



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:41 am BST

PDB ID : 1L0V
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

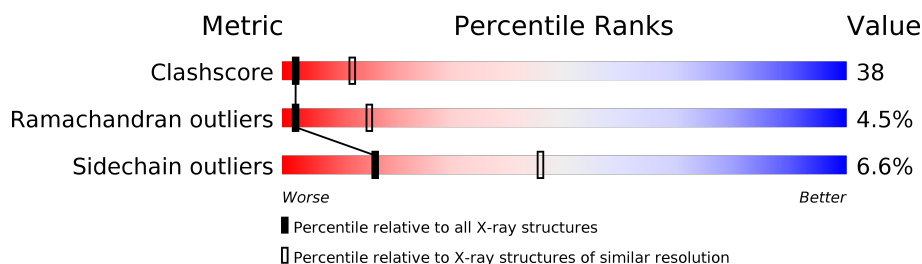
1 Overall quality at a glance

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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 on 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			

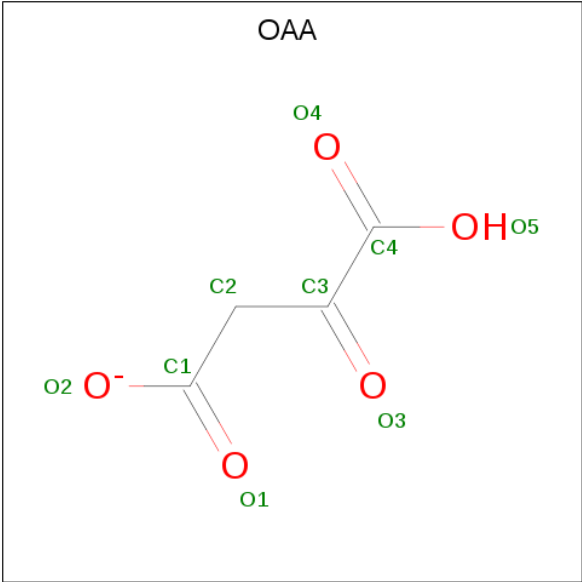
- Molecule 3 is a protein called Fumarate reductase 15 kDa hydrophobic protein.

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 (three-letter code: OAA) (formula: C₄H₃O₅).



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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



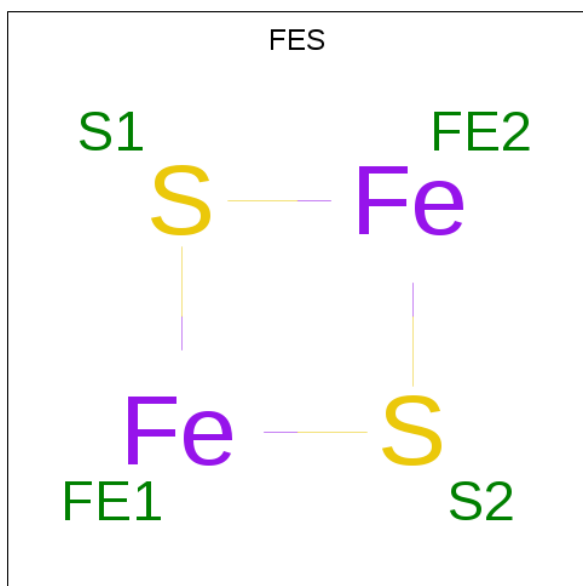
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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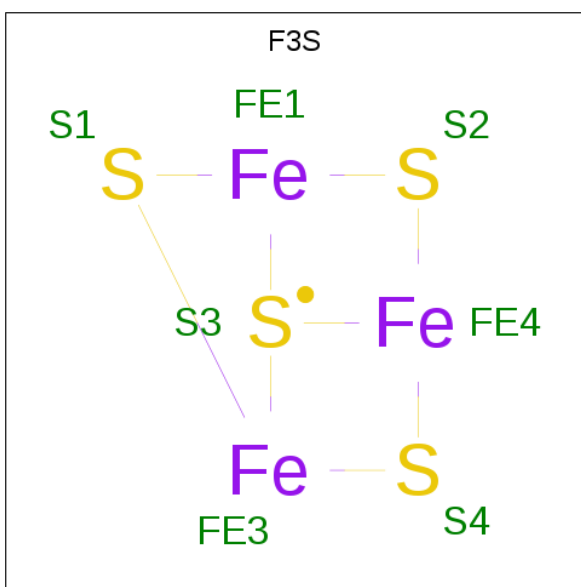
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



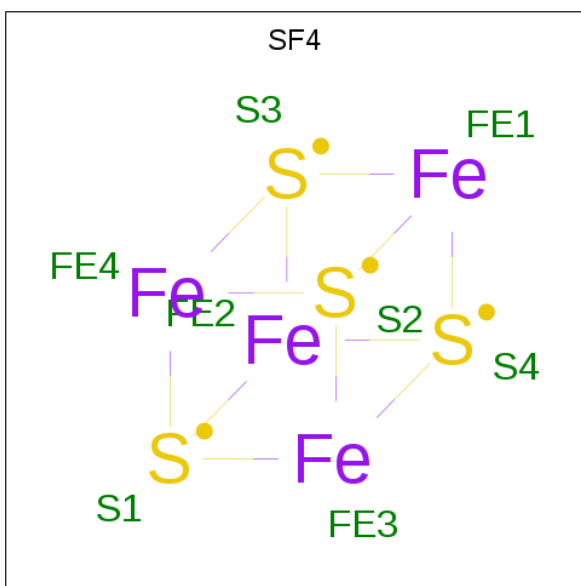
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



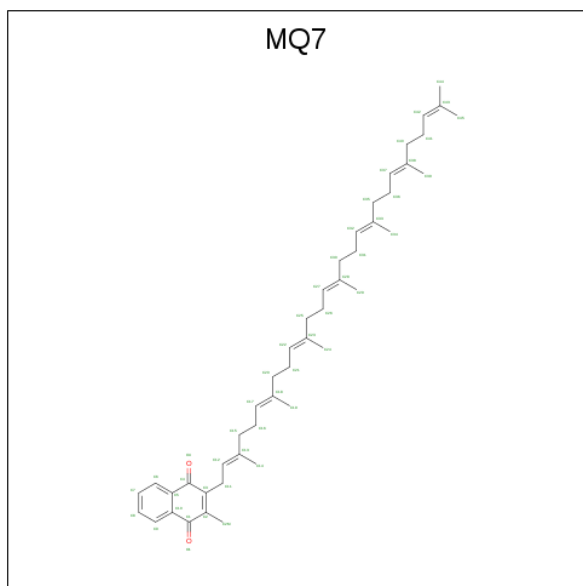
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



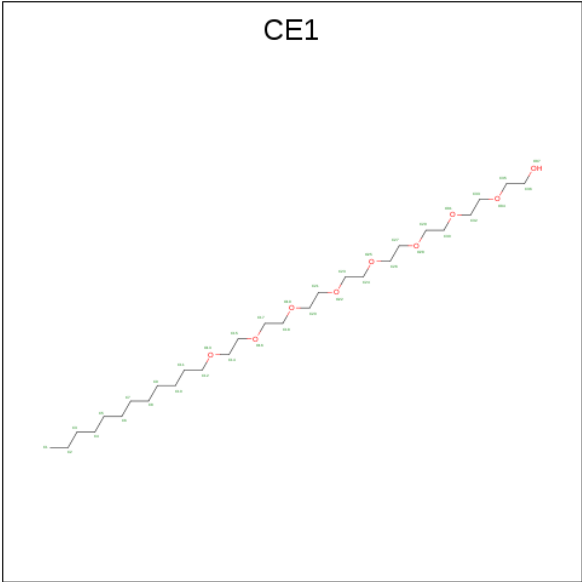
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



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 (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).



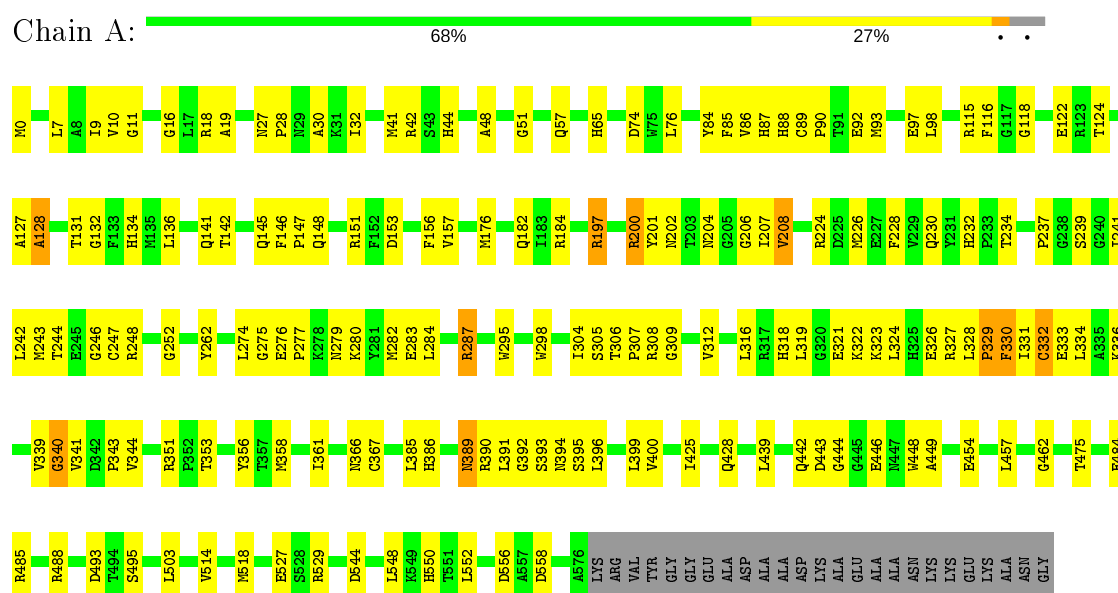
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			37	28	9		
11	D	1	Total	C	O	0	0
			37	28	9		
11	O	1	Total	C	O	0	0
			37	28	9		
11	O	1	Total	C	O	0	0
			37	28	9		

3 Residue-property plots

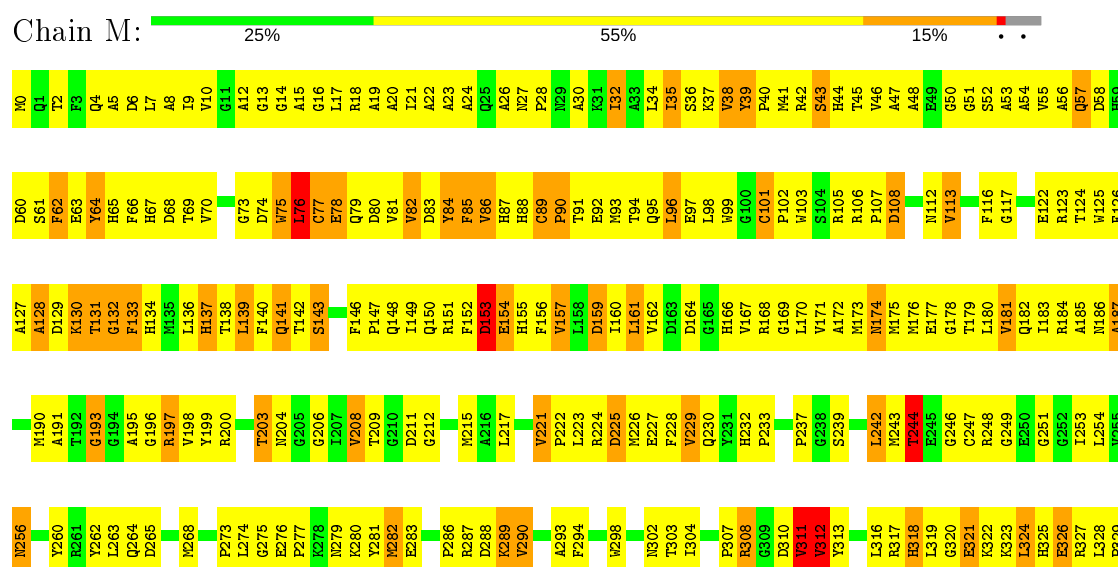
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

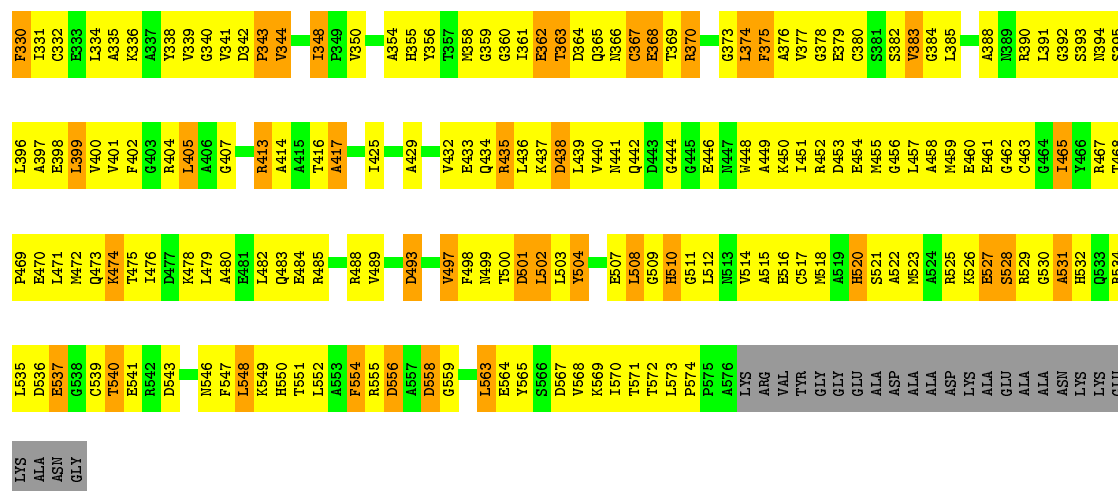
Note EDS was not executed.

• Molecule 1: Fumarate reductase flavoprotein subunit



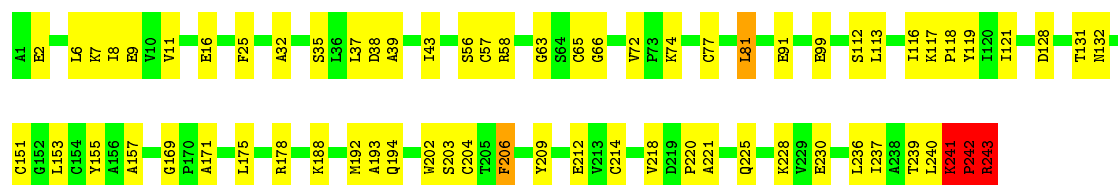
• Molecule 1: Fumarate reductase flavoprotein subunit





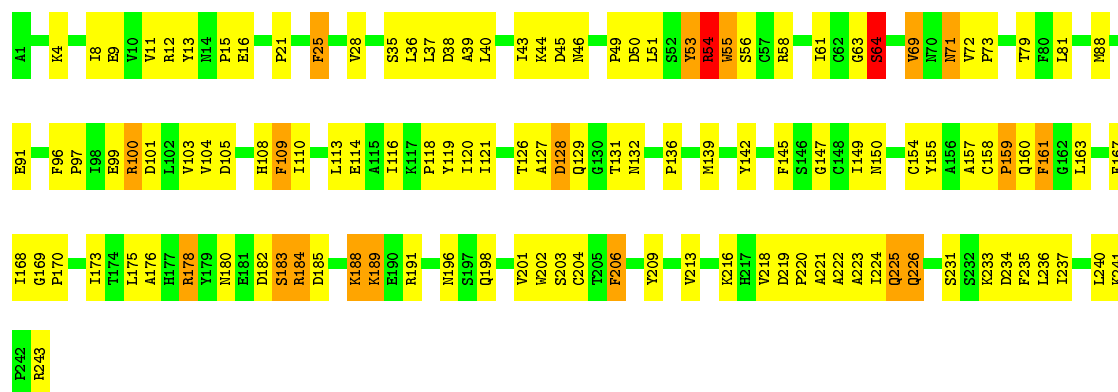
- Molecule 2: Fumarate reductase iron-sulfur protein

Chain B: 72% 26%



- Molecule 2: Fumarate reductase iron-sulfur protein

Chain N: 49% 42% 7%



- Molecule 3: Fumarate reductase 15 kDa hydrophobic protein

Chain C: 62% 35%





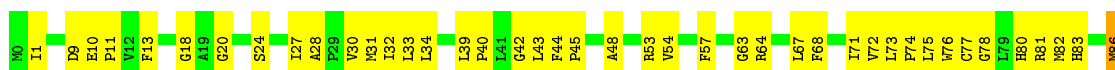
- Molecule 3: Fumarate reductase 15 kDa hydrophobic protein

Chain O: 53% 42% 5%



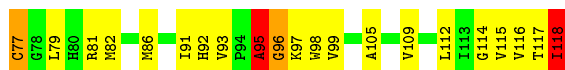
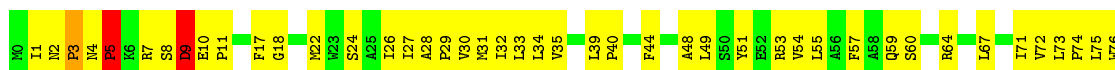
- Molecule 4: Fumarate reductase 13 kDa hydrophobic protein

Chain D: 50% 47% 2%



- Molecule 4: Fumarate reductase 13 kDa hydrophobic protein

Chain P: 45% 49% 2%



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	96.59 Å 138.09 Å 275.25 Å 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: MQ7, OAA, SF4, F3S, FES, CE1, FAD

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	0.59	0/4540	0.80	2/6139 (0.0%)
1	M	0.48	0/4540	0.75	1/6139 (0.0%)
2	B	0.98	6/1931 (0.3%)	1.04	11/2617 (0.4%)
2	N	0.80	9/1931 (0.5%)	0.89	8/2617 (0.3%)
3	C	0.50	0/1094	0.69	1/1496 (0.1%)
3	O	0.52	0/1094	0.68	0/1496
4	D	0.53	0/956	0.74	0/1303
4	P	0.99	2/956 (0.2%)	0.78	1/1303 (0.1%)
All	All	0.66	17/17042 (0.1%)	0.81	24/23110 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	N	0	3
4	P	0	1
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	9	ASP	C-N	-21.89	0.83	1.34
2	B	243	ARG	CA-C	19.61	2.04	1.52
2	B	243	ARG	C-O	17.19	1.56	1.23
4	P	95	ALA	C-N	13.40	1.57	1.33
2	N	69	VAL	C-N	-13.14	1.03	1.34
2	B	242	PRO	CB-CG	-12.84	0.85	1.50
2	N	159	PRO	C-N	-12.79	1.04	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	64	SER	C-N	11.23	1.59	1.34
2	B	242	PRO	CA-C	-10.22	1.32	1.52
2	N	161	PHE	C-N	8.92	1.49	1.33
2	N	4	LYS	C-N	-8.65	1.14	1.34
2	B	243	ARG	CZ-NH1	-7.21	1.23	1.33
2	N	54	ARG	C-N	6.46	1.49	1.34
2	B	243	ARG	CA-CB	6.23	1.67	1.53
2	N	184	ARG	C-O	5.49	1.33	1.23
2	N	63	GLY	C-N	-5.33	1.21	1.34
2	N	55	TRP	C-N	5.08	1.45	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	243	ARG	CB-CG-CD	16.45	154.36	111.60
2	B	243	ARG	NE-CZ-NH1	-11.92	114.34	120.30
2	N	54	ARG	O-C-N	-11.67	104.03	122.70
2	B	242	PRO	CA-N-CD	-11.40	95.53	111.50
2	B	243	ARG	NE-CZ-NH2	11.02	125.81	120.30
2	N	69	VAL	C-N-CA	10.54	148.05	121.70
2	B	242	PRO	CA-C-N	-10.01	95.19	117.20
1	A	128	ALA	N-CA-C	-9.11	86.41	111.00
2	B	242	PRO	O-C-N	7.91	135.35	122.70
2	N	183	SER	O-C-N	-7.66	110.45	122.70
2	N	69	VAL	O-C-N	-7.44	110.80	122.70
2	N	4	LYS	O-C-N	-7.21	111.17	122.70
2	B	242	PRO	N-CA-C	-7.17	93.45	112.10
2	B	241	LYS	C-N-CA	7.00	151.42	122.00
2	B	241	LYS	C-N-CD	-6.39	106.54	120.60
2	B	243	ARG	CA-C-O	6.22	133.17	120.10
1	M	38	VAL	N-CA-C	-5.92	95.01	111.00
3	C	65	ASN	N-CA-C	5.72	126.44	111.00
4	P	118	ILE	N-CA-C	5.66	126.28	111.00
1	A	312	VAL	N-CA-C	-5.49	96.18	111.00
2	N	4	LYS	CA-C-N	5.29	128.83	117.20
2	N	184	ARG	O-C-N	-5.19	114.40	122.70
2	N	69	VAL	CA-C-N	5.11	128.44	117.20
2	B	243	ARG	CD-NE-CZ	-5.08	116.49	123.60

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	143	0
1	M	4448	0	4333	662	0
2	B	1888	0	1837	72	0
2	N	1888	0	1833	172	0
3	C	1058	0	1108	52	0
3	O	1058	0	1108	82	0
4	D	926	0	971	90	0
4	P	926	0	970	106	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	4	0
10	D	24	0	23	26	0
10	N	24	0	23	14	0
10	P	24	0	23	20	0
11	D	74	0	116	8	0
11	O	74	0	116	1	0
All	All	17046	0	16885	1285	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 38.

All (1285) 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:A:44:HIS:NE2	6:A:703:FAD:HM82	1.16	1.45
1:M:98:LEU:CD2	2:N:132:ASN:HD21	1.28	1.42
1:M:44:HIS:NE2	6:M:803:FAD:HM82	1.06	1.32
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
2:N:11:VAL:CG2	2:N:91:GLU:HG2	1.63	1.27
4:P:9:ASP:C	4:P:10:GLU:CA	2.01	1.27
2:B:243:ARG:C	2:B:243:ARG:CA	2.03	1.26
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
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
1:A:44:HIS:CE1	6:A:703:FAD:HM82	1.82	1.12
4:D:53:ARG:HH12	10:D:700:MQ7:C14	1.62	1.11
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.24	1.11
4:D:53:ARG:HH12	10:D:700:MQ7:C15	1.63	1.11
4:P:86:MET:CE	4:P:91:ILE:HG21	1.81	1.10
1:M:287:ARG:NH2	5:M:802:OAA:O3	1.85	1.10
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
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
4:D:31:MET:HE1	10:D:700:MQ7:O1	1.58	1.02
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.42	1.02
4:D:53:ARG:HH12	10:D:700:MQ7:C13	1.72	1.01
1:A:308:ARG:HH12	1:A:339:VAL:HA	1.25	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:HB3	2:B:242:PRO:CG	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:537:GLU:CD	1:M:537:GLU:H	1.59	0.99
1:M:573:LEU:HD12	1:M:574:PRO:HD2	1.40	0.99
4:D:31:MET:CE	10:D:700:MQ7:O1	2.12	0.98
2:B:242:PRO:HG2	2:B:242:PRO:CB	1.48	0.98
1:M:223:LEU:HB3	1:M:226:MET:HG3	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:PRO:HG3	2:B:242:PRO:CB	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
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
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
4:P:31:MET:CE	10:P:800:MQ7:O1	2.19	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
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
2:N:36:LEU:HD13	2:N:88:MET:HE2	1.52	0.89
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:9:ASP:C	4:P:10:GLU:N	0.83	0.88
4:D:54:VAL:CG1	10:D:700:MQ7:H6	2.03	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
2:B:242:PRO:HG2	2:B:243:ARG:HD3	1.55	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:98:LEU:HD22	2:N:132:ASN:HD21	1.39	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
3:O:86:TRP:HE1	4:P:22:MET:HE2	1.40	0.86
4:P:31:MET:HE3	10:P:800:MQ7:O1	1.74	0.86
1:A:44:HIS:NE2	6:A:703:FAD:HM81	1.89	0.86
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
10:N:801:MQ7:H143	10:N:801:MQ7:H2M1	1.59	0.84
2:B:242:PRO:CG	2:B:243:ARG:HD3	2.07	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
1:M:256:ASN:H	1:M:256:ASN:HD22	1.27	0.82
1:M:242:LEU:O	1:M:242:LEU:HD13	1.80	0.82
1:M:80:ASP:OD2	1:M:365:GLN:HG2	1.79	0.82
4:P:64:ARG:NH2	4:P:118:ILE:H	1.76	0.82
3:O:50:LYS:HZ2	4:P:117:THR:HG21	1.43	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
1:M:396:LEU:HA	1:M:399:LEU:HD12	1.63	0.81
10:N:801:MQ7:H2M2	3:O:28:ARG:NH1	1.96	0.81
4:P:86:MET:HE3	4:P:91:ILE:HG21	1.62	0.80
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:263:LEU:HD12	1:M:283:GLU:HA	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168:ARG:HG3	1:M:425:ILE:CD1	2.12	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
1:M:42:ARG:HH11	1:M:42:ARG:HG2	1.47	0.79
1:M:222:PRO:CG	1:M:362:GLU:HB2	2.11	0.79
1:M:537:GLU:CD	1:M:537:GLU:N	2.34	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
2:N:109:PHE:C	2:N:109:PHE:HD2	1.86	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
1:M:493:ASP:OD2	2:N:50:ASP:CA	2.21	0.78
1:M:211:ASP:HB3	1:M:510:HIS:ND1	1.98	0.78
2:N:40:LEU:CB	2:N:53:TYR:CE2	2.65	0.78
1:A:327:ARG:C	1:A:328:LEU:HD23	2.02	0.77
2:N:53:TYR:HE1	2:N:55:TRP:CD1	2.01	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:187:ALA:HB2	1:M:414:ALA:HB2	1.65	0.77
1:M:46:VAL:HG22	2:N:61:ILE:HG13	1.66	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
2:N:36:LEU:CD1	2:N:88:MET:HE2	2.13	0.76
1:M:73:GLY:O	1:M:388:ALA:HB3	1.86	0.76
1:M:44:HIS:CE1	6:M:803:FAD:HM82	2.12	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
4:P:86:MET:HE3	4:P:91:ILE:CG2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:LYS:O	2:B:241:LYS:HG3	1.84	0.75
1:M:569:LYS:O	1:M:570:ILE:HD13	1.86	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
1:M:304:ILE:HG13	1:M:313:TYR:CE2	2.21	0.74
1:M:203:THR:HG23	1:M:354:ALA:O	1.87	0.74
3:O:65:ASN:C	3:O:65:ASN:HD22	1.90	0.74
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:M:84:TYR:CE1	1:M:405:LEU:HD21	2.23	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:151:ARG:NH1	1:M:153:ASP:OD2	2.21	0.73
1:M:94:THR:HG23	2:N:131:THR:CG2	2.18	0.73
2:N:39:ALA:O	2:N:43:ILE:HG12	1.87	0.73
2:N:109:PHE:C	2:N:109:PHE:CD2	2.60	0.73
2:N:109:PHE:HD2	2:N:109:PHE:O	1.72	0.73
1:M:44:HIS:CD2	6:M:803:FAD:HM82	2.18	0.72
3:C:104:GLY:HA2	3:C:107:PRO:HD2	1.71	0.72
1:M:317:ARG:O	1:M:319:LEU:N	2.15	0.72
1:M:81:VAL:HG11	1:M:383:VAL:O	1.89	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
4:P:31:MET:HE1	10:P:800:MQ7:O1	1.88	0.71
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: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: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:176:MET:SD	2:N:99:GLU:HG3	2.31	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:149:ILE:HG22	1:M:150:GLN:N	2.06	0.70
1:M:195:ALA:O	1:M:198:VAL:HG13	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:GLU:O	3:C:91:PRO:HD2	1.90	0.70
1:M:177:GLU:OE1	3:O:4:ARG:HG2	1.91	0.70
4:P:86:MET:HE1	4:P:91:ILE:HG21	1.74	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
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:183:ILE:N	1:M:183:ILE:HD12	2.07	0.69
1:M:5:ALA:HB3	1:M:185:ALA:HB2	1.74	0.69
1:M:308:ARG:N	1:M:308:ARG:HD2	2.08	0.69
1:M:35:ILE:HG12	1:M:36:SER:N	2.07	0.69
1:M:7:LEU:HA	1:M:187:ALA:HB3	1.73	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:CD2	3:O:19:LEU:H	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: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: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
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:15:ALA:HB2	1:M:399:LEU:HA	1.76	0.67
1:M:373:GLY:O	1:M:375:PHE:HD1	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:500:THR:O	1:M:502:LEU:N	2.23	0.67
1:M:66:PHE:O	1:M:69:THR:HB	1.94	0.67
2:N:36:LEU:HD13	2:N:88:MET:HE1	1.73	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
4:D:31:MET:HE3	10:D:700:MQ7:O1	1.93	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:321:GLU:C	1:M:323:LYS:H	1.97	0.66
1:M:62:PHE:H	1:M:62:PHE:HD1	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:175:LEU:O	2:N:178:ARG:HB3	1.95	0.66
2:N:73:PRO:HG2	2:N:213:VAL:HG11	1.76	0.66
1:A:287:ARG:HH11	1:A:287:ARG:CG	1.95	0.66
1:M:331:ILE:HD12	1:M:331:ILE:H	1.59	0.66
1:M:40:PRO:HB2	1:M:140:PHE:CE1	2.31	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: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
1:M:509:GLY:C	1:M:511:GLY:H	1.98	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
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:HH11	1:A:184:ARG:HG2	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: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:35:ILE:CG1	1:M:36:SER:N	2.59	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: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
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:275:GLY:C	1:M:277:PRO:HD3	2.18	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
1:M:159:ASP:CG	1:M:160:ILE:H	2.02	0.63
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:256:ASN:HD21	1:M:260:TYR:CB	2.10	0.63
1:M:32:ILE:O	1:M:150:GLN:HB3	1.98	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
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
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: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:527:GLU:HG3	1:M:528:SER:N	2.14	0.62
1:M:52:SER:O	1:M:125:TRP:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:327:ARG:C	1:A:329:PRO:HD3	2.20	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:37:LYS:HZ1	1:M:507:GLU:CD	2.02	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
1:M:365:GLN:C	1:M:366:ASN:HD22	2.02	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
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
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: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:208:VAL:HG12	1:M:208:VAL:O	2.01	0.60
1:M:2:THR:HG23	1:M:184:ARG:CG	2.31	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: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:9:ILE:HD13	1:M:19:ALA:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:PRO:HB2	2:B:243:ARG:CG	2.32	0.60
1:M:263:LEU:HD22	1:M:268:MET:HE3	1.84	0.60
1:A:306:THR:HB	1:A:309:GLY:O	2.00	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
1:M:70:VAL:C	1:M:73:GLY:H	2.05	0.60
1:M:42:ARG:HD3	2:N:64:SER:HB2	1.83	0.60
1:M:509:GLY:O	1:M:511:GLY:N	2.35	0.60
2:B:241:LYS:C	2:B:242:PRO:O	2.33	0.59
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
1:M:440:VAL:C	1:M:442:GLN:H	2.05	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:509:GLY:C	1:M:511:GLY:N	2.55	0.59
1:M:14:GLY:N	6:M:803:FAD:O2P	2.35	0.59
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.37	0.59
1:M:206:GLY:HA3	2:N:55:TRP:CZ3	2.36	0.59
10:N:801:MQ7:H2M2	3:O:28:ARG:HH12	1.66	0.59
3:O:106:GLU:H	3:O:106:GLU:CD	2.05	0.59
3:O:98:VAL:HG23	3:O:98:VAL:O	2.02	0.59
4:P:9:ASP:O	4:P:10:GLU:C	2.40	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:M:67:HIS:C	1:M:69:THR:H	2.06	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:N:236:LEU:HD23	2:N:236:LEU:C	2.24	0.58
4:P:64:ARG:HB3	4:P:115:VAL:HG22	1.85	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: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: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:74:ASP:HA	1:M:75:TRP:CE3	2.38	0.58
3:O:65:ASN:HB3	3:O:66:PRO:C	2.25	0.58
1:M:127:ALA:O	1:M:128:ALA:O	2.21	0.57
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
1:M:24:ALA:C	1:M:26:ALA:H	2.08	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:C:33:VAL:HA	4:D:82:MET:HE3	1.86	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
1:M:88:HIS:CB	1:M:401:VAL:HG13	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:53:TYR:C	2:N:53:TYR:CD1	2.78	0.57
2:B:116:ILE:HD12	2:B:116:ILE:C	2.26	0.57
1:M:175:MET:HE2	1:M:503:LEU:HD13	1.87	0.57
1:M:396:LEU:HA	1:M:399:LEU:CD1	2.34	0.57
1:M:46:VAL:HA	1:M:133:PHE:HA	1.86	0.57
1:M:514:VAL:O	1:M:518:MET:HG2	2.04	0.57
1:M:39:TYR:HE1	2:N:54:ARG:HH12	1.53	0.57
4:D:34:LEU:HD13	10:D:700:MQ7:H2M3	1.86	0.57
1:M:217:LEU:HD11	1:M:223:LEU:HD11	1.87	0.57
1:M:62:PHE:HD2	1:M:87:HIS:HD1	1.52	0.57
4:D:113:ILE:O	4:D:116:VAL:CG2	2.53	0.56
1:M:161:LEU:HG	1:M:169:GLY:O	2.05	0.56
1:M:22:ALA:HB1	1:M:404:ARG:HG3	1.86	0.56
1:M:312:VAL:CG2	1:M:350:VAL:HG23	2.30	0.56
2:N:109:PHE:CE2	2:N:113:LEU:HD22	2.40	0.56
1:M:497:VAL:HG11	2:N:15:PRO:HG3	1.87	0.56
3:O:50:LYS:HZ2	4:P:117:THR:CG2	2.15	0.56
1:A:282:MET:HB3	1:A:283:GLU:OE1	2.05	0.56
4:D:102:GLY:HA2	11:D:710:CE1:H62	1.87	0.56
1:M:82:VAL:HG22	1:M:385:LEU:HA	1.87	0.56
1:M:67:HIS:O	1:M:69:THR:N	2.38	0.56
4:P:64:ARG:HH12	4:P:118:ILE:C	2.09	0.56
4:D:13:PHE:HE2	4:D:97:LYS:HE2	1.70	0.56
1:M:396:LEU:C	1:M:398:GLU:H	2.08	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:366:ASN:O	1:A:367:CYS:HB2	2.06	0.56
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.88	0.56
1:A:439:LEU:HD12	1:A:442:GLN:NE2	2.20	0.56
2:B:2:GLU:OE2	2:B:2:GLU:HA	2.05	0.56
4:D:27:ILE:HG22	4:D:27:ILE:O	2.05	0.56
1:M:193:GLY:HA2	1:M:379:GLU:HB3	1.86	0.56
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.41	0.56
2:B:7:LYS:HE2	2:B:25:PHE:CD2	2.41	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:O	1:M:436:LEU:HD12	2.06	0.56
1:M:46:VAL:HG13	1:M:47:ALA:N	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:P:86:MET:HE3	4:P:91:ILE:HB	1.87	0.56
2:B:113:LEU:O	2:B:113:LEU:HD23	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:HG3	1:M:150:GLN:O	2.05	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
1:M:502:LEU:C	1:M:504:TYR:H	2.10	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
2:N:81:LEU:HD12	2:N:81:LEU:N	2.21	0.55
1:M:382:SER:C	1:M:384:GLY:H	2.09	0.55
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.22	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
1:M:6:ASP:OD1	1:M:30:ALA:HA	2.07	0.55
2:N:201:VAL:HG23	2:N:202:TRP:N	2.20	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
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
1:M:77:CYS:O	1:M:79:GLN:N	2.40	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:A:7:LEU:CD2	1:A:32:ILE:HG12	2.36	0.55
1:M:204:ASN:HD22	6:M:803:FAD:HM83	1.70	0.55
1:M:308:ARG:H	1:M:308:ARG:HD2	1.70	0.55
1:M:520:HIS:O	1:M:521:SER:C	2.45	0.55
1:M:81:VAL:HG22	1:M:365:GLN:HA	1.89	0.55
4:D:114:GLY:O	4:D:117:THR:HA	2.07	0.55
1:M:211:ASP:O	1:M:215:MET:N	2.39	0.55
1:M:21:ILE:HG21	1:M:99:TRP:CH2	2.42	0.55
1:M:204:ASN:ND2	6:M:803:FAD:HM81	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:7:ARG:HG2	4:P:8:SER:N	2.21	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
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:251:GLY:HA2	1:M:277:PRO:CG	2.35	0.54
1:M:62:PHE:CD1	1:M:62:PHE:N	2.75	0.54
1:A:316:LEU:O	1:A:319:LEU:HG	2.07	0.54
1:M:468:THR:CG2	1:M:535:LEU:HD12	2.37	0.54
1:M:356:TYR:HE2	6:M:803:FAD:HO3'	1.53	0.54
2:N:168:ILE:HD11	2:N:173:ILE:HG12	1.90	0.54
1:M:15:ALA:HB2	1:M:399:LEU:HB3	1.89	0.54
1:M:8:ALA:O	1:M:9:ILE:HG13	2.08	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
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:M:551:THR:C	1:M:552:LEU:HD23	2.28	0.54
1:A:306:THR:CG2	1:A:307:PRO:HD2	2.38	0.54
4:D:53:ARG:HG2	4:D:53:ARG:HH11	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:HD12	4:P:26:ILE:N	2.23	0.54
3:C:130:TRP:CD1	3:C:130:TRP:N	2.76	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:HA	1:M:434:GLN:HE21	1.73	0.54
1:M:448:TRP:HB2	1:M:508:LEU:HD23	1.90	0.54
1:M:382:SER:O	1:M:384:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:MET:O	1:A:518:MET:HG2	2.08	0.53
3:C:19:LEU:HD12	3:C:20:PRO:CD	2.31	0.53
1:M:169:GLY:HA3	1:M:184:ARG:HD3	1.89	0.53
1:M:42:ARG:CG	1:M:42:ARG:HH11	2.20	0.53
1:M:43:SER:HB2	1:M:136:LEU:HD22	1.91	0.53
1:M:525:ARG:O	1:M:534:ARG:NH1	2.41	0.53
1:M:21:ILE:HG21	1:M:99:TRP:CZ3	2.43	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
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
1:M:127:ALA:HB3	1:M:131:THR:HA	1.89	0.53
1:M:10:VAL:HG11	1:M:157:VAL:HG21	1.90	0.53
1:M:484:GLU:O	1:M:488:ARG:HD2	2.07	0.53
1:M:7:LEU:O	1:M:32:ILE:HG23	2.08	0.53
1:M:82:VAL:O	1:M:82:VAL:HG12	2.09	0.53
2:N:53:TYR:C	2:N:53:TYR:HD1	2.11	0.53
4:P:1:ILE:HG23	4:P:1:ILE:O	2.08	0.53
2:B:6:LEU:HD23	2:B:81:LEU:HD13	1.90	0.53
4:D:115:VAL:C	4:D:117:THR:H	2.07	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
1:A:228:PHE:O	1:A:358:MET:HB2	2.09	0.53
2:B:16:GLU:OE2	3:C:3:LYS:HD2	2.09	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:102:PRO:O	1:M:103:TRP:C	2.46	0.53
1:M:279:ASN:ND2	1:M:280:LYS:N	2.56	0.53
2:N:109:PHE:CD2	2:N:109:PHE:O	2.58	0.53
2:N:44:LYS:HD3	2:N:51:LEU:O	2.09	0.53
1:M:336:LYS:O	1:M:340:GLY:HA2	2.09	0.53
1:M:15:ALA:HA	1:M:399:LEU:O	2.08	0.53
10:N:801:MQ7:C14	10:N:801:MQ7:H2M1	2.36	0.53
3:O:65:ASN:HB3	3:O:68:ILE:H	1.73	0.53
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:162:VAL:HG13	1:M:166:HIS:C	2.30	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:256:ASN:H	1:M:256:ASN:ND2	2.03	0.52
1:M:530:GLY:O	1:M:532:HIS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLN:CD	1:A:287:ARG:HH21	2.13	0.52
1:M:103:TRP:HZ3	1:M:131:THR:HG23	1.74	0.52
1:M:373:GLY:O	1:M:375:PHE:CD1	2.62	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
4:D:53:ARG:CZ	10:D:700:MQ7:H151	2.34	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: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:212:GLY:HA2	1:M:215:MET:HG2	1.92	0.52
1:M:237:PRO:HB2	1:M:308:ARG:HB3	1.90	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:H171	11:D:710:CE1:H211	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:34:LEU:HD13	1:M:149:ILE:CG2	2.40	0.51
1:M:7:LEU:CB	1:M:187:ALA:HB3	2.41	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:256:ASN:HB2	1:M:302:ASN:HB3	1.91	0.51
1:M:230:GLN:NE2	1:M:390:ARG:HB3	2.20	0.51
3:O:65:ASN:HB2	3:O:68:ILE:CB	2.41	0.51
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.91	0.51
1:A:44:HIS:NE2	6:A:703:FAD:C8	2.69	0.51
4:D:54:VAL:HG13	10:D:700:MQ7:C4	2.37	0.51
1:M:382:SER:C	1:M:384:GLY:N	2.60	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
3:C:98:VAL:O	3:C:99:LYS:HB2	2.11	0.51
3:C:33:VAL:HG22	4:D:82:MET:CE	2.41	0.51
1:M:444:GLY:HA3	1:M:488:ARG:O	2.11	0.51
1:M:96:LEU:O	1:M:101:CYS:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:137:HIS:O	1:M:138:THR:C	2.49	0.51
1:M:251:GLY:CA	1:M:277:PRO:HG2	2.38	0.51
1:M:35:ILE:HD13	1:M:157:VAL:CG2	2.37	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
10:B:701:MQ7:H2M2	3:C:28:ARG:NH1	2.26	0.51
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
4:P:86:MET:HE2	4:P:91:ILE:CG2	2.41	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
1:M:16:GLY:O	1:M:19:ALA:HB3	2.11	0.51
1:M:396:LEU:C	1:M:398:GLU:N	2.63	0.51
1:M:15:ALA:HB2	1:M:399:LEU:CB	2.41	0.51
1:M:502:LEU:C	1:M:504:TYR:N	2.64	0.51
1:M:483:GLN:OE1	1:M:555:ARG:NH2	2.44	0.51
3:O:50:LYS:HZ3	11:O:812:CE1:C3	2.24	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:454:GLU:O	1:M:455:MET:C	2.48	0.50
2:N:202:TRP:HE1	2:N:231:SER:HG	1.57	0.50
1:M:321:GLU:C	1:M:323:LYS:N	2.64	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: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: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:NH1	1:M:42:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:P:3:PRO:C	4:P:4:ASN:HD22	2.15	0.50
1:A:42:ARG:HD2	1:A:42:ARG:N	2.26	0.50
1:M:89:CYS:C	1:M:91:THR:H	2.15	0.50
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.47	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
4:D:27:ILE:CG2	4:D:27:ILE:O	2.60	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:105:PRO:HD2	3:O:106:GLU:OE2	2.12	0.50
3:O:65:ASN:HB2	3:O:68:ILE:CG1	2.42	0.50
1:M:256:ASN:HD21	1:M:260:TYR:N	2.09	0.49
1:M:56:ALA:O	1:M:57:GLN:O	2.31	0.49
2:N:72:VAL:HG13	2:N:73:PRO:HD2	1.94	0.49
1:M:479:LEU:HA	1:M:482:LEU:HD12	1.93	0.49
1:M:7:LEU:HD11	1:M:23:ALA:HB1	1.93	0.49
2:N:132:ASN:HB2	2:N:184:ARG:HD3	1.94	0.49
2:N:56:SER:O	2:N:58:ARG:HG3	2.12	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:133:PHE:O	1:M:137:HIS:HB2	2.11	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:479:LEU:HD13	1:M:516:GLU:N	2.27	0.49
1:M:53:ALA:HA	1:M:124:THR:HA	1.94	0.49
1:A:232:HIS:HD2	1:A:234:THR:H	1.61	0.49
1:A:51:GLY:HA3	1:A:124:THR:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:ARG:HG2	1:M:112:ASN:CB	2.43	0.49
1:M:20:ALA:CB	1:M:34:LEU:HD11	2.42	0.49
4:D:39:LEU:HB3	4:D:40:PRO:CD	2.42	0.49
1:M:18:ARG:HH11	1:M:18:ARG:HG2	1.78	0.49
1:M:416:THR:OG1	1:M:417:ALA:N	2.46	0.49
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:321:GLU:O	1:M:323:LYS:N	2.43	0.49
1:M:479:LEU:HD13	1:M:516:GLU:HA	1.94	0.49
1:M:54:ALA:O	1:M:55:VAL:C	2.51	0.49
1:M:44:HIS:CD2	6:M:803:FAD:C8M	2.86	0.49
3:O:99:LYS:O	3:O:100:ASP:HB2	2.13	0.49
3:O:96:ILE:HD12	3:O:103:MET:CE	2.43	0.49
3:O:36:VAL:HG12	4:P:75:LEU:HD23	1.95	0.49
1:A:321:GLU:O	1:A:322:LYS:C	2.51	0.49
3:C:128:LEU:O	4:D:45:PRO:HG2	2.13	0.49
1:A:307:PRO:C	1:A:309:GLY:H	2.16	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
1:M:212:GLY:C	1:M:215:MET:HG2	2.33	0.48
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:H	1:M:465:ILE:HD13	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:NH1	1:A:184:ARG:HG2	2.28	0.48
1:A:448:TRP:CG	1:A:449:ALA:N	2.81	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: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
3:C:98:VAL:HG22	3:C:103:MET:HB3	1.96	0.48
1:M:63:GLU:O	1:M:64:TYR:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HH11	1:M:413:ARG:HB2	1.79	0.48
1:M:67:HIS:C	1:M:69:THR:N	2.66	0.48
1:M:136:LEU:O	1:M:136:LEU:HG	2.14	0.48
1:M:527:GLU:CG	1:M:528:SER:N	2.77	0.48
2:N:25:PHE:HD1	2:N:25:PHE:N	2.11	0.48
1:M:327:ARG:O	1:M:328:LEU:HD12	2.14	0.48
1:M:324:LEU:HG	1:M:344:VAL:HG12	1.95	0.48
1:M:525:ARG:O	1:M:534:ARG:HD2	2.14	0.48
1:M:81:VAL:C	1:M:83:ASP:H	2.17	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:153:ASP:O	1:M:155:HIS:ND1	2.46	0.47
1:M:508:LEU:HD12	1:M:508:LEU:O	2.14	0.47
1:M:9:ILE:CD1	1:M:19:ALA:CB	2.92	0.47
1:M:146:PHE:O	1:M:149:ILE:HD13	2.13	0.47
1:M:196:GLY:O	1:M:198:VAL:N	2.48	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
1:M:356:TYR:CE2	6:M:803:FAD:O3'	2.66	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
4:P:35:VAL:O	4:P:40:PRO:HD3	2.13	0.47
3:C:33:VAL:HG22	4:D:82:MET:HE1	1.95	0.47
1:M:18:ARG:HD2	1:M:18:ARG:O	2.14	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
1:M:63:GLU:OE1	1:M:66:PHE:HB3	2.14	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
1:M:288:ASP:O	1:M:289:LYS:C	2.51	0.47
1:M:564:GLU:C	1:M:565:TYR:CD1	2.88	0.47
2:N:37:LEU:HD11	2:N:55:TRP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HD13	1:A:344:VAL:CG2	2.43	0.47
3:O:65:ASN:CG	3:O:67:VAL:N	2.67	0.47
1:A:330:PHE:O	1:A:331:ILE:C	2.53	0.47
2:B:113:LEU:C	2:B:113:LEU:HD23	2.35	0.47
4:D:57:PHE:HB2	10:D:700:MQ7:H152	1.97	0.47
1:M:318:HIS:O	1:M:319:LEU:HD23	2.15	0.47
1:M:46:VAL:HA	1:M:133:PHE:CA	2.45	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:M:146:PHE:HA	1:M:147:PRO:HD2	1.76	0.47
1:M:27:ASN:CG	1:M:30:ALA:HB2	2.35	0.47
1:M:469:PRO:HG2	1:M:536:ASP:HB3	1.97	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:317:ARG:C	1:M:319:LEU:H	2.10	0.47
1:M:433:GLU:O	1:M:436:LEU:HB3	2.15	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:A:127:ALA:HB2	1:A:131:THR:HA	1.96	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:75:TRP:O	1:M:76:LEU:HB2	2.14	0.47
1:M:182:GLN:NE2	1:M:184:ARG:HH22	2.11	0.47
3:C:106:GLU:CD	3:C:106:GLU:H	2.17	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
1:M:449:ALA:C	1:M:451:ILE:N	2.66	0.46
4:P:72:VAL:HG12	4:P:76:TRP:CD1	2.50	0.46
1:M:60:ASP:CG	1:M:123:ARG:HE	2.19	0.46
1:M:198:VAL:HG23	1:M:199:TYR:N	2.30	0.46
1:M:452:ARG:C	1:M:454:GLU:H	2.19	0.46
1:M:95:GLN:C	1:M:97:GLU:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLY:O	1:A:277:PRO:HD3	2.16	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:310:ASP:C	1:M:311:VAL:HG12	2.35	0.46
1:M:52:SER:OG	1:M:397:ALA:N	2.49	0.46
4:P:86:MET:HE2	4:P:91:ILE:HG21	1.87	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:HG13	2:N:149:ILE:O	2.14	0.46
1:A:361:ILE:H	1:A:361:ILE:HG13	1.51	0.46
1:A:392:GLY:O	1:A:393:SER:OG	2.21	0.46
2:B:151:CYS:SG	2:B:153:LEU:HG	2.56	0.46
1:M:440:VAL:C	1:M:442:GLN:N	2.67	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
2:B:236:LEU:O	2:B:237:ILE:C	2.54	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:101:CYS:H	1:M:138:THR:CG2	2.29	0.46
1:M:45:THR:CB	1:M:136:LEU:HB2	2.42	0.46
1:M:364:ASP:OD2	1:M:368:GLU:N	2.49	0.46
1:M:82:VAL:HG13	1:M:385:LEU:HD12	1.97	0.46
1:M:483:GLN:HE21	1:M:512:LEU:HB3	1.81	0.46
1:M:555:ARG:O	1:M:556:ASP:C	2.54	0.46
4:D:9:ASP:HB3	11:D:810:CE1:H242	1.98	0.46
1:M:279:ASN:C	1:M:281:TYR:H	2.19	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
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:M:149:ILE:CD1	1:M:149:ILE:H	2.28	0.46
1:M:356:TYR:HB2	1:M:390:ARG:NH2	2.31	0.46
1:M:482:LEU:O	1:M:483:GLN:C	2.53	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

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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:51:GLY:C	1:M:396:LEU:HD12	2.37	0.45
1:M:429:ALA:HA	1:M:432:VAL:CG2	2.46	0.45
1:M:42:ARG:CG	1:M:42:ARG:NH1	2.78	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
2:N:11:VAL:HG23	2:N:91:GLU:CG	2.39	0.45
1:A:358:MET:CE	1:A:389:ASN:HA	2.47	0.45
2:B:155:TYR:CE2	2:B:169:GLY:HA3	2.51	0.45
2:B:37:LEU:HD22	2:B:77:CYS:HB3	1.98	0.45
4:D:30:VAL:O	4:D:33:LEU:HB3	2.17	0.45
1:M:364:ASP:OD2	1:M:364:ASP:N	2.50	0.45
1:M:117:GLY:HA3	1:M:392:GLY:HA3	1.97	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:118:GLY:HA2	1:A:279:ASN:HD21	1.81	0.45
1:A:97:GLU:CD	2:B:131:THR:HB	2.36	0.45
1:A:98:LEU:HD23	2:B:132:ASN:ND2	2.31	0.45
2:B:175:LEU:HA	2:B:175:LEU:HD12	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:356:TYR:CB	1:M:390:ARG:HH21	2.29	0.45
1:M:356:TYR:HE2	6:M:803:FAD:O3'	1.99	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: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:HH11	1:M:151:ARG:HB3	1.82	0.45
1:M:263:LEU:HD22	1:M:268:MET:CE	2.45	0.45
1:M:358:MET:HE3	1:M:388:ALA:O	2.16	0.45
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
1:M:78:GLU:HB3	1:M:81:VAL:HG23	1.98	0.45
2:N:159:PRO:HB3	3:O:15:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:329:PRO:O	1:M:330:PHE:C	2.55	0.45
1:M:521:SER:HA	1:M:563:LEU:HD23	1.98	0.45
1:M:204:ASN:ND2	6:M:803:FAD:HM83	2.30	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:H	2:N:81:LEU:HD12	1.82	0.45
4:D:68:PHE:CD1	4:D:111:THR:HG22	2.49	0.45
1:M:161:LEU:HD21	1:M:171:VAL:HG23	1.98	0.45
1:M:88:HIS:O	1:M:401:VAL:HG13	2.17	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: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:A:76:LEU:HA	1:A:76:LEU:HD23	1.78	0.45
1:M:168:ARG:O	1:M:185:ALA:O	2.35	0.45
2:N:219:ASP:N	2:N:220:PRO:CD	2.80	0.45
2:N:55:TRP:CZ3	2:N:58:ARG:HD3	2.52	0.45
1:M:2:THR:HA	1:M:182:GLN:O	2.17	0.44
1:M:311:VAL:HG23	1:M:350:VAL:N	2.32	0.44
1:M:539:CYS:C	1:M:541:GLU:H	2.19	0.44
4:P:96:GLY:O	4:P:97:LYS:C	2.55	0.44
1:M:127:ALA:C	1:M:128:ALA:O	2.54	0.44
1:M:173:MET:CE	1:M:178:GLY:HA2	2.46	0.44
1:M:253:ILE:HA	1:M:283:GLU:HG2	1.99	0.44
1:M:89:CYS:SG	1:M:401:VAL:HG21	2.57	0.44
1:M:227:GLU:HB2	1:M:522:ALA:HB2	1.99	0.44
1:M:7:LEU:HD23	1:M:7:LEU:N	2.32	0.44
1:M:89:CYS:H	1:M:90:PRO:HD2	1.83	0.44
3:C:29:GLU:OE1	4:D:81:ARG:HG2	2.17	0.44
1:M:398:GLU:O	1:M:402:PHE:HB2	2.17	0.44
1:M:69:THR:HG22	1:M:70:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:M:416:THR:O	1:M:417:ALA:C	2.55	0.44
1:M:63:GLU:HA	1:M:63:GLU:OE1	2.17	0.44
1:M:500:THR:HG1	2:N:44:LYS:NZ	2.04	0.44
3:O:47:PHE:HE2	4:P:114:GLY:CA	2.30	0.44
3:O:65:ASN:CG	3:O:68:ILE:H	2.20	0.44
1:A:307:PRO:C	1:A:309:GLY:N	2.69	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:294:PHE:CD2	1:M:294:PHE:C	2.90	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
4:P:79:LEU:HD23	4:P:82:MET:CE	2.47	0.44
1:M:268:MET:HE1	1:M:290:VAL:N	2.33	0.44
1:M:334:LEU:HD23	1:M:338:TYR:CE1	2.52	0.44
2:N:216:LYS:HG3	2:N:216:LYS:O	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
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: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
4:P:57:PHE:CB	10:P:800:MQ7:H152	2.33	0.44
1:M:221:VAL:CG2	1:M:369:THR:HB	2.48	0.44
1:M:199:TYR:CE2	1:M:459:MET:HB3	2.53	0.44
1:A:425:ILE:O	1:A:428:GLN:HB2	2.17	0.44
1:M:174:ASN:HB3	1:M:177:GLU:HB2	2.00	0.44
1:M:152:PHE:HZ	1:M:181:VAL:HG11	1.82	0.44
1:M:242:LEU:HD22	1:M:242:LEU:C	2.38	0.44
1:M:311:VAL:HG23	1:M:350:VAL:H	1.83	0.44
1:M:473:GLN:O	1:M:475:THR:N	2.51	0.44
10:N:801:MQ7:H2M2	3:O:28:ARG:HH11	1.77	0.44
3:O:96:ILE:HD12	3:O:103:MET:HE2	2.00	0.44
1:A:9:ILE:HD13	1:A:19:ALA:HB3	1.99	0.43
1:M:12:ALA:HA	1:M:17:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:38:VAL:O	1:M:39:TYR:O	2.36	0.43
1:M:413:ARG:CB	1:M:413:ARG:HH11	2.31	0.43
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.83	0.43
1:M:37:LYS:NZ	1:M:507:GLU:CD	2.71	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:321:GLU:HG3	1:M:325:HIS:HD2	1.83	0.43
1:M:18:ARG:NH2	1:M:404:ARG:HB2	2.34	0.43
1:M:452:ARG:HH12	2:N:45:ASP:CG	2.21	0.43
1:M:469:PRO:CG	1:M:536:ASP:OD2	2.65	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:N	1:M:256:ASN:HD22	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
1:M:177:GLU:CD	3:O:2:THR:OG1	2.55	0.43
3:O:65:ASN:C	3:O:65:ASN:ND2	2.59	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:556:ASP:HB3	1:M:558:ASP:CG	2.38	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
1:M:449:ALA:C	1:M:451:ILE:H	2.20	0.43
1:M:493:ASP:CG	2:N:50:ASP:HA	2.23	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:89:CYS:HA	1:M:401:VAL:CG2	2.48	0.43
1:M:84:TYR:CE2	1:M:88:HIS:CG	3.06	0.43
2:N:220:PRO:O	2:N:221:ALA:C	2.56	0.43
2:B:228:LYS:HZ3	10:B:701:MQ7:H6	1.84	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:195:ALA:O	1:M:196:GLY:C	2.57	0.43
1:M:500:THR:C	1:M:502:LEU:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:53:ALA:HB2	1:M:393:SER:OG	2.19	0.43
1:M:93:MET:HB3	1:M:125:TRP:CH2	2.53	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:C:125:PHE:CD1	3:C:129:TYR:CG	3.06	0.43
1:M:190:MET:HE1	1:M:215:MET:SD	2.59	0.43
1:M:237:PRO:HB2	1:M:308:ARG:CB	2.48	0.43
1:M:62:PHE:CD2	1:M:87:HIS:ND1	2.86	0.43
2:N:35:SER:O	2:N:38:ASP:HB2	2.18	0.43
2:B:206:PHE:CE1	2:B:225:GLN:HG3	2.54	0.43
2:B:63:GLY:N	7:B:244:FES:S1	2.84	0.43
1:M:182:GLN:C	1:M:183:ILE:HD12	2.39	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:86:MET:HE3	4:P:91:ILE:CD1	2.49	0.43
4:P:91:ILE:HG22	4:P:93:VAL:HG23	2.01	0.43
1:A:44:HIS:CD2	6:A:703:FAD:HM81	2.51	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:14:GLY:HA3	1:M:399:LEU:HD13	2.01	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:108:THR:O	4:D:111:THR:HB	2.19	0.42
1:M:248:ARG:O	1:M:251:GLY:N	2.49	0.42
1:M:469:PRO:HG3	1:M:534:ARG:NH2	2.33	0.42
1:M:467:ARG:NH1	1:M:531:ALA:O	2.46	0.42
1:M:156:PHE:HE2	6:M:803:FAD:H62A	1.63	0.42
1:M:88:HIS:HB2	1:M:401:VAL:HG11	1.99	0.42
4:D:93:VAL:N	2:N:243:ARG:O	2.51	0.42
4:P:7:ARG:CB	4:P:7:ARG:HH11	2.31	0.42
1:A:454:GLU:CD	1:A:485:ARG:HH22	2.23	0.42
2:B:241:LYS:O	2:B:241:LYS:CG	2.61	0.42
1:M:392:GLY:O	1:M:393:SER:OG	2.35	0.42
2:N:226:GLN:HE21	2:N:226:GLN:HB2	1.57	0.42
2:N:54:ARG:HB3	2:N:64:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:O	1:A:247:CYS:C	2.58	0.42
1:M:367:CYS:HB3	1:M:376:ALA:O	2.20	0.42
1:M:76:LEU:HA	1:M:76:LEU:HD22	1.87	0.42
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:155:HIS:HA	1:M:173:MET:O	2.19	0.42
1:M:322:LYS:HG3	1:M:322:LYS:O	2.19	0.42
1:M:130:LYS:HZ1	2:N:216:LYS:HD2	1.81	0.42
3:O:65:ASN:OD1	3:O:68:ILE:N	2.51	0.42
1:A:514:VAL:HG12	1:A:518:MET:CE	2.50	0.42
4:D:72:VAL:O	4:D:75:LEU:HB2	2.20	0.42
1:M:139:LEU:O	1:M:140:PHE:C	2.57	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
1:M:77:CYS:HA	1:M:550:HIS:CE1	2.52	0.42
1:M:48:ALA:HA	6:M:803:FAD:C5X	2.50	0.42
1:M:130:LYS:HZ3	2:N:216:LYS:HD2	1.84	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: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
1:M:507:GLU:O	1:M:508:LEU:C	2.57	0.42
1:M:62:PHE:O	1:M:86:VAL:HG21	2.19	0.42
1:M:50:GLY:N	6:M:803:FAD:O4	2.52	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:254:LEU:HD13	1:M:262:TYR:OH	2.20	0.42
1:M:186:ASN:O	1:M:414:ALA:CB	2.68	0.42
1:M:534:ARG:O	1:M:540:THR:HG22	2.19	0.42
4:P:28:ALA:N	4:P:29:PRO:HD2	2.35	0.42
3:O:128:LEU:HD22	4:P:44:PHE:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HD2	1:A:283:GLU:O	2.20	0.42
1:M:15:ALA:CA	1:M:399:LEU:HB3	2.49	0.42
1:M:456:GLY:C	1:M:458:ALA:N	2.74	0.42
1:M:465:ILE:H	1:M:465:ILE:CD1	2.28	0.42
1:M:570:ILE:CG2	1:M:571:THR:H	2.31	0.42
3:O:91:PRO:HB3	3:O:108:ILE:HG21	2.02	0.42
3:O:56:TRP:O	3:O:59:PHE:HB3	2.20	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:M:87:HIS:C	1:M:89:CYS:H	2.23	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
1:M:93:MET:HE2	1:M:103:TRP:HZ2	1.85	0.41
1:M:131:THR:O	1:M:132:GLY:O	2.38	0.41
1:M:83:ASP:O	1:M:84:TYR:C	2.58	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
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.52	0.41
1:A:10:VAL:HG13	1:A:157:VAL:HG21	2.02	0.41
2:B:192:MET:O	2:B:193:ALA:C	2.59	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
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: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:182:GLN:CB	1:M:184:ARG:HH12	2.33	0.41
1:M:436:LEU:O	1:M:440:VAL:HG23	2.20	0.41
1:M:65:HIS:CD2	1:M:123:ARG:NH1	2.88	0.41
3:O:91:PRO:HB3	3:O:108:ILE:CG2	2.50	0.41
1:A:358:MET:HE3	1:A:389:ASN:HA	2.03	0.41
2:B:117:LYS:O	2:B:119:TYR:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:159:ASP:CG	1:M:160:ILE:N	2.72	0.41
1:M:335:ALA:O	1:M:339:VAL:HG22	2.20	0.41
1:M:471:LEU:O	1:M:472:MET:C	2.56	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:324:LEU:HD11	1:M:343:PRO:HB2	2.01	0.41
1:M:405:LEU:C	1:M:407:GLY:N	2.74	0.41
1:M:437:LYS:O	1:M:441:ASN:N	2.47	0.41
1:M:65:HIS:CD2	1:M:123:ARG:HH11	2.38	0.41
2:N:81:LEU:CD1	2:N:81:LEU:N	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
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
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
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
1:M:361:ILE:O	1:M:362:GLU:C	2.59	0.41
1:M:396:LEU:O	1:M:399:LEU:N	2.53	0.41
3:O:87:PHE:CD2	3:O:112:LEU:HD13	2.56	0.41
4:P:30:VAL:HG13	4:P:31:MET:N	2.35	0.41
1:A:27:ASN:OD1	1:A:27:ASN:C	2.59	0.41
1:M:127:ALA:N	1:M:131:THR:OG1	2.38	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
3:O:66:PRO:HA	3:O:69:VAL:HG23	2.02	0.41
1:A:16:GLY:O	1:A:19:ALA:HB3	2.20	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
1:A:156:PHE:CD1	1:A:503:LEU:HD22	2.55	0.41
3:C:15:TRP:CD2	3:C:16:TRP:N	2.89	0.41
1:M:246:GLY:O	1:M:247:CYS:C	2.60	0.41
1:M:396:LEU:O	1:M:398:GLU:N	2.54	0.41
1:M:550:HIS:CD2	1:M:568:VAL:HG22	2.55	0.41
1:M:70:VAL:O	1:M:73:GLY:N	2.51	0.41
2:N:158:CYS:HA	2:N:159:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LEU:O	1:A:442:GLN:HB3	2.21	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: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
1:M:60:ASP:OD1	1:M:61:SER:N	2.53	0.41
2:N:71:ASN:ND2	3:O:18:LYS:HD3	2.36	0.41
2:N:8:ILE:HD11	2:N:81:LEU:CD2	2.48	0.41
3:O:74:ILE:O	3:O:75:THR:C	2.59	0.41
1:A:330:PHE:O	1:A:333:GLU:HB2	2.22	0.40
1:M:195:ALA:HA	1:M:208:VAL:O	2.22	0.40
1:M:195:ALA:O	1:M:198:VAL:HG22	2.21	0.40
1:M:26:ALA:C	1:M:28:PRO:HD3	2.41	0.40
1:M:460:GLU:O	1:M:461:GLU:C	2.59	0.40
1:M:85:PHE:O	1:M:86:VAL:C	2.59	0.40
1:A:239:SER:HB2	1:A:241:ILE:HG13	2.02	0.40
1:A:331:ILE:HA	1:A:331:ILE:HD13	1.80	0.40
2:B:220:PRO:O	2:B:221:ALA:C	2.58	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:51:GLY:HA2	1:M:131:THR:HG21	2.04	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
1:M:58:ASP:C	1:M:60:ASP:H	2.25	0.40
1:M:46:VAL:CG2	2:N:61:ILE:HG13	2.42	0.40
2:N:97:PRO:HG2	2:N:105:ASP:CB	2.51	0.40
1:A:324:LEU:HB3	1:A:344:VAL:HG22	2.02	0.40
2:B:204:CYS:O	2:B:228:LYS:NZ	2.52	0.40
3:C:36:VAL:O	3:C:39:SER:N	2.54	0.40
4:D:31:MET:HE2	4:D:31:MET:HB3	1.85	0.40
2:N:54:ARG:NE	2:N:103:VAL:HG13	2.19	0.40
4:P:64:ARG:HB3	4:P:115:VAL:CG2	2.51	0.40
1:A:552:LEU:HA	1:A:552:LEU:HD23	1.84	0.40
2:B:72:VAL:O	2:B:74:LYS:HG3	2.21	0.40
3:C:50:LYS:HB3	4:D:118:ILE:CG2	2.51	0.40
4:D:30:VAL:HG13	4:D:31:MET:N	2.37	0.40
3:C:128:LEU:O	4:D:45:PRO:CG	2.69	0.40
1:M:167:VAL:O	1:M:167:VAL:HG13	2.21	0.40
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:50:LYS:HZ2	4:P:117:THR:CB	2.35	0.40
4:P:57:PHE:HB2	10:P:800:MQ7:C15	2.34	0.40
1:A:274:LEU:HA	1:A:274:LEU:HD23	1.81	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
2:B:236:LEU:HA	2:B:236:LEU:HD12	1.89	0.40
1:M:322:LYS:HZ2	1:M:326:GLU:HG3	1.87	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:479:LEU:CD1	1:M:516:GLU:HA	2.51	0.40
1:M:539:CYS:C	1:M:541:GLU:N	2.75	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
3:O:65:ASN:CG	3:O:67:VAL:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/602 (96%)	529 (92%)	37 (6%)	9 (2%)	9	36
1	M	575/602 (96%)	355 (62%)	153 (27%)	67 (12%)	0	2
2	B	241/243 (99%)	215 (89%)	22 (9%)	4 (2%)	9	35
2	N	241/243 (99%)	205 (85%)	34 (14%)	2 (1%)	19	51
3	C	128/130 (98%)	121 (94%)	5 (4%)	2 (2%)	9	36
3	O	128/130 (98%)	113 (88%)	12 (9%)	3 (2%)	6	29
4	D	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	5	27
4	P	117/119 (98%)	99 (85%)	12 (10%)	6 (5%)	2	13
All	All	2122/2188 (97%)	1738 (82%)	288 (14%)	96 (4%)	2	15

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	448 (97%)	12 (3%)	46	71
1	M	460/475 (97%)	400 (87%)	60 (13%)	4	17
2	B	205/205 (100%)	197 (96%)	8 (4%)	32	62
2	N	205/205 (100%)	191 (93%)	14 (7%)	16	44
3	C	111/111 (100%)	104 (94%)	7 (6%)	18	47
3	O	111/111 (100%)	103 (93%)	8 (7%)	14	41
4	D	97/97 (100%)	94 (97%)	3 (3%)	40	67
4	P	97/97 (100%)	93 (96%)	4 (4%)	30	61
All	All	1746/1776 (98%)	1630 (93%)	116 (7%)	16	46

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	A	93	MET
1	A	197	ARG

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Mol	Chain	Res	Type
1	A	200	ARG
1	A	207	ILE
1	A	276	GLU
1	A	287	ARG
1	A	305	SER
1	A	330	PHE
1	A	332	CYS
1	A	351	ARG
1	A	443	ASP
2	B	65	CYS
2	B	81	LEU
2	B	128	ASP
2	B	178	ARG
2	B	203	SER
2	B	206	PHE
2	B	212	GLU
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
4	D	86	MET
4	D	117	THR
4	D	118	ILE
1	M	0	MET
1	M	4	GLN
1	M	32	ILE
1	M	35	ILE
1	M	62	PHE
1	M	64	TYR
1	M	76	LEU
1	M	77	CYS
1	M	84	TYR
1	M	89	CYS
1	M	96	LEU
1	M	108	ASP
1	M	113	VAL
1	M	116	PHE
1	M	122	GLU

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Mol	Chain	Res	Type
1	M	126	PHE
1	M	133	PHE
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	174	ASN
1	M	197	ARG
1	M	203	THR
1	M	225	ASP
1	M	242	LEU
1	M	243	MET
1	M	244	THR
1	M	256	ASN
1	M	274	LEU
1	M	308	ARG
1	M	311	VAL
1	M	312	VAL
1	M	321	GLU
1	M	324	LEU
1	M	326	GLU
1	M	330	PHE
1	M	348	ILE
1	M	363	THR
1	M	370	ARG
1	M	399	LEU
1	M	413	ARG
1	M	435	ARG
1	M	438	ASP
1	M	457	LEU
1	M	465	ILE
1	M	470	GLU
1	M	493	ASP
1	M	497	VAL
1	M	504	TYR
1	M	508	LEU
1	M	527	GLU
1	M	528	SER
1	M	537	GLU

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Mol	Chain	Res	Type
1	M	554	PHE
1	M	558	ASP
1	M	563	LEU
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	178	ARG
2	N	185	ASP
2	N	188	LYS
2	N	189	LYS
2	N	206	PHE
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	37	TRP
3	O	39	SER
3	O	61	ASP
3	O	65	ASN
3	O	84	LYS
4	P	5	PRO
4	P	17	PHE
4	P	77	CYS
4	P	118	ILE

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

Mol	Chain	Res	Type
1	A	57	GLN
1	A	59	HIS
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

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Mol	Chain	Res	Type
1	A	434	GLN
1	A	442	GLN
2	B	134	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
1	M	4	GLN
1	M	65	HIS
1	M	137	HIS
1	M	145	GLN
1	M	148	GLN
1	M	174	ASN
1	M	182	GLN
1	M	204	ASN
1	M	230	GLN
1	M	256	ASN
1	M	264	GLN
1	M	279	ASN
1	M	292	GLN
1	M	296	HIS
1	M	325	HIS
1	M	366	ASN
1	M	394	ASN
1	M	409	GLN
1	M	434	GLN
1	M	441	ASN
1	M	442	GLN
2	N	70	ASN
2	N	71	ASN
2	N	95	ASN
2	N	108	HIS
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

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 carbohydrates 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	$\# Z > 2$
8	F3S	N	245	2	0,9,9	0.00	-	-		
6	FAD	A	703	1	51,58,58	1.85	16 (31%)	60,89,89	1.90	14 (23%)
11	CE1	D	810	-	36,36,36	1.10	0	35,35,35	1.70	15 (42%)
5	OAA	M	802	-	2,8,8	1.77	1 (50%)	2,10,10	1.98	1 (50%)
11	CE1	O	812	-	36,36,36	1.12	0	35,35,35	1.57	7 (20%)
8	F3S	B	245	2	0,9,9	0.00	-	-		
10	MQ7	N	801	-	25,25,49	3.47	6 (24%)	31,34,63	2.48	9 (29%)
9	SF4	N	246	2	0,12,12	0.00	-	-		
11	CE1	D	710	-	36,36,36	1.00	0	35,35,35	1.67	14 (40%)
9	SF4	B	246	2	0,12,12	0.00	-	-		
10	MQ7	P	800	-	25,25,49	3.23	5 (20%)	31,34,63	2.31	11 (35%)
7	FES	B	244	2	0,4,4	0.00	-	-		
5	OAA	A	702	-	2,8,8	2.08	1 (50%)	2,10,10	0.97	0
7	FES	N	244	2	0,4,4	0.00	-	-		
11	CE1	O	811	-	36,36,36	1.23	4 (11%)	35,35,35	1.82	13 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MQ7	D	700	-	25,25,49	3.29	5 (20%)	31,34,63	2.32	10 (32%)
6	FAD	M	803	1	51,58,58	1.80	13 (25%)	60,89,89	1.76	9 (15%)
10	MQ7	B	701	-	25,25,49	3.27	6 (24%)	31,34,63	2.32	8 (25%)

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
8	F3S	N	245	2	-	-	0/3/3/3
11	CE1	O	811	-	-	15/34/34/34	-
11	CE1	D	810	-	-	16/34/34/34	-
5	OAA	M	802	-	-	2/2/8/8	-
9	SF4	B	246	2	-	-	0/6/5/5
8	F3S	B	245	2	-	-	0/3/3/3
10	MQ7	N	801	-	-	3/13/33/61	0/2/2/2
9	SF4	N	246	2	-	-	0/6/5/5
11	CE1	D	710	-	-	16/34/34/34	-
11	CE1	O	812	-	-	18/34/34/34	-
10	MQ7	P	800	-	-	1/13/33/61	0/2/2/2
7	FES	B	244	2	-	-	0/1/1/1
5	OAA	A	702	-	-	2/2/8/8	-
7	FES	N	244	2	-	-	0/1/1/1
6	FAD	A	703	1	-	8/30/50/50	0/6/6/6
10	MQ7	D	700	-	-	2/13/33/61	0/2/2/2
6	FAD	M	803	1	-	10/30/50/50	0/6/6/6
10	MQ7	B	701	-	-	3/13/33/61	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	801	MQ7	C11-C12	-11.95	1.33	1.50
10	D	700	MQ7	C11-C12	-11.04	1.34	1.50
10	P	800	MQ7	C11-C12	-10.87	1.34	1.50
10	B	701	MQ7	C11-C12	-10.24	1.35	1.50
10	N	801	MQ7	C12-C13	9.78	1.56	1.33
10	B	701	MQ7	C12-C13	9.60	1.56	1.33
10	D	700	MQ7	C12-C13	8.96	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	800	MQ7	C12-C13	8.73	1.53	1.33
6	M	803	FAD	C9A-N10	5.74	1.46	1.38
10	P	800	MQ7	C14-C13	-5.36	1.36	1.50
10	B	701	MQ7	C14-C13	-5.34	1.37	1.50
10	N	801	MQ7	C14-C13	-5.25	1.37	1.50
10	D	700	MQ7	C14-C13	-5.14	1.37	1.50
6	M	803	FAD	C4-N3	4.81	1.41	1.33
6	A	703	FAD	C4-N3	4.20	1.40	1.33
6	A	703	FAD	C9A-N10	3.76	1.43	1.38
6	A	703	FAD	C4X-N5	3.49	1.38	1.33
10	P	800	MQ7	C7-C6	3.49	1.46	1.38
6	A	703	FAD	C2-N1	-3.46	1.31	1.38
6	A	703	FAD	C4A-N3A	3.44	1.40	1.35
10	D	700	MQ7	C7-C6	3.38	1.46	1.38
6	A	703	FAD	C2B-C1B	-3.37	1.48	1.53
6	A	703	FAD	C9A-C5X	3.28	1.49	1.42
10	B	701	MQ7	C7-C6	3.18	1.45	1.38
6	M	803	FAD	C5'-C4'	3.10	1.56	1.51
6	M	803	FAD	C1'-N10	3.07	1.51	1.48
10	B	701	MQ7	C2-C1	2.92	1.54	1.48
6	M	803	FAD	O4B-C1B	2.83	1.45	1.41
6	A	703	FAD	O4B-C1B	2.82	1.45	1.41
6	M	803	FAD	C4X-N5	2.80	1.37	1.33
5	A	702	OAA	C2-C3	2.78	1.54	1.51
6	A	703	FAD	C6-C5X	-2.75	1.37	1.41
6	A	703	FAD	C2'-C3'	-2.69	1.48	1.53
6	M	803	FAD	C2-N3	2.68	1.43	1.38
10	P	800	MQ7	C2-C1	2.60	1.53	1.48
6	M	803	FAD	C6-C5X	-2.52	1.37	1.41
6	M	803	FAD	C4A-N3A	2.48	1.39	1.35
10	N	801	MQ7	C7-C6	2.45	1.44	1.38
6	A	703	FAD	C4X-C10	2.42	1.41	1.38
6	A	703	FAD	P-O5'	-2.39	1.49	1.59
10	N	801	MQ7	C5-C4	2.34	1.52	1.48
6	A	703	FAD	C2-N3	2.31	1.42	1.38
11	O	811	CE1	C24-C23	2.27	1.60	1.49
6	M	803	FAD	C4'-C3'	2.26	1.57	1.53
5	M	802	OAA	C2-C3	2.24	1.53	1.51
10	D	700	MQ7	C17-C18	2.21	1.38	1.33
6	M	803	FAD	C9A-C5X	2.16	1.46	1.42
11	O	811	CE1	C21-C20	2.15	1.60	1.49
6	A	703	FAD	C5X-N5	2.14	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	801	MQ7	C3-C4	2.13	1.52	1.47
10	B	701	MQ7	O4-C4	2.11	1.27	1.23
6	A	703	FAD	C5A-N7A	-2.10	1.32	1.39
6	M	803	FAD	C2A-N3A	2.09	1.35	1.32
11	O	811	CE1	O13-C12	2.09	1.51	1.42
11	O	811	CE1	O22-C21	2.07	1.51	1.42
6	M	803	FAD	C8M-C8	2.07	1.55	1.51
6	A	703	FAD	O4B-C4B	-2.00	1.40	1.45

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	801	MQ7	C11-C3-C4	-7.64	110.33	118.50
10	D	700	MQ7	C11-C3-C4	-7.39	110.59	118.50
10	B	701	MQ7	C11-C3-C4	-7.37	110.61	118.50
6	M	803	FAD	C4X-N5-C5X	7.18	123.94	116.77
10	P	800	MQ7	C11-C3-C4	-7.02	110.99	118.50
6	A	703	FAD	C4X-N5-C5X	6.41	123.18	116.77
10	P	800	MQ7	C12-C11-C3	6.17	128.69	112.05
6	A	703	FAD	N3A-C2A-N1A	-6.01	119.29	128.68
10	N	801	MQ7	C12-C11-C3	5.82	127.73	112.05
10	D	700	MQ7	C12-C11-C3	5.58	127.08	112.05
6	M	803	FAD	C4-N3-C2	5.50	119.79	115.14
10	B	701	MQ7	C12-C11-C3	5.49	126.84	112.05
6	M	803	FAD	N3A-C2A-N1A	-5.01	120.84	128.68
6	A	703	FAD	C4-N3-C2	4.66	119.08	115.14
10	N	801	MQ7	C2M-C2-C1	-4.31	109.13	116.27
10	B	701	MQ7	O1-C1-C10	-4.28	114.64	121.56
10	N	801	MQ7	O1-C1-C10	-3.94	115.19	121.56
10	D	700	MQ7	O1-C1-C10	-3.92	115.22	121.56
6	A	703	FAD	C4-C4X-C10	-3.87	117.39	119.95
10	P	800	MQ7	O1-C1-C10	-3.68	115.60	121.56
11	O	811	CE1	O31-C30-C29	3.54	126.36	110.39
6	A	703	FAD	C5'-C4'-C3'	3.51	118.99	112.20
10	B	701	MQ7	C11-C12-C13	3.51	132.63	126.79
6	M	803	FAD	C4X-C4-N3	-3.50	118.65	123.43
11	O	811	CE1	O13-C12-C11	3.44	128.34	110.26
10	B	701	MQ7	O1-C1-C2	3.32	124.57	120.25
10	N	801	MQ7	O1-C1-C2	3.30	124.54	120.25
10	N	801	MQ7	C11-C12-C13	3.25	132.21	126.79
11	O	811	CE1	O19-C18-C17	3.21	124.89	110.39
11	O	812	CE1	O34-C35-C36	3.12	123.77	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	811	CE1	O22-C23-C24	3.11	124.43	110.39
6	A	703	FAD	C4X-C4-N3	-3.11	119.18	123.43
6	A	703	FAD	C4-C4X-N5	3.05	122.09	118.60
10	N	801	MQ7	C2M-C2-C3	3.03	129.34	124.40
10	N	801	MQ7	C9-C10-C5	2.97	122.56	119.26
10	P	800	MQ7	C2M-C2-C1	-2.96	111.37	116.27
11	O	812	CE1	O22-C21-C20	2.92	123.55	110.39
11	O	811	CE1	O16-C17-C18	2.87	123.34	110.39
10	D	700	MQ7	C11-C12-C13	2.86	131.56	126.79
11	O	812	CE1	O19-C18-C17	2.85	123.26	110.39
11	O	812	CE1	O16-C17-C18	2.85	123.25	110.39
6	A	703	FAD	C7-C6-C5X	-2.84	117.20	121.22
6	A	703	FAD	C1'-N10-C10	2.72	120.85	118.41
5	M	802	OAA	C1-C2-C3	2.72	120.35	115.51
11	O	811	CE1	O19-C20-C21	2.72	122.64	110.39
11	O	812	CE1	O34-C33-C32	2.69	122.50	110.39
10	D	700	MQ7	C2M-C2-C1	-2.64	111.89	116.27
10	B	701	MQ7	C2M-C2-C1	-2.61	111.94	116.27
11	O	811	CE1	O16-C15-C14	2.60	122.14	110.39
10	N	801	MQ7	C19-C18-C20	2.58	118.94	115.98
11	O	811	CE1	O28-C27-C26	2.57	121.97	110.39
11	D	810	CE1	O34-C35-C36	2.57	121.35	110.07
11	D	810	CE1	O25-C24-C23	2.53	121.81	110.39
11	D	710	CE1	O13-C14-C15	2.52	121.77	110.39
10	P	800	MQ7	C11-C12-C13	2.49	130.93	126.79
11	D	810	CE1	O16-C15-C14	2.48	121.59	110.39
11	O	811	CE1	O34-C33-C32	2.45	121.45	110.39
10	B	701	MQ7	C19-C18-C20	2.42	118.75	115.98
6	M	803	FAD	C6-C5X-C9A	2.41	122.21	119.05
11	D	810	CE1	O19-C18-C17	2.39	121.19	110.39
6	M	803	FAD	C5'-C4'-C3'	2.39	116.82	112.20
10	D	700	MQ7	C14-C13-C15	2.39	119.29	115.27
11	D	810	CE1	O19-C20-C21	2.38	121.14	110.39
6	A	703	FAD	C4'-C3'-C2'	-2.37	108.43	113.36
11	D	710	CE1	O31-C30-C29	2.37	121.08	110.39
10	B	701	MQ7	C9-C10-C5	2.36	121.89	119.26
11	D	710	CE1	O22-C21-C20	2.36	121.03	110.39
11	D	810	CE1	O13-C14-C15	2.34	120.95	110.39
10	D	700	MQ7	C9-C10-C5	2.34	121.86	119.26
10	D	700	MQ7	O1-C1-C2	2.33	123.28	120.25
11	D	810	CE1	O31-C32-C33	2.32	120.86	110.39
10	P	800	MQ7	O1-C1-C2	2.32	123.27	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	803	FAD	C1'-N10-C10	2.32	120.48	118.41
6	A	703	FAD	C9A-C5X-N5	-2.32	118.74	122.36
11	O	811	CE1	O25-C26-C27	2.31	120.82	110.39
11	D	710	CE1	O19-C20-C21	2.30	120.79	110.39
11	D	710	CE1	O16-C17-C18	2.30	120.78	110.39
11	D	810	CE1	O28-C29-C30	2.29	120.73	110.39
10	D	700	MQ7	C5-C10-C1	-2.29	118.20	120.68
11	D	710	CE1	O31-C32-C33	2.29	120.73	110.39
10	P	800	MQ7	C5-C10-C1	-2.28	118.21	120.68
11	D	710	CE1	O28-C29-C30	2.28	120.67	110.39
11	D	810	CE1	O22-C21-C20	2.27	120.64	110.39
11	D	710	CE1	O28-C27-C26	2.27	120.63	110.39
11	D	710	CE1	O16-C15-C14	2.27	120.62	110.39
11	D	810	CE1	O28-C27-C26	2.25	120.56	110.39
6	A	703	FAD	C7M-C7-C6	-2.25	114.97	120.34
11	D	710	CE1	O34-C35-C36	2.25	119.94	110.07
11	D	710	CE1	O22-C23-C24	2.24	120.51	110.39
11	O	811	CE1	O31-C32-C33	2.24	120.50	110.39
11	D	810	CE1	O31-C30-C29	2.21	120.36	110.39
11	D	810	CE1	O25-C26-C27	2.20	120.30	110.39
11	O	811	CE1	O22-C21-C20	2.19	120.28	110.39
10	P	800	MQ7	C9-C10-C5	2.19	121.69	119.26
11	D	710	CE1	O25-C24-C23	2.19	120.26	110.39
11	D	810	CE1	O22-C23-C24	2.17	120.20	110.39
6	M	803	FAD	C9A-C5X-N5	-2.17	118.97	122.36
6	A	703	FAD	O4'-C4'-C5'	-2.16	105.06	109.92
11	D	810	CE1	O16-C17-C18	2.16	120.14	110.39
10	P	800	MQ7	C14-C13-C15	2.15	118.89	115.27
11	O	811	CE1	O13-C14-C15	2.15	120.07	110.39
10	D	700	MQ7	O4-C4-C3	-2.12	117.15	120.56
11	D	710	CE1	O25-C26-C27	2.12	119.93	110.39
6	M	803	FAD	C7M-C7-C6	-2.09	115.35	120.34
10	P	800	MQ7	C2M-C2-C3	2.07	127.78	124.40
6	A	703	FAD	O4'-C4'-C3'	-2.07	104.08	109.10
10	P	800	MQ7	O4-C4-C3	-2.06	117.24	120.56
11	O	812	CE1	O31-C30-C29	2.06	119.69	110.39
11	D	710	CE1	O19-C18-C17	2.03	119.53	110.39
11	O	812	CE1	O19-C20-C21	2.02	119.51	110.39
11	D	810	CE1	O13-C12-C11	2.01	120.81	110.26

There are no chirality outliers.

All (96) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
10	N	801	MQ7	C14-C13-C15-C16
10	B	701	MQ7	C14-C13-C15-C16
10	N	801	MQ7	C12-C13-C15-C16
10	B	701	MQ7	C12-C13-C15-C16
11	D	810	CE1	C36-C35-O34-C33
11	O	812	CE1	C24-C23-O22-C21
11	O	812	CE1	C14-C15-O16-C17
11	O	812	CE1	C2-C3-C4-C5
11	D	710	CE1	C11-C12-O13-C14
11	O	811	CE1	C33-C32-O31-C30
6	A	703	FAD	C5'-O5'-P-O3P
6	M	803	FAD	C5'-O5'-P-O3P
11	O	811	CE1	C7-C8-C9-C10
11	D	710	CE1	C30-C29-O28-C27
11	O	811	CE1	O28-C29-C30-O31
6	A	703	FAD	C5'-O5'-P-O1P
6	M	803	FAD	C5'-O5'-P-O2P
11	D	710	CE1	C36-C35-O34-C33
11	D	810	CE1	C33-C32-O31-C30
10	D	700	MQ7	C17-C18-C20-C21
11	O	811	CE1	C4-C5-C6-C7
11	O	811	CE1	C29-C30-O31-C32
11	D	710	CE1	C11-C10-C9-C8
11	D	810	CE1	C11-C12-O13-C14
11	O	812	CE1	O31-C32-C33-O34
11	D	810	CE1	C1-C2-C3-C4
11	O	811	CE1	C36-C35-O34-C33
11	D	710	CE1	C24-C23-O22-C21
11	O	812	CE1	C7-C8-C9-C10
6	M	803	FAD	O4B-C4B-C5B-O5B
11	O	812	CE1	C32-C33-O34-C35
11	O	811	CE1	O19-C20-C21-O22
10	P	800	MQ7	C19-C18-C20-C21
11	O	812	CE1	C4-C5-C6-C7
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	812	CE1	C21-C20-O19-C18
11	D	710	CE1	O31-C32-C33-O34
11	D	810	CE1	O31-C32-C33-O34
11	O	812	CE1	O19-C20-C21-O22
11	D	810	CE1	C32-C33-O34-C35

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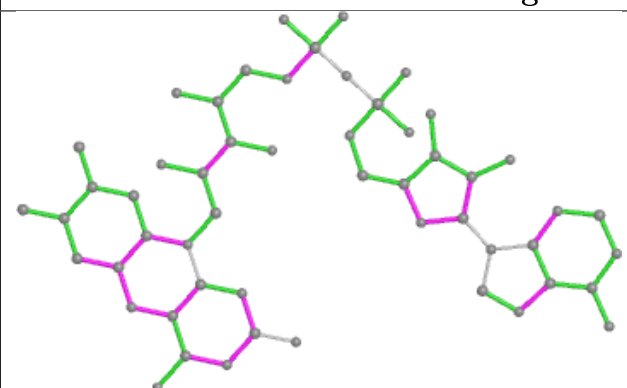
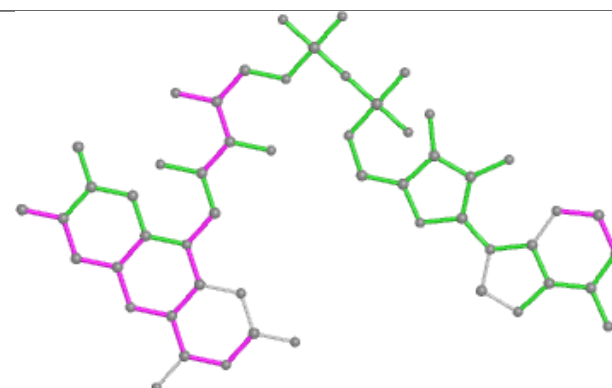
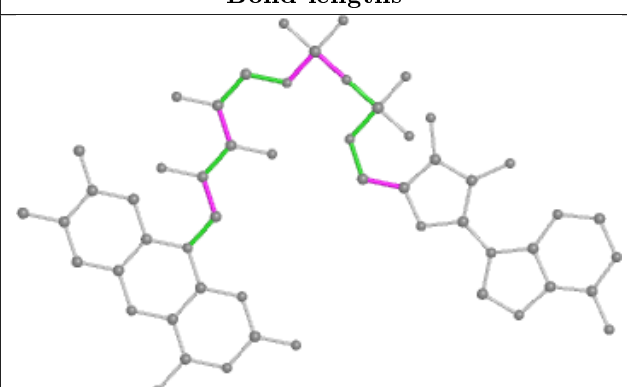
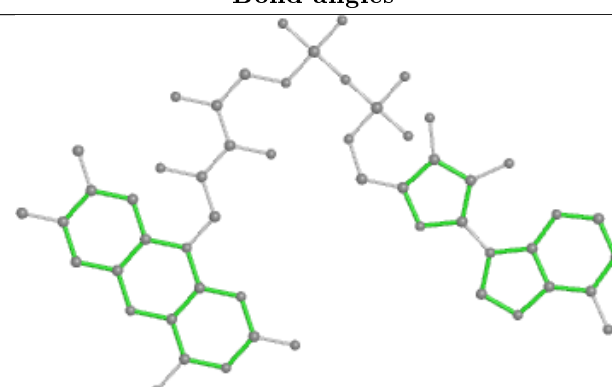
Mol	Chain	Res	Type	Atoms
11	D	710	CE1	O22-C23-C24-O25
11	O	811	CE1	O16-C17-C18-O19
6	A	703	FAD	O4B-C4B-C5B-O5B
11	O	812	CE1	C33-C32-O31-C30
6	M	803	FAD	PA-O3P-P-O2P
11	D	810	CE1	O19-C20-C21-O22
11	O	812	CE1	O16-C17-C18-O19
11	O	811	CE1	C14-C15-O16-C17
11	D	810	CE1	O16-C17-C18-O19
11	D	710	CE1	O19-C20-C21-O22
11	D	710	CE1	O16-C17-C18-O19




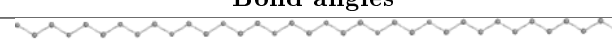
There are no ring outliers.

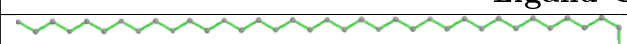
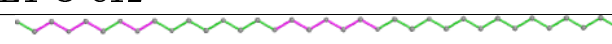

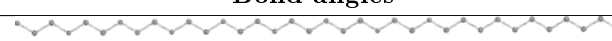
13 monomers are involved in 109 short contacts:

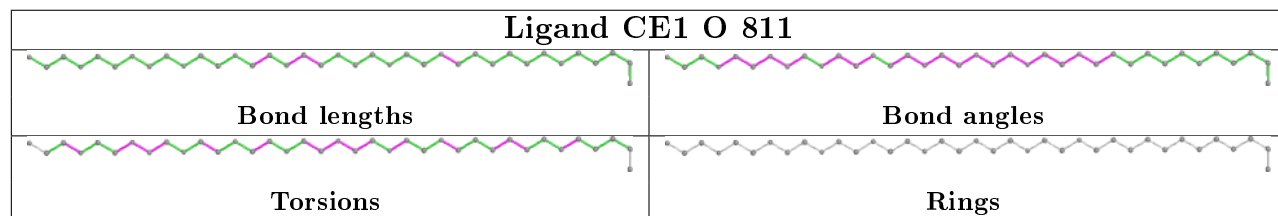
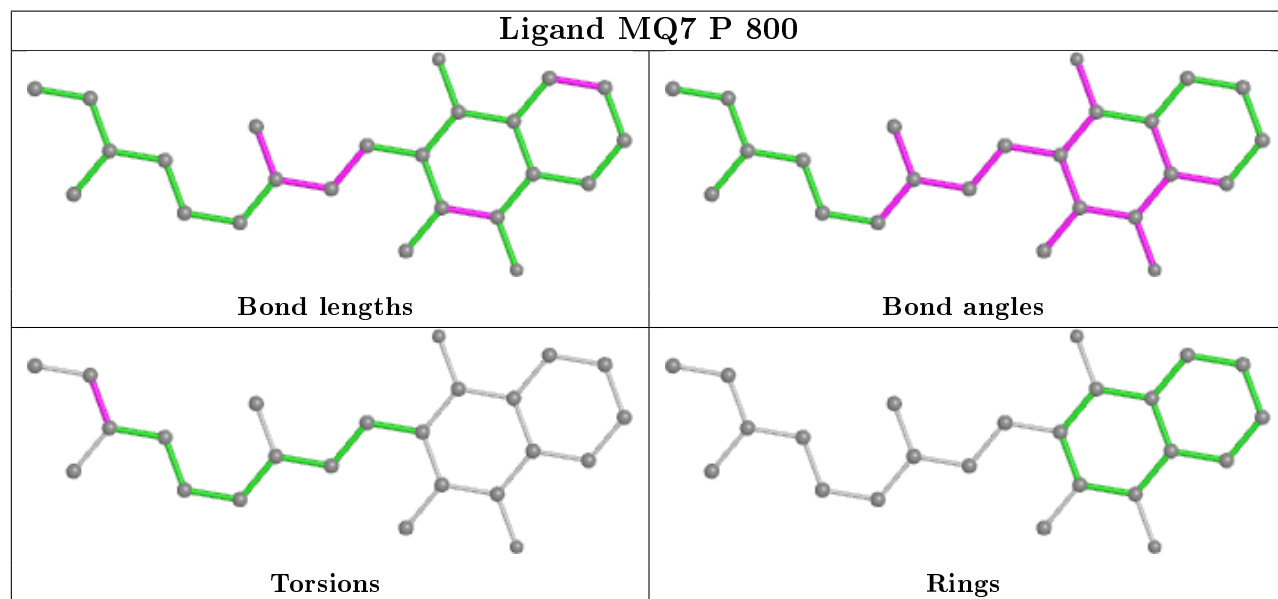
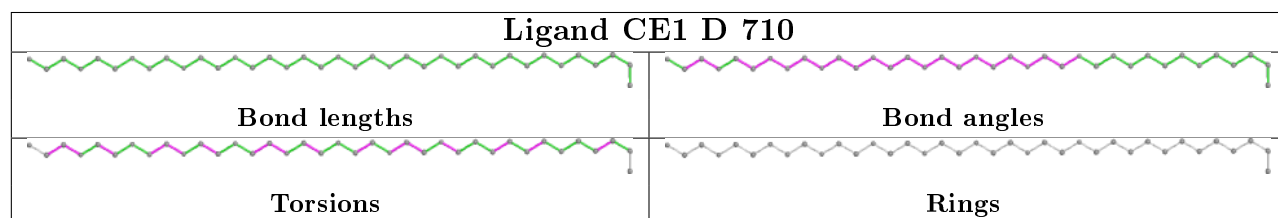
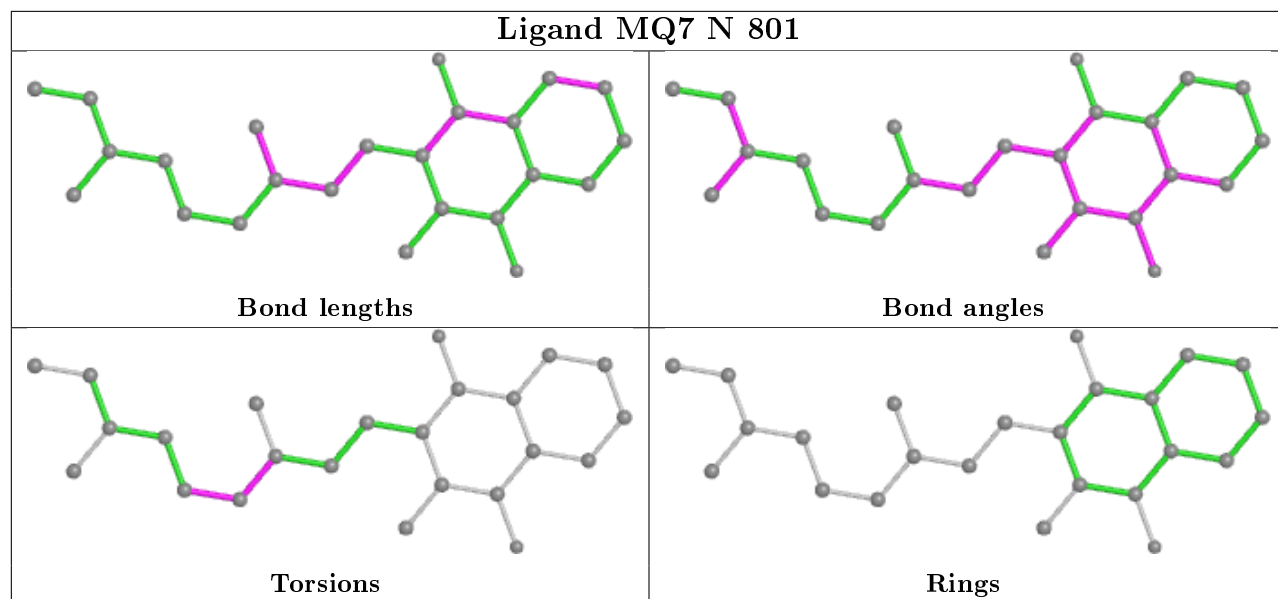
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	245	F3S	1	0
6	A	703	FAD	8	0
11	D	810	CE1	5	0
5	M	802	OAA	1	0
11	O	812	CE1	1	0
10	N	801	MQ7	14	0
11	D	710	CE1	3	0
10	P	800	MQ7	20	0
7	B	244	FES	1	0
5	A	702	OAA	1	0
10	D	700	MQ7	26	0
6	M	803	FAD	24	0
10	B	701	MQ7	4	0

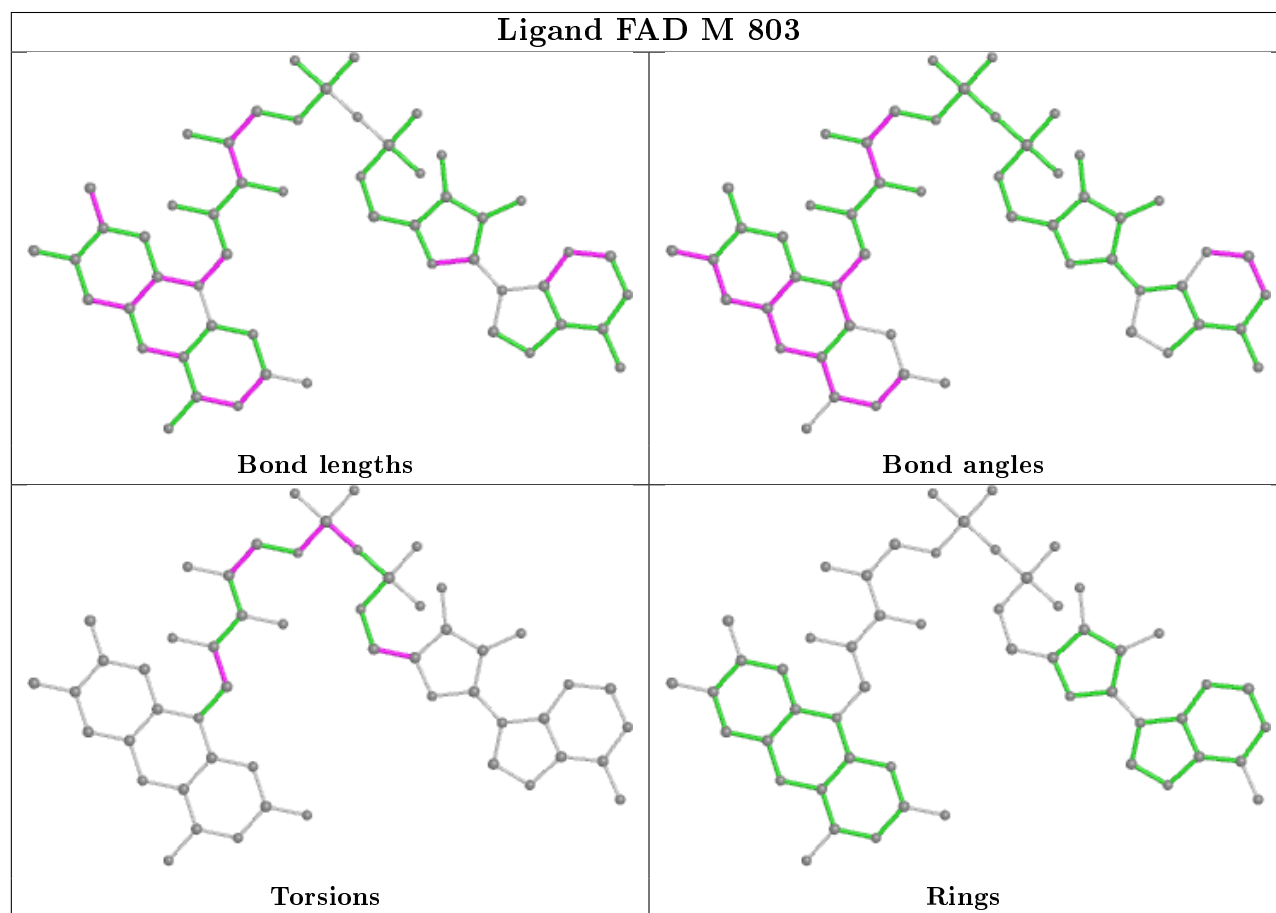
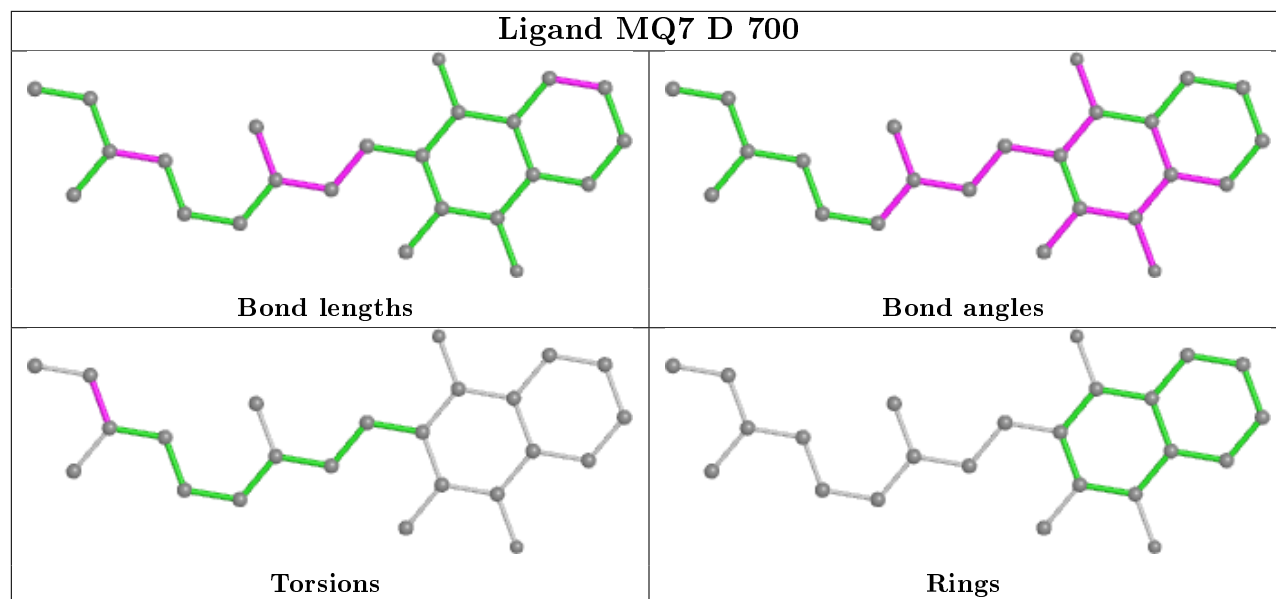
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

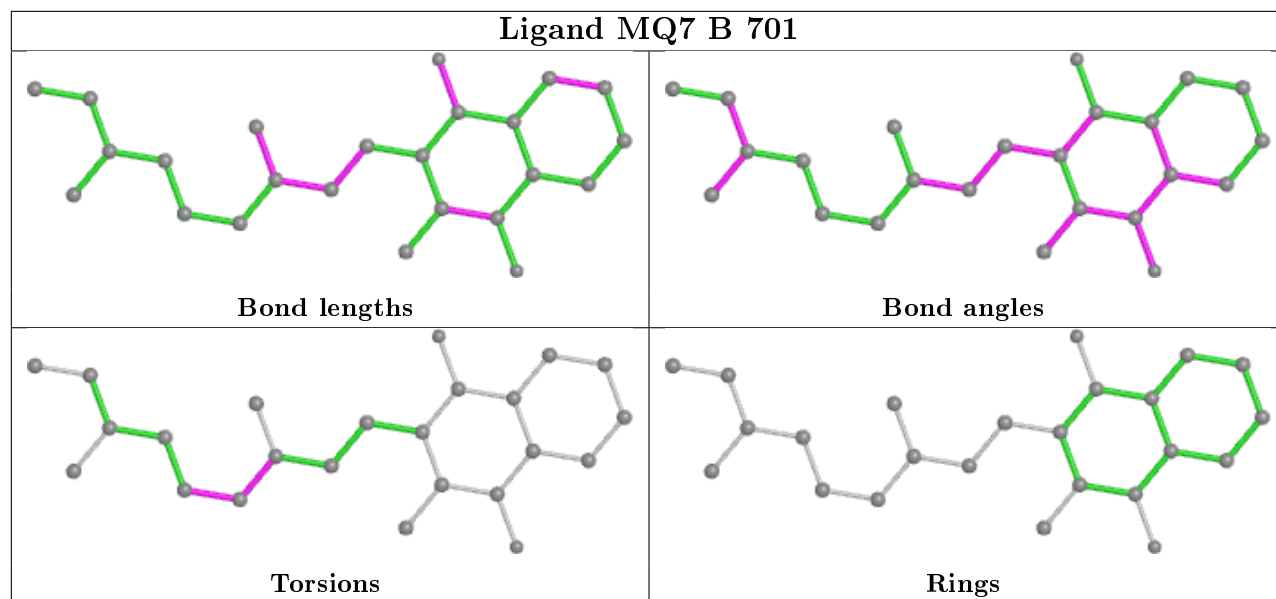
Ligand FAD A 703	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CE1 D 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CE1 O 812	
	
Bond lengths	Bond angles
	
Torsions	Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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.