



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:09 AM UTC

PDB ID : 1OFE / pdb_00001ofe
Title : Glutamate Synthase from Synechocystis sp in complex with 2-Oxoglutarate and L-DON at 2.45 Angstrom resolution
Authors : Van Den heuvel, R.H.H.; Mattevi, A.
Deposited on : 2003-04-14
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

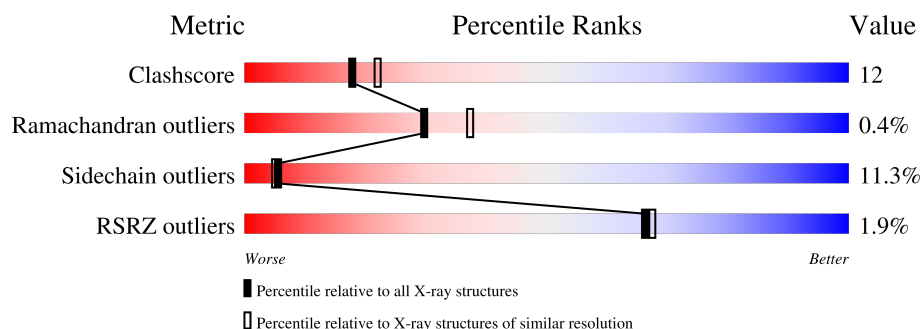
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	1520	2% 69% 24% 5%
1	B	1520	2% 72% 20% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AKG	A	2510	-	X	-	-
5	ONL	B	2511	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23181 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.

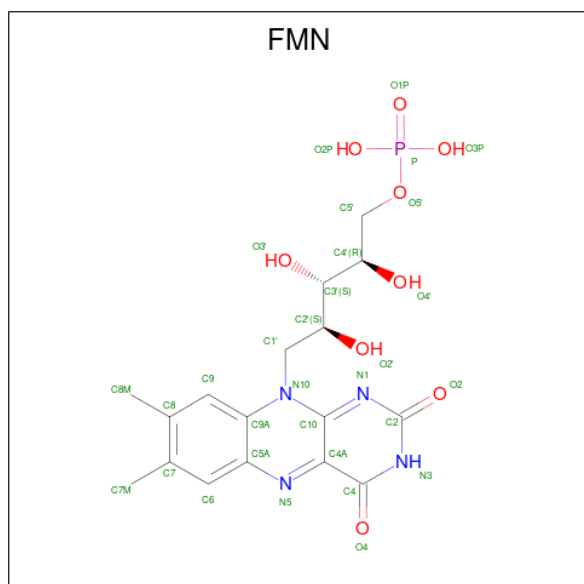
- Molecule 1 is a protein called FERREDONIN-DEPENDENT GLUTAMATE SYNTHASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1485	Total	C	N	O	S	0	0	0
			11388	7184	1986	2163	55			
1	B	1485	Total	C	N	O	S	0	0	0
			11388	7184	1986	2163	55			

There are 6 discrepancies between the modelled and reference sequences:

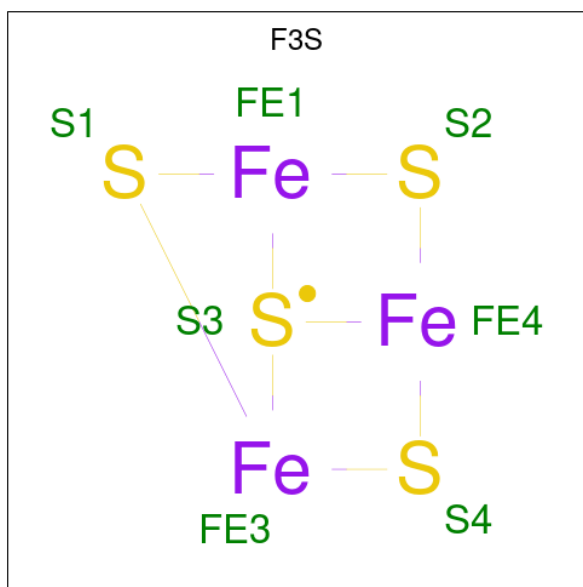
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	conflict	UNP P55038
A	581	THR	ASP	conflict	UNP P55038
A	1507	ASN	GLY	conflict	UNP P55038
B	578	ASP	THR	conflict	UNP P55038
B	581	THR	ASP	conflict	UNP P55038
B	1507	ASN	GLY	conflict	UNP P55038

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



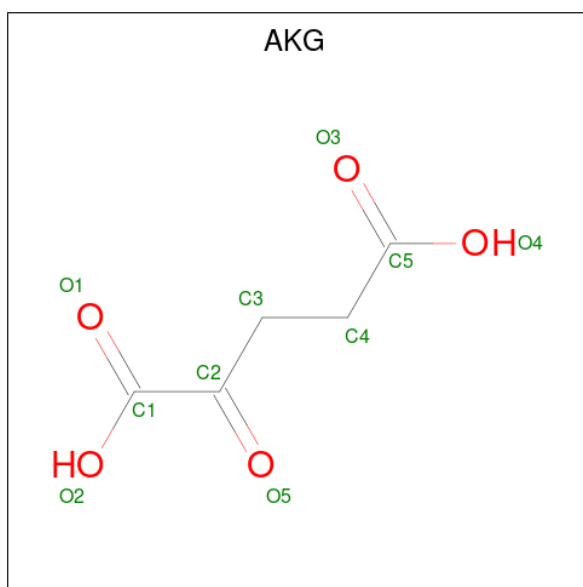
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



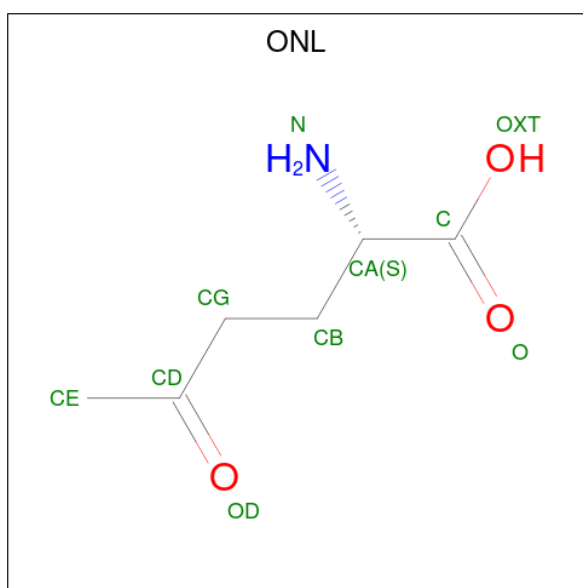
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	4		
3	B	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $\text{C}_5\text{H}_6\text{O}_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is 5-OXO-L-NORLEUCINE (CCD ID: ONL) (formula: $C_6H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	1	3		
5	B	1	Total	C	N	O	0	0
			10	6	1	3		

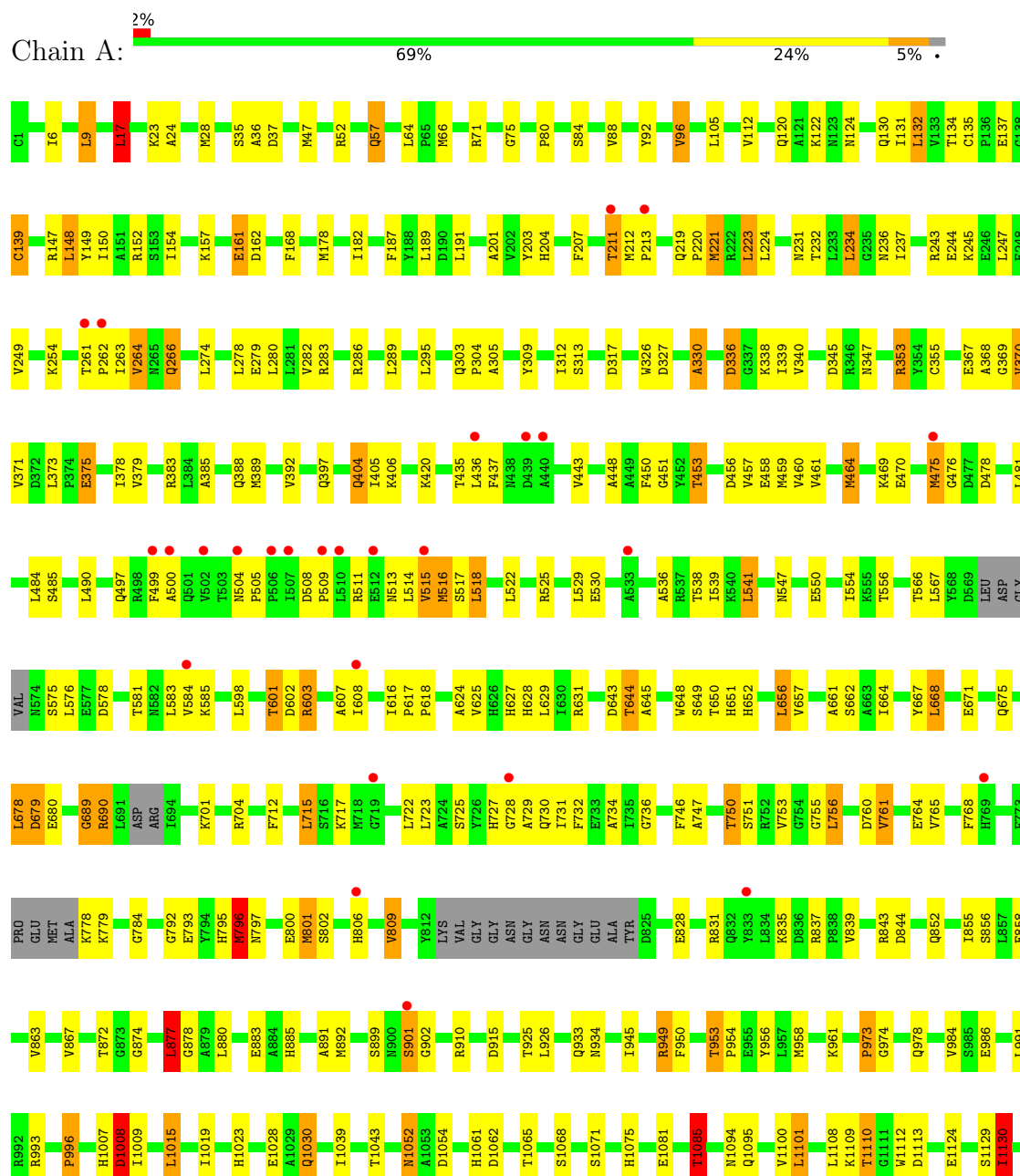
- Molecule 6 is water.

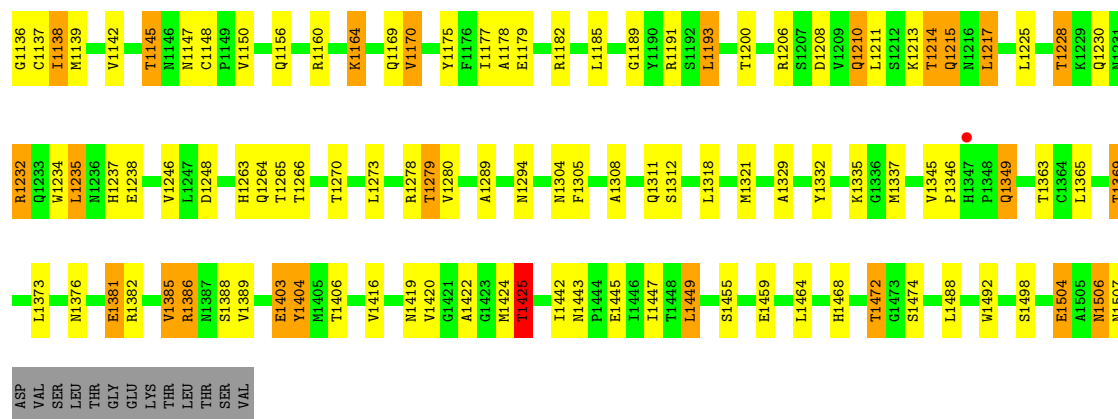
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total 208	O 208	0	0
6	B	81	Total 81	O 81	0	0

3 Residue-property plots

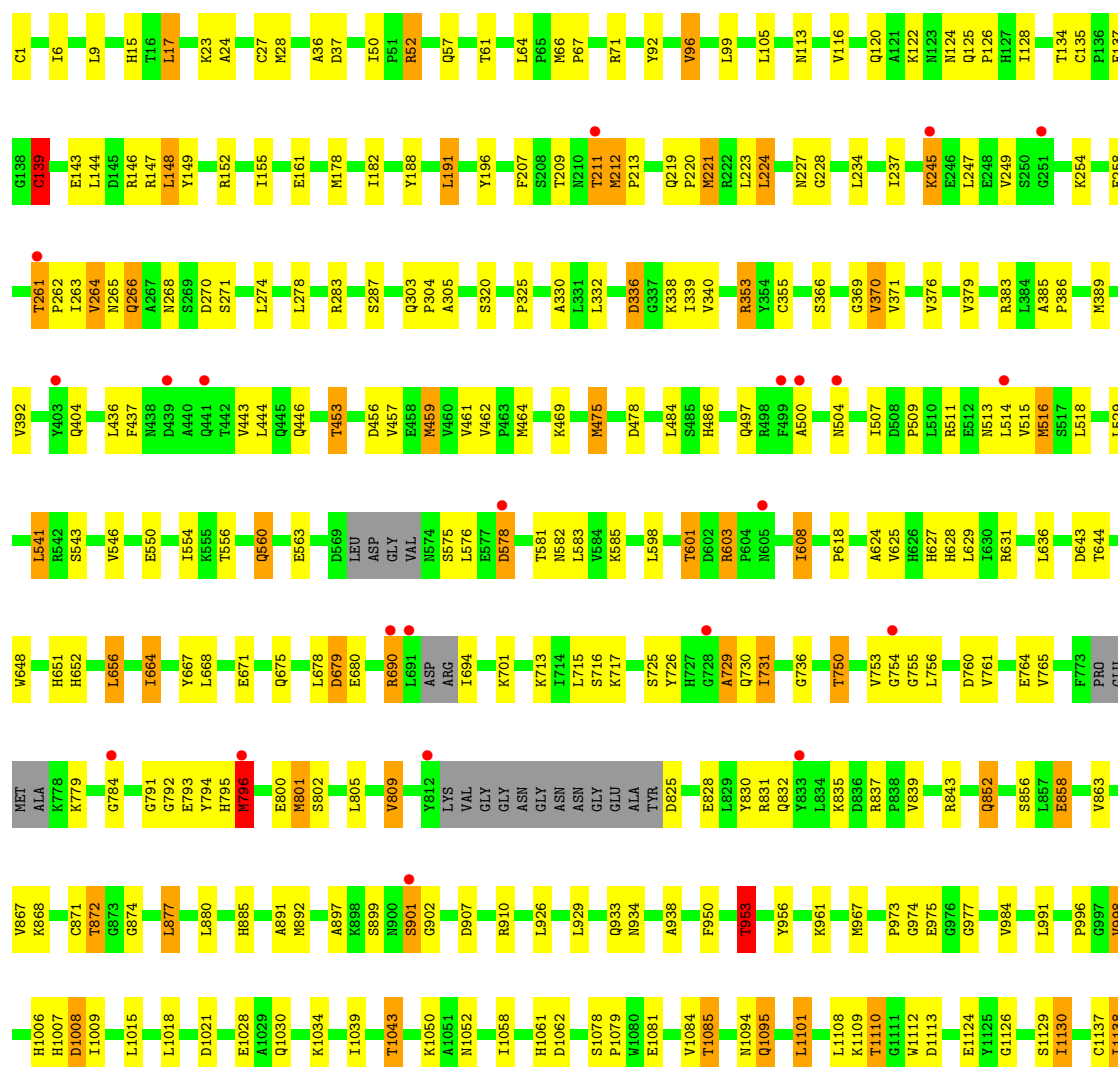
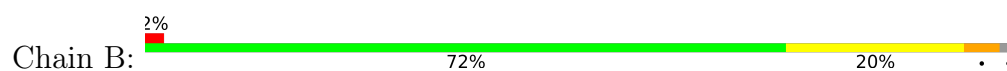
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

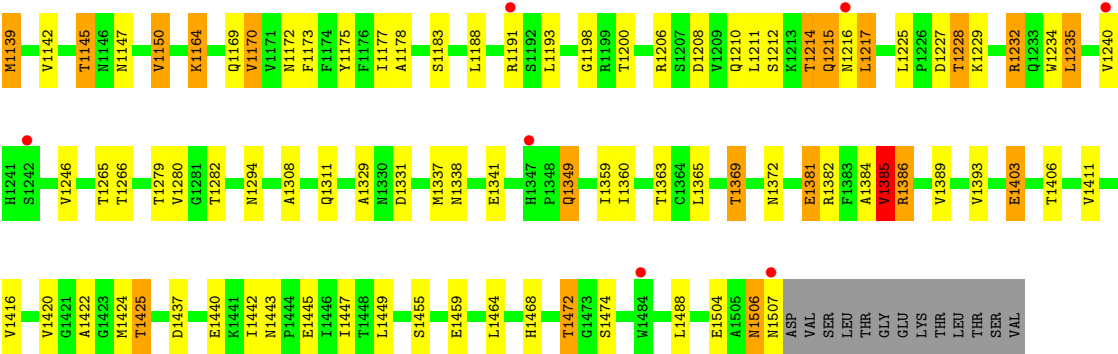
• Molecule 1: FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE 2





Molecule 1: FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.67Å 134.38Å 198.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 20.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.45) 99.2 (20.00-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.207 , 0.257 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23181	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: FMN, ONL, AKG, F3S

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	1.00	16/11609 (0.1%)	1.23	52/15739 (0.3%)
1	B	0.85	7/11609 (0.1%)	1.12	31/15739 (0.2%)
All	All	0.93	23/23218 (0.1%)	1.18	83/31478 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	475	MET	SD-CE	12.08	2.09	1.79
1	A	796	MET	SD-CE	10.73	2.06	1.79
1	B	516	MET	SD-CE	-10.11	1.54	1.79
1	A	950	PHE	C-O	9.39	1.35	1.24
1	B	796	MET	SD-CE	8.31	2.00	1.79
1	A	464	MET	SD-CE	-7.86	1.59	1.79
1	A	516	MET	SD-CE	-7.67	1.60	1.79
1	B	475	MET	SD-CE	7.30	1.97	1.79
1	A	1138	ILE	CA-CB	-7.09	1.44	1.54
1	A	1321	MET	SD-CE	6.84	1.96	1.79
1	A	1177	ILE	CA-CB	6.67	1.61	1.54
1	B	462	VAL	CA-CB	6.28	1.57	1.54
1	A	901	SER	CA-C	-6.07	1.45	1.52
1	A	761	VAL	CA-CB	6.02	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	459	MET	SD-CE	5.95	1.94	1.79
1	A	1130	ILE	CG1-CD1	5.91	1.74	1.51
1	A	1404	TYR	N-CA	5.85	1.53	1.46
1	A	690	ARG	N-CA	5.56	1.53	1.45
1	A	690	ARG	NE-CZ	5.52	1.39	1.33
1	A	1345	VAL	CA-CB	5.47	1.61	1.54
1	B	389	MET	SD-CE	-5.45	1.66	1.79
1	B	221	MET	SD-CE	5.17	1.92	1.79
1	A	945	ILE	CA-CB	5.00	1.60	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	ALA	CA-C-N	-10.33	109.18	123.03
1	A	729	ALA	C-N-CA	-10.33	109.18	123.03
1	A	1061	HIS	CA-C-N	10.14	134.27	120.38
1	A	1061	HIS	C-N-CA	10.14	134.27	120.38
1	A	1164	LYS	N-CA-C	-9.64	96.26	110.52
1	A	878	GLY	N-CA-C	9.35	123.95	112.73
1	A	901	SER	N-CA-C	-8.95	95.55	109.25
1	A	1062	ASP	N-CA-C	8.67	121.82	111.33
1	B	1164	LYS	N-CA-C	-8.36	97.47	110.42
1	A	1007	HIS	CA-C-N	8.33	136.33	121.92
1	A	1007	HIS	C-N-CA	8.33	136.33	121.92
1	A	792	GLY	N-CA-C	7.93	125.50	112.66
1	A	973	PRO	CA-C-N	-7.88	105.97	121.41
1	A	973	PRO	C-N-CA	-7.88	105.97	121.41
1	B	1061	HIS	CA-C-N	7.52	131.11	120.28
1	B	1061	HIS	C-N-CA	7.52	131.11	120.28
1	B	934	ASN	N-CA-C	7.42	119.36	111.28
1	A	368	ALA	N-CA-C	7.39	119.12	111.14
1	B	478	ASP	N-CA-C	-7.16	104.42	113.72
1	B	729	ALA	CA-C-N	-7.04	112.73	122.87
1	B	729	ALA	C-N-CA	-7.04	112.73	122.87
1	A	1008	ASP	N-CA-CB	-6.88	100.42	110.53
1	B	336	ASP	N-CA-C	-6.87	105.43	113.88
1	A	996	PRO	CA-C-N	-6.87	107.95	121.41
1	A	996	PRO	C-N-CA	-6.87	107.95	121.41
1	B	1139	MET	N-CA-C	-6.79	100.23	109.54
1	A	371	VAL	CA-C-N	-6.76	114.05	122.84
1	A	371	VAL	C-N-CA	-6.76	114.05	122.84
1	A	1385	VAL	CB-CA-C	-6.73	100.25	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	877	LEU	CA-C-N	-6.53	112.73	119.98
1	A	877	LEU	C-N-CA	-6.53	112.73	119.98
1	A	353	ARG	CG-CD-NE	-6.36	98.00	112.00
1	A	1425	THR	N-CA-CB	-6.25	102.58	110.90
1	B	973	PRO	CA-C-N	-6.06	109.53	121.41
1	B	973	PRO	C-N-CA	-6.06	109.53	121.41
1	A	729	ALA	N-CA-C	-6.02	101.86	110.59
1	A	727	HIS	CA-C-N	-6.00	112.61	120.22
1	A	727	HIS	C-N-CA	-6.00	112.61	120.22
1	B	1062	ASP	N-CA-CB	-5.98	101.02	110.22
1	A	934	ASN	N-CA-C	5.96	118.56	111.71
1	B	1008	ASP	N-CA-CB	-5.90	103.05	110.90
1	A	478	ASP	N-CA-CB	-5.89	101.75	110.53
1	A	678	LEU	N-CA-C	-5.87	101.59	110.28
1	A	370	VAL	N-CA-CB	-5.83	105.79	112.21
1	A	355	CYS	N-CA-CB	-5.82	100.73	110.57
1	A	616	ILE	N-CA-C	-5.80	101.90	107.76
1	A	373	LEU	N-CA-C	-5.77	102.14	110.40
1	B	371	VAL	CA-C-N	-5.76	114.76	122.42
1	B	371	VAL	C-N-CA	-5.76	114.76	122.42
1	A	1403	GLU	CA-C-N	-5.76	110.54	121.54
1	A	1403	GLU	C-N-CA	-5.76	110.54	121.54
1	B	973	PRO	O-C-N	-5.75	115.97	122.18
1	A	353	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	1062	ASP	N-CA-CB	-5.68	101.53	110.06
1	B	690	ARG	N-CA-C	-5.65	102.15	110.52
1	B	1403	GLU	CA-C-N	-5.65	113.57	122.95
1	B	1403	GLU	C-N-CA	-5.65	113.57	122.95
1	B	953	THR	N-CA-CB	-5.62	101.90	109.88
1	B	901	SER	N-CA-C	-5.60	100.68	109.25
1	B	998	VAL	N-CA-C	5.57	116.32	108.36
1	B	754	GLY	N-CA-C	5.56	126.36	113.18
1	A	1130	ILE	CB-CG1-CD1	5.52	125.39	113.80
1	A	644	THR	N-CA-C	5.52	117.78	109.23
1	A	607	ALA	N-CA-C	5.50	118.25	110.50
1	A	1230	GLN	CA-C-N	-5.49	115.46	122.77
1	A	1230	GLN	C-N-CA	-5.49	115.46	122.77
1	A	1403	GLU	O-C-N	-5.49	115.29	122.59
1	B	128	ILE	N-CA-C	5.48	115.48	107.37
1	B	1008	ASP	N-CA-C	-5.46	107.27	114.31
1	A	161	GLU	CA-C-N	5.44	131.24	121.66
1	A	161	GLU	C-N-CA	5.44	131.24	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1007	HIS	CA-C-N	5.37	130.68	122.24
1	B	1007	HIS	C-N-CA	5.37	130.68	122.24
1	B	832	GLN	N-CA-C	5.32	117.82	111.71
1	A	17	LEU	CA-CB-CG	5.29	134.83	116.30
1	A	689	GLY	N-CA-C	5.26	124.63	116.01
1	A	949	ARG	CG-CD-NE	-5.10	100.78	112.00
1	A	1238	GLU	CB-CA-C	5.09	117.42	109.42
1	A	1085	THR	N-CA-CB	-5.09	102.36	109.94
1	B	950	PHE	N-CA-C	5.09	116.51	111.07
1	B	792	GLY	N-CA-C	5.08	120.04	112.41
1	A	949	ARG	NE-CZ-NH2	-5.06	114.65	119.20
1	B	478	ASP	N-CA-CB	-5.00	103.30	110.65

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	ALA	Peptide
1	A	689	GLY	Peptide
1	A	728	GLY	Peptide
1	B	330	ALA	Peptide

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	11388	0	11335	310	0
1	B	11388	0	11336	248	0
2	A	31	0	19	1	0
2	B	31	0	19	3	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
4	A	10	0	4	1	0
4	B	10	0	4	0	0
5	A	10	0	9	0	0
5	B	10	0	10	6	0
6	A	208	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	81	0	0	12	0
All	All	23181	0	22736	560	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 12.

All (560) 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:1130:ILE:CD1	1:A:1130:ILE:CG1	1.74	1.56
1:A:796:MET:SD	1:A:796:MET:CE	2.06	1.43
1:A:475:MET:SD	1:A:475:MET:CE	2.09	1.40
1:B:1:CYS:SG	5:B:2511:ONL:CE	2.20	1.29
1:B:1:CYS:SG	5:B:2511:ONL:CD	2.27	1.22
1:B:475:MET:HE1	1:B:1129:SER:OG	1.33	1.22
1:A:1228:THR:CG2	1:A:1232:ARG:HH21	1.54	1.21
1:B:1:CYS:SG	5:B:2511:ONL:HE2	1.78	1.21
1:B:1138:ILE:HG22	1:B:1139:MET:H	1.04	1.15
1:A:872:THR:HG22	1:A:899:SER:HA	1.29	1.15
1:B:1228:THR:HG22	1:B:1232:ARG:HH21	1.06	1.14
1:B:825:ASP:HB3	6:B:2051:HOH:O	1.47	1.12
1:A:1138:ILE:HG22	1:A:1139:MET:N	1.56	1.11
1:A:509:PRO:HA	1:A:516:MET:HE1	1.13	1.10
1:B:825:ASP:CB	6:B:2051:HOH:O	1.94	1.09
1:B:1228:THR:CG2	1:B:1232:ARG:HH21	1.65	1.08
1:A:1138:ILE:CG2	1:A:1139:MET:H	1.67	1.07
1:A:885:HIS:CD2	1:A:910:ARG:HH22	1.72	1.07
1:B:1228:THR:CG2	1:B:1232:ARG:NH2	2.18	1.05
1:B:885:HIS:CD2	1:B:910:ARG:HH22	1.75	1.04
1:A:1228:THR:HG22	1:A:1232:ARG:HH21	1.22	1.03
1:A:1424:MET:HE3	1:A:1447:ILE:HG21	1.38	1.03
1:A:497:GLN:HE21	1:A:651:HIS:HD2	1.05	1.01
1:B:1130:ILE:HD13	1:B:1130:ILE:H	1.25	1.01
1:B:509:PRO:HA	1:B:516:MET:HE1	1.43	1.00
1:A:1228:THR:CG2	1:A:1232:ARG:NH2	2.24	0.99
1:B:1137:CYS:SG	1:B:1138:ILE:O	2.21	0.98
1:A:717:LYS:HG2	1:A:974:GLY:HA3	1.47	0.97
1:B:1206:ARG:NH1	6:B:2075:HOH:O	1.98	0.96
1:A:135:CYS:SG	1:A:139:CYS:HB2	2.06	0.96
1:A:1337:MET:HE2	1:A:1365:LEU:HD22	1.50	0.93
1:A:509:PRO:HA	1:A:516:MET:CE	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:THR:HG21	1:B:1294:ASN:HD21	1.34	0.93
1:A:885:HIS:HD2	1:A:910:ARG:HH22	1.05	0.92
1:B:1138:ILE:HG22	1:B:1139:MET:N	1.85	0.91
1:A:1110:THR:HG22	1:A:1113:ASP:H	1.35	0.91
1:A:1138:ILE:HG22	1:A:1139:MET:H	0.76	0.91
1:A:509:PRO:CA	1:A:516:MET:HE1	2.01	0.90
1:A:603:ARG:O	1:A:603:ARG:HG2	1.68	0.90
1:B:1472:THR:HG22	1:B:1474:SER:H	1.37	0.89
1:A:475:MET:HE1	1:A:1129:SER:OG	1.70	0.89
1:A:1468:HIS:O	1:A:1472:THR:HB	1.74	0.88
1:A:1381:GLU:HG3	6:A:2041:HOH:O	1.73	0.88
1:A:1137:CYS:SG	1:A:1138:ILE:O	2.34	0.86
1:A:336:ASP:HB3	1:A:338:LYS:H	1.40	0.85
1:B:603:ARG:O	1:B:603:ARG:HG2	1.74	0.85
1:A:1145:THR:HG21	6:A:2156:HOH:O	1.77	0.85
1:B:953:THR:CG2	1:B:1294:ASN:HD21	1.90	0.85
1:B:1506:ASN:O	1:B:1507:ASN:HB2	1.76	0.84
1:A:756:LEU:HA	1:A:1214:THR:HG21	1.57	0.84
1:B:1228:THR:HG22	1:B:1232:ARG:NH2	1.85	0.83
1:A:652:HIS:HE1	6:A:2068:HOH:O	1.59	0.83
1:A:656:LEU:HD23	1:A:664:ILE:HD12	1.61	0.83
1:A:1472:THR:HG22	1:A:1474:SER:H	1.41	0.83
1:A:1337:MET:HE2	1:A:1365:LEU:CD2	2.09	0.82
1:A:1265:THR:HG22	1:A:1266:THR:H	1.42	0.82
1:B:497:GLN:HE21	1:B:651:HIS:HD2	1.28	0.82
1:A:1211:LEU:HD11	1:A:1217:LEU:HD22	1.62	0.81
1:B:825:ASP:HB2	6:B:2051:HOH:O	1.68	0.81
1:A:756:LEU:HA	1:A:1214:THR:CG2	2.09	0.81
1:A:953:THR:CG2	1:A:1294:ASN:HD21	1.94	0.80
1:A:1385:VAL:O	1:A:1404:TYR:N	2.12	0.80
1:A:648:TRP:H	1:A:652:HIS:HD2	1.26	0.80
1:B:1138:ILE:CG2	1:B:1139:MET:H	1.87	0.80
1:A:135:CYS:CB	1:A:139:CYS:HB2	2.11	0.80
1:A:1110:THR:HG21	6:A:2104:HOH:O	1.82	0.80
1:A:497:GLN:HE21	1:A:651:HIS:CD2	1.97	0.79
1:A:547:ASN:OD1	1:A:550:GLU:HG3	1.82	0.79
1:B:1425:THR:HG21	6:B:2060:HOH:O	1.83	0.79
1:A:953:THR:HG22	1:A:956:TYR:H	1.47	0.78
1:B:1130:ILE:H	1:B:1130:ILE:CD1	1.93	0.78
1:A:237:ILE:HG23	1:A:264:VAL:HG13	1.65	0.78
1:B:1468:HIS:O	1:B:1472:THR:HB	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:THR:O	1:A:263:ILE:N	2.17	0.78
1:A:453:THR:HG23	6:A:2061:HOH:O	1.83	0.78
1:A:678:LEU:O	1:A:679:ASP:CB	2.30	0.77
1:A:901:SER:O	1:A:901:SER:OG	1.99	0.77
1:A:1108:LEU:O	1:A:1130:ILE:HG13	1.84	0.77
1:B:675:GLN:O	1:B:678:LEU:O	2.02	0.77
1:B:1081:GLU:O	1:B:1085:THR:HB	1.84	0.77
1:A:1130:ILE:HD13	1:A:1130:ILE:H	1.50	0.76
1:B:713:LYS:NZ	1:B:975:GLU:OE1	2.19	0.76
1:B:784:GLY:O	1:B:795:HIS:NE2	2.17	0.76
1:B:791:GLY:HA3	6:B:2050:HOH:O	1.86	0.76
1:B:627:HIS:O	1:B:631:ARG:HG3	1.86	0.75
1:B:135:CYS:SG	1:B:139:CYS:HB2	2.25	0.75
1:A:601:THR:HG22	1:A:643:ASP:OD2	1.86	0.74
1:A:461:VAL:HA	1:A:464:MET:CE	2.17	0.74
1:B:1382:ARG:O	1:B:1385:VAL:HG22	1.88	0.74
1:A:756:LEU:HD12	1:A:1214:THR:HG23	1.70	0.73
1:A:436:LEU:HD11	6:A:2084:HOH:O	1.89	0.72
1:A:717:LYS:CG	1:A:974:GLY:HA3	2.19	0.72
1:A:953:THR:HG23	1:A:1294:ASN:HD21	1.54	0.72
1:B:237:ILE:HG23	1:B:264:VAL:CG1	2.19	0.72
1:B:303:GLN:HE21	1:B:305:ALA:H	1.36	0.72
1:A:736:GLY:O	1:A:755:GLY:HA3	1.90	0.72
1:A:872:THR:HG22	1:A:899:SER:CA	2.17	0.71
1:B:910:ARG:HD3	1:B:938:ALA:HB1	1.71	0.71
1:B:953:THR:HG22	1:B:956:TYR:H	1.55	0.71
1:B:1363:THR:HG22	1:B:1363:THR:O	1.90	0.71
1:B:648:TRP:H	1:B:652:HIS:HD2	1.37	0.71
1:B:353:ARG:NH2	1:B:1329:ALA:O	2.23	0.70
1:A:9:LEU:O	1:A:397:GLN:HG2	1.91	0.70
1:A:124:ASN:ND2	1:A:213:PRO:O	2.24	0.70
1:A:885:HIS:HD2	1:A:910:ARG:NH2	1.85	0.70
1:A:461:VAL:HA	1:A:464:MET:HE2	1.74	0.70
1:A:247:LEU:HD22	1:A:529:LEU:HD11	1.72	0.70
1:B:717:LYS:HG2	1:B:974:GLY:HA3	1.74	0.69
1:A:601:THR:CG2	1:A:643:ASP:OD2	2.39	0.69
1:B:237:ILE:HG23	1:B:264:VAL:HG13	1.74	0.69
1:A:453:THR:HB	1:A:456:ASP:OD2	1.92	0.69
1:B:304:PRO:HB3	1:B:1440:GLU:OE1	1.91	0.69
1:A:404:GLN:HG3	6:A:2057:HOH:O	1.93	0.69
1:A:1337:MET:CE	1:A:1365:LEU:HD22	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:MET:HG3	1:A:1139:MET:HE1	1.73	0.69
1:A:1138:ILE:CG2	1:A:1139:MET:N	2.32	0.69
1:A:303:GLN:HE21	1:A:305:ALA:H	1.40	0.68
1:A:1228:THR:HG23	1:A:1232:ARG:HH21	1.54	0.68
1:B:247:LEU:HD22	1:B:529:LEU:HD11	1.74	0.68
1:B:756:LEU:HD12	1:B:1214:THR:HG23	1.76	0.68
1:B:885:HIS:CD2	1:B:910:ARG:NH2	2.58	0.67
1:A:1228:THR:HG22	1:A:1232:ARG:NH2	2.02	0.67
1:B:261:THR:HB	1:B:262:PRO:HD3	1.76	0.67
1:A:1420:VAL:HB	1:A:1442:ILE:HD13	1.76	0.67
1:B:1228:THR:HG21	1:B:1232:ARG:NH2	2.09	0.66
1:B:1424:MET:HE3	1:B:1447:ILE:HG21	1.77	0.66
1:A:453:THR:CG2	6:A:2061:HOH:O	2.42	0.66
1:B:266:GLN:HG2	6:B:2021:HOH:O	1.94	0.66
1:B:261:THR:O	1:B:263:ILE:N	2.28	0.66
1:A:475:MET:HE3	1:A:476:GLY:H	1.60	0.65
1:A:1265:THR:HG22	1:A:1266:THR:N	2.10	0.65
1:A:1403:GLU:O	1:A:1422:ALA:O	2.13	0.65
1:B:1108:LEU:O	1:B:1130:ILE:HG13	1.97	0.65
1:B:760:ASP:OD2	1:B:1214:THR:HG22	1.97	0.65
1:A:37:ASP:H	1:A:120:GLN:NE2	1.94	0.65
1:A:52:ARG:CZ	1:A:66:MET:HE3	2.27	0.65
1:B:541:LEU:HD11	1:B:554:ILE:HD11	1.77	0.65
1:A:648:TRP:H	1:A:652:HIS:CD2	2.11	0.65
1:B:1110:THR:HG21	6:B:2052:HOH:O	1.96	0.64
1:B:1211:LEU:HD11	1:B:1217:LEU:HD22	1.80	0.64
1:A:1110:THR:CG2	1:A:1113:ASP:H	2.08	0.64
1:A:1506:ASN:O	1:A:1507:ASN:HB2	1.97	0.64
1:B:756:LEU:HA	1:B:1214:THR:CG2	2.27	0.64
1:B:1130:ILE:HD13	1:B:1130:ILE:N	2.07	0.64
1:A:1210:GLN:HA	1:A:1210:GLN:HE21	1.62	0.64
1:A:550:GLU:OE2	1:A:704:ARG:NH2	2.30	0.64
1:B:135:CYS:CB	1:B:139:CYS:HB2	2.27	0.64
1:B:124:ASN:ND2	1:B:213:PRO:O	2.31	0.64
1:B:497:GLN:HE21	1:B:651:HIS:CD2	2.12	0.64
1:B:984:VAL:O	1:B:996:PRO:O	2.16	0.64
1:A:1142:VAL:O	1:A:1145:THR:HB	1.97	0.63
1:A:717:LYS:HG2	1:A:974:GLY:CA	2.27	0.63
1:A:925:THR:O	1:A:926:LEU:HD23	1.98	0.63
1:A:736:GLY:C	1:A:755:GLY:HA3	2.23	0.63
1:B:369:GLY:HA3	1:B:1308:ALA:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1110:THR:HG22	1:B:1113:ASP:H	1.63	0.63
1:A:152:ARG:HG2	1:A:152:ARG:HH11	1.64	0.62
1:B:877:LEU:O	1:B:880:LEU:O	2.17	0.62
2:B:2508:FMN:O1P	2:B:2508:FMN:O4'	2.17	0.62
1:A:178:MET:HE2	1:A:213:PRO:HA	1.81	0.62
1:A:1130:ILE:CD1	1:A:1130:ILE:H	2.12	0.62
1:B:461:VAL:HA	1:B:464:MET:HE2	1.79	0.62
1:A:796:MET:HG2	1:A:1109:LYS:HZ2	1.63	0.62
1:A:1337:MET:CE	1:A:1365:LEU:CD2	2.76	0.62
1:A:263:ILE:HD12	1:A:280:LEU:HD22	1.81	0.62
1:A:1145:THR:CG2	1:A:1147:ASN:ND2	2.62	0.62
1:A:883:GLU:OE2	1:A:1160:ARG:NH1	2.32	0.62
1:A:1145:THR:CG2	1:A:1147:ASN:HD22	2.12	0.62
1:B:336:ASP:HB3	1:B:338:LYS:H	1.65	0.62
1:A:1455:SER:O	1:A:1459:GLU:HG2	1.99	0.62
1:B:1455:SER:O	1:B:1459:GLU:HG2	1.99	0.62
1:A:1424:MET:CE	1:A:1447:ILE:HG21	2.22	0.62
1:A:1109:LYS:HD2	6:A:2151:HOH:O	1.99	0.61
1:B:796:MET:CG	1:B:1109:LYS:HZ2	2.13	0.61
1:A:1419:ASN:HD21	1:A:1443:ASN:HD22	1.47	0.61
1:A:863:VAL:HG11	1:A:1175:TYR:CD2	2.36	0.61
1:B:500:ALA:HB1	1:B:504:ASN:O	2.01	0.61
1:B:891:ALA:HB1	1:B:1170:VAL:HG22	1.82	0.60
1:A:678:LEU:O	1:A:679:ASP:HB2	2.00	0.60
1:A:953:THR:HG21	1:A:1294:ASN:HD21	1.65	0.60
1:A:28:MET:HE2	1:A:203:TYR:HE1	1.67	0.60
1:B:1110:THR:CG2	1:B:1113:ASP:H	2.15	0.60
1:B:178:MET:HE2	1:B:213:PRO:HA	1.84	0.59
1:B:891:ALA:CB	1:B:1170:VAL:HG22	2.31	0.59
1:B:1006:HIS:C	1:B:1008:ASP:H	2.11	0.59
1:A:211:THR:HB	1:A:1094:ASN:OD1	2.01	0.59
1:B:1420:VAL:HB	1:B:1442:ILE:HD13	1.85	0.59
1:B:1337:MET:HE2	1:B:1365:LEU:CD2	2.32	0.59
1:B:92:TYR:O	1:B:96:VAL:HG13	2.03	0.59
1:B:1265:THR:HG22	1:B:1266:THR:H	1.68	0.59
1:A:508:ASP:OD2	1:A:1404:TYR:OH	2.13	0.59
1:A:389:MET:HG3	1:A:406:LYS:HE3	1.85	0.58
1:A:678:LEU:O	1:A:679:ASP:HB3	2.03	0.58
1:A:986:GLU:CD	6:A:2130:HOH:O	2.46	0.58
1:B:1009:ILE:HD11	1:B:1018:LEU:CD2	2.33	0.58
1:A:37:ASP:H	1:A:120:GLN:HE21	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:THR:CG2	1:A:1112:TRP:HB3	2.34	0.58
1:A:1110:THR:HG23	1:A:1112:TRP:HB3	1.86	0.58
1:B:1095:GLN:HE21	1:B:1095:GLN:HA	1.69	0.58
1:B:1403:GLU:O	1:B:1422:ALA:O	2.22	0.58
1:A:675:GLN:O	1:A:678:LEU:O	2.21	0.58
1:A:541:LEU:HD11	1:A:554:ILE:HD11	1.86	0.57
1:A:750:THR:HG21	1:A:1039:ILE:HG12	1.85	0.57
1:B:885:HIS:HD2	1:B:910:ARG:HH22	1.47	0.57
1:A:885:HIS:CD2	1:A:910:ARG:NH2	2.58	0.57
1:A:369:GLY:HA3	1:A:1308:ALA:CB	2.34	0.57
1:A:618:PRO:HD2	6:A:2087:HOH:O	2.04	0.57
1:A:219:GLN:HB3	1:A:220:PRO:HA	1.87	0.57
1:A:237:ILE:HG23	1:A:264:VAL:CG1	2.32	0.57
1:B:443:VAL:HG21	1:B:675:GLN:HG3	1.86	0.57
1:B:461:VAL:HA	1:B:464:MET:CE	2.35	0.57
1:A:1346:PRO:HD2	1:A:1376:ASN:HD22	1.69	0.57
1:A:178:MET:HE2	1:A:213:PRO:CA	2.33	0.57
1:A:436:LEU:HD12	1:A:671:GLU:HB2	1.87	0.57
1:A:35:SER:HB3	1:A:120:GLN:NE2	2.20	0.57
1:A:178:MET:HG3	1:A:213:PRO:HB2	1.85	0.57
1:B:910:ARG:HD3	1:B:938:ALA:CB	2.35	0.57
1:A:717:LYS:CB	1:A:974:GLY:HA3	2.35	0.56
1:A:984:VAL:O	1:A:996:PRO:O	2.22	0.56
1:B:603:ARG:HD2	1:B:667:TYR:CE2	2.40	0.56
1:B:1425:THR:CG2	6:B:2060:HOH:O	2.48	0.56
1:A:261:THR:HB	1:A:262:PRO:HD3	1.88	0.56
1:B:224:LEU:HD11	1:B:332:LEU:HD22	1.86	0.56
1:B:1130:ILE:CD1	1:B:1130:ILE:N	2.67	0.56
1:B:601:THR:CG2	1:B:643:ASP:OD2	2.54	0.56
1:B:863:VAL:HG13	1:B:1178:ALA:HB3	1.88	0.56
1:A:1234:TRP:CZ3	1:A:1235:LEU:HD13	2.41	0.56
1:B:796:MET:HG2	1:B:1109:LYS:HZ2	1.71	0.56
1:B:1101:LEU:HD11	1:B:1124:GLU:HG3	1.87	0.56
1:B:1265:THR:HG22	1:B:1266:THR:N	2.20	0.56
1:B:113:ASN:O	1:B:116:VAL:HG22	2.07	0.55
1:A:837:ARG:NH1	1:A:844:ASP:OD1	2.40	0.55
1:A:1228:THR:HG23	1:A:1232:ARG:NH2	2.16	0.55
1:A:1200:THR:HG21	1:A:1225:LEU:HB2	1.89	0.55
1:B:178:MET:HE2	1:B:213:PRO:CA	2.36	0.55
1:B:437:PHE:CE2	1:B:608:ILE:HD11	2.41	0.55
1:A:760:ASP:OD2	1:A:1214:THR:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:CYS:SG	5:B:2511:ONL:HE1	2.39	0.55
1:B:1384:ALA:O	1:B:1385:VAL:C	2.50	0.55
1:B:1472:THR:CG2	1:B:1474:SER:HB2	2.37	0.55
1:A:1085:THR:CG2	6:A:2167:HOH:O	2.55	0.55
1:B:678:LEU:O	1:B:679:ASP:HB2	2.06	0.55
1:A:801:MET:HE3	1:A:802:SER:N	2.21	0.55
1:B:784:GLY:H	1:B:793:GLU:H	1.54	0.55
1:A:303:GLN:NE2	1:A:304:PRO:HD2	2.21	0.54
1:A:234:LEU:C	1:A:234:LEU:HD13	2.32	0.54
1:A:389:MET:HE3	1:A:405:ILE:HG21	1.89	0.54
1:A:891:ALA:HB1	1:A:1170:VAL:HG22	1.89	0.54
1:A:1030:GLN:HG2	1:A:1054:ASP:HB3	1.90	0.54
1:A:1363:THR:O	1:A:1363:THR:HG22	2.07	0.54
1:A:223:LEU:HD22	1:A:279:GLU:HB2	1.90	0.54
1:B:910:ARG:HD2	1:B:938:ALA:O	2.08	0.54
1:B:601:THR:HA	1:B:643:ASP:HB3	1.88	0.54
1:B:1:CYS:HB2	1:B:227:ASN:ND2	2.22	0.53
1:A:784:GLY:H	1:A:793:GLU:H	1.56	0.53
1:B:715:LEU:HD22	1:B:726:TYR:CG	2.43	0.53
1:A:1145:THR:HG23	1:A:1147:ASN:ND2	2.24	0.53
1:B:717:LYS:HG2	1:B:974:GLY:CA	2.38	0.53
1:A:1081:GLU:O	1:A:1085:THR:HB	2.09	0.53
1:B:736:GLY:O	1:B:755:GLY:HA3	2.09	0.53
1:B:1110:THR:HG23	1:B:1112:TRP:H	1.73	0.53
1:A:500:ALA:HB1	1:A:504:ASN:O	2.09	0.53
1:B:219:GLN:HB3	1:B:220:PRO:HA	1.90	0.53
1:B:383:ARG:HH22	1:B:1381:GLU:CD	2.16	0.53
1:B:756:LEU:HA	1:B:1214:THR:HG21	1.91	0.53
1:B:801:MET:HE3	1:B:802:SER:N	2.23	0.53
1:A:1228:THR:HG21	1:A:1232:ARG:NH2	2.21	0.52
1:B:1050:LYS:HE3	6:B:2002:HOH:O	2.09	0.52
1:B:1142:VAL:O	1:B:1145:THR:HB	2.08	0.52
1:A:289:LEU:HD13	1:A:405:ILE:HG23	1.90	0.52
1:B:228:GLY:O	5:B:2511:ONL:HB1	2.09	0.52
1:B:578:ASP:O	1:B:582:ASN:ND2	2.40	0.52
1:B:648:TRP:H	1:B:652:HIS:CD2	2.24	0.52
1:A:1085:THR:HG22	6:A:2167:HOH:O	2.09	0.52
1:B:872:THR:HG22	1:B:899:SER:HA	1.91	0.52
1:B:1338:ASN:HA	1:B:1369:THR:HG22	1.92	0.52
1:A:883:GLU:CD	1:A:1160:ARG:HH11	2.18	0.52
1:B:1110:THR:HG23	1:B:1112:TRP:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:LEU:O	1:B:679:ASP:CB	2.57	0.52
1:B:1294:ASN:HB3	1:B:1338:ASN:HD21	1.75	0.52
1:A:797:ASN:HB3	1:A:1139:MET:HG3	1.92	0.51
1:A:1015:LEU:HD13	1:A:1019:ILE:HD12	1.92	0.51
1:A:1382:ARG:O	1:A:1385:VAL:HG22	2.10	0.51
1:B:1:CYS:HB2	1:B:227:ASN:HD22	1.74	0.51
1:B:1506:ASN:HD22	1:B:1506:ASN:C	2.18	0.51
1:A:505:PRO:HD2	6:A:2076:HOH:O	2.10	0.51
1:A:484:LEU:HD13	1:A:839:VAL:HG22	1.92	0.51
1:A:734:ALA:O	1:A:751:SER:HA	2.10	0.51
1:B:1:CYS:SG	5:B:2511:ONL:OD	2.66	0.51
1:A:207:PHE:HD2	1:A:207:PHE:C	2.18	0.51
1:A:877:LEU:O	1:A:880:LEU:O	2.28	0.51
1:A:993:ARG:HB3	1:A:1388:SER:HB3	1.93	0.51
1:B:261:THR:HB	1:B:262:PRO:CD	2.41	0.51
1:A:1147:ASN:O	1:A:1148:CYS:C	2.54	0.51
1:A:309:TYR:HB3	1:A:312:ILE:HD12	1.93	0.51
1:A:730:GLN:O	1:A:732:PHE:N	2.40	0.50
1:A:513:ASN:HA	1:A:516:MET:HE3	1.92	0.50
1:A:1472:THR:CG2	1:A:1474:SER:H	2.17	0.50
1:B:15:HIS:HD2	1:B:196:TYR:O	1.94	0.50
1:B:1206:ARG:HG2	1:B:1208:ASP:OD2	2.11	0.50
1:A:715:LEU:HD11	1:A:723:LEU:HA	1.94	0.50
1:A:953:THR:HG23	1:A:1294:ASN:ND2	2.24	0.50
1:B:211:THR:O	1:B:211:THR:CG2	2.58	0.50
1:B:1145:THR:CG2	1:B:1147:ASN:ND2	2.75	0.50
1:A:232:THR:HG21	1:A:725:SER:HB3	1.92	0.50
1:A:603:ARG:HD3	1:A:643:ASP:OD2	2.10	0.50
1:A:1382:ARG:HB3	1:A:1385:VAL:HG22	1.93	0.50
1:A:1108:LEU:O	1:A:1130:ILE:CG1	2.57	0.50
1:B:1337:MET:HE2	1:B:1365:LEU:HD22	1.92	0.50
1:B:436:LEU:HD12	1:B:671:GLU:HB2	1.93	0.50
1:A:575:SER:O	1:A:576:LEU:C	2.54	0.50
1:B:36:ALA:HB2	1:B:211:THR:CG2	2.42	0.50
1:A:207:PHE:C	1:A:207:PHE:CD2	2.89	0.49
1:A:383:ARG:HH22	1:A:1381:GLU:CD	2.21	0.49
1:A:485:SER:OG	1:A:793:GLU:OE2	2.28	0.49
1:A:1210:GLN:HA	1:A:1210:GLN:NE2	2.25	0.49
1:B:105:LEU:HD11	1:B:134:THR:HG23	1.93	0.49
1:B:446:GLN:NE2	1:B:608:ILE:HG23	2.26	0.49
1:A:437:PHE:HD1	1:A:443:VAL:HG22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:GLY:O	2:A:2508:FMN:C4A	2.60	0.49
1:B:852:GLN:HB2	1:B:1188:LEU:O	2.12	0.49
1:A:149:TYR:CE1	1:A:279:GLU:HG2	2.48	0.49
1:B:211:THR:O	1:B:211:THR:HG23	2.13	0.49
1:B:385:ALA:HB1	1:B:386:PRO:HD2	1.94	0.49
1:B:1009:ILE:HD11	1:B:1018:LEU:HD23	1.94	0.49
1:A:627:HIS:O	1:A:631:ARG:HG3	2.13	0.49
1:B:37:ASP:H	1:B:120:GLN:NE2	2.11	0.49
1:B:486:HIS:HD2	1:B:1212:SER:OG	1.96	0.49
1:B:325:PRO:HD2	1:B:725:SER:OG	2.13	0.48
1:A:105:LEU:HD11	1:A:134:THR:HG23	1.95	0.48
1:B:135:CYS:HB3	1:B:139:CYS:HB2	1.94	0.48
1:B:453:THR:HB	1:B:456:ASP:OD2	2.14	0.48
1:A:624:ALA:O	1:A:628:HIS:HD2	1.97	0.48
1:A:9:LEU:HD22	1:A:392:VAL:HG11	1.95	0.48
1:A:891:ALA:CB	1:A:1170:VAL:HG22	2.43	0.48
1:B:624:ALA:O	1:B:628:HIS:HD2	1.97	0.48
1:B:9:LEU:CD2	1:B:392:VAL:HG11	2.44	0.48
1:B:717:LYS:CG	1:B:974:GLY:HA3	2.41	0.48
1:A:1100:VAL:O	1:A:1237:HIS:CE1	2.67	0.48
1:A:35:SER:HB3	1:A:120:GLN:HE22	1.78	0.48
1:A:52:ARG:NH2	1:A:66:MET:HE3	2.29	0.48
1:A:460:VAL:C	1:A:464:MET:HE2	2.38	0.48
1:B:212:MET:HE3	1:B:1094:ASN:OD1	2.14	0.48
1:B:901:SER:O	1:B:901:SER:OG	2.30	0.48
1:A:347:ASN:OD1	1:A:515:VAL:HG11	2.13	0.48
1:A:461:VAL:HA	1:A:464:MET:HE3	1.94	0.48
1:A:1065:THR:HG21	1:A:1068:SER:OG	2.14	0.48
1:B:998:VAL:HG11	1:B:1425:THR:OG1	2.14	0.47
1:A:796:MET:CG	1:A:1109:LYS:HZ2	2.26	0.47
1:A:236:ASN:ND2	1:A:326:TRP:HA	2.29	0.47
1:A:460:VAL:O	1:A:464:MET:HG3	2.14	0.47
1:A:603:ARG:O	1:A:603:ARG:CG	2.51	0.47
1:B:1095:GLN:HE21	1:B:1095:GLN:CA	2.27	0.47
1:A:57:GLN:H	1:A:57:GLN:HG2	1.56	0.47
1:A:219:GLN:HG2	1:A:221:MET:HE2	1.96	0.47
1:A:756:LEU:CA	1:A:1214:THR:HG21	2.38	0.47
1:A:135:CYS:HB3	1:A:139:CYS:HB2	1.94	0.47
1:A:282:VAL:HA	1:A:286:ARG:O	2.14	0.47
1:A:796:MET:CE	1:A:796:MET:CG	2.91	0.47
1:A:1278:ARG:NH2	6:A:2174:HOH:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:THR:HG23	1:B:1294:ASN:HD21	1.78	0.47
1:B:258:GLU:O	1:B:261:THR:OG1	2.28	0.47
1:B:730:GLN:NE2	6:B:2048:HOH:O	2.44	0.47
1:A:330:ALA:HB3	1:A:345:ASP:HB3	1.95	0.47
1:A:1008:ASP:OD1	1:A:1335:LYS:HE2	2.14	0.47
1:A:1443:ASN:OD1	1:A:1445:GLU:HG2	2.15	0.47
1:A:375:GLU:H	1:A:375:GLU:CD	2.22	0.46
1:A:518:LEU:HD13	1:A:712:PHE:CE2	2.50	0.46
1:A:266:GLN:H	1:A:266:GLN:HG2	1.53	0.46
1:A:618:PRO:HG3	1:A:644:THR:OG1	2.16	0.46
1:B:1110:THR:HG22	1:B:1113:ASP:CG	2.39	0.46
1:A:993:ARG:HD3	1:A:1369:THR:OG1	2.15	0.46
1:A:223:LEU:HD23	1:A:278:LEU:HD23	1.98	0.46
1:A:522:LEU:HB2	1:A:539:ILE:HB	1.98	0.46
1:A:651:HIS:CD2	1:A:1075:HIS:HB3	2.51	0.46
1:B:1058:ILE:HD13	1:B:1084:VAL:HA	1.98	0.46
1:A:649:SER:H	1:A:652:HIS:CD2	2.33	0.46
1:B:581:THR:O	1:B:585:LYS:HG3	2.16	0.46
1:A:978:GLN:H	4:A:2510:AKG:H41	1.80	0.46
1:B:209:THR:OG1	1:B:1043:THR:HG23	2.16	0.46
1:B:715:LEU:HD22	1:B:726:TYR:CD1	2.51	0.46
1:A:36:ALA:N	1:A:120:GLN:HE22	2.14	0.46
1:B:143:GLU:OE1	1:B:143:GLU:HA	2.16	0.46
1:B:546:VAL:HA	1:B:550:GLU:OE2	2.16	0.46
1:A:112:VAL:HA	1:A:187:PHE:O	2.15	0.46
1:B:28:MET:HE1	1:B:366:SER:HB2	1.97	0.46
1:A:75:GLY:O	1:A:130:GLN:HA	2.16	0.46
1:A:80:PRO:HA	1:A:162:ASP:OD1	2.16	0.46
1:A:313:SER:O	1:A:317:ASP:HB2	2.16	0.46
1:A:954:PRO:O	1:A:958:MET:HG2	2.16	0.46
1:B:717:LYS:CB	1:B:974:GLY:HA3	2.45	0.46
1:B:1234:TRP:CZ3	1:B:1235:LEU:HD13	2.51	0.45
1:B:1393:VAL:HG22	1:B:1411:VAL:HB	1.98	0.45
2:B:2508:FMN:HO4'	2:B:2508:FMN:P	2.38	0.45
1:A:385:ALA:HB3	1:A:388:GLN:NE2	2.31	0.45
1:A:567:LEU:HD21	1:A:602:ASP:HB2	1.99	0.45
1:B:27:CYS:CB	1:B:370:VAL:HG22	2.47	0.45
1:B:871:CYS:O	1:B:1126:GLY:HA2	2.16	0.45
1:B:188:TYR:HB2	1:B:191:LEU:HD22	1.98	0.45
1:B:245:LYS:HB2	1:B:245:LYS:NZ	2.31	0.45
1:B:794:TYR:CE2	1:B:837:ARG:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1363:THR:O	1:B:1363:THR:CG2	2.61	0.45
1:A:6:ILE:HG22	1:A:17:LEU:HD22	1.98	0.45
1:B:750:THR:HG21	1:B:1039:ILE:HG12	1.97	0.45
1:A:9:LEU:CD2	1:A:392:VAL:HG11	2.46	0.45
1:A:1185:LEU:HD21	1:A:1193:LEU:HD13	1.99	0.45
1:A:1279:THR:HA	1:A:1312:SER:O	2.17	0.45
1:A:353:ARG:NH2	1:A:1329:ALA:O	2.36	0.45
1:B:270:ASP:OD1	1:B:271:SER:N	2.50	0.45
1:A:47:MET:O	1:A:201:ALA:HA	2.17	0.45
1:A:1228:THR:CG2	1:A:1228:THR:O	2.65	0.45
1:A:451:GLY:HA2	1:A:768:PHE:CD2	2.52	0.45
1:A:1386:ARG:HG2	1:A:1404:TYR:HB2	1.99	0.45
1:A:278:LEU:HD12	1:A:295:LEU:HD12	1.98	0.44
1:B:1406:THR:HG22	1:B:1425:THR:HG22	1.98	0.44
1:A:1265:THR:CG2	1:A:1266:THR:H	2.20	0.44
1:B:1145:THR:HG22	1:B:1147:ASN:HB2	1.99	0.44
1:B:603:ARG:HD3	1:B:643:ASP:OD2	2.16	0.44
1:B:618:PRO:HG3	1:B:644:THR:OG1	2.18	0.44
1:A:152:ARG:HG2	1:A:152:ARG:NH1	2.30	0.44
1:A:1442:ILE:HD13	1:A:1442:ILE:HA	1.66	0.44
1:B:320:SER:HB2	6:B:2026:HOH:O	2.16	0.44
1:B:385:ALA:HB1	1:B:386:PRO:CD	2.48	0.44
1:B:729:ALA:HB1	1:B:731:ILE:HD11	1.99	0.44
1:A:178:MET:HE2	1:A:213:PRO:CB	2.48	0.44
1:B:507:ILE:O	1:B:716:SER:HB2	2.17	0.44
1:B:926:LEU:HD13	1:B:929:LEU:CD1	2.48	0.44
1:B:1108:LEU:O	1:B:1130:ILE:CG1	2.64	0.44
1:A:149:TYR:CD2	1:A:283:ARG:HG3	2.53	0.44
1:B:1506:ASN:O	1:B:1507:ASN:CB	2.58	0.44
1:A:499:PHE:CG	1:A:973:PRO:HB2	2.52	0.44
1:A:764:GLU:OE1	1:A:1213:LYS:NZ	2.50	0.44
1:A:1179:GLU:OE2	1:A:1182:ARG:HD3	2.18	0.44
1:B:892:MET:HE3	1:B:897:ALA:HB3	1.99	0.44
1:B:1349:GLN:H	1:B:1349:GLN:HG3	1.42	0.44
1:A:1110:THR:HG22	1:A:1113:ASP:N	2.17	0.44
1:B:96:VAL:HG21	1:B:155:ILE:HG13	2.00	0.44
1:B:1215:GLN:O	1:B:1216:ASN:HB3	2.18	0.44
1:A:1349:GLN:H	1:A:1349:GLN:HG3	1.50	0.43
1:B:1279:THR:HG22	1:B:1282:THR:CB	2.48	0.43
1:A:92:TYR:O	1:A:96:VAL:HG13	2.18	0.43
1:A:784:GLY:O	1:A:795:HIS:NE2	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:THR:HG23	1:A:1385:VAL:HG21	1.99	0.43
1:B:1443:ASN:OD1	1:B:1445:GLU:HG2	2.17	0.43
1:A:148:LEU:HD12	1:A:148:LEU:HA	1.88	0.43
1:A:517:SER:HB3	1:A:722:LEU:HD22	1.99	0.43
1:A:1156:GLN:O	1:A:1160:ARG:HG3	2.18	0.43
1:A:1381:GLU:H	1:A:1381:GLU:HG2	1.55	0.43
1:A:243:ARG:HH22	1:A:525:ARG:HH11	1.66	0.43
1:B:1198:GLY:O	1:B:1200:THR:N	2.51	0.43
1:B:36:ALA:HB2	1:B:211:THR:HG21	1.99	0.43
1:B:601:THR:HG23	1:B:643:ASP:OD2	2.17	0.43
1:B:1078:SER:HB3	1:B:1079:PRO:HD2	2.00	0.43
1:A:378:ILE:HD12	6:A:2051:HOH:O	2.18	0.43
1:B:484:LEU:HD13	1:B:839:VAL:HG22	1.99	0.43
1:A:470:GLU:OE1	1:A:1071:SER:OG	2.33	0.43
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.85	0.43
1:A:809:VAL:CG1	1:A:1169:GLN:HB3	2.49	0.43
1:A:863:VAL:CG1	1:A:1175:TYR:CD2	3.01	0.43
1:A:668:LEU:HD23	1:A:668:LEU:HA	1.92	0.43
1:A:746:PHE:O	1:A:747:ALA:C	2.60	0.43
1:B:560:GLN:HE21	1:B:560:GLN:HB2	1.55	0.43
1:B:1437:ASP:O	1:B:1440:GLU:HB2	2.19	0.43
1:A:124:ASN:ND2	1:A:213:PRO:HG2	2.34	0.43
1:A:1419:ASN:ND2	1:A:1443:ASN:HD22	2.16	0.43
1:B:66:MET:HA	1:B:67:PRO:HD3	1.90	0.43
1:A:883:GLU:CD	1:A:1160:ARG:NH1	2.75	0.43
1:A:1449:LEU:HG	1:A:1492:TRP:HB3	2.00	0.43
1:B:755:GLY:C	1:B:1214:THR:HG21	2.44	0.43
1:B:1172:ASN:O	1:B:1175:TYR:HB2	2.19	0.43
1:A:1263:HIS:O	1:A:1264:GLN:C	2.60	0.42
1:B:874:GLY:O	2:B:2508:FMN:C10	2.66	0.42
1:B:967:MET:HB2	1:B:1034:LYS:O	2.18	0.42
1:B:1341:GLU:HA	1:B:1372:ASN:O	2.18	0.42
1:A:657:VAL:HA	1:A:661:ALA:O	2.19	0.42
1:A:872:THR:HB	1:A:892:MET:HG3	2.01	0.42
1:A:1215:GLN:HE21	1:A:1215:GLN:HA	1.84	0.42
1:A:1472:THR:CG2	1:A:1474:SER:HB2	2.49	0.42
1:B:863:VAL:HG11	1:B:1175:TYR:CD2	2.55	0.42
1:B:1472:THR:HG21	1:B:1474:SER:HB2	2.02	0.42
1:A:28:MET:HE2	1:A:203:TYR:CE1	2.52	0.42
1:B:1279:THR:HG22	1:B:1282:THR:HB	2.00	0.42
1:A:84:SER:O	1:A:88:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:LEU:HD11	1:A:1124:GLU:HG3	2.01	0.42
1:A:1273:LEU:HG	1:A:1305:PHE:HB3	2.01	0.42
1:A:1289:ALA:HB2	1:A:1318:LEU:HD11	2.00	0.42
1:A:1504:GLU:CD	1:A:1504:GLU:H	2.28	0.42
1:B:369:GLY:HA3	1:B:1308:ALA:HB1	2.00	0.42
1:B:513:ASN:HA	1:B:516:MET:CE	2.50	0.42
1:B:624:ALA:O	1:B:628:HIS:CD2	2.73	0.42
1:A:450:PHE:CD2	1:A:645:ALA:HB3	2.55	0.42
1:B:24:ALA:O	1:B:28:MET:HG2	2.20	0.42
1:B:143:GLU:OE1	1:B:146:ARG:HD3	2.19	0.42
1:B:1150:VAL:O	1:B:1150:VAL:HG13	2.19	0.42
1:A:150:ILE:O	1:A:154:ILE:HG13	2.20	0.42
1:A:536:ALA:O	1:A:538:THR:HG22	2.19	0.42
1:A:872:THR:CG2	1:A:899:SER:HA	2.21	0.42
1:A:1008:ASP:HB3	1:A:1009:ILE:HG13	2.00	0.42
1:A:1270:THR:HA	1:A:1304:ASN:O	2.20	0.42
1:B:149:TYR:CD2	1:B:283:ARG:HG3	2.54	0.42
1:B:805:LEU:HB2	1:B:830:TYR:CD1	2.54	0.42
1:B:125:GLN:HA	1:B:126:PRO:HD2	1.86	0.42
1:B:446:GLN:HE22	1:B:608:ILE:HG23	1.85	0.42
1:A:231:ASN:OD1	1:A:327:ASP:HB3	2.20	0.42
1:A:490:LEU:HD11	1:A:648:TRP:CH2	2.55	0.42
1:B:52:ARG:NH2	1:B:66:MET:HE3	2.35	0.42
1:B:144:LEU:HG	1:B:148:LEU:HD22	2.01	0.42
1:A:261:THR:HB	1:A:262:PRO:CD	2.49	0.42
1:B:575:SER:O	1:B:576:LEU:C	2.63	0.42
1:B:907:ASP:O	1:B:910:ARG:HB2	2.20	0.42
1:B:1200:THR:HG21	1:B:1225:LEU:H	1.85	0.42
1:A:617:PRO:HA	1:A:618:PRO:HD3	1.91	0.41
1:A:1023:HIS:HE1	1:A:1054:ASP:OD2	2.03	0.41
1:A:1206:ARG:HG2	1:A:1208:ASP:OD2	2.20	0.41
1:B:178:MET:HG3	1:B:213:PRO:HB2	2.01	0.41
1:A:796:MET:C	1:A:1109:LYS:HZ1	2.29	0.41
1:A:855:ILE:HG12	1:A:1189:GLY:HA2	2.03	0.41
1:A:204:HIS:ND1	1:A:219:GLN:HB2	2.35	0.41
1:A:420:LYS:HE3	1:A:420:LYS:HB2	1.84	0.41
1:A:863:VAL:HG13	1:A:1178:ALA:HB3	2.01	0.41
1:B:1009:ILE:HD11	1:B:1018:LEU:HD22	2.01	0.41
1:B:1363:THR:HG23	1:B:1385:VAL:HG21	2.03	0.41
1:B:1385:VAL:HB	1:B:1386:ARG:H	1.73	0.41
1:A:801:MET:HE2	1:A:801:MET:HB3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:HIS:CE1	6:A:2105:HOH:O	2.73	0.41
1:A:1030:GLN:HG2	1:A:1054:ASP:CB	2.51	0.41
1:A:1406:THR:HG22	1:A:1425:THR:HG22	2.02	0.41
1:A:1425:THR:HG21	6:A:2133:HOH:O	2.20	0.41
1:A:1145:THR:HG22	1:A:1147:ASN:H	1.85	0.41
1:B:1145:THR:HG22	1:B:1147:ASN:CB	2.50	0.41
1:B:1359:ILE:HG23	1:B:1360:ILE:HG23	2.03	0.41
1:A:309:TYR:CB	1:A:312:ILE:HD12	2.51	0.41
1:B:152:ARG:HG2	1:B:152:ARG:HH11	1.85	0.41
1:B:872:THR:HB	1:B:892:MET:HG3	2.02	0.41
1:B:1021:ASP:HA	1:B:1279:THR:HG21	2.01	0.41
1:A:806:HIS:CE1	1:A:1136:GLY:HA2	2.56	0.41
1:B:6:ILE:HG22	1:B:17:LEU:HD22	2.03	0.41
1:B:27:CYS:HB2	1:B:370:VAL:HG22	2.01	0.41
1:B:265:ASN:HB3	1:B:268:ASN:ND2	2.36	0.41
1:B:1227:ASP:OD1	1:B:1229:LYS:HG3	2.20	0.41
1:B:219:GLN:HG2	1:B:221:MET:HE2	2.03	0.41
1:B:656:LEU:HD23	1:B:664:ILE:HD12	2.02	0.41
1:B:809:VAL:HG21	1:B:1173:PHE:HB2	2.03	0.41
1:B:809:VAL:CG1	1:B:1169:GLN:HB3	2.51	0.41
1:B:1311:GLN:OE1	1:B:1331:ASP:HB2	2.21	0.41
1:A:448:ALA:HA	6:A:2060:HOH:O	2.20	0.40
1:A:581:THR:O	1:A:585:LYS:HG3	2.21	0.40
1:A:1425:THR:CG2	6:A:2133:HOH:O	2.68	0.40
1:A:24:ALA:O	1:A:28:MET:HG2	2.22	0.40
1:A:603:ARG:HD2	1:A:667:TYR:CE2	2.56	0.40
1:A:131:ILE:C	1:A:132:LEU:HD23	2.47	0.40
1:A:244:GLU:OE1	1:A:261:THR:O	2.39	0.40
1:A:261:THR:O	1:A:262:PRO:C	2.63	0.40
1:A:566:THR:OG1	1:A:602:ASP:HB3	2.21	0.40
1:A:1052:ASN:HD22	1:A:1052:ASN:HA	1.75	0.40
1:B:858:GLU:H	1:B:858:GLU:HG2	1.47	0.40
1:B:953:THR:CG2	1:B:1294:ASN:ND2	2.71	0.40
1:A:1332:TYR:HB3	1:A:1335:LYS:HE3	2.03	0.40
1:B:135:CYS:HG	1:B:139:CYS:HB2	1.86	0.40
1:B:1382:ARG:HB3	1:B:1385:VAL:HG22	2.03	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	1475/1520 (97%)	1398 (95%)	72 (5%)	5 (0%)	36	45
1	B	1475/1520 (97%)	1394 (94%)	73 (5%)	8 (0%)	24	32
All	All	2950/3040 (97%)	2792 (95%)	145 (5%)	13 (0%)	30	37

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	679	ASP
1	B	679	ASP
1	B	1385	VAL
1	B	902	GLY
1	B	977	GLY
1	A	731	ILE
1	A	1498	SER
1	B	731	ILE
1	A	221	MET
1	B	139	CYS
1	B	261	THR
1	A	902	GLY
1	B	1138	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1209/1236 (98%)	1072 (89%)	137 (11%)	5	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1209/1236 (98%)	1072 (89%)	137 (11%)	5	5
All	All	2418/2472 (98%)	2144 (89%)	274 (11%)	5	5

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	17	LEU
1	A	23	LYS
1	A	57	GLN
1	A	64	LEU
1	A	71	ARG
1	A	96	VAL
1	A	122	LYS
1	A	132	LEU
1	A	137	GLU
1	A	139	CYS
1	A	147	ARG
1	A	148	LEU
1	A	157	LYS
1	A	161	GLU
1	A	168	PHE
1	A	182	ILE
1	A	189	LEU
1	A	191	LEU
1	A	211	THR
1	A	212	MET
1	A	223	LEU
1	A	224	LEU
1	A	234	LEU
1	A	245	LYS
1	A	249	VAL
1	A	254	LYS
1	A	264	VAL
1	A	266	GLN
1	A	274	LEU
1	A	336	ASP
1	A	339	ILE
1	A	340	VAL
1	A	367	GLU
1	A	370	VAL
1	A	375	GLU

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Mol	Chain	Res	Type
1	A	379	VAL
1	A	404	GLN
1	A	435	THR
1	A	453	THR
1	A	457	VAL
1	A	458	GLU
1	A	459	MET
1	A	469	LYS
1	A	511	ARG
1	A	514	LEU
1	A	515	VAL
1	A	518	LEU
1	A	530	GLU
1	A	541	LEU
1	A	556	THR
1	A	578	ASP
1	A	583	LEU
1	A	584	VAL
1	A	598	LEU
1	A	601	THR
1	A	603	ARG
1	A	608	ILE
1	A	625	VAL
1	A	629	LEU
1	A	650	THR
1	A	656	LEU
1	A	662	SER
1	A	668	LEU
1	A	680	GLU
1	A	690	ARG
1	A	701	LYS
1	A	715	LEU
1	A	750	THR
1	A	753	VAL
1	A	756	LEU
1	A	761	VAL
1	A	765	VAL
1	A	778	LYS
1	A	779	LYS
1	A	796	MET
1	A	800	GLU
1	A	801	MET

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Mol	Chain	Res	Type
1	A	809	VAL
1	A	828	GLU
1	A	831	ARG
1	A	835	LYS
1	A	843	ARG
1	A	852	GLN
1	A	856	SER
1	A	858	GLU
1	A	867	VAL
1	A	877	LEU
1	A	915	ASP
1	A	933	GLN
1	A	949	ARG
1	A	953	THR
1	A	961	LYS
1	A	991	LEU
1	A	1008	ASP
1	A	1015	LEU
1	A	1028	GLU
1	A	1030	GLN
1	A	1043	THR
1	A	1052	ASN
1	A	1085	THR
1	A	1095	GLN
1	A	1101	LEU
1	A	1110	THR
1	A	1130	ILE
1	A	1145	THR
1	A	1150	VAL
1	A	1164	LYS
1	A	1170	VAL
1	A	1191	ARG
1	A	1193	LEU
1	A	1210	GLN
1	A	1214	THR
1	A	1215	GLN
1	A	1217	LEU
1	A	1228	THR
1	A	1232	ARG
1	A	1235	LEU
1	A	1246	VAL
1	A	1248	ASP

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Mol	Chain	Res	Type
1	A	1279	THR
1	A	1280	VAL
1	A	1311	GLN
1	A	1349	GLN
1	A	1369	THR
1	A	1373	LEU
1	A	1381	GLU
1	A	1386	ARG
1	A	1389	VAL
1	A	1416	VAL
1	A	1425	THR
1	A	1449	LEU
1	A	1464	LEU
1	A	1472	THR
1	A	1488	LEU
1	A	1504	GLU
1	A	1506	ASN
1	B	17	LEU
1	B	23	LYS
1	B	50	ILE
1	B	52	ARG
1	B	57	GLN
1	B	61	THR
1	B	64	LEU
1	B	71	ARG
1	B	96	VAL
1	B	99	LEU
1	B	122	LYS
1	B	137	GLU
1	B	139	CYS
1	B	147	ARG
1	B	148	LEU
1	B	161	GLU
1	B	182	ILE
1	B	191	LEU
1	B	207	PHE
1	B	211	THR
1	B	212	MET
1	B	223	LEU
1	B	224	LEU
1	B	234	LEU
1	B	245	LYS

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Mol	Chain	Res	Type
1	B	249	VAL
1	B	254	LYS
1	B	264	VAL
1	B	266	GLN
1	B	274	LEU
1	B	278	LEU
1	B	287	SER
1	B	339	ILE
1	B	340	VAL
1	B	353	ARG
1	B	355	CYS
1	B	370	VAL
1	B	376	VAL
1	B	379	VAL
1	B	404	GLN
1	B	444	LEU
1	B	453	THR
1	B	457	VAL
1	B	459	MET
1	B	469	LYS
1	B	511	ARG
1	B	514	LEU
1	B	515	VAL
1	B	518	LEU
1	B	541	LEU
1	B	543	SER
1	B	556	THR
1	B	560	GLN
1	B	563	GLU
1	B	578	ASP
1	B	583	LEU
1	B	598	LEU
1	B	601	THR
1	B	603	ARG
1	B	608	ILE
1	B	625	VAL
1	B	629	LEU
1	B	636	LEU
1	B	656	LEU
1	B	664	ILE
1	B	668	LEU
1	B	680	GLU

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Mol	Chain	Res	Type
1	B	690	ARG
1	B	694	ILE
1	B	701	LYS
1	B	750	THR
1	B	753	VAL
1	B	761	VAL
1	B	764	GLU
1	B	765	VAL
1	B	779	LYS
1	B	796	MET
1	B	800	GLU
1	B	801	MET
1	B	809	VAL
1	B	828	GLU
1	B	831	ARG
1	B	835	LYS
1	B	843	ARG
1	B	852	GLN
1	B	856	SER
1	B	858	GLU
1	B	867	VAL
1	B	868	LYS
1	B	872	THR
1	B	877	LEU
1	B	933	GLN
1	B	953	THR
1	B	961	LYS
1	B	991	LEU
1	B	1015	LEU
1	B	1028	GLU
1	B	1030	GLN
1	B	1043	THR
1	B	1052	ASN
1	B	1085	THR
1	B	1095	GLN
1	B	1101	LEU
1	B	1110	THR
1	B	1130	ILE
1	B	1145	THR
1	B	1150	VAL
1	B	1164	LYS
1	B	1170	VAL

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Mol	Chain	Res	Type
1	B	1177	ILE
1	B	1183	SER
1	B	1191	ARG
1	B	1193	LEU
1	B	1210	GLN
1	B	1214	THR
1	B	1215	GLN
1	B	1217	LEU
1	B	1228	THR
1	B	1232	ARG
1	B	1235	LEU
1	B	1240	VAL
1	B	1246	VAL
1	B	1280	VAL
1	B	1349	GLN
1	B	1369	THR
1	B	1381	GLU
1	B	1385	VAL
1	B	1386	ARG
1	B	1389	VAL
1	B	1416	VAL
1	B	1425	THR
1	B	1449	LEU
1	B	1464	LEU
1	B	1472	THR
1	B	1488	LEU
1	B	1504	GLU
1	B	1506	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	57	GLN
1	A	120	GLN
1	A	124	ASN
1	A	199	ASN
1	A	227	ASN
1	A	236	ASN
1	A	303	GLN
1	A	422	GLN
1	A	486	HIS

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Mol	Chain	Res	Type
1	A	513	ASN
1	A	560	GLN
1	A	582	ASN
1	A	627	HIS
1	A	628	HIS
1	A	651	HIS
1	A	652	HIS
1	A	730	GLN
1	A	806	HIS
1	A	885	HIS
1	A	934	ASN
1	A	978	GLN
1	A	1023	HIS
1	A	1052	ASN
1	A	1095	GLN
1	A	1147	ASN
1	A	1210	GLN
1	A	1215	GLN
1	A	1216	ASN
1	A	1294	ASN
1	A	1317	ASN
1	A	1372	ASN
1	A	1376	ASN
1	A	1419	ASN
1	A	1450	GLN
1	A	1493	GLN
1	A	1506	ASN
1	A	1507	ASN
1	B	15	HIS
1	B	57	GLN
1	B	120	GLN
1	B	199	ASN
1	B	266	GLN
1	B	268	ASN
1	B	303	GLN
1	B	422	GLN
1	B	446	GLN
1	B	486	HIS
1	B	513	ASN
1	B	560	GLN
1	B	628	HIS
1	B	651	HIS

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Mol	Chain	Res	Type
1	B	652	HIS
1	B	730	GLN
1	B	885	HIS
1	B	933	GLN
1	B	978	GLN
1	B	1023	HIS
1	B	1052	ASN
1	B	1095	GLN
1	B	1147	ASN
1	B	1215	GLN
1	B	1216	ASN
1	B	1275	ASN
1	B	1294	ASN
1	B	1372	ASN
1	B	1376	ASN
1	B	1450	GLN
1	B	1460	GLN
1	B	1493	GLN
1	B	1506	ASN
1	B	1507	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
4	AKG	A	2510	-	9,9,9	3.24	4 (44%)	11,11,11	3.86	6 (54%)
3	F3S	B	2509	1	0,9,9	-	-	-	-	-
5	ONL	B	2511	-	8,9,9	0.71	0	8,11,11	2.45	3 (37%)
3	F3S	A	2509	1	0,9,9	-	-	-	-	-
2	FMN	B	2508	-	33,33,33	1.31	3 (9%)	48,50,50	1.67	13 (27%)
5	ONL	A	2511	1	8,9,9	0.83	0	8,11,11	2.54	5 (62%)
2	FMN	A	2508	-	33,33,33	1.11	3 (9%)	48,50,50	1.43	9 (18%)
4	AKG	B	2510	-	9,9,9	2.99	3 (33%)	11,11,11	4.90	5 (45%)

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
4	AKG	A	2510	-	-	4/9/9/9	-
5	ONL	B	2511	-	-	1/9/9/9	-
3	F3S	B	2509	1	-	-	0/3/3/3
3	F3S	A	2509	1	-	-	0/3/3/3
2	FMN	B	2508	-	-	2/18/18/18	0/3/3/3
5	ONL	A	2511	1	-	3/9/9/9	-
2	FMN	A	2508	-	-	6/18/18/18	0/3/3/3
4	AKG	B	2510	-	-	3/9/9/9	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2510	AKG	O5-C2	6.72	1.36	1.23
4	B	2510	AKG	O5-C2	5.73	1.34	1.23
4	A	2510	AKG	O1-C1	5.52	1.36	1.22
4	B	2510	AKG	O1-C1	5.51	1.36	1.22
2	B	2508	FMN	C4A-N5	4.25	1.39	1.30
4	B	2510	AKG	O3-C5	3.73	1.34	1.22
4	A	2510	AKG	O3-C5	2.89	1.31	1.22
2	A	2508	FMN	C4A-N5	2.64	1.36	1.30
2	A	2508	FMN	C10-N1	2.50	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2508	FMN	C1'-N10	2.44	1.53	1.47
2	A	2508	FMN	P-O1P	2.28	1.57	1.50
4	A	2510	AKG	C2-C1	2.21	1.56	1.53
2	B	2508	FMN	P-O2P	-2.01	1.47	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2510	AKG	C4-C3-C2	-10.45	93.30	112.91
4	B	2510	AKG	O5-C2-C1	-7.89	108.39	119.67
4	A	2510	AKG	C4-C3-C2	-7.51	98.81	112.91
4	B	2510	AKG	C3-C2-C1	6.77	127.36	115.86
4	A	2510	AKG	O1-C1-C2	-5.57	114.88	121.81
4	B	2510	AKG	O1-C1-C2	-5.56	114.90	121.81
4	A	2510	AKG	C3-C2-C1	4.99	124.33	115.86
5	B	2511	ONL	OXT-C-O	-4.66	113.51	124.08
5	A	2511	ONL	OD-CD-CG	4.31	133.78	121.47
5	B	2511	ONL	CB-CG-CD	-4.10	108.38	114.77
4	A	2510	AKG	O4-C5-O3	-4.09	112.82	123.33
2	B	2508	FMN	O4'-C4'-C5'	-4.03	101.10	109.99
4	A	2510	AKG	O5-C2-C1	-3.87	114.13	119.67
4	A	2510	AKG	O4-C5-C4	3.85	126.15	114.00
5	A	2511	ONL	OXT-C-O	-3.74	115.59	124.08
2	A	2508	FMN	C10-C4A-N5	-3.73	117.20	124.81
2	A	2508	FMN	C4A-C10-N10	3.12	120.95	116.48
5	A	2511	ONL	CB-CG-CD	-2.92	110.21	114.77
2	A	2508	FMN	O4-C4-N3	-2.91	114.65	120.11
2	B	2508	FMN	C10-C4A-N5	-2.88	118.92	124.81
2	B	2508	FMN	O3P-P-O5'	2.87	114.15	106.67
2	A	2508	FMN	C4-C4A-C10	2.82	121.77	116.93
2	B	2508	FMN	C1'-N10-C9A	-2.72	115.34	120.63
2	B	2508	FMN	C9-C9A-N10	-2.72	118.20	121.85
4	B	2510	AKG	O2-C1-O1	2.71	130.35	123.90
2	B	2508	FMN	C4A-C10-N10	2.69	120.34	116.48
2	A	2508	FMN	C9A-C5A-N5	-2.67	119.62	122.45
2	B	2508	FMN	C5'-C4'-C3'	-2.52	107.46	112.22
2	B	2508	FMN	C4-N3-C2	-2.46	121.27	125.64
2	B	2508	FMN	O4-C4-N3	-2.42	115.56	120.11
5	B	2511	ONL	CB-CA-N	-2.32	104.06	110.12
2	A	2508	FMN	O4-C4-C4A	-2.26	120.57	126.53
2	B	2508	FMN	C5A-C9A-N10	2.25	120.00	117.97
2	A	2508	FMN	C4-N3-C2	-2.25	121.65	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2511	ONL	OD-CD-CE	-2.24	115.87	121.48
2	B	2508	FMN	C9A-C5A-N5	-2.22	120.10	122.45
2	B	2508	FMN	C1'-C2'-C3'	2.19	115.58	109.66
2	A	2508	FMN	C9A-N10-C10	-2.17	117.44	120.75
2	B	2508	FMN	C4-C4A-N5	2.16	121.20	118.21
5	A	2511	ONL	CE-CD-CG	-2.15	110.31	116.85
2	A	2508	FMN	C6-C5A-C9A	2.11	121.95	119.05

There are no chirality outliers.

All (19) torsion outliers are listed below:

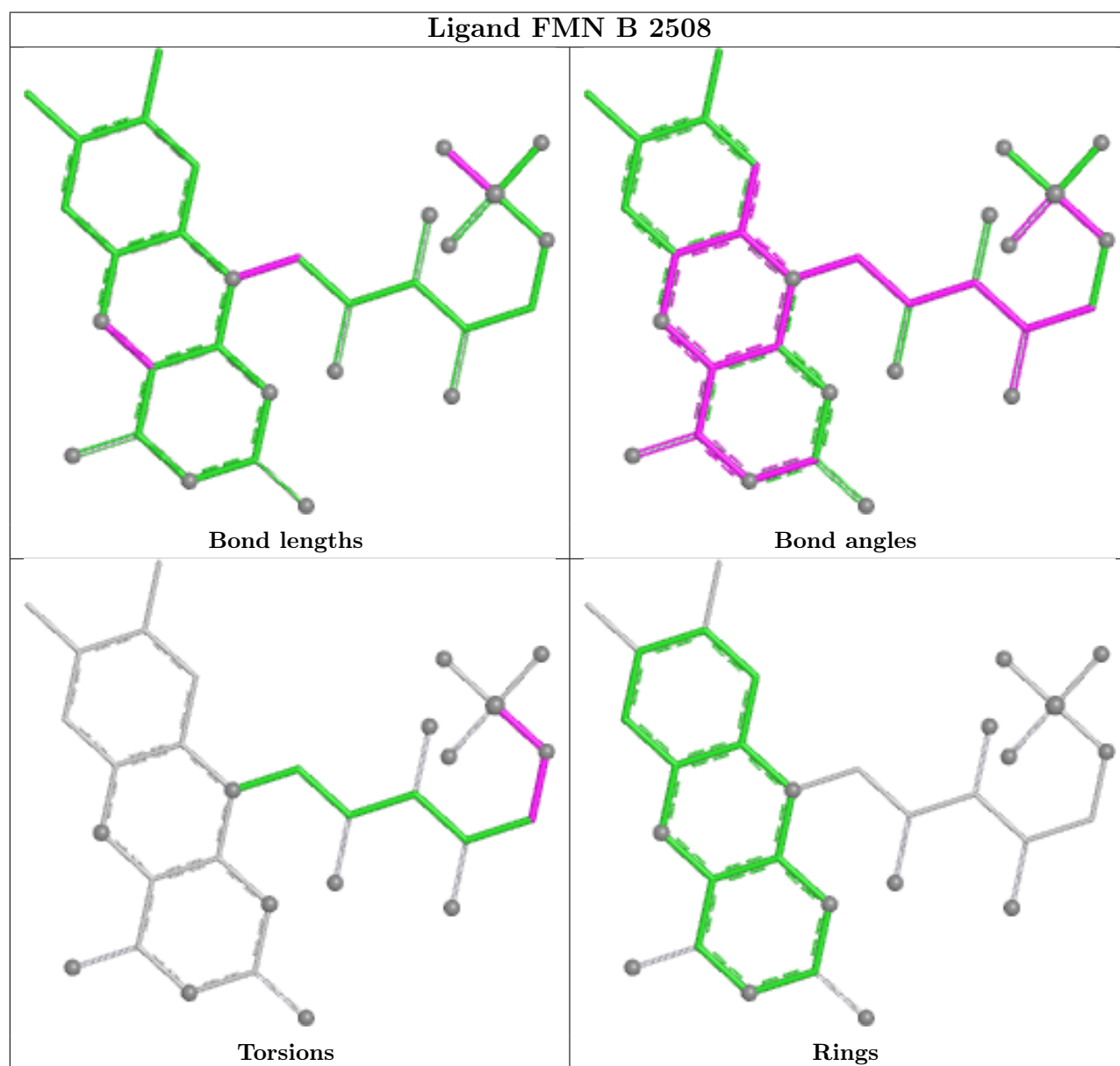
Mol	Chain	Res	Type	Atoms
4	A	2510	AKG	O2-C1-C2-C3
2	A	2508	FMN	O3'-C3'-C4'-C5'
2	A	2508	FMN	C2'-C3'-C4'-O4'
2	A	2508	FMN	O3'-C3'-C4'-O4'
2	B	2508	FMN	C4'-C5'-O5'-P
4	A	2510	AKG	O1-C1-C2-C3
5	A	2511	ONL	OD-CD-CG-CB
2	A	2508	FMN	C2'-C3'-C4'-C5'
4	A	2510	AKG	O2-C1-C2-O5
4	B	2510	AKG	O2-C1-C2-O5
2	A	2508	FMN	C4'-C5'-O5'-P
2	A	2508	FMN	C5'-O5'-P-O1P
2	B	2508	FMN	C5'-O5'-P-O1P
5	A	2511	ONL	CE-CD-CG-CB
5	B	2511	ONL	O-C-CA-N
4	A	2510	AKG	O1-C1-C2-O5
5	A	2511	ONL	CA-CB-CG-CD
4	B	2510	AKG	C3-C4-C5-O4
4	B	2510	AKG	C3-C4-C5-O3

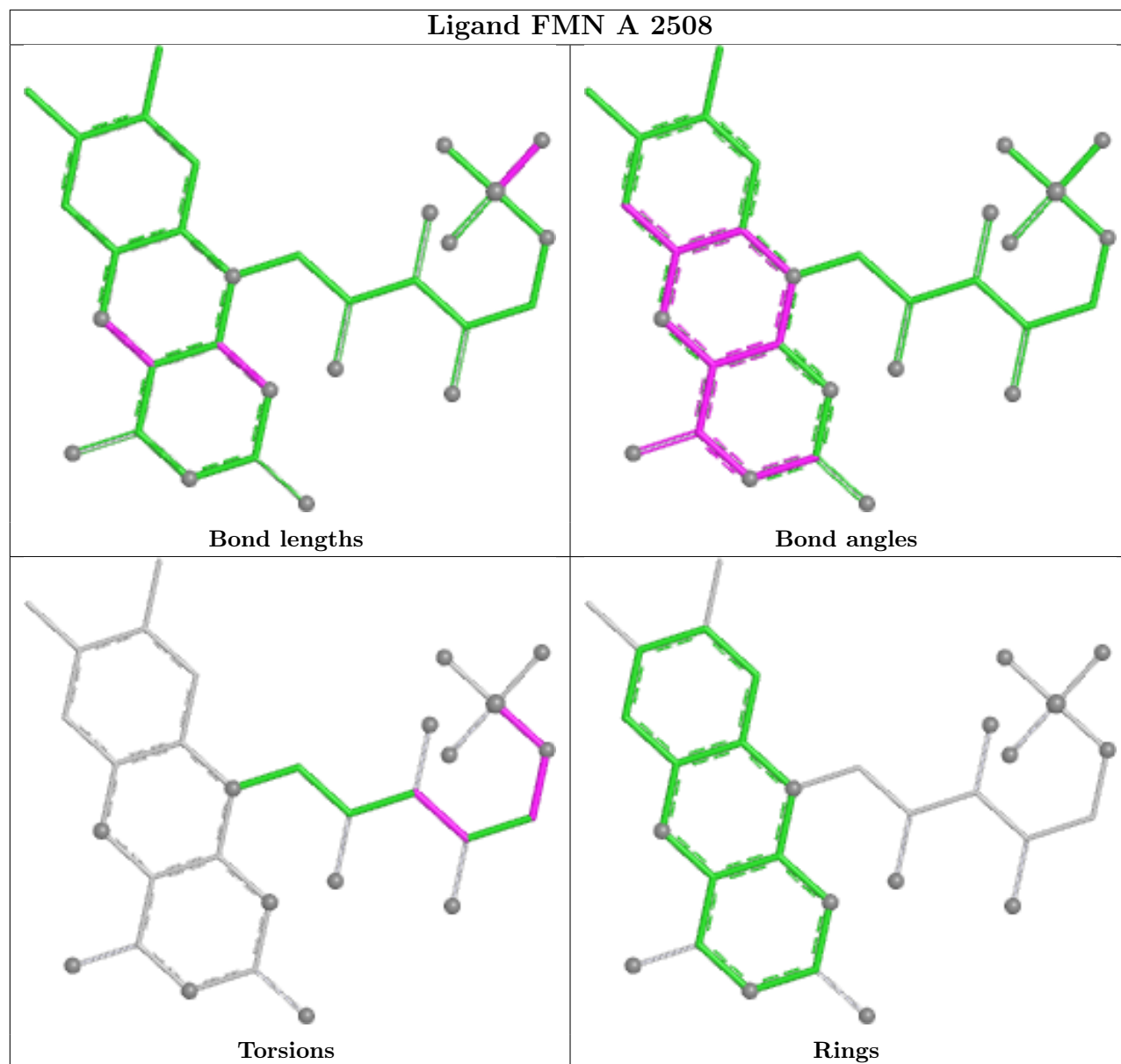
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2510	AKG	1	0
5	B	2511	ONL	6	0
2	B	2508	FMN	3	0
2	A	2508	FMN	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1485/1520 (97%)	-0.01	28 (1%) 66 67	8, 16, 23, 29	0
1	B	1485/1520 (97%)	0.20	29 (1%) 65 66	7, 17, 23, 31	0
All	All	2970/3040 (97%)	0.10	57 (1%) 66 67	7, 16, 23, 31	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	439	ASP	3.5
1	B	784	GLY	3.4
1	B	403	TYR	3.2
1	B	833	TYR	3.2
1	A	211	THR	3.2
1	B	1240	VAL	3.1
1	A	502	VAL	3.1
1	B	728	GLY	3.1
1	B	812	TYR	3.0
1	A	439	ASP	3.0
1	A	510	LEU	3.0
1	A	261	THR	3.0
1	B	251	GLY	2.9
1	A	506	PRO	2.8
1	B	578	ASP	2.7
1	B	1216	ASN	2.7
1	B	245	LYS	2.7
1	A	728	GLY	2.7
1	B	261	THR	2.6
1	A	833	TYR	2.6
1	B	901	SER	2.6
1	B	605	ASN	2.5
1	A	533	ALA	2.5
1	A	1347	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	440	ALA	2.5
1	B	211	THR	2.4
1	A	499	PHE	2.4
1	A	507	ILE	2.4
1	A	719	GLY	2.3
1	B	1347	HIS	2.3
1	A	504	ASN	2.3
1	B	754	GLY	2.3
1	A	262	PRO	2.3
1	A	509	PRO	2.3
1	A	500	ALA	2.2
1	A	436	LEU	2.2
1	B	1242	SER	2.2
1	B	1484	TRP	2.2
1	B	499	PHE	2.2
1	A	475	MET	2.2
1	A	806	HIS	2.2
1	B	514	LEU	2.2
1	B	691	LEU	2.1
1	A	901	SER	2.1
1	A	769	HIS	2.1
1	B	504	ASN	2.1
1	A	512	GLU	2.1
1	A	515	VAL	2.1
1	B	441	GLN	2.1
1	B	500	ALA	2.1
1	B	1191	ARG	2.1
1	A	584	VAL	2.1
1	B	690	ARG	2.1
1	B	796	MET	2.1
1	B	1507	ASN	2.0
1	A	608	ILE	2.0
1	A	213	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

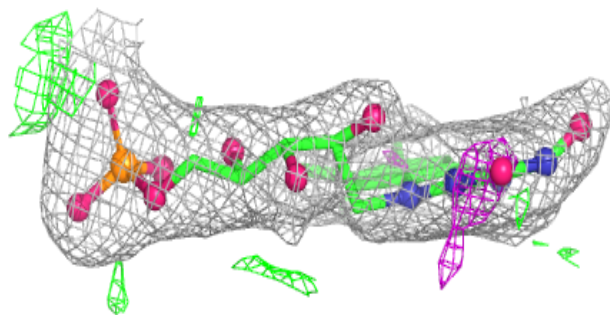
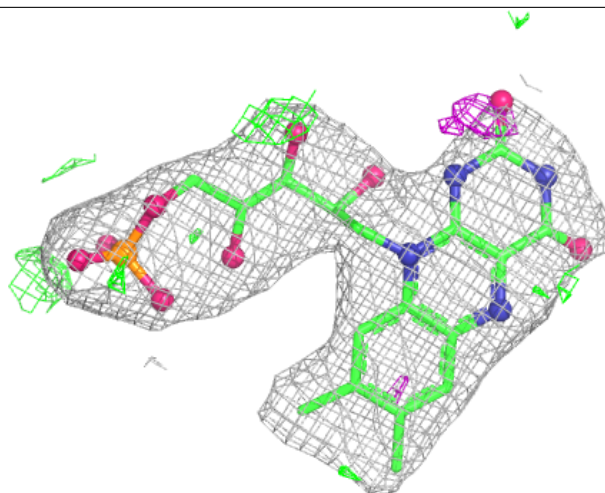
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AKG	B	2510	10/10	0.86	0.16	36,37,40,41	0
5	ONL	B	2511	10/10	0.88	0.16	32,36,37,38	0
5	ONL	A	2511	10/10	0.90	0.12	24,32,34,36	0
4	AKG	A	2510	10/10	0.92	0.09	24,27,35,37	0
2	FMN	B	2508	31/31	0.93	0.09	22,29,32,35	0
2	FMN	A	2508	31/31	0.94	0.08	18,23,28,31	0
3	F3S	A	2509	7/7	0.98	0.04	19,22,24,24	0
3	F3S	B	2509	7/7	0.98	0.07	27,29,30,31	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.

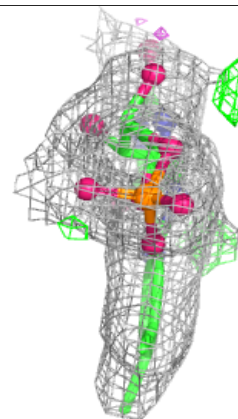
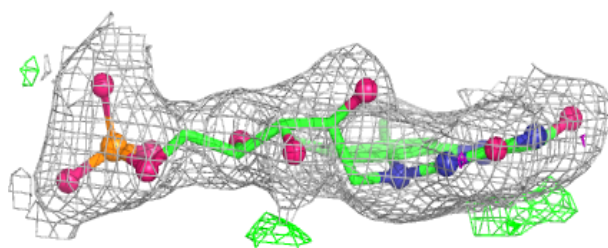
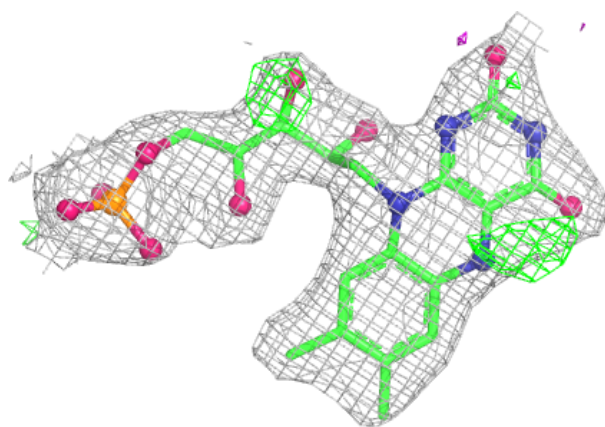
Electron density around FMN B 2508:

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



Electron density around FMN A 2508:

$2mF_o - DF_c$ (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.