



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:27 am BST

PDB ID : 3P4P
Title : Crystal structure of Menaquinol:fumarate oxidoreductase in complex with fumarate
Authors : Tomasiak, T.M.; Archuleta, T.L.; Andr ll, J.; Luna-Ch vez, C.; Davis, T.A.; Sarwar, M.; Ham, A.J.; McDonald, W.H.; Yankowskaya, V.; Stern, H.A.; Johnston, J.N.; Maklashina, E.; Cecchini, G.; Iverson, T.M.
Deposited on : 2010-10-06
Resolution : 2.80 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

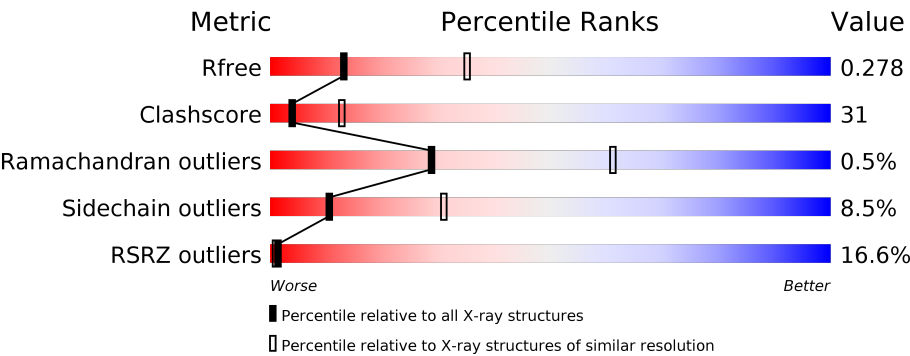
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	577	<div><div></div><div>66%31%.</div></div>
1	M	577	<div><div>50%</div><div>47%47%5%</div></div>
2	B	243	<div><div>2%</div><div>68%29%.</div></div>
2	N	243	<div><div>20%</div><div>44%47%9%</div></div>
3	C	130	<div><div></div><div>58%38%5%</div></div>
3	O	130	<div><div>4%</div><div>58%38%. </div></div>

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Mol	Chain	Length	Quality of chain
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
5	FAD	M	601	-	-	X	-
7	FES	B	244	-	-	X	-
8	F3S	B	245	-	-	X	-
9	SF4	B	246	-	-	X	-
9	SF4	N	246	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16873 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
			4449	2775	802	841	31			
1	M	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	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 subunit C.

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 subunit D.

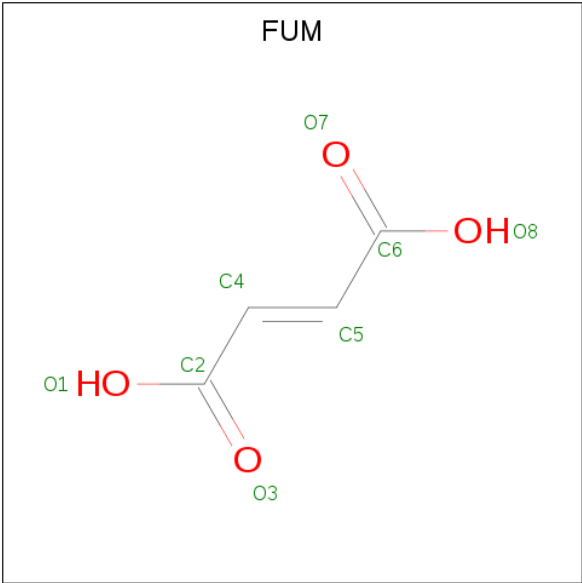
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is FUMARIC ACID (three-letter code: FUM) (formula: C₄H₄O₄).



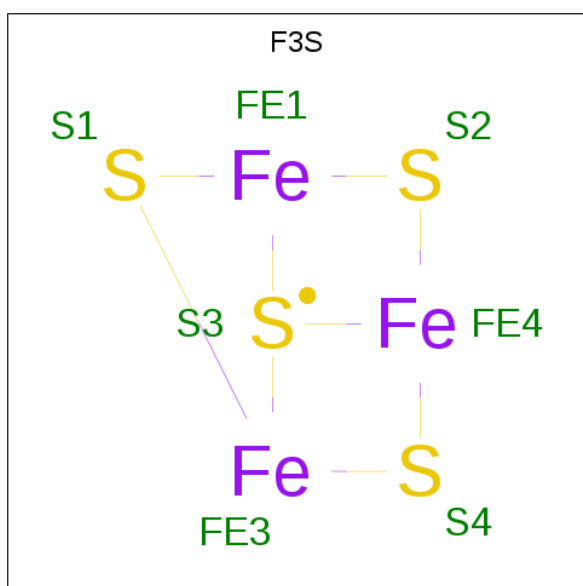
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	4	4		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



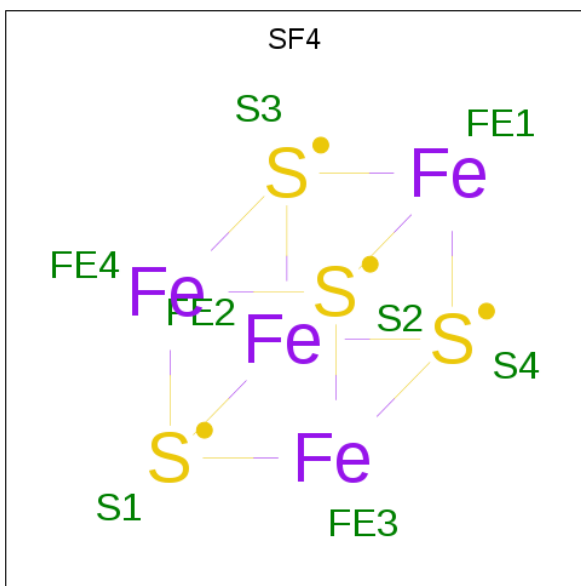
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- 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		

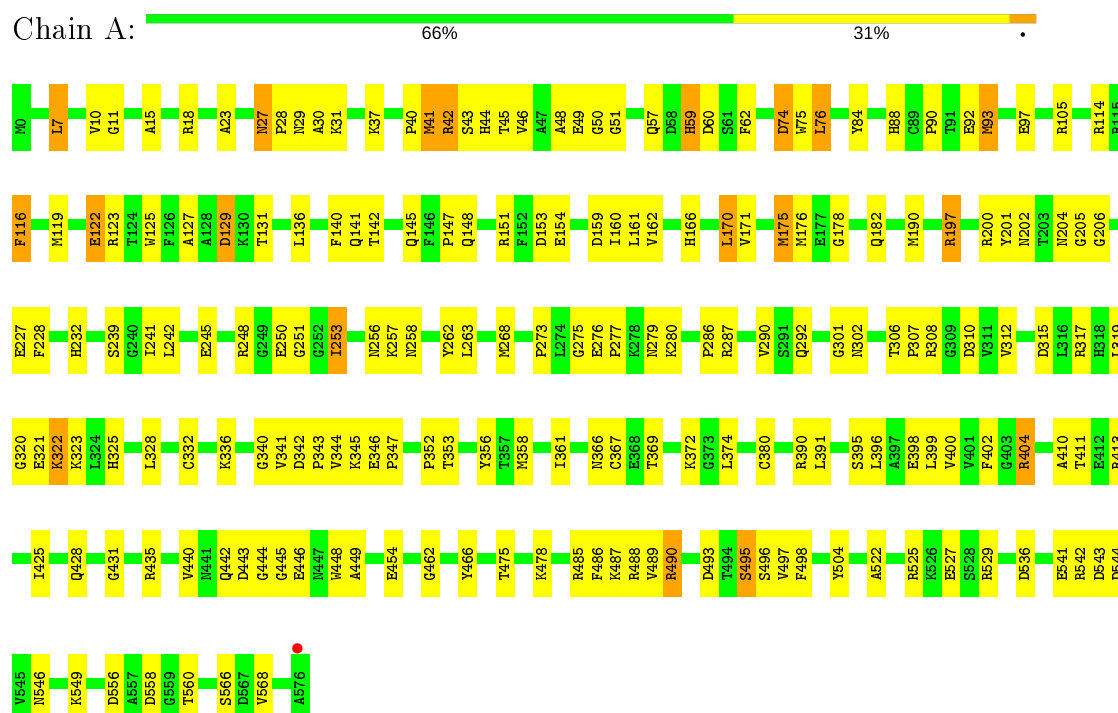
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	60	Total	O	0	0
			60	60		
10	B	10	Total	O	0	0
			10	10		
10	C	2	Total	O	0	0
			2	2		
10	D	4	Total	O	0	0
			4	4		
10	M	1	Total	O	0	0
			1	1		
10	N	2	Total	O	0	0
			2	2		

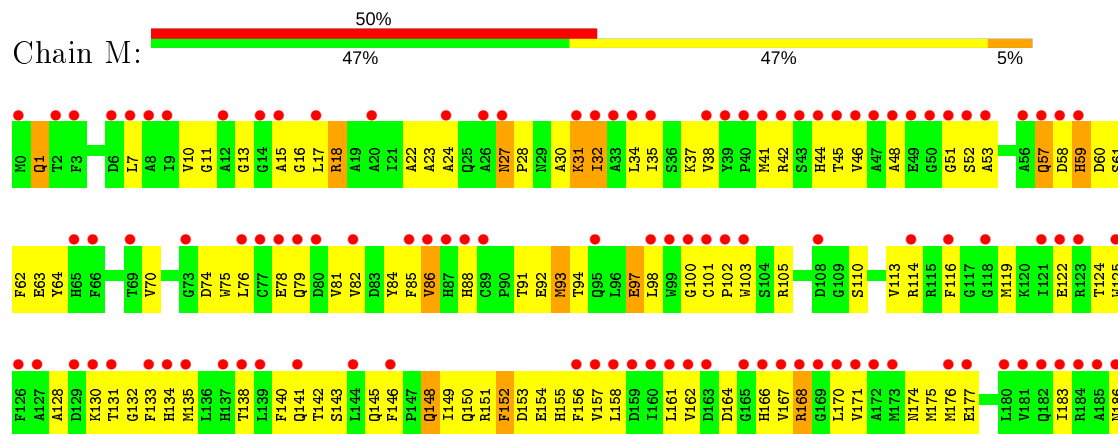
3 Residue-property plots

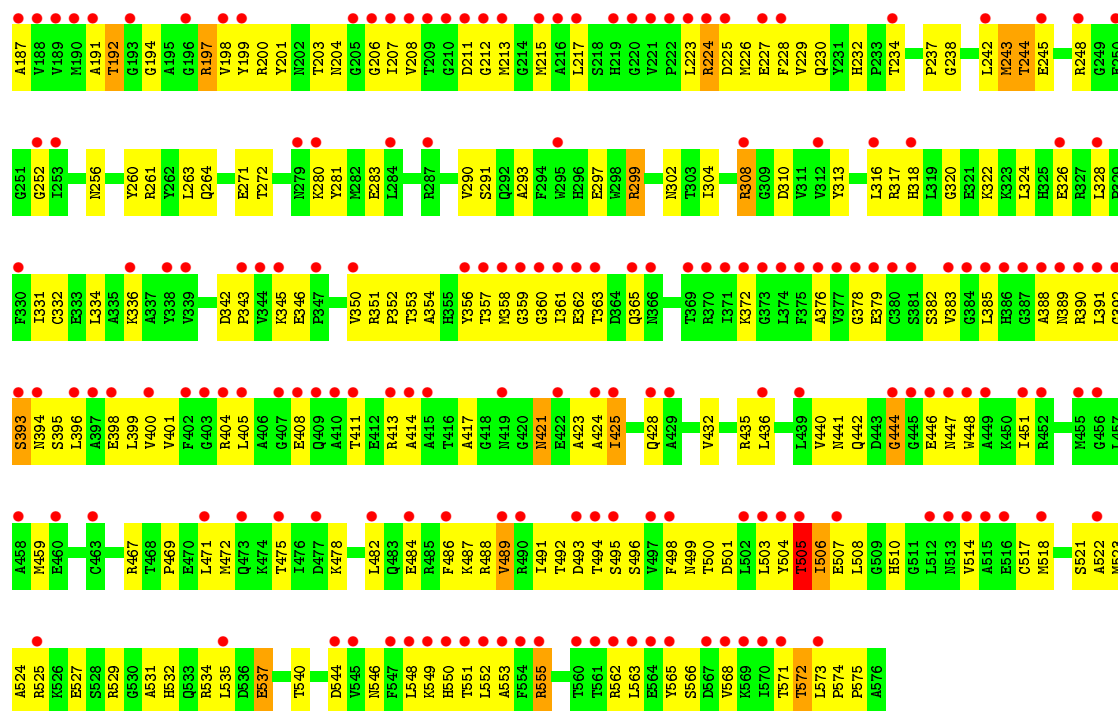
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Fumarate reductase flavoprotein subunit

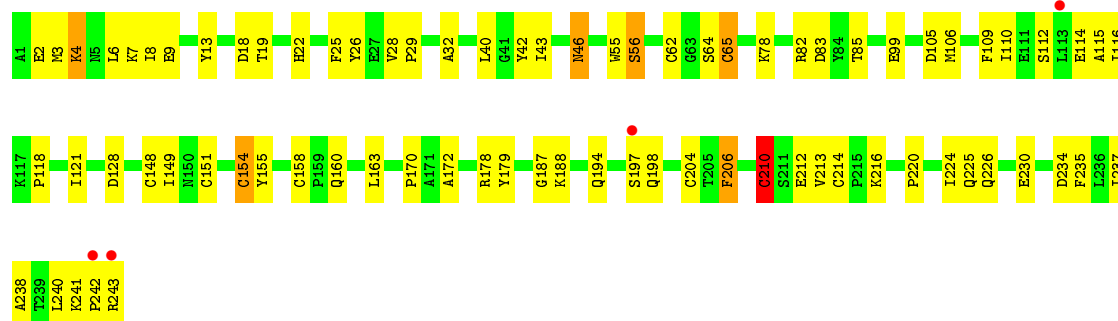


- Molecule 1: Fumarate reductase flavoprotein subunit

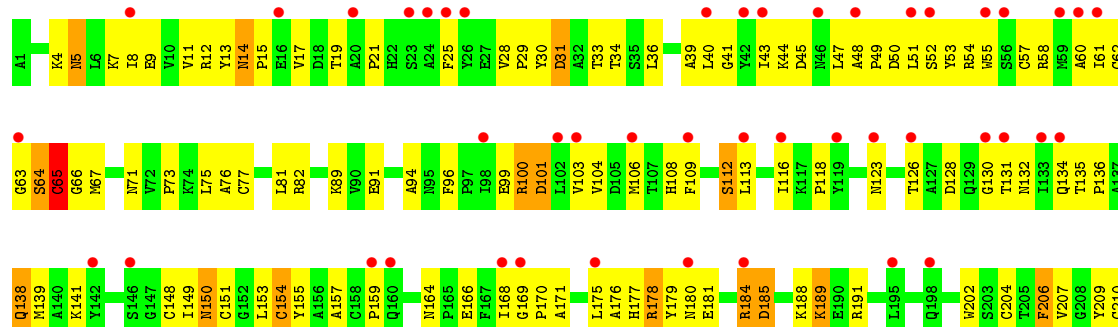
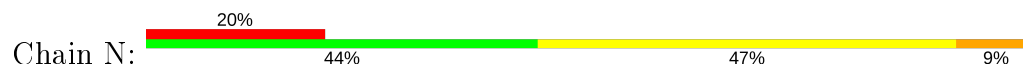




• Molecule 2: Fumarate reductase iron-sulfur protein

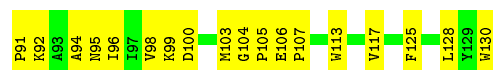


• Molecule 2: Fumarate reductase iron-sulfur protein





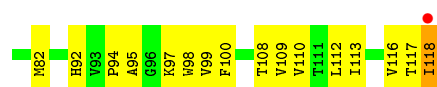
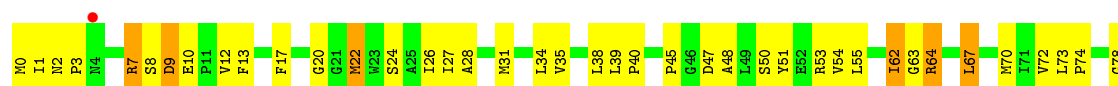
• Molecule 3: Fumarate reductase subunit C



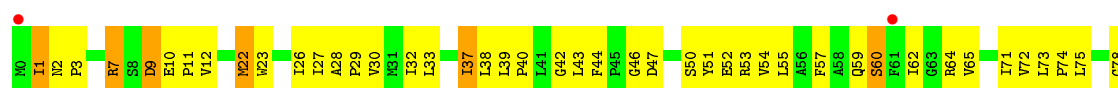
• Molecule 3: Fumarate reductase subunit C



• Molecule 4: Fumarate reductase subunit D



• Molecule 4: Fumarate reductase subunit D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.32Å 137.63Å 270.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 2.80 90.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.92-2.80) 94.9 (90.74-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.249 , 0.272 0.258 , 0.278	Depositor DCC
R_{free} test set	1408 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16873	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, F3S, FUM, FES, 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	0.77	0/4541	0.83	3/6139 (0.0%)
1	M	0.53	1/4541 (0.0%)	0.64	2/6139 (0.0%)
2	B	0.76	1/1931 (0.1%)	0.84	3/2617 (0.1%)
2	N	0.58	3/1931 (0.2%)	0.73	3/2617 (0.1%)
3	C	0.60	0/1094	0.70	2/1496 (0.1%)
3	O	0.57	0/1094	0.65	0/1496
4	D	0.60	0/956	0.72	0/1303
4	P	0.55	0/956	0.68	0/1303
All	All	0.65	5/17044 (0.0%)	0.74	13/23110 (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	N	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	210	CYS	C-N	10.72	1.58	1.34
2	N	77	CYS	C-N	8.04	1.52	1.34
2	N	65	CYS	CB-SG	7.05	1.94	1.82
1	M	505	THR	C-N	6.89	1.49	1.34
2	N	77	CYS	CB-SG	5.33	1.91	1.82

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	CYS	O-C-N	10.16	138.96	122.70
2	B	210	CYS	CA-C-N	-8.65	98.16	117.20
2	N	65	CYS	N-CA-CB	-7.65	96.83	110.60
2	B	210	CYS	C-N-CA	-7.21	103.66	121.70
3	C	28	ARG	NE-CZ-NH1	6.72	123.66	120.30
3	C	28	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	404	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	170	LEU	CA-CB-CG	6.37	129.95	115.30
2	N	77	CYS	CA-CB-SG	5.63	124.14	114.00
2	N	65	CYS	O-C-N	-5.39	114.04	123.20
1	A	404	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	M	1	GLN	N-CA-C	-5.14	97.13	111.00
1	M	1	GLN	N-CA-CB	5.00	119.61	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	64	SER	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	4449	0	4335	169	0
1	M	4449	0	4335	401	0
2	B	1888	0	1844	91	0
2	N	1888	0	1839	199	0
3	C	1058	0	1108	63	0
3	O	1058	0	1108	74	0
4	D	926	0	971	79	0
4	P	926	0	970	68	0
5	A	53	0	30	14	0
5	M	53	0	30	25	0
6	A	8	0	2	1	0
7	B	4	0	0	3	0
7	N	4	0	0	1	0
8	B	7	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	7	0	0	1	0
9	B	8	0	0	12	0
9	N	8	0	0	6	0
10	A	60	0	0	2	0
10	B	10	0	0	0	0
10	C	2	0	0	0	0
10	D	4	0	0	0	0
10	M	1	0	0	5	0
10	N	2	0	0	0	0
All	All	16873	0	16572	1016	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 31.

All (1016) 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	5:A:601:FAD:C8M	1.77	1.45
1:A:44:HIS:CE1	5:A:601:FAD:HM82	1.53	1.44
1:M:44:HIS:NE2	5:M:601:FAD:HM82	1.41	1.34
2:N:31:ASP:OD2	2:N:33:THR:N	1.57	1.33
1:M:168:ARG:HD2	10:M:577:HOH:O	1.19	1.27
1:M:527:GLU:OE1	1:M:529:ARG:NH1	1.72	1.21
1:A:44:HIS:NE2	5:A:601:FAD:HM81	1.50	1.13
1:A:44:HIS:NE2	5:A:601:FAD:HM82	1.44	1.12
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.17	1.09
2:N:189:LYS:HD2	2:N:189:LYS:H	0.99	1.08
3:C:86:TRP:HE1	4:D:22:MET:CE	1.67	1.07
4:P:1:ILE:HD12	4:P:1:ILE:H	1.16	1.06
1:A:346:GLU:HG3	1:A:347:PRO:HD2	1.31	1.06
1:M:44:HIS:NE2	5:M:601:FAD:C8M	2.20	1.04
2:N:71:ASN:HB3	3:O:18:LYS:HE3	1.33	1.04
1:M:100:GLY:C	2:N:184:ARG:NH2	2.12	1.02
1:M:155:HIS:CE1	1:M:174:ASN:HD22	1.76	1.02
1:M:146:PHE:HB2	1:M:149:ILE:HD13	1.39	1.02
2:B:204:CYS:SG	8:B:245:F3S:FE1	1.51	1.02
1:M:168:ARG:CD	10:M:577:HOH:O	1.81	1.01
2:N:178:ARG:HH11	2:N:178:ARG:HG2	1.22	1.01
3:C:86:TRP:NE1	4:D:22:MET:CE	2.24	1.01
3:C:86:TRP:HE1	4:D:22:MET:HE3	1.25	1.01
1:A:151:ARG:NH1	1:A:153:ASP:OD2	1.95	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:192:THR:HG21	1:M:212:GLY:HA3	1.42	1.00
3:C:50:LYS:HE2	3:C:50:LYS:HA	1.44	0.99
1:M:451:ILE:HG23	1:M:482:LEU:HD12	1.38	0.99
2:B:198:GLN:HE22	4:D:10:GLU:HG3	1.27	0.99
2:N:13:TYR:HB2	2:N:21:PRO:HB3	1.45	0.99
2:N:159:PRO:HG2	2:N:207:VAL:HG21	1.45	0.99
1:M:549:LYS:HD2	1:M:565:TYR:HB3	1.45	0.98
2:B:151:CYS:SG	9:B:246:SF4:FE1	1.55	0.98
2:B:214:CYS:HG	9:B:246:SF4:FE4	0.80	0.97
1:A:57:GLN:HE22	1:A:122:GLU:HG2	1.25	0.97
1:M:100:GLY:CA	2:N:184:ARG:HH21	1.76	0.97
1:A:44:HIS:CE1	5:A:601:FAD:C8M	2.37	0.97
1:M:425:ILE:HD11	10:M:577:HOH:O	1.63	0.96
3:C:86:TRP:CD1	4:D:22:MET:HE2	2.01	0.96
1:M:421:ASN:OD1	1:M:424:ALA:N	1.96	0.96
2:B:151:CYS:HG	9:B:246:SF4:FE1	0.78	0.95
2:B:198:GLN:OE1	4:D:8:SER:OG	1.85	0.95
3:O:130:TRP:O	4:P:53:ARG:NH2	2.00	0.95
1:M:81:VAL:HG11	1:M:383:VAL:HG12	1.48	0.94
1:M:537:GLU:CD	1:M:537:GLU:H	1.71	0.93
1:M:328:LEU:O	1:M:332:CYS:SG	2.26	0.93
2:N:189:LYS:HD2	2:N:189:LYS:N	1.84	0.92
2:N:154:CYS:HB2	2:N:170:PRO:HG2	1.50	0.92
2:N:71:ASN:HB3	3:O:18:LYS:CE	1.98	0.92
1:A:328:LEU:O	1:A:332:CYS:SG	2.29	0.91
1:M:197:ARG:HD2	1:M:206:GLY:HA2	1.51	0.91
1:M:155:HIS:CE1	1:M:174:ASN:HA	2.04	0.91
2:N:189:LYS:H	2:N:189:LYS:CD	1.84	0.91
1:M:42:ARG:NH2	2:N:150:ASN:O	2.04	0.90
2:N:116:ILE:HG21	2:N:176:ALA:CB	2.00	0.90
2:N:151:CYS:HG	9:N:246:SF4:FE1	0.76	0.90
1:M:192:THR:HG21	1:M:212:GLY:CA	2.02	0.90
2:B:154:CYS:SG	9:B:246:SF4:FE2	1.64	0.89
1:M:149:ILE:HD12	1:M:149:ILE:H	1.36	0.89
1:M:100:GLY:HA2	2:N:184:ARG:HH21	1.36	0.89
1:M:11:GLY:HA2	5:M:601:FAD:O4B	1.72	0.89
1:M:93:MET:HE2	1:M:93:MET:HA	1.55	0.88
3:C:86:TRP:CD1	4:D:22:MET:CE	2.55	0.88
1:M:525:ARG:O	1:M:534:ARG:NH1	2.07	0.88
3:C:50:LYS:HA	3:C:50:LYS:CE	2.05	0.87
1:M:42:ARG:HD2	2:N:64:SER:HB3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:PRO:HB2	4:P:92:HIS:HB3	1.55	0.87
4:D:92:HIS:HB3	2:N:243:ARG:HB2	1.56	0.87
1:M:146:PHE:HB2	1:M:149:ILE:CD1	2.05	0.87
1:M:444:GLY:HA3	1:M:488:ARG:C	1.95	0.86
4:D:0:MET:HG3	4:D:1:ILE:H	1.40	0.86
1:A:60:ASP:OD1	1:A:123:ARG:NH2	2.08	0.86
1:A:57:GLN:NE2	1:A:122:GLU:HG2	1.89	0.86
4:P:22:MET:HA	4:P:22:MET:HE3	1.56	0.85
2:N:222:ALA:O	2:N:226:GLN:NE2	2.10	0.85
2:N:149:ILE:HG23	2:N:216:LYS:HG3	1.58	0.85
1:A:60:ASP:CG	1:A:123:ARG:HH21	1.80	0.84
1:M:44:HIS:CE1	5:M:601:FAD:HM82	2.11	0.84
4:D:64:ARG:HG2	4:D:64:ARG:HH11	1.40	0.84
2:N:63:GLY:O	2:N:151:CYS:HA	1.77	0.84
4:P:1:ILE:CD1	4:P:1:ILE:H	1.92	0.83
2:B:4:LYS:H	2:B:4:LYS:CE	1.90	0.83
1:M:24:ALA:HB2	1:M:32:ILE:HD11	1.59	0.83
3:C:86:TRP:NE1	4:D:22:MET:HE2	1.91	0.82
1:M:155:HIS:CE1	1:M:174:ASN:ND2	2.47	0.82
2:N:148:CYS:SG	9:N:246:SF4:FE3	1.70	0.82
1:M:360:GLY:C	1:M:382:SER:OG	2.17	0.82
2:B:214:CYS:SG	9:B:246:SF4:FE4	1.70	0.82
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.61	0.82
2:B:46:ASN:N	2:B:46:ASN:HD22	1.78	0.82
1:M:425:ILE:CD1	10:M:577:HOH:O	2.22	0.82
2:N:116:ILE:CG2	2:N:176:ALA:HB2	2.07	0.82
1:M:157:VAL:HG22	5:M:601:FAD:N1A	1.95	0.81
2:N:71:ASN:CB	3:O:18:LYS:HE3	2.11	0.81
2:N:148:CYS:HG	9:N:246:SF4:FE3	0.92	0.81
3:O:120:THR:HG23	4:P:30:VAL:HB	1.62	0.81
1:M:100:GLY:CA	2:N:184:ARG:NH2	2.42	0.81
1:M:260:TYR:CE1	1:M:264:GLN:NE2	2.47	0.81
1:M:297:GLU:OE1	1:M:297:GLU:HA	1.81	0.81
1:M:97:GLU:OE2	2:N:132:ASN:N	2.14	0.81
1:M:390:ARG:HD2	1:M:391:LEU:O	1.81	0.80
1:A:154:GLU:O	1:A:175:MET:HG3	1.81	0.80
1:M:62:PHE:HB3	1:M:86:VAL:CG1	2.11	0.80
2:B:46:ASN:HD22	2:B:46:ASN:H	1.27	0.80
1:M:155:HIS:NE2	1:M:174:ASN:ND2	2.28	0.80
1:M:7:LEU:HB2	1:M:32:ILE:HG22	1.63	0.80
1:M:155:HIS:ND1	1:M:174:ASN:HA	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:146:PHE:CB	1:M:149:ILE:HD13	2.11	0.79
1:M:152:PHE:HB3	1:M:155:HIS:CD2	2.17	0.79
1:M:158:LEU:HG	1:M:506:ILE:HD12	1.62	0.79
1:M:92:GLU:HB3	1:M:400:VAL:HB	1.63	0.78
3:C:50:LYS:CA	3:C:50:LYS:HE2	2.14	0.78
4:D:92:HIS:HB3	2:N:243:ARG:CB	2.13	0.78
1:M:79:GLN:NE2	1:M:571:THR:H	1.81	0.78
2:B:32:ALA:O	2:B:82:ARG:NH1	2.17	0.77
1:M:152:PHE:O	1:M:155:HIS:HB2	1.83	0.77
1:A:232:HIS:CE1	1:A:242:LEU:HD11	2.19	0.77
2:N:12:ARG:NH2	2:N:50:ASP:OD1	2.18	0.77
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.67	0.77
1:M:100:GLY:HA2	2:N:184:ARG:NH2	1.98	0.77
1:A:321:GLU:HG2	1:A:344:VAL:HG11	1.67	0.77
2:B:9:GLU:HB2	2:B:25:PHE:CE2	2.20	0.76
2:N:116:ILE:O	2:N:191:ARG:HG2	1.85	0.76
1:A:44:HIS:HE1	5:A:601:FAD:HM82	1.44	0.76
1:M:102:PRO:HG2	1:M:134:HIS:CD2	2.21	0.76
1:M:230:GLN:HB3	1:M:356:TYR:H	1.51	0.76
1:M:156:PHE:CE1	5:M:601:FAD:N6A	2.53	0.76
1:M:237:PRO:HB2	1:M:308:ARG:HB3	1.68	0.76
1:M:146:PHE:CB	1:M:149:ILE:CD1	2.65	0.75
1:M:24:ALA:CA	1:M:32:ILE:HD11	2.16	0.75
1:M:62:PHE:HB3	1:M:86:VAL:HG13	1.67	0.75
1:M:81:VAL:HG11	1:M:383:VAL:CG1	2.17	0.75
4:D:34:LEU:HD23	4:D:38:LEU:HD12	1.68	0.75
4:P:9:ASP:C	4:P:11:PRO:HD2	2.07	0.75
4:D:26:ILE:HG22	4:D:27:ILE:HG13	1.69	0.74
1:M:155:HIS:CE1	1:M:174:ASN:CA	2.70	0.74
1:M:11:GLY:HA2	5:M:601:FAD:C1B	2.16	0.74
1:M:24:ALA:CB	1:M:32:ILE:HD11	2.17	0.74
2:B:46:ASN:N	2:B:46:ASN:ND2	2.35	0.74
1:M:114:ARG:O	1:M:124:THR:HB	1.88	0.74
2:N:31:ASP:OD2	2:N:33:THR:CA	2.35	0.74
2:N:177:HIS:O	2:N:181:GLU:HB2	1.87	0.74
2:N:12:ARG:NH1	2:N:50:ASP:OD1	2.21	0.74
2:N:96:PHE:O	3:O:9:ARG:NH1	2.20	0.74
3:C:54:GLU:HA	3:C:54:GLU:OE1	1.87	0.74
1:M:328:LEU:HD22	1:M:331:ILE:CD1	2.16	0.73
2:B:65:CYS:SG	7:B:244:FES:FE1	1.79	0.73
1:M:444:GLY:HA3	1:M:488:ARG:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:OG1	5:A:601:FAD:O2A	2.06	0.73
1:M:527:GLU:CD	1:M:529:ARG:NH1	2.41	0.73
1:M:360:GLY:O	1:M:382:SER:OG	2.07	0.72
2:B:99:GLU:OE2	3:C:4:ARG:NH1	2.23	0.72
3:O:19:LEU:HD21	3:O:22:TYR:CE2	2.25	0.72
2:B:154:CYS:HG	9:B:246:SF4:FE2	0.90	0.72
1:M:192:THR:HG21	1:M:212:GLY:N	2.03	0.72
1:A:49:GLU:HG2	1:A:129:ASP:O	1.89	0.72
1:M:224:ARG:HB2	1:M:552:LEU:HD23	1.72	0.72
1:M:546:ASN:O	1:M:549:LYS:NZ	2.23	0.72
1:M:13:GLY:H	5:M:601:FAD:H4B	1.54	0.72
1:M:212:GLY:HA2	1:M:215:MET:HE3	1.71	0.72
1:M:549:LYS:HD2	1:M:565:TYR:CB	2.19	0.72
1:A:275:GLY:O	1:A:277:PRO:HD3	1.89	0.72
1:M:166:HIS:CD2	1:M:372:LYS:HB3	2.24	0.72
1:A:200:ARG:HD3	1:A:201:TYR:CZ	2.24	0.71
1:M:176:MET:HE2	2:N:99:GLU:HG3	1.72	0.71
1:M:93:MET:CE	1:M:93:MET:HA	2.20	0.71
1:A:151:ARG:NH2	2:B:114:GLU:OE1	2.23	0.71
1:A:346:GLU:HG3	1:A:347:PRO:CD	2.14	0.71
1:M:100:GLY:C	2:N:184:ARG:HH22	1.94	0.71
1:A:18:ARG:NH1	1:A:92:GLU:OE2	2.23	0.71
2:B:241:LYS:O	2:B:241:LYS:CG	2.39	0.71
1:M:141:GLN:HB3	2:N:118:PRO:O	1.90	0.70
3:O:54:GLU:H	3:O:54:GLU:CD	1.94	0.70
1:A:366:ASN:O	1:A:367:CYS:HB2	1.90	0.70
1:M:242:LEU:HG	1:M:244:THR:H	1.56	0.70
1:A:497:VAL:HG12	1:A:497:VAL:O	1.90	0.70
1:M:212:GLY:HA2	1:M:215:MET:CE	2.22	0.70
1:M:192:THR:HG21	1:M:212:GLY:H	1.56	0.70
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.72	0.70
2:B:148:CYS:HG	9:B:246:SF4:FE3	1.07	0.70
2:B:148:CYS:SG	9:B:246:SF4:FE3	1.84	0.70
3:C:19:LEU:HD13	3:C:20:PRO:HD2	1.73	0.70
1:M:217:LEU:HG	1:M:555:ARG:HB2	1.72	0.70
2:N:15:PRO:HB3	3:O:5:LYS:H	1.54	0.70
1:A:119:MET:CE	1:A:391:LEU:HD23	2.21	0.70
1:M:243:MET:HA	1:M:243:MET:HE2	1.72	0.70
1:M:467:ARG:NH1	1:M:532:HIS:ND1	2.39	0.70
1:M:37:LYS:HE2	5:M:601:FAD:C8A	2.22	0.70
1:M:149:ILE:HD12	1:M:149:ILE:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:ARG:HD3	2:N:134:GLN:O	1.92	0.69
1:A:200:ARG:HD3	1:A:201:TYR:CE1	2.27	0.69
4:D:92:HIS:CB	2:N:243:ARG:HB2	2.22	0.69
3:O:75:THR:HG22	4:P:32:ILE:HD13	1.74	0.69
4:D:0:MET:HG3	4:D:1:ILE:N	2.08	0.69
1:M:213:MET:HB3	1:M:223:LEU:HD21	1.74	0.69
3:O:49:LEU:HD21	4:P:55:LEU:HA	1.73	0.69
4:P:33:LEU:HD12	4:P:37:ILE:HD12	1.73	0.69
1:A:342:ASP:OD2	1:A:344:VAL:HG23	1.93	0.68
1:M:243:MET:HA	1:M:243:MET:CE	2.22	0.68
1:M:357:THR:HG22	1:M:359:GLY:O	1.93	0.68
2:N:240:LEU:O	2:N:243:ARG:CZ	2.41	0.68
1:A:125:TRP:CD1	1:A:125:TRP:N	2.54	0.68
1:M:553:ALA:HA	1:M:562:ARG:O	1.93	0.68
4:P:79:LEU:HD12	4:P:104:ALA:HB2	1.75	0.68
4:D:9:ASP:OD2	4:D:97:LYS:NZ	2.24	0.68
1:M:421:ASN:OD1	1:M:421:ASN:C	2.30	0.68
2:N:109:PHE:CE2	2:N:113:LEU:HD11	2.28	0.68
3:C:59:PHE:HE2	3:C:63:LEU:HD11	1.59	0.68
1:M:84:TYR:CE2	1:M:405:LEU:HD22	2.29	0.68
1:M:342:ASP:HB3	1:M:345:LYS:CB	2.24	0.68
2:B:4:LYS:H	2:B:4:LYS:HE3	1.58	0.68
4:D:64:ARG:HH12	4:D:117:THR:HG23	1.58	0.68
1:M:102:PRO:C	2:N:139:MET:HE1	2.15	0.68
1:M:227:GLU:HB2	1:M:522:ALA:HB2	1.76	0.68
1:M:260:TYR:OH	1:M:264:GLN:NE2	2.27	0.67
4:P:105:ALA:O	4:P:109:VAL:HG23	1.94	0.67
1:A:10:VAL:HB	1:A:190:MET:CE	2.24	0.67
1:M:244:THR:HG23	1:M:245:GLU:N	2.08	0.67
4:P:55:LEU:O	4:P:59:GLN:HG3	1.93	0.67
1:A:341:VAL:HG13	1:A:346:GLU:HB3	1.75	0.67
2:N:214:CYS:SG	2:N:218:VAL:HG23	2.35	0.67
2:N:41:GLY:HA2	2:N:53:TYR:OH	1.94	0.67
3:C:50:LYS:HD3	4:D:118:ILE:H	1.60	0.67
1:A:346:GLU:CG	1:A:347:PRO:HD2	2.17	0.67
4:D:95:ALA:HB1	4:D:98:TRP:HB2	1.76	0.66
2:N:31:ASP:OD1	2:N:33:THR:OG1	2.12	0.66
3:O:18:LYS:HE2	3:O:19:LEU:HD22	1.75	0.66
1:M:158:LEU:O	1:M:158:LEU:HD23	1.95	0.66
3:O:54:GLU:N	3:O:54:GLU:CD	2.48	0.66
3:C:50:LYS:HB3	4:D:118:ILE:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TRP:HD1	1:A:125:TRP:N	1.93	0.66
1:A:306:THR:HB	1:A:307:PRO:HD2	1.78	0.66
1:A:166:HIS:CD2	1:A:372:LYS:HB3	2.30	0.66
1:A:549:LYS:HB2	1:A:566:SER:O	1.96	0.66
2:N:210:CYS:SG	2:N:221:ALA:HB2	2.36	0.66
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.22	0.66
1:M:146:PHE:HB3	1:M:148:GLN:HE22	1.61	0.65
1:M:358:MET:SD	1:M:389:ASN:HA	2.37	0.65
1:M:53:ALA:HB2	1:M:393:SER:OG	1.95	0.65
1:A:37:LYS:HE2	5:A:601:FAD:N7A	2.11	0.65
1:M:299:ARG:HE	1:M:299:ARG:CA	2.06	0.65
1:M:332:CYS:HA	1:M:343:PRO:HG2	1.77	0.65
1:A:321:GLU:HG2	1:A:344:VAL:CG1	2.27	0.65
1:M:37:LYS:HD3	1:M:156:PHE:CE1	2.31	0.65
1:A:322:LYS:HA	1:A:322:LYS:HE3	1.78	0.65
1:M:436:LEU:O	1:M:440:VAL:HG23	1.97	0.65
1:A:27:ASN:OD1	1:A:27:ASN:C	2.35	0.65
1:A:341:VAL:O	1:A:343:PRO:HD3	1.96	0.65
2:B:65:CYS:SG	7:B:244:FES:S1	2.94	0.65
1:M:51:GLY:O	1:M:396:LEU:HD12	1.97	0.65
1:M:328:LEU:HB3	1:M:331:ILE:HD12	1.78	0.65
1:M:44:HIS:CD2	1:M:44:HIS:O	2.50	0.64
1:M:573:LEU:HD12	1:M:574:PRO:HD2	1.78	0.64
2:B:4:LYS:HE2	2:B:4:LYS:H	1.60	0.64
4:D:92:HIS:HA	2:N:243:ARG:O	1.97	0.64
2:N:108:HIS:O	2:N:112:SER:OG	2.13	0.64
2:N:164:ASN:C	2:N:164:ASN:OD1	2.36	0.64
1:M:478:LYS:O	1:M:482:LEU:HD23	1.97	0.64
4:P:95:ALA:HB1	4:P:98:TRP:HB2	1.79	0.64
1:A:361:ILE:HG13	1:A:380:CYS:O	1.97	0.64
1:M:320:GLY:O	1:M:324:LEU:HB2	1.98	0.64
2:B:198:GLN:HE22	4:D:10:GLU:CG	2.06	0.64
4:D:64:ARG:CG	4:D:64:ARG:HH11	2.10	0.64
1:M:226:MET:O	1:M:518:MET:HG2	1.98	0.64
3:O:53:PRO:HG3	4:P:51:TYR:CE2	2.33	0.64
3:C:125:PHE:CE2	3:C:130:TRP:HH2	2.16	0.64
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.62	0.63
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.79	0.63
1:M:97:GLU:OE2	2:N:132:ASN:O	2.15	0.63
1:A:59:HIS:H	1:A:59:HIS:CD2	2.15	0.63
1:M:192:THR:CG2	1:M:212:GLY:HA3	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:11:GLY:CA	5:M:601:FAD:O4B	2.46	0.63
1:M:155:HIS:CE1	1:M:174:ASN:CB	2.82	0.63
1:A:425:ILE:O	1:A:428:GLN:HB2	1.98	0.63
1:A:37:LYS:HE2	5:A:601:FAD:C8A	2.29	0.63
1:M:342:ASP:HB3	1:M:345:LYS:HB3	1.81	0.63
1:A:443:ASP:OD1	1:A:444:GLY:N	2.32	0.63
1:M:70:VAL:HG11	1:M:573:LEU:HD23	1.81	0.63
2:N:141:LYS:HB3	2:N:181:GLU:OE1	1.99	0.63
2:B:28:VAL:CG2	2:B:43:ILE:HD11	2.29	0.63
1:M:156:PHE:HE1	5:M:601:FAD:N6A	1.96	0.63
2:N:151:CYS:SG	9:N:246:SF4:FE1	1.85	0.62
1:M:234:THR:HA	1:M:350:VAL:HG13	1.80	0.62
1:A:10:VAL:HB	1:A:190:MET:HE3	1.80	0.62
3:C:33:VAL:HA	4:D:82:MET:HE2	1.80	0.62
1:M:360:GLY:C	1:M:382:SER:HG	2.00	0.62
3:C:50:LYS:HD3	4:D:118:ILE:HG22	1.81	0.62
1:M:61:SER:N	1:M:64:TYR:HD1	1.97	0.62
2:N:73:PRO:HG2	2:N:213:VAL:HG11	1.79	0.62
4:P:1:ILE:N	4:P:1:ILE:HD12	2.00	0.62
1:A:529:ARG:CZ	1:A:542:ARG:HD2	2.29	0.62
2:N:12:ARG:CZ	2:N:50:ASP:OD1	2.47	0.62
1:A:542:ARG:NH1	1:A:544:ASP:OD2	2.32	0.61
1:A:556:ASP:HB2	1:A:558:ASP:OD2	2.00	0.61
3:C:90:ALA:N	3:C:91:PRO:HD2	2.15	0.61
1:M:149:ILE:CD1	1:M:149:ILE:H	2.11	0.61
1:M:102:PRO:CG	1:M:134:HIS:HD2	2.12	0.61
1:M:361:ILE:O	1:M:363:THR:HG23	2.00	0.61
3:C:12:THR:HG23	3:C:14:THR:H	1.66	0.61
1:M:38:VAL:HG11	1:M:207:ILE:HG21	1.82	0.61
1:M:299:ARG:NE	1:M:299:ARG:HA	2.14	0.61
1:A:41:MET:HE3	1:A:140:PHE:CE2	2.36	0.61
1:A:202:ASN:HA	1:A:353:THR:HG22	1.80	0.61
4:D:48:ALA:O	4:D:53:ARG:HD3	2.01	0.61
1:M:113:VAL:HG12	1:M:125:TRP:HA	1.82	0.61
4:P:10:GLU:OE2	4:P:84:HIS:NE2	2.32	0.61
1:A:176:MET:HG3	3:C:4:ARG:HD3	1.83	0.61
4:D:13:PHE:HE2	4:D:97:LYS:HZ1	1.49	0.61
1:M:15:ALA:HB2	1:M:399:LEU:HD22	1.82	0.61
1:M:304:ILE:HD12	1:M:304:ILE:H	1.65	0.61
1:M:51:GLY:O	5:M:601:FAD:N3	2.33	0.61
3:C:15:TRP:O	3:C:18:LYS:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:34:THR:HG22	2:N:81:LEU:HD13	1.83	0.60
4:P:28:ALA:N	4:P:29:PRO:HD2	2.16	0.60
1:M:15:ALA:HB2	1:M:399:LEU:CD2	2.31	0.60
1:A:11:GLY:HA2	5:A:601:FAD:H1B	1.82	0.60
1:M:176:MET:CE	2:N:99:GLU:HG3	2.30	0.60
1:M:76:LEU:HG	1:M:529:ARG:HD3	1.83	0.60
4:P:10:GLU:N	4:P:11:PRO:CD	2.64	0.60
4:P:22:MET:CE	4:P:22:MET:HA	2.31	0.60
3:O:75:THR:HG22	4:P:32:ILE:CD1	2.31	0.60
2:B:240:LEU:O	2:B:242:PRO:HD3	2.00	0.60
1:M:134:HIS:O	1:M:138:THR:OG1	2.15	0.60
2:B:28:VAL:HG22	2:B:43:ILE:HD11	1.84	0.60
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.37	0.60
1:M:151:ARG:HH12	1:M:153:ASP:CG	2.03	0.60
2:N:12:ARG:NH2	2:N:101:ASP:OD1	2.31	0.60
2:B:9:GLU:HB2	2:B:25:PHE:CD2	2.37	0.60
3:O:86:TRP:CD1	4:P:22:MET:HE3	2.37	0.60
1:A:148:GLN:N	1:A:148:GLN:OE1	2.33	0.60
4:D:0:MET:CG	4:D:1:ILE:H	2.14	0.60
2:N:65:CYS:HB3	2:N:75:LEU:HD22	1.82	0.60
1:M:152:PHE:HB3	1:M:155:HIS:HD2	1.61	0.60
1:M:500:THR:HA	1:M:503:LEU:HB2	1.84	0.60
1:M:232:HIS:O	1:M:352:PRO:HA	2.01	0.59
1:M:491:ILE:HD13	1:M:491:ILE:N	2.15	0.59
2:N:9:GLU:HG3	2:N:25:PHE:CZ	2.37	0.59
3:O:33:VAL:O	3:O:36:VAL:HG22	2.01	0.59
1:M:102:PRO:CG	1:M:134:HIS:CD2	2.84	0.59
1:A:250:GLU:O	1:A:319:LEU:HD11	2.01	0.59
1:A:546:ASN:O	1:A:549:LYS:HE2	2.02	0.59
1:M:208:VAL:HG12	1:M:208:VAL:O	2.01	0.59
3:O:103:MET:HG2	3:O:104:GLY:N	2.17	0.59
2:B:3:MET:CE	2:B:29:PRO:HB2	2.31	0.59
4:D:92:HIS:HA	2:N:243:ARG:C	2.23	0.59
3:C:50:LYS:HB3	4:D:118:ILE:CG2	2.31	0.59
2:N:5:ASN:HD22	2:N:5:ASN:N	2.00	0.59
1:M:234:THR:HG22	1:M:350:VAL:HG11	1.85	0.59
2:B:170:PRO:HA	2:B:224:ILE:HD11	1.85	0.59
1:A:27:ASN:OD1	1:A:29:ASN:N	2.36	0.58
1:M:11:GLY:O	1:M:16:GLY:HA3	2.03	0.58
1:M:217:LEU:HD13	1:M:223:LEU:HG	1.84	0.58
2:N:157:ALA:HB1	2:N:209:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:74:ASP:O	1:M:75:TRP:HB2	2.02	0.58
3:O:118:VAL:O	3:O:122:VAL:HG23	2.03	0.58
1:A:493:ASP:OD1	1:A:495:SER:OG	2.20	0.58
1:A:527:GLU:CD	1:A:529:ARG:HH11	2.07	0.58
1:M:224:ARG:NH1	1:M:382:SER:O	2.36	0.58
2:N:238:ALA:O	2:N:242:PRO:HD3	2.02	0.58
1:M:34:LEU:O	1:M:151:ARG:HA	2.03	0.58
1:M:260:TYR:HE1	1:M:264:GLN:NE2	2.00	0.58
2:N:36:LEU:HD23	2:N:76:ALA:HA	1.85	0.58
1:A:119:MET:HE2	1:A:391:LEU:HD23	1.86	0.58
2:B:206:PHE:CE1	2:B:225:GLN:HG3	2.38	0.58
1:M:360:GLY:CA	1:M:382:SER:OG	2.51	0.58
1:M:392:GLY:O	1:M:393:SER:HB3	2.03	0.58
1:M:155:HIS:HE1	1:M:174:ASN:HB2	1.69	0.58
3:C:59:PHE:CE2	3:C:63:LEU:HD11	2.39	0.57
1:M:245:GLU:HG2	1:M:245:GLU:O	2.04	0.57
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.70	0.57
1:A:306:THR:HB	1:A:307:PRO:CD	2.34	0.57
1:M:198:VAL:CG1	1:M:459:MET:HG3	2.33	0.57
2:N:206:PHE:CE1	2:N:225:GLN:HG3	2.39	0.57
4:P:60:SER:O	4:P:64:ARG:HG3	2.04	0.57
1:A:336:LYS:O	1:A:340:GLY:HA2	2.04	0.57
1:A:228:PHE:O	1:A:358:MET:HB2	2.05	0.57
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.87	0.57
1:M:280:LYS:C	1:M:281:TYR:HD2	2.08	0.57
2:N:178:ARG:NH1	2:N:178:ARG:HG2	2.00	0.57
1:A:142:THR:O	1:A:145:GLN:HG2	2.04	0.57
1:A:116:PHE:HE2	6:A:577:FUM:H4	1.68	0.57
3:C:50:LYS:CG	4:D:118:ILE:HG22	2.35	0.57
2:N:235:PHE:C	2:N:235:PHE:CD2	2.78	0.57
1:A:286:PRO:O	1:A:290:VAL:HG23	2.04	0.57
3:C:33:VAL:HA	4:D:82:MET:CE	2.35	0.57
1:M:444:GLY:CA	1:M:488:ARG:O	2.53	0.57
1:M:552:LEU:HD11	1:M:566:SER:HB2	1.86	0.57
3:O:68:ILE:HD12	3:O:68:ILE:N	2.18	0.57
4:P:78:GLY:O	4:P:82:MET:HG3	2.05	0.57
1:A:10:VAL:CB	1:A:190:MET:CE	2.82	0.56
3:O:15:TRP:CD2	3:O:16:TRP:N	2.73	0.56
1:A:178:GLY:HA3	1:A:496:SER:O	2.05	0.56
3:C:94:ALA:HB1	3:C:96:ILE:HD11	1.86	0.56
4:D:112:LEU:O	4:D:116:VAL:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:342:ASP:HB3	1:M:345:LYS:HB2	1.86	0.56
4:D:92:HIS:HB3	2:N:243:ARG:CG	2.34	0.56
2:B:241:LYS:O	2:B:241:LYS:HG2	2.05	0.56
1:M:146:PHE:HB3	1:M:148:GLN:NE2	2.19	0.56
1:M:151:ARG:NH1	1:M:153:ASP:OD1	2.37	0.56
1:M:24:ALA:HA	1:M:32:ILE:HD11	1.86	0.56
3:C:54:GLU:CA	3:C:54:GLU:OE1	2.54	0.56
1:M:85:PHE:HE1	1:M:398:GLU:HA	1.71	0.56
4:P:113:ILE:O	4:P:117:THR:OG1	2.24	0.56
2:N:14:ASN:HD22	2:N:15:PRO:HD2	1.69	0.56
1:A:44:HIS:NE2	5:A:601:FAD:C8	2.65	0.56
2:N:180:ASN:ND2	2:N:188:LYS:HG3	2.20	0.56
2:N:202:TRP:CZ2	4:P:11:PRO:HG3	2.41	0.56
3:O:86:TRP:CD1	4:P:22:MET:CE	2.89	0.56
2:B:210:CYS:O	2:B:213:VAL:HG22	2.04	0.56
1:M:13:GLY:N	5:M:601:FAD:H4B	2.19	0.56
1:M:61:SER:H	1:M:64:TYR:HD1	1.51	0.56
2:N:31:ASP:OD2	2:N:31:ASP:C	2.42	0.56
3:O:15:TRP:CE3	3:O:16:TRP:HA	2.41	0.56
1:A:141:GLN:HB3	2:B:118:PRO:O	2.05	0.56
1:M:27:ASN:C	1:M:27:ASN:HD22	2.09	0.56
2:N:21:PRO:HD3	3:O:7:TYR:CE2	2.41	0.56
4:P:112:LEU:O	4:P:116:VAL:HG22	2.07	0.55
1:M:225:ASP:HB3	1:M:228:PHE:CD2	2.41	0.55
1:A:119:MET:HE1	1:A:391:LEU:HD23	1.88	0.55
1:A:529:ARG:HG3	1:A:542:ARG:HD3	1.87	0.55
4:P:51:TYR:CZ	4:P:55:LEU:HD22	2.41	0.55
2:B:194:GLN:O	2:B:197:SER:HB3	2.05	0.55
1:M:243:MET:HE2	1:M:331:ILE:HG23	1.88	0.55
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.70	0.55
1:M:243:MET:O	1:M:244:THR:HG22	2.06	0.55
1:M:24:ALA:N	1:M:32:ILE:CD1	2.69	0.55
4:P:62:ILE:O	4:P:65:VAL:HG22	2.06	0.55
3:C:130:TRP:HB2	4:D:53:ARG:NH2	2.22	0.55
3:O:33:VAL:CB	3:O:34:PRO:HD3	2.36	0.55
4:D:51:TYR:C	4:D:51:TYR:CD2	2.80	0.55
1:M:27:ASN:ND2	1:M:27:ASN:C	2.60	0.55
2:N:71:ASN:HD22	3:O:18:LYS:NZ	2.04	0.55
3:O:39:SER:OG	4:P:71:ILE:O	2.25	0.55
1:A:127:ALA:HB3	1:A:131:THR:HA	1.89	0.55
1:M:10:VAL:HG13	5:M:601:FAD:C2A	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:389:ASN:OD1	1:M:531:ALA:HB2	2.07	0.55
1:M:18:ARG:NH1	1:M:92:GLU:OE2	2.40	0.55
1:M:62:PHE:HB3	1:M:86:VAL:HG11	1.89	0.55
2:N:13:TYR:HB2	2:N:21:PRO:CB	2.29	0.55
2:B:154:CYS:HB2	2:B:170:PRO:HG2	1.88	0.54
1:M:322:LYS:O	1:M:326:GLU:HB3	2.06	0.54
1:M:93:MET:CE	1:M:400:VAL:HG21	2.37	0.54
2:N:71:ASN:HD22	3:O:18:LYS:HZ2	1.55	0.54
1:M:225:ASP:HB3	1:M:228:PHE:HD2	1.72	0.54
1:M:52:SER:O	1:M:125:TRP:N	2.39	0.54
1:M:24:ALA:HB2	1:M:32:ILE:CD1	2.35	0.54
1:M:299:ARG:HA	1:M:299:ARG:HE	1.69	0.54
2:N:241:LYS:O	2:N:243:ARG:HG2	2.06	0.54
1:A:42:ARG:HG2	2:B:64:SER:HB3	1.88	0.54
2:B:154:CYS:SG	9:B:246:SF4:S4	3.04	0.54
1:M:30:ALA:O	1:M:148:GLN:HB3	2.08	0.54
1:A:440:VAL:HG13	10:A:606:HOH:O	2.08	0.54
1:M:299:ARG:NE	1:M:299:ARG:CA	2.71	0.54
1:M:7:LEU:HD11	1:M:411:THR:CG2	2.37	0.54
1:M:97:GLU:C	1:M:97:GLU:OE1	2.46	0.54
2:N:135:THR:HB	2:N:138:GLN:HB2	1.90	0.54
2:N:8:ILE:HD11	2:N:81:LEU:HD21	1.89	0.54
1:A:273:PRO:HG2	1:A:276:GLU:HB2	1.89	0.54
1:M:151:ARG:NH1	1:M:153:ASP:CG	2.61	0.54
1:M:472:MET:SD	1:M:523:MET:HA	2.48	0.54
1:M:308:ARG:NH2	2:N:33:THR:HB	2.22	0.54
1:A:59:HIS:HD2	1:A:59:HIS:H	1.56	0.54
3:O:50:LYS:HD2	4:P:117:THR:HB	1.89	0.54
1:M:448:TRP:CH2	1:M:504:TYR:HB3	2.43	0.54
1:M:88:HIS:CB	1:M:401:VAL:HG13	2.38	0.53
1:M:94:THR:HA	2:N:131:THR:CG2	2.38	0.53
1:A:15:ALA:HB2	1:A:399:LEU:HD22	1.90	0.53
2:N:31:ASP:CG	2:N:33:THR:OG1	2.46	0.53
2:N:73:PRO:HB2	2:N:153:LEU:HD22	1.90	0.53
3:O:68:ILE:N	3:O:68:ILE:CD1	2.70	0.53
1:M:152:PHE:N	1:M:152:PHE:CD2	2.77	0.53
1:M:194:GLY:O	1:M:208:VAL:HG13	2.09	0.53
4:D:92:HIS:HD2	2:N:243:ARG:OXT	1.91	0.53
2:N:51:LEU:HD23	2:N:52:SER:N	2.23	0.53
1:A:493:ASP:C	1:A:493:ASP:OD1	2.47	0.53
2:N:236:LEU:HD23	2:N:236:LEU:C	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:19:LEU:CD2	3:O:22:TYR:CD2	2.91	0.53
1:M:94:THR:O	1:M:98:LEU:HG	2.08	0.53
2:N:153:LEU:HD12	2:N:215:PRO:HD3	1.89	0.53
3:O:33:VAL:HB	3:O:34:PRO:CD	2.37	0.53
3:C:86:TRP:CD1	4:D:22:MET:HE1	2.42	0.53
2:N:54:ARG:NH2	2:N:104:VAL:O	2.42	0.53
1:A:542:ARG:HG3	1:A:543:ASP:N	2.24	0.53
1:M:207:ILE:HG13	1:M:208:VAL:HG23	1.91	0.53
1:M:81:VAL:CG1	1:M:383:VAL:CG1	2.87	0.53
2:B:151:CYS:SG	9:B:246:SF4:S3	3.07	0.53
1:M:11:GLY:HA2	5:M:601:FAD:H1B	1.91	0.53
1:M:198:VAL:HG12	1:M:459:MET:HG3	1.89	0.53
3:O:38:PHE:HB2	3:O:75:THR:HG21	1.90	0.53
3:C:50:LYS:CB	4:D:118:ILE:HG22	2.39	0.53
1:M:396:LEU:HG	5:M:601:FAD:C2	2.38	0.53
2:N:60:ALA:HA	7:N:244:FES:S1	2.49	0.53
1:A:442:GLN:NE2	1:A:487:LYS:C	2.63	0.53
1:M:421:ASN:OD1	1:M:423:ALA:N	2.42	0.53
1:M:451:ILE:HG22	1:M:508:LEU:HD11	1.91	0.53
2:N:116:ILE:CG2	2:N:176:ALA:CB	2.78	0.53
1:A:527:GLU:OE1	1:A:529:ARG:HD2	2.10	0.52
2:N:135:THR:CG2	2:N:136:PRO:HD2	2.39	0.52
1:M:119:MET:CE	1:M:391:LEU:HD23	2.40	0.52
2:N:240:LEU:O	2:N:243:ARG:NH2	2.42	0.52
1:A:200:ARG:NH1	1:A:201:TYR:OH	2.42	0.52
1:M:42:ARG:HH22	2:N:150:ASN:C	2.10	0.52
1:M:37:LYS:HE2	5:M:601:FAD:N7A	2.24	0.52
1:M:97:GLU:OE1	1:M:98:LEU:HD23	2.10	0.52
4:P:22:MET:HE2	4:P:26:ILE:CD1	2.38	0.52
1:A:442:GLN:HE21	1:A:489:VAL:H	1.57	0.52
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.91	0.52
1:M:486:PHE:O	1:M:489:VAL:HB	2.10	0.52
1:M:211:ASP:OD2	1:M:507:GLU:HG2	2.09	0.52
1:M:524:ALA:HB2	1:M:563:LEU:CD1	2.39	0.52
1:A:154:GLU:C	1:A:175:MET:HG3	2.30	0.52
2:N:175:LEU:O	2:N:178:ARG:HB3	2.10	0.52
4:P:50:SER:O	4:P:53:ARG:N	2.43	0.52
1:M:146:PHE:HB3	1:M:149:ILE:CD1	2.38	0.52
2:N:123:ASN:ND2	2:N:184:ARG:O	2.43	0.52
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.45	0.52
1:M:101:CYS:N	2:N:184:ARG:NH2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:103:TRP:O	1:M:105:ARG:HG3	2.10	0.52
1:M:243:MET:CE	1:M:331:ILE:HG23	2.39	0.52
1:M:93:MET:CE	1:M:93:MET:CA	2.87	0.52
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.10	0.52
2:B:188:LYS:HZ3	2:B:230:GLU:HG3	1.75	0.52
2:N:178:ARG:CG	2:N:178:ARG:HH11	2.07	0.52
1:A:43:SER:O	1:A:46:VAL:HG12	2.10	0.51
1:A:317:ARG:HD3	1:A:345:LYS:O	2.10	0.51
3:C:59:PHE:O	3:C:62:PHE:HB3	2.11	0.51
1:M:23:ALA:CB	1:M:32:ILE:HG21	2.40	0.51
1:M:225:ASP:OD2	1:M:550:HIS:HD2	1.93	0.51
4:P:33:LEU:HA	4:P:37:ILE:HG13	1.91	0.51
3:C:63:LEU:HB3	4:D:40:PRO:HG3	1.93	0.51
4:D:62:ILE:CG2	4:D:63:GLY:N	2.74	0.51
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.46	0.51
1:M:525:ARG:NH2	1:M:549:LYS:O	2.36	0.51
1:M:24:ALA:CA	1:M:32:ILE:CD1	2.87	0.51
1:M:527:GLU:CD	1:M:529:ARG:HH12	2.09	0.51
4:D:92:HIS:CD2	2:N:243:ARG:OXT	2.64	0.51
3:O:9:ARG:HB3	3:O:10:PRO:HD2	1.91	0.51
1:A:448:TRP:CG	1:A:449:ALA:N	2.78	0.51
1:A:356:TYR:HE1	5:A:601:FAD:O3'	1.93	0.51
1:M:510:HIS:O	1:M:514:VAL:HG23	2.11	0.51
1:M:100:GLY:C	2:N:184:ARG:HH21	1.92	0.51
1:A:50:GLY:HA3	1:A:116:PHE:CZ	2.46	0.51
1:A:257:LYS:NZ	1:A:301:GLY:O	2.39	0.51
2:N:151:CYS:SG	9:N:246:SF4:S3	3.09	0.51
2:N:57:CYS:O	2:N:58:ARG:HB2	2.11	0.51
2:B:188:LYS:NZ	2:B:230:GLU:HG3	2.25	0.51
1:M:34:LEU:N	1:M:150:GLN:O	2.36	0.51
1:M:414:ALA:HA	1:M:417:ALA:HB2	1.93	0.51
1:M:211:ASP:OD1	1:M:507:GLU:HA	2.11	0.51
1:M:51:GLY:N	5:M:601:FAD:O4	2.44	0.51
2:N:155:TYR:CE1	2:N:170:PRO:HD2	2.46	0.51
1:M:447:ASN:ND2	2:N:45:ASP:O	2.44	0.51
2:N:206:PHE:HA	8:N:245:F3S:S1	2.51	0.51
1:A:525:ARG:NH2	1:A:549:LYS:O	2.39	0.51
1:M:524:ALA:CB	1:M:563:LEU:CD1	2.89	0.51
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.93	0.50
3:C:130:TRP:HB2	4:D:53:ARG:HH21	1.75	0.50
2:N:112:SER:O	2:N:116:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:ARG:NH1	2:N:62:CYS:O	2.44	0.50
3:O:59:PHE:O	3:O:62:PHE:HB3	2.11	0.50
4:P:64:ARG:HH21	4:P:116:VAL:HA	1.77	0.50
1:A:493:ASP:OD2	1:A:495:SER:OG	2.29	0.50
1:M:263:LEU:CD1	1:M:283:GLU:HA	2.41	0.50
1:M:535:LEU:O	1:M:540:THR:HG22	2.11	0.50
1:M:61:SER:HB3	1:M:64:TYR:CD1	2.47	0.50
1:A:527:GLU:OE1	1:A:529:ARG:NH1	2.41	0.50
2:N:64:SER:O	2:N:66:GLY:N	2.45	0.50
1:A:279:ASN:O	1:A:280:LYS:HB2	2.12	0.50
1:A:442:GLN:HG2	1:A:489:VAL:O	2.11	0.50
2:B:204:CYS:SG	8:B:245:F3S:S2	2.90	0.50
4:D:92:HIS:HB3	2:N:243:ARG:HG3	1.94	0.50
1:M:155:HIS:HE1	1:M:174:ASN:CB	2.20	0.50
1:M:232:HIS:HE1	1:M:244:THR:O	1.93	0.50
1:M:342:ASP:O	1:M:346:GLU:N	2.44	0.50
1:M:48:ALA:HA	5:M:601:FAD:C6	2.42	0.50
1:M:388:ALA:HB2	1:M:529:ARG:HD3	1.93	0.50
4:D:92:HIS:C	2:N:243:ARG:HB2	2.32	0.50
3:O:28:ARG:O	3:O:31:THR:HB	2.11	0.50
1:A:84:TYR:CE1	1:A:88:HIS:CE1	2.99	0.50
2:B:115:ALA:HB2	4:D:1:ILE:HD12	1.94	0.50
2:B:234:ASP:OD1	4:D:7:ARG:NH2	2.45	0.50
2:B:13:TYR:OH	3:C:5:LYS:O	2.25	0.50
1:M:158:LEU:HD13	1:M:436:LEU:HD23	1.94	0.50
1:M:168:ARG:HD3	10:M:577:HOH:O	1.78	0.50
4:P:50:SER:O	4:P:51:TYR:C	2.50	0.50
1:A:97:GLU:OE1	1:A:105:ARG:NH2	2.45	0.50
2:B:3:MET:HE1	2:B:29:PRO:HB2	1.94	0.50
1:M:224:ARG:CB	1:M:552:LEU:HD23	2.41	0.50
2:N:28:VAL:CG1	2:N:29:PRO:HD2	2.42	0.50
1:M:521:SER:HA	1:M:551:THR:HG21	1.94	0.50
1:M:7:LEU:HD22	1:M:187:ALA:HB3	1.93	0.50
1:M:256:ASN:HB2	1:M:302:ASN:O	2.12	0.50
4:D:22:MET:HE2	4:D:22:MET:HA	1.94	0.49
1:M:113:VAL:HB	1:M:124:THR:O	2.11	0.49
1:M:70:VAL:CG1	1:M:573:LEU:HD23	2.41	0.49
2:B:149:ILE:HG23	2:B:216:LYS:HG3	1.93	0.49
2:B:241:LYS:O	2:B:241:LYS:HG3	2.12	0.49
3:C:2:THR:HG1	3:C:4:ARG:H	1.60	0.49
1:M:105:ARG:NH1	2:N:134:GLN:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:44:LYS:HA	2:N:48:ALA:O	2.12	0.49
2:N:51:LEU:HA	2:N:101:ASP:OD1	2.13	0.49
4:P:27:ILE:C	4:P:29:PRO:HD2	2.33	0.49
1:A:262:TYR:OH	1:A:312:VAL:HG11	2.13	0.49
1:A:493:ASP:CG	1:A:495:SER:OG	2.51	0.49
1:A:556:ASP:CB	1:A:558:ASP:OD2	2.59	0.49
2:B:154:CYS:SG	9:B:246:SF4:S3	2.95	0.49
1:M:114:ARG:NE	1:M:116:PHE:HE1	2.11	0.49
1:M:48:ALA:O	1:M:132:GLY:N	2.43	0.49
1:M:177:GLU:OE1	1:M:177:GLU:HA	2.11	0.49
1:M:331:ILE:HA	1:M:334:LEU:HD12	1.95	0.49
2:N:135:THR:HG22	2:N:136:PRO:HD2	1.95	0.49
2:N:155:TYR:HE1	2:N:171:ALA:CB	2.25	0.49
3:O:56:TRP:CD1	4:P:51:TYR:HB2	2.47	0.49
3:C:98:VAL:HG23	3:C:98:VAL:O	2.12	0.49
1:M:85:PHE:CD2	1:M:385:LEU:HD11	2.48	0.49
4:P:10:GLU:N	4:P:11:PRO:HD2	2.28	0.49
1:A:10:VAL:CB	1:A:190:MET:HE3	2.41	0.49
1:A:27:ASN:OD1	1:A:30:ALA:N	2.42	0.49
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.94	0.49
1:M:17:LEU:HD22	1:M:140:PHE:HA	1.94	0.49
1:M:245:GLU:HG3	1:M:248:ARG:NH2	2.28	0.49
1:M:395:SER:OG	5:M:601:FAD:H2'	2.12	0.49
4:P:2:ASN:HB2	4:P:3:PRO:CD	2.42	0.49
1:M:158:LEU:CD1	1:M:436:LEU:HD23	2.42	0.49
2:N:5:ASN:N	2:N:5:ASN:ND2	2.60	0.49
1:M:378:GLY:HA2	1:M:399:LEU:HD23	1.94	0.49
2:N:28:VAL:HG13	2:N:29:PRO:HD2	1.94	0.49
3:O:28:ARG:HG3	3:O:85:THR:HG21	1.95	0.49
1:A:536:ASP:OD1	1:A:536:ASP:N	2.40	0.49
4:D:39:LEU:HB3	4:D:40:PRO:HD3	1.95	0.49
1:M:7:LEU:HD21	1:M:411:THR:HA	1.94	0.49
3:O:19:LEU:HD23	3:O:22:TYR:CD2	2.48	0.49
4:P:22:MET:HE2	4:P:26:ILE:HD12	1.95	0.49
1:M:161:LEU:HD21	1:M:171:VAL:HG23	1.95	0.49
1:M:365:GLN:H	1:M:365:GLN:CD	2.16	0.49
1:M:186:ASN:HB3	1:M:417:ALA:HB1	1.95	0.49
1:M:472:MET:HE1	1:M:532:HIS:CE1	2.48	0.49
1:M:78:GLU:OE1	1:M:550:HIS:HE1	1.96	0.49
1:A:256:ASN:HB2	1:A:302:ASN:O	2.12	0.48
1:M:499:ASN:O	1:M:503:LEU:HG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:86:MET:CE	4:P:91:ILE:HG21	2.42	0.48
2:B:188:LYS:NZ	2:B:230:GLU:CG	2.77	0.48
2:N:185:ASP:OD2	2:N:185:ASP:C	2.52	0.48
1:A:44:HIS:CE1	1:A:204:ASN:HA	2.48	0.48
1:M:28:PRO:O	1:M:148:GLN:HG2	2.12	0.48
1:M:442:GLN:NE2	1:M:487:LYS:HA	2.29	0.48
1:M:225:ASP:OD1	1:M:550:HIS:HB3	2.13	0.48
4:P:30:VAL:O	4:P:33:LEU:HB3	2.13	0.48
4:P:42:GLY:C	4:P:44:PHE:H	2.16	0.48
3:C:50:LYS:CD	4:D:118:ILE:HG22	2.43	0.48
1:M:85:PHE:CE1	1:M:398:GLU:HA	2.49	0.48
2:N:109:PHE:CZ	2:N:113:LEU:HD11	2.48	0.48
1:M:31:LYS:O	1:M:31:LYS:HD3	2.14	0.48
1:M:232:HIS:CE1	1:M:242:LEU:CD1	2.97	0.48
1:M:75:TRP:O	1:M:568:VAL:HG11	2.14	0.48
2:N:134:GLN:NE2	2:N:184:ARG:HH11	2.11	0.48
1:A:292:GLN:HG2	1:A:466:TYR:CZ	2.48	0.48
3:C:50:LYS:CD	4:D:118:ILE:H	2.26	0.48
1:M:363:THR:HG21	1:M:376:ALA:HB3	1.94	0.48
2:N:54:ARG:HH21	2:N:103:VAL:HG12	1.78	0.48
3:O:114:ALA:O	3:O:118:VAL:HG23	2.14	0.48
3:O:63:LEU:O	3:O:69:VAL:HG22	2.13	0.48
1:A:40:PRO:HG2	1:A:140:PHE:CE1	2.48	0.48
1:M:82:VAL:HG22	1:M:385:LEU:HD12	1.96	0.48
2:B:3:MET:HE2	2:B:29:PRO:HB2	1.96	0.48
2:B:28:VAL:HG22	2:B:43:ILE:CD1	2.42	0.48
1:A:62:PHE:CZ	1:A:90:PRO:HG2	2.49	0.47
3:O:18:LYS:HG2	3:O:19:LEU:HD22	1.94	0.47
3:O:65:ASN:O	3:O:69:VAL:HG23	2.14	0.47
4:P:9:ASP:C	4:P:11:PRO:CD	2.79	0.47
1:M:102:PRO:CD	1:M:134:HIS:HD2	2.27	0.47
1:M:223:LEU:HD13	1:M:226:MET:HE2	1.96	0.47
2:N:5:ASN:HA	2:N:28:VAL:O	2.14	0.47
2:N:57:CYS:HB3	2:N:62:CYS:HB3	1.96	0.47
2:N:7:LYS:HE2	2:N:25:PHE:CD1	2.49	0.47
3:O:68:ILE:H	3:O:68:ILE:CD1	2.26	0.47
2:B:42:TYR:CD2	2:B:42:TYR:C	2.87	0.47
1:M:194:GLY:HA2	1:M:379:GLU:HG2	1.95	0.47
1:M:88:HIS:HB3	1:M:401:VAL:HG13	1.95	0.47
3:O:43:ILE:HG13	4:P:71:ILE:HD13	1.96	0.47
1:A:529:ARG:NH2	1:A:542:ARG:HD2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:GLY:N	3:C:59:PHE:CE1	2.82	0.47
1:M:37:LYS:HD3	1:M:156:PHE:CD1	2.49	0.47
1:M:290:VAL:O	1:M:293:ALA:HB3	2.14	0.47
2:N:14:ASN:HD22	2:N:15:PRO:CD	2.27	0.47
3:C:56:TRP:O	3:C:59:PHE:HB3	2.15	0.47
1:M:101:CYS:C	2:N:184:ARG:HH22	2.18	0.47
1:M:76:LEU:HD12	1:M:228:PHE:CZ	2.50	0.47
1:M:252:GLY:HA3	1:M:316:LEU:CD2	2.44	0.47
1:M:332:CYS:O	1:M:336:LYS:HG3	2.15	0.47
2:N:30:TYR:HA	2:N:34:THR:OG1	2.14	0.47
1:A:396:LEU:HG	5:A:601:FAD:C2	2.45	0.47
3:C:113:TRP:O	3:C:117:VAL:HG23	2.15	0.47
1:M:146:PHE:CB	1:M:149:ILE:HD11	2.44	0.47
1:M:194:GLY:CA	1:M:379:GLU:HG2	2.44	0.47
1:M:432:VAL:HA	1:M:435:ARG:HH11	1.79	0.47
4:P:38:LEU:HD22	4:P:43:LEU:HB2	1.96	0.47
2:B:116:ILE:HD12	2:B:172:ALA:O	2.15	0.47
3:C:125:PHE:CE2	3:C:130:TRP:CH2	3.01	0.47
4:D:109:VAL:O	4:D:112:LEU:HB3	2.15	0.47
2:N:226:GLN:HE21	2:N:226:GLN:HB2	1.57	0.47
1:M:38:VAL:HG11	1:M:207:ILE:CG2	2.44	0.47
1:M:261:ARG:HD3	1:M:271:GLU:OE1	2.15	0.47
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.95	0.47
3:O:15:TRP:HZ3	3:O:22:TYR:CG	2.33	0.47
1:M:114:ARG:NE	1:M:116:PHE:CE1	2.83	0.47
3:O:53:PRO:HG3	4:P:51:TYR:CD2	2.49	0.47
1:A:398:GLU:HG3	1:A:402:PHE:CD1	2.50	0.46
1:M:101:CYS:N	2:N:184:ARG:HH22	2.14	0.46
2:N:36:LEU:HD21	2:N:67:MET:SD	2.55	0.46
1:M:224:ARG:HG2	1:M:362:GLU:HA	1.97	0.46
1:M:7:LEU:HD12	1:M:23:ALA:HB1	1.96	0.46
1:A:159:ASP:OD1	1:A:160:ILE:N	2.48	0.46
1:M:57:GLN:HB2	1:M:59:HIS:CD2	2.51	0.46
1:A:232:HIS:O	1:A:352:PRO:HA	2.15	0.46
3:C:49:LEU:HG	4:D:55:LEU:HD12	1.96	0.46
1:M:177:GLU:OE1	3:O:2:THR:HB	2.16	0.46
1:M:94:THR:HA	2:N:131:THR:HG22	1.97	0.46
4:D:92:HIS:CA	2:N:243:ARG:HB2	2.44	0.46
4:D:64:ARG:HH22	4:D:117:THR:CG2	2.28	0.46
2:N:96:PHE:HB3	2:N:104:VAL:HB	1.97	0.46
1:A:454:GLU:CD	1:A:485:ARG:HH22	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:CYS:HG	7:B:244:FES:FE2	1.31	0.46
3:C:36:VAL:HG23	4:D:78:GLY:HA3	1.96	0.46
2:N:15:PRO:HG3	2:N:99:GLU:O	2.15	0.46
1:M:203:THR:CG2	1:M:353:THR:HG23	2.46	0.46
4:P:72:VAL:O	4:P:75:LEU:HB2	2.16	0.46
1:A:10:VAL:CG2	1:A:190:MET:HE3	2.46	0.46
1:M:130:LYS:NZ	2:N:216:LYS:HD2	2.31	0.46
1:M:154:GLU:O	1:M:175:MET:HB2	2.16	0.46
1:M:203:THR:HG22	1:M:353:THR:HG23	1.98	0.46
2:B:204:CYS:SG	8:B:245:F3S:S3	3.14	0.46
1:M:122:GLU:HG2	1:M:122:GLU:O	2.15	0.46
1:M:158:LEU:HG	1:M:506:ILE:CD1	2.40	0.46
1:M:444:GLY:CA	1:M:488:ARG:C	2.78	0.46
2:B:6:LEU:HD23	2:B:8:ILE:HG12	1.99	0.45
2:B:99:GLU:CD	3:C:4:ARG:HH11	2.20	0.45
1:M:320:GLY:O	1:M:324:LEU:CB	2.63	0.45
1:M:358:MET:SD	1:M:390:ARG:N	2.89	0.45
1:M:227:GLU:HB3	1:M:521:SER:HB2	1.98	0.45
2:N:36:LEU:HB3	2:N:76:ALA:O	2.17	0.45
1:A:398:GLU:HG3	1:A:402:PHE:HD1	1.80	0.45
1:A:395:SER:O	1:A:399:LEU:HG	2.15	0.45
1:M:51:GLY:HA2	1:M:131:THR:HG21	1.97	0.45
1:M:98:LEU:CD2	2:N:132:ASN:ND2	2.79	0.45
4:D:31:MET:HG3	4:D:70:MET:SD	2.57	0.45
1:M:113:VAL:HG23	1:M:122:GLU:O	2.16	0.45
2:B:26:TYR:HB3	2:B:43:ILE:HD12	1.97	0.45
4:D:35:VAL:O	4:D:40:PRO:HD3	2.16	0.45
1:A:7:LEU:HD21	1:A:410:ALA:HB1	1.99	0.45
2:B:112:SER:HA	4:D:1:ILE:CD1	2.46	0.45
2:N:219:ASP:N	2:N:220:PRO:CD	2.79	0.45
4:P:2:ASN:HB2	4:P:3:PRO:HD2	1.99	0.45
1:A:549:LYS:HA	1:A:568:VAL:HG23	1.98	0.45
2:B:226:GLN:OE1	3:C:95:ASN:ND2	2.49	0.45
2:N:155:TYR:HE1	2:N:171:ALA:HB3	1.81	0.45
1:A:93:MET:HB3	1:A:125:TRP:CZ3	2.52	0.45
2:N:17:VAL:O	2:N:17:VAL:HG12	2.16	0.45
2:N:204:CYS:CB	2:N:224:ILE:HG21	2.47	0.45
1:A:74:ASP:O	1:A:75:TRP:HB2	2.16	0.45
2:B:2:GLU:CD	2:B:2:GLU:N	2.70	0.45
4:D:63:GLY:O	4:D:67:LEU:HD22	2.17	0.45
1:M:243:MET:O	1:M:244:THR:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:27:ASN:O	1:M:30:ALA:HB3	2.17	0.45
2:N:149:ILE:HD11	2:N:151:CYS:HB3	1.99	0.45
4:D:94:PRO:HG3	2:N:243:ARG:HE	1.82	0.45
2:N:65:CYS:HB3	2:N:75:LEU:CD2	2.46	0.45
3:O:15:TRP:CE3	3:O:16:TRP:CA	3.00	0.45
4:P:42:GLY:O	4:P:44:PHE:N	2.38	0.45
1:A:227:GLU:HB2	1:A:522:ALA:HB2	1.98	0.45
4:D:110:VAL:O	4:D:113:ILE:HB	2.17	0.45
1:M:242:LEU:CG	1:M:244:THR:H	2.25	0.45
3:O:53:PRO:HA	3:O:56:TRP:HB3	1.98	0.45
1:A:251:GLY:HA2	10:A:617:HOH:O	2.17	0.45
1:A:317:ARG:HD3	1:A:345:LYS:C	2.37	0.45
2:B:18:ASP:OD1	2:B:22:HIS:NE2	2.50	0.45
1:M:176:MET:CE	2:N:99:GLU:CG	2.94	0.45
1:M:245:GLU:HG3	1:M:248:ARG:CZ	2.47	0.45
1:M:38:VAL:HB	1:M:42:ARG:HB2	1.98	0.45
2:N:164:ASN:OD1	2:N:166:GLU:N	2.50	0.45
1:M:206:GLY:HA3	2:N:55:TRP:CZ3	2.52	0.45
1:A:253:ILE:HG13	1:A:315:ASP:HB3	1.99	0.44
3:O:127:ALA:C	3:O:128:LEU:HD23	2.37	0.44
2:B:238:ALA:HA	2:B:241:LYS:HD3	1.99	0.44
1:M:446:GLU:O	1:M:489:VAL:HG22	2.18	0.44
2:N:226:GLN:OE1	3:O:95:ASN:HB2	2.17	0.44
3:O:90:ALA:N	3:O:91:PRO:CD	2.79	0.44
2:B:109:PHE:HE1	2:B:155:TYR:CE1	2.35	0.44
2:B:82:ARG:HG3	2:B:83:ASP:N	2.32	0.44
3:C:103:MET:HG2	3:C:104:GLY:O	2.17	0.44
1:M:223:LEU:HB3	1:M:226:MET:CG	2.47	0.44
1:M:44:HIS:HD2	1:M:44:HIS:O	1.98	0.44
1:M:472:MET:CE	1:M:532:HIS:HE1	2.30	0.44
2:N:5:ASN:C	2:N:30:TYR:HE2	2.21	0.44
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.53	0.44
1:M:212:GLY:HA2	1:M:215:MET:HE2	1.99	0.44
1:M:304:ILE:HG12	1:M:313:TYR:CE1	2.53	0.44
1:M:98:LEU:HD21	2:N:130:GLY:O	2.17	0.44
1:A:162:VAL:HA	1:A:166:HIS:O	2.17	0.44
3:C:99:LYS:O	3:C:100:ASP:HB2	2.17	0.44
1:M:237:PRO:HB2	1:M:308:ARG:CB	2.44	0.44
2:N:154:CYS:HB2	2:N:170:PRO:CG	2.36	0.44
3:O:112:LEU:HD23	3:O:112:LEU:HA	1.85	0.44
2:B:204:CYS:SG	8:B:245:F3S:S1	3.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:161:LEU:HA	1:M:428:GLN:OE1	2.17	0.44
1:M:35:ILE:CD1	1:M:170:LEU:HD21	2.47	0.44
2:N:155:TYR:CE1	2:N:171:ALA:HB3	2.52	0.44
4:D:95:ALA:HB2	2:N:240:LEU:HD23	2.00	0.44
1:M:135:MET:CE	1:M:396:LEU:HD22	2.48	0.44
1:M:18:ARG:HH21	1:M:22:ALA:HB2	1.81	0.44
1:M:322:LYS:O	1:M:326:GLU:N	2.40	0.44
1:M:478:LYS:HA	1:M:478:LYS:HD2	1.80	0.44
1:A:46:VAL:HB	1:A:136:LEU:CD2	2.48	0.43
1:M:135:MET:HE1	1:M:396:LEU:HB3	1.99	0.43
2:N:178:ARG:CG	2:N:178:ARG:NH1	2.71	0.43
3:C:45:GLY:O	3:C:49:LEU:HB2	2.17	0.43
1:M:150:GLN:HG3	1:M:152:PHE:CE2	2.54	0.43
2:N:89:LYS:NZ	2:N:91:GLU:OE2	2.38	0.43
3:O:15:TRP:CE3	3:O:16:TRP:N	2.86	0.43
4:P:9:ASP:O	4:P:12:VAL:HG23	2.17	0.43
1:A:256:ASN:OD1	1:A:258:ASN:N	2.48	0.43
1:A:525:ARG:NH1	1:A:527:GLU:OE1	2.51	0.43
1:A:527:GLU:OE2	1:A:529:ARG:NH1	2.51	0.43
1:M:113:VAL:HG11	1:M:125:TRP:CD1	2.54	0.43
1:M:162:VAL:HG22	1:M:167:VAL:HA	2.00	0.43
1:M:27:ASN:O	1:M:30:ALA:CB	2.66	0.43
1:M:322:LYS:O	1:M:326:GLU:CB	2.66	0.43
1:M:11:GLY:HA3	1:M:191:ALA:O	2.18	0.43
2:N:51:LEU:HD22	2:N:53:TYR:HD2	1.82	0.43
1:A:442:GLN:HE22	1:A:487:LYS:HA	1.82	0.43
2:B:163:LEU:HG	3:C:11:MET:CE	2.47	0.43
1:M:88:HIS:HB2	1:M:401:VAL:HG13	1.99	0.43
2:N:214:CYS:SG	2:N:218:VAL:CG2	3.06	0.43
4:D:2:ASN:HA	4:D:3:PRO:HD2	1.74	0.43
1:M:10:VAL:HG22	1:M:157:VAL:HG11	1.99	0.43
1:M:203:THR:HG22	1:M:353:THR:CG2	2.48	0.43
1:M:203:THR:HG23	1:M:354:ALA:O	2.18	0.43
1:M:441:ASN:O	1:M:442:GLN:C	2.57	0.43
4:P:50:SER:C	4:P:52:GLU:N	2.72	0.43
2:B:121:ILE:HB	2:B:187:GLY:HA3	2.01	0.43
2:B:18:ASP:OD1	2:B:22:HIS:CD2	2.71	0.43
4:D:72:VAL:HG22	4:D:108:THR:HA	2.01	0.43
1:M:10:VAL:CG2	1:M:157:VAL:HG11	2.49	0.43
1:M:76:LEU:CD1	1:M:228:PHE:CZ	3.02	0.43
2:B:4:LYS:HE3	2:B:4:LYS:N	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLY:HA3	2:B:55:TRP:CH2	2.54	0.43
4:P:28:ALA:N	4:P:29:PRO:CD	2.81	0.43
1:A:369:THR:HG23	1:A:374:LEU:O	2.19	0.43
1:M:7:LEU:CD2	1:M:187:ALA:HB3	2.49	0.43
2:N:211:SER:OG	2:N:219:ASP:HA	2.19	0.43
3:O:86:TRP:HD1	4:P:22:MET:HE1	1.83	0.43
2:B:158:CYS:SG	2:B:160:GLN:HB2	2.59	0.43
1:M:7:LEU:HD11	1:M:411:THR:HG23	2.01	0.43
2:N:39:ALA:O	2:N:43:ILE:HG12	2.19	0.43
2:N:12:ARG:NH2	2:N:51:LEU:HA	2.34	0.43
1:A:308:ARG:HE	1:A:308:ARG:HB2	1.68	0.42
1:A:7:LEU:HD12	1:A:23:ALA:HB1	2.01	0.42
4:D:50:SER:O	4:D:51:TYR:C	2.56	0.42
1:M:93:MET:HE3	1:M:400:VAL:HG21	1.99	0.42
1:M:471:LEU:HD23	1:M:471:LEU:HA	1.93	0.42
1:M:399:LEU:CD2	5:M:601:FAD:O2P	2.67	0.42
2:N:241:LYS:HG3	2:N:242:PRO:N	2.34	0.42
2:N:64:SER:C	2:N:66:GLY:H	2.22	0.42
1:A:245:GLU:O	1:A:248:ARG:N	2.40	0.42
1:A:76:LEU:HD22	1:A:568:VAL:HG21	2.01	0.42
2:B:7:LYS:HE3	2:B:25:PHE:HB3	2.00	0.42
4:D:13:PHE:HE2	4:D:97:LYS:NZ	2.15	0.42
1:M:200:ARG:NH1	1:M:201:TYR:OH	2.52	0.42
1:M:501:ASP:O	1:M:505:THR:OG1	2.23	0.42
1:M:58:ASP:C	1:M:60:ASP:H	2.22	0.42
2:N:153:LEU:HB2	9:N:246:SF4:S3	2.59	0.42
3:O:36:VAL:HG23	3:O:37:TRP:N	2.34	0.42
4:P:54:VAL:O	4:P:57:PHE:HB3	2.19	0.42
2:B:106:MET:O	2:B:109:PHE:HB3	2.19	0.42
3:C:31:THR:O	3:C:34:PRO:HD2	2.19	0.42
4:D:113:ILE:HG12	4:P:113:ILE:HG12	2.01	0.42
1:M:176:MET:HB3	1:M:176:MET:HE3	1.68	0.42
1:M:498:PHE:CD2	2:N:103:VAL:HG21	2.54	0.42
2:B:235:PHE:C	2:B:235:PHE:CD2	2.93	0.42
2:B:220:PRO:HG3	9:B:246:SF4:S1	2.58	0.42
1:M:495:SER:O	1:M:499:ASN:HB2	2.20	0.42
1:M:537:GLU:CD	1:M:537:GLU:N	2.51	0.42
3:C:105:PRO:HD2	3:C:106:GLU:CD	2.39	0.42
3:C:91:PRO:HB2	3:C:105:PRO:HB3	2.01	0.42
1:M:98:LEU:HD22	2:N:132:ASN:ND2	2.35	0.42
2:N:43:ILE:HD13	2:N:47:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:SER:OG	1:A:241:ILE:HG13	2.19	0.42
1:M:232:HIS:CE1	1:M:242:LEU:HD11	2.55	0.42
1:M:421:ASN:O	1:M:425:ILE:HG12	2.19	0.42
2:N:150:ASN:OD1	2:N:150:ASN:N	2.53	0.42
1:M:493:ASP:OD1	2:N:50:ASP:CB	2.68	0.42
1:M:200:ARG:HD3	1:M:201:TYR:CE1	2.54	0.42
1:M:52:SER:O	1:M:125:TRP:HB2	2.20	0.42
1:M:544:ASP:O	1:M:548:LEU:HB2	2.20	0.42
1:M:572:THR:O	1:M:574:PRO:HD3	2.19	0.42
1:M:45:THR:OG1	5:M:601:FAD:O2A	2.33	0.42
2:N:40:LEU:HB3	2:N:53:TYR:CE2	2.55	0.42
1:A:48:ALA:HA	5:A:601:FAD:C6	2.50	0.42
1:M:223:LEU:HB3	1:M:226:MET:HG3	2.01	0.42
1:M:78:GLU:OE1	1:M:568:VAL:HA	2.19	0.42
2:N:185:ASP:OD1	2:N:191:ARG:NH2	2.45	0.42
3:O:86:TRP:NE1	4:P:22:MET:HE3	2.34	0.42
1:A:332:CYS:HA	1:A:343:PRO:HG2	2.01	0.42
1:A:446:GLU:HB2	1:A:488:ARG:O	2.20	0.42
1:A:442:GLN:NE2	1:A:486:PHE:O	2.53	0.42
1:M:203:THR:OG1	5:M:601:FAD:HM83	2.20	0.42
1:M:23:ALA:HB3	1:M:32:ILE:HG21	2.02	0.42
2:N:65:CYS:O	2:N:66:GLY:C	2.57	0.42
4:P:23:TRP:CD2	4:P:27:ILE:HD13	2.55	0.42
1:A:161:LEU:HD21	1:A:171:VAL:HG23	2.02	0.42
1:A:446:GLU:HB2	1:A:489:VAL:HA	2.02	0.42
4:D:24:SER:O	4:D:28:ALA:HB3	2.20	0.42
2:N:204:CYS:HB2	2:N:224:ILE:HG21	2.01	0.42
2:N:235:PHE:HA	4:P:7:ARG:NH2	2.34	0.42
2:N:48:ALA:HA	2:N:49:PRO:HD3	1.80	0.42
4:P:26:ILE:HG22	4:P:27:ILE:HG13	2.01	0.42
3:C:63:LEU:CD1	4:D:39:LEU:HD23	2.50	0.41
1:M:260:TYR:CZ	1:M:264:GLN:NE2	2.62	0.41
1:M:38:VAL:HG22	5:M:601:FAD:O2B	2.20	0.41
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.55	0.41
1:A:205:GLY:HA2	2:B:56:SER:O	2.20	0.41
1:M:23:ALA:HB1	1:M:32:ILE:HG21	2.02	0.41
1:M:46:VAL:HG23	1:M:133:PHE:HA	2.02	0.41
2:N:151:CYS:SG	2:N:153:LEU:HB2	2.60	0.41
2:N:99:GLU:HA	2:N:99:GLU:OE1	2.21	0.41
3:O:106:GLU:N	3:O:107:PRO:CD	2.83	0.41
4:P:39:LEU:N	4:P:40:PRO:HD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:238:GLY:HA3	1:M:308:ARG:HD2	2.02	0.41
2:N:61:ILE:O	2:N:61:ILE:HG13	2.19	0.41
4:P:42:GLY:HA2	4:P:44:PHE:CE2	2.54	0.41
1:A:306:THR:CB	1:A:307:PRO:CD	2.95	0.41
1:M:213:MET:CB	1:M:223:LEU:HD21	2.48	0.41
2:N:242:PRO:O	2:N:243:ARG:OXT	2.38	0.41
4:P:73:LEU:HB2	4:P:74:PRO:HD3	2.02	0.41
1:A:10:VAL:HG11	1:A:190:MET:HE1	2.03	0.41
2:B:110:ILE:O	2:B:114:GLU:HG3	2.21	0.41
3:C:65:ASN:O	3:C:69:VAL:HG23	2.20	0.41
1:M:404:ARG:HG2	1:M:408:GLU:OE1	2.21	0.41
2:N:216:LYS:HA	2:N:216:LYS:HD3	1.78	0.41
2:N:94:ALA:HA	3:O:9:ARG:NH2	2.36	0.41
3:O:15:TRP:CZ3	3:O:16:TRP:HA	2.55	0.41
3:O:33:VAL:CB	3:O:34:PRO:CD	2.97	0.41
3:O:49:LEU:HD21	4:P:55:LEU:CA	2.48	0.41
1:A:232:HIS:ND1	1:A:242:LEU:HD11	2.34	0.41
1:M:170:LEU:HG	1:M:183:ILE:HB	2.02	0.41
1:M:232:HIS:CE1	1:M:244:THR:O	2.73	0.41
1:M:392:GLY:O	1:M:393:SER:CB	2.67	0.41
3:O:98:VAL:HG23	3:O:103:MET:HB2	2.02	0.41
3:C:72:ASN:HA	3:C:72:ASN:HD22	1.62	0.41
1:M:174:ASN:HB3	1:M:177:GLU:HB2	2.01	0.41
1:M:18:ARG:NH2	1:M:404:ARG:HG3	2.36	0.41
1:M:261:ARG:NH1	1:M:272:THR:O	2.35	0.41
1:M:79:GLN:NE2	1:M:571:THR:N	2.60	0.41
1:M:91:THR:HG22	1:M:92:GLU:OE1	2.21	0.41
2:N:149:ILE:CG2	2:N:216:LYS:HG3	2.39	0.41
2:N:4:LYS:HB3	2:N:30:TYR:CE2	2.56	0.41
1:A:442:GLN:NE2	1:A:487:LYS:HA	2.36	0.41
4:D:50:SER:O	4:D:54:VAL:HG23	2.20	0.41
1:M:142:THR:O	1:M:145:GLN:HB3	2.20	0.41
1:M:328:LEU:CB	1:M:331:ILE:HD12	2.49	0.41
1:M:206:GLY:HA3	2:N:55:TRP:CH2	2.56	0.41
3:O:18:LYS:CE	3:O:19:LEU:HD22	2.47	0.41
1:A:147:PRO:HD2	1:A:148:GLN:OE1	2.21	0.41
1:A:542:ARG:HH11	1:A:544:ASP:CG	2.23	0.41
3:C:47:PHE:HA	3:C:50:LYS:HB2	2.03	0.41
1:M:57:GLN:NE2	1:M:122:GLU:O	2.47	0.41
1:M:243:MET:O	1:M:244:THR:CG2	2.68	0.41
1:M:408:GLU:O	1:M:411:THR:OG1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LYS:HE3	1:A:322:LYS:CA	2.48	0.41
2:B:216:LYS:HA	2:B:216:LYS:HD3	1.91	0.41
3:C:106:GLU:HB2	3:C:107:PRO:HD3	2.02	0.41
3:C:56:TRP:O	3:C:60:VAL:HG23	2.20	0.41
1:M:324:LEU:O	1:M:328:LEU:N	2.50	0.41
1:M:492:THR:HG21	2:N:49:PRO:HG2	2.03	0.41
2:N:106:MET:HE3	2:N:109:PHE:CD2	2.56	0.41
2:N:116:ILE:HD11	2:N:168:ILE:HD12	2.03	0.41
2:N:159:PRO:CG	2:N:207:VAL:HG21	2.31	0.41
3:O:7:TYR:CD1	3:O:7:TYR:C	2.94	0.41
1:A:445:GLY:H	1:A:490:ARG:HB2	1.86	0.41
1:A:141:GLN:NE2	2:B:179:TYR:OH	2.54	0.41
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.82	0.41
1:M:44:HIS:H	1:M:207:ILE:HD11	1.86	0.41
2:N:100:ARG:O	2:N:101:ASP:C	2.59	0.41
3:O:50:LYS:CG	4:P:118:ILE:HA	2.51	0.41
2:B:6:LEU:HD23	2:B:8:ILE:CG1	2.51	0.40
1:M:574:PRO:HA	1:M:575:PRO:HD2	1.99	0.40
2:N:236:LEU:HD22	2:N:237:ILE:HD12	2.01	0.40
3:O:16:TRP:HA	3:O:22:TYR:HB3	2.03	0.40
3:O:25:TYR:HD1	3:O:28:ARG:NH2	2.19	0.40
1:A:15:ALA:HB2	1:A:399:LEU:CD2	2.50	0.40
1:A:319:LEU:O	1:A:323:LYS:HB2	2.21	0.40
1:A:92:GLU:OE1	1:A:404:ARG:HD2	2.22	0.40
1:A:431:GLY:O	1:A:435:ARG:HB2	2.21	0.40
2:B:105:ASP:C	2:B:105:ASP:OD1	2.60	0.40
4:D:99:VAL:HG12	4:D:100:PHE:N	2.36	0.40
2:B:198:GLN:NE2	4:D:10:GLU:HG3	2.11	0.40
3:C:56:TRP:CD1	4:D:51:TYR:HB2	2.57	0.40
1:M:224:ARG:HG3	1:M:382:SER:CB	2.51	0.40
3:O:50:LYS:HG2	4:P:118:ILE:HA	2.03	0.40
1:A:10:VAL:HG21	1:A:190:MET:CE	2.52	0.40
1:A:263:LEU:HB3	1:A:268:MET:HE3	2.03	0.40
1:M:503:LEU:O	1:M:507:GLU:HG3	2.21	0.40
2:N:44:LYS:NZ	2:N:49:PRO:O	2.47	0.40
3:O:19:LEU:HA	3:O:20:PRO:HD3	1.90	0.40
2:B:112:SER:HA	4:D:1:ILE:HD11	2.03	0.40
1:M:119:MET:HE2	1:M:391:LEU:HD23	2.03	0.40
1:M:522:ALA:HB1	1:M:532:HIS:CE1	2.56	0.40
2:N:113:LEU:HD22	2:N:175:LEU:HD22	2.03	0.40
2:N:179:TYR:C	2:N:181:GLU:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:45:GLY:HA3	3:O:59:PHE:CZ	2.57	0.40
2:B:116:ILE:CD1	2:B:172:ALA:O	2.69	0.40
2:B:242:PRO:HD2	2:B:243:ARG:HG2	2.03	0.40
3:C:128:LEU:HD22	4:D:45:PRO:HD2	2.02	0.40
1:M:328:LEU:HD22	1:M:331:ILE:HD11	1.99	0.40
1:M:192:THR:OG1	5:M:601:FAD:N7A	2.55	0.40
1:M:88:HIS:HB2	1:M:401:VAL:CG1	2.51	0.40
2:N:180:ASN:OD1	2:N:191:ARG:NH1	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/577 (100%)	551 (96%)	23 (4%)	1 (0%)	47	78
1	M	575/577 (100%)	546 (95%)	24 (4%)	5 (1%)	17	46
2	B	241/243 (99%)	225 (93%)	15 (6%)	1 (0%)	34	66
2	N	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	19	49
3	C	128/130 (98%)	124 (97%)	3 (2%)	1 (1%)	19	49
3	O	128/130 (98%)	118 (92%)	10 (8%)	0	100	100
4	D	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
4	P	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	17	46
All	All	2122/2138 (99%)	2008 (95%)	103 (5%)	11 (0%)	29	61

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	65	CYS
1	M	1	GLN

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Mol	Chain	Res	Type
1	M	244	THR
4	P	46	GLY
1	M	128	ALA
3	C	18	LYS
1	M	59	HIS
2	N	101	ASP
2	B	56	SER
1	M	444	GLY
1	A	320	GLY

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	460/460 (100%)	430 (94%)	30 (6%)	17	44
1	M	460/460 (100%)	417 (91%)	43 (9%)	9	26
2	B	205/205 (100%)	193 (94%)	12 (6%)	19	49
2	N	205/205 (100%)	180 (88%)	25 (12%)	5	15
3	C	111/111 (100%)	99 (89%)	12 (11%)	6	19
3	O	111/111 (100%)	104 (94%)	7 (6%)	18	46
4	D	97/97 (100%)	87 (90%)	10 (10%)	7	21
4	P	97/97 (100%)	88 (91%)	9 (9%)	9	26
All	All	1746/1746 (100%)	1598 (92%)	148 (8%)	10	31

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	27	ASN
1	A	31	LYS
1	A	41	MET
1	A	42	ARG
1	A	59	HIS

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Mol	Chain	Res	Type
1	A	74	ASP
1	A	76	LEU
1	A	93	MET
1	A	114	ARG
1	A	116	PHE
1	A	122	GLU
1	A	129	ASP
1	A	170	LEU
1	A	175	MET
1	A	182	GLN
1	A	197	ARG
1	A	253	ILE
1	A	287	ARG
1	A	310	ASP
1	A	322	LYS
1	A	325	HIS
1	A	411	THR
1	A	413	ARG
1	A	478	LYS
1	A	490	ARG
1	A	495	SER
1	A	498	PHE
1	A	541	GLU
1	A	560	THR
2	B	4	LYS
2	B	19	THR
2	B	46	ASN
2	B	65	CYS
2	B	78	LYS
2	B	85	THR
2	B	128	ASP
2	B	154	CYS
2	B	178	ARG
2	B	206	PHE
2	B	210	CYS
2	B	237	ILE
3	C	2	THR
3	C	5	LYS
3	C	19	LEU
3	C	27	LEU
3	C	37	TRP
3	C	39	SER

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Mol	Chain	Res	Type
3	C	50	LYS
3	C	54	GLU
3	C	76	LEU
3	C	84	LYS
3	C	85	THR
3	C	92	LYS
4	D	7	ARG
4	D	9	ASP
4	D	12	VAL
4	D	17	PHE
4	D	22	MET
4	D	47	ASP
4	D	62	ILE
4	D	64	ARG
4	D	67	LEU
4	D	118	ILE
1	M	18	ARG
1	M	27	ASN
1	M	31	LYS
1	M	32	ILE
1	M	41	MET
1	M	57	GLN
1	M	63	GLU
1	M	86	VAL
1	M	93	MET
1	M	97	GLU
1	M	110	SER
1	M	143	SER
1	M	148	GLN
1	M	152	PHE
1	M	164	ASP
1	M	168	ARG
1	M	192	THR
1	M	197	ARG
1	M	224	ARG
1	M	243	MET
1	M	291	SER
1	M	299	ARG
1	M	308	ARG
1	M	310	ASP
1	M	317	ARG
1	M	318	HIS

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Mol	Chain	Res	Type
1	M	351	ARG
1	M	393	SER
1	M	394	ASN
1	M	413	ARG
1	M	421	ASN
1	M	425	ILE
1	M	475	THR
1	M	484	GLU
1	M	489	VAL
1	M	494	THR
1	M	496	SER
1	M	505	THR
1	M	506	ILE
1	M	517	CYS
1	M	537	GLU
1	M	555	ARG
1	M	572	THR
2	N	5	ASN
2	N	14	ASN
2	N	19	THR
2	N	31	ASP
2	N	65	CYS
2	N	82	ARG
2	N	100	ARG
2	N	112	SER
2	N	126	THR
2	N	128	ASP
2	N	138	GLN
2	N	150	ASN
2	N	154	CYS
2	N	178	ARG
2	N	184	ARG
2	N	185	ASP
2	N	189	LYS
2	N	206	PHE
2	N	219	ASP
2	N	226	GLN
2	N	233	LYS
2	N	235	PHE
2	N	240	LEU
2	N	241	LYS
2	N	243	ARG

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Mol	Chain	Res	Type
3	O	2	THR
3	O	12	THR
3	O	31	THR
3	O	39	SER
3	O	40	ILE
3	O	50	LYS
3	O	98	VAL
4	P	1	ILE
4	P	7	ARG
4	P	9	ASP
4	P	22	MET
4	P	37	ILE
4	P	47	ASP
4	P	60	SER
4	P	115	VAL
4	P	117	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	166	HIS
1	A	204	ASN
1	A	230	GLN
1	A	292	GLN
1	A	409	GLN
1	A	442	GLN
2	B	5	ASN
2	B	46	ASN
2	B	134	GLN
2	B	143	HIS
2	B	150	ASN
2	B	194	GLN
3	C	51	ASN
3	C	72	ASN
4	D	59	GLN
4	D	92	HIS
1	M	27	ASN
1	M	59	HIS
1	M	79	GLN
1	M	134	HIS
1	M	145	GLN

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Mol	Chain	Res	Type
1	M	148	GLN
1	M	166	HIS
1	M	264	GLN
1	M	442	GLN
1	M	546	ASN
1	M	550	HIS
2	N	5	ASN
2	N	14	ASN
2	N	22	HIS
2	N	71	ASN
2	N	95	ASN
2	N	123	ASN
2	N	132	ASN
2	N	160	GLN
3	O	95	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 ⓘ

9 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	B	245	2	0,9,9	0.00	-	-		
9	SF4	N	246	2	0,12,12	0.00	-	-		
7	FES	B	244	2	0,4,4	0.00	-	-		
5	FAD	M	601	-	51,58,58	2.08	9 (17%)	60,89,89	1.96	14 (23%)
8	F3S	N	245	2	0,9,9	0.00	-	-		
6	FUM	A	577	-	1,7,7	4.15	1 (100%)	2,8,8	3.82	1 (50%)
7	FES	N	244	2	0,4,4	0.00	-	-		
5	FAD	A	601	-	51,58,58	2.19	8 (15%)	60,89,89	2.07	17 (28%)
9	SF4	B	246	-	0,12,12	0.00	-	-		

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	B	245	2	-	-	0/3/3/3
9	SF4	N	246	2	-	-	0/6/5/5
7	FES	B	244	2	-	-	0/1/1/1
5	FAD	M	601	-	-	7/30/50/50	0/6/6/6
8	F3S	N	245	2	-	-	0/3/3/3
6	FUM	A	577	-	-	0/0/5/5	-
7	FES	N	244	2	-	-	0/1/1/1
5	FAD	A	601	-	-	9/30/50/50	0/6/6/6
9	SF4	B	246	-	-	-	0/6/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	O2B-C2B	-10.06	1.19	1.43
5	M	601	FAD	O2B-C2B	-9.28	1.21	1.43
5	A	601	FAD	C2B-C1B	6.44	1.63	1.53
5	M	601	FAD	C2B-C1B	5.33	1.61	1.53
5	A	601	FAD	C9A-N10	4.76	1.45	1.38
5	M	601	FAD	C9A-N10	4.61	1.44	1.38
6	A	577	FUM	C5-C4	4.15	1.52	1.31
5	A	601	FAD	C10-N1	3.93	1.38	1.33
5	M	601	FAD	C4X-N5	3.81	1.38	1.33
5	A	601	FAD	C4X-N5	3.63	1.38	1.33
5	M	601	FAD	C2B-C3B	3.36	1.62	1.53
5	M	601	FAD	C5X-N5	2.99	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	C10-N1	2.78	1.36	1.33
5	M	601	FAD	C4-N3	2.72	1.37	1.33
5	A	601	FAD	C2B-C3B	2.49	1.60	1.53
5	A	601	FAD	C4-N3	2.44	1.37	1.33
5	A	601	FAD	O3B-C3B	2.38	1.48	1.43
5	M	601	FAD	O4B-C1B	2.33	1.44	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C4X-N5-C5X	7.09	123.85	116.77
5	M	601	FAD	C4-N3-C2	5.82	120.06	115.14
5	M	601	FAD	C4X-N5-C5X	5.82	122.58	116.77
5	A	601	FAD	C4-N3-C2	5.43	119.72	115.14
6	A	577	FUM	C6-C5-C4	-5.30	112.36	123.69
5	M	601	FAD	N3A-C2A-N1A	-5.09	120.72	128.68
5	M	601	FAD	C4-C4X-C10	-4.18	117.18	119.95
5	A	601	FAD	N3A-C2A-N1A	-4.15	122.20	128.68
5	M	601	FAD	C3B-C2B-C1B	-4.14	94.75	100.98
5	A	601	FAD	C3B-C2B-C1B	-3.97	95.01	100.98
5	A	601	FAD	O3'-C3'-C2'	-3.94	99.28	108.81
5	A	601	FAD	C1'-N10-C9A	3.75	121.25	118.29
5	M	601	FAD	C4-C4X-N5	3.50	122.60	118.60
5	M	601	FAD	C1B-N9A-C4A	-3.15	121.10	126.64
5	A	601	FAD	O4'-C4'-C5'	-3.06	103.03	109.92
5	A	601	FAD	C1B-N9A-C4A	-2.90	121.55	126.64
5	A	601	FAD	C4-C4X-N5	2.75	121.73	118.60
5	A	601	FAD	O2'-C2'-C3'	-2.70	102.54	109.10
5	M	601	FAD	C1'-N10-C10	2.63	120.77	118.41
5	M	601	FAD	O2B-C2B-C3B	2.58	120.17	111.82
5	M	601	FAD	O2B-C2B-C1B	-2.45	101.79	110.85
5	A	601	FAD	C6-C5X-C9A	2.42	122.23	119.05
5	A	601	FAD	C1'-C2'-C3'	2.41	116.52	109.79
5	M	601	FAD	C6-C5X-N5	2.40	121.69	119.05
5	A	601	FAD	O4B-C4B-C3B	2.28	109.62	105.11
5	M	601	FAD	P-O3P-PA	-2.22	125.22	132.83
5	A	601	FAD	C4-C4X-C10	-2.19	118.50	119.95
5	A	601	FAD	C10-C4X-N5	-2.17	119.75	121.26
5	M	601	FAD	C5X-C9A-N10	2.13	119.26	117.72
5	A	601	FAD	O3B-C3B-C4B	2.10	117.12	111.05
5	M	601	FAD	C9A-C5X-N5	-2.09	119.10	122.36
5	A	601	FAD	C9A-C5X-N5	-2.08	119.11	122.36

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	P-O3P-PA-O1A
5	M	601	FAD	PA-O3P-P-O5'
5	A	601	FAD	PA-O3P-P-O5'
5	M	601	FAD	P-O3P-PA-O2A
5	M	601	FAD	O4'-C4'-C5'-O5'
5	A	601	FAD	N10-C1'-C2'-C3'
5	M	601	FAD	O4B-C4B-C5B-O5B
5	A	601	FAD	C5'-O5'-P-O3P
5	A	601	FAD	O4B-C4B-C5B-O5B
5	A	601	FAD	PA-O3P-P-O1P
5	A	601	FAD	PA-O3P-P-O2P
5	A	601	FAD	C5'-O5'-P-O1P
5	A	601	FAD	O4'-C4'-C5'-O5'

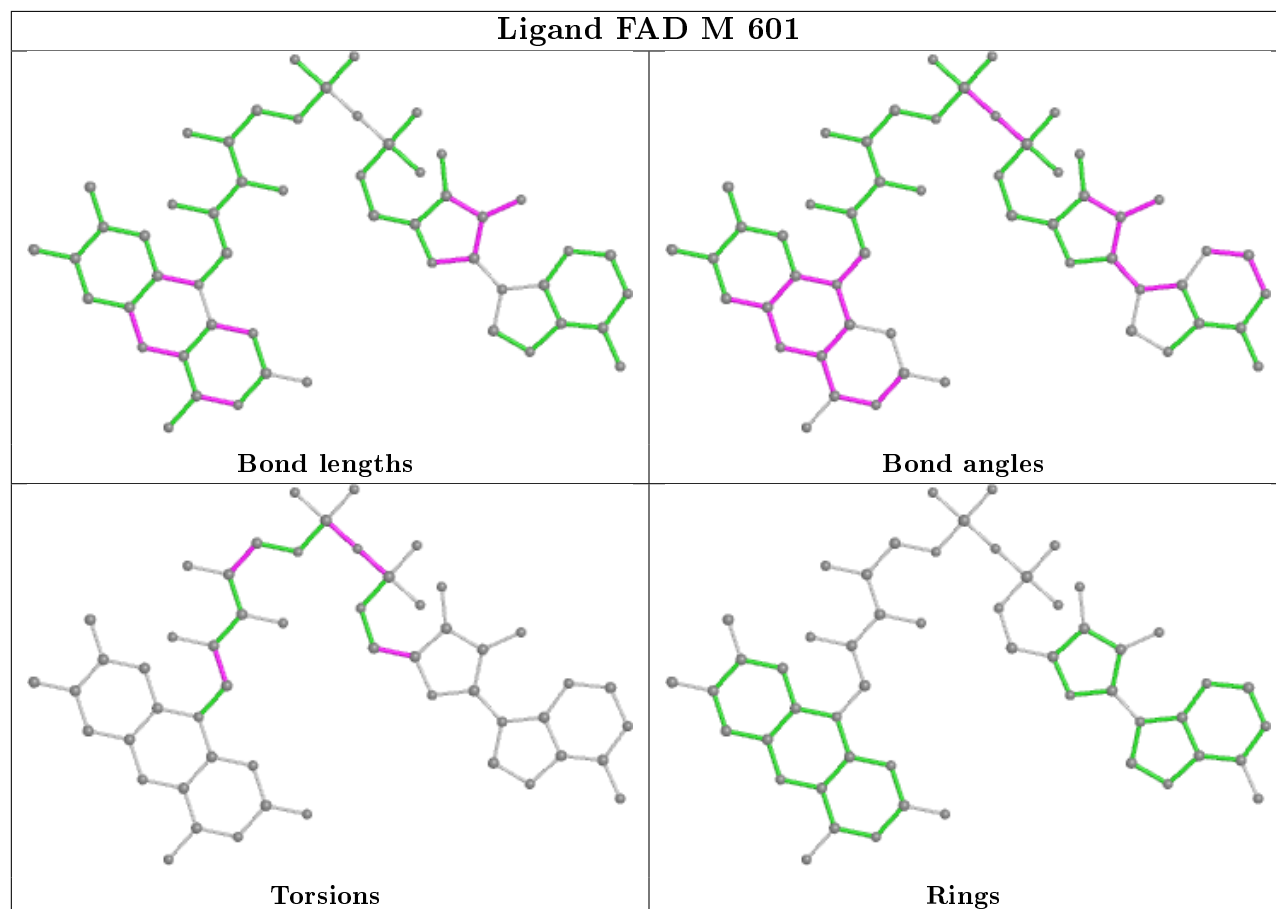
There are no ring outliers.

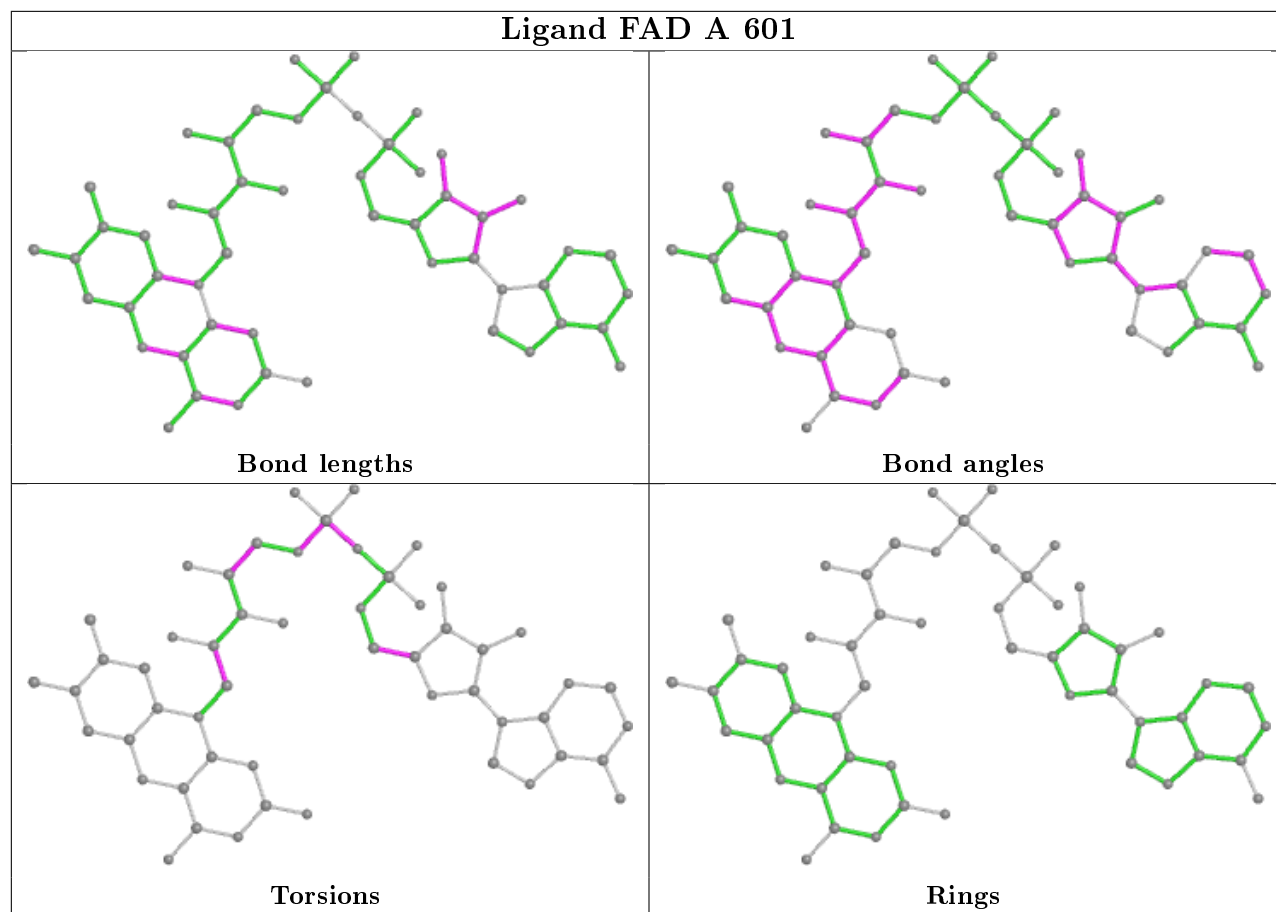
9 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	245	F3S	4	0
9	N	246	SF4	6	0
7	B	244	FES	3	0
5	M	601	FAD	25	0
8	N	245	F3S	1	0
6	A	577	FUM	1	0
7	N	244	FES	1	0
5	A	601	FAD	14	0
9	B	246	SF4	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	577/577 (100%)	0.47	1 (0%) 95 94	38, 56, 93, 138	0
1	M	577/577 (100%)	2.35	290 (50%) 0 0	68, 160, 235, 266	0
2	B	243/243 (100%)	0.71	4 (1%) 72 66	39, 71, 104, 151	0
2	N	243/243 (100%)	1.35	49 (20%) 1 0	64, 131, 202, 235	0
3	C	130/130 (100%)	0.22	0 100 100	51, 74, 110, 136	0
3	O	130/130 (100%)	0.44	5 (3%) 40 30	60, 93, 154, 215	0
4	D	119/119 (100%)	0.34	2 (1%) 70 63	55, 76, 107, 144	0
4	P	119/119 (100%)	0.46	3 (2%) 57 47	64, 86, 144, 224	0
All	All	2138/2138 (100%)	1.08	354 (16%) 1 1	38, 88, 208, 266	0

All (354) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	407	GLY	15.2
1	M	219	HIS	10.7
1	M	167	VAL	10.3
1	M	386	HIS	10.2
1	M	411	THR	10.2
1	M	188	VAL	9.7
1	M	17	LEU	9.5
1	M	170	LEU	9.2
1	M	125	TRP	8.8
1	M	361	ILE	8.4
1	M	396	LEU	8.2
1	M	165	GLY	7.9
1	M	376	ALA	7.7
1	M	489	VAL	7.5
4	P	0	MET	7.2
1	M	573	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
1	M	43	SER	7.0
1	M	385	LEU	7.0
1	M	375	PHE	6.8
1	M	217	LEU	6.8
1	M	220	GLY	6.6
1	M	129	ASP	6.5
2	B	243	ARG	6.4
1	M	172	ALA	6.4
1	M	89	CYS	6.4
1	M	77	CYS	6.4
1	M	169	GLY	6.4
1	M	215	MET	6.3
1	M	187	ALA	5.8
1	M	101	CYS	5.7
1	M	356	TYR	5.7
1	M	362	GLU	5.7
1	M	121	ILE	5.7
1	M	8	ALA	5.7
1	M	0	MET	5.6
1	M	486	PHE	5.5
1	M	502	LEU	5.5
1	M	191	ALA	5.4
1	M	130	LYS	5.3
1	M	189	VAL	5.3
1	M	7	LEU	5.3
1	M	377	VAL	5.3
1	M	494	THR	5.2
1	M	429	ALA	5.1
1	M	212	GLY	5.1
1	M	378	GLY	5.1
1	M	224	ARG	5.0
4	D	118	ILE	5.0
1	M	373	GLY	5.0
1	M	99	TRP	4.9
1	M	160	ILE	4.9
1	M	482	LEU	4.9
2	N	198	GLN	4.8
2	N	184	ARG	4.8
1	M	228	PHE	4.8
1	M	222	PRO	4.8
1	M	48	ALA	4.8
1	M	46	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	M	14	GLY	4.7
1	M	223	LEU	4.7
1	M	383	VAL	4.7
1	M	6	ASP	4.7
2	N	130	GLY	4.6
1	M	400	VAL	4.6
1	M	182	GLN	4.6
1	M	161	LEU	4.6
1	M	545	VAL	4.6
1	M	449	ALA	4.6
1	M	137	HIS	4.6
1	M	78	GLU	4.6
1	M	374	LEU	4.5
1	M	392	GLY	4.5
1	M	102	PRO	4.5
1	M	190	MET	4.5
2	N	63	GLY	4.5
1	M	181	VAL	4.4
1	M	425	ILE	4.4
2	N	52	SER	4.4
1	M	475	THR	4.4
1	M	571	THR	4.4
1	M	44	HIS	4.4
1	M	330	PHE	4.4
2	N	142	TYR	4.3
1	M	34	LEU	4.3
1	M	544	ASP	4.3
1	M	551	THR	4.2
1	M	32	ILE	4.2
1	M	210	GLY	4.2
1	M	384	GLY	4.2
1	M	498	PHE	4.2
1	M	495	SER	4.1
1	M	369	THR	4.1
1	M	422	GLU	4.1
1	M	380	CYS	4.1
1	M	424	ALA	4.1
1	M	490	ARG	4.1
1	M	553	ALA	4.1
1	M	452	ARG	4.1
1	M	135	MET	4.1
1	M	308	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	M	513	ASN	4.0
2	N	55	TRP	4.1
1	M	24	ALA	4.0
1	M	162	VAL	4.0
1	M	88	HIS	4.0
1	M	444	GLY	4.0
1	M	456	GLY	4.0
1	M	394	ASN	4.0
1	M	387	GLY	4.0
1	M	565	TYR	4.0
1	M	345	LYS	3.9
1	M	198	VAL	3.9
1	M	177	GLU	3.9
1	M	552	LEU	3.9
2	N	26	TYR	3.9
2	N	98	ILE	3.9
2	N	146	SER	3.9
1	M	183	ILE	3.9
1	M	316	LEU	3.9
1	M	370	ARG	3.8
1	M	41	MET	3.8
1	M	402	PHE	3.8
1	M	463	CYS	3.8
1	M	27	ASN	3.8
1	M	448	TRP	3.8
1	M	381	SER	3.7
1	M	404	ARG	3.7
1	M	144	LEU	3.7
1	M	40	PRO	3.7
1	M	358	MET	3.7
1	M	134	HIS	3.7
1	M	166	HIS	3.7
1	M	141	GLN	3.7
1	M	569	LYS	3.6
1	M	390	ARG	3.6
1	M	122	GLU	3.6
2	N	48	ALA	3.6
1	M	549	LYS	3.5
1	M	199	TYR	3.5
2	N	25	PHE	3.5
1	M	473	GLN	3.5
1	M	66	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	N	113	LEU	3.5
1	M	405	LEU	3.4
1	M	139	LEU	3.4
1	M	455	MET	3.4
1	M	458	ALA	3.4
2	N	23	SER	3.4
1	M	3	PHE	3.4
1	M	398	GLU	3.4
1	M	252	GLY	3.4
1	M	15	ALA	3.4
1	M	253	ILE	3.3
1	M	250	GLU	3.3
1	M	391	LEU	3.3
1	M	379	GLU	3.3
1	M	560	THR	3.3
1	M	216	ALA	3.3
1	M	410	ALA	3.3
1	M	497	VAL	3.3
1	M	39	TYR	3.3
1	M	159	ASP	3.3
1	M	248	ARG	3.3
1	M	518	MET	3.3
1	M	163	ASP	3.3
1	M	413	ARG	3.2
1	M	79	GLN	3.2
1	M	207	ILE	3.2
1	M	393	SER	3.2
1	M	49	GLU	3.2
1	M	103	TRP	3.2
2	N	40	LEU	3.2
1	M	80	ASP	3.2
2	N	126	THR	3.2
1	M	554	PHE	3.1
1	M	328	LEU	3.1
1	M	389	ASN	3.1
1	M	33	ALA	3.1
1	M	221	VAL	3.1
1	M	504	TYR	3.1
2	N	102	LEU	3.1
2	N	180	ASN	3.1
1	M	359	GLY	3.1
1	M	360	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	38	VAL	3.0
2	N	20	ALA	3.0
1	M	209	THR	3.0
1	M	12	ALA	3.0
1	M	168	ARG	3.0
1	M	138	THR	3.0
1	M	50	GLY	3.0
2	N	43	ILE	3.0
1	M	205	GLY	3.0
2	N	217	HIS	3.0
1	M	9	ILE	3.0
1	M	516	GLU	3.0
2	N	175	LEU	3.0
1	M	51	GLY	3.0
1	M	114	ARG	3.0
1	M	59	HIS	3.0
1	M	85	PHE	3.0
1	M	206	GLY	3.0
1	M	31	LYS	3.0
1	M	460	GLU	3.0
1	M	568	VAL	3.0
2	N	109	PHE	2.9
2	N	238	ALA	2.9
1	M	493	ASP	2.9
1	M	451	ILE	2.9
2	N	195	LEU	2.9
1	M	445	GLY	2.9
2	N	237	ILE	2.9
1	M	371	ILE	2.8
1	M	567	ASP	2.8
4	D	4	ASN	2.8
1	M	514	VAL	2.8
2	N	16	GLU	2.8
1	M	156	PHE	2.8
1	M	56	ALA	2.8
1	M	42	ARG	2.8
4	P	88	ASP	2.8
1	M	45	THR	2.8
1	M	133	PHE	2.7
1	M	180	LEU	2.7
1	M	347	PRO	2.7
1	M	171	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	116	PHE	2.7
1	M	186	ASN	2.7
1	M	208	VAL	2.7
1	M	338	TYR	2.7
2	N	131	THR	2.7
1	M	211	ASP	2.7
1	M	312	VAL	2.7
1	M	2	THR	2.7
1	M	287	ARG	2.7
1	M	58	ASP	2.7
1	M	100	GLY	2.7
1	M	213	MET	2.7
1	M	409	GLN	2.7
1	M	173	MET	2.7
1	M	184	ARG	2.7
1	M	570	ILE	2.6
3	O	96	ILE	2.6
2	N	123	ASN	2.6
2	N	24	ALA	2.6
1	M	446	GLU	2.6
1	M	98	LEU	2.6
1	A	576	ALA	2.6
1	M	53	ALA	2.6
1	M	535	LEU	2.6
1	M	227	GLU	2.6
2	N	46	ASN	2.6
1	M	447	ASN	2.6
1	M	318	HIS	2.6
1	M	87	HIS	2.6
2	N	119	TYR	2.6
1	M	515	ALA	2.6
2	N	8	ILE	2.5
2	B	113	LEU	2.5
1	M	339	VAL	2.5
1	M	350	VAL	2.5
1	M	555	ARG	2.5
1	M	343	PRO	2.5
1	M	118	GLY	2.5
4	P	61	PHE	2.5
1	M	366	ASN	2.5
2	N	133	ILE	2.5
2	B	242	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	169	GLY	2.5
1	M	336	LYS	2.5
1	M	414	ALA	2.5
1	M	403	GLY	2.5
1	M	126	PHE	2.5
1	M	127	ALA	2.5
1	M	176	MET	2.4
1	M	57	GLN	2.4
1	M	522	ALA	2.4
3	O	1	THR	2.4
1	M	82	VAL	2.4
1	M	26	ALA	2.4
2	N	159	PRO	2.4
1	M	525	ARG	2.4
1	M	484	GLU	2.4
1	M	564	GLU	2.4
1	M	245	GLU	2.4
1	M	561	THR	2.4
2	N	61	ILE	2.4
1	M	225	ASP	2.3
2	N	59	MET	2.3
1	M	419	ASN	2.3
1	M	372	LYS	2.3
1	M	47	ALA	2.3
1	M	439	LEU	2.3
1	M	295	TRP	2.3
1	M	65	HIS	2.3
1	M	505	THR	2.3
1	M	52	SER	2.3
3	O	16	TRP	2.3
1	M	363	THR	2.3
1	M	242	LEU	2.3
1	M	280	LYS	2.3
2	B	197	SER	2.3
2	N	56	SER	2.3
1	M	507	GLU	2.3
1	M	76	LEU	2.3
2	N	106	MET	2.3
2	N	160	GLN	2.3
1	M	69	THR	2.2
1	M	234	THR	2.2
2	N	134	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	279	ASN	2.2
1	M	146	PHE	2.2
1	M	185	ALA	2.2
1	M	503	LEU	2.2
2	N	51	LEU	2.2
1	M	562	ARG	2.2
2	N	234	ASP	2.2
1	M	123	ARG	2.2
1	M	158	LEU	2.2
1	M	157	VAL	2.2
2	N	103	VAL	2.2
2	N	116	ILE	2.1
1	M	550	HIS	2.1
2	N	42	TYR	2.1
1	M	193	GLY	2.1
1	M	357	THR	2.1
1	M	512	LEU	2.1
1	M	415	ALA	2.1
1	M	344	VAL	2.1
1	M	131	THR	2.1
1	M	284	LEU	2.1
1	M	548	LEU	2.1
1	M	397	ALA	2.1
1	M	196	GLY	2.1
3	O	4	ARG	2.1
1	M	326	GLU	2.1
1	M	477	ASP	2.1
1	M	388	ALA	2.1
1	M	86	VAL	2.1
3	O	8	VAL	2.1
1	M	436	LEU	2.1
2	N	60	ALA	2.1
1	M	471	LEU	2.1
1	M	20	ALA	2.1
1	M	547	PHE	2.1
1	M	563	LEU	2.0
2	N	168	ILE	2.0
1	M	365	GLN	2.0
1	M	408	GLU	2.0
1	M	108	ASP	2.0
1	M	95	GLN	2.0
1	M	428	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	35	ILE	2.0
1	M	73	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

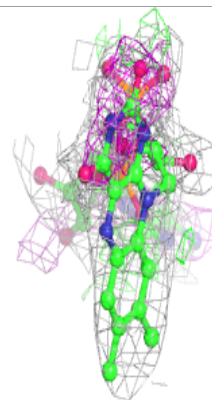
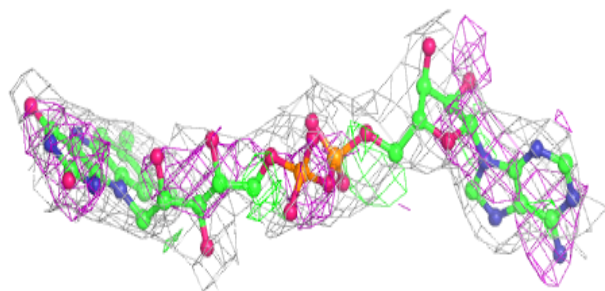
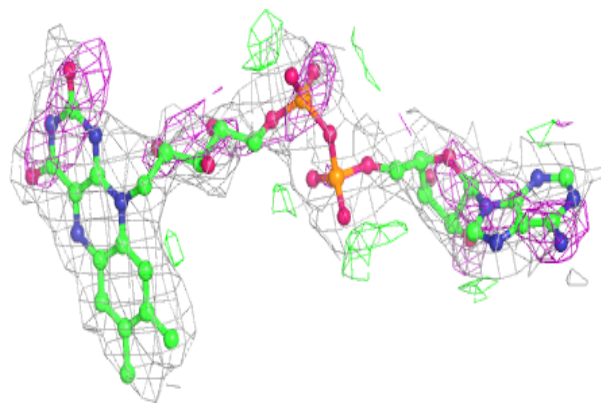
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FAD	M	601	53/53	0.87	0.29	49,74,85,86	0
6	FUM	A	577	8/8	0.89	0.38	66,67,70,103	0
9	SF4	B	246	8/8	0.92	0.27	86,104,134,134	0
7	FES	B	244	4/4	0.94	0.31	98,107,110,114	0
7	FES	N	244	4/4	0.96	0.22	76,90,94,104	0
8	F3S	N	245	7/7	0.96	0.20	86,90,101,134	0
9	SF4	N	246	8/8	0.97	0.19	103,112,131,134	0
5	FAD	A	601	53/53	0.98	0.25	34,41,78,78	0
8	F3S	B	245	7/7	0.98	0.20	60,64,70,93	0

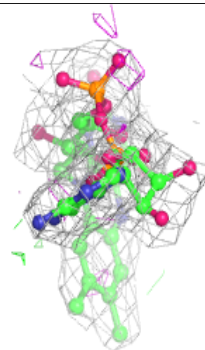
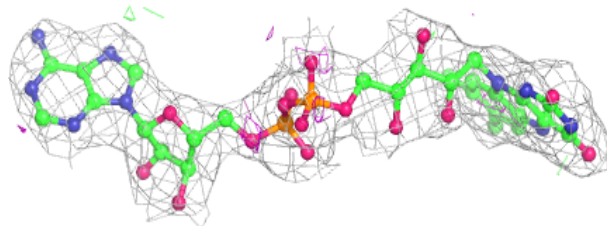
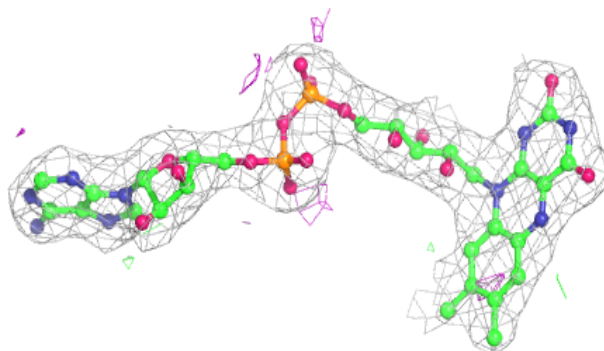
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD M 601:

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

**Electron density around FAD A 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.