



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:15 AM UTC

PDB ID : 1CX2 / pdb_00001cx2
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-
PLEXED WITH A SELECTIVE INHIBITOR, SC-558
Authors : Kurumbail, R.; Stallings, W.
Deposited on : 1996-12-17
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

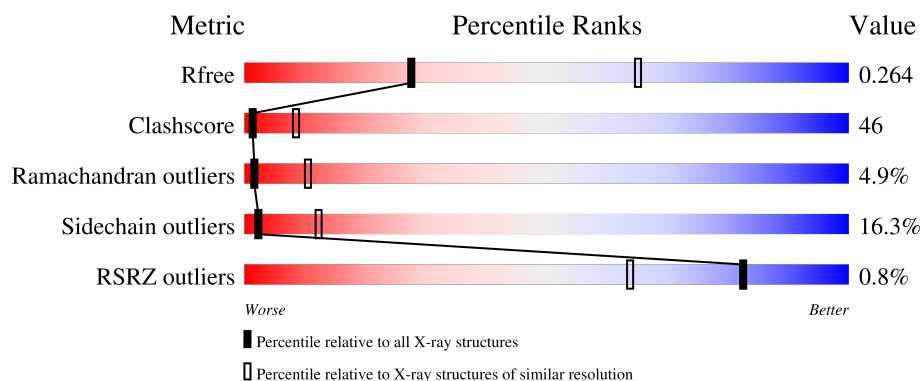
1 Overall quality at a glance

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	587	
1	B	587	
1	C	587	
1	D	587	

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
4	S58	A	701	-	-	X	-
4	S58	C	701	-	-	X	-
4	S58	D	701	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22376 atoms, of which 4040 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.

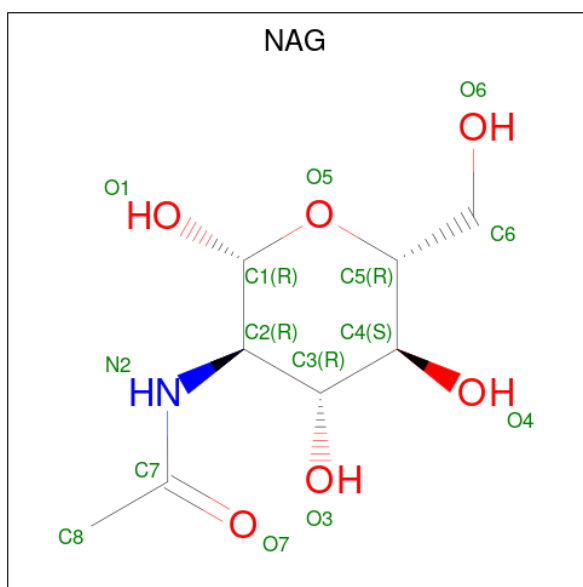
- Molecule 1 is a protein called CYCLOOXYGENASE-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	552	Total	C	H	N	O	S	0	0	0
			5439	2886	966	748	814	25			
1	B	552	Total	C	H	N	O	S	0	0	0
			5439	2886	966	748	814	25			
1	C	552	Total	C	H	N	O	S	0	0	0
			5439	2886	966	748	814	25			
1	D	552	Total	C	H	N	O	S	0	0	0
			5439	2886	966	748	814	25			

There are 8 discrepancies between the modelled and reference sequences:

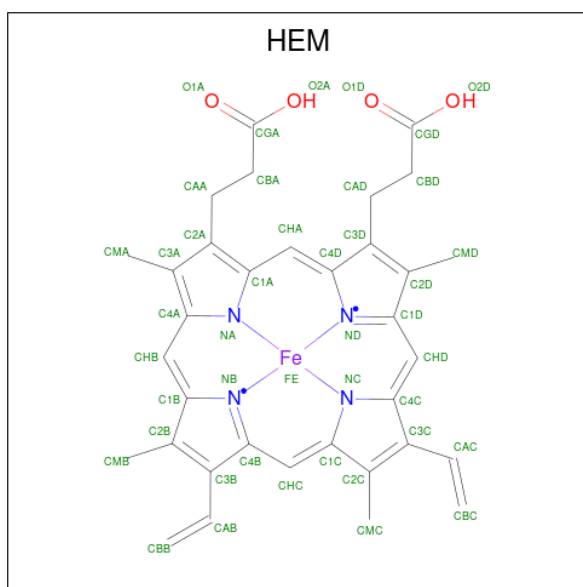
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	conflict	UNP Q05769
A	333	LYS	ARG	conflict	UNP Q05769
B	310	GLN	ASN	conflict	UNP Q05769
B	333	LYS	ARG	conflict	UNP Q05769
C	310	GLN	ASN	conflict	UNP Q05769
C	333	LYS	ARG	conflict	UNP Q05769
D	310	GLN	ASN	conflict	UNP Q05769
D	333	LYS	ARG	conflict	UNP Q05769

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



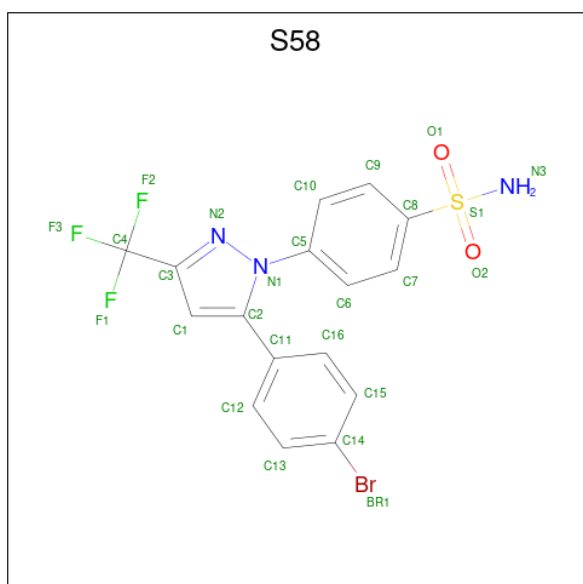
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	D	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 1-PHENYLSULFONAMIDE-3-TRIFLUOROMETHYL-5-PARABROMOPHENYLPYRAZOLE (CCD ID: S58) (formula: $\text{C}_{16}\text{H}_{11}\text{BrF}_3\text{N}_3\text{O}_2\text{S}$).

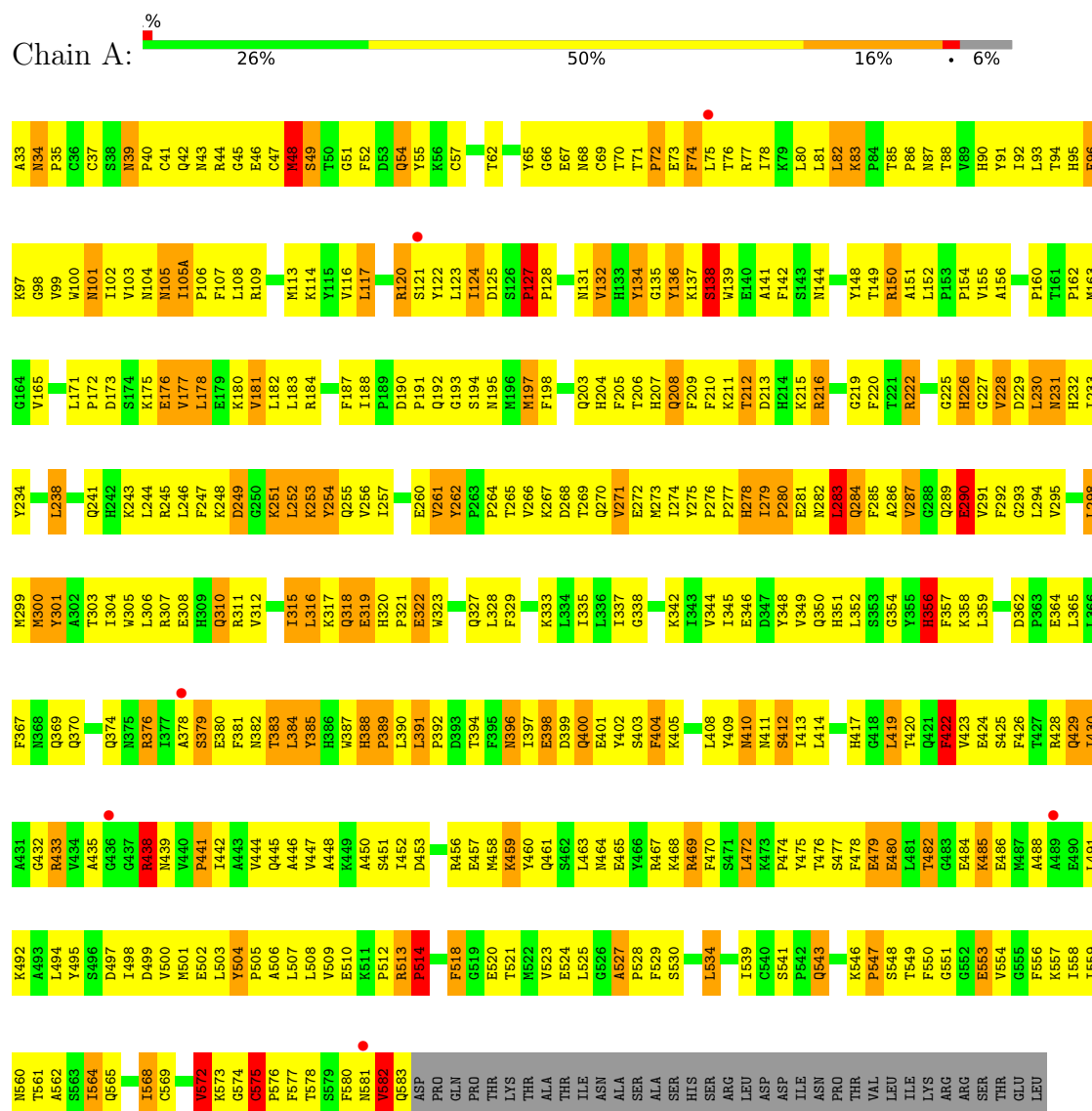


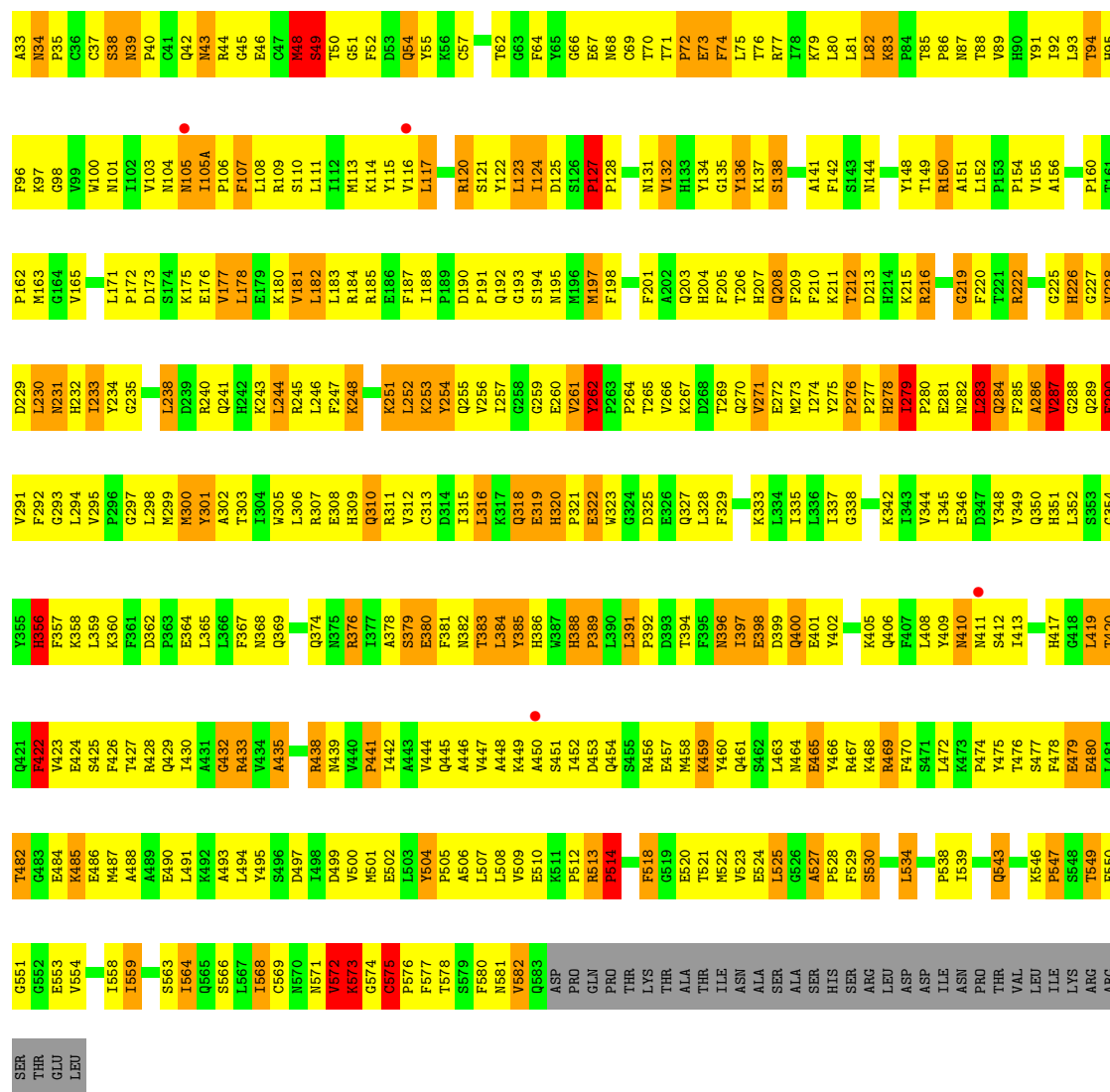
Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
4	A	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	B	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	C	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		
4	D	1	Total	Br	C	F	H	N	O	S	0	0
			28	1	16	3	2	3	2	1		

3 Residue-property plots

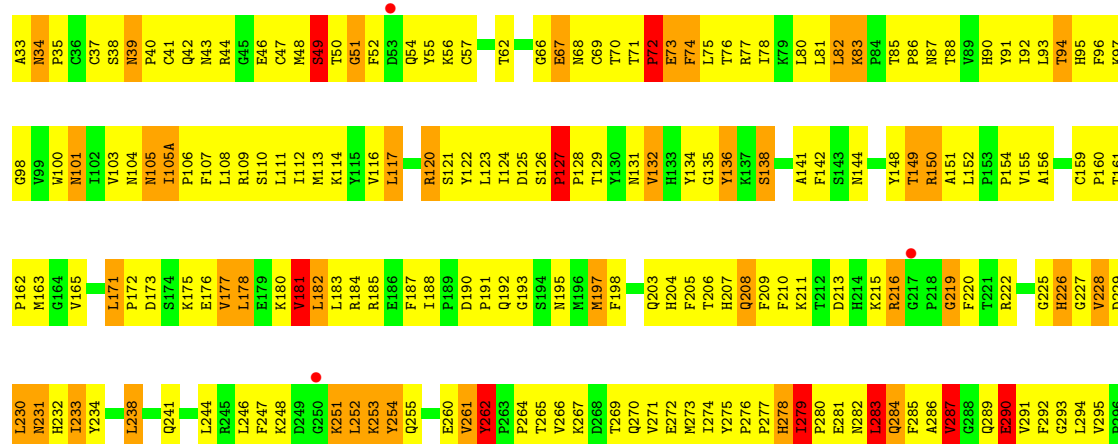
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

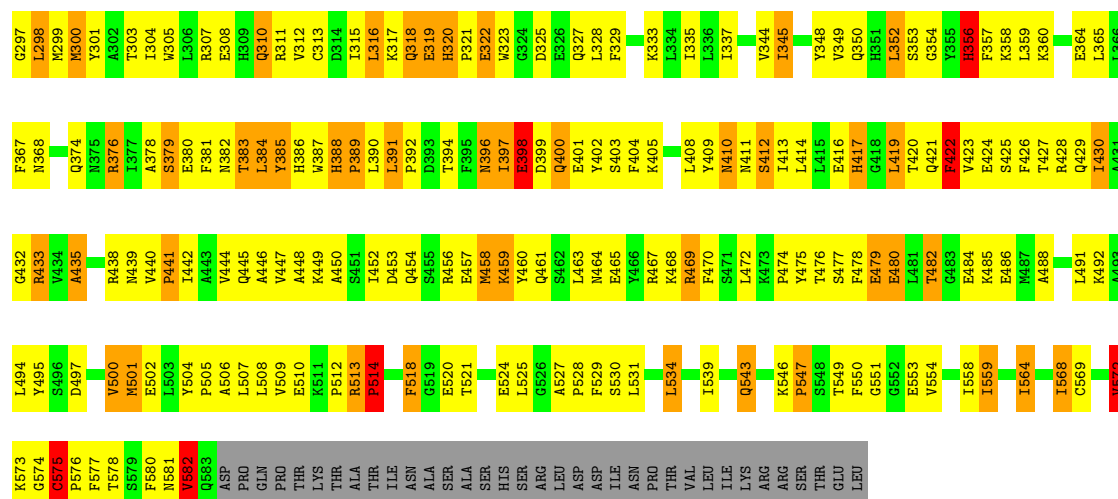
• Molecule 1: CYCLOOXYGENASE-2



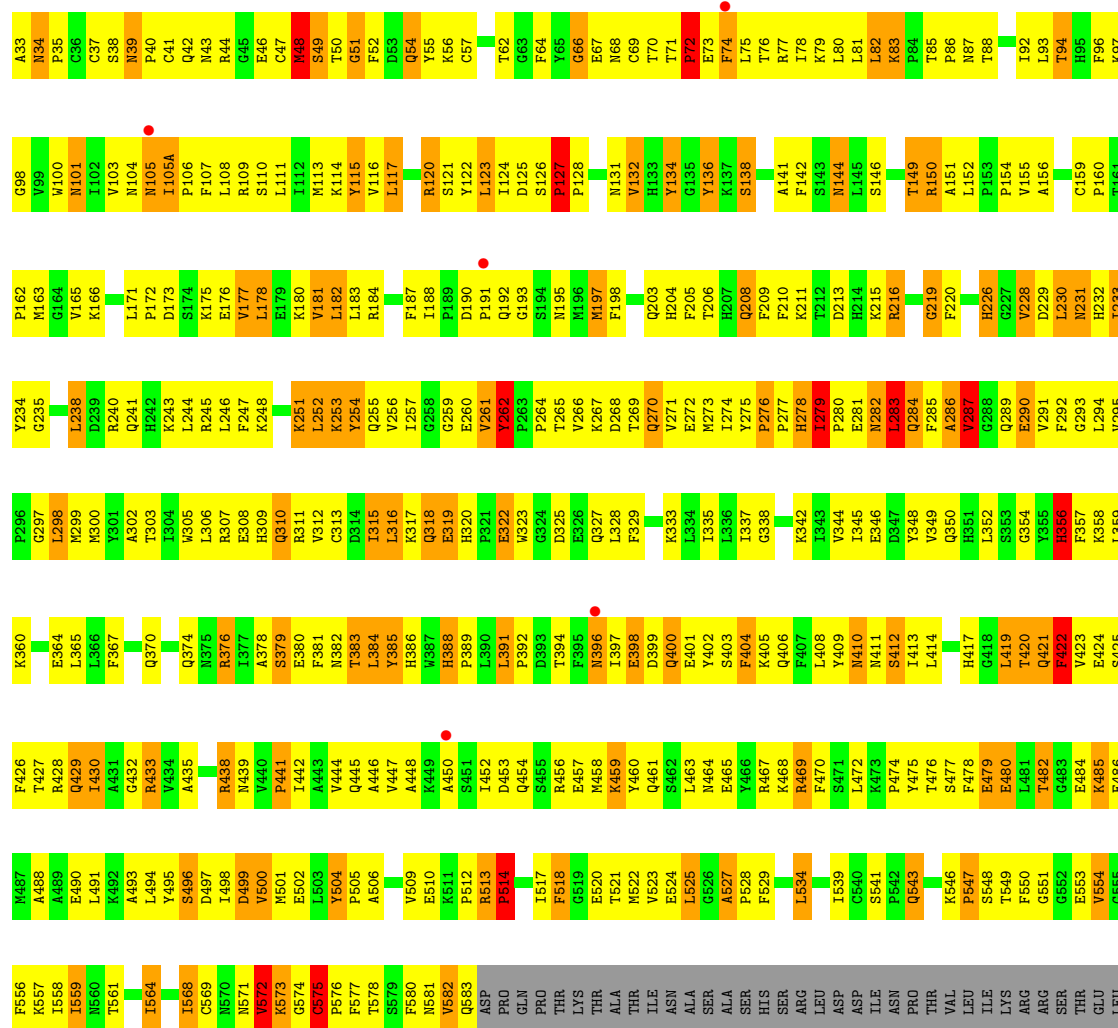


• Molecule 1: CYCLOOXYGENASE-2





- Molecule 1: CYCLOOXYGENASE-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	180.34Å 133.92Å 121.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 8.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	54.0 (8.00-3.00) 57.4 (8.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.98Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.216 , 0.218 (Not available) , 0.264	Depositor DCC
R_{free} test set	3652 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtrriage
Anisotropy	0.960	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	22376	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3164e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, S58, HEM

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	0.86	0/4600	1.33	59/6237 (0.9%)
1	B	0.86	1/4600 (0.0%)	1.34	71/6237 (1.1%)
1	C	0.87	3/4600 (0.1%)	1.34	60/6237 (1.0%)
1	D	0.86	3/4600 (0.1%)	1.35	69/6237 (1.1%)
All	All	0.86	7/18400 (0.0%)	1.34	259/24948 (1.0%)

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	A	0	3
1	B	0	2
1	C	0	2
1	D	0	4
All	All	0	11

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	559	ILE	CA-CB	6.32	1.61	1.54
1	C	279	ILE	CA-CB	5.72	1.61	1.54
1	D	430	ILE	CA-CB	5.42	1.59	1.54
1	C	345	ILE	CA-CB	5.38	1.59	1.55
1	B	397	ILE	CA-CB	5.10	1.59	1.53
1	C	501	MET	SD-CE	-5.09	1.66	1.79
1	D	197	MET	SD-CE	-5.04	1.67	1.79

All (259) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	558	ILE	N-CA-C	-15.83	99.12	111.62
1	A	558	ILE	N-CA-C	-15.22	99.59	111.62
1	B	558	ILE	N-CA-C	-14.95	99.81	111.62
1	D	558	ILE	N-CA-C	-14.49	99.10	111.56
1	D	234	TYR	N-CA-C	10.56	124.76	112.93
1	D	319	GLU	N-CA-C	-10.22	101.36	114.04
1	B	234	TYR	N-CA-C	10.15	124.30	112.93
1	D	282	ASN	N-CA-C	-9.81	101.41	113.97
1	C	282	ASN	N-CA-C	-9.66	102.00	113.88
1	A	234	TYR	N-CA-C	9.61	123.69	112.93
1	B	319	GLU	N-CA-C	-9.54	101.76	113.97
1	C	234	TYR	N-CA-C	9.54	123.61	112.93
1	A	482	THR	N-CA-C	9.37	124.04	112.23
1	C	553	GLU	N-CA-C	-9.13	100.73	112.23
1	C	319	GLU	N-CA-C	-9.01	102.86	114.04
1	A	319	GLU	N-CA-C	-8.98	102.90	114.04
1	B	279	ILE	CA-C-N	8.96	131.04	119.84
1	B	279	ILE	C-N-CA	8.96	131.04	119.84
1	B	177	VAL	N-CA-C	-8.93	104.62	112.12
1	A	553	GLU	N-CA-C	-8.92	101.00	112.23
1	D	482	THR	N-CA-C	8.90	123.44	112.23
1	C	482	THR	N-CA-C	8.89	123.43	112.23
1	B	282	ASN	N-CA-C	-8.86	102.63	113.97
1	A	282	ASN	N-CA-C	-8.79	102.71	113.97
1	C	391	LEU	N-CA-C	8.75	122.07	109.48
1	D	391	LEU	N-CA-C	8.70	122.00	109.48
1	C	238	LEU	N-CA-C	-8.68	101.38	112.93
1	C	62	THR	N-CA-C	-8.52	97.69	109.95
1	B	482	THR	N-CA-C	8.51	124.04	112.90
1	D	287	VAL	N-CA-C	8.51	127.03	109.34
1	D	513	ARG	N-CA-C	-8.48	98.05	109.84
1	A	73	GLU	N-CA-C	-8.46	96.88	110.32
1	D	279	ILE	CA-C-N	8.43	130.38	119.84
1	D	279	ILE	C-N-CA	8.43	130.38	119.84
1	B	287	VAL	N-CA-C	8.42	126.86	109.34
1	A	238	LEU	N-CA-C	-8.40	101.76	112.93
1	A	62	THR	N-CA-C	-8.38	97.89	109.95
1	C	287	VAL	N-CA-C	8.34	126.69	109.34
1	D	62	THR	N-CA-C	-8.19	98.16	109.95
1	B	73	GLU	N-CA-C	-8.11	97.42	110.32
1	B	553	GLU	N-CA-C	-8.10	102.03	112.23
1	A	287	VAL	N-CA-C	8.07	126.12	109.34
1	A	279	ILE	CA-C-N	8.06	129.92	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ILE	C-N-CA	8.06	129.92	119.84
1	D	73	GLU	N-CA-C	-8.06	97.51	110.32
1	B	391	LEU	N-CA-C	8.02	121.03	109.48
1	A	513	ARG	N-CA-C	-7.88	98.88	109.84
1	D	283	LEU	N-CA-C	-7.85	102.66	111.14
1	C	34	ASN	CA-C-N	7.85	127.56	119.56
1	C	34	ASN	C-N-CA	7.85	127.56	119.56
1	C	513	ARG	N-CA-C	-7.83	98.96	109.84
1	D	238	LEU	N-CA-C	-7.78	102.58	112.93
1	C	73	GLU	N-CA-C	-7.77	97.96	110.32
1	D	553	GLU	N-CA-C	-7.76	102.14	111.69
1	C	283	LEU	N-CA-C	-7.69	102.49	111.03
1	A	177	VAL	N-CA-C	-7.68	105.55	111.62
1	B	513	ARG	N-CA-C	-7.68	99.17	109.84
1	A	575	CYS	N-CA-C	-7.60	93.02	109.81
1	B	62	THR	N-CA-C	-7.59	97.97	109.96
1	A	391	LEU	N-CA-C	7.57	120.38	109.48
1	B	238	LEU	N-CA-C	-7.54	102.90	112.93
1	B	48	MET	N-CA-C	7.42	121.83	108.69
1	D	575	CYS	N-CA-C	-7.36	93.54	109.81
1	C	575	CYS	N-CA-C	-7.26	93.78	109.81
1	A	127	PRO	CA-C-N	7.23	127.27	119.90
1	A	127	PRO	C-N-CA	7.23	127.27	119.90
1	B	575	CYS	N-CA-C	-7.22	93.85	109.81
1	C	433	ARG	N-CA-C	-7.19	99.83	110.48
1	D	500	VAL	N-CA-C	-7.19	106.30	113.20
1	C	127	PRO	CA-C-N	7.13	127.18	119.90
1	C	127	PRO	C-N-CA	7.13	127.18	119.90
1	B	433	ARG	N-CA-C	-7.10	99.98	110.48
1	C	177	VAL	N-CA-C	-7.08	106.17	112.12
1	B	34	ASN	CA-C-N	7.07	126.77	119.56
1	B	34	ASN	C-N-CA	7.07	126.77	119.56
1	D	34	ASN	CA-C-N	7.06	126.74	119.82
1	D	34	ASN	C-N-CA	7.06	126.74	119.82
1	A	197	MET	N-CA-C	-6.96	103.62	111.14
1	C	279	ILE	CA-C-N	6.96	128.54	119.84
1	C	279	ILE	C-N-CA	6.96	128.54	119.84
1	A	433	ARG	N-CA-C	-6.96	100.19	110.48
1	A	208	GLN	N-CA-C	-6.88	102.14	112.04
1	C	388	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	C	197	MET	N-CA-C	-6.73	103.88	111.14
1	D	197	MET	N-CA-C	-6.67	103.94	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	PRO	CA-C-N	6.66	126.69	119.90
1	D	127	PRO	C-N-CA	6.66	126.69	119.90
1	B	251	LYS	N-CA-C	6.61	119.34	110.35
1	C	132	VAL	N-CA-C	6.60	118.15	110.62
1	A	388	HIS	CA-CB-CG	-6.58	107.22	113.80
1	C	572	VAL	N-CA-C	6.53	117.31	108.17
1	A	283	LEU	N-CA-C	-6.50	103.81	111.03
1	D	388	HIS	ND1-CG-CD2	6.49	112.59	106.10
1	D	177	VAL	N-CA-C	-6.48	106.50	111.62
1	A	572	VAL	N-CA-C	6.47	117.18	107.80
1	B	185	ARG	N-CA-C	-6.42	101.77	111.34
1	B	182	LEU	N-CA-C	6.39	121.74	113.88
1	B	127	PRO	CA-C-N	6.38	126.41	119.90
1	B	127	PRO	C-N-CA	6.38	126.41	119.90
1	C	440	VAL	N-CA-C	6.36	114.18	107.76
1	B	148	TYR	N-CA-C	-6.35	99.05	109.40
1	C	500	VAL	N-CA-C	-6.32	106.97	113.10
1	B	208	GLN	N-CA-C	-6.27	103.74	112.45
1	B	197	MET	N-CA-C	-6.26	104.38	111.14
1	D	388	HIS	CA-CB-CG	-6.24	107.56	113.80
1	A	34	ASN	CA-C-N	6.24	127.64	119.84
1	A	34	ASN	C-N-CA	6.24	127.64	119.84
1	B	320	HIS	CA-C-N	6.21	125.91	119.82
1	B	320	HIS	C-N-CA	6.21	125.91	119.82
1	A	148	TYR	N-CA-C	-6.20	99.30	109.40
1	D	433	ARG	N-CA-C	-6.18	101.33	110.48
1	B	559	ILE	N-CA-C	-6.16	104.50	110.42
1	B	572	VAL	N-CA-C	6.15	117.16	108.36
1	D	572	VAL	N-CA-C	6.15	117.15	108.36
1	B	577	PHE	N-CA-C	-6.15	101.83	110.50
1	D	527	ALA	CA-C-N	6.14	125.36	118.97
1	D	527	ALA	C-N-CA	6.14	125.36	118.97
1	C	148	TYR	N-CA-C	-6.13	99.40	109.40
1	A	132	VAL	N-CA-C	6.10	117.58	110.62
1	B	422	PHE	N-CA-C	-6.10	97.81	110.80
1	D	388	HIS	CB-CG-CD2	-6.09	123.29	131.20
1	B	262	TYR	CA-C-N	6.08	126.64	120.38
1	B	262	TYR	C-N-CA	6.08	126.64	120.38
1	C	422	PHE	N-CA-C	-6.05	97.92	110.80
1	D	48	MET	N-CA-C	5.99	118.89	108.76
1	A	182	LEU	N-CA-C	5.98	121.24	113.88
1	D	370	GLN	N-CA-C	-5.97	101.00	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	PRO	N-CA-C	5.96	120.62	111.57
1	B	549	THR	N-CA-C	-5.95	104.87	111.71
1	A	527	ALA	CA-C-N	5.95	125.16	118.97
1	A	527	ALA	C-N-CA	5.95	125.16	118.97
1	B	138	SER	N-CA-C	5.95	123.46	110.80
1	C	233	ILE	CB-CA-C	-5.91	104.49	111.94
1	D	208	GLN	N-CA-C	-5.90	103.54	112.04
1	A	124	ILE	N-CA-C	5.90	116.43	108.17
1	B	571	ASN	N-CA-C	5.89	121.51	113.97
1	D	121	SER	N-CA-C	5.88	120.15	112.92
1	C	149	THR	N-CA-C	-5.87	102.91	110.19
1	B	283	LEU	N-CA-C	-5.87	103.67	111.24
1	B	410	ASN	N-CA-C	5.86	118.79	109.24
1	C	388	HIS	CA-CB-CG	-5.86	107.94	113.80
1	D	410	ASN	N-CA-C	5.85	118.78	109.24
1	D	561	THR	N-CA-C	-5.84	105.52	114.16
1	D	286	ALA	N-CA-C	5.84	120.45	112.04
1	C	388	HIS	ND1-CG-CD2	5.84	111.94	106.10
1	B	121	SER	N-CA-C	5.83	120.09	112.92
1	B	504	TYR	N-CA-C	5.79	120.37	112.55
1	D	577	PHE	N-CA-C	-5.79	102.34	110.50
1	A	315	ILE	N-CA-C	-5.77	104.88	110.42
1	C	124	ILE	N-CA-C	5.77	116.25	108.17
1	D	356	HIS	N-CA-C	-5.76	98.52	110.80
1	D	72	PRO	N-CA-C	5.75	120.31	111.57
1	A	388	HIS	ND1-CG-CD2	5.74	111.83	106.10
1	D	422	PHE	N-CA-C	-5.73	98.59	110.80
1	C	290	GLU	N-CA-C	5.71	122.97	110.80
1	A	410	ASN	N-CA-C	5.70	118.53	109.24
1	D	276	PRO	CA-C-N	5.70	126.96	119.84
1	D	276	PRO	C-N-CA	5.70	126.96	119.84
1	C	251	LYS	N-CA-C	5.69	118.52	110.50
1	C	262	TYR	CA-C-N	5.68	126.23	120.38
1	C	262	TYR	C-N-CA	5.68	126.23	120.38
1	D	182	LEU	N-CA-C	5.67	120.85	113.88
1	D	132	VAL	N-CA-C	5.65	117.06	110.62
1	A	498	ILE	N-CA-C	-5.65	105.02	110.72
1	C	577	PHE	N-CA-C	-5.63	102.55	110.50
1	C	559	ILE	N-CA-C	-5.63	105.02	110.42
1	A	422	PHE	N-CA-C	-5.61	98.86	110.80
1	C	138	SER	N-CA-C	5.58	122.69	110.80
1	B	286	ALA	N-CA-C	5.57	120.06	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	GLY	N-CA-C	-5.56	107.69	114.92
1	A	121	SER	N-CA-C	5.56	119.76	112.92
1	C	410	ASN	N-CA-C	5.53	118.25	109.24
1	A	438	ARG	N-CA-C	5.51	118.80	111.30
1	B	396	ASN	N-CA-C	5.51	118.34	107.98
1	C	182	LEU	N-CA-C	5.51	120.66	113.88
1	D	262	TYR	CA-C-N	5.50	126.04	120.38
1	D	262	TYR	C-N-CA	5.50	126.04	120.38
1	B	256	VAL	N-CA-C	5.49	116.01	107.99
1	C	135	GLY	N-CA-C	-5.49	107.10	115.66
1	A	504	TYR	N-CA-C	5.47	119.94	112.55
1	D	66	GLY	N-CA-C	-5.47	105.86	112.48
1	C	161	THR	CA-C-N	5.47	125.14	119.56
1	C	161	THR	C-N-CA	5.47	125.14	119.56
1	D	256	VAL	N-CA-C	5.46	115.96	107.99
1	D	315	ILE	N-CA-C	-5.46	105.18	110.42
1	A	138	SER	N-CA-C	5.45	122.41	110.80
1	C	208	GLN	N-CA-C	-5.43	104.22	112.04
1	D	149	THR	N-CA-C	-5.42	103.47	110.19
1	D	388	HIS	CG-CD2-NE2	-5.41	101.79	107.20
1	B	233	ILE	CB-CA-C	-5.39	105.15	111.94
1	A	176	GLU	N-CA-C	-5.38	106.78	113.19
1	A	561	THR	N-CA-C	-5.38	104.62	113.50
1	A	48	MET	N-CA-C	5.38	118.21	108.69
1	D	571	ASN	N-CA-C	5.37	120.85	113.97
1	A	404	PHE	N-CA-C	-5.37	104.67	111.11
1	C	417	HIS	N-CA-C	5.37	117.13	111.28
1	D	251	LYS	N-CA-C	5.36	118.06	110.50
1	B	219	GLY	N-CA-C	-5.36	108.31	114.69
1	B	222	ARG	N-CA-C	-5.36	105.42	113.89
1	A	251	LYS	N-CA-C	5.34	118.04	110.50
1	B	132	VAL	N-CA-C	5.34	116.71	110.62
1	C	388	HIS	CG-CD2-NE2	-5.34	101.86	107.20
1	D	559	ILE	N-CA-C	-5.30	104.79	110.36
1	A	96	PHE	N-CA-C	5.30	118.75	111.54
1	C	356	HIS	N-CA-C	-5.30	99.51	110.80
1	B	290	GLU	N-CA-C	5.28	122.05	110.80
1	C	320	HIS	CA-C-N	5.26	124.98	119.82
1	C	320	HIS	C-N-CA	5.26	124.98	119.82
1	A	135	GLY	N-CA-C	-5.25	107.48	115.66
1	A	290	GLU	N-CA-C	5.24	121.97	110.80
1	B	435	ALA	N-CA-C	5.24	117.25	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	HIS	CB-CG-CD2	-5.24	124.39	131.20
1	B	527	ALA	CA-C-N	5.24	124.42	118.97
1	B	527	ALA	C-N-CA	5.24	124.42	118.97
1	D	101	ASN	N-CA-C	-5.24	105.48	111.14
1	D	138	SER	N-CA-C	5.23	121.94	110.80
1	C	435	ALA	N-CA-C	5.21	117.22	110.65
1	D	290	GLU	N-CA-C	5.21	121.90	110.80
1	B	485	LYS	N-CA-C	5.20	119.75	113.41
1	A	222	ARG	N-CA-C	-5.19	105.69	113.89
1	B	356	HIS	N-CA-C	-5.19	99.75	110.80
1	C	121	SER	N-CA-C	5.18	119.30	112.92
1	D	396	ASN	N-CA-C	5.18	117.72	107.98
1	A	388	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	D	233	ILE	CB-CA-C	-5.16	105.16	111.92
1	A	472	LEU	N-CA-C	-5.15	101.71	109.85
1	B	135	GLY	N-CA-C	-5.15	107.63	115.66
1	C	72	PRO	N-CA-C	5.13	119.37	111.57
1	B	276	PRO	CA-C-N	5.13	126.25	119.84
1	B	276	PRO	C-N-CA	5.13	126.25	119.84
1	B	124	ILE	N-CA-C	5.12	115.34	108.17
1	B	43	ASN	N-CA-C	5.12	118.82	112.47
1	D	219	GLY	N-CA-C	-5.12	107.92	114.37
1	D	504	TYR	N-CA-C	5.12	119.46	112.55
1	B	465	GLU	N-CA-C	-5.12	105.70	111.28
1	A	396	ASN	N-CA-C	5.12	117.60	107.98
1	A	256	VAL	N-CA-C	5.11	115.45	107.99
1	A	356	HIS	N-CA-C	-5.10	99.94	110.80
1	D	404	PHE	N-CA-C	-5.09	105.00	111.11
1	B	89	VAL	N-CA-C	-5.08	105.89	110.82
1	A	252	LEU	N-CA-C	-5.08	102.24	110.32
1	B	302	ALA	N-CA-C	-5.08	105.66	111.14
1	D	279	ILE	N-CA-C	-5.08	103.43	108.96
1	C	181	VAL	N-CA-C	5.07	119.46	113.22
1	D	421	GLN	N-CA-CB	5.07	116.72	110.53
1	A	370	GLN	N-CA-C	-5.06	102.37	109.96
1	B	432	GLY	N-CA-C	5.06	117.75	111.93
1	B	388	HIS	CA-CB-CG	-5.06	108.74	113.80
1	B	244	LEU	N-CA-C	-5.05	107.80	114.31
1	C	129	THR	N-CA-C	-5.05	101.53	109.50
1	D	252	LEU	N-CA-C	-5.05	102.30	110.32
1	D	302	ALA	N-CA-C	-5.04	105.86	111.36
1	D	270	GLN	N-CA-C	5.04	121.53	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	573	LYS	N-CA-C	5.04	121.53	110.80
1	B	573	LYS	N-CA-C	5.03	121.51	110.80
1	C	101	ASN	N-CA-C	-5.03	105.71	111.14
1	A	101	ASN	N-CA-C	-5.01	105.73	111.14
1	B	227	GLY	N-CA-C	5.01	117.37	110.56
1	A	72	PRO	N-CA-C	5.00	120.13	111.77

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	TYR	Sidechain
1	A	262	TYR	Sidechain
1	A	348	TYR	Sidechain
1	B	262	TYR	Sidechain
1	B	348	TYR	Sidechain
1	C	262	TYR	Sidechain
1	C	348	TYR	Sidechain
1	D	115	TYR	Sidechain
1	D	134	TYR	Sidechain
1	D	262	TYR	Sidechain
1	D	348	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	4473	966	4375	426	0
1	B	4473	966	4375	434	0
1	C	4473	966	4375	408	0
1	D	4473	966	4375	413	0
2	A	42	42	39	1	0
2	B	42	42	39	6	0
2	C	42	42	39	1	0
2	D	42	42	39	6	0
3	A	43	0	30	3	0
3	B	43	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	43	0	30	7	0
3	D	43	0	30	5	0
4	A	26	2	11	9	0
4	B	26	2	11	5	0
4	C	26	2	11	11	0
4	D	26	2	11	7	0
All	All	18336	4040	17820	1645	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 46.

All (1645) 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)
1:C:52:PHE:N	1:D:322:GLU:HG2	1.80	0.96
1:C:322:GLU:HG2	1:D:52:PHE:N	1.83	0.93
1:A:275:TYR:CE2	1:A:284:GLN:HA	2.04	0.93
1:C:184:ARG:HA	1:C:438:ARG:O	1.71	0.89
1:C:275:TYR:CE2	1:C:284:GLN:HA	2.07	0.89
1:D:279:ILE:HG12	1:D:283:LEU:HD23	1.55	0.89
1:D:391:LEU:HD21	3:D:682:HEM:HAB	1.53	0.88
1:A:479:GLU:HG2	1:A:485:LYS:HE3	1.55	0.87
1:A:322:GLU:HG2	1:B:52:PHE:N	1.90	0.86
1:A:281:GLU:HA	1:A:284:GLN:HG3	1.55	0.86
1:C:453:ASP:HA	1:C:456:ARG:HD2	1.57	0.86
1:D:184:ARG:HA	1:D:438:ARG:O	1.75	0.85
1:C:322:GLU:HG2	1:D:52:PHE:H	1.40	0.84
1:D:342:LYS:HD2	1:D:346:GLU:HG3	1.57	0.84
1:B:134:TYR:HD1	1:B:136:TYR:HE1	1.24	0.83
1:B:396:ASN:HB2	1:B:401:GLU:HG2	1.59	0.83
1:B:275:TYR:CE2	1:B:284:GLN:HA	2.13	0.83
1:C:479:GLU:HG2	1:C:485:LYS:CE	2.08	0.83
1:D:275:TYR:CE2	1:D:284:GLN:HA	2.14	0.82
1:C:198:PHE:HZ	1:C:352:LEU:HD12	1.44	0.82
1:B:276:PRO:HD2	1:B:279:ILE:HD13	1.58	0.82
1:A:479:GLU:HG2	1:A:485:LYS:CE	2.09	0.82
1:C:52:PHE:H	1:D:322:GLU:HG2	1.43	0.82
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.15	0.81
1:B:435:ALA:HB3	1:B:518:PHE:HA	1.62	0.81
1:B:184:ARG:HA	1:B:438:ARG:O	1.79	0.81
1:C:405:LYS:H	1:C:405:LYS:HD2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:THR:HG21	1:D:385:TYR:CE1	2.15	0.81
1:B:323:TRP:HH2	1:B:551:GLY:HA2	1.46	0.81
1:B:435:ALA:O	1:B:512:PRO:HG3	1.80	0.81
1:D:134:TYR:HD1	1:D:136:TYR:HE1	1.28	0.81
1:D:208:GLN:HB3	1:D:232:HIS:CD2	2.16	0.81
1:B:345:ILE:HD11	1:B:534:LEU:HD23	1.62	0.80
1:D:276:PRO:HD2	1:D:279:ILE:HD13	1.62	0.80
1:C:279:ILE:HG23	1:C:283:LEU:HB3	1.60	0.80
1:C:206:THR:HG21	1:C:385:TYR:CE1	2.16	0.80
1:B:134:TYR:HD1	1:B:136:TYR:CE1	1.99	0.80
1:C:345:ILE:HD11	1:C:534:LEU:HD23	1.65	0.79
1:D:323:TRP:HH2	1:D:551:GLY:HA2	1.47	0.79
1:B:134:TYR:CD1	1:B:136:TYR:HE1	2.01	0.79
1:D:458:MET:HE3	1:D:460:TYR:HE1	1.47	0.79
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.63	0.79
1:A:197:MET:HE1	1:A:423:VAL:HA	1.63	0.79
1:D:479:GLU:HG2	1:D:485:LYS:HE3	1.64	0.79
1:B:120:ARG:HD3	1:B:527:ALA:HB1	1.64	0.78
1:B:406:GLN:HG2	2:B:681:NAG:O7	1.83	0.78
1:C:134:TYR:HD1	1:C:136:TYR:HE1	1.31	0.78
1:A:453:ASP:HA	1:A:456:ARG:HD2	1.64	0.78
1:D:396:ASN:HB2	1:D:401:GLU:HG2	1.65	0.78
1:A:206:THR:HG21	1:A:385:TYR:CE1	2.19	0.78
1:D:318:GLN:NE2	1:D:318:GLN:HA	1.98	0.78
1:D:435:ALA:O	1:D:512:PRO:HG3	1.83	0.78
1:C:197:MET:HE1	1:C:423:VAL:HA	1.65	0.78
1:C:323:TRP:HH2	1:C:551:GLY:HA2	1.49	0.77
1:C:120:ARG:HD3	1:C:527:ALA:HB1	1.66	0.77
1:D:198:PHE:HZ	1:D:352:LEU:HD12	1.50	0.77
1:A:279:ILE:HG23	1:A:283:LEU:HB3	1.64	0.77
1:D:435:ALA:HB3	1:D:518:PHE:HA	1.66	0.77
1:B:197:MET:HE1	1:B:423:VAL:HA	1.67	0.77
1:A:184:ARG:HA	1:A:438:ARG:O	1.85	0.77
1:A:345:ILE:HD11	1:A:534:LEU:HD23	1.66	0.77
1:D:345:ILE:HD11	1:D:534:LEU:HD23	1.67	0.77
1:C:281:GLU:HA	1:C:284:GLN:HG3	1.66	0.76
1:A:120:ARG:HD3	1:A:527:ALA:HB1	1.67	0.76
1:D:453:ASP:HA	1:D:456:ARG:HD2	1.66	0.76
1:D:385:TYR:CE2	4:D:701:S58:BR1	2.94	0.76
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.21	0.76
1:D:120:ARG:HD3	1:D:527:ALA:HB1	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PHE:N	1:B:322:GLU:HG2	2.00	0.75
1:A:323:TRP:HH2	1:A:551:GLY:HA2	1.50	0.75
1:D:40:PRO:HA	2:D:661:NAG:H61	1.66	0.75
1:C:134:TYR:HD1	1:C:136:TYR:CE1	2.04	0.75
1:B:208:GLN:HB3	1:B:232:HIS:CD2	2.20	0.75
1:B:198:PHE:HZ	1:B:352:LEU:HD12	1.49	0.75
1:C:479:GLU:HG2	1:C:485:LYS:HE3	1.67	0.75
1:C:497:ASP:HB3	1:C:500:VAL:HG23	1.69	0.75
1:A:435:ALA:O	1:A:512:PRO:HG3	1.87	0.75
1:A:405:LYS:H	1:A:405:LYS:HD2	1.52	0.74
1:B:405:LYS:H	1:B:405:LYS:HD2	1.52	0.74
1:C:109:ARG:HG3	1:C:357:PHE:CE1	2.22	0.74
1:D:134:TYR:HD1	1:D:136:TYR:CE1	2.04	0.74
1:D:210:PHE:CE1	1:D:382:ASN:HA	2.23	0.74
1:D:208:GLN:HB3	1:D:232:HIS:HD2	1.52	0.74
1:A:109:ARG:HG3	1:A:357:PHE:CE1	2.22	0.74
1:B:478:PHE:CZ	1:B:495:TYR:HB2	2.23	0.74
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.22	0.74
1:C:424:GLU:HA	1:C:428:ARG:HH11	1.53	0.74
1:A:160:PRO:HG3	1:A:165:VAL:HG12	1.69	0.74
1:A:198:PHE:HZ	1:A:352:LEU:HD12	1.51	0.74
1:A:281:GLU:HG2	1:A:284:GLN:HE21	1.53	0.74
1:B:279:ILE:HG12	1:B:283:LEU:HD23	1.68	0.74
1:B:479:GLU:HG2	1:B:485:LYS:HE3	1.70	0.74
1:A:344:VAL:O	1:A:349:VAL:HG23	1.89	0.73
1:C:208:GLN:HB3	1:C:232:HIS:CD2	2.22	0.73
1:A:134:TYR:HD1	1:A:136:TYR:HE1	1.36	0.73
1:B:479:GLU:HG2	1:B:485:LYS:CE	2.18	0.73
1:C:435:ALA:HB3	1:C:518:PHE:HA	1.68	0.73
1:D:134:TYR:CD1	1:D:136:TYR:HE1	2.05	0.73
1:D:97:LYS:HB2	1:D:356:HIS:NE2	2.02	0.73
1:C:276:PRO:HD2	1:C:279:ILE:HD13	1.69	0.73
1:C:424:GLU:HA	1:C:428:ARG:NH1	2.04	0.73
1:D:197:MET:HE1	1:D:423:VAL:HA	1.70	0.73
1:C:478:PHE:CZ	1:C:495:TYR:HB2	2.23	0.72
1:D:279:ILE:HG23	1:D:283:LEU:HB3	1.70	0.72
1:D:458:MET:HE3	1:D:460:TYR:CE1	2.25	0.72
1:C:160:PRO:HG3	1:C:165:VAL:HG12	1.71	0.72
1:A:478:PHE:CZ	1:A:495:TYR:HB2	2.25	0.72
1:D:479:GLU:HG2	1:D:485:LYS:CE	2.20	0.72
1:B:206:THR:HB	1:B:210:PHE:CD2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:ILE:CG1	1:D:283:LEU:HD23	2.19	0.72
1:C:344:VAL:O	1:C:349:VAL:HG23	1.89	0.72
1:D:344:VAL:O	1:D:349:VAL:HG23	1.90	0.72
1:C:352:LEU:HD23	4:C:701:S58:C10	2.20	0.71
1:D:206:THR:HB	1:D:210:PHE:CD2	2.24	0.71
1:C:134:TYR:CD1	1:C:136:TYR:HE1	2.08	0.71
1:B:295:VAL:HG22	1:B:408:LEU:HD22	1.73	0.71
1:B:453:ASP:HA	1:B:456:ARG:HD2	1.71	0.71
1:C:50:THR:HG21	1:C:56:LYS:HG3	1.72	0.71
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.26	0.71
1:A:396:ASN:HB2	1:A:401:GLU:HG2	1.73	0.70
1:A:318:GLN:HA	1:A:318:GLN:NE2	2.05	0.70
1:D:109:ARG:HG3	1:D:357:PHE:CE1	2.26	0.70
1:C:352:LEU:HD23	4:C:701:S58:H10	1.73	0.70
1:B:406:GLN:HA	2:B:681:NAG:C7	2.20	0.70
1:B:344:VAL:O	1:B:349:VAL:HG23	1.91	0.70
1:A:206:THR:HB	1:A:210:PHE:CD2	2.27	0.70
1:B:497:ASP:HB3	1:B:500:VAL:HG23	1.73	0.70
1:B:210:PHE:CE1	1:B:382:ASN:HA	2.26	0.70
1:A:134:TYR:HD1	1:A:136:TYR:CE1	2.09	0.69
1:D:264:PRO:HG2	1:D:286:ALA:HB3	1.73	0.69
1:D:464:ASN:ND2	1:D:475:TYR:H	1.89	0.69
1:A:295:VAL:HG22	1:A:408:LEU:HD22	1.74	0.69
1:A:35:PRO:HD3	1:A:52:PHE:O	1.93	0.69
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.28	0.69
1:A:435:ALA:HB3	1:A:518:PHE:HA	1.72	0.69
1:D:527:ALA:HB3	1:D:528:PRO:HD3	1.74	0.69
1:B:180:LYS:HD2	1:B:490:GLU:OE2	1.92	0.69
1:A:191:PRO:HG3	1:A:433:ARG:CZ	2.23	0.69
1:C:39:ASN:N	1:C:40:PRO:HD3	2.08	0.69
1:B:98:GLY:O	1:B:101:ASN:HB2	1.93	0.69
1:A:150:ARG:NH2	1:A:154:PRO:HB3	2.08	0.69
1:A:251:LYS:HG2	1:A:310:GLN:HG3	1.76	0.69
1:B:419:LEU:HB3	1:B:572:VAL:HG13	1.75	0.69
1:B:150:ARG:NH2	1:B:154:PRO:HB3	2.08	0.68
1:C:97:LYS:HB2	1:C:356:HIS:NE2	2.07	0.68
1:D:246:LEU:HG	1:D:248:LYS:HB2	1.74	0.68
1:C:173:ASP:O	1:C:177:VAL:HG23	1.94	0.68
1:C:279:ILE:HG12	1:C:283:LEU:HD23	1.76	0.68
1:A:564:ILE:HG13	1:A:580:PHE:CZ	2.28	0.68
1:B:113:MET:SD	1:B:360:LYS:N	2.64	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PHE:CE1	1:C:382:ASN:HA	2.29	0.68
1:A:419:LEU:HB3	1:A:572:VAL:HG13	1.74	0.68
1:D:333:LYS:O	1:D:337:ILE:HG13	1.93	0.68
1:C:295:VAL:HG22	1:C:408:LEU:HD22	1.76	0.68
1:B:68:ASN:H	2:B:661:NAG:H82	1.58	0.68
1:C:564:ILE:HG13	1:C:580:PHE:CZ	2.29	0.68
1:B:181:VAL:HG21	1:B:491:LEU:HG	1.76	0.68
1:D:254:TYR:HD1	1:D:254:TYR:C	2.01	0.68
1:A:134:TYR:CD1	1:A:136:TYR:HE1	2.12	0.67
1:C:198:PHE:CZ	1:C:352:LEU:HD12	2.28	0.67
1:A:173:ASP:O	1:A:177:VAL:HG23	1.93	0.67
1:D:295:VAL:HG22	1:D:408:LEU:HD22	1.75	0.67
1:D:478:PHE:CZ	1:D:495:TYR:HB2	2.29	0.67
1:A:464:ASN:ND2	1:A:475:TYR:H	1.93	0.67
1:A:94:THR:HG23	1:A:354:GLY:O	1.95	0.67
1:B:193:GLY:O	1:B:581:ASN:HA	1.95	0.67
1:D:94:THR:HG23	1:D:354:GLY:O	1.95	0.67
1:C:385:TYR:CE2	4:C:701:S58:BR1	3.03	0.67
1:D:39:ASN:N	1:D:40:PRO:HD3	2.10	0.67
1:D:281:GLU:HG2	1:D:284:GLN:NE2	2.10	0.67
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.30	0.67
1:C:184:ARG:HH21	1:C:187:PHE:HA	1.60	0.67
1:D:254:TYR:HB2	1:D:261:VAL:HG13	1.76	0.67
1:B:113:MET:O	1:B:116:VAL:HG22	1.95	0.66
1:B:564:ILE:HG13	1:B:580:PHE:CZ	2.30	0.66
1:A:254:TYR:HB2	1:A:261:VAL:HG13	1.76	0.66
1:A:458:MET:HE3	1:A:460:TYR:HE1	1.60	0.66
1:A:160:PRO:HG2	1:A:165:VAL:HA	1.77	0.66
1:C:181:VAL:HG21	1:C:491:LEU:HG	1.76	0.66
1:C:435:ALA:O	1:C:512:PRO:HG3	1.95	0.66
1:B:39:ASN:N	1:B:40:PRO:HD3	2.11	0.66
1:C:470:PHE:CD1	1:C:525:LEU:HD22	2.30	0.66
1:A:109:ARG:HG3	1:A:357:PHE:HE1	1.60	0.66
1:A:583:GLN:HE21	1:D:282:ASN:CG	2.04	0.66
1:C:206:THR:HB	1:C:210:PHE:CD2	2.30	0.66
1:D:283:LEU:HD22	1:D:411:ASN:HB2	1.78	0.66
1:D:419:LEU:HB3	1:D:572:VAL:HG13	1.78	0.66
1:B:279:ILE:CG1	1:B:283:LEU:HD23	2.25	0.66
1:C:150:ARG:NH2	1:C:154:PRO:HB3	2.10	0.66
1:A:193:GLY:O	1:A:581:ASN:HA	1.95	0.66
1:A:458:MET:HE3	1:A:460:TYR:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PRO:HG3	1:B:165:VAL:HG12	1.76	0.66
1:B:352:LEU:HD23	4:B:701:S58:H10	1.78	0.66
1:C:142:PHE:O	1:C:376:ARG:NH2	2.29	0.66
1:C:205:PHE:CZ	1:C:344:VAL:HG11	2.31	0.66
1:C:333:LYS:O	1:C:337:ILE:HG13	1.95	0.66
1:D:160:PRO:HG3	1:D:165:VAL:HG12	1.78	0.66
1:B:109:ARG:HG3	1:B:357:PHE:CE1	2.31	0.66
1:B:254:TYR:HB2	1:B:261:VAL:HG13	1.78	0.66
1:D:470:PHE:CD1	1:D:525:LEU:HD22	2.31	0.66
1:B:255:GLN:HE22	1:B:265:THR:HG23	1.61	0.65
1:A:142:PHE:O	1:A:376:ARG:NH2	2.28	0.65
1:A:281:GLU:HG2	1:A:284:GLN:NE2	2.10	0.65
1:D:195:ASN:HB2	1:D:426:PHE:O	1.95	0.65
1:A:97:LYS:HB2	1:A:356:HIS:NE2	2.12	0.65
1:A:266:VAL:HG23	1:A:271:VAL:O	1.97	0.65
1:C:183:LEU:HD21	1:C:445:GLN:HB3	1.77	0.65
1:D:160:PRO:HG2	1:D:165:VAL:HA	1.78	0.65
1:A:208:GLN:HB3	1:A:232:HIS:HD2	1.62	0.65
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.11	0.65
1:C:388:HIS:CE1	1:C:447:VAL:HG11	2.32	0.65
1:D:150:ARG:HH22	1:D:154:PRO:HB3	1.62	0.65
1:B:208:GLN:HE22	1:B:228:VAL:HG13	1.62	0.65
1:B:479:GLU:HG3	1:B:488:ALA:HB1	1.79	0.65
1:C:109:ARG:HG3	1:C:357:PHE:HE1	1.61	0.65
1:C:279:ILE:CG1	1:C:283:LEU:HD23	2.27	0.65
1:D:406:GLN:HA	2:D:681:NAG:O7	1.95	0.65
1:B:75:LEU:HG	1:B:79:LYS:HE2	1.78	0.65
1:A:464:ASN:HD21	1:A:475:TYR:H	1.44	0.65
1:B:264:PRO:HG2	1:B:286:ALA:HB3	1.76	0.65
1:C:109:ARG:NH2	1:C:360:LYS:HB2	2.11	0.65
1:C:505:PRO:O	1:C:509:VAL:HG12	1.97	0.65
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.79	0.65
1:D:251:LYS:HG2	1:D:310:GLN:HG3	1.78	0.65
1:B:160:PRO:HG2	1:B:165:VAL:HA	1.79	0.65
1:B:352:LEU:HD21	1:B:518:PHE:HZ	1.62	0.65
1:C:251:LYS:HG2	1:C:310:GLN:HG3	1.79	0.65
1:D:155:VAL:HB	1:D:459:LYS:HZ2	1.61	0.65
1:D:464:ASN:HD21	1:D:475:TYR:H	1.42	0.65
1:D:497:ASP:HB3	1:D:500:VAL:HG23	1.80	0.65
1:C:208:GLN:HB3	1:C:232:HIS:HD2	1.63	0.64
1:D:173:ASP:O	1:D:177:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ILE:HG13	1:A:572:VAL:HG21	1.79	0.64
1:B:195:ASN:HB2	1:B:426:PHE:O	1.97	0.64
1:B:208:GLN:HB3	1:B:232:HIS:HD2	1.61	0.64
1:C:193:GLY:O	1:C:581:ASN:HA	1.97	0.64
1:C:482:THR:HG22	1:C:509:VAL:HG22	1.80	0.64
1:D:497:ASP:OD2	1:D:499:ASP:HB2	1.97	0.64
1:B:94:THR:HG23	1:B:354:GLY:O	1.98	0.64
1:C:391:LEU:HD21	3:C:682:HEM:HAB	1.78	0.64
1:A:518:PHE:HE1	4:A:701:S58:H9	1.63	0.64
1:B:35:PRO:HD3	1:B:52:PHE:O	1.97	0.64
1:B:150:ARG:HH22	1:B:154:PRO:HB3	1.62	0.64
1:B:279:ILE:HG23	1:B:283:LEU:HB3	1.79	0.64
1:C:35:PRO:HD3	1:C:52:PHE:O	1.98	0.64
1:C:273:MET:SD	1:C:290:GLU:HA	2.37	0.64
1:C:479:GLU:HG2	1:C:485:LYS:NZ	2.13	0.64
1:A:198:PHE:CZ	1:A:352:LEU:HD12	2.33	0.64
1:A:352:LEU:HD21	1:A:518:PHE:HZ	1.63	0.64
1:B:198:PHE:HD2	1:B:580:PHE:HB3	1.63	0.64
1:B:452:ILE:O	1:B:456:ARG:HG3	1.98	0.64
1:D:230:LEU:HG	1:D:337:ILE:HG12	1.80	0.64
1:D:447:VAL:HG13	3:D:682:HEM:HBA2	1.78	0.64
1:A:150:ARG:HH22	1:A:154:PRO:HB3	1.61	0.64
1:B:205:PHE:CZ	1:B:344:VAL:HG11	2.32	0.64
1:C:527:ALA:HB3	1:C:528:PRO:HD3	1.80	0.64
1:A:104:ASN:ND2	1:A:358:LYS:HB2	2.13	0.64
1:A:181:VAL:HG21	1:A:491:LEU:HG	1.80	0.64
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.80	0.64
1:C:419:LEU:HB3	1:C:572:VAL:HG13	1.80	0.64
1:D:150:ARG:NH2	1:D:154:PRO:HB3	2.12	0.64
1:D:281:GLU:HA	1:D:284:GLN:HE21	1.63	0.63
1:B:497:ASP:OD2	1:B:499:ASP:HB2	1.99	0.63
1:C:255:GLN:HE22	1:C:265:THR:HG23	1.63	0.63
1:D:193:GLY:O	1:D:581:ASN:HA	1.98	0.63
1:A:113:MET:HE3	1:A:117:LEU:HD13	1.81	0.63
1:A:322:GLU:HG2	1:B:52:PHE:H	1.61	0.63
1:C:198:PHE:HD2	1:C:580:PHE:HB3	1.63	0.63
1:A:505:PRO:O	1:A:509:VAL:HG12	1.98	0.63
1:C:113:MET:O	1:C:116:VAL:HG22	1.99	0.63
1:D:266:VAL:HG23	1:D:271:VAL:O	1.99	0.63
1:B:198:PHE:CZ	1:B:352:LEU:HD12	2.31	0.62
1:C:264:PRO:HG2	1:C:286:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASN:N	1:A:39:ASN:HD22	1.98	0.62
1:A:205:PHE:CZ	1:A:344:VAL:HG11	2.34	0.62
1:A:333:LYS:O	1:A:337:ILE:HG13	1.99	0.62
1:C:74:PHE:HA	1:C:77:ARG:NE	2.14	0.62
1:C:160:PRO:HG2	1:C:165:VAL:HA	1.78	0.62
1:A:98:GLY:O	1:A:101:ASN:HB2	1.99	0.62
1:A:391:LEU:HD21	3:A:682:HEM:HAB	1.81	0.62
1:C:150:ARG:HH22	1:C:154:PRO:HB3	1.63	0.62
1:D:151:ALA:HB2	1:D:529:PHE:HZ	1.65	0.62
1:D:181:VAL:HG21	1:D:491:LEU:HG	1.81	0.62
1:A:113:MET:O	1:A:116:VAL:HG22	2.00	0.62
1:B:243:LYS:O	1:B:269:THR:HB	1.99	0.62
1:C:100:TRP:CE3	1:C:357:PHE:HB2	2.34	0.62
1:A:452:ILE:O	1:A:456:ARG:HG3	2.00	0.62
1:B:216:ARG:HB3	1:B:220:PHE:CD2	2.34	0.62
1:B:230:LEU:HG	1:B:337:ILE:HG12	1.81	0.62
1:D:43:ASN:ND2	1:D:70:THR:HA	2.14	0.62
1:B:281:GLU:HG2	1:B:284:GLN:HE21	1.64	0.62
1:A:98:GLY:HA2	1:A:101:ASN:HD22	1.64	0.62
1:A:100:TRP:CE3	1:A:357:PHE:HB2	2.34	0.62
1:B:333:LYS:O	1:B:337:ILE:HG13	1.99	0.62
1:A:198:PHE:HD2	1:A:580:PHE:HB3	1.65	0.62
1:A:312:VAL:HA	1:A:315:ILE:HD12	1.82	0.62
1:B:100:TRP:CE3	1:B:357:PHE:HB2	2.35	0.62
1:D:568:ILE:HG13	1:D:572:VAL:HG21	1.82	0.62
1:A:72:PRO:HB2	1:A:76:THR:HB	1.80	0.62
1:D:281:GLU:HA	1:D:284:GLN:HG3	1.81	0.62
1:A:470:PHE:CD1	1:A:525:LEU:HD22	2.34	0.61
1:A:583:GLN:NE2	1:D:282:ASN:ND2	2.48	0.61
1:A:155:VAL:HB	1:A:459:LYS:HZ2	1.65	0.61
1:C:501:MET:HG3	1:C:506:ALA:HB2	1.81	0.61
1:A:197:MET:CE	1:A:423:VAL:HA	2.29	0.61
1:B:464:ASN:ND2	1:B:475:TYR:H	1.97	0.61
1:D:98:GLY:O	1:D:101:ASN:HB2	2.00	0.61
1:D:198:PHE:HD2	1:D:580:PHE:HB3	1.66	0.61
1:D:255:GLN:HE22	1:D:265:THR:HG23	1.64	0.61
1:D:269:THR:O	1:D:271:VAL:HG12	2.00	0.61
1:A:229:ASP:OD1	1:A:231:ASN:HB3	2.00	0.61
1:A:342:LYS:HD2	1:A:346:GLU:HG3	1.82	0.61
1:A:482:THR:HG22	1:A:509:VAL:HG22	1.81	0.61
1:C:43:ASN:ND2	1:C:70:THR:HA	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:CG1	1:A:283:LEU:HD23	2.31	0.61
1:D:38:SER:HB2	2:D:661:NAG:O6	1.99	0.61
1:D:183:LEU:HD21	1:D:445:GLN:HB3	1.82	0.61
1:D:420:THR:O	1:D:424:GLU:HG3	1.99	0.61
1:A:246:LEU:HG	1:A:248:LYS:HB2	1.83	0.61
1:A:52:PHE:CD1	1:B:322:GLU:HB3	2.36	0.61
1:D:35:PRO:HD3	1:D:52:PHE:O	2.01	0.61
1:C:155:VAL:HB	1:C:459:LYS:HZ2	1.65	0.61
1:C:230:LEU:HG	1:C:337:ILE:HG12	1.83	0.61
1:A:195:ASN:HB2	1:A:426:PHE:O	2.00	0.61
1:B:85:THR:HB	1:B:88:THR:HG23	1.82	0.61
1:C:254:TYR:HB2	1:C:261:VAL:HG13	1.81	0.61
1:B:175:LYS:HA	1:B:178:LEU:HB3	1.82	0.61
1:D:100:TRP:CE3	1:D:357:PHE:HB2	2.35	0.61
1:A:105(A):ILE:HG22	1:A:108:LEU:HB2	1.82	0.60
1:B:205:PHE:CE1	1:B:344:VAL:HG21	2.36	0.60
1:C:464:ASN:ND2	1:C:475:TYR:H	1.98	0.60
1:D:85:THR:CG2	1:D:86:PRO:HD2	2.30	0.60
1:A:479:GLU:HG3	1:A:488:ALA:HB1	1.82	0.60
1:B:120:ARG:HD3	1:B:527:ALA:CB	2.30	0.60
1:B:568:ILE:HG13	1:B:572:VAL:HG21	1.82	0.60
1:C:444:VAL:HG12	1:C:444:VAL:O	2.01	0.60
1:C:478:PHE:HZ	1:C:495:TYR:HB2	1.65	0.60
1:D:72:PRO:HB2	1:D:76:THR:HB	1.83	0.60
1:D:208:GLN:HE22	1:D:228:VAL:HG13	1.65	0.60
1:B:197:MET:CE	1:B:423:VAL:HA	2.31	0.60
1:A:205:PHE:CE1	1:A:344:VAL:HG21	2.36	0.60
1:D:182:LEU:O	1:D:438:ARG:HA	2.00	0.60
1:B:505:PRO:O	1:B:509:VAL:HG12	1.99	0.60
1:D:113:MET:HE3	1:D:117:LEU:HD13	1.83	0.60
1:B:173:ASP:O	1:B:177:VAL:HG23	2.01	0.60
1:B:216:ARG:HB3	1:B:220:PHE:CG	2.37	0.60
1:B:281:GLU:HG2	1:B:284:GLN:NE2	2.17	0.60
1:C:72:PRO:HB2	1:C:76:THR:HB	1.83	0.60
1:A:184:ARG:HH21	1:A:187:PHE:HA	1.66	0.60
1:A:497:ASP:HB3	1:A:500:VAL:CG2	2.32	0.60
1:C:568:ILE:HG13	1:C:572:VAL:HG21	1.83	0.60
1:D:281:GLU:HG2	1:D:284:GLN:HE21	1.65	0.60
1:B:229:ASP:OD1	1:B:231:ASN:HB3	2.02	0.60
1:B:245:ARG:HG2	1:B:247:PHE:H	1.66	0.60
1:B:253:LYS:HE2	1:B:269:THR:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:THR:HG22	1:C:384:LEU:N	2.16	0.60
1:B:283:LEU:HD22	1:B:411:ASN:HB2	1.83	0.60
1:B:458:MET:HE3	1:B:460:TYR:CE1	2.37	0.60
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.83	0.60
1:C:120:ARG:O	1:C:123:LEU:HD23	2.01	0.60
1:C:386:HIS:CE1	3:C:682:HEM:HAD2	2.36	0.60
1:B:37:CYS:O	1:B:39:ASN:ND2	2.34	0.60
1:B:149:THR:O	1:B:378:ALA:HA	2.02	0.60
1:C:458:MET:HE3	1:C:460:TYR:CE1	2.37	0.60
1:D:198:PHE:CZ	1:D:352:LEU:HD12	2.34	0.60
1:A:269:THR:O	1:A:271:VAL:N	2.34	0.59
1:B:97:LYS:HB2	1:B:356:HIS:NE2	2.17	0.59
1:D:113:MET:O	1:D:116:VAL:HG22	2.02	0.59
1:D:269:THR:O	1:D:271:VAL:N	2.35	0.59
1:A:385:TYR:CE2	4:A:701:S58:BR1	3.10	0.59
1:B:43:ASN:ND2	1:B:70:THR:HA	2.17	0.59
1:B:104:ASN:ND2	1:B:358:LYS:HB2	2.17	0.59
1:B:155:VAL:HB	1:B:459:LYS:HZ2	1.67	0.59
1:B:458:MET:HE3	1:B:460:TYR:HE1	1.66	0.59
1:A:43:ASN:ND2	1:A:70:THR:HA	2.18	0.59
1:C:210:PHE:O	1:C:211:LYS:HG3	2.03	0.59
1:C:472:LEU:HD21	1:C:524:GLU:HG3	1.85	0.59
1:D:55:TYR:HE2	1:D:57:CYS:SG	2.25	0.59
1:D:109:ARG:HG3	1:D:357:PHE:HE1	1.67	0.59
1:D:452:ILE:O	1:D:456:ARG:HG3	2.02	0.59
1:B:182:LEU:O	1:B:438:ARG:HA	2.03	0.59
1:B:273:MET:SD	1:B:290:GLU:HA	2.43	0.59
1:B:386:HIS:CE1	3:B:682:HEM:HAD2	2.37	0.59
1:C:352:LEU:HD21	1:C:518:PHE:HZ	1.68	0.59
1:D:191:PRO:HG3	1:D:433:ARG:CZ	2.33	0.59
1:A:582:VAL:O	1:A:582:VAL:HG13	2.03	0.59
1:C:151:ALA:HB2	1:C:529:PHE:HZ	1.68	0.59
1:C:274:ILE:HG13	1:C:290:GLU:HG2	1.85	0.59
1:D:105(A):ILE:HG23	1:D:107:PHE:CE1	2.38	0.59
1:B:446:ALA:O	1:B:449:LYS:HB3	2.03	0.59
1:C:464:ASN:HD21	1:C:475:TYR:H	1.49	0.59
1:C:504:TYR:HB3	1:C:505:PRO:HD3	1.85	0.59
1:D:205:PHE:CZ	1:D:344:VAL:HG11	2.38	0.59
1:A:206:THR:HB	1:A:210:PHE:CE2	2.38	0.58
1:C:104:ASN:ND2	1:C:358:LYS:HB2	2.17	0.58
1:C:197:MET:CE	1:C:423:VAL:HA	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PRO:HG2	1:A:286:ALA:HB3	1.84	0.58
1:B:198:PHE:HZ	1:B:352:LEU:CD1	2.16	0.58
1:C:85:THR:CG2	1:C:86:PRO:HD2	2.33	0.58
1:C:246:LEU:HG	1:C:248:LYS:HB2	1.84	0.58
1:B:206:THR:HB	1:B:210:PHE:CE2	2.39	0.58
1:C:327:GLN:NE2	1:D:136:TYR:HD2	2.02	0.58
1:D:386:HIS:CE1	3:D:682:HEM:HAD2	2.38	0.58
1:D:444:VAL:HG12	1:D:444:VAL:O	2.04	0.58
1:A:293:GLY:HA2	1:A:299:MET:HE2	1.86	0.58
1:B:72:PRO:HB2	1:B:76:THR:HB	1.83	0.58
1:B:105(A):ILE:HG22	1:B:108:LEU:HB2	1.85	0.58
1:B:506:ALA:O	1:B:510:GLU:HB2	2.04	0.58
1:C:318:GLN:NE2	1:C:318:GLN:HA	2.19	0.58
1:A:405:LYS:HD2	1:A:405:LYS:N	2.16	0.58
1:B:251:LYS:HG2	1:B:310:GLN:HG3	1.85	0.58
1:C:216:ARG:HB3	1:C:220:PHE:CG	2.39	0.58
1:C:353:SER:HA	4:C:701:S58:C7	2.33	0.58
1:D:105(A):ILE:HG22	1:D:108:LEU:HB2	1.85	0.58
1:B:381:PHE:CD1	1:B:529:PHE:CB	2.87	0.58
1:A:506:ALA:O	1:A:510:GLU:HB2	2.03	0.58
1:C:90:HIS:NE2	4:C:701:S58:N3	2.51	0.58
1:D:40:PRO:HB3	2:D:661:NAG:H5	1.86	0.58
1:D:183:LEU:O	1:D:438:ARG:HB3	2.03	0.58
1:B:184:ARG:HH11	1:B:441:PRO:HG3	1.68	0.58
1:B:385:TYR:CE2	4:B:701:S58:BR1	3.12	0.58
1:C:67:GLU:HB3	2:C:661:NAG:H82	1.86	0.58
1:C:272:GLU:HB3	1:C:290:GLU:OE2	2.04	0.58
1:C:452:ILE:O	1:C:456:ARG:HG3	2.03	0.58
1:D:104:ASN:ND2	1:D:358:LYS:HB2	2.19	0.58
1:A:501:MET:HG3	1:A:506:ALA:HB2	1.86	0.57
1:B:203:GLN:HB2	3:B:682:HEM:HMC2	1.86	0.57
1:D:206:THR:HB	1:D:210:PHE:CE2	2.38	0.57
1:D:216:ARG:HB3	1:D:220:PHE:CD2	2.40	0.57
1:A:183:LEU:HD22	1:A:442:ILE:HG13	1.85	0.57
1:B:464:ASN:HD21	1:B:475:TYR:H	1.51	0.57
1:B:582:VAL:O	1:B:582:VAL:HG13	2.04	0.57
1:C:479:GLU:HG3	1:C:488:ALA:HB1	1.87	0.57
1:C:195:ASN:HB2	1:C:426:PHE:O	2.03	0.57
1:C:198:PHE:HZ	1:C:352:LEU:CD1	2.14	0.57
1:B:470:PHE:CD1	1:B:525:LEU:HD22	2.40	0.57
1:B:477:SER:O	1:B:480:GLU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:PRO:HA	2:D:661:NAG:C6	2.33	0.57
1:D:205:PHE:CE1	1:D:344:VAL:HG21	2.38	0.57
1:D:254:TYR:C	1:D:254:TYR:CD1	2.75	0.57
1:A:74:PHE:CD1	1:A:77:ARG:HD2	2.39	0.57
1:C:94:THR:HG23	1:C:354:GLY:O	2.04	0.57
1:D:427:THR:HB	1:D:428:ARG:HD2	1.86	0.57
1:A:335:ILE:HA	1:A:559:ILE:HD11	1.87	0.57
1:A:565:GLN:HG2	1:D:268:ASP:HA	1.87	0.57
1:B:92:ILE:HA	1:B:96:PHE:HE1	1.69	0.57
1:B:244:LEU:HD21	1:B:271:VAL:HG11	1.85	0.57
1:A:577:PHE:HE2	1:D:267:LYS:HD3	1.69	0.57
1:B:142:PHE:O	1:B:376:ARG:NH2	2.37	0.57
1:D:273:MET:SD	1:D:290:GLU:HA	2.45	0.57
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.87	0.56
1:A:276:PRO:HD2	1:A:279:ILE:HD13	1.86	0.56
1:B:184:ARG:HH21	1:B:187:PHE:HA	1.70	0.56
1:D:291:VAL:HG22	1:D:294:LEU:HD12	1.86	0.56
1:D:410:ASN:CG	1:D:413:ILE:HG13	2.30	0.56
1:B:151:ALA:HB2	1:B:529:PHE:HZ	1.68	0.56
1:C:105(A):ILE:HG22	1:C:108:LEU:HB2	1.88	0.56
1:D:142:PHE:O	1:D:376:ARG:NH2	2.37	0.56
1:A:151:ALA:HB2	1:A:529:PHE:HZ	1.70	0.56
1:A:176:GLU:O	1:A:180:LYS:HG3	2.05	0.56
1:A:322:GLU:HB3	1:B:52:PHE:CD1	2.40	0.56
1:B:183:LEU:HD21	1:B:445:GLN:HB3	1.86	0.56
1:B:352:LEU:HD21	1:B:518:PHE:CZ	2.41	0.56
1:C:105(A):ILE:HG23	1:C:107:PHE:CE1	2.41	0.56
1:C:109:ARG:HH21	1:C:360:LYS:HB2	1.71	0.56
1:C:120:ARG:HD3	1:C:527:ALA:CB	2.34	0.56
1:C:276:PRO:HB2	1:C:278:HIS:CE1	2.41	0.56
1:C:279:ILE:CG2	1:C:283:LEU:HB3	2.34	0.56
1:D:198:PHE:HZ	1:D:352:LEU:CD1	2.18	0.56
1:D:399:ASP:O	1:D:400:GLN:HB2	2.04	0.56
1:A:105(A):ILE:HG23	1:A:107:PHE:CE1	2.40	0.56
1:B:352:LEU:HD23	4:B:701:S58:C10	2.36	0.56
1:D:105(A):ILE:HG23	1:D:107:PHE:CD1	2.41	0.56
1:D:271:VAL:HG11	1:D:286:ALA:HB1	1.87	0.56
1:A:213:ASP:OD1	1:A:215:LYS:HG2	2.06	0.56
1:B:283:LEU:HB2	1:B:411:ASN:HB2	1.86	0.56
1:D:564:ILE:HG13	1:D:580:PHE:CZ	2.41	0.56
1:D:48:MET:HE3	1:D:49:SER:OG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:GLN:HA	2:B:681:NAG:O7	2.05	0.56
1:C:216:ARG:HB3	1:C:220:PHE:CD2	2.40	0.56
1:C:253:LYS:HE2	1:C:269:THR:HG22	1.88	0.56
1:D:253:LYS:HE2	1:D:269:THR:HG22	1.87	0.56
1:D:338:GLY:HA3	1:D:559:ILE:HG13	1.88	0.56
1:A:546:LYS:C	1:A:547:PRO:O	2.48	0.56
1:C:206:THR:HB	1:C:210:PHE:CE2	2.41	0.56
1:C:506:ALA:O	1:C:510:GLU:HB2	2.04	0.56
1:D:83:LYS:HG3	1:D:83:LYS:O	2.04	0.56
1:A:127:PRO:HD2	1:B:543:GLN:OE1	2.06	0.56
1:A:175:LYS:HG2	1:A:178:LEU:HD13	1.88	0.56
1:A:255:GLN:HE22	1:A:265:THR:HG23	1.71	0.56
1:A:445:GLN:HG3	1:A:446:ALA:N	2.21	0.56
1:B:253:LYS:NZ	1:B:269:THR:HG21	2.21	0.56
1:B:482:THR:HG22	1:B:509:VAL:HG22	1.88	0.56
1:C:464:ASN:HB3	1:C:474:PRO:HB3	1.87	0.56
1:C:477:SER:O	1:C:480:GLU:HB2	2.06	0.56
1:A:241:GLN:NE2	1:A:329:PHE:CE1	2.74	0.56
1:B:447:VAL:HG13	3:B:682:HEM:HBA2	1.88	0.56
1:D:85:THR:HB	1:D:88:THR:HG23	1.88	0.56
1:D:184:ARG:HH11	1:D:441:PRO:HG3	1.70	0.56
1:D:335:ILE:HA	1:D:559:ILE:HD11	1.87	0.56
1:A:444:VAL:O	1:A:444:VAL:HG12	2.06	0.55
1:C:183:LEU:HD22	1:C:442:ILE:HG13	1.88	0.55
1:C:229:ASP:OD1	1:C:231:ASN:HB3	2.06	0.55
1:C:458:MET:HE3	1:C:460:TYR:HE1	1.71	0.55
1:C:205:PHE:CE1	1:C:344:VAL:HG21	2.42	0.55
1:D:352:LEU:HD23	4:D:701:S58:H10	1.88	0.55
1:A:136:TYR:HD2	1:B:327:GLN:NE2	2.05	0.55
1:A:183:LEU:HD21	1:A:445:GLN:HB3	1.89	0.55
1:A:279:ILE:HG13	1:A:283:LEU:HD23	1.86	0.55
1:C:92:ILE:HA	1:C:96:PHE:HE1	1.70	0.55
1:D:216:ARG:HB3	1:D:220:PHE:CG	2.40	0.55
1:D:419:LEU:O	1:D:423:VAL:HG23	2.06	0.55
1:A:41:CYS:SG	1:A:47:CYS:HB2	2.47	0.55
1:A:43:ASN:HD22	1:A:70:THR:HA	1.72	0.55
1:D:188:ILE:O	1:D:432:GLY:HA2	2.07	0.55
1:D:385:TYR:HE2	4:D:701:S58:BR1	2.44	0.55
1:A:37:CYS:O	1:A:39:ASN:ND2	2.39	0.55
1:C:57:CYS:HB3	1:C:69:CYS:SG	2.47	0.55
1:C:445:GLN:HG3	1:C:446:ALA:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:ASP:O	1:B:400:GLN:HB2	2.07	0.55
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.89	0.55
1:C:48:MET:HE3	1:C:49:SER:OG	2.06	0.55
1:C:51:GLY:O	1:C:52:PHE:HB2	2.07	0.55
1:C:476:THR:OG1	1:C:480:GLU:HG3	2.06	0.55
1:D:197:MET:CE	1:D:423:VAL:HA	2.36	0.55
1:D:313:CYS:O	1:D:317:LYS:HB2	2.06	0.55
1:A:345:ILE:CD1	1:A:534:LEU:HD23	2.35	0.55
1:A:478:PHE:HZ	1:A:495:TYR:HB2	1.67	0.55
1:C:254:TYR:CD1	1:C:254:TYR:C	2.84	0.55
1:D:283:LEU:HB2	1:D:411:ASN:CG	2.31	0.55
1:A:208:GLN:HE22	1:A:228:VAL:HG13	1.71	0.55
1:A:419:LEU:HB3	1:A:572:VAL:CG1	2.37	0.55
1:B:51:GLY:O	1:B:52:PHE:HB2	2.07	0.55
1:D:241:GLN:NE2	1:D:329:PHE:CE1	2.75	0.55
1:A:85:THR:HB	1:A:88:THR:HG23	1.88	0.55
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.89	0.55
1:C:43:ASN:HD22	1:C:70:THR:HA	1.71	0.55
1:C:497:ASP:HB3	1:C:500:VAL:CG2	2.36	0.55
1:D:184:ARG:HH21	1:D:187:PHE:HA	1.72	0.55
1:D:501:MET:HG3	1:D:506:ALA:HB2	1.89	0.55
1:D:513:ARG:HH11	4:D:701:S58:HN31	1.55	0.55
1:A:39:ASN:N	1:A:40:PRO:HD3	2.21	0.55
1:B:254:TYR:HD1	1:B:254:TYR:C	2.15	0.55
1:B:283:LEU:O	1:B:285:PHE:N	2.40	0.55
1:B:364:GLU:HG2	1:B:367:PHE:CE2	2.41	0.55
1:D:388:HIS:CE1	1:D:447:VAL:HG11	2.41	0.55
1:A:120:ARG:HD3	1:A:527:ALA:CB	2.36	0.54
1:A:123:LEU:O	1:A:469:ARG:NH2	2.40	0.54
1:A:352:LEU:HD23	4:A:701:S58:H10	1.89	0.54
1:B:34:ASN:HD22	1:B:156:ALA:HB2	1.72	0.54
1:B:464:ASN:HB3	1:B:474:PRO:HB3	1.88	0.54
1:C:316:LEU:HB3	1:C:328:LEU:CD2	2.37	0.54
1:A:52:PHE:CE1	1:B:322:GLU:HB3	2.43	0.54
1:A:269:THR:O	1:A:271:VAL:HG12	2.06	0.54
1:B:197:MET:CE	1:B:423:VAL:HG13	2.37	0.54
1:B:272:GLU:HB3	1:B:290:GLU:OE2	2.07	0.54
1:C:463:LEU:HD13	1:C:506:ALA:HB3	1.89	0.54
1:A:276:PRO:HB2	1:A:279:ILE:HD13	1.89	0.54
1:B:244:LEU:O	1:B:253:LYS:HB2	2.07	0.54
1:B:398:GLU:HG2	1:B:425:SER:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LYS:HG3	1:C:365:LEU:HB3	1.89	0.54
1:D:210:PHE:O	1:D:211:LYS:HG3	2.08	0.54
1:B:335:ILE:HA	1:B:559:ILE:HD11	1.88	0.54
1:B:448:ALA:O	1:B:452:ILE:HG13	2.08	0.54
1:D:98:GLY:HA2	1:D:101:ASN:HD22	1.72	0.54
1:B:57:CYS:HB3	1:B:69:CYS:SG	2.47	0.54
1:B:546:LYS:C	1:B:547:PRO:O	2.49	0.54
1:C:123:LEU:O	1:C:469:ARG:NH2	2.40	0.54
1:D:244:LEU:O	1:D:253:LYS:HB2	2.06	0.54
1:A:152:LEU:HD13	1:A:461:GLN:OE1	2.07	0.54
1:A:335:ILE:HG23	1:A:559:ILE:HD12	1.90	0.54
1:B:345:ILE:CD1	1:B:534:LEU:HD23	2.34	0.54
1:B:572:VAL:O	1:B:574:GLY:N	2.40	0.54
1:C:572:VAL:O	1:C:574:GLY:N	2.41	0.54
1:D:208:GLN:NE2	1:D:228:VAL:HG13	2.23	0.54
1:D:260:GLU:HB2	1:D:262:TYR:CE2	2.42	0.54
1:A:66:GLY:O	1:A:68:ASN:N	2.40	0.54
1:B:34:ASN:HD22	1:B:156:ALA:CB	2.21	0.54
1:B:213:ASP:OD2	1:B:216:ARG:HB2	2.08	0.54
1:C:323:TRP:HH2	1:C:551:GLY:CA	2.19	0.54
1:D:182:LEU:C	1:D:438:ARG:HA	2.33	0.54
1:D:391:LEU:CD2	3:D:682:HEM:HAB	2.30	0.54
1:C:273:MET:HA	1:C:290:GLU:CG	2.38	0.54
1:A:424:GLU:HG2	1:A:428:ARG:HH12	1.73	0.54
1:D:34:ASN:HD22	1:D:156:ALA:CB	2.21	0.54
1:D:479:GLU:HG3	1:D:488:ALA:HB1	1.89	0.54
1:A:198:PHE:CD1	1:A:198:PHE:C	2.86	0.54
1:A:291:VAL:HG22	1:A:294:LEU:HD12	1.90	0.54
1:B:232:HIS:CE1	1:B:233:ILE:HG13	2.43	0.54
1:B:472:LEU:HD21	1:B:524:GLU:HG3	1.90	0.54
1:C:85:THR:HB	1:C:88:THR:HG23	1.89	0.54
1:C:113:MET:HE3	1:C:117:LEU:HD13	1.90	0.54
1:C:582:VAL:O	1:C:582:VAL:HG13	2.06	0.54
1:D:350:GLN:HE22	1:D:359:LEU:H	1.56	0.54
1:A:92:ILE:HA	1:A:96:PHE:HE1	1.72	0.53
1:A:399:ASP:O	1:A:400:GLN:HB2	2.08	0.53
1:B:182:LEU:C	1:B:438:ARG:HA	2.32	0.53
1:B:281:GLU:HA	1:B:284:GLN:HG3	1.90	0.53
1:D:572:VAL:O	1:D:574:GLY:N	2.42	0.53
1:A:175:LYS:HA	1:A:178:LEU:HB3	1.88	0.53
1:B:254:TYR:C	1:B:254:TYR:CD1	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:THR:HG22	1:B:384:LEU:N	2.24	0.53
1:B:396:ASN:CB	1:B:401:GLU:HG2	2.36	0.53
1:D:272:GLU:HB3	1:D:290:GLU:OE2	2.08	0.53
1:D:283:LEU:HB2	1:D:411:ASN:HB2	1.89	0.53
1:D:381:PHE:CD1	1:D:529:PHE:CB	2.91	0.53
1:A:320:HIS:CE1	1:A:551:GLY:O	2.61	0.53
1:A:387:TRP:HB2	3:A:682:HEM:HBC2	1.90	0.53
1:B:232:HIS:ND1	1:B:233:ILE:HG13	2.24	0.53
1:B:478:PHE:HZ	1:B:495:TYR:HB2	1.69	0.53
1:D:541:SER:HB2	1:D:543:GLN:OE1	2.08	0.53
1:A:134:TYR:CD1	1:A:136:TYR:CE1	2.92	0.53
1:A:463:LEU:HD22	1:A:506:ALA:CB	2.37	0.53
1:D:34:ASN:HD22	1:D:156:ALA:HB2	1.73	0.53
1:D:39:ASN:N	1:D:39:ASN:HD22	2.06	0.53
1:D:279:ILE:CG2	1:D:283:LEU:HB3	2.38	0.53
1:B:244:LEU:CD2	1:B:271:VAL:HG11	2.38	0.53
1:C:232:HIS:CE1	1:C:233:ILE:HG13	2.44	0.53
1:C:311:ARG:O	1:C:315:ILE:HG13	2.08	0.53
1:D:134:TYR:CD1	1:D:136:TYR:CE1	2.89	0.53
1:D:197:MET:CE	1:D:423:VAL:HG13	2.38	0.53
1:D:213:ASP:OD2	1:D:216:ARG:HB2	2.09	0.53
1:A:364:GLU:HA	1:A:367:PHE:CD2	2.44	0.53
1:A:383:THR:HG22	1:A:384:LEU:N	2.23	0.53
1:B:105(A):ILE:HG23	1:B:107:PHE:CE1	2.44	0.53
1:B:210:PHE:O	1:B:211:LYS:HG3	2.09	0.53
1:B:246:LEU:HG	1:B:248:LYS:HB2	1.89	0.53
1:B:513:ARG:NH1	1:B:523:VAL:HG11	2.23	0.53
1:C:350:GLN:HE22	1:C:359:LEU:H	1.56	0.53
1:D:183:LEU:HD22	1:D:442:ILE:HG13	1.91	0.53
1:D:518:PHE:HE1	4:D:701:S58:H9	1.73	0.53
1:A:136:TYR:CD2	1:B:327:GLN:NE2	2.76	0.53
1:A:216:ARG:HB3	1:A:220:PHE:CD2	2.44	0.53
1:A:253:LYS:HE2	1:A:269:THR:HG22	1.91	0.53
1:B:191:PRO:HG3	1:B:433:ARG:CZ	2.39	0.53
1:C:322:GLU:HB3	1:D:52:PHE:CD1	2.44	0.53
1:D:482:THR:HG22	1:D:509:VAL:HG22	1.89	0.53
1:D:504:TYR:HB3	1:D:505:PRO:HD3	1.90	0.53
1:B:55:TYR:HE2	1:B:57:CYS:SG	2.32	0.53
1:C:208:GLN:HE22	1:C:228:VAL:HG13	1.73	0.53
1:A:464:ASN:HB3	1:A:474:PRO:HB3	1.91	0.53
1:B:206:THR:HB	1:B:210:PHE:HD2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:VAL:HG23	1:B:271:VAL:O	2.08	0.53
1:C:335:ILE:HG12	1:C:550:PHE:HB3	1.91	0.53
1:D:43:ASN:HD22	1:D:70:THR:HA	1.73	0.53
1:D:43:ASN:O	1:D:44:ARG:HB2	2.08	0.53
1:D:162:PRO:O	1:D:163:MET:HE2	2.09	0.53
1:D:291:VAL:O	1:D:293:GLY:N	2.42	0.53
1:A:260:GLU:HB2	1:A:262:TYR:CE2	2.43	0.53
1:B:150:ARG:NH2	1:B:458:MET:O	2.42	0.53
1:C:254:TYR:HD2	1:C:310:GLN:HE21	1.57	0.53
1:C:266:VAL:HG23	1:C:271:VAL:O	2.09	0.53
1:C:345:ILE:CD1	1:C:534:LEU:HD23	2.36	0.53
1:C:381:PHE:CD1	1:C:529:PHE:CB	2.92	0.53
1:D:505:PRO:O	1:D:509:VAL:HG12	2.09	0.53
1:A:105(A):ILE:CG2	1:A:108:LEU:HB2	2.39	0.52
1:A:188:ILE:O	1:A:432:GLY:HA2	2.09	0.52
1:B:75:LEU:O	1:B:79:LYS:HG3	2.10	0.52
1:C:273:MET:HA	1:C:290:GLU:HG3	1.91	0.52
1:C:281:GLU:HG2	1:C:284:GLN:HE21	1.74	0.52
1:A:210:PHE:O	1:A:211:LYS:HG3	2.08	0.52
1:B:66:GLY:O	1:B:68:ASN:N	2.43	0.52
1:B:198:PHE:CD1	1:B:198:PHE:C	2.87	0.52
1:C:260:GLU:HB2	1:C:262:TYR:CE2	2.44	0.52
1:C:291:VAL:HG22	1:C:294:LEU:HD12	1.90	0.52
1:D:273:MET:HA	1:D:290:GLU:CG	2.39	0.52
1:D:383:THR:HG22	1:D:384:LEU:N	2.23	0.52
1:D:546:LYS:C	1:D:547:PRO:O	2.51	0.52
1:A:398:GLU:HG2	1:A:425:SER:HA	1.92	0.52
1:C:253:LYS:NZ	1:C:269:THR:HG21	2.23	0.52
1:D:150:ARG:NH2	1:D:458:MET:O	2.42	0.52
1:D:352:LEU:HD21	1:D:518:PHE:HZ	1.75	0.52
1:A:57:CYS:HB3	1:A:69:CYS:SG	2.49	0.52
1:A:476:THR:OG1	1:A:480:GLU:HG3	2.09	0.52
1:A:572:VAL:O	1:A:574:GLY:N	2.43	0.52
1:B:316:LEU:HB3	1:B:328:LEU:CD2	2.39	0.52
1:B:381:PHE:CD1	1:B:529:PHE:HB2	2.44	0.52
1:C:39:ASN:N	1:C:39:ASN:HD22	2.07	0.52
1:C:427:THR:HB	1:C:428:ARG:HD2	1.90	0.52
1:C:448:ALA:O	1:C:452:ILE:HG13	2.10	0.52
1:D:274:ILE:HG13	1:D:290:GLU:HG2	1.90	0.52
1:B:273:MET:HA	1:B:290:GLU:CG	2.39	0.52
1:B:274:ILE:HG13	1:B:290:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:TYR:CZ	1:C:284:GLN:HA	2.44	0.52
1:D:464:ASN:HB3	1:D:474:PRO:HB3	1.91	0.52
1:A:48:MET:HE3	1:A:49:SER:OG	2.10	0.52
1:A:232:HIS:ND1	1:A:233:ILE:HG13	2.25	0.52
1:B:134:TYR:CD1	1:B:136:TYR:CE1	2.84	0.52
1:B:381:PHE:O	1:B:385:TYR:HB2	2.09	0.52
1:C:136:TYR:HD2	1:D:327:GLN:NE2	2.06	0.52
1:D:490:GLU:O	1:D:493:ALA:HB3	2.09	0.52
1:A:150:ARG:HD3	1:A:379:SER:OG	2.09	0.52
1:A:293:GLY:HA2	1:A:299:MET:CE	2.40	0.52
1:B:183:LEU:HD22	1:B:442:ILE:HG13	1.92	0.52
1:B:445:GLN:HG3	1:B:446:ALA:N	2.24	0.52
1:C:253:LYS:HZ3	1:C:269:THR:HG21	1.75	0.52
1:D:381:PHE:O	1:D:385:TYR:HB2	2.10	0.52
1:A:204:HIS:HE2	1:A:305:TRP:CD1	2.28	0.52
1:A:482:THR:CG2	1:A:509:VAL:HG22	2.40	0.52
1:B:175:LYS:HG2	1:B:178:LEU:HD13	1.91	0.52
1:B:433:ARG:HH21	1:B:512:PRO:CB	2.23	0.52
1:D:198:PHE:CD1	1:D:198:PHE:C	2.87	0.52
1:D:419:LEU:HB3	1:D:572:VAL:CG1	2.38	0.52
1:D:477:SER:O	1:D:480:GLU:HB2	2.10	0.52
1:B:320:HIS:CE1	1:B:551:GLY:O	2.63	0.52
1:B:442:ILE:O	1:B:445:GLN:HG2	2.10	0.52
1:C:312:VAL:HA	1:C:315:ILE:HD12	1.90	0.52
1:D:120:ARG:HD3	1:D:527:ALA:CB	2.36	0.52
1:A:55:TYR:HE2	1:A:57:CYS:SG	2.33	0.52
1:A:120:ARG:O	1:A:123:LEU:HD23	2.10	0.52
1:A:279:ILE:CG2	1:A:283:LEU:HB3	2.37	0.52
1:A:553:GLU:O	1:A:557:LYS:HG2	2.10	0.52
1:B:109:ARG:HG3	1:B:357:PHE:HE1	1.72	0.52
1:B:389:PRO:HG2	1:B:508:LEU:HD22	1.91	0.52
1:C:350:GLN:NE2	1:C:359:LEU:H	2.08	0.52
1:C:442:ILE:O	1:C:445:GLN:HG2	2.10	0.52
1:D:316:LEU:HB3	1:D:328:LEU:CD2	2.40	0.52
1:A:176:GLU:HB3	1:A:494:LEU:HD21	1.91	0.51
1:A:254:TYR:CD1	1:A:254:TYR:C	2.89	0.51
1:A:335:ILE:HG12	1:A:550:PHE:HB3	1.93	0.51
1:A:448:ALA:O	1:A:452:ILE:HG13	2.10	0.51
1:B:136:TYR:O	1:B:136:TYR:HD1	1.91	0.51
1:C:327:GLN:NE2	1:D:136:TYR:CD2	2.78	0.51
1:D:582:VAL:O	1:D:582:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ILE:HG21	1:B:417:HIS:ND1	2.25	0.51
1:C:232:HIS:ND1	1:C:233:ILE:HG13	2.25	0.51
1:C:254:TYR:C	1:C:254:TYR:HD1	2.17	0.51
1:C:269:THR:O	1:C:271:VAL:N	2.44	0.51
1:D:152:LEU:HD13	1:D:461:GLN:OE1	2.10	0.51
1:A:35:PRO:HG3	1:A:54:GLN:O	2.09	0.51
1:A:52:PHE:H	1:B:322:GLU:HG2	1.75	0.51
1:A:105:ASN:O	1:A:106:PRO:HD3	2.10	0.51
1:A:335:ILE:HG23	1:A:559:ILE:CD1	2.40	0.51
1:D:253:LYS:NZ	1:D:269:THR:HG21	2.25	0.51
1:B:381:PHE:CD1	1:B:529:PHE:HB3	2.46	0.51
1:B:495:TYR:HE2	1:B:502:GLU:HG3	1.76	0.51
1:C:252:LEU:O	1:C:310:GLN:NE2	2.43	0.51
1:C:269:THR:O	1:C:271:VAL:HG12	2.11	0.51
1:D:445:GLN:HG3	1:D:446:ALA:N	2.26	0.51
1:A:51:GLY:O	1:A:52:PHE:HB2	2.10	0.51
1:A:91:TYR:O	1:A:95:HIS:HD2	1.92	0.51
1:B:39:ASN:N	1:B:39:ASN:HD22	2.09	0.51
1:B:203:GLN:HB2	3:B:682:HEM:CMC	2.41	0.51
1:D:80:LEU:C	1:D:82:LEU:H	2.18	0.51
1:D:513:ARG:O	1:D:514:PRO:C	2.54	0.51
1:A:43:ASN:O	1:A:44:ARG:HB2	2.10	0.51
1:A:216:ARG:HB3	1:A:220:PHE:CG	2.45	0.51
1:B:43:ASN:HD22	1:B:70:THR:HA	1.75	0.51
1:B:132:VAL:HG21	1:B:219:GLY:HA3	1.92	0.51
1:D:75:LEU:HG	1:D:79:LYS:HE2	1.93	0.51
1:C:42:GLN:O	1:C:69:CYS:HB2	2.10	0.51
1:C:241:GLN:NE2	1:C:329:PHE:CE1	2.78	0.51
1:A:74:PHE:HA	1:A:77:ARG:NE	2.26	0.51
1:A:105(A):ILE:HG23	1:A:107:PHE:CD1	2.46	0.51
1:A:273:MET:SD	1:A:290:GLU:HA	2.51	0.51
1:A:274:ILE:HG13	1:A:290:GLU:HG2	1.92	0.51
1:A:352:LEU:HD21	1:A:518:PHE:CZ	2.44	0.51
1:A:477:SER:O	1:A:480:GLU:HB2	2.11	0.51
1:B:171:LEU:HD23	1:B:502:GLU:OE2	2.11	0.51
1:B:184:ARG:NH1	1:B:441:PRO:HG3	2.26	0.51
1:B:187:PHE:HE2	1:B:392:PRO:HA	1.76	0.51
1:B:391:LEU:HD21	3:B:682:HEM:HAB	1.93	0.51
1:B:463:LEU:HD13	1:B:506:ALA:HB3	1.92	0.51
1:D:405:LYS:H	1:D:405:LYS:HD2	1.76	0.51
1:A:541:SER:HB2	1:A:543:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105(A):ILE:HG23	1:B:107:PHE:CD1	2.45	0.51
1:B:291:VAL:O	1:B:293:GLY:N	2.44	0.51
1:B:419:LEU:HB3	1:B:572:VAL:CG1	2.39	0.51
1:C:335:ILE:HA	1:C:559:ILE:HD11	1.92	0.51
1:C:543:GLN:OE1	1:D:127:PRO:HD2	2.11	0.51
1:D:345:ILE:CD1	1:D:534:LEU:HD23	2.38	0.51
1:A:513:ARG:O	1:A:514:PRO:C	2.53	0.51
1:B:35:PRO:HG3	1:B:54:GLN:O	2.12	0.51
1:C:34:ASN:HD22	1:C:156:ALA:HB2	1.76	0.51
1:C:109:ARG:NH2	1:C:359:LEU:O	2.43	0.51
1:C:150:ARG:HD3	1:C:379:SER:OG	2.11	0.51
1:C:175:LYS:HA	1:C:178:LEU:HB3	1.91	0.51
1:C:198:PHE:C	1:C:198:PHE:CD1	2.89	0.51
1:C:274:ILE:HG13	1:C:290:GLU:O	2.10	0.51
1:D:253:LYS:HZ3	1:D:269:THR:HG21	1.75	0.51
1:D:323:TRP:HH2	1:D:551:GLY:CA	2.22	0.51
1:A:80:LEU:C	1:A:82:LEU:H	2.18	0.50
1:A:424:GLU:O	1:A:428:ARG:HD2	2.10	0.50
1:A:509:VAL:HG13	1:A:509:VAL:O	2.11	0.50
1:C:150:ARG:NH2	1:C:458:MET:O	2.43	0.50
1:D:276:PRO:HB2	1:D:278:HIS:CE1	2.45	0.50
1:D:478:PHE:HZ	1:D:495:TYR:HB2	1.74	0.50
1:A:283:LEU:HD22	1:A:411:ASN:HB2	1.92	0.50
1:A:397:ILE:O	1:A:397:ILE:HG22	2.11	0.50
1:B:42:GLN:O	1:B:69:CYS:HB2	2.11	0.50
1:B:48:MET:HE3	1:B:49:SER:OG	2.11	0.50
1:B:427:THR:HB	1:B:428:ARG:HD2	1.94	0.50
1:D:273:MET:HA	1:D:290:GLU:HG3	1.94	0.50
1:A:197:MET:CE	1:A:423:VAL:HG13	2.42	0.50
1:A:410:ASN:CG	1:A:413:ILE:HG13	2.35	0.50
1:A:85:THR:CG2	1:A:86:PRO:HD2	2.41	0.50
1:A:198:PHE:HZ	1:A:352:LEU:CD1	2.20	0.50
1:A:215:LYS:HE3	1:A:222:ARG:HH12	1.77	0.50
1:A:291:VAL:O	1:A:293:GLY:N	2.44	0.50
1:B:197:MET:HE2	1:B:423:VAL:HG13	1.93	0.50
1:B:342:LYS:HD2	1:B:346:GLU:HG3	1.94	0.50
1:B:444:VAL:HG12	1:B:444:VAL:O	2.09	0.50
1:C:43:ASN:O	1:C:44:ARG:HB2	2.11	0.50
1:C:55:TYR:HE2	1:C:57:CYS:SG	2.34	0.50
1:C:530:SER:O	1:C:534:LEU:HD13	2.11	0.50
1:B:501:MET:HG3	1:B:506:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:VAL:HG21	1:C:219:GLY:HA3	1.92	0.50
1:C:513:ARG:O	1:C:514:PRO:C	2.54	0.50
1:D:206:THR:HB	1:D:210:PHE:HD2	1.71	0.50
1:D:350:GLN:NE2	1:D:359:LEU:H	2.09	0.50
1:A:39:ASN:OD1	1:A:461:GLN:NE2	2.44	0.50
1:A:40:PRO:HB2	1:A:55:TYR:CE2	2.47	0.50
1:B:150:ARG:HD3	1:B:379:SER:OG	2.11	0.50
1:C:41:CYS:SG	1:C:47:CYS:HB2	2.52	0.50
1:C:381:PHE:O	1:C:385:TYR:HB2	2.12	0.50
1:C:397:ILE:HG21	1:C:417:HIS:ND1	2.27	0.50
1:A:137:LYS:HG3	1:B:549:THR:HG23	1.94	0.50
1:A:565:GLN:HG3	1:D:268:ASP:OD1	2.12	0.50
1:B:311:ARG:O	1:B:315:ILE:HG13	2.11	0.50
1:C:501:MET:CE	1:C:505:PRO:HB2	2.42	0.50
1:D:41:CYS:SG	1:D:47:CYS:HB2	2.51	0.50
1:D:187:PHE:CD1	1:D:187:PHE:C	2.90	0.50
1:D:335:ILE:HG12	1:D:550:PHE:HB3	1.93	0.50
1:A:568:ILE:HG13	1:A:572:VAL:CG2	2.40	0.50
1:D:506:ALA:O	1:D:510:GLU:HB2	2.12	0.50
1:A:206:THR:HB	1:A:210:PHE:HD2	1.76	0.50
1:C:509:VAL:HG22	1:C:509:VAL:O	2.12	0.50
1:D:105:ASN:O	1:D:106:PRO:HD3	2.12	0.50
1:D:187:PHE:HE2	1:D:392:PRO:HA	1.77	0.50
1:D:501:MET:CE	1:D:505:PRO:HB2	2.42	0.50
1:B:208:GLN:NE2	1:B:228:VAL:HA	2.26	0.49
1:B:323:TRP:CH2	1:B:551:GLY:HA2	2.36	0.49
1:B:350:GLN:HE22	1:B:359:LEU:H	1.60	0.49
1:C:190:ASP:CG	1:C:192:GLN:H	2.20	0.49
1:D:37:CYS:O	1:D:39:ASN:ND2	2.45	0.49
1:D:171:LEU:HD23	1:D:502:GLU:OE2	2.12	0.49
1:D:247:PHE:HA	1:D:325:ASP:OD2	2.12	0.49
1:B:391:LEU:HB2	1:B:441:PRO:HG2	1.94	0.49
1:D:120:ARG:O	1:D:123:LEU:HD23	2.12	0.49
1:D:509:VAL:HG22	1:D:509:VAL:O	2.12	0.49
1:B:293:GLY:HA2	1:B:299:MET:HE2	1.94	0.49
1:C:105:ASN:O	1:C:106:PRO:HD3	2.12	0.49
1:D:114:LYS:HG3	1:D:365:LEU:HB3	1.94	0.49
1:A:556:PHE:CD2	1:A:557:LYS:HE2	2.48	0.49
1:B:172:PRO:HG2	1:B:495:TYR:CD1	2.48	0.49
1:B:497:ASP:HB3	1:B:500:VAL:CG2	2.42	0.49
1:B:509:VAL:HG22	1:B:509:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:GLN:NE2	1:B:136:TYR:HD2	2.09	0.49
1:D:150:ARG:HG2	1:D:152:LEU:O	2.11	0.49
1:D:430:ILE:HG13	1:D:582:VAL:HG21	1.95	0.49
1:D:472:LEU:HD21	1:D:524:GLU:HG3	1.93	0.49
1:A:34:ASN:HD22	1:A:156:ALA:CB	2.25	0.49
1:B:80:LEU:C	1:B:82:LEU:H	2.20	0.49
1:B:150:ARG:HG2	1:B:152:LEU:O	2.12	0.49
1:C:276:PRO:CB	1:C:278:HIS:CE1	2.95	0.49
1:D:210:PHE:CE1	1:D:382:ASN:CA	2.94	0.49
1:A:308:GLU:HA	1:A:308:GLU:OE1	2.13	0.49
1:A:342:LYS:NZ	1:A:560:ASN:HA	2.27	0.49
1:B:191:PRO:HD2	1:B:433:ARG:HG3	1.95	0.49
1:B:273:MET:HA	1:B:290:GLU:HG3	1.95	0.49
1:C:48:MET:HE3	1:C:49:SER:HG	1.76	0.49
1:C:182:LEU:C	1:C:438:ARG:HA	2.38	0.49
1:D:176:GLU:HB3	1:D:494:LEU:HD21	1.95	0.49
1:A:34:ASN:HD22	1:A:156:ALA:HB2	1.76	0.49
1:B:260:GLU:HB2	1:B:262:TYR:CE2	2.48	0.49
1:C:105:ASN:CG	1:C:105(A):ILE:N	2.71	0.49
1:C:183:LEU:HD21	1:C:445:GLN:CB	2.42	0.49
1:A:405:LYS:H	1:A:405:LYS:CD	2.23	0.49
1:A:430:ILE:HG13	1:A:582:VAL:HG21	1.95	0.49
1:A:583:GLN:NE2	1:D:282:ASN:CG	2.69	0.49
1:B:241:GLN:NE2	1:B:329:PHE:CE1	2.81	0.49
1:B:350:GLN:NE2	1:B:359:LEU:H	2.10	0.49
1:B:501:MET:CE	1:B:505:PRO:HB2	2.42	0.49
1:B:513:ARG:O	1:B:514:PRO:C	2.56	0.49
1:C:80:LEU:C	1:C:82:LEU:H	2.21	0.49
1:C:419:LEU:HB3	1:C:572:VAL:CG1	2.42	0.49
1:D:150:ARG:HD3	1:D:379:SER:OG	2.13	0.49
1:A:39:ASN:N	1:A:39:ASN:ND2	2.61	0.49
1:A:509:VAL:HG22	1:A:509:VAL:O	2.13	0.49
1:B:43:ASN:O	1:B:44:ARG:HB2	2.12	0.49
1:B:176:GLU:CD	1:B:180:LYS:HE3	2.37	0.49
1:B:402:TYR:CE1	1:B:417:HIS:HE1	2.30	0.49
1:C:66:GLY:O	1:C:68:ASN:N	2.46	0.49
1:C:105(A):ILE:CG2	1:C:108:LEU:HB2	2.43	0.49
1:D:197:MET:HE2	1:D:423:VAL:HG13	1.93	0.49
1:C:381:PHE:CD1	1:C:529:PHE:HB3	2.48	0.48
1:C:430:ILE:HG13	1:C:582:VAL:HG21	1.94	0.48
1:C:543:GLN:HE22	1:D:127:PRO:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:PHE:CD1	1:D:529:PHE:HB2	2.48	0.48
1:D:402:TYR:CE1	1:D:417:HIS:HE1	2.31	0.48
1:A:323:TRP:HH2	1:A:551:GLY:CA	2.24	0.48
1:B:105(A):ILE:CG2	1:B:108:LEU:HB2	2.42	0.48
1:B:253:LYS:HZ3	1:B:269:THR:HG21	1.78	0.48
1:C:283:LEU:HA	1:C:411:ASN:OD1	2.13	0.48
1:D:124:ILE:HD11	1:D:528:PRO:HB3	1.94	0.48
1:A:210:PHE:CE1	1:A:382:ASN:CA	2.94	0.48
1:A:245:ARG:HD2	1:A:247:PHE:CD1	2.48	0.48
1:A:283:LEU:HD13	1:A:411:ASN:HA	1.94	0.48
1:B:183:LEU:O	1:B:438:ARG:HB3	2.13	0.48
1:C:335:ILE:HG23	1:C:559:ILE:CD1	2.43	0.48
1:D:320:HIS:CE1	1:D:551:GLY:O	2.67	0.48
1:A:197:MET:HE1	1:A:300:MET:HE1	1.94	0.48
1:A:556:PHE:HD2	1:A:557:LYS:HE2	1.78	0.48
1:B:208:GLN:NE2	1:B:228:VAL:HG13	2.26	0.48
1:B:419:LEU:O	1:B:423:VAL:HG23	2.13	0.48
1:C:136:TYR:CD2	1:D:327:GLN:NE2	2.81	0.48
1:C:419:LEU:O	1:C:423:VAL:HG23	2.13	0.48
1:D:283:LEU:O	1:D:285:PHE:N	2.46	0.48
1:A:124:ILE:N	1:A:124:ILE:HD12	2.28	0.48
1:B:467:ARG:NH1	1:B:521:THR:OG1	2.46	0.48
1:C:197:MET:CE	1:C:423:VAL:HG13	2.44	0.48
1:C:546:LYS:C	1:C:547:PRO:O	2.53	0.48
1:D:35:PRO:HG3	1:D:54:GLN:O	2.14	0.48
1:D:556:PHE:CD2	1:D:557:LYS:HE2	2.49	0.48
1:A:48:MET:HE3	1:A:49:SER:HG	1.79	0.48
1:A:338:GLY:HA3	1:A:559:ILE:HG13	1.96	0.48
1:B:40:PRO:HB2	1:B:55:TYR:CE2	2.48	0.48
1:C:106:PRO:C	1:C:108:LEU:H	2.22	0.48
1:D:229:ASP:OD1	1:D:231:ASN:HB3	2.13	0.48
1:A:322:GLU:HB3	1:B:52:PHE:CE1	2.49	0.48
1:A:463:LEU:HD22	1:A:506:ALA:HB1	1.95	0.48
1:B:424:GLU:O	1:B:428:ARG:HD2	2.13	0.48
1:C:204:HIS:HE2	1:C:305:TRP:CD1	2.32	0.48
1:C:291:VAL:O	1:C:293:GLY:N	2.46	0.48
1:C:424:GLU:O	1:C:428:ARG:HD2	2.13	0.48
1:A:106:PRO:C	1:A:108:LEU:H	2.21	0.48
1:A:150:ARG:NH2	1:A:458:MET:O	2.46	0.48
1:B:295:VAL:HG12	1:B:297:GLY:H	1.79	0.48
1:C:273:MET:HE2	1:C:287:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLY:HA2	1:C:299:MET:CE	2.44	0.48
1:C:482:THR:CG2	1:C:509:VAL:HG22	2.43	0.48
1:D:85:THR:HG23	1:D:86:PRO:HD2	1.94	0.48
1:D:149:THR:O	1:D:378:ALA:HA	2.13	0.48
1:D:312:VAL:HA	1:D:315:ILE:HD12	1.95	0.48
1:D:335:ILE:HG23	1:D:559:ILE:CD1	2.44	0.48
1:D:338:GLY:HA3	1:D:559:ILE:CG1	2.44	0.48
1:D:463:LEU:HD22	1:D:506:ALA:CB	2.44	0.48
1:A:283:LEU:HB2	1:A:411:ASN:HB2	1.95	0.48
1:B:48:MET:SD	1:B:49:SER:N	2.86	0.48
1:B:187:PHE:CE2	1:B:392:PRO:HA	2.49	0.48
1:B:386:HIS:CE1	3:B:682:HEM:CAD	2.96	0.48
1:D:132:VAL:HG21	1:D:219:GLY:HA3	1.96	0.48
1:D:136:TYR:O	1:D:136:TYR:HD1	1.97	0.48
1:A:114:LYS:HG3	1:A:365:LEU:HB3	1.95	0.48
1:B:124:ILE:HD12	1:B:124:ILE:N	2.29	0.48
1:B:127:PRO:HA	1:B:128:PRO:HD2	1.74	0.48
1:C:34:ASN:HD22	1:C:156:ALA:CB	2.26	0.48
1:C:91:TYR:O	1:C:95:HIS:HD2	1.97	0.48
1:C:320:HIS:CE1	1:C:551:GLY:O	2.67	0.48
1:C:389:PRO:HG2	1:C:508:LEU:HD22	1.96	0.48
1:D:175:LYS:HA	1:D:178:LEU:HB3	1.95	0.48
1:D:513:ARG:NH1	1:D:523:VAL:HG11	2.29	0.48
1:A:132:VAL:HG21	1:A:219:GLY:HA3	1.96	0.47
1:A:213:ASP:OD2	1:A:216:ARG:HB2	2.13	0.47
1:B:187:PHE:CD1	1:B:187:PHE:C	2.92	0.47
1:C:187:PHE:HE2	1:C:392:PRO:HA	1.78	0.47
1:C:433:ARG:HH21	1:C:512:PRO:HB3	1.79	0.47
1:C:457:GLU:C	1:C:459:LYS:H	2.22	0.47
1:C:478:PHE:HZ	1:C:495:TYR:CB	2.26	0.47
1:D:335:ILE:HG23	1:D:559:ILE:HD12	1.95	0.47
1:A:264:PRO:HB2	1:A:269:THR:CG2	2.44	0.47
1:A:513:ARG:NH1	1:A:523:VAL:HG11	2.29	0.47
1:B:38:SER:C	1:B:40:PRO:HD3	2.38	0.47
1:B:91:TYR:O	1:B:95:HIS:HD2	1.96	0.47
1:B:410:ASN:CG	1:B:413:ILE:HG13	2.39	0.47
1:C:105(A):ILE:HG23	1:C:107:PHE:CD1	2.49	0.47
1:C:128:PRO:HG3	1:C:376:ARG:CZ	2.44	0.47
1:D:92:ILE:HA	1:D:96:PHE:HE1	1.78	0.47
1:D:109:ARG:NH2	1:D:360:LYS:HB2	2.30	0.47
1:D:495:TYR:HE2	1:D:502:GLU:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:CE1	1:A:233:ILE:HG13	2.49	0.47
1:A:253:LYS:HZ3	1:A:269:THR:HG21	1.79	0.47
1:A:364:GLU:HA	1:A:367:PHE:CG	2.49	0.47
1:B:335:ILE:HG23	1:B:559:ILE:CD1	2.44	0.47
1:B:463:LEU:HD22	1:B:506:ALA:CB	2.44	0.47
1:D:253:LYS:HB2	1:D:253:LYS:NZ	2.29	0.47
1:D:303:THR:HG22	1:D:307:ARG:HD2	1.96	0.47
1:D:397:ILE:HG21	1:D:417:HIS:ND1	2.28	0.47
1:A:387:TRP:HB2	3:A:682:HEM:CBC	2.45	0.47
1:A:403:SER:O	1:A:404:PHE:C	2.56	0.47
1:B:106:PRO:C	1:B:108:LEU:H	2.22	0.47
1:B:253:LYS:HE2	1:B:269:THR:CG2	2.43	0.47
1:B:338:GLY:HA3	1:B:559:ILE:HG13	1.96	0.47
1:C:98:GLY:HA2	1:C:101:ASN:HD22	1.79	0.47
1:A:342:LYS:HZ3	1:A:560:ASN:HA	1.79	0.47
1:A:381:PHE:O	1:A:385:TYR:HB2	2.14	0.47
1:A:387:TRP:O	1:A:390:LEU:HB2	2.15	0.47
1:A:497:ASP:OD2	1:A:499:ASP:HB2	2.14	0.47
1:B:244:LEU:C	1:B:253:LYS:HZ2	2.23	0.47
1:C:283:LEU:O	1:C:285:PHE:N	2.47	0.47
1:C:352:LEU:HD23	4:C:701:S58:C9	2.44	0.47
1:C:397:ILE:O	1:C:398:GLU:C	2.57	0.47
1:A:273:MET:HA	1:A:290:GLU:CG	2.44	0.47
1:B:197:MET:HE1	1:B:300:MET:HE1	1.97	0.47
1:C:98:GLY:O	1:C:101:ASN:HB2	2.14	0.47
1:C:122:TYR:CE1	1:C:123:LEU:HD13	2.50	0.47
1:C:213:ASP:OD2	1:C:216:ARG:HB2	2.14	0.47
1:D:264:PRO:HG2	1:D:286:ALA:CB	2.42	0.47
1:A:42:GLN:O	1:A:69:CYS:HB2	2.14	0.47
1:A:150:ARG:NH1	1:A:150:ARG:HG2	2.30	0.47
1:A:197:MET:HE2	1:A:423:VAL:HG13	1.96	0.47
1:A:397:ILE:O	1:A:398:GLU:C	2.57	0.47
1:A:501:MET:CE	1:A:505:PRO:HB2	2.43	0.47
1:A:518:PHE:CE1	4:A:701:S58:H9	2.45	0.47
1:B:397:ILE:O	1:B:398:GLU:C	2.57	0.47
1:B:465:GLU:OE2	1:B:468:LYS:HE2	2.15	0.47
1:B:476:THR:OG1	1:B:480:GLU:HG3	2.15	0.47
1:C:403:SER:O	1:C:404:PHE:C	2.58	0.47
1:D:57:CYS:HB3	1:D:69:CYS:SG	2.55	0.47
1:D:131:ASN:ND2	1:D:141:ALA:HA	2.29	0.47
1:A:124:ILE:HD11	1:A:528:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:O	1:A:378:ALA:HA	2.14	0.47
1:A:254:TYR:C	1:A:254:TYR:HD1	2.22	0.47
1:A:397:ILE:HG21	1:A:417:HIS:ND1	2.30	0.47
1:C:110:SER:O	1:C:114:LYS:HB2	2.15	0.47
1:D:42:GLN:O	1:D:69:CYS:HB2	2.14	0.47
1:D:172:PRO:HG2	1:D:495:TYR:CD1	2.50	0.47
1:D:204:HIS:HE2	1:D:305:TRP:CD1	2.33	0.47
1:A:48:MET:O	1:A:55:TYR:HA	2.15	0.47
1:A:184:ARG:HH11	1:A:441:PRO:HG3	1.80	0.47
1:A:245:ARG:HG2	1:A:246:LEU:N	2.30	0.47
1:B:152:LEU:HB2	1:B:466:TYR:CZ	2.50	0.47
1:B:254:TYR:HD2	1:B:310:GLN:HE21	1.63	0.47
1:B:478:PHE:HZ	1:B:495:TYR:CB	2.28	0.47
1:B:518:PHE:HE1	4:B:701:S58:H9	1.80	0.47
1:C:136:TYR:HD1	1:C:136:TYR:O	1.98	0.47
1:C:149:THR:O	1:C:378:ALA:HA	2.15	0.47
1:C:162:PRO:O	1:C:163:MET:HE2	2.15	0.47
1:D:235:GLY:HA3	1:D:240:ARG:HG2	1.97	0.47
1:A:187:PHE:HE2	1:A:392:PRO:HA	1.80	0.47
1:A:513:ARG:HH11	4:A:701:S58:HN31	1.63	0.47
1:B:85:THR:CG2	1:B:86:PRO:HD2	2.44	0.47
1:B:312:VAL:HA	1:B:315:ILE:HD12	1.97	0.47
1:B:457:GLU:C	1:B:459:LYS:H	2.23	0.47
1:B:482:THR:CG2	1:B:509:VAL:HG22	2.45	0.47
1:C:125:ASP:O	1:C:128:PRO:HA	2.15	0.47
1:D:381:PHE:CD1	1:D:529:PHE:HB3	2.49	0.47
1:B:269:THR:O	1:B:271:VAL:N	2.45	0.46
1:C:134:TYR:CD1	1:C:136:TYR:CE1	2.89	0.46
1:D:48:MET:O	1:D:55:TYR:HA	2.15	0.46
1:D:176:GLU:O	1:D:494:LEU:HD11	2.15	0.46
1:D:257:ILE:HD12	1:D:262:TYR:CD2	2.49	0.46
1:A:275:TYR:CZ	1:A:284:GLN:HA	2.48	0.46
1:A:502:GLU:HB2	1:A:505:PRO:HD2	1.98	0.46
1:A:546:LYS:O	1:A:547:PRO:O	2.34	0.46
1:B:92:ILE:HA	1:B:96:PHE:CE1	2.50	0.46
1:B:116:VAL:HG23	1:B:117:LEU:N	2.31	0.46
1:B:188:ILE:O	1:B:432:GLY:HA2	2.14	0.46
1:B:210:PHE:CE1	1:B:382:ASN:CA	2.98	0.46
1:B:276:PRO:CD	1:B:279:ILE:HD13	2.37	0.46
1:C:509:VAL:O	1:C:509:VAL:HG13	2.14	0.46
1:D:187:PHE:CE2	1:D:392:PRO:HA	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:O	1:A:306:LEU:HD11	2.14	0.46
1:B:162:PRO:O	1:B:163:MET:HE2	2.16	0.46
1:B:176:GLU:O	1:B:180:LYS:HG3	2.15	0.46
1:B:194:SER:OG	1:B:351:HIS:HE1	1.98	0.46
1:B:257:ILE:HD12	1:B:262:TYR:CD2	2.51	0.46
1:C:182:LEU:O	1:C:438:ARG:HA	2.15	0.46
1:C:278:HIS:CD2	1:C:279:ILE:HD12	2.51	0.46
1:A:34:ASN:HA	1:A:35:PRO:HD2	1.73	0.46
1:A:283:LEU:O	1:A:285:PHE:N	2.48	0.46
1:A:549:THR:HG23	1:B:137:LYS:HG3	1.98	0.46
1:C:225:GLY:O	1:C:226:HIS:C	2.58	0.46
1:C:386:HIS:CE1	3:C:682:HEM:CAD	2.98	0.46
1:C:414:LEU:HD11	1:C:419:LEU:HD22	1.97	0.46
1:A:184:ARG:O	1:A:442:ILE:HD11	2.15	0.46
1:A:478:PHE:HZ	1:A:495:TYR:CB	2.28	0.46
1:B:48:MET:O	1:B:50:THR:HG23	2.15	0.46
1:B:213:ASP:CG	1:B:216:ARG:HB2	2.40	0.46
1:C:399:ASP:O	1:C:400:GLN:HB2	2.14	0.46
1:C:402:TYR:CE1	1:C:417:HIS:HE1	2.33	0.46
1:D:232:HIS:ND1	1:D:233:ILE:HG13	2.31	0.46
1:D:450:ALA:O	1:D:454:GLN:HB2	2.15	0.46
1:A:136:TYR:HD1	1:A:136:TYR:O	1.97	0.46
1:B:98:GLY:HA2	1:B:101:ASN:HD22	1.81	0.46
1:C:175:LYS:HG2	1:C:178:LEU:HD13	1.96	0.46
1:D:463:LEU:HD13	1:D:506:ALA:HB3	1.98	0.46
1:A:113:MET:CE	1:A:117:LEU:HD13	2.46	0.46
1:A:244:LEU:C	1:A:253:LYS:HZ2	2.23	0.46
1:A:381:PHE:CD1	1:A:529:PHE:CB	2.99	0.46
1:B:176:GLU:OE2	1:B:180:LYS:HE3	2.16	0.46
1:C:131:ASN:ND2	1:C:141:ALA:HA	2.30	0.46
1:A:198:PHE:CD2	1:A:580:PHE:HB3	2.50	0.46
1:C:39:ASN:N	1:C:40:PRO:CD	2.77	0.46
1:C:97:LYS:HG2	1:C:101:ASN:ND2	2.31	0.46
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.84	0.46
1:C:308:GLU:OE1	1:C:308:GLU:HA	2.16	0.46
1:A:281:GLU:CA	1:A:284:GLN:HG3	2.37	0.46
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.98	0.46
1:B:190:ASP:CG	1:B:192:GLN:H	2.24	0.46
1:C:281:GLU:HG2	1:C:284:GLN:NE2	2.31	0.46
1:C:323:TRP:CH2	1:C:551:GLY:HA2	2.40	0.46
1:D:184:ARG:O	1:D:442:ILE:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:ILE:HG13	1:D:572:VAL:CG2	2.46	0.46
1:A:274:ILE:HG13	1:A:290:GLU:O	2.16	0.46
1:B:230:LEU:N	1:B:230:LEU:CD2	2.79	0.46
1:C:198:PHE:CD2	1:C:580:PHE:HB3	2.47	0.46
1:C:291:VAL:CG2	1:C:294:LEU:HD12	2.46	0.46
1:C:319:GLU:CD	1:C:554:VAL:HG21	2.41	0.46
1:D:509:VAL:O	1:D:509:VAL:HG13	2.16	0.46
1:A:402:TYR:CE1	1:A:417:HIS:HE1	2.35	0.45
1:B:64:PHE:CD2	1:B:70:THR:O	2.69	0.45
1:B:123:LEU:N	1:B:123:LEU:HD22	2.31	0.45
1:B:513:ARG:HH12	1:B:523:VAL:HG11	1.79	0.45
1:C:184:ARG:HH11	1:C:441:PRO:HG3	1.81	0.45
1:C:208:GLN:OE1	1:C:230:LEU:HA	2.15	0.45
1:D:105(A):ILE:CG2	1:D:108:LEU:HB2	2.45	0.45
1:D:152:LEU:HD23	1:D:152:LEU:HA	1.80	0.45
1:D:184:ARG:NH1	1:D:441:PRO:HG3	2.30	0.45
1:A:123:LEU:N	1:A:123:LEU:HD22	2.30	0.45
1:B:275:TYR:CZ	1:B:284:GLN:HA	2.48	0.45
1:B:449:LYS:O	1:B:452:ILE:N	2.50	0.45
1:B:461:GLN:HB2	1:B:466:TYR:CE1	2.52	0.45
1:C:150:ARG:NH1	1:C:150:ARG:HG2	2.30	0.45
1:C:171:LEU:HD23	1:C:502:GLU:OE2	2.16	0.45
1:C:184:ARG:HB3	1:C:439:ASN:C	2.40	0.45
1:D:40:PRO:HB2	1:D:55:TYR:CE2	2.51	0.45
1:B:191:PRO:HG3	1:B:433:ARG:NH1	2.32	0.45
1:B:319:GLU:CD	1:B:554:VAL:HG21	2.41	0.45
1:C:191:PRO:HG3	1:C:433:ARG:CZ	2.47	0.45
1:C:575:CYS:N	1:C:576:PRO:CD	2.79	0.45
1:D:467:ARG:NH1	1:D:521:THR:OG1	2.48	0.45
1:B:303:THR:HG22	1:B:307:ARG:HD2	1.99	0.45
1:B:490:GLU:O	1:B:493:ALA:HB3	2.16	0.45
1:C:495:TYR:HE2	1:C:502:GLU:HG3	1.82	0.45
1:D:111:LEU:HD23	1:D:111:LEU:HA	1.81	0.45
1:D:122:TYR:CD1	1:D:122:TYR:C	2.94	0.45
1:D:123:LEU:O	1:D:469:ARG:NH2	2.47	0.45
1:D:172:PRO:HG2	1:D:495:TYR:CE1	2.52	0.45
1:D:266:VAL:HG13	1:D:267:LYS:N	2.32	0.45
1:D:291:VAL:CG2	1:D:294:LEU:HD12	2.46	0.45
1:D:352:LEU:HD23	4:D:701:S58:C10	2.47	0.45
1:D:386:HIS:CE1	3:D:682:HEM:CAD	2.99	0.45
1:D:575:CYS:N	1:D:576:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:CG1	1:A:267:LYS:N	2.80	0.45
1:A:397:ILE:O	1:A:398:GLU:O	2.35	0.45
1:C:206:THR:HB	1:C:210:PHE:HD2	1.80	0.45
1:C:271:VAL:HG11	1:C:286:ALA:HB1	1.98	0.45
1:D:128:PRO:HG3	1:D:376:ARG:CZ	2.47	0.45
1:D:293:GLY:HA2	1:D:299:MET:HE2	1.98	0.45
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.86	0.45
1:A:264:PRO:HB2	1:A:269:THR:HG23	1.99	0.45
1:A:281:GLU:HA	1:A:284:GLN:HE21	1.81	0.45
1:B:183:LEU:HD21	1:B:445:GLN:CB	2.46	0.45
1:C:122:TYR:CD1	1:C:122:TYR:C	2.95	0.45
1:C:352:LEU:O	4:C:701:S58:C9	2.65	0.45
1:D:106:PRO:C	1:D:108:LEU:H	2.24	0.45
1:D:150:ARG:HG2	1:D:150:ARG:NH1	2.30	0.45
1:D:398:GLU:HG2	1:D:425:SER:HA	1.99	0.45
1:D:448:ALA:O	1:D:452:ILE:HG13	2.15	0.45
1:A:311:ARG:O	1:A:315:ILE:HG13	2.16	0.45
1:A:414:LEU:HD11	1:A:419:LEU:HD22	1.98	0.45
1:B:573:LYS:O	1:B:573:LYS:HG3	2.15	0.45
1:C:253:LYS:HE2	1:C:269:THR:CG2	2.47	0.45
1:C:295:VAL:HB	1:C:298:LEU:HD22	1.98	0.45
1:D:43:ASN:O	1:D:44:ARG:CB	2.64	0.45
1:D:213:ASP:OD1	1:D:215:LYS:HG2	2.17	0.45
1:D:388:HIS:CD2	1:D:444:VAL:HG11	2.52	0.45
1:D:397:ILE:O	1:D:397:ILE:HG22	2.16	0.45
1:A:128:PRO:HG3	1:A:376:ARG:CZ	2.47	0.45
1:A:266:VAL:HG13	1:A:267:LYS:N	2.31	0.45
1:B:110:SER:O	1:B:114:LYS:HB2	2.16	0.45
1:C:75:LEU:HA	1:C:78:ILE:HD12	1.97	0.45
1:D:230:LEU:CD2	1:D:230:LEU:N	2.80	0.45
1:D:275:TYR:CZ	1:D:284:GLN:HA	2.52	0.45
1:A:43:ASN:HB2	1:A:69:CYS:O	2.16	0.45
1:B:276:PRO:HB2	1:B:278:HIS:CE1	2.52	0.45
1:C:40:PRO:HB2	1:C:55:TYR:CE2	2.52	0.45
1:C:172:PRO:HG2	1:C:495:TYR:CD1	2.52	0.45
1:D:246:LEU:O	1:D:247:PHE:HB2	2.17	0.45
1:D:323:TRP:CH2	1:D:551:GLY:HA2	2.39	0.45
1:D:364:GLU:HA	1:D:367:PHE:CD2	2.52	0.45
1:A:172:PRO:HG2	1:A:495:TYR:CD1	2.52	0.45
4:A:701:S58:H10	4:A:701:S58:C11	2.47	0.45
1:B:568:ILE:HG13	1:B:572:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:LEU:N	1:C:123:LEU:HD22	2.32	0.45
1:C:308:GLU:OE1	1:C:311:ARG:NH1	2.50	0.45
1:D:110:SER:O	1:D:114:LYS:HB2	2.17	0.45
1:D:190:ASP:HA	1:D:433:ARG:HB2	1.98	0.45
1:D:518:PHE:CG	1:D:522:MET:HG2	2.52	0.45
1:D:527:ALA:N	1:D:528:PRO:CD	2.80	0.45
1:A:279:ILE:HG12	1:A:283:LEU:HD23	1.99	0.44
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.81	0.44
1:B:335:ILE:HG23	1:B:559:ILE:HD12	1.98	0.44
1:C:478:PHE:CE1	1:C:492:LYS:HA	2.52	0.44
1:D:203:GLN:NE2	1:D:298:LEU:HD13	2.33	0.44
1:D:463:LEU:HD22	1:D:506:ALA:HB1	1.97	0.44
1:A:33:ALA:O	1:A:34:ASN:C	2.60	0.44
1:A:323:TRP:CH2	1:A:551:GLY:HA2	2.41	0.44
1:A:391:LEU:HB2	1:A:441:PRO:HG2	1.98	0.44
1:B:97:LYS:HG2	1:B:101:ASN:ND2	2.32	0.44
1:B:211:LYS:O	1:B:212:THR:C	2.60	0.44
1:C:381:PHE:CD1	1:C:529:PHE:HB2	2.52	0.44
1:D:213:ASP:CG	1:D:216:ARG:HB2	2.42	0.44
1:A:272:GLU:HB3	1:A:290:GLU:OE2	2.16	0.44
1:B:235:GLY:HA3	1:B:240:ARG:HG2	1.98	0.44
1:B:253:LYS:O	1:B:306:LEU:HD11	2.17	0.44
1:B:283:LEU:HB2	1:B:411:ASN:CG	2.43	0.44
1:B:364:GLU:HA	1:B:367:PHE:CD2	2.52	0.44
1:B:450:ALA:O	1:B:454:GLN:HB2	2.17	0.44
1:B:546:LYS:O	1:B:547:PRO:O	2.34	0.44
1:C:83:LYS:O	1:C:83:LYS:HG3	2.17	0.44
1:C:176:GLU:O	1:C:494:LEU:HD11	2.17	0.44
1:C:188:ILE:O	1:C:432:GLY:HA2	2.17	0.44
1:C:293:GLY:HA2	1:C:299:MET:HE2	1.99	0.44
1:D:33:ALA:O	1:D:34:ASN:C	2.60	0.44
1:A:122:TYR:CD1	1:A:122:TYR:C	2.95	0.44
1:A:273:MET:HA	1:A:290:GLU:HG3	1.99	0.44
1:A:327:GLN:HE22	1:B:48:MET:HE2	1.82	0.44
1:A:547:PRO:O	1:A:549:THR:N	2.48	0.44
1:B:131:ASN:ND2	1:B:141:ALA:HA	2.32	0.44
1:B:247:PHE:HA	1:B:325:ASP:OD2	2.18	0.44
1:C:126:SER:HA	1:C:127:PRO:C	2.42	0.44
1:C:208:GLN:NE2	1:C:228:VAL:HG13	2.32	0.44
1:C:312:VAL:O	1:C:315:ILE:N	2.51	0.44
1:D:397:ILE:O	1:D:398:GLU:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASN:O	1:A:44:ARG:CB	2.65	0.44
1:A:125:ASP:O	1:A:128:PRO:HA	2.18	0.44
1:B:433:ARG:HH21	1:B:512:PRO:HB2	1.82	0.44
1:B:463:LEU:HD22	1:B:506:ALA:HB1	2.00	0.44
1:C:105(A):ILE:HD12	1:C:108:LEU:HD12	1.99	0.44
1:C:283:LEU:C	1:C:283:LEU:HD12	2.43	0.44
1:C:283:LEU:HB2	1:C:411:ASN:HB2	1.99	0.44
1:A:291:VAL:CG2	1:A:294:LEU:HD12	2.48	0.44
1:A:396:ASN:CB	1:A:401:GLU:HG2	2.44	0.44
1:B:39:ASN:N	1:B:40:PRO:CD	2.80	0.44
1:B:291:VAL:HG22	1:B:294:LEU:HD12	2.00	0.44
1:B:384:LEU:HD12	1:B:384:LEU:C	2.42	0.44
1:B:450:ALA:O	1:B:451:SER:C	2.61	0.44
1:C:48:MET:O	1:C:55:TYR:HA	2.17	0.44
1:C:183:LEU:O	1:C:438:ARG:HB3	2.17	0.44
1:C:184:ARG:HB3	1:C:439:ASN:HA	2.00	0.44
1:A:171:LEU:HD23	1:A:502:GLU:OE2	2.17	0.44
1:A:184:ARG:HB3	1:A:439:ASN:C	2.43	0.44
1:A:187:PHE:CE2	1:A:392:PRO:HA	2.53	0.44
1:A:465:GLU:OE2	1:A:468:LYS:HE2	2.17	0.44
1:B:34:ASN:HA	1:B:35:PRO:HD2	1.69	0.44
1:B:152:LEU:HD21	1:B:469:ARG:HD3	2.00	0.44
1:B:338:GLY:HA3	1:B:559:ILE:CG1	2.48	0.44
1:B:518:PHE:CG	1:B:522:MET:HG2	2.52	0.44
1:B:575:CYS:N	1:B:576:PRO:CD	2.80	0.44
1:D:39:ASN:N	1:D:40:PRO:CD	2.80	0.44
1:D:403:SER:O	1:D:404:PHE:C	2.60	0.44
1:A:83:LYS:O	1:A:83:LYS:HG3	2.17	0.44
1:A:131:ASN:ND2	1:A:141:ALA:HA	2.33	0.44
1:A:308:GLU:OE1	1:A:311:ARG:NH1	2.51	0.44
1:A:527:ALA:N	1:A:528:PRO:CD	2.80	0.44
1:B:122:TYR:CD1	1:B:122:TYR:C	2.95	0.44
1:C:187:PHE:CD1	1:C:187:PHE:C	2.95	0.44
1:C:253:LYS:NZ	1:C:253:LYS:HB2	2.32	0.44
1:C:281:GLU:HA	1:C:284:GLN:HE21	1.82	0.44
1:C:287:VAL:HG11	1:C:299:MET:SD	2.58	0.44
1:C:335:ILE:HG23	1:C:559:ILE:HD12	1.98	0.44
1:C:353:SER:HA	4:C:701:S58:C8	2.47	0.44
1:D:244:LEU:C	1:D:253:LYS:HZ2	2.26	0.44
1:D:283:LEU:HB2	1:D:411:ASN:CB	2.47	0.44
1:D:412:SER:O	1:D:413:ILE:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLN:NE2	1:A:329:PHE:CZ	2.86	0.44
1:A:303:THR:HG22	1:A:307:ARG:HD2	2.00	0.44
1:A:316:LEU:HB3	1:A:328:LEU:CD2	2.48	0.44
1:A:338:GLY:HA3	1:A:559:ILE:CG1	2.48	0.44
1:A:389:PRO:HG2	1:A:508:LEU:HD22	2.00	0.44
1:B:113:MET:HE3	1:B:117:LEU:HD13	1.99	0.44
1:C:255:GLN:NE2	1:C:265:THR:HG23	2.32	0.44
1:C:352:LEU:HD21	1:C:518:PHE:CZ	2.50	0.44
1:B:125:ASP:O	1:B:128:PRO:HA	2.18	0.43
1:B:203:GLN:O	1:B:207:HIS:ND1	2.51	0.43
1:B:293:GLY:HA2	1:B:299:MET:CE	2.48	0.43
1:B:362:ASP:HB3	1:B:365:LEU:HG	1.99	0.43
1:C:91:TYR:CE2	1:C:95:HIS:NE2	2.86	0.43
1:C:266:VAL:HG13	1:C:267:LYS:N	2.32	0.43
1:C:568:ILE:HG13	1:C:572:VAL:CG2	2.47	0.43
1:D:122:TYR:CE1	1:D:123:LEU:HD13	2.53	0.43
1:D:190:ASP:CG	1:D:192:GLN:H	2.26	0.43
1:D:266:VAL:CG1	1:D:267:LYS:N	2.81	0.43
1:D:308:GLU:HA	1:D:308:GLU:OE1	2.18	0.43
1:D:476:THR:OG1	1:D:480:GLU:HG3	2.16	0.43
1:D:478:PHE:HZ	1:D:495:TYR:CB	2.31	0.43
1:A:184:ARG:CB	1:A:439:ASN:HA	2.48	0.43
1:B:115:TYR:CD1	1:B:115:TYR:C	2.96	0.43
1:B:309:HIS:CD2	1:B:313:CYS:SG	3.11	0.43
1:B:321:PRO:HG2	1:B:322:GLU:HG3	1.99	0.43
1:C:185:ARG:HH21	1:C:438:ARG:HE	1.64	0.43
1:C:187:PHE:CE2	1:C:392:PRO:HA	2.52	0.43
1:C:210:PHE:CE1	1:C:382:ASN:CA	3.00	0.43
1:D:421:GLN:O	1:D:422:PHE:HD1	2.00	0.43
1:A:253:LYS:HB2	1:A:253:LYS:NZ	2.32	0.43
1:B:281:GLU:HA	1:B:284:GLN:HE21	1.83	0.43
1:C:37:CYS:O	1:C:39:ASN:ND2	2.51	0.43
1:C:203:GLN:O	1:C:207:HIS:ND1	2.50	0.43
1:C:495:TYR:CE2	1:C:502:GLU:HG3	2.53	0.43
1:D:34:ASN:HA	1:D:35:PRO:HD2	1.72	0.43
1:D:305:TRP:O	1:D:306:LEU:C	2.58	0.43
1:A:243:LYS:O	1:A:269:THR:HB	2.17	0.43
1:B:150:ARG:HG2	1:B:150:ARG:NH1	2.32	0.43
1:C:85:THR:HG22	1:C:86:PRO:HD2	2.00	0.43
1:C:453:ASP:HA	1:C:456:ARG:CD	2.40	0.43
1:C:467:ARG:NH1	1:C:521:THR:OG1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:PRO:CB	2:D:661:NAG:H5	2.47	0.43
1:A:187:PHE:CD1	1:A:187:PHE:C	2.96	0.43
1:A:225:GLY:O	1:A:226:HIS:C	2.60	0.43
1:B:43:ASN:ND2	1:B:64:PHE:CG	2.87	0.43
1:B:176:GLU:HB3	1:B:494:LEU:HD21	1.99	0.43
1:B:319:GLU:OE1	1:B:554:VAL:HG21	2.18	0.43
1:C:108:LEU:O	1:C:112:ILE:HG12	2.19	0.43
1:C:412:SER:OG	1:C:416:GLU:HG2	2.18	0.43
1:D:457:GLU:C	1:D:459:LYS:H	2.27	0.43
1:D:498:ILE:C	1:D:500:VAL:H	2.26	0.43
1:A:127:PRO:HA	1:A:128:PRO:HD2	1.74	0.43
1:A:208:GLN:NE2	1:A:228:VAL:HG13	2.32	0.43
1:A:276:PRO:HD2	1:A:279:ILE:CD1	2.49	0.43
1:B:402:TYR:OH	1:B:417:HIS:CE1	2.71	0.43
1:C:43:ASN:O	1:C:44:ARG:CB	2.66	0.43
1:C:176:GLU:O	1:C:180:LYS:HG3	2.18	0.43
1:C:447:VAL:HG13	3:C:682:HEM:HBA2	2.00	0.43
1:D:183:LEU:HD21	1:D:445:GLN:CB	2.48	0.43
1:D:253:LYS:HE2	1:D:269:THR:CG2	2.49	0.43
1:D:442:ILE:HG22	1:D:442:ILE:O	2.18	0.43
1:D:547:PRO:O	1:D:549:THR:N	2.47	0.43
1:A:244:LEU:O	1:A:253:LYS:HB2	2.18	0.43
1:A:301:TYR:HA	1:A:304:ILE:HG12	2.00	0.43
1:A:352:LEU:HD23	4:A:701:S58:C10	2.48	0.43
1:A:479:GLU:HG2	1:A:485:LYS:NZ	2.34	0.43
1:B:43:ASN:HB2	1:B:69:CYS:O	2.19	0.43
1:B:123:LEU:HD22	1:B:123:LEU:H	1.84	0.43
1:B:495:TYR:CE2	1:B:502:GLU:HG3	2.54	0.43
1:D:414:LEU:HD11	1:D:419:LEU:HD22	2.01	0.43
1:A:76:THR:O	1:A:77:ARG:C	2.62	0.43
1:A:116:VAL:O	1:A:120:ARG:HB2	2.18	0.43
1:A:246:LEU:O	1:A:247:PHE:HB2	2.19	0.43
1:A:271:VAL:HG11	1:A:286:ALA:HB1	2.00	0.43
1:A:327:GLN:NE2	1:B:136:TYR:CD2	2.86	0.43
1:A:450:ALA:O	1:A:451:SER:C	2.62	0.43
1:B:184:ARG:HB3	1:B:439:ASN:C	2.43	0.43
1:B:226:HIS:ND1	1:B:376:ARG:HG3	2.34	0.43
1:C:152:LEU:HD13	1:C:461:GLN:OE1	2.18	0.43
1:C:241:GLN:NE2	1:C:329:PHE:CZ	2.87	0.43
1:C:283:LEU:HD22	1:C:411:ASN:HB2	2.00	0.43
1:D:85:THR:CG2	1:D:87:ASN:HD22	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:LYS:HD3	1:D:497:ASP:OD2	2.18	0.43
1:D:279:ILE:HG12	1:D:283:LEU:CD2	2.38	0.43
1:A:190:ASP:CG	1:A:192:GLN:H	2.26	0.43
1:A:387:TRP:HB3	1:A:390:LEU:HD12	2.01	0.43
1:B:120:ARG:O	1:B:123:LEU:HD23	2.19	0.43
1:B:266:VAL:CG1	1:B:267:LYS:N	2.81	0.43
1:B:381:PHE:CE1	1:B:529:PHE:HB2	2.54	0.43
1:C:105:ASN:OD1	1:C:105:ASN:C	2.61	0.43
1:C:266:VAL:CG1	1:C:267:LYS:N	2.82	0.43
1:C:295:VAL:HG12	1:C:297:GLY:H	1.83	0.43
1:A:530:SER:O	1:A:534:LEU:HD13	2.19	0.43
1:B:204:HIS:HE2	1:B:305:TRP:CD1	2.36	0.43
1:B:252:LEU:O	1:B:310:GLN:NE2	2.52	0.43
1:D:206:THR:HG21	1:D:385:TYR:CD1	2.52	0.43
1:D:245:ARG:HG2	1:D:247:PHE:H	1.84	0.43
1:D:269:THR:C	1:D:271:VAL:H	2.27	0.43
1:D:295:VAL:HB	1:D:298:LEU:HD22	2.01	0.43
1:D:497:ASP:HB3	1:D:500:VAL:CG2	2.46	0.43
1:B:287:VAL:HG11	1:B:299:MET:SD	2.59	0.42
1:B:335:ILE:HG12	1:B:550:PHE:HB3	2.01	0.42
1:B:509:VAL:O	1:B:509:VAL:HG13	2.19	0.42
1:C:150:ARG:HG2	1:C:152:LEU:O	2.19	0.42
1:C:176:GLU:HB3	1:C:494:LEU:HD21	2.01	0.42
1:C:412:SER:O	1:C:416:GLU:HB2	2.19	0.42
1:D:66:GLY:O	1:D:68:ASN:N	2.51	0.42
1:D:116:VAL:HG23	1:D:117:LEU:N	2.34	0.42
1:D:156:ALA:HB3	1:D:159:CYS:SG	2.58	0.42
1:A:254:TYR:HD2	1:A:310:GLN:HE21	1.67	0.42
1:A:388:HIS:C	1:A:390:LEU:N	2.77	0.42
1:A:543:GLN:NE2	1:B:127:PRO:O	2.51	0.42
1:B:113:MET:HE3	1:B:116:VAL:CG2	2.48	0.42
1:C:276:PRO:CD	1:C:279:ILE:HD13	2.44	0.42
1:C:303:THR:HG22	1:C:307:ARG:HD2	2.01	0.42
1:C:402:TYR:OH	1:C:417:HIS:CE1	2.72	0.42
1:C:504:TYR:O	1:C:507:LEU:HB2	2.18	0.42
1:D:43:ASN:HB2	1:D:69:CYS:O	2.18	0.42
1:D:421:GLN:O	1:D:422:PHE:CD1	2.72	0.42
1:A:85:THR:CG2	1:A:87:ASN:HD22	2.32	0.42
1:A:211:LYS:O	1:A:212:THR:C	2.61	0.42
1:B:43:ASN:O	1:B:44:ARG:CB	2.67	0.42
1:B:117:LEU:HD12	1:B:117:LEU:HA	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HB2	1:B:466:TYR:OH	2.18	0.42
1:C:386:HIS:HE1	3:C:682:HEM:HAD2	1.82	0.42
1:C:387:TRP:O	1:C:390:LEU:HB2	2.19	0.42
4:C:701:S58:H10	4:C:701:S58:C11	2.50	0.42
1:D:74:PHE:HA	1:D:77:ARG:NE	2.34	0.42
1:D:120:ARG:HD2	4:D:701:S58:F2	2.10	0.42
1:D:232:HIS:CE1	1:D:233:ILE:HG13	2.54	0.42
1:D:295:VAL:HG12	1:D:297:GLY:H	1.83	0.42
1:D:305:TRP:O	1:D:308:GLU:N	2.52	0.42
1:A:127:PRO:O	1:B:543:GLN:NE2	2.52	0.42
1:A:320:HIS:HD2	1:B:49:SER:O	2.03	0.42
1:A:467:ARG:NH1	1:A:521:THR:OG1	2.51	0.42
1:B:255:GLN:O	1:B:255:GLN:HG3	2.19	0.42
1:B:527:ALA:N	1:B:528:PRO:CD	2.82	0.42
1:C:85:THR:HG23	1:C:86:PRO:HD2	2.00	0.42
1:C:116:VAL:HG23	1:C:117:LEU:N	2.33	0.42
1:C:152:LEU:HA	1:C:152:LEU:HD23	1.75	0.42
1:C:388:HIS:N	1:C:389:PRO:CD	2.81	0.42
1:D:402:TYR:HE1	1:D:417:HIS:HE1	1.67	0.42
1:A:83:LYS:HE3	1:A:83:LYS:HB2	1.82	0.42
1:A:362:ASP:HB3	1:A:365:LEU:HG	2.02	0.42
1:A:457:GLU:C	1:A:459:LYS:H	2.28	0.42
1:B:124:ILE:HD11	1:B:528:PRO:HB3	2.00	0.42
1:B:172:PRO:HG2	1:B:495:TYR:CE1	2.55	0.42
1:B:308:GLU:OE1	1:B:308:GLU:HA	2.20	0.42
1:C:213:ASP:HB2	1:C:222:ARG:HG2	2.02	0.42
1:C:382:ASN:HD21	3:C:682:HEM:CGD	2.33	0.42
1:A:248:LYS:HE2	1:A:248:LYS:HB3	1.87	0.42
1:A:257:ILE:HD12	1:A:262:TYR:CD2	2.55	0.42
1:A:479:GLU:CG	1:A:485:LYS:HE3	2.39	0.42
1:B:68:ASN:N	2:B:661:NAG:H82	2.30	0.42
1:B:388:HIS:N	1:B:389:PRO:CD	2.82	0.42
1:B:396:ASN:HA	1:B:401:GLU:HA	2.02	0.42
1:C:35:PRO:HG3	1:C:54:GLN:O	2.19	0.42
1:C:109:ARG:CZ	1:C:360:LYS:HB2	2.50	0.42
1:C:531:LEU:HD11	4:C:701:S58:F2	2.10	0.42
1:C:559:ILE:HD12	1:C:559:ILE:N	2.35	0.42
1:D:126:SER:HA	1:D:127:PRO:C	2.44	0.42
1:A:183:LEU:HD21	1:A:445:GLN:CB	2.50	0.42
1:B:83:LYS:O	1:B:83:LYS:HG3	2.18	0.42
1:B:206:THR:HG21	1:B:385:TYR:CD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:GLU:HB2	1:B:505:PRO:HD2	2.02	0.42
1:C:156:ALA:HB3	1:C:159:CYS:SG	2.59	0.42
1:C:396:ASN:HB2	1:C:401:GLU:HG2	2.02	0.42
1:D:582:VAL:O	1:D:583:GLN:HB2	2.19	0.42
1:A:75:LEU:HA	1:A:78:ILE:HD12	2.01	0.42
1:A:279:ILE:HA	1:A:280:PRO:HD2	1.77	0.42
1:B:478:PHE:CD2	1:B:491:LEU:HB3	2.55	0.42
1:C:225:GLY:O	1:C:227:GLY:N	2.53	0.42
1:C:321:PRO:HG2	1:C:322:GLU:HG3	2.02	0.42
1:D:391:LEU:HB2	1:D:441:PRO:HG2	2.01	0.42
1:D:465:GLU:OE2	1:D:468:LYS:HE2	2.20	0.42
1:A:92:ILE:HA	1:A:96:PHE:CE1	2.53	0.42
1:A:137:LYS:O	1:A:138:SER:O	2.38	0.42
1:A:253:LYS:NZ	1:A:269:THR:CG2	2.83	0.42
1:A:301:TYR:O	1:A:304:ILE:HB	2.20	0.42
1:A:463:LEU:HD13	1:A:506:ALA:HB3	2.00	0.42
1:B:316:LEU:HD12	1:B:316:LEU:HA	1.82	0.42
1:B:449:LYS:O	1:B:450:ALA:C	2.62	0.42
1:C:405:LYS:HD2	1:C:405:LYS:N	2.26	0.42
1:C:433:ARG:HH21	1:C:512:PRO:CB	2.33	0.42
1:D:83:LYS:HB2	1:D:83:LYS:HE3	1.75	0.42
1:D:208:GLN:OE1	1:D:232:HIS:CD2	2.73	0.42
1:D:495:TYR:CE2	1:D:502:GLU:HG3	2.55	0.42
1:A:123:LEU:HD22	1:A:123:LEU:H	1.85	0.42
1:A:150:ARG:HG2	1:A:152:LEU:O	2.20	0.42
1:A:176:GLU:O	1:A:494:LEU:HD11	2.20	0.42
1:A:276:PRO:O	1:A:278:HIS:N	2.49	0.42
1:C:197:MET:HE1	1:C:300:MET:HE1	2.02	0.42
1:C:203:GLN:HB2	3:C:682:HEM:CMC	2.49	0.42
1:C:244:LEU:O	1:C:253:LYS:HB2	2.20	0.42
1:C:449:LYS:O	1:C:450:ALA:C	2.63	0.42
1:C:547:PRO:O	1:C:549:THR:N	2.47	0.42
1:D:253:LYS:NZ	1:D:269:THR:CG2	2.83	0.42
1:D:281:GLU:HA	1:D:284:GLN:NE2	2.33	0.42
1:A:442:ILE:O	1:A:445:GLN:HG2	2.20	0.41
1:A:523:VAL:HG22	4:A:701:S58:C9	2.49	0.41
1:A:575:CYS:N	1:A:576:PRO:CD	2.82	0.41
1:B:64:PHE:HD2	1:B:70:THR:O	2.03	0.41
1:B:225:GLY:O	1:B:226:HIS:C	2.62	0.41
1:B:305:TRP:O	1:B:306:LEU:C	2.63	0.41
1:B:406:GLN:CG	2:B:681:NAG:O7	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:THR:O	1:B:424:GLU:HG3	2.20	0.41
1:B:530:SER:O	1:B:534:LEU:HD22	2.20	0.41
1:C:283:LEU:O	1:C:283:LEU:HD12	2.20	0.41
1:C:397:ILE:HA	1:C:425:SER:CB	2.50	0.41
1:C:465:GLU:OE2	1:C:468:LYS:HE2	2.20	0.41
1:D:85:THR:HG22	1:D:86:PRO:HD2	2.01	0.41
1:D:166:LYS:NZ	1:D:499:ASP:OD2	2.52	0.41
1:A:85:THR:HG23	1:A:86:PRO:HD2	2.02	0.41
1:A:184:ARG:NH2	1:A:187:PHE:HA	2.34	0.41
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.35	0.41
1:B:105:ASN:O	1:B:106:PRO:HD3	2.20	0.41
1:B:283:LEU:HB2	1:B:411:ASN:CB	2.50	0.41
1:C:92:ILE:HA	1:C:96:PHE:CE1	2.53	0.41
1:C:184:ARG:CB	1:C:439:ASN:HA	2.50	0.41
1:C:477:SER:H	1:C:480:GLU:HB2	1.85	0.41
1:D:311:ARG:O	1:D:315:ILE:HG13	2.20	0.41
1:A:122:TYR:CE1	1:A:123:LEU:HD13	2.55	0.41
1:A:139:TRP:CZ3	1:B:538:PRO:HG2	2.54	0.41
1:A:249:ASP:OD1	1:A:249:ASP:N	2.54	0.41
1:A:264:PRO:HG2	1:A:286:ALA:CB	2.50	0.41
1:B:45:GLY:HA3	1:B:69:CYS:SG	2.60	0.41
1:B:213:ASP:OD1	1:B:215:LYS:HG2	2.20	0.41
1:D:64:PHE:CD2	1:D:70:THR:O	2.74	0.41
1:D:253:LYS:NZ	1:D:253:LYS:CB	2.84	0.41
1:D:344:VAL:O	1:D:344:VAL:CG1	2.68	0.41
1:D:352:LEU:HD21	1:D:518:PHE:CZ	2.53	0.41
1:A:225:GLY:O	1:A:227:GLY:N	2.53	0.41
1:A:388:HIS:N	1:A:389:PRO:CD	2.83	0.41
1:A:504:TYR:O	1:A:507:LEU:HB2	2.20	0.41
1:B:309:HIS:O	1:B:310:GLN:C	2.63	0.41
1:B:563:SER:OG	1:B:566:SER:OG	2.37	0.41
1:C:279:ILE:CG2	1:C:284:GLN:HG2	2.51	0.41
1:C:279:ILE:HG13	1:C:283:LEU:HD23	1.99	0.41
1:C:424:GLU:CA	1:C:428:ARG:HH11	2.26	0.41
1:D:144:ASN:OD1	1:D:146:SER:HB2	2.20	0.41
1:D:193:GLY:O	1:D:582:VAL:N	2.53	0.41
1:D:208:GLN:OE1	1:D:230:LEU:HA	2.20	0.41
1:A:321:PRO:HG2	1:A:322:GLU:HG3	2.03	0.41
1:A:329:PHE:CD1	1:A:329:PHE:C	2.99	0.41
1:A:396:ASN:HB2	1:A:401:GLU:CG	2.46	0.41
1:C:181:VAL:HG12	1:C:182:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:LEU:C	1:C:253:LYS:HZ2	2.28	0.41
1:C:329:PHE:CD1	1:C:329:PHE:C	2.97	0.41
1:C:352:LEU:CD2	4:C:701:S58:H10	2.45	0.41
1:C:364:GLU:HA	1:C:367:PHE:CD2	2.56	0.41
1:D:495:TYR:O	1:D:496:SER:HB2	2.21	0.41
1:D:517:ILE:HG23	1:D:518:PHE:CD2	2.55	0.41
1:A:90:HIS:NE2	4:A:701:S58:N3	2.69	0.41
1:A:216:ARG:HH21	2:A:671:NAG:H3	1.85	0.41
1:A:577:PHE:CE2	1:D:267:LYS:HD3	2.54	0.41
1:B:272:GLU:O	1:B:290:GLU:HG3	2.21	0.41
1:B:273:MET:HA	1:B:290:GLU:HG2	2.02	0.41
1:C:33:ALA:O	1:C:34:ASN:C	2.63	0.41
1:C:172:PRO:HG2	1:C:495:TYR:CE1	2.55	0.41
1:C:247:PHE:HA	1:C:325:ASP:OD2	2.21	0.41
1:C:319:GLU:OE1	1:C:554:VAL:HG21	2.19	0.41
1:C:397:ILE:O	1:C:397:ILE:HG22	2.20	0.41
1:C:527:ALA:N	1:C:528:PRO:CD	2.83	0.41
1:D:85:THR:HG21	1:D:87:ASN:HD22	1.85	0.41
1:A:350:GLN:HE22	1:A:359:LEU:H	1.69	0.41
1:B:329:PHE:CD1	1:B:329:PHE:C	2.98	0.41
1:B:478:PHE:CE2	1:B:495:TYR:HB2	2.55	0.41
1:C:48:MET:HE3	1:C:49:SER:H	1.85	0.41
1:D:205:PHE:CZ	1:D:344:VAL:HG21	2.56	0.41
1:D:226:HIS:CE1	1:D:376:ARG:HD2	2.56	0.41
1:D:253:LYS:O	1:D:306:LEU:HD11	2.21	0.41
1:A:35:PRO:CG	1:A:54:GLN:O	2.68	0.41
1:A:175:LYS:C	1:A:177:VAL:H	2.29	0.41
1:A:323:TRP:HE3	1:A:328:LEU:HD23	1.85	0.41
1:A:495:TYR:CE2	1:A:502:GLU:HG3	2.55	0.41
1:B:74:PHE:HA	1:B:77:ARG:NE	2.36	0.41
1:B:123:LEU:O	1:B:469:ARG:NH2	2.49	0.41
1:B:530:SER:O	1:B:534:LEU:HD13	2.21	0.41
1:C:73:GLU:O	1:C:74:PHE:C	2.63	0.41
1:D:51:GLY:O	1:D:52:PHE:HB2	2.21	0.41
1:D:176:GLU:O	1:D:180:LYS:HG3	2.21	0.41
1:D:243:LYS:O	1:D:269:THR:HB	2.21	0.41
1:A:127:PRO:HB2	1:B:543:GLN:HE22	1.86	0.41
1:A:162:PRO:O	1:A:163:MET:HE2	2.20	0.41
1:A:176:GLU:C	1:A:180:LYS:HG3	2.46	0.41
1:A:381:PHE:CD1	1:A:529:PHE:HB3	2.55	0.41
1:A:419:LEU:O	1:A:422:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:PHE:CE1	1:A:492:LYS:HA	2.56	0.41
1:A:548:SER:C	1:A:550:PHE:N	2.76	0.41
1:B:73:GLU:O	1:B:74:PHE:C	2.63	0.41
1:B:91:TYR:O	1:B:92:ILE:C	2.64	0.41
1:B:176:GLU:O	1:B:494:LEU:HD11	2.20	0.41
1:B:190:ASP:HA	1:B:433:ARG:HB2	2.03	0.41
1:B:226:HIS:HB3	1:B:376:ARG:HA	2.03	0.41
1:B:253:LYS:NZ	1:B:253:LYS:HB2	2.35	0.41
1:B:283:LEU:O	1:B:283:LEU:HD12	2.21	0.41
1:C:38:SER:C	1:C:40:PRO:HD3	2.46	0.41
1:C:184:ARG:NH2	1:C:187:PHE:CD2	2.89	0.41
1:C:300:MET:O	1:C:304:ILE:HG12	2.21	0.41
1:C:419:LEU:O	1:C:422:PHE:HB2	2.21	0.41
1:C:435:ALA:HB3	1:C:518:PHE:CA	2.46	0.41
1:C:463:LEU:HD22	1:C:506:ALA:CB	2.50	0.41
1:D:50:THR:HG21	1:D:56:LYS:HG3	2.03	0.41
1:D:96:PHE:O	1:D:97:LYS:C	2.64	0.41
1:D:293:GLY:HA2	1:D:299:MET:CE	2.50	0.41
1:D:309:HIS:O	1:D:310:GLN:C	2.62	0.41
1:D:477:SER:HB2	1:D:479:GLU:CD	2.46	0.41
1:D:502:GLU:HB2	1:D:505:PRO:HD2	2.02	0.41
1:A:269:THR:C	1:A:271:VAL:H	2.28	0.41
1:B:213:ASP:HB2	1:B:222:ARG:HG2	2.03	0.41
1:B:255:GLN:HG2	1:B:262:TYR:O	2.21	0.41
1:B:266:VAL:HG13	1:B:267:LYS:N	2.35	0.41
1:B:402:TYR:HE1	1:B:417:HIS:HE1	1.67	0.41
1:C:410:ASN:CG	1:C:413:ILE:HG13	2.46	0.41
1:D:115:TYR:CD2	1:D:115:TYR:C	2.99	0.41
1:D:181:VAL:HG12	1:D:182:LEU:HG	2.02	0.41
1:D:184:ARG:HB3	1:D:439:ASN:C	2.45	0.41
1:D:287:VAL:HG11	1:D:299:MET:SD	2.61	0.41
1:D:548:SER:C	1:D:550:PHE:N	2.76	0.41
1:A:65:TYR:CD1	1:A:65:TYR:N	2.88	0.40
1:A:116:VAL:HG23	1:A:117:LEU:N	2.35	0.40
1:A:128:PRO:HG3	1:A:376:ARG:NH1	2.36	0.40
1:A:203:GLN:O	1:A:207:HIS:ND1	2.55	0.40
1:A:230:LEU:N	1:A:230:LEU:CD2	2.84	0.40
1:A:265:THR:OG1	1:A:268:ASP:HB2	2.21	0.40
1:A:503:LEU:O	1:A:507:LEU:HD12	2.21	0.40
1:B:96:PHE:O	1:B:97:LYS:C	2.63	0.40
1:B:128:PRO:HG3	1:B:376:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLN:NE2	1:B:265:THR:HG23	2.32	0.40
1:B:286:ALA:O	1:B:288:GLY:N	2.54	0.40
1:B:487:MET:O	1:B:490:GLU:N	2.54	0.40
1:C:43:ASN:HB2	1:C:69:CYS:O	2.21	0.40
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.86	0.40
1:C:123:LEU:HD22	1:C:123:LEU:H	1.85	0.40
1:C:450:ALA:O	1:C:454:GLN:HB2	2.20	0.40
1:D:162:PRO:HG2	1:D:171:LEU:HD13	2.02	0.40
1:D:319:GLU:CD	1:D:554:VAL:HG21	2.46	0.40
1:D:429:GLN:H	1:D:582:VAL:HG23	1.86	0.40
1:D:482:THR:CG2	1:D:509:VAL:HG22	2.50	0.40
1:A:99:VAL:O	1:A:102:ILE:N	2.55	0.40
1:A:381:PHE:CD1	1:A:529:PHE:HB2	2.57	0.40
1:A:429:GLN:H	1:A:582:VAL:HG23	1.86	0.40
1:B:33:ALA:O	1:B:34:ASN:C	2.64	0.40
1:B:85:THR:CG2	1:B:87:ASN:HD22	2.34	0.40
1:B:405:LYS:HD2	1:B:405:LYS:N	2.26	0.40
1:B:419:LEU:O	1:B:422:PHE:HB2	2.20	0.40
1:C:175:LYS:C	1:C:177:VAL:H	2.28	0.40
1:C:198:PHE:HB2	1:C:580:PHE:HB3	2.03	0.40
1:C:559:ILE:HD12	1:C:559:ILE:H	1.86	0.40
1:D:109:ARG:NH2	1:D:359:LEU:O	2.46	0.40
1:D:272:GLU:O	1:D:290:GLU:HG3	2.22	0.40
1:D:433:ARG:HH21	1:D:512:PRO:CB	2.33	0.40
1:A:184:ARG:NH1	1:A:441:PRO:HG3	2.35	0.40
1:B:111:LEU:HA	1:B:111:LEU:HD23	1.77	0.40
1:B:184:ARG:CB	1:B:439:ASN:HA	2.52	0.40
1:B:291:VAL:CG2	1:B:294:LEU:HD12	2.51	0.40
1:B:477:SER:H	1:B:480:GLU:HB2	1.86	0.40
4:B:701:S58:H10	4:B:701:S58:C11	2.51	0.40
1:C:116:VAL:O	1:C:120:ARG:HB2	2.20	0.40
1:C:421:GLN:O	1:C:422:PHE:CD1	2.75	0.40
1:C:554:VAL:H	1:C:554:VAL:HG23	1.67	0.40
1:D:176:GLU:HB3	1:D:494:LEU:CD2	2.52	0.40
1:D:396:ASN:HA	1:D:401:GLU:HA	2.03	0.40
1:A:203:GLN:NE2	1:A:298:LEU:HD13	2.36	0.40
1:A:319:GLU:OE1	1:A:554:VAL:HG21	2.22	0.40
1:B:184:ARG:O	1:B:442:ILE:HD11	2.21	0.40
1:B:230:LEU:N	1:B:230:LEU:HD23	2.37	0.40
1:B:429:GLN:H	1:B:582:VAL:HG23	1.86	0.40
1:B:504:TYR:O	1:B:507:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ILE:HA	1:C:425:SER:HB3	2.03	0.40
1:D:75:LEU:HA	1:D:78:ILE:HD12	2.02	0.40
1:D:245:ARG:HG2	1:D:246:LEU:N	2.37	0.40
1:D:479:GLU:HG2	1:D:485:LYS:NZ	2.36	0.40
1:D:485:LYS:HD3	1:D:485:LYS:HA	1.92	0.40
1:D:559:ILE:HD12	1:D:559:ILE:N	2.37	0.40
1:A:45:GLY:HA3	1:A:69:CYS:SG	2.62	0.40
1:A:194:SER:OG	1:A:351:HIS:HE1	2.05	0.40
1:A:412:SER:O	1:A:413:ILE:C	2.65	0.40
1:B:201:PHE:HD2	1:B:301:TYR:CZ	2.39	0.40
1:B:283:LEU:O	1:B:285:PHE:CD1	2.75	0.40
1:B:380:GLU:O	1:B:381:PHE:C	2.63	0.40
1:C:85:THR:HG21	1:C:87:ASN:HD22	1.87	0.40
1:C:108:LEU:HD23	1:C:108:LEU:HA	1.97	0.40
1:C:313:CYS:O	1:C:317:LYS:HB2	2.21	0.40
1:C:397:ILE:HD11	1:C:426:PHE:CE1	2.56	0.40
1:D:125:ASP:O	1:D:128:PRO:HA	2.21	0.40
1:D:283:LEU:HA	1:D:411:ASN:OD1	2.21	0.40
1:D:442:ILE:O	1:D:445:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	550/587 (94%)	439 (80%)	86 (16%)	25 (4%)	2	12
1	B	550/587 (94%)	438 (80%)	85 (16%)	27 (5%)	1	10
1	C	550/587 (94%)	439 (80%)	84 (15%)	27 (5%)	1	10
1	D	550/587 (94%)	444 (81%)	78 (14%)	28 (5%)	1	10
All	All	2200/2348 (94%)	1760 (80%)	333 (15%)	107 (5%)	1	10

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	138	SER
1	A	226	HIS
1	A	270	GLN
1	A	284	GLN
1	A	292	PHE
1	A	356	HIS
1	A	398	GLU
1	A	514	PRO
1	A	573	LYS
1	B	67	GLU
1	B	138	SER
1	B	226	HIS
1	B	270	GLN
1	B	284	GLN
1	B	287	VAL
1	B	292	PHE
1	B	356	HIS
1	B	514	PRO
1	B	573	LYS
1	C	67	GLU
1	C	138	SER
1	C	226	HIS
1	C	270	GLN
1	C	284	GLN
1	C	292	PHE
1	C	356	HIS
1	C	398	GLU
1	C	514	PRO
1	C	573	LYS
1	C	575	CYS
1	D	67	GLU
1	D	138	SER
1	D	226	HIS
1	D	270	GLN
1	D	284	GLN
1	D	287	VAL
1	D	292	PHE
1	D	356	HIS
1	D	398	GLU
1	D	514	PRO
1	D	573	LYS

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Mol	Chain	Res	Type
1	A	278	HIS
1	A	287	VAL
1	A	575	CYS
1	A	582	VAL
1	B	144	ASN
1	B	278	HIS
1	B	280	PRO
1	B	290	GLU
1	B	398	GLU
1	B	422	PHE
1	B	575	CYS
1	B	582	VAL
1	C	144	ASN
1	C	278	HIS
1	C	287	VAL
1	C	422	PHE
1	C	582	VAL
1	D	144	ASN
1	D	278	HIS
1	D	280	PRO
1	D	400	GLN
1	D	422	PHE
1	D	575	CYS
1	D	582	VAL
1	A	144	ASN
1	A	280	PRO
1	A	422	PHE
1	A	547	PRO
1	B	49	SER
1	B	81	LEU
1	B	547	PRO
1	C	81	LEU
1	C	280	PRO
1	C	290	GLU
1	D	81	LEU
1	D	429	GLN
1	A	81	LEU
1	B	212	THR
1	B	400	GLN
1	C	429	GLN
1	C	547	PRO
1	D	547	PRO

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Mol	Chain	Res	Type
1	A	212	THR
1	A	290	GLU
1	A	400	GLN
1	A	429	GLN
1	B	107	PHE
1	C	400	GLN
1	C	458	MET
1	D	496	SER
1	B	228	VAL
1	B	277	PRO
1	C	49	SER
1	D	499	ASP
1	A	277	PRO
1	C	228	VAL
1	D	259	GLY
1	A	228	VAL
1	C	277	PRO
1	D	228	VAL
1	D	277	PRO
1	C	51	GLY
1	B	259	GLY
1	D	51	GLY
1	D	554	VAL

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	493/525 (94%)	413 (84%)	80 (16%)	2	12
1	B	493/525 (94%)	410 (83%)	83 (17%)	2	11
1	C	493/525 (94%)	412 (84%)	81 (16%)	2	12
1	D	493/525 (94%)	416 (84%)	77 (16%)	2	13
All	All	1972/2100 (94%)	1651 (84%)	321 (16%)	2	12

All (321) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	46	GLU
1	A	48	MET
1	A	49	SER
1	A	54	GLN
1	A	71	THR
1	A	74	PHE
1	A	82	LEU
1	A	83	LYS
1	A	93	LEU
1	A	103	VAL
1	A	105	ASN
1	A	105(A)	ILE
1	A	117	LEU
1	A	120	ARG
1	A	127	PRO
1	A	136	TYR
1	A	138	SER
1	A	150	ARG
1	A	178	LEU
1	A	181	VAL
1	A	209	PHE
1	A	216	ARG
1	A	230	LEU
1	A	231	ASN
1	A	238	LEU
1	A	249	ASP
1	A	252	LEU
1	A	253	LYS
1	A	254	TYR
1	A	261	VAL
1	A	271	VAL
1	A	283	LEU
1	A	289	GLN
1	A	298	LEU
1	A	300	MET
1	A	301	TYR
1	A	310	GLN
1	A	316	LEU
1	A	317	LYS
1	A	318	GLN
1	A	322	GLU
1	A	356	HIS

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Mol	Chain	Res	Type
1	A	369	GLN
1	A	374	GLN
1	A	376	ARG
1	A	379	SER
1	A	380	GLU
1	A	383	THR
1	A	384	LEU
1	A	385	TYR
1	A	389	PRO
1	A	394	THR
1	A	409	TYR
1	A	412	SER
1	A	419	LEU
1	A	420	THR
1	A	422	PHE
1	A	430	ILE
1	A	438	ARG
1	A	441	PRO
1	A	459	LYS
1	A	469	ARG
1	A	479	GLU
1	A	480	GLU
1	A	484	GLU
1	A	485	LYS
1	A	486	GLU
1	A	514	PRO
1	A	518	PHE
1	A	520	GLU
1	A	534	LEU
1	A	539	ILE
1	A	543	GLN
1	A	564	ILE
1	A	568	ILE
1	A	569	CYS
1	A	572	VAL
1	A	578	THR
1	A	582	VAL
1	B	38	SER
1	B	39	ASN
1	B	46	GLU
1	B	48	MET
1	B	49	SER

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Mol	Chain	Res	Type
1	B	54	GLN
1	B	71	THR
1	B	74	PHE
1	B	82	LEU
1	B	83	LYS
1	B	93	LEU
1	B	94	THR
1	B	103	VAL
1	B	105	ASN
1	B	105(A)	ILE
1	B	117	LEU
1	B	120	ARG
1	B	123	LEU
1	B	127	PRO
1	B	136	TYR
1	B	150	ARG
1	B	178	LEU
1	B	181	VAL
1	B	209	PHE
1	B	216	ARG
1	B	230	LEU
1	B	231	ASN
1	B	238	LEU
1	B	248	LYS
1	B	252	LEU
1	B	253	LYS
1	B	254	TYR
1	B	261	VAL
1	B	271	VAL
1	B	279	ILE
1	B	283	LEU
1	B	289	GLN
1	B	298	LEU
1	B	300	MET
1	B	301	TYR
1	B	310	GLN
1	B	316	LEU
1	B	318	GLN
1	B	322	GLU
1	B	356	HIS
1	B	368	ASN
1	B	369	GLN

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Mol	Chain	Res	Type
1	B	374	GLN
1	B	376	ARG
1	B	379	SER
1	B	380	GLU
1	B	383	THR
1	B	384	LEU
1	B	385	TYR
1	B	389	PRO
1	B	394	THR
1	B	409	TYR
1	B	412	SER
1	B	419	LEU
1	B	420	THR
1	B	422	PHE
1	B	430	ILE
1	B	438	ARG
1	B	441	PRO
1	B	459	LYS
1	B	469	ARG
1	B	479	GLU
1	B	480	GLU
1	B	484	GLU
1	B	486	GLU
1	B	514	PRO
1	B	518	PHE
1	B	520	GLU
1	B	525	LEU
1	B	530	SER
1	B	534	LEU
1	B	539	ILE
1	B	543	GLN
1	B	564	ILE
1	B	568	ILE
1	B	569	CYS
1	B	572	VAL
1	B	578	THR
1	C	39	ASN
1	C	46	GLU
1	C	49	SER
1	C	71	THR
1	C	72	PRO
1	C	74	PHE

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Mol	Chain	Res	Type
1	C	82	LEU
1	C	83	LYS
1	C	93	LEU
1	C	94	THR
1	C	103	VAL
1	C	105	ASN
1	C	105(A)	ILE
1	C	117	LEU
1	C	120	ARG
1	C	127	PRO
1	C	136	TYR
1	C	150	ARG
1	C	171	LEU
1	C	178	LEU
1	C	181	VAL
1	C	209	PHE
1	C	215	LYS
1	C	216	ARG
1	C	230	LEU
1	C	231	ASN
1	C	238	LEU
1	C	252	LEU
1	C	253	LYS
1	C	254	TYR
1	C	261	VAL
1	C	279	ILE
1	C	283	LEU
1	C	289	GLN
1	C	298	LEU
1	C	300	MET
1	C	301	TYR
1	C	310	GLN
1	C	316	LEU
1	C	318	GLN
1	C	322	GLU
1	C	352	LEU
1	C	356	HIS
1	C	368	ASN
1	C	374	GLN
1	C	376	ARG
1	C	379	SER
1	C	380	GLU

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Mol	Chain	Res	Type
1	C	383	THR
1	C	384	LEU
1	C	385	TYR
1	C	389	PRO
1	C	394	THR
1	C	396	ASN
1	C	397	ILE
1	C	398	GLU
1	C	409	TYR
1	C	412	SER
1	C	419	LEU
1	C	420	THR
1	C	422	PHE
1	C	430	ILE
1	C	441	PRO
1	C	459	LYS
1	C	469	ARG
1	C	479	GLU
1	C	480	GLU
1	C	484	GLU
1	C	486	GLU
1	C	514	PRO
1	C	518	PHE
1	C	520	GLU
1	C	534	LEU
1	C	539	ILE
1	C	543	GLN
1	C	564	ILE
1	C	568	ILE
1	C	569	CYS
1	C	572	VAL
1	C	578	THR
1	C	582	VAL
1	D	39	ASN
1	D	46	GLU
1	D	48	MET
1	D	49	SER
1	D	54	GLN
1	D	71	THR
1	D	72	PRO
1	D	74	PHE
1	D	82	LEU

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Mol	Chain	Res	Type
1	D	83	LYS
1	D	93	LEU
1	D	94	THR
1	D	103	VAL
1	D	105	ASN
1	D	105(A)	ILE
1	D	117	LEU
1	D	120	ARG
1	D	123	LEU
1	D	127	PRO
1	D	136	TYR
1	D	150	ARG
1	D	178	LEU
1	D	181	VAL
1	D	209	PHE
1	D	216	ARG
1	D	230	LEU
1	D	231	ASN
1	D	238	LEU
1	D	252	LEU
1	D	253	LYS
1	D	254	TYR
1	D	261	VAL
1	D	279	ILE
1	D	283	LEU
1	D	289	GLN
1	D	298	LEU
1	D	300	MET
1	D	310	GLN
1	D	316	LEU
1	D	318	GLN
1	D	322	GLU
1	D	356	HIS
1	D	374	GLN
1	D	376	ARG
1	D	379	SER
1	D	380	GLU
1	D	383	THR
1	D	384	LEU
1	D	385	TYR
1	D	389	PRO
1	D	394	THR

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Mol	Chain	Res	Type
1	D	409	TYR
1	D	412	SER
1	D	419	LEU
1	D	420	THR
1	D	422	PHE
1	D	438	ARG
1	D	441	PRO
1	D	459	LYS
1	D	469	ARG
1	D	479	GLU
1	D	480	GLU
1	D	484	GLU
1	D	485	LYS
1	D	486	GLU
1	D	514	PRO
1	D	518	PHE
1	D	520	GLU
1	D	525	LEU
1	D	534	LEU
1	D	539	ILE
1	D	543	GLN
1	D	564	ILE
1	D	568	ILE
1	D	569	CYS
1	D	572	VAL
1	D	578	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	43	ASN
1	A	87	ASN
1	A	101	ASN
1	A	203	GLN
1	A	214	HIS
1	A	255	GLN
1	A	282	ASN
1	A	284	GLN
1	A	320	HIS
1	A	327	GLN
1	A	350	GLN

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Mol	Chain	Res	Type
1	A	351	HIS
1	A	368	ASN
1	A	369	GLN
1	A	417	HIS
1	A	461	GLN
1	A	464	ASN
1	A	537	ASN
1	A	583	GLN
1	B	39	ASN
1	B	43	ASN
1	B	87	ASN
1	B	101	ASN
1	B	203	GLN
1	B	255	GLN
1	B	278	HIS
1	B	282	ASN
1	B	284	GLN
1	B	320	HIS
1	B	350	GLN
1	B	351	HIS
1	B	382	ASN
1	B	400	GLN
1	B	417	HIS
1	B	461	GLN
1	B	464	ASN
1	B	537	ASN
1	B	571	ASN
1	C	39	ASN
1	C	43	ASN
1	C	87	ASN
1	C	101	ASN
1	C	203	GLN
1	C	255	GLN
1	C	278	HIS
1	C	282	ASN
1	C	284	GLN
1	C	320	HIS
1	C	327	GLN
1	C	350	GLN
1	C	351	HIS
1	C	382	ASN
1	C	400	GLN

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Mol	Chain	Res	Type
1	C	417	HIS
1	C	461	GLN
1	C	464	ASN
1	C	537	ASN
1	C	560	ASN
1	D	39	ASN
1	D	43	ASN
1	D	87	ASN
1	D	101	ASN
1	D	203	GLN
1	D	255	GLN
1	D	278	HIS
1	D	282	ASN
1	D	284	GLN
1	D	350	GLN
1	D	368	ASN
1	D	382	ASN
1	D	400	GLN
1	D	417	HIS
1	D	461	GLN
1	D	464	ASN
1	D	537	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](#)

20 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
2	NAG	C	661	1	14,14,15	0.95	0	17,19,21	0.76	1 (5%)
4	S58	C	701	-	28,28,28	2.44	5 (17%)	43,43,43	2.00	10 (23%)
3	HEM	A	682	1	50,50,50	1.19	4 (8%)	67,82,82	0.92	1 (1%)
2	NAG	C	681	1	14,14,15	0.88	1 (7%)	17,19,21	0.91	1 (5%)
3	HEM	D	682	1	50,50,50	1.18	5 (10%)	67,82,82	0.93	1 (1%)
2	NAG	D	671	1	14,14,15	0.62	0	17,19,21	1.16	2 (11%)
2	NAG	A	661	1	14,14,15	0.76	0	17,19,21	0.90	0
4	S58	B	701	-	28,28,28	2.52	7 (25%)	43,43,43	2.17	9 (20%)
3	HEM	C	682	1	50,50,50	1.24	5 (10%)	67,82,82	1.06	2 (2%)
2	NAG	A	681	1	14,14,15	0.84	0	17,19,21	0.97	1 (5%)
2	NAG	D	681	1	14,14,15	0.57	0	17,19,21	0.95	1 (5%)
2	NAG	A	671	1	14,14,15	0.55	0	17,19,21	1.15	2 (11%)
4	S58	D	701	-	28,28,28	2.61	9 (32%)	43,43,43	2.05	10 (23%)
2	NAG	B	661	1	14,14,15	0.63	0	17,19,21	0.88	1 (5%)
2	NAG	B	671	1	14,14,15	0.62	0	17,19,21	0.94	1 (5%)
2	NAG	B	681	1	14,14,15	0.71	0	17,19,21	0.82	1 (5%)
2	NAG	C	671	1	14,14,15	0.91	1 (7%)	17,19,21	1.19	1 (5%)
4	S58	A	701	-	28,28,28	2.43	7 (25%)	43,43,43	2.08	9 (20%)
2	NAG	D	661	1	14,14,15	0.65	0	17,19,21	0.78	1 (5%)
3	HEM	B	682	1	50,50,50	1.22	6 (12%)	67,82,82	0.93	1 (1%)

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
2	NAG	C	661	1	-	2/6/23/26	0/1/1/1
4	S58	C	701	-	-	7/20/20/20	0/3/3/3
3	HEM	A	682	1	-	5/14/54/54	-
2	NAG	C	681	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	D	682	1	-	6/14/54/54	-
2	NAG	D	671	1	-	1/6/23/26	0/1/1/1
2	NAG	A	661	1	-	2/6/23/26	0/1/1/1
4	S58	B	701	-	-	8/20/20/20	0/3/3/3
3	HEM	C	682	1	-	5/14/54/54	-
2	NAG	A	681	1	-	2/6/23/26	0/1/1/1
2	NAG	D	681	1	-	2/6/23/26	0/1/1/1
2	NAG	A	671	1	-	0/6/23/26	0/1/1/1
4	S58	D	701	-	-	7/20/20/20	0/3/3/3
2	NAG	B	661	1	-	2/6/23/26	0/1/1/1
2	NAG	B	671	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	2/6/23/26	0/1/1/1
2	NAG	C	671	1	-	0/6/23/26	0/1/1/1
4	S58	A	701	-	-	8/20/20/20	0/3/3/3
2	NAG	D	661	1	-	1/6/23/26	0/1/1/1
3	HEM	B	682	1	-	5/14/54/54	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	701	S58	S1-N3	8.18	1.76	1.60
4	B	701	S58	S1-N3	8.08	1.76	1.60
4	A	701	S58	S1-N3	7.98	1.76	1.60
4	C	701	S58	S1-N3	7.85	1.75	1.60
4	C	701	S58	C1-C3	6.69	1.50	1.39
4	D	701	S58	C1-C3	6.65	1.50	1.39
4	A	701	S58	C1-C3	6.20	1.49	1.39
4	B	701	S58	C1-C3	5.39	1.48	1.39
4	B	701	S58	BR1-C14	-5.06	1.80	1.90
3	B	682	HEM	CAB-C3B	-3.75	1.37	1.47
4	A	701	S58	C8-S1	3.71	1.82	1.77
4	D	701	S58	C8-S1	3.68	1.82	1.77
4	C	701	S58	C3-N2	-3.47	1.28	1.34
4	D	701	S58	C3-N2	-3.42	1.29	1.34
3	A	682	HEM	CBC-CAC	3.35	1.46	1.30
3	D	682	HEM	CAB-C3B	-3.32	1.38	1.47
4	B	701	S58	C3-N2	-3.29	1.29	1.34
3	B	682	HEM	CAC-C3C	-3.21	1.38	1.47
4	A	701	S58	C5-N1	-3.05	1.37	1.43
3	C	682	HEM	CBB-CAB	3.05	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	CAB-C3B	-3.04	1.39	1.47
3	D	682	HEM	CAC-C3C	-3.02	1.39	1.47
3	C	682	HEM	CAC-C3C	-2.97	1.39	1.47
3	C	682	HEM	CAB-C3B	-2.93	1.39	1.47
4	D	701	S58	C16-C15	2.85	1.43	1.38
4	C	701	S58	N1-N2	2.84	1.45	1.39
3	A	682	HEM	CAC-C3C	-2.77	1.40	1.47
4	D	701	S58	C5-N1	-2.69	1.38	1.43
4	B	701	S58	C5-N1	-2.67	1.38	1.43
4	A	701	S58	BR1-C14	-2.67	1.85	1.90
3	B	682	HEM	CBC-CAC	2.66	1.43	1.30
4	B	701	S58	C8-S1	2.59	1.81	1.77
3	B	682	HEM	CBB-CAB	2.54	1.42	1.30
2	C	671	NAG	C1-C2	2.50	1.55	1.52
4	D	701	S58	C13-C12	2.49	1.42	1.38
3	C	682	HEM	C1B-NB	-2.44	1.36	1.40
3	C	682	HEM	C4A-NA	-2.37	1.35	1.39
3	B	682	HEM	CBA-CGA	2.28	1.55	1.50
4	D	701	S58	C1-C2	-2.22	1.34	1.38
3	D	682	HEM	CBB-CAB	2.20	1.41	1.30
4	C	701	S58	O1-S1	2.18	1.47	1.43
4	D	701	S58	N1-N2	2.16	1.43	1.39
3	D	682	HEM	O2D-CGD	-2.15	1.23	1.30
4	B	701	S58	N1-N2	2.14	1.43	1.39
4	A	701	S58	C3-N2	-2.12	1.31	1.34
2	C	681	NAG	C3-C2	2.10	1.56	1.52
4	A	701	S58	N1-N2	2.06	1.43	1.39
3	A	682	HEM	CBB-CAB	2.06	1.40	1.30
3	D	682	HEM	CBC-CAC	2.03	1.40	1.30
3	B	682	HEM	O2D-CGD	-2.02	1.24	1.30

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	S58	C2-N1-N2	-7.24	107.60	112.19
4	C	701	S58	C2-N1-N2	-6.36	108.16	112.19
4	A	701	S58	C2-N1-N2	-6.17	108.28	112.19
4	D	701	S58	C2-N1-N2	-6.04	108.36	112.19
4	A	701	S58	O2-S1-O1	-5.91	109.71	118.80
4	B	701	S58	C3-N2-N1	5.82	109.15	104.27
4	B	701	S58	O2-S1-O1	-5.71	110.02	118.80
4	D	701	S58	O2-S1-O1	-5.47	110.38	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	S58	C3-N2-N1	5.44	108.83	104.27
4	A	701	S58	C3-N2-N1	5.34	108.74	104.27
4	D	701	S58	C3-N2-N1	5.11	108.56	104.27
4	C	701	S58	O2-S1-O1	-4.71	111.55	118.80
3	C	682	HEM	C3B-C4B-NB	3.88	112.26	109.47
4	B	701	S58	C4-C3-N2	3.62	124.06	119.20
4	D	701	S58	C4-C3-N2	3.59	124.02	119.20
3	B	682	HEM	C3B-C4B-NB	3.47	111.96	109.47
4	A	701	S58	C1-C2-N1	3.44	108.85	105.84
3	D	682	HEM	C3B-C4B-NB	3.44	111.94	109.47
4	C	701	S58	C1-C2-N1	3.32	108.74	105.84
4	C	701	S58	C1-C3-N2	-3.32	107.94	111.86
4	A	701	S58	C1-C3-N2	-3.26	108.01	111.86
4	A	701	S58	O1-S1-N3	3.23	112.01	107.35
2	D	671	NAG	C2-N2-C7	-3.22	118.59	122.90
4	D	701	S58	C1-C3-N2	-3.21	108.07	111.86
2	A	671	NAG	C2-N2-C7	-3.14	118.69	122.90
3	A	682	HEM	C3B-C4B-NB	3.14	111.72	109.47
4	A	701	S58	C4-C3-N2	3.08	123.33	119.20
4	B	701	S58	C1-C2-N1	3.06	108.51	105.84
4	D	701	S58	C1-C2-N1	3.05	108.50	105.84
2	C	671	NAG	C2-N2-C7	-3.03	118.84	122.90
4	B	701	S58	C1-C3-N2	-2.83	108.52	111.86
4	B	701	S58	F2-C4-C3	-2.69	107.35	112.86
4	B	701	S58	O1-S1-N3	2.63	111.15	107.35
4	C	701	S58	C4-C3-N2	2.60	122.68	119.20
2	C	681	NAG	C1-C2-N2	-2.55	106.41	110.43
2	B	671	NAG	C2-N2-C7	-2.55	119.49	122.90
4	B	701	S58	F1-C4-C3	-2.48	107.78	112.86
2	B	661	NAG	C2-N2-C7	-2.45	119.62	122.90
4	A	701	S58	F3-C4-C3	-2.41	107.92	112.86
4	D	701	S58	F1-C4-C3	-2.35	108.05	112.86
4	D	701	S58	O2-S1-N3	2.33	110.72	107.35
2	C	661	NAG	C2-N2-C7	-2.29	119.83	122.90
2	A	681	NAG	C2-N2-C7	-2.25	119.88	122.90
4	D	701	S58	O1-S1-C8	2.22	109.86	107.35
2	D	681	NAG	C1-C2-N2	-2.21	106.95	110.43
4	D	701	S58	C2-C1-C3	2.20	106.49	104.05
4	C	701	S58	F1-C4-C3	-2.16	108.43	112.86
3	C	682	HEM	C4C-C3C-C2C	-2.13	104.97	106.81
4	A	701	S58	O2-S1-N3	2.09	110.37	107.35
4	C	701	S58	F3-C4-C3	-2.08	108.58	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	681	NAG	C1-C2-N2	-2.08	107.16	110.43
2	A	671	NAG	C1-O5-C5	2.06	114.95	112.19
2	D	671	NAG	C1-O5-C5	2.06	114.95	112.19
2	D	661	NAG	C2-N2-C7	-2.06	120.14	122.90
4	C	701	S58	O2-S1-N3	2.05	110.31	107.35
4	C	701	S58	C2-C1-C3	2.04	106.32	104.05

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	682	HEM	C2C-C3C-CAC-CBC
2	B	681	NAG	O5-C5-C6-O6
2	D	681	NAG	O5-C5-C6-O6
2	A	681	NAG	O5-C5-C6-O6
2	C	681	NAG	O5-C5-C6-O6
2	C	681	NAG	C4-C5-C6-O6
2	D	681	NAG	C4-C5-C6-O6
2	A	681	NAG	C4-C5-C6-O6
2	B	681	NAG	C4-C5-C6-O6
2	B	661	NAG	O5-C5-C6-O6
2	A	661	NAG	O5-C5-C6-O6
3	A	682	HEM	C2A-CAA-CBA-CGA
3	B	682	HEM	C2A-CAA-CBA-CGA
3	C	682	HEM	C2A-CAA-CBA-CGA
3	D	682	HEM	C2A-CAA-CBA-CGA
2	D	661	NAG	O5-C5-C6-O6
2	C	661	NAG	O5-C5-C6-O6
4	B	701	S58	C9-C8-S1-O2
4	D	701	S58	C7-C8-S1-O2
4	D	701	S58	C9-C8-S1-O2
3	A	682	HEM	C2C-C3C-CAC-CBC
3	B	682	HEM	C2C-C3C-CAC-CBC
3	D	682	HEM	C2C-C3C-CAC-CBC
4	A	701	S58	C7-C8-S1-O2
4	A	701	S58	C9-C8-S1-O2
4	B	701	S58	C7-C8-S1-O2
4	C	701	S58	C7-C8-S1-O2
4	C	701	S58	C9-C8-S1-O2
4	A	701	S58	C7-C8-S1-N3
4	D	701	S58	C7-C8-S1-N3
4	B	701	S58	C7-C8-S1-N3

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Mol	Chain	Res	Type	Atoms
4	A	701	S58	C9-C8-S1-N3
4	B	701	S58	C9-C8-S1-N3
4	D	701	S58	C9-C8-S1-N3
4	C	701	S58	C7-C8-S1-N3
2	B	661	NAG	C4-C5-C6-O6
2	A	661	NAG	C4-C5-C6-O6
4	A	701	S58	C16-C11-C2-C1
4	B	701	S58	C16-C11-C2-C1
4	C	701	S58	C9-C8-S1-N3
4	D	701	S58	C16-C11-C2-C1
4	C	701	S58	C16-C11-C2-C1
4	B	701	S58	C12-C11-C2-C1
4	D	701	S58	C12-C11-C2-C1
4	C	701	S58	C12-C11-C2-C1
4	A	701	S58	C12-C11-C2-C1
2	C	661	NAG	C1-C2-N2-C7
3	D	682	HEM	C2B-C3B-CAB-CBB
4	C	701	S58	C16-C11-C2-N1
2	D	671	NAG	O5-C5-C6-O6
3	B	682	HEM	CAA-CBA-CGA-O2A
4	A	701	S58	C16-C11-C2-N1
4	B	701	S58	C16-C11-C2-N1
4	D	701	S58	C16-C11-C2-N1
3	C	682	HEM	CAA-CBA-CGA-O2A
3	A	682	HEM	CAA-CBA-CGA-O2A
3	B	682	HEM	CAA-CBA-CGA-O1A
3	D	682	HEM	CAA-CBA-CGA-O2A
3	C	682	HEM	CAA-CBA-CGA-O1A
4	B	701	S58	C12-C11-C2-N1
3	A	682	HEM	CAA-CBA-CGA-O1A
3	D	682	HEM	CAA-CBA-CGA-O1A
3	A	682	HEM	CAD-CBD-CGD-O2D
3	D	682	HEM	CAD-CBD-CGD-O2D
4	A	701	S58	C12-C11-C2-N1
3	B	682	HEM	C2B-C3B-CAB-CBB
3	C	682	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

14 monomers are involved in 67 short contacts:

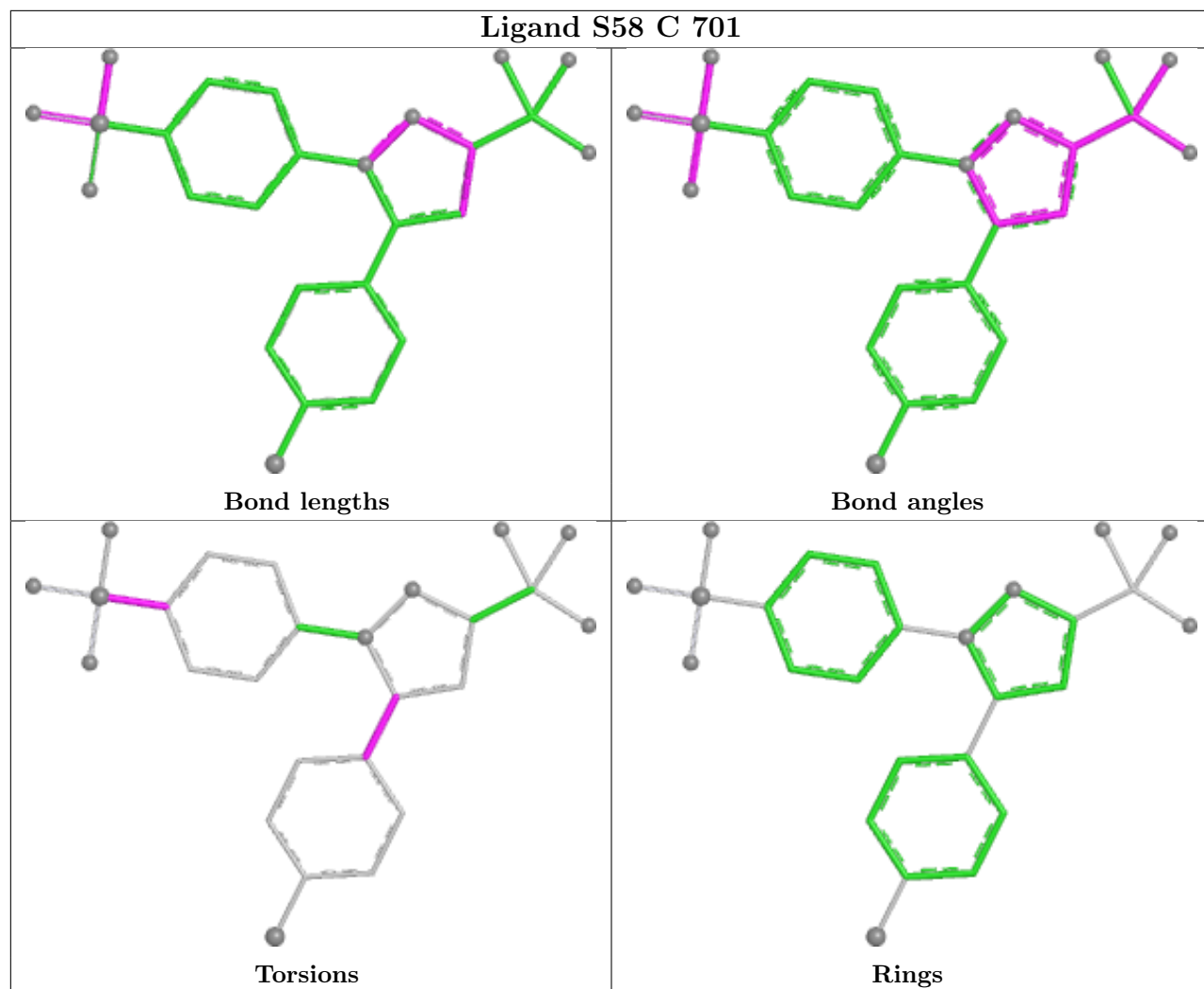
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	661	NAG	1	0

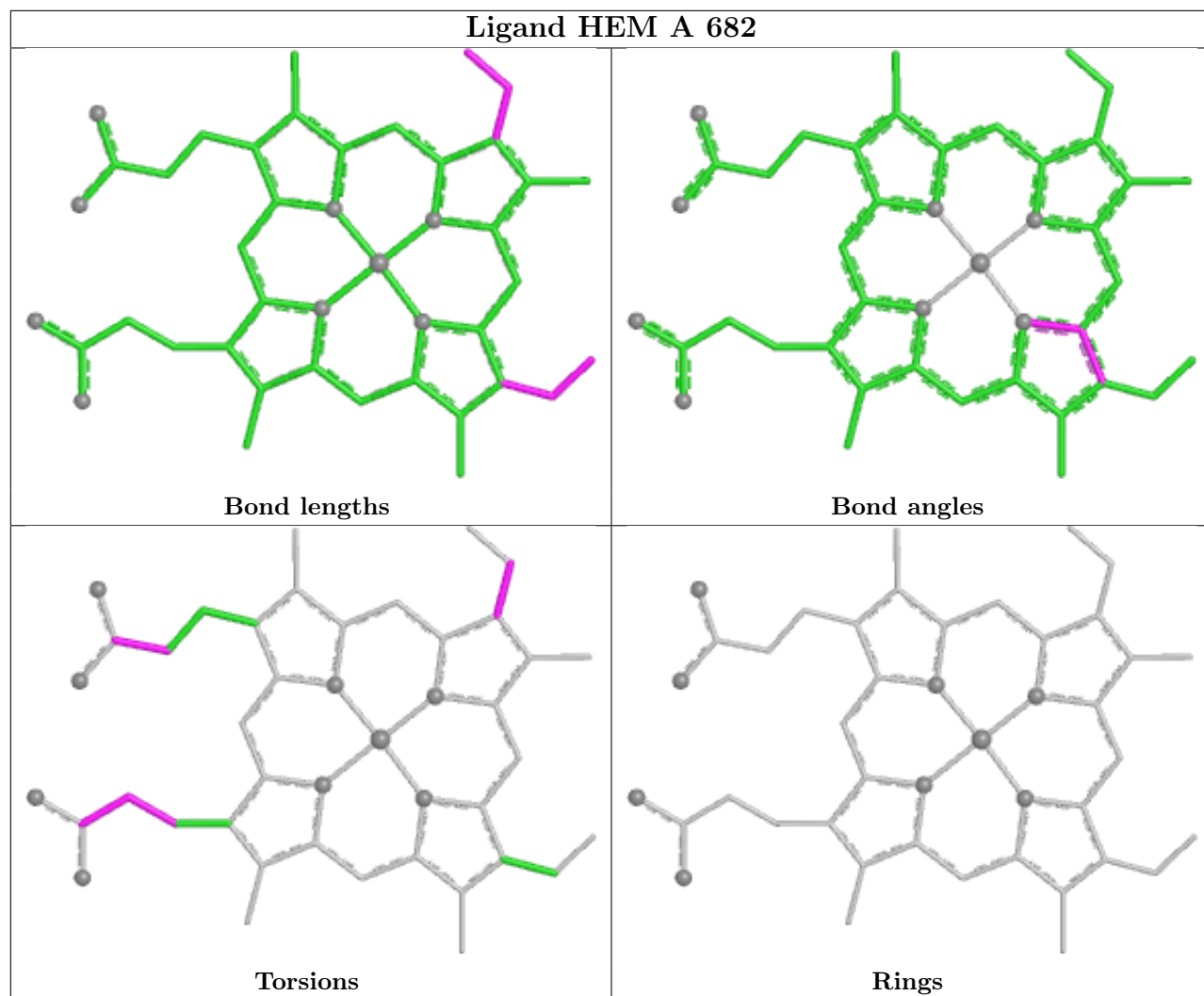
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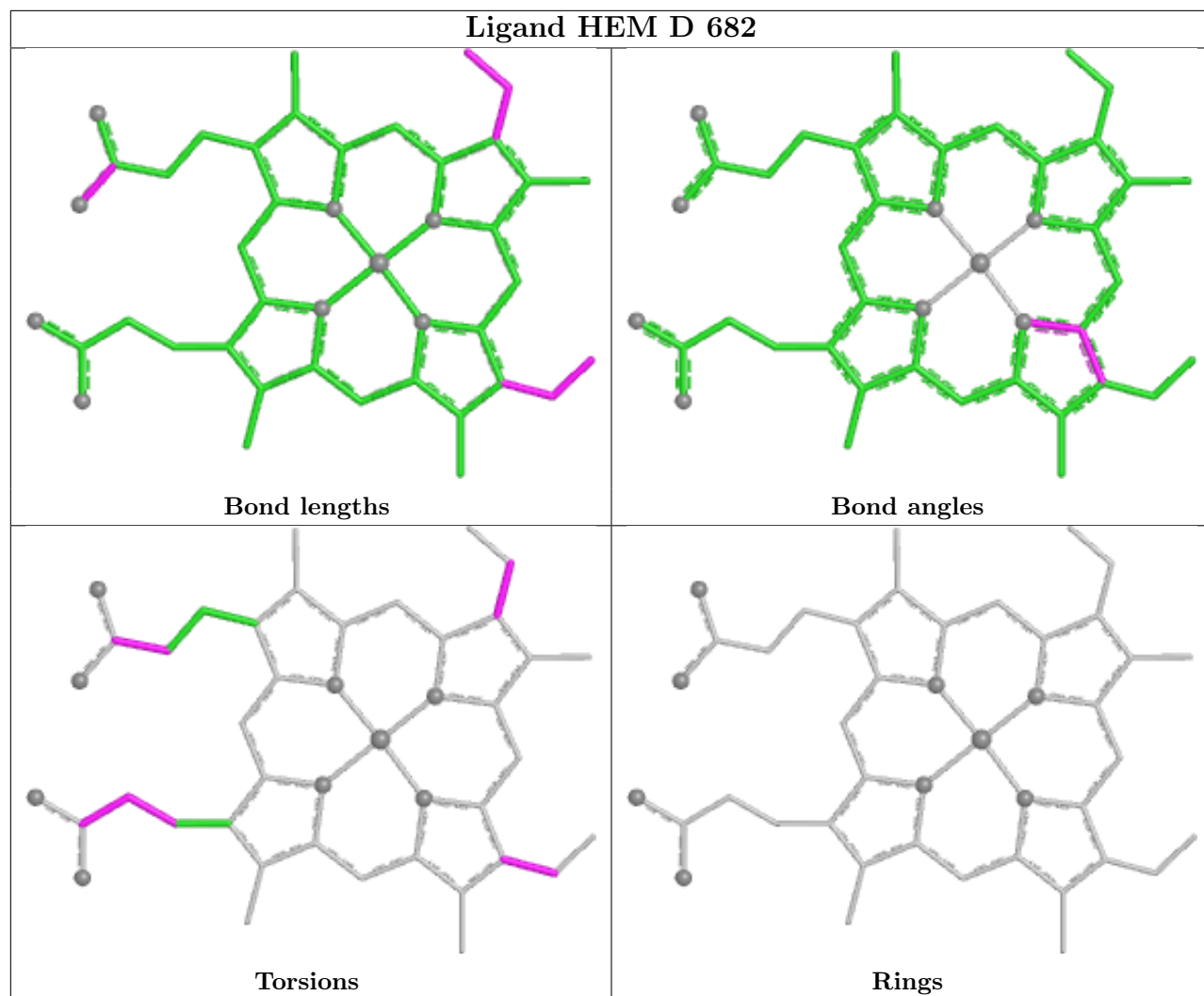
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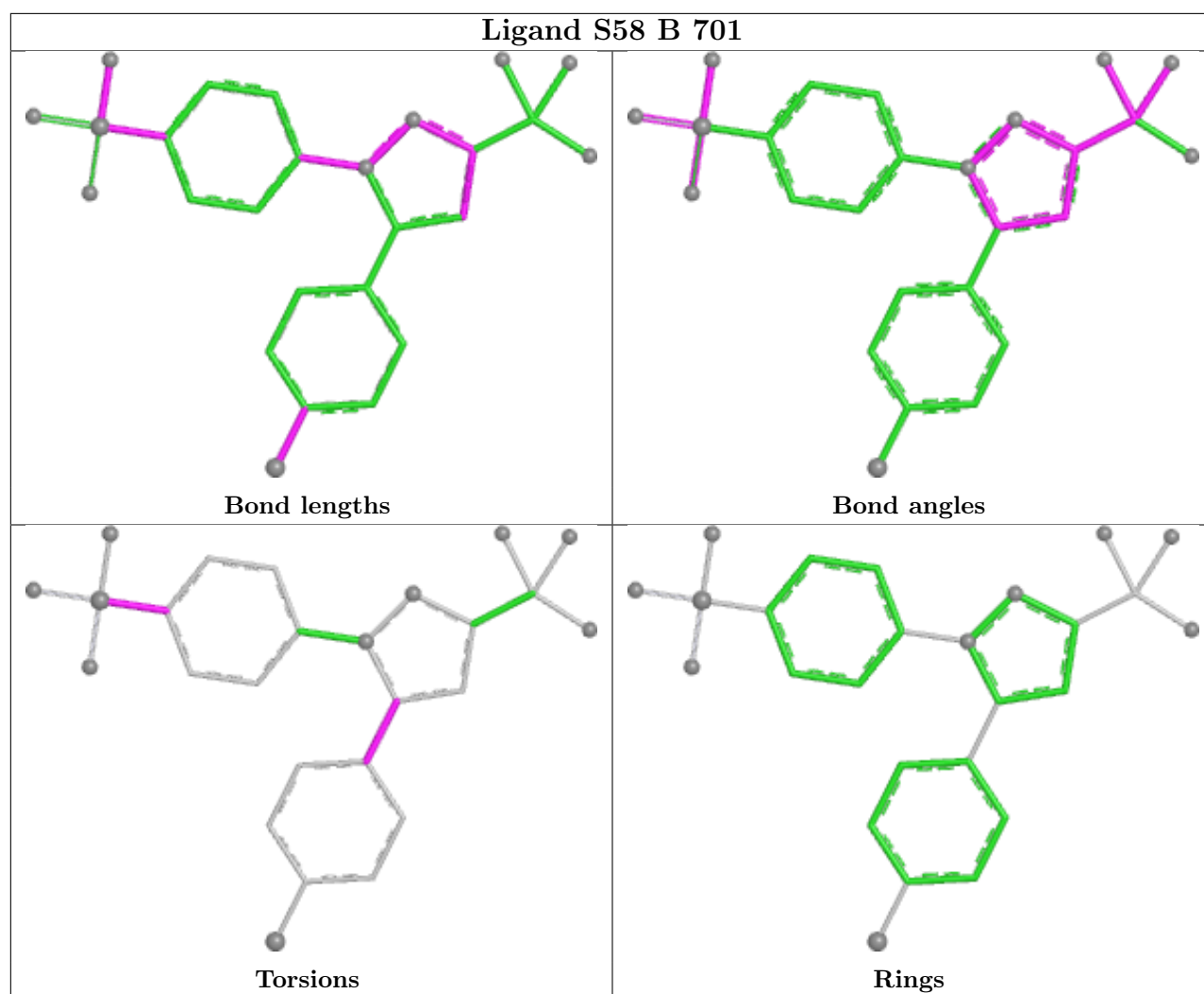
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	701	S58	11	0
3	A	682	HEM	3	0
3	D	682	HEM	5	0
4	B	701	S58	5	0
3	C	682	HEM	7	0
2	D	681	NAG	1	0
2	A	671	NAG	1	0
4	D	701	S58	7	0
2	B	661	NAG	2	0
2	B	681	NAG	4	0
4	A	701	S58	9	0
2	D	661	NAG	5	0
3	B	682	HEM	6	0

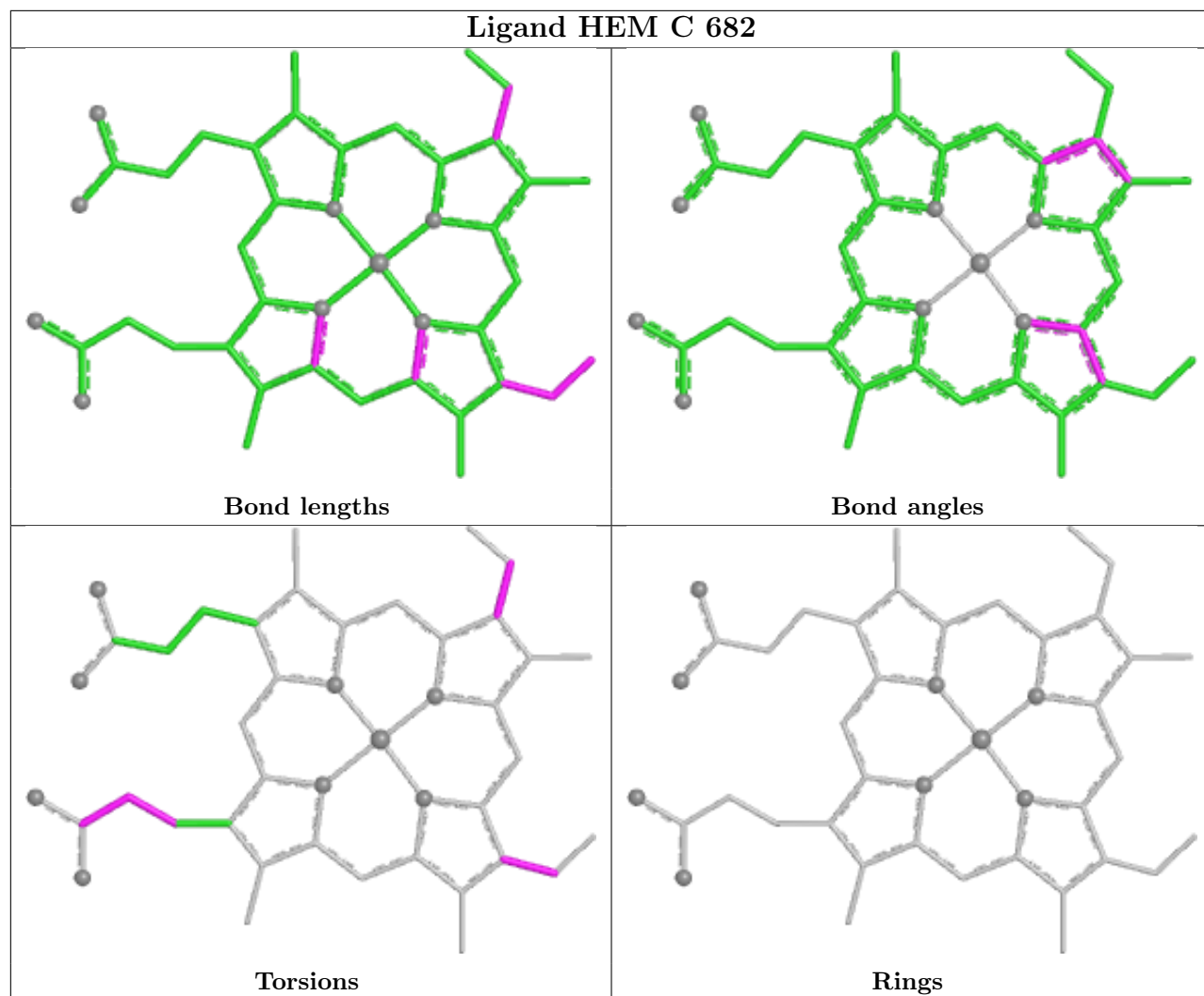
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

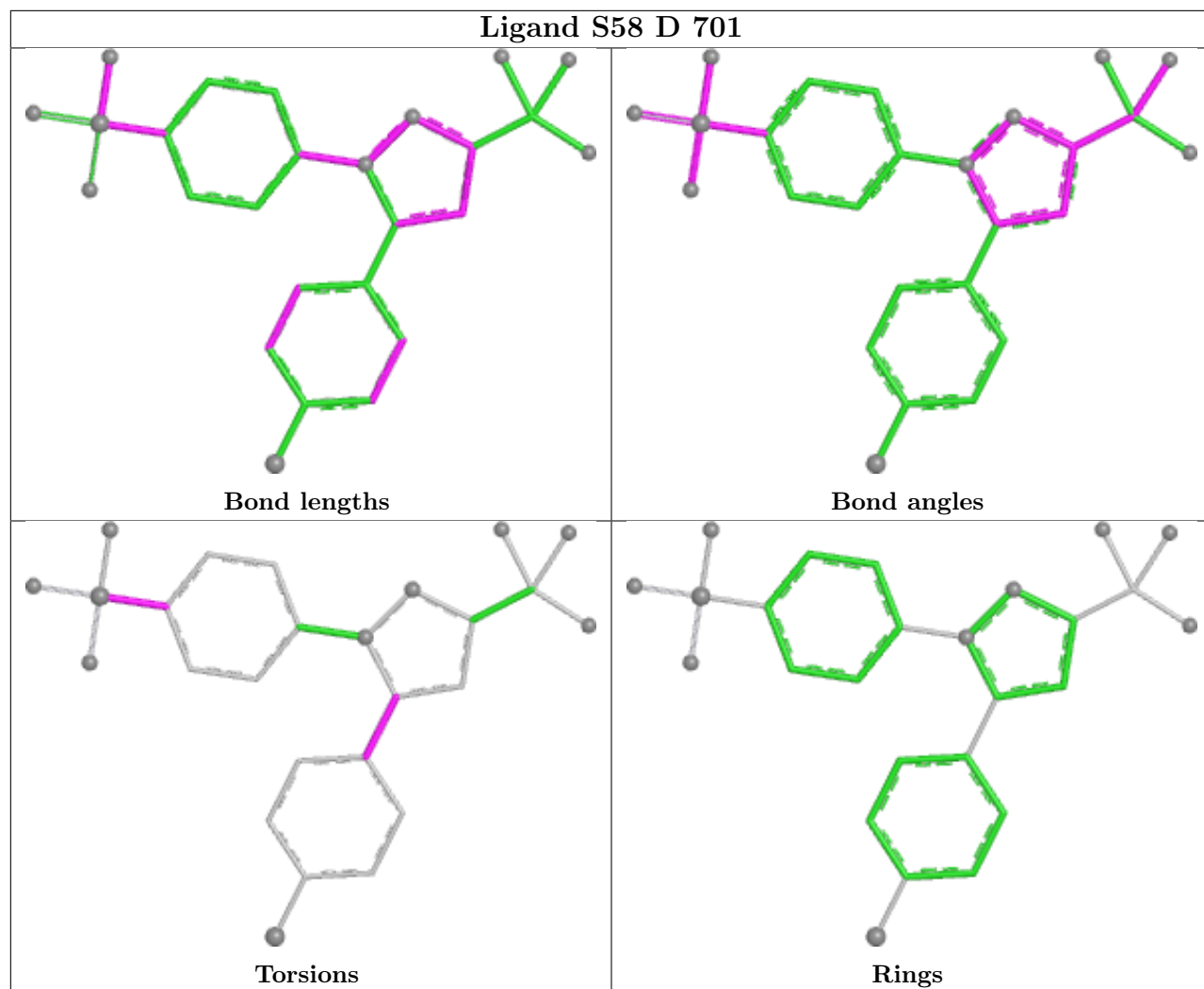


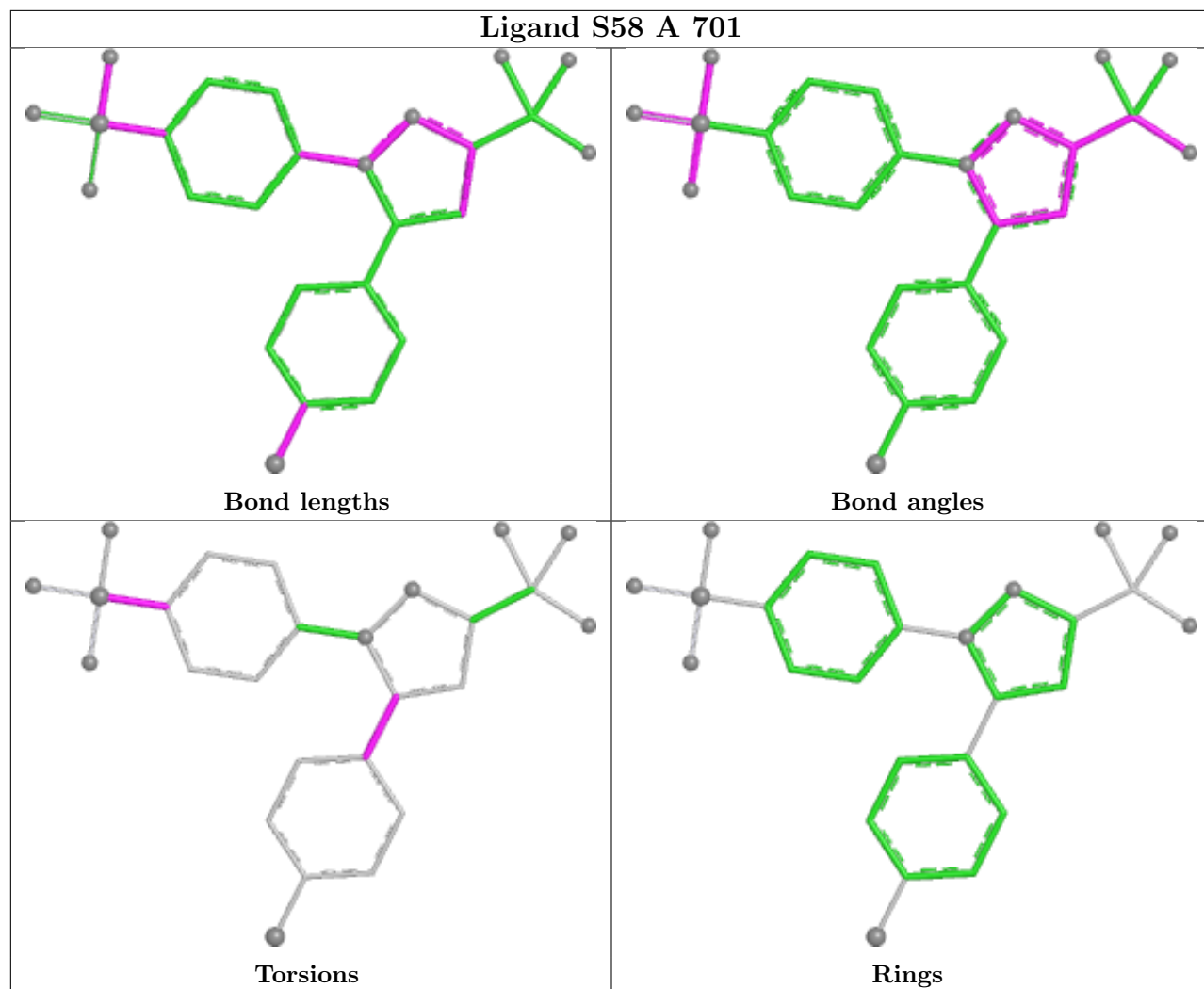


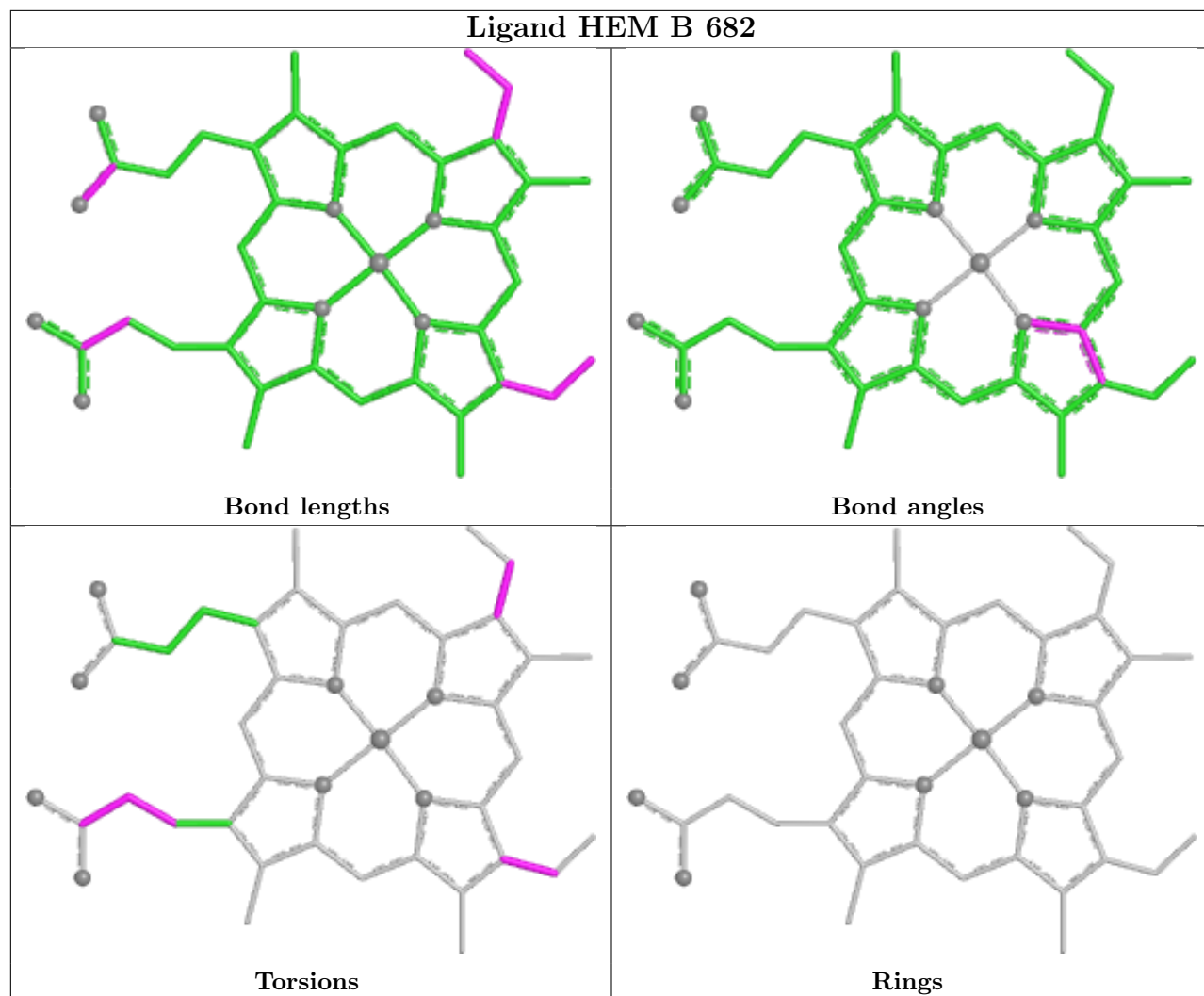












5.7 Other polymers [i](#)

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	552/587 (94%)	-0.05	6 (1%) 78 57	2, 8, 16, 29	0
1	B	552/587 (94%)	-0.06	4 (0%) 84 66	2, 8, 16, 24	0
1	C	552/587 (94%)	-0.07	3 (0%) 87 72	2, 8, 16, 25	0
1	D	552/587 (94%)	-0.05	5 (0%) 81 61	3, 8, 17, 29	0
All	All	2208/2348 (94%)	-0.06	18 (0%) 82 64	2, 8, 16, 29	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	SER	4.1
1	D	105	ASN	4.1
1	C	217	GLY	3.3
1	B	450	ALA	2.8
1	B	105	ASN	2.7
1	B	116	VAL	2.6
1	A	378	ALA	2.5
1	C	250	GLY	2.4
1	D	191	PRO	2.4
1	D	450	ALA	2.4
1	B	411	ASN	2.3
1	A	75	LEU	2.3
1	A	581	ASN	2.1
1	A	489	ALA	2.1
1	A	436	GLY	2.1
1	D	74	PHE	2.1
1	C	53	ASP	2.0
1	D	396	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

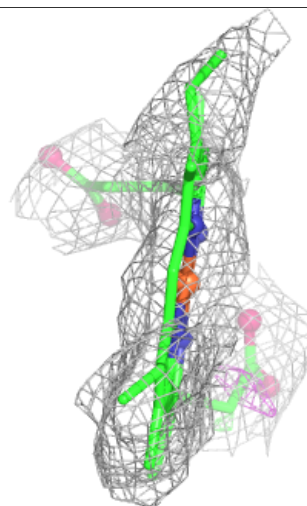
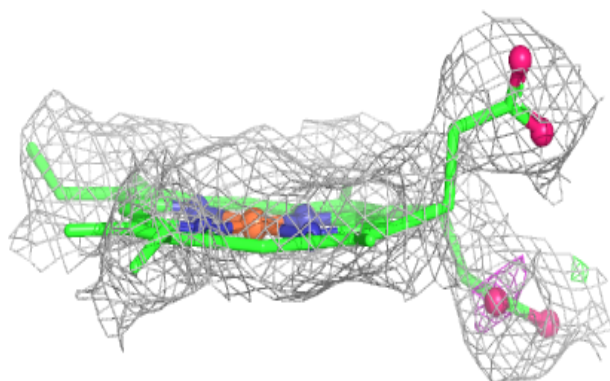
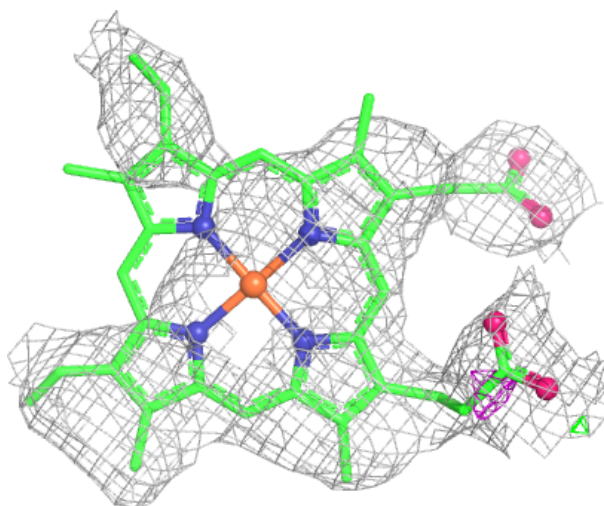
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	NAG	A	661	14/15	0.69	0.17	12,17,20,21	0
2	NAG	B	681	14/15	0.70	0.17	11,17,22,24	0
2	NAG	D	661	14/15	0.70	0.15	15,17,19,21	0
2	NAG	D	681	14/15	0.80	0.20	12,17,20,24	0
2	NAG	C	661	14/15	0.82	0.15	12,17,21,22	0
2	NAG	B	661	14/15	0.84	0.14	15,17,19,20	0
2	NAG	A	681	14/15	0.85	0.11	7,17,18,21	0
2	NAG	B	671	14/15	0.85	0.10	5,12,17,17	0
2	NAG	C	681	14/15	0.86	0.13	11,17,21,22	0
2	NAG	C	671	14/15	0.88	0.07	7,13,17,17	0
2	NAG	D	671	14/15	0.89	0.09	5,11,17,17	0
2	NAG	A	671	14/15	0.91	0.09	4,12,17,17	0
3	HEM	D	682	43/43	0.91	0.10	2,3,7,9	0
3	HEM	B	682	43/43	0.93	0.10	2,3,7,9	0
3	HEM	A	682	43/43	0.93	0.09	2,3,8,10	0
3	HEM	C	682	43/43	0.95	0.08	2,3,7,8	0
4	S58	D	701	26/26	0.95	0.09	2,8,13,17	0
4	S58	C	701	26/26	0.96	0.09	2,8,15,17	0
4	S58	B	701	26/26	0.96	0.08	2,8,14,17	0
4	S58	A	701	26/26	0.98	0.06	2,9,15,17	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.

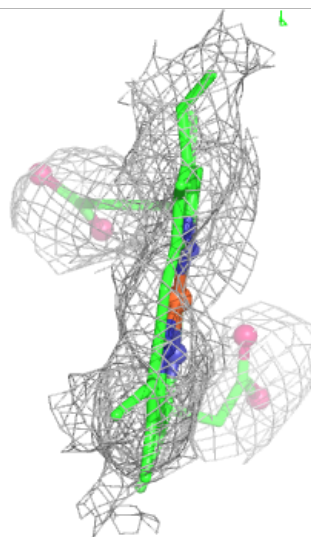
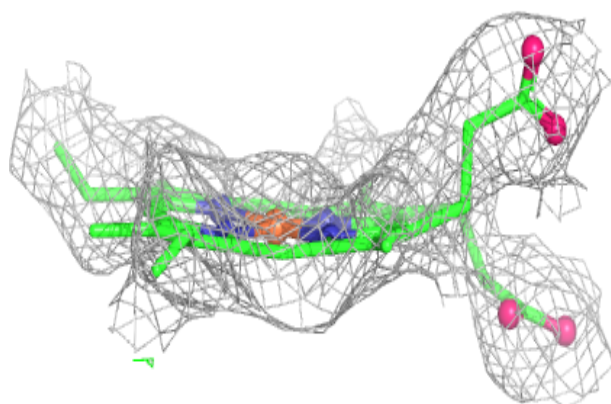
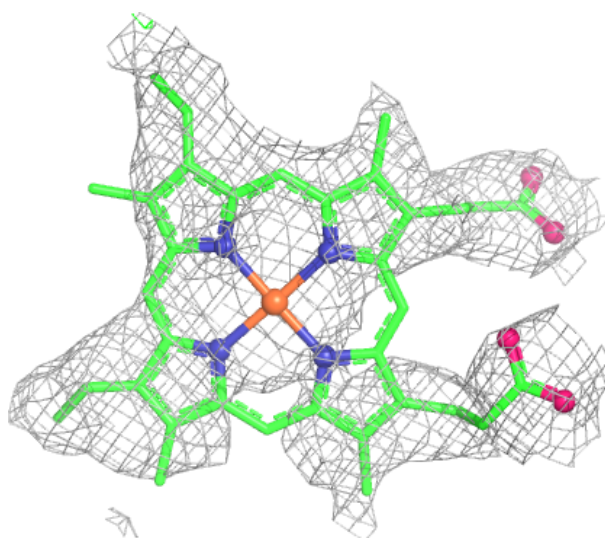
Electron density around HEM D 682:

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



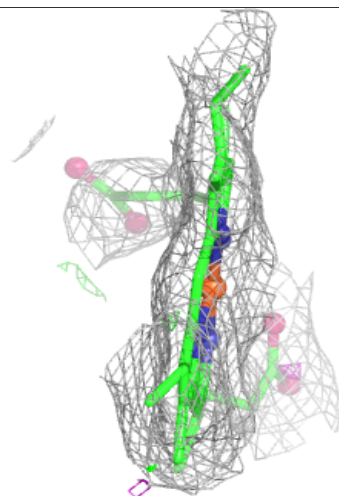
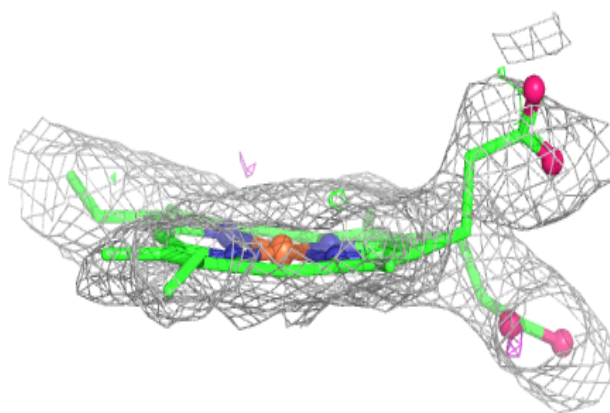
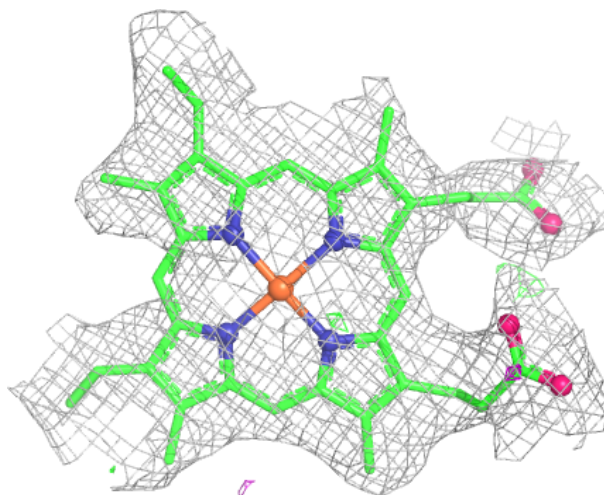
Electron density around HEM B 682:

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



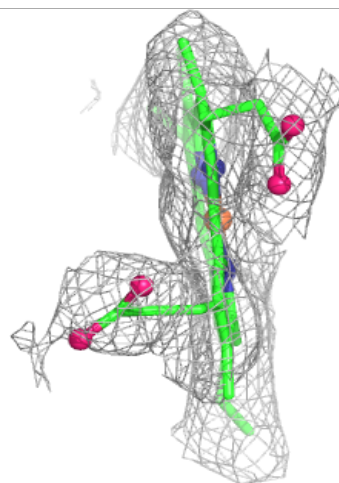
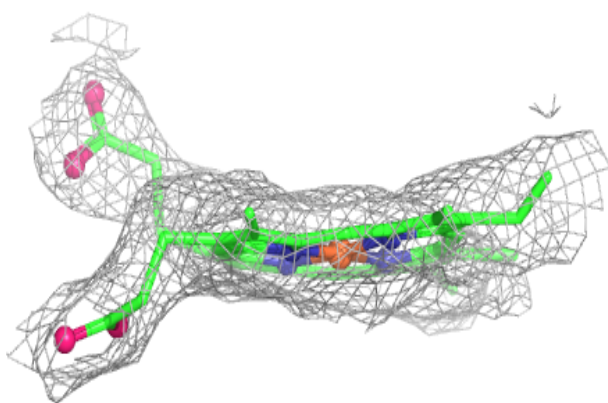
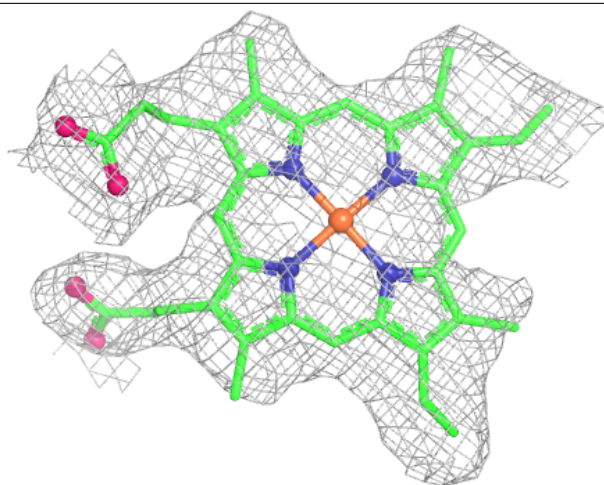
Electron density around HEM A 682:

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



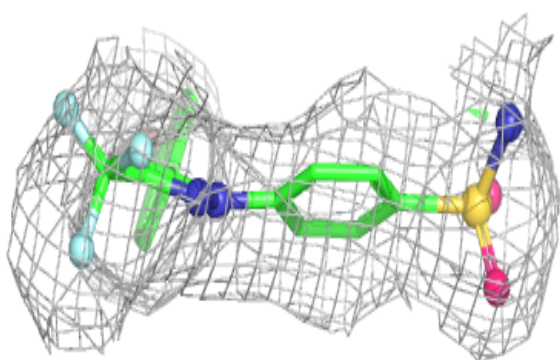
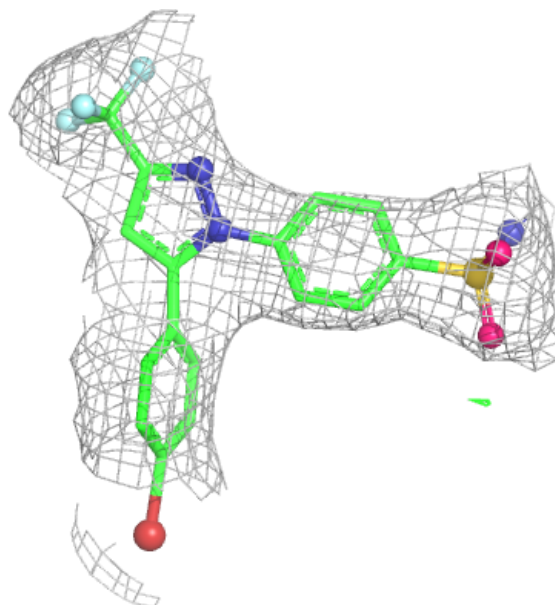
Electron density around HEM C 682:

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



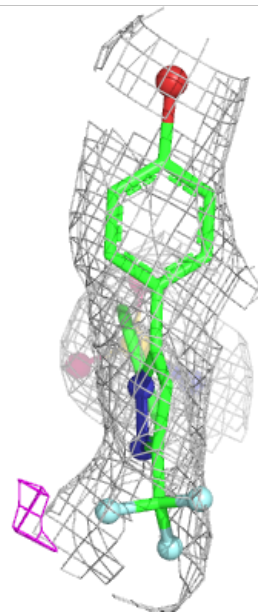
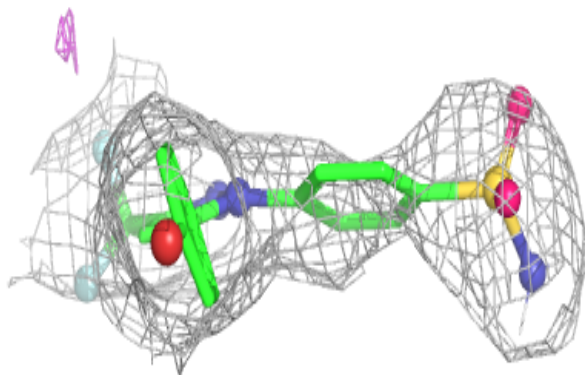
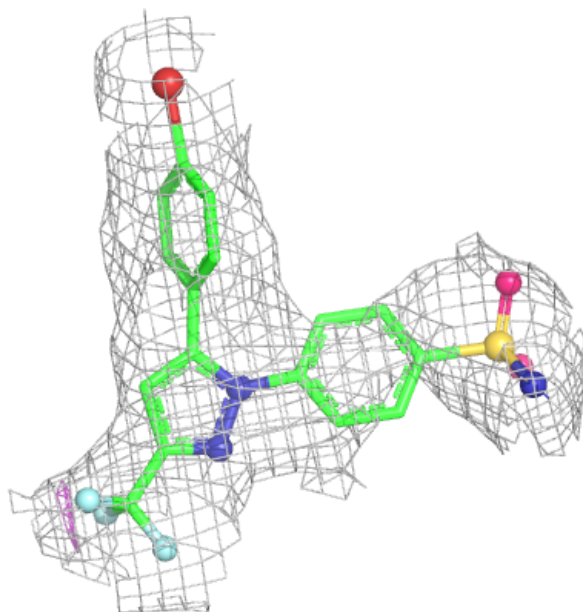
Electron density around S58 D 701:

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



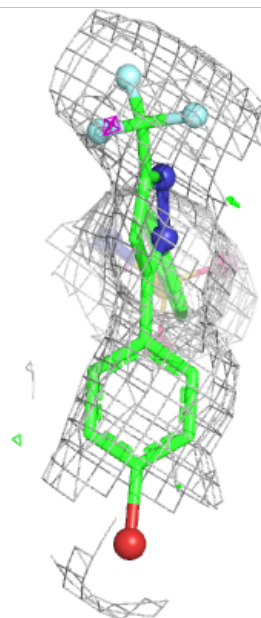
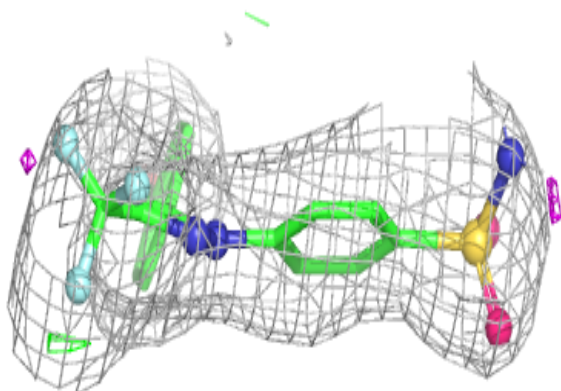
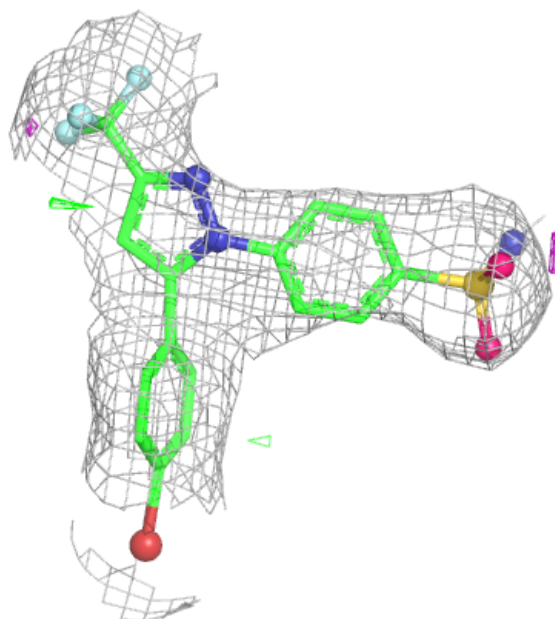
Electron density around S58 C 701:

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



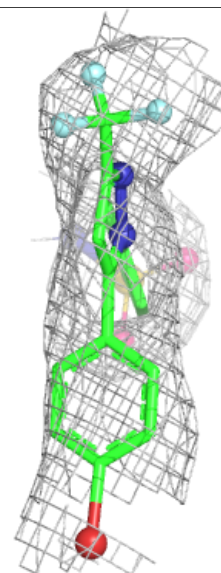
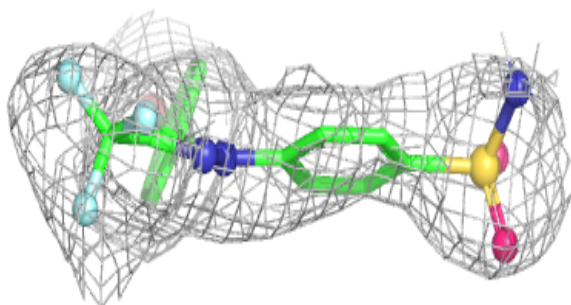
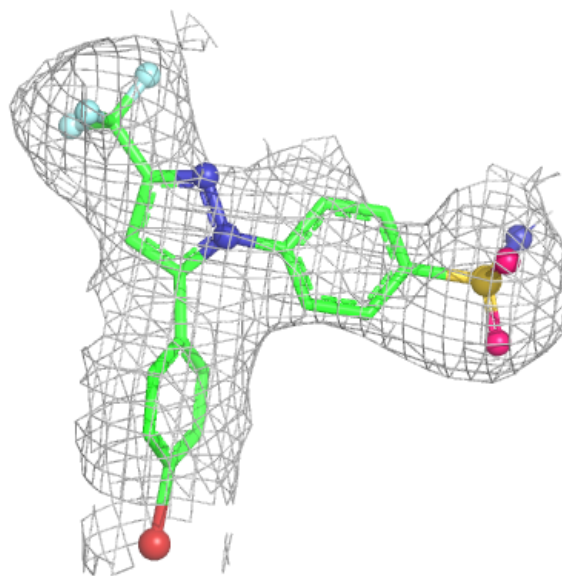
Electron density around S58 B 701:

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



Electron density around S58 A 701:

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.