



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:41 PM UTC

PDB ID : 1OFD / pdb_00001ofd
Title : Glutamate Synthase from Synechocystis sp in complex with 2-Oxoglutarate at 2.0 Angstrom resolution
Authors : Van Den heuvel, R.H.H.; Mattevi, A.
Deposited on : 2003-04-14
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

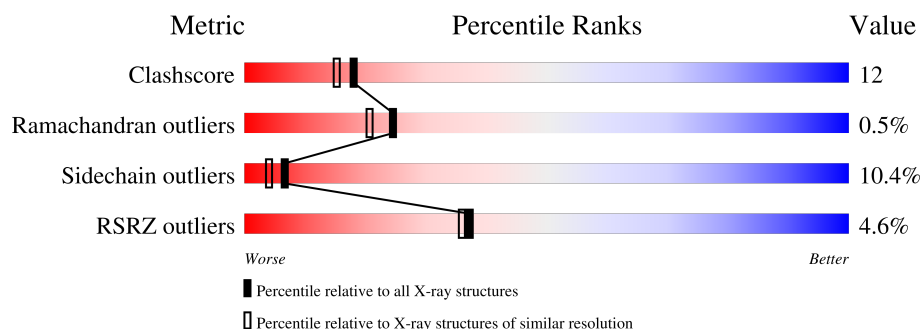
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	1520	4% 73% 20% ...
1	B	1520	5% 74% 19% ...

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	3510	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24388 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.

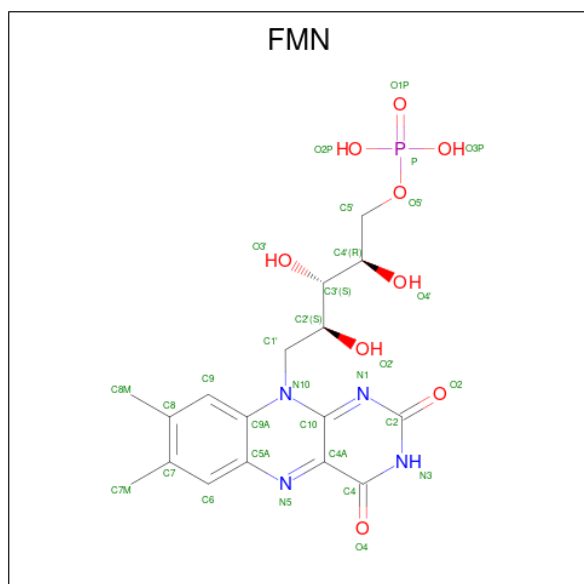
- Molecule 1 is a protein called FERREDONIN-DEPENDENT GLUTAMATE SYNTHASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1491	Total	C	N	O	S	0	0	0
			11434	7211	1995	2173	55			
1	B	1491	Total	C	N	O	S	0	0	0
			11434	7211	1995	2173	55			

There are 6 discrepancies between the modelled and reference sequences:

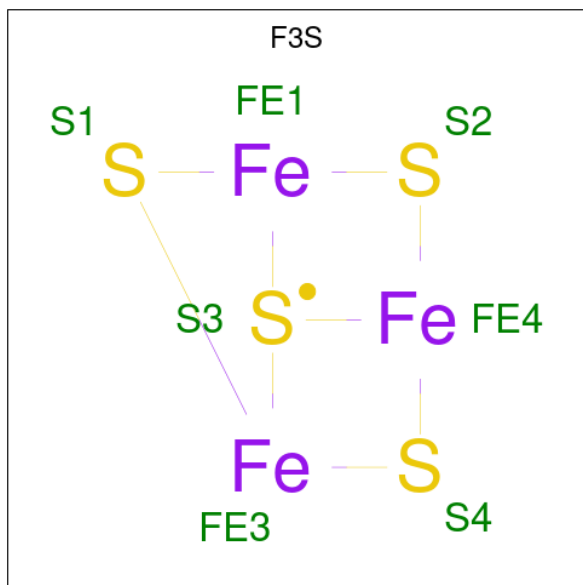
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	conflict	UNP P55038
A	581	THR	ASP	conflict	UNP P55038
A	1507	ASN	GLY	conflict	UNP P55038
B	578	ASP	THR	conflict	UNP P55038
B	581	THR	ASP	conflict	UNP P55038
B	1507	ASN	GLY	conflict	UNP P55038

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



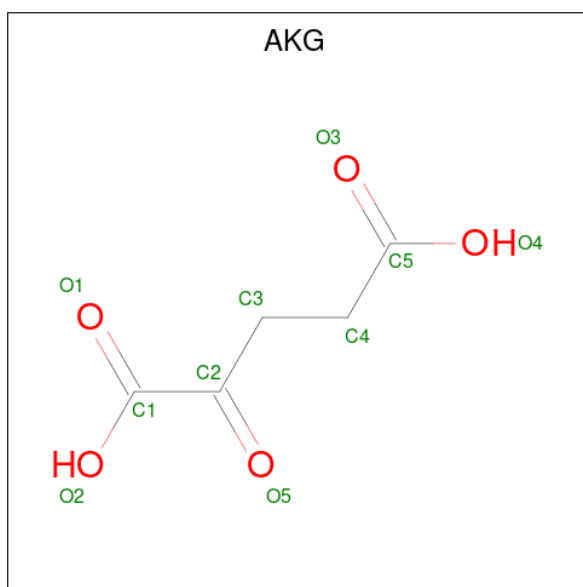
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- 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		

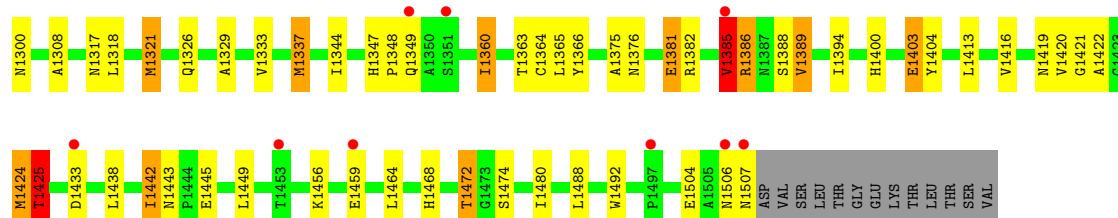
- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $\text{C}_5\text{H}_6\text{O}_5$).



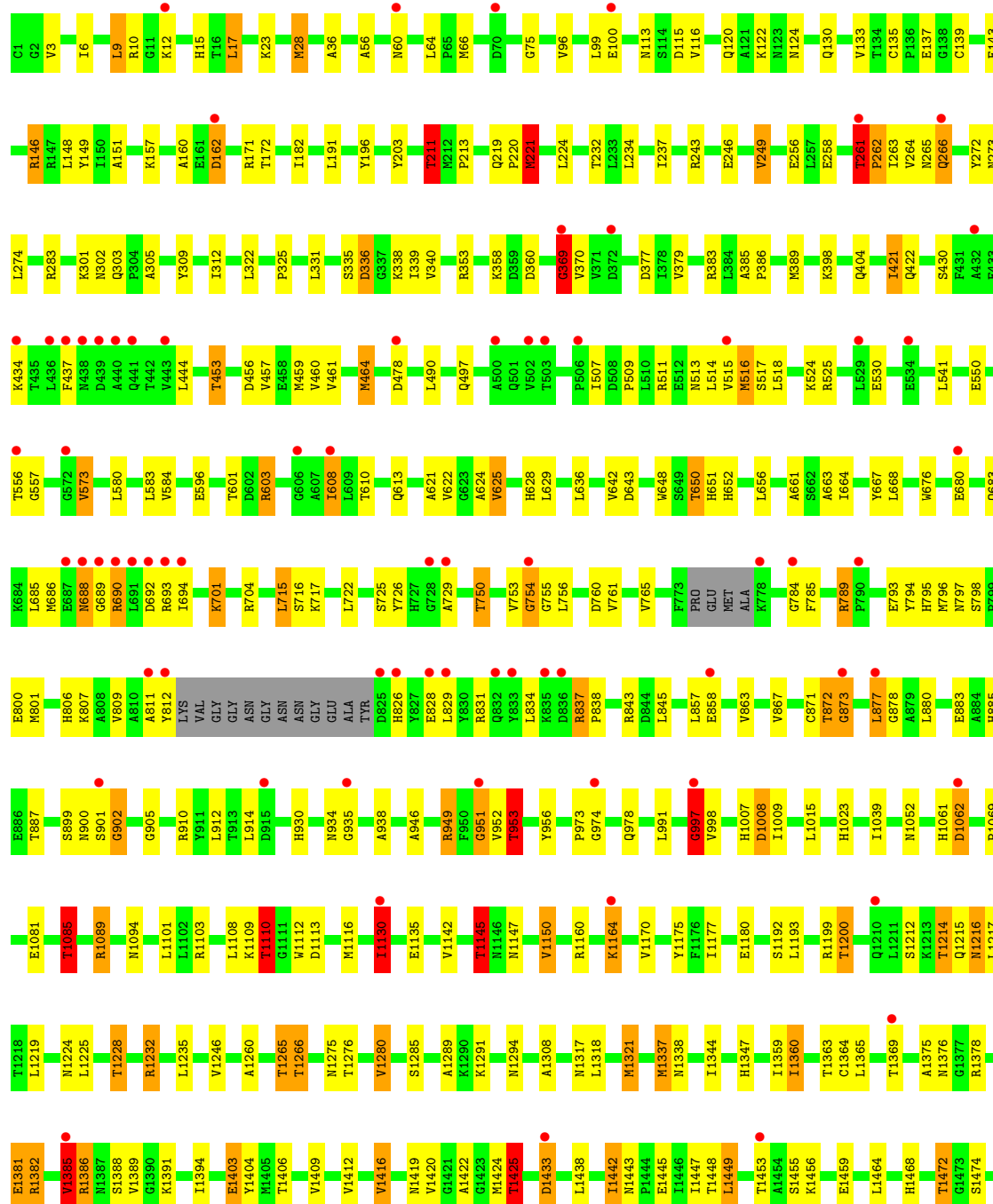
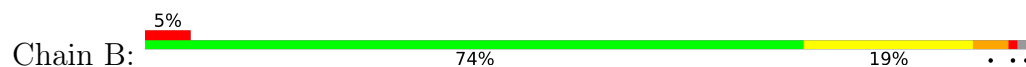
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	705	Total	O	0	0
			705	705		
5	B	719	Total	O	0	0
			719	719		



● Molecule 1: FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE 2



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.02Å 149.66Å 195.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.00) 96.2 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.192 , 0.231 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24388	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: F3S, FMN, AKG

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	0.74	11/11657 (0.1%)	1.03	40/15807 (0.3%)
1	B	0.72	9/11657 (0.1%)	1.02	39/15807 (0.2%)
All	All	0.73	20/23314 (0.1%)	1.03	79/31614 (0.2%)

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	4
1	B	0	4
All	All	0	8

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	MET	SD-CE	-13.25	1.46	1.79
1	B	464	MET	SD-CE	-11.89	1.49	1.79
1	B	1321	MET	SD-CE	-11.70	1.50	1.79
1	A	1321	MET	SD-CE	-10.15	1.54	1.79
1	A	1337	MET	SD-CE	-9.83	1.54	1.79
1	A	1116	MET	SD-CE	-9.32	1.56	1.79
1	B	516	MET	SD-CE	-8.26	1.58	1.79
1	B	1337	MET	SD-CE	-7.22	1.61	1.79
1	B	28	MET	SD-CE	-6.69	1.62	1.79
1	A	1385	VAL	C-O	6.63	1.31	1.24
1	A	462	VAL	CA-CB	6.25	1.57	1.54
1	B	389	MET	SD-CE	-6.11	1.64	1.79
1	B	221	MET	CG-SD	-5.82	1.66	1.80
1	A	1424	MET	SD-CE	-5.65	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1130	ILE	CG1-CD1	5.43	1.73	1.51
1	A	475	MET	SD-CE	-5.34	1.66	1.79
1	B	1130	ILE	CG1-CD1	5.27	1.72	1.51
1	A	1139	MET	SD-CE	-5.16	1.66	1.79
1	B	1116	MET	SD-CE	-5.08	1.66	1.79
1	A	1008	ASP	CB-CG	-5.00	1.39	1.52

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	ALA	CA-C-N	-14.20	101.38	123.24
1	A	729	ALA	C-N-CA	-14.20	101.38	123.24
1	A	693	ARG	N-CA-C	-11.69	96.41	112.30
1	B	729	ALA	CA-C-N	-11.65	105.30	123.24
1	B	729	ALA	C-N-CA	-11.65	105.30	123.24
1	B	1403	GLU	CA-C-N	-10.70	106.49	122.86
1	B	1403	GLU	C-N-CA	-10.70	106.49	122.86
1	A	1403	GLU	CA-C-N	-9.36	107.44	123.25
1	A	1403	GLU	C-N-CA	-9.36	107.44	123.25
1	B	693	ARG	N-CA-C	-8.84	101.80	112.59
1	B	878	GLY	N-CA-C	8.48	122.90	112.73
1	B	949	ARG	NE-CZ-NH1	-8.10	113.40	121.50
1	A	878	GLY	N-CA-C	7.82	122.11	112.64
1	A	1164	LYS	N-CA-C	-7.80	98.34	110.42
1	B	1498	SER	N-CA-C	-7.77	104.70	114.56
1	A	1062	ASP	N-CA-C	7.43	120.44	111.82
1	B	1150	VAL	CB-CA-C	7.17	117.79	110.70
1	A	221	MET	CG-SD-CE	-7.09	85.30	100.90
1	A	1425	THR	N-CA-CB	-6.96	101.27	110.88
1	B	221	MET	CG-SD-CE	-6.81	85.92	100.90
1	A	729	ALA	O-C-N	-6.73	115.42	123.03
1	B	335	SER	CA-C-N	6.71	131.92	120.72
1	B	335	SER	C-N-CA	6.71	131.92	120.72
1	B	1385	VAL	CB-CA-C	-6.60	100.47	111.29
1	A	877	LEU	CA-C-N	-6.59	112.54	119.99
1	A	877	LEU	C-N-CA	-6.59	112.54	119.99
1	A	785	PHE	N-CA-C	6.58	118.11	111.07
1	A	1085	THR	N-CA-CB	-6.58	100.47	110.01
1	B	370	VAL	N-CA-C	6.50	122.95	113.39
1	A	370	VAL	N-CA-C	6.44	122.86	113.39
1	B	1403	GLU	O-C-N	-6.31	114.57	122.20
1	B	1164	LYS	N-CA-C	-6.21	100.18	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	973	PRO	CA-C-N	-6.14	109.37	121.41
1	A	973	PRO	C-N-CA	-6.14	109.37	121.41
1	A	934	ASN	N-CA-C	6.13	118.75	111.33
1	A	650	THR	N-CA-CB	-6.12	100.81	109.94
1	A	1403	GLU	O-C-N	-6.10	114.82	122.20
1	A	1061	HIS	CA-C-N	6.09	129.56	120.31
1	A	1061	HIS	C-N-CA	6.09	129.56	120.31
1	B	1007	HIS	CA-C-N	6.07	131.77	121.14
1	B	1007	HIS	C-N-CA	6.07	131.77	121.14
1	A	172	THR	OG1-CB-CG2	-6.07	97.17	109.30
1	B	949	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	A	935	GLY	N-CA-C	6.05	121.11	114.40
1	B	1425	THR	N-CA-CB	-6.03	103.02	110.98
1	A	877	LEU	O-C-N	-6.03	115.73	122.12
1	B	1145	THR	N-CA-CB	-5.86	101.92	110.53
1	A	1385	VAL	CB-CA-C	-5.85	101.70	111.29
1	A	1232	ARG	NE-CZ-NH2	-5.83	113.96	119.20
1	B	729	ALA	O-C-N	-5.75	116.50	122.94
1	B	1085	THR	N-CA-CB	-5.71	101.72	110.01
1	B	952	VAL	N-CA-C	5.71	115.89	107.15
1	A	1007	HIS	CA-C-N	5.71	131.71	121.66
1	A	1007	HIS	C-N-CA	5.71	131.71	121.66
1	B	729	ALA	N-CA-C	-5.70	102.09	110.52
1	A	952	VAL	N-CA-C	5.68	115.84	107.15
1	A	901	SER	CB-CA-C	-5.55	101.67	111.05
1	A	335	SER	CA-C-N	5.53	130.82	121.14
1	A	335	SER	C-N-CA	5.53	130.82	121.14
1	A	123	ASN	CA-C-N	5.51	130.79	121.14
1	A	123	ASN	C-N-CA	5.51	130.79	121.14
1	B	997	GLY	N-CA-C	5.49	120.81	114.16
1	A	211	THR	N-CA-CB	-5.48	101.93	110.98
1	B	953	THR	N-CA-CB	-5.46	101.12	110.72
1	B	369	GLY	N-CA-C	5.35	125.85	113.18
1	A	369	GLY	N-CA-C	5.31	125.76	113.18
1	B	211	THR	N-CA-CB	-5.29	102.50	111.27
1	B	1110	THR	N-CA-CB	-5.20	102.64	111.69
1	B	1061	HIS	CA-C-N	5.18	129.38	120.72
1	B	1061	HIS	C-N-CA	5.18	129.38	120.72
1	B	935	GLY	N-CA-C	5.17	120.36	114.67
1	B	998	VAL	N-CA-C	5.15	115.26	107.80
1	A	953	THR	N-CA-CB	-5.06	101.27	110.63
1	B	1062	ASP	N-CA-C	5.05	118.70	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1110	THR	N-CA-CB	-5.05	102.14	111.53
1	B	973	PRO	CA-C-N	-5.04	108.95	121.60
1	B	973	PRO	C-N-CA	-5.04	108.95	121.60
1	B	785	PHE	N-CA-C	5.01	116.82	111.36
1	B	353	ARG	CG-CD-NE	-5.00	100.99	112.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	GLY	Peptide
1	A	728	GLY	Peptide
1	A	784	GLY	Peptide
1	A	951	GLY	Peptide
1	B	369	GLY	Peptide
1	B	873	GLY	Peptide
1	B	951	GLY	Peptide
1	B	997	GLY	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	11434	0	11382	289	0
1	B	11434	0	11382	270	0
2	A	31	0	19	1	0
2	B	31	0	19	0	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
5	A	705	0	0	44	0
5	B	719	0	0	44	0
All	All	24388	0	22810	559	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 (559) 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:261:THR:HB	1:A:262:PRO:CD	1.52	1.38
1:B:261:THR:HB	1:B:262:PRO:CD	1.53	1.30
1:A:1385:VAL:O	1:A:1404:TYR:N	1.71	1.21
1:B:1385:VAL:O	1:B:1404:TYR:N	1.74	1.18
1:B:258:GLU:O	1:B:261:THR:HG23	1.44	1.18
1:B:261:THR:CB	1:B:262:PRO:HD2	1.73	1.17
1:B:997:GLY:HA3	5:B:2497:HOH:O	1.42	1.17
1:A:1318:LEU:H	1:A:1321:MET:CE	1.57	1.15
1:B:1424:MET:HE2	1:B:1447:ILE:HG21	1.26	1.15
1:A:1344:ILE:HD12	1:A:1360:ILE:HD11	1.22	1.14
1:B:1318:LEU:H	1:B:1321:MET:CE	1.58	1.14
1:A:261:THR:HB	1:A:262:PRO:HD2	1.12	1.11
1:B:1318:LEU:H	1:B:1321:MET:HE2	1.05	1.09
1:B:1228:THR:HG23	1:B:1232:ARG:HH21	1.11	1.09
1:A:258:GLU:O	1:A:261:THR:HG23	1.52	1.08
1:A:1318:LEU:H	1:A:1321:MET:HE2	1.12	1.07
1:B:509:PRO:HA	1:B:516:MET:HE1	1.10	1.07
1:A:1228:THR:HG23	1:A:1232:ARG:HH21	1.10	1.07
1:B:1228:THR:HG23	1:B:1232:ARG:NH2	1.70	1.06
1:A:601:THR:HG22	1:A:603:ARG:H	1.23	1.03
1:A:261:THR:CB	1:A:262:PRO:HD2	1.87	1.03
1:B:901:SER:OG	1:B:901:SER:O	1.72	1.02
1:B:885:HIS:CD2	1:B:910:ARG:HH22	1.77	1.01
1:A:1228:THR:HG23	1:A:1232:ARG:NH2	1.73	1.00
1:B:1344:ILE:HD12	1:B:1360:ILE:HD11	1.44	0.99
1:A:901:SER:O	1:A:901:SER:OG	1.69	0.99
1:B:650:THR:HG21	5:B:2253:HOH:O	1.61	0.99
1:B:601:THR:HG22	1:B:603:ARG:H	1.28	0.96
1:A:157:LYS:NZ	1:A:261:THR:OG1	2.01	0.94
1:B:261:THR:HB	1:B:262:PRO:HD2	0.93	0.93
1:A:1381:GLU:HG3	5:A:2175:HOH:O	1.69	0.91
1:B:1318:LEU:N	1:B:1321:MET:HE2	1.84	0.91
1:B:1228:THR:CG2	1:B:1232:ARG:HH21	1.83	0.90
1:A:1318:LEU:N	1:A:1321:MET:HE2	1.85	0.90
1:A:885:HIS:CD2	1:A:910:ARG:HH22	1.90	0.89
1:B:513:ASN:HA	1:B:516:MET:HE3	1.54	0.89
1:A:1130:ILE:H	1:A:1130:ILE:HD12	1.35	0.89
1:B:883:GLU:OE1	1:B:1160:ARG:HD2	1.73	0.89
1:B:1130:ILE:HD12	1:B:1130:ILE:H	1.38	0.88
1:B:460:VAL:HG12	1:B:464:MET:HE2	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:LEU:N	1:A:1321:MET:CE	2.39	0.86
1:A:223:LEU:HD23	1:A:278:LEU:HG	1.57	0.86
1:A:27:CYS:HB2	1:A:370:VAL:HG23	1.59	0.85
1:A:1228:THR:CG2	1:A:1232:ARG:HH21	1.90	0.85
1:A:211:THR:HG21	1:A:1094:ASN:O	1.75	0.84
1:A:453:THR:HG23	5:A:2227:HOH:O	1.78	0.84
1:A:459:MET:HE1	5:A:2387:HOH:O	1.78	0.83
1:A:460:VAL:HG12	1:A:464:MET:CE	2.07	0.83
1:A:797:ASN:HA	1:A:801:MET:HE2	1.59	0.82
1:A:1085:THR:HG23	5:A:2569:HOH:O	1.78	0.82
1:A:872:THR:CG2	5:A:2409:HOH:O	2.26	0.82
1:B:760:ASP:OD2	1:B:1214:THR:HG22	1.80	0.82
1:B:1228:THR:CG2	1:B:1232:ARG:NH2	2.42	0.82
1:B:784:GLY:HA3	5:B:2406:HOH:O	1.79	0.81
1:B:460:VAL:HG12	1:B:464:MET:CE	2.10	0.80
1:B:211:THR:HG21	1:B:1094:ASN:O	1.81	0.80
1:B:100:GLU:OE1	1:B:151:ALA:HB2	1.82	0.80
1:B:1110:THR:HG22	1:B:1113:ASP:H	1.47	0.80
1:A:1285:SER:OG	1:A:1321:MET:HE1	1.81	0.79
1:A:261:THR:HB	1:A:262:PRO:HD3	1.62	0.79
1:B:1318:LEU:N	1:B:1321:MET:CE	2.42	0.79
1:A:497:GLN:HE21	1:A:651:HIS:HD2	1.28	0.79
1:B:797:ASN:HA	1:B:801:MET:HE2	1.64	0.78
1:B:953:THR:HG22	1:B:956:TYR:H	1.48	0.78
1:B:1468:HIS:O	1:B:1472:THR:HB	1.84	0.77
1:A:1419:ASN:HD21	1:A:1443:ASN:HD22	1.33	0.77
1:A:278:LEU:HD13	5:A:2138:HOH:O	1.84	0.77
1:B:828:GLU:HA	5:B:2414:HOH:O	1.83	0.77
1:B:872:THR:HG23	5:B:2430:HOH:O	1.85	0.77
1:A:1337:MET:HE3	1:A:1365:LEU:HD22	1.67	0.77
1:B:1420:VAL:HB	1:B:1442:ILE:HD12	1.66	0.77
1:B:421:ILE:HG22	1:B:422:GLN:HG2	1.65	0.76
1:A:1403:GLU:O	1:A:1422:ALA:O	2.03	0.76
1:A:987:TYR:O	1:A:991:LEU:HD13	1.86	0.76
1:B:1424:MET:CE	1:B:1447:ILE:HG21	2.14	0.76
1:A:648:TRP:H	1:A:652:HIS:HD2	1.34	0.76
1:B:237:ILE:HG12	1:B:264:VAL:HG11	1.65	0.75
1:B:877:LEU:O	1:B:880:LEU:O	2.03	0.75
1:B:1337:MET:HE2	1:B:1365:LEU:HD22	1.67	0.75
1:A:953:THR:CG2	1:A:1294:ASN:HD21	1.98	0.75
1:A:404:GLN:OE1	5:A:2206:HOH:O	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:ARG:HG2	1:A:838:PRO:O	1.87	0.74
1:A:24:ALA:HA	1:A:370:VAL:HG22	1.69	0.74
1:B:157:LYS:NZ	1:B:261:THR:OG1	2.20	0.74
1:A:1228:THR:CG2	1:A:1232:ARG:NH2	2.48	0.74
1:A:1337:MET:CE	1:A:1365:LEU:CD2	2.64	0.74
1:B:885:HIS:HD2	1:B:910:ARG:HH22	1.33	0.74
1:B:461:VAL:HA	1:B:464:MET:HE3	1.69	0.73
1:B:1145:THR:HG22	1:B:1147:ASN:H	1.54	0.73
1:A:513:ASN:HA	1:A:516:MET:HE2	1.68	0.73
1:A:953:THR:HG22	1:A:956:TYR:H	1.53	0.73
1:B:905:GLY:HA2	1:B:951:GLY:HA3	1.70	0.73
1:B:453:THR:HG23	5:B:2242:HOH:O	1.87	0.73
1:A:1376:ASN:HB2	1:A:1472:THR:CG2	2.18	0.73
1:B:237:ILE:HG12	1:B:264:VAL:CG1	2.19	0.73
1:B:459:MET:HE1	5:B:2403:HOH:O	1.89	0.73
1:A:603:ARG:HD2	1:A:667:TYR:CE2	2.24	0.72
1:A:1200:THR:HG22	5:A:2570:HOH:O	1.89	0.72
1:B:750:THR:HG22	5:B:2379:HOH:O	1.89	0.72
1:A:1130:ILE:H	1:A:1130:ILE:CD1	2.02	0.72
1:A:650:THR:HG21	5:A:2237:HOH:O	1.90	0.72
1:A:27:CYS:CB	1:A:370:VAL:HG23	2.20	0.71
1:B:261:THR:O	1:B:263:ILE:N	2.23	0.71
1:A:70:ASP:HB2	5:A:2023:HOH:O	1.91	0.71
1:A:1376:ASN:HB2	1:A:1472:THR:HG21	1.73	0.71
1:B:753:VAL:O	1:B:754:GLY:O	2.09	0.71
1:A:953:THR:HG21	1:A:1294:ASN:HD21	1.56	0.70
1:B:831:ARG:HB3	5:B:2415:HOH:O	1.91	0.70
1:B:249:VAL:HG12	1:B:530:GLU:HG2	1.74	0.70
1:A:1089:ARG:NH1	1:A:1224:ASN:O	2.24	0.70
1:B:264:VAL:HG13	1:B:273:ASN:OD1	1.92	0.70
1:B:1506:ASN:O	1:B:1507:ASN:HB2	1.91	0.70
1:B:872:THR:CG2	5:B:2430:HOH:O	2.40	0.69
1:A:1145:THR:HG22	1:A:1147:ASN:H	1.57	0.69
1:B:1403:GLU:O	1:B:1422:ALA:O	2.11	0.69
1:A:1081:GLU:O	1:A:1085:THR:HB	1.92	0.69
1:A:883:GLU:OE1	1:A:1160:ARG:HD2	1.91	0.69
1:B:1391:LYS:NZ	5:B:2668:HOH:O	2.25	0.69
1:A:1030:GLN:HG3	1:A:1240:VAL:HG22	1.73	0.69
1:B:421:ILE:HG21	5:B:2230:HOH:O	1.93	0.69
1:A:1337:MET:HE3	1:A:1365:LEU:CD2	2.23	0.69
1:B:750:THR:HG21	1:B:1039:ILE:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:THR:HG23	5:A:2409:HOH:O	1.88	0.68
1:A:1300:ASN:OD1	5:A:2609:HOH:O	2.10	0.68
1:A:67:PRO:HG2	1:A:72:LEU:HB2	1.75	0.68
1:B:460:VAL:CG1	1:B:464:MET:HE2	2.24	0.68
1:B:1130:ILE:H	1:B:1130:ILE:CD1	2.06	0.68
1:A:873:GLY:HA2	5:A:2422:HOH:O	1.94	0.68
1:A:1337:MET:HE1	1:A:1365:LEU:HD21	1.76	0.68
1:A:237:ILE:HG12	1:A:264:VAL:CG1	2.24	0.67
1:B:1386:ARG:HG2	1:B:1404:TYR:HB2	1.74	0.67
1:A:686:MET:HB3	1:A:692:ASP:HB2	1.76	0.67
1:B:628:HIS:HE1	5:B:2330:HOH:O	1.76	0.67
1:B:237:ILE:HG23	1:B:264:VAL:HG12	1.75	0.67
1:B:369:GLY:HA3	1:B:1275:ASN:HB3	1.77	0.67
1:A:789:ARG:HG3	5:A:2388:HOH:O	1.94	0.67
1:B:497:GLN:HE21	1:B:651:HIS:HD2	1.42	0.67
1:B:953:THR:CG2	1:B:1294:ASN:HD21	2.07	0.67
1:A:1326:GLN:CD	1:A:1348:PRO:HD3	2.19	0.66
1:B:1081:GLU:O	1:B:1085:THR:HB	1.94	0.66
1:A:460:VAL:HG12	1:A:464:MET:HE1	1.76	0.66
1:B:261:THR:O	1:B:262:PRO:C	2.38	0.66
1:A:1333:VAL:HG21	1:A:1360:ILE:HG12	1.78	0.65
1:A:784:GLY:HA3	5:A:2390:HOH:O	1.96	0.65
1:A:453:THR:CG2	5:A:2227:HOH:O	2.41	0.65
1:A:453:THR:HB	1:A:456:ASP:OD2	1.96	0.65
1:B:1337:MET:CE	1:B:1365:LEU:HD22	2.26	0.65
1:A:27:CYS:HB2	1:A:370:VAL:CG2	2.25	0.65
1:B:760:ASP:OD2	1:B:1214:THR:CG2	2.45	0.65
1:A:676:TRP:HE1	1:A:690:ARG:NH1	1.94	0.65
1:A:1110:THR:HG22	1:A:1113:ASP:H	1.62	0.65
1:B:336:ASP:HB3	1:B:338:LYS:H	1.61	0.65
1:B:1419:ASN:HD21	1:B:1443:ASN:HD22	1.44	0.65
1:A:124:ASN:ND2	5:A:2051:HOH:O	2.30	0.64
1:B:873:GLY:HA2	5:B:2440:HOH:O	1.95	0.64
1:A:1421:GLY:HA2	1:A:1424:MET:CE	2.28	0.64
1:A:834:LEU:HD21	1:A:1109:LYS:NZ	2.12	0.64
1:A:37:ASP:H	1:A:120:GLN:NE2	1.96	0.64
1:A:389:MET:HE2	1:A:406:LYS:HE3	1.80	0.64
1:A:685:LEU:HD13	1:A:690:ARG:HD2	1.79	0.64
1:B:1285:SER:OG	1:B:1321:MET:HE1	1.98	0.64
1:B:509:PRO:CA	1:B:516:MET:HE1	2.06	0.63
1:B:1337:MET:HE2	1:B:1365:LEU:CD2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:VAL:CG1	1:A:464:MET:HE2	2.28	0.63
1:B:10:ARG:NH2	1:B:360:ASP:OD2	2.28	0.63
1:B:834:LEU:O	1:B:837:ARG:HB3	1.98	0.62
1:B:603:ARG:HD3	1:B:643:ASP:OD2	1.99	0.62
1:A:863:VAL:HG13	1:A:1178:ALA:HB3	1.81	0.62
1:B:1085:THR:CG2	5:B:2588:HOH:O	2.46	0.62
1:B:872:THR:HG22	1:B:899:SER:HA	1.81	0.62
1:A:264:VAL:HG13	1:A:273:ASN:OD1	1.99	0.62
1:A:1199:ARG:HD2	1:A:1228:THR:HG22	1.81	0.62
1:A:603:ARG:HD3	1:A:643:ASP:OD2	1.98	0.62
1:A:497:GLN:HE21	1:A:651:HIS:CD2	2.15	0.62
1:B:648:TRP:H	1:B:652:HIS:HD2	1.46	0.62
1:A:358:LYS:HG2	1:A:377:ASP:HB2	1.81	0.62
1:A:261:THR:CB	1:A:262:PRO:CD	2.42	0.62
1:A:1421:GLY:HA2	1:A:1424:MET:HE2	1.82	0.62
1:B:794:TYR:CZ	1:B:837:ARG:HB2	2.34	0.62
1:B:1344:ILE:CD1	1:B:1360:ILE:HD11	2.24	0.62
1:B:509:PRO:HA	1:B:516:MET:CE	2.06	0.61
1:B:946:ALA:O	1:B:949:ARG:NH1	2.33	0.61
1:B:1424:MET:HE2	1:B:1447:ILE:CG2	2.17	0.61
1:B:1085:THR:HG23	5:B:2588:HOH:O	2.00	0.61
1:A:28:MET:CE	1:A:203:TYR:HE1	2.13	0.61
1:A:172:THR:HG21	5:A:2106:HOH:O	2.01	0.61
1:A:784:GLY:CA	5:A:2390:HOH:O	2.48	0.61
1:B:953:THR:HG23	1:B:1294:ASN:HD21	1.65	0.61
1:A:901:SER:O	1:A:902:GLY:O	2.19	0.60
1:A:1085:THR:CG2	5:A:2569:HOH:O	2.44	0.60
1:B:550:GLU:OE2	1:B:704:ARG:NH2	2.34	0.60
1:B:930:HIS:HD2	5:B:2453:HOH:O	1.83	0.60
1:B:1276:THR:HB	5:B:2611:HOH:O	2.00	0.60
1:A:237:ILE:HG12	1:A:264:VAL:HG11	1.83	0.60
1:B:219:GLN:HB3	1:B:220:PRO:HA	1.83	0.60
1:B:1359:ILE:HG23	1:B:1360:ILE:HD12	1.84	0.60
1:B:1145:THR:HG21	5:B:2551:HOH:O	2.01	0.60
1:B:1145:THR:HG23	1:B:1147:ASN:ND2	2.16	0.60
1:A:461:VAL:HA	1:A:464:MET:HE3	1.83	0.60
1:A:1420:VAL:HB	1:A:1442:ILE:HD12	1.84	0.60
1:B:135:CYS:SG	1:B:139:CYS:HB2	2.41	0.60
1:A:237:ILE:HG23	1:A:264:VAL:HG12	1.84	0.60
1:B:6:ILE:HG22	1:B:17:LEU:HD22	1.83	0.59
1:B:261:THR:HG21	5:B:2077:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:LYS:HG2	1:B:974:GLY:HA3	1.84	0.59
1:A:475:MET:HE1	1:A:1129:SER:HB3	1.84	0.59
1:B:1376:ASN:HB2	1:B:1472:THR:HG23	1.84	0.59
1:A:1062:ASP:OD2	5:A:2508:HOH:O	2.16	0.59
1:A:261:THR:HG21	5:A:2071:HOH:O	2.01	0.59
1:B:901:SER:O	1:B:902:GLY:O	2.19	0.59
1:A:769:HIS:HD2	5:A:2379:HOH:O	1.86	0.59
1:B:596:GLU:OE1	5:B:2324:HOH:O	2.17	0.59
1:B:1199:ARG:HD2	1:B:1228:THR:HG22	1.83	0.59
1:A:642:VAL:HG13	1:A:664:ILE:HG23	1.85	0.59
1:A:460:VAL:CG1	1:A:464:MET:CE	2.78	0.59
1:B:237:ILE:HG23	1:B:264:VAL:CG1	2.33	0.58
1:B:1265:THR:CG2	1:B:1266:THR:N	2.66	0.58
1:A:353:ARG:NH2	1:A:1329:ALA:O	2.31	0.58
1:B:685:LEU:O	1:B:690:ARG:N	2.37	0.58
1:B:453:THR:CG2	5:B:2242:HOH:O	2.47	0.58
1:B:1455:SER:O	1:B:1459:GLU:HG2	2.02	0.58
1:B:885:HIS:CD2	1:B:910:ARG:NH2	2.61	0.58
1:A:146:ARG:HH22	1:A:256:GLU:CD	2.12	0.58
1:A:914:LEU:O	1:A:934:ASN:O	2.20	0.58
1:B:1337:MET:CE	1:B:1365:LEU:CD2	2.82	0.58
1:A:580:LEU:HD21	1:A:620:LEU:HD21	1.85	0.58
1:A:37:ASP:H	1:A:120:GLN:HE21	1.52	0.58
1:B:120:GLN:O	1:B:124:ASN:HB2	2.03	0.58
1:B:211:THR:CG2	5:B:2108:HOH:O	2.51	0.58
1:B:1265:THR:HG22	1:B:1266:THR:N	2.19	0.57
1:A:286:ARG:NH1	1:A:290:GLU:OE2	2.36	0.57
1:B:100:GLU:OE2	1:B:151:ALA:N	2.37	0.57
1:B:601:THR:HG22	1:B:603:ARG:N	2.11	0.57
1:B:386:PRO:HD3	1:B:1381:GLU:OE2	2.05	0.56
1:A:27:CYS:HB3	1:A:1275:ASN:HD21	1.70	0.56
1:A:171:ARG:CZ	1:A:338:LYS:HD2	2.35	0.56
1:A:863:VAL:CG1	1:A:1175:TYR:CD2	2.88	0.56
1:A:905:GLY:HA3	1:A:951:GLY:HA2	1.88	0.56
1:B:1443:ASN:OD1	1:B:1445:GLU:HG2	2.06	0.56
1:B:784:GLY:O	1:B:795:HIS:NE2	2.30	0.56
1:A:232:THR:HG21	1:A:725:SER:HB3	1.86	0.56
1:B:172:THR:HG21	5:B:2115:HOH:O	2.06	0.56
1:A:717:LYS:HG2	1:A:974:GLY:HA3	1.87	0.56
1:A:910:ARG:HD3	1:A:938:ALA:CB	2.36	0.56
1:B:603:ARG:HD2	1:B:667:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:GLY:CA	1:A:951:GLY:HA2	2.35	0.56
1:B:160:ALA:C	1:B:162:ASP:H	2.11	0.56
1:A:811:ALA:O	1:A:812:TYR:HB2	2.06	0.56
1:A:877:LEU:O	1:A:880:LEU:O	2.23	0.56
1:A:910:ARG:HD3	1:A:938:ALA:HB1	1.88	0.56
1:A:1468:HIS:O	1:A:1472:THR:HB	2.06	0.56
1:B:905:GLY:HA2	1:B:951:GLY:CA	2.36	0.56
1:B:701:LYS:HG2	5:B:2349:HOH:O	2.05	0.56
1:A:987:TYR:O	1:A:991:LEU:CD1	2.54	0.55
1:B:266:GLN:HG2	5:B:2137:HOH:O	2.04	0.55
1:B:525:ARG:NH2	5:B:2295:HOH:O	2.39	0.55
1:B:784:GLY:H	1:B:793:GLU:H	1.55	0.55
1:B:146:ARG:HH22	1:B:256:GLU:CD	2.13	0.55
1:B:211:THR:HG22	5:B:2108:HOH:O	2.06	0.55
1:A:556:THR:O	1:A:557:GLY:O	2.24	0.55
1:B:686:MET:HB3	1:B:692:ASP:HB2	1.89	0.55
1:B:1317:ASN:HA	1:B:1321:MET:HE1	1.88	0.55
1:A:863:VAL:CG1	1:A:1175:TYR:HD2	2.20	0.55
1:A:953:THR:HG23	1:A:1294:ASN:HD21	1.69	0.55
1:A:1386:ARG:HG2	1:A:1404:TYR:HB2	1.89	0.55
1:A:603:ARG:CG	1:A:603:ARG:O	2.54	0.55
1:B:1433:ASP:CG	1:B:1438:LEU:HB2	2.32	0.55
1:A:160:ALA:C	1:A:162:ASP:H	2.15	0.54
1:A:715:LEU:HD22	1:A:726:TYR:CD1	2.43	0.54
1:B:1472:THR:HG22	1:B:1474:SER:H	1.72	0.54
1:B:837:ARG:HG2	1:B:838:PRO:O	2.06	0.54
1:A:1376:ASN:HB2	1:A:1472:THR:HG23	1.89	0.54
1:B:811:ALA:O	1:B:812:TYR:HB2	2.07	0.54
1:A:1506:ASN:O	1:A:1507:ASN:HB2	2.06	0.54
1:B:1472:THR:HG22	1:B:1474:SER:N	2.23	0.54
1:A:278:LEU:HB2	5:A:2138:HOH:O	2.07	0.54
1:B:1376:ASN:HB2	1:B:1472:THR:CG2	2.37	0.54
1:B:843:ARG:HG3	1:B:1112:TRP:CH2	2.43	0.54
1:A:223:LEU:CD2	1:A:278:LEU:HG	2.35	0.53
1:A:784:GLY:H	1:A:793:GLU:H	1.56	0.53
1:B:243:ARG:NH2	1:B:322:LEU:O	2.41	0.53
1:B:863:VAL:CG1	1:B:1175:TYR:CD2	2.91	0.53
1:A:787:ASN:HB2	5:A:2387:HOH:O	2.07	0.53
1:B:325:PRO:HD2	1:B:725:SER:OG	2.08	0.53
1:B:910:ARG:HD3	1:B:938:ALA:HB1	1.91	0.53
1:A:601:THR:HG22	1:A:603:ARG:N	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ALA:N	1:A:120:GLN:HE22	2.06	0.53
1:A:869:ARG:HD2	1:A:1193:LEU:HD23	1.90	0.53
1:B:36:ALA:HB2	1:B:211:THR:HG23	1.91	0.53
1:A:648:TRP:H	1:A:652:HIS:CD2	2.21	0.53
1:A:796:MET:HE1	1:A:834:LEU:HD22	1.91	0.53
1:A:750:THR:HG21	1:A:1039:ILE:HG12	1.91	0.53
1:A:601:THR:CG2	1:A:603:ARG:HG2	2.39	0.53
1:B:621:ALA:O	1:B:625:VAL:HG13	2.08	0.53
1:B:694:ILE:HD12	5:B:2346:HOH:O	2.08	0.53
1:A:15:HIS:HD2	1:A:196:TYR:O	1.91	0.52
1:B:28:MET:HE2	1:B:203:TYR:HE1	1.73	0.52
1:B:232:THR:HG21	1:B:725:SER:HB3	1.90	0.52
1:B:497:GLN:HE21	1:B:651:HIS:CD2	2.26	0.52
1:A:475:MET:HE1	1:A:1129:SER:CB	2.39	0.52
1:B:1280:VAL:HG13	5:B:2610:HOH:O	2.10	0.52
1:B:1363:THR:HG22	1:B:1363:THR:O	2.09	0.52
1:A:650:THR:CG2	5:A:2237:HOH:O	2.51	0.52
1:A:1108:LEU:O	1:A:1130:ILE:HG12	2.09	0.52
1:B:905:GLY:CA	1:B:951:GLY:CA	2.87	0.52
1:A:863:VAL:HG12	1:A:1175:TYR:CD2	2.44	0.52
1:B:685:LEU:HB3	1:B:690:ARG:HB2	1.91	0.52
1:A:28:MET:HE2	1:A:203:TYR:HE1	1.72	0.52
1:B:717:LYS:CG	1:B:974:GLY:HA3	2.39	0.52
1:B:978:GLN:HE22	1:B:1069:PRO:HD3	1.74	0.52
1:B:1360:ILE:HG23	1:B:1364:CYS:SG	2.50	0.52
1:B:1378:ARG:HD2	5:B:2679:HOH:O	2.09	0.52
1:A:417:GLU:O	1:A:421:ILE:HG22	2.10	0.51
1:B:113:ASN:O	1:B:116:VAL:HG22	2.10	0.51
1:B:642:VAL:CG1	1:B:664:ILE:HD12	2.39	0.51
1:B:603:ARG:O	1:B:603:ARG:CG	2.57	0.51
1:A:1326:GLN:NE2	1:A:1348:PRO:HD3	2.25	0.51
1:A:1177:ILE:HD11	5:A:2527:HOH:O	2.10	0.51
1:B:798:SER:H	1:B:801:MET:HE2	1.76	0.51
1:A:13:PRO:HB3	1:A:199:ASN:ND2	2.26	0.51
1:B:796:MET:HE1	1:B:834:LEU:HD22	1.93	0.51
1:A:219:GLN:HB3	1:A:220:PRO:HA	1.93	0.51
1:A:834:LEU:HD21	1:A:1109:LYS:HZ2	1.74	0.51
1:A:872:THR:HG22	5:A:2409:HOH:O	2.04	0.51
1:A:1265:THR:CG2	1:A:1266:THR:N	2.74	0.51
1:B:160:ALA:C	1:B:162:ASP:N	2.69	0.51
1:B:676:TRP:HE1	1:B:690:ARG:NH1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1369:THR:HG22	5:B:2635:HOH:O	2.11	0.51
1:B:873:GLY:C	1:B:900:ASN:HB3	2.36	0.50
1:A:1318:LEU:HB2	1:A:1321:MET:HE2	1.93	0.50
1:B:603:ARG:O	1:B:603:ARG:HG2	2.12	0.50
1:B:755:GLY:C	1:B:1214:THR:HG21	2.36	0.50
1:B:1317:ASN:OD1	1:B:1321:MET:HE3	2.11	0.50
1:A:1413:LEU:HD22	1:A:1480:ILE:HD13	1.94	0.50
1:B:1425:THR:CG2	5:B:2491:HOH:O	2.60	0.50
1:A:385:ALA:HB1	1:A:386:PRO:CD	2.42	0.50
1:A:460:VAL:HG13	1:A:464:MET:HE2	1.92	0.50
1:A:462:VAL:HG11	1:A:690:ARG:NH2	2.27	0.50
1:A:717:LYS:CG	1:A:974:GLY:HA3	2.42	0.50
1:A:1449:LEU:HG	1:A:1492:TRP:HB3	1.94	0.50
1:A:601:THR:HG21	1:A:603:ARG:HG2	1.94	0.50
1:B:905:GLY:HA3	1:B:951:GLY:HA2	1.92	0.50
1:A:9:LEU:HG	1:A:360:ASP:O	2.12	0.49
1:A:36:ALA:HB2	1:A:211:THR:HG23	1.95	0.49
1:A:239:TRP:NE1	1:A:728:GLY:HA3	2.27	0.49
1:B:550:GLU:CD	1:B:704:ARG:HH22	2.20	0.49
1:B:1023:HIS:HD2	5:B:2596:HOH:O	1.93	0.49
1:A:652:HIS:HE1	5:A:2251:HOH:O	1.94	0.49
1:A:1363:THR:O	1:A:1363:THR:HG22	2.12	0.49
1:A:834:LEU:O	1:A:837:ARG:HB3	2.13	0.49
1:A:1023:HIS:HD2	5:A:2579:HOH:O	1.95	0.49
1:B:663:ALA:C	1:B:664:ILE:HD13	2.38	0.49
1:A:764:GLU:HG2	5:A:2377:HOH:O	2.13	0.49
1:A:953:THR:HG21	5:A:2605:HOH:O	2.12	0.49
1:A:1210:GLN:HG3	5:A:2563:HOH:O	2.11	0.49
1:B:1289:ALA:HB2	1:B:1318:LEU:HD11	1.94	0.49
1:A:874:GLY:O	2:A:3508:FMN:C10	2.61	0.49
1:B:1142:VAL:O	1:B:1145:THR:HB	2.13	0.49
1:B:1419:ASN:ND2	1:B:1443:ASN:HD22	2.10	0.49
1:A:1337:MET:CE	1:A:1365:LEU:HD21	2.33	0.49
1:B:15:HIS:HD2	1:B:196:TYR:O	1.95	0.49
1:B:1200:THR:HG21	1:B:1225:LEU:HB2	1.94	0.49
1:B:358:LYS:HG2	1:B:377:ASP:HB2	1.95	0.48
1:B:517:SER:HB3	1:B:722:LEU:HD22	1.95	0.48
1:B:1338:ASN:OD1	1:B:1369:THR:HG23	2.13	0.48
1:A:693:ARG:C	1:A:694:ILE:HG12	2.37	0.48
1:A:1317:ASN:OD1	1:A:1321:MET:HE3	2.13	0.48
1:B:1449:LEU:HG	1:B:1492:TRP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:HIS:HD2	1:A:910:ARG:HH22	1.52	0.48
1:A:1382:ARG:HD2	1:A:1400:HIS:HB2	1.95	0.48
1:B:369:GLY:HA2	1:B:1308:ALA:CB	2.43	0.48
1:B:383:ARG:HH22	1:B:1381:GLU:CD	2.21	0.48
1:B:953:THR:HG21	1:B:1294:ASN:HD21	1.76	0.48
1:B:9:LEU:HG	1:B:360:ASP:O	2.14	0.48
1:B:157:LYS:CE	1:B:261:THR:OG1	2.61	0.48
1:A:6:ILE:HG22	1:A:17:LEU:HD22	1.94	0.48
1:A:984:VAL:O	1:A:996:PRO:O	2.32	0.48
1:A:28:MET:HE2	1:A:203:TYR:CE1	2.48	0.48
1:A:680:GLU:O	1:A:684:LYS:HB2	2.14	0.48
1:A:75:GLY:O	1:A:130:GLN:HA	2.14	0.48
1:A:437:PHE:HD1	1:A:443:VAL:HG22	1.78	0.48
1:A:1382:ARG:O	1:A:1385:VAL:HG22	2.14	0.48
1:B:624:ALA:O	1:B:628:HIS:HD2	1.97	0.48
1:A:765:VAL:CG2	5:A:2312:HOH:O	2.62	0.47
1:A:1433:ASP:CG	1:A:1438:LEU:HB2	2.39	0.47
1:B:1375:ALA:HB3	1:B:1394:ILE:HG22	1.95	0.47
1:B:1378:ARG:CD	5:B:2679:HOH:O	2.61	0.47
1:A:798:SER:H	1:A:801:MET:CE	2.27	0.47
1:B:1412:VAL:HG11	1:B:1416:VAL:HG23	1.97	0.47
1:A:649:SER:H	1:A:652:HIS:CD2	2.32	0.47
1:A:1008:ASP:HB3	1:A:1009:ILE:HG13	1.95	0.47
1:B:171:ARG:CZ	1:B:338:LYS:HD2	2.43	0.47
1:A:625:VAL:HG23	1:A:629:LEU:HD22	1.96	0.47
1:B:303:GLN:HE21	1:B:305:ALA:H	1.61	0.47
1:A:92:TYR:CZ	1:A:158:LYS:HE3	2.50	0.47
1:A:237:ILE:HA	1:A:264:VAL:HG11	1.96	0.47
1:A:261:THR:O	1:A:263:ILE:N	2.47	0.47
1:A:389:MET:HE2	1:A:406:LYS:CE	2.44	0.47
1:A:505:PRO:HD2	5:A:2261:HOH:O	2.13	0.47
1:A:873:GLY:C	1:A:900:ASN:HB3	2.40	0.47
1:B:309:TYR:HB3	1:B:312:ILE:HD12	1.95	0.47
1:B:753:VAL:HG23	1:B:1219:LEU:HD23	1.97	0.47
1:B:930:HIS:CD2	5:B:2453:HOH:O	2.64	0.47
1:A:1375:ALA:HB3	1:A:1394:ILE:HG22	1.97	0.47
1:A:261:THR:CG2	5:A:2123:HOH:O	2.62	0.46
1:A:695:ASP:HB2	5:A:2334:HOH:O	2.13	0.46
1:A:905:GLY:HA2	1:A:951:GLY:HA3	1.97	0.46
1:A:550:GLU:OE2	1:A:704:ARG:NH2	2.48	0.46
1:A:760:ASP:OD2	1:A:1214:THR:CG2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ALA:HB2	1:B:66:MET:HE1	1.98	0.46
1:A:266:GLN:HE21	1:A:266:GLN:HB3	1.55	0.46
1:A:336:ASP:HB3	1:A:338:LYS:H	1.81	0.46
1:B:756:LEU:HD12	1:B:1214:THR:HG23	1.96	0.46
1:B:905:GLY:CA	1:B:951:GLY:HA2	2.45	0.46
1:B:249:VAL:CG1	1:B:530:GLU:HG2	2.45	0.46
1:A:243:ARG:NH2	1:A:322:LEU:O	2.47	0.46
1:A:805:LEU:HD23	1:A:1133:ILE:HG22	1.98	0.46
1:B:75:GLY:O	1:B:130:GLN:HA	2.16	0.46
1:B:1008:ASP:HB3	1:B:1009:ILE:HG13	1.96	0.46
1:B:1089:ARG:NH1	1:B:1224:ASN:O	2.49	0.46
1:A:1318:LEU:CA	1:A:1321:MET:HE2	2.46	0.46
1:B:628:HIS:CE1	5:B:2330:HOH:O	2.61	0.46
1:A:485:SER:O	1:A:1213:LYS:HE3	2.17	0.45
1:A:872:THR:HG22	1:A:899:SER:HA	1.98	0.45
1:A:905:GLY:CA	1:A:951:GLY:CA	2.94	0.45
1:A:223:LEU:HD12	1:A:335:SER:O	2.16	0.45
1:A:1265:THR:HG22	1:A:1266:THR:N	2.31	0.45
1:A:905:GLY:HA2	1:A:951:GLY:CA	2.46	0.45
1:A:1280:VAL:HG13	5:A:2597:HOH:O	2.16	0.45
1:A:1443:ASN:OD1	1:A:1445:GLU:HG2	2.17	0.45
1:A:1472:THR:HG22	1:A:1474:SER:N	2.31	0.45
1:A:871:CYS:SG	1:A:1103:ARG:HD2	2.56	0.45
1:A:1008:ASP:HB2	1:A:1366:TYR:HE1	1.82	0.45
1:B:1406:THR:HG22	1:B:1425:THR:HG22	1.98	0.45
1:A:546:VAL:HG23	1:A:665:CYS:HB2	1.98	0.45
1:B:453:THR:HB	1:B:456:ASP:OD2	2.17	0.45
1:B:715:LEU:HD22	1:B:726:TYR:CD1	2.52	0.45
1:B:789:ARG:HG3	5:B:2402:HOH:O	2.16	0.45
1:B:798:SER:H	1:B:801:MET:CE	2.29	0.45
1:A:509:PRO:HA	1:A:516:MET:CE	2.47	0.45
1:A:843:ARG:HG3	1:A:1112:TRP:CH2	2.52	0.45
1:B:221:MET:HE1	1:B:272:TYR:HA	1.98	0.45
1:A:50:ILE:CD1	1:A:170:CYS:C	2.89	0.45
1:A:1004:PRO:HB2	1:A:1005:PRO:HD3	1.99	0.45
1:B:490:LEU:HD11	1:B:648:TRP:CH2	2.51	0.45
1:B:1108:LEU:O	1:B:1130:ILE:CD1	2.65	0.45
1:A:23:LYS:HB3	5:A:2007:HOH:O	2.17	0.45
1:A:516:MET:HE3	1:A:712:PHE:CD2	2.52	0.45
1:A:621:ALA:O	1:A:625:VAL:HG13	2.16	0.45
1:A:1318:LEU:H	1:A:1321:MET:HE3	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1157:GLU:O	1:A:1161:GLN:HG3	2.17	0.45
1:A:28:MET:CE	1:A:203:TYR:CE1	2.97	0.45
1:A:36:ALA:H	1:A:120:GLN:HE22	1.64	0.45
1:A:863:VAL:HG13	1:A:1178:ALA:CB	2.45	0.45
1:B:910:ARG:HD3	1:B:938:ALA:CB	2.46	0.45
1:B:901:SER:C	1:B:902:GLY:O	2.61	0.44
1:A:375:GLU:HG2	1:A:1347:HIS:CD2	2.52	0.44
1:A:1425:THR:CG2	5:A:2477:HOH:O	2.65	0.44
1:A:809:VAL:CG1	1:A:1169:GLN:HB3	2.47	0.44
1:B:266:GLN:HE21	1:B:266:GLN:HB3	1.65	0.44
1:B:796:MET:C	1:B:1109:LYS:HZ1	2.25	0.44
1:A:369:GLY:HA2	1:A:1308:ALA:CB	2.47	0.44
1:A:1419:ASN:ND2	1:A:1443:ASN:HD22	2.10	0.44
1:B:1504:GLU:H	1:B:1504:GLU:CD	2.26	0.44
1:B:459:MET:HE1	5:B:2241:HOH:O	2.16	0.44
1:B:642:VAL:HG11	1:B:664:ILE:HD12	2.00	0.44
1:B:807:LYS:HB3	1:B:826:HIS:CD2	2.52	0.44
1:B:143:GLU:OE1	1:B:146:ARG:HD3	2.18	0.44
1:B:264:VAL:HG12	1:B:265:ASN:N	2.33	0.43
1:B:1318:LEU:HB2	1:B:1321:MET:HE2	2.00	0.43
1:A:901:SER:C	1:A:902:GLY:O	2.61	0.43
1:B:157:LYS:HE2	1:B:261:THR:OG1	2.18	0.43
1:B:885:HIS:HD2	1:B:910:ARG:NH2	2.05	0.43
1:A:1085:THR:HG21	1:A:1222:LEU:HD23	2.00	0.43
1:A:517:SER:HB3	1:A:722:LEU:HD22	2.00	0.43
1:A:1145:THR:CG2	1:A:1147:ASN:HB2	2.48	0.43
1:B:685:LEU:O	1:B:689:GLY:N	2.52	0.43
1:B:887:THR:HB	1:B:1135:GLU:OE2	2.18	0.43
1:B:1109:LYS:HG2	1:B:1130:ILE:HG12	1.99	0.43
1:B:36:ALA:H	1:B:120:GLN:HE22	1.65	0.43
1:B:648:TRP:H	1:B:652:HIS:CD2	2.32	0.43
1:B:1265:THR:CG2	1:B:1266:THR:H	2.30	0.43
1:A:146:ARG:NH2	1:A:256:GLU:OE1	2.30	0.43
1:A:717:LYS:CB	1:A:974:GLY:HA3	2.48	0.43
1:A:1317:ASN:HA	1:A:1321:MET:HE1	2.00	0.43
1:B:622:VAL:HG21	1:B:661:ALA:HB2	2.00	0.43
1:A:784:GLY:N	1:A:793:GLU:H	2.15	0.43
1:A:1347:HIS:HB3	5:A:2628:HOH:O	2.17	0.43
1:A:760:ASP:OD2	1:A:1214:THR:HG23	2.18	0.43
1:A:1060:GLY:C	1:A:1062:ASP:H	2.27	0.43
1:A:891:ALA:CB	1:A:1170:VAL:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:GLN:HE22	1:A:1069:PRO:HD3	1.84	0.42
1:A:642:VAL:HG11	1:A:656:LEU:HG	2.00	0.42
1:A:690:ARG:NH2	5:A:2332:HOH:O	2.53	0.42
1:B:642:VAL:HG13	1:B:664:ILE:HG23	2.00	0.42
1:B:1347:HIS:HB3	5:B:2639:HOH:O	2.18	0.42
1:A:274:LEU:O	1:A:278:LEU:HB3	2.19	0.42
1:A:885:HIS:HD2	1:A:910:ARG:HH12	1.68	0.42
1:A:1079:PRO:HD2	1:A:1082:LEU:HD12	2.01	0.42
1:A:1360:ILE:HG23	1:A:1364:CYS:SG	2.59	0.42
1:B:1317:ASN:CG	1:B:1321:MET:HE3	2.44	0.42
1:A:686:MET:C	1:A:688:ASN:H	2.26	0.42
1:B:845:LEU:HD11	1:B:1217:LEU:HD22	2.02	0.42
1:B:1110:THR:HG23	1:B:1112:TRP:H	1.84	0.42
1:A:1056:ILE:HD12	1:A:1100:VAL:HG21	2.00	0.42
1:B:796:MET:CE	1:B:834:LEU:HD22	2.50	0.42
1:A:239:TRP:HE1	1:A:728:GLY:HA3	1.85	0.42
1:A:1254:ASP:HA	1:A:1255:PRO:HD2	1.93	0.42
1:B:601:THR:HG23	1:B:643:ASP:OD2	2.19	0.42
1:B:796:MET:O	1:B:1109:LYS:NZ	2.51	0.42
1:A:160:ALA:C	1:A:162:ASP:N	2.74	0.42
1:B:385:ALA:HB1	1:B:386:PRO:HD2	2.02	0.42
1:B:437:PHE:CE2	1:B:608:ILE:HD11	2.54	0.42
1:B:863:VAL:HG11	1:B:1175:TYR:CD2	2.54	0.42
1:B:1391:LYS:HA	1:B:1409:VAL:O	2.20	0.42
1:B:871:CYS:SG	1:B:1103:ARG:HD2	2.60	0.42
1:A:863:VAL:HG11	1:A:1175:TYR:CD2	2.55	0.42
1:B:36:ALA:N	1:B:120:GLN:HE22	2.18	0.42
1:B:172:THR:HG23	5:B:2114:HOH:O	2.19	0.42
1:B:1317:ASN:HA	1:B:1321:MET:CE	2.50	0.42
1:A:603:ARG:O	1:A:603:ARG:HG2	2.19	0.41
1:A:870:PHE:O	1:A:897:ALA:HB1	2.19	0.41
1:B:652:HIS:HE1	5:B:2267:HOH:O	2.01	0.41
1:B:1442:ILE:HG12	1:B:1449:LEU:HD22	2.02	0.41
1:A:437:PHE:CE1	1:A:671:GLU:HG2	2.55	0.41
1:A:475:MET:HE2	1:A:1139:MET:SD	2.60	0.41
1:B:3:VAL:CG1	1:B:331:LEU:HD23	2.50	0.41
1:B:688:ASN:HD22	1:B:689:GLY:N	2.17	0.41
1:A:1382:ARG:HG3	1:A:1385:VAL:HG13	2.01	0.41
1:B:831:ARG:NH1	1:B:1180:GLU:OE1	2.54	0.41
1:B:806:HIS:HB2	5:B:2543:HOH:O	2.20	0.41
1:B:149:TYR:CD2	1:B:283:ARG:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:914:LEU:O	1:B:934:ASN:O	2.38	0.41
1:A:266:GLN:HG2	5:A:2128:HOH:O	2.20	0.41
1:A:811:ALA:O	1:A:812:TYR:CB	2.69	0.41
1:A:784:GLY:HA3	1:A:793:GLU:N	2.35	0.41
1:B:507:ILE:O	1:B:716:SER:HB2	2.20	0.41
1:B:1382:ARG:O	1:B:1385:VAL:HG22	2.20	0.41
1:A:518:LEU:HD23	1:A:708:GLU:HG2	2.02	0.41
1:A:685:LEU:CD1	1:A:690:ARG:HD2	2.47	0.41
1:A:1089:ARG:CZ	1:A:1224:ASN:O	2.69	0.41
1:A:1232:ARG:HD3	5:A:2553:HOH:O	2.20	0.41
1:B:124:ASN:ND2	1:B:213:PRO:O	2.54	0.41
1:B:650:THR:CG2	5:B:2253:HOH:O	2.43	0.41
1:B:717:LYS:CB	1:B:974:GLY:HA3	2.51	0.41
1:A:383:ARG:HH22	1:A:1381:GLU:CD	2.29	0.41
1:B:610:THR:H	1:B:613:GLN:HE21	1.69	0.41
1:A:404:GLN:O	1:A:408:GLN:HG3	2.20	0.40
1:A:1248:ASP:HB3	1:A:1283:ARG:HB3	2.03	0.40
1:A:261:THR:O	1:A:262:PRO:C	2.63	0.40
1:A:349:LEU:O	1:A:350:ARG:HD2	2.21	0.40
1:B:301:LYS:HZ3	1:B:301:LYS:HG3	1.74	0.40
1:B:1216:ASN:C	1:B:1216:ASN:HD22	2.29	0.40
1:A:221:MET:HE1	1:A:272:TYR:HA	2.04	0.40
1:A:660:GLY:O	1:A:727:HIS:HE1	2.05	0.40
1:A:1273:LEU:HD23	1:A:1273:LEU:HA	1.89	0.40
1:B:385:ALA:HB1	1:B:386:PRO:CD	2.51	0.40
1:B:1260:ALA:HA	1:B:1265:THR:HB	2.03	0.40
1:A:1179:GLU:OE2	1:A:1182:ARG:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1485/1520 (98%)	1430 (96%)	46 (3%)	9 (1%)	21	17
1	B	1485/1520 (98%)	1437 (97%)	41 (3%)	7 (0%)	24	21
All	All	2970/3040 (98%)	2867 (96%)	87 (3%)	16 (0%)	24	21

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	THR
1	A	557	GLY
1	A	902	GLY
1	B	261	THR
1	B	754	GLY
1	B	902	GLY
1	A	1385	VAL
1	A	687	GLU
1	B	262	PRO
1	A	369	GLY
1	A	688	ASN
1	B	1385	VAL
1	A	262	PRO
1	B	557	GLY
1	B	573	VAL
1	A	1389	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1214/1236 (98%)	1089 (90%)	125 (10%)	7	4
1	B	1214/1236 (98%)	1086 (90%)	128 (10%)	6	4
All	All	2428/2472 (98%)	2175 (90%)	253 (10%)	7	4

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	LYS
1	A	17	LEU
1	A	23	LYS
1	A	60	ASN
1	A	64	LEU
1	A	66	MET
1	A	96	VAL
1	A	99	LEU
1	A	124	ASN
1	A	148	LEU
1	A	182	ILE
1	A	189	LEU
1	A	191	LEU
1	A	211	THR
1	A	224	LEU
1	A	234	LEU
1	A	246	GLU
1	A	249	VAL
1	A	254	LYS
1	A	261	THR
1	A	266	GLN
1	A	274	LEU
1	A	278	LEU
1	A	301	LYS
1	A	339	ILE
1	A	340	VAL
1	A	355	CYS
1	A	379	VAL
1	A	421	ILE
1	A	430	SER
1	A	439	ASP
1	A	441	GLN
1	A	453	THR
1	A	457	VAL
1	A	469	LYS
1	A	511	ARG
1	A	514	LEU
1	A	515	VAL
1	A	518	LEU
1	A	532	LYS
1	A	541	LEU
1	A	580	LEU

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Mol	Chain	Res	Type
1	A	582	ASN
1	A	583	LEU
1	A	584	VAL
1	A	598	LEU
1	A	603	ARG
1	A	608	ILE
1	A	625	VAL
1	A	629	LEU
1	A	636	LEU
1	A	642	VAL
1	A	650	THR
1	A	656	LEU
1	A	664	ILE
1	A	668	LEU
1	A	680	GLU
1	A	681	LYS
1	A	684	LYS
1	A	688	ASN
1	A	693	ARG
1	A	694	ILE
1	A	701	LYS
1	A	715	LEU
1	A	735	ILE
1	A	750	THR
1	A	761	VAL
1	A	765	VAL
1	A	800	GLU
1	A	804	SER
1	A	809	VAL
1	A	837	ARG
1	A	857	LEU
1	A	858	GLU
1	A	867	VAL
1	A	872	THR
1	A	877	LEU
1	A	912	LEU
1	A	915	ASP
1	A	953	THR
1	A	1015	LEU
1	A	1028	GLU
1	A	1052	ASN
1	A	1062	ASP

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Mol	Chain	Res	Type
1	A	1085	THR
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	1177	ILE
1	A	1193	LEU
1	A	1210	GLN
1	A	1212	SER
1	A	1214	THR
1	A	1215	GLN
1	A	1217	LEU
1	A	1228	THR
1	A	1230	GLN
1	A	1232	ARG
1	A	1235	LEU
1	A	1238	GLU
1	A	1246	VAL
1	A	1265	THR
1	A	1279	THR
1	A	1280	VAL
1	A	1291	LYS
1	A	1349	GLN
1	A	1360	ILE
1	A	1381	GLU
1	A	1386	ARG
1	A	1388	SER
1	A	1389	VAL
1	A	1416	VAL
1	A	1425	THR
1	A	1442	ILE
1	A	1456	LYS
1	A	1459	GLU
1	A	1464	LEU
1	A	1472	THR
1	A	1488	LEU
1	A	1504	GLU
1	B	9	LEU
1	B	12	LYS

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Mol	Chain	Res	Type
1	B	17	LEU
1	B	23	LYS
1	B	60	ASN
1	B	64	LEU
1	B	96	VAL
1	B	99	LEU
1	B	115	ASP
1	B	122	LYS
1	B	133	VAL
1	B	137	GLU
1	B	146	ARG
1	B	148	LEU
1	B	162	ASP
1	B	182	ILE
1	B	191	LEU
1	B	211	THR
1	B	221	MET
1	B	224	LEU
1	B	234	LEU
1	B	246	GLU
1	B	249	VAL
1	B	261	THR
1	B	266	GLN
1	B	274	LEU
1	B	302	ASN
1	B	336	ASP
1	B	339	ILE
1	B	340	VAL
1	B	379	VAL
1	B	398	LYS
1	B	404	GLN
1	B	421	ILE
1	B	430	SER
1	B	434	LYS
1	B	444	LEU
1	B	453	THR
1	B	457	VAL
1	B	478	ASP
1	B	511	ARG
1	B	514	LEU
1	B	515	VAL
1	B	518	LEU

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Mol	Chain	Res	Type
1	B	524	LYS
1	B	541	LEU
1	B	556	THR
1	B	573	VAL
1	B	580	LEU
1	B	583	LEU
1	B	584	VAL
1	B	603	ARG
1	B	608	ILE
1	B	625	VAL
1	B	629	LEU
1	B	636	LEU
1	B	650	THR
1	B	656	LEU
1	B	668	LEU
1	B	680	GLU
1	B	683	GLN
1	B	688	ASN
1	B	690	ARG
1	B	701	LYS
1	B	715	LEU
1	B	750	THR
1	B	761	VAL
1	B	765	VAL
1	B	789	ARG
1	B	800	GLU
1	B	809	VAL
1	B	829	LEU
1	B	837	ARG
1	B	857	LEU
1	B	858	GLU
1	B	867	VAL
1	B	872	THR
1	B	877	LEU
1	B	912	LEU
1	B	953	THR
1	B	991	LEU
1	B	1008	ASP
1	B	1015	LEU
1	B	1052	ASN
1	B	1062	ASP
1	B	1085	THR

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Mol	Chain	Res	Type
1	B	1089	ARG
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
1	B	1177	ILE
1	B	1192	SER
1	B	1193	LEU
1	B	1200	THR
1	B	1212	SER
1	B	1214	THR
1	B	1215	GLN
1	B	1216	ASN
1	B	1228	THR
1	B	1232	ARG
1	B	1235	LEU
1	B	1246	VAL
1	B	1265	THR
1	B	1266	THR
1	B	1280	VAL
1	B	1291	LYS
1	B	1360	ILE
1	B	1381	GLU
1	B	1382	ARG
1	B	1386	ARG
1	B	1388	SER
1	B	1389	VAL
1	B	1416	VAL
1	B	1425	THR
1	B	1433	ASP
1	B	1442	ILE
1	B	1448	THR
1	B	1449	LEU
1	B	1453	THR
1	B	1456	LYS
1	B	1464	LEU
1	B	1472	THR
1	B	1488	LEU
1	B	1504	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	57	GLN
1	A	120	GLN
1	A	199	ASN
1	A	236	ASN
1	A	266	GLN
1	A	303	GLN
1	A	404	GLN
1	A	446	GLN
1	A	486	HIS
1	A	613	GLN
1	A	628	HIS
1	A	646	GLN
1	A	651	HIS
1	A	652	HIS
1	A	727	HIS
1	A	769	HIS
1	A	852	GLN
1	A	885	HIS
1	A	978	GLN
1	A	1023	HIS
1	A	1030	GLN
1	A	1052	ASN
1	A	1210	GLN
1	A	1215	GLN
1	A	1216	ASN
1	A	1230	GLN
1	A	1258	GLN
1	A	1275	ASN
1	A	1419	ASN
1	A	1450	GLN
1	A	1460	GLN
1	A	1493	GLN
1	B	15	HIS
1	B	120	GLN
1	B	124	ASN
1	B	266	GLN
1	B	447	GLN
1	B	513	ASN
1	B	613	GLN
1	B	628	HIS

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Mol	Chain	Res	Type
1	B	646	GLN
1	B	651	HIS
1	B	652	HIS
1	B	688	ASN
1	B	727	HIS
1	B	730	GLN
1	B	826	HIS
1	B	852	GLN
1	B	885	HIS
1	B	930	HIS
1	B	933	GLN
1	B	978	GLN
1	B	1023	HIS
1	B	1030	GLN
1	B	1052	ASN
1	B	1216	ASN
1	B	1275	ASN
1	B	1419	ASN
1	B	1450	GLN
1	B	1460	GLN
1	B	1493	GLN

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	B	3508	-	33,33,33	1.07	2 (6%)	48,50,50	1.43	11 (22%)
4	AKG	A	3510	-	9,9,9	2.49	3 (33%)	11,11,11	1.84	4 (36%)
2	FMN	A	3508	-	33,33,33	1.08	3 (9%)	48,50,50	1.43	9 (18%)
3	F3S	B	3509	1	0,9,9	-	-	-	-	-
4	AKG	B	3510	-	9,9,9	2.55	3 (33%)	11,11,11	1.73	2 (18%)
3	F3S	A	3509	1	0,9,9	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	3508	-	-	1/18/18/18	0/3/3/3
4	AKG	A	3510	-	-	5/9/9/9	-
2	FMN	A	3508	-	-	1/18/18/18	0/3/3/3
3	F3S	B	3509	1	-	-	0/3/3/3
4	AKG	B	3510	-	-	5/9/9/9	-
3	F3S	A	3509	1	-	-	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3510	AKG	O5-C2	5.50	1.34	1.23
4	A	3510	AKG	O5-C2	5.41	1.34	1.23
4	B	3510	AKG	O1-C1	4.23	1.33	1.22
4	A	3510	AKG	O1-C1	4.14	1.32	1.22
2	B	3508	FMN	C4A-N5	3.51	1.38	1.30
2	A	3508	FMN	C4A-N5	3.12	1.37	1.30
4	B	3510	AKG	O3-C5	3.02	1.32	1.22
4	A	3510	AKG	O3-C5	2.75	1.31	1.22
2	B	3508	FMN	C10-N1	2.63	1.38	1.33
2	A	3508	FMN	C10-N1	2.24	1.37	1.33
2	A	3508	FMN	P-O2P	-2.19	1.46	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3508	FMN	C4A-C10-N10	3.88	122.04	116.48
2	B	3508	FMN	C4A-C10-N10	3.56	121.57	116.48
4	A	3510	AKG	O4-C5-C4	3.33	124.53	114.00
2	A	3508	FMN	C10-C4A-N5	-3.15	118.38	124.81
4	B	3510	AKG	O4-C5-C4	3.09	123.75	114.00
2	B	3508	FMN	C10-C4A-N5	-3.04	118.61	124.81
2	B	3508	FMN	O4-C4-N3	-2.83	114.80	120.11
2	B	3508	FMN	C9A-C5A-N5	-2.58	119.71	122.45
2	A	3508	FMN	O4-C4-N3	-2.55	115.31	120.11
2	A	3508	FMN	O4-C4-C4A	-2.55	119.81	126.53
2	B	3508	FMN	O4-C4-C4A	-2.49	119.96	126.53
4	A	3510	AKG	C4-C3-C2	-2.38	108.45	112.91
2	A	3508	FMN	C9A-C5A-N5	-2.37	119.94	122.45
2	B	3508	FMN	C9A-N10-C10	-2.32	117.22	120.75
2	B	3508	FMN	C4A-C10-N1	-2.29	118.97	124.59
2	B	3508	FMN	O3P-P-O5'	2.27	112.60	106.67
2	B	3508	FMN	C4-N3-C2	-2.26	121.63	125.64
2	A	3508	FMN	C9A-N10-C10	-2.19	117.42	120.75
2	A	3508	FMN	C4-C4A-N5	2.17	121.20	118.21
4	A	3510	AKG	O4-C5-O3	-2.13	117.85	123.33
4	B	3510	AKG	C4-C3-C2	-2.06	109.04	112.91
2	B	3508	FMN	C4-C4A-N5	2.04	121.02	118.21
2	A	3508	FMN	C4-C4A-C10	2.03	120.42	116.93
2	B	3508	FMN	C10-N1-C2	2.02	121.23	116.85
4	A	3510	AKG	O2-C1-C2	2.02	119.19	113.59
2	A	3508	FMN	C4-N3-C2	-2.01	122.07	125.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

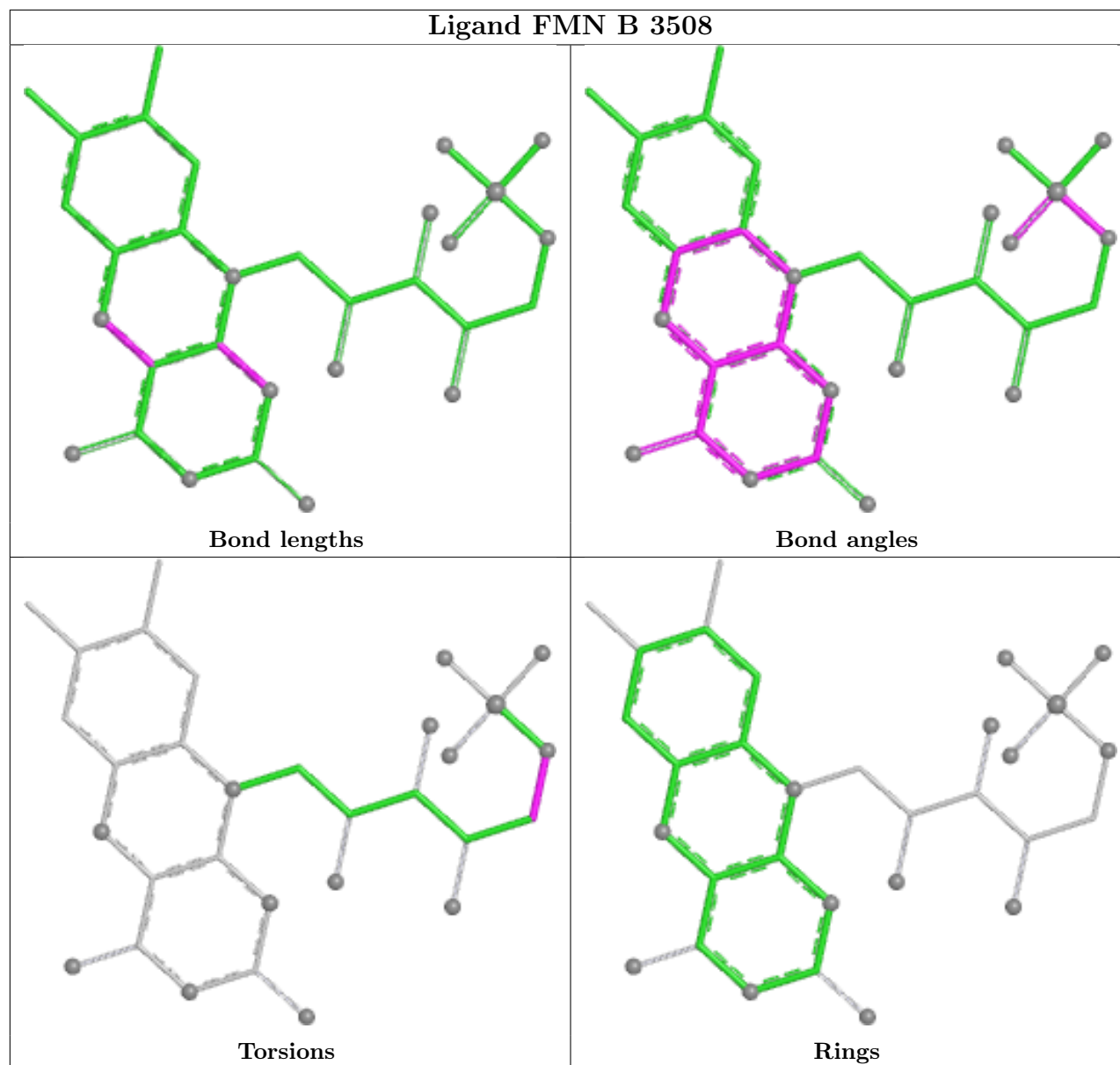
Mol	Chain	Res	Type	Atoms
4	A	3510	AKG	O1-C1-C2-C3
4	A	3510	AKG	O2-C1-C2-O5
4	A	3510	AKG	O2-C1-C2-C3
4	B	3510	AKG	O2-C1-C2-C3
4	A	3510	AKG	C2-C3-C4-C5
4	B	3510	AKG	C2-C3-C4-C5
2	A	3508	FMN	C4'-C5'-O5'-P
4	A	3510	AKG	O1-C1-C2-O5
4	B	3510	AKG	O1-C1-C2-O5
4	B	3510	AKG	O1-C1-C2-C3
2	B	3508	FMN	C4'-C5'-O5'-P
4	B	3510	AKG	O2-C1-C2-O5

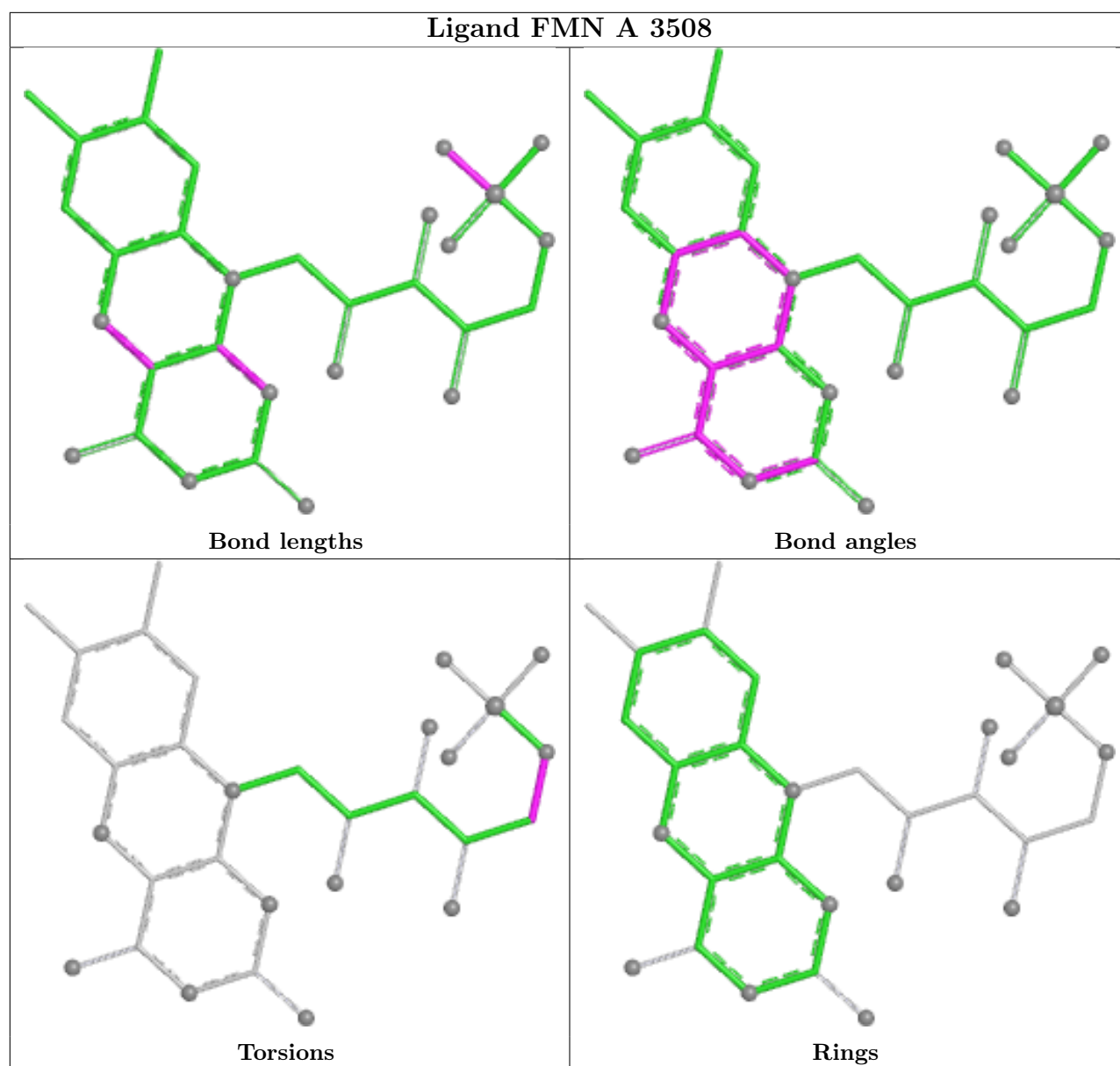
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3508	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 ⓘ

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	1491/1520 (98%)	0.01	63 (4%) 40 39	2, 7, 14, 21	0
1	B	1491/1520 (98%)	0.09	73 (4%) 35 34	2, 7, 13, 22	0
All	All	2982/3040 (98%)	0.05	136 (4%) 37 36	2, 7, 13, 22	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	693	ARG	6.5
1	A	261	THR	6.4
1	A	693	ARG	5.8
1	A	728	GLY	5.8
1	A	692	ASP	5.6
1	B	692	ASP	5.1
1	B	1433	ASP	5.0
1	A	690	ARG	4.9
1	A	1433	ASP	4.8
1	B	812	TYR	4.8
1	A	833	TYR	4.7
1	B	261	THR	4.7
1	B	829	LEU	4.6
1	B	833	TYR	4.6
1	A	1507	ASN	4.5
1	B	915	ASP	4.4
1	A	678	LEU	4.4
1	B	690	ARG	4.3
1	B	689	GLY	4.3
1	B	974	GLY	4.2
1	B	828	GLU	4.2
1	B	438	ASN	4.1
1	B	439	ASP	4.1
1	A	440	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	728	GLY	4.0
1	A	694	ILE	3.9
1	B	1507	ASN	3.8
1	A	829	LEU	3.8
1	B	901	SER	3.8
1	B	572	GLY	3.8
1	A	828	GLU	3.6
1	B	100	GLU	3.6
1	B	873	GLY	3.6
1	B	369	GLY	3.6
1	B	441	GLN	3.6
1	B	608	ILE	3.5
1	A	1497	PRO	3.5
1	B	1164	LYS	3.4
1	A	687	GLU	3.3
1	B	826	HIS	3.3
1	A	951	GLY	3.3
1	A	556	THR	3.3
1	A	997	GLY	3.3
1	A	1385	VAL	3.3
1	A	438	ASN	3.2
1	B	70	ASP	3.2
1	A	689	GLY	3.1
1	B	951	GLY	3.1
1	A	502	VAL	3.1
1	A	784	GLY	3.1
1	A	439	ASP	3.1
1	A	915	ASP	3.0
1	B	1385	VAL	3.0
1	A	1147	ASN	3.0
1	B	754	GLY	2.9
1	B	688	ASN	2.9
1	B	478	ASP	2.9
1	A	12	LYS	2.9
1	A	684	LYS	2.9
1	A	1351	SER	2.8
1	B	680	GLU	2.8
1	B	790	PRO	2.8
1	A	70	ASP	2.8
1	B	825	ASP	2.8
1	B	997	GLY	2.8
1	A	729	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	502	VAL	2.8
1	A	901	SER	2.7
1	A	873	GLY	2.7
1	B	877	LEU	2.7
1	A	806	HIS	2.7
1	B	694	ILE	2.7
1	A	369	GLY	2.6
1	A	832	GLN	2.6
1	B	832	GLN	2.6
1	A	826	HIS	2.6
1	B	162	ASP	2.6
1	B	1453	THR	2.6
1	B	687	GLU	2.6
1	B	1369	THR	2.6
1	B	506	PRO	2.6
1	B	529	LEU	2.6
1	B	437	PHE	2.5
1	B	784	GLY	2.5
1	B	691	LEU	2.5
1	B	1130	ILE	2.5
1	A	831	ARG	2.5
1	A	1349	GLN	2.5
1	B	500	ALA	2.5
1	B	858	GLU	2.5
1	A	974	GLY	2.5
1	A	441	GLN	2.5
1	B	266	GLN	2.5
1	B	440	ALA	2.5
1	A	691	LEU	2.5
1	A	812	TYR	2.4
1	A	432	ALA	2.4
1	A	572	GLY	2.4
1	A	811	ALA	2.4
1	B	729	ALA	2.4
1	B	534	GLU	2.4
1	A	731	ILE	2.4
1	A	686	MET	2.4
1	A	139	CYS	2.4
1	A	1453	THR	2.4
1	A	443	VAL	2.3
1	B	443	VAL	2.3
1	B	556	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	835	LYS	2.3
1	B	432	ALA	2.3
1	B	811	ALA	2.3
1	B	606	GLY	2.3
1	A	608	ILE	2.2
1	B	515	VAL	2.2
1	B	836	ASP	2.2
1	A	935	GLY	2.2
1	A	246	GLU	2.2
1	A	437	PHE	2.2
1	B	503	THR	2.2
1	B	778	LYS	2.2
1	A	790	PRO	2.2
1	B	935	GLY	2.2
1	B	372	ASP	2.2
1	B	434	LYS	2.1
1	A	1506	ASN	2.1
1	B	1210	GLN	2.1
1	A	421	ILE	2.1
1	B	436	LEU	2.1
1	A	478	ASP	2.1
1	B	1062	ASP	2.1
1	A	503	THR	2.1
1	A	499	PHE	2.1
1	A	1028	GLU	2.0
1	B	12	LYS	2.0
1	A	1459	GLU	2.0
1	B	60	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

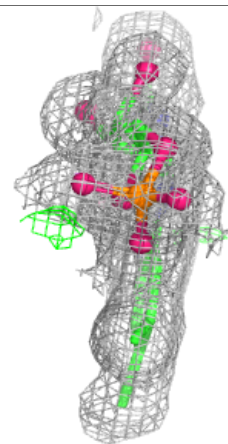
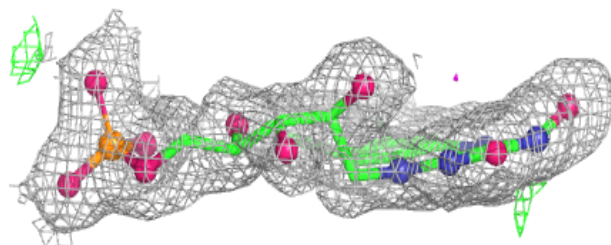
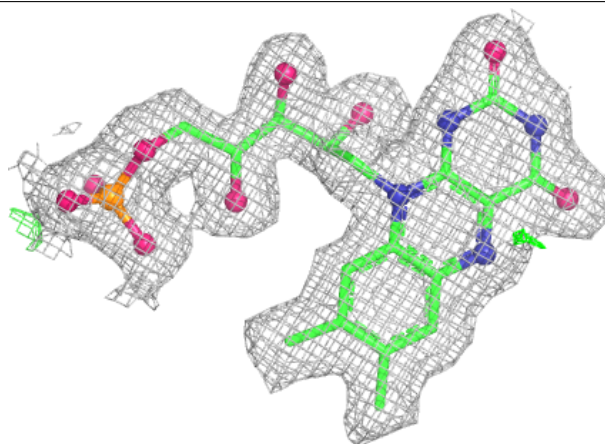
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AKG	B	3510	10/10	0.91	0.14	12,15,19,21	0
4	AKG	A	3510	10/10	0.95	0.09	11,15,18,19	0
2	FMN	A	3508	31/31	0.97	0.06	8,10,14,15	0
2	FMN	B	3508	31/31	0.97	0.05	9,13,15,17	0
3	F3S	A	3509	7/7	0.99	0.02	10,11,11,12	0
3	F3S	B	3509	7/7	0.99	0.03	11,11,11,13	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.

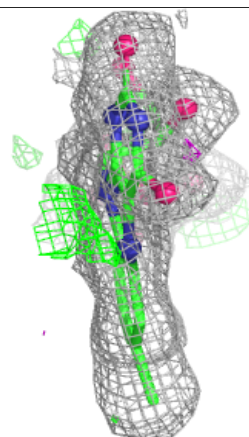
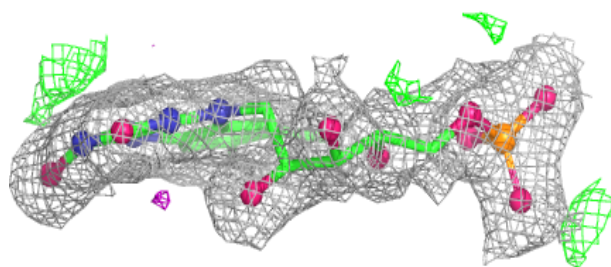
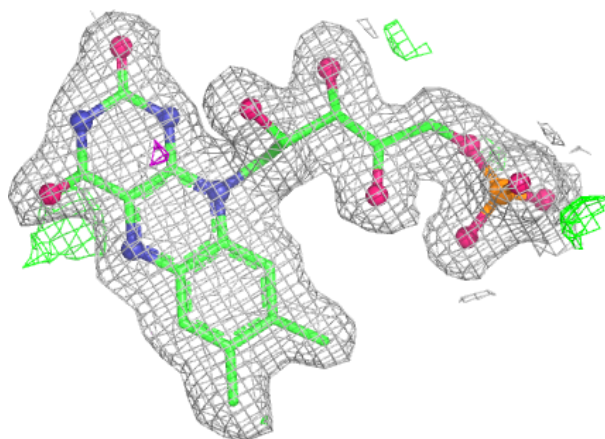
Electron density around FMN A 3508:

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 B 3508:

$2mF_o - DF_c$ (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.