



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:38 AM EDT

PDB ID : 1L0V / pdb_0000110v
Title : Quinol-Fumarate Reductase with Menaquinol Molecules
Authors : Iverson, T.M.; Luna-Chavez, C.; Croal, L.R.; Cecchini, G.; Rees, D.C.
Deposited on : 2002-02-13
Resolution : 3.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

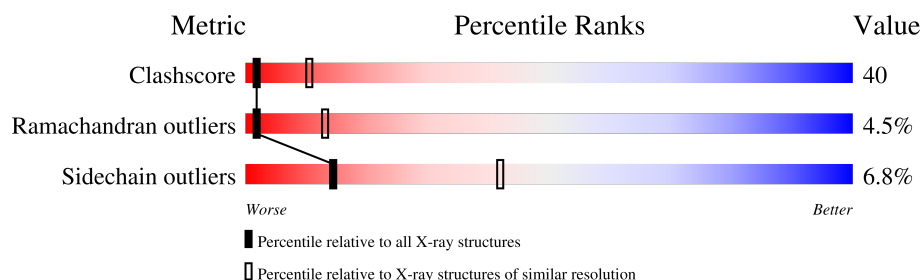
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	602	
1	M	602	
2	B	243	
2	N	243	
3	C	130	
3	O	130	
4	D	119	
4	P	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MQ7	D	700	-	-	X	-
6	FAD	M	803	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17046 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			
1	M	577	Total	C	N	O	S	0	0	0
			4448	2775	802	840	31			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			

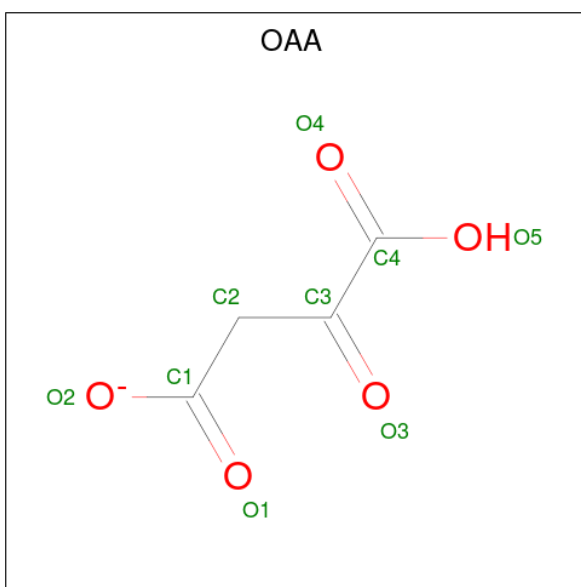
- Molecule 3 is a protein called Fumarate reductase 15 kDa hydrophobic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

- Molecule 4 is a protein called Fumarate reductase 13 kDa hydrophobic protein.

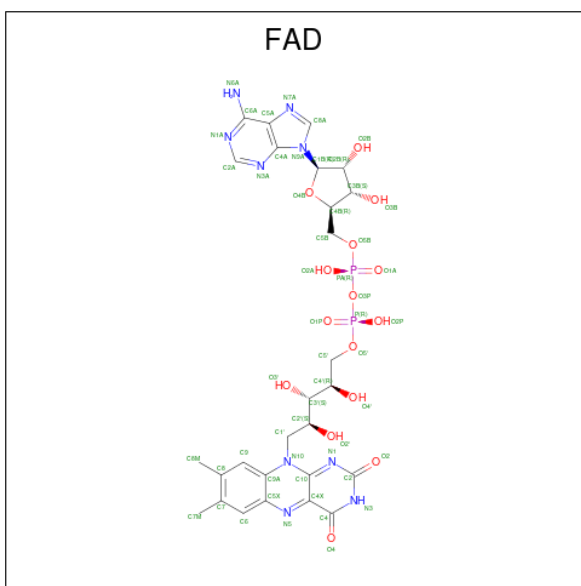
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



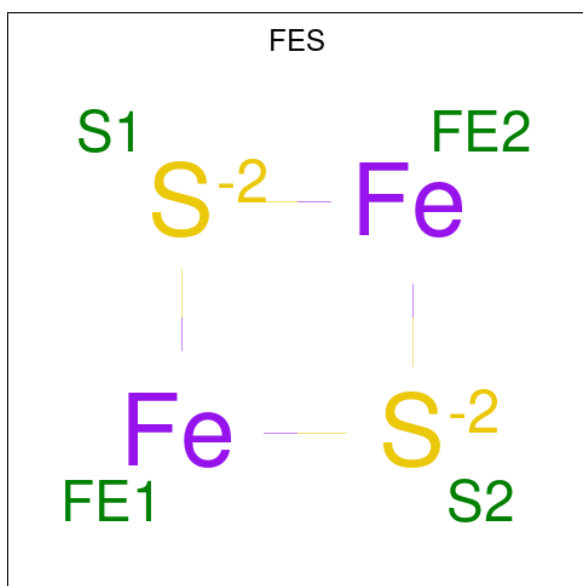
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 4 5	0	0
5	M	1	Total C O 9 4 5	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



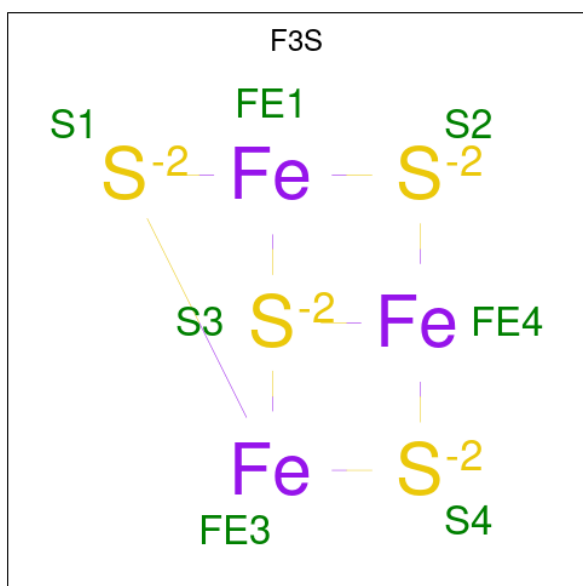
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
6	M	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



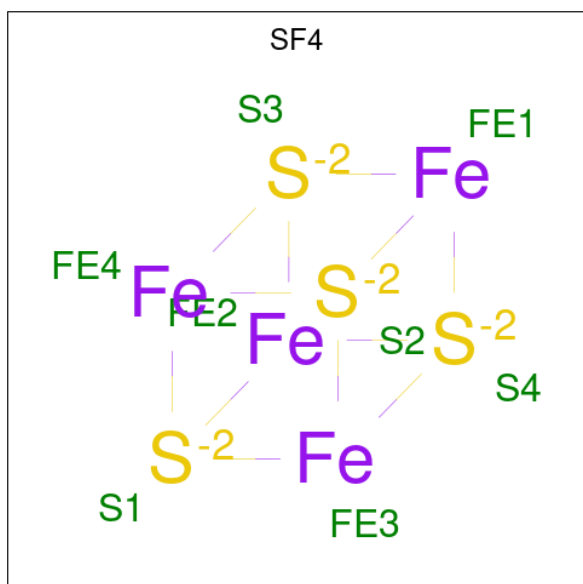
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

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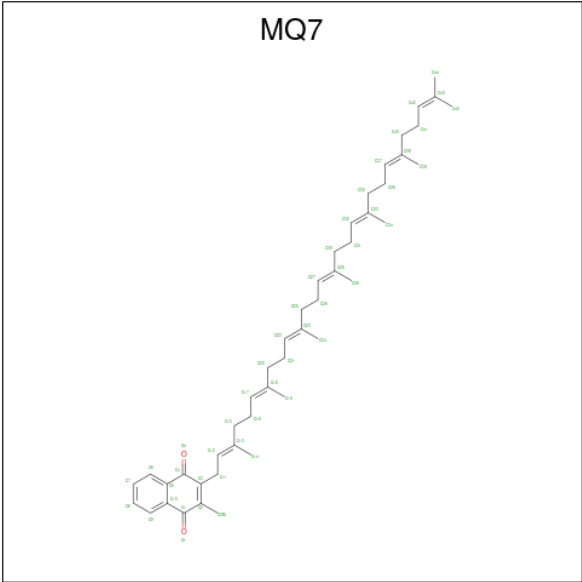
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



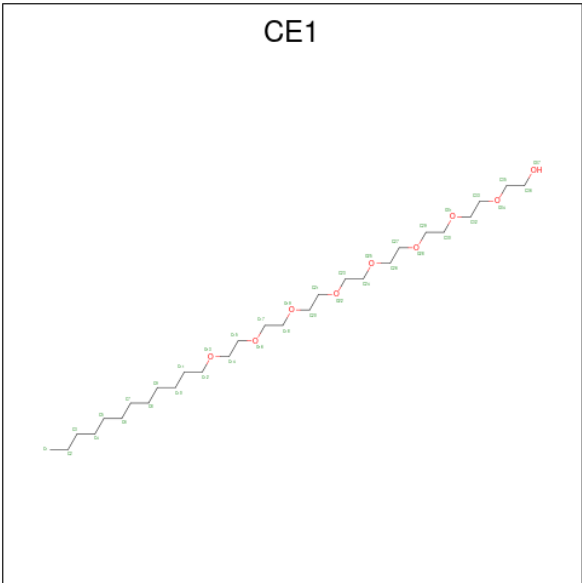
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $\text{C}_{46}\text{H}_{64}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			24	22	2		
10	D	1	Total	C	O	0	0
			24	22	2		
10	N	1	Total	C	O	0	0
			24	22	2		
10	P	1	Total	C	O	0	0
			24	22	2		

- Molecule 11 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: $C_{28}H_{58}O_9$).



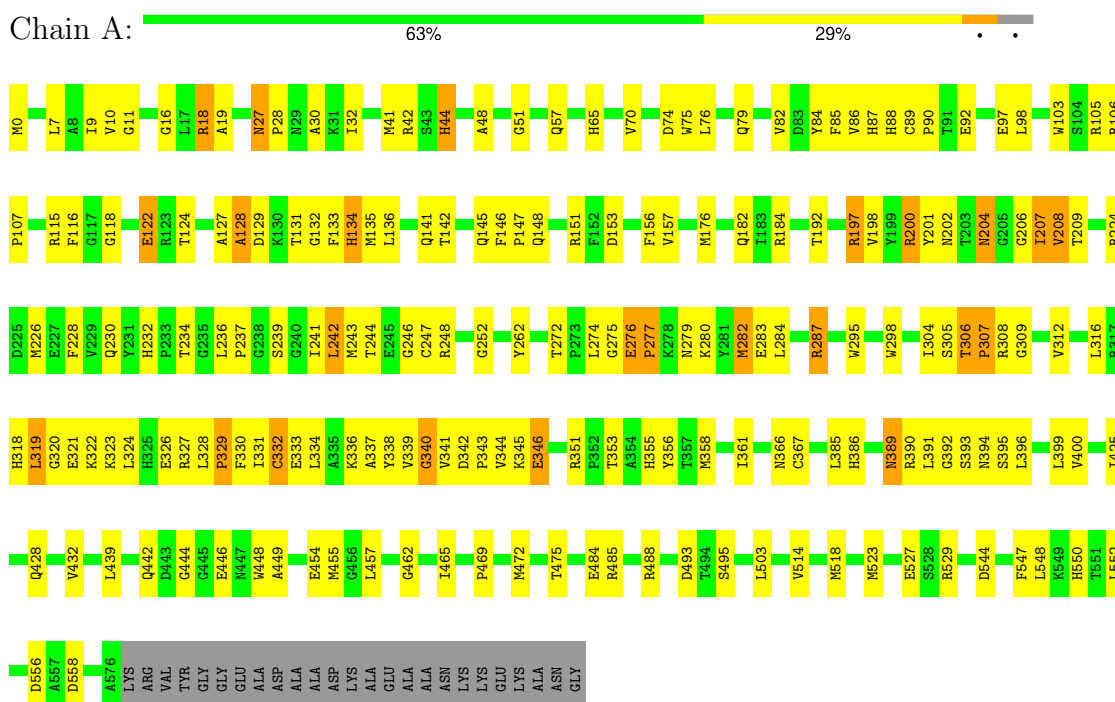
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			37	28	9		
11	D	1	Total	C	O	0	0
			37	28	9		
11	O	1	Total	C	O	0	0
			37	28	9		
11	O	1	Total	C	O	0	0
			37	28	9		

3 Residue-property plots

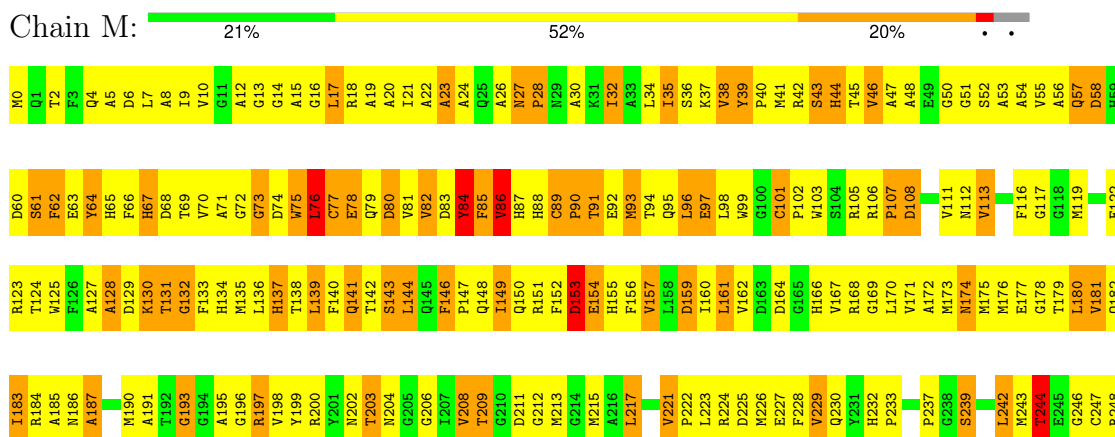
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

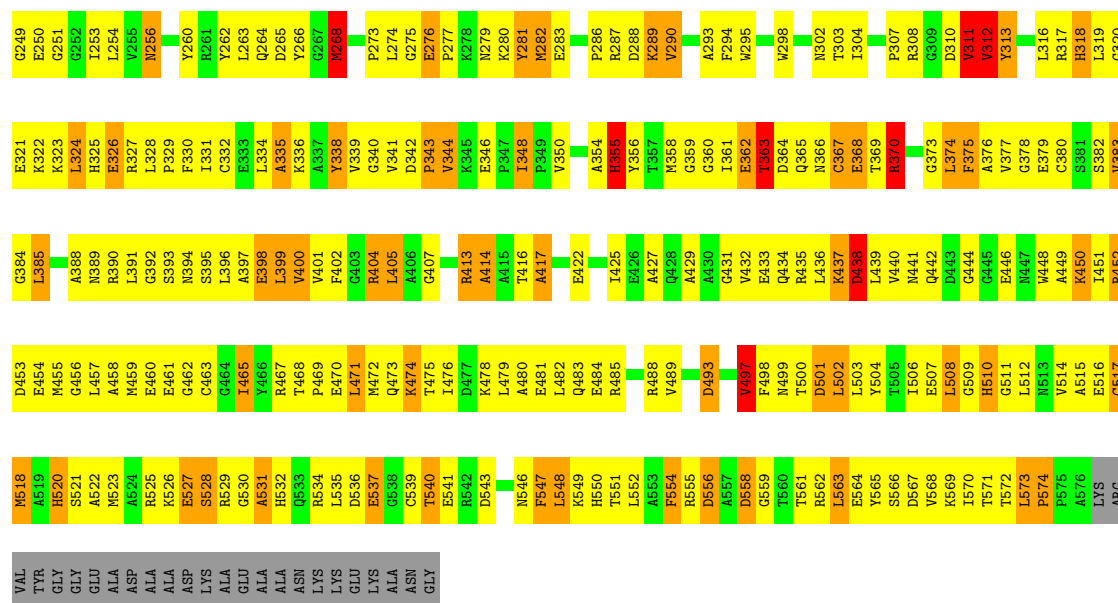
Note EDS was not executed.

- Molecule 1: Fumarate reductase flavoprotein subunit

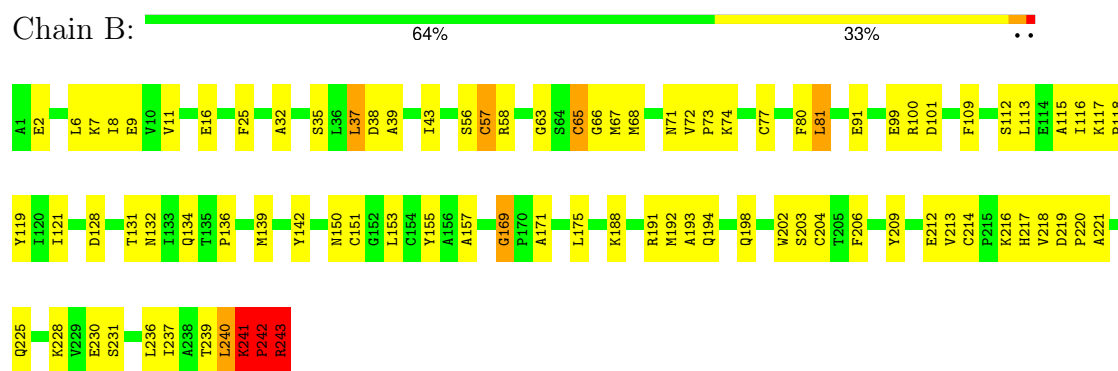


- Molecule 1: Fumarate reductase flavoprotein subunit

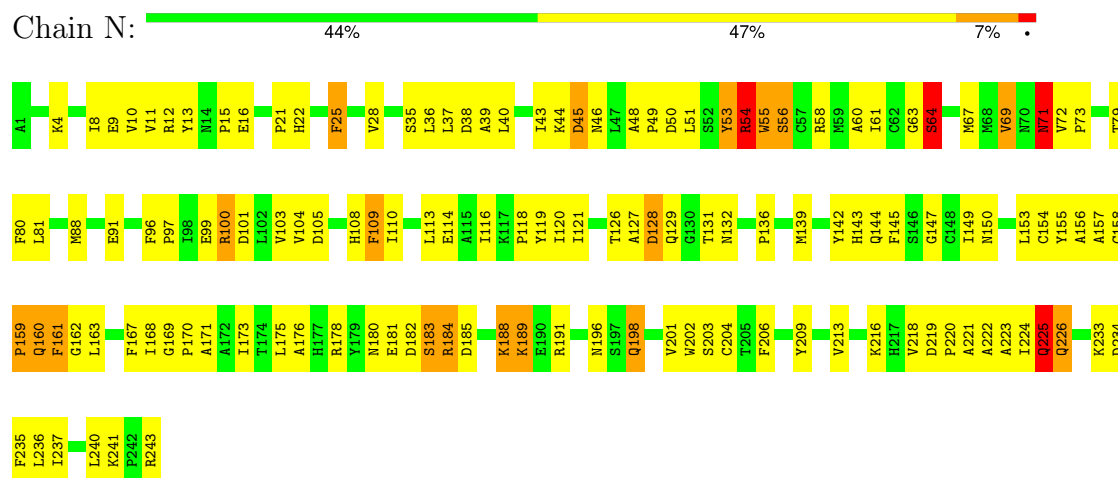




- Molecule 2: Fumarate reductase iron-sulfur protein

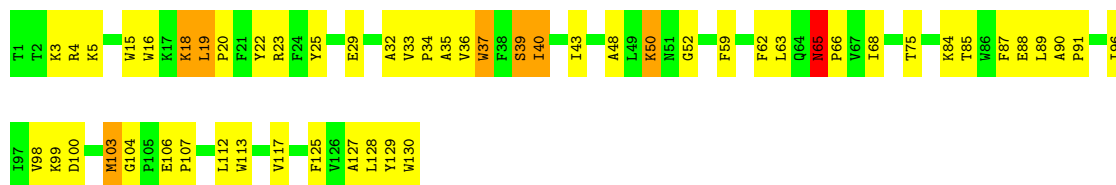


- Molecule 2: Fumarate reductase iron-sulfur protein



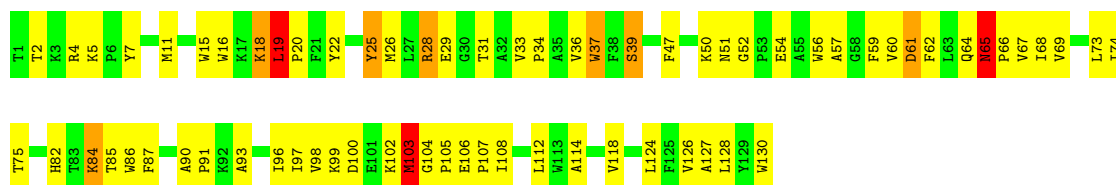
- Molecule 3: Fumarate reductase 15 kDa hydrophobic protein

Chain C:  58% 35% 5% •

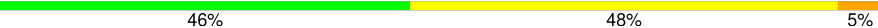


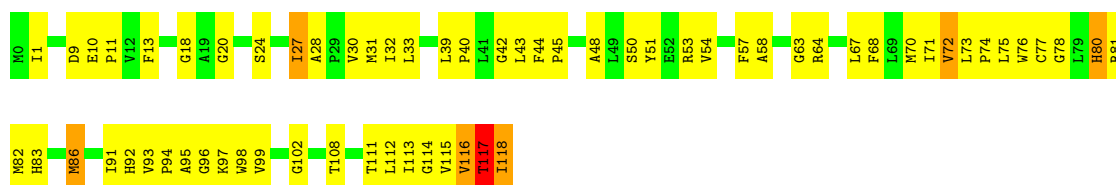
- Molecule 3: Fumarate reductase 15 kDa hydrophobic protein

Chain O:  47% 45% 5% •



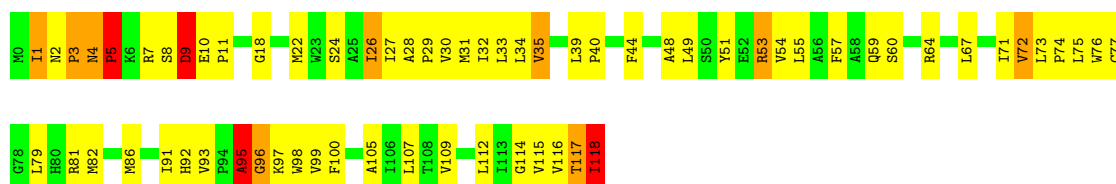
- Molecule 4: Fumarate reductase 13 kDa hydrophobic protein

Chain D:  46% 48% 5% •



- Molecule 4: Fumarate reductase 13 kDa hydrophobic protein

Chain P:  45% 45% 8% •



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.59Å 138.09Å 275.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17046	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, SF4, FES, OAA, MQ7, FAD, CE1

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	0.79	2/4540 (0.0%)	1.16	33/6139 (0.5%)
1	M	0.58	1/4540 (0.0%)	1.18	54/6139 (0.9%)
2	B	1.17	10/1931 (0.5%)	1.48	24/2617 (0.9%)
2	N	1.21	10/1931 (0.5%)	1.39	26/2617 (1.0%)
3	C	0.66	0/1094	1.07	8/1496 (0.5%)
3	O	0.66	0/1094	1.10	8/1496 (0.5%)
4	D	0.70	0/956	1.08	4/1303 (0.3%)
4	P	1.49	3/956 (0.3%)	1.18	11/1303 (0.8%)
All	All	0.89	26/17042 (0.2%)	1.22	168/23110 (0.7%)

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
2	B	0	1
2	N	0	3
4	P	0	1
All	All	0	5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	9	ASP	C-N	-37.54	0.83	1.33
2	B	243	ARG	CA-C	24.28	2.04	1.52
2	N	69	VAL	C-N	-21.89	1.03	1.33
2	N	159	PRO	C-N	-21.54	1.04	1.33
2	N	64	SER	C-N	18.66	1.59	1.33
2	B	243	ARG	C-O	16.23	1.56	1.23
4	P	95	ALA	C-N	16.21	1.57	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	242	PRO	CA-C	-14.08	1.32	1.52
2	N	4	LYS	C-N	-13.32	1.14	1.33
2	B	242	PRO	CB-CG	-12.78	0.85	1.49
2	N	161	PHE	C-N	12.66	1.49	1.33
2	N	54	ARG	C-N	10.98	1.49	1.33
2	N	55	TRP	C-N	8.60	1.45	1.33
2	N	63	GLY	C-N	-8.22	1.21	1.33
2	N	184	ARG	C-O	7.13	1.33	1.23
2	B	243	ARG	CA-CB	7.10	1.67	1.53
1	A	82	VAL	CA-CB	-7.06	1.46	1.54
2	B	243	ARG	CZ-NH1	-6.48	1.23	1.32
2	B	242	PRO	N-CA	-5.89	1.39	1.47
2	B	242	PRO	C-O	-5.51	1.16	1.24
1	A	135	MET	SD-CE	-5.50	1.65	1.79
4	P	4	ASN	CG-OD1	5.29	1.33	1.23
1	M	27	ASN	CG-OD1	5.19	1.33	1.23
2	N	67	MET	SD-CE	5.16	1.92	1.79
2	B	243	ARG	NE-CZ	-5.13	1.27	1.33
2	B	243	ARG	N-CA	5.06	1.55	1.46

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	LYS	CA-C-N	25.27	151.42	119.84
2	B	241	LYS	C-N-CA	25.27	151.42	119.84
2	B	243	ARG	CB-CG-CD	18.72	154.36	111.30
2	N	69	VAL	CA-C-N	18.09	148.05	122.36
2	N	69	VAL	C-N-CA	18.09	148.05	122.36
2	N	54	ARG	O-C-N	-15.99	104.03	123.05
1	M	268	MET	N-CA-C	-12.96	97.94	112.72
2	B	242	PRO	CA-N-CD	-11.76	95.53	112.00
1	A	128	ALA	N-CA-C	-11.45	86.41	110.80
1	M	97	GLU	N-CA-C	-11.23	99.56	113.38
2	N	4	LYS	O-C-N	-10.20	111.17	122.79
4	P	4	ASN	CA-C-N	10.08	132.44	119.84
4	P	4	ASN	C-N-CA	10.08	132.44	119.84
1	M	84	TYR	N-CA-C	-9.83	99.43	111.33
2	B	242	PRO	O-C-N	9.41	135.35	122.64
2	B	242	PRO	N-CA-C	-9.23	93.45	112.47
1	A	204	ASN	N-CA-C	9.20	121.72	110.41
2	N	183	SER	O-C-N	-9.13	110.45	122.59
3	O	52	GLY	CA-C-N	8.83	129.38	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	52	GLY	C-N-CA	8.83	129.38	119.32
1	A	337	ALA	N-CA-C	8.82	120.67	111.14
1	M	566	SER	N-CA-C	8.75	122.37	107.93
1	A	312	VAL	N-CA-C	-8.65	96.18	108.80
2	N	225	GLN	OE1-CD-NE2	-8.61	113.99	122.60
1	M	355	HIS	N-CA-C	8.51	121.66	108.12
2	N	160	GLN	OE1-CD-NE2	-8.49	114.11	122.60
2	B	65	CYS	N-CA-C	8.49	122.61	111.75
2	N	69	VAL	O-C-N	-8.44	110.80	122.62
1	M	80	ASP	N-CA-C	-7.98	101.88	111.69
1	M	93	MET	N-CA-C	-7.76	102.35	112.68
2	B	198	GLN	N-CA-C	-7.67	103.00	111.36
1	M	404	ARG	N-CA-C	-7.64	102.95	111.28
3	C	65	ASN	N-CA-C	7.52	126.44	109.81
2	B	243	ARG	NE-CZ-NH2	7.35	125.81	119.20
4	D	72	VAL	N-CA-C	7.28	117.36	110.30
1	M	146	PHE	CA-C-N	7.26	127.26	119.28
1	M	146	PHE	C-N-CA	7.26	127.26	119.28
1	M	398	GLU	N-CA-C	-7.21	101.94	111.24
2	B	243	ARG	NE-CZ-NH1	-7.16	114.34	121.50
1	M	346	GLU	N-CA-C	7.01	114.31	108.07
1	M	437	LYS	N-CA-C	-6.97	103.73	111.82
1	M	38	VAL	N-CA-C	-6.89	95.01	109.34
1	A	105	ARG	N-CA-C	6.84	120.66	109.85
3	O	25	TYR	N-CA-C	-6.74	103.86	111.14
1	M	174	ASN	N-CA-C	-6.72	97.88	108.63
1	A	282	MET	CB-CA-C	-6.62	108.92	116.54
1	M	438	ASP	N-CA-C	-6.61	105.18	113.18
4	D	27	ILE	N-CA-C	6.60	121.34	113.22
2	B	57	CYS	N-CA-C	6.59	118.47	111.28
4	P	72	VAL	N-CA-C	6.55	116.58	110.42
1	M	213	MET	N-CA-C	-6.50	103.89	110.97
1	M	281	TYR	N-CA-C	6.47	120.03	110.46
1	A	276	GLU	N-CA-C	6.43	119.98	108.47
4	P	35	VAL	N-CA-C	6.41	116.57	110.42
1	A	133	PHE	N-CA-C	-6.38	104.24	111.07
1	A	272	THR	N-CA-C	-6.37	102.11	110.39
2	N	184	ARG	O-C-N	-6.35	114.40	122.34
1	A	134	HIS	N-CA-C	6.35	119.01	111.71
1	A	319	LEU	N-CA-C	-6.34	105.44	113.43
1	M	313	TYR	N-CA-C	6.34	118.74	108.34
1	A	106	ARG	N-CA-C	-6.34	101.87	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	MET	N-CA-C	-6.32	104.02	111.03
4	P	1	ILE	N-CA-C	6.31	115.70	106.55
2	B	37	LEU	N-CA-C	-6.30	104.33	111.07
2	N	48	ALA	CA-C-N	6.27	125.97	119.82
2	N	48	ALA	C-N-CA	6.27	125.97	119.82
1	M	338	TYR	N-CA-C	6.23	119.05	111.82
1	A	432	VAL	N-CA-C	-6.22	104.45	110.42
3	O	19	LEU	CA-C-N	6.16	127.54	119.84
3	O	19	LEU	C-N-CA	6.16	127.54	119.84
1	A	338	TYR	N-CA-C	6.15	120.78	113.28
2	B	169	GLY	N-CA-C	6.15	124.88	112.34
3	O	103	MET	N-CA-C	6.12	117.99	109.31
3	C	89	LEU	N-CA-C	6.10	117.93	111.28
2	N	225	GLN	CG-CD-NE2	6.08	125.53	116.40
1	M	422	GLU	N-CA-C	6.07	118.87	111.82
1	M	452	ARG	N-CA-C	-6.06	104.58	111.07
1	M	17	LEU	N-CA-C	-6.06	104.59	111.07
1	M	295	TRP	N-CA-C	-6.06	104.68	111.28
1	M	370	ARG	N-CA-C	-6.06	104.68	111.28
2	N	160	GLN	CG-CD-NE2	6.05	125.47	116.40
3	O	73	LEU	N-CA-C	-6.05	104.61	111.14
3	C	48	ALA	N-CA-C	-6.04	104.77	111.36
4	P	100	PHE	N-CA-C	6.04	117.53	111.07
1	A	277	PRO	N-CA-C	-6.02	101.62	111.68
1	M	276	GLU	CA-C-N	6.02	125.78	119.76
1	M	276	GLU	C-N-CA	6.02	125.78	119.76
1	A	79	GLN	N-CA-C	5.99	118.57	111.33
2	N	4	LYS	CA-C-N	5.89	132.06	122.81
2	N	4	LYS	C-N-CA	5.89	132.06	122.81
4	D	80	HIS	N-CA-C	-5.87	104.79	111.07
2	N	80	PHE	N-CA-C	5.86	118.50	109.07
1	M	202	ASN	N-CA-C	5.85	118.18	108.99
1	M	471	LEU	N-CA-C	5.84	117.32	111.07
1	A	547	PHE	N-CA-C	5.82	121.15	112.94
1	M	71	ALA	N-CA-C	-5.74	105.11	111.71
1	M	23	ALA	N-CA-C	-5.73	106.09	112.57
2	B	241	LYS	O-C-N	5.72	125.84	121.27
1	M	209	THR	N-CA-C	-5.71	106.30	113.20
1	A	70	VAL	N-CA-C	5.70	116.48	110.72
1	M	73	GLY	N-CA-C	-5.70	105.82	115.34
2	N	71	ASN	CA-CB-CG	-5.69	106.91	112.60
1	M	414	ALA	N-CA-C	-5.68	107.34	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	46	VAL	N-CA-C	-5.68	105.19	110.53
1	M	547	PHE	N-CA-C	5.67	121.09	113.72
1	A	192	THR	N-CA-C	5.66	120.03	113.18
2	B	243	ARG	CD-NE-CZ	-5.65	116.49	124.40
2	N	56	SER	O-C-N	-5.61	115.13	122.59
1	A	44	HIS	N-CA-C	5.58	118.08	111.33
1	M	61	SER	N-CA-C	5.56	116.98	108.42
2	B	80	PHE	N-CA-C	5.54	117.94	108.90
2	B	71	ASN	N-CA-C	5.53	119.85	113.38
2	B	136	PRO	N-CA-C	-5.52	105.85	113.53
3	C	85	THR	N-CA-C	5.50	117.28	111.28
1	M	506	ILE	N-CA-C	-5.50	105.36	110.53
1	M	44	HIS	N-CA-C	-5.47	107.25	114.31
2	B	115	ALA	N-CA-C	5.47	119.05	112.38
1	A	207	ILE	N-CA-C	5.46	119.69	112.04
4	P	118	ILE	N-CA-C	5.46	126.28	111.00
1	A	306	THR	CA-C-N	5.44	124.62	118.97
1	A	306	THR	C-N-CA	5.44	124.62	118.97
1	M	335	ALA	N-CA-C	5.43	116.88	111.07
1	M	400	VAL	N-CA-C	5.41	116.81	111.67
1	A	465	ILE	N-CA-C	5.39	116.12	110.62
3	C	5	LYS	CA-C-N	5.39	126.23	119.98
3	C	5	LYS	C-N-CA	5.39	126.23	119.98
1	M	497	VAL	CB-CA-C	-5.36	106.57	112.68
2	N	60	ALA	N-CA-C	5.35	118.57	111.30
2	N	198	GLN	N-CA-C	-5.33	106.61	113.01
1	M	427	ALA	N-CA-C	-5.31	106.30	112.89
1	A	242	LEU	N-CA-C	5.31	117.93	110.23
1	M	149	ILE	CB-CA-C	-5.29	105.77	111.59
1	M	58	ASP	N-CA-C	5.27	119.63	112.04
3	O	65	ASN	N-CA-C	5.25	121.40	109.81
1	M	450	LYS	N-CA-C	-5.24	106.58	112.87
4	D	116	VAL	N-CA-C	-5.22	98.47	109.34
1	M	363	THR	N-CA-C	5.22	117.22	107.99
4	P	117	THR	N-CA-C	5.20	121.93	114.39
1	M	497	VAL	N-CA-C	5.20	114.08	106.55
2	B	242	PRO	N-CA-CB	5.19	108.70	103.25
2	N	153	LEU	N-CA-C	-5.19	105.80	111.82
4	P	107	LEU	N-CA-C	-5.16	105.65	111.28
1	M	385	LEU	N-CA-C	-5.15	107.16	113.50
1	A	355	HIS	N-CA-C	5.15	121.77	110.80
2	N	156	ALA	N-CA-C	-5.15	107.05	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	5	PRO	N-CA-C	5.13	123.04	112.47
2	N	181	GLU	CA-C-N	5.12	131.33	121.54
2	N	181	GLU	C-N-CA	5.12	131.33	121.54
1	A	129	ASP	N-CA-C	-5.11	106.79	112.57
1	M	573	LEU	CA-C-N	5.11	125.65	120.38
1	M	573	LEU	C-N-CA	5.11	125.65	120.38
1	M	144	LEU	N-CA-C	-5.11	107.72	114.31
3	C	19	LEU	N-CA-C	5.10	116.08	109.65
2	B	243	ARG	CB-CA-C	5.08	119.76	110.10
1	M	574	PRO	N-CA-C	5.08	116.89	110.70
3	C	40	ILE	N-CA-C	-5.07	105.38	110.30
2	N	45	ASP	N-CA-C	5.07	116.62	111.14
1	A	27	ASN	CA-C-N	5.07	126.18	119.84
1	A	27	ASN	C-N-CA	5.07	126.18	119.84
1	A	209	THR	N-CA-C	5.06	119.55	113.17
2	B	191	ARG	N-CA-C	5.06	119.72	113.50
4	P	26	ILE	N-CA-C	5.06	115.34	110.74
1	M	517	CYS	N-CA-C	-5.06	107.06	113.18
1	A	346	GLU	N-CA-C	5.05	113.95	108.14
2	B	204	CYS	N-CA-C	5.05	116.99	108.96
2	N	10	VAL	N-CA-C	5.03	115.10	107.75
1	A	75	TRP	N-CA-C	5.03	119.26	113.38
2	B	231	SER	N-CA-C	-5.01	105.10	111.11

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	243	ARG	Sidechain
2	N	183	SER	Mainchain
2	N	54	ARG	Mainchain
2	N	64	SER	Mainchain
4	P	9	ASP	Mainchain

5.2 Too-close contacts ⓘ

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	4448	0	4335	156	0
1	M	4448	0	4333	695	0
2	B	1888	0	1837	84	0
2	N	1888	0	1834	176	0
3	C	1058	0	1108	54	0
3	O	1058	0	1108	88	0
4	D	926	0	971	93	0
4	P	926	0	970	105	0
5	A	9	0	2	1	0
5	M	9	0	2	1	0
6	A	53	0	31	8	0
6	M	53	0	31	24	0
7	B	4	0	0	1	0
7	N	4	0	0	0	0
8	B	7	0	0	0	0
8	N	7	0	0	1	0
9	B	8	0	0	0	0
9	N	8	0	0	0	0
10	B	24	0	23	3	0
10	D	24	0	23	24	0
10	N	24	0	23	13	0
10	P	24	0	23	19	0
11	D	74	0	116	8	0
11	O	74	0	116	1	0
All	All	17046	0	16886	1353	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 40.

All (1353) 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:M:98:LEU:CD2	2:N:132:ASN:HD21	1.28	1.42
1:A:44:HIS:NE2	6:A:703:FAD:C8M	1.82	1.41
4:P:31:MET:HE1	10:P:800:MQ7:O1	1.23	1.34
1:M:44:HIS:NE2	6:M:803:FAD:HM81	1.41	1.34
1:M:493:ASP:OD2	2:N:50:ASP:HA	1.27	1.31
1:M:98:LEU:HD23	2:N:132:ASN:ND2	1.42	1.31
4:P:9:ASP:C	4:P:10:GLU:CA	2.01	1.31
2:B:243:ARG:CA	2:B:243:ARG:C	2.03	1.30
2:N:11:VAL:CG2	2:N:91:GLU:HG2	1.63	1.27
4:D:31:MET:HE1	10:D:700:MQ7:O1	1.27	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:44:HIS:NE2	6:M:803:FAD:C8M	1.99	1.25
4:P:9:ASP:CA	4:P:10:GLU:N	1.99	1.25
1:M:98:LEU:CD2	2:N:132:ASN:ND2	1.91	1.25
1:A:44:HIS:NE2	6:A:703:FAD:HM82	0.86	1.18
2:N:40:LEU:HB3	2:N:53:TYR:CE2	1.78	1.18
4:D:53:ARG:NH1	10:D:700:MQ7:H141	1.56	1.17
1:M:500:THR:OG1	2:N:44:LYS:NZ	1.78	1.17
4:D:53:ARG:NH1	10:D:700:MQ7:H151	1.61	1.16
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.08	1.13
4:D:53:ARG:NH1	10:D:700:MQ7:C14	2.10	1.13
4:P:9:ASP:O	4:P:10:GLU:N	1.80	1.13
4:D:53:ARG:HH12	10:D:700:MQ7:C14	1.62	1.11
4:D:53:ARG:HH12	10:D:700:MQ7:C15	1.63	1.11
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.24	1.11
4:P:86:MET:CE	4:P:91:ILE:HG21	1.81	1.10
2:N:36:LEU:HD13	2:N:88:MET:HE1	1.31	1.10
1:M:287:ARG:NH2	5:M:802:OAA:O3	1.85	1.10
1:A:44:HIS:CE1	6:A:703:FAD:HM82	1.85	1.09
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.32	1.07
4:P:59:GLN:HG2	4:P:118:ILE:HB	1.34	1.05
1:M:537:GLU:H	1:M:537:GLU:CD	1.59	1.04
4:P:53:ARG:NH1	10:P:800:MQ7:H141	1.75	1.02
2:B:242:PRO:CG	2:B:242:PRO:HB2	1.51	1.02
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.42	1.02
1:A:308:ARG:HH12	1:A:339:VAL:HA	1.25	1.01
4:D:53:ARG:HH12	10:D:700:MQ7:C13	1.72	1.01
2:N:36:LEU:HD13	2:N:88:MET:CE	1.90	1.01
4:P:64:ARG:HH22	4:P:118:ILE:N	1.56	1.01
2:B:242:PRO:CG	2:B:242:PRO:HB3	1.51	1.01
1:M:65:HIS:HD2	1:M:123:ARG:HD2	1.25	1.00
1:M:95:GLN:OE1	2:N:127:ALA:HB2	1.60	0.99
1:M:573:LEU:HD12	1:M:574:PRO:HD2	1.40	0.99
10:N:801:MQ7:H2M1	10:N:801:MQ7:H143	1.44	0.99
4:D:31:MET:CE	10:D:700:MQ7:O1	2.12	0.98
2:B:242:PRO:CB	2:B:242:PRO:HG2	1.48	0.98
1:M:223:LEU:HB3	1:M:226:MET:HG3	1.45	0.98
2:B:242:PRO:CB	2:B:242:PRO:HG3	1.48	0.97
1:M:222:PRO:HG2	1:M:362:GLU:HB2	1.43	0.97
4:P:53:ARG:HH12	10:P:800:MQ7:C14	1.75	0.97
1:M:501:ASP:OD2	2:N:49:PRO:HB3	1.63	0.97
3:O:19:LEU:H	3:O:19:LEU:HD23	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:75:THR:HG22	4:P:32:ILE:HD13	1.43	0.96
1:M:377:VAL:HG21	1:M:402:PHE:O	1.65	0.96
4:P:2:ASN:HB3	4:P:3:PRO:HD2	1.46	0.96
1:A:332:CYS:O	1:A:336:LYS:HG3	1.66	0.96
4:D:54:VAL:HG11	10:D:700:MQ7:H6	1.46	0.95
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.02	0.95
1:M:312:VAL:HG23	1:M:350:VAL:HG23	1.49	0.95
4:P:57:PHE:HB2	10:P:800:MQ7:H152	1.46	0.94
1:M:41:MET:SD	2:N:150:ASN:ND2	2.39	0.94
1:M:298:TRP:HD1	1:M:303:THR:HG21	1.33	0.94
4:D:54:VAL:HG13	10:D:700:MQ7:O4	1.68	0.94
2:N:225:GLN:OE1	3:O:93:ALA:HB2	1.66	0.93
1:M:177:GLU:OE1	3:O:2:THR:OG1	1.86	0.93
4:P:9:ASP:C	4:P:10:GLU:N	0.83	0.93
1:M:55:VAL:HA	1:M:123:ARG:HD3	1.50	0.92
3:C:19:LEU:HD12	3:C:20:PRO:HD2	1.49	0.92
1:M:98:LEU:HD23	2:N:132:ASN:HD21	0.97	0.92
4:P:64:ARG:NH1	4:P:118:ILE:OXT	2.00	0.92
1:M:167:VAL:HG11	1:M:374:LEU:HD13	1.52	0.91
1:A:321:GLU:HG2	1:A:344:VAL:HG11	1.52	0.91
2:N:11:VAL:HG21	2:N:91:GLU:CG	1.99	0.91
1:A:44:HIS:CD2	6:A:703:FAD:HM82	2.05	0.91
4:D:54:VAL:HG22	10:D:700:MQ7:O4	1.71	0.91
4:D:53:ARG:HH12	10:D:700:MQ7:H141	1.14	0.91
4:P:53:ARG:HH12	10:P:800:MQ7:H141	1.28	0.91
1:M:13:GLY:HA3	6:M:803:FAD:O2P	1.71	0.91
2:N:116:ILE:HG21	2:N:176:ALA:CB	2.02	0.90
1:A:324:LEU:HD13	1:A:344:VAL:HA	1.54	0.89
1:M:438:ASP:O	1:M:442:GLN:HB2	1.71	0.89
3:O:86:TRP:HE1	4:P:22:MET:HE2	1.37	0.89
1:A:287:ARG:HG3	1:A:287:ARG:NH1	1.82	0.89
4:P:64:ARG:HH22	4:P:118:ILE:H	1.14	0.89
1:M:497:VAL:HG21	2:N:15:PRO:HG2	1.53	0.89
4:P:53:ARG:NH1	10:P:800:MQ7:C14	2.34	0.89
4:D:53:ARG:NH1	10:D:700:MQ7:C15	2.28	0.89
1:M:17:LEU:HD22	1:M:139:LEU:HB3	1.54	0.88
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.37	0.88
4:D:54:VAL:CG1	10:D:700:MQ7:H6	2.03	0.88
4:P:31:MET:CE	10:P:800:MQ7:O1	2.19	0.88
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.55	0.88
1:A:327:ARG:O	1:A:328:LEU:HD23	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:PRO:HG2	2:B:243:ARG:HD3	1.55	0.87
1:M:98:LEU:HD22	2:N:132:ASN:HD21	1.39	0.87
1:M:467:ARG:NH1	1:M:532:HIS:HA	1.89	0.87
1:M:501:ASP:OD2	2:N:49:PRO:CB	2.22	0.87
1:M:35:ILE:HD13	1:M:157:VAL:HG23	1.57	0.87
2:N:40:LEU:HB3	2:N:53:TYR:HE2	1.34	0.87
1:M:44:HIS:NE2	6:M:803:FAD:HM83	1.91	0.85
1:M:537:GLU:CD	1:M:537:GLU:N	2.34	0.85
1:M:256:ASN:HD21	1:M:260:TYR:HB3	1.39	0.84
1:M:98:LEU:HD21	2:N:132:ASN:ND2	1.90	0.84
4:P:86:MET:CE	4:P:91:ILE:CG2	2.55	0.84
2:B:242:PRO:CG	2:B:243:ARG:HD3	2.07	0.83
3:C:33:VAL:HG22	4:D:82:MET:HE2	1.60	0.83
2:N:109:PHE:C	2:N:109:PHE:HD2	1.86	0.83
3:C:50:LYS:HD2	4:D:118:ILE:O	1.78	0.83
2:B:242:PRO:CG	2:B:242:PRO:CB	0.85	0.83
2:B:242:PRO:HB2	2:B:243:ARG:HD3	1.61	0.82
4:D:53:ARG:NH1	10:D:700:MQ7:C13	2.38	0.82
3:O:50:LYS:HZ2	4:P:117:THR:HG21	1.42	0.82
1:A:327:ARG:C	1:A:328:LEU:HD23	2.02	0.82
1:A:358:MET:HE3	1:A:389:ASN:HA	1.60	0.82
1:M:256:ASN:HD22	1:M:256:ASN:H	1.27	0.82
1:M:80:ASP:OD2	1:M:365:GLN:HG2	1.79	0.82
1:M:242:LEU:HD13	1:M:242:LEU:O	1.80	0.82
4:P:64:ARG:NH2	4:P:118:ILE:H	1.76	0.82
1:M:48:ALA:HB3	1:M:132:GLY:HA3	1.62	0.81
1:M:48:ALA:HB3	1:M:132:GLY:CA	2.10	0.81
3:O:127:ALA:HA	10:P:800:MQ7:H142	1.62	0.81
4:P:54:VAL:HG13	10:P:800:MQ7:H6	1.60	0.81
4:P:86:MET:HE3	4:P:91:ILE:CG2	2.11	0.81
1:M:396:LEU:HA	1:M:399:LEU:HD12	1.63	0.81
1:M:88:HIS:HB2	1:M:401:VAL:CG1	2.10	0.80
1:M:251:GLY:HA2	1:M:277:PRO:HG2	1.64	0.80
2:B:242:PRO:HB2	2:B:243:ARG:CD	2.11	0.80
1:M:286:PRO:HD2	1:M:289:LYS:HD2	1.64	0.80
2:N:36:LEU:CD1	2:N:88:MET:CE	2.60	0.80
2:N:11:VAL:HG23	2:N:91:GLU:HG2	1.59	0.80
1:M:168:ARG:HG3	1:M:425:ILE:CD1	2.12	0.80
1:M:263:LEU:HD12	1:M:283:GLU:HA	1.63	0.80
1:M:230:GLN:HE22	1:M:390:ARG:HB3	1.45	0.80
2:N:225:GLN:HE22	10:N:801:MQ7:H161	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:ARG:HG2	1:M:42:ARG:HH11	1.47	0.79
1:M:222:PRO:CG	1:M:362:GLU:HB2	2.11	0.79
1:M:206:GLY:HA3	2:N:55:TRP:CH2	2.17	0.79
3:O:50:LYS:NZ	4:P:117:THR:HG21	1.97	0.79
1:M:27:ASN:ND2	1:M:30:ALA:HB2	1.98	0.79
3:O:65:ASN:C	3:O:65:ASN:HD22	1.90	0.79
1:M:468:THR:HG22	1:M:535:LEU:HB2	1.64	0.79
1:M:551:THR:O	1:M:552:LEU:HD23	1.82	0.79
1:M:45:THR:HB	1:M:136:LEU:HB2	1.63	0.78
2:N:53:TYR:HE1	2:N:55:TRP:HD1	1.29	0.78
1:A:308:ARG:NH1	1:A:339:VAL:HA	1.97	0.78
1:M:263:LEU:CD1	1:M:283:GLU:HA	2.13	0.78
3:O:96:ILE:HD12	3:O:103:MET:HE2	1.65	0.78
2:N:109:PHE:C	2:N:109:PHE:CD2	2.60	0.78
1:M:211:ASP:HB3	1:M:510:HIS:ND1	1.98	0.78
1:M:493:ASP:OD2	2:N:50:ASP:CA	2.21	0.78
2:N:40:LEU:CB	2:N:53:TYR:CE2	2.65	0.78
2:N:53:TYR:HE1	2:N:55:TRP:CD1	2.01	0.77
1:A:41:MET:HE2	2:B:150:ASN:HD22	1.48	0.77
1:M:176:MET:O	1:M:497:VAL:HA	1.84	0.77
1:M:211:ASP:OD1	1:M:510:HIS:HB2	1.85	0.77
1:M:217:LEU:HD21	1:M:517:CYS:SG	2.24	0.77
1:A:327:ARG:O	1:A:329:PRO:HD3	1.85	0.77
1:M:46:VAL:HG22	2:N:61:ILE:HG13	1.66	0.77
1:M:187:ALA:HB2	1:M:414:ALA:HB2	1.65	0.77
1:M:168:ARG:HG3	1:M:425:ILE:HD13	1.66	0.77
1:M:227:GLU:OE1	1:M:522:ALA:HA	1.85	0.77
1:M:311:VAL:HG23	1:M:350:VAL:O	1.84	0.77
1:M:298:TRP:HA	1:M:303:THR:CG2	2.15	0.76
1:M:73:GLY:O	1:M:388:ALA:HB3	1.86	0.76
1:M:199:TYR:HE1	1:M:229:VAL:HG11	1.47	0.76
1:M:141:GLN:HG2	2:N:118:PRO:HB2	1.68	0.76
1:M:256:ASN:ND2	1:M:260:TYR:H	1.83	0.76
1:M:140:PHE:HA	1:M:143:SER:HB3	1.68	0.76
1:M:312:VAL:HG23	1:M:350:VAL:CG2	2.16	0.75
1:M:501:ASP:HB2	2:N:49:PRO:O	1.86	0.75
2:B:241:LYS:HG3	2:B:241:LYS:O	1.84	0.75
1:M:569:LYS:O	1:M:570:ILE:HD13	1.86	0.75
4:P:86:MET:HE3	4:P:91:ILE:HG21	1.66	0.75
1:M:128:ALA:O	1:M:130:LYS:N	2.20	0.74
1:M:556:ASP:HB3	1:M:558:ASP:OD1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:203:THR:HG23	1:M:354:ALA:O	1.87	0.74
1:M:304:ILE:HG13	1:M:313:TYR:CE2	2.21	0.74
1:M:263:LEU:HD22	1:M:268:MET:HE3	1.70	0.73
1:M:478:LYS:O	1:M:482:LEU:HG	1.88	0.73
1:M:139:LEU:O	1:M:142:THR:N	2.21	0.73
1:M:482:LEU:O	1:M:485:ARG:N	2.19	0.73
1:A:514:VAL:HG12	1:A:518:MET:HE3	1.68	0.73
1:M:84:TYR:CE1	1:M:405:LEU:HD21	2.23	0.73
4:P:86:MET:HE1	4:P:91:ILE:HG21	1.68	0.73
1:M:46:VAL:HG23	1:M:133:PHE:HB2	1.69	0.73
1:M:363:THR:HG22	1:M:367:CYS:HA	1.70	0.73
1:M:298:TRP:CD1	1:M:303:THR:HG21	2.20	0.73
1:M:515:ALA:O	1:M:518:MET:HB2	1.88	0.73
1:M:94:THR:HG23	2:N:131:THR:CG2	2.18	0.73
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.21	0.73
2:N:39:ALA:O	2:N:43:ILE:HG12	1.87	0.73
2:N:109:PHE:HD2	2:N:109:PHE:O	1.72	0.73
3:C:104:GLY:HA2	3:C:107:PRO:HD2	1.71	0.72
1:M:81:VAL:HG11	1:M:383:VAL:O	1.89	0.72
1:M:317:ARG:O	1:M:319:LEU:N	2.15	0.72
2:B:112:SER:HA	4:D:1:ILE:HD12	1.70	0.72
1:M:279:ASN:ND2	1:M:280:LYS:H	1.87	0.72
2:N:225:GLN:HE21	10:N:801:MQ7:C12	2.02	0.71
3:O:65:ASN:OD1	3:O:67:VAL:HB	1.89	0.71
1:M:435:ARG:HA	1:M:438:ASP:HB2	1.71	0.71
1:M:141:GLN:HB3	2:N:118:PRO:O	1.90	0.71
1:M:321:GLU:C	1:M:323:LYS:H	1.97	0.71
1:A:279:ASN:O	1:A:280:LYS:HB2	1.91	0.71
2:N:202:TRP:CZ2	4:P:11:PRO:HG3	2.26	0.71
1:M:176:MET:SD	2:N:99:GLU:HG3	2.31	0.71
1:M:256:ASN:ND2	1:M:260:TYR:HB3	2.05	0.71
1:M:324:LEU:HD12	1:M:332:CYS:SG	2.30	0.71
1:M:40:PRO:HB2	1:M:140:PHE:CD1	2.24	0.71
1:M:149:ILE:HD12	1:M:149:ILE:H	1.56	0.71
1:M:78:GLU:O	1:M:81:VAL:HB	1.91	0.70
1:M:195:ALA:O	1:M:198:VAL:HG13	1.91	0.70
3:C:88:GLU:O	3:C:91:PRO:HD2	1.90	0.70
1:M:509:GLY:C	1:M:511:GLY:H	1.98	0.70
1:M:177:GLU:OE1	3:O:4:ARG:HG2	1.91	0.70
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.27	0.70
1:M:467:ARG:HH12	1:M:532:HIS:HA	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:549:LYS:HE3	1:M:565:TYR:CD2	2.27	0.70
1:M:94:THR:HG23	2:N:131:THR:HG22	1.74	0.70
1:A:324:LEU:HD13	1:A:344:VAL:HG22	1.73	0.70
1:M:51:GLY:O	1:M:396:LEU:HD12	1.92	0.70
1:M:528:SER:HB2	1:M:539:CYS:O	1.92	0.70
3:O:65:ASN:CB	3:O:68:ILE:H	2.05	0.69
2:B:242:PRO:CB	2:B:243:ARG:HD3	2.20	0.69
1:M:113:VAL:HG12	1:M:124:THR:O	1.92	0.69
2:B:112:SER:HA	4:D:1:ILE:CD1	2.22	0.69
1:M:5:ALA:HB3	1:M:185:ALA:HB2	1.74	0.69
1:M:149:ILE:HG22	1:M:150:GLN:N	2.06	0.69
1:M:183:ILE:HD12	1:M:183:ILE:N	2.07	0.69
1:M:308:ARG:HD2	1:M:308:ARG:N	2.08	0.69
1:M:7:LEU:HA	1:M:187:ALA:HB3	1.73	0.69
1:M:35:ILE:HG12	1:M:36:SER:N	2.07	0.69
1:M:356:TYR:HE2	6:M:803:FAD:HO3'	1.38	0.69
2:N:225:GLN:NE2	10:N:801:MQ7:H161	2.07	0.69
1:M:479:LEU:HB3	1:M:516:GLU:HG2	1.74	0.69
3:O:19:LEU:H	3:O:19:LEU:CD2	2.05	0.69
3:O:106:GLU:HB2	3:O:107:PRO:HD3	1.73	0.68
2:B:236:LEU:HG	2:B:240:LEU:HD11	1.75	0.68
1:M:275:GLY:C	1:M:277:PRO:HD3	2.18	0.68
1:M:298:TRP:HA	1:M:303:THR:HG23	1.72	0.68
3:O:75:THR:HG22	4:P:32:ILE:CD1	2.20	0.68
2:N:11:VAL:CG2	2:N:91:GLU:CG	2.55	0.68
1:A:7:LEU:HD21	1:A:32:ILE:HG12	1.75	0.68
1:M:65:HIS:CD2	1:M:123:ARG:HD2	2.17	0.68
1:M:223:LEU:HB3	1:M:226:MET:CG	2.23	0.68
4:D:63:GLY:O	4:D:67:LEU:HD23	1.94	0.68
1:M:570:ILE:HG22	1:M:571:THR:H	1.58	0.68
3:O:104:GLY:HA2	3:O:107:PRO:HD2	1.75	0.68
1:M:182:GLN:HE21	1:M:184:ARG:HH22	1.42	0.68
1:A:327:ARG:C	1:A:329:PRO:HD3	2.20	0.68
1:M:536:ASP:O	1:M:540:THR:HG23	1.93	0.68
1:M:55:VAL:HG13	1:M:60:ASP:OD1	1.94	0.67
2:N:36:LEU:CD1	2:N:88:MET:HE1	2.16	0.67
1:A:321:GLU:HG2	1:A:344:VAL:CG1	2.23	0.67
1:M:469:PRO:HG3	1:M:536:ASP:OD2	1.94	0.67
2:N:225:GLN:HE22	10:N:801:MQ7:C16	2.08	0.67
1:M:204:ASN:ND2	6:M:803:FAD:HM82	2.09	0.67
1:M:15:ALA:HB2	1:M:399:LEU:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:66:PHE:O	1:M:69:THR:HB	1.94	0.67
1:M:373:GLY:O	1:M:375:PHE:HD1	1.77	0.67
1:M:500:THR:O	1:M:502:LEU:N	2.23	0.67
1:M:105:ARG:NH2	2:N:132:ASN:O	2.27	0.67
1:M:98:LEU:HD23	2:N:132:ASN:HD22	1.52	0.67
3:C:59:PHE:CZ	3:C:63:LEU:HD11	2.30	0.67
1:M:2:THR:HG23	1:M:184:ARG:HG3	1.77	0.67
1:M:256:ASN:HD21	1:M:260:TYR:H	1.43	0.67
4:D:54:VAL:CG1	10:D:700:MQ7:O4	2.43	0.66
4:D:68:PHE:CE1	4:D:72:VAL:HG21	2.29	0.66
1:M:358:MET:SD	1:M:390:ARG:N	2.68	0.66
4:P:39:LEU:HD13	4:P:49:LEU:HB3	1.77	0.66
1:M:228:PHE:CE2	1:M:388:ALA:HA	2.29	0.66
1:M:62:PHE:HD1	1:M:62:PHE:H	1.40	0.66
1:M:212:GLY:O	1:M:215:MET:HG2	1.94	0.66
1:M:263:LEU:HD13	1:M:282:MET:O	1.95	0.66
2:N:73:PRO:HG2	2:N:213:VAL:HG11	1.76	0.66
2:N:175:LEU:O	2:N:178:ARG:HB3	1.95	0.66
1:A:287:ARG:HH11	1:A:287:ARG:CG	1.95	0.66
1:M:40:PRO:HB2	1:M:140:PHE:CE1	2.31	0.66
1:M:159:ASP:CG	1:M:160:ILE:H	2.02	0.66
1:M:331:ILE:HD12	1:M:331:ILE:H	1.59	0.66
2:N:147:GLY:O	2:N:216:LYS:HG2	1.95	0.66
2:B:241:LYS:O	2:B:242:PRO:O	2.14	0.66
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.76	0.66
1:M:365:GLN:C	1:M:366:ASN:HD22	2.02	0.66
1:A:322:LYS:O	1:A:326:GLU:HB3	1.96	0.66
3:C:59:PHE:CE1	3:C:63:LEU:HD11	2.30	0.66
1:M:391:LEU:HB3	1:M:394:ASN:ND2	2.11	0.66
2:N:225:GLN:NE2	10:N:801:MQ7:C12	2.59	0.66
3:C:128:LEU:HD22	4:D:45:PRO:HD2	1.78	0.66
1:M:358:MET:HE1	1:M:389:ASN:HA	1.77	0.66
4:P:105:ALA:O	4:P:109:VAL:HG23	1.95	0.66
2:B:11:VAL:HG21	2:B:91:GLU:HG2	1.77	0.66
1:M:162:VAL:HG13	1:M:166:HIS:O	1.96	0.66
4:P:9:ASP:O	4:P:10:GLU:CA	2.31	0.65
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.60	0.65
1:M:97:GLU:OE1	2:N:131:THR:HB	1.96	0.65
2:N:169:GLY:O	2:N:173:ILE:HG13	1.96	0.65
1:M:46:VAL:CG2	1:M:133:PHE:HB2	2.26	0.65
1:M:15:ALA:N	1:M:399:LEU:HB3	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:54:VAL:CG2	10:D:700:MQ7:O4	2.45	0.65
4:P:79:LEU:HD23	4:P:82:MET:HE3	1.78	0.65
4:P:86:MET:HE3	4:P:91:ILE:CB	2.27	0.65
1:M:200:ARG:HG2	1:M:200:ARG:O	1.96	0.65
1:M:510:HIS:O	1:M:514:VAL:HG23	1.97	0.65
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.60	0.65
1:M:307:PRO:HD2	1:M:308:ARG:NH1	2.11	0.65
1:M:497:VAL:HG23	2:N:16:GLU:OE1	1.97	0.65
1:M:17:LEU:HD13	1:M:139:LEU:HB2	1.78	0.65
1:M:70:VAL:C	1:M:73:GLY:H	2.05	0.65
1:M:35:ILE:CG1	1:M:36:SER:N	2.59	0.64
2:B:241:LYS:C	2:B:242:PRO:O	2.33	0.64
1:M:440:VAL:C	1:M:442:GLN:H	2.05	0.64
2:N:28:VAL:HG22	2:N:43:ILE:HD11	1.80	0.64
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.78	0.64
1:M:67:HIS:C	1:M:69:THR:H	2.06	0.64
1:M:570:ILE:HG22	1:M:571:THR:N	2.13	0.64
2:N:8:ILE:HD11	2:N:81:LEU:HD21	1.79	0.64
4:P:9:ASP:O	4:P:10:GLU:C	2.40	0.64
1:M:37:LYS:HZ1	1:M:507:GLU:CD	2.05	0.64
3:O:106:GLU:H	3:O:106:GLU:CD	2.05	0.64
1:M:360:GLY:HA2	1:M:380:CYS:O	1.98	0.64
1:A:324:LEU:CD1	1:A:344:VAL:HA	2.27	0.64
1:M:341:VAL:O	1:M:343:PRO:HD3	1.98	0.64
2:B:243:ARG:NH1	4:P:92:HIS:ND1	2.46	0.64
1:M:88:HIS:HB2	1:M:401:VAL:HG13	1.78	0.64
2:N:69:VAL:HG11	2:N:79:THR:HG21	1.79	0.64
4:P:95:ALA:O	4:P:98:TRP:N	2.30	0.63
1:A:27:ASN:ND2	1:A:30:ALA:HB2	2.13	0.63
1:M:32:ILE:O	1:M:150:GLN:HB3	1.98	0.63
1:M:256:ASN:HD21	1:M:260:TYR:CB	2.10	0.63
1:M:499:ASN:ND2	1:M:502:LEU:HB3	2.13	0.63
1:M:525:ARG:CG	1:M:527:GLU:HB3	2.28	0.63
3:O:25:TYR:HD1	3:O:28:ARG:HH21	1.46	0.63
1:M:413:ARG:NH1	1:M:413:ARG:HB2	2.13	0.63
1:A:321:GLU:CG	1:A:344:VAL:HG11	2.27	0.63
1:M:162:VAL:HG22	1:M:167:VAL:CB	2.28	0.63
4:D:68:PHE:HD1	4:D:111:THR:HG22	1.64	0.63
2:N:236:LEU:HD23	2:N:236:LEU:C	2.24	0.63
1:M:191:ALA:HA	1:M:380:CYS:SG	2.38	0.63
4:D:76:TRP:CZ2	11:D:810:CE1:H351	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:60:SER:O	4:P:64:ARG:HG3	1.99	0.63
1:M:204:ASN:ND2	6:M:803:FAD:C8M	2.61	0.63
1:M:509:GLY:C	1:M:511:GLY:N	2.55	0.63
1:A:306:THR:HG23	1:A:307:PRO:HD2	1.81	0.62
3:O:97:ILE:HD13	3:O:102:LYS:HA	1.79	0.62
1:A:204:ASN:N	1:A:204:ASN:HD22	1.95	0.62
1:M:52:SER:O	1:M:125:TRP:HB2	1.99	0.62
1:M:527:GLU:HG3	1:M:528:SER:N	2.14	0.62
1:M:563:LEU:HD12	1:M:563:LEU:N	2.13	0.62
1:M:463:CYS:SG	1:M:467:ARG:NE	2.71	0.62
3:O:65:ASN:HB3	3:O:66:PRO:C	2.25	0.62
4:P:51:TYR:CE2	4:P:55:LEU:HD22	2.34	0.62
1:A:323:LYS:O	1:A:327:ARG:HB2	1.99	0.62
3:C:33:VAL:HA	4:D:82:MET:CE	2.30	0.62
1:M:511:GLY:O	1:M:515:ALA:N	2.32	0.62
2:N:28:VAL:CG2	2:N:43:ILE:HD11	2.30	0.62
1:M:24:ALA:C	1:M:26:ALA:H	2.08	0.62
1:M:44:HIS:HE1	1:M:204:ASN:HA	1.62	0.62
1:M:156:PHE:HE2	6:M:803:FAD:N6A	1.97	0.62
1:M:151:ARG:HB3	1:M:153:ASP:OD1	1.99	0.62
1:M:181:VAL:HG12	1:M:182:GLN:N	2.15	0.62
2:N:96:PHE:HB3	2:N:104:VAL:HB	1.82	0.62
1:M:548:LEU:O	1:M:548:LEU:HD23	2.00	0.62
3:O:65:ASN:HB2	3:O:68:ILE:HB	1.81	0.61
1:A:336:LYS:O	1:A:340:GLY:HA2	2.00	0.61
2:N:53:TYR:CD1	2:N:53:TYR:C	2.78	0.61
4:P:86:MET:HE3	4:P:91:ILE:HB	1.81	0.61
10:B:701:MQ7:H202	4:D:18:GLY:HA3	1.80	0.61
1:M:103:TRP:CZ3	1:M:131:THR:HG23	2.35	0.61
2:N:73:PRO:CG	2:N:213:VAL:HG11	2.30	0.61
4:P:55:LEU:O	4:P:59:GLN:HG3	2.00	0.61
4:P:64:ARG:HH12	4:P:118:ILE:C	2.09	0.61
1:A:141:GLN:HB3	2:B:118:PRO:O	2.01	0.61
1:M:149:ILE:HD12	1:M:149:ILE:N	2.16	0.61
1:M:331:ILE:HD12	1:M:331:ILE:N	2.16	0.61
2:B:116:ILE:HD12	2:B:116:ILE:C	2.26	0.61
1:M:226:MET:SD	1:M:359:GLY:HA3	2.40	0.61
1:M:479:LEU:HD23	1:M:482:LEU:HD12	1.82	0.61
4:P:53:ARG:NH1	10:P:800:MQ7:H143	2.16	0.61
3:C:22:TYR:O	3:C:25:TYR:HB3	2.00	0.61
1:M:396:LEU:C	1:M:398:GLU:H	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:44:HIS:CE1	6:M:803:FAD:HM81	2.29	0.60
1:M:221:VAL:HG22	1:M:369:THR:HB	1.83	0.60
1:A:324:LEU:HD13	1:A:344:VAL:CA	2.27	0.60
1:M:2:THR:HG23	1:M:184:ARG:CG	2.31	0.60
1:M:208:VAL:O	1:M:208:VAL:HG12	2.01	0.60
3:O:86:TRP:HE1	4:P:22:MET:CE	2.12	0.60
1:A:446:GLU:HB2	1:A:488:ARG:O	2.01	0.60
1:M:331:ILE:H	1:M:331:ILE:CD1	2.14	0.60
2:N:11:VAL:HG21	2:N:91:GLU:CB	2.31	0.60
3:C:87:PHE:CD2	3:C:112:LEU:HD13	2.36	0.60
1:M:204:ASN:HD22	6:M:803:FAD:HM82	1.64	0.60
1:M:356:TYR:CZ	1:M:379:GLU:HG3	2.37	0.60
1:M:526:LYS:HA	1:M:534:ARG:HH11	1.64	0.60
1:M:502:LEU:C	1:M:504:TYR:H	2.10	0.60
1:M:9:ILE:HD13	1:M:19:ALA:HB3	1.84	0.60
2:B:242:PRO:HB2	2:B:243:ARG:CG	2.32	0.60
1:A:306:THR:HB	1:A:309:GLY:O	2.00	0.60
1:M:42:ARG:HD3	2:N:64:SER:HB2	1.83	0.60
1:M:116:PHE:O	1:M:119:MET:HE3	2.02	0.60
1:M:356:TYR:OH	1:M:379:GLU:HA	2.01	0.60
1:M:480:ALA:HA	1:M:516:GLU:OE2	2.01	0.60
1:M:525:ARG:HG3	1:M:527:GLU:HB3	1.83	0.60
4:D:86:MET:HE3	4:D:86:MET:HA	1.84	0.60
1:M:509:GLY:O	1:M:511:GLY:N	2.35	0.60
1:M:520:HIS:O	1:M:521:SER:C	2.45	0.60
4:D:92:HIS:HB3	2:N:243:ARG:CB	2.31	0.59
1:M:34:LEU:HD13	1:M:149:ILE:HG23	1.84	0.59
4:P:9:ASP:N	4:P:10:GLU:N	2.48	0.59
1:A:41:MET:HA	1:A:136:LEU:HD21	1.83	0.59
4:D:117:THR:HG23	4:D:118:ILE:O	2.01	0.59
1:M:14:GLY:N	6:M:803:FAD:O2P	2.35	0.59
1:M:206:GLY:HA3	2:N:55:TRP:CZ3	2.36	0.59
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.37	0.59
1:M:382:SER:C	1:M:384:GLY:N	2.60	0.59
3:O:98:VAL:O	3:O:98:VAL:HG23	2.02	0.59
1:M:154:GLU:O	1:M:175:MET:HG3	2.02	0.59
1:M:183:ILE:HG22	1:M:184:ARG:N	2.17	0.59
1:M:512:LEU:O	1:M:515:ALA:HB3	2.02	0.59
1:A:304:ILE:HD12	1:A:304:ILE:H	1.66	0.59
1:M:13:GLY:CA	6:M:803:FAD:O2P	2.49	0.59
1:M:159:ASP:OD2	1:M:160:ILE:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:2:ASN:HB3	4:P:3:PRO:CD	2.28	0.59
4:P:57:PHE:CD2	10:P:800:MQ7:H12	2.36	0.59
1:M:204:ASN:HD22	6:M:803:FAD:C8M	2.16	0.59
1:M:375:PHE:HE1	1:M:413:ARG:HG2	1.67	0.59
1:M:391:LEU:HG	1:M:392:GLY:H	1.67	0.59
2:N:53:TYR:C	2:N:53:TYR:HD1	2.11	0.59
4:D:113:ILE:O	4:D:116:VAL:HG22	2.03	0.59
2:N:233:LYS:O	2:N:237:ILE:HD13	2.02	0.59
4:P:57:PHE:HD1	10:P:800:MQ7:H192	1.68	0.59
1:M:382:SER:C	1:M:384:GLY:H	2.09	0.58
3:C:33:VAL:HA	4:D:82:MET:HE3	1.85	0.58
1:M:20:ALA:HB3	1:M:34:LEU:HD21	1.85	0.58
1:M:221:VAL:HA	1:M:370:ARG:HG3	1.85	0.58
1:M:446:GLU:HB2	1:M:489:VAL:HG22	1.86	0.58
1:M:547:PHE:O	1:M:549:LYS:N	2.37	0.58
1:M:551:THR:C	1:M:552:LEU:HD23	2.28	0.58
2:N:119:TYR:CE1	2:N:121:ILE:HD11	2.38	0.58
1:A:341:VAL:O	1:A:343:PRO:HD3	2.03	0.58
1:M:9:ILE:HD13	1:M:19:ALA:CB	2.33	0.58
1:M:77:CYS:HA	1:M:550:HIS:HE1	1.67	0.58
2:N:40:LEU:HB3	2:N:53:TYR:CD2	2.37	0.58
4:P:64:ARG:HB3	4:P:115:VAL:HG22	1.85	0.58
2:B:68:MET:HE1	2:B:73:PRO:HD3	1.84	0.58
3:C:87:PHE:O	3:C:91:PRO:HD3	2.04	0.58
1:M:17:LEU:CD2	1:M:139:LEU:HB3	2.31	0.58
1:A:356:TYR:CE2	1:A:390:ARG:HD3	2.39	0.58
1:A:395:SER:O	1:A:399:LEU:HG	2.04	0.58
1:M:162:VAL:HG22	1:M:167:VAL:HB	1.84	0.58
4:P:53:ARG:CZ	10:P:800:MQ7:H141	2.34	0.58
1:M:15:ALA:HB2	1:M:399:LEU:CA	2.34	0.58
1:M:175:MET:HE2	1:M:503:LEU:HD13	1.85	0.58
1:M:44:HIS:CD2	6:M:803:FAD:C8M	2.86	0.58
1:M:181:VAL:HG12	1:M:182:GLN:H	1.69	0.58
2:N:220:PRO:O	2:N:223:ALA:N	2.37	0.58
1:A:469:PRO:HB3	1:A:523:MET:HE1	1.86	0.58
1:M:74:ASP:HA	1:M:75:TRP:CE3	2.38	0.58
1:M:155:HIS:CD2	1:M:174:ASN:HA	2.39	0.58
1:M:276:GLU:N	1:M:277:PRO:HD3	2.18	0.58
1:M:368:GLU:HA	1:M:375:PHE:HA	1.85	0.58
1:M:102:PRO:O	1:M:103:TRP:C	2.46	0.57
1:M:127:ALA:O	1:M:128:ALA:O	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:130:LYS:NZ	2:N:216:LYS:HD2	2.19	0.57
2:N:204:CYS:SG	2:N:224:ILE:HG21	2.43	0.57
3:O:50:LYS:HZ2	4:P:117:THR:CG2	2.14	0.57
4:P:77:CYS:O	4:P:81:ARG:HG3	2.04	0.57
4:P:95:ALA:HB1	4:P:98:TRP:HB2	1.85	0.57
3:O:65:ASN:OD1	3:O:68:ILE:HG12	2.03	0.57
4:P:4:ASN:N	4:P:5:PRO:HD3	2.18	0.57
4:D:42:GLY:O	4:D:44:PHE:N	2.35	0.57
1:M:10:VAL:CG1	1:M:157:VAL:HG21	2.35	0.57
1:M:304:ILE:HG13	1:M:313:TYR:HE2	1.68	0.57
1:M:316:LEU:HD12	1:M:348:ILE:HD11	1.85	0.57
3:O:19:LEU:HD21	3:O:22:TYR:CE2	2.39	0.57
1:A:48:ALA:HB3	1:A:132:GLY:HA3	1.86	0.57
4:D:115:VAL:C	4:D:117:THR:H	2.07	0.57
1:M:88:HIS:CB	1:M:401:VAL:HG13	2.34	0.57
1:M:162:VAL:HG13	1:M:166:HIS:C	2.30	0.57
1:M:48:ALA:HB3	1:M:132:GLY:HA2	1.84	0.57
1:M:211:ASP:OD1	1:M:507:GLU:HA	2.04	0.57
1:M:39:TYR:HE1	2:N:54:ARG:HH12	1.53	0.57
1:M:46:VAL:HA	1:M:133:PHE:HA	1.86	0.57
1:M:396:LEU:HA	1:M:399:LEU:CD1	2.34	0.57
1:M:514:VAL:O	1:M:518:MET:HG2	2.04	0.57
1:A:230:GLN:CD	1:A:287:ARG:HH21	2.13	0.57
1:M:62:PHE:HD2	1:M:87:HIS:HD1	1.52	0.57
1:M:217:LEU:HD11	1:M:223:LEU:HD11	1.87	0.57
4:D:113:ILE:O	4:D:116:VAL:CG2	2.53	0.56
1:M:22:ALA:HB1	1:M:404:ARG:HG3	1.86	0.56
1:M:161:LEU:HG	1:M:169:GLY:O	2.05	0.56
1:M:312:VAL:CG2	1:M:350:VAL:HG23	2.30	0.56
1:M:497:VAL:HG11	2:N:15:PRO:HG3	1.87	0.56
2:N:109:PHE:CE2	2:N:113:LEU:HD22	2.40	0.56
1:A:282:MET:HB3	1:A:283:GLU:OE1	2.05	0.56
1:M:396:LEU:C	1:M:398:GLU:N	2.63	0.56
1:A:392:GLY:O	1:A:393:SER:OG	2.21	0.56
4:D:102:GLY:HA2	11:D:710:CE1:H62	1.87	0.56
1:M:67:HIS:O	1:M:69:THR:N	2.38	0.56
1:M:82:VAL:HG22	1:M:385:LEU:HA	1.87	0.56
4:D:13:PHE:HE2	4:D:97:LYS:HE2	1.70	0.56
2:N:145:PHE:HA	2:N:218:VAL:HG13	1.88	0.56
3:O:19:LEU:HD23	3:O:19:LEU:N	2.09	0.56
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASN:O	1:A:367:CYS:HB2	2.06	0.56
1:A:439:LEU:HD12	1:A:442:GLN:NE2	2.20	0.56
2:B:2:GLU:HA	2:B:2:GLU:OE2	2.05	0.56
4:D:27:ILE:O	4:D:27:ILE:HG22	2.05	0.56
1:M:193:GLY:HA2	1:M:379:GLU:HB3	1.86	0.56
2:B:7:LYS:HE2	2:B:25:PHE:CD2	2.41	0.56
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.41	0.56
1:M:46:VAL:HG13	1:M:47:ALA:N	2.21	0.56
1:M:159:ASP:O	1:M:160:ILE:HG23	2.06	0.56
1:M:322:LYS:NZ	1:M:326:GLU:HG3	2.21	0.56
1:M:391:LEU:HG	1:M:392:GLY:N	2.20	0.56
1:M:436:LEU:HD12	1:M:436:LEU:O	2.06	0.56
1:M:137:HIS:O	1:M:138:THR:C	2.49	0.56
1:M:170:LEU:HD12	1:M:171:VAL:N	2.21	0.56
4:D:42:GLY:HA2	4:D:44:PHE:CE2	2.40	0.56
1:M:311:VAL:HG22	1:M:312:VAL:O	2.05	0.56
1:M:554:PHE:N	1:M:554:PHE:CD1	2.74	0.56
2:B:113:LEU:HD23	2:B:113:LEU:O	2.06	0.56
1:M:499:ASN:HA	2:N:100:ARG:HH21	1.71	0.56
3:C:98:VAL:HG23	3:C:98:VAL:O	2.05	0.56
1:M:323:LYS:HD3	1:M:327:ARG:CZ	2.36	0.56
3:O:65:ASN:HB2	3:O:68:ILE:HG12	1.87	0.56
1:A:57:GLN:NE2	1:A:122:GLU:HG2	2.20	0.55
1:M:150:GLN:O	1:M:150:GLN:HG3	2.05	0.55
1:M:230:GLN:NE2	1:M:358:MET:HE2	2.21	0.55
1:M:436:LEU:O	1:M:439:LEU:HB3	2.05	0.55
1:M:493:ASP:HB2	1:M:501:ASP:HB3	1.87	0.55
2:N:81:LEU:N	2:N:81:LEU:HD12	2.21	0.55
2:N:113:LEU:HD11	2:N:175:LEU:HD22	1.88	0.55
2:N:225:GLN:NE2	10:N:801:MQ7:C13	2.69	0.55
1:M:518:MET:HA	1:M:518:MET:HE2	1.87	0.55
2:N:69:VAL:CG1	2:N:88:MET:HE2	2.36	0.55
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.22	0.55
1:M:6:ASP:OD1	1:M:30:ALA:HA	2.07	0.55
1:M:186:ASN:O	1:M:414:ALA:HB2	2.06	0.55
1:M:504:TYR:HD2	1:M:507:GLU:HB2	1.70	0.55
2:N:201:VAL:HG23	2:N:202:TRP:N	2.20	0.55
1:M:77:CYS:O	1:M:79:GLN:N	2.40	0.55
1:M:190:MET:HE1	1:M:215:MET:SD	2.47	0.55
1:M:326:GLU:OE1	1:M:326:GLU:O	2.23	0.55
1:M:342:ASP:OD1	1:M:344:VAL:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:526:LYS:HA	1:M:534:ARG:NH1	2.21	0.55
1:M:549:LYS:HD2	1:M:565:TYR:HB3	1.87	0.55
3:O:65:ASN:HB3	3:O:66:PRO:CA	2.36	0.55
1:M:328:LEU:N	1:M:329:PRO:HD3	2.21	0.55
1:M:364:ASP:OD1	1:M:368:GLU:HB3	2.06	0.55
1:M:454:GLU:O	1:M:455:MET:C	2.48	0.55
1:A:7:LEU:CD2	1:A:32:ILE:HG12	2.36	0.55
1:M:81:VAL:HG22	1:M:365:GLN:HA	1.89	0.55
1:M:308:ARG:HD2	1:M:308:ARG:H	1.70	0.55
4:D:114:GLY:O	4:D:117:THR:HA	2.07	0.55
1:M:21:ILE:HG21	1:M:99:TRP:CH2	2.42	0.55
1:M:211:ASP:O	1:M:215:MET:N	2.39	0.55
3:O:25:TYR:HD1	3:O:28:ARG:NH2	2.04	0.55
4:P:7:ARG:HH11	4:P:7:ARG:HB2	1.72	0.55
4:P:7:ARG:HG2	4:P:8:SER:N	2.21	0.55
1:M:89:CYS:C	1:M:91:THR:H	2.15	0.55
2:N:25:PHE:N	2:N:25:PHE:CD1	2.72	0.55
3:O:126:VAL:HA	3:O:130:TRP:HB3	1.88	0.55
4:P:3:PRO:C	4:P:4:ASN:HD22	2.15	0.55
2:B:99:GLU:OE2	3:C:4:ARG:NH1	2.40	0.55
4:D:67:LEU:O	4:D:71:ILE:HG13	2.07	0.55
1:M:504:TYR:CD2	1:M:507:GLU:HB2	2.42	0.55
1:A:237:PRO:HB2	1:A:308:ARG:HB2	1.89	0.54
1:A:529:ARG:NH2	1:A:544:ASP:OD1	2.38	0.54
2:B:39:ALA:O	2:B:43:ILE:HG13	2.07	0.54
2:N:36:LEU:CD1	2:N:88:MET:SD	2.96	0.54
4:P:53:ARG:HH12	10:P:800:MQ7:H143	1.64	0.54
1:A:127:ALA:HB1	1:A:134:HIS:CD2	2.43	0.54
1:M:62:PHE:CD1	1:M:62:PHE:N	2.75	0.54
1:M:251:GLY:HA2	1:M:277:PRO:CG	2.35	0.54
1:A:316:LEU:O	1:A:319:LEU:HG	2.07	0.54
1:M:322:LYS:HZ2	1:M:326:GLU:HG3	1.73	0.54
1:M:468:THR:CG2	1:M:535:LEU:HD12	2.37	0.54
2:N:168:ILE:HD11	2:N:173:ILE:HG12	1.90	0.54
1:M:8:ALA:O	1:M:9:ILE:HG13	2.08	0.54
1:M:15:ALA:HB2	1:M:399:LEU:HB3	1.89	0.54
4:D:48:ALA:HA	4:D:53:ARG:HD3	1.89	0.54
1:M:94:THR:HG23	2:N:131:THR:HG23	1.88	0.54
2:N:40:LEU:HD13	2:N:53:TYR:CD2	2.43	0.54
1:A:127:ALA:HB1	1:A:134:HIS:HD2	1.73	0.54
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:HIS:HB3	2:N:243:ARG:HB3	1.88	0.54
1:M:539:CYS:O	1:M:541:GLU:N	2.40	0.54
2:B:214:CYS:SG	2:B:218:VAL:HG23	2.48	0.54
1:M:446:GLU:O	1:M:489:VAL:HG13	2.08	0.54
1:A:306:THR:CG2	1:A:307:PRO:HD2	2.38	0.54
4:D:53:ARG:HH11	4:D:53:ARG:HG2	1.73	0.54
1:M:335:ALA:O	1:M:339:VAL:CG2	2.56	0.54
4:P:24:SER:O	4:P:28:ALA:HB3	2.08	0.54
4:P:26:ILE:N	4:P:26:ILE:HD12	2.23	0.54
3:C:130:TRP:N	3:C:130:TRP:CD1	2.76	0.54
1:M:54:ALA:O	1:M:55:VAL:C	2.51	0.54
1:M:140:PHE:CA	1:M:143:SER:HB3	2.37	0.54
1:M:332:CYS:SG	1:M:343:PRO:HB2	2.48	0.54
1:M:434:GLN:HE21	1:M:434:GLN:HA	1.73	0.54
1:M:448:TRP:HB2	1:M:508:LEU:HD23	1.90	0.54
1:A:321:GLU:O	1:A:322:LYS:C	2.51	0.53
1:M:382:SER:O	1:M:384:GLY:N	2.42	0.53
1:A:226:MET:O	1:A:518:MET:HG2	2.08	0.53
1:A:307:PRO:C	1:A:309:GLY:H	2.16	0.53
3:C:19:LEU:HD12	3:C:20:PRO:CD	2.31	0.53
1:M:21:ILE:HG21	1:M:99:TRP:CZ3	2.43	0.53
1:M:42:ARG:HH11	1:M:42:ARG:CG	2.20	0.53
1:M:43:SER:HB2	1:M:136:LEU:HD22	1.91	0.53
1:M:169:GLY:HA3	1:M:184:ARG:HD3	1.89	0.53
1:M:525:ARG:O	1:M:534:ARG:NH1	2.41	0.53
1:A:142:THR:O	1:A:145:GLN:HG2	2.08	0.53
1:M:53:ALA:HB1	1:M:123:ARG:O	2.09	0.53
1:M:212:GLY:C	1:M:215:MET:HG2	2.33	0.53
2:N:73:PRO:HG2	2:N:213:VAL:CG1	2.38	0.53
1:A:176:MET:HG3	3:C:4:ARG:HD3	1.89	0.53
2:B:228:LYS:HZ3	10:B:701:MQ7:H6	1.74	0.53
1:M:7:LEU:O	1:M:32:ILE:HG23	2.08	0.53
1:M:10:VAL:HG11	1:M:157:VAL:HG21	1.90	0.53
1:M:44:HIS:CD2	6:M:803:FAD:HM83	2.43	0.53
1:M:82:VAL:O	1:M:82:VAL:HG12	2.09	0.53
1:M:127:ALA:HB3	1:M:131:THR:HA	1.89	0.53
1:M:321:GLU:C	1:M:323:LYS:N	2.64	0.53
1:M:484:GLU:O	1:M:488:ARG:HD2	2.07	0.53
2:B:6:LEU:HD23	2:B:81:LEU:HD13	1.90	0.53
1:M:149:ILE:CG2	1:M:150:GLN:N	2.71	0.53
1:M:40:PRO:HG2	1:M:151:ARG:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:449:ALA:C	1:M:451:ILE:N	2.66	0.53
1:A:228:PHE:O	1:A:358:MET:HB2	2.09	0.53
1:A:469:PRO:CB	1:A:523:MET:HE1	2.39	0.53
2:B:16:GLU:OE2	3:C:3:LYS:HD2	2.09	0.53
1:M:63:GLU:O	1:M:64:TYR:C	2.52	0.53
1:M:502:LEU:C	1:M:504:TYR:N	2.64	0.53
3:O:60:VAL:O	3:O:64:GLN:HG3	2.09	0.53
1:A:204:ASN:N	1:A:204:ASN:ND2	2.57	0.53
1:M:279:ASN:ND2	1:M:280:LYS:N	2.56	0.53
2:N:44:LYS:HD3	2:N:51:LEU:O	2.09	0.53
2:N:109:PHE:CD2	2:N:109:PHE:O	2.58	0.53
1:M:15:ALA:HA	1:M:399:LEU:O	2.08	0.53
1:M:336:LYS:O	1:M:340:GLY:HA2	2.09	0.53
3:O:65:ASN:HB3	3:O:68:ILE:H	1.73	0.53
1:A:236:LEU:CG	1:A:243:MET:HE3	2.38	0.52
1:M:81:VAL:C	1:M:83:ASP:H	2.17	0.52
1:M:440:VAL:C	1:M:442:GLN:N	2.67	0.52
4:P:3:PRO:O	4:P:4:ASN:ND2	2.42	0.52
1:A:324:LEU:CD1	1:A:344:VAL:HG22	2.37	0.52
1:M:67:HIS:C	1:M:69:THR:N	2.66	0.52
1:M:51:GLY:O	6:M:803:FAD:N3	2.43	0.52
1:A:399:LEU:HD11	6:A:703:FAD:H4'	1.91	0.52
1:M:530:GLY:O	1:M:532:HIS:N	2.42	0.52
1:M:103:TRP:HZ3	1:M:131:THR:HG23	1.74	0.52
1:M:288:ASP:O	1:M:289:LYS:C	2.51	0.52
1:M:373:GLY:O	1:M:375:PHE:CD1	2.62	0.52
1:M:564:GLU:C	1:M:565:TYR:CD1	2.88	0.52
1:M:183:ILE:N	1:M:183:ILE:CD1	2.72	0.52
1:M:429:ALA:HA	1:M:432:VAL:HG23	1.91	0.52
1:M:463:CYS:SG	1:M:467:ARG:NH2	2.83	0.52
3:O:65:ASN:CG	3:O:67:VAL:N	2.67	0.52
2:B:113:LEU:HD23	2:B:113:LEU:C	2.35	0.52
4:D:53:ARG:CZ	10:D:700:MQ7:H151	2.34	0.52
1:A:330:PHE:O	1:A:331:ILE:C	2.53	0.52
1:M:211:ASP:HA	1:M:510:HIS:HB3	1.92	0.52
2:N:206:PHE:HD1	10:N:801:MQ7:H112	1.75	0.52
4:P:1:ILE:HG23	4:P:1:ILE:O	2.08	0.52
4:P:10:GLU:N	4:P:11:PRO:CD	2.73	0.52
2:B:57:CYS:O	2:B:58:ARG:HB2	2.09	0.52
1:M:27:ASN:CG	1:M:30:ALA:HB2	2.35	0.52
1:M:212:GLY:HA2	1:M:215:MET:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:237:PRO:HB2	1:M:308:ARG:HB3	1.90	0.52
1:M:317:ARG:C	1:M:319:LEU:H	2.10	0.52
2:N:36:LEU:HD11	2:N:88:MET:SD	2.50	0.52
1:A:200:ARG:NH1	1:A:201:TYR:OH	2.43	0.52
3:C:75:THR:HG22	4:D:32:ILE:HD13	1.91	0.52
11:D:710:CE1:H211	11:D:710:CE1:H171	1.92	0.52
1:M:395:SER:OG	6:M:803:FAD:H1'2	2.10	0.52
2:N:109:PHE:HE2	2:N:113:LEU:HD22	1.75	0.52
2:N:196:ASN:ND2	2:N:234:ASP:OD1	2.40	0.52
3:O:39:SER:OG	4:P:71:ILE:O	2.27	0.52
1:A:304:ILE:HD12	1:A:304:ILE:N	2.25	0.51
1:M:7:LEU:CB	1:M:187:ALA:HB3	2.41	0.51
1:M:34:LEU:HD13	1:M:149:ILE:CG2	2.40	0.51
2:N:136:PRO:HG2	3:O:100:ASP:OD1	2.11	0.51
3:O:84:LYS:HG3	3:O:85:THR:N	2.25	0.51
4:P:54:VAL:CG1	10:P:800:MQ7:H6	2.37	0.51
4:D:57:PHE:CE1	10:D:700:MQ7:H192	2.45	0.51
1:M:230:GLN:NE2	1:M:390:ARG:HB3	2.20	0.51
1:M:256:ASN:HB2	1:M:302:ASN:HB3	1.91	0.51
3:O:65:ASN:HB2	3:O:68:ILE:CB	2.41	0.51
1:A:44:HIS:NE2	6:A:703:FAD:C8	2.69	0.51
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.91	0.51
4:D:54:VAL:HG13	10:D:700:MQ7:C4	2.37	0.51
1:M:62:PHE:HD2	1:M:87:HIS:ND1	2.08	0.51
2:N:108:HIS:HD2	2:N:161:PHE:HZ	1.57	0.51
1:M:444:GLY:HA3	1:M:488:ARG:O	2.11	0.51
1:M:452:ARG:C	1:M:454:GLU:H	2.19	0.51
3:C:106:GLU:CD	3:C:106:GLU:H	2.17	0.51
1:M:35:ILE:HD13	1:M:157:VAL:CG2	2.37	0.51
1:M:60:ASP:CG	1:M:123:ARG:HE	2.19	0.51
1:M:95:GLN:C	1:M:97:GLU:H	2.19	0.51
1:M:96:LEU:O	1:M:101:CYS:HB3	2.10	0.51
1:M:251:GLY:CA	1:M:277:PRO:HG2	2.38	0.51
1:M:554:PHE:N	1:M:554:PHE:HD1	2.08	0.51
1:A:202:ASN:HA	1:A:353:THR:HG22	1.93	0.51
2:B:236:LEU:O	2:B:239:THR:N	2.43	0.51
4:D:53:ARG:NH1	4:D:53:ARG:HG2	2.25	0.51
1:M:199:TYR:HE2	1:M:459:MET:O	1.94	0.51
1:M:474:LYS:O	1:M:474:LYS:HD3	2.11	0.51
2:N:72:VAL:CG1	2:N:73:PRO:HD2	2.41	0.51
1:A:484:GLU:HG3	1:A:488:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:478:LYS:O	1:M:482:LEU:N	2.44	0.51
4:D:9:ASP:CB	11:D:810:CE1:H242	2.41	0.51
1:M:360:GLY:HA3	1:M:382:SER:N	2.26	0.51
1:M:310:ASP:C	1:M:311:VAL:HG12	2.35	0.51
1:M:555:ARG:O	1:M:556:ASP:C	2.54	0.51
2:N:37:LEU:HD11	2:N:55:TRP:CB	2.40	0.51
3:O:33:VAL:HB	3:O:34:PRO:CD	2.34	0.51
2:B:236:LEU:O	2:B:237:ILE:C	2.54	0.51
1:M:15:ALA:HB2	1:M:399:LEU:CB	2.41	0.51
1:M:16:GLY:O	1:M:19:ALA:HB3	2.11	0.51
1:M:483:GLN:OE1	1:M:555:ARG:NH2	2.44	0.51
1:A:84:TYR:CE1	1:A:88:HIS:CE1	2.99	0.50
2:B:11:VAL:CG2	2:B:91:GLU:HG2	2.40	0.50
1:M:279:ASN:C	1:M:281:TYR:H	2.19	0.50
3:C:98:VAL:O	3:C:99:LYS:HB2	2.11	0.50
1:M:536:ASP:OD1	1:M:539:CYS:HB2	2.11	0.50
2:N:53:TYR:CE1	2:N:55:TRP:HD1	2.19	0.50
1:M:334:LEU:HD23	1:M:338:TYR:HE1	1.77	0.50
1:M:482:LEU:O	1:M:483:GLN:C	2.53	0.50
1:M:525:ARG:HG2	1:M:527:GLU:H	1.77	0.50
1:M:547:PHE:O	1:M:549:LYS:HG2	2.11	0.50
3:O:18:LYS:HD2	3:O:19:LEU:HD22	1.93	0.50
4:P:53:ARG:HH11	4:P:53:ARG:HG2	1.76	0.50
1:A:97:GLU:CD	2:B:131:THR:HB	2.36	0.50
1:A:556:ASP:HB2	1:A:558:ASP:OD2	2.11	0.50
4:D:24:SER:O	4:D:28:ALA:HB3	2.11	0.50
1:M:42:ARG:HG2	1:M:42:ARG:NH1	2.22	0.50
2:N:116:ILE:HG22	2:N:191:ARG:HD3	1.92	0.50
1:M:21:ILE:O	1:M:24:ALA:HB3	2.11	0.50
1:M:51:GLY:C	1:M:396:LEU:HD12	2.37	0.50
2:N:139:MET:HA	2:N:142:TYR:CE2	2.46	0.50
4:P:30:VAL:O	4:P:33:LEU:HB3	2.12	0.50
1:M:212:GLY:HA2	1:M:215:MET:SD	2.52	0.50
1:M:499:ASN:HD22	1:M:502:LEU:HB3	1.75	0.50
1:A:42:ARG:HD2	1:A:42:ARG:N	2.26	0.50
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.47	0.50
3:O:50:LYS:HZ3	11:O:812:CE1:C3	2.25	0.50
1:A:236:LEU:HG	1:A:243:MET:HE3	1.94	0.50
1:A:331:ILE:HD13	1:A:334:LEU:HD12	1.93	0.50
2:B:242:PRO:CD	2:B:243:ARG:HD3	2.42	0.50
3:C:15:TRP:O	3:C:18:LYS:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:ILE:O	4:D:27:ILE:CG2	2.60	0.50
4:D:70:MET:HE3	4:D:70:MET:O	2.12	0.50
1:M:93:MET:HG2	1:M:125:TRP:CD2	2.46	0.50
1:M:335:ALA:O	1:M:339:VAL:HG23	2.12	0.50
3:O:65:ASN:HB2	3:O:68:ILE:CG1	2.42	0.50
3:O:105:PRO:HD2	3:O:106:GLU:OE2	2.12	0.50
1:M:56:ALA:O	1:M:57:GLN:O	2.31	0.49
1:M:256:ASN:HD21	1:M:260:TYR:N	2.09	0.49
1:M:329:PRO:O	1:M:330:PHE:C	2.55	0.49
2:N:72:VAL:HG13	2:N:73:PRO:HD2	1.94	0.49
1:M:7:LEU:HD11	1:M:23:ALA:HB1	1.93	0.49
1:M:479:LEU:HA	1:M:482:LEU:HD12	1.93	0.49
2:N:56:SER:O	2:N:58:ARG:HG3	2.12	0.49
2:N:132:ASN:HB2	2:N:184:ARG:HD3	1.94	0.49
4:P:4:ASN:N	4:P:5:PRO:CD	2.74	0.49
1:A:0:MET:SD	1:A:182:GLN:HG3	2.52	0.49
1:A:391:LEU:O	1:A:394:ASN:HB2	2.12	0.49
2:B:6:LEU:CD2	2:B:81:LEU:HD13	2.43	0.49
3:C:65:ASN:HB3	3:C:68:ILE:H	1.77	0.49
4:D:98:TRP:NE1	11:D:710:CE1:H141	2.27	0.49
1:M:7:LEU:CA	1:M:187:ALA:HB3	2.41	0.49
1:M:20:ALA:HB2	1:M:34:LEU:HD11	1.94	0.49
1:M:525:ARG:HD3	1:M:527:GLU:CG	2.42	0.49
2:N:198:GLN:O	2:N:203:SER:HB2	2.12	0.49
4:D:78:GLY:O	4:D:82:MET:HG3	2.12	0.49
1:M:17:LEU:HD11	1:M:140:PHE:H	1.77	0.49
1:M:22:ALA:CB	1:M:404:ARG:HA	2.42	0.49
1:M:53:ALA:HA	1:M:124:THR:HA	1.94	0.49
1:M:133:PHE:O	1:M:137:HIS:HB2	2.11	0.49
1:M:479:LEU:HD13	1:M:516:GLU:N	2.27	0.49
1:M:539:CYS:C	1:M:541:GLU:H	2.19	0.49
4:P:96:GLY:O	4:P:97:LYS:C	2.55	0.49
1:A:51:GLY:HA3	1:A:124:THR:CG2	2.43	0.49
1:A:232:HIS:HD2	1:A:234:THR:H	1.61	0.49
1:M:20:ALA:CB	1:M:34:LEU:HD11	2.42	0.49
1:M:106:ARG:HG2	1:M:112:ASN:CB	2.43	0.49
1:M:127:ALA:C	1:M:128:ALA:O	2.54	0.49
1:A:307:PRO:C	1:A:309:GLY:N	2.69	0.49
4:D:39:LEU:HB3	4:D:40:PRO:CD	2.42	0.49
1:M:18:ARG:HG2	1:M:18:ARG:HH11	1.78	0.49
1:M:416:THR:OG1	1:M:417:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:501:ASP:OD2	2:N:49:PRO:HB2	2.11	0.49
3:O:130:TRP:O	4:P:53:ARG:NH2	2.45	0.49
1:M:162:VAL:HG22	1:M:167:VAL:HA	1.93	0.49
1:M:294:PHE:C	1:M:294:PHE:CD2	2.90	0.49
1:M:321:GLU:O	1:M:323:LYS:N	2.43	0.49
1:M:416:THR:O	1:M:417:ALA:C	2.55	0.49
1:M:479:LEU:HD13	1:M:516:GLU:HA	1.94	0.49
3:O:36:VAL:HG12	4:P:75:LEU:HD23	1.95	0.49
3:O:65:ASN:CG	3:O:68:ILE:H	2.20	0.49
3:C:128:LEU:O	4:D:45:PRO:HG2	2.13	0.49
3:C:127:ALA:HA	10:D:700:MQ7:H142	1.94	0.49
2:N:201:VAL:CG2	2:N:202:TRP:N	2.75	0.49
4:P:22:MET:O	4:P:26:ILE:HD13	2.13	0.49
2:N:154:CYS:SG	2:N:170:PRO:HG2	2.53	0.48
1:A:340:GLY:O	1:A:341:VAL:HG23	2.13	0.48
2:B:119:TYR:O	2:B:121:ILE:HG13	2.14	0.48
1:M:209:THR:O	1:M:209:THR:HG22	2.13	0.48
1:M:465:ILE:HD13	1:M:465:ILE:H	1.77	0.48
3:C:39:SER:O	3:C:43:ILE:HG13	2.12	0.48
1:M:88:HIS:O	1:M:401:VAL:HG22	2.14	0.48
1:M:89:CYS:HA	1:M:401:VAL:HG21	1.95	0.48
1:A:184:ARG:HG2	1:A:184:ARG:NH1	2.28	0.48
1:A:448:TRP:CG	1:A:449:ALA:N	2.81	0.48
1:M:37:LYS:NZ	1:M:507:GLU:CD	2.71	0.48
1:M:360:GLY:CA	1:M:380:CYS:O	2.60	0.48
1:M:360:GLY:O	1:M:361:ILE:HG23	2.13	0.48
1:M:375:PHE:CE1	1:M:413:ARG:HG2	2.45	0.48
1:M:452:ARG:HH12	2:N:45:ASP:CG	2.21	0.48
1:M:543:ASP:OD1	1:M:546:ASN:N	2.47	0.48
4:P:73:LEU:HB2	4:P:74:PRO:HD3	1.94	0.48
1:A:103:TRP:O	2:B:139:MET:HE1	2.14	0.48
3:C:98:VAL:HG22	3:C:103:MET:HB3	1.96	0.48
1:M:242:LEU:C	1:M:242:LEU:HD22	2.38	0.48
1:M:450:LYS:NZ	2:N:46:ASN:OD1	2.29	0.48
1:A:529:ARG:HH21	1:A:548:LEU:HD12	1.79	0.48
2:B:117:LYS:HD2	2:B:119:TYR:OH	2.13	0.48
3:C:50:LYS:HB3	4:D:118:ILE:HG22	1.95	0.48
1:M:177:GLU:CD	3:O:2:THR:OG1	2.55	0.48
1:M:499:ASN:HA	2:N:100:ARG:NH2	2.28	0.48
2:N:9:GLU:HG2	2:N:25:PHE:CE2	2.48	0.48
4:P:7:ARG:HB2	4:P:7:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:ILE:CG2	1:M:184:ARG:N	2.76	0.48
1:M:256:ASN:ND2	1:M:260:TYR:N	2.57	0.48
1:M:413:ARG:HB2	1:M:413:ARG:HH11	1.79	0.48
1:M:556:ASP:HB3	1:M:558:ASP:CG	2.38	0.48
1:M:136:LEU:O	1:M:136:LEU:HG	2.14	0.48
1:M:493:ASP:CG	2:N:50:ASP:HA	2.23	0.48
1:M:527:GLU:CG	1:M:528:SER:N	2.77	0.48
2:N:25:PHE:N	2:N:25:PHE:HD1	2.11	0.48
1:M:324:LEU:HG	1:M:344:VAL:HG12	1.95	0.48
1:M:327:ARG:O	1:M:328:LEU:HD12	2.14	0.48
1:M:525:ARG:O	1:M:534:ARG:HD2	2.14	0.48
2:N:162:GLY:HA3	3:O:11:MET:HE1	1.95	0.48
2:N:220:PRO:O	2:N:221:ALA:C	2.56	0.48
1:A:295:TRP:O	1:A:298:TRP:HB3	2.14	0.48
1:A:493:ASP:OD1	1:A:495:SER:OG	2.20	0.48
1:M:449:ALA:C	1:M:451:ILE:H	2.20	0.48
1:M:9:ILE:CD1	1:M:19:ALA:CB	2.92	0.47
1:M:153:ASP:O	1:M:155:HIS:ND1	2.46	0.47
1:M:500:THR:C	1:M:502:LEU:N	2.72	0.47
1:M:508:LEU:O	1:M:508:LEU:HD12	2.14	0.47
3:O:99:LYS:O	3:O:100:ASP:HB2	2.13	0.47
1:M:85:PHE:O	1:M:87:HIS:N	2.47	0.47
1:M:88:HIS:O	1:M:92:GLU:HB2	2.13	0.47
1:M:94:THR:O	1:M:94:THR:HG22	2.14	0.47
1:M:146:PHE:O	1:M:149:ILE:HD13	2.13	0.47
1:M:195:ALA:O	1:M:196:GLY:C	2.57	0.47
1:M:196:GLY:O	1:M:198:VAL:N	2.48	0.47
1:M:356:TYR:CE2	6:M:803:FAD:O3'	2.66	0.47
1:M:383:VAL:HG21	1:M:402:PHE:CE2	2.49	0.47
1:M:479:LEU:HD13	1:M:516:GLU:CA	2.44	0.47
4:P:35:VAL:O	4:P:40:PRO:HD3	2.13	0.47
1:M:18:ARG:HD2	1:M:18:ARG:O	2.14	0.47
1:M:63:GLU:OE1	1:M:66:PHE:HB3	2.14	0.47
1:M:182:GLN:C	1:M:183:ILE:HD12	2.39	0.47
1:M:212:GLY:CA	1:M:215:MET:HG2	2.44	0.47
1:M:373:GLY:O	1:M:375:PHE:N	2.39	0.47
4:P:67:LEU:O	4:P:71:ILE:HG13	2.14	0.47
2:B:35:SER:O	2:B:38:ASP:HB2	2.15	0.47
1:M:156:PHE:CE1	1:M:503:LEU:O	2.68	0.47
2:N:37:LEU:HD11	2:N:55:TRP:HB3	1.96	0.47
1:A:324:LEU:HD13	1:A:344:VAL:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:GLU:CD	1:A:485:ARG:HH22	2.23	0.47
3:O:65:ASN:C	3:O:65:ASN:ND2	2.59	0.47
3:C:33:VAL:HG22	4:D:82:MET:CE	2.41	0.47
4:D:57:PHE:HB2	10:D:700:MQ7:H152	1.97	0.47
1:M:46:VAL:HA	1:M:133:PHE:CA	2.45	0.47
1:M:318:HIS:O	1:M:319:LEU:HD23	2.15	0.47
1:M:523:MET:HE3	1:M:523:MET:O	2.14	0.47
1:M:525:ARG:HD3	1:M:527:GLU:HG2	1.95	0.47
2:N:189:LYS:H	2:N:189:LYS:HD3	1.79	0.47
3:O:90:ALA:N	3:O:91:PRO:HD2	2.30	0.47
1:A:89:CYS:HB2	1:A:90:PRO:HD3	1.96	0.47
1:A:246:GLY:O	1:A:247:CYS:C	2.58	0.47
3:C:59:PHE:O	3:C:62:PHE:HB3	2.15	0.47
1:M:9:ILE:CD1	1:M:19:ALA:HB1	2.44	0.47
1:M:146:PHE:HA	1:M:147:PRO:HD2	1.76	0.47
1:M:433:GLU:O	1:M:436:LEU:HB3	2.15	0.47
1:M:469:PRO:HG2	1:M:536:ASP:HB3	1.97	0.47
3:O:114:ALA:O	3:O:118:VAL:HG23	2.15	0.47
1:A:330:PHE:O	1:A:333:GLU:N	2.48	0.47
4:D:64:ARG:NH1	4:D:115:VAL:O	2.45	0.47
1:M:35:ILE:HG13	1:M:155:HIS:HB2	1.95	0.47
1:M:206:GLY:O	1:M:504:TYR:OH	2.32	0.47
1:M:507:GLU:O	1:M:508:LEU:C	2.57	0.47
1:A:127:ALA:HB2	1:A:131:THR:HA	1.96	0.47
1:M:75:TRP:O	1:M:76:LEU:HB2	2.14	0.47
1:M:246:GLY:O	1:M:249:GLY:N	2.48	0.47
1:M:316:LEU:CD1	1:M:348:ILE:HD11	2.44	0.47
1:M:182:GLN:NE2	1:M:184:ARG:HH22	2.11	0.47
1:A:236:LEU:HD21	1:A:243:MET:HE3	1.97	0.46
4:D:10:GLU:N	4:D:11:PRO:HD2	2.29	0.46
1:M:244:THR:HG23	1:M:247:CYS:SG	2.55	0.46
1:M:435:ARG:O	1:M:439:LEU:N	2.48	0.46
4:P:72:VAL:HG12	4:P:76:TRP:CD1	2.50	0.46
1:M:198:VAL:HG23	1:M:199:TYR:N	2.30	0.46
1:M:456:GLY:C	1:M:458:ALA:N	2.74	0.46
2:N:157:ALA:HB1	2:N:209:TYR:CD2	2.51	0.46
2:N:206:PHE:HA	8:N:245:F3S:S1	2.55	0.46
3:O:65:ASN:HB3	3:O:66:PRO:HA	1.96	0.46
1:A:11:GLY:O	1:A:16:GLY:HA3	2.16	0.46
1:A:275:GLY:O	1:A:277:PRO:HD3	2.16	0.46
1:M:52:SER:OG	1:M:397:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:87:HIS:C	1:M:89:CYS:H	2.23	0.46
1:M:139:LEU:O	1:M:143:SER:N	2.48	0.46
1:M:222:PRO:HG3	1:M:362:GLU:OE1	2.16	0.46
1:M:500:THR:HG1	2:N:44:LYS:NZ	2.02	0.46
1:A:230:GLN:HB2	1:A:358:MET:HE1	1.97	0.46
1:M:400:VAL:HG23	1:M:401:VAL:N	2.29	0.46
1:M:469:PRO:CG	1:M:536:ASP:HB3	2.46	0.46
2:N:149:ILE:O	2:N:149:ILE:HG13	2.14	0.46
1:A:361:ILE:H	1:A:361:ILE:HG13	1.51	0.46
2:B:151:CYS:SG	2:B:153:LEU:HG	2.56	0.46
2:B:192:MET:O	2:B:193:ALA:C	2.59	0.46
1:M:224:ARG:HG3	1:M:550:HIS:HB3	1.98	0.46
3:O:25:TYR:CD1	3:O:28:ARG:NH2	2.83	0.46
2:B:9:GLU:HG3	2:B:25:PHE:CZ	2.51	0.46
1:M:77:CYS:O	1:M:79:GLN:HG3	2.16	0.46
3:O:97:ILE:CD1	3:O:102:LYS:HA	2.45	0.46
3:C:113:TRP:O	3:C:117:VAL:HG23	2.15	0.46
4:D:54:VAL:HG13	10:D:700:MQ7:H6	1.93	0.46
1:M:45:THR:CB	1:M:136:LEU:HB2	2.42	0.46
1:M:82:VAL:HG13	1:M:385:LEU:HD12	1.97	0.46
1:M:101:CYS:H	1:M:138:THR:CG2	2.29	0.46
1:M:364:ASP:OD2	1:M:368:GLU:N	2.49	0.46
1:M:471:LEU:O	1:M:472:MET:C	2.56	0.46
1:M:483:GLN:HE21	1:M:512:LEU:HB3	1.81	0.46
4:D:9:ASP:HB3	11:D:810:CE1:H242	1.98	0.46
1:M:37:LYS:NZ	1:M:507:GLU:OE1	2.49	0.46
2:N:13:TYR:HB2	2:N:21:PRO:HB3	1.97	0.46
3:O:124:LEU:HD23	3:O:124:LEU:HA	1.84	0.46
1:A:319:LEU:HB3	1:A:323:LYS:HD3	1.98	0.46
1:A:328:LEU:HD23	1:A:328:LEU:N	2.25	0.46
4:D:115:VAL:C	4:D:117:THR:N	2.69	0.46
1:M:46:VAL:CG1	1:M:47:ALA:N	2.79	0.46
2:N:110:ILE:O	2:N:114:GLU:HG3	2.15	0.46
1:A:27:ASN:OD1	1:A:27:ASN:C	2.59	0.46
1:M:139:LEU:O	1:M:140:PHE:C	2.57	0.46
1:M:149:ILE:H	1:M:149:ILE:CD1	2.28	0.46
1:M:356:TYR:HB2	1:M:390:ARG:NH2	2.31	0.46
1:M:361:ILE:O	1:M:362:GLU:C	2.59	0.46
3:O:18:LYS:HD2	3:O:19:LEU:CD2	2.46	0.46
1:A:127:ALA:CB	1:A:131:THR:HA	2.45	0.45
1:A:198:VAL:HA	1:A:455:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:356:TYR:HB3	1:M:390:ARG:HH21	1.81	0.45
4:P:57:PHE:CG	10:P:800:MQ7:H12	2.51	0.45
1:A:252:GLY:HA3	1:A:316:LEU:HD23	1.98	0.45
3:C:50:LYS:CG	4:D:118:ILE:HG22	2.47	0.45
4:D:77:CYS:O	4:D:80:HIS:HB3	2.17	0.45
1:M:42:ARG:CG	1:M:42:ARG:NH1	2.78	0.45
1:M:246:GLY:O	1:M:247:CYS:C	2.60	0.45
1:M:429:ALA:HA	1:M:432:VAL:CG2	2.46	0.45
3:C:36:VAL:HG23	3:C:37:TRP:N	2.32	0.45
1:M:78:GLU:HG3	1:M:224:ARG:HH12	1.82	0.45
1:M:232:HIS:CE1	1:M:242:LEU:HD23	2.51	0.45
1:M:405:LEU:C	1:M:407:GLY:N	2.74	0.45
2:N:11:VAL:HG23	2:N:91:GLU:CG	2.39	0.45
3:O:74:ILE:O	3:O:75:THR:C	2.59	0.45
2:B:37:LEU:HD22	2:B:77:CYS:HB3	1.98	0.45
2:B:155:TYR:CE2	2:B:169:GLY:HA3	2.51	0.45
2:B:220:PRO:O	2:B:221:ALA:C	2.58	0.45
4:D:30:VAL:O	4:D:33:LEU:HB3	2.17	0.45
1:M:26:ALA:C	1:M:28:PRO:HD3	2.41	0.45
1:M:85:PHE:O	1:M:86:VAL:C	2.59	0.45
1:M:117:GLY:HA3	1:M:392:GLY:HA3	1.97	0.45
1:M:364:ASP:OD2	1:M:364:ASP:N	2.50	0.45
1:M:460:GLU:O	1:M:461:GLU:C	2.59	0.45
2:N:12:ARG:NH2	2:N:101:ASP:OD1	2.46	0.45
4:P:112:LEU:O	4:P:116:VAL:HG22	2.16	0.45
1:A:98:LEU:HD23	2:B:132:ASN:ND2	2.31	0.45
1:A:118:GLY:HA2	1:A:279:ASN:HD21	1.81	0.45
2:B:175:LEU:HD12	2:B:175:LEU:HA	1.83	0.45
2:B:243:ARG:HD2	4:P:92:HIS:CG	2.51	0.45
3:C:37:TRP:O	3:C:40:ILE:HB	2.16	0.45
1:M:20:ALA:CB	1:M:34:LEU:HD21	2.46	0.45
1:M:58:ASP:C	1:M:60:ASP:H	2.25	0.45
1:M:356:TYR:CB	1:M:390:ARG:HH21	2.29	0.45
4:D:76:TRP:CH2	11:D:810:CE1:H331	2.51	0.45
4:D:83:HIS:O	4:D:86:MET:HB2	2.17	0.45
4:D:92:HIS:HB3	2:N:243:ARG:HB2	1.98	0.45
1:M:78:GLU:HB3	1:M:81:VAL:HG23	1.98	0.45
1:M:133:PHE:HE2	1:M:134:HIS:CE1	2.34	0.45
1:M:140:PHE:O	1:M:143:SER:HB3	2.17	0.45
1:M:151:ARG:HB3	1:M:151:ARG:HH11	1.82	0.45
1:M:263:LEU:HD22	1:M:268:MET:CE	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:377:VAL:CG2	1:M:402:PHE:O	2.52	0.45
1:M:493:ASP:HB3	1:M:499:ASN:OD1	2.15	0.45
2:N:159:PRO:HB3	3:O:15:TRP:CZ3	2.51	0.45
2:N:235:PHE:HE1	4:P:8:SER:O	1.98	0.45
2:B:155:TYR:HE1	2:B:171:ALA:HB3	1.82	0.45
1:M:298:TRP:HA	1:M:303:THR:HG21	1.97	0.45
1:M:521:SER:HA	1:M:563:LEU:HD23	1.98	0.45
2:N:97:PRO:HG2	2:N:105:ASP:HB3	1.98	0.45
10:N:801:MQ7:H202	4:P:18:GLY:HA3	1.98	0.45
1:A:115:ARG:O	1:A:116:PHE:CD1	2.70	0.45
2:B:81:LEU:HD23	2:B:81:LEU:N	2.32	0.45
4:D:54:VAL:CG1	10:D:700:MQ7:C6	2.87	0.45
1:M:439:LEU:O	1:M:442:GLN:HB3	2.17	0.45
2:N:81:LEU:HD12	2:N:81:LEU:H	1.82	0.45
3:O:65:ASN:CG	3:O:67:VAL:H	2.25	0.45
4:D:68:PHE:CD1	4:D:111:THR:HG22	2.49	0.45
1:M:88:HIS:O	1:M:401:VAL:HG13	2.17	0.45
1:M:161:LEU:HD21	1:M:171:VAL:HG23	1.98	0.45
1:M:476:ILE:HG23	1:M:520:HIS:HE1	1.81	0.45
1:M:502:LEU:O	1:M:504:TYR:N	2.50	0.45
2:N:126:THR:OG1	2:N:129:GLN:HG3	2.17	0.45
2:N:206:PHE:O	2:N:206:PHE:CD2	2.70	0.45
4:P:64:ARG:NH2	4:P:118:ILE:N	2.37	0.45
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.78	0.45
1:A:145:GLN:HB3	2:B:119:TYR:CZ	2.52	0.45
1:A:395:SER:OG	6:A:703:FAD:H2'	2.17	0.45
1:M:168:ARG:O	1:M:185:ALA:O	2.35	0.45
2:N:55:TRP:CZ3	2:N:58:ARG:HD3	2.52	0.45
2:N:219:ASP:N	2:N:220:PRO:CD	2.80	0.45
2:B:109:PHE:C	2:B:109:PHE:CD2	2.94	0.44
1:M:2:THR:HA	1:M:182:GLN:O	2.17	0.44
1:M:14:GLY:C	1:M:399:LEU:HB3	2.41	0.44
1:M:72:GLY:C	1:M:74:ASP:H	2.24	0.44
1:M:135:MET:C	1:M:137:HIS:N	2.74	0.44
1:M:311:VAL:HG23	1:M:350:VAL:N	2.32	0.44
1:M:7:LEU:N	1:M:7:LEU:HD23	2.32	0.44
1:M:89:CYS:H	1:M:90:PRO:HD2	1.83	0.44
1:M:89:CYS:SG	1:M:401:VAL:HG21	2.57	0.44
1:M:173:MET:CE	1:M:178:GLY:HA2	2.46	0.44
1:M:227:GLU:HB2	1:M:522:ALA:HB2	1.99	0.44
1:M:253:ILE:HA	1:M:283:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:264:GLN:C	1:M:266:TYR:H	2.25	0.44
3:C:29:GLU:OE1	4:D:81:ARG:HG2	2.17	0.44
1:M:69:THR:HG22	1:M:70:VAL:HG23	1.98	0.44
1:M:398:GLU:O	1:M:402:PHE:HB2	2.17	0.44
3:O:50:LYS:NZ	4:P:117:THR:CG2	2.74	0.44
4:P:72:VAL:HG12	4:P:76:TRP:HD1	1.81	0.44
1:A:396:LEU:HG	6:A:703:FAD:C2	2.47	0.44
1:M:63:GLU:OE1	1:M:63:GLU:HA	2.17	0.44
1:M:179:THR:O	1:M:181:VAL:HG23	2.17	0.44
1:M:182:GLN:HB3	1:M:184:ARG:HH12	1.83	0.44
3:O:47:PHE:HE2	4:P:114:GLY:CA	2.30	0.44
4:D:86:MET:CE	4:D:91:ILE:HD12	2.47	0.44
1:M:18:ARG:HE	1:M:22:ALA:HB2	1.82	0.44
1:M:227:GLU:C	1:M:228:PHE:CD1	2.96	0.44
2:N:108:HIS:HD2	2:N:161:PHE:CZ	2.34	0.44
3:O:50:LYS:HE3	4:P:117:THR:HB	1.99	0.44
3:O:57:ALA:O	3:O:61:ASP:HB2	2.18	0.44
1:M:334:LEU:HD23	1:M:338:TYR:CE1	2.52	0.44
1:M:456:GLY:C	1:M:458:ALA:H	2.26	0.44
2:N:216:LYS:O	2:N:216:LYS:HG3	2.17	0.44
2:N:241:LYS:O	2:N:243:ARG:HG3	2.16	0.44
1:A:18:ARG:NH1	1:A:92:GLU:OE1	2.50	0.44
2:B:213:VAL:O	2:B:214:CYS:C	2.60	0.44
3:C:32:ALA:O	3:C:35:ALA:HB3	2.18	0.44
3:C:50:LYS:CD	4:D:118:ILE:HG22	2.47	0.44
1:M:106:ARG:O	1:M:107:PRO:C	2.59	0.44
1:M:162:VAL:HG22	1:M:167:VAL:CA	2.48	0.44
1:M:198:VAL:HA	1:M:455:MET:CE	2.48	0.44
1:M:260:TYR:CE1	1:M:264:GLN:NE2	2.85	0.44
1:M:539:CYS:C	1:M:541:GLU:N	2.75	0.44
10:N:801:MQ7:H2M2	3:O:28:ARG:NH1	2.33	0.44
3:O:16:TRP:CD1	3:O:26:MET:HE2	2.53	0.44
4:P:57:PHE:CB	10:P:800:MQ7:H152	2.33	0.44
1:M:77:CYS:O	1:M:78:GLU:C	2.61	0.44
1:M:199:TYR:CE2	1:M:459:MET:HB3	2.53	0.44
1:M:221:VAL:CG2	1:M:369:THR:HB	2.48	0.44
1:A:425:ILE:O	1:A:428:GLN:HB2	2.17	0.44
1:M:83:ASP:O	1:M:84:TYR:C	2.58	0.44
1:M:152:PHE:HZ	1:M:181:VAL:HG11	1.82	0.44
1:M:174:ASN:HB3	1:M:177:GLU:HB2	2.00	0.44
1:M:311:VAL:HG23	1:M:350:VAL:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:473:GLN:O	1:M:475:THR:N	2.51	0.44
1:A:9:ILE:HD13	1:A:19:ALA:HB3	1.99	0.43
1:A:320:GLY:O	1:A:321:GLU:C	2.61	0.43
1:M:12:ALA:HA	1:M:17:LEU:N	2.33	0.43
1:M:38:VAL:O	1:M:39:TYR:O	2.36	0.43
1:M:413:ARG:HH11	1:M:413:ARG:CB	2.31	0.43
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.83	0.43
1:A:65:HIS:ND1	1:A:86:VAL:HG12	2.33	0.43
2:B:155:TYR:CZ	2:B:169:GLY:HA3	2.53	0.43
2:B:194:GLN:HA	2:B:194:GLN:NE2	2.34	0.43
2:B:241:LYS:HA	2:B:242:PRO:HD3	1.48	0.43
3:C:87:PHE:O	3:C:91:PRO:CD	2.66	0.43
1:M:18:ARG:NH2	1:M:404:ARG:HB2	2.34	0.43
1:M:316:LEU:O	1:M:317:ARG:C	2.61	0.43
1:M:321:GLU:HG3	1:M:325:HIS:HD2	1.83	0.43
1:M:469:PRO:CG	1:M:536:ASP:OD2	2.65	0.43
1:M:483:GLN:HG3	1:M:516:GLU:CD	2.43	0.43
2:N:225:GLN:HE21	10:N:801:MQ7:C11	2.31	0.43
2:B:188:LYS:NZ	2:B:230:GLU:HG3	2.33	0.43
1:M:172:ALA:O	1:M:173:MET:HB2	2.18	0.43
1:M:256:ASN:HD22	1:M:256:ASN:N	2.04	0.43
1:M:395:SER:O	1:M:399:LEU:HG	2.18	0.43
1:M:437:LYS:HB3	1:M:441:ASN:ND2	2.33	0.43
4:D:112:LEU:O	4:D:116:VAL:HG22	2.18	0.43
1:M:149:ILE:HG22	1:M:150:GLN:H	1.82	0.43
1:M:437:LYS:HA	1:M:440:VAL:HB	1.99	0.43
1:M:483:GLN:HG3	1:M:516:GLU:OE2	2.18	0.43
1:M:530:GLY:C	1:M:532:HIS:N	2.76	0.43
3:C:90:ALA:N	3:C:91:PRO:CD	2.82	0.43
1:M:361:ILE:H	1:M:382:SER:H	1.66	0.43
1:M:435:ARG:CA	1:M:438:ASP:HB2	2.44	0.43
2:N:54:ARG:CB	2:N:64:SER:OG	2.66	0.43
4:P:64:ARG:O	4:P:115:VAL:HG21	2.18	0.43
1:M:84:TYR:CE2	1:M:88:HIS:CG	3.06	0.43
1:M:89:CYS:HA	1:M:401:VAL:CG2	2.48	0.43
1:M:144:LEU:C	1:M:146:PHE:N	2.75	0.43
1:M:63:GLU:C	1:M:65:HIS:N	2.77	0.43
1:M:237:PRO:C	1:M:239:SER:H	2.27	0.43
1:M:499:ASN:ND2	1:M:502:LEU:CB	2.82	0.43
1:M:15:ALA:O	1:M:19:ALA:N	2.50	0.43
1:M:53:ALA:HB2	1:M:393:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:93:MET:HB3	1:M:125:TRP:CH2	2.53	0.43
1:M:286:PRO:O	1:M:287:ARG:C	2.62	0.43
2:N:120:ILE:HG22	2:N:121:ILE:N	2.33	0.43
2:N:160:GLN:OE1	2:N:163:LEU:HD12	2.19	0.43
3:O:96:ILE:HD12	3:O:103:MET:CE	2.43	0.43
1:A:342:ASP:C	1:A:344:VAL:H	2.27	0.43
3:C:125:PHE:CD1	3:C:129:TYR:CG	3.06	0.43
1:M:62:PHE:CD2	1:M:87:HIS:ND1	2.86	0.43
1:M:131:THR:O	1:M:132:GLY:C	2.59	0.43
1:M:237:PRO:HB2	1:M:308:ARG:CB	2.48	0.43
2:N:35:SER:O	2:N:38:ASP:HB2	2.18	0.43
2:B:63:GLY:N	7:B:244:FES:S1	2.84	0.43
2:B:206:PHE:CE1	2:B:225:GLN:HG3	2.54	0.43
1:M:570:ILE:O	1:M:571:THR:HG23	2.19	0.43
2:N:53:TYR:CD1	2:N:53:TYR:O	2.72	0.43
4:P:91:ILE:HG22	4:P:93:VAL:HG23	2.01	0.43
1:M:14:GLY:HA3	1:M:399:LEU:HD13	2.01	0.42
1:M:96:LEU:HD23	1:M:139:LEU:HD21	2.01	0.42
1:M:143:SER:O	1:M:143:SER:OG	2.37	0.42
1:M:225:ASP:OD1	1:M:550:HIS:HB3	2.19	0.42
1:M:570:ILE:CG2	1:M:571:THR:N	2.82	0.42
2:N:167:PHE:CD1	2:N:203:SER:HB3	2.54	0.42
2:N:180:ASN:OD1	2:N:188:LYS:HA	2.19	0.42
4:P:48:ALA:HA	4:P:53:ARG:HD3	2.01	0.42
1:A:527:GLU:OE1	1:A:529:ARG:HD2	2.19	0.42
2:B:214:CYS:SG	2:B:218:VAL:CG2	3.07	0.42
2:B:242:PRO:HD2	2:B:243:ARG:HD3	2.01	0.42
4:D:93:VAL:N	2:N:243:ARG:O	2.51	0.42
4:D:108:THR:O	4:D:111:THR:HB	2.19	0.42
1:M:88:HIS:HB2	1:M:401:VAL:HG11	1.99	0.42
1:M:156:PHE:HE2	6:M:803:FAD:H62A	1.63	0.42
1:M:248:ARG:O	1:M:251:GLY:N	2.49	0.42
1:M:467:ARG:NH1	1:M:531:ALA:O	2.46	0.42
1:M:469:PRO:HG3	1:M:534:ARG:NH2	2.33	0.42
4:P:7:ARG:HH11	4:P:7:ARG:CB	2.31	0.42
2:B:241:LYS:O	2:B:241:LYS:CG	2.61	0.42
2:N:54:ARG:HB3	2:N:64:SER:OG	2.19	0.42
2:N:157:ALA:O	3:O:22:TYR:OH	2.32	0.42
2:N:226:GLN:HE21	2:N:226:GLN:HB2	1.57	0.42
1:M:76:LEU:HD22	1:M:76:LEU:HA	1.87	0.42
1:M:367:CYS:HB3	1:M:376:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:28:VAL:HG22	2:N:43:ILE:CD1	2.47	0.42
1:A:197:ARG:HB2	1:A:208:VAL:O	2.19	0.42
1:A:200:ARG:HG3	1:A:457:LEU:HD23	2.02	0.42
3:C:99:LYS:O	3:C:100:ASP:HB2	2.19	0.42
1:M:130:LYS:HZ1	2:N:216:LYS:HD2	1.81	0.42
1:M:155:HIS:HA	1:M:173:MET:O	2.19	0.42
1:M:248:ARG:C	1:M:250:GLU:N	2.78	0.42
1:M:322:LYS:HG3	1:M:322:LYS:O	2.19	0.42
3:O:65:ASN:OD1	3:O:68:ILE:N	2.51	0.42
4:D:72:VAL:O	4:D:75:LEU:HB2	2.20	0.42
1:M:48:ALA:HA	6:M:803:FAD:C5X	2.50	0.42
1:M:77:CYS:HA	1:M:550:HIS:CE1	2.52	0.42
1:M:130:LYS:HZ3	2:N:216:LYS:HD2	1.84	0.42
1:M:156:PHE:HD1	1:M:503:LEU:HD23	1.85	0.42
1:M:323:LYS:O	1:M:327:ARG:HG3	2.19	0.42
1:M:324:LEU:HG	1:M:344:VAL:CG1	2.50	0.42
1:M:472:MET:SD	1:M:523:MET:HA	2.60	0.42
1:M:527:GLU:OE1	1:M:529:ARG:NH2	2.52	0.42
3:C:37:TRP:CD1	3:C:37:TRP:C	2.97	0.42
3:C:59:PHE:O	3:C:62:PHE:N	2.53	0.42
1:M:15:ALA:O	1:M:18:ARG:N	2.53	0.42
1:M:50:GLY:N	6:M:803:FAD:O4	2.52	0.42
1:M:62:PHE:O	1:M:86:VAL:HG21	2.19	0.42
1:M:324:LEU:CD1	1:M:332:CYS:SG	3.06	0.42
1:M:472:MET:O	1:M:476:ILE:HG13	2.19	0.42
4:P:55:LEU:HG	4:P:59:GLN:OE1	2.19	0.42
1:A:242:LEU:HD12	1:A:243:MET:H	1.85	0.42
1:A:247:CYS:HB3	1:A:316:LEU:HD21	2.01	0.42
1:M:186:ASN:O	1:M:414:ALA:CB	2.68	0.42
1:M:254:LEU:HD13	1:M:262:TYR:OH	2.20	0.42
1:M:405:LEU:C	1:M:407:GLY:H	2.26	0.42
1:M:534:ARG:O	1:M:540:THR:HG22	2.19	0.42
3:O:29:GLU:C	3:O:31:THR:H	2.28	0.42
3:O:128:LEU:HD22	4:P:44:PHE:HB2	2.02	0.42
4:P:28:ALA:N	4:P:29:PRO:HD2	2.35	0.42
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.85	0.42
1:M:12:ALA:O	1:M:17:LEU:HB2	2.20	0.42
1:M:54:ALA:HB3	1:M:125:TRP:NE1	2.35	0.42
1:M:395:SER:OG	6:M:803:FAD:H2'	2.20	0.42
4:P:72:VAL:O	4:P:73:LEU:C	2.62	0.42
1:A:248:ARG:HD2	1:A:283:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:ALA:CA	1:M:399:LEU:HB3	2.49	0.42
1:M:74:ASP:C	1:M:75:TRP:CE3	2.98	0.42
1:M:465:ILE:H	1:M:465:ILE:CD1	2.28	0.42
1:M:562:ARG:C	1:M:563:LEU:HD12	2.45	0.42
1:M:570:ILE:CG2	1:M:571:THR:H	2.31	0.42
10:N:801:MQ7:C2M	3:O:28:ARG:NH1	2.83	0.42
3:O:7:TYR:CD1	3:O:7:TYR:C	2.97	0.42
3:O:56:TRP:O	3:O:59:PHE:HB3	2.20	0.42
3:O:91:PRO:HB3	3:O:108:ILE:HG21	2.02	0.42
3:C:18:LYS:HB2	3:C:19:LEU:H	1.69	0.41
4:D:9:ASP:HB2	11:D:810:CE1:H242	2.02	0.41
1:M:175:MET:O	1:M:498:PHE:HA	2.19	0.41
1:M:203:THR:HG21	1:M:355:HIS:ND1	2.35	0.41
1:M:246:GLY:O	1:M:248:ARG:N	2.53	0.41
1:M:320:GLY:O	1:M:324:LEU:HB2	2.20	0.41
1:A:146:PHE:HA	1:A:147:PRO:HD2	1.85	0.41
1:A:390:ARG:HH22	5:A:702:OAA:C4	2.28	0.41
1:A:529:ARG:NH2	1:A:548:LEU:HD12	2.35	0.41
2:B:134:GLN:HE21	2:B:139:MET:HE3	1.85	0.41
2:B:142:TYR:CD1	2:B:142:TYR:C	2.97	0.41
1:M:131:THR:O	1:M:132:GLY:O	2.38	0.41
3:O:36:VAL:HG23	3:O:37:TRP:N	2.35	0.41
4:P:27:ILE:O	4:P:30:VAL:HG12	2.20	0.41
4:P:86:MET:HE1	4:P:91:ILE:HD13	2.00	0.41
1:A:10:VAL:HG13	1:A:157:VAL:HG21	2.02	0.41
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.52	0.41
1:A:345:LYS:C	1:A:346:GLU:HG3	2.46	0.41
2:B:67:MET:HB3	2:B:67:MET:HE2	1.87	0.41
2:B:202:TRP:CE2	4:D:11:PRO:HD3	2.56	0.41
3:C:106:GLU:HB2	3:C:107:PRO:HD3	2.02	0.41
4:D:42:GLY:HA2	4:D:44:PHE:HE2	1.81	0.41
4:D:50:SER:O	4:D:51:TYR:C	2.63	0.41
1:M:256:ASN:ND2	1:M:260:TYR:O	2.53	0.41
1:M:436:LEU:O	1:M:440:VAL:N	2.49	0.41
1:M:448:TRP:HA	1:M:451:ILE:HD12	2.02	0.41
1:M:459:MET:HE1	1:M:518:MET:HG3	2.02	0.41
1:A:197:ARG:HD2	1:A:206:GLY:HA2	2.02	0.41
1:A:224:ARG:HD2	1:A:550:HIS:CG	2.55	0.41
2:B:214:CYS:SG	2:B:218:VAL:HB	2.60	0.41
1:M:13:GLY:HA3	6:M:803:FAD:P	2.58	0.41
1:M:65:HIS:CD2	1:M:123:ARG:NH1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:182:GLN:CB	1:M:184:ARG:HH12	2.33	0.41
1:M:246:GLY:C	1:M:248:ARG:N	2.77	0.41
1:M:366:ASN:O	1:M:367:CYS:C	2.63	0.41
1:M:436:LEU:O	1:M:440:VAL:HG23	2.20	0.41
3:O:50:LYS:HZ2	4:P:117:THR:CB	2.34	0.41
3:O:91:PRO:HB3	3:O:108:ILE:CG2	2.50	0.41
2:B:117:LYS:O	2:B:119:TYR:N	2.50	0.41
2:B:228:LYS:NZ	10:B:701:MQ7:H6	2.35	0.41
1:M:17:LEU:CD1	1:M:139:LEU:HB2	2.49	0.41
1:M:155:HIS:HA	1:M:175:MET:HG3	2.01	0.41
1:M:335:ALA:O	1:M:339:VAL:HG22	2.20	0.41
2:N:159:PRO:O	2:N:163:LEU:HG	2.20	0.41
3:O:59:PHE:O	3:O:62:PHE:HB3	2.21	0.41
1:M:65:HIS:CD2	1:M:123:ARG:HH11	2.38	0.41
1:M:196:GLY:C	1:M:198:VAL:N	2.78	0.41
1:M:324:LEU:HD11	1:M:343:PRO:HB2	2.01	0.41
1:M:437:LYS:O	1:M:441:ASN:N	2.47	0.41
2:N:81:LEU:N	2:N:81:LEU:CD1	2.84	0.41
4:P:39:LEU:N	4:P:40:PRO:HD2	2.35	0.41
4:P:54:VAL:HG13	10:P:800:MQ7:C6	2.43	0.41
4:P:79:LEU:HD23	4:P:82:MET:CE	2.47	0.41
1:M:92:GLU:HB2	1:M:401:VAL:HG22	2.02	0.41
1:M:98:LEU:O	2:N:120:ILE:HG13	2.20	0.41
1:M:181:VAL:CG1	1:M:182:GLN:N	2.84	0.41
1:M:290:VAL:O	1:M:293:ALA:HB3	2.20	0.41
1:M:393:SER:HA	6:M:803:FAD:O2	2.21	0.41
2:N:36:LEU:HD12	2:N:36:LEU:HA	1.88	0.41
2:N:81:LEU:H	2:N:81:LEU:CD1	2.33	0.41
2:B:216:LYS:O	2:B:217:HIS:C	2.64	0.41
4:D:95:ALA:O	4:D:96:GLY:C	2.63	0.41
1:M:396:LEU:O	1:M:399:LEU:N	2.53	0.41
2:N:170:PRO:O	2:N:171:ALA:C	2.64	0.41
3:O:87:PHE:CD2	3:O:112:LEU:HD13	2.56	0.41
1:A:16:GLY:O	1:A:19:ALA:HB3	2.20	0.41
1:A:156:PHE:CD1	1:A:503:LEU:HD22	2.55	0.41
1:A:202:ASN:OD1	1:A:204:ASN:HB2	2.20	0.41
1:A:232:HIS:CE1	1:A:242:LEU:HD11	2.55	0.41
2:B:219:ASP:O	2:B:220:PRO:C	2.62	0.41
3:C:15:TRP:CD2	3:C:16:TRP:N	2.89	0.41
3:C:50:LYS:C	3:C:52:GLY:H	2.28	0.41
1:M:67:HIS:C	1:M:67:HIS:ND1	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:70:VAL:O	1:M:73:GLY:N	2.51	0.41
1:M:127:ALA:N	1:M:131:THR:OG1	2.38	0.41
1:M:181:VAL:C	1:M:182:GLN:HG3	2.46	0.41
1:M:396:LEU:O	1:M:398:GLU:N	2.54	0.41
1:M:397:ALA:HA	1:M:400:VAL:HG22	2.03	0.41
1:M:511:GLY:O	1:M:514:VAL:N	2.53	0.41
1:M:550:HIS:CD2	1:M:568:VAL:HG22	2.55	0.41
2:N:143:HIS:O	2:N:144:GLN:C	2.64	0.41
2:N:158:CYS:HA	2:N:159:PRO:HD3	1.85	0.41
10:N:801:MQ7:H2M1	10:N:801:MQ7:C14	2.32	0.41
3:O:66:PRO:HA	3:O:69:VAL:HG23	2.02	0.41
4:P:30:VAL:HG13	4:P:31:MET:N	2.35	0.41
1:A:236:LEU:CD2	1:A:243:MET:HE3	2.51	0.41
1:A:439:LEU:O	1:A:442:GLN:HB3	2.21	0.41
2:B:239:THR:C	2:B:241:LYS:H	2.29	0.41
3:C:87:PHE:CE2	3:C:112:LEU:HB3	2.56	0.41
4:D:20:GLY:HA2	4:D:73:LEU:HB3	2.03	0.41
1:M:60:ASP:OD1	1:M:61:SER:N	2.53	0.41
1:M:155:HIS:O	1:M:175:MET:SD	2.79	0.41
1:M:463:CYS:SG	1:M:467:ARG:CZ	3.08	0.41
1:M:475:THR:O	1:M:478:LYS:HB3	2.21	0.41
2:N:8:ILE:HD11	2:N:81:LEU:CD2	2.48	0.41
2:N:71:ASN:ND2	3:O:18:LYS:HD3	2.36	0.41
3:O:29:GLU:C	3:O:31:THR:N	2.77	0.41
1:A:330:PHE:O	1:A:333:GLU:HB2	2.22	0.40
1:M:195:ALA:O	1:M:198:VAL:HG22	2.21	0.40
1:M:195:ALA:HA	1:M:208:VAL:O	2.22	0.40
1:A:239:SER:HB2	1:A:241:ILE:HG13	2.02	0.40
1:A:331:ILE:HD13	1:A:331:ILE:HA	1.80	0.40
1:A:493:ASP:OD1	1:A:493:ASP:C	2.64	0.40
2:B:8:ILE:HD11	2:B:81:LEU:HD11	2.03	0.40
4:D:93:VAL:HA	4:D:94:PRO:HD2	1.84	0.40
1:M:46:VAL:CG2	2:N:61:ILE:HG13	2.42	0.40
1:M:51:GLY:HA2	1:M:131:THR:HG21	2.04	0.40
1:M:81:VAL:C	1:M:83:ASP:N	2.79	0.40
1:M:106:ARG:HG3	1:M:111:VAL:C	2.45	0.40
1:M:170:LEU:HD12	1:M:171:VAL:C	2.46	0.40
1:M:279:ASN:O	1:M:281:TYR:N	2.52	0.40
1:M:304:ILE:HG21	1:M:313:TYR:OH	2.21	0.40
1:M:377:VAL:HG22	1:M:378:GLY:N	2.36	0.40
2:N:97:PRO:HG2	2:N:105:ASP:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HB3	1:A:344:VAL:HG22	2.02	0.40
2:B:116:ILE:C	2:B:116:ILE:CD1	2.94	0.40
3:C:36:VAL:O	3:C:39:SER:N	2.54	0.40
1:M:38:VAL:O	1:M:39:TYR:C	2.63	0.40
1:M:151:ARG:NH1	1:M:153:ASP:CG	2.78	0.40
2:N:54:ARG:NE	2:N:103:VAL:HG13	2.19	0.40
2:N:206:PHE:CD2	2:N:206:PHE:C	2.99	0.40
4:P:64:ARG:HB3	4:P:115:VAL:CG2	2.51	0.40
1:A:552:LEU:HD23	1:A:552:LEU:HA	1.84	0.40
2:B:72:VAL:O	2:B:74:LYS:HG3	2.21	0.40
2:B:100:ARG:O	2:B:101:ASP:C	2.64	0.40
3:C:16:TRP:CD1	3:C:16:TRP:H	2.39	0.40
3:C:50:LYS:HB3	4:D:118:ILE:CG2	2.51	0.40
3:C:128:LEU:O	4:D:45:PRO:CG	2.69	0.40
4:D:30:VAL:HG13	4:D:31:MET:N	2.37	0.40
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.56	0.40
1:M:167:VAL:O	1:M:167:VAL:HG13	2.21	0.40
1:M:170:LEU:HD12	1:M:170:LEU:C	2.46	0.40
3:O:91:PRO:C	3:O:93:ALA:H	2.28	0.40
4:P:57:PHE:HB2	10:P:800:MQ7:C15	2.34	0.40
1:A:85:PHE:CD2	1:A:385:LEU:HD11	2.57	0.40
1:A:86:VAL:HG23	1:A:87:HIS:N	2.36	0.40
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.81	0.40
2:B:236:LEU:HD12	2:B:236:LEU:HA	1.89	0.40
4:D:57:PHE:O	4:D:58:ALA:C	2.63	0.40
1:M:15:ALA:CB	1:M:399:LEU:HB3	2.51	0.40
1:M:43:SER:HB2	1:M:136:LEU:CD2	2.51	0.40
1:M:431:GLY:O	1:M:432:VAL:C	2.64	0.40
1:M:479:LEU:CD1	1:M:516:GLU:HA	2.51	0.40
2:N:222:ALA:O	2:N:226:GLN:NE2	2.55	0.40
3:O:127:ALA:O	3:O:128:LEU:HD23	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	575/602 (96%)	529 (92%)	37 (6%)	9 (2%)	7	31
1	M	575/602 (96%)	355 (62%)	153 (27%)	67 (12%)	0	1
2	B	241/243 (99%)	215 (89%)	22 (9%)	4 (2%)	7	30
2	N	241/243 (99%)	205 (85%)	34 (14%)	2 (1%)	16	45
3	C	128/130 (98%)	121 (94%)	5 (4%)	2 (2%)	7	31
3	O	128/130 (98%)	113 (88%)	12 (9%)	3 (2%)	5	25
4	D	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	4	23
4	P	117/119 (98%)	99 (85%)	12 (10%)	6 (5%)	1	11
All	All	2122/2188 (97%)	1738 (82%)	288 (14%)	96 (4%)	2	13

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	242	PRO
4	D	99	VAL
1	M	57	GLN
1	M	76	LEU
1	M	85	PHE
1	M	153	ASP
1	M	154	GLU
1	M	180	LEU
1	M	318	HIS
1	M	362	GLU
1	M	375	PHE
1	M	531	ALA
1	M	548	LEU
3	O	18	LYS
3	O	65	ASN
4	P	3	PRO
4	P	5	PRO
1	A	128	ALA
2	B	56	SER
3	C	18	LYS
3	C	65	ASN
4	D	43	LEU
1	M	43	SER
1	M	68	ASP

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Mol	Chain	Res	Type
1	M	75	TRP
1	M	78	GLU
1	M	82	VAL
1	M	86	VAL
1	M	128	ALA
1	M	129	ASP
1	M	157	VAL
1	M	159	ASP
1	M	181	VAL
1	M	187	ALA
1	M	193	GLY
1	M	239	SER
1	M	244	THR
1	M	289	LYS
1	M	367	CYS
1	M	417	ALA
1	M	501	ASP
1	M	502	LEU
1	M	540	THR
1	M	556	ASP
1	M	567	ASP
4	P	34	LEU
1	A	244	THR
1	A	262	TYR
1	A	318	HIS
1	A	389	ASN
2	B	32	ALA
4	D	117	THR
1	M	108	ASP
1	M	139	LEU
1	M	197	ARG
1	M	221	VAL
1	M	273	PRO
1	M	282	MET
1	M	368	GLU
1	M	453	ASP
1	M	474	LYS
1	M	510	HIS
2	N	128	ASP
4	P	95	ALA
2	B	66	GLY
1	M	130	LYS

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Mol	Chain	Res	Type
1	M	405	LEU
1	M	520	HIS
1	M	559	GLY
1	M	572	THR
3	O	51	ASN
1	M	107	PRO
1	M	208	VAL
1	M	344	VAL
1	M	374	LEU
1	M	462	GLY
2	N	182	ASP
1	M	90	PRO
1	M	131	THR
1	M	233	PRO
1	M	265	ASP
1	M	290	VAL
1	M	39	TYR
1	M	343	PRO
4	P	96	GLY
1	A	329	PRO
1	A	340	GLY
1	A	444	GLY
1	M	311	VAL
1	M	383	VAL
1	M	229	VAL
4	P	99	VAL
1	A	208	VAL
1	M	101	CYS
1	M	132	GLY
1	M	312	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	460/475 (97%)	447 (97%)	13 (3%)	38 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	460/475 (97%)	398 (86%)	62 (14%)	4	16
2	B	205/205 (100%)	198 (97%)	7 (3%)	32	59
2	N	205/205 (100%)	192 (94%)	13 (6%)	16	44
3	C	111/111 (100%)	103 (93%)	8 (7%)	13	40
3	O	111/111 (100%)	101 (91%)	10 (9%)	9	31
4	D	97/97 (100%)	94 (97%)	3 (3%)	35	60
4	P	97/97 (100%)	94 (97%)	3 (3%)	35	60
All	All	1746/1776 (98%)	1627 (93%)	119 (7%)	14	42

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	74	ASP
1	A	107	PRO
1	A	122	GLU
1	A	197	ARG
1	A	200	ARG
1	A	207	ILE
1	A	276	GLU
1	A	287	ARG
1	A	305	SER
1	A	307	PRO
1	A	332	CYS
1	A	351	ARG
2	B	65	CYS
2	B	81	LEU
2	B	128	ASP
2	B	203	SER
2	B	212	GLU
2	B	240	LEU
2	B	241	LYS
3	C	23	ARG
3	C	37	TRP
3	C	39	SER
3	C	50	LYS
3	C	66	PRO
3	C	84	LYS
3	C	96	ILE
3	C	103	MET

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Mol	Chain	Res	Type
4	D	86	MET
4	D	117	THR
4	D	118	ILE
1	M	0	MET
1	M	4	GLN
1	M	28	PRO
1	M	32	ILE
1	M	35	ILE
1	M	62	PHE
1	M	64	TYR
1	M	67	HIS
1	M	76	LEU
1	M	77	CYS
1	M	84	TYR
1	M	86	VAL
1	M	89	CYS
1	M	91	THR
1	M	96	LEU
1	M	108	ASP
1	M	113	VAL
1	M	122	GLU
1	M	137	HIS
1	M	141	GLN
1	M	143	SER
1	M	148	GLN
1	M	153	ASP
1	M	161	LEU
1	M	164	ASP
1	M	180	LEU
1	M	183	ILE
1	M	197	ARG
1	M	203	THR
1	M	217	LEU
1	M	242	LEU
1	M	243	MET
1	M	244	THR
1	M	256	ASN
1	M	268	MET
1	M	274	LEU
1	M	311	VAL
1	M	312	VAL
1	M	324	LEU

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Mol	Chain	Res	Type
1	M	326	GLU
1	M	348	ILE
1	M	355	HIS
1	M	363	THR
1	M	370	ARG
1	M	399	LEU
1	M	413	ARG
1	M	438	ASP
1	M	457	LEU
1	M	465	ILE
1	M	470	GLU
1	M	481	GLU
1	M	493	ASP
1	M	497	VAL
1	M	508	LEU
1	M	518	MET
1	M	527	GLU
1	M	528	SER
1	M	537	GLU
1	M	554	PHE
1	M	558	ASP
1	M	561	THR
1	M	563	LEU
2	N	22	HIS
2	N	25	PHE
2	N	53	TYR
2	N	71	ASN
2	N	100	ARG
2	N	109	PHE
2	N	128	ASP
2	N	185	ASP
2	N	188	LYS
2	N	189	LYS
2	N	225	GLN
2	N	226	GLN
2	N	240	LEU
3	O	5	LYS
3	O	19	LEU
3	O	20	PRO
3	O	28	ARG
3	O	37	TRP
3	O	39	SER

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Mol	Chain	Res	Type
3	O	54	GLU
3	O	61	ASP
3	O	84	LYS
3	O	103	MET
4	P	5	PRO
4	P	53	ARG
4	P	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	95	GLN
1	A	134	HIS
1	A	141	GLN
1	A	204	ASN
1	A	232	HIS
1	A	279	ASN
1	A	292	GLN
1	A	325	HIS
1	A	428	GLN
1	A	434	GLN
1	A	442	GLN
2	B	108	HIS
2	B	134	GLN
2	B	144	GLN
2	B	150	ASN
2	B	194	GLN
3	C	51	ASN
3	C	72	ASN
4	D	4	ASN
4	D	59	GLN
4	D	83	HIS
1	M	4	GLN
1	M	65	HIS
1	M	137	HIS
1	M	141	GLN
1	M	145	GLN
1	M	174	ASN
1	M	182	GLN
1	M	204	ASN
1	M	230	GLN

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Mol	Chain	Res	Type
1	M	256	ASN
1	M	264	GLN
1	M	279	ASN
1	M	292	GLN
1	M	325	HIS
1	M	366	ASN
1	M	386	HIS
1	M	394	ASN
1	M	409	GLN
1	M	434	GLN
1	M	441	ASN
1	M	520	HIS
2	N	5	ASN
2	N	70	ASN
2	N	71	ASN
2	N	95	ASN
2	N	108	HIS
2	N	123	ASN
2	N	129	GLN
2	N	132	ASN
2	N	177	HIS
2	N	225	GLN
2	N	226	GLN
3	O	72	ASN
4	P	4	ASN
4	P	83	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MQ7	B	701	-	25,25,49	3.27	6 (24%)	31,34,63	2.44	9 (29%)
6	FAD	M	803	-	58,58,58	1.69	14 (24%)	85,89,89	1.63	18 (21%)
5	OAA	M	802	-	8,8,8	1.24	1 (12%)	8,10,10	1.24	1 (12%)
7	FES	B	244	2	0,4,4	-	-	-	-	-
8	F3S	B	245	2	0,9,9	-	-	-	-	-
10	MQ7	N	801	-	25,25,49	3.43	7 (28%)	31,34,63	2.55	10 (32%)
10	MQ7	D	700	-	25,25,49	3.27	5 (20%)	31,34,63	2.44	11 (35%)
9	SF4	N	246	2	0,12,12	-	-	-	-	-
10	MQ7	P	800	-	25,25,49	3.22	5 (20%)	31,34,63	2.43	12 (38%)
5	OAA	A	702	-	8,8,8	1.15	0	8,10,10	1.06	1 (12%)
7	FES	N	244	2	0,4,4	-	-	-	-	-
11	CE1	D	710	-	36,36,36	1.04	0	35,35,35	1.66	14 (40%)
11	CE1	O	812	-	36,36,36	1.16	0	35,35,35	1.56	7 (20%)
9	SF4	B	246	2	0,12,12	-	-	-	-	-
11	CE1	D	810	-	36,36,36	1.15	0	35,35,35	1.69	14 (40%)
8	F3S	N	245	2	0,9,9	-	-	-	-	-
11	CE1	O	811	-	36,36,36	1.24	4 (11%)	35,35,35	1.81	13 (37%)
6	FAD	A	703	-	58,58,58	1.99	15 (25%)	85,89,89	1.83	21 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MQ7	B	701	-	-	3/13/33/61	0/2/2/2
6	FAD	M	803	-	-	10/34/50/50	0/6/6/6
5	OAA	M	802	-	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	B	244	2	-	-	0/1/1/1
8	F3S	B	245	2	-	-	0/3/3/3
10	MQ7	N	801	-	-	3/13/33/61	0/2/2/2
10	MQ7	D	700	-	-	2/13/33/61	0/2/2/2
10	MQ7	P	800	-	-	1/13/33/61	0/2/2/2
9	SF4	N	246	2	-	-	0/6/5/5
5	OAA	A	702	-	-	6/8/8/8	-
11	CE1	D	710	-	-	14/34/34/34	-
11	CE1	O	812	-	-	18/34/34/34	-
7	FES	N	244	2	-	-	0/1/1/1
9	SF4	B	246	2	-	-	0/6/5/5
11	CE1	D	810	-	-	15/34/34/34	-
8	F3S	N	245	2	-	-	0/3/3/3
11	CE1	O	811	-	-	15/34/34/34	-
6	FAD	A	703	-	-	11/34/50/50	0/6/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	801	MQ7	C11-C12	-10.94	1.33	1.50
10	N	801	MQ7	C12-C13	10.15	1.56	1.33
10	D	700	MQ7	C11-C12	-10.11	1.34	1.50
10	B	701	MQ7	C12-C13	9.96	1.56	1.33
10	P	800	MQ7	C11-C12	-9.94	1.34	1.50
10	B	701	MQ7	C11-C12	-9.37	1.35	1.50
10	D	700	MQ7	C12-C13	9.30	1.54	1.33
10	P	800	MQ7	C12-C13	9.06	1.53	1.33
6	A	703	FAD	PA-O3P	-7.38	1.51	1.59
10	P	800	MQ7	C14-C13	-5.65	1.36	1.50
10	B	701	MQ7	C14-C13	-5.63	1.37	1.50
10	N	801	MQ7	C14-C13	-5.53	1.37	1.50
10	D	700	MQ7	C14-C13	-5.42	1.37	1.50
6	A	703	FAD	C9A-C5X	4.95	1.49	1.41
6	M	803	FAD	PA-O3P	-4.35	1.54	1.59
10	P	800	MQ7	C7-C6	4.30	1.46	1.38
10	D	700	MQ7	C7-C6	4.17	1.46	1.38
6	A	703	FAD	P-O3P	-4.15	1.55	1.59
10	B	701	MQ7	C7-C6	3.93	1.45	1.38
6	A	703	FAD	C5A-N7A	-3.82	1.32	1.39
6	M	803	FAD	C9A-C5X	3.54	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	FAD	C4X-N5	3.51	1.38	1.30
6	M	803	FAD	C5A-C4A	3.28	1.44	1.39
6	M	803	FAD	C5'-C4'	3.21	1.56	1.51
6	A	703	FAD	C4A-N3A	3.20	1.40	1.34
6	M	803	FAD	C4X-N5	3.05	1.37	1.30
10	N	801	MQ7	C7-C6	3.02	1.44	1.38
6	M	803	FAD	C10-N10	2.96	1.43	1.37
6	M	803	FAD	C9A-N10	2.95	1.46	1.41
10	B	701	MQ7	C2-C1	2.92	1.54	1.47
6	A	703	FAD	C2'-C3'	-2.87	1.48	1.53
6	A	703	FAD	C8A-N7A	2.74	1.37	1.31
6	M	803	FAD	C5A-N7A	-2.68	1.34	1.39
6	A	703	FAD	C10-N10	2.68	1.43	1.37
6	A	703	FAD	C4A-N9A	-2.68	1.32	1.37
10	P	800	MQ7	C2-C1	2.63	1.53	1.47
6	A	703	FAD	P-O5'	-2.50	1.49	1.59
6	M	803	FAD	C4A-N3A	2.49	1.39	1.34
6	M	803	FAD	C4'-C3'	2.46	1.57	1.53
6	A	703	FAD	C2-N1	-2.35	1.31	1.36
11	O	811	CE1	C24-C23	2.33	1.60	1.49
10	N	801	MQ7	C5-C4	2.31	1.52	1.48
10	D	700	MQ7	C17-C18	2.26	1.38	1.33
6	M	803	FAD	C8M-C8	2.22	1.55	1.51
11	O	811	CE1	C21-C20	2.19	1.60	1.49
6	A	703	FAD	C5A-C4A	2.14	1.42	1.39
10	N	801	MQ7	C3-C4	2.13	1.52	1.47
10	B	701	MQ7	O4-C4	2.13	1.27	1.23
6	M	803	FAD	C7M-C7	2.11	1.55	1.51
11	O	811	CE1	O13-C12	2.09	1.51	1.42
6	M	803	FAD	C9-C8	2.07	1.42	1.39
11	O	811	CE1	O22-C21	2.06	1.51	1.42
6	M	803	FAD	C2-N3	2.06	1.43	1.39
10	N	801	MQ7	C8-C9	2.05	1.42	1.38
6	A	703	FAD	O4-C4	2.04	1.27	1.23
5	M	802	OAA	C2-C1	2.01	1.54	1.51
6	A	703	FAD	O4B-C4B	-2.01	1.40	1.45

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	801	MQ7	C11-C3-C4	-7.83	110.33	118.58
10	D	700	MQ7	C11-C3-C4	-7.58	110.59	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	701	MQ7	C11-C3-C4	-7.56	110.61	118.58
10	P	800	MQ7	C11-C3-C4	-7.20	110.99	118.58
10	P	800	MQ7	C12-C11-C3	6.74	128.69	112.08
10	N	801	MQ7	C12-C11-C3	6.35	127.73	112.08
6	A	703	FAD	N3A-C2A-N1A	-6.14	119.29	128.58
10	D	700	MQ7	C12-C11-C3	6.09	127.08	112.08
10	B	701	MQ7	C12-C11-C3	5.99	126.84	112.08
6	A	703	FAD	C5A-C4A-N3A	-5.16	119.61	126.72
6	M	803	FAD	N3A-C2A-N1A	-5.11	120.84	128.58
10	B	701	MQ7	O1-C1-C10	-4.33	114.64	121.57
10	N	801	MQ7	C2M-C2-C1	-4.10	109.13	116.68
10	N	801	MQ7	O1-C1-C10	-3.99	115.19	121.57
6	A	703	FAD	C2A-N3A-C4A	3.99	121.56	111.83
10	D	700	MQ7	O1-C1-C10	-3.97	115.22	121.57
6	A	703	FAD	N3A-C4A-N9A	3.84	133.70	127.17
10	P	800	MQ7	O1-C1-C10	-3.73	115.60	121.57
6	A	703	FAD	C4-N3-C2	-3.70	119.08	125.64
6	M	803	FAD	N3A-C4A-N9A	3.67	133.41	127.17
6	M	803	FAD	C5A-C4A-N3A	-3.62	121.73	126.72
6	M	803	FAD	C5X-N5-C4X	3.62	123.94	118.09
6	A	703	FAD	C5'-C4'-C3'	3.59	118.99	112.22
11	O	811	CE1	O31-C30-C29	3.51	126.36	110.35
6	A	703	FAD	C9A-C5X-N5	-3.50	118.74	122.45
10	D	700	MQ7	C11-C3-C2	3.48	130.87	124.89
11	O	811	CE1	O13-C12-C11	3.43	128.34	110.32
10	B	701	MQ7	C11-C3-C2	3.40	130.72	124.89
10	B	701	MQ7	C11-C12-C13	3.36	132.63	126.83
10	P	800	MQ7	C11-C3-C2	3.31	130.58	124.89
6	M	803	FAD	C4-N3-C2	-3.30	119.79	125.64
6	M	803	FAD	C9A-C5X-N5	-3.29	118.97	122.45
6	M	803	FAD	C4A-N9A-C8A	3.27	109.17	105.74
11	O	811	CE1	O19-C18-C17	3.19	124.89	110.35
6	M	803	FAD	C2A-N3A-C4A	3.17	119.58	111.83
6	A	703	FAD	C5X-N5-C4X	3.15	123.18	118.09
10	B	701	MQ7	O1-C1-C2	3.13	124.57	120.45
10	N	801	MQ7	C11-C12-C13	3.12	132.21	126.83
10	N	801	MQ7	O1-C1-C2	3.11	124.54	120.45
11	O	812	CE1	O34-C35-C36	3.10	123.77	110.11
6	A	703	FAD	C4'-C3'-C2'	-3.09	108.43	113.57
11	O	811	CE1	O22-C23-C24	3.09	124.43	110.35
6	A	703	FAD	N9A-C8A-N7A	-3.05	109.60	113.94
10	N	801	MQ7	C2M-C2-C3	2.97	129.34	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	803	FAD	N9A-C8A-N7A	-2.96	109.73	113.94
10	N	801	MQ7	C9-C10-C5	2.94	122.56	119.26
11	O	812	CE1	O22-C21-C20	2.90	123.55	110.35
10	N	801	MQ7	C11-C3-C2	2.88	129.84	124.89
10	P	800	MQ7	C2M-C2-C1	-2.88	111.37	116.68
6	A	703	FAD	O4-C4-C4X	-2.86	118.98	126.53
6	A	703	FAD	C10-N1-C2	2.85	123.02	116.85
11	O	811	CE1	O16-C17-C18	2.85	123.34	110.35
11	O	812	CE1	O19-C18-C17	2.83	123.26	110.35
11	O	812	CE1	O16-C17-C18	2.83	123.25	110.35
6	A	703	FAD	C4-C4X-N5	2.81	122.09	118.21
10	D	700	MQ7	C11-C12-C13	2.74	131.56	126.83
11	O	811	CE1	O19-C20-C21	2.70	122.64	110.35
11	O	812	CE1	O34-C33-C32	2.67	122.50	110.35
5	M	802	OAA	O4-C4-C3	2.62	125.07	121.81
6	A	703	FAD	C7M-C7-C6	-2.61	114.97	119.57
6	M	803	FAD	C9-C9A-N10	2.61	125.36	121.85
10	D	700	MQ7	C2M-C2-C1	-2.60	111.89	116.68
11	O	811	CE1	O16-C15-C14	2.59	122.14	110.35
10	B	701	MQ7	C2M-C2-C1	-2.57	111.94	116.68
11	O	811	CE1	O28-C27-C26	2.55	121.97	110.35
11	D	810	CE1	O34-C35-C36	2.55	121.35	110.11
11	D	810	CE1	O25-C24-C23	2.51	121.81	110.35
6	M	803	FAD	C5A-N7A-C8A	2.51	107.39	103.45
11	D	710	CE1	O13-C14-C15	2.51	121.77	110.35
11	D	810	CE1	O16-C15-C14	2.47	121.59	110.35
6	M	803	FAD	C5'-C4'-C3'	2.44	116.82	112.22
11	O	811	CE1	O34-C33-C32	2.43	121.45	110.35
6	M	803	FAD	C7M-C7-C6	-2.40	115.35	119.57
10	N	801	MQ7	C19-C18-C20	2.39	118.94	116.13
10	P	800	MQ7	C11-C12-C13	2.38	130.93	126.83
11	D	810	CE1	O19-C18-C17	2.38	121.19	110.35
11	D	810	CE1	O19-C20-C21	2.37	121.14	110.35
11	D	710	CE1	O31-C30-C29	2.35	121.08	110.35
11	D	710	CE1	O22-C21-C20	2.34	121.03	110.35
10	B	701	MQ7	C9-C10-C5	2.34	121.89	119.26
10	D	700	MQ7	C5-C10-C1	-2.34	118.20	120.71
10	D	700	MQ7	C14-C13-C15	2.34	119.29	115.23
6	M	803	FAD	O4-C4-C4X	-2.34	120.36	126.53
10	P	800	MQ7	C5-C10-C1	-2.33	118.21	120.71
6	A	703	FAD	C4X-C4-N3	2.33	119.18	113.25
11	D	810	CE1	O13-C14-C15	2.33	120.95	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	700	MQ7	C9-C10-C5	2.32	121.86	119.26
11	D	810	CE1	O31-C32-C33	2.31	120.86	110.35
6	M	803	FAD	C6-C5X-C9A	2.30	122.21	119.05
11	O	811	CE1	O25-C26-C27	2.30	120.82	110.35
11	D	710	CE1	O19-C20-C21	2.29	120.79	110.35
11	D	710	CE1	O16-C17-C18	2.29	120.78	110.35
6	M	803	FAD	C4'-C3'-C2'	-2.28	109.77	113.57
11	D	810	CE1	O28-C29-C30	2.28	120.73	110.35
11	D	710	CE1	O31-C32-C33	2.28	120.73	110.35
6	A	703	FAD	C4A-N9A-C8A	2.26	108.11	105.74
11	D	710	CE1	O28-C29-C30	2.26	120.67	110.35
11	D	810	CE1	O22-C21-C20	2.26	120.64	110.35
11	D	710	CE1	O28-C27-C26	2.25	120.63	110.35
11	D	710	CE1	O16-C15-C14	2.25	120.62	110.35
11	D	810	CE1	O28-C27-C26	2.24	120.56	110.35
6	A	703	FAD	O4'-C4'-C5'	-2.23	105.06	109.99
11	D	710	CE1	O34-C35-C36	2.23	119.94	110.11
11	D	710	CE1	O22-C23-C24	2.23	120.51	110.35
11	O	811	CE1	O31-C32-C33	2.23	120.50	110.35
10	B	701	MQ7	C19-C18-C20	2.23	118.75	116.13
6	A	703	FAD	O4'-C4'-C3'	-2.21	104.08	109.25
11	D	810	CE1	O31-C30-C29	2.20	120.36	110.35
10	D	700	MQ7	O4-C4-C3	-2.19	117.15	120.67
11	D	810	CE1	O25-C26-C27	2.18	120.30	110.35
11	O	811	CE1	O22-C21-C20	2.18	120.28	110.35
11	D	710	CE1	O25-C24-C23	2.17	120.26	110.35
5	A	702	OAA	O4-C4-C3	2.17	124.51	121.81
10	P	800	MQ7	C9-C10-C5	2.17	121.69	119.26
11	D	810	CE1	O22-C23-C24	2.16	120.20	110.35
6	A	703	FAD	O4B-C1B-N9A	2.16	112.23	108.09
10	D	700	MQ7	O1-C1-C2	2.15	123.28	120.45
11	D	810	CE1	O16-C17-C18	2.15	120.14	110.35
10	P	800	MQ7	O1-C1-C2	2.14	123.27	120.45
10	P	800	MQ7	O4-C4-C3	-2.14	117.24	120.67
6	A	703	FAD	C10-C4X-N5	-2.13	120.45	124.81
11	O	811	CE1	O13-C14-C15	2.13	120.07	110.35
6	M	803	FAD	C4X-C4-N3	2.12	118.65	113.25
10	P	800	MQ7	C14-C13-C15	2.11	118.89	115.23
11	D	710	CE1	O25-C26-C27	2.10	119.93	110.35
11	O	812	CE1	O31-C30-C29	2.05	119.69	110.35
6	M	803	FAD	O4B-C1B-N9A	2.02	111.98	108.09
10	P	800	MQ7	C2M-C2-C3	2.02	127.78	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	FAD	C5A-N7A-C8A	2.02	106.62	103.45
11	D	710	CE1	O19-C18-C17	2.01	119.53	110.35
11	O	812	CE1	O19-C20-C21	2.01	119.51	110.35

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	OAA	O3-C3-C4-O4
5	A	702	OAA	O3-C3-C4-O5
5	A	702	OAA	C2-C3-C4-O4
5	A	702	OAA	C2-C3-C4-O5
5	M	802	OAA	C1-C2-C3-O3
5	M	802	OAA	O3-C3-C4-O4
5	M	802	OAA	O3-C3-C4-O5
5	M	802	OAA	C2-C3-C4-O4
5	M	802	OAA	C2-C3-C4-O5
6	A	703	FAD	N10-C1'-C2'-O2'
6	A	703	FAD	N10-C1'-C2'-C3'
6	A	703	FAD	C5'-O5'-P-O2P
6	A	703	FAD	PA-O3P-P-O5'
6	M	803	FAD	N10-C1'-C2'-O2'
6	M	803	FAD	N10-C1'-C2'-C3'
6	M	803	FAD	C3'-C4'-C5'-O5'
6	M	803	FAD	O4'-C4'-C5'-O5'
6	M	803	FAD	C5'-O5'-P-O1P
6	M	803	FAD	C5'-O5'-P-O3P
6	M	803	FAD	PA-O3P-P-O5'
10	D	700	MQ7	C19-C18-C20-C21
11	O	811	CE1	C17-C18-O19-C20
11	O	812	CE1	C17-C18-O19-C20
10	B	701	MQ7	C13-C15-C16-C17
10	N	801	MQ7	C13-C15-C16-C17
11	D	810	CE1	O28-C29-C30-O31
11	O	812	CE1	C18-C17-O16-C15
11	O	811	CE1	C11-C12-O13-C14
11	O	812	CE1	O22-C23-C24-O25
11	D	810	CE1	O13-C14-C15-O16
11	D	710	CE1	O25-C26-C27-O28
11	D	710	CE1	O34-C35-C36-O37
11	D	710	CE1	O28-C29-C30-O31
11	O	811	CE1	O22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
11	D	810	CE1	O22-C23-C24-O25
11	D	710	CE1	O13-C14-C15-O16
11	O	812	CE1	O25-C26-C27-O28
11	D	810	CE1	O34-C35-C36-O37
11	O	812	CE1	C6-C7-C8-C9
11	D	810	CE1	C11-C10-C9-C8
11	D	810	CE1	O25-C26-C27-O28
11	O	812	CE1	O34-C35-C36-O37
6	A	703	FAD	C2'-C3'-C4'-O4'
11	D	810	CE1	C4-C5-C6-C7
11	O	811	CE1	C11-C10-C9-C8
11	D	710	CE1	C6-C7-C8-C9
11	O	811	CE1	O25-C26-C27-O28
11	D	710	CE1	C2-C3-C4-C5
10	B	701	MQ7	C14-C13-C15-C16
10	N	801	MQ7	C14-C13-C15-C16
11	O	812	CE1	C3-C4-C5-C6
10	N	801	MQ7	C12-C13-C15-C16
11	D	810	CE1	C36-C35-O34-C33
5	A	702	OAA	C1-C2-C3-O3
11	O	812	CE1	C24-C23-O22-C21
11	O	812	CE1	C14-C15-O16-C17
10	B	701	MQ7	C12-C13-C15-C16
11	O	811	CE1	C33-C32-O31-C30
11	D	710	CE1	C30-C29-O28-C27
11	O	812	CE1	C2-C3-C4-C5
11	D	710	CE1	C11-C12-O13-C14
11	D	710	CE1	C36-C35-O34-C33
11	O	811	CE1	C7-C8-C9-C10
10	D	700	MQ7	C17-C18-C20-C21
11	D	810	CE1	C33-C32-O31-C30
11	O	811	CE1	O28-C29-C30-O31
11	O	811	CE1	C4-C5-C6-C7
5	A	702	OAA	C1-C2-C3-C4
5	M	802	OAA	C1-C2-C3-C4
6	A	703	FAD	C5'-O5'-P-O1P
6	A	703	FAD	C5'-O5'-P-O3P
6	M	803	FAD	C5'-O5'-P-O2P
11	D	810	CE1	C11-C12-O13-C14
11	O	811	CE1	C29-C30-O31-C32
11	D	710	CE1	C11-C10-C9-C8
11	O	811	CE1	C36-C35-O34-C33

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Mol	Chain	Res	Type	Atoms
10	P	800	MQ7	C19-C18-C20-C21
11	O	812	CE1	O31-C32-C33-O34
11	D	710	CE1	C24-C23-O22-C21
11	D	810	CE1	C1-C2-C3-C4
11	O	812	CE1	C32-C33-O34-C35
11	O	812	CE1	C7-C8-C9-C10
11	O	811	CE1	C21-C20-O19-C18
11	D	710	CE1	C14-C15-O16-C17
11	D	810	CE1	C24-C23-O22-C21
11	O	811	CE1	O19-C20-C21-O22
11	O	812	CE1	C4-C5-C6-C7
11	O	812	CE1	C21-C20-O19-C18
11	D	810	CE1	C32-C33-O34-C35
11	D	710	CE1	O31-C32-C33-O34
11	D	810	CE1	O31-C32-C33-O34
6	M	803	FAD	PA-O3P-P-O2P
11	O	812	CE1	O19-C20-C21-O22
11	O	811	CE1	O16-C17-C18-O19
6	A	703	FAD	O3'-C3'-C4'-O4'
11	D	710	CE1	O22-C23-C24-O25
6	M	803	FAD	O4B-C4B-C5B-O5B
11	O	812	CE1	C33-C32-O31-C30
6	A	703	FAD	C2'-C3'-C4'-C5'
11	D	810	CE1	O19-C20-C21-O22
11	O	811	CE1	C14-C15-O16-C17
11	O	812	CE1	O16-C17-C18-O19
6	A	703	FAD	PA-O3P-P-O2P
6	A	703	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

13 monomers are involved in 104 short contacts:

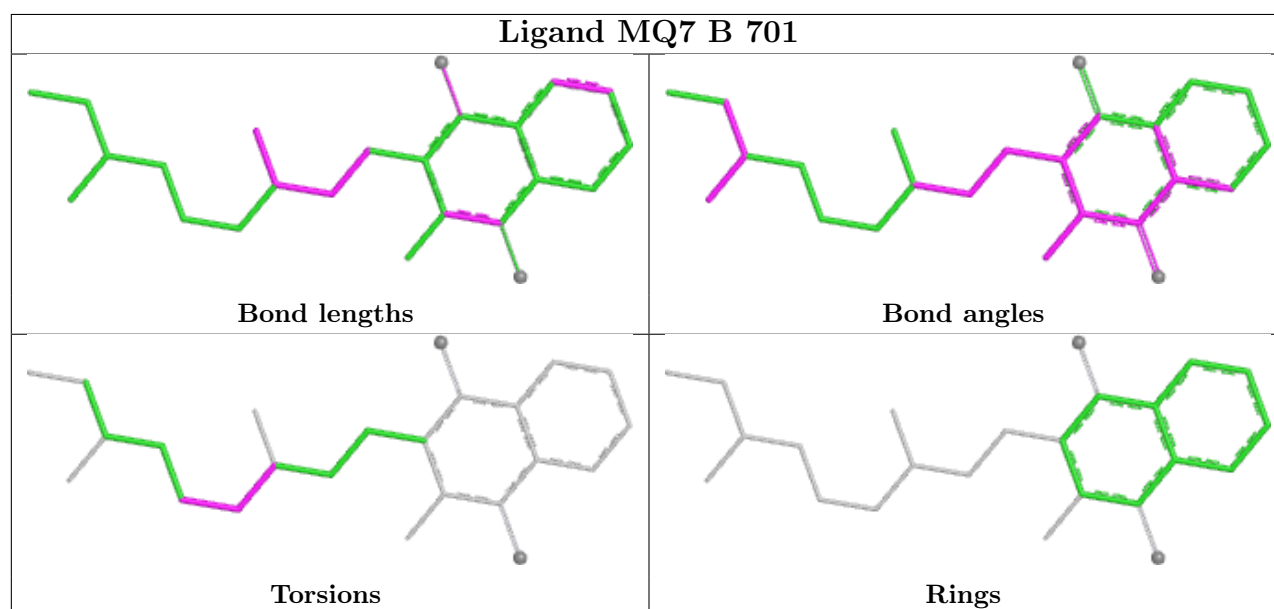
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	701	MQ7	3	0
6	M	803	FAD	24	0
5	M	802	OAA	1	0
7	B	244	FES	1	0
10	N	801	MQ7	13	0
10	D	700	MQ7	24	0
10	P	800	MQ7	19	0
5	A	702	OAA	1	0
11	D	710	CE1	3	0

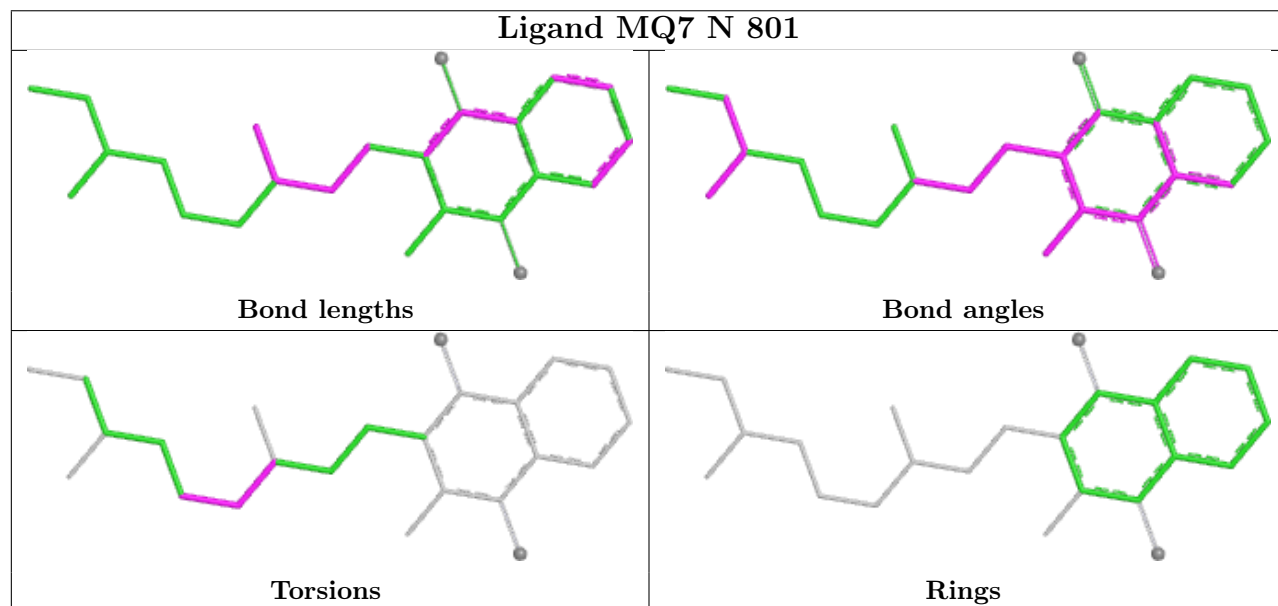
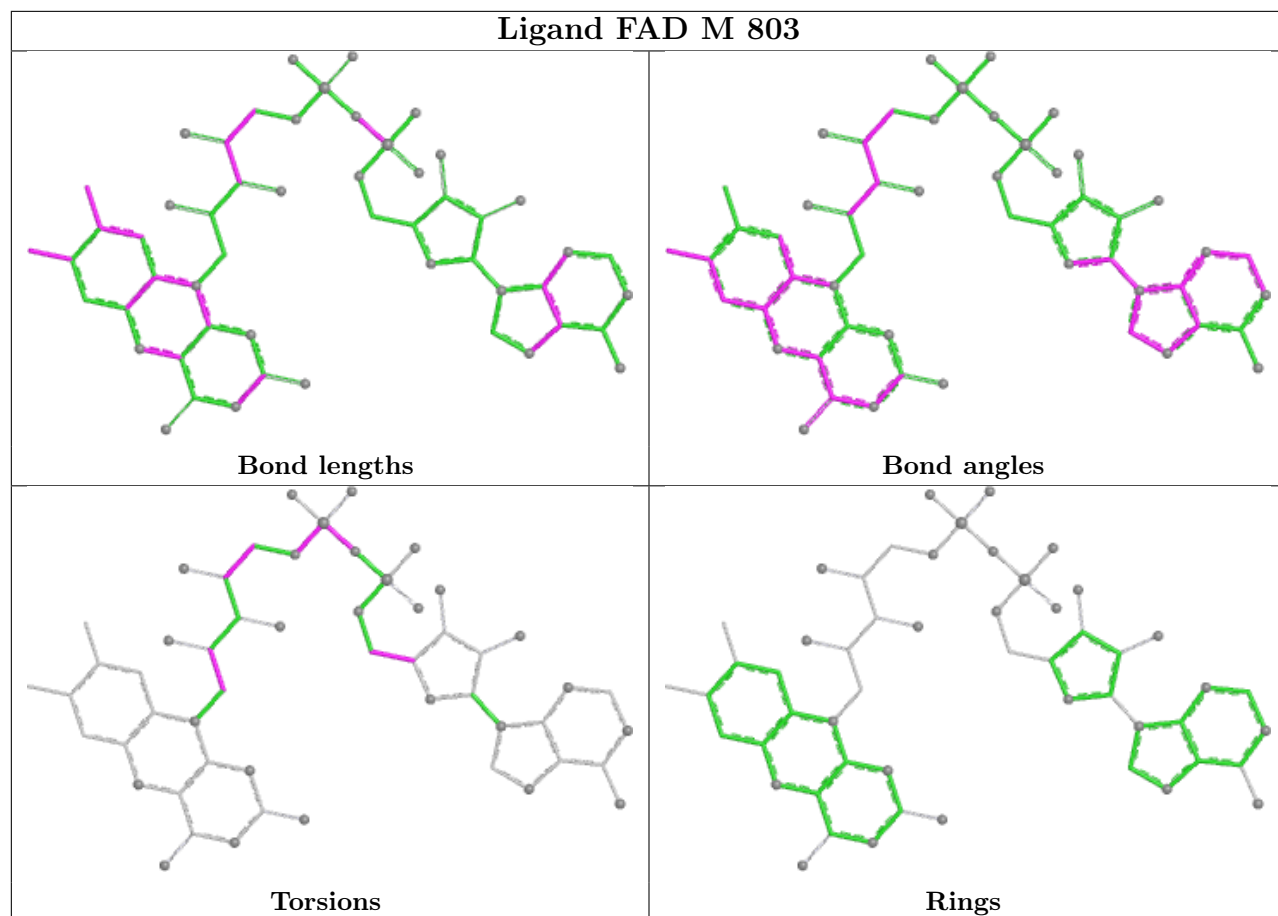
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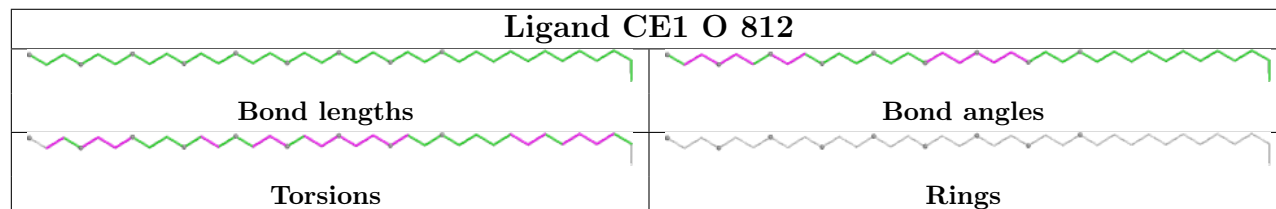
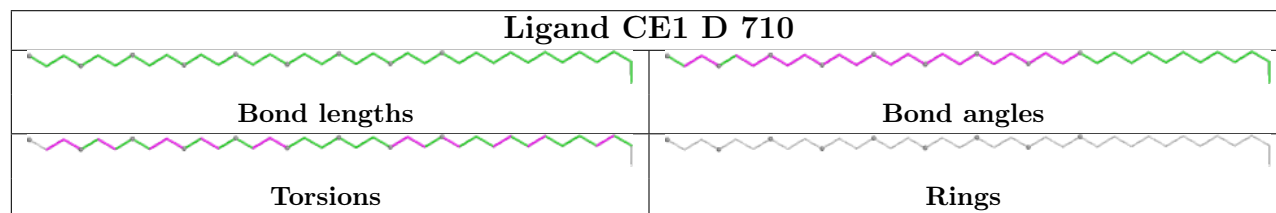
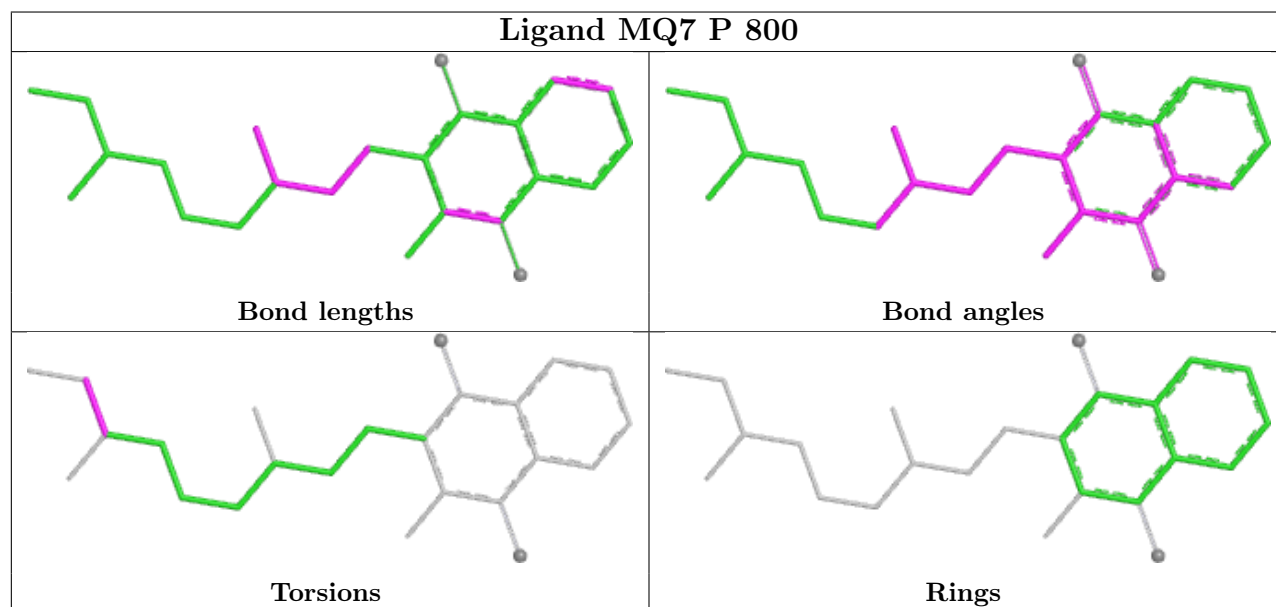
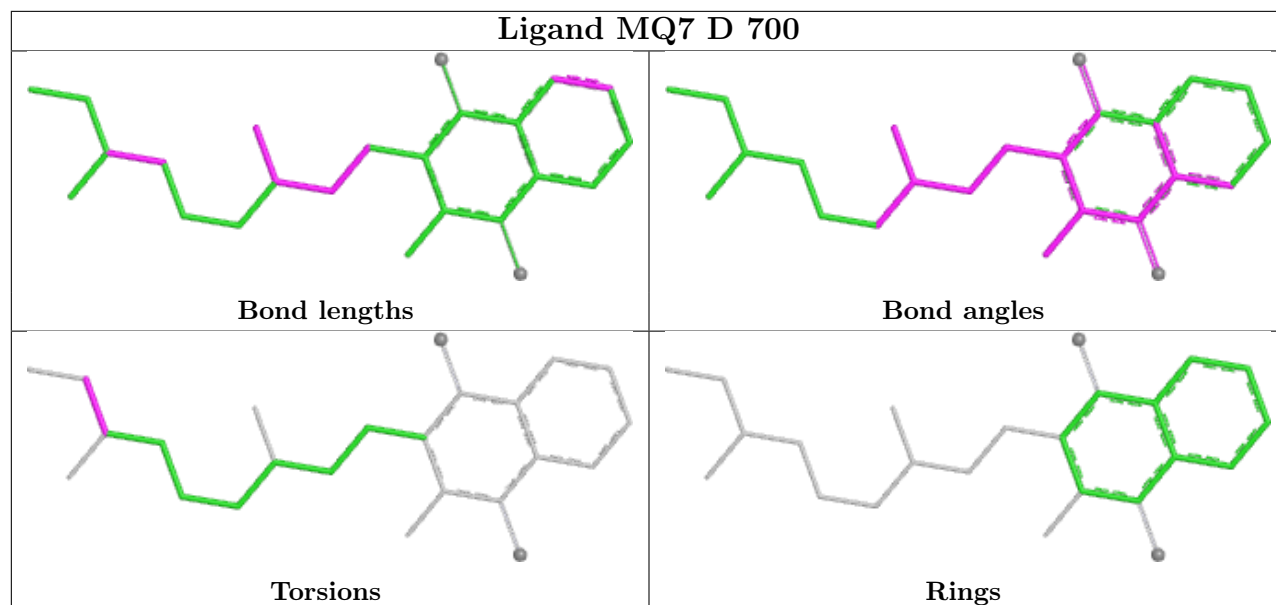
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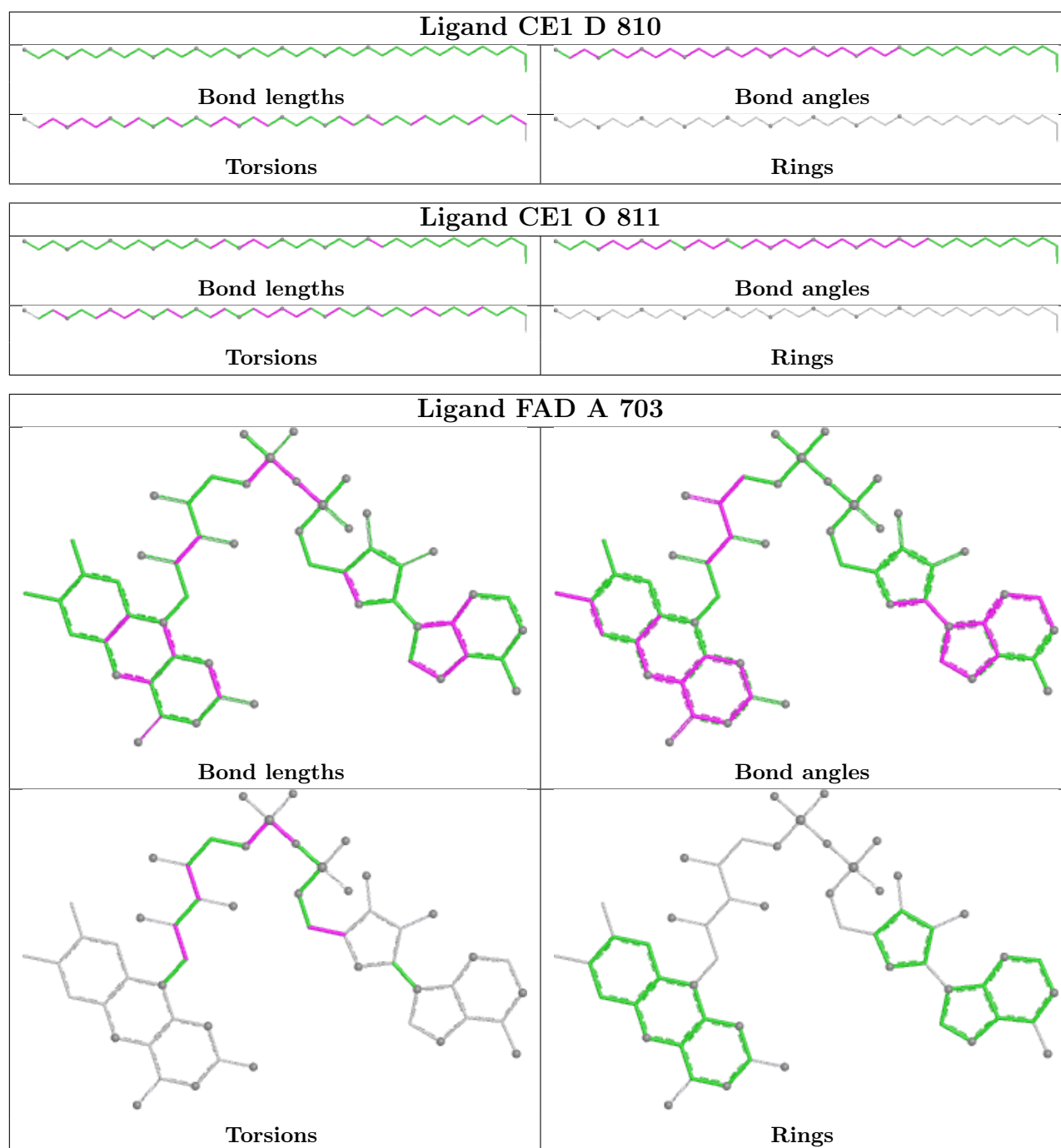
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	O	812	CE1	1	0
11	D	810	CE1	5	0
8	N	245	F3S	1	0
6	A	703	FAD	8	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	N	3
4	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	4:LYS	C	5:ASN	N	1.14
1	N	159:PRO	C	160:GLN	N	1.04
1	N	69:VAL	C	70:ASN	N	1.03
1	P	9:ASP	C	10:GLU	N	0.83

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.