:132:GLN:H	4:D:144:ALA:HB2	1.68	0.59
7:G:11:LEU:HA	7:G:14:VAL:HG13	1.85	0.59
3:P:28:ALA:O	3:P:239:GLY:HA3	2.03	0.59
3:P:105:PRO:HB3	3:P:110:GLN:O	2.02	0.59
3:P:278:GLN:O	3:P:281:LYS:HE2	2.03	0.59
4:Q:94:GLU:HG2	4:Q:95:SER:N	2.18	0.59
2:B:71:THR:CB	2:B:72:PRO:HD3	2.11	0.59
3:C:171:VAL:HG13	3:C:234:ASN:HD22	1.68	0.59
3:P:40:VAL:HG13	3:P:247:ILE:HD11	1.85	0.59
4:Q:66:VAL:HG22	4:Q:160:ILE:HG12	1.85	0.59
2:B:32:TRP:CZ3	2:B:36:LEU:HG	2.37	0.59
2:B:86:GLN:HG2	2:B:143:LEU:HA	1.84	0.59
3:C:269:GLN:NE2	7:G:24:ALA:HA	2.17	0.59
4:D:123:LYS:HZ1	4:D:140:ILE:HG13	1.67	0.59
5:E:3:LEU:HA	5:E:6:VAL:HG23	1.85	0.59
6:F:12:SER:O	6:F:16:ILE:HG12	2.02	0.59
3:P:195:TYR:O	3:P:196:GLN:O	2.21	0.59
4:Q:55:THR:O	4:Q:56:ALA:HB3	2.03	0.59
4:Q:91:ILE:HG23	4:Q:160:ILE:CD1	2.32	0.59
3:C:49:VAL:HG22	3:C:128:VAL:HG22	1.85	0.59
3:C:54:TYR:HD2	3:C:70:LEU:HD13	1.66	0.59
3:C:226:LYS:HZ1	3:C:230:ALA:HB3	1.65	0.59
4:D:65:LYS:O	4:D:68:LYS:HB2	2.03	0.59
4:D:99:ILE:HD12	4:D:99:ILE:O	2.03	0.59
8:H:17:TRP:O	8:H:20:ALA:HB3	2.03	0.59
1:N:141:ASP:C	2:O:64:GLU:HG2	2.27	0.59
3:P:86:PRO:HG2	3:P:89:ARG:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:216:GLU:HB2	3:P:233:ASN:OD1	2.03	0.59
4:Q:93:VAL:HG22	4:Q:94:GLU:N	2.17	0.59
7:T:31:ARG:HD3	7:T:32:PRO:HD3	1.85	0.59
11:A:304:TDS:CBC	2:B:85:PHE:HD2	2.15	0.59
2:B:124:PHE:C	2:B:124:PHE:CD1	2.80	0.59
5:E:5:ALA:HA	5:E:8:TYR:HB2	1.85	0.59
8:H:11:LEU:HB3	8:H:15:PHE:HZ	1.66	0.59
1:N:154:VAL:HG11	11:N:1304:TDS:HAX1	1.84	0.59
2:O:25:ASN:OD1	2:O:26:TYR:N	2.35	0.59
5:R:16:PHE:O	5:R:20:VAL:HB	2.03	0.59
1:A:35:CYS:O	1:A:39:ILE:HG12	2.02	0.59
3:C:117:GLY:O	3:C:118:PRO:C	2.45	0.59
3:C:118:PRO:C	3:C:120:PRO:HD3	2.28	0.59
5:E:26:ILE:HA	5:E:29:ILE:HG13	1.84	0.59
4:Q:134:ASP:OD1	4:Q:138:ARG:HB2	2.03	0.59
4:Q:138:ARG:HB3	4:Q:138:ARG:NH1	2.18	0.59
4:Q:156:GLN:CB	4:Q:161:VAL:HG21	2.23	0.59
5:R:9:ILE:HG12	6:S:13:PHE:HB2	1.85	0.59
7:T:21:LEU:C	7:T:23:TYR:N	2.58	0.59
2:O:148:ALA:C	2:O:149:LEU:O	2.44	0.58
7:T:17:THR:O	7:T:21:LEU:HB2	2.03	0.58
2:B:118:ASN:CB	2:B:121:GLN:O	2.49	0.58
2:B:149:LEU:HD12	2:B:149:LEU:N	2.18	0.58
3:C:194:LYS:HE3	3:C:212:PRO:HB3	1.85	0.58
3:C:221:GLU:CD	3:C:221:GLU:H	2.12	0.58
4:D:80:LEU:HD13	4:D:88:PRO:HB2	1.85	0.58
4:D:131:SER:OG	4:D:144:ALA:HA	2.02	0.58
3:P:49:VAL:HG22	3:P:128:VAL:HG22	1.85	0.58
3:P:116:VAL:O	3:P:116:VAL:HG12	2.03	0.58
1:A:23:SER:HB2	1:A:24:LYS:HD3	1.86	0.58
2:B:151:LEU:C	2:B:153:LYS:N	2.62	0.58
3:C:59:GLN:CB	3:C:67:LYS:HB3	2.33	0.58
4:D:65:LYS:HD3	4:D:68:LYS:HZ1	1.68	0.58
5:E:3:LEU:O	5:E:4:GLY:C	2.47	0.58
4:Q:66:VAL:HG12	4:Q:70:LEU:HD12	1.85	0.58
4:Q:73:HIS:HA	4:Q:77:ASP:CG	2.28	0.58
13:Q:1307:OPC:HAT1	13:Q:1307:OPC:CAX	2.33	0.58
7:T:27:GLN:HA	7:T:27:GLN:NE2	2.18	0.58
1:A:33:PHE:CE1	5:E:14:LEU:HD22	2.39	0.58
12:A:305:PL9:H162	13:B:307:OPC:HBU1	1.84	0.58
3:C:50:VAL:HG13	3:C:151:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:LYS:CD	3:C:229:GLU:HB3	2.33	0.58
4:D:104:ILE:CG2	4:D:148:LEU:HB3	2.34	0.58
4:D:134:ASP:N	4:D:138:ARG:O	2.36	0.58
7:G:30:LYS:O	7:G:31:ARG:CZ	2.50	0.58
1:N:23:SER:HA	1:N:25:TYR:CE2	2.39	0.58
2:O:24:HIS:N	2:O:24:HIS:ND1	2.50	0.58
3:P:218:ILE:HG12	3:P:232:THR:CA	2.33	0.58
3:P:275:LYS:CE	4:Q:17:GLN:HB2	2.32	0.58
4:Q:142:GLY:CA	4:Q:144:ALA:H	2.17	0.58
16:R:1101:BCR:H362	6:S:17:PHE:CZ	2.38	0.58
3:C:91:PRO:HD2	3:C:95:LYS:CG	2.33	0.58
3:C:216:GLU:O	3:C:233:ASN:CB	2.51	0.58
4:D:50:VAL:HG12	4:D:164:PRO:HB3	1.84	0.58
1:N:95:LEU:HD13	1:N:96:MET:CE	2.33	0.58
3:P:231:LEU:HD12	3:P:231:LEU:H	1.68	0.58
4:Q:78:ARG:NH2	4:Q:100:ARG:NH2	2.46	0.58
1:A:196:ALA:O	1:A:200:LEU:HB2	2.04	0.58
1:A:207:ARG:C	1:A:208:LYS:HD2	2.28	0.58
3:C:255:VAL:CG1	7:G:14:VAL:CG1	2.74	0.58
8:H:12:LEU:HA	8:H:15:PHE:CD1	2.38	0.58
3:P:59:GLN:CB	3:P:67:LYS:HB3	2.34	0.58
4:Q:168:THR:HG23	4:Q:175:LYS:N	2.17	0.58
8:U:6:LEU:C	8:U:8:TRP:N	2.57	0.58
1:A:159:PRO:C	1:A:161:VAL:H	2.06	0.58
6:F:7:TYR:O	6:F:11:LEU:HD12	2.04	0.58
7:G:26:TYR:N	7:G:26:TYR:HD1	2.00	0.58
8:U:7:GLY:O	8:U:11:LEU:HD11	2.03	0.58
8:U:23:VAL:O	8:U:27:ASN:ND2	2.36	0.58
3:C:120:PRO:HB3	3:C:124:TYR:CD1	2.39	0.58
3:C:261:PHE:CE2	4:D:30:VAL:HG13	2.38	0.58
4:D:129:HIS:O	4:D:143:PRO:HG3	2.03	0.58
4:D:137:GLY:HA3	4:D:148:LEU:HB2	1.85	0.58
7:G:9:LEU:HG	7:G:10:VAL:H	1.69	0.58
1:A:193:TRP:O	1:A:197:VAL:HG23	2.03	0.58
4:Q:152:HIS:H	4:Q:162:LEU:HD23	1.69	0.58
2:B:38:TYR:HB3	3:C:276:LYS:CG	2.32	0.58
4:D:93:VAL:HG13	4:D:94:GLU:O	2.03	0.58
4:D:116:PRO:CG	4:D:126:CYS:HA	2.34	0.58
1:N:188:THR:CG2	9:N:301:HEM:HBC2	2.33	0.58
3:P:188:ASP:O	3:P:189:GLU:HB2	2.03	0.58
12:A:305:PL9:H513	4:D:28:THR:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:C	2:B:38:TYR:H	2.11	0.57
3:C:283:GLN:C	3:C:285:ALA:H	2.10	0.57
7:G:26:TYR:HA	7:G:29:TYR:HD1	1.61	0.57
1:N:142:GLN:HE21	2:O:64:GLU:CD	2.12	0.57
2:O:21:GLY:C	2:O:24:HIS:CD2	2.82	0.57
2:B:119:LYS:HD3	2:B:119:LYS:O	2.03	0.57
4:D:134:ASP:HB3	4:D:138:ARG:HG2	1.85	0.57
4:Q:123:LYS:HB2	4:Q:125:LYS:HE2	1.86	0.57
13:Q:1307:OPC:HBG3	13:Q:1307:OPC:CAQ	2.34	0.57
8:U:6:LEU:HA	8:U:9:VAL:HG12	1.86	0.57
3:C:3:PHE:HZ	3:C:119:LEU:HD11	1.69	0.57
3:C:93:GLU:O	3:C:94:LEU:C	2.48	0.57
4:Q:178:TRP:N	4:Q:178:TRP:CE3	2.69	0.57
4:D:84:LEU:O	4:D:86:GLY:N	2.37	0.57
7:G:25:ALA:O	7:G:29:TYR:CD2	2.57	0.57
1:N:29:HIS:HE2	1:N:209:GLN:CG	2.16	0.57
1:N:112:LYS:HB2	1:N:113:PRO:CD	2.27	0.57
3:P:52:ILE:HG12	3:P:153:ALA:CB	2.34	0.57
3:P:255:VAL:CG1	7:T:14:VAL:HG12	2.34	0.57
4:Q:88:PRO:HG3	4:Q:106:ALA:N	2.20	0.57
4:Q:123:LYS:O	4:Q:125:LYS:HG2	2.03	0.57
1:A:27:PRO:HG3	2:B:33:PRO:HG3	1.87	0.57
4:D:150:LEU:HD13	4:D:171:ARG:HD3	1.86	0.57
3:P:84:ILE:HD12	3:P:130:PRO:HD2	1.86	0.57
3:P:217:LEU:HA	3:P:232:THR:CB	2.33	0.57
3:C:278:GLN:O	3:C:281:LYS:HE2	2.04	0.57
4:D:110:HIS:CE1	4:D:129:HIS:HB2	2.39	0.57
4:D:136:THR:HG22	4:D:136:THR:O	2.04	0.57
3:P:202:ASP:HA	3:P:206:THR:CB	2.25	0.57
4:Q:64:VAL:O	4:Q:91:ILE:HD11	2.04	0.57
1:A:32:ILE:C	1:A:34:TYR:H	2.13	0.57
3:C:79:PRO:HG2	3:C:82:PHE:CE1	2.39	0.57
3:C:117:GLY:O	3:C:119:LEU:HG	2.05	0.57
4:D:124:PHE:CB	4:D:133:TYR:HB2	2.22	0.57
2:O:72:PRO:O	2:O:73:LEU:HB3	2.04	0.57
3:P:216:GLU:O	3:P:233:ASN:HB2	2.03	0.57
3:P:258:MET:O	3:P:262:ILE:HD13	2.04	0.57
7:T:28:GLN:C	7:T:30:LYS:N	2.61	0.57
1:A:62:VAL:HG13	1:A:177:GLN:CB	2.34	0.57
1:A:154:VAL:HG11	2:B:101:MET:HE1	1.84	0.57
3:C:202:ASP:HA	3:C:206:THR:CB	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:231:LEU:HD22	3:C:232:THR:N	2.19	0.57
1:N:79:GLY:HA2	4:Q:41:TYR:HE1	1.69	0.57
2:O:133:PHE:HA	14:O:1201:CLA:HMB2	1.86	0.57
3:P:61:VAL:O	3:P:157:ARG:NH1	2.37	0.57
1:A:207:ARG:O	1:A:208:LYS:HD2	2.05	0.57
2:B:134:LEU:O	2:B:138:LEU:HD13	2.05	0.57
3:C:276:LYS:HA	3:C:276:LYS:HE3	1.87	0.57
4:D:128:CYS:HB3	4:D:129:HIS:CE1	2.40	0.57
4:D:166:THR:HG23	4:D:179:VAL:HG11	1.86	0.57
2:O:74:GLU:O	2:O:75:ILE:HB	2.05	0.57
3:P:91:PRO:HD2	3:P:95:LYS:HG2	1.86	0.57
2:B:32:TRP:H	2:B:33:PRO:HD3	1.70	0.57
3:C:271:MET:HB3	4:D:23:ALA:HA	1.87	0.57
5:E:3:LEU:HA	5:E:6:VAL:CG2	2.34	0.57
5:E:27:LYS:O	5:E:31:LEU:HB2	2.05	0.57
8:H:23:VAL:O	8:H:27:ASN:ND2	2.37	0.57
4:Q:116:PRO:HD2	4:Q:126:CYS:CA	2.26	0.57
2:B:18:LEU:O	2:B:19:ALA:CB	2.51	0.56
2:B:84:VAL:O	2:B:88:LEU:HD13	2.04	0.56
1:N:33:PHE:HB3	1:N:103:ARG:HG2	1.87	0.56
1:N:95:LEU:HG	5:R:7:PHE:CB	2.34	0.56
1:N:111:LYS:CB	1:N:114:ARG:NH1	2.68	0.56
1:N:209:GLN:CB	2:O:27:TYR:HB2	2.35	0.56
2:O:80:TYR:N	2:O:80:TYR:CD1	2.73	0.56
1:A:88:TRP:HZ2	2:B:58:ASP:HB3	1.69	0.56
2:B:155:LEU:HD23	2:B:155:LEU:O	2.04	0.56
1:N:149:LYS:HD2	1:N:175:VAL:CG2	2.34	0.56
2:O:79:TRP:CZ2	5:R:1:MET:N	2.66	0.56
2:O:127:PRO:C	2:O:129:ALA:N	2.63	0.56
12:Q:1305:PL9:C32	13:Q:1307:OPC:HBW2	2.34	0.56
7:T:17:THR:O	7:T:21:LEU:CB	2.52	0.56
1:A:26:VAL:HB	2:B:29:GLU:CG	2.35	0.56
1:A:106:LEU:HD12	5:E:18:ILE:HD12	1.85	0.56
1:A:177:GLN:H	1:A:177:GLN:CD	2.13	0.56
2:B:41:PRO:O	2:B:45:MET:HG3	2.06	0.56
3:C:185:LYS:HE2	3:C:195:TYR:CB	2.35	0.56
5:E:5:ALA:HB2	6:F:5:MET:HB2	1.87	0.56
5:E:9:ILE:HG23	6:F:12:SER:HB2	1.88	0.56
7:G:30:LYS:CB	7:G:31:ARG:NH2	2.66	0.56
1:N:213:GLY:O	5:R:30:LYS:CD	2.49	0.56
2:O:32:TRP:N	2:O:33:PRO:CD	2.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:141:ILE:O	2:O:144:GLY:N	2.39	0.56
3:P:93:GLU:CA	3:P:97:GLU:HB2	2.28	0.56
3:P:219:VAL:HG11	3:P:223:GLN:NE2	2.19	0.56
4:Q:13:MET:N	4:Q:13:MET:SD	2.78	0.56
7:T:28:GLN:O	7:T:31:ARG:HB3	2.06	0.56
8:U:6:LEU:C	8:U:8:TRP:H	2.13	0.56
1:A:81:LEU:HD13	1:A:81:LEU:C	2.30	0.56
4:D:65:LYS:NZ	4:D:158:ASP:HB3	2.20	0.56
5:E:6:VAL:O	5:E:10:VAL:HB	2.04	0.56
1:N:118:TRP:CZ3	2:O:108:LEU:O	2.58	0.56
3:P:12:THR:OG1	3:P:13:PRO:HD2	2.06	0.56
3:P:38:GLN:OE1	7:T:15:PHE:CE1	2.59	0.56
3:P:54:TYR:OH	3:P:58:LEU:HD22	2.05	0.56
5:R:9:ILE:HG23	6:S:12:SER:HB2	1.88	0.56
1:A:14:ILE:CD1	1:A:15:GLN:N	2.67	0.56
6:F:15:LEU:HD12	7:G:26:TYR:OH	2.05	0.56
3:P:221:GLU:H	3:P:221:GLU:CD	2.14	0.56
3:P:223:GLN:O	3:P:224:ALA:HB3	2.05	0.56
4:Q:73:HIS:O	4:Q:74:ASN:HB2	2.04	0.56
7:T:11:LEU:HA	7:T:14:VAL:CG1	2.36	0.56
1:A:13:GLU:O	1:A:17:LEU:HD12	2.06	0.56
1:A:172:GLY:O	1:A:173:SER:C	2.48	0.56
3:C:271:MET:HG3	4:D:22:LEU:CD2	2.26	0.56
4:D:19:MET:HE3	4:D:22:LEU:HD22	1.88	0.56
8:H:6:LEU:HA	8:H:9:VAL:HG12	1.87	0.56
2:O:86:GLN:HG2	2:O:143:LEU:HA	1.87	0.56
2:O:112:PRO:O	2:O:116:ASN:CB	2.53	0.56
5:R:6:VAL:O	5:R:10:VAL:HB	2.05	0.56
1:A:77:SER:O	1:A:78:PHE:HB2	2.05	0.56
2:B:37:LEU:HD23	2:B:40:PHE:CE2	2.41	0.56
3:C:86:PRO:CG	3:C:89:ARG:HG3	2.36	0.56
7:G:25:ALA:O	7:G:29:TYR:CG	2.59	0.56
1:N:15:GLN:O	1:N:17:LEU:N	2.39	0.56
2:O:32:TRP:N	2:O:33:PRO:HD3	2.20	0.56
3:C:94:LEU:H	3:C:94:LEU:CD2	2.12	0.56
7:G:11:LEU:CA	7:G:14:VAL:HG13	2.36	0.56
4:Q:100:ARG:HD2	4:Q:102:TYR:CZ	2.40	0.56
6:S:12:SER:O	6:S:16:ILE:HG12	2.05	0.56
1:A:72:ILE:O	1:A:79:GLY:HA3	2.06	0.56
2:B:36:LEU:O	2:B:39:VAL:HG22	2.06	0.56
3:C:178:GLY:HA2	3:C:225:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:SER:CB	4:D:144:ALA:HA	2.36	0.56
2:O:74:GLU:CG	2:O:75:ILE:H	2.18	0.56
2:O:96:LEU:O	2:O:100:LEU:HB2	2.05	0.56
4:Q:137:GLY:C	4:Q:171:ARG:HH12	2.14	0.56
4:Q:152:HIS:O	4:Q:153:ALA:HB2	2.05	0.56
5:R:7:PHE:CA	5:R:10:VAL:HG12	2.23	0.56
13:B:307:OPC:HAP1	13:B:307:OPC:CBI	2.26	0.56
7:G:15:PHE:C	7:G:17:THR:N	2.63	0.56
13:N:1306:OPC:HBQ2	13:N:1306:OPC:CAT	2.36	0.56
4:Q:156:GLN:HB2	4:Q:161:VAL:HG11	1.88	0.56
6:S:26:LEU:HD21	8:U:17:TRP:HE1	1.70	0.56
7:G:17:THR:O	7:G:21:LEU:CB	2.54	0.55
7:G:30:LYS:O	7:G:31:ARG:NE	2.39	0.55
2:O:91:LEU:HD22	2:O:96:LEU:HD13	1.88	0.55
3:P:134:PRO:CB	3:P:142:ILE:HD13	2.35	0.55
5:R:3:LEU:O	5:R:4:GLY:C	2.49	0.55
3:C:269:GLN:HE22	7:G:24:ALA:CA	2.19	0.55
4:D:57:LYS:H	4:D:82:GLN:CG	2.20	0.55
2:O:75:ILE:N	2:O:75:ILE:HD12	2.22	0.55
4:Q:16:ARG:C	4:Q:18:PHE:N	2.64	0.55
4:Q:138:ARG:HB3	4:Q:138:ARG:HH11	1.69	0.55
6:S:11:LEU:O	6:S:15:LEU:HD23	2.06	0.55
1:A:166:SER:O	1:A:170:ARG:HG2	2.06	0.55
4:D:100:ARG:C	4:D:153:ALA:HB2	2.31	0.55
5:E:26:ILE:HD12	5:E:26:ILE:N	2.22	0.55
1:N:31:ASN:HB3	1:N:34:TYR:CD2	2.41	0.55
2:O:30:PRO:HG2	2:O:31:ALA:H	1.71	0.55
3:P:194:LYS:HD3	3:P:212:PRO:HA	1.89	0.55
3:P:255:VAL:O	3:P:258:MET:HG3	2.07	0.55
3:P:276:LYS:HA	3:P:276:LYS:HE3	1.89	0.55
13:Q:1307:OPC:CBF	13:Q:1307:OPC:HBZ2	2.37	0.55
8:U:3:ILE:HG13	8:U:4:ASP:OD1	2.06	0.55
2:B:79:TRP:C	2:B:81:LEU:H	2.14	0.55
2:B:142:TRP:CD1	2:B:155:LEU:C	2.85	0.55
2:B:150:PRO:HG2	2:B:151:LEU:H	1.72	0.55
3:C:216:GLU:HB2	3:C:233:ASN:OD1	2.06	0.55
3:C:218:ILE:CG1	3:C:232:THR:HG22	2.36	0.55
4:D:73:HIS:HE2	4:D:91:ILE:CG2	2.19	0.55
3:P:26:HIS:ND1	3:P:154:ASN:OD1	2.39	0.55
3:P:168:ASN:HA	3:P:172:PHE:CE1	2.40	0.55
4:Q:155:VAL:HA	4:Q:159:ASN:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:14:VAL:HG23	7:T:15:PHE:N	2.21	0.55
1:A:108:GLY:HA2	1:A:110:PHE:CE2	2.41	0.55
2:B:31:ALA:O	2:B:32:TRP:CB	2.46	0.55
4:D:118:ASN:OD1	4:D:123:LYS:C	2.50	0.55
7:G:28:GLN:O	7:G:30:LYS:N	2.39	0.55
13:N:1306:OPC:HBQ2	13:N:1306:OPC:HAU2	1.89	0.55
2:O:73:LEU:C	2:O:73:LEU:HD12	2.31	0.55
4:Q:101:ASP:HA	4:Q:153:ALA:CB	2.37	0.55
1:A:88:TRP:CZ2	2:B:58:ASP:HB3	2.42	0.55
3:C:111:ASP:O	3:C:114:LEU:HD21	2.06	0.55
3:C:185:LYS:HE3	3:C:217:LEU:HD11	1.89	0.55
3:C:226:LYS:CG	3:C:229:GLU:HB3	2.36	0.55
3:C:266:MET:HE3	7:G:23:TYR:HB3	1.88	0.55
4:D:95:SER:C	4:D:97:GLU:H	2.14	0.55
4:D:168:THR:HA	4:D:176:PRO:CD	2.36	0.55
1:N:28:PRO:O	2:O:30:PRO:HG2	2.07	0.55
1:N:141:ASP:HA	2:O:65:PRO:CD	2.35	0.55
2:O:32:TRP:CZ3	2:O:36:LEU:HG	2.42	0.55
4:Q:92:VAL:HG21	4:Q:100:ARG:HB2	1.87	0.55
5:R:27:LYS:O	5:R:31:LEU:HD22	2.06	0.55
1:A:95:LEU:HD11	5:E:10:VAL:HG11	1.88	0.55
2:B:149:LEU:CD1	2:B:149:LEU:N	2.66	0.55
1:N:193:TRP:O	1:N:197:VAL:HG23	2.07	0.55
1:N:213:GLY:O	5:R:26:ILE:HG23	2.06	0.55
2:O:133:PHE:CD2	14:O:1201:CLA:HMB2	2.42	0.55
3:P:82:PHE:O	3:P:112:ASN:HB3	2.07	0.55
3:P:119:LEU:HD12	3:P:119:LEU:H	1.69	0.55
4:Q:115:VAL:CG1	4:Q:124:PHE:HB3	2.35	0.55
7:T:22:PHE:C	7:T:26:TYR:CE1	2.85	0.55
1:A:211:ILE:HD12	1:A:211:ILE:N	2.14	0.55
2:B:42:VAL:CG2	3:C:272:LEU:HD13	2.37	0.55
4:D:104:ILE:HG21	4:D:148:LEU:HB3	1.89	0.55
4:D:134:ASP:CG	4:D:135:GLU:N	2.61	0.55
4:D:138:ARG:HB3	4:D:138:ARG:CZ	2.37	0.55
5:R:5:ALA:HB2	6:S:5:MET:HB2	1.89	0.55
2:B:88:LEU:HD11	2:B:101:MET:SD	2.46	0.55
2:O:86:GLN:HG3	2:O:143:LEU:HD22	1.89	0.55
3:P:185:LYS:HD3	3:P:195:TYR:CD2	2.41	0.55
4:Q:104:ILE:HG21	4:Q:124:PHE:HE2	1.71	0.55
3:C:40:VAL:HG13	3:C:247:ILE:HD11	1.89	0.55
3:C:178:GLY:C	3:C:225:VAL:HA	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:GLU:HG3	3:C:188:ASP:N	2.22	0.55
4:D:88:PRO:O	4:D:105:ASN:HA	2.07	0.55
7:G:21:LEU:C	7:G:23:TYR:H	2.13	0.55
2:O:122:ASN:ND2	2:O:125:ARG:NH1	2.54	0.55
4:Q:80:LEU:C	4:Q:80:LEU:HD23	2.32	0.55
1:A:47:GLN:HG2	9:A:301:HEM:C3B	2.42	0.54
4:D:121:GLU:CD	4:D:123:LYS:HE2	2.32	0.54
13:D:306:OPC:HAR2	13:D:306:OPC:CBM	2.38	0.54
7:G:21:LEU:C	7:G:23:TYR:N	2.63	0.54
8:H:3:ILE:HG13	8:H:4:ASP:OD1	2.06	0.54
3:P:171:VAL:HG12	3:P:233:ASN:O	2.07	0.54
3:P:275:LYS:NZ	3:P:276:LYS:NZ	2.55	0.54
4:Q:120:ALA:C	4:Q:122:ASN:H	2.16	0.54
13:Q:1307:OPC:HBP2	13:Q:1307:OPC:HBA1	1.89	0.54
1:A:62:VAL:HG12	1:A:140:TRP:CH2	2.42	0.54
2:B:79:TRP:C	2:B:81:LEU:N	2.64	0.54
5:R:27:LYS:O	5:R:31:LEU:HB2	2.07	0.54
4:D:87:ASP:HB3	4:D:105:ASN:HB3	1.89	0.54
3:P:174:ALA:HB3	3:P:228:GLY:HA2	1.89	0.54
4:Q:134:ASP:C	4:Q:136:THR:H	2.14	0.54
8:U:3:ILE:HG23	8:U:4:ASP:N	2.22	0.54
4:D:106:ALA:HB1	4:D:115:VAL:HB	1.89	0.54
2:O:106:LEU:CD2	14:O:1201:CLA:H151	2.36	0.54
3:P:171:VAL:HB	3:P:231:LEU:HD12	1.90	0.54
3:P:199:ILE:HB	3:P:208:VAL:HA	1.90	0.54
3:P:231:LEU:HD13	3:P:233:ASN:H	1.71	0.54
4:Q:90:TYR:O	4:Q:91:ILE:HD13	2.08	0.54
13:Q:1307:OPC:HAH2	13:Q:1307:OPC:HAP2	1.88	0.54
1:A:33:PHE:HE1	5:E:14:LEU:HD22	1.71	0.54
13:B:307:OPC:CAP	13:B:307:OPC:HAL2	2.37	0.54
3:C:20:ILE:HG21	3:C:75:VAL:HG11	1.88	0.54
3:C:273:ILE:O	3:C:278:GLN:HG2	2.08	0.54
4:D:133:TYR:CD2	4:D:148:LEU:HG	2.42	0.54
7:G:11:LEU:C	7:G:14:VAL:HG13	2.33	0.54
2:O:79:TRP:HB3	5:R:7:PHE:HZ	1.73	0.54
3:P:93:GLU:O	3:P:94:LEU:C	2.49	0.54
4:Q:74:ASN:O	4:Q:94:GLU:O	2.25	0.54
4:Q:84:LEU:HD21	4:Q:164:PRO:HA	1.89	0.54
2:B:114:ILE:O	2:B:116:ASN:N	2.40	0.54
3:C:219:VAL:O	3:C:232:THR:HG21	2.07	0.54
3:P:231:LEU:HD22	3:P:232:THR:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:275:LYS:O	3:P:279:VAL:HB	2.08	0.54
4:Q:73:HIS:NE2	4:Q:77:ASP:O	2.40	0.54
8:U:8:TRP:HA	8:U:11:LEU:HG	1.89	0.54
8:U:11:LEU:HB3	8:U:15:PHE:HZ	1.72	0.54
3:C:62:ALA:HB2	3:C:68:VAL:HG11	1.90	0.54
4:D:147:SER:CB	4:D:171:ARG:NH2	2.70	0.54
8:H:3:ILE:HG23	8:H:4:ASP:N	2.21	0.54
1:N:144:GLY:O	1:N:148:VAL:HG12	2.08	0.54
4:Q:81:VAL:O	4:Q:82:GLN:HG2	2.08	0.54
4:Q:121:GLU:O	4:Q:123:LYS:HG3	2.08	0.54
3:C:281:LYS:H	3:C:281:LYS:HD2	1.73	0.54
4:D:76:GLY:O	4:D:117:TRP:CH2	2.60	0.54
5:E:9:ILE:HG12	6:F:13:PHE:HB2	1.90	0.54
3:P:79:PRO:HD3	3:P:149:ILE:HG12	1.89	0.54
4:Q:157:ASP:O	4:Q:158:ASP:HB2	2.08	0.54
1:A:14:ILE:CD1	1:A:15:GLN:H	2.18	0.54
1:A:146:TRP:CH2	2:B:71:THR:OG1	2.59	0.54
7:G:30:LYS:HB3	7:G:31:ARG:HH22	1.71	0.54
1:N:116:LEU:HD11	1:N:208:LYS:NZ	2.23	0.54
7:T:22:PHE:O	7:T:26:TYR:CE1	2.61	0.54
2:B:96:LEU:HD22	2:B:100:LEU:HG	1.90	0.54
3:C:194:LYS:HD3	3:C:212:PRO:HA	1.89	0.54
3:P:178:GLY:O	3:P:225:VAL:HA	2.07	0.54
4:Q:57:LYS:O	4:Q:64:VAL:HG23	2.08	0.54
7:T:9:LEU:HG	7:T:10:VAL:H	1.72	0.54
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.22	0.53
2:B:40:PHE:N	2:B:41:PRO:HD2	2.22	0.53
2:B:146:GLY:O	2:B:147:ALA:HB3	2.08	0.53
3:C:55:ASP:OD1	3:C:57:LYS:CG	2.56	0.53
3:C:185:LYS:CG	3:C:195:TYR:HB3	2.30	0.53
3:C:273:ILE:HG21	7:G:27:GLN:HB3	1.89	0.53
4:D:19:MET:C	4:D:21:LEU:H	2.14	0.53
2:O:39:VAL:O	2:O:42:VAL:HB	2.09	0.53
4:Q:132:GLN:NE2	4:Q:141:ARG:HB2	2.23	0.53
8:U:10:ALA:O	8:U:14:VAL:HG23	2.08	0.53
1:A:102:PHE:O	1:A:103:ARG:C	2.50	0.53
2:B:48:PHE:CE2	2:B:52:VAL:HG21	2.43	0.53
2:B:79:TRP:C	2:B:79:TRP:CD1	2.86	0.53
3:C:54:TYR:OH	3:C:58:LEU:HD22	2.09	0.53
3:C:226:LYS:CE	3:C:229:GLU:HB3	2.37	0.53
4:D:19:MET:C	4:D:21:LEU:N	2.65	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:VAL:O	8:H:9:VAL:HB	2.08	0.53
2:O:96:LEU:HD22	2:O:100:LEU:HG	1.89	0.53
4:Q:84:LEU:O	4:Q:85:LYS:HB2	2.07	0.53
6:S:15:LEU:HD12	7:T:26:TYR:OH	2.09	0.53
7:T:10:VAL:O	7:T:14:VAL:HG13	2.08	0.53
3:C:9:TYR:C	3:C:11:PRO:HD2	2.33	0.53
4:D:16:ARG:C	4:D:18:PHE:N	2.60	0.53
13:D:306:OPC:HBL1	13:D:306:OPC:CAR	2.28	0.53
3:P:9:TYR:C	3:P:11:PRO:HD2	2.33	0.53
3:P:216:GLU:O	3:P:233:ASN:CB	2.56	0.53
4:Q:81:VAL:HB	4:Q:89:THR:CB	2.38	0.53
5:R:18:ILE:HG22	5:R:22:ILE:HD11	1.91	0.53
1:A:28:PRO:HD2	2:B:32:TRP:HB2	1.91	0.53
2:B:20:LYS:CG	2:B:21:GLY:N	2.55	0.53
5:E:23:ILE:CG2	5:E:24:PHE:N	2.71	0.53
5:E:30:LYS:HB2	5:E:30:LYS:HZ2	1.74	0.53
11:A:304:TDS:HBC1	2:B:85:PHE:CD2	2.43	0.53
3:C:79:PRO:HD3	3:C:149:ILE:HG12	1.90	0.53
3:C:187:GLU:HG3	3:C:188:ASP:H	1.74	0.53
7:T:11:LEU:HA	7:T:14:VAL:HG13	1.91	0.53
4:D:19:MET:O	4:D:21:LEU:N	2.41	0.53
4:D:64:VAL:HG12	4:D:69:PHE:HE2	1.73	0.53
4:D:66:VAL:CG2	4:D:158:ASP:C	2.82	0.53
4:D:94:GLU:OE1	4:D:98:ALA:O	2.26	0.53
1:N:200:LEU:HD22	13:N:1306:OPC:HBC1	1.90	0.53
4:Q:64:VAL:CG1	4:Q:91:ILE:HG12	2.36	0.53
4:Q:109:THR:OG1	4:Q:145:PRO:HG2	2.09	0.53
4:Q:150:LEU:HD23	4:Q:178:TRP:CH2	2.44	0.53
2:B:72:PRO:HB3	4:Q:127:PRO:CG	2.39	0.53
3:C:40:VAL:HG11	3:C:46:PHE:CD2	2.44	0.53
3:C:119:LEU:HD12	3:C:119:LEU:H	1.72	0.53
3:C:146:LYS:CD	3:C:246:GLU:HG3	2.32	0.53
3:C:275:LYS:O	3:C:279:VAL:HB	2.07	0.53
4:D:73:HIS:HB3	4:D:93:VAL:HG12	1.90	0.53
2:O:38:TYR:CG	3:P:276:LYS:HD3	2.43	0.53
3:P:146:LYS:CD	3:P:246:GLU:HG3	2.29	0.53
4:Q:178:TRP:HE3	4:Q:178:TRP:H	1.57	0.53
5:R:23:ILE:CG2	5:R:24:PHE:N	2.71	0.53
2:B:136:GLY:HA3	14:B:201:CLA:C2C	2.39	0.53
3:C:219:VAL:HG11	3:C:223:GLN:NE2	2.21	0.53
4:D:108:CYS:C	4:D:110:HIS:N	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:130:GLY:C	4:D:143:PRO:HG2	2.34	0.53
4:Q:109:THR:CG2	4:Q:177:TRP:CH2	2.92	0.53
12:Q:1305:PL9:H301	13:Q:1307:OPC:HBU1	1.89	0.53
4:D:20:ASN:C	4:D:22:LEU:N	2.63	0.53
7:G:15:PHE:C	7:G:17:THR:H	2.15	0.53
1:N:83:ARG:NH1	9:N:301:HEM:O1A	2.41	0.53
4:Q:15:ARG:HH12	4:Q:18:PHE:HE2	1.56	0.53
4:Q:136:THR:O	4:Q:171:ARG:NH2	2.41	0.53
2:B:26:TYR:HB2	2:B:27:TYR:CE1	2.43	0.53
13:D:306:OPC:HBC2	13:D:306:OPC:CAY	2.40	0.53
6:F:20:TRP:O	6:F:24:VAL:HG23	2.09	0.53
6:F:26:LEU:HD21	8:H:17:TRP:NE1	2.24	0.53
2:O:133:PHE:HA	14:O:1201:CLA:CMB	2.39	0.53
3:P:191:GLY:O	3:P:192:ASN:HB2	2.08	0.53
3:P:283:GLN:C	3:P:285:ALA:N	2.62	0.53
5:R:9:ILE:HG21	6:S:9:ALA:C	2.33	0.53
1:A:211:ILE:CD1	1:A:211:ILE:N	2.70	0.52
3:C:194:LYS:HB3	3:C:196:GLN:HE21	1.74	0.52
1:N:28:PRO:CG	2:O:32:TRP:HB3	2.39	0.52
1:N:93:MET:HE2	1:N:128:THR:CG2	2.38	0.52
1:N:104:VAL:CG1	9:N:302:HEM:HMD3	2.39	0.52
2:O:79:TRP:HZ2	5:R:1:MET:N	2.03	0.52
3:P:117:GLY:O	3:P:118:PRO:C	2.51	0.52
3:P:185:LYS:HE3	3:P:217:LEU:HD11	1.90	0.52
3:C:202:ASP:O	3:C:204:GLY:N	2.42	0.52
3:C:217:LEU:CA	3:C:232:THR:HB	2.38	0.52
1:N:61:THR:HG22	1:N:62:VAL:N	2.23	0.52
1:N:182:ARG:HB3	11:N:1304:TDS:HAA1	1.92	0.52
2:O:20:LYS:HG3	2:O:21:GLY:N	2.24	0.52
2:O:36:LEU:C	2:O:38:TYR:H	2.17	0.52
2:O:153:LYS:C	2:O:155:LEU:H	2.17	0.52
4:Q:142:GLY:HA2	4:Q:144:ALA:H	1.73	0.52
8:U:6:LEU:O	8:U:8:TRP:N	2.42	0.52
8:U:8:TRP:O	8:U:8:TRP:HE3	1.93	0.52
1:A:93:MET:HE2	1:A:128:THR:CG2	2.40	0.52
11:A:304:TDS:HAX2	14:B:201:CLA:H93	1.90	0.52
13:B:307:OPC:HAP1	13:B:307:OPC:HAL2	1.91	0.52
7:G:14:VAL:HG23	7:G:15:PHE:N	2.25	0.52
1:N:104:VAL:HA	1:N:107:THR:HG22	1.91	0.52
1:N:142:GLN:HG2	2:O:64:GLU:CB	2.39	0.52
2:O:22:MET:C	2:O:24:HIS:H	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:218:ILE:H	3:P:232:THR:CG2	2.23	0.52
3:P:282:VAL:CG2	4:Q:15:ARG:HE	2.23	0.52
4:Q:92:VAL:O	4:Q:99:ILE:HA	2.09	0.52
4:Q:153:ALA:HA	4:Q:162:LEU:HD11	1.92	0.52
5:R:18:ILE:HB	5:R:22:ILE:HD12	1.92	0.52
1:A:189:PHE:CE2	1:N:52:PHE:HB2	2.45	0.52
2:B:125:ARG:O	2:B:127:PRO:HD3	2.09	0.52
3:C:105:PRO:HB3	3:C:110:GLN:O	2.10	0.52
3:C:277:LYS:HB3	3:C:277:LYS:NZ	2.25	0.52
4:D:138:ARG:NH2	4:D:147:SER:HB3	2.24	0.52
3:P:62:ALA:HB2	3:P:68:VAL:HG11	1.92	0.52
3:P:94:LEU:HD22	3:P:94:LEU:N	2.12	0.52
3:P:117:GLY:N	3:P:118:PRO:HD2	2.24	0.52
3:P:226:LYS:HG2	3:P:229:GLU:CB	2.39	0.52
8:U:12:LEU:HA	8:U:15:PHE:CD1	2.44	0.52
2:B:38:TYR:CD1	3:C:276:LYS:HD3	2.44	0.52
3:C:180:ILE:HG13	3:C:199:ILE:HA	1.91	0.52
1:N:23:SER:O	1:N:25:TYR:CE1	2.61	0.52
1:N:141:ASP:C	2:O:64:GLU:CG	2.83	0.52
2:O:78:GLU:HG2	2:O:80:TYR:H	1.74	0.52
2:O:79:TRP:HB3	5:R:7:PHE:CZ	2.45	0.52
3:P:277:LYS:NZ	3:P:277:LYS:HB3	2.25	0.52
4:D:19:MET:HG3	4:D:20:ASN:N	2.25	0.52
2:O:24:HIS:O	2:O:25:ASN:CB	2.57	0.52
2:O:32:TRP:CE3	2:O:36:LEU:HG	2.44	0.52
2:O:75:ILE:HG22	2:O:77:PRO:HD3	1.91	0.52
4:Q:104:ILE:HD11	4:Q:136:THR:HA	1.90	0.52
4:Q:152:HIS:HB2	4:Q:162:LEU:HG	1.90	0.52
4:Q:154:THR:O	4:Q:160:ILE:HG23	2.08	0.52
9:A:301:HEM:HHA	9:A:301:HEM:HBD1	1.92	0.52
3:C:231:LEU:HD12	3:C:231:LEU:H	1.75	0.52
8:H:8:TRP:HE3	8:H:8:TRP:O	1.92	0.52
3:P:124:TYR:HB3	3:P:127:ILE:HG12	1.92	0.52
4:Q:76:GLY:CA	4:Q:93:VAL:HG13	2.40	0.52
4:Q:100:ARG:HD2	4:Q:102:TYR:HH	1.74	0.52
5:R:26:ILE:HD12	5:R:26:ILE:N	2.24	0.52
1:A:41:LEU:O	1:A:44:PHE:HB3	2.09	0.52
3:C:11:PRO:HA	3:C:107:LYS:NZ	2.25	0.52
3:C:28:ALA:HB3	3:C:238:GLY:O	2.10	0.52
4:D:73:HIS:CE1	4:D:91:ILE:O	2.63	0.52
8:H:6:LEU:O	8:H:8:TRP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:209:GLN:HB3	2:O:27:TYR:HB2	1.92	0.52
3:P:218:ILE:HG13	3:P:232:THR:HG22	1.90	0.52
3:P:233:ASN:ND2	3:P:234:ASN:H	2.08	0.52
4:Q:64:VAL:HG13	4:Q:69:PHE:CD2	2.45	0.52
4:Q:78:ARG:NH1	4:Q:100:ARG:HH21	2.06	0.52
12:Q:1305:PL9:H302	13:Q:1307:OPC:CBB	2.39	0.52
12:Q:1305:PL9:H201	13:Q:1307:OPC:OCC	2.08	0.52
8:U:22:VAL:O	8:U:26:ARG:HG3	2.10	0.52
1:A:44:PHE:HD1	9:A:301:HEM:CBB	2.21	0.52
2:B:72:PRO:HB3	4:Q:127:PRO:HG2	1.90	0.52
3:C:91:PRO:HD2	3:C:95:LYS:HG3	1.92	0.52
3:C:201:THR:O	3:C:203:SER:N	2.43	0.52
4:D:55:THR:OG1	4:D:57:LYS:NZ	2.36	0.52
4:D:116:PRO:CD	4:D:126:CYS:HA	2.40	0.52
5:E:21:GLY:O	5:E:25:ALA:HB2	2.10	0.52
2:O:85:PHE:O	2:O:89:ARG:HG2	2.10	0.52
13:Q:1307:OPC:HBX2	13:Q:1307:OPC:CBE	2.39	0.52
7:T:25:ALA:CB	7:T:29:TYR:OH	2.57	0.52
2:B:79:TRP:CG	2:B:80:TYR:N	2.78	0.52
4:D:84:LEU:H	4:D:89:THR:HG23	1.75	0.52
4:D:105:ASN:C	4:D:107:VAL:HG23	2.34	0.52
1:N:102:PHE:O	1:N:103:ARG:C	2.53	0.52
2:O:95:LEU:N	2:O:95:LEU:CD2	2.67	0.52
3:P:52:ILE:HG21	3:P:154:ASN:O	2.10	0.52
3:P:185:LYS:CD	3:P:195:TYR:HD2	2.23	0.52
4:Q:84:LEU:HD13	4:Q:164:PRO:HD3	1.91	0.52
6:S:17:PHE:CD1	6:S:17:PHE:N	2.78	0.52
1:A:33:PHE:CZ	5:E:17:GLY:HA3	2.45	0.51
2:B:150:PRO:O	2:B:153:LYS:NZ	2.43	0.51
14:B:201:CLA:HHC	14:B:201:CLA:HBB1	1.93	0.51
3:C:59:GLN:HB2	3:C:67:LYS:HB3	1.93	0.51
5:E:18:ILE:HG22	5:E:22:ILE:HD11	1.92	0.51
3:P:55:ASP:OD1	3:P:57:LYS:HG3	2.10	0.51
3:P:202:ASP:O	3:P:204:GLY:N	2.44	0.51
4:Q:116:PRO:HD3	4:Q:127:PRO:HD3	1.92	0.51
2:B:127:PRO:C	2:B:129:ALA:N	2.63	0.51
3:C:218:ILE:H	3:C:232:THR:CG2	2.22	0.51
4:D:78:ARG:HG3	4:D:117:TRP:CG	2.45	0.51
4:D:84:LEU:HD23	4:D:84:LEU:C	2.35	0.51
1:N:29:HIS:O	1:N:30:VAL:CG1	2.45	0.51
1:N:106:LEU:HD12	5:R:18:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:114:ARG:NH2	1:N:209:GLN:H	2.08	0.51
1:N:204:LEU:C	1:N:206:ILE:N	2.68	0.51
5:E:25:ALA:C	5:E:27:LYS:H	2.18	0.51
1:N:110:PHE:CD1	2:O:112:PRO:HB3	2.42	0.51
4:Q:150:LEU:HD11	4:Q:171:ARG:NH2	2.22	0.51
1:A:39:ILE:HD11	2:B:43:VAL:CG1	2.40	0.51
2:B:39:VAL:O	2:B:42:VAL:HB	2.10	0.51
2:B:79:TRP:HA	2:B:82:TYR:CD2	2.46	0.51
3:C:50:VAL:HG12	3:C:50:VAL:O	2.10	0.51
3:C:102:TYR:N	3:C:118:PRO:HG3	2.22	0.51
3:C:134:PRO:CB	3:C:142:ILE:HD13	2.39	0.51
5:E:20:VAL:CG1	5:E:21:GLY:N	2.69	0.51
16:E:101:BCR:H362	6:F:17:PHE:HZ	1.75	0.51
2:O:143:LEU:O	2:O:145:ILE:N	2.43	0.51
3:P:50:VAL:HG13	3:P:151:LEU:HD21	1.92	0.51
1:A:75:GLU:HA	1:A:75:GLU:OE1	2.11	0.51
1:A:99:LEU:HD21	5:E:11:PHE:HB2	1.92	0.51
2:B:96:LEU:O	2:B:100:LEU:HB2	2.11	0.51
2:B:150:PRO:O	2:B:153:LYS:HD2	2.09	0.51
4:D:115:VAL:HG21	4:D:148:LEU:CD2	2.41	0.51
3:P:118:PRO:O	3:P:120:PRO:HD3	2.11	0.51
8:U:17:TRP:O	8:U:20:ALA:HB3	2.10	0.51
1:A:204:LEU:C	1:A:206:ILE:N	2.68	0.51
4:D:155:VAL:HG12	4:D:156:GLN:N	2.25	0.51
8:H:22:VAL:C	8:H:24:TRP:N	2.67	0.51
1:N:26:VAL:O	1:N:26:VAL:HG23	2.11	0.51
2:O:118:ASN:ND2	2:O:121:GLN:NE2	2.37	0.51
4:Q:77:ASP:N	4:Q:93:VAL:HG12	2.18	0.51
4:Q:88:PRO:CD	4:Q:107:VAL:HG23	2.41	0.51
2:B:32:TRP:H	2:B:33:PRO:CD	2.24	0.51
3:C:178:GLY:O	3:C:225:VAL:HA	2.11	0.51
3:C:283:GLN:C	3:C:285:ALA:N	2.67	0.51
5:E:23:ILE:HG23	5:E:24:PHE:HD2	1.75	0.51
7:G:30:LYS:C	7:G:31:ARG:CZ	2.84	0.51
4:Q:35:LEU:O	4:Q:39:VAL:HG23	2.11	0.51
4:Q:133:TYR:CD2	4:Q:139:VAL:HB	2.46	0.51
4:Q:152:HIS:CA	4:Q:162:LEU:HG	2.41	0.51
5:R:23:ILE:O	5:R:27:LYS:CB	2.58	0.51
1:A:103:ARG:HG3	1:A:103:ARG:NH1	2.25	0.51
1:A:105:TYR:C	1:A:107:THR:H	2.19	0.51
4:D:35:LEU:HD12	4:D:35:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:PHE:CD1	3:P:3:PHE:N	2.78	0.51
3:P:201:THR:O	3:P:203:SER:N	2.43	0.51
4:Q:109:THR:HG22	4:Q:177:TRP:CH2	2.45	0.51
7:T:15:PHE:C	7:T:17:THR:N	2.68	0.51
1:A:118:TRP:CZ3	2:B:108:LEU:O	2.64	0.51
3:C:262:ILE:HG12	7:G:17:THR:HG22	1.92	0.51
4:D:90:TYR:HD2	4:D:104:ILE:O	1.93	0.51
5:E:9:ILE:HG21	6:F:9:ALA:C	2.34	0.51
1:N:29:HIS:HE1	2:O:29:GLU:OE2	1.94	0.51
2:O:74:GLU:CG	2:O:75:ILE:N	2.73	0.51
3:P:20:ILE:HG21	3:P:75:VAL:HG11	1.91	0.51
4:Q:78:ARG:HD3	4:Q:78:ARG:N	2.25	0.51
4:Q:152:HIS:HB2	4:Q:162:LEU:CB	2.41	0.51
3:C:181:THR:C	3:C:221:GLU:HB3	2.35	0.51
3:C:221:GLU:CD	3:C:221:GLU:N	2.68	0.51
5:E:16:PHE:O	5:E:20:VAL:HB	2.11	0.51
1:N:14:ILE:O	1:N:14:ILE:HG13	2.11	0.51
3:P:226:LYS:CD	3:P:229:GLU:HB3	2.40	0.51
4:Q:133:TYR:HA	4:Q:138:ARG:C	2.35	0.51
4:Q:152:HIS:CB	4:Q:162:LEU:HG	2.40	0.51
4:Q:162:LEU:O	4:Q:163:THR:HB	2.11	0.51
5:R:25:ALA:C	5:R:27:LYS:H	2.17	0.51
7:T:15:PHE:C	7:T:17:THR:H	2.18	0.51
8:U:5:VAL:O	8:U:9:VAL:HB	2.11	0.51
3:C:61:VAL:O	3:C:157:ARG:NH1	2.42	0.50
4:D:115:VAL:HG12	4:D:124:PHE:HB3	1.92	0.50
1:N:95:LEU:HG	5:R:7:PHE:HB3	1.94	0.50
1:N:150:ILE:HD12	2:O:75:ILE:HG12	1.93	0.50
2:O:78:GLU:OE1	2:O:80:TYR:HB2	2.11	0.50
2:O:91:LEU:HD12	2:O:91:LEU:O	2.11	0.50
2:O:122:ASN:OD1	5:R:26:ILE:HG21	2.10	0.50
3:P:187:GLU:HG3	3:P:188:ASP:N	2.26	0.50
3:C:34:VAL:HG22	3:C:151:LEU:HD22	1.93	0.50
3:C:53:PRO:O	3:C:54:TYR:HB2	2.10	0.50
4:D:59:LYS:HB3	4:D:80:LEU:O	2.10	0.50
2:O:21:GLY:C	2:O:24:HIS:HD2	2.19	0.50
2:O:24:HIS:O	2:O:25:ASN:HB3	2.10	0.50
2:O:57:LEU:O	3:P:38:GLN:NE2	2.45	0.50
3:P:181:THR:C	3:P:221:GLU:HB3	2.36	0.50
3:P:194:LYS:HB3	3:P:196:GLN:HE21	1.75	0.50
3:P:231:LEU:CD1	3:P:231:LEU:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:123:LYS:O	4:Q:125:LYS:N	2.44	0.50
4:Q:132:GLN:NE2	4:Q:141:ARG:HD3	2.22	0.50
4:Q:149:ALA:O	4:Q:150:LEU:HD13	2.11	0.50
5:R:5:ALA:HB1	6:S:9:ALA:CB	2.21	0.50
8:U:24:TRP:CD2	8:U:25:GLY:N	2.79	0.50
2:B:142:TRP:NE1	2:B:154:THR:O	2.41	0.50
3:C:3:PHE:N	3:C:3:PHE:CD1	2.78	0.50
3:C:134:PRO:HB3	3:C:142:ILE:CD1	2.40	0.50
4:D:78:ARG:NE	4:D:92:VAL:HG11	2.23	0.50
6:F:7:TYR:CD1	6:F:7:TYR:C	2.89	0.50
7:G:26:TYR:HD1	7:G:26:TYR:H	1.59	0.50
1:N:58:TYR:OH	1:N:138:LEU:O	2.25	0.50
1:N:140:TRP:O	2:O:65:PRO:HG3	2.11	0.50
1:N:214:PRO:HA	5:R:29:ILE:O	2.12	0.50
4:Q:70:LEU:HD22	4:Q:71:GLU:OE1	2.12	0.50
1:A:14:ILE:O	1:A:15:GLN:C	2.54	0.50
3:C:199:ILE:HG22	3:C:200:GLN:N	2.26	0.50
3:C:231:LEU:CD1	3:C:232:THR:H	2.23	0.50
7:G:28:GLN:C	7:G:30:LYS:N	2.68	0.50
2:O:76:LEU:HD23	2:O:76:LEU:H	1.75	0.50
4:Q:94:GLU:HB3	4:Q:100:ARG:CD	2.12	0.50
4:Q:156:GLN:O	4:Q:157:ASP:CB	2.59	0.50
8:U:9:VAL:HG22	8:U:13:VAL:CG2	2.41	0.50
3:C:231:LEU:HD22	3:C:232:THR:H	1.77	0.50
3:C:233:ASN:ND2	3:C:234:ASN:H	2.09	0.50
4:D:106:ALA:HB3	4:D:114:VAL:HG13	1.94	0.50
16:E:101:BCR:H362	6:F:17:PHE:CZ	2.46	0.50
1:N:33:PHE:O	1:N:36:LEU:HD23	2.11	0.50
4:Q:19:MET:C	4:Q:21:LEU:N	2.68	0.50
4:Q:22:LEU:HD23	4:Q:22:LEU:C	2.36	0.50
4:Q:147:SER:HB3	4:Q:171:ARG:NH1	2.26	0.50
2:B:86:GLN:HG3	2:B:143:LEU:HD22	1.94	0.50
4:D:68:LYS:H	4:D:68:LYS:HD2	1.75	0.50
2:O:22:MET:O	2:O:24:HIS:N	2.44	0.50
2:O:36:LEU:O	2:O:39:VAL:HG22	2.11	0.50
4:Q:116:PRO:CD	4:Q:127:PRO:HD3	2.41	0.50
4:Q:121:GLU:CD	4:Q:125:LYS:HE3	2.37	0.50
4:Q:156:GLN:HB2	4:Q:161:VAL:CG1	2.42	0.50
1:A:14:ILE:HA	1:A:17:LEU:HD12	1.94	0.50
1:A:23:SER:C	1:A:25:TYR:H	2.18	0.50
1:A:158:ILE:HB	1:A:162:GLY:HA2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:HIS:HE1	4:D:129:HIS:HB2	1.77	0.50
13:D:306:OPC:HBW2	13:D:306:OPC:CCA	2.39	0.50
4:Q:123:LYS:HA	4:Q:133:TYR:O	2.11	0.50
1:A:27:PRO:HG3	2:B:33:PRO:CG	2.41	0.50
2:B:79:TRP:CD1	2:B:80:TYR:N	2.80	0.50
3:C:52:ILE:HG12	3:C:153:ALA:CB	2.40	0.50
3:C:56:THR:HG22	3:C:122:GLU:HB3	1.92	0.50
3:C:199:ILE:HB	3:C:208:VAL:HA	1.94	0.50
3:C:274:LEU:HD11	8:H:23:VAL:HG21	1.92	0.50
4:D:51:GLY:C	4:D:85:LYS:NZ	2.70	0.50
4:D:149:ALA:HA	4:D:178:TRP:CE2	2.47	0.50
4:D:167:GLU:O	4:D:176:PRO:CB	2.59	0.50
4:D:167:GLU:O	4:D:176:PRO:HB3	2.11	0.50
3:P:86:PRO:CG	3:P:89:ARG:HG3	2.41	0.50
3:P:173:THR:HB	3:P:229:GLU:HA	1.92	0.50
6:S:7:TYR:CD1	6:S:7:TYR:C	2.89	0.50
1:A:32:ILE:C	1:A:34:TYR:N	2.68	0.50
1:N:41:LEU:O	1:N:44:PHE:HB3	2.12	0.50
4:Q:56:ALA:HA	4:Q:81:VAL:CG1	2.25	0.50
4:Q:100:ARG:CD	4:Q:102:TYR:OH	2.57	0.50
2:B:32:TRP:CH2	3:C:277:LYS:HD2	2.43	0.49
2:B:117:VAL:O	2:B:117:VAL:HG22	2.11	0.49
3:C:229:GLU:O	3:C:230:ALA:C	2.55	0.49
3:C:269:GLN:HE22	7:G:24:ALA:HA	1.75	0.49
3:C:277:LYS:HE3	7:G:31:ARG:CG	2.42	0.49
4:D:99:ILE:HD12	4:D:153:ALA:HB3	1.94	0.49
6:F:17:PHE:CD1	6:F:17:PHE:N	2.80	0.49
1:N:115:GLU:O	1:N:119:ILE:HG13	2.12	0.49
3:P:3:PHE:CZ	3:P:119:LEU:HD11	2.41	0.49
3:P:134:PRO:HB3	3:P:142:ILE:CD1	2.36	0.49
4:Q:64:VAL:HA	4:Q:69:PHE:CE1	2.47	0.49
4:Q:123:LYS:HE3	4:Q:125:LYS:HZ3	1.75	0.49
1:A:28:PRO:HD2	2:B:31:ALA:C	2.36	0.49
1:A:36:LEU:CD2	1:A:103:ARG:HB2	2.43	0.49
2:B:58:ASP:OD1	3:C:146:LYS:NZ	2.45	0.49
2:B:127:PRO:O	2:B:129:ALA:N	2.42	0.49
2:B:148:ALA:C	2:B:149:LEU:HD12	2.36	0.49
4:D:59:LYS:CD	4:D:79:VAL:HB	2.42	0.49
4:D:165:TRP:HA	4:D:167:GLU:OE2	2.12	0.49
5:E:30:LYS:CB	5:E:30:LYS:NZ	2.75	0.49
1:N:31:ASN:O	1:N:32:ILE:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:60:ALA:C	2:O:61:MET:HG2	2.36	0.49
4:Q:19:MET:C	4:Q:21:LEU:H	2.19	0.49
4:Q:99:ILE:HD12	4:Q:160:ILE:HD13	1.94	0.49
12:Q:1305:PL9:C30	13:Q:1307:OPC:HBU1	2.42	0.49
5:R:9:ILE:HB	6:S:9:ALA:HB1	1.94	0.49
1:A:91:SER:CB	2:B:79:TRP:HZ3	2.25	0.49
3:C:26:HIS:ND1	3:C:154:ASN:OD1	2.46	0.49
4:D:19:MET:HE3	4:D:22:LEU:CD2	2.42	0.49
1:N:106:LEU:HD12	5:R:18:ILE:HD12	1.95	0.49
3:P:91:PRO:HD2	3:P:95:LYS:HG3	1.94	0.49
4:Q:141:ARG:HG2	4:Q:141:ARG:HH11	1.77	0.49
4:Q:154:THR:O	4:Q:160:ILE:CA	2.58	0.49
4:Q:170:PHE:H	4:Q:170:PHE:HD1	1.60	0.49
2:B:22:MET:O	2:B:22:MET:SD	2.70	0.49
3:C:124:TYR:HB3	3:C:127:ILE:HG12	1.95	0.49
4:D:102:TYR:CE2	4:D:136:THR:HG23	2.47	0.49
4:D:104:ILE:HG23	4:D:149:ALA:O	2.13	0.49
1:N:212:SER:HB2	2:O:122:ASN:OD1	2.12	0.49
3:P:59:GLN:HB2	3:P:67:LYS:HB3	1.94	0.49
1:A:66:TYR:CZ	2:B:65:PRO:HD3	2.47	0.49
2:B:147:ALA:HB1	2:B:152:ASP:HA	1.95	0.49
3:C:262:ILE:HG13	7:G:21:LEU:CG	2.27	0.49
8:H:11:LEU:O	8:H:12:LEU:C	2.54	0.49
1:N:71:TYR:O	1:N:76:VAL:HG23	2.12	0.49
3:P:275:LYS:NZ	3:P:276:LYS:HZ1	2.10	0.49
6:S:7:TYR:O	6:S:11:LEU:HD12	2.12	0.49
8:U:6:LEU:O	8:U:10:ALA:HB3	2.12	0.49
1:A:114:ARG:NH1	1:A:208:LYS:HB3	2.28	0.49
2:B:32:TRP:N	2:B:33:PRO:CD	2.76	0.49
2:B:82:TYR:N	2:B:83:PRO:HD2	2.28	0.49
3:C:174:ALA:HB3	3:C:228:GLY:HA2	1.93	0.49
4:D:84:LEU:O	4:D:87:ASP:N	2.46	0.49
4:D:126:CYS:N	4:D:131:SER:O	2.38	0.49
8:H:11:LEU:C	8:H:15:PHE:CE1	2.91	0.49
13:N:1306:OPC:HBQ2	13:N:1306:OPC:CAU	2.42	0.49
2:O:64:GLU:CG	2:O:65:PRO:N	2.75	0.49
2:O:79:TRP:CH2	5:R:1:MET:N	2.79	0.49
2:O:114:ILE:C	2:O:116:ASN:N	2.70	0.49
3:P:171:VAL:HG13	3:P:234:ASN:HB2	1.93	0.49
3:P:199:ILE:HG22	3:P:200:GLN:N	2.27	0.49
3:P:270:LEU:HG	3:P:274:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:281:LYS:HA	3:P:284:ALA:CB	2.25	0.49
4:Q:94:GLU:OE2	4:Q:100:ARG:HG2	2.12	0.49
4:Q:109:THR:C	4:Q:145:PRO:HG3	2.37	0.49
8:U:9:VAL:C	8:U:11:LEU:N	2.69	0.49
1:A:97:MET:O	1:A:101:VAL:HG23	2.13	0.49
2:B:141:ILE:O	2:B:144:GLY:N	2.45	0.49
3:C:217:LEU:HA	3:C:232:THR:CB	2.39	0.49
5:E:26:ILE:HG13	5:E:29:ILE:HD12	1.95	0.49
7:G:30:LYS:C	7:G:31:ARG:NE	2.71	0.49
1:N:111:LYS:HB2	1:N:114:ARG:NH1	2.26	0.49
4:Q:169:ASP:HB3	4:Q:172:THR:OG1	2.13	0.49
1:A:142:GLN:HE22	2:B:67:ASN:H	1.59	0.49
2:B:118:ASN:O	2:B:121:GLN:O	2.30	0.49
2:O:147:ALA:O	2:O:149:LEU:N	2.45	0.49
3:P:226:LYS:O	3:P:227:ALA:HB2	2.12	0.49
4:Q:20:ASN:C	4:Q:22:LEU:N	2.60	0.49
1:A:178:ALA:O	1:A:182:ARG:HG3	2.13	0.49
2:B:32:TRP:N	2:B:33:PRO:HD3	2.28	0.49
2:B:102:ALA:O	2:B:105:PRO:HD2	2.12	0.49
4:D:174:GLU:HG2	4:D:175:LYS:O	2.13	0.49
5:E:15:PHE:O	5:E:16:PHE:C	2.56	0.49
2:O:146:GLY:O	2:O:149:LEU:CB	2.61	0.49
3:P:26:HIS:ND1	3:P:154:ASN:ND2	2.61	0.49
4:Q:161:VAL:C	4:Q:162:LEU:HD12	2.38	0.49
4:Q:163:THR:O	4:Q:164:PRO:O	2.31	0.49
1:A:114:ARG:HB3	1:A:208:LYS:NZ	2.27	0.49
3:C:182:LYS:CG	3:C:198:SER:HB2	2.40	0.49
3:C:199:ILE:HB	3:C:207:VAL:O	2.13	0.49
4:D:35:LEU:O	4:D:39:VAL:HG23	2.13	0.49
4:D:166:THR:CA	4:D:179:VAL:HG22	2.43	0.49
7:G:25:ALA:CB	7:G:29:TYR:OH	2.61	0.49
2:O:153:LYS:O	2:O:155:LEU:N	2.40	0.49
1:A:27:PRO:HB3	2:B:31:ALA:C	2.38	0.48
1:A:99:LEU:CD2	5:E:11:PHE:HB2	2.43	0.48
3:C:98:VAL:O	3:C:99:GLY:O	2.31	0.48
3:C:191:GLY:O	3:C:192:ASN:HB2	2.13	0.48
4:D:54:THR:HG23	4:D:82:GLN:HG3	1.95	0.48
4:D:77:ASP:C	4:D:77:ASP:OD2	2.56	0.48
5:E:26:ILE:O	5:E:26:ILE:HG22	2.12	0.48
1:N:28:PRO:C	1:N:29:HIS:ND1	2.71	0.48
1:N:97:MET:O	1:N:101:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:110:PHE:O	1:N:111:LYS:O	2.31	0.48
2:O:18:LEU:HD13	2:O:31:ALA:HB2	1.93	0.48
2:O:59:PRO:HD2	3:P:248:VAL:HG21	1.95	0.48
4:Q:81:VAL:C	4:Q:82:GLN:HG2	2.38	0.48
7:T:28:GLN:C	7:T:30:LYS:H	2.21	0.48
1:A:105:TYR:C	1:A:107:THR:N	2.71	0.48
7:G:17:THR:O	7:G:21:LEU:HB2	2.13	0.48
7:G:21:LEU:O	7:G:21:LEU:HD13	2.12	0.48
7:G:27:GLN:HA	7:G:27:GLN:NE2	2.28	0.48
1:N:135:GLY:HA2	1:N:138:LEU:HG	1.96	0.48
2:O:46:GLY:HA3	7:T:24:ALA:HB1	1.95	0.48
2:O:79:TRP:HA	2:O:82:TYR:CZ	2.48	0.48
2:O:146:GLY:O	2:O:147:ALA:C	2.55	0.48
3:P:219:VAL:O	3:P:232:THR:HG21	2.13	0.48
3:P:226:LYS:CG	3:P:229:GLU:HB3	2.43	0.48
4:Q:102:TYR:H	4:Q:153:ALA:HB2	1.78	0.48
6:S:26:LEU:HD22	8:U:17:TRP:HE1	1.75	0.48
8:U:8:TRP:O	8:U:11:LEU:HB2	2.13	0.48
1:A:159:PRO:C	1:A:161:VAL:N	2.68	0.48
4:Q:28:THR:OG1	12:Q:1305:PL9:H23	2.13	0.48
4:Q:154:THR:C	4:Q:155:VAL:HG23	2.38	0.48
1:A:104:VAL:O	1:A:107:THR:HG22	2.14	0.48
2:B:91:LEU:HD12	2:B:91:LEU:O	2.13	0.48
2:B:135:PHE:O	2:B:138:LEU:HB2	2.13	0.48
2:B:149:LEU:O	2:B:150:PRO:C	2.56	0.48
3:C:12:THR:OG1	3:C:13:PRO:HD2	2.12	0.48
4:D:139:VAL:HG23	4:D:144:ALA:HB3	1.96	0.48
8:H:7:GLY:O	8:H:11:LEU:HD11	2.13	0.48
3:P:34:VAL:HG22	3:P:151:LEU:HD22	1.95	0.48
3:P:88:GLU:H	3:P:88:GLU:CD	2.21	0.48
4:Q:74:ASN:N	4:Q:93:VAL:HG11	2.13	0.48
4:Q:88:PRO:O	4:Q:89:THR:HG23	2.13	0.48
4:Q:163:THR:O	4:Q:164:PRO:C	2.57	0.48
5:R:9:ILE:CG1	6:S:13:PHE:HB2	2.43	0.48
2:B:99:LEU:C	2:B:99:LEU:HD13	2.39	0.48
3:C:266:MET:HG3	7:G:21:LEU:HD23	1.95	0.48
4:D:107:VAL:HG12	4:D:109:THR:HG23	1.94	0.48
4:D:147:SER:HB2	4:D:171:ARG:NH2	2.28	0.48
1:N:104:VAL:O	1:N:107:THR:HG22	2.12	0.48
1:N:118:TRP:CZ3	2:O:108:LEU:C	2.91	0.48
2:O:82:TYR:N	2:O:83:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:21:MET:O	8:U:24:TRP:HE3	1.96	0.48
1:A:95:LEU:HD13	1:A:96:MET:HE2	1.94	0.48
3:C:91:PRO:HD2	3:C:95:LYS:HG2	1.94	0.48
1:N:66:TYR:CG	2:O:65:PRO:HG2	2.48	0.48
1:N:141:ASP:O	1:N:145:TYR:HB3	2.13	0.48
3:P:180:ILE:HG23	3:P:220:SER:C	2.38	0.48
3:P:231:LEU:CD1	3:P:231:LEU:N	2.77	0.48
3:P:273:ILE:O	3:P:278:GLN:HG2	2.13	0.48
3:C:220:SER:HB2	3:C:221:GLU:CD	2.39	0.48
4:D:116:PRO:HD2	4:D:126:CYS:SG	2.54	0.48
1:N:72:ILE:O	1:N:79:GLY:HA3	2.13	0.48
1:N:109:GLY:HA3	9:N:302:HEM:HBD2	1.96	0.48
1:N:118:TRP:CH2	2:O:108:LEU:HB3	2.49	0.48
3:P:104:GLN:HG2	3:P:115:LEU:HB2	1.96	0.48
3:P:213:ALA:C	3:P:215:PRO:HD2	2.38	0.48
4:Q:66:VAL:O	4:Q:70:LEU:N	2.46	0.48
4:Q:159:ASN:O	4:Q:161:VAL:N	2.46	0.48
2:B:148:ALA:O	2:B:149:LEU:C	2.57	0.48
3:C:1:TYR:CD2	3:C:119:LEU:HD21	2.46	0.48
3:C:41:LEU:HD21	7:G:11:LEU:HD21	1.96	0.48
3:C:226:LYS:O	3:C:227:ALA:HB2	2.12	0.48
3:C:251:ASP:HB3	3:C:254:ARG:HD2	1.94	0.48
4:D:15:ARG:HH22	4:D:17:GLN:HG2	1.75	0.48
4:D:138:ARG:HB3	4:D:138:ARG:HH11	1.75	0.48
5:E:7:PHE:CD1	5:E:7:PHE:C	2.92	0.48
8:H:24:TRP:CD2	8:H:25:GLY:N	2.82	0.48
1:N:99:LEU:HD21	5:R:11:PHE:HB2	1.96	0.48
1:N:107:THR:O	2:O:123:PRO:HG2	2.13	0.48
2:O:18:LEU:CB	2:O:31:ALA:HB2	2.43	0.48
2:O:58:ASP:OD1	5:R:2:ILE:HG21	2.13	0.48
4:Q:77:ASP:OD1	4:Q:93:VAL:HG11	2.14	0.48
4:Q:115:VAL:HG13	4:Q:126:CYS:CA	2.43	0.48
4:Q:155:VAL:HG12	4:Q:156:GLN:H	1.79	0.48
3:C:275:LYS:HE2	4:D:17:GLN:HB2	1.95	0.48
4:D:61:GLY:HA2	2:O:66:ALA:O	2.14	0.48
4:D:138:ARG:HE	4:D:171:ARG:HD2	1.77	0.48
5:E:5:ALA:HB2	6:F:5:MET:CB	2.43	0.48
7:G:14:VAL:HG22	7:G:15:PHE:H	1.78	0.48
1:N:58:TYR:HE2	1:N:60:PRO:HB3	1.79	0.48
3:P:226:LYS:CE	3:P:229:GLU:HB3	2.44	0.48
4:Q:92:VAL:HG23	4:Q:100:ARG:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:94:GLU:CG	4:Q:95:SER:N	2.76	0.48
4:Q:120:ALA:C	4:Q:122:ASN:N	2.71	0.48
6:S:22:LEU:O	6:S:26:LEU:HD23	2.14	0.48
1:A:23:SER:O	1:A:25:TYR:HD1	1.97	0.48
1:A:30:VAL:HG23	1:A:30:VAL:O	2.14	0.48
1:A:104:VAL:CG1	9:A:302:HEM:HMD3	2.44	0.48
2:B:85:PHE:O	2:B:89:ARG:HG2	2.14	0.48
4:D:118:ASN:HB2	4:D:122:ASN:H	1.78	0.48
4:D:138:ARG:HH21	4:D:147:SER:HB3	1.79	0.48
1:N:191:LEU:HD11	11:N:1304:TDS:OBD	2.14	0.48
10:N:303:HEC:CBC	2:O:44:ILE:HD11	2.39	0.48
2:O:22:MET:O	2:O:23:GLY:C	2.56	0.48
3:P:187:GLU:HG3	3:P:188:ASP:H	1.79	0.48
1:A:119:ILE:C	1:A:121:GLY:N	2.67	0.47
3:C:266:MET:HE3	7:G:20:GLY:O	2.14	0.47
4:D:68:LYS:HD2	4:D:68:LYS:N	2.29	0.47
4:D:70:LEU:HD23	4:D:70:LEU:O	2.14	0.47
4:D:94:GLU:OE1	4:D:94:GLU:N	2.40	0.47
1:N:109:GLY:C	1:N:111:LYS:N	2.72	0.47
1:N:112:LYS:CB	1:N:113:PRO:HD3	2.31	0.47
1:N:163:VAL:CG1	1:N:164:LEU:N	2.77	0.47
3:P:218:ILE:CG1	3:P:232:THR:HG22	2.43	0.47
3:P:275:LYS:HG3	4:Q:20:ASN:CA	2.43	0.47
5:R:26:ILE:HG22	5:R:26:ILE:O	2.12	0.47
7:T:14:VAL:HG22	7:T:15:PHE:H	1.79	0.47
1:A:158:ILE:CB	1:A:162:GLY:HA3	2.40	0.47
2:B:126:ARG:O	2:B:129:ALA:HB3	2.14	0.47
4:D:66:VAL:CG2	4:D:160:ILE:N	2.77	0.47
4:D:147:SER:HB3	4:D:171:ARG:NH2	2.29	0.47
1:N:20:ASP:O	1:N:21:VAL:O	2.32	0.47
2:O:18:LEU:HD21	7:T:35:LEU:O	2.14	0.47
2:O:79:TRP:CH2	5:R:4:GLY:CA	2.92	0.47
3:P:47:LYS:HG3	3:P:128:VAL:HG13	1.96	0.47
4:Q:93:VAL:HG22	4:Q:94:GLU:H	1.79	0.47
7:T:28:GLN:O	7:T:29:TYR:C	2.57	0.47
11:A:304:TDS:HBC1	2:B:85:PHE:CA	2.41	0.47
2:B:38:TYR:CG	3:C:276:LYS:HD3	2.50	0.47
2:B:84:VAL:HG21	14:B:201:CLA:H41	1.96	0.47
1:N:34:TYR:CE2	1:N:103:ARG:HD3	2.48	0.47
1:N:79:GLY:HA2	4:Q:41:TYR:CE1	2.49	0.47
1:N:159:PRO:C	1:N:160:VAL:HG23	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:147:ALA:C	2:O:149:LEU:N	2.69	0.47
3:P:77:MET:HG2	3:P:113:VAL:HG13	1.95	0.47
3:P:177:THR:CA	3:P:227:ALA:HA	2.44	0.47
1:A:39:ILE:CD1	16:E:101:BCR:H312	2.41	0.47
1:A:188:THR:HG22	9:A:301:HEM:HBC2	1.95	0.47
2:B:122:ASN:ND2	2:B:124:PHE:CD2	2.78	0.47
2:B:142:TRP:HD1	2:B:155:LEU:C	2.20	0.47
3:C:198:SER:HA	3:C:208:VAL:HB	1.96	0.47
3:C:211:ILE:HD11	3:C:231:LEU:HD23	1.95	0.47
3:C:223:GLN:O	3:C:224:ALA:HB3	2.14	0.47
2:O:91:LEU:CD2	2:O:100:LEU:HD12	2.44	0.47
2:O:135:PHE:O	2:O:138:LEU:HB2	2.13	0.47
3:P:56:THR:HG22	3:P:122:GLU:HB3	1.95	0.47
4:Q:27:VAL:C	4:Q:29:GLY:N	2.71	0.47
2:B:27:TYR:CD1	2:B:27:TYR:N	2.83	0.47
3:C:185:LYS:CD	3:C:195:TYR:HD2	2.26	0.47
4:D:55:THR:O	4:D:57:LYS:HG3	2.14	0.47
7:G:11:LEU:O	7:G:14:VAL:HG13	2.15	0.47
8:H:8:TRP:HA	8:H:11:LEU:HG	1.96	0.47
1:N:21:VAL:CG1	1:N:22:THR:H	2.21	0.47
2:O:41:PRO:O	2:O:45:MET:HG3	2.15	0.47
2:O:95:LEU:HD23	2:O:95:LEU:H	1.77	0.47
3:P:53:PRO:O	3:P:54:TYR:HB2	2.14	0.47
3:P:54:TYR:OH	3:P:58:LEU:HB2	2.14	0.47
1:A:62:VAL:HG11	1:A:177:GLN:HB3	1.96	0.47
1:A:170:ARG:HG3	1:A:172:GLY:H	1.79	0.47
2:B:118:ASN:HB2	2:B:123:PRO:HG3	1.95	0.47
3:C:26:HIS:ND1	3:C:154:ASN:ND2	2.62	0.47
3:C:41:LEU:HD22	3:C:41:LEU:H	1.79	0.47
4:D:52:GLY:CA	4:D:85:LYS:NZ	2.77	0.47
1:N:47:GLN:HG2	9:N:301:HEM:HBB2	1.95	0.47
2:O:91:LEU:HD21	2:O:100:LEU:HD12	1.97	0.47
2:O:116:ASN:C	2:O:116:ASN:HD22	2.21	0.47
2:O:127:PRO:O	2:O:129:ALA:N	2.41	0.47
2:O:144:GLY:O	2:O:145:ILE:CD1	2.62	0.47
3:P:281:LYS:H	3:P:281:LYS:HD2	1.79	0.47
13:Q:1307:OPC:HAL2	13:Q:1307:OPC:HAP2	1.93	0.47
1:A:103:ARG:NH2	9:A:302:HEM:HBD1	2.29	0.47
1:A:202:HIS:O	1:A:206:ILE:HG13	2.15	0.47
3:C:82:PHE:O	3:C:112:ASN:HB3	2.15	0.47
4:D:78:ARG:HB3	4:D:90:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:5:VAL:O	8:H:9:VAL:CB	2.63	0.47
1:N:28:PRO:CG	2:O:32:TRP:CB	2.93	0.47
1:N:186:ALA:HB2	11:N:1304:TDS:HAA3	1.97	0.47
10:N:303:HEC:CBB	2:O:43:VAL:HG21	2.44	0.47
2:O:37:LEU:HD23	2:O:40:PHE:CE2	2.49	0.47
3:P:50:VAL:O	3:P:50:VAL:HG12	2.14	0.47
3:P:161:TYR:C	3:P:163:THR:H	2.21	0.47
3:P:279:VAL:HG12	3:P:279:VAL:O	2.14	0.47
4:Q:35:LEU:O	4:Q:35:LEU:HD12	2.15	0.47
4:Q:73:HIS:HD2	4:Q:92:VAL:C	2.23	0.47
4:Q:134:ASP:HB2	4:Q:138:ARG:CB	2.43	0.47
13:Q:1307:OPC:HBN2	13:Q:1307:OPC:HAZ2	1.97	0.47
7:T:25:ALA:O	7:T:29:TYR:CD2	2.68	0.47
7:T:26:TYR:CA	7:T:29:TYR:CD1	2.90	0.47
12:A:305:PL9:H121	12:A:305:PL9:HC71	1.96	0.47
2:B:144:GLY:O	2:B:145:ILE:CG1	2.63	0.47
2:B:148:ALA:O	2:B:152:ASP:N	2.48	0.47
3:C:13:PRO:O	3:C:21:VAL:HG22	2.14	0.47
4:D:65:LYS:HB3	4:D:68:LYS:CD	2.42	0.47
4:D:150:LEU:HD11	4:D:171:ARG:HD3	1.96	0.47
4:D:169:ASP:HB3	4:D:178:TRP:CZ2	2.50	0.47
1:N:27:PRO:HB3	2:O:33:PRO:HD3	1.97	0.47
2:O:58:ASP:OD2	3:P:146:LYS:HE2	2.14	0.47
2:O:148:ALA:O	2:O:149:LEU:O	2.32	0.47
1:A:91:SER:HB3	2:B:79:TRP:CZ3	2.50	0.47
1:A:125:ALA:HB2	9:A:302:HEM:CMC	2.45	0.47
1:A:138:LEU:C	1:A:140:TRP:H	2.23	0.47
1:A:141:ASP:O	1:A:145:TYR:N	2.42	0.47
1:A:144:GLY:O	1:A:148:VAL:HG12	2.14	0.47
2:B:53:ALA:O	2:B:57:LEU:HG	2.14	0.47
2:B:154:THR:HG22	2:B:155:LEU:N	2.30	0.47
3:C:1:TYR:O	3:C:4:TRP:HB2	2.15	0.47
3:C:49:VAL:HG12	3:C:51:LYS:HD2	1.96	0.47
4:D:93:VAL:CA	4:D:100:ARG:HB2	2.39	0.47
7:G:23:TYR:O	7:G:24:ALA:C	2.58	0.47
1:N:66:TYR:HE1	2:O:63:GLY:H	1.63	0.47
1:N:120:SER:HA	1:N:123:ILE:HD12	1.97	0.47
3:P:41:LEU:H	3:P:41:LEU:HD22	1.79	0.47
3:P:161:TYR:C	3:P:163:THR:N	2.73	0.47
7:T:33:ASN:CG	7:T:34:GLU:H	2.23	0.47
1:A:15:GLN:CG	1:N:113:PRO:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:SER:O	2:B:79:TRP:HH2	1.98	0.47
1:A:103:ARG:HH22	9:A:302:HEM:HBD1	1.80	0.47
1:A:146:TRP:HB2	2:B:75:ILE:CD1	2.43	0.47
11:A:304:TDS:CBC	2:B:88:LEU:HD22	2.45	0.47
3:C:88:GLU:H	3:C:88:GLU:CD	2.23	0.47
3:C:205:LYS:HZ3	3:C:205:LYS:HA	1.80	0.47
6:F:26:LEU:HD22	8:H:17:TRP:HE1	1.80	0.47
8:H:6:LEU:O	8:H:10:ALA:HB3	2.15	0.47
2:O:87:ILE:O	2:O:88:LEU:C	2.58	0.47
3:P:11:PRO:HA	3:P:107:LYS:NZ	2.29	0.47
3:P:167:SER:O	3:P:172:PHE:CZ	2.68	0.47
3:P:198:SER:HA	3:P:208:VAL:HB	1.97	0.47
6:S:26:LEU:HD21	8:U:17:TRP:NE1	2.29	0.47
8:U:11:LEU:O	8:U:12:LEU:C	2.56	0.47
1:A:95:LEU:HD21	5:E:7:PHE:HB2	1.98	0.46
1:A:105:TYR:O	1:A:107:THR:N	2.48	0.46
2:B:77:PRO:O	2:B:78:GLU:C	2.57	0.46
4:D:99:ILE:HD13	4:D:153:ALA:O	2.15	0.46
4:Q:147:SER:HB3	4:Q:171:ARG:HH12	1.80	0.46
5:R:23:ILE:HG23	5:R:24:PHE:HD2	1.76	0.46
1:A:15:GLN:HG3	1:N:113:PRO:HA	1.97	0.46
1:A:200:LEU:HD22	1:A:200:LEU:HA	1.76	0.46
4:D:50:VAL:O	4:D:164:PRO:HB2	2.15	0.46
4:D:133:TYR:HE2	4:D:146:LEU:O	1.99	0.46
5:E:18:ILE:HG22	5:E:22:ILE:CD1	2.45	0.46
1:N:118:TRP:HZ3	2:O:108:LEU:C	2.23	0.46
2:O:27:TYR:O	2:O:27:TYR:CD2	2.65	0.46
3:P:79:PRO:HG2	3:P:82:PHE:CD1	2.50	0.46
3:P:201:THR:C	3:P:203:SER:N	2.73	0.46
3:P:231:LEU:CD1	3:P:233:ASN:H	2.28	0.46
1:A:39:ILE:CD1	2:B:43:VAL:CG1	2.93	0.46
1:A:104:VAL:HG11	9:A:302:HEM:HMD3	1.96	0.46
2:B:73:LEU:O	2:B:74:GLU:HB2	2.15	0.46
3:C:270:LEU:HG	3:C:274:LEU:CD1	2.45	0.46
4:D:156:GLN:HB2	4:D:161:VAL:CG2	2.45	0.46
2:O:145:ILE:HG23	2:O:149:LEU:HB2	1.98	0.46
3:P:199:ILE:HB	3:P:207:VAL:O	2.14	0.46
4:Q:63:ASN:O	4:Q:69:PHE:CE1	2.68	0.46
13:Q:1307:OPC:HB2	13:Q:1307:OPC:CBX	2.38	0.46
12:A:305:PL9:H512	12:A:305:PL9:C40	2.42	0.46
3:C:250:GLN:NE2	3:C:251:ASP:H	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:275:LYS:HE3	4:D:20:ASN:HB3	1.96	0.46
3:C:277:LYS:HE3	7:G:31:ARG:CD	2.45	0.46
4:D:55:THR:O	4:D:56:ALA:C	2.58	0.46
8:H:9:VAL:CG1	8:H:10:ALA:N	2.79	0.46
3:P:26:HIS:CB	3:P:154:ASN:HD21	2.29	0.46
6:S:26:LEU:HB3	7:T:30:LYS:HE3	1.98	0.46
3:C:93:GLU:CA	3:C:97:GLU:CB	2.87	0.46
3:C:195:TYR:O	3:C:196:GLN:O	2.34	0.46
3:C:268:ALA:HA	4:D:26:THR:OG1	2.15	0.46
4:D:168:THR:HA	4:D:176:PRO:HB3	1.97	0.46
7:G:14:VAL:HG22	7:G:15:PHE:N	2.28	0.46
1:N:95:LEU:HG	5:R:7:PHE:HB2	1.97	0.46
2:O:31:ALA:O	2:O:32:TRP:CB	2.54	0.46
4:Q:53:GLY:O	4:Q:54:THR:OG1	2.27	0.46
4:Q:65:LYS:HB2	4:Q:68:LYS:HD3	1.98	0.46
2:B:42:VAL:CG1	7:G:28:GLN:HE22	2.28	0.46
3:C:213:ALA:C	3:C:215:PRO:HD2	2.40	0.46
3:C:231:LEU:CD1	3:C:231:LEU:H	2.29	0.46
4:D:15:ARG:NE	4:D:15:ARG:HA	2.31	0.46
4:D:141:ARG:HG2	4:D:141:ARG:HH11	1.81	0.46
4:D:151:CYS:SG	4:D:162:LEU:HD23	2.55	0.46
5:E:5:ALA:HB2	6:F:5:MET:CG	2.46	0.46
6:F:3:GLU:HA	6:F:6:LEU:HD12	1.96	0.46
3:P:221:GLU:CD	3:P:221:GLU:N	2.74	0.46
3:P:229:GLU:O	3:P:230:ALA:C	2.58	0.46
5:R:7:PHE:CD1	5:R:7:PHE:C	2.94	0.46
1:A:188:THR:CG2	9:A:301:HEM:HBC2	2.46	0.46
8:H:5:VAL:O	8:H:9:VAL:HG12	2.15	0.46
1:N:104:VAL:HG11	9:N:302:HEM:HMD3	1.97	0.46
1:N:178:ALA:O	1:N:182:ARG:HG3	2.16	0.46
2:O:72:PRO:O	2:O:73:LEU:CB	2.62	0.46
3:P:163:THR:OG1	3:P:165:GLU:HG2	2.16	0.46
4:Q:12:ASP:O	4:Q:14:GLY:N	2.48	0.46
8:U:5:VAL:O	8:U:9:VAL:HG12	2.16	0.46
1:A:61:THR:HA	1:N:59:LYS:HZ2	1.81	0.46
1:A:114:ARG:HB3	1:A:208:LYS:HZ3	1.81	0.46
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.97	0.46
3:C:273:ILE:CG2	7:G:27:GLN:HB3	2.46	0.46
4:D:168:THR:HG22	4:D:169:ASP:N	2.30	0.46
5:E:5:ALA:HB3	6:F:5:MET:HB2	1.98	0.46
1:N:27:PRO:HB3	2:O:31:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:38:GLY:HA3	10:N:303:HEC:C4C	2.46	0.46
3:P:180:ILE:HG13	3:P:199:ILE:HA	1.97	0.46
4:Q:64:VAL:HA	4:Q:69:PHE:CG	2.51	0.46
4:Q:125:LYS:CD	4:Q:132:GLN:HG2	2.46	0.46
4:Q:165:TRP:HE1	4:Q:176:PRO:HB2	1.81	0.46
3:C:59:GLN:OE1	3:C:67:LYS:HE3	2.16	0.46
3:C:265:VAL:O	3:C:269:GLN:HG3	2.14	0.46
4:D:36:TYR:O	4:D:40:LYS:HG2	2.16	0.46
4:D:99:ILE:CD1	4:D:153:ALA:HB3	2.46	0.46
2:O:57:LEU:CD2	3:P:258:MET:HE2	2.43	0.46
3:P:167:SER:O	3:P:172:PHE:HZ	1.98	0.46
4:Q:91:ILE:HD12	4:Q:160:ILE:CD1	2.38	0.46
4:Q:117:TRP:HE1	4:Q:135:GLU:CB	2.29	0.46
4:Q:133:TYR:CA	4:Q:139:VAL:HA	2.38	0.46
5:R:9:ILE:CG2	6:S:12:SER:HB2	2.46	0.46
5:R:18:ILE:HG22	5:R:22:ILE:CD1	2.46	0.46
1:A:33:PHE:CD1	5:E:18:ILE:HG23	2.51	0.46
2:B:91:LEU:HD21	2:B:100:LEU:HD12	1.97	0.46
4:D:57:LYS:H	4:D:82:GLN:HG2	1.81	0.46
1:N:141:ASP:HA	2:O:64:GLU:HG3	1.98	0.46
2:O:57:LEU:HD11	7:T:18:LEU:HB2	1.97	0.46
2:O:87:ILE:HG13	2:O:143:LEU:HD13	1.98	0.46
4:Q:133:TYR:CD2	4:Q:148:LEU:HG	2.51	0.46
4:Q:137:GLY:C	4:Q:171:ARG:NH1	2.73	0.46
12:A:305:PL9:H18	13:B:307:OPC:HBU1	1.97	0.45
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.97	0.45
2:B:149:LEU:H	2:B:149:LEU:HG	1.26	0.45
3:P:93:GLU:HG3	3:P:94:LEU:N	2.31	0.45
13:Q:1307:OPC:HAR2	13:Q:1307:OPC:HBM1	1.97	0.45
5:R:7:PHE:O	5:R:11:PHE:HD2	1.98	0.45
6:S:25:LEU:HD23	6:S:25:LEU:C	2.40	0.45
1:A:14:ILE:CG1	1:A:15:GLN:N	2.77	0.45
1:A:68:SER:O	1:A:71:TYR:HB3	2.15	0.45
3:C:163:THR:OG1	3:C:165:GLU:HG2	2.16	0.45
3:C:177:THR:CA	3:C:227:ALA:HA	2.45	0.45
4:D:123:LYS:CB	4:D:134:ASP:HA	2.46	0.45
6:F:25:LEU:HD23	6:F:25:LEU:C	2.41	0.45
8:H:3:ILE:HG23	8:H:4:ASP:H	1.81	0.45
1:N:17:LEU:C	1:N:17:LEU:HD13	2.41	0.45
1:N:98:ILE:CD1	14:O:1201:CLA:HED3	2.45	0.45
2:O:102:ALA:O	2:O:105:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:1:TYR:HD2	3:P:119:LEU:CD2	2.25	0.45
4:Q:115:VAL:HG13	4:Q:126:CYS:CB	2.44	0.45
6:S:30:GLN:HE21	6:S:30:GLN:HB2	1.55	0.45
1:A:15:GLN:HE21	1:A:15:GLN:HB2	1.57	0.45
1:A:106:LEU:HD12	5:E:18:ILE:HG13	1.99	0.45
1:A:112:LYS:HG3	1:A:113:PRO:N	2.31	0.45
1:A:143:VAL:HA	2:B:75:ILE:CD1	2.46	0.45
2:B:149:LEU:HD13	2:B:150:PRO:CD	2.43	0.45
2:B:152:ASP:OD2	2:B:152:ASP:C	2.58	0.45
3:C:161:TYR:C	3:C:163:THR:H	2.25	0.45
4:D:66:VAL:HG23	4:D:159:ASN:N	2.32	0.45
4:D:168:THR:HG23	4:D:174:GLU:O	2.17	0.45
5:E:23:ILE:O	5:E:27:LYS:CB	2.60	0.45
7:G:10:VAL:O	7:G:14:VAL:HG13	2.17	0.45
2:O:79:TRP:CZ2	5:R:1:MET:CB	2.86	0.45
2:O:122:ASN:CG	5:R:26:ILE:HG22	2.40	0.45
3:P:3:PHE:HE1	3:P:117:GLY:CA	2.29	0.45
3:P:282:VAL:HG22	4:Q:15:ARG:HE	1.82	0.45
1:A:142:GLN:HG2	2:B:65:PRO:O	2.16	0.45
2:B:26:TYR:O	2:B:27:TYR:HD1	1.98	0.45
2:B:36:LEU:C	2:B:38:TYR:N	2.74	0.45
2:O:40:PHE:N	2:O:41:PRO:HD2	2.31	0.45
4:Q:100:ARG:HB3	4:Q:102:TYR:CE2	2.52	0.45
4:Q:175:LYS:HB3	4:Q:175:LYS:HZ3	1.82	0.45
2:B:83:PRO:O	2:B:87:ILE:HG13	2.15	0.45
3:C:52:ILE:HG21	3:C:154:ASN:O	2.16	0.45
3:C:79:PRO:O	3:C:80:GLU:C	2.60	0.45
4:D:95:SER:C	4:D:97:GLU:N	2.75	0.45
4:D:108:CYS:O	4:D:110:HIS:N	2.50	0.45
4:D:123:LYS:NZ	4:D:140:ILE:CD1	2.80	0.45
1:N:28:PRO:HD2	2:O:32:TRP:C	2.40	0.45
1:N:119:ILE:C	1:N:121:GLY:N	2.69	0.45
2:O:28:GLY:O	2:O:29:GLU:OE2	2.35	0.45
4:Q:81:VAL:HB	4:Q:89:THR:HB	1.97	0.45
7:T:25:ALA:O	7:T:29:TYR:CG	2.70	0.45
8:U:9:VAL:HG22	8:U:13:VAL:HG23	1.97	0.45
2:B:77:PRO:HG3	2:B:85:PHE:CB	2.47	0.45
2:B:84:VAL:HG13	2:B:101:MET:HB2	1.99	0.45
4:D:55:THR:O	4:D:82:GLN:HG3	2.16	0.45
4:D:58:ASP:HB3	4:D:62:ASN:H	1.82	0.45
4:D:98:ALA:O	4:D:100:ARG:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:PRO:HG3	4:D:126:CYS:HA	1.97	0.45
1:N:154:VAL:HG11	2:O:101:MET:HE1	1.97	0.45
1:N:209:GLN:HB2	2:O:27:TYR:HB2	1.98	0.45
3:P:55:ASP:OD1	3:P:57:LYS:CG	2.64	0.45
3:P:98:VAL:O	3:P:99:GLY:O	2.34	0.45
3:P:219:VAL:HG12	3:P:220:SER:N	2.32	0.45
4:Q:56:ALA:O	4:Q:57:LYS:O	2.34	0.45
4:Q:118:ASN:O	4:Q:122:ASN:HA	2.17	0.45
8:U:8:TRP:CE3	8:U:11:LEU:HB2	2.52	0.45
1:A:26:VAL:HB	2:B:29:GLU:HB2	1.98	0.45
1:A:106:LEU:HD21	2:B:133:PHE:CZ	2.52	0.45
3:C:3:PHE:CZ	3:C:119:LEU:HD11	2.49	0.45
3:C:59:GLN:HB2	3:C:67:LYS:HE3	1.97	0.45
3:C:197:VAL:HG12	3:C:198:SER:N	2.32	0.45
4:D:38:LEU:HG	13:D:306:OPC:OBH	2.17	0.45
4:D:65:LYS:CB	4:D:68:LYS:HD3	2.41	0.45
4:D:123:LYS:HB3	4:D:134:ASP:HA	1.99	0.45
1:N:202:HIS:O	1:N:206:ILE:HG13	2.16	0.45
2:O:86:GLN:NE2	2:O:145:ILE:HB	2.31	0.45
3:P:28:ALA:HB3	3:P:238:GLY:O	2.17	0.45
3:P:40:VAL:HG11	3:P:46:PHE:CD2	2.51	0.45
3:P:185:LYS:HE3	3:P:217:LEU:HD21	1.98	0.45
3:P:190:TYR:HB3	3:P:191:GLY:H	1.44	0.45
3:P:251:ASP:HB3	3:P:254:ARG:HD2	1.98	0.45
4:Q:12:ASP:HB2	4:Q:13:MET:CE	2.47	0.45
4:Q:16:ARG:HG2	4:Q:16:ARG:HH11	1.80	0.45
4:Q:105:ASN:O	4:Q:149:ALA:HB3	2.16	0.45
8:U:7:GLY:O	8:U:11:LEU:CD1	2.64	0.45
3:C:171:VAL:HG13	3:C:234:ASN:CB	2.45	0.45
4:D:57:LYS:N	4:D:82:GLN:HG2	2.32	0.45
4:D:58:ASP:OD1	4:D:69:PHE:CE2	2.70	0.45
4:D:99:ILE:CB	4:D:153:ALA:HB1	2.36	0.45
4:D:124:PHE:CD2	4:D:148:LEU:HD12	2.52	0.45
7:G:21:LEU:C	7:G:21:LEU:HD13	2.41	0.45
3:P:4:TRP:CE3	3:P:4:TRP:N	2.85	0.45
4:Q:19:MET:O	4:Q:21:LEU:N	2.50	0.45
12:Q:1305:PL9:H412	12:Q:1305:PL9:H512	1.99	0.45
8:U:24:TRP:CG	8:U:25:GLY:N	2.83	0.45
1:A:17:LEU:HA	1:A:20:ASP:OD1	2.17	0.45
3:C:1:TYR:HD2	3:C:119:LEU:CD2	2.29	0.45
3:C:180:ILE:HG23	3:C:220:SER:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:29:TYR:C	7:G:31:ARG:H	2.24	0.45
1:N:137:SER:O	1:N:140:TRP:CD1	2.64	0.45
1:N:154:VAL:CG1	11:N:1304:TDS:HAX1	2.47	0.45
4:Q:156:GLN:CB	4:Q:161:VAL:HG11	2.47	0.45
4:Q:165:TRP:HA	4:Q:167:GLU:OE2	2.17	0.45
5:R:30:LYS:CB	5:R:30:LYS:NZ	2.80	0.45
7:T:14:VAL:HG22	7:T:15:PHE:N	2.32	0.45
1:A:114:ARG:NH1	1:A:209:GLN:N	2.55	0.45
2:B:53:ALA:HB2	3:C:262:ILE:HD11	1.99	0.45
3:C:218:ILE:HG23	3:C:232:THR:O	2.17	0.45
4:D:64:VAL:HG21	4:D:81:VAL:CG1	2.47	0.45
2:O:57:LEU:HD22	7:T:14:VAL:CB	2.47	0.45
2:O:57:LEU:HD22	7:T:14:VAL:HB	1.99	0.45
3:P:93:GLU:HG3	3:P:94:LEU:H	1.82	0.45
4:Q:16:ARG:HG2	4:Q:16:ARG:NH1	2.32	0.45
1:A:71:TYR:CE1	1:A:75:GLU:HG2	2.52	0.44
3:C:84:ILE:HD12	3:C:130:PRO:HD2	1.99	0.44
3:C:187:GLU:CG	3:C:188:ASP:H	2.28	0.44
1:N:111:LYS:HB3	1:N:113:PRO:HD2	1.99	0.44
1:N:209:GLN:HE21	2:O:28:GLY:C	2.26	0.44
4:Q:59:LYS:HG2	4:Q:79:VAL:HG13	1.99	0.44
4:Q:88:PRO:HD3	4:Q:107:VAL:HG23	1.99	0.44
4:Q:117:TRP:HE1	4:Q:135:GLU:CA	2.25	0.44
2:B:145:ILE:O	2:B:147:ALA:N	2.50	0.44
3:C:41:LEU:HD22	3:C:41:LEU:N	2.32	0.44
3:C:60:GLN:OE1	3:C:156:GLY:HA2	2.17	0.44
4:D:147:SER:HB2	4:D:177:TRP:CH2	2.45	0.44
11:N:1304:TDS:CB	2:O:81:LEU:HB3	2.47	0.44
2:O:32:TRP:CZ3	2:O:36:LEU:HA	2.50	0.44
2:O:122:ASN:HD22	2:O:125:ARG:NH1	2.14	0.44
3:P:86:PRO:HB2	3:P:88:GLU:OE1	2.17	0.44
4:Q:81:VAL:HG12	4:Q:82:GLN:N	2.32	0.44
4:Q:90:TYR:O	4:Q:91:ILE:CD1	2.65	0.44
4:Q:149:ALA:O	4:Q:150:LEU:HD22	2.17	0.44
8:U:5:VAL:O	8:U:9:VAL:CB	2.64	0.44
2:B:26:TYR:C	2:B:27:TYR:HD1	2.24	0.44
3:C:281:LYS:C	3:C:284:ALA:HB3	2.41	0.44
1:N:58:TYR:CE2	1:N:60:PRO:HB3	2.53	0.44
1:N:77:SER:O	1:N:78:PHE:HB2	2.17	0.44
1:N:115:GLU:OE1	1:N:115:GLU:N	2.46	0.44
2:O:73:LEU:C	2:O:73:LEU:CD1	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:77:PRO:O	2:O:78:GLU:C	2.59	0.44
3:P:62:ALA:C	3:P:157:ARG:NH1	2.75	0.44
3:P:218:ILE:HG23	3:P:232:THR:O	2.17	0.44
4:Q:15:ARG:NE	4:Q:15:ARG:HA	2.32	0.44
4:Q:121:GLU:O	4:Q:122:ASN:C	2.60	0.44
1:A:19:ASP:O	1:A:20:ASP:C	2.60	0.44
1:A:52:PHE:HB2	1:N:189:PHE:CE2	2.52	0.44
2:B:38:TYR:HB3	3:C:276:LYS:HD3	1.99	0.44
2:B:86:GLN:HG2	2:B:143:LEU:CA	2.47	0.44
3:C:48:ALA:HB3	3:C:129:PHE:HB2	1.98	0.44
3:C:124:TYR:C	3:C:126:GLU:H	2.24	0.44
3:C:154:ASN:OD1	3:C:155:ARG:N	2.49	0.44
3:C:185:LYS:HD3	3:C:195:TYR:CD2	2.47	0.44
3:C:277:LYS:CE	7:G:31:ARG:NE	2.81	0.44
4:D:55:THR:HG1	4:D:57:LYS:HZ2	1.60	0.44
8:H:9:VAL:C	8:H:11:LEU:N	2.74	0.44
1:N:29:HIS:HE2	1:N:209:GLN:NE2	2.15	0.44
3:P:41:LEU:HD22	3:P:41:LEU:N	2.32	0.44
4:Q:102:TYR:N	4:Q:153:ALA:HB2	2.32	0.44
1:A:78:PHE:O	1:A:79:GLY:C	2.58	0.44
2:B:86:GLN:O	2:B:90:SER:HB2	2.18	0.44
1:N:77:SER:O	4:Q:41:TYR:HA	2.18	0.44
3:P:61:VAL:HG11	3:P:214:GLY:C	2.43	0.44
3:P:71:ASN:HB2	10:P:301:HEC:CGA	2.47	0.44
3:P:120:PRO:CB	3:P:124:TYR:CD1	3.01	0.44
7:T:26:TYR:HA	7:T:29:TYR:HD1	1.71	0.44
1:A:114:ARG:NH1	1:A:209:GLN:O	2.51	0.44
1:A:189:PHE:O	1:A:192:PRO:HG2	2.17	0.44
3:C:45:VAL:HG22	3:C:85:ALA:CB	2.48	0.44
3:C:190:TYR:HB3	3:C:191:GLY:H	1.42	0.44
3:C:201:THR:C	3:C:203:SER:N	2.75	0.44
4:D:22:LEU:O	4:D:26:THR:HG23	2.17	0.44
4:D:57:LYS:CG	4:D:82:GLN:HG2	2.48	0.44
13:N:1306:OPC:HBG1	4:Q:39:VAL:HG13	1.99	0.44
4:Q:68:LYS:N	4:Q:68:LYS:CD	2.78	0.44
5:R:23:ILE:O	5:R:27:LYS:HG2	2.17	0.44
1:A:119:ILE:O	1:A:123:ILE:HG13	2.18	0.44
2:B:75:ILE:O	2:B:76:LEU:C	2.61	0.44
3:C:275:LYS:HZ3	3:C:276:LYS:NZ	2.16	0.44
4:D:16:ARG:O	4:D:18:PHE:N	2.48	0.44
2:O:25:ASN:OD1	2:O:26:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:57:LEU:HD13	7:T:15:PHE:CD2	2.53	0.44
2:O:81:LEU:O	2:O:85:PHE:CB	2.66	0.44
2:O:96:LEU:O	2:O:100:LEU:CB	2.66	0.44
2:O:146:GLY:O	2:O:149:LEU:CG	2.65	0.44
4:Q:103:GLY:O	4:Q:105:ASN:N	2.50	0.44
4:Q:123:LYS:CD	4:Q:140:ILE:HD12	2.33	0.44
4:Q:174:GLU:O	4:Q:175:LYS:C	2.60	0.44
8:U:22:VAL:HG12	8:U:26:ARG:HE	1.82	0.44
1:A:29:HIS:CG	1:A:30:VAL:N	2.85	0.44
2:B:74:GLU:O	2:B:75:ILE:HB	2.18	0.44
3:C:54:TYR:OH	3:C:58:LEU:HB2	2.18	0.44
3:C:173:THR:HB	3:C:229:GLU:HA	1.99	0.44
4:D:59:LYS:HD2	4:D:79:VAL:HB	1.99	0.44
4:D:117:TRP:CG	4:D:118:ASN:N	2.85	0.44
4:D:177:TRP:CE3	4:D:178:TRP:HE3	2.36	0.44
5:E:30:LYS:HZ2	5:E:30:LYS:CB	2.28	0.44
7:G:28:GLN:O	7:G:29:TYR:C	2.60	0.44
1:N:44:PHE:HD1	9:N:301:HEM:HBB1	1.82	0.44
1:N:81:LEU:HD13	1:N:81:LEU:O	2.18	0.44
1:N:92:MET:O	1:N:96:MET:HG2	2.18	0.44
2:O:99:LEU:C	2:O:99:LEU:HD13	2.43	0.44
2:O:146:GLY:H	2:O:149:LEU:CD1	2.22	0.44
3:P:61:VAL:O	3:P:61:VAL:HG23	2.17	0.44
4:Q:78:ARG:HG2	4:Q:117:TRP:CE3	2.53	0.44
4:Q:83:GLY:HA3	4:Q:87:ASP:O	2.17	0.44
4:Q:124:PHE:HD2	4:Q:133:TYR:HB2	1.82	0.44
5:R:26:ILE:N	5:R:26:ILE:CD1	2.80	0.44
8:U:9:VAL:CG1	8:U:10:ALA:N	2.81	0.44
10:A:303:HEC:HBD2	10:A:303:HEC:HHA	2.00	0.44
2:B:32:TRP:CZ3	2:B:36:LEU:HA	2.47	0.44
2:B:122:ASN:HA	2:B:123:PRO:HD3	1.69	0.44
4:D:138:ARG:CZ	4:D:138:ARG:CB	2.96	0.44
4:D:152:HIS:N	4:D:152:HIS:CD2	2.86	0.44
7:G:9:LEU:CG	7:G:10:VAL:H	2.31	0.44
3:P:233:ASN:HD22	3:P:234:ASN:H	1.66	0.44
3:P:251:ASP:O	3:P:252:PRO:C	2.61	0.44
7:T:11:LEU:CA	7:T:14:VAL:HG13	2.47	0.44
8:U:17:TRP:CZ3	8:U:21:MET:HE3	2.53	0.44
8:U:22:VAL:C	8:U:24:TRP:N	2.74	0.44
1:A:28:PRO:CD	2:B:32:TRP:HB2	2.48	0.43
2:B:151:LEU:HA	2:B:153:LYS:CD	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:THR:O	3:C:201:THR:HG22	2.18	0.43
3:C:231:LEU:CD1	3:C:231:LEU:N	2.80	0.43
3:C:279:VAL:O	3:C:279:VAL:HG12	2.16	0.43
4:D:100:ARG:HD3	4:D:101:ASP:N	2.33	0.43
4:D:118:ASN:HB3	4:D:121:GLU:H	1.83	0.43
4:D:129:HIS:O	4:D:143:PRO:CG	2.65	0.43
5:E:22:ILE:O	5:E:23:ILE:C	2.58	0.43
1:N:200:LEU:HD22	1:N:200:LEU:HA	1.76	0.43
3:P:48:ALA:HB3	3:P:129:PHE:HB2	1.99	0.43
3:P:262:ILE:HG13	7:T:21:LEU:HG	2.00	0.43
4:Q:64:VAL:HB	4:Q:81:VAL:HG23	1.98	0.43
5:R:5:ALA:HB2	6:S:5:MET:CB	2.48	0.43
8:U:27:ASN:C	8:U:29:LEU:H	2.22	0.43
1:A:111:LYS:CG	1:A:112:LYS:N	2.73	0.43
11:A:304:TDS:HBC3	2:B:88:LEU:HD22	2.00	0.43
3:C:26:HIS:CB	3:C:154:ASN:HD21	2.31	0.43
3:C:161:TYR:C	3:C:163:THR:N	2.74	0.43
3:C:231:LEU:HD13	3:C:232:THR:N	2.26	0.43
3:C:275:LYS:O	3:C:276:LYS:O	2.36	0.43
4:D:99:ILE:HD12	4:D:101:ASP:OD1	2.17	0.43
1:N:140:TRP:O	2:O:65:PRO:CG	2.65	0.43
2:O:153:LYS:C	2:O:155:LEU:N	2.76	0.43
3:P:29:ALA:O	3:P:30:LYS:HG2	2.18	0.43
3:P:45:VAL:HG22	3:P:85:ALA:CB	2.47	0.43
4:Q:94:GLU:N	4:Q:94:GLU:OE1	2.52	0.43
4:Q:115:VAL:CG2	4:Q:126:CYS:HB2	2.47	0.43
5:R:2:ILE:HG23	5:R:3:LEU:H	1.83	0.43
5:R:27:LYS:HD3	5:R:27:LYS:HA	1.71	0.43
2:B:73:LEU:HD22	2:B:73:LEU:N	2.33	0.43
2:B:114:ILE:C	2:B:116:ASN:N	2.75	0.43
2:B:149:LEU:CB	2:B:150:PRO:CD	2.95	0.43
4:D:22:LEU:HD23	4:D:22:LEU:C	2.41	0.43
13:D:306:OPC:HBX1	1:N:201:LEU:HD13	1.99	0.43
5:E:9:ILE:HB	6:F:9:ALA:HB1	2.00	0.43
6:F:10:LEU:N	6:F:10:LEU:HD23	2.32	0.43
7:G:22:PHE:C	7:G:26:TYR:CE1	2.96	0.43
8:H:21:MET:O	8:H:24:TRP:HE3	2.01	0.43
1:N:103:ARG:NE	1:N:107:THR:HG21	2.19	0.43
1:N:119:ILE:O	1:N:123:ILE:HG13	2.18	0.43
2:O:67:ASN:HD22	3:P:16:PRO:HB3	1.80	0.43
2:O:149:LEU:C	2:O:151:LEU:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:O	1:A:30:VAL:CG2	2.66	0.43
9:A:301:HEM:HBD1	9:A:301:HEM:CHA	2.47	0.43
2:B:24:HIS:O	2:B:25:ASN:HB3	2.18	0.43
2:B:45:MET:HE1	4:D:27:VAL:HA	2.00	0.43
2:B:67:ASN:HA	2:B:68:PRO:HD2	1.80	0.43
13:B:307:OPC:HAP1	13:B:307:OPC:CAL	2.45	0.43
3:C:251:ASP:C	3:C:253:ASN:N	2.75	0.43
4:D:78:ARG:HH21	4:D:92:VAL:HG11	1.83	0.43
1:N:30:VAL:HG23	1:N:30:VAL:O	2.17	0.43
3:P:1:TYR:CD2	3:P:119:LEU:HD21	2.48	0.43
4:Q:76:GLY:CA	4:Q:93:VAL:O	2.62	0.43
4:Q:91:ILE:O	4:Q:91:ILE:HG22	2.18	0.43
4:D:57:LYS:H	4:D:82:GLN:HB2	1.84	0.43
4:D:81:VAL:HG21	4:D:91:ILE:CD1	2.43	0.43
4:D:105:ASN:CB	4:D:107:VAL:HG23	2.49	0.43
5:E:9:ILE:CG1	6:F:13:PHE:HB2	2.47	0.43
8:H:8:TRP:O	8:H:11:LEU:HB2	2.17	0.43
2:O:57:LEU:HD12	7:T:18:LEU:HD12	2.00	0.43
2:O:94:LYS:HB3	2:O:95:LEU:H	1.66	0.43
2:O:136:GLY:HA3	14:O:1201:CLA:C4B	2.48	0.43
4:Q:16:ARG:NH2	4:Q:18:PHE:HE1	2.16	0.43
4:Q:19:MET:HG3	4:Q:20:ASN:N	2.34	0.43
4:Q:91:ILE:O	4:Q:92:VAL:O	2.35	0.43
4:Q:134:ASP:H	4:Q:138:ARG:C	2.26	0.43
5:R:18:ILE:HA	5:R:22:ILE:HG13	2.01	0.43
1:A:142:GLN:HE21	2:B:66:ALA:CA	2.22	0.43
2:B:25:ASN:N	2:B:25:ASN:ND2	2.66	0.43
3:C:14:ARG:HB3	3:C:20:ILE:HD13	2.01	0.43
3:C:255:VAL:O	3:C:258:MET:HG3	2.18	0.43
4:D:68:LYS:H	4:D:68:LYS:CD	2.32	0.43
4:D:73:HIS:ND1	4:D:77:ASP:CG	2.76	0.43
4:D:73:HIS:ND1	4:D:77:ASP:OD1	2.52	0.43
5:E:27:LYS:HD3	5:E:27:LYS:HA	1.75	0.43
1:N:22:THR:O	1:N:25:TYR:CE2	2.71	0.43
3:P:41:LEU:HB3	3:P:42:PRO:HD2	2.00	0.43
3:P:231:LEU:O	3:P:232:THR:CG2	2.58	0.43
4:Q:82:GLN:O	4:Q:87:ASP:O	2.37	0.43
4:Q:152:HIS:HB2	4:Q:162:LEU:HB3	2.01	0.43
13:Q:1307:OPC:HBE1	13:Q:1307:OPC:HBX2	2.01	0.43
8:U:6:LEU:O	8:U:7:GLY:C	2.61	0.43
8:U:27:ASN:C	8:U:29:LEU:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TYR:O	1:A:26:VAL:HG13	2.19	0.43
1:A:35:CYS:HA	10:A:303:HEC:C3B	2.49	0.43
1:A:106:LEU:HD12	5:E:18:ILE:CG1	2.48	0.43
2:B:24:HIS:O	2:B:25:ASN:CB	2.66	0.43
3:C:262:ILE:HG21	7:G:17:THR:HG22	1.99	0.43
4:D:16:ARG:NH2	4:D:18:PHE:HE1	2.17	0.43
4:D:78:ARG:HG3	4:D:117:TRP:CD1	2.54	0.43
4:D:118:ASN:HB2	4:D:122:ASN:N	2.34	0.43
4:D:118:ASN:CB	4:D:122:ASN:H	2.31	0.43
5:E:9:ILE:CG2	6:F:12:SER:HB2	2.47	0.43
1:N:34:TYR:CD2	1:N:34:TYR:N	2.87	0.43
2:O:141:ILE:CD1	5:R:11:PHE:CZ	3.01	0.43
3:P:211:ILE:HD11	3:P:231:LEU:HD23	1.99	0.43
3:P:251:ASP:C	3:P:253:ASN:N	2.75	0.43
3:P:262:ILE:HG22	3:P:263:CYS:N	2.34	0.43
4:Q:92:VAL:HG23	4:Q:100:ARG:H	1.83	0.43
4:Q:115:VAL:CG1	4:Q:126:CYS:HB2	2.46	0.43
4:Q:118:ASN:C	4:Q:120:ALA:H	2.25	0.43
4:Q:134:ASP:N	4:Q:138:ARG:O	2.51	0.43
4:Q:155:VAL:HG13	4:Q:159:ASN:O	2.18	0.43
1:A:91:SER:OG	2:B:79:TRP:HZ3	2.02	0.43
1:A:105:TYR:C	1:A:105:TYR:CD2	2.96	0.43
1:A:119:ILE:O	1:A:120:SER:C	2.62	0.43
2:B:94:LYS:HE2	2:B:94:LYS:HB2	1.82	0.43
4:D:12:ASP:HB2	4:D:13:MET:CE	2.49	0.43
4:D:165:TRP:CZ2	4:D:178:TRP:NE1	2.87	0.43
1:N:35:CYS:O	1:N:39:ILE:HG12	2.18	0.43
4:Q:36:TYR:O	4:Q:40:LYS:HG2	2.18	0.43
4:Q:152:HIS:NE2	4:Q:167:GLU:CD	2.76	0.43
6:S:14:GLY:O	6:S:15:LEU:C	2.61	0.43
1:A:27:PRO:HD2	2:B:29:GLU:HB2	2.00	0.43
1:A:44:PHE:CD1	9:A:301:HEM:HBB1	2.37	0.43
12:A:305:PL9:C10	13:D:306:OPC:HBF2	2.45	0.43
2:B:126:ARG:HG2	2:B:128:VAL:HG23	2.01	0.43
3:C:193:VAL:HG12	3:C:195:TYR:CE1	2.53	0.43
3:C:250:GLN:NE2	3:C:251:ASP:N	2.67	0.43
4:D:50:VAL:O	4:D:164:PRO:CB	2.66	0.43
4:D:117:TRP:CZ2	4:D:122:ASN:HA	2.54	0.43
8:H:22:VAL:O	8:H:26:ARG:HG3	2.19	0.43
1:N:110:PHE:HB3	1:N:118:TRP:CD1	2.54	0.43
1:N:118:TRP:HZ3	2:O:108:LEU:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:275:LYS:O	3:P:276:LYS:O	2.36	0.43
4:Q:78:ARG:HH12	4:Q:100:ARG:NH2	2.12	0.43
7:T:33:ASN:ND2	7:T:34:GLU:H	2.17	0.43
1:A:189:PHE:O	1:A:193:TRP:CE3	2.65	0.43
3:C:176:ALA:HB1	3:C:201:THR:HG21	2.00	0.43
4:D:73:HIS:CE1	4:D:77:ASP:OD1	2.72	0.43
2:O:126:ARG:NH1	2:O:129:ALA:HB2	2.33	0.43
2:O:145:ILE:HG22	2:O:146:GLY:N	2.33	0.43
4:Q:73:HIS:CE1	4:Q:77:ASP:HB2	2.53	0.43
4:Q:133:TYR:HA	4:Q:139:VAL:N	2.34	0.43
1:A:91:SER:CB	2:B:79:TRP:CZ3	3.02	0.42
1:A:186:ALA:HA	1:A:190:VAL:HB	1.99	0.42
9:A:301:HEM:HMA1	9:A:301:HEM:HAA2	1.87	0.42
10:A:303:HEC:HBC1	12:A:305:PL9:H161	2.01	0.42
2:B:95:LEU:N	2:B:95:LEU:CD2	2.71	0.42
3:C:270:LEU:HG	3:C:274:LEU:HD11	2.00	0.42
4:D:55:THR:OG1	4:D:55:THR:O	2.32	0.42
4:D:66:VAL:O	4:D:70:LEU:HB2	2.18	0.42
4:D:78:ARG:NE	4:D:92:VAL:CG1	2.78	0.42
5:E:16:PHE:CD2	16:E:101:BCR:H361	2.54	0.42
6:F:22:LEU:O	6:F:26:LEU:HB2	2.18	0.42
1:N:131:PHE:CD1	9:N:301:HEM:HAB	2.53	0.42
2:O:18:LEU:HD22	2:O:31:ALA:CB	2.49	0.42
4:Q:146:LEU:O	4:Q:147:SER:O	2.37	0.42
4:Q:175:LYS:NZ	4:Q:175:LYS:CB	2.82	0.42
1:A:14:ILE:HD13	1:A:15:GLN:CA	2.49	0.42
1:A:141:ASP:OD2	1:A:144:GLY:N	2.49	0.42
3:C:54:TYR:CD2	3:C:70:LEU:HD13	2.52	0.42
3:C:117:GLY:N	3:C:118:PRO:HD2	2.33	0.42
4:D:123:LYS:HZ2	4:D:140:ILE:CD1	2.32	0.42
4:D:168:THR:OG1	4:D:176:PRO:HD3	2.18	0.42
1:N:13:GLU:HB3	1:N:14:ILE:H	1.53	0.42
1:N:68:SER:O	1:N:71:TYR:HB3	2.19	0.42
1:N:95:LEU:HD21	5:R:7:PHE:HB2	2.01	0.42
1:N:111:LYS:O	1:N:112:LYS:C	2.62	0.42
1:N:112:LYS:H	1:N:112:LYS:HG2	1.43	0.42
1:N:154:VAL:N	1:N:155:PRO:HD2	2.34	0.42
1:N:186:ALA:HA	1:N:190:VAL:HB	2.00	0.42
3:P:27:LEU:H	3:P:27:LEU:HG	1.26	0.42
3:P:154:ASN:OD1	3:P:155:ARG:N	2.51	0.42
4:Q:15:ARG:C	4:Q:16:ARG:HG2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:73:HIS:CD2	4:Q:92:VAL:C	2.97	0.42
5:R:25:ALA:C	5:R:27:LYS:N	2.77	0.42
2:B:145:ILE:O	2:B:145:ILE:HG22	2.20	0.42
4:D:27:VAL:C	4:D:29:GLY:N	2.75	0.42
4:D:166:THR:HA	4:D:179:VAL:HG22	2.01	0.42
1:N:154:VAL:CG1	2:O:101:MET:HE1	2.49	0.42
2:O:130:THR:O	2:O:131:THR:C	2.62	0.42
3:P:116:VAL:O	3:P:117:GLY:C	2.62	0.42
3:P:197:VAL:HG12	3:P:198:SER:N	2.33	0.42
4:Q:138:ARG:HA	4:Q:138:ARG:CZ	2.48	0.42
1:A:135:GLY:HA2	1:A:138:LEU:HG	2.00	0.42
5:E:18:ILE:HB	5:E:22:ILE:HD12	2.01	0.42
5:E:25:ALA:C	5:E:27:LYS:N	2.77	0.42
6:F:30:GLN:HE21	6:F:30:GLN:HB2	1.56	0.42
1:N:21:VAL:C	1:N:23:SER:N	2.77	0.42
1:N:34:TYR:CD2	1:N:103:ARG:HD3	2.54	0.42
2:O:82:TYR:O	2:O:83:PRO:C	2.62	0.42
3:P:153:ALA:O	3:P:240:PHE:CD1	2.72	0.42
4:Q:91:ILE:O	4:Q:99:ILE:HB	2.20	0.42
4:Q:155:VAL:CG1	4:Q:156:GLN:N	2.82	0.42
8:U:3:ILE:HG23	8:U:4:ASP:H	1.85	0.42
1:A:21:VAL:O	1:A:21:VAL:HG12	2.18	0.42
3:C:11:PRO:HA	3:C:107:LYS:HZ3	1.83	0.42
4:D:52:GLY:CA	4:D:85:LYS:HZ3	2.33	0.42
4:D:155:VAL:CG1	4:D:156:GLN:N	2.83	0.42
8:H:27:ASN:C	8:H:29:LEU:N	2.75	0.42
2:O:64:GLU:CG	2:O:65:PRO:CD	2.86	0.42
2:O:86:GLN:HG2	2:O:143:LEU:CA	2.48	0.42
2:O:141:ILE:O	2:O:142:TRP:C	2.62	0.42
4:Q:73:HIS:HB3	4:Q:93:VAL:CB	2.50	0.42
6:S:18:VAL:O	6:S:22:LEU:HG	2.18	0.42
1:A:182:ARG:HH21	1:N:57:TYR:HE2	1.67	0.42
1:A:189:PHE:CD1	1:A:193:TRP:CZ3	3.08	0.42
3:C:92:GLU:N	3:C:94:LEU:HD23	2.35	0.42
7:G:17:THR:O	7:G:21:LEU:HB3	2.19	0.42
1:N:83:ARG:HD2	9:N:301:HEM:O2D	2.19	0.42
1:N:95:LEU:CD2	5:R:7:PHE:HB2	2.50	0.42
1:N:149:LYS:HD2	1:N:175:VAL:HG21	2.01	0.42
1:N:211:ILE:HB	1:N:212:SER:H	1.62	0.42
3:P:275:LYS:HG3	4:Q:20:ASN:HB3	2.00	0.42
4:Q:36:TYR:N	4:Q:37:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:65:LYS:HD3	4:Q:68:LYS:CG	2.48	0.42
4:Q:76:GLY:N	4:Q:93:VAL:CG1	2.72	0.42
4:Q:174:GLU:C	4:Q:174:GLU:CD	2.88	0.42
6:S:32:ALA:O	6:S:33:GLU:C	2.63	0.42
7:T:33:ASN:ND2	7:T:34:GLU:N	2.68	0.42
1:A:141:ASP:O	1:A:145:TYR:HB3	2.20	0.42
1:A:173:SER:HB2	1:A:174:SER:H	1.60	0.42
2:B:135:PHE:O	2:B:139:VAL:HG23	2.20	0.42
3:C:172:PHE:H	3:C:231:LEU:CG	2.08	0.42
3:C:177:THR:CB	3:C:227:ALA:HA	2.49	0.42
3:C:273:ILE:CG2	7:G:31:ARG:HH12	2.32	0.42
5:E:23:ILE:CG2	5:E:24:PHE:H	2.32	0.42
7:G:18:LEU:C	7:G:18:LEU:CD2	2.93	0.42
1:N:59:LYS:O	1:N:65:ALA:HA	2.19	0.42
1:N:81:LEU:O	1:N:85:ILE:HG13	2.20	0.42
2:O:80:TYR:HB3	14:O:1201:CLA:CED	2.38	0.42
4:Q:155:VAL:HG22	4:Q:160:ILE:HA	2.02	0.42
1:A:88:TRP:HZ2	2:B:58:ASP:CB	2.31	0.42
2:B:38:TYR:HD2	2:B:38:TYR:HA	1.62	0.42
2:B:87:ILE:O	2:B:88:LEU:C	2.61	0.42
2:B:91:LEU:CD2	2:B:100:LEU:HD12	2.50	0.42
3:C:277:LYS:O	3:C:280:GLU:HB3	2.20	0.42
3:C:280:GLU:O	3:C:284:ALA:HB2	2.20	0.42
4:D:138:ARG:HG2	4:D:138:ARG:H	1.45	0.42
7:G:22:PHE:O	7:G:26:TYR:CE1	2.73	0.42
2:O:94:LYS:HB2	2:O:94:LYS:HE2	1.84	0.42
2:O:122:ASN:ND2	2:O:125:ARG:CZ	2.74	0.42
3:P:54:TYR:CD2	3:P:70:LEU:HD13	2.48	0.42
3:P:79:PRO:O	3:P:80:GLU:C	2.61	0.42
3:P:84:ILE:HG13	3:P:103:PHE:HD1	1.84	0.42
3:P:92:GLU:N	3:P:94:LEU:HD23	2.33	0.42
3:P:171:VAL:HB	3:P:231:LEU:CD1	2.49	0.42
3:P:185:LYS:CG	3:P:195:TYR:HB3	2.32	0.42
3:P:275:LYS:HD3	3:P:276:LYS:N	2.34	0.42
4:Q:165:TRP:HE1	4:Q:176:PRO:CB	2.33	0.42
6:S:34:LYS:HE2	6:S:34:LYS:N	2.35	0.42
7:T:27:GLN:NE2	7:T:27:GLN:CA	2.83	0.42
1:A:29:HIS:CD2	1:A:30:VAL:CG2	3.00	0.42
1:A:191:LEU:N	1:A:192:PRO:HD2	2.35	0.42
2:B:37:LEU:O	2:B:38:TYR:CD2	2.73	0.42
3:C:22:CYS:O	3:C:24:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:ASP:O	3:C:252:PRO:C	2.62	0.42
4:D:147:SER:CB	4:D:171:ARG:HH22	2.33	0.42
7:G:28:GLN:O	7:G:31:ARG:HD2	2.20	0.42
1:N:116:LEU:H	1:N:116:LEU:CD1	2.16	0.42
2:O:29:GLU:OE2	2:O:29:GLU:HA	2.19	0.42
3:P:50:VAL:HG21	3:P:76:LEU:HD22	2.02	0.42
3:P:52:ILE:HD12	3:P:127:ILE:HD12	2.02	0.42
3:P:248:VAL:HG12	3:P:250:GLN:HG2	2.01	0.42
3:P:268:ALA:HA	4:Q:26:THR:OG1	2.20	0.42
4:Q:55:THR:O	4:Q:56:ALA:CB	2.67	0.42
4:Q:73:HIS:CD2	4:Q:77:ASP:CB	2.92	0.42
4:Q:87:ASP:HB3	4:Q:88:PRO:CD	2.43	0.42
4:Q:88:PRO:HD2	4:Q:107:VAL:HG23	2.02	0.42
4:Q:90:TYR:C	4:Q:91:ILE:HG12	2.45	0.42
12:Q:1305:PL9:C41	12:Q:1305:PL9:H512	2.50	0.42
3:C:248:VAL:HG12	3:C:250:GLN:HG2	2.01	0.42
4:D:84:LEU:O	4:D:85:LYS:C	2.62	0.42
4:D:131:SER:HB3	4:D:144:ALA:HA	2.01	0.42
4:D:165:TRP:CE2	4:D:167:GLU:O	2.72	0.42
4:D:177:TRP:CZ2	4:D:178:TRP:HZ3	2.38	0.42
1:N:114:ARG:HH21	1:N:209:GLN:CA	2.33	0.42
3:P:59:GLN:HB2	3:P:67:LYS:CE	2.50	0.42
4:Q:109:THR:OG1	4:Q:146:LEU:O	2.30	0.42
1:A:153:GLY:O	1:A:154:VAL:C	2.63	0.41
11:A:304:TDS:HBC2	2:B:85:PHE:HD2	1.84	0.41
4:D:16:ARG:HG2	4:D:16:ARG:HH11	1.85	0.41
4:D:20:ASN:C	4:D:20:ASN:OD1	2.63	0.41
4:D:108:CYS:HB3	4:D:115:VAL:HG22	2.01	0.41
8:H:27:ASN:C	8:H:29:LEU:H	2.25	0.41
1:N:95:LEU:HD11	5:R:10:VAL:CG1	2.36	0.41
1:N:110:PHE:HB3	1:N:118:TRP:HB2	2.02	0.41
3:P:59:GLN:HB2	3:P:67:LYS:HE3	2.01	0.41
3:P:154:ASN:O	3:P:155:ARG:HB3	2.19	0.41
3:P:182:LYS:CG	3:P:198:SER:HB2	2.46	0.41
4:Q:64:VAL:O	4:Q:81:VAL:HG22	2.19	0.41
4:Q:66:VAL:C	4:Q:68:LYS:N	2.76	0.41
1:A:53:ALA:O	4:D:41:TYR:OH	2.34	0.41
1:A:103:ARG:O	1:A:107:THR:HG22	2.20	0.41
2:B:79:TRP:HA	2:B:82:TYR:CZ	2.54	0.41
3:C:183:ILE:H	3:C:183:ILE:HG13	1.72	0.41
3:C:231:LEU:HD13	3:C:233:ASN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:ARG:HH21	4:D:17:GLN:HG2	1.82	0.41
4:D:118:ASN:N	4:D:123:LYS:O	2.53	0.41
4:D:156:GLN:OE1	4:D:161:VAL:HG11	2.20	0.41
2:O:104:VAL:HB	2:O:105:PRO:HD3	2.02	0.41
2:O:124:PHE:HB2	5:R:23:ILE:HA	2.01	0.41
3:P:201:THR:O	3:P:201:THR:HG22	2.20	0.41
3:P:220:SER:HB2	3:P:221:GLU:CD	2.45	0.41
4:Q:100:ARG:NH2	4:Q:135:GLU:O	2.50	0.41
5:R:23:ILE:O	5:R:27:LYS:CG	2.68	0.41
1:A:50:THR:O	1:A:54:MET:HG3	2.21	0.41
1:A:77:SER:O	1:A:78:PHE:CB	2.67	0.41
1:A:156:GLU:C	1:A:158:ILE:H	2.28	0.41
3:C:59:GLN:HB2	3:C:67:LYS:CE	2.51	0.41
3:C:93:GLU:HG3	3:C:94:LEU:N	2.35	0.41
5:E:26:ILE:N	5:E:26:ILE:CD1	2.83	0.41
6:F:14:GLY:O	6:F:15:LEU:C	2.63	0.41
1:N:21:VAL:O	1:N:22:THR:C	2.63	0.41
1:N:101:VAL:HG11	14:O:1201:CLA:HMA1	2.02	0.41
3:P:185:LYS:CD	3:P:217:LEU:HD11	2.49	0.41
3:P:231:LEU:HD21	3:P:233:ASN:O	2.20	0.41
4:Q:77:ASP:N	4:Q:77:ASP:OD1	2.53	0.41
4:Q:109:THR:HG21	4:Q:177:TRP:CH2	2.54	0.41
12:Q:1305:PL9:H302	13:Q:1307:OPC:HBB2	2.02	0.41
12:Q:1305:PL9:H151	12:Q:1305:PL9:H171	1.68	0.41
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.29	0.41
2:B:22:MET:N	2:B:24:HIS:CE1	2.88	0.41
2:B:150:PRO:O	2:B:153:LYS:CD	2.68	0.41
4:D:100:ARG:C	4:D:100:ARG:HD3	2.45	0.41
11:N:1304:TDS:CBB	2:O:81:LEU:HD13	2.47	0.41
3:P:84:ILE:HG23	3:P:130:PRO:HG2	2.01	0.41
3:P:231:LEU:HD22	3:P:232:THR:H	1.82	0.41
4:Q:154:THR:C	4:Q:155:VAL:CG2	2.94	0.41
8:U:11:LEU:C	8:U:15:PHE:CE1	2.99	0.41
1:A:14:ILE:HA	1:A:17:LEU:CD1	2.50	0.41
2:B:71:THR:CB	2:B:72:PRO:CD	2.80	0.41
2:B:110:LEU:O	2:B:113:PHE:HB2	2.20	0.41
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.54	0.41
3:C:118:PRO:O	3:C:120:PRO:HD3	2.20	0.41
4:D:93:VAL:HG22	4:D:98:ALA:O	2.21	0.41
4:D:98:ALA:O	4:D:99:ILE:C	2.61	0.41
8:H:25:GLY:O	8:H:29:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:158:ILE:HD11	2:O:98:VAL:HG11	2.03	0.41
2:O:78:GLU:HG2	2:O:80:TYR:HD1	1.85	0.41
2:O:123:PRO:C	2:O:124:PHE:CD2	2.98	0.41
2:O:151:LEU:O	2:O:152:ASP:C	2.62	0.41
2:O:155:LEU:HG	2:O:155:LEU:O	2.21	0.41
3:P:93:GLU:CA	3:P:97:GLU:CB	2.94	0.41
4:Q:15:ARG:HH21	4:Q:17:GLN:HG2	1.84	0.41
4:Q:50:VAL:O	4:Q:50:VAL:HG12	2.21	0.41
6:S:34:LYS:HD2	6:S:35:GLU:N	2.35	0.41
1:A:105:TYR:CE1	14:B:201:CLA:HAB	2.55	0.41
1:A:156:GLU:HG2	1:A:163:VAL:HG22	2.02	0.41
3:C:159:GLN:HG3	3:C:170:ASN:HB3	2.02	0.41
4:D:78:ARG:NH1	4:D:124:PHE:CZ	2.88	0.41
1:N:34:TYR:N	1:N:34:TYR:HD2	2.19	0.41
1:N:140:TRP:CZ2	1:N:145:TYR:HD2	2.39	0.41
1:N:142:GLN:HG2	2:O:64:GLU:HB3	2.03	0.41
2:O:81:LEU:O	2:O:85:PHE:HB2	2.20	0.41
3:P:52:ILE:CG1	3:P:153:ALA:HB1	2.44	0.41
4:Q:70:LEU:HD23	4:Q:70:LEU:C	2.45	0.41
4:Q:139:VAL:O	4:Q:139:VAL:HG13	2.21	0.41
7:T:11:LEU:H	7:T:11:LEU:CD2	2.24	0.41
1:A:20:ASP:C	1:A:22:THR:H	2.28	0.41
1:A:33:PHE:HZ	5:E:17:GLY:HA3	1.85	0.41
1:A:47:GLN:OE1	1:A:86:HIS:O	2.39	0.41
2:B:89:ARG:NH2	2:B:147:ALA:O	2.51	0.41
13:B:307:OPC:HBC1	13:B:307:OPC:HBS	2.02	0.41
3:C:116:VAL:O	3:C:117:GLY:C	2.62	0.41
3:C:177:THR:OG1	3:C:227:ALA:HA	2.21	0.41
4:D:39:VAL:O	4:D:43:ILE:HD13	2.20	0.41
4:D:167:GLU:OE2	4:D:167:GLU:N	2.53	0.41
8:H:15:PHE:O	8:H:19:ILE:HG13	2.21	0.41
2:O:34:ASN:OD1	2:O:35:ASP:N	2.54	0.41
3:P:73:GLY:O	3:P:74:ALA:HB2	2.21	0.41
3:P:187:GLU:CG	3:P:188:ASP:H	2.32	0.41
4:Q:78:ARG:HH21	4:Q:135:GLU:HB2	1.85	0.41
7:T:33:ASN:H	7:T:33:ASN:HD22	1.68	0.41
1:A:29:HIS:CE1	1:A:210:GLY:O	2.74	0.41
1:A:120:SER:HA	1:A:123:ILE:HD12	2.03	0.41
2:B:40:PHE:N	2:B:41:PRO:CD	2.84	0.41
3:C:86:PRO:HB2	3:C:88:GLU:OE1	2.21	0.41
4:D:126:CYS:HB2	4:D:131:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:LEU:H	7:G:11:LEU:CD2	2.23	0.41
1:N:148:VAL:HA	1:N:151:VAL:HG22	2.03	0.41
3:P:10:PRO:N	3:P:11:PRO:HD2	2.36	0.41
3:P:161:TYR:CE1	3:P:167:SER:CA	2.96	0.41
3:P:180:ILE:HG12	3:P:181:THR:N	2.36	0.41
3:P:183:ILE:H	3:P:183:ILE:HG13	1.72	0.41
3:P:192:ASN:OD1	3:P:193:VAL:N	2.54	0.41
3:P:264:LEU:HD13	4:Q:30:VAL:HA	2.02	0.41
4:Q:98:ALA:O	4:Q:99:ILE:C	2.63	0.41
4:Q:168:THR:HG23	4:Q:175:LYS:CA	2.50	0.41
5:R:22:ILE:HA	5:R:25:ALA:HB2	2.02	0.41
1:A:142:GLN:HE21	2:B:67:ASN:N	2.16	0.41
3:C:3:PHE:HE1	3:C:117:GLY:CA	2.33	0.41
3:C:6:GLN:HG3	3:C:106:TYR:O	2.20	0.41
3:C:10:PRO:HG2	3:C:11:PRO:CD	2.49	0.41
3:C:20:ILE:HB	3:C:240:PHE:CZ	2.56	0.41
3:C:66:SER:O	3:C:68:VAL:HG13	2.21	0.41
3:C:131:VAL:CG2	3:C:132:LEU:N	2.83	0.41
3:C:140:LYS:HD3	3:C:140:LYS:HA	1.96	0.41
3:C:275:LYS:HE3	4:D:17:GLN:HB2	2.02	0.41
3:C:277:LYS:HE3	7:G:31:ARG:NE	2.35	0.41
3:C:281:LYS:O	3:C:284:ALA:HB3	2.21	0.41
4:D:81:VAL:CG1	4:D:82:GLN:H	2.20	0.41
4:D:138:ARG:NH2	4:D:147:SER:CB	2.83	0.41
13:D:306:OPC:HBL1	13:D:306:OPC:CAP	2.44	0.41
5:E:2:ILE:O	5:E:2:ILE:HD12	2.21	0.41
5:E:15:PHE:HD2	5:E:15:PHE:HA	1.65	0.41
5:E:23:ILE:O	5:E:27:LYS:HG2	2.21	0.41
6:F:26:LEU:HD13	6:F:26:LEU:HA	1.77	0.41
8:H:24:TRP:CE3	8:H:25:GLY:N	2.89	0.41
1:N:39:ILE:CD1	16:R:1101:BCR:H312	2.50	0.41
1:N:156:GLU:HG3	1:N:166:SER:OG	2.21	0.41
2:O:75:ILE:O	2:O:77:PRO:CD	2.67	0.41
2:O:106:LEU:HD21	14:O:1201:CLA:C15	2.48	0.41
2:O:126:ARG:HA	2:O:127:PRO:HD2	1.78	0.41
3:P:4:TRP:N	3:P:4:TRP:HE3	2.18	0.41
3:P:192:ASN:O	3:P:193:VAL:HG23	2.21	0.41
3:P:270:LEU:HG	3:P:274:LEU:HD11	2.03	0.41
4:Q:44:PRO:HA	4:Q:45:PRO:HD2	1.51	0.41
4:Q:78:ARG:N	4:Q:78:ARG:CD	2.82	0.41
4:Q:80:LEU:HA	4:Q:89:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:104:ILE:O	4:Q:106:ALA:N	2.54	0.41
5:R:23:ILE:CG2	5:R:24:PHE:H	2.34	0.41
7:T:11:LEU:HA	7:T:14:VAL:HG11	2.03	0.41
1:A:14:ILE:HG23	1:A:15:GLN:N	2.31	0.41
1:A:22:THR:C	1:A:25:TYR:HE1	2.29	0.41
1:A:154:VAL:N	1:A:155:PRO:HD2	2.36	0.41
10:A:303:HEC:HBC3	12:A:305:PL9:C15	2.51	0.41
2:B:42:VAL:CG1	7:G:28:GLN:NE2	2.83	0.41
3:C:52:ILE:HD12	3:C:127:ILE:HD12	2.03	0.41
3:C:231:LEU:HD21	3:C:233:ASN:O	2.20	0.41
4:D:92:VAL:O	4:D:100:ARG:HB2	2.21	0.41
1:N:23:SER:O	1:N:25:TYR:CZ	2.74	0.41
1:N:190:VAL:HG11	11:N:1304:TDS:OAK	2.21	0.41
2:O:94:LYS:C	2:O:95:LEU:HD23	2.46	0.41
3:P:4:TRP:CE3	3:P:4:TRP:CA	3.03	0.41
3:P:124:TYR:C	3:P:126:GLU:H	2.26	0.41
3:P:130:PRO:HG2	3:P:130:PRO:O	2.21	0.41
4:Q:123:LYS:HE3	4:Q:125:LYS:CE	2.51	0.41
16:R:1101:BCR:C14	6:S:16:ILE:HG21	2.51	0.41
2:B:84:VAL:CG1	2:B:101:MET:HB2	2.50	0.40
2:B:92:PRO:O	2:B:93:ASN:C	2.64	0.40
2:B:118:ASN:HB3	2:B:121:GLN:HG3	2.02	0.40
3:C:127:ILE:HG22	3:C:129:PHE:CE1	2.57	0.40
3:C:188:ASP:O	3:C:189:GLU:CB	2.68	0.40
4:D:15:ARG:C	4:D:16:ARG:HG2	2.47	0.40
4:D:87:ASP:CG	4:D:107:VAL:HG21	2.46	0.40
4:D:160:ILE:HG22	4:D:162:LEU:HD13	2.04	0.40
8:H:22:VAL:HG12	8:H:26:ARG:HE	1.85	0.40
1:N:25:TYR:HB2	1:N:26:VAL:H	1.51	0.40
1:N:28:PRO:HD2	2:O:32:TRP:CA	2.51	0.40
1:N:50:THR:O	1:N:54:MET:HG3	2.20	0.40
1:N:112:LYS:CB	1:N:113:PRO:CD	2.95	0.40
3:P:273:ILE:C	3:P:273:ILE:HD12	2.46	0.40
4:Q:15:ARG:HH22	4:Q:17:GLN:HG2	1.86	0.40
4:Q:41:TYR:CD2	4:Q:41:TYR:C	2.98	0.40
4:Q:64:VAL:HG13	4:Q:69:PHE:CE2	2.56	0.40
4:Q:84:LEU:O	4:Q:87:ASP:OD1	2.38	0.40
1:A:20:ASP:C	1:A:22:THR:N	2.79	0.40
1:A:34:TYR:N	1:A:34:TYR:CD2	2.87	0.40
11:A:304:TDS:HBC1	2:B:85:PHE:CB	2.51	0.40
2:B:149:LEU:HD23	4:Q:129:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:CYS:C	3:C:24:ASN:N	2.80	0.40
3:C:192:ASN:O	3:C:193:VAL:HG23	2.21	0.40
3:C:275:LYS:HG3	4:D:20:ASN:HB3	2.02	0.40
4:D:58:ASP:C	4:D:60:LEU:N	2.79	0.40
4:D:59:LYS:HD3	4:D:79:VAL:HB	2.03	0.40
1:N:102:PHE:HB3	5:R:18:ILE:CD1	2.49	0.40
3:P:275:LYS:CE	4:Q:20:ASN:HD22	2.34	0.40
6:S:3:GLU:HA	6:S:6:LEU:HD12	2.02	0.40
1:A:116:LEU:H	1:A:116:LEU:CD1	2.18	0.40
1:A:134:THR:HG23	11:A:304:TDS:HAQ2	2.03	0.40
2:B:57:LEU:HD13	7:G:15:PHE:CD2	2.56	0.40
2:B:126:ARG:HG2	2:B:128:VAL:CG2	2.51	0.40
3:C:14:ARG:NH2	3:C:150:HIS:CD2	2.89	0.40
3:C:93:GLU:HG3	3:C:94:LEU:H	1.86	0.40
3:C:173:THR:HB	3:C:229:GLU:C	2.46	0.40
3:C:185:LYS:CD	3:C:217:LEU:HD11	2.51	0.40
3:C:226:LYS:HB3	3:C:227:ALA:H	1.69	0.40
4:D:50:VAL:HG12	4:D:164:PRO:CB	2.49	0.40
4:D:165:TRP:HA	4:D:167:GLU:CD	2.46	0.40
7:G:9:LEU:HG	7:G:10:VAL:N	2.36	0.40
1:N:83:ARG:NH2	2:O:61:MET:O	2.54	0.40
1:N:189:PHE:CD1	1:N:193:TRP:CZ3	3.09	0.40
2:O:135:PHE:O	2:O:139:VAL:HG23	2.22	0.40
3:P:59:GLN:OE1	3:P:67:LYS:HE3	2.21	0.40
4:Q:66:VAL:CG2	4:Q:160:ILE:HG13	2.46	0.40
4:Q:81:VAL:C	4:Q:82:GLN:CG	2.94	0.40
4:Q:83:GLY:CA	4:Q:87:ASP:O	2.69	0.40
4:Q:111:LEU:HD23	4:Q:129:HIS:CE1	2.57	0.40
4:Q:131:SER:CB	4:Q:144:ALA:HB2	2.51	0.40
4:Q:138:ARG:CD	4:Q:171:ARG:HD3	2.51	0.40
4:Q:165:TRP:CE2	4:Q:178:TRP:CH2	3.10	0.40
3:C:61:VAL:O	3:C:61:VAL:HG23	2.21	0.40
3:C:234:ASN:C	3:C:236:ASN:H	2.30	0.40
1:N:104:VAL:HG13	9:N:302:HEM:HMD3	2.02	0.40
1:N:163:VAL:HG12	1:N:164:LEU:N	2.36	0.40
3:P:76:LEU:HG	3:P:78:LEU:HD21	2.03	0.40
4:Q:96:LYS:O	4:Q:96:LYS:HD2	2.22	0.40
5:R:5:ALA:HB3	6:S:5:MET:HB2	2.01	0.40
8:U:17:TRP:O	8:U:21:MET:HG3	2.22	0.40
1:A:105:TYR:CD1	14:B:201:CLA:HMB1	2.55	0.40
3:C:109:GLY:O	3:C:111:ASP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:TYR:OH	4:D:135:GLU:HG3	2.21	0.40
4:D:149:ALA:HB1	4:D:178:TRP:CD1	2.57	0.40
7:G:25:ALA:HA	7:G:28:GLN:OE1	2.22	0.40
3:P:188:ASP:O	3:P:189:GLU:CB	2.69	0.40
3:P:193:VAL:HG12	3:P:195:TYR:CE1	2.57	0.40
4:Q:155:VAL:HA	4:Q:161:VAL:N	2.24	0.40
6:S:32:ALA:O	6:S:34:LYS:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/215 (93%)	152 (76%)	29 (14%)	19 (10%)	0	2
1	N	200/215 (93%)	155 (78%)	32 (16%)	13 (6%)	1	5
2	B	136/160 (85%)	80 (59%)	31 (23%)	25 (18%)	0	0
2	O	136/160 (85%)	67 (49%)	38 (28%)	31 (23%)	0	0
3	C	284/289 (98%)	206 (72%)	47 (16%)	31 (11%)	0	1
3	P	284/289 (98%)	213 (75%)	44 (16%)	27 (10%)	0	2
4	D	166/179 (93%)	123 (74%)	25 (15%)	18 (11%)	0	1
4	Q	166/179 (93%)	85 (51%)	49 (30%)	32 (19%)	0	0
5	E	30/32 (94%)	22 (73%)	6 (20%)	2 (7%)	1	5
5	R	30/32 (94%)	23 (77%)	5 (17%)	2 (7%)	1	5
6	F	31/35 (89%)	25 (81%)	5 (16%)	1 (3%)	3	18
6	S	33/35 (94%)	25 (76%)	5 (15%)	3 (9%)	0	2
7	G	21/37 (57%)	15 (71%)	5 (24%)	1 (5%)	2	11
7	T	25/37 (68%)	18 (72%)	6 (24%)	1 (4%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	25/29 (86%)	18 (72%)	7 (28%)	0	100	100
8	U	25/29 (86%)	19 (76%)	6 (24%)	0	100	100
All	All	1792/1952 (92%)	1246 (70%)	340 (19%)	206 (12%)	0	1

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	TYR
1	A	28	PRO
1	A	111	LYS
1	A	160	VAL
1	A	173	SER
1	A	211	ILE
2	B	22	MET
2	B	25	ASN
2	B	32	TRP
2	B	33	PRO
2	B	34	ASN
2	B	35	ASP
2	B	72	PRO
2	B	75	ILE
2	B	76	LEU
2	B	149	LEU
2	B	154	THR
3	C	54	TYR
3	C	92	GLU
3	C	99	GLY
3	C	110	GLN
3	C	189	GLU
3	C	196	GLN
3	C	203	SER
3	C	227	ALA
3	C	232	THR
3	C	276	LYS
4	D	66	VAL
4	D	85	LYS
4	D	110	HIS
1	N	19	ASP
1	N	21	VAL
1	N	22	THR
1	N	30	VAL

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Mol	Chain	Res	Type
1	N	32	ILE
1	N	111	LYS
2	O	25	ASN
2	O	26	TYR
2	O	30	PRO
2	O	32	TRP
2	O	33	PRO
2	O	34	ASN
2	O	35	ASP
2	O	65	PRO
2	O	72	PRO
2	O	73	LEU
2	O	115	GLU
2	O	121	GLN
2	O	123	PRO
2	O	124	PHE
2	O	150	PRO
2	O	151	LEU
3	P	54	TYR
3	P	92	GLU
3	P	99	GLY
3	P	110	GLN
3	P	189	GLU
3	P	196	GLN
3	P	203	SER
3	P	227	ALA
3	P	232	THR
3	P	276	LYS
4	Q	46	SER
4	Q	57	LYS
4	Q	73	HIS
4	Q	74	ASN
4	Q	92	VAL
4	Q	106	ALA
4	Q	124	PHE
4	Q	145	PRO
4	Q	153	ALA
4	Q	164	PRO
1	A	14	ILE
1	A	20	ASP
1	A	27	PRO
1	A	75	GLU

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Mol	Chain	Res	Type
1	A	106	LEU
2	B	19	ALA
2	B	71	THR
2	B	78	GLU
2	B	93	ASN
2	B	115	GLU
2	B	128	VAL
2	B	145	ILE
2	B	146	GLY
2	B	153	LYS
3	C	56	THR
3	C	94	LEU
3	C	188	ASP
3	C	202	ASP
3	C	230	ALA
4	D	14	GLY
4	D	20	ASN
4	D	75	ALA
4	D	106	ALA
4	D	109	THR
7	G	29	TYR
1	N	16	ALA
1	N	110	PHE
1	N	177	GLN
1	N	190	VAL
2	O	20	LYS
2	O	93	ASN
2	O	128	VAL
2	O	147	ALA
2	O	148	ALA
2	O	149	LEU
2	O	153	LYS
3	P	56	THR
3	P	188	ASP
3	P	202	ASP
3	P	230	ALA
4	Q	14	GLY
4	Q	56	ALA
4	Q	81	VAL
4	Q	91	ILE
4	Q	93	VAL
4	Q	104	ILE

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Mol	Chain	Res	Type
4	Q	105	ASN
4	Q	147	SER
4	Q	157	ASP
5	R	25	ALA
6	S	33	GLU
7	T	29	TYR
1	A	112	LYS
1	A	140	TRP
1	A	190	VAL
2	B	92	PRO
3	C	23	ALA
3	C	127	ILE
3	C	220	SER
3	C	233	ASN
4	D	68	LYS
4	D	99	ILE
4	D	141	ARG
5	E	25	ALA
1	N	205	MET
2	O	63	GLY
2	O	64	GLU
2	O	92	PRO
2	O	114	ILE
2	O	118	ASN
3	P	94	LEU
3	P	193	VAL
3	P	220	SER
3	P	233	ASN
4	Q	48	GLY
4	Q	175	LYS
1	A	15	GLN
1	A	205	MET
2	B	30	PRO
2	B	79	TRP
3	C	87	GLU
3	C	130	PRO
3	C	187	GLU
3	C	193	VAL
4	D	56	ALA
2	O	75	ILE
3	P	23	ALA
3	P	87	GLU

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Mol	Chain	Res	Type
3	P	91	PRO
3	P	127	ILE
3	P	130	PRO
3	P	187	GLU
4	Q	13	MET
4	Q	20	ASN
4	Q	45	PRO
4	Q	67	SER
4	Q	143	PRO
1	A	24	LYS
1	A	105	TYR
2	B	114	ILE
3	C	221	GLU
4	D	47	GLY
4	D	50	VAL
4	D	101	ASP
4	D	143	PRO
2	O	76	LEU
3	P	224	ALA
4	Q	50	VAL
4	Q	98	ALA
4	Q	151	CYS
4	Q	160	ILE
6	S	30	GLN
1	A	21	VAL
3	C	58	LEU
3	C	191	GLY
3	C	224	ALA
3	C	282	VAL
4	D	13	MET
1	N	26	VAL
4	Q	102	TYR
3	C	31	PRO
5	E	20	VAL
3	P	282	VAL
3	P	191	GLY
6	S	29	ILE
3	C	91	PRO
6	F	29	ILE
2	O	109	ILE
5	R	20	VAL
2	B	123	PRO

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Mol	Chain	Res	Type
3	C	117	GLY
4	D	145	PRO
4	Q	64	VAL
1	N	211	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/184 (94%)	144 (84%)	28 (16%)	2	12
1	N	172/184 (94%)	150 (87%)	22 (13%)	4	19
2	B	117/136 (86%)	92 (79%)	25 (21%)	1	6
2	O	117/136 (86%)	96 (82%)	21 (18%)	2	10
3	C	240/243 (99%)	205 (85%)	35 (15%)	3	15
3	P	240/243 (99%)	202 (84%)	38 (16%)	2	13
4	D	136/146 (93%)	117 (86%)	19 (14%)	3	16
4	Q	136/146 (93%)	116 (85%)	20 (15%)	3	15
5	E	25/25 (100%)	14 (56%)	11 (44%)	0	0
5	R	25/25 (100%)	13 (52%)	12 (48%)	0	0
6	F	25/27 (93%)	22 (88%)	3 (12%)	5	22
6	S	27/27 (100%)	23 (85%)	4 (15%)	3	15
7	G	17/28 (61%)	9 (53%)	8 (47%)	0	0
7	T	21/28 (75%)	12 (57%)	9 (43%)	0	0
8	H	22/24 (92%)	19 (86%)	3 (14%)	3	17
8	U	22/24 (92%)	19 (86%)	3 (14%)	3	17
All	All	1514/1626 (93%)	1253 (83%)	261 (17%)	2	11

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	15	GLN
1	A	19	ASP
1	A	24	LYS
1	A	26	VAL
1	A	28	PRO
1	A	36	LEU
1	A	47	GLN
1	A	63	THR
1	A	74	ASN
1	A	75	GLU
1	A	95	LEU
1	A	103	ARG
1	A	115	GLU
1	A	116	LEU
1	A	140	TRP
1	A	143	VAL
1	A	148	VAL
1	A	150	ILE
1	A	164	LEU
1	A	167	ASP
1	A	173	SER
1	A	177	GLN
1	A	193	TRP
1	A	195	ILE
1	A	200	LEU
1	A	207	ARG
1	A	211	ILE
2	B	20	LYS
2	B	22	MET
2	B	25	ASN
2	B	26	TYR
2	B	27	TYR
2	B	29	GLU
2	B	32	TRP
2	B	33	PRO
2	B	35	ASP
2	B	36	LEU
2	B	39	VAL
2	B	62	VAL
2	B	74	GLU
2	B	78	GLU
2	B	79	TRP

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Mol	Chain	Res	Type
2	B	81	LEU
2	B	84	VAL
2	B	90	SER
2	B	92	PRO
2	B	95	LEU
2	B	96	LEU
2	B	108	LEU
2	B	121	GLN
2	B	124	PHE
2	B	149	LEU
3	C	3	PHE
3	C	4	TRP
3	C	14	ARG
3	C	17	THR
3	C	19	ARG
3	C	27	LEU
3	C	51	LYS
3	C	83	LYS
3	C	91	PRO
3	C	93	GLU
3	C	94	LEU
3	C	98	VAL
3	C	100	ASP
3	C	104	GLN
3	C	114	LEU
3	C	119	LEU
3	C	122	GLU
3	C	131	VAL
3	C	155	ARG
3	C	165	GLU
3	C	182	LYS
3	C	183	ILE
3	C	205	LYS
3	C	211	ILE
3	C	231	LEU
3	C	232	THR
3	C	249	LEU
3	C	250	GLN
3	C	258	MET
3	C	262	ILE
3	C	264	LEU
3	C	271	MET

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Mol	Chain	Res	Type
3	C	276	LYS
3	C	281	LYS
3	C	283	GLN
4	D	13	MET
4	D	16	ARG
4	D	22	LEU
4	D	62	ASN
4	D	63	ASN
4	D	92	VAL
4	D	93	VAL
4	D	99	ILE
4	D	100	ARG
4	D	101	ASP
4	D	126	CYS
4	D	138	ARG
4	D	139	VAL
4	D	154	THR
4	D	161	VAL
4	D	170	PHE
4	D	174	GLU
4	D	175	LYS
4	D	177	TRP
5	E	2	ILE
5	E	8	TYR
5	E	11	PHE
5	E	12	ILE
5	E	14	LEU
5	E	15	PHE
5	E	16	PHE
5	E	18	ILE
5	E	27	LYS
5	E	29	ILE
5	E	30	LYS
6	F	7	TYR
6	F	26	LEU
6	F	30	GLN
7	G	9	LEU
7	G	11	LEU
7	G	13	LEU
7	G	14	VAL
7	G	18	LEU
7	G	21	LEU

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Mol	Chain	Res	Type
7	G	26	TYR
7	G	31	ARG
8	H	8	TRP
8	H	16	THR
8	H	21	MET
1	N	13	GLU
1	N	17	LEU
1	N	21	VAL
1	N	25	TYR
1	N	29	HIS
1	N	47	GLN
1	N	63	THR
1	N	95	LEU
1	N	103	ARG
1	N	110	PHE
1	N	112	LYS
1	N	116	LEU
1	N	140	TRP
1	N	143	VAL
1	N	148	VAL
1	N	150	ILE
1	N	163	VAL
1	N	164	LEU
1	N	167	ASP
1	N	193	TRP
1	N	195	ILE
1	N	200	LEU
2	O	20	LYS
2	O	24	HIS
2	O	27	TYR
2	O	30	PRO
2	O	32	TRP
2	O	33	PRO
2	O	35	ASP
2	O	36	LEU
2	O	39	VAL
2	O	52	VAL
2	O	57	LEU
2	O	65	PRO
2	O	74	GLU
2	O	84	VAL
2	O	90	SER

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Mol	Chain	Res	Type
2	O	92	PRO
2	O	95	LEU
2	O	96	LEU
2	O	108	LEU
2	O	126	ARG
2	O	152	ASP
3	P	3	PHE
3	P	4	TRP
3	P	14	ARG
3	P	17	THR
3	P	19	ARG
3	P	27	LEU
3	P	34	VAL
3	P	51	LYS
3	P	83	LYS
3	P	91	PRO
3	P	93	GLU
3	P	94	LEU
3	P	98	VAL
3	P	100	ASP
3	P	104	GLN
3	P	114	LEU
3	P	119	LEU
3	P	122	GLU
3	P	131	VAL
3	P	155	ARG
3	P	165	GLU
3	P	182	LYS
3	P	183	ILE
3	P	205	LYS
3	P	206	THR
3	P	211	ILE
3	P	231	LEU
3	P	232	THR
3	P	249	LEU
3	P	250	GLN
3	P	258	MET
3	P	262	ILE
3	P	264	LEU
3	P	271	MET
3	P	276	LYS
3	P	280	GLU

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Mol	Chain	Res	Type
3	P	281	LYS
3	P	283	GLN
4	Q	13	MET
4	Q	16	ARG
4	Q	22	LEU
4	Q	58	ASP
4	Q	59	LYS
4	Q	63	ASN
4	Q	64	VAL
4	Q	70	LEU
4	Q	71	GLU
4	Q	94	GLU
4	Q	97	GLU
4	Q	132	GLN
4	Q	138	ARG
4	Q	159	ASN
4	Q	161	VAL
4	Q	162	LEU
4	Q	164	PRO
4	Q	167	GLU
4	Q	175	LYS
4	Q	178	TRP
5	R	2	ILE
5	R	8	TYR
5	R	11	PHE
5	R	12	ILE
5	R	14	LEU
5	R	15	PHE
5	R	16	PHE
5	R	18	ILE
5	R	26	ILE
5	R	27	LYS
5	R	29	ILE
5	R	30	LYS
6	S	7	TYR
6	S	26	LEU
6	S	30	GLN
6	S	34	LYS
7	T	9	LEU
7	T	11	LEU
7	T	13	LEU
7	T	14	VAL

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Mol	Chain	Res	Type
7	T	18	LEU
7	T	21	LEU
7	T	26	TYR
7	T	31	ARG
7	T	33	ASN
8	U	8	TRP
8	U	16	THR
8	U	21	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	29	HIS
1	A	47	GLN
1	A	142	GLN
2	B	25	ASN
2	B	86	GLN
2	B	116	ASN
2	B	118	ASN
2	B	121	GLN
3	C	7	GLN
3	C	60	GLN
3	C	71	ASN
3	C	125	GLN
3	C	150	HIS
3	C	159	GLN
3	C	223	GLN
3	C	236	ASN
3	C	250	GLN
3	C	269	GLN
4	D	82	GLN
4	D	132	GLN
4	D	152	HIS
7	G	28	GLN
8	H	27	ASN
1	N	47	GLN
1	N	142	GLN
1	N	209	GLN
2	O	86	GLN
2	O	116	ASN
2	O	121	GLN

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Mol	Chain	Res	Type
2	O	122	ASN
3	P	7	GLN
3	P	60	GLN
3	P	125	GLN
3	P	159	GLN
3	P	223	GLN
3	P	234	ASN
3	P	236	ASN
3	P	250	GLN
4	Q	20	ASN
4	Q	62	ASN
4	Q	63	ASN
4	Q	73	HIS
4	Q	82	GLN
4	Q	105	ASN
4	Q	122	ASN
4	Q	132	GLN
7	T	27	GLN
7	T	33	ASN
8	U	27	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HEC	P	301	3	50,50,50	1.71	11 (22%)	68,82,82	1.75	11 (16%)
16	BCR	R	1101	-	41,41,41	2.08	9 (21%)	56,56,56	2.52	22 (39%)
14	CLA	B	201	-	69,73,73	1.61	9 (13%)	82,113,113	2.22	17 (20%)
11	TDS	N	1304	-	31,31,31	2.82	9 (29%)	37,40,40	2.05	9 (24%)
11	TDS	A	304	-	31,31,31	2.83	9 (29%)	37,40,40	1.96	9 (24%)
9	HEM	N	302	1	50,50,50	1.79	8 (16%)	67,82,82	2.01	12 (17%)
9	HEM	N	301	1	50,50,50	1.81	11 (22%)	67,82,82	1.37	8 (11%)
13	OPC	N	1306	-	53,53,54	1.42	9 (16%)	59,61,64	1.37	6 (10%)
10	HEC	N	303	1,17	50,50,50	1.35	9 (18%)	68,82,82	1.32	10 (14%)
12	PL9	A	305	-	55,55,55	3.41	21 (38%)	68,69,69	2.30	18 (26%)
10	HEC	C	301	3	50,50,50	1.63	8 (16%)	68,82,82	1.70	10 (14%)
13	OPC	D	306	-	53,53,54	1.43	9 (16%)	59,61,64	1.17	5 (8%)
10	HEC	A	303	1,17	50,50,50	1.32	4 (8%)	68,82,82	1.81	16 (23%)
14	CLA	O	1201	-	69,73,73	1.55	11 (15%)	82,113,113	2.31	15 (18%)
15	FES	D	200	4	0,4,4	-	-	-	-	-
9	HEM	A	301	1	50,50,50	1.77	11 (22%)	67,82,82	1.39	10 (14%)
12	PL9	Q	1305	-	55,55,55	3.40	21 (38%)	68,69,69	2.39	16 (23%)
16	BCR	E	101	-	41,41,41	2.16	8 (19%)	56,56,56	2.51	23 (41%)
13	OPC	Q	1307	-	53,53,54	1.43	9 (16%)	59,61,64	1.19	3 (5%)
13	OPC	B	307	-	53,53,54	1.43	9 (16%)	59,61,64	1.07	4 (6%)
15	FES	Q	1200	4	0,4,4	-	-	-	-	-
9	HEM	A	302	1	50,50,50	1.76	14 (28%)	67,82,82	1.99	10 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEC	P	301	3	1/1/3/7	4/14/54/54	-
16	BCR	R	1101	-	-	5/29/63/63	0/2/2/2
14	CLA	B	201	-	2/2/15/20	18/39/115/115	-
11	TDS	N	1304	-	-	7/17/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	TDS	A	304	-	-	6/17/17/17	0/2/2/2
9	HEM	N	302	1	-	4/14/54/54	-
9	HEM	N	301	1	-	9/14/54/54	-
13	OPC	N	1306	-	-	11/57/57/60	-
10	HEC	N	303	1,17	1/1/3/7	2/14/54/54	-
12	PL9	A	305	-	-	28/53/73/73	0/1/1/1
10	HEC	C	301	3	1/1/3/7	4/14/54/54	-
13	OPC	D	306	-	-	10/57/57/60	-
10	HEC	A	303	1,17	1/1/3/7	2/14/54/54	-
14	CLA	O	1201	-	3/3/15/20	10/39/115/115	-
15	FES	D	200	4	-	-	0/1/1/1
9	HEM	A	301	1	-	6/14/54/54	-
12	PL9	Q	1305	-	-	30/53/73/73	0/1/1/1
16	BCR	E	101	-	-	5/29/63/63	0/2/2/2
13	OPC	Q	1307	-	-	11/57/57/60	-
13	OPC	B	307	-	-	14/57/57/60	-
15	FES	Q	1200	4	-	-	0/1/1/1
9	HEM	A	302	1	-	4/14/54/54	-

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	1304	TDS	CAL-CAM	9.34	1.53	1.40
11	A	304	TDS	CAL-CAM	9.33	1.53	1.40
12	A	305	PL9	C13-C14	8.98	1.53	1.33
12	A	305	PL9	C33-C34	8.92	1.53	1.33
12	A	305	PL9	C18-C19	8.91	1.53	1.33
12	Q	1305	PL9	C13-C14	8.91	1.53	1.33
12	Q	1305	PL9	C33-C34	8.88	1.53	1.33
12	Q	1305	PL9	C18-C19	8.86	1.53	1.33
11	A	304	TDS	CAM-CAN	8.72	1.53	1.39
11	N	1304	TDS	CAM-CAN	8.72	1.53	1.39
12	Q	1305	PL9	C48-C49	7.11	1.53	1.32
12	A	305	PL9	C48-C49	7.08	1.53	1.32
16	E	101	BCR	C30-C25	7.00	1.62	1.53
12	A	305	PL9	C7-C8	-6.98	1.39	1.50
12	Q	1305	PL9	C7-C8	-6.96	1.39	1.50
14	B	201	CLA	C3A-C2A	-6.50	1.36	1.54
12	Q	1305	PL9	C3-C4	-6.37	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	305	PL9	C3-C4	-6.27	1.39	1.49
16	E	101	BCR	C26-C25	6.13	1.44	1.34
16	R	1101	BCR	C26-C25	5.84	1.44	1.34
16	R	1101	BCR	C30-C25	5.76	1.61	1.53
12	A	305	PL9	C11-C9	-5.63	1.39	1.51
12	A	305	PL9	C41-C39	-5.63	1.39	1.51
12	Q	1305	PL9	C11-C9	-5.62	1.39	1.51
14	O	1201	CLA	C3A-C2A	-5.61	1.39	1.54
12	Q	1305	PL9	C41-C39	-5.59	1.39	1.51
12	Q	1305	PL9	C6-C1	-5.28	1.39	1.48
9	N	302	HEM	FE-NB	5.23	2.11	1.94
16	R	1101	BCR	C1-C6	5.16	1.60	1.53
12	A	305	PL9	C6-C1	-5.12	1.40	1.48
16	E	101	BCR	C1-C6	5.05	1.60	1.53
9	A	302	HEM	FE-NB	5.02	2.10	1.94
9	N	302	HEM	CBC-CAC	4.95	1.54	1.30
10	P	301	HEC	FE-NB	4.87	2.09	1.94
9	A	302	HEM	CBC-CAC	4.76	1.53	1.30
9	N	301	HEM	C4D-ND	-4.61	1.32	1.40
9	A	301	HEM	CBC-CAC	4.58	1.52	1.30
10	C	301	HEC	FE-NC	4.57	2.10	1.95
9	N	301	HEM	FE-NB	4.48	2.08	1.94
10	P	301	HEC	CBB-CAB	-4.44	1.32	1.51
9	N	301	HEM	CBC-CAC	4.44	1.51	1.30
10	C	301	HEC	CBB-CAB	-4.41	1.32	1.51
14	O	1201	CLA	O2D-CGD	4.37	1.44	1.33
9	A	301	HEM	C4D-ND	-4.33	1.32	1.40
10	C	301	HEC	FE-NB	4.31	2.08	1.94
14	B	201	CLA	O2D-CGD	4.31	1.43	1.33
12	Q	1305	PL9	C41-C42	-4.29	1.39	1.53
12	A	305	PL9	C41-C42	-4.28	1.39	1.53
11	A	304	TDS	CAQ-CAP	-4.12	1.39	1.49
10	P	301	HEC	FE-NC	4.11	2.08	1.95
12	Q	1305	PL9	C51-C49	-4.10	1.39	1.50
11	N	1304	TDS	CAQ-CAP	-4.09	1.39	1.49
14	B	201	CLA	C3D-C4D	-4.09	1.35	1.44
12	A	305	PL9	C51-C49	-4.06	1.39	1.50
16	R	1101	BCR	C38-C26	3.96	1.57	1.50
9	N	302	HEM	C4D-ND	-3.94	1.33	1.40
13	Q	1307	OPC	CAV-CAW	3.89	1.53	1.31
13	D	306	OPC	CAG-CAH	-3.87	1.39	1.51
9	N	302	HEM	FE-NC	3.85	2.07	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	306	OPC	CAV-CAW	3.85	1.53	1.31
11	A	304	TDS	OAK-CAL	3.85	1.43	1.37
13	Q	1307	OPC	CAG-CAH	-3.84	1.39	1.51
13	N	1306	OPC	CAV-CAW	3.84	1.53	1.31
13	B	307	OPC	CAV-CAW	3.82	1.53	1.31
13	B	307	OPC	CAG-CAH	-3.81	1.39	1.51
11	N	1304	TDS	OAK-CAL	3.79	1.43	1.37
13	N	1306	OPC	CAG-CAH	-3.78	1.39	1.51
9	A	302	HEM	C4D-ND	-3.75	1.33	1.40
14	O	1201	CLA	C3D-C4D	-3.72	1.35	1.44
16	E	101	BCR	C29-C30	3.69	1.62	1.54
9	N	301	HEM	FE-NC	3.69	2.07	1.95
9	A	301	HEM	C4A-C3A	3.68	1.51	1.43
9	A	302	HEM	FE-NC	3.66	2.07	1.95
16	E	101	BCR	C38-C26	3.64	1.56	1.50
16	R	1101	BCR	C29-C30	3.63	1.62	1.54
12	A	305	PL9	C47-C48	-3.61	1.39	1.50
12	A	305	PL9	C27-C28	-3.60	1.39	1.50
12	Q	1305	PL9	C47-C48	-3.60	1.39	1.50
12	A	305	PL9	C22-C23	-3.60	1.39	1.50
11	A	304	TDS	CAH-CAG	-3.60	1.39	1.47
12	Q	1305	PL9	C27-C28	-3.59	1.39	1.50
12	Q	1305	PL9	C22-C23	-3.59	1.39	1.50
9	A	301	HEM	FE-NC	3.58	2.07	1.95
12	A	305	PL9	C42-C43	-3.53	1.39	1.50
9	A	301	HEM	FE-NA	3.53	2.06	1.95
16	R	1101	BCR	C2-C1	3.52	1.62	1.54
12	Q	1305	PL9	C42-C43	-3.50	1.39	1.50
13	D	306	OPC	CAQ-CAP	-3.48	1.39	1.52
13	B	307	OPC	CAQ-CAP	-3.48	1.39	1.52
11	N	1304	TDS	CAR-CAQ	-3.47	1.39	1.52
14	O	1201	CLA	C2-C3	3.45	1.41	1.33
9	N	301	HEM	FE-NA	3.45	2.06	1.95
13	N	1306	OPC	CAQ-CAP	-3.45	1.39	1.52
13	Q	1307	OPC	CAQ-CAP	-3.44	1.39	1.52
11	N	1304	TDS	CAH-CAG	-3.43	1.39	1.47
11	A	304	TDS	CAR-CAQ	-3.43	1.39	1.52
16	E	101	BCR	C2-C1	3.30	1.61	1.54
14	B	201	CLA	O1D-CGD	3.28	1.29	1.21
14	O	1201	CLA	O1D-CGD	3.19	1.29	1.21
9	N	302	HEM	CAC-C3C	3.18	1.55	1.47
9	A	301	HEM	FE-NB	3.18	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	1201	CLA	MG-ND	-3.17	1.99	2.05
10	N	303	HEC	CMD-C2D	3.14	1.57	1.50
10	P	301	HEC	FE-NA	3.06	2.05	1.95
13	D	306	OPC	CBP-CBQ	-3.04	1.39	1.52
13	Q	1307	OPC	CBP-CBQ	-3.03	1.39	1.52
13	B	307	OPC	CBP-CBQ	-3.03	1.39	1.52
9	A	301	HEM	FE-ND	3.03	2.04	1.94
13	N	1306	OPC	CBP-CBQ	-2.98	1.39	1.52
12	A	305	PL9	C43-C44	2.93	1.39	1.33
16	R	1101	BCR	C5-C6	2.89	1.39	1.34
14	B	201	CLA	C2-C3	2.89	1.39	1.33
12	Q	1305	PL9	C43-C44	2.88	1.39	1.33
12	Q	1305	PL9	C38-C39	2.88	1.39	1.33
12	A	305	PL9	C23-C24	2.87	1.39	1.33
12	Q	1305	PL9	C23-C24	2.86	1.39	1.33
12	A	305	PL9	C38-C39	2.86	1.39	1.33
10	A	303	HEC	FE-NC	2.85	2.04	1.95
12	A	305	PL9	C28-C29	2.85	1.39	1.33
14	O	1201	CLA	MG-NC	2.83	2.13	2.06
12	A	305	PL9	C8-C9	2.82	1.39	1.33
12	Q	1305	PL9	C8-C9	2.81	1.39	1.33
9	N	302	HEM	CMA-C3A	2.81	1.56	1.50
12	Q	1305	PL9	C28-C29	2.80	1.39	1.33
10	A	303	HEC	C4B-C3B	2.78	1.49	1.45
11	A	304	TDS	CAH-CAP	2.78	1.40	1.34
10	C	301	HEC	FE-ND	2.77	2.03	1.94
11	N	1304	TDS	CAF-CAG	-2.75	1.39	1.46
9	A	301	HEM	C1D-C2D	2.74	1.50	1.44
11	A	304	TDS	CAF-CAG	-2.72	1.39	1.46
11	N	1304	TDS	CAH-CAP	2.70	1.39	1.34
14	B	201	CLA	MG-ND	-2.67	2.00	2.05
14	B	201	CLA	MG-NC	2.66	2.12	2.06
9	A	302	HEM	CMA-C3A	2.66	1.56	1.50
10	C	301	HEC	FE-NA	2.65	2.03	1.95
9	N	302	HEM	FE-ND	2.65	2.03	1.94
9	A	302	HEM	FE-ND	2.61	2.02	1.94
9	N	301	HEM	CMA-C3A	2.59	1.56	1.50
10	P	301	HEC	CHA-C1A	2.59	1.43	1.38
9	A	301	HEM	CMA-C3A	2.56	1.56	1.50
9	A	302	HEM	C3B-C4B	2.54	1.49	1.44
13	D	306	OPC	CBC-CBD	-2.51	1.39	1.51
10	N	303	HEC	C4B-C3B	2.51	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	307	OPC	CBC-CBD	-2.50	1.39	1.51
13	B	307	OPC	CAR-CAS	-2.48	1.39	1.51
11	A	304	TDS	CAR-CAS	-2.48	1.39	1.51
13	N	1306	OPC	CAQ-CAR	-2.48	1.39	1.51
13	Q	1307	OPC	CBP-CBO	-2.48	1.39	1.51
13	N	1306	OPC	CBB-CBC	-2.48	1.39	1.51
13	D	306	OPC	CBB-CBC	-2.48	1.39	1.51
10	N	303	HEC	C1B-NB	2.48	1.43	1.38
16	E	101	BCR	C5-C6	2.48	1.38	1.34
13	D	306	OPC	CAR-CAS	-2.47	1.39	1.51
13	D	306	OPC	CBP-CBO	-2.47	1.39	1.51
13	B	307	OPC	CAQ-CAR	-2.47	1.39	1.51
13	N	1306	OPC	CAR-CAS	-2.47	1.39	1.51
13	Q	1307	OPC	CBB-CBC	-2.47	1.39	1.51
10	N	303	HEC	FE-ND	2.47	2.02	1.94
13	Q	1307	OPC	CBC-CBD	-2.46	1.39	1.51
13	Q	1307	OPC	CAQ-CAR	-2.46	1.39	1.51
13	N	1306	OPC	CBP-CBO	-2.46	1.39	1.51
11	N	1304	TDS	CAR-CAS	-2.46	1.39	1.51
13	D	306	OPC	CAQ-CAR	-2.46	1.39	1.51
13	N	1306	OPC	CBC-CBD	-2.46	1.39	1.51
13	B	307	OPC	CBB-CBC	-2.46	1.39	1.51
13	Q	1307	OPC	CAR-CAS	-2.45	1.39	1.51
13	B	307	OPC	CBP-CBO	-2.45	1.39	1.51
9	N	301	HEM	FE-ND	2.44	2.02	1.94
9	N	301	HEM	C4A-C3A	2.43	1.48	1.43
10	P	301	HEC	FE-ND	2.42	2.02	1.94
10	A	303	HEC	FE-ND	2.41	2.02	1.94
10	C	301	HEC	CHA-C1A	2.40	1.43	1.38
9	A	302	HEM	CAC-C3C	2.35	1.53	1.47
9	N	301	HEM	CAC-C3C	2.34	1.53	1.47
9	A	302	HEM	CBA-CAA	2.32	1.60	1.51
10	P	301	HEC	CBA-CGA	2.32	1.55	1.50
9	N	301	HEM	CHC-C1C	2.30	1.42	1.38
9	A	302	HEM	C1D-C2D	2.28	1.49	1.44
14	O	1201	CLA	CBD-CHA	2.28	1.63	1.51
9	A	302	HEM	CHC-C1C	2.25	1.42	1.38
10	P	301	HEC	C4B-C3B	2.24	1.48	1.45
14	O	1201	CLA	CAC-C3C	2.24	1.56	1.51
10	N	303	HEC	FE-NC	2.23	2.02	1.95
16	E	101	BCR	C8-C9	2.23	1.50	1.46
10	C	301	HEC	CMA-C3A	2.21	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	303	HEC	C1D-C2D	2.19	1.49	1.44
9	A	301	HEM	C1B-NB	-2.19	1.36	1.40
10	P	301	HEC	CMA-C3A	2.18	1.55	1.50
10	P	301	HEC	C1A-C2A	2.15	1.49	1.45
14	B	201	CLA	CBA-CGA	2.15	1.56	1.50
14	O	1201	CLA	C3B-C4B	2.12	1.48	1.42
10	C	301	HEC	CAC-C3C	2.12	1.56	1.51
9	N	301	HEM	C1D-C2D	2.12	1.48	1.44
9	A	302	HEM	C4A-C3A	2.11	1.48	1.43
10	A	303	HEC	CMD-C2D	2.11	1.55	1.50
10	N	303	HEC	FE-NA	2.09	2.02	1.95
10	N	303	HEC	C1C-NC	-2.09	1.35	1.39
9	A	302	HEM	FE-NA	2.08	2.02	1.95
12	Q	1305	PL9	C2-C3	2.08	1.39	1.34
9	A	302	HEM	O2A-CGA	-2.07	1.24	1.30
16	R	1101	BCR	C7-C6	2.07	1.52	1.45
14	B	201	CLA	C3B-C4B	2.06	1.48	1.42
12	A	305	PL9	C2-C3	2.05	1.39	1.34
9	A	301	HEM	CAC-C3C	2.04	1.52	1.47
9	N	302	HEM	CBD-CGD	2.03	1.55	1.50
10	P	301	HEC	CAC-C3C	2.03	1.56	1.51
16	R	1101	BCR	C23-C22	-2.02	1.41	1.46
10	N	303	HEC	C4D-C3D	2.01	1.48	1.45
14	O	1201	CLA	C4-C3	2.01	1.55	1.50

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	1201	CLA	C4A-NA-C1A	10.47	111.46	106.68
9	N	302	HEM	CBA-CAA-C2A	-9.63	85.90	112.53
9	A	302	HEM	CBA-CAA-C2A	-9.44	86.43	112.53
14	B	201	CLA	C4A-NA-C1A	8.89	110.73	106.68
14	O	1201	CLA	C4D-C3D-CAD	8.28	117.10	108.11
12	A	305	PL9	C7-C8-C9	-7.90	113.23	126.83
12	Q	1305	PL9	C7-C8-C9	-7.83	113.34	126.83
14	B	201	CLA	C4D-C3D-CAD	7.60	116.36	108.11
14	B	201	CLA	CMA-C3A-C4A	7.44	131.78	111.77
9	A	302	HEM	CAA-CBA-CGA	7.39	133.27	113.67
16	R	1101	BCR	C38-C26-C25	7.23	132.37	124.48
12	Q	1305	PL9	C17-C18-C19	-7.01	111.57	127.62
14	O	1201	CLA	CMA-C3A-C4A	6.96	130.49	111.77
9	N	302	HEM	CAA-CBA-CGA	6.89	131.95	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	E	101	BCR	C38-C26-C25	6.83	131.94	124.48
12	A	305	PL9	C22-C23-C24	-6.78	112.11	127.62
12	Q	1305	PL9	C12-C13-C14	-6.72	112.24	127.62
12	Q	1305	PL9	C37-C38-C39	-6.56	112.62	127.62
12	A	305	PL9	C17-C18-C19	-6.52	112.69	127.62
12	A	305	PL9	C37-C38-C39	-6.46	112.84	127.62
13	N	1306	OPC	OAN-CAO-CAP	6.36	125.24	111.48
12	A	305	PL9	C12-C13-C14	-6.32	113.15	127.62
12	Q	1305	PL9	C22-C23-C24	-6.25	113.31	127.62
14	O	1201	CLA	CAA-C2A-C1A	6.06	131.82	111.97
10	A	303	HEC	C1D-C2D-C3D	5.98	113.27	106.98
10	P	301	HEC	CBC-CAC-C3C	5.91	128.45	112.42
10	C	301	HEC	CBC-CAC-C3C	5.89	128.38	112.42
14	B	201	CLA	CAA-C2A-C1A	5.84	131.10	111.97
16	R	1101	BCR	C24-C23-C22	5.62	134.54	126.23
13	Q	1307	OPC	OAN-CAO-CAP	5.58	123.56	111.48
10	P	301	HEC	CBB-CAB-C3B	5.48	127.27	112.42
14	B	201	CLA	CBC-CAC-C3C	5.38	127.01	112.42
11	A	304	TDS	CAJ-OAK-CAL	-5.35	109.67	117.51
13	D	306	OPC	OAN-CAO-CAP	5.31	122.96	111.48
10	C	301	HEC	CBB-CAB-C3B	5.25	126.66	112.42
16	E	101	BCR	C24-C23-C22	5.24	133.98	126.23
11	N	1304	TDS	CAJ-OAK-CAL	-5.19	109.90	117.51
12	Q	1305	PL9	C25-C24-C26	5.14	124.16	115.23
16	E	101	BCR	C20-C21-C22	5.07	134.39	127.28
16	E	101	BCR	C33-C5-C6	5.07	130.01	124.48
16	R	1101	BCR	C33-C5-C6	5.04	129.98	124.48
16	R	1101	BCR	C20-C21-C22	4.93	134.20	127.28
13	B	307	OPC	OAN-CAO-CAP	4.87	122.02	111.48
14	O	1201	CLA	CBC-CAC-C3C	4.70	125.17	112.42
9	A	302	HEM	CMA-C3A-C4A	4.61	132.43	125.42
10	P	301	HEC	CAB-C3B-C4B	4.55	130.71	124.79
10	A	303	HEC	CAD-C3D-C4D	4.40	132.37	124.70
10	A	303	HEC	C2D-C1D-ND	-4.33	104.86	109.84
11	A	304	TDS	CAA-OAB-CAE	-4.29	111.22	117.51
11	A	304	TDS	CAL-CAM-CAN	-4.21	112.94	118.91
9	N	302	HEM	CMA-C3A-C4A	4.21	131.82	125.42
14	O	1201	CLA	C3A-C2A-C1A	4.19	107.61	101.34
10	P	301	HEC	CAA-C2A-C3A	-4.18	120.03	127.87
9	A	301	HEM	CMA-C3A-C4A	4.18	131.78	125.42
12	A	305	PL9	C25-C24-C26	4.14	122.42	115.23
11	N	1304	TDS	CAL-CAM-CAN	-4.11	113.07	118.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	E	101	BCR	C7-C8-C9	4.08	132.28	126.23
16	R	1101	BCR	C29-C30-C25	4.07	116.35	110.44
10	C	301	HEC	CAB-C3B-C4B	4.06	130.08	124.79
10	C	301	HEC	CAA-C2A-C3A	-4.03	120.31	127.87
16	E	101	BCR	C29-C30-C25	4.02	116.28	110.44
16	R	1101	BCR	C30-C25-C26	-3.99	117.18	122.64
11	N	1304	TDS	OAO-CAP-CAH	-3.99	118.31	121.81
16	E	101	BCR	C30-C25-C26	-3.98	117.20	122.64
10	A	303	HEC	CMD-C2D-C1D	-3.87	118.98	125.03
16	R	1101	BCR	C23-C22-C21	-3.87	112.93	119.01
13	N	1306	OPC	OBJ-CBK-CBL	3.84	123.55	111.83
14	B	201	CLA	C1-C2-C3	3.82	132.46	126.20
16	R	1101	BCR	C7-C8-C9	3.82	131.89	126.23
11	N	1304	TDS	CAA-OAB-CAE	-3.81	111.93	117.51
14	B	201	CLA	C3A-C2A-C1A	3.80	107.03	101.34
10	P	301	HEC	CAA-C2A-C1A	3.77	132.53	124.85
14	O	1201	CLA	C2A-C1A-CHA	3.77	130.41	123.87
9	A	301	HEM	CAA-C2A-C1A	3.73	132.22	124.94
10	P	301	HEC	CMA-C3A-C4A	3.73	131.29	124.73
10	A	303	HEC	CAD-CBD-CGD	3.69	123.46	113.67
9	N	301	HEM	CAA-C2A-C1A	3.69	132.15	124.94
16	R	1101	BCR	C38-C26-C27	-3.67	105.77	113.60
9	N	301	HEM	CMA-C3A-C4A	3.67	131.01	125.42
16	E	101	BCR	C23-C22-C21	-3.67	113.24	119.01
11	A	304	TDS	OAO-CAP-CAH	-3.66	118.59	121.81
11	N	1304	TDS	OAB-CAE-CAD	-3.66	117.78	124.08
14	B	201	CLA	C2A-C3A-C4A	3.64	107.75	101.87
14	O	1201	CLA	C1-C2-C3	3.63	132.14	126.20
9	A	301	HEM	CHA-C4D-C3D	-3.62	118.55	125.23
16	E	101	BCR	C2-C1-C6	3.62	115.70	110.44
16	R	1101	BCR	C2-C1-C6	3.55	115.59	110.44
10	C	301	HEC	CAA-C2A-C1A	3.54	132.05	124.85
16	E	101	BCR	C38-C26-C27	-3.53	106.08	113.60
10	C	301	HEC	CMA-C3A-C4A	3.49	130.87	124.73
10	A	303	HEC	C4D-C3D-C2D	-3.49	101.82	106.89
14	O	1201	CLA	C2A-C3A-C4A	3.48	107.48	101.87
9	N	302	HEM	C2A-C1A-NA	-3.44	106.33	110.15
16	E	101	BCR	C23-C24-C25	3.44	136.18	127.00
12	Q	1305	PL9	C15-C14-C16	3.43	121.18	115.23
10	A	303	HEC	CAA-CBA-CGA	3.42	122.75	113.67
16	E	101	BCR	C1-C6-C5	-3.42	117.96	122.64
10	N	303	HEC	C2A-C1A-NA	3.39	113.60	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	301	HEM	CHA-C4D-C3D	-3.39	118.97	125.23
16	R	1101	BCR	C33-C5-C4	-3.39	106.37	113.60
11	N	1304	TDS	OAB-CAE-CAF	3.38	120.63	115.84
16	E	101	BCR	C33-C5-C4	-3.36	106.43	113.60
16	R	1101	BCR	C1-C6-C5	-3.35	118.05	122.64
16	R	1101	BCR	C23-C24-C25	3.33	135.88	127.00
11	N	1304	TDS	OAO-CAP-CAQ	3.32	117.17	110.12
13	D	306	OPC	OBJ-CBK-CBL	3.31	121.94	111.83
12	Q	1305	PL9	C30-C29-C31	3.27	120.90	115.23
10	N	303	HEC	C1D-C2D-C3D	3.26	110.41	106.98
12	Q	1305	PL9	C26-C24-C23	-3.24	113.89	121.17
10	A	303	HEC	C2A-C1A-NA	3.20	113.41	110.32
16	R	1101	BCR	C11-C10-C9	3.18	131.73	127.28
10	C	301	HEC	C2A-C1A-NA	-3.12	107.31	110.32
11	N	1304	TDS	CAE-CAF-CAN	3.11	122.41	116.87
9	A	301	HEM	CHA-C4D-ND	3.07	128.17	124.37
10	N	303	HEC	C2D-C1D-ND	-3.06	106.33	109.84
9	N	301	HEM	CHA-C4D-ND	3.06	128.15	124.37
14	B	201	CLA	O2D-CGD-CBD	3.05	116.57	111.23
12	A	305	PL9	C30-C29-C31	3.04	120.50	115.23
10	P	301	HEC	CHA-C4D-ND	3.01	127.66	124.42
10	N	303	HEC	CAA-C2A-C1A	2.97	130.90	124.85
9	N	302	HEM	CAA-C2A-C3A	-2.96	120.43	127.07
14	B	201	CLA	C2A-C1A-CHA	2.96	129.00	123.87
11	A	304	TDS	OAB-CAE-CAD	-2.92	119.06	124.08
11	A	304	TDS	OAO-CAP-CAQ	2.91	116.29	110.12
9	A	302	HEM	C4B-C3B-C2B	-2.86	104.65	107.28
11	A	304	TDS	CAE-CAF-CAN	2.85	121.94	116.87
9	N	302	HEM	C4B-C3B-C2B	-2.85	104.66	107.28
13	N	1306	OPC	OAN-CAO-OAD	-2.84	117.06	123.70
10	P	301	HEC	C2A-C1A-NA	-2.84	107.58	110.32
9	A	301	HEM	C3D-C4D-ND	2.84	113.28	110.17
10	C	301	HEC	CHA-C4D-ND	2.83	127.47	124.42
16	E	101	BCR	C1-C6-C7	2.83	123.32	115.65
9	A	302	HEM	C2A-C1A-NA	-2.82	107.02	110.15
9	N	301	HEM	CAA-C2A-C3A	-2.82	120.74	127.07
13	Q	1307	OPC	OAN-CAO-OAD	-2.81	117.13	123.70
12	Q	1305	PL9	C35-C34-C36	2.80	120.09	115.23
16	R	1101	BCR	C1-C6-C7	2.80	123.24	115.65
16	E	101	BCR	C15-C14-C13	2.80	131.20	127.28
16	E	101	BCR	C11-C10-C9	2.77	131.17	127.28
16	E	101	BCR	C35-C13-C12	2.77	122.32	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	R	1101	BCR	C8-C7-C6	2.77	134.41	127.00
9	A	301	HEM	CAA-C2A-C3A	-2.74	120.92	127.07
14	B	201	CLA	OBD-CAD-C3D	2.73	134.81	128.42
14	B	201	CLA	O2A-CGA-CBA	2.73	120.15	111.83
9	N	302	HEM	C4A-NA-C1A	2.71	110.24	105.82
13	B	307	OPC	CBM-CBL-CBK	2.71	123.62	113.69
10	A	303	HEC	CAA-C2A-C1A	2.70	130.35	124.85
16	R	1101	BCR	C35-C13-C12	2.70	122.21	118.09
16	E	101	BCR	C37-C22-C23	2.69	122.20	118.09
16	E	101	BCR	C8-C7-C6	2.69	134.18	127.00
16	R	1101	BCR	C37-C22-C23	2.69	122.19	118.09
13	Q	1307	OPC	OBJ-CBK-CBL	2.68	120.02	111.83
10	P	301	HEC	CHA-C4D-C3D	-2.67	120.88	124.77
16	E	101	BCR	C32-C1-C6	2.66	114.42	110.24
16	R	1101	BCR	C15-C14-C13	2.66	131.01	127.28
12	A	305	PL9	C26-C24-C23	-2.65	115.21	121.17
14	O	1201	CLA	O2A-CGA-CBA	2.63	119.85	111.83
10	A	303	HEC	CBA-CAA-C2A	-2.60	105.35	112.53
12	Q	1305	PL9	C42-C43-C44	2.60	133.57	127.62
9	A	302	HEM	CHA-C4D-C3D	-2.57	120.48	125.23
10	N	303	HEC	CAD-CBD-CGD	2.55	120.43	113.67
10	A	303	HEC	CAA-C2A-C3A	-2.55	123.09	127.87
13	D	306	OPC	OAN-CAO-OAD	-2.55	117.75	123.70
14	O	1201	CLA	CAA-C2A-C3A	2.55	119.88	113.00
14	B	201	CLA	C3D-C4D-ND	2.52	114.08	109.99
12	A	305	PL9	C42-C43-C44	2.52	133.39	127.62
11	A	304	TDS	CAS-CAR-CAQ	2.50	122.31	113.13
9	N	302	HEM	CAA-C2A-C1A	2.50	129.81	124.94
13	N	1306	OPC	CAM-OAN-CAO	2.49	123.76	117.80
10	C	301	HEC	CHA-C4D-C3D	-2.48	121.16	124.77
12	A	305	PL9	C35-C34-C36	2.48	119.53	115.23
10	N	303	HEC	CMD-C2D-C1D	-2.48	121.16	125.03
16	R	1101	BCR	C32-C1-C6	2.47	114.12	110.24
16	E	101	BCR	C12-C13-C14	-2.47	115.12	119.01
9	N	301	HEM	C3D-C4D-ND	2.47	112.88	110.17
16	R	1101	BCR	C12-C13-C14	-2.46	115.14	119.01
14	O	1201	CLA	CED-O2D-CGD	2.44	121.46	115.92
10	N	303	HEC	CAA-C2A-C3A	-2.44	123.30	127.87
12	Q	1305	PL9	C10-C9-C11	2.42	119.43	115.23
9	N	301	HEM	CAA-CBA-CGA	2.41	120.07	113.67
14	O	1201	CLA	OBD-CAD-C3D	2.40	134.03	128.42
13	N	1306	OPC	OBJ-CBK-OCC	-2.39	117.65	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Q	1305	PL9	C20-C19-C21	2.39	119.37	115.23
12	A	305	PL9	C20-C19-C21	2.38	119.36	115.23
9	A	302	HEM	C4A-NA-C1A	2.38	109.70	105.82
9	A	302	HEM	C3D-C4D-ND	2.38	112.78	110.17
12	A	305	PL9	C7-C3-C4	-2.37	114.96	116.91
9	A	302	HEM	O2A-CGA-CBA	2.35	121.43	114.00
14	B	201	CLA	CAA-C2A-C3A	2.34	119.33	113.00
14	B	201	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
10	C	301	HEC	C4A-NA-C1A	2.32	109.61	105.82
10	A	303	HEC	C2B-C1B-NB	2.31	112.57	109.90
11	A	304	TDS	OAB-CAE-CAF	2.30	119.10	115.84
12	Q	1305	PL9	C40-C39-C41	2.30	119.22	115.23
12	A	305	PL9	C40-C39-C41	2.30	119.22	115.23
9	A	302	HEM	CAA-C2A-C3A	-2.30	121.92	127.07
13	B	307	OPC	OAN-CAO-OAD	-2.30	118.34	123.70
16	E	101	BCR	C34-C9-C8	2.29	121.58	118.09
10	A	303	HEC	C3D-C4D-ND	2.26	112.54	110.35
12	A	305	PL9	C10-C9-C8	-2.25	117.84	123.63
11	N	1304	TDS	CAS-CAR-CAQ	2.25	121.39	113.13
9	N	301	HEM	CBA-CAA-C2A	-2.24	106.35	112.53
9	A	301	HEM	CMA-C3A-C2A	-2.22	120.91	125.62
13	N	1306	OPC	CBM-CBL-CBK	2.21	121.80	113.69
9	N	302	HEM	CHA-C4D-C3D	-2.20	121.17	125.23
10	P	301	HEC	O2A-CGA-CBA	2.20	120.95	114.00
9	N	302	HEM	O1A-CGA-CBA	-2.19	116.13	123.09
16	R	1101	BCR	C34-C9-C8	2.18	121.42	118.09
9	A	301	HEM	C1D-C2D-C3D	-2.18	104.69	106.98
10	A	303	HEC	CHA-C4D-C3D	-2.18	121.60	124.77
12	A	305	PL9	C10-C9-C11	2.17	119.00	115.23
9	A	301	HEM	O2A-CGA-CBA	2.15	120.81	114.00
14	B	201	CLA	C12-C11-C10	-2.15	103.66	113.28
12	A	305	PL9	C51-C49-C50	2.14	119.52	114.59
10	N	303	HEC	CAA-CBA-CGA	2.14	119.34	113.67
10	N	303	HEC	CHA-C4D-ND	2.13	126.71	124.42
14	B	201	CLA	CED-O2D-CGD	2.11	120.71	115.92
9	N	302	HEM	C3D-C4D-ND	2.11	112.48	110.17
14	O	1201	CLA	C4B-C3B-C2B	-2.11	104.68	107.30
12	A	305	PL9	C53-C6-C1	2.10	119.58	115.28
9	A	301	HEM	O1D-CGD-CBD	-2.09	116.46	123.09
13	D	306	OPC	OBJ-CBK-OCC	-2.09	118.41	123.63
10	A	303	HEC	CBC-CAC-C3C	2.08	118.06	112.42
16	E	101	BCR	C34-C9-C10	-2.08	119.44	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	306	OPC	CBM-CBL-CBK	2.08	121.32	113.69
10	N	303	HEC	CBD-CAD-C3D	-2.08	106.78	112.53
13	B	307	OPC	CBQ-CBR-CBS	-2.08	109.28	124.83
14	O	1201	CLA	C3D-C4D-ND	2.05	113.32	109.99
9	N	302	HEM	O2A-CGA-CBA	2.04	120.46	114.00
12	A	305	PL9	C45-C44-C43	-2.04	118.38	123.63
12	Q	1305	PL9	C53-C6-C1	2.04	119.46	115.28
12	Q	1305	PL9	C2-C1-C6	2.04	121.42	119.00
10	P	301	HEC	C4A-NA-C1A	2.03	109.12	105.82
10	A	303	HEC	CHB-C1B-NB	-2.02	122.25	124.42

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	303	HEC	NA
10	C	301	HEC	NA
10	N	303	HEC	NA
10	P	301	HEC	NA
14	B	201	CLA	C3A
14	B	201	CLA	C8
14	O	1201	CLA	C3A
14	O	1201	CLA	C2A
14	O	1201	CLA	C8

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	301	HEM	C2B-C3B-CAB-CBB
9	A	301	HEM	C4B-C3B-CAB-CBB
9	A	302	HEM	C2C-C3C-CAC-CBC
9	A	302	HEM	C4C-C3C-CAC-CBC
9	N	301	HEM	C2B-C3B-CAB-CBB
9	N	301	HEM	C4B-C3B-CAB-CBB
9	N	302	HEM	C2B-C3B-CAB-CBB
11	N	1304	TDS	OAQ-CAP-CAQ-CAR
11	N	1304	TDS	CAH-CAP-CAQ-CAR
12	A	305	PL9	C7-C8-C9-C10
12	A	305	PL9	C7-C8-C9-C11
12	A	305	PL9	C12-C13-C14-C15
12	A	305	PL9	C12-C13-C14-C16
12	A	305	PL9	C17-C18-C19-C20
12	A	305	PL9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
12	A	305	PL9	C22-C23-C24-C25
12	A	305	PL9	C22-C23-C24-C26
12	A	305	PL9	C32-C33-C34-C35
12	A	305	PL9	C32-C33-C34-C36
12	A	305	PL9	C37-C38-C39-C40
12	A	305	PL9	C37-C38-C39-C41
12	A	305	PL9	C41-C42-C43-C44
12	Q	1305	PL9	C7-C8-C9-C10
12	Q	1305	PL9	C7-C8-C9-C11
12	Q	1305	PL9	C12-C13-C14-C16
12	Q	1305	PL9	C17-C18-C19-C20
12	Q	1305	PL9	C17-C18-C19-C21
12	Q	1305	PL9	C22-C23-C24-C25
12	Q	1305	PL9	C22-C23-C24-C26
12	Q	1305	PL9	C32-C33-C34-C35
12	Q	1305	PL9	C32-C33-C34-C36
12	Q	1305	PL9	C37-C38-C39-C40
12	Q	1305	PL9	C37-C38-C39-C41
12	Q	1305	PL9	C41-C42-C43-C44
13	B	307	OPC	CAP-CAO-OAN-CAM
13	B	307	OPC	OAD-CAO-OAN-CAM
13	B	307	OPC	CAL-OAK-PAJ-OAB
13	B	307	OPC	CAL-OAK-PAJ-OAI
13	B	307	OPC	CAH-OAI-PAJ-OAK
13	B	307	OPC	CAH-OAI-PAJ-OAB
13	D	306	OPC	CAP-CAO-OAN-CAM
13	D	306	OPC	OAD-CAO-OAN-CAM
13	D	306	OPC	CAH-OAI-PAJ-OAK
13	D	306	OPC	CAH-OAI-PAJ-OBH
13	D	306	OPC	OCC-CBK-OBJ-CBI
13	D	306	OPC	CBL-CBK-OBJ-CBI
13	N	1306	OPC	CAP-CAO-OAN-CAM
13	N	1306	OPC	OAD-CAO-OAN-CAM
13	N	1306	OPC	OCC-CBK-OBJ-CBI
13	N	1306	OPC	CBL-CBK-OBJ-CBI
13	Q	1307	OPC	CAP-CAO-OAN-CAM
13	Q	1307	OPC	OAD-CAO-OAN-CAM
13	Q	1307	OPC	CAH-OAI-PAJ-OAK
13	Q	1307	OPC	CAH-OAI-PAJ-OAB
14	B	201	CLA	C1A-C2A-CAA-CBA
14	O	1201	CLA	C1A-C2A-CAA-CBA
16	E	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	E	101	BCR	C5-C6-C7-C8
16	E	101	BCR	C11-C10-C9-C8
16	E	101	BCR	C11-C10-C9-C34
16	E	101	BCR	C22-C23-C24-C25
16	R	1101	BCR	C1-C6-C7-C8
16	R	1101	BCR	C5-C6-C7-C8
16	R	1101	BCR	C11-C10-C9-C8
16	R	1101	BCR	C11-C10-C9-C34
16	R	1101	BCR	C22-C23-C24-C25
14	O	1201	CLA	C3-C5-C6-C7
12	Q	1305	PL9	C30-C29-C31-C32
12	Q	1305	PL9	C12-C13-C14-C15
10	P	301	HEC	C2C-C3C-CAC-CBC
12	Q	1305	PL9	C15-C14-C16-C17
12	Q	1305	PL9	C13-C14-C16-C17
12	Q	1305	PL9	C23-C24-C26-C27
12	Q	1305	PL9	C28-C29-C31-C32
12	A	305	PL9	C39-C41-C42-C43
10	C	301	HEC	C2C-C3C-CAC-CBC
11	A	304	TDS	CAF-CAE-OAB-CAA
11	N	1304	TDS	CAD-CAL-OAK-CAJ
11	N	1304	TDS	CAF-CAE-OAB-CAA
11	A	304	TDS	CAD-CAE-OAB-CAA
12	Q	1305	PL9	C25-C24-C26-C27
14	B	201	CLA	C3-C5-C6-C7
14	O	1201	CLA	C11-C12-C13-C14
11	N	1304	TDS	CAD-CAE-OAB-CAA
10	P	301	HEC	C4C-C3C-CAC-CBC
12	Q	1305	PL9	C14-C16-C17-C18
11	A	304	TDS	CAD-CAL-OAK-CAJ
14	O	1201	CLA	C2A-CAA-CBA-CGA
14	B	201	CLA	C10-C11-C12-C13
10	C	301	HEC	C4C-C3C-CAC-CBC
11	N	1304	TDS	CAM-CAL-OAK-CAJ
12	A	305	PL9	C14-C16-C17-C18
11	A	304	TDS	CAM-CAL-OAK-CAJ
11	A	304	TDS	CAV-CAW-CAX-CAY
14	B	201	CLA	C2C-C3C-CAC-CBC
11	N	1304	TDS	CAT-CAU-CAV-CAW
12	Q	1305	PL9	C39-C41-C42-C43
9	N	302	HEM	C4B-C3B-CAB-CBB
13	N	1306	OPC	CAS-CAT-CAU-CAV

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Mol	Chain	Res	Type	Atoms
12	A	305	PL9	C31-C32-C33-C34
10	A	303	HEC	C4D-C3D-CAD-CBD
14	B	201	CLA	O2A-C1-C2-C3
12	Q	1305	PL9	C31-C32-C33-C34
13	Q	1307	OPC	CAT-CAU-CAV-CAW
14	B	201	CLA	CBA-CGA-O2A-C1
14	B	201	CLA	C6-C7-C8-C9
14	B	201	CLA	C6-C7-C8-C10
11	A	304	TDS	CAT-CAU-CAV-CAW
10	N	303	HEC	C1A-C2A-CAA-CBA
14	O	1201	CLA	C12-C13-C15-C16
10	A	303	HEC	C2D-C3D-CAD-CBD
14	B	201	CLA	O1A-CGA-O2A-C1
9	A	302	HEM	C2B-C3B-CAB-CBB
9	N	301	HEM	C2C-C3C-CAC-CBC
9	N	301	HEM	C4C-C3C-CAC-CBC
13	B	307	OPC	NAF-CAG-CAH-OAI
13	D	306	OPC	NAF-CAG-CAH-OAI
13	N	1306	OPC	NAF-CAG-CAH-OAI
13	Q	1307	OPC	NAF-CAG-CAH-OAI
14	B	201	CLA	C13-C15-C16-C17
14	B	201	CLA	C11-C12-C13-C15
13	B	307	OPC	CAL-OAK-PAJ-OBH
13	B	307	OPC	CAH-OAI-PAJ-OBH
13	N	1306	OPC	CAH-OAI-PAJ-OAK
13	Q	1307	OPC	CAH-OAI-PAJ-OBH
14	B	201	CLA	C4-C3-C5-C6
13	N	1306	OPC	CBI-CAM-OAN-CAO
13	Q	1307	OPC	CAL-CAM-OAN-CAO
12	A	305	PL9	C12-C11-C9-C10
14	B	201	CLA	C4C-C3C-CAC-CBC
14	O	1201	CLA	C14-C13-C15-C16
14	B	201	CLA	C2-C3-C5-C6
12	Q	1305	PL9	C20-C19-C21-C22
10	N	303	HEC	C3A-C2A-CAA-CBA
12	A	305	PL9	C35-C34-C36-C37
12	A	305	PL9	C40-C39-C41-C42
14	B	201	CLA	C11-C12-C13-C14
13	B	307	OPC	CBI-CAM-OAN-CAO
13	D	306	OPC	CBI-CAM-OAN-CAO
9	N	301	HEM	CAA-CBA-CGA-O2A
12	A	305	PL9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
9	N	301	HEM	CAA-CBA-CGA-O1A
9	N	301	HEM	CAD-CBD-CGD-O1D
12	Q	1305	PL9	C18-C19-C21-C22
14	O	1201	CLA	C11-C12-C13-C15
9	N	301	HEM	CAD-CBD-CGD-O2D
12	A	305	PL9	C25-C24-C26-C27
12	Q	1305	PL9	C35-C34-C36-C37
12	A	305	PL9	C33-C34-C36-C37
12	A	305	PL9	C20-C19-C21-C22
13	B	307	OPC	CAM-CAL-OAK-PAJ
12	A	305	PL9	C38-C39-C41-C42
10	P	301	HEC	CAD-CBD-CGD-O2D
12	A	305	PL9	C24-C26-C27-C28
10	C	301	HEC	CAD-CBD-CGD-O2D
12	Q	1305	PL9	C12-C11-C9-C10
9	A	301	HEM	C1A-C2A-CAA-CBA
9	A	301	HEM	CAA-CBA-CGA-O2A
13	B	307	OPC	CBP-CBQ-CBR-CBS
13	D	306	OPC	CBR-CBS-CBT-CBU
12	A	305	PL9	C18-C19-C21-C22
13	Q	1307	OPC	CAV-CAW-CAX-CAY
10	C	301	HEC	CAD-CBD-CGD-O1D
9	A	301	HEM	CAA-CBA-CGA-O1A
10	P	301	HEC	CAD-CBD-CGD-O1D
9	N	301	HEM	C4D-C3D-CAD-CBD
13	N	1306	OPC	CAT-CAU-CAV-CAW
9	A	302	HEM	C4B-C3B-CAB-CBB
13	B	307	OPC	CBR-CBS-CBT-CBU
13	N	1306	OPC	OBJ-CBK-CBL-CBM
12	A	305	PL9	C23-C24-C26-C27
13	D	306	OPC	CBW-CBX-CBY-CBZ
9	N	302	HEM	CAA-CBA-CGA-O2A
12	Q	1305	PL9	C46-C47-C48-C49
9	N	302	HEM	CAA-CBA-CGA-O1A
14	O	1201	CLA	CAA-CBA-CGA-O2A
14	B	201	CLA	CAA-CBA-CGA-O2A
14	B	201	CLA	C2A-CAA-CBA-CGA
12	Q	1305	PL9	C33-C34-C36-C37
13	B	307	OPC	CAL-CAM-OAN-CAO
9	A	301	HEM	CAD-CBD-CGD-O1D
12	Q	1305	PL9	C36-C37-C38-C39
13	N	1306	OPC	OCC-CBK-CBL-CBM

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Mol	Chain	Res	Type	Atoms
14	B	201	CLA	CAA-CBA-CGA-O1A
14	O	1201	CLA	CAA-CBA-CGA-O1A
13	Q	1307	OPC	OAN-CAM-CBI-OBJ
13	Q	1307	OPC	CAR-CAS-CAT-CAU
12	A	305	PL9	C36-C37-C38-C39
12	Q	1305	PL9	C21-C22-C23-C24
14	O	1201	CLA	CAD-CBD-CGD-O2D

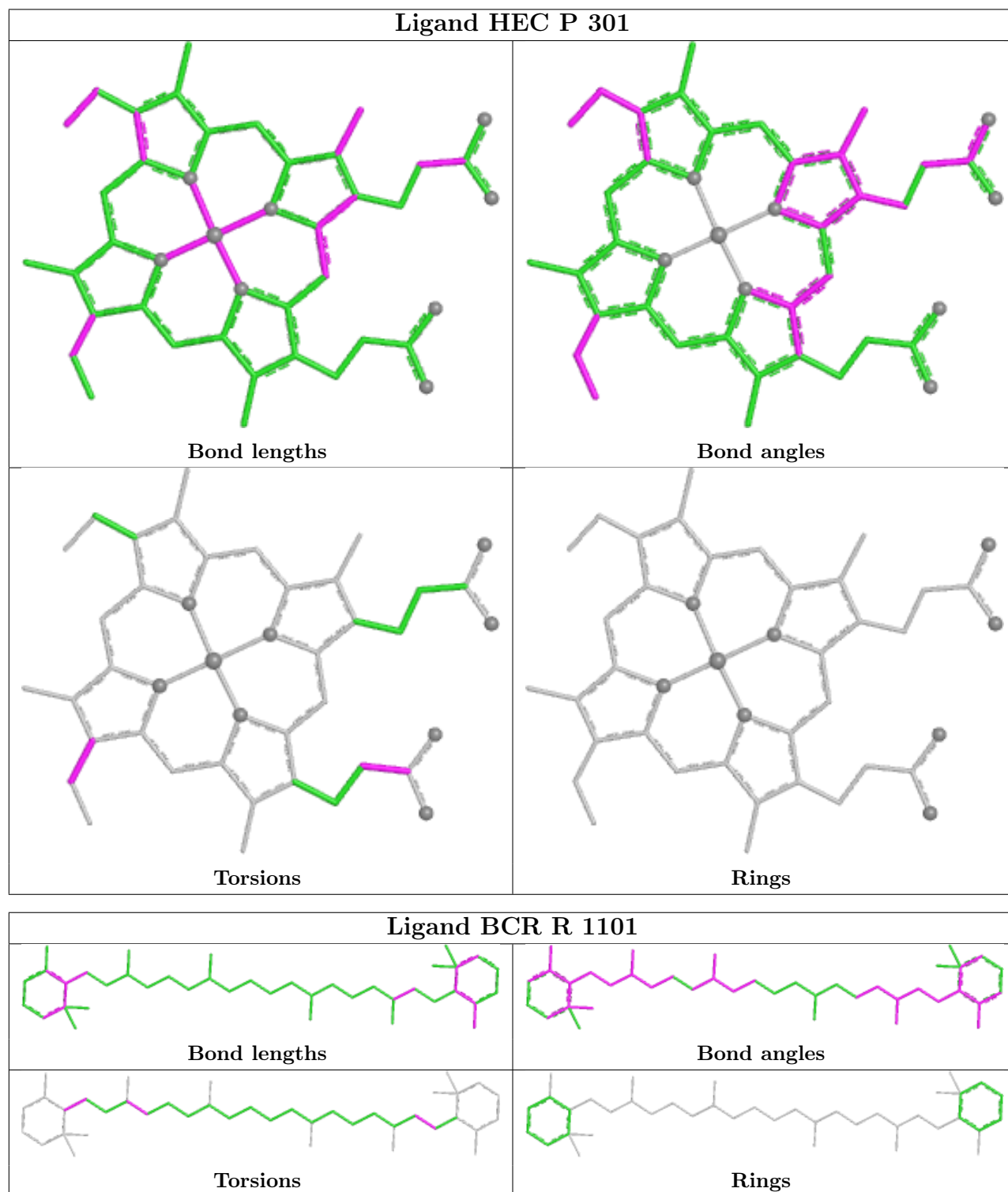
There are no ring outliers.

21 monomers are involved in 202 short contacts:

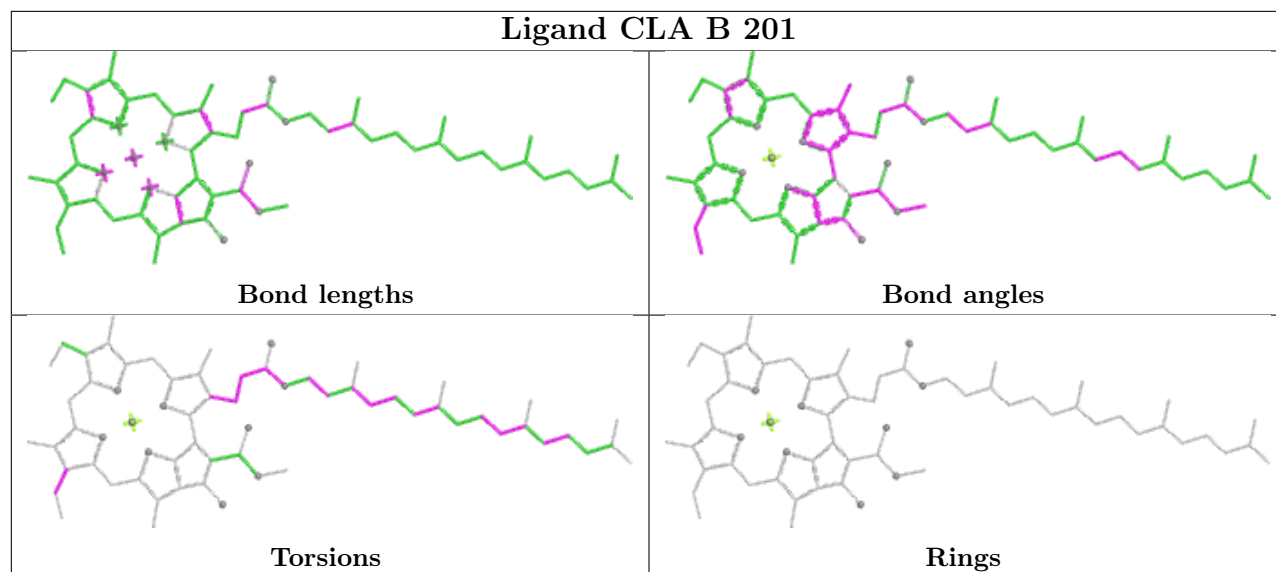
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	301	HEC	1	0
16	R	1101	BCR	7	0
14	B	201	CLA	8	0
11	N	1304	TDS	12	0
11	A	304	TDS	13	0
9	N	302	HEM	5	0
9	N	301	HEM	9	0
13	N	1306	OPC	10	0
10	N	303	HEC	4	0
12	A	305	PL9	19	0
13	D	306	OPC	24	0
10	A	303	HEC	4	0
14	O	1201	CLA	19	0
15	D	200	FES	1	0
9	A	301	HEM	10	0
12	Q	1305	PL9	22	0
16	E	101	BCR	7	0
13	Q	1307	OPC	30	0
13	B	307	OPC	14	0
15	Q	1200	FES	1	0
9	A	302	HEM	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

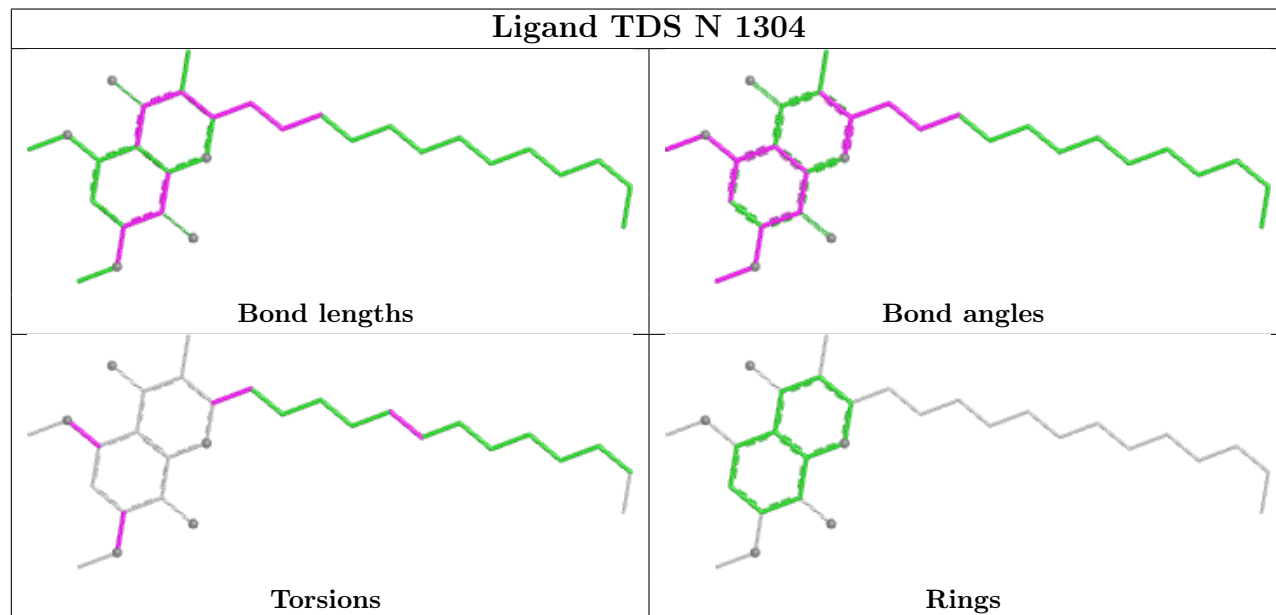
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



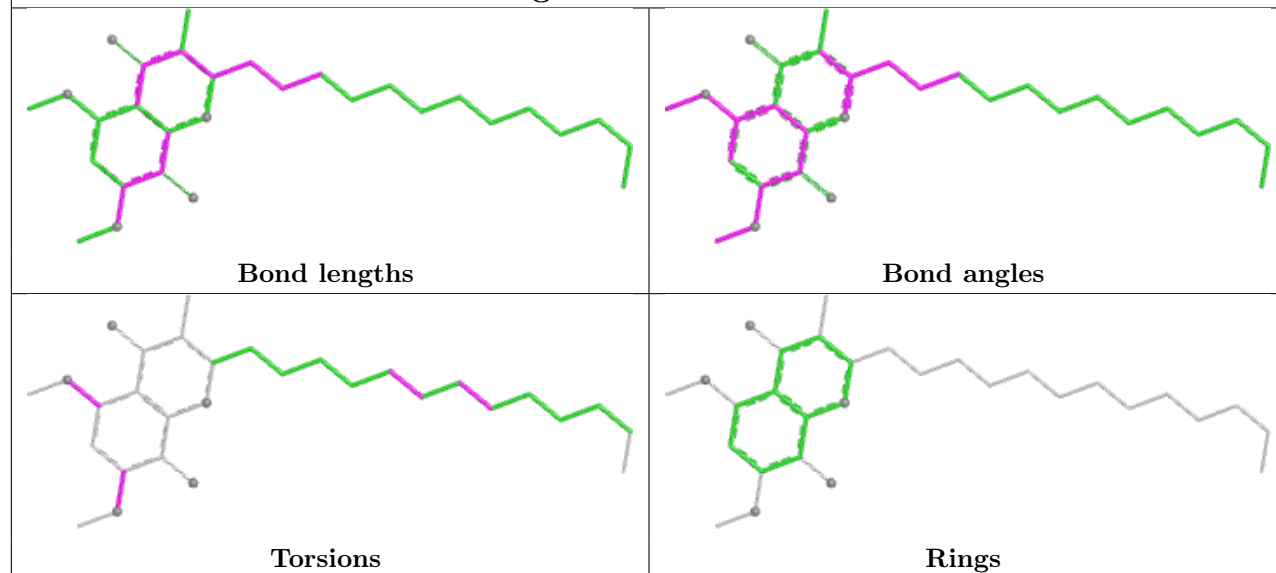
Ligand CLA B 201



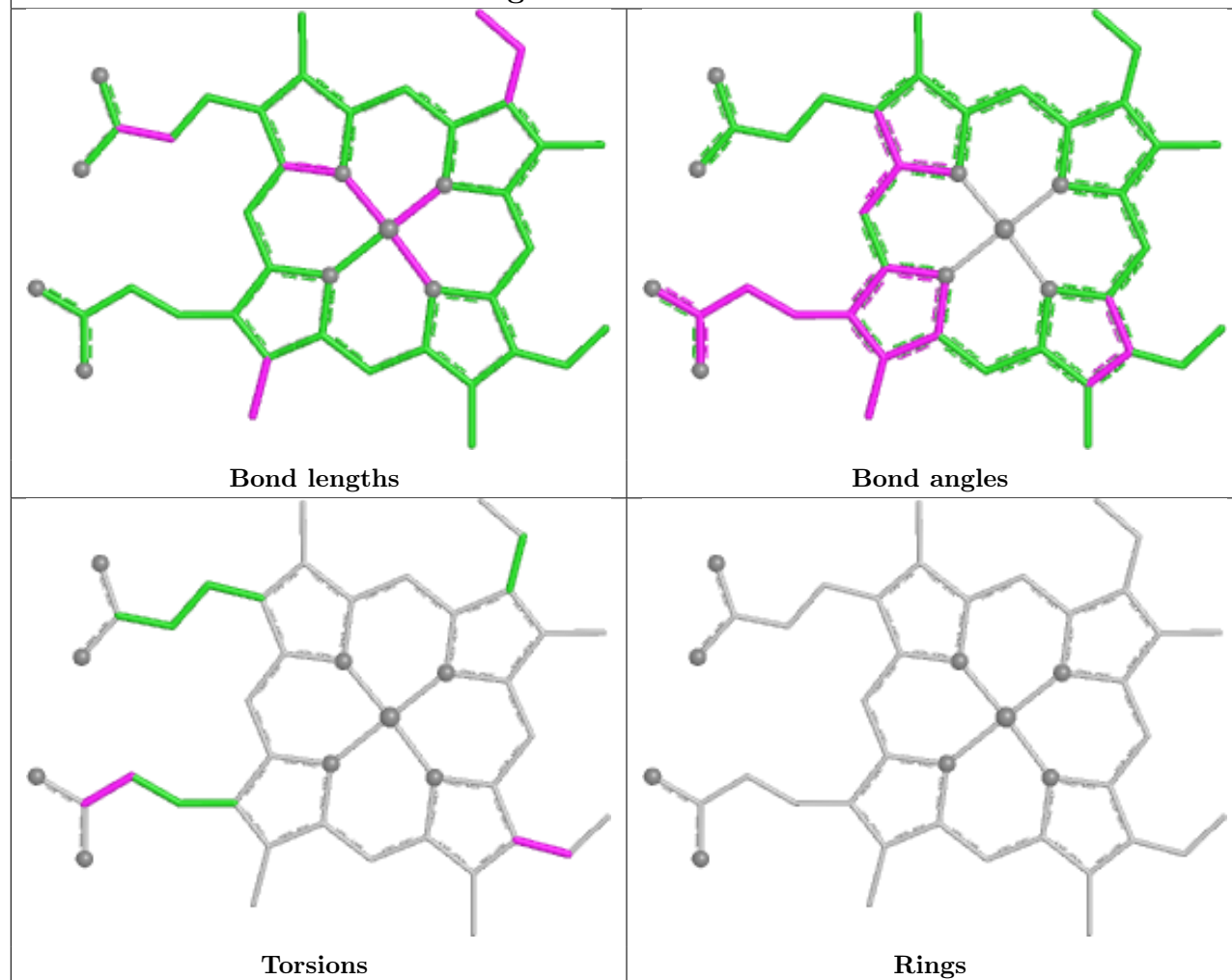
Ligand TDS N 1304



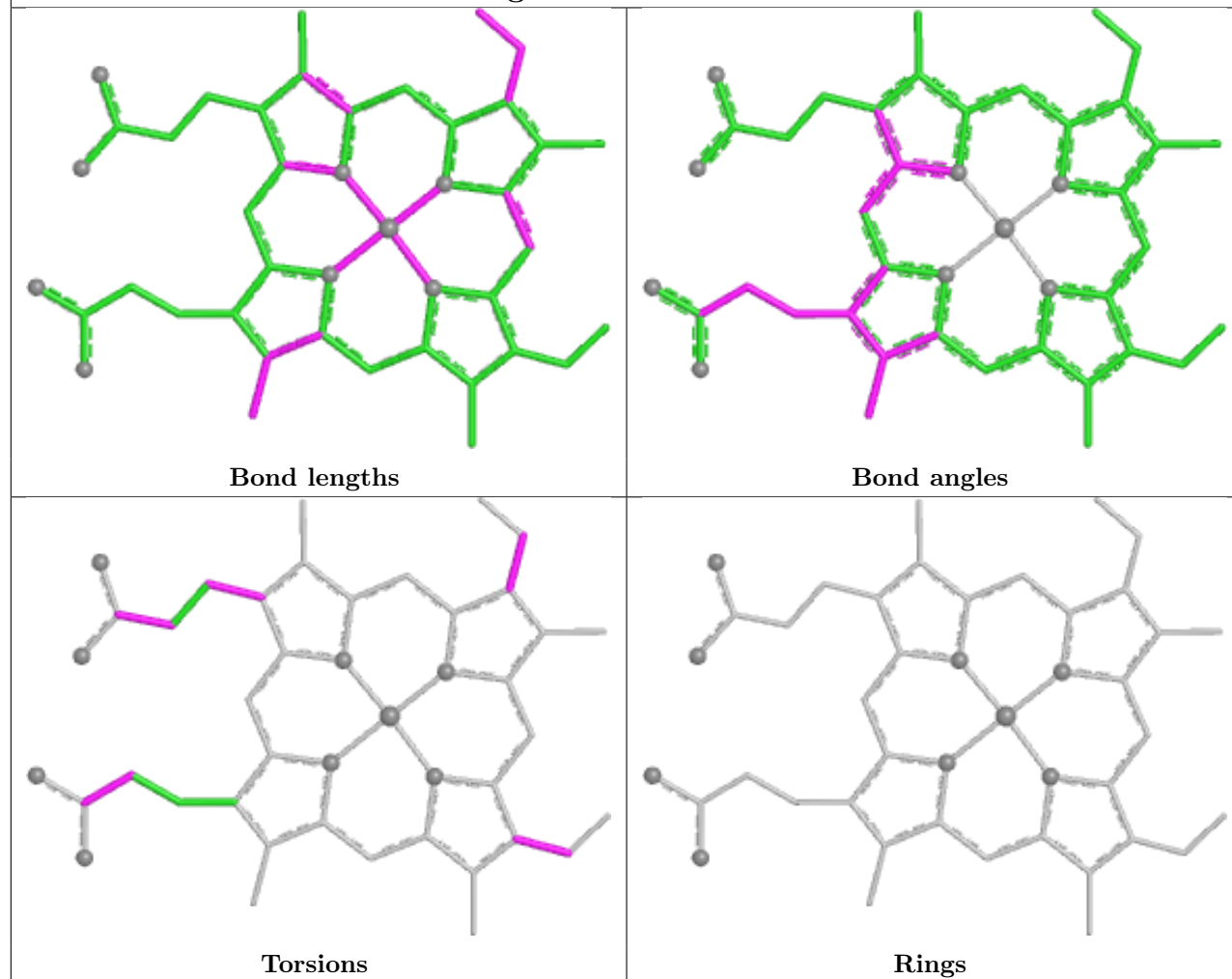
Ligand TDS A 304



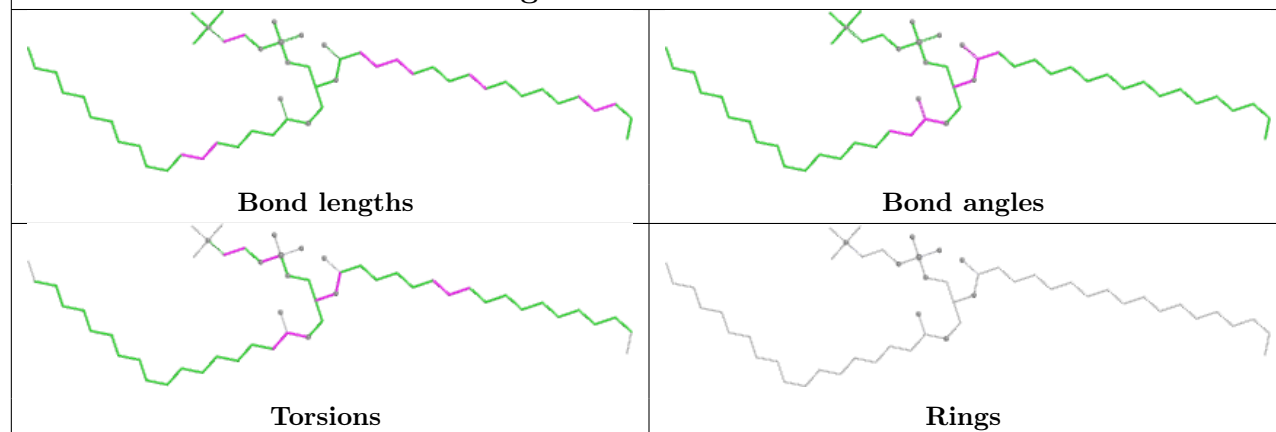
Ligand HEM N 302



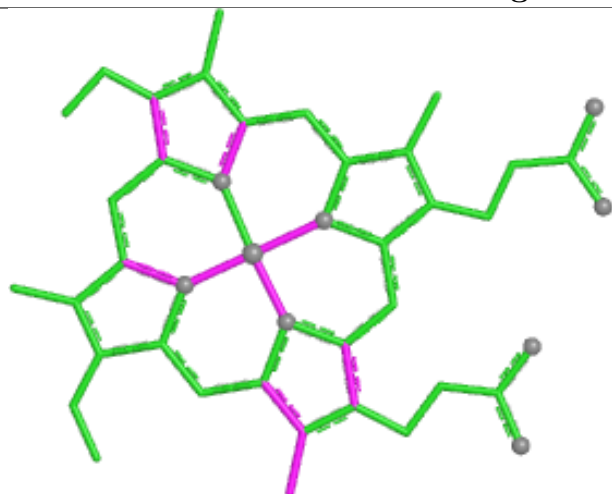
Ligand HEM N 301



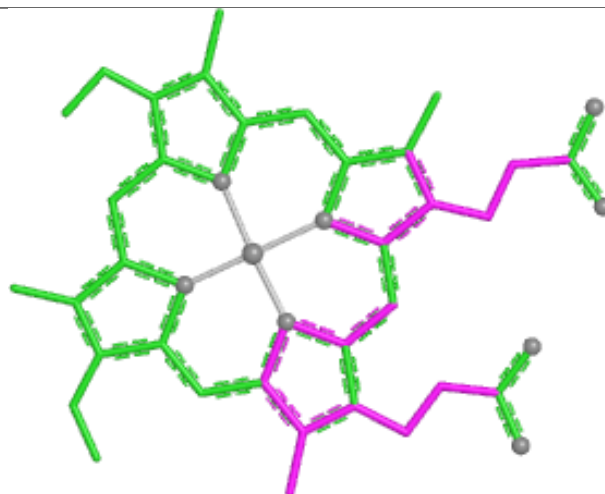
Ligand OPC N 1306



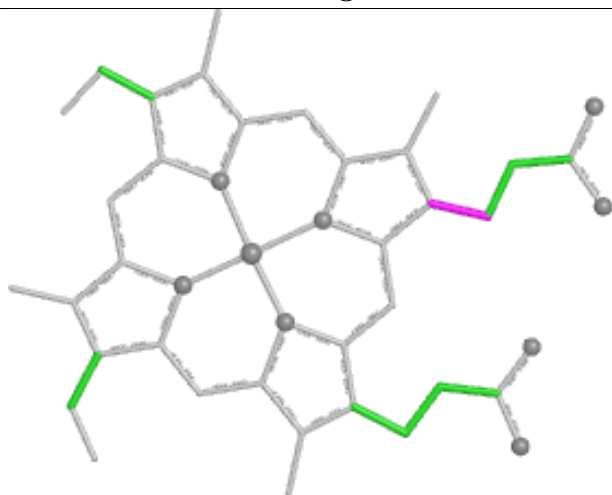
Ligand HEC N 303



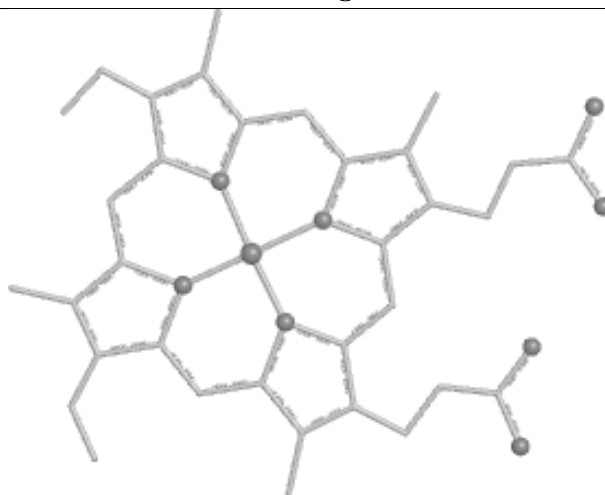
Bond lengths



Bond angles



Torsions

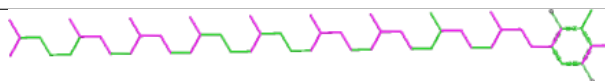


Rings

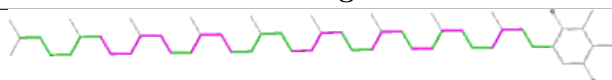
Ligand PL9 A 305



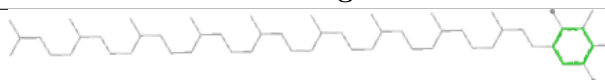
Bond lengths



Bond angles

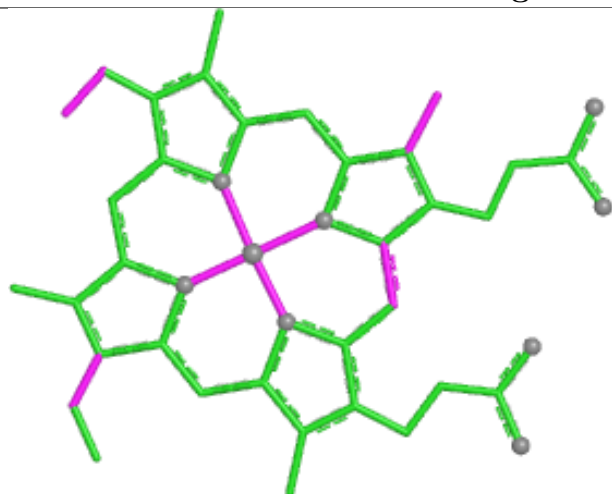


Torsions

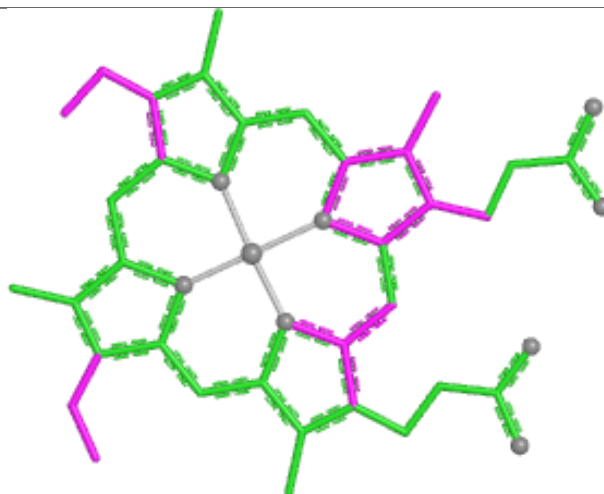


Rings

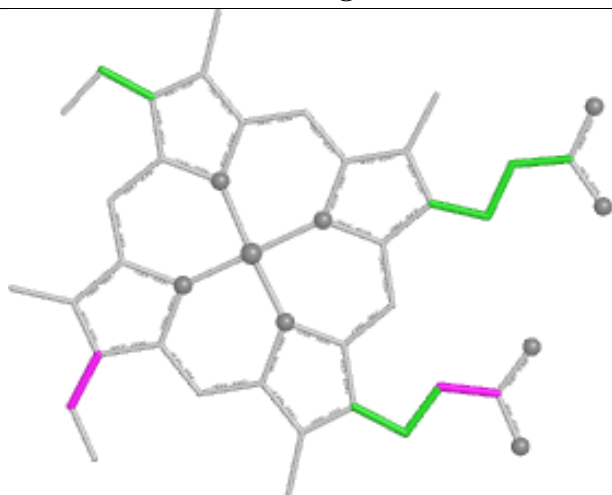
Ligand HEC C 301



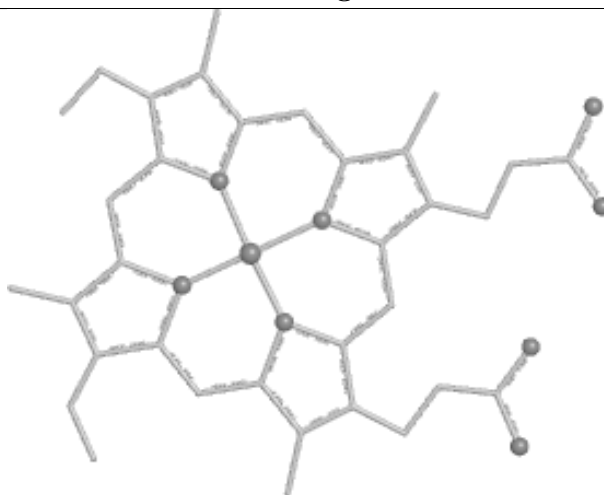
Bond lengths



Bond angles

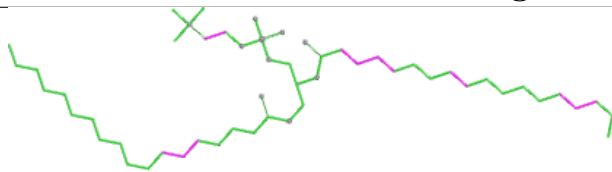


Torsions

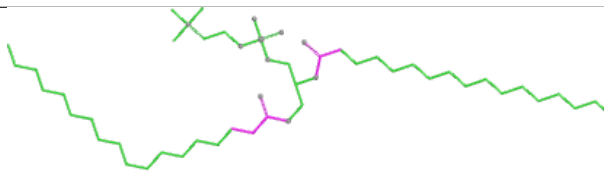


Rings

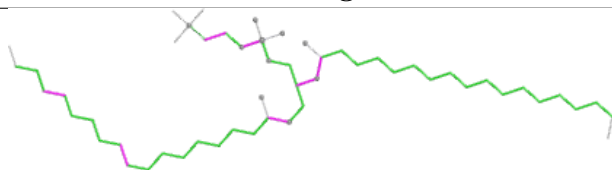
Ligand OPC D 306



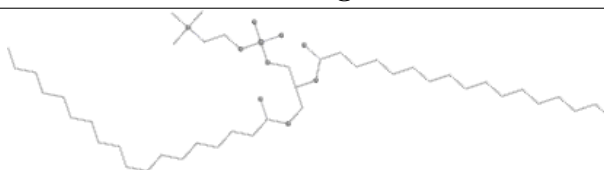
Bond lengths



Bond angles

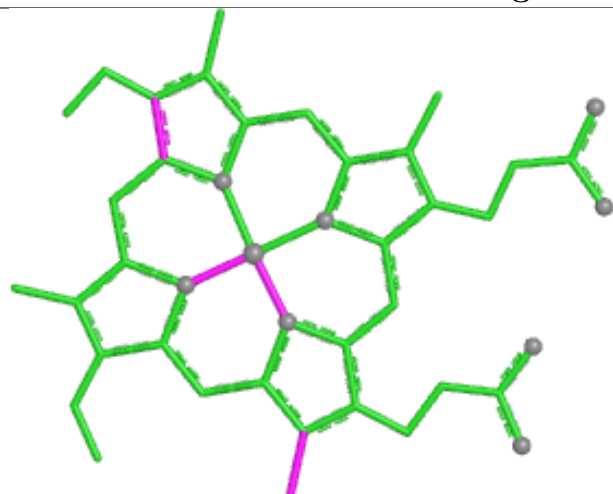


Torsions

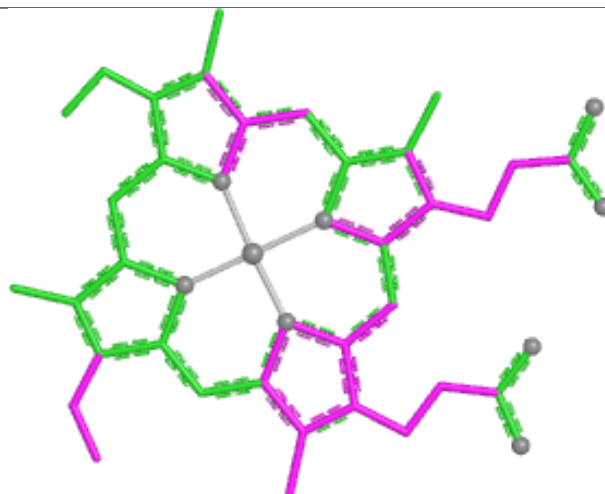


Rings

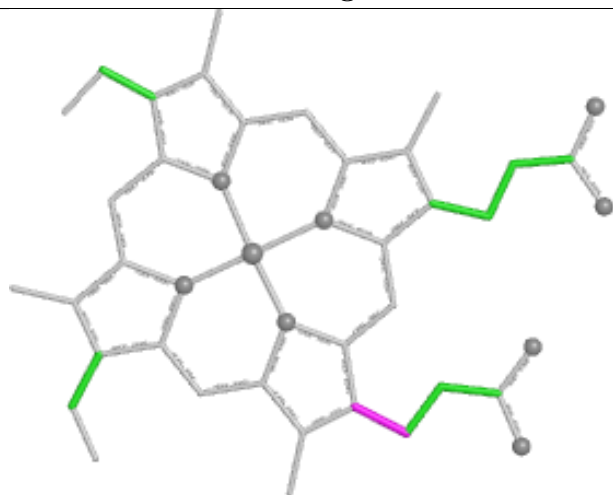
Ligand HEC A 303



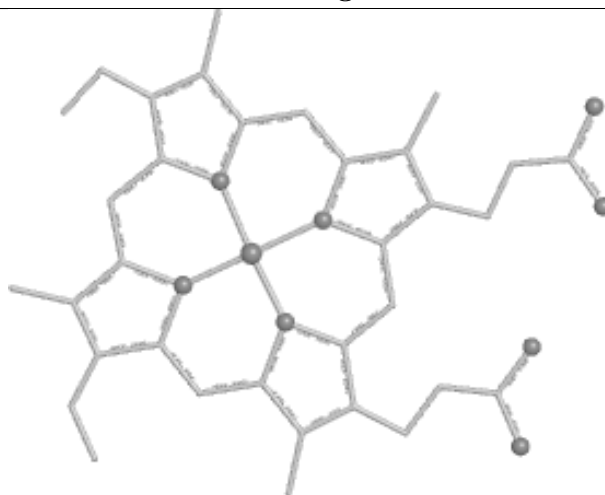
Bond lengths



Bond angles

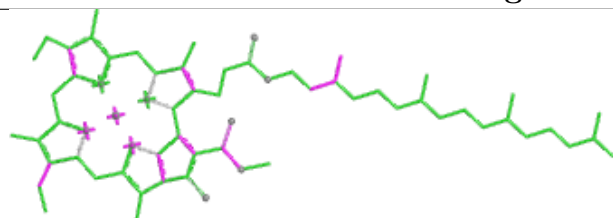


Torsions

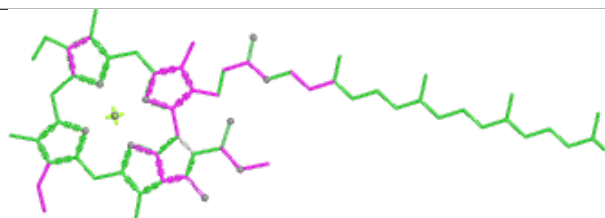


Rings

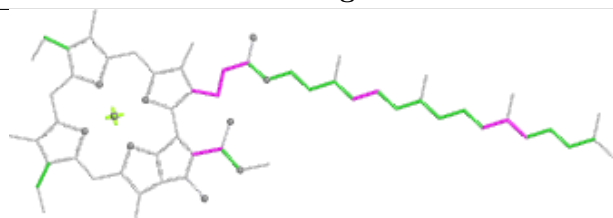
Ligand CLA O 1201



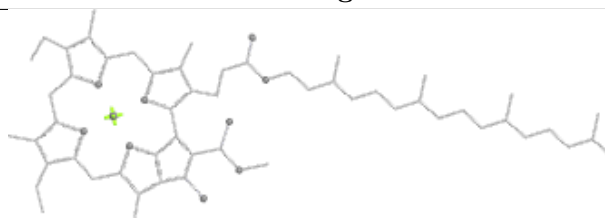
Bond lengths



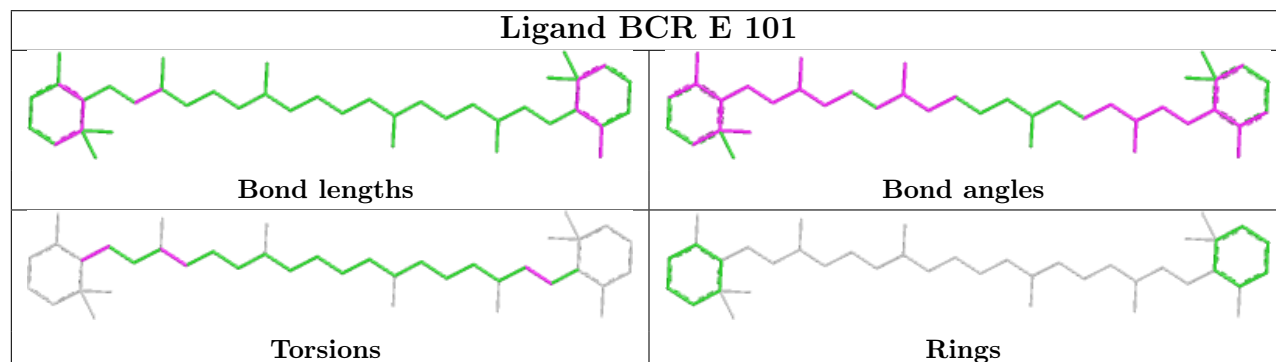
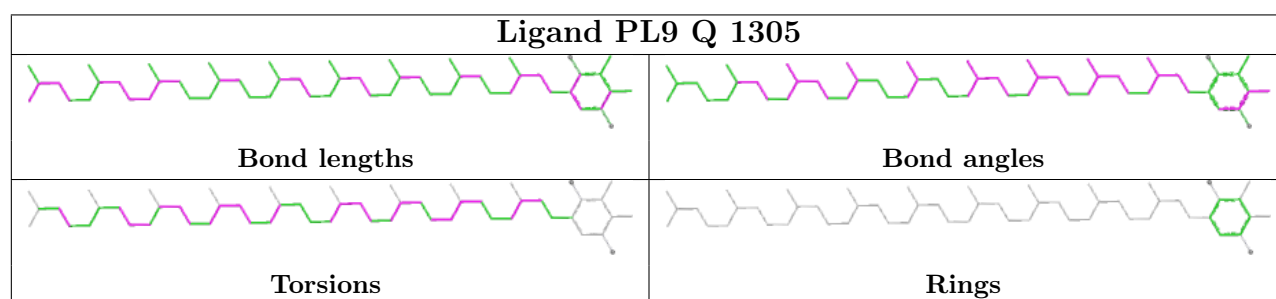
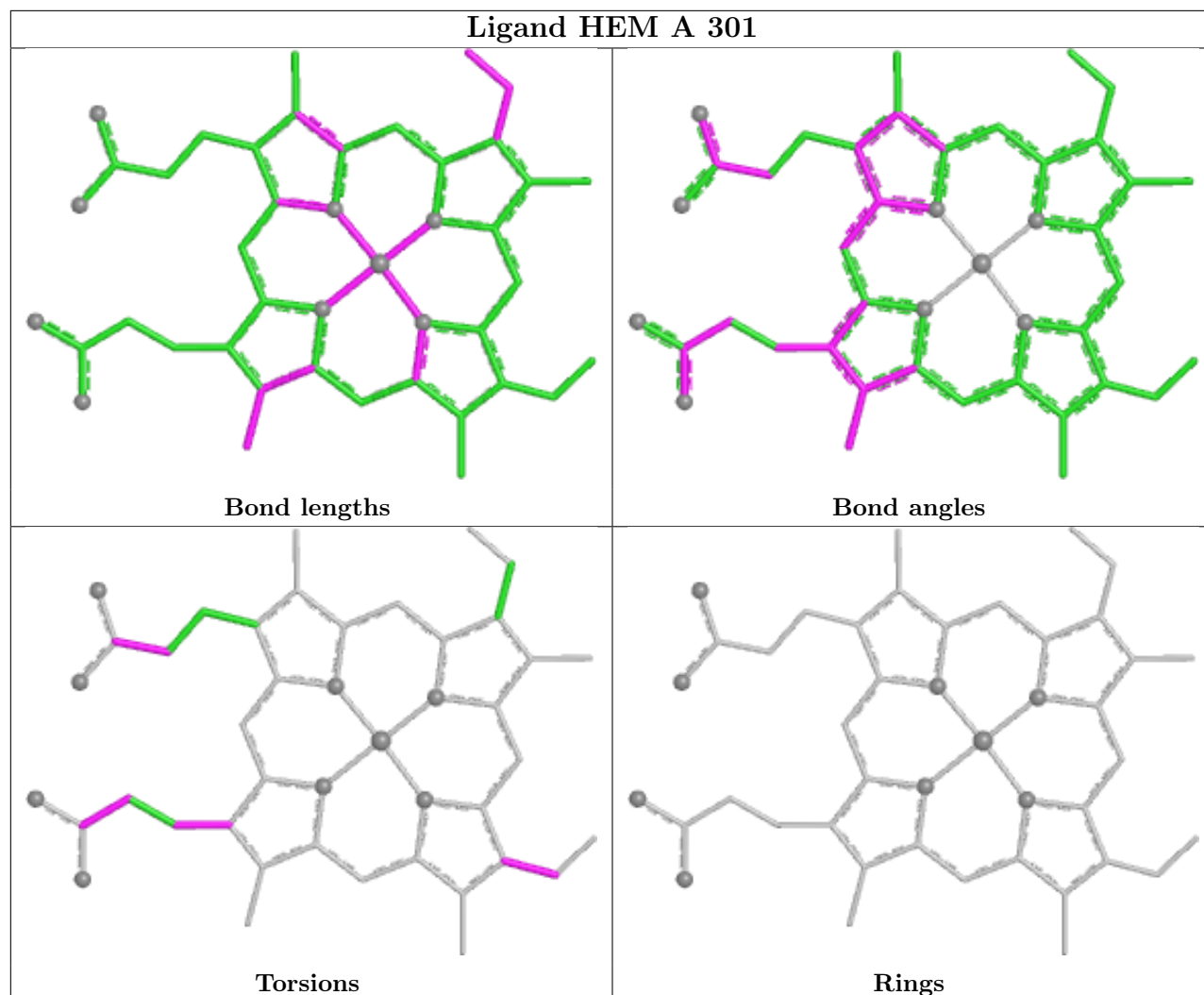
Bond angles

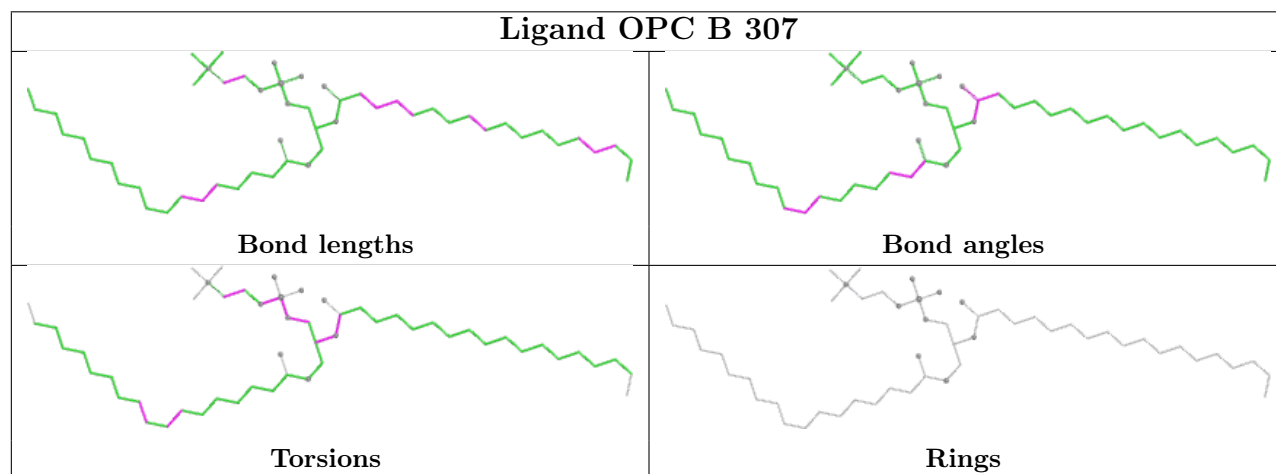
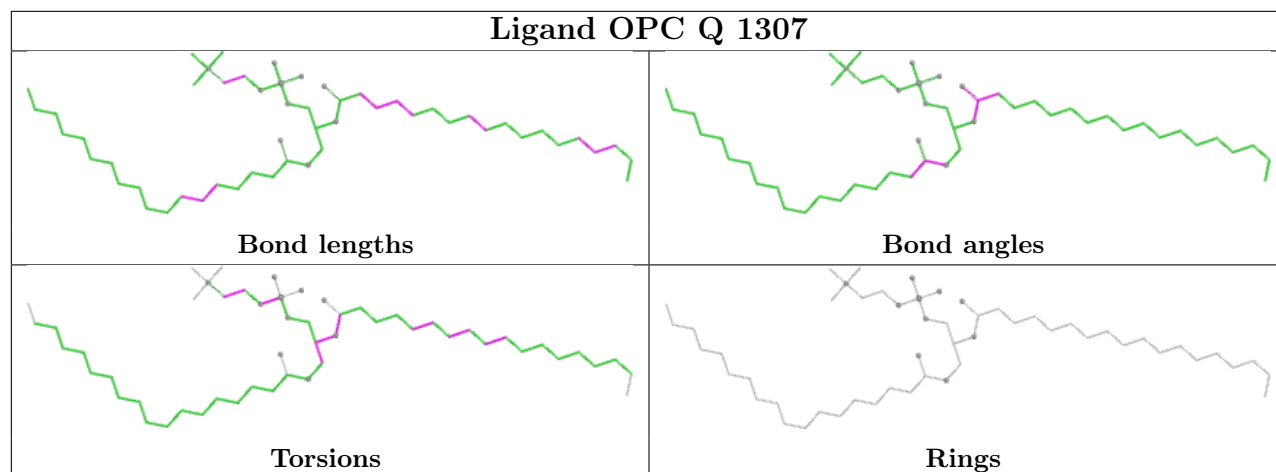


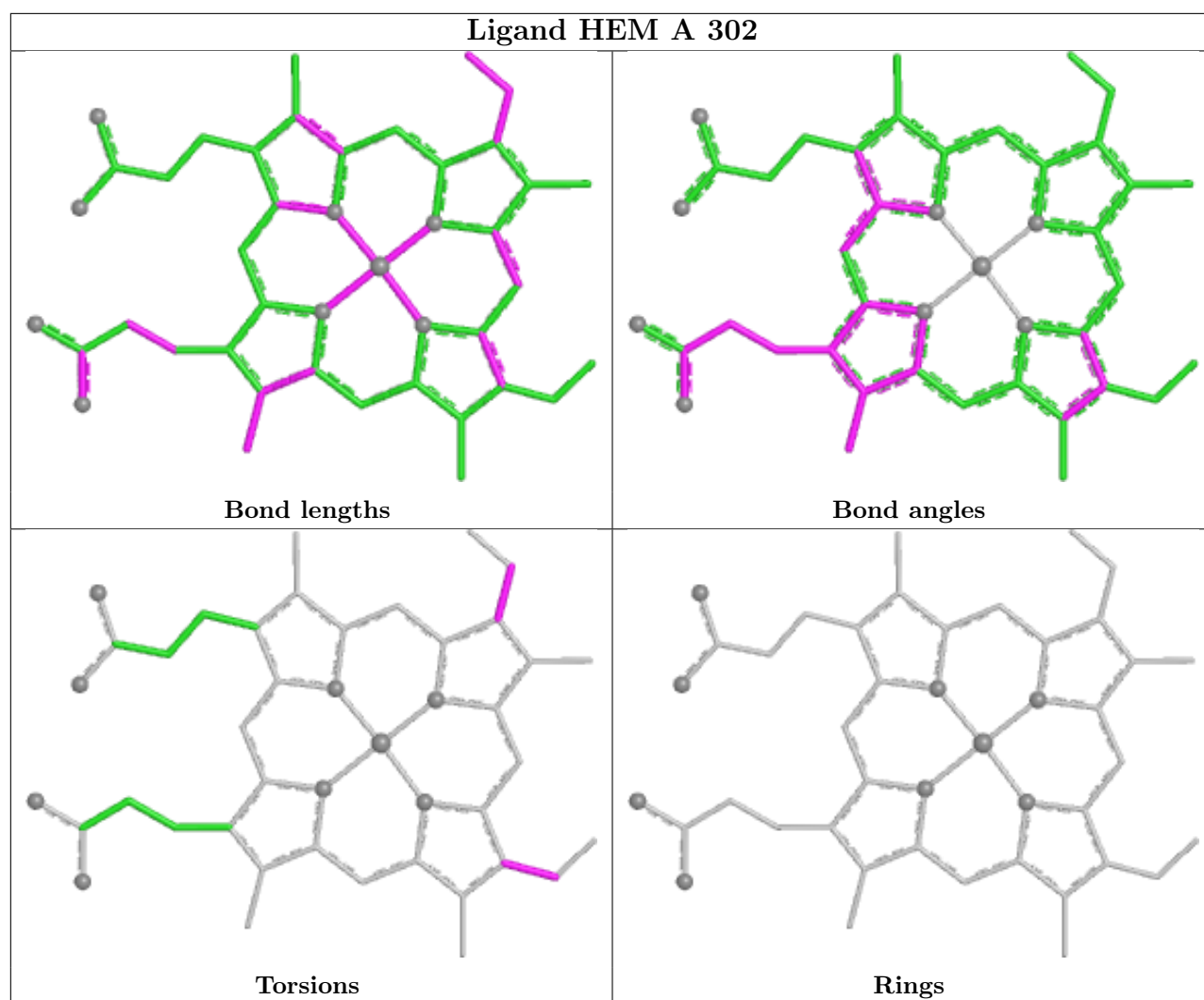
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	202/215 (93%)	-1.46	0 100 100	22, 55, 101, 174	0
1	N	202/215 (93%)	-1.50	0 100 100	19, 53, 86, 121	0
2	B	138/160 (86%)	-1.35	0 100 100	24, 65, 122, 194	0
2	O	138/160 (86%)	-1.31	0 100 100	28, 62, 139, 184	0
3	C	286/289 (98%)	-1.21	0 100 100	3, 82, 153, 200	1 (0%)
3	P	286/289 (98%)	-1.24	0 100 100	7, 85, 154, 200	1 (0%)
4	D	168/179 (93%)	-1.09	0 100 100	36, 117, 179, 200	0
4	Q	168/179 (93%)	-1.12	0 100 100	33, 109, 165, 192	0
5	E	32/32 (100%)	-1.14	0 100 100	30, 76, 149, 177	0
5	R	32/32 (100%)	-1.23	0 100 100	37, 81, 149, 171	0
6	F	33/35 (94%)	-1.27	0 100 100	39, 63, 140, 177	0
6	S	35/35 (100%)	-1.12	0 100 100	41, 78, 152, 167	0
7	G	23/37 (62%)	-1.45	0 100 100	33, 71, 128, 171	0
7	T	27/37 (72%)	-1.36	0 100 100	37, 65, 100, 152	0
8	H	27/29 (93%)	-1.29	0 100 100	33, 71, 130, 165	0
8	U	27/29 (93%)	-1.13	0 100 100	46, 81, 152, 157	0
All	All	1824/1952 (93%)	-1.28	0 100 100	3, 74, 155, 200	2 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

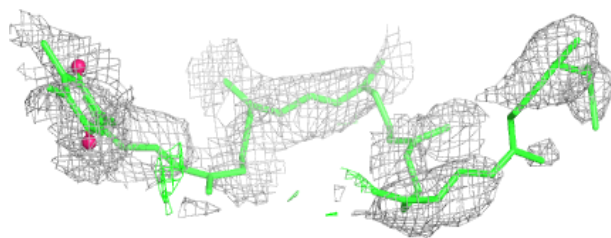
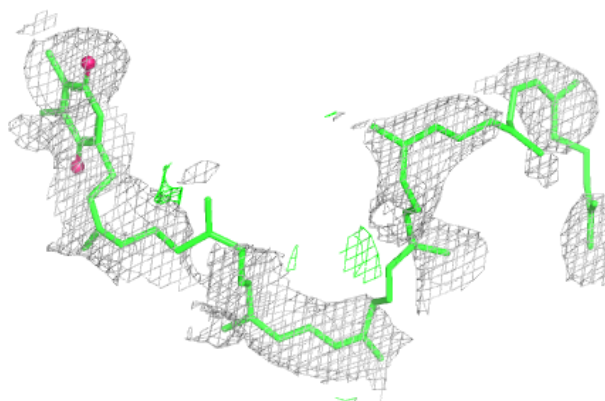
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	PL9	A	305	55/55	0.98	0.08	98,98,98,98	0
12	PL9	Q	1305	55/55	0.98	0.06	85,85,85,85	0
13	OPC	B	307	54/55	0.98	0.06	84,84,84,84	0
13	OPC	N	1306	54/55	0.98	0.07	87,87,87,87	0
11	TDS	A	304	30/30	0.99	0.06	52,52,52,52	0
13	OPC	D	306	54/55	0.99	0.06	86,86,86,86	0
11	TDS	N	1304	30/30	0.99	0.07	80,80,80,80	0
13	OPC	Q	1307	54/55	0.99	0.05	72,72,72,72	0
14	CLA	B	201	65/65	0.99	0.04	45,56,56,56	0
14	CLA	O	1201	65/65	0.99	0.05	22,72,72,72	0
16	BCR	E	101	40/40	0.99	0.06	77,77,77,77	0
16	BCR	R	1101	40/40	0.99	0.07	91,91,91,91	0
10	HEC	A	303	43/43	1.00	0.04	55,81,81,81	0
10	HEC	C	301	43/43	1.00	0.04	62,83,83,83	0
10	HEC	N	303	43/43	1.00	0.03	61,61,61,64	0
10	HEC	P	301	43/43	1.00	0.03	47,56,56,56	0
9	HEM	A	301	43/43	1.00	0.04	45,45,45,45	0
9	HEM	A	302	43/43	1.00	0.04	62,62,62,62	0
15	FES	D	200	4/4	1.00	0.04	144,144,170,170	0
15	FES	Q	1200	4/4	1.00	0.04	94,94,98,98	0
9	HEM	N	301	43/43	1.00	0.04	41,50,50,50	0
9	HEM	N	302	43/43	1.00	0.03	48,56,56,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

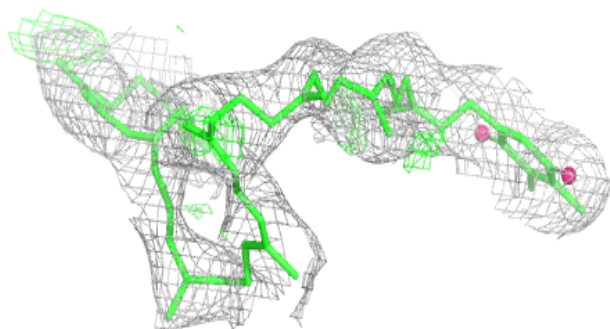
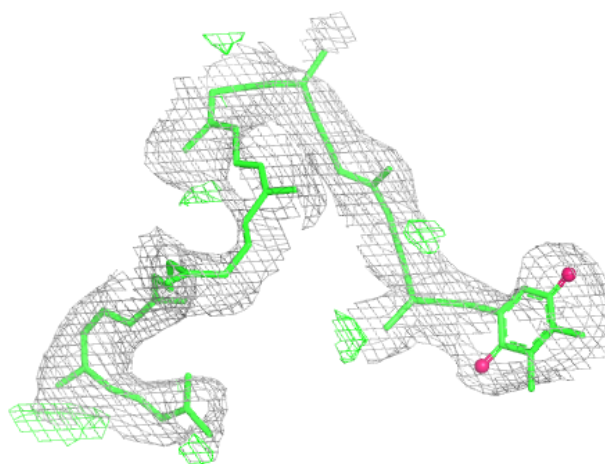
Electron density around PL9 A 305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



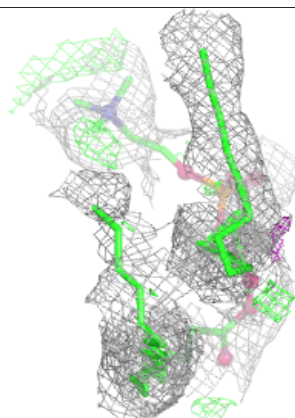
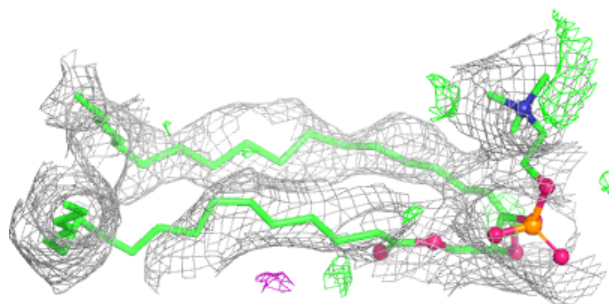
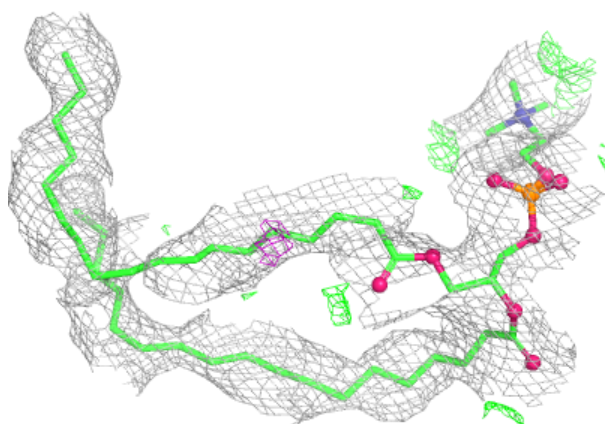
Electron density around PL9 Q 1305:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

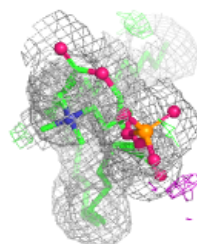
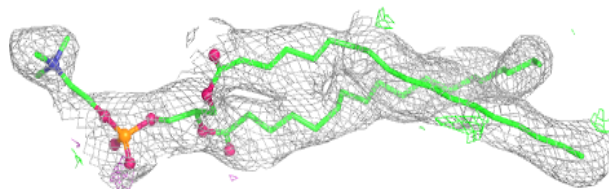
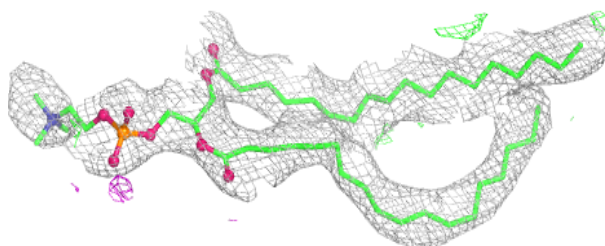


Electron density around OPC B 307:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

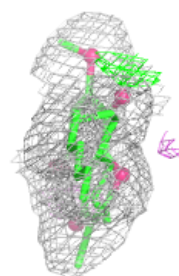
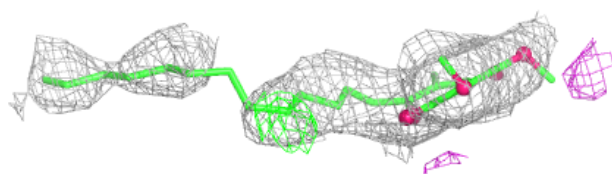
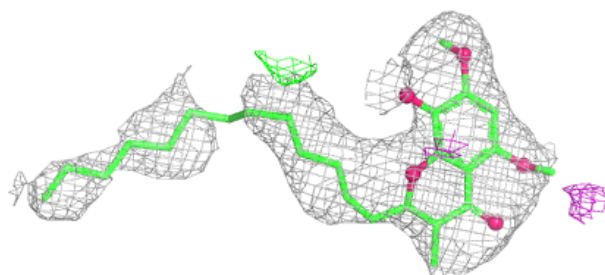
**Electron density around OPC N 1306:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

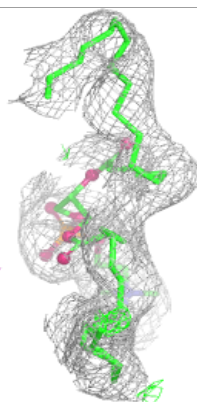
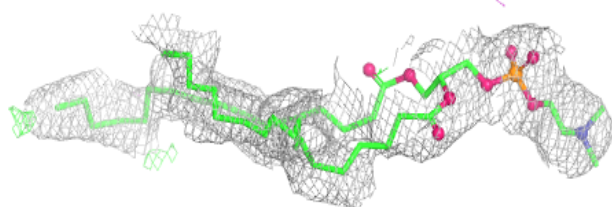
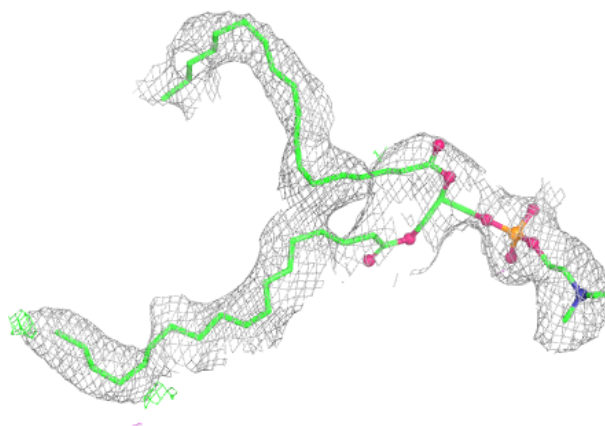


Electron density around TDS A 304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

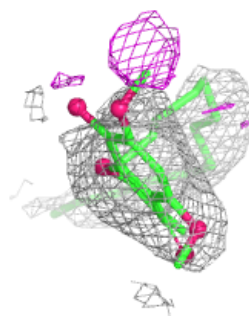
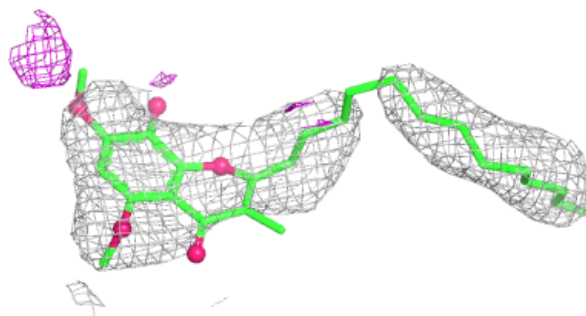
**Electron density around OPC D 306:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

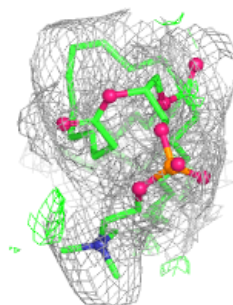
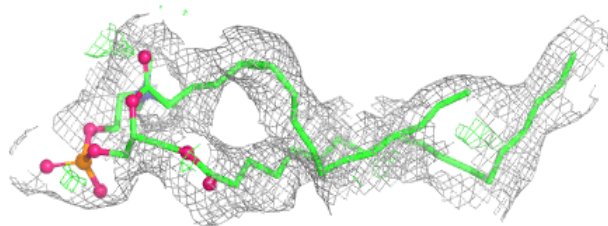
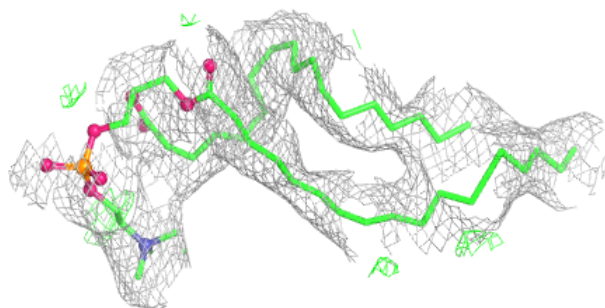


Electron density around TDS N 1304:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

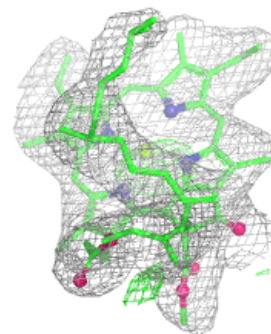
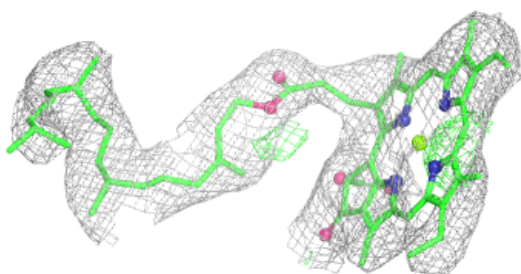
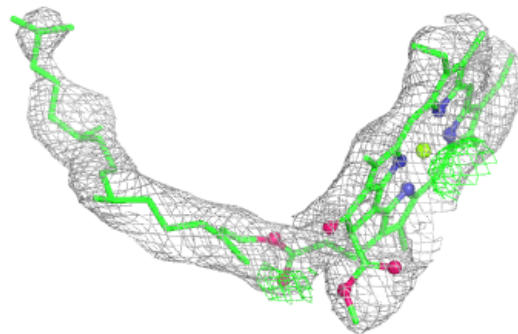
**Electron density around OPC Q 1307:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

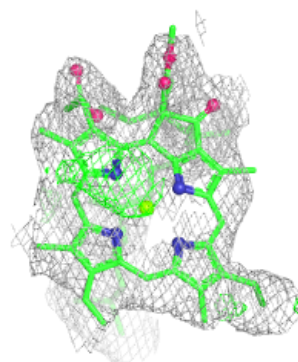
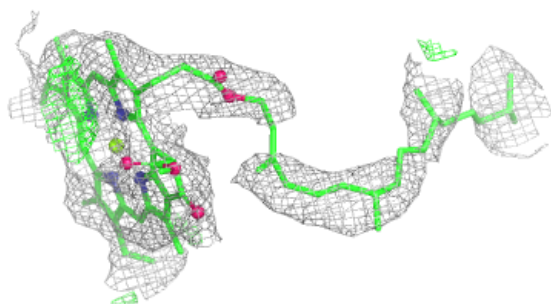
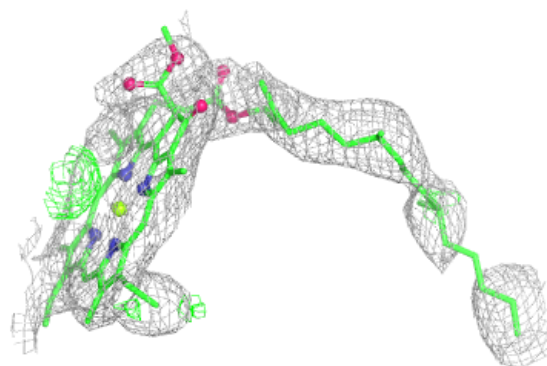


Electron density around CLA B 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

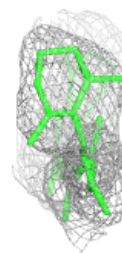
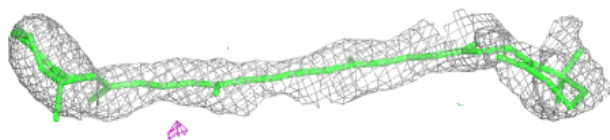
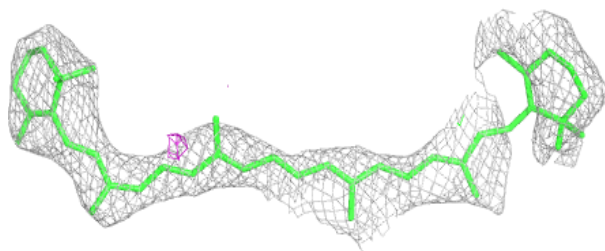
**Electron density around CLA O 1201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

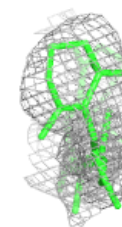
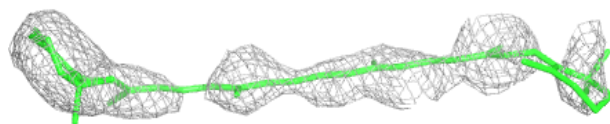
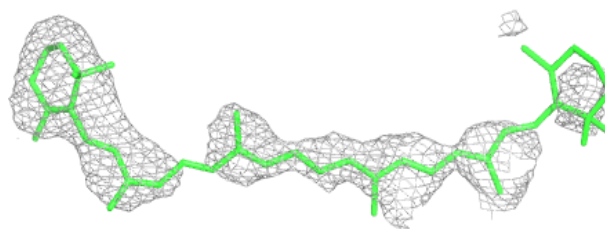


Electron density around BCR E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

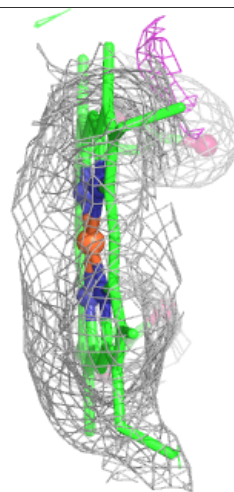
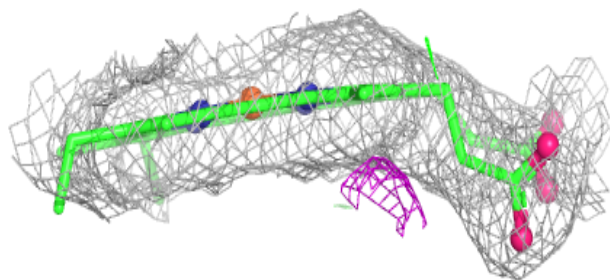
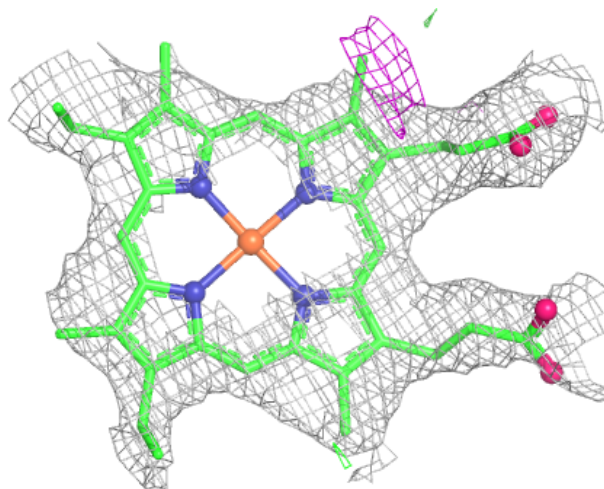
**Electron density around BCR R 1101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



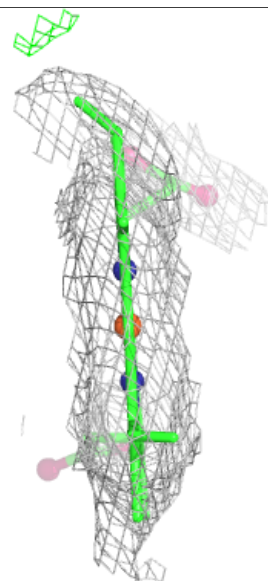
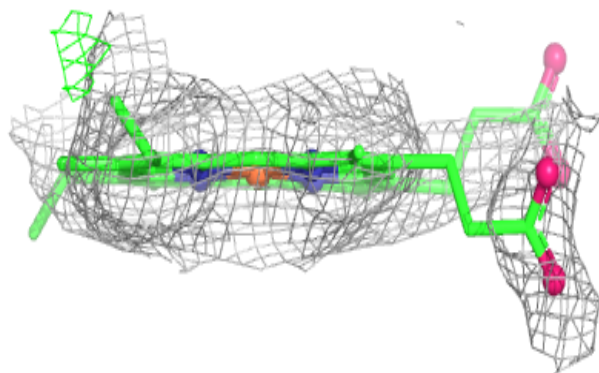
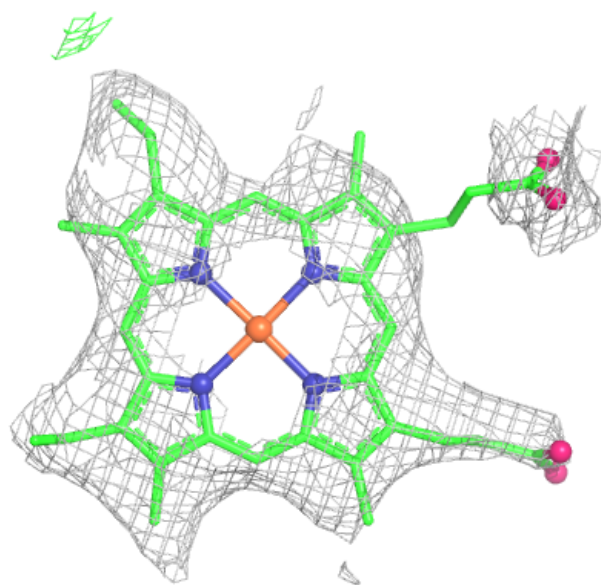
Electron density around HEC A 303:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



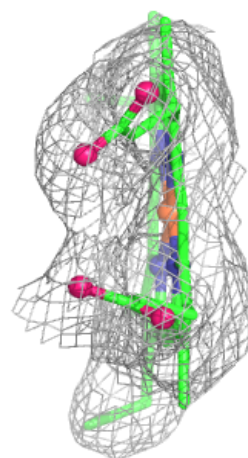
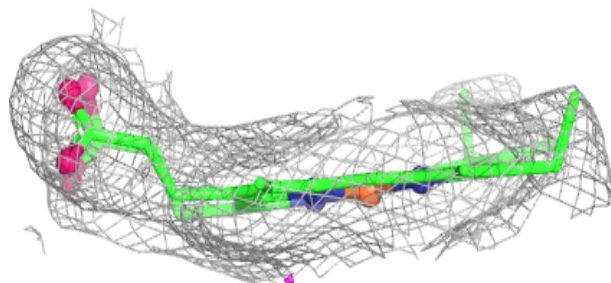
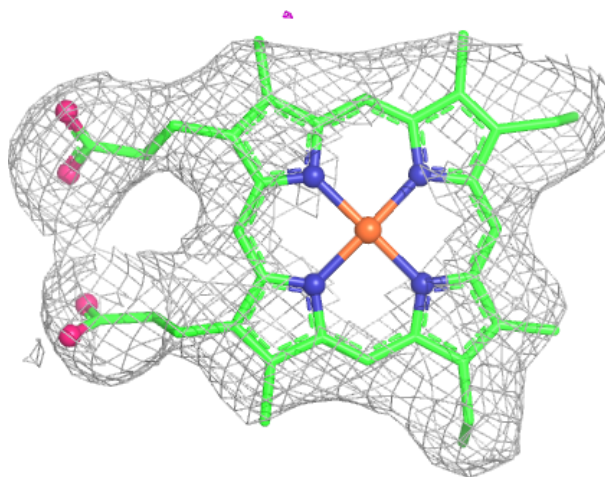
Electron density around HEC C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



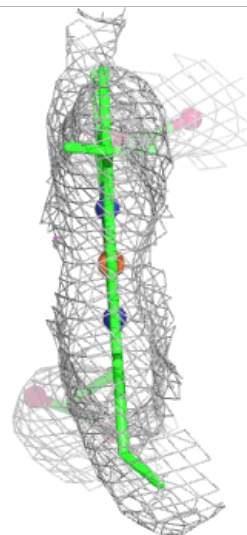
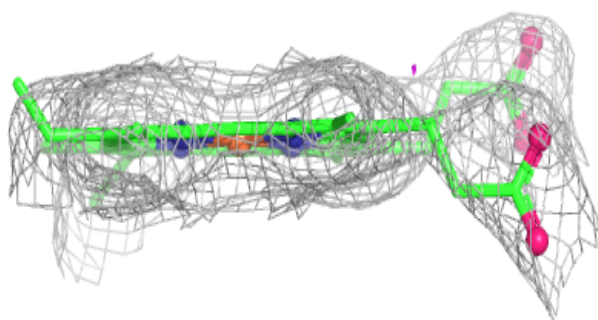
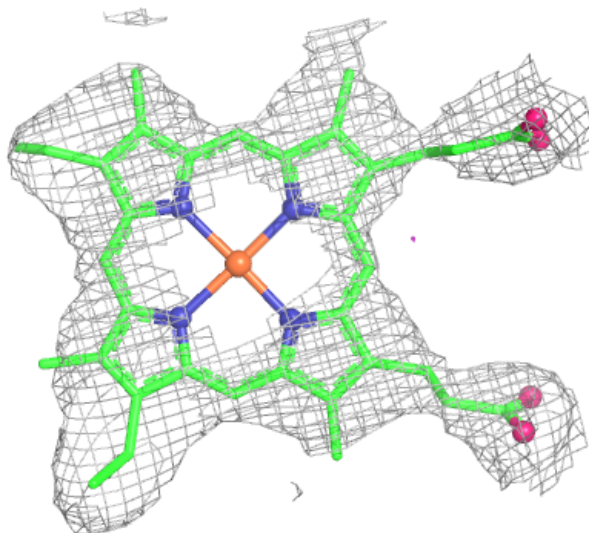
Electron density around HEC N 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



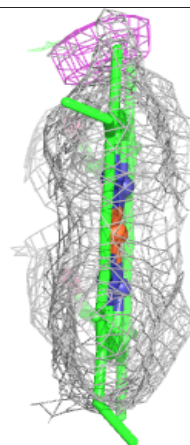
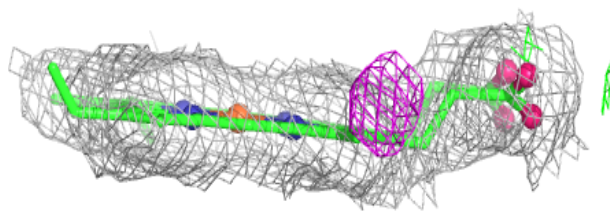
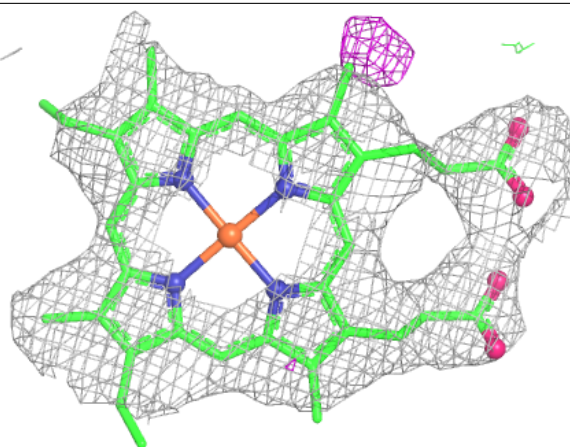
Electron density around HEC P 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



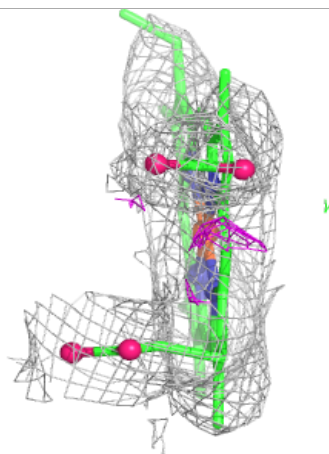
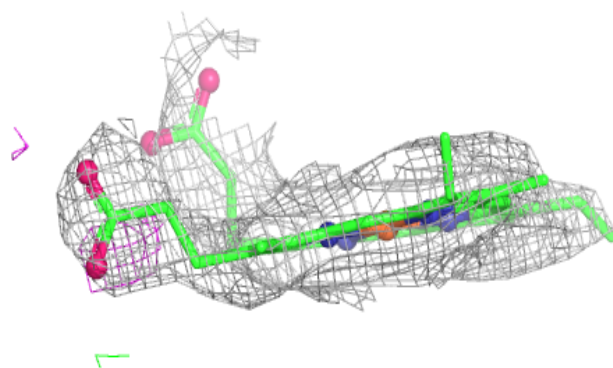
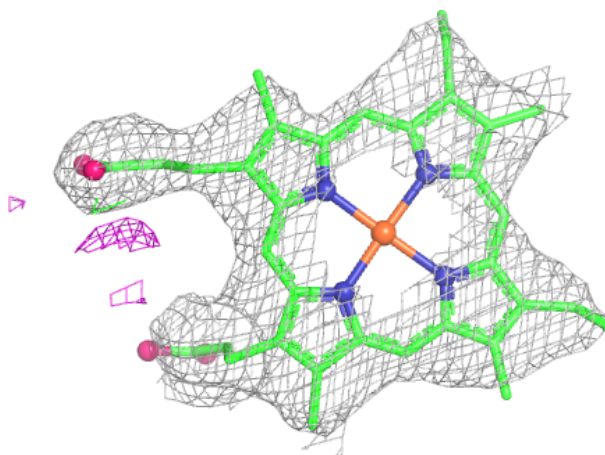
Electron density around HEM A 301:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



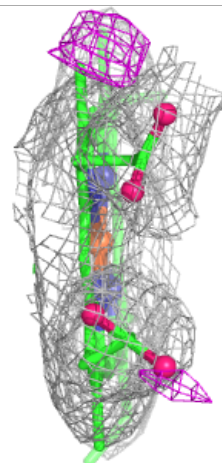
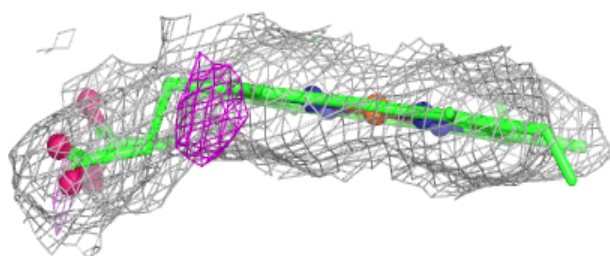
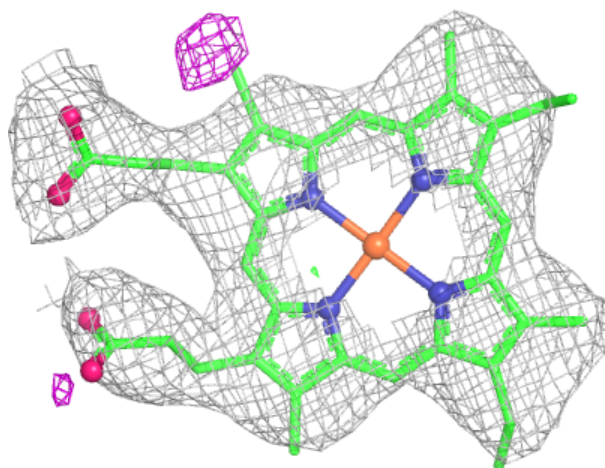
Electron density around HEM A 302:

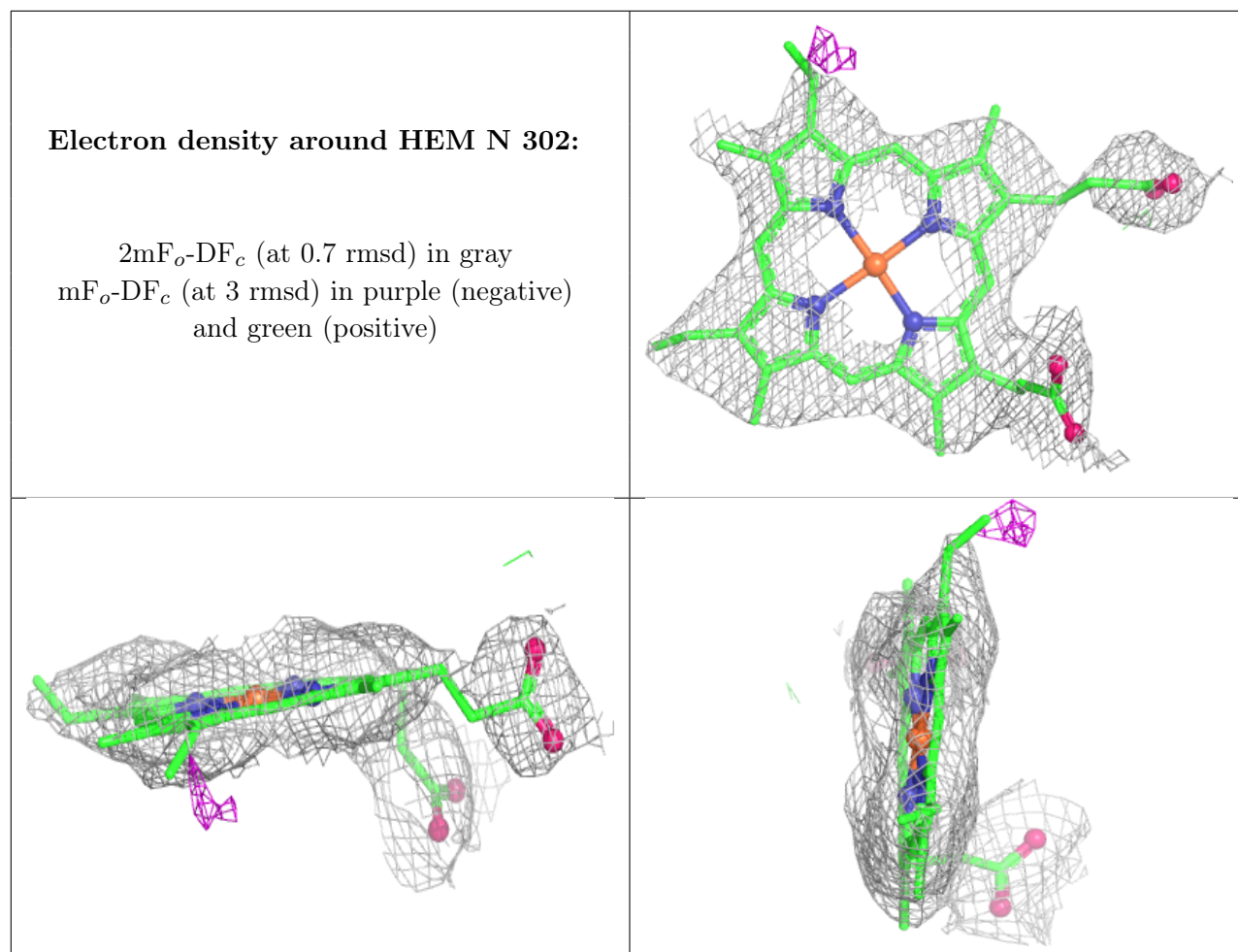
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM N 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.