



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:45 am GMT

PDB ID : 1OFE  
Title : GLUTAMATE SYNTHASE FROM SYNECHOCYSTIS SP IN COMPLEX WITH 2-OXOGLUTARATE AND L-DON AT 2.45 ANGSTROM RESOLUTION  
Authors : Van Den Heuvel, R.H.H.; Mattevi, A.  
Deposited on : 2003-04-14  
Resolution : 2.45 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

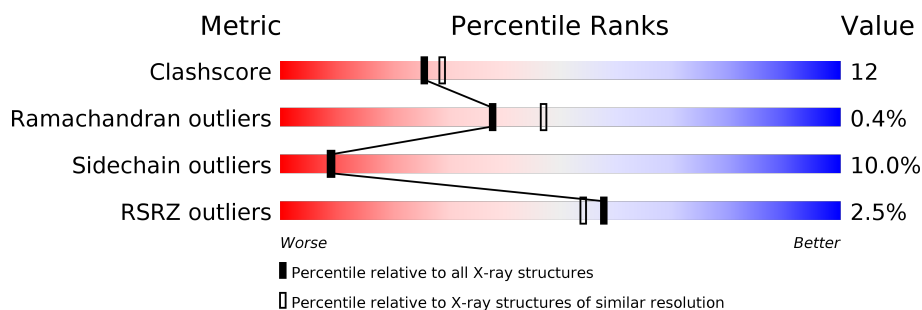
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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. 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	
1	B	1520	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ONL	B	2511	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23181 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

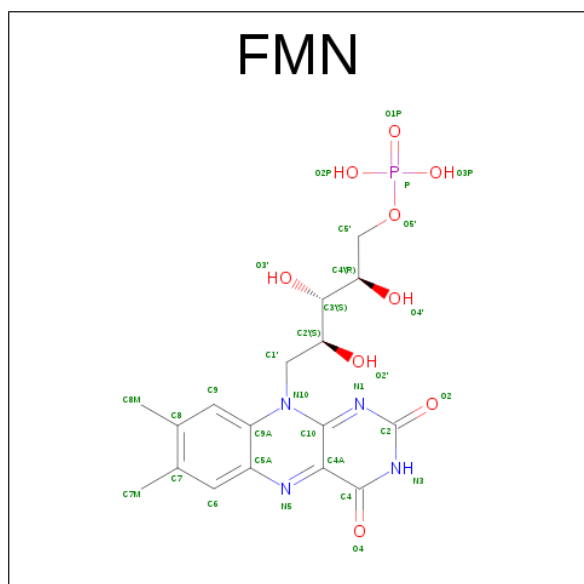
- Molecule 1 is a protein called FERREDONIN-DEPENDENT GLUTAMATE SYNTHASE 2.

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

There are 6 discrepancies between the modelled and reference sequences:

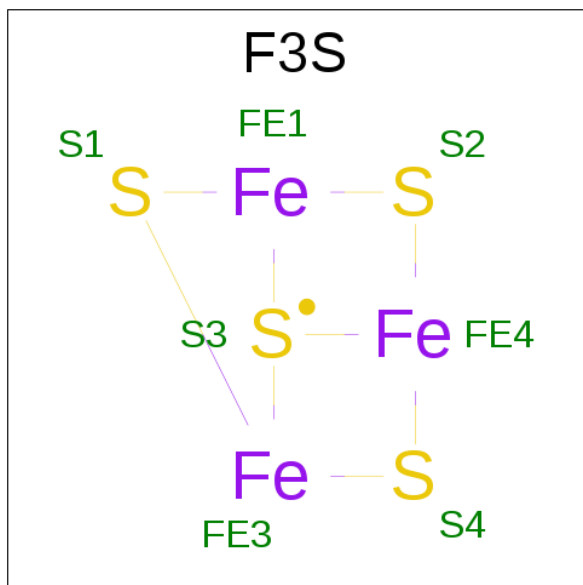
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	CONFLICT	UNP P55038
A	581	THR	ASP	CONFLICT	UNP P55038
A	1507	ASN	GLY	CONFLICT	UNP P55038
B	578	ASP	THR	CONFLICT	UNP P55038
B	581	THR	ASP	CONFLICT	UNP P55038
B	1507	ASN	GLY	CONFLICT	UNP P55038

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



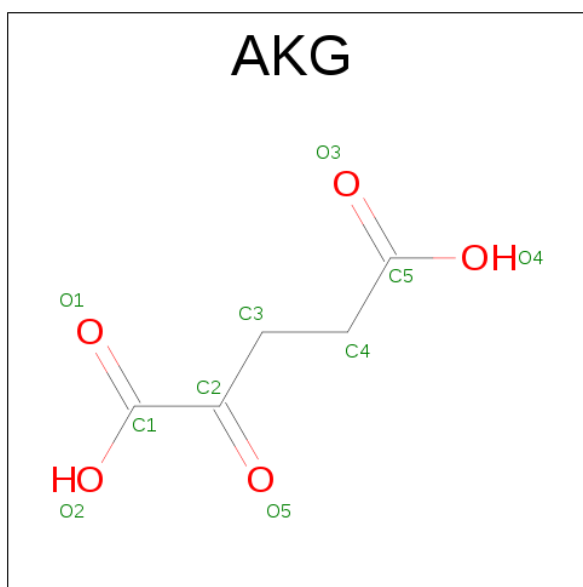
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



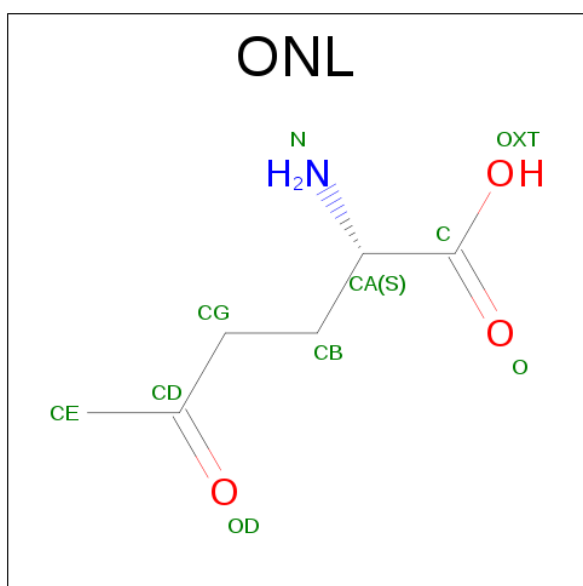
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	4		
3	B	1	Total	Fe	S	0	0
			7	3	4		

- 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 5-OXO-L-NORLEUCINE (three-letter code: ONL) (formula:  $C_6H_{11}NO_3$ ).



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

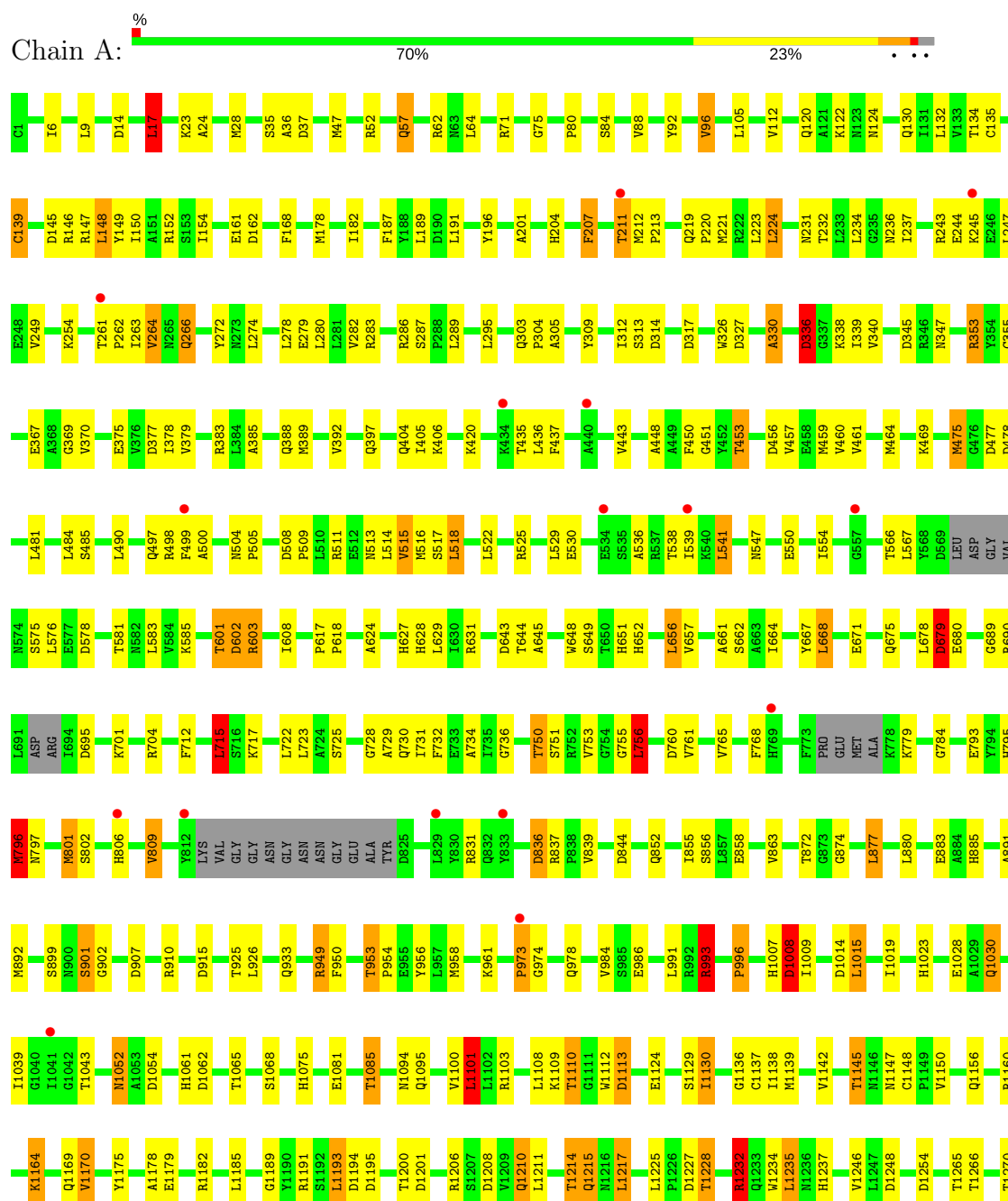
- Molecule 6 is water.

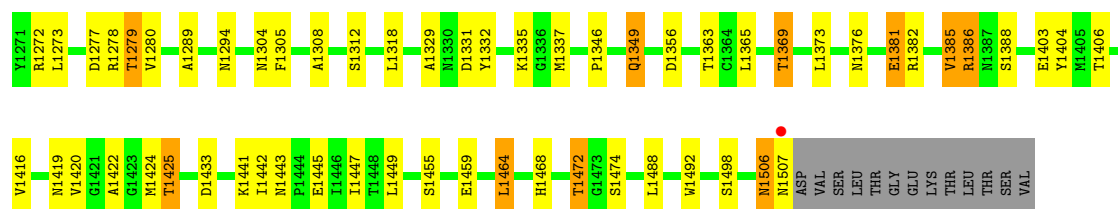
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total 208	O 208	0	0
6	B	81	Total 81	O 81	0	0

### 3 Residue-property plots

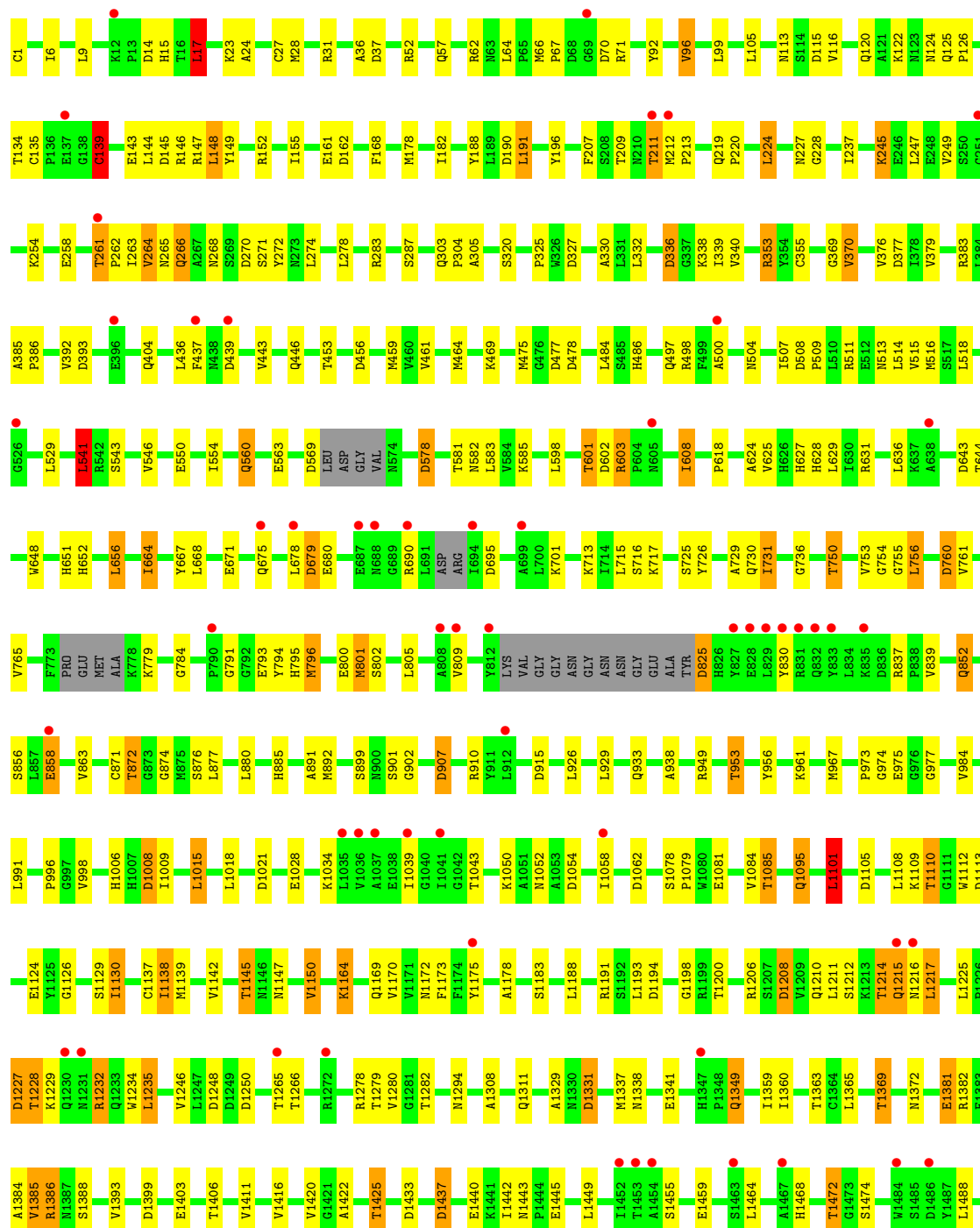
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE 2

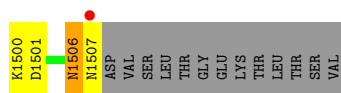




● Molecule 1: FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.67Å 134.38Å 198.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.45 46.61 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.45) 99.4 (46.61-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.207 , 0.257 0.205 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, ONL

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	0.80	4/11609 (0.0%)	1.02	56/15739 (0.4%)
1	B	0.67	0/11609	0.92	46/15739 (0.3%)
All	All	0.74	4/23218 (0.0%)	0.97	102/31478 (0.3%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	950	PHE	C-O	6.56	1.35	1.23
1	A	355	CYS	CB-SG	-5.72	1.72	1.81
1	A	475	MET	SD-CE	5.70	2.09	1.77
1	A	796	MET	SD-CE	5.09	2.06	1.77

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	949	ARG	NE-CZ-NH2	-11.31	114.65	120.30
1	A	1062	ASP	CB-CG-OD2	8.98	126.38	118.30
1	B	695	ASP	CB-CG-OD2	8.69	126.12	118.30
1	A	17	LEU	CA-CB-CG	8.49	134.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	ASP	CB-CG-OD2	8.35	125.81	118.30
1	A	695	ASP	CB-CG-OD2	8.15	125.64	118.30
1	A	949	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	1277	ASP	CB-CG-OD2	7.98	125.48	118.30
1	A	353	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	B	1105	ASP	CB-CG-OD1	7.80	125.32	118.30
1	A	973	PRO	C-N-CA	-7.78	105.97	122.30
1	A	1008	ASP	CB-CG-OD2	7.54	125.08	118.30
1	A	1433	ASP	CB-CG-OD2	7.42	124.98	118.30
1	B	498	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	B	377	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	1101	LEU	CA-CB-CG	7.28	132.05	115.30
1	B	907	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	1227	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	1062	ASP	CB-CG-OD1	-7.16	111.86	118.30
1	A	836	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	14	ASP	CB-CG-OD2	7.03	124.62	118.30
1	B	353	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	1331	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	377	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	439	ASP	CB-CG-OD2	6.84	124.46	118.30
1	A	907	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	996	PRO	C-N-CA	-6.83	107.95	122.30
1	B	1101	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	145	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	146	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	825	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	353	ARG	CG-CD-NE	-6.57	98.00	111.80
1	B	14	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	17	LEU	CA-CB-CG	6.37	129.94	115.30
1	B	145	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	1227	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	541	LEU	CA-CB-CG	6.28	129.74	115.30
1	A	1201	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	224	LEU	CB-CG-CD1	-6.22	100.43	111.00
1	A	679	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	478	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	602	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	1014	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	1194	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	973	PRO	C-N-CA	-6.08	109.53	122.30
1	B	336	ASP	CB-CG-OD2	6.04	123.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	393	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	1103	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	1054	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	756	LEU	CA-CB-CG	5.96	129.02	115.30
1	A	1254	ASP	CB-CG-OD2	5.96	123.67	118.30
1	B	327	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	1194	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	1385	VAL	CB-CA-C	-5.87	100.25	111.40
1	B	1437	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	1007	HIS	C-N-CA	5.85	136.33	121.70
1	B	477	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	901	SER	N-CA-C	-5.72	95.55	111.00
1	B	1331	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	993	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	1008	ASP	N-CA-CB	-5.65	100.42	110.60
1	A	1195	ASP	CB-CG-OD2	5.61	123.34	118.30
1	A	1464	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	314	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	336	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	B	508	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	760	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	569	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	355	CYS	N-CA-CB	-5.48	100.73	110.60
1	B	115	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	1164	LYS	N-CA-C	-5.46	96.26	111.00
1	B	1008	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	478	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	1250	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	1208	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	31	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	715	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	336	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	1062	ASP	N-CA-CB	-5.32	101.02	110.60
1	B	754	GLY	N-CA-C	5.30	126.36	113.10
1	A	1356	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	190	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	949	ARG	CG-CD-NE	-5.25	100.78	111.80
1	B	1278	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	1015	LEU	CA-CB-CG	5.19	127.25	115.30
1	A	1232	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	915	ASP	CB-CG-OD2	5.16	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	1113	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	146	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	1399	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	1501	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	477	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	1062	ASP	N-CA-CB	-5.04	101.53	110.60
1	A	1441	LYS	CD-CE-NZ	-5.04	100.11	111.70
1	A	1061	HIS	C-N-CA	5.03	134.27	121.70
1	B	1433	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	1164	LYS	N-CA-C	-5.01	97.47	111.00
1	B	756	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	729	ALA	C-N-CA	-5.01	109.18	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11388	0	11335	296	0
1	B	11388	0	11336	245	0
2	A	31	0	19	1	0
2	B	31	0	19	3	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
4	A	10	0	4	1	0
4	B	10	0	4	0	0
5	A	10	0	9	0	0
5	B	10	0	10	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	208	0	0	20	0
6	B	81	0	0	12	0
All	All	23181	0	22736	543	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 (543) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ILE:CG1	1:A:1130:ILE:CD1	1.74	1.56
1:A:796:MET:CE	1:A:796:MET:SD	2.06	1.43
1:A:475:MET:CE	1:A:475:MET:SD	2.09	1.40
1:B:1:CYS:SG	5:B:2511:ONL:CE	2.20	1.29
1:B:1:CYS:SG	5:B:2511:ONL:CD	2.27	1.22
1:A:1228:THR:CG2	1:A:1232:ARG:HH21	1.54	1.21
1:B:1:CYS:SG	5:B:2511:ONL:HE2	1.78	1.21
1:B:1138:ILE:HG22	1:B:1139:MET:H	1.04	1.15
1:A:872:THR:HG22	1:A:899:SER:HA	1.29	1.15
1:B:1228:THR:HG22	1:B:1232:ARG:HH21	1.06	1.14
1:B:825:ASP:HB3	6:B:2051:HOH:O	1.47	1.12
1:A:1138:ILE:HG22	1:A:1139:MET:N	1.56	1.11
1:B:825:ASP:CB	6:B:2051:HOH:O	1.94	1.09
1:B:1228:THR:CG2	1:B:1232:ARG:HH21	1.65	1.08
1:A:1138:ILE:CG2	1:A:1139:MET:H	1.67	1.07
1:A:885:HIS:CD2	1:A:910:ARG:HH22	1.72	1.07
1:B:1228:THR:CG2	1:B:1232:ARG:NH2	2.18	1.05
1:B:885:HIS:CD2	1:B:910:ARG:HH22	1.75	1.04
1:A:1228:THR:HG22	1:A:1232:ARG:HH21	1.22	1.03
1:A:497:GLN:HE21	1:A:651:HIS:HD2	1.05	1.01
1:B:1130:ILE:HD13	1:B:1130:ILE:H	1.25	1.01
1:A:1228:THR:CG2	1:A:1232:ARG:NH2	2.24	0.99
1:B:1137:CYS:SG	1:B:1138:ILE:O	2.21	0.98
1:A:717:LYS:HG2	1:A:974:GLY:HA3	1.47	0.97
1:B:1206:ARG:NH1	6:B:2075:HOH:O	1.98	0.96
1:A:135:CYS:SG	1:A:139:CYS:HB2	2.06	0.96
1:A:509:PRO:HA	1:A:516:MET:HE1	1.49	0.95
1:A:509:PRO:HA	1:A:516:MET:CE	1.98	0.93
1:B:953:THR:HG21	1:B:1294:ASN:HD21	1.34	0.93
1:A:1337:MET:HE2	1:A:1365:LEU:HD22	1.52	0.92
1:A:885:HIS:HD2	1:A:910:ARG:HH22	1.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1138:ILE:HG22	1:B:1139:MET:N	1.85	0.91
1:A:1110:THR:HG22	1:A:1113:ASP:H	1.35	0.91
1:A:1138:ILE:HG22	1:A:1139:MET:H	0.76	0.91
1:A:603:ARG:HG2	1:A:603:ARG:O	1.68	0.90
1:B:1472:THR:HG22	1:B:1474:SER:H	1.37	0.89
1:A:1468:HIS:O	1:A:1472:THR:HB	1.74	0.88
1:A:1381:GLU:HG3	6:A:2041:HOH:O	1.73	0.88
1:A:1137:CYS:SG	1:A:1138:ILE:O	2.34	0.86
1:A:336:ASP:HB3	1:A:338:LYS:H	1.40	0.85
1:B:603:ARG:O	1:B:603:ARG:HG2	1.74	0.85
1:A:1145:THR:HG21	6:A:2156:HOH:O	1.77	0.85
1:B:953:THR:CG2	1:B:1294:ASN:HD21	1.90	0.85
1:B:1506:ASN:O	1:B:1507:ASN:HB2	1.76	0.84
1:A:756:LEU:HA	1:A:1214:THR:HG21	1.57	0.84
1:B:1228:THR:HG22	1:B:1232:ARG:NH2	1.85	0.83
1:A:652:HIS:HE1	6:A:2068:HOH:O	1.59	0.83
1:A:656:LEU:HD23	1:A:664:ILE:HD12	1.61	0.83
1:A:1472:THR:HG22	1:A:1474:SER:H	1.41	0.83
1:A:1265:THR:HG22	1:A:1266:THR:H	1.42	0.82
1:B:497:GLN:HE21	1:B:651:HIS:HD2	1.28	0.82
1:A:1211:LEU:HD11	1:A:1217:LEU:HD22	1.62	0.81
1:B:825:ASP:HB2	6:B:2051:HOH:O	1.68	0.81
1:A:756:LEU:HA	1:A:1214:THR:CG2	2.09	0.81
1:A:1385:VAL:O	1:A:1404:TYR:N	2.12	0.80
1:A:953:THR:CG2	1:A:1294:ASN:HD21	1.94	0.80
1:B:475:MET:CE	1:B:1129:SER:OG	2.30	0.80
1:A:648:TRP:H	1:A:652:HIS:HD2	1.26	0.80
1:B:1138:ILE:CG2	1:B:1139:MET:H	1.87	0.80
1:A:1110:THR:HG21	6:A:2104:HOH:O	1.82	0.80
1:A:135:CYS:CB	1:A:139:CYS:HB2	2.11	0.80
1:A:497:GLN:HE21	1:A:651:HIS:CD2	1.97	0.79
1:A:547:ASN:OD1	1:A:550:GLU:HG3	1.82	0.79
1:B:1425:THR:HG21	6:B:2060:HOH:O	1.83	0.79
1:A:953:THR:HG22	1:A:956:TYR:H	1.47	0.78
1:B:1130:ILE:H	1:B:1130:ILE:CD1	1.93	0.78
1:A:237:ILE:HG23	1:A:264:VAL:HG13	1.65	0.78
1:A:1337:MET:HE2	1:A:1365:LEU:CD2	2.13	0.78
1:B:1468:HIS:O	1:B:1472:THR:HB	1.84	0.78
1:A:261:THR:O	1:A:263:ILE:N	2.17	0.78
1:A:453:THR:HG23	6:A:2061:HOH:O	1.83	0.78
1:A:678:LEU:O	1:A:679:ASP:CB	2.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:SER:OG	1:A:901:SER:O	1.99	0.77
1:A:1108:LEU:O	1:A:1130:ILE:HG13	1.84	0.77
1:B:675:GLN:O	1:B:678:LEU:O	2.02	0.77
1:B:1081:GLU:O	1:B:1085:THR:HB	1.84	0.77
1:A:1130:ILE:H	1:A:1130:ILE:HD13	1.50	0.76
1:B:713:LYS:NZ	1:B:975:GLU:OE1	2.19	0.76
1:B:784:GLY:O	1:B:795:HIS:NE2	2.17	0.76
1:B:791:GLY:HA3	6:B:2050:HOH:O	1.86	0.76
1:B:627:HIS:O	1:B:631:ARG:HG3	1.86	0.75
1:B:135:CYS:SG	1:B:139:CYS:HB2	2.25	0.75
1:B:475:MET:HE1	1:B:1129:SER:OG	1.85	0.75
1:A:601:THR:HG22	1:A:643:ASP:OD2	1.86	0.74
1:A:461:VAL:HA	1:A:464:MET:CE	2.17	0.74
1:B:1382:ARG:O	1:B:1385:VAL:HG22	1.88	0.74
1:A:756:LEU:HD12	1:A:1214:THR:HG23	1.70	0.73
1:A:436:LEU:HD11	6:A:2084:HOH:O	1.89	0.72
1:A:717:LYS:CG	1:A:974:GLY:HA3	2.19	0.72
1:A:953:THR:HG23	1:A:1294:ASN:HD21	1.54	0.72
1:B:237:ILE:HG23	1:B:264:VAL:CG1	2.19	0.72
1:B:303:GLN:HE21	1:B:305:ALA:H	1.36	0.72
1:A:736:GLY:O	1:A:755:GLY:HA3	1.90	0.72
1:A:872:THR:HG22	1:A:899:SER:CA	2.17	0.71
1:B:910:ARG:HD3	1:B:938:ALA:HB1	1.71	0.71
1:B:953:THR:HG22	1:B:956:TYR:H	1.55	0.71
1:B:1363:THR:HG22	1:B:1363:THR:O	1.90	0.71
1:B:648:TRP:H	1:B:652:HIS:HD2	1.37	0.71
1:B:353:ARG:NH2	1:B:1329:ALA:O	2.23	0.70
1:A:9:LEU:O	1:A:397:GLN:HG2	1.91	0.70
1:A:124:ASN:ND2	1:A:213:PRO:O	2.24	0.70
1:A:885:HIS:HD2	1:A:910:ARG:NH2	1.85	0.70
1:A:247:LEU:HD22	1:A:529:LEU:HD11	1.72	0.70
1:B:717:LYS:HG2	1:B:974:GLY:HA3	1.74	0.69
1:A:1424:MET:CE	1:A:1447:ILE:HG21	2.22	0.69
1:A:601:THR:CG2	1:A:643:ASP:OD2	2.39	0.69
1:B:237:ILE:HG23	1:B:264:VAL:HG13	1.74	0.69
1:A:453:THR:HB	1:A:456:ASP:OD2	1.92	0.69
1:B:304:PRO:HB3	1:B:1440:GLU:OE1	1.91	0.69
1:A:1337:MET:CE	1:A:1365:LEU:HD22	2.21	0.69
1:A:404:GLN:HG3	6:A:2057:HOH:O	1.93	0.69
1:A:1138:ILE:CG2	1:A:1139:MET:N	2.32	0.69
1:A:303:GLN:HE21	1:A:305:ALA:H	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:THR:HG23	1:A:1232:ARG:HH21	1.54	0.68
1:B:247:LEU:HD22	1:B:529:LEU:HD11	1.74	0.68
1:B:756:LEU:HD12	1:B:1214:THR:HG23	1.76	0.68
1:B:509:PRO:HA	1:B:516:MET:HE1	1.75	0.67
1:B:885:HIS:CD2	1:B:910:ARG:NH2	2.58	0.67
1:A:1228:THR:HG22	1:A:1232:ARG:NH2	2.02	0.67
1:B:261:THR:HB	1:B:262:PRO:HD3	1.76	0.67
1:A:1420:VAL:HB	1:A:1442:ILE:HD13	1.76	0.67
1:A:801:MET:HE3	1:A:802:SER:N	2.10	0.66
1:B:1228:THR:HG21	1:B:1232:ARG:NH2	2.09	0.66
1:A:453:THR:CG2	6:A:2061:HOH:O	2.42	0.66
1:B:266:GLN:HG2	6:B:2021:HOH:O	1.94	0.66
1:B:261:THR:O	1:B:263:ILE:N	2.28	0.66
1:A:1265:THR:HG22	1:A:1266:THR:N	2.10	0.65
1:A:1403:GLU:O	1:A:1422:ALA:O	2.13	0.65
1:B:1108:LEU:O	1:B:1130:ILE:HG13	1.97	0.65
1:B:760:ASP:OD2	1:B:1214:THR:HG22	1.97	0.65
1:A:37:ASP:H	1:A:120:GLN:NE2	1.94	0.65
1:B:541:LEU:HD11	1:B:554:ILE:HD11	1.77	0.65
1:A:648:TRP:H	1:A:652:HIS:CD2	2.11	0.65
1:B:1110:THR:HG21	6:B:2052:HOH:O	1.96	0.64
1:B:1211:LEU:HD11	1:B:1217:LEU:HD22	1.80	0.64
1:A:1110:THR:CG2	1:A:1113:ASP:H	2.08	0.64
1:A:509:PRO:HA	1:A:516:MET:HE3	1.78	0.64
1:B:1337:MET:HE2	1:B:1365:LEU:CD2	2.27	0.64
1:A:1424:MET:HE2	1:A:1447:ILE:HG21	1.79	0.64
1:A:1506:ASN:O	1:A:1507:ASN:HB2	1.97	0.64
1:B:756:LEU:HA	1:B:1214:THR:CG2	2.27	0.64
1:B:1130:ILE:N	1:B:1130:ILE:HD13	2.07	0.64
1:A:1210:GLN:HE21	1:A:1210:GLN:HA	1.62	0.64
1:A:461:VAL:HA	1:A:464:MET:HE2	1.80	0.64
1:A:550:GLU:OE2	1:A:704:ARG:NH2	2.30	0.64
1:B:135:CYS:CB	1:B:139:CYS:HB2	2.27	0.64
1:B:124:ASN:ND2	1:B:213:PRO:O	2.31	0.64
1:B:497:GLN:HE21	1:B:651:HIS:CD2	2.12	0.64
1:B:984:VAL:O	1:B:996:PRO:O	2.16	0.64
1:A:1142:VAL:O	1:A:1145:THR:HB	1.97	0.63
1:A:1337:MET:CE	1:A:1365:LEU:CD2	2.76	0.63
1:A:717:LYS:HG2	1:A:974:GLY:CA	2.27	0.63
1:A:925:THR:O	1:A:926:LEU:HD23	1.98	0.63
1:B:1110:THR:HG22	1:B:1113:ASP:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLY:HA3	1:B:1308:ALA:CB	2.28	0.63
1:A:152:ARG:HH11	1:A:152:ARG:HG2	1.64	0.62
2:B:2508:FMN:O1P	2:B:2508:FMN:O4'	2.17	0.62
1:B:877:LEU:O	1:B:880:LEU:O	2.17	0.62
1:A:1130:ILE:H	1:A:1130:ILE:CD1	2.12	0.62
1:A:796:MET:HG2	1:A:1109:LYS:HZ2	1.63	0.62
1:A:263:ILE:HD12	1:A:280:LEU:HD22	1.81	0.62
1:A:1145:THR:CG2	1:A:1147:ASN:ND2	2.62	0.62
1:A:1145:THR:CG2	1:A:1147:ASN:HD22	2.12	0.62
1:A:883:GLU:OE2	1:A:1160:ARG:NH1	2.32	0.62
1:B:336:ASP:HB3	1:B:338:LYS:H	1.65	0.62
1:A:513:ASN:HA	1:A:516:MET:HE2	1.81	0.62
1:A:1455:SER:O	1:A:1459:GLU:HG2	1.99	0.62
1:B:1455:SER:O	1:B:1459:GLU:HG2	1.99	0.62
1:A:1109:LYS:HD2	6:A:2151:HOH:O	1.99	0.61
1:A:1419:ASN:HD21	1:A:1443:ASN:HD22	1.47	0.61
1:A:863:VAL:HG11	1:A:1175:TYR:CD2	2.36	0.61
1:B:178:MET:HE2	1:B:213:PRO:HA	1.83	0.61
1:B:500:ALA:HB1	1:B:504:ASN:O	2.01	0.61
1:B:891:ALA:HB1	1:B:1170:VAL:HG22	1.82	0.60
1:A:678:LEU:O	1:A:679:ASP:HB2	2.00	0.60
1:B:461:VAL:HA	1:B:464:MET:HE2	1.82	0.60
1:A:953:THR:HG21	1:A:1294:ASN:HD21	1.65	0.60
1:A:178:MET:HE2	1:A:213:PRO:HA	1.83	0.60
1:B:1110:THR:CG2	1:B:1113:ASP:H	2.15	0.60
1:B:178:MET:HE2	1:B:213:PRO:CA	2.32	0.60
1:B:891:ALA:CB	1:B:1170:VAL:HG22	2.31	0.59
1:A:211:THR:HB	1:A:1094:ASN:OD1	2.01	0.59
1:A:475:MET:HB3	1:A:475:MET:HE2	1.84	0.59
1:B:1420:VAL:HB	1:B:1442:ILE:HD13	1.85	0.59
1:B:1265:THR:HG22	1:B:1266:THR:H	1.68	0.59
1:B:92:TYR:O	1:B:96:VAL:HG13	2.03	0.59
1:B:475:MET:HE3	1:B:1129:SER:OG	2.03	0.58
1:A:389:MET:HG3	1:A:406:LYS:HE3	1.85	0.58
1:B:509:PRO:HA	1:B:516:MET:CE	2.32	0.58
1:A:678:LEU:O	1:A:679:ASP:HB3	2.03	0.58
1:A:736:GLY:C	1:A:755:GLY:HA3	2.23	0.58
1:B:1009:ILE:HD11	1:B:1018:LEU:CD2	2.33	0.58
1:A:1110:THR:CG2	1:A:1112:TRP:HB3	2.34	0.58
1:A:1110:THR:HG23	1:A:1112:TRP:HB3	1.86	0.58
1:A:37:ASP:H	1:A:120:GLN:HE21	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1095:GLN:HA	1:B:1095:GLN:HE21	1.69	0.58
1:B:1403:GLU:O	1:B:1422:ALA:O	2.22	0.58
1:A:675:GLN:O	1:A:678:LEU:O	2.21	0.58
1:A:541:LEU:HD11	1:A:554:ILE:HD11	1.86	0.57
1:A:750:THR:HG21	1:A:1039:ILE:HG12	1.85	0.57
1:B:885:HIS:HD2	1:B:910:ARG:HH22	1.47	0.57
1:A:885:HIS:CD2	1:A:910:ARG:NH2	2.58	0.57
1:A:369:GLY:HA3	1:A:1308:ALA:CB	2.34	0.57
1:A:618:PRO:HD2	6:A:2087:HOH:O	2.04	0.57
1:A:219:GLN:HB3	1:A:220:PRO:HA	1.87	0.57
1:A:237:ILE:HG23	1:A:264:VAL:CG1	2.32	0.57
1:B:443:VAL:HG21	1:B:675:GLN:HG3	1.86	0.57
1:B:461:VAL:HA	1:B:464:MET:CE	2.35	0.57
1:A:1346:PRO:HD2	1:A:1376:ASN:HD22	1.69	0.57
1:A:436:LEU:HD12	1:A:671:GLU:HB2	1.87	0.57
1:A:35:SER:HB3	1:A:120:GLN:NE2	2.20	0.57
1:A:178:MET:HG3	1:A:213:PRO:HB2	1.85	0.57
1:B:910:ARG:HD3	1:B:938:ALA:CB	2.35	0.57
1:A:717:LYS:CB	1:A:974:GLY:HA3	2.35	0.56
1:A:984:VAL:O	1:A:996:PRO:O	2.22	0.56
1:B:1425:THR:CG2	6:B:2060:HOH:O	2.48	0.56
1:B:603:ARG:HD2	1:B:667:TYR:CE2	2.40	0.56
1:A:261:THR:HB	1:A:262:PRO:HD3	1.88	0.56
1:B:224:LEU:HD11	1:B:332:LEU:HD22	1.86	0.56
1:B:1130:ILE:N	1:B:1130:ILE:CD1	2.67	0.56
1:B:601:THR:CG2	1:B:643:ASP:OD2	2.54	0.56
1:B:863:VAL:HG13	1:B:1178:ALA:HB3	1.88	0.56
1:A:1234:TRP:CZ3	1:A:1235:LEU:HD13	2.41	0.56
1:B:1101:LEU:HD11	1:B:1124:GLU:HG3	1.87	0.56
1:B:1265:THR:HG22	1:B:1266:THR:N	2.20	0.56
1:B:513:ASN:HA	1:B:516:MET:HE3	1.87	0.56
1:B:113:ASN:O	1:B:116:VAL:HG22	2.07	0.55
1:A:1228:THR:HG23	1:A:1232:ARG:NH2	2.16	0.55
1:A:837:ARG:NH1	1:A:844:ASP:OD1	2.40	0.55
1:A:1200:THR:HG21	1:A:1225:LEU:HB2	1.89	0.55
1:B:437:PHE:CE2	1:B:608:ILE:HD11	2.41	0.55
1:A:760:ASP:OD2	1:A:1214:THR:HG22	2.06	0.55
1:B:1:CYS:SG	5:B:2511:ONL:HE1	2.39	0.55
1:B:1472:THR:CG2	1:B:1474:SER:HB2	2.37	0.55
1:A:1085:THR:CG2	6:A:2167:HOH:O	2.55	0.55
1:B:678:LEU:O	1:B:679:ASP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:GLY:H	1:B:793:GLU:H	1.54	0.55
1:A:303:GLN:NE2	1:A:304:PRO:HD2	2.21	0.54
1:A:1030:GLN:HG2	1:A:1054:ASP:HB3	1.90	0.54
1:A:891:ALA:HB1	1:A:1170:VAL:HG22	1.89	0.54
1:A:1363:THR:HG22	1:A:1363:THR:O	2.07	0.54
1:A:461:VAL:HA	1:A:464:MET:HE3	1.87	0.54
1:A:223:LEU:HD22	1:A:279:GLU:HB2	1.90	0.54
1:B:1006:HIS:C	1:B:1008:ASP:H	2.11	0.54
1:A:986:GLU:CD	6:A:2130:HOH:O	2.46	0.54
1:B:910:ARG:HD2	1:B:938:ALA:O	2.08	0.54
1:B:601:THR:HA	1:B:643:ASP:HB3	1.88	0.54
1:B:1:CYS:HB2	1:B:227:ASN:ND2	2.22	0.53
1:A:784:GLY:H	1:A:793:GLU:H	1.56	0.53
1:B:715:LEU:HD22	1:B:726:TYR:CG	2.43	0.53
1:A:1145:THR:HG23	1:A:1147:ASN:ND2	2.24	0.53
1:B:717:LYS:HG2	1:B:974:GLY:CA	2.38	0.53
1:A:1081:GLU:O	1:A:1085:THR:HB	2.09	0.53
1:B:1110:THR:HG23	1:B:1112:TRP:H	1.73	0.53
1:B:736:GLY:O	1:B:755:GLY:HA3	2.09	0.53
1:A:500:ALA:HB1	1:A:504:ASN:O	2.09	0.53
1:B:219:GLN:HB3	1:B:220:PRO:HA	1.90	0.53
1:A:389:MET:HE3	1:A:405:ILE:HG21	1.90	0.53
1:B:756:LEU:HA	1:B:1214:THR:HG21	1.91	0.53
1:A:1228:THR:HG21	1:A:1232:ARG:NH2	2.21	0.52
1:B:1050:LYS:HE3	6:B:2002:HOH:O	2.09	0.52
1:B:1142:VAL:O	1:B:1145:THR:HB	2.08	0.52
1:A:1424:MET:HE3	1:A:1447:ILE:HG21	1.89	0.52
1:A:289:LEU:HD13	1:A:405:ILE:HG23	1.90	0.52
1:B:228:GLY:O	5:B:2511:ONL:HB1	2.09	0.52
1:B:578:ASP:O	1:B:582:ASN:ND2	2.40	0.52
1:B:648:TRP:H	1:B:652:HIS:CD2	2.24	0.52
1:A:1085:THR:HG22	6:A:2167:HOH:O	2.09	0.52
1:B:1338:ASN:HA	1:B:1369:THR:HG22	1.92	0.52
1:B:872:THR:HG22	1:B:899:SER:HA	1.91	0.52
1:B:1110:THR:HG23	1:B:1112:TRP:N	2.25	0.52
1:B:1294:ASN:HB3	1:B:1338:ASN:HD21	1.75	0.52
1:B:678:LEU:O	1:B:679:ASP:CB	2.57	0.52
1:A:1015:LEU:HD13	1:A:1019:ILE:HD12	1.92	0.51
1:A:1382:ARG:O	1:A:1385:VAL:HG22	2.10	0.51
1:A:797:ASN:HB3	1:A:1139:MET:HG3	1.92	0.51
1:B:1:CYS:HB2	1:B:227:ASN:HD22	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:PRO:HD2	6:A:2076:HOH:O	2.10	0.51
1:A:734:ALA:O	1:A:751:SER:HA	2.10	0.51
1:A:484:LEU:HD13	1:A:839:VAL:HG22	1.92	0.51
1:B:1:CYS:SG	5:B:2511:ONL:OD	2.66	0.51
1:A:877:LEU:O	1:A:880:LEU:O	2.28	0.51
1:A:993:ARG:HB3	1:A:1388:SER:HB3	1.93	0.51
1:B:261:THR:HB	1:B:262:PRO:CD	2.41	0.51
1:A:309:TYR:HB3	1:A:312:ILE:HD12	1.93	0.51
1:A:730:GLN:O	1:A:732:PHE:N	2.40	0.50
1:A:1472:THR:CG2	1:A:1474:SER:H	2.17	0.50
1:B:1206:ARG:HG2	1:B:1208:ASP:OD2	2.11	0.50
1:B:1384:ALA:O	1:B:1385:VAL:C	2.50	0.50
1:B:15:HIS:HD2	1:B:196:TYR:O	1.94	0.50
1:A:715:LEU:HD11	1:A:723:LEU:HA	1.94	0.50
1:B:211:THR:O	1:B:211:THR:CG2	2.58	0.50
1:A:953:THR:HG23	1:A:1294:ASN:ND2	2.24	0.50
1:B:1145:THR:CG2	1:B:1147:ASN:ND2	2.75	0.50
1:A:1382:ARG:HB3	1:A:1385:VAL:HG22	1.93	0.50
1:A:232:THR:HG21	1:A:725:SER:HB3	1.92	0.50
1:A:603:ARG:HD3	1:A:643:ASP:OD2	2.10	0.50
1:A:1108:LEU:O	1:A:1130:ILE:CG1	2.57	0.50
1:A:178:MET:HE2	1:A:213:PRO:CA	2.41	0.50
1:B:436:LEU:HD12	1:B:671:GLU:HB2	1.93	0.50
1:A:508:ASP:OD2	1:A:1404:TYR:OH	2.13	0.50
1:B:36:ALA:HB2	1:B:211:THR:CG2	2.42	0.50
1:A:1210:GLN:NE2	1:A:1210:GLN:HA	2.25	0.49
1:A:234:LEU:HD13	1:A:234:LEU:C	2.32	0.49
1:A:485:SER:OG	1:A:793:GLU:OE2	2.28	0.49
1:B:105:LEU:HD11	1:B:134:THR:HG23	1.93	0.49
1:B:446:GLN:NE2	1:B:608:ILE:HG23	2.26	0.49
1:A:874:GLY:O	2:A:2508:FMN:C4A	2.60	0.49
1:A:437:PHE:HD1	1:A:443:VAL:HG22	1.76	0.49
1:B:796:MET:CG	1:B:1109:LYS:HZ2	2.24	0.49
1:B:852:GLN:HB2	1:B:1188:LEU:O	2.12	0.49
1:A:149:TYR:CE1	1:A:279:GLU:HG2	2.48	0.49
1:B:1009:ILE:HD11	1:B:1018:LEU:HD23	1.94	0.49
1:B:211:THR:O	1:B:211:THR:HG23	2.13	0.49
1:B:385:ALA:HB1	1:B:386:PRO:HD2	1.94	0.49
1:A:627:HIS:O	1:A:631:ARG:HG3	2.13	0.49
1:B:486:HIS:HD2	1:B:1212:SER:OG	1.96	0.49
1:B:37:ASP:H	1:B:120:GLN:NE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:PRO:HD2	1:B:725:SER:OG	2.13	0.48
1:A:105:LEU:HD11	1:A:134:THR:HG23	1.95	0.48
1:B:135:CYS:HB3	1:B:139:CYS:HB2	1.94	0.48
1:B:453:THR:HB	1:B:456:ASP:OD2	2.14	0.48
1:A:624:ALA:O	1:A:628:HIS:HD2	1.97	0.48
1:A:891:ALA:CB	1:A:1170:VAL:HG22	2.43	0.48
1:A:9:LEU:HD22	1:A:392:VAL:HG11	1.95	0.48
1:B:383:ARG:HH22	1:B:1381:GLU:CD	2.16	0.48
1:B:624:ALA:O	1:B:628:HIS:HD2	1.97	0.48
1:B:9:LEU:CD2	1:B:392:VAL:HG11	2.44	0.48
1:B:717:LYS:CG	1:B:974:GLY:HA3	2.41	0.48
1:A:1100:VAL:O	1:A:1237:HIS:CE1	2.67	0.48
1:A:35:SER:HB3	1:A:120:GLN:HE22	1.78	0.48
1:B:901:SER:O	1:B:901:SER:OG	2.30	0.48
1:A:1065:THR:HG21	1:A:1068:SER:OG	2.14	0.48
1:A:347:ASN:OD1	1:A:515:VAL:HG11	2.13	0.48
1:B:1:CYS:HG	5:B:2511:ONL:CD	2.23	0.48
1:B:998:VAL:HG11	1:B:1425:THR:OG1	2.14	0.47
1:A:796:MET:CG	1:A:1109:LYS:HZ2	2.26	0.47
1:A:236:ASN:ND2	1:A:326:TRP:HA	2.29	0.47
1:A:460:VAL:O	1:A:464:MET:HG3	2.14	0.47
1:A:603:ARG:O	1:A:603:ARG:CG	2.51	0.47
1:B:1095:GLN:CA	1:B:1095:GLN:HE21	2.27	0.47
1:A:756:LEU:CA	1:A:1214:THR:HG21	2.38	0.47
1:A:57:GLN:H	1:A:57:GLN:HG2	1.56	0.47
1:A:883:GLU:CD	1:A:1160:ARG:HH11	2.18	0.47
1:A:1278:ARG:NH2	6:A:2174:HOH:O	2.43	0.47
1:A:282:VAL:HA	1:A:286:ARG:O	2.14	0.47
1:B:953:THR:HG23	1:B:1294:ASN:HD21	1.78	0.47
1:A:135:CYS:HB3	1:A:139:CYS:HB2	1.94	0.47
1:A:796:MET:CE	1:A:796:MET:CG	2.91	0.47
1:B:1506:ASN:HD22	1:B:1506:ASN:C	2.18	0.47
1:B:258:GLU:O	1:B:261:THR:OG1	2.28	0.47
1:B:730:GLN:NE2	6:B:2048:HOH:O	2.44	0.47
1:A:1008:ASP:OD1	1:A:1335:LYS:HE2	2.14	0.47
1:A:1443:ASN:OD1	1:A:1445:GLU:HG2	2.15	0.47
1:A:330:ALA:HB3	1:A:345:ASP:HB3	1.95	0.47
1:B:796:MET:HG2	1:B:1109:LYS:HZ2	1.80	0.47
1:A:207:PHE:HD2	1:A:207:PHE:C	2.18	0.46
1:A:518:LEU:HD13	1:A:712:PHE:CE2	2.50	0.46
1:A:266:GLN:H	1:A:266:GLN:HG2	1.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:PRO:HG3	1:A:644:THR:OG1	2.16	0.46
1:A:993:ARG:HD3	1:A:1369:THR:OG1	2.15	0.46
1:A:651:HIS:CD2	1:A:1075:HIS:HB3	2.51	0.46
1:A:223:LEU:HD23	1:A:278:LEU:HD23	1.98	0.46
1:A:522:LEU:HB2	1:A:539:ILE:HB	1.98	0.46
1:B:1058:ILE:HD13	1:B:1084:VAL:HA	1.98	0.46
1:B:1337:MET:HE2	1:B:1365:LEU:HD22	1.96	0.46
1:A:1147:ASN:O	1:A:1148:CYS:C	2.54	0.46
1:A:649:SER:H	1:A:652:HIS:CD2	2.33	0.46
1:B:581:THR:O	1:B:585:LYS:HG3	2.16	0.46
1:A:978:GLN:H	4:A:2510:AKG:H41	1.80	0.46
1:B:209:THR:OG1	1:B:1043:THR:HG23	2.16	0.46
1:B:715:LEU:HD22	1:B:726:TYR:CD1	2.51	0.46
1:A:36:ALA:N	1:A:120:GLN:HE22	2.14	0.46
1:B:143:GLU:HA	1:B:143:GLU:OE1	2.16	0.46
1:B:546:VAL:HA	1:B:550:GLU:OE2	2.16	0.46
1:A:112:VAL:HA	1:A:187:PHE:O	2.15	0.46
1:A:75:GLY:O	1:A:130:GLN:HA	2.16	0.46
1:A:313:SER:O	1:A:317:ASP:HB2	2.16	0.46
1:A:80:PRO:HA	1:A:162:ASP:OD1	2.16	0.46
1:A:954:PRO:O	1:A:958:MET:HG2	2.16	0.46
1:B:717:LYS:CB	1:B:974:GLY:HA3	2.45	0.46
1:A:207:PHE:CD2	1:A:207:PHE:C	2.89	0.45
1:B:1234:TRP:CZ3	1:B:1235:LEU:HD13	2.51	0.45
1:B:1393:VAL:HG22	1:B:1411:VAL:HB	1.98	0.45
1:A:385:ALA:HB3	1:A:388:GLN:NE2	2.31	0.45
1:A:567:LEU:HD21	1:A:602:ASP:HB2	1.99	0.45
1:B:27:CYS:CB	1:B:370:VAL:HG22	2.47	0.45
1:B:871:CYS:O	1:B:1126:GLY:HA2	2.16	0.45
1:B:188:TYR:HB2	1:B:191:LEU:HD22	1.98	0.45
1:B:245:LYS:HB2	1:B:245:LYS:NZ	2.31	0.45
1:B:1363:THR:CG2	1:B:1363:THR:O	2.61	0.45
1:B:794:TYR:CE2	1:B:837:ARG:HB2	2.52	0.45
1:A:6:ILE:HG22	1:A:17:LEU:HD22	1.98	0.45
1:B:750:THR:HG21	1:B:1039:ILE:HG12	1.97	0.45
1:A:1185:LEU:HD21	1:A:1193:LEU:HD13	1.99	0.45
1:A:1279:THR:HA	1:A:1312:SER:O	2.17	0.45
1:A:9:LEU:CD2	1:A:392:VAL:HG11	2.46	0.45
1:A:575:SER:O	1:A:576:LEU:C	2.54	0.45
1:A:353:ARG:NH2	1:A:1329:ALA:O	2.36	0.45
1:B:270:ASP:OD1	1:B:271:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:THR:O	1:A:1228:THR:CG2	2.65	0.45
1:A:47:MET:O	1:A:201:ALA:HA	2.17	0.45
1:A:1386:ARG:HG2	1:A:1404:TYR:HB2	1.99	0.45
1:A:451:GLY:HA2	1:A:768:PHE:CD2	2.52	0.45
1:A:278:LEU:HD12	1:A:295:LEU:HD12	1.98	0.44
1:A:383:ARG:HH22	1:A:1381:GLU:CD	2.21	0.44
1:B:1406:THR:HG22	1:B:1425:THR:HG22	1.98	0.44
1:A:1265:THR:CG2	1:A:1266:THR:H	2.20	0.44
1:B:1145:THR:HG22	1:B:1147:ASN:HB2	1.99	0.44
1:B:603:ARG:HD3	1:B:643:ASP:OD2	2.16	0.44
1:B:618:PRO:HG3	1:B:644:THR:OG1	2.18	0.44
1:A:1442:ILE:HD13	1:A:1442:ILE:HA	1.66	0.44
1:A:152:ARG:HG2	1:A:152:ARG:NH1	2.30	0.44
1:B:320:SER:HB2	6:B:2026:HOH:O	2.16	0.44
1:B:385:ALA:HB1	1:B:386:PRO:CD	2.48	0.44
1:B:729:ALA:HB1	1:B:731:ILE:HD11	1.99	0.44
1:A:475:MET:CE	1:A:1129:SER:OG	2.65	0.44
1:B:1108:LEU:O	1:B:1130:ILE:CG1	2.64	0.44
1:B:507:ILE:O	1:B:716:SER:HB2	2.17	0.44
1:B:926:LEU:HD13	1:B:929:LEU:CD1	2.48	0.44
1:A:149:TYR:CD2	1:A:283:ARG:HG3	2.53	0.44
1:B:1506:ASN:O	1:B:1507:ASN:CB	2.58	0.44
1:A:1179:GLU:OE2	1:A:1182:ARG:HD3	2.18	0.44
1:A:499:PHE:CG	1:A:973:PRO:HB2	2.52	0.44
1:B:1349:GLN:HG3	1:B:1349:GLN:H	1.42	0.44
1:A:1110:THR:HG22	1:A:1113:ASP:N	2.17	0.44
1:B:1215:GLN:O	1:B:1216:ASN:HB3	2.18	0.44
1:B:96:VAL:HG21	1:B:155:ILE:HG13	2.00	0.44
1:A:1349:GLN:H	1:A:1349:GLN:HG3	1.50	0.43
1:B:1279:THR:HG22	1:B:1282:THR:CB	2.48	0.43
1:A:1363:THR:HG23	1:A:1385:VAL:HG21	1.99	0.43
1:A:784:GLY:O	1:A:795:HIS:NE2	2.29	0.43
1:A:92:TYR:O	1:A:96:VAL:HG13	2.18	0.43
1:B:1443:ASN:OD1	1:B:1445:GLU:HG2	2.17	0.43
1:A:1156:GLN:O	1:A:1160:ARG:HG3	2.18	0.43
1:A:1381:GLU:HG2	1:A:1381:GLU:H	1.55	0.43
1:A:148:LEU:HA	1:A:148:LEU:HD12	1.88	0.43
1:A:517:SER:HB3	1:A:722:LEU:HD22	1.99	0.43
1:A:243:ARG:HH22	1:A:525:ARG:HH11	1.66	0.43
1:B:1198:GLY:O	1:B:1200:THR:N	2.51	0.43
1:B:1078:SER:HB3	1:B:1079:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ALA:HB2	1:B:211:THR:HG21	1.99	0.43
2:B:2508:FMN:HO4'	2:B:2508:FMN:P	2.40	0.43
1:B:601:THR:HG23	1:B:643:ASP:OD2	2.17	0.43
1:A:378:ILE:HD12	6:A:2051:HOH:O	2.18	0.43
1:B:484:LEU:HD13	1:B:839:VAL:HG22	1.99	0.43
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.85	0.43
1:A:809:VAL:CG1	1:A:1169:GLN:HB3	2.49	0.43
1:A:863:VAL:CG1	1:A:1175:TYR:CD2	3.01	0.43
1:A:668:LEU:HD23	1:A:668:LEU:HA	1.92	0.43
1:B:1437:ASP:O	1:B:1440:GLU:HB2	2.19	0.43
1:B:560:GLN:HB2	1:B:560:GLN:HE21	1.55	0.43
1:A:124:ASN:ND2	1:A:213:PRO:HG2	2.34	0.43
1:A:1419:ASN:ND2	1:A:1443:ASN:HD22	2.16	0.43
1:B:66:MET:HA	1:B:67:PRO:HD3	1.90	0.43
1:A:1449:LEU:HG	1:A:1492:TRP:HB3	2.00	0.43
1:B:1172:ASN:O	1:B:1175:TYR:HB2	2.19	0.43
1:B:475:MET:HB3	1:B:475:MET:HE2	1.86	0.43
1:B:967:MET:HB2	1:B:1034:LYS:O	2.18	0.42
1:B:1341:GLU:HA	1:B:1372:ASN:O	2.18	0.42
1:B:874:GLY:O	2:B:2508:FMN:C10	2.66	0.42
1:A:1215:GLN:HA	1:A:1215:GLN:HE21	1.84	0.42
1:A:1472:THR:CG2	1:A:1474:SER:HB2	2.49	0.42
1:A:657:VAL:HA	1:A:661:ALA:O	2.19	0.42
1:A:872:THR:HB	1:A:892:MET:HG3	2.01	0.42
1:B:1110:THR:HG22	1:B:1113:ASP:CG	2.39	0.42
1:B:1472:THR:HG21	1:B:1474:SER:HB2	2.02	0.42
1:B:863:VAL:HG11	1:B:1175:TYR:CD2	2.55	0.42
1:B:1279:THR:HG22	1:B:1282:THR:HB	2.00	0.42
1:A:1101:LEU:HD11	1:A:1124:GLU:HG3	2.01	0.42
1:A:1273:LEU:HG	1:A:1305:PHE:HB3	2.01	0.42
1:A:1289:ALA:HB2	1:A:1318:LEU:HD11	2.00	0.42
1:A:84:SER:O	1:A:88:VAL:HG23	2.20	0.42
1:B:369:GLY:HA3	1:B:1308:ALA:HB1	2.00	0.42
1:B:624:ALA:O	1:B:628:HIS:CD2	2.73	0.42
1:A:450:PHE:CD2	1:A:645:ALA:HB3	2.55	0.42
1:B:1150:VAL:HG13	1:B:1150:VAL:O	2.19	0.42
1:B:143:GLU:OE1	1:B:146:ARG:HD3	2.19	0.42
1:B:24:ALA:O	1:B:28:MET:HG2	2.20	0.42
1:A:1008:ASP:HB3	1:A:1009:ILE:HG13	2.00	0.42
1:A:1270:THR:HA	1:A:1304:ASN:O	2.20	0.42
1:A:1424:MET:HB3	1:A:1424:MET:HE2	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:O	1:A:154:ILE:HG13	2.20	0.42
1:A:375:GLU:CD	1:A:375:GLU:H	2.22	0.42
1:A:536:ALA:O	1:A:538:THR:HG22	2.19	0.42
1:A:872:THR:CG2	1:A:899:SER:HA	2.21	0.42
1:B:149:TYR:CD2	1:B:283:ARG:HG3	2.54	0.42
1:B:801:MET:HB3	1:B:801:MET:HE2	1.85	0.42
1:B:805:LEU:HB2	1:B:830:TYR:CD1	2.54	0.42
1:B:125:GLN:HA	1:B:126:PRO:HD2	1.86	0.42
1:B:446:GLN:HE22	1:B:608:ILE:HG23	1.85	0.42
1:A:231:ASN:OD1	1:A:327:ASP:HB3	2.20	0.42
1:A:490:LEU:HD11	1:A:648:TRP:CH2	2.55	0.42
1:B:144:LEU:HG	1:B:148:LEU:HD22	2.01	0.42
1:A:261:THR:HB	1:A:262:PRO:CD	2.49	0.42
1:B:1200:THR:HG21	1:B:1225:LEU:H	1.85	0.42
1:B:907:ASP:O	1:B:910:ARG:HB2	2.20	0.42
1:A:1023:HIS:HE1	1:A:1054:ASP:OD2	2.03	0.41
1:A:1206:ARG:HG2	1:A:1208:ASP:OD2	2.20	0.41
1:A:617:PRO:HA	1:A:618:PRO:HD3	1.91	0.41
1:B:178:MET:HG3	1:B:213:PRO:HB2	2.01	0.41
1:A:855:ILE:HG12	1:A:1189:GLY:HA2	2.03	0.41
1:A:204:HIS:ND1	1:A:219:GLN:HB2	2.35	0.41
1:A:420:LYS:HB2	1:A:420:LYS:HE3	1.84	0.41
1:A:863:VAL:HG13	1:A:1178:ALA:HB3	2.01	0.41
1:B:1009:ILE:HD11	1:B:1018:LEU:HD22	2.01	0.41
1:B:1363:THR:HG23	1:B:1385:VAL:HG21	2.03	0.41
1:B:1385:VAL:HB	1:B:1386:ARG:H	1.73	0.41
1:A:1030:GLN:HG2	1:A:1054:ASP:CB	2.51	0.41
1:A:1425:THR:HG21	6:A:2133:HOH:O	2.20	0.41
1:A:1406:THR:HG22	1:A:1425:THR:HG22	2.02	0.41
1:A:885:HIS:CE1	6:A:2105:HOH:O	2.73	0.41
1:B:801:MET:HE3	1:B:802:SER:N	2.36	0.41
1:A:1145:THR:HG22	1:A:1147:ASN:H	1.85	0.41
1:B:1145:THR:HG22	1:B:1147:ASN:CB	2.50	0.41
1:B:1359:ILE:HG23	1:B:1360:ILE:HG23	2.03	0.41
1:A:309:TYR:CB	1:A:312:ILE:HD12	2.51	0.41
1:B:1021:ASP:HA	1:B:1279:THR:HG21	2.01	0.41
1:B:152:ARG:HH11	1:B:152:ARG:HG2	1.85	0.41
1:B:872:THR:HB	1:B:892:MET:HG3	2.02	0.41
1:B:1227:ASP:OD1	1:B:1229:LYS:HG3	2.20	0.41
1:A:806:HIS:CE1	1:A:1136:GLY:HA2	2.56	0.41
1:B:265:ASN:HB3	1:B:268:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:CYS:HB2	1:B:370:VAL:HG22	2.01	0.41
1:B:6:ILE:HG22	1:B:17:LEU:HD22	2.03	0.41
1:A:460:VAL:C	1:A:464:MET:HE2	2.41	0.41
1:B:809:VAL:CG1	1:B:1169:GLN:HB3	2.51	0.41
1:B:1311:GLN:OE1	1:B:1331:ASP:HB2	2.21	0.41
1:B:656:LEU:HD23	1:B:664:ILE:HD12	2.02	0.41
1:B:809:VAL:HG21	1:B:1173:PHE:HB2	2.03	0.41
1:A:1425:THR:CG2	6:A:2133:HOH:O	2.68	0.40
1:A:448:ALA:HA	6:A:2060:HOH:O	2.20	0.40
1:A:581:THR:O	1:A:585:LYS:HG3	2.21	0.40
1:A:475:MET:HE1	1:A:1129:SER:OG	2.21	0.40
1:A:24:ALA:O	1:A:28:MET:HG2	2.22	0.40
1:A:603:ARG:HD2	1:A:667:TYR:CE2	2.56	0.40
1:A:1052:ASN:HD22	1:A:1052:ASN:HA	1.75	0.40
1:A:244:GLU:OE1	1:A:261:THR:O	2.39	0.40
1:A:566:THR:OG1	1:A:602:ASP:HB3	2.21	0.40
1:B:858:GLU:HG2	1:B:858:GLU:H	1.47	0.40
1:B:953:THR:CG2	1:B:1294:ASN:ND2	2.71	0.40
1:A:1332:TYR:HB3	1:A:1335:LYS:HE3	2.03	0.40
1:B:1382:ARG:HB3	1:B:1385:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1475/1520 (97%)	1398 (95%)	72 (5%)	5 (0%)	44	55
1	B	1475/1520 (97%)	1394 (94%)	73 (5%)	8 (0%)	32	39
All	All	2950/3040 (97%)	2792 (95%)	145 (5%)	13 (0%)	38	47

All (13) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1209/1236 (98%)	1085 (90%)	124 (10%)	8	9
1	B	1209/1236 (98%)	1092 (90%)	117 (10%)	9	10
All	All	2418/2472 (98%)	2177 (90%)	241 (10%)	9	9

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	23	LYS
1	A	52	ARG
1	A	57	GLN
1	A	62	ARG
1	A	64	LEU
1	A	71	ARG
1	A	96	VAL
1	A	122	LYS
1	A	132	LEU
1	A	139	CYS

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Mol	Chain	Res	Type
1	A	147	ARG
1	A	148	LEU
1	A	161	GLU
1	A	168	PHE
1	A	182	ILE
1	A	189	LEU
1	A	191	LEU
1	A	196	TYR
1	A	207	PHE
1	A	211	THR
1	A	212	MET
1	A	224	LEU
1	A	245	LYS
1	A	249	VAL
1	A	254	LYS
1	A	264	VAL
1	A	266	GLN
1	A	272	TYR
1	A	274	LEU
1	A	287	SER
1	A	336	ASP
1	A	339	ILE
1	A	340	VAL
1	A	367	GLU
1	A	370	VAL
1	A	379	VAL
1	A	435	THR
1	A	453	THR
1	A	457	VAL
1	A	459	MET
1	A	469	LYS
1	A	498	ARG
1	A	511	ARG
1	A	514	LEU
1	A	515	VAL
1	A	518	LEU
1	A	530	GLU
1	A	541	LEU
1	A	578	ASP
1	A	583	LEU
1	A	601	THR
1	A	603	ARG

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Mol	Chain	Res	Type
1	A	608	ILE
1	A	629	LEU
1	A	656	LEU
1	A	662	SER
1	A	668	LEU
1	A	680	GLU
1	A	690	ARG
1	A	701	LYS
1	A	715	LEU
1	A	750	THR
1	A	753	VAL
1	A	756	LEU
1	A	761	VAL
1	A	765	VAL
1	A	779	LYS
1	A	796	MET
1	A	801	MET
1	A	809	VAL
1	A	831	ARG
1	A	836	ASP
1	A	852	GLN
1	A	856	SER
1	A	858	GLU
1	A	877	LEU
1	A	915	ASP
1	A	933	GLN
1	A	949	ARG
1	A	953	THR
1	A	961	LYS
1	A	991	LEU
1	A	993	ARG
1	A	1008	ASP
1	A	1015	LEU
1	A	1028	GLU
1	A	1030	GLN
1	A	1043	THR
1	A	1052	ASN
1	A	1085	THR
1	A	1095	GLN
1	A	1101	LEU
1	A	1110	THR
1	A	1130	ILE

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Mol	Chain	Res	Type
1	A	1145	THR
1	A	1150	VAL
1	A	1164	LYS
1	A	1170	VAL
1	A	1191	ARG
1	A	1193	LEU
1	A	1210	GLN
1	A	1214	THR
1	A	1215	GLN
1	A	1217	LEU
1	A	1228	THR
1	A	1232	ARG
1	A	1235	LEU
1	A	1246	VAL
1	A	1248	ASP
1	A	1272	ARG
1	A	1279	THR
1	A	1280	VAL
1	A	1349	GLN
1	A	1369	THR
1	A	1373	LEU
1	A	1381	GLU
1	A	1386	ARG
1	A	1416	VAL
1	A	1425	THR
1	A	1464	LEU
1	A	1472	THR
1	A	1488	LEU
1	A	1506	ASN
1	B	17	LEU
1	B	23	LYS
1	B	52	ARG
1	B	57	GLN
1	B	62	ARG
1	B	64	LEU
1	B	71	ARG
1	B	96	VAL
1	B	99	LEU
1	B	122	LYS
1	B	139	CYS
1	B	147	ARG
1	B	148	LEU

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Mol	Chain	Res	Type
1	B	161	GLU
1	B	168	PHE
1	B	182	ILE
1	B	191	LEU
1	B	207	PHE
1	B	211	THR
1	B	212	MET
1	B	224	LEU
1	B	245	LYS
1	B	249	VAL
1	B	254	LYS
1	B	264	VAL
1	B	266	GLN
1	B	272	TYR
1	B	274	LEU
1	B	278	LEU
1	B	287	SER
1	B	339	ILE
1	B	340	VAL
1	B	355	CYS
1	B	370	VAL
1	B	376	VAL
1	B	379	VAL
1	B	404	GLN
1	B	459	MET
1	B	469	LYS
1	B	511	ARG
1	B	514	LEU
1	B	515	VAL
1	B	518	LEU
1	B	541	LEU
1	B	543	SER
1	B	560	GLN
1	B	563	GLU
1	B	578	ASP
1	B	583	LEU
1	B	598	LEU
1	B	601	THR
1	B	603	ARG
1	B	608	ILE
1	B	625	VAL
1	B	629	LEU

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Mol	Chain	Res	Type
1	B	636	LEU
1	B	656	LEU
1	B	664	ILE
1	B	668	LEU
1	B	680	GLU
1	B	690	ARG
1	B	701	LYS
1	B	750	THR
1	B	753	VAL
1	B	761	VAL
1	B	765	VAL
1	B	779	LYS
1	B	796	MET
1	B	800	GLU
1	B	801	MET
1	B	852	GLN
1	B	856	SER
1	B	858	GLU
1	B	872	THR
1	B	876	SER
1	B	933	GLN
1	B	949	ARG
1	B	953	THR
1	B	961	LYS
1	B	991	LEU
1	B	1015	LEU
1	B	1028	GLU
1	B	1052	ASN
1	B	1085	THR
1	B	1095	GLN
1	B	1101	LEU
1	B	1110	THR
1	B	1130	ILE
1	B	1145	THR
1	B	1150	VAL
1	B	1164	LYS
1	B	1183	SER
1	B	1191	ARG
1	B	1193	LEU
1	B	1210	GLN
1	B	1214	THR
1	B	1215	GLN

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Mol	Chain	Res	Type
1	B	1217	LEU
1	B	1228	THR
1	B	1232	ARG
1	B	1235	LEU
1	B	1246	VAL
1	B	1248	ASP
1	B	1280	VAL
1	B	1349	GLN
1	B	1369	THR
1	B	1381	GLU
1	B	1386	ARG
1	B	1388	SER
1	B	1416	VAL
1	B	1425	THR
1	B	1449	LEU
1	B	1464	LEU
1	B	1472	THR
1	B	1488	LEU
1	B	1500	LYS
1	B	1506	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	57	GLN
1	A	120	GLN
1	A	227	ASN
1	A	236	ASN
1	A	266	GLN
1	A	303	GLN
1	A	323	GLN
1	A	446	GLN
1	A	486	HIS
1	A	560	GLN
1	A	627	HIS
1	A	628	HIS
1	A	651	HIS
1	A	652	HIS
1	A	730	GLN
1	A	806	HIS
1	A	885	HIS

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Mol	Chain	Res	Type
1	A	978	GLN
1	A	1023	HIS
1	A	1052	ASN
1	A	1095	GLN
1	A	1147	ASN
1	A	1210	GLN
1	A	1215	GLN
1	A	1294	ASN
1	A	1326	GLN
1	A	1372	ASN
1	A	1376	ASN
1	A	1419	ASN
1	A	1450	GLN
1	A	1493	GLN
1	A	1506	ASN
1	B	15	HIS
1	B	57	GLN
1	B	120	GLN
1	B	199	ASN
1	B	236	ASN
1	B	266	GLN
1	B	303	GLN
1	B	323	GLN
1	B	446	GLN
1	B	486	HIS
1	B	560	GLN
1	B	628	HIS
1	B	651	HIS
1	B	652	HIS
1	B	730	GLN
1	B	852	GLN
1	B	885	HIS
1	B	933	GLN
1	B	978	GLN
1	B	1023	HIS
1	B	1052	ASN
1	B	1095	GLN
1	B	1147	ASN
1	B	1215	GLN
1	B	1294	ASN
1	B	1372	ASN
1	B	1419	ASN

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Mol	Chain	Res	Type
1	B	1450	GLN
1	B	1493	GLN
1	B	1506	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FMN	A	2508	-	31,33,33	1.45	5 (16%)	38,50,50	2.22	8 (21%)
3	F3S	A	2509	1	0,9,9	0.00	-	0,15,15	0.00	-
4	AKG	A	2510	-	3,9,9	5.03	1 (33%)	4,11,11	3.16	1 (25%)
5	ONL	A	2511	1	4,9,9	0.97	0	5,11,11	3.35	4 (80%)
2	FMN	B	2508	-	31,33,33	1.76	5 (16%)	38,50,50	2.21	10 (26%)
3	F3S	B	2509	1	0,9,9	0.00	-	0,15,15	0.00	-
4	AKG	B	2510	-	3,9,9	4.30	1 (33%)	4,11,11	4.59	3 (75%)
5	ONL	B	2511	-	4,9,9	0.55	0	5,11,11	2.73	1 (20%)

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	A	2508	-	-	0/16/18/18	0/3/3/3
3	F3S	A	2509	1	-	0/0/24/24	0/0/3/3
4	AKG	A	2510	-	-	0/3/9/9	0/0/0/0
5	ONL	A	2511	1	-	0/5/9/9	0/0/0/0
2	FMN	B	2508	-	-	0/16/18/18	0/3/3/3
3	F3S	B	2509	1	-	0/0/24/24	0/0/3/3
4	AKG	B	2510	-	-	0/3/9/9	0/0/0/0
5	ONL	B	2511	-	-	0/5/9/9	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2508	FMN	C4A-N5	2.19	1.36	1.33
2	B	2508	FMN	C10-N1	2.33	1.36	1.33
2	A	2508	FMN	C4-N3	2.82	1.38	1.33
2	A	2508	FMN	C1'-N10	2.90	1.51	1.48
2	B	2508	FMN	C4-N3	3.05	1.38	1.33
2	A	2508	FMN	C5A-N5	3.12	1.40	1.35
2	A	2508	FMN	C10-N1	3.57	1.38	1.33
2	B	2508	FMN	C5A-N5	3.58	1.40	1.35
2	B	2508	FMN	C4A-N5	4.58	1.39	1.33
2	B	2508	FMN	C1'-N10	5.21	1.53	1.48
4	B	2510	AKG	O5-C2	7.43	1.34	1.22
4	A	2510	AKG	O5-C2	8.63	1.36	1.22

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2510	AKG	C4-C3-C2	-8.55	93.30	113.04
4	A	2510	AKG	C4-C3-C2	-6.16	98.81	113.04
2	A	2508	FMN	C4A-C4-N3	-6.07	114.83	123.48
2	A	2508	FMN	C1'-N10-C10	-5.86	112.49	118.50
5	B	2511	ONL	CB-CG-CD	-5.65	108.38	114.47
2	B	2508	FMN	O4'-C4'-C5'	-3.99	101.10	110.00
5	A	2511	ONL	CB-CG-CD	-3.95	110.21	114.47
2	B	2508	FMN	C4A-C4-N3	-3.76	118.13	123.48
2	B	2508	FMN	C1'-N10-C9A	-3.28	115.34	118.35
2	B	2508	FMN	O2'-C2'-C1'	-3.05	102.74	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2508	FMN	C10-C4A-N5	-2.95	117.20	120.59
5	A	2511	ONL	CE-CD-CG	-2.60	110.31	116.87
5	A	2511	ONL	OD-CD-CE	-2.15	115.87	121.37
2	B	2508	FMN	C1'-C2'-C3'	2.02	115.58	109.82
4	B	2510	AKG	O5-C2-C3	2.19	124.23	120.32
2	A	2508	FMN	C4-C4A-C10	2.24	121.77	119.96
2	A	2508	FMN	C6-C5A-C9A	2.28	121.95	119.00
2	B	2508	FMN	C4-C4A-N5	2.30	121.20	118.68
4	B	2510	AKG	C3-C2-C1	2.54	127.36	121.60
2	A	2508	FMN	C4A-N5-C5A	2.55	119.45	116.76
2	B	2508	FMN	O3P-P-O5'	2.79	114.15	106.73
2	A	2508	FMN	C1'-N10-C9A	3.04	121.13	118.35
2	B	2508	FMN	C5A-C9A-N10	3.16	120.00	117.66
5	A	2511	ONL	OD-CD-CG	5.40	133.78	121.54
2	B	2508	FMN	C1'-N10-C10	5.88	124.53	118.50
2	B	2508	FMN	C4-N3-C2	6.99	121.27	115.16
2	A	2508	FMN	C4-N3-C2	7.42	121.65	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2508	FMN	1	0
4	A	2510	AKG	1	0
2	B	2508	FMN	3	0
5	B	2511	ONL	7	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	1485/1520 (97%)	-0.21	17 (1%) 80 81	8, 16, 23, 29	0
1	B	1485/1520 (97%)	0.08	57 (3%) 41 38	7, 17, 23, 31	0
All	All	2970/3040 (97%)	-0.06	74 (2%) 58 54	7, 16, 23, 31	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1507	ASN	5.1
1	B	812	TYR	5.0
1	B	1453	THR	3.9
1	B	833	TYR	3.9
1	B	261	THR	3.6
1	B	827	TYR	3.5
1	B	211	THR	3.5
1	A	211	THR	3.2
1	B	1484	TRP	3.2
1	A	539	ILE	3.2
1	B	1452	ILE	3.2
1	B	694	ILE	3.2
1	B	251	GLY	3.1
1	A	440	ALA	3.1
1	B	690	ARG	3.0
1	B	687	GLU	2.9
1	A	1507	ASN	2.9
1	B	678	LEU	2.9
1	B	69	GLY	2.9
1	A	261	THR	2.9
1	B	396	GLU	2.8
1	B	675	GLN	2.8
1	B	437	PHE	2.8
1	B	835	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	638	ALA	2.8
1	B	439	ASP	2.8
1	B	526	GLY	2.7
1	A	557	GLY	2.7
1	B	1058	ILE	2.7
1	B	1265	THR	2.7
1	B	1036	VAL	2.6
1	B	1230	GLN	2.6
1	B	1215	GLN	2.6
1	A	499	PHE	2.6
1	B	1347	HIS	2.6
1	B	1454	ALA	2.5
1	B	137	GLU	2.5
1	B	699	ALA	2.5
1	A	812	TYR	2.4
1	A	769	HIS	2.4
1	A	534	GLU	2.4
1	B	605	ASN	2.4
1	B	1175	TYR	2.4
1	A	806	HIS	2.4
1	B	830	TYR	2.3
1	B	1463	SER	2.3
1	B	828	GLU	2.3
1	A	833	TYR	2.3
1	A	829	LEU	2.3
1	B	1039	ILE	2.3
1	B	832	GLN	2.3
1	B	912	LEU	2.3
1	B	1216	ASN	2.2
1	B	1037	ALA	2.2
1	B	1467	ALA	2.2
1	B	831	ARG	2.2
1	A	434	LYS	2.2
1	B	500	ALA	2.2
1	A	245	LYS	2.2
1	B	1035	LEU	2.2
1	B	858	GLU	2.2
1	B	808	ALA	2.1
1	A	1041	ILE	2.1
1	B	212	MET	2.1
1	B	790	PRO	2.1
1	A	973	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	688	ASN	2.1
1	B	1041	ILE	2.1
1	B	12	LYS	2.1
1	B	1486	ASP	2.1
1	B	1231	ASN	2.1
1	B	829	LEU	2.1
1	B	1272	ARG	2.1
1	B	809	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ONL	A	2511	10/10	0.91	0.16	-0.12	24,32,34,36	0
4	AKG	B	2510	10/10	0.93	0.17	-0.13	36,37,40,41	0
5	ONL	B	2511	10/10	0.92	0.14	-0.70	32,36,37,38	0
2	FMN	A	2508	31/31	0.97	0.14	-0.88	18,23,28,31	0
2	FMN	B	2508	31/31	0.96	0.13	-1.02	22,29,32,35	0
4	AKG	A	2510	10/10	0.96	0.11	-1.05	24,27,35,37	0
3	F3S	A	2509	7/7	0.99	0.09	-1.60	19,22,24,24	0
3	F3S	B	2509	7/7	0.97	0.04	-3.28	27,29,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.