



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:24 am BST

PDB ID : 1OFD  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

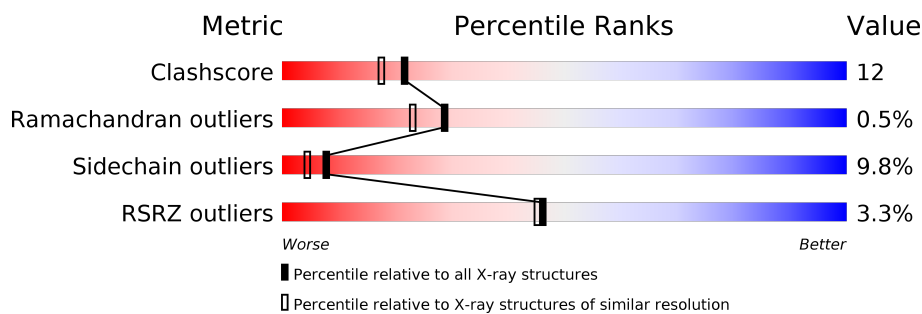
# 1 Overall quality at a glance

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div>73%</div> <div>19%</div> <div>5%</div> <div>..</div> </div>
1	B	1520	<div> <div>3%</div> <div>75%</div> <div>19%</div> <div>..</div> <div>..</div> </div>

## 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.

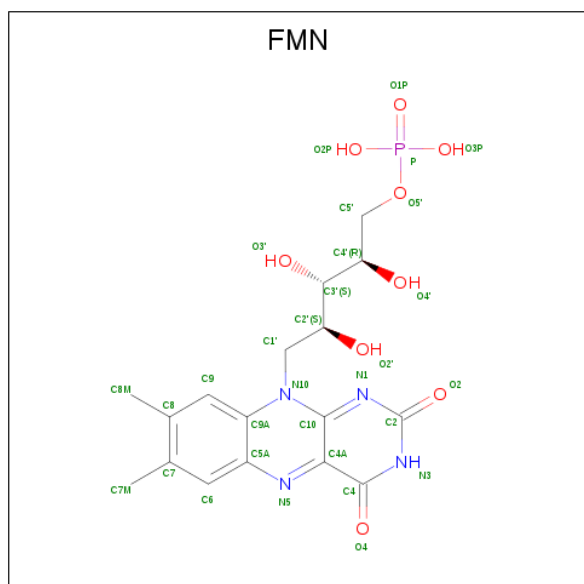
- Molecule 1 is a protein called FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE 2.

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:

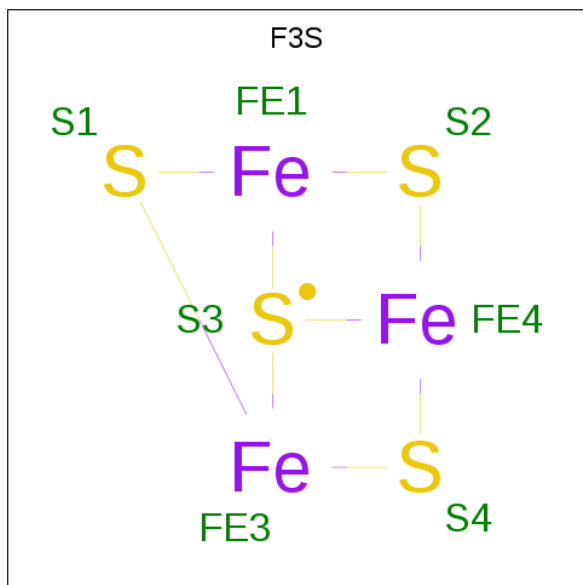
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	conflict	UNP P55038
A	581	THR	ASP	conflict	UNP P55038
A	1507	ASN	GLY	conflict	UNP P55038
B	578	ASP	THR	conflict	UNP P55038
B	581	THR	ASP	conflict	UNP P55038
B	1507	ASN	GLY	conflict	UNP P55038

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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 (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



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 (three-letter code: AKG) (formula:  $\text{C}_5\text{H}_6\text{O}_5$ ).

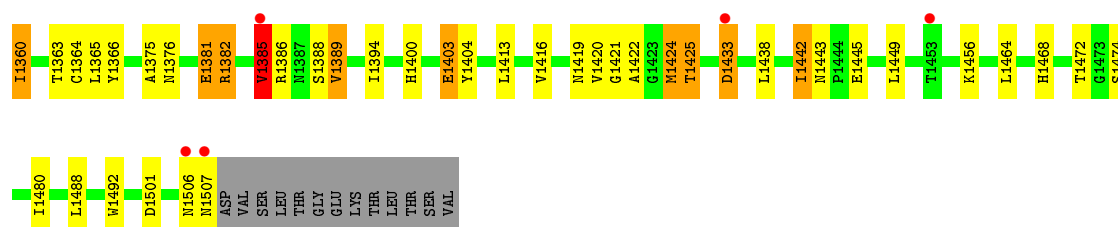


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

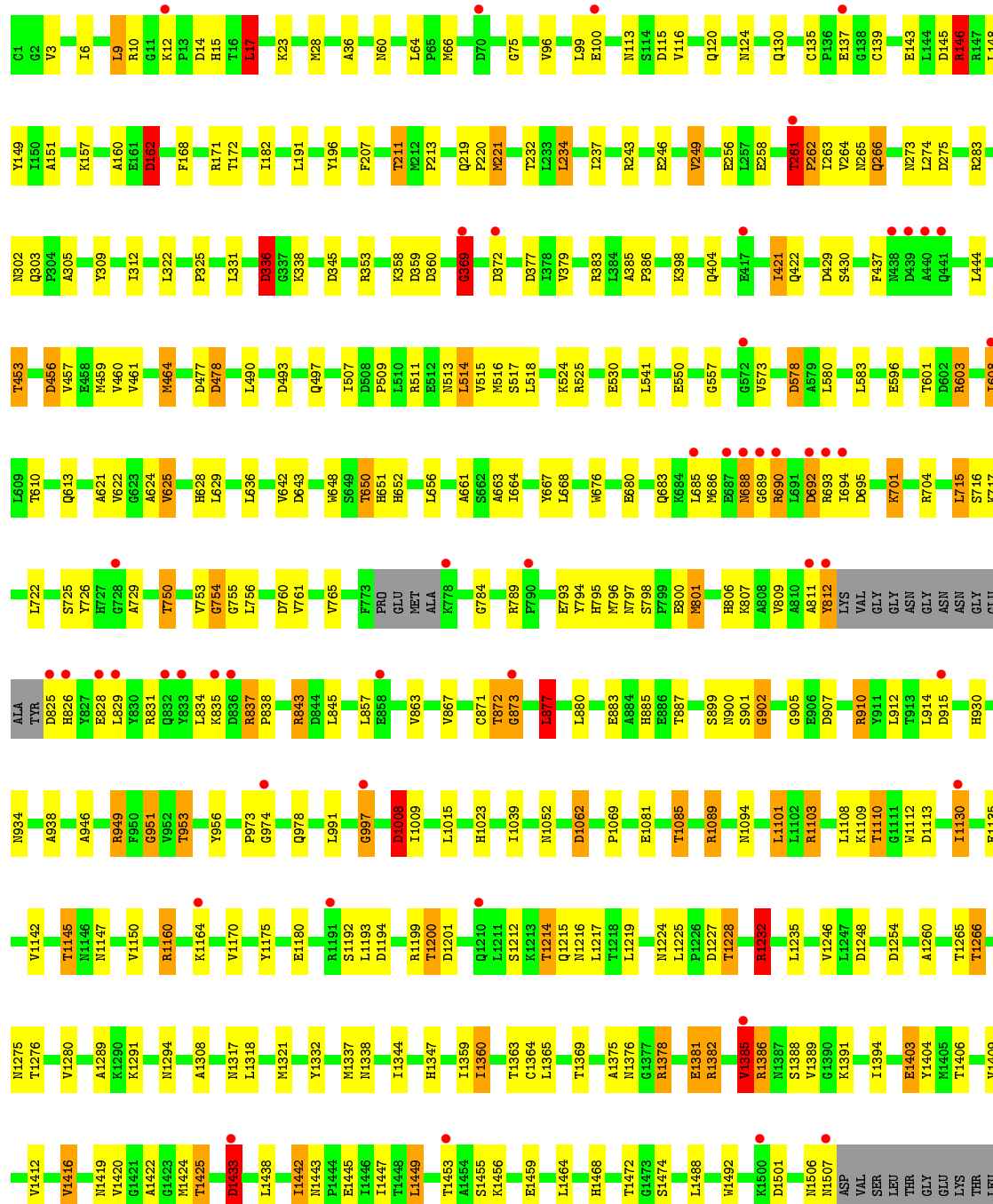
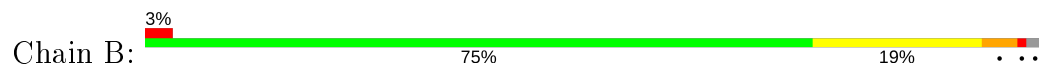
- Molecule 5 is water.

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



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.02Å 149.66Å 195.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 43.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.00) 96.3 (43.23-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, F3S, 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	0.59	3/11657 (0.0%)	0.91	57/15807 (0.4%)
1	B	0.57	3/11657 (0.0%)	0.90	57/15807 (0.4%)
All	All	0.58	6/23314 (0.0%)	0.90	114/31614 (0.4%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	CYS	CB-SG	-6.89	1.70	1.82
1	A	1008	ASP	CB-CG	-5.81	1.39	1.51
1	B	221	MET	CG-SD	-5.75	1.66	1.81
1	A	464	MET	SD-CE	-5.61	1.46	1.77
1	B	1008	ASP	CB-CG	-5.11	1.41	1.51
1	B	464	MET	SD-CE	-5.01	1.49	1.77

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	949	ARG	NE-CZ-NH1	-13.79	113.40	120.30
1	A	1232	ARG	NE-CZ-NH2	-12.69	113.96	120.30
1	B	353	ARG	NE-CZ-NH2	-11.04	114.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1008	ASP	CB-CG-OD2	10.47	127.72	118.30
1	A	1008	ASP	CB-CG-OD2	10.17	127.45	118.30
1	A	1008	ASP	CB-CG-OD1	-9.95	109.34	118.30
1	B	1008	ASP	CB-CG-OD1	-9.90	109.39	118.30
1	B	843	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	843	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	A	1232	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	B	1232	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	A	221	MET	CG-SD-CE	-9.31	85.30	100.20
1	A	1103	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	1062	ASP	CB-CG-OD2	9.07	126.47	118.30
1	B	221	MET	CG-SD-CE	-8.92	85.92	100.20
1	A	1103	ARG	NE-CZ-NH2	-8.91	115.85	120.30
1	A	353	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	B	949	ARG	NE-CZ-NH2	8.71	124.65	120.30
1	A	162	ASP	CB-CG-OD2	8.32	125.79	118.30
1	A	146	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	B	1232	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	729	ALA	C-N-CA	-8.13	101.38	121.70
1	B	1062	ASP	CB-CG-OD2	7.99	125.49	118.30
1	B	1101	LEU	CA-CB-CG	7.91	133.50	115.30
1	B	162	ASP	CB-CG-OD2	7.89	125.40	118.30
1	B	17	LEU	CA-CB-CG	7.83	133.30	115.30
1	A	910	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	B	336	ASP	CB-CG-OD2	7.57	125.12	118.30
1	B	843	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	17	LEU	CA-CB-CG	7.49	132.51	115.30
1	A	1062	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	B	910	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	145	ASP	CB-CG-OD2	7.35	124.91	118.30
1	B	146	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	234	LEU	CA-CB-CG	7.16	131.77	115.30
1	B	14	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	478	ASP	CB-CG-OD2	7.06	124.66	118.30
1	A	278	LEU	CA-CB-CG	7.02	131.44	115.30
1	B	234	LEU	CA-CB-CG	7.01	131.43	115.30
1	A	1101	LEU	CA-CB-CG	6.86	131.07	115.30
1	A	843	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	B	1103	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	14	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	336	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	910	ARG	NE-CZ-NH1	6.61	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	ASP	CB-CG-OD2	6.59	124.23	118.30
1	B	729	ALA	C-N-CA	-6.56	105.30	121.70
1	A	695	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	973	PRO	C-N-CA	-6.36	108.95	122.30
1	A	514	LEU	CA-CB-CG	6.30	129.79	115.30
1	B	1227	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	973	PRO	C-N-CA	-6.16	109.37	122.30
1	B	877	LEU	CA-CB-CG	-6.12	101.23	115.30
1	B	1403	GLU	C-N-CA	-6.08	106.49	121.70
1	B	695	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	1103	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	1194	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	477	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	1433	ASP	CB-CG-OD2	5.94	123.64	118.30
1	B	1433	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	145	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	580	LEU	CA-CB-CG	5.87	128.79	115.30
1	B	514	LEU	CA-CB-CG	5.87	128.79	115.30
1	B	275	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	1208	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	353	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	1385	VAL	CB-CA-C	-5.75	100.47	111.40
1	A	429	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	1403	GLU	C-N-CA	-5.71	107.44	121.70
1	B	1501	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	1160	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	162	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	A	146	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	172	THR	OG1-CB-CG2	-5.58	97.17	110.00
1	A	602	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	907	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	679	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	825	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	578	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	1501	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	1250	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	693	ARG	N-CA-C	-5.41	96.41	111.00
1	A	353	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	1098	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	692	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	456	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	345	ASP	CB-CG-OD2	5.26	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	825	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	1160	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	1378	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	372	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	429	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	146	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	17	LEU	CB-CG-CD1	5.21	119.85	111.00
1	A	1331	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	915	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	478	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	1085	THR	N-CA-CB	-5.17	100.47	110.30
1	A	877	LEU	CA-CB-CG	-5.16	103.42	115.30
1	B	907	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	353	ARG	CG-CD-NE	-5.15	100.99	111.80
1	B	359	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	1385	VAL	CB-CA-C	-5.11	101.70	111.40
1	B	369	GLY	N-CA-C	5.10	125.85	113.10
1	B	1254	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	1254	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	1403	GLU	O-C-N	-5.08	114.57	122.70
1	A	369	GLY	N-CA-C	5.06	125.76	113.10
1	B	1201	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	1160	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	514	LEU	CB-CG-CD1	5.03	119.55	111.00
1	B	456	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	493	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	578	ASP	CB-CG-OD2	5.00	122.80	118.30

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	280	0
1	B	11434	0	11382	264	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	43	0
5	B	719	0	0	44	0
All	All	24388	0	22810	544	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 (544) 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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:SER:O	1:B:901:SER:OG	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:OG	1:A:901:SER:O	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:1318:LEU:H	1:A:1321:MET:HE2	1.28	0.96
1:A:157:LYS:NZ	1:A:261:THR:OG1	2.01	0.94
1:B:1318:LEU:H	1:B:1321:MET:HE1	1.33	0.93
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:509:PRO:HA	1:B:516:MET:HE1	1.52	0.91
1:B:1228:THR:CG2	1:B:1232:ARG:HH21	1.83	0.90
1:A:885:HIS:CD2	1:A:910:ARG:HH22	1.90	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:1318:LEU:H	1:B:1321:MET:HE2	1.38	0.88
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:1228:THR:CG2	1:A:1232:ARG:HH21	1.90	0.85
1:A:27:CYS:HB2	1:A:370:VAL:HG23	1.59	0.85
1:A:211:THR:HG21	1:A:1094:ASN:O	1.75	0.84
1:B:509:PRO:HA	1:B:516:MET:CE	2.06	0.84
1:A:453:THR:HG23	5:A:2227:HOH:O	1.78	0.84
1:A:460:VAL:HG12	1:A:464:MET:CE	2.07	0.83
1:B:460:VAL:HG12	1:B:464:MET:HE2	1.58	0.83
1:B:1318:LEU:N	1:B:1321:MET:CE	2.42	0.83
1:A:1085:THR:HG23	5:A:2569:HOH:O	1.78	0.82
1:A:1318:LEU:H	1:A:1321:MET:HE1	1.45	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:261:THR:HB	1:A:262:PRO:HD3	1.62	0.79
1:A:497:GLN:HE21	1:A:651:HIS:HD2	1.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1424:MET:CE	1:B:1447:ILE:HG21	2.14	0.78
1:A:1337:MET:HE3	1:A:1365:LEU:HD22	1.64	0.78
1:B:953:THR:HG22	1:B:956:TYR:H	1.48	0.78
1:B:1337:MET:HE2	1:B:1365:LEU:HD22	1.65	0.77
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: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: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: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
1:B:1318:LEU:N	1:B:1321:MET:HE1	1.99	0.74
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:B:461:VAL:HA	1:B:464:MET:HE3	1.69	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:1145:THR:HG22	1:B:1147:ASN:H	1.54	0.73
1:B:1424:MET:HE2	1:B:1447:ILE:HG21	1.70	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:A:1200:THR:HG22	5:A:2570:HOH:O	1.89	0.72
1:A:603:ARG:HD2	1:A:667:TYR:CE2	2.24	0.72
1:B:750:THR:HG22	5:B:2379:HOH:O	1.89	0.72
1:A:1337:MET:HE3	1:A:1365:LEU:CD2	2.19	0.72
1:B:1337:MET:HE2	1:B:1365:LEU:CD2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:460:VAL:HG12	1:A:464:MET:HE1	1.73	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:B:750:THR:HG21	1:B:1039:ILE:HG12	1.74	0.69
1:A:1300:ASN:OD1	5:A:2609:HOH:O	2.10	0.68
1:A:872:THR:HG23	5:A:2409:HOH:O	1.88	0.68
1:A:67:PRO:HG2	1:A:72:LEU:HB2	1.75	0.68
1:B:1130:ILE:H	1:B:1130:ILE:CD1	2.06	0.68
1:B:459:MET:HE1	5:B:2403:HOH:O	1.93	0.68
1:A:873:GLY:HA2	5:A:2422:HOH:O	1.94	0.68
1:A:1318:LEU:N	1:A:1321:MET:HE1	2.05	0.67
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:369:GLY:HA3	1:B:1275:ASN:HB3	1.77	0.67
1:B:237:ILE:HG23	1:B:264:VAL:HG12	1.75	0.67
1:A:789:ARG:HG3	5:A:2388:HOH:O	1.94	0.67
1:B:953:THR:CG2	1:B:1294:ASN:HD21	2.07	0.67
1:B:497:GLN:HE21	1:B:651:HIS:HD2	1.42	0.67
1:B:1081:GLU:O	1:B:1085:THR:HB	1.94	0.66
1:B:798:SER:H	1:B:801:MET:HE2	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1419:ASN:HD21	1:B:1443:ASN:HD22	1.44	0.65
1:B:336:ASP:HB3	1:B:338:LYS:H	1.61	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:B:460:VAL:CG1	1:B:464:MET:HE2	2.27	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:685:LEU:HD13	1:A:690:ARG:HD2	1.79	0.64
1:A:389:MET:HE2	1:A:406:LYS:HE3	1.78	0.63
1:A:461:VAL:HA	1:A:464:MET:HE3	1.81	0.63
1:B:10:ARG:NH2	1:B:360:ASP:OD2	2.28	0.63
1:A:1337:MET:HE1	1:A:1365:LEU:HD21	1.81	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:1199:ARG:HD2	1:A:1228:THR:HG22	1.81	0.62
1:A:264:VAL:HG13	1:A:273:ASN:OD1	1.99	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:1326:GLN:CD	1:A:1348:PRO:HD3	2.19	0.62
1:A:261:THR:CB	1:A:262:PRO:CD	2.42	0.62
1:B:1344:ILE:CD1	1:B:1360:ILE:HD11	2.24	0.62
1:B:794:TYR:CZ	1:B:837:ARG:HB2	2.34	0.62
1:B:946:ALA:O	1:B:949:ARG:NH1	2.33	0.61
1:B:1085:THR:HG23	5:B:2588:HOH:O	2.00	0.61
1:A:172:THR:HG21	5:A:2106:HOH:O	2.01	0.61
1:A:28:MET:CE	1:A:203:TYR:HE1	2.13	0.61
1:A:784:GLY:CA	5:A:2390:HOH:O	2.48	0.61
1:B:261:THR:O	1:B:262:PRO:C	2.38	0.61
1:B:953:THR:HG23	1:B:1294:ASN:HD21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:THR:CG2	5:A:2569:HOH:O	2.44	0.60
1:A:901:SER:O	1:A:902:GLY:O	2.19	0.60
1:B:550:GLU:OE2	1:B:704:ARG:NH2	2.34	0.60
1:B:1276:THR:HB	5:B:2611:HOH:O	2.00	0.60
1:B:930:HIS:HD2	5:B:2453:HOH:O	1.83	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: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:A:460:VAL:CG1	1:A:464:MET:CE	2.78	0.59
1:B:6:ILE:HG22	1:B:17:LEU:HD22	1.83	0.59
1:A:797:ASN:HA	1:A:801:MET:HE2	1.83	0.59
1:B:261:THR:HG21	5:B:2077:HOH:O	2.03	0.59
1:B:717:LYS:HG2	1:B:974:GLY:HA3	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:1199:ARG:HD2	1:B:1228:THR:HG22	1.83	0.59
1:B:596:GLU:OE1	5:B:2324:HOH:O	2.17	0.59
1:A:642:VAL:HG13	1:A:664:ILE:HG23	1.85	0.59
1:B:1424:MET:HE3	1:B:1447:ILE:HG21	1.85	0.58
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:A:1337:MET:CE	1:A:1365:LEU:HD21	2.33	0.58
1:B:1455:SER:O	1:B:1459:GLU:HG2	2.02	0.58
1:B:453:THR:CG2	5:B:2242:HOH:O	2.47	0.58
1:B:885:HIS:CD2	1:B:910:ARG:NH2	2.61	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:A:460:VAL:CG1	1:A:464:MET:HE2	2.33	0.58
1:B:120:GLN:O	1:B:124:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1421:GLY:HA2	1:A:1424:MET:HE2	1.86	0.57
1:A:513:ASN:HA	1:A:516:MET:HE2	1.87	0.56
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: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:1317:ASN:HA	1:B:1321:MET:HE3	1.86	0.56
1:B:1443:ASN:OD1	1:B:1445:GLU:HG2	2.06	0.56
1:A:171:ARG:CZ	1:A:338:LYS:HD2	2.35	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
1:A:905:GLY:CA	1:A:951:GLY:HA2	2.35	0.56
1:A:1468:HIS:O	1:A:1472:THR:HB	2.06	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: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:211:THR:HG22	5:B:2108:HOH:O	2.06	0.55
1:A:1317:ASN:HA	1:A:1321:MET:HE3	1.87	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:A:1506:ASN:O	1:A:1507:ASN:HB2	2.06	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:863:VAL:CG1	1:A:1175:TYR:HD2	2.20	0.55
1:A:603:ARG:O	1:A:603:ARG:CG	2.54	0.55
1:A:715:LEU:HD22	1:A:726:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:475:MET:HE2	1:A:1139:MET:SD	2.47	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:1424:MET:HE3	1:B:1447:ILE:CG2	2.37	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:146:ARG:HH22	1:A:256:GLU:CD	2.12	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
1:A:869:ARG:HD2	1:A:1193:LEU:HD23	1.90	0.53
1:A:36:ALA:N	1:A:120:GLN:HE22	2.06	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: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:497:GLN:HE21	1:B:651:HIS:CD2	2.26	0.52
1:B:232:THR:HG21	1:B:725:SER:HB3	1.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ALA:C	1:B:162:ASP:H	2.11	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:CG	1:B:603:ARG:O	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:A:13:PRO:HB3	1:A:199:ASN:ND2	2.26	0.51
1:A:834:LEU:HD21	1:A:1109:LYS:HZ2	1.74	0.51
1:A:219:GLN:HB3	1:A:220:PRO:HA	1.93	0.51
1:B:513:ASN:HA	1:B:516:MET:CE	2.41	0.51
1:A:1265:THR:CG2	1:A:1266:THR:N	2.74	0.51
1:A:872:THR:HG22	5:A:2409:HOH:O	2.04	0.51
1:B:1369:THR:HG22	5:B:2635:HOH:O	2.11	0.51
1:B:676:TRP:HE1	1:B:690:ARG:NH1	2.09	0.51
1:B:146:ARG:HH22	1:B:256:GLU:CD	2.13	0.50
1:B:603:ARG:O	1:B:603:ARG:HG2	2.12	0.50
1:B:797:ASN:HA	1:B:801:MET:HE2	1.93	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:1449:LEU:HG	1:A:1492:TRP:HB3	1.94	0.50
1:A:385:ALA:HB1	1:A:386:PRO:CD	2.42	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:B:1433:ASP:CG	1:B:1438:LEU:HB2	2.32	0.50
1:A:601:THR:HG21	1:A:603:ARG:HG2	1.94	0.50
1:B:459:MET:HE3	5:B:2241:HOH:O	2.11	0.50
1:B:905:GLY:HA3	1:B:951:GLY:HA2	1.92	0.50
1:A:1318:LEU:N	1:A:1321:MET:HE2	2.11	0.49
1:A:239:TRP:NE1	1:A:728:GLY:HA3	2.27	0.49
1:A:36:ALA:HB2	1:A:211:THR:HG23	1.95	0.49
1:A:9:LEU:HG	1:A:360:ASP:O	2.12	0.49
1:B:1023:HIS:HD2	5:B:2596:HOH:O	1.93	0.49
1:A:1363:THR:O	1:A:1363:THR:HG22	2.12	0.49
1:A:652:HIS:HE1	5:A:2251:HOH:O	1.94	0.49
1:B:460:VAL:HG12	1:B:464:MET:HE1	1.93	0.49
1:A:160:ALA:C	1:A:162:ASP:H	2.15	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:A:797:ASN:HA	1:A:801:MET:CE	2.42	0.49
1:A:1210:GLN:HG3	5:A:2563:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1200:THR:HG21	1:B:1225:LEU:HB2	1.94	0.49
1:B:15:HIS:HD2	1:B:196:TYR:O	1.95	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:A:516:MET:HE1	1:A:712:PHE:HB3	1.95	0.48
1:B:1338:ASN:OD1	1:B:1369:THR:HG23	2.13	0.48
1:A:798:SER:H	1:A:801:MET:HE2	1.79	0.48
1:B:1449:LEU:HG	1:B:1492:TRP:HB3	1.95	0.48
1:A:1382:ARG:HD2	1:A:1400:HIS:HB2	1.95	0.48
1:A:885:HIS:HD2	1:A:910:ARG:HH22	1.52	0.48
1:B:369:GLY:HA2	1:B:1308:ALA:CB	2.43	0.48
1:B:953:THR:HG21	1:B:1294:ASN:HD21	1.76	0.48
1:B:157:LYS:CE	1:B:261:THR:OG1	2.61	0.48
1:B:9:LEU:HG	1:B:360:ASP:O	2.14	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: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:1382:ARG:O	1:A:1385:VAL:HG22	2.14	0.48
1:A:437:PHE:HD1	1:A:443:VAL:HG22	1.78	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:B:1378:ARG:CD	5:B:2679:HOH:O	2.61	0.47
1:B:1375:ALA:HB3	1:B:1394:ILE:HG22	1.95	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:1008:ASP:HB3	1:A:1009:ILE:HG13	1.95	0.47
1:A:649:SER:H	1:A:652:HIS:CD2	2.32	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:261:THR:O	1:A:263:ILE:N	2.47	0.47
1:A:505:PRO:HD2	5:A:2261:HOH:O	2.13	0.47
1:B:753:VAL:HG23	1:B:1219:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:TYR:HB3	1:B:312:ILE:HD12	1.95	0.47
1:A:237:ILE:HA	1:A:264:VAL:HG11	1.96	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:760:ASP:OD2	1:A:1214:THR:CG2	2.64	0.46
1:A:550:GLU:OE2	1:A:704:ARG:NH2	2.48	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:B:755:GLY:C	1:B:1214:THR:HG21	2.36	0.46
1:A:243:ARG:NH2	1:A:322:LEU:O	2.47	0.46
1:B:160:ALA:C	1:B:162:ASP:N	2.69	0.46
1:A:805:LEU:HD23	1:A:1133:ILE:HG22	1.98	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:B:75:GLY:O	1:B:130:GLN:HA	2.16	0.46
1:B:873:GLY:C	1:B:900:ASN:HB3	2.36	0.46
1:A:796:MET:HE1	1:A:834:LEU:HD22	1.98	0.46
1:B:509:PRO:HA	1:B:516:MET:HE3	1.92	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:1265:THR:HG22	1:A:1266:THR:N	2.31	0.45
1:A:223:LEU:HD12	1:A:335:SER:O	2.16	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:905:GLY:HA2	1:A:951:GLY:CA	2.46	0.45
1:A:1008:ASP:HB2	1:A:1366:TYR:HE1	1.82	0.45
1:A:871:CYS:SG	1:A:1103:ARG:HD2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:ARG:HG3	1:A:1112:TRP:CH2	2.52	0.45
1:A:509:PRO:HA	1:A:516:MET:CE	2.47	0.45
1:A:1004:PRO:HB2	1:A:1005:PRO:HD3	1.99	0.45
1:B:1108:LEU:O	1:B:1130:ILE:CD1	2.65	0.45
1:B:490:LEU:HD11	1:B:648:TRP:CH2	2.51	0.45
1:A:23:LYS:HB3	5:A:2007:HOH:O	2.17	0.45
1:A:621:ALA:O	1:A:625:VAL:HG13	2.16	0.45
1:B:550:GLU:CD	1:B:704:ARG:HH22	2.20	0.45
1:A:1157:GLU:O	1:A:1161:GLN:HG3	2.17	0.45
1:A:36:ALA:H	1:A:120:GLN:HE22	1.64	0.45
1:A:28:MET:CE	1:A:203:TYR:CE1	2.97	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:513:ASN:HA	1:B:516:MET:HE2	1.98	0.44
1:B:798:SER:H	1:B:801:MET:CE	2.29	0.44
1:B:663:ALA:C	1:B:664:ILE:HD13	2.38	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:A:1419:ASN:ND2	1:A:1443:ASN:HD22	2.10	0.44
1:A:369:GLY:HA2	1:A:1308:ALA:CB	2.47	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:A:1285:SER:OG	1:A:1321:MET:CE	2.65	0.44
1:B:143:GLU:OE1	1:B:146:ARG:HD3	2.18	0.44
1:B:383:ARG:HH22	1:B:1381:GLU:CD	2.21	0.44
1:B:264:VAL:HG12	1:B:265:ASN:N	2.33	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:1145:THR:CG2	1:A:1147:ASN:HB2	2.48	0.43
1:A:517:SER:HB3	1:A:722:LEU:HD22	2.00	0.43
1:B:887:THR:HB	1:B:1135:GLU:OE2	2.18	0.43
1:B:685:LEU:O	1:B:689:GLY:N	2.52	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:1265:THR:CG2	1:B:1266:THR:H	2.30	0.43
1:B:648:TRP:H	1:B:652:HIS:CD2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:VAL:HG21	1:B:661:ALA:HB2	2.00	0.43
1:A:1347:HIS:HB3	5:A:2628:HOH:O	2.17	0.43
1:A:1433:ASP:CG	1:A:1438:LEU:HB2	2.39	0.43
1:A:693:ARG:C	1:A:694:ILE:HG12	2.37	0.43
1:A:784:GLY:N	1:A:793:GLU:H	2.15	0.43
1:A:460:VAL:HG13	1:A:464:MET:HE2	1.99	0.43
1:A:760:ASP:OD2	1:A:1214:THR:HG23	2.18	0.43
1:B:1318:LEU:N	1:B:1321:MET:HE2	2.20	0.43
1:A:978:GLN:HE22	1:A:1069:PRO:HD3	1.84	0.42
1:A:891:ALA:CB	1:A:1170:VAL:HG22	2.50	0.42
1:B:3:VAL:N	1:B:28:MET:HE1	2.34	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:1347:HIS:HB3	5:B:2639:HOH:O	2.18	0.42
1:B:642:VAL:HG13	1:B:664:ILE:HG23	2.00	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: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:B:1110:THR:HG23	1:B:1112:TRP:H	1.84	0.42
1:B:845:LEU:HD11	1:B:1217:LEU:HD22	2.02	0.42
1:A:1056:ILE:HD12	1:A:1100:VAL:HG21	2.00	0.42
1:A:28:MET:HE1	1:A:203:TYR:CE1	2.54	0.42
1:B:796:MET:CE	1:B:834:LEU:HD22	2.50	0.42
1:A:1254:ASP:HA	1:A:1255:PRO:HD2	1.93	0.42
1:A:239:TRP:HE1	1:A:728:GLY:HA3	1.85	0.42
1:A:873:GLY:C	1:A:900:ASN:HB3	2.40	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:B:1391:LYS:HA	1:B:1409:VAL:O	2.20	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:A:603:ARG:O	1:A:603:ARG:HG2	2.19	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:1317:ASN:HA	1:B:1321:MET:CE	2.50	0.42
1:B:172:THR:HG23	5:B:2114:HOH:O	2.19	0.42
1:B:36:ALA:N	1:B:120:GLN:HE22	2.18	0.42
1:A:389:MET:HE3	1:A:405:ILE:HG21	2.02	0.41
1:A:870:PHE:O	1:A:897:ALA:HB1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1442:ILE:HG12	1:B:1449:LEU:HD22	2.02	0.41
1:B:652:HIS:HE1	5:B:2267:HOH:O	2.01	0.41
1:A:437:PHE:CE1	1:A:671:GLU:HG2	2.55	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
1:B:460:VAL:O	1:B:464:MET:HE2	2.20	0.41
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:1382:ARG:O	1:B:1385:VAL:HG22	2.20	0.41
1:B:507:ILE:O	1:B:716:SER:HB2	2.20	0.41
1:A:1089:ARG:CZ	1:A:1224:ASN:O	2.69	0.41
1:A:28:MET:HE1	1:A:203:TYR:HE1	1.82	0.41
1:A:685:LEU:CD1	1:A:690:ARG:HD2	2.47	0.41
1:B:650:THR:CG2	5:B:2253:HOH:O	2.43	0.41
1:A:1232:ARG:HD3	5:A:2553:HOH:O	2.20	0.41
1:A:518:LEU:HD23	1:A:708:GLU:HG2	2.02	0.41
1:B:124:ASN:ND2	1:B:213:PRO:O	2.54	0.41
1:B:717:LYS:CB	1:B:974:GLY:HA3	2.51	0.41
1:B:610:THR:H	1:B:613:GLN:HE21	1.69	0.41
1:A:1248:ASP:HB3	1:A:1283:ARG:HB3	2.03	0.40
1:A:389:MET:HE2	1:A:406:LYS:CE	2.50	0.40
1:A:404:GLN:O	1:A:408:GLN:HG3	2.20	0.40
1:A:349:LEU:O	1:A:350:ARG:HD2	2.21	0.40
1:A:1273:LEU:HD23	1:A:1273:LEU:HA	1.89	0.40
1:A:50:ILE:CD1	1:A:170:CYS:C	2.89	0.40
1:A:660:GLY:O	1:A:727:HIS:HE1	2.05	0.40
1:B:1260:ALA:HA	1:B:1265:THR:HB	2.03	0.40
1:B:385:ALA:HB1	1:B:386:PRO:CD	2.51	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%)	25	19
1	B	1485/1520 (98%)	1437 (97%)	41 (3%)	7 (0%)	29	23
All	All	2970/3040 (98%)	2867 (96%)	87 (3%)	16 (0%)	29	23

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 [i](#)

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%)	1097 (90%)	117 (10%)	8	5
1	B	1214/1236 (98%)	1092 (90%)	122 (10%)	7	4
All	All	2428/2472 (98%)	2189 (90%)	239 (10%)	8	4

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	99	LEU
1	A	124	ASN
1	A	148	LEU
1	A	168	PHE
1	A	182	ILE
1	A	191	LEU
1	A	207	PHE
1	A	211	THR
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	336	ASP
1	A	339	ILE
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	478	ASP
1	A	511	ARG
1	A	514	LEU

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Mol	Chain	Res	Type
1	A	515	VAL
1	A	518	LEU
1	A	532	LYS
1	A	541	LEU
1	A	580	LEU
1	A	583	LEU
1	A	603	ARG
1	A	608	ILE
1	A	625	VAL
1	A	629	LEU
1	A	636	LEU
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	690	ARG
1	A	693	ARG
1	A	694	ILE
1	A	715	LEU
1	A	750	THR
1	A	779	LYS
1	A	804	SER
1	A	809	VAL
1	A	825	ASP
1	A	837	ARG
1	A	857	LEU
1	A	858	GLU
1	A	872	THR
1	A	877	LEU
1	A	912	LEU
1	A	915	ASP
1	A	953	THR
1	A	1008	ASP
1	A	1015	LEU
1	A	1028	GLU
1	A	1052	ASN
1	A	1062	ASP
1	A	1085	THR

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Mol	Chain	Res	Type
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	1216	ASN
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	1248	ASP
1	A	1265	THR
1	A	1279	THR
1	A	1280	VAL
1	A	1291	LYS
1	A	1332	TYR
1	A	1349	GLN
1	A	1360	ILE
1	A	1381	GLU
1	A	1382	ARG
1	A	1388	SER
1	A	1389	VAL
1	A	1416	VAL
1	A	1424	MET
1	A	1425	THR
1	A	1442	ILE
1	A	1456	LYS
1	A	1464	LEU
1	A	1488	LEU
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	66	MET
1	B	96	VAL
1	B	99	LEU
1	B	115	ASP
1	B	137	GLU
1	B	146	ARG
1	B	148	LEU
1	B	162	ASP
1	B	168	PHE
1	B	182	ILE
1	B	191	LEU
1	B	207	PHE
1	B	211	THR
1	B	221	MET
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	379	VAL
1	B	398	LYS
1	B	404	GLN
1	B	421	ILE
1	B	430	SER
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
1	B	524	LYS
1	B	541	LEU
1	B	578	ASP

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Mol	Chain	Res	Type
1	B	580	LEU
1	B	583	LEU
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	693	ARG
1	B	701	LYS
1	B	715	LEU
1	B	750	THR
1	B	761	VAL
1	B	765	VAL
1	B	800	GLU
1	B	801	MET
1	B	809	VAL
1	B	812	TYR
1	B	829	LEU
1	B	835	LYS
1	B	837	ARG
1	B	857	LEU
1	B	867	VAL
1	B	872	THR
1	B	877	LEU
1	B	912	LEU
1	B	915	ASP
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
1	B	1089	ARG
1	B	1101	LEU

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Mol	Chain	Res	Type
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	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	1248	ASP
1	B	1266	THR
1	B	1291	LYS
1	B	1332	TYR
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	1449	LEU
1	B	1453	THR
1	B	1456	LYS
1	B	1464	LEU
1	B	1488	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	120	GLN

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Mol	Chain	Res	Type
1	A	199	ASN
1	A	236	ASN
1	A	266	GLN
1	A	303	GLN
1	A	323	GLN
1	A	404	GLN
1	A	467	GLN
1	A	486	HIS
1	A	613	GLN
1	A	651	HIS
1	A	652	HIS
1	A	727	HIS
1	A	730	GLN
1	A	769	HIS
1	A	885	HIS
1	A	978	GLN
1	A	1023	HIS
1	A	1052	ASN
1	A	1210	GLN
1	A	1215	GLN
1	A	1216	ASN
1	A	1275	ASN
1	A	1338	ASN
1	A	1419	ASN
1	A	1450	GLN
1	A	1493	GLN
1	B	15	HIS
1	B	120	GLN
1	B	236	ASN
1	B	266	GLN
1	B	303	GLN
1	B	323	GLN
1	B	486	HIS
1	B	513	ASN
1	B	613	GLN
1	B	628	HIS
1	B	651	HIS
1	B	652	HIS
1	B	688	ASN
1	B	727	HIS
1	B	730	GLN
1	B	826	HIS

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Mol	Chain	Res	Type
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	1147	ASN
1	B	1156	GLN
1	B	1216	ASN
1	B	1275	ASN
1	B	1376	ASN
1	B	1419	ASN
1	B	1450	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 carbohydrates 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
3	F3S	A	3509	1	0,9,9	0.00	-	-		
2	FMN	B	3508	-	31,33,33	1.62	5 (16%)	40,50,50	1.90	8 (20%)
4	AKG	A	3510	-	3,9,9	4.25	1 (33%)	4,11,11	1.63	1 (25%)
4	AKG	B	3510	-	3,9,9	4.33	1 (33%)	4,11,11	1.55	1 (25%)
3	F3S	B	3509	1	0,9,9	0.00	-	-		
2	FMN	A	3508	-	31,33,33	1.57	7 (22%)	40,50,50	2.09	9 (22%)

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	B	3510	-	-	1/3/9/9	-
2	FMN	B	3508	-	-	1/18/18/18	0/3/3/3
4	AKG	A	3510	-	-	1/3/9/9	-
3	F3S	A	3509	1	-	-	0/3/3/3
3	F3S	B	3509	1	-	-	0/3/3/3
2	FMN	A	3508	-	-	1/18/18/18	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3510	AKG	O5-C2	7.47	1.34	1.22
4	A	3510	AKG	O5-C2	7.35	1.34	1.22
2	B	3508	FMN	C1'-N10	4.26	1.52	1.48
2	B	3508	FMN	C10-N1	4.10	1.38	1.33
2	A	3508	FMN	C1'-N10	3.88	1.52	1.48
2	B	3508	FMN	C4A-N5	3.50	1.38	1.33
2	A	3508	FMN	C10-N1	3.49	1.37	1.33
2	B	3508	FMN	C4-N3	3.37	1.38	1.33
2	A	3508	FMN	C4-N3	3.29	1.38	1.33
2	A	3508	FMN	C4A-N5	2.91	1.37	1.33
2	A	3508	FMN	C5A-N5	2.55	1.39	1.35
2	A	3508	FMN	C4A-C10	2.47	1.41	1.38
2	A	3508	FMN	P-O2P	-2.12	1.46	1.54
2	B	3508	FMN	C5A-N5	2.12	1.38	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3508	FMN	C4-N3-C2	8.20	122.07	115.14
2	B	3508	FMN	C4-N3-C2	7.69	121.63	115.14
2	A	3508	FMN	C4A-C4-N3	-4.52	117.25	123.43
2	A	3508	FMN	C10-C4A-N5	-4.16	118.38	121.26
2	B	3508	FMN	C10-C4A-N5	-3.84	118.61	121.26
2	B	3508	FMN	C4A-C4-N3	-3.76	118.29	123.43
2	B	3508	FMN	C9A-N10-C10	-3.58	117.22	121.91
2	A	3508	FMN	C9A-N10-C10	-3.43	117.42	121.91
2	A	3508	FMN	C1'-N10-C9A	3.35	120.93	118.29
2	B	3508	FMN	C5A-C9A-N10	2.82	119.76	117.72
2	A	3508	FMN	C5A-C9A-N10	2.70	119.67	117.72
2	A	3508	FMN	C4A-N5-C5A	2.48	119.25	116.77
2	B	3508	FMN	C4A-N5-C5A	2.43	119.20	116.77
2	A	3508	FMN	P-O5'-C5'	2.32	124.69	118.30
2	A	3508	FMN	C4-C4A-N5	2.28	121.20	118.60
2	B	3508	FMN	O3P-P-O5'	2.20	112.60	106.73
4	A	3510	AKG	C4-C3-C2	-2.18	108.45	113.14
2	B	3508	FMN	C4-C4A-N5	2.12	121.02	118.60
4	B	3510	AKG	O5-C2-C3	2.11	123.98	120.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

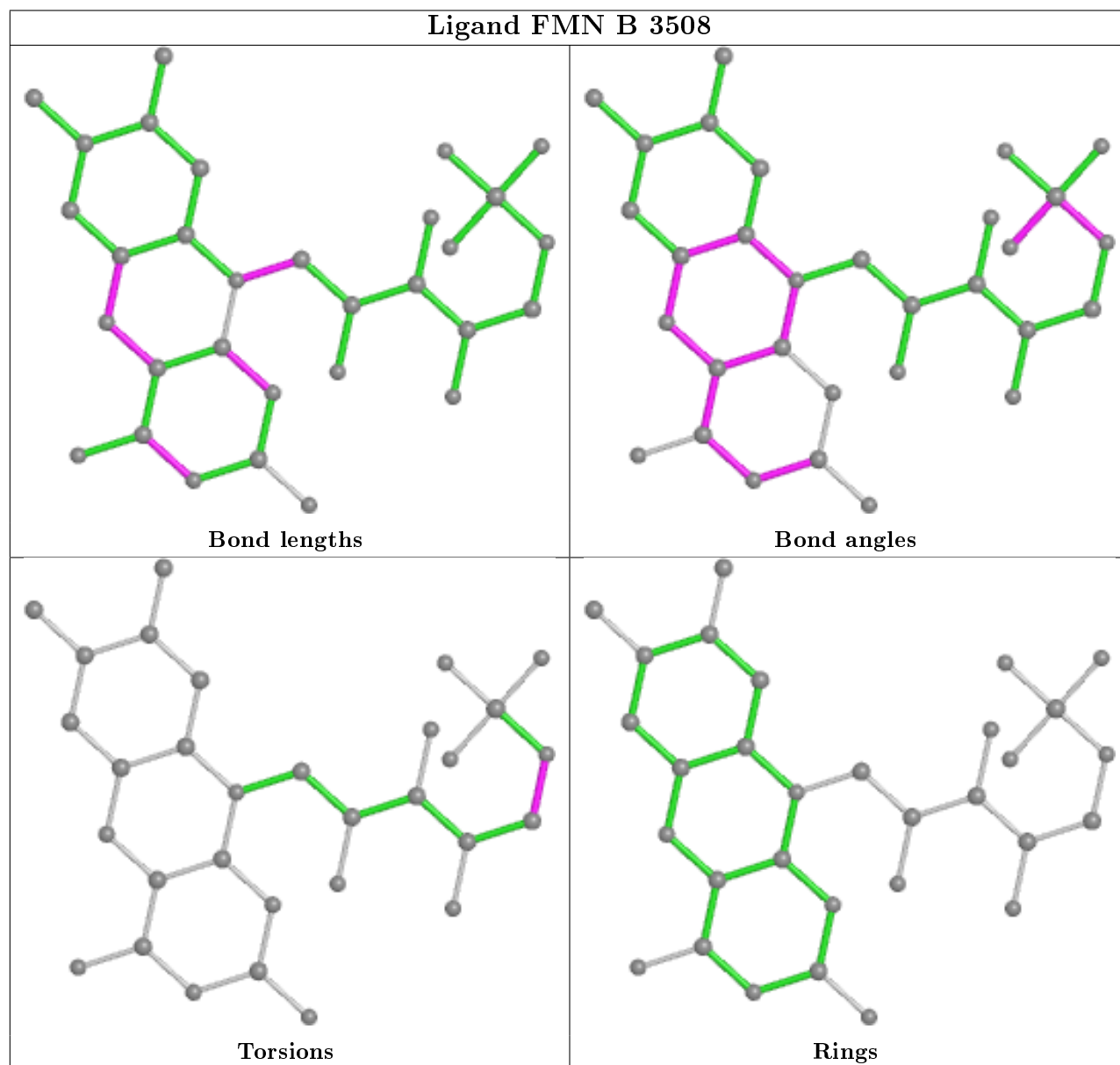
There are no ring outliers.

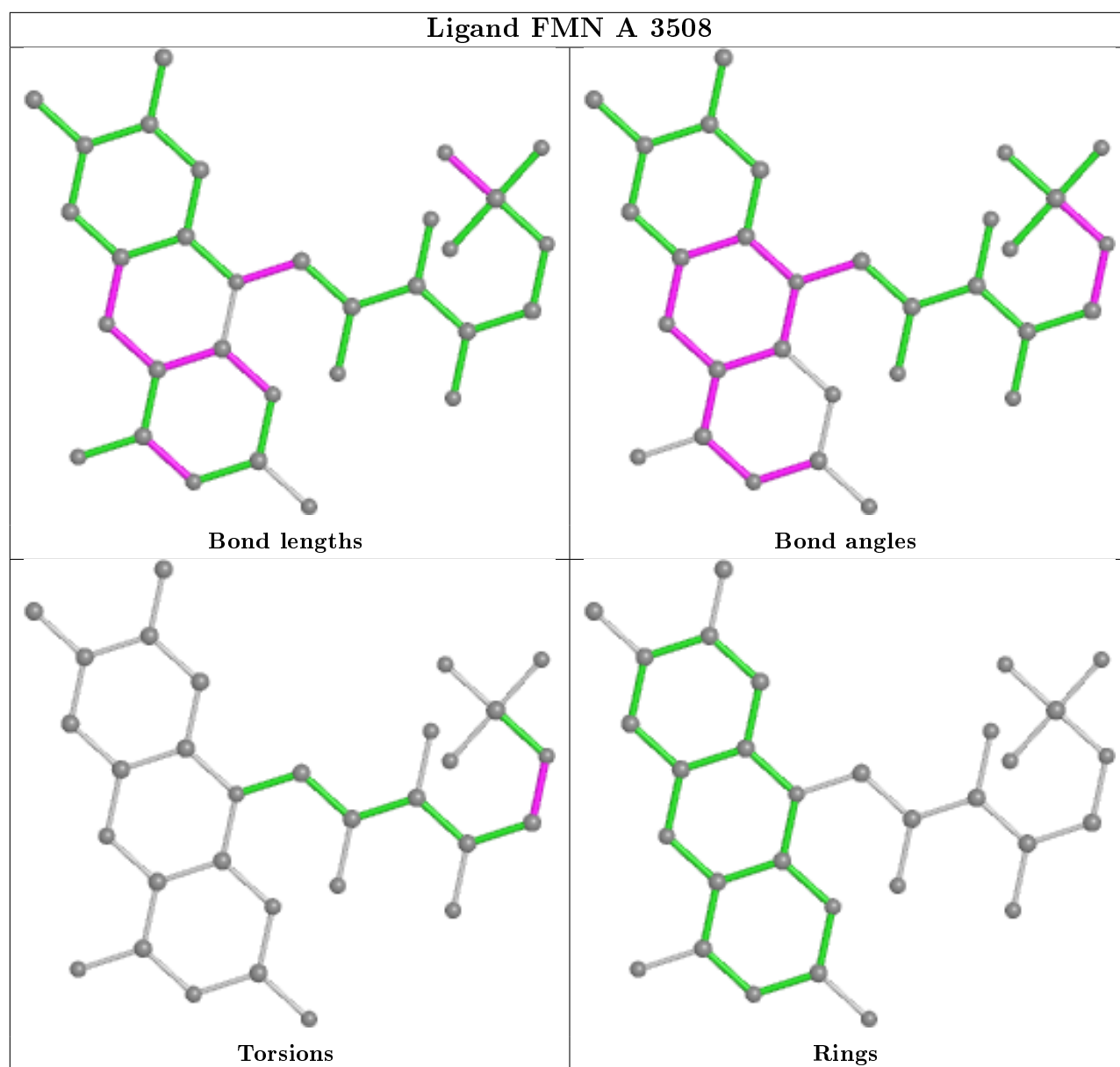
1 monomer is involved in 1 short contact:

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1491/1520 (98%)	-0.06	49 (3%) 46 45	2, 7, 14, 21	0
1	B	1491/1520 (98%)	-0.08	49 (3%) 46 45	2, 7, 13, 22	0
All	All	2982/3040 (98%)	-0.07	98 (3%) 46 45	2, 7, 13, 22	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	693	ARG	7.1
1	A	693	ARG	6.8
1	B	829	LEU	5.9
1	B	833	TYR	5.7
1	A	833	TYR	5.7
1	B	812	TYR	5.2
1	A	261	THR	5.0
1	A	692	ASP	4.9
1	A	690	ARG	4.8
1	B	1507	ASN	4.7
1	B	692	ASP	4.4
1	A	1507	ASN	4.4
1	B	690	ARG	4.4
1	B	1453	THR	4.4
1	A	440	ALA	4.2
1	A	829	LEU	4.1
1	B	438	ASN	3.8
1	A	678	LEU	3.8
1	A	694	ILE	3.7
1	A	1453	THR	3.7
1	B	915	ASP	3.7
1	B	441	GLN	3.7
1	B	608	ILE	3.6
1	B	826	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	572	GLY	3.4
1	B	689	GLY	3.3
1	A	12	LYS	3.2
1	B	261	THR	3.2
1	A	687	GLU	3.2
1	B	1433	ASP	3.2
1	B	1130	ILE	3.2
1	A	832	GLN	3.1
1	A	812	TYR	3.1
1	B	832	GLN	3.0
1	B	369	GLY	3.0
1	A	873	GLY	2.9
1	A	691	LEU	2.9
1	B	828	GLU	2.9
1	B	685	LEU	2.9
1	A	728	GLY	2.9
1	A	686	MET	2.8
1	B	873	GLY	2.8
1	A	828	GLU	2.8
1	B	439	ASP	2.8
1	A	421	ILE	2.8
1	B	440	ALA	2.8
1	B	417	GLU	2.8
1	B	974	GLY	2.7
1	A	836	ASP	2.7
1	A	915	ASP	2.7
1	A	1433	ASP	2.7
1	B	572	GLY	2.7
1	B	728	GLY	2.7
1	B	687	GLU	2.7
1	B	1385	VAL	2.7
1	B	778	LYS	2.7
1	A	441	GLN	2.7
1	B	811	ALA	2.7
1	A	439	ASP	2.6
1	A	1385	VAL	2.6
1	B	694	ILE	2.5
1	B	70	ASP	2.5
1	B	372	ASP	2.5
1	A	369	GLY	2.5
1	A	778	LYS	2.5
1	A	689	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	912	LEU	2.4
1	A	826	HIS	2.4
1	B	825	ASP	2.4
1	B	12	LYS	2.4
1	B	1164	LYS	2.4
1	A	1349	GLN	2.4
1	A	858	GLU	2.3
1	B	100	GLU	2.3
1	A	811	ALA	2.3
1	B	858	GLU	2.3
1	A	1506	ASN	2.3
1	A	684	LYS	2.3
1	B	790	PRO	2.3
1	A	788	TYR	2.3
1	A	139	CYS	2.3
1	A	919	SER	2.3
1	B	688	ASN	2.3
1	A	556	THR	2.2
1	A	246	GLU	2.2
1	B	836	ASP	2.2
1	B	137	GLU	2.2
1	A	974	GLY	2.1
1	A	438	ASN	2.1
1	B	835	LYS	2.1
1	B	1191	ARG	2.1
1	A	680	GLU	2.1
1	B	997	GLY	2.1
1	A	877	LEU	2.1
1	A	951	GLY	2.1
1	A	831	ARG	2.0
1	B	1210	GLN	2.0
1	B	1500	LYS	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

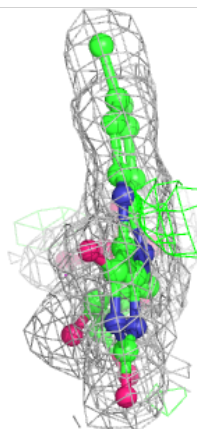
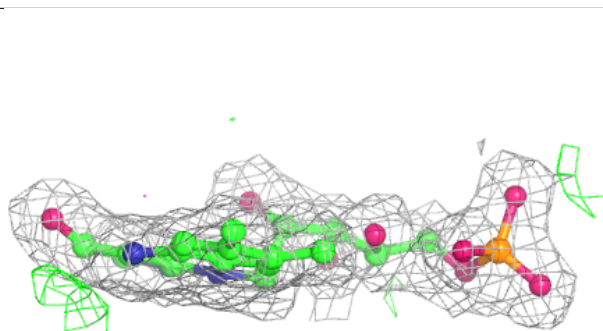
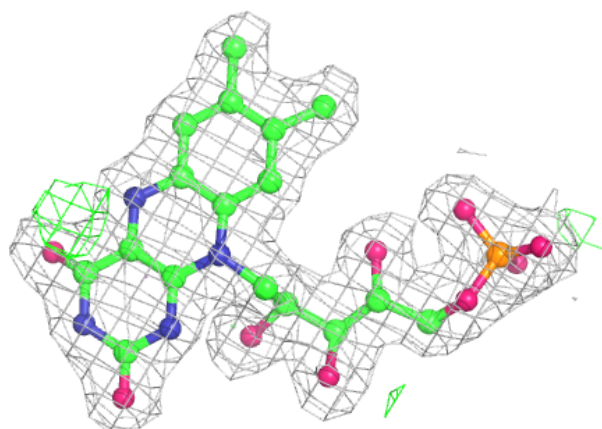
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	0.95	0.12	12,15,19,21	0
4	AKG	A	3510	10/10	0.97	0.10	11,15,18,19	0
2	FMN	B	3508	31/31	0.98	0.14	9,13,15,17	0
2	FMN	A	3508	31/31	0.98	0.14	8,10,14,15	0
3	F3S	B	3509	7/7	0.99	0.07	11,11,11,13	0
3	F3S	A	3509	7/7	0.99	0.07	10,11,11,12	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.

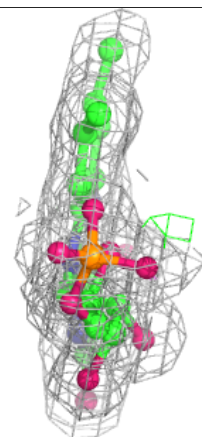
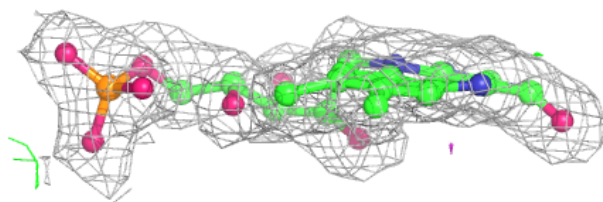
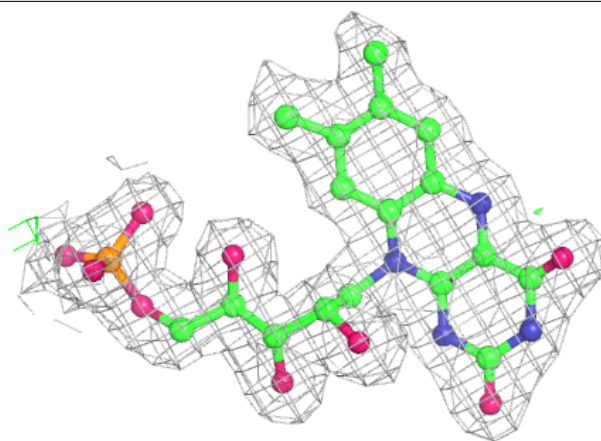
### Electron density around FMN B 3508:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)



**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.