



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:54 PM GMT

PDB ID : 4Q86  
Title : YcaO with AMP Bound  
Authors : Chekan, J.R.; Nair, S.K.  
Deposited on : 2014-04-25  
Resolution : 2.25 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:

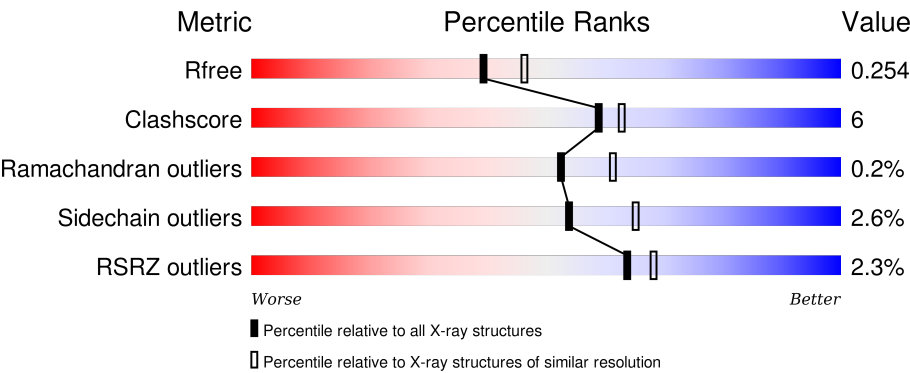
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	586	<div><div></div><div>91%7% ..</div></div>
1	B	586	<div><div></div><div>90%8% ...</div></div>
1	C	586	<div><div></div><div>88%9% ..</div></div>
1	D	586	<div><div>%</div><div>91%7% ..</div></div>
1	E	586	<div><div></div><div>89%9% ..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	586	
1	G	586	
1	H	586	

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
3	MG	A	602	-	-	-	X
3	MG	B	602	-	-	-	X
3	MG	D	602	-	-	-	X

## 2 Entry composition

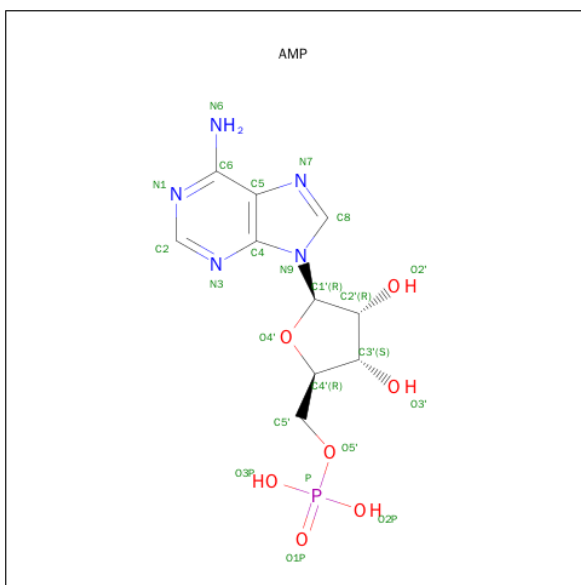
There are 4 unique types of molecules in this entry. The entry contains 38743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribosomal protein S12 methylthiotransferase accessory factor YcaO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4599	2935	748	899	17			
1	B	583	Total	C	N	O	S	0	0	0
			4613	2946	750	900	17			
1	C	570	Total	C	N	O	S	0	0	0
			4508	2875	734	882	17			
1	D	582	Total	C	N	O	S	0	0	0
			4599	2935	748	899	17			
1	E	578	Total	C	N	O	S	0	0	0
			4567	2914	743	893	17			
1	F	574	Total	C	N	O	S	0	0	0
			4534	2890	739	888	17			
1	G	575	Total	C	N	O	S	0	0	0
			4541	2895	740	889	17			
1	H	583	Total	C	N	O	S	0	0	0
			4613	2946	750	900	17			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total	Mg	0	0
			3	3		
3	D	3	Total	Mg	0	0
			3	3		
3	E	3	Total	Mg	0	0
			3	3		
3	H	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total 3	Mg 3	0	0
3	A	3	Total 3	Mg 3	0	0

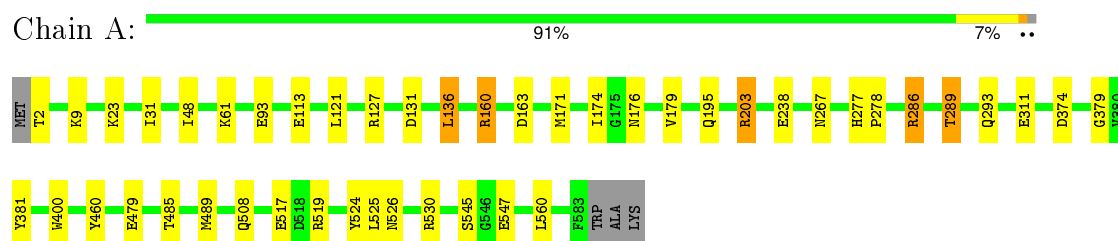
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	334	Total 334	O 334	0	0
4	B	336	Total 336	O 336	0	0
4	C	231	Total 231	O 231	0	0
4	D	255	Total 255	O 255	0	0
4	E	215	Total 215	O 215	0	0
4	F	111	Total 111	O 111	0	0
4	G	197	Total 197	O 197	0	0
4	H	308	Total 308	O 308	0	0

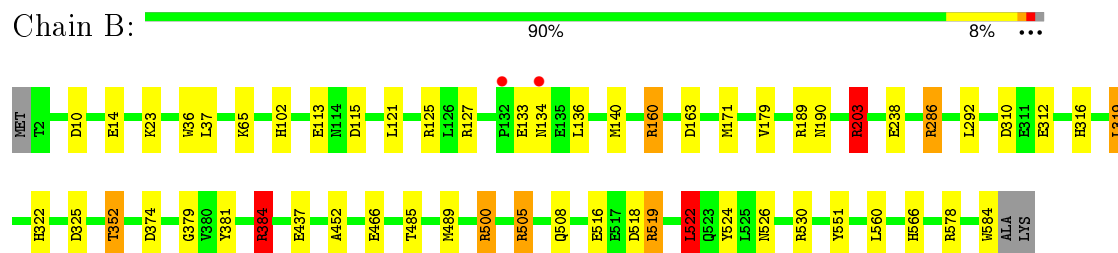
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

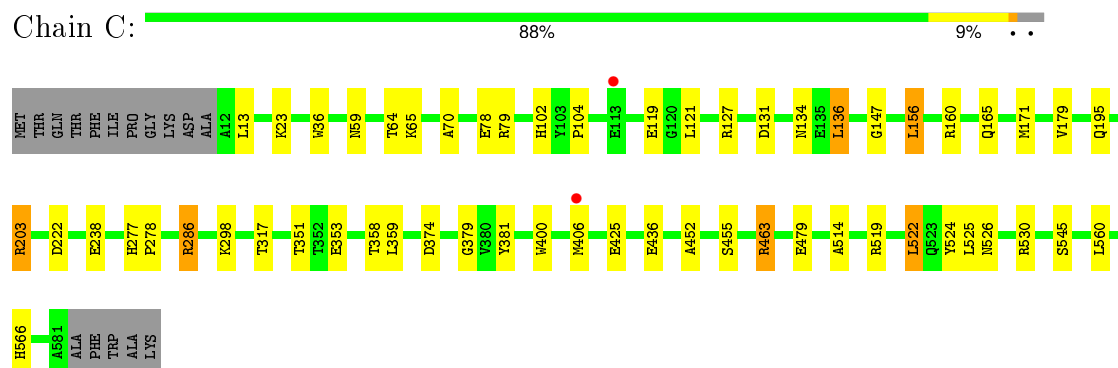
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

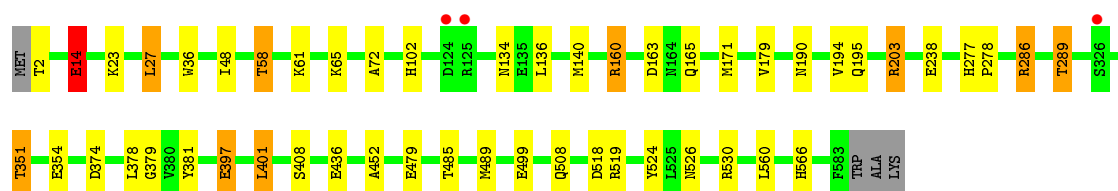


- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO



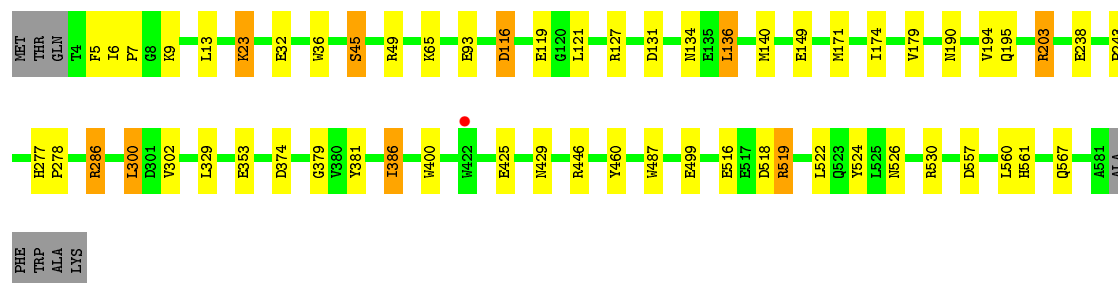
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO





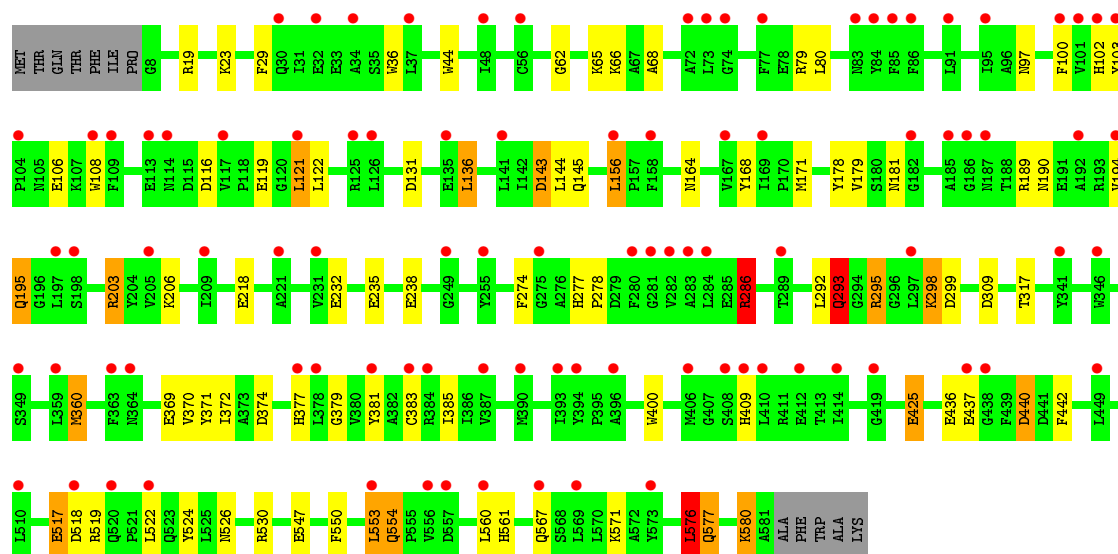
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain E: 89% 9% ..



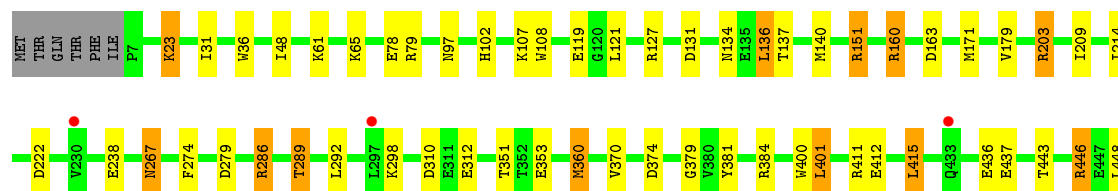
- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain F: 16% 83% 12% ...



- Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

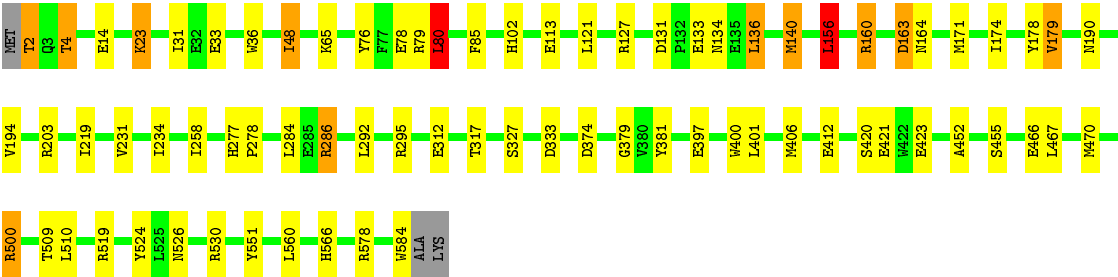
Chain G: 86% 10% ..





● Molecule 1: Ribosomal protein S12 methylthiotransferase accessory factor YcaO

Chain H: 87% 11% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.25Å 112.95Å 132.89Å 89.94° 73.51° 77.23°	Depositor
Resolution (Å)	127.14 – 2.25 127.14 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.1 (127.14-2.25) 92.0 (127.14-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.218 , 0.250 0.221 , 0.254	Depositor DCC
$R_{free}$ test set	13386 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 264918 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	38743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AMP, MG

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	0.66	0/4713	0.74	8/6411 (0.1%)
1	B	0.70	0/4729	0.81	19/6434 (0.3%)
1	C	0.56	0/4619	0.74	11/6283 (0.2%)
1	D	0.63	1/4713 (0.0%)	0.76	12/6411 (0.2%)
1	E	0.58	0/4680	0.76	12/6366 (0.2%)
1	F	0.53	1/4645 (0.0%)	0.81	21/6317 (0.3%)
1	G	0.58	0/4653	0.81	17/6328 (0.3%)
1	H	0.70	2/4729 (0.0%)	0.89	16/6434 (0.2%)
All	All	0.62	4/37481 (0.0%)	0.79	116/50984 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	397	GLU	CB-CG	6.21	1.64	1.52
1	F	143	ASP	CB-CG	-5.68	1.39	1.51
1	H	412	GLU	CD-OE2	5.52	1.31	1.25
1	D	397	GLU	CB-CG	5.34	1.62	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	203	ARG	NE-CZ-NH2	27.57	134.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	203	ARG	NE-CZ-NH1	-21.36	109.62	120.30
1	G	151	ARG	NE-CZ-NH1	15.26	127.93	120.30
1	G	151	ARG	NE-CZ-NH2	-14.21	113.19	120.30
1	B	203	ARG	NE-CZ-NH2	-13.07	113.77	120.30
1	A	203	ARG	NE-CZ-NH2	-12.33	114.14	120.30
1	E	203	ARG	NE-CZ-NH2	-12.15	114.22	120.30
1	D	203	ARG	NE-CZ-NH2	-12.00	114.30	120.30
1	A	203	ARG	NE-CZ-NH1	11.77	126.19	120.30
1	G	203	ARG	NE-CZ-NH2	-11.73	114.43	120.30
1	B	203	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	E	203	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	C	203	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	D	203	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	C	203	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	G	203	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	F	203	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	G	384	ARG	CG-CD-NE	10.67	134.21	111.80
1	F	203	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	F	440	ASP	CB-CG-OD1	-9.90	109.39	118.30
1	F	576	LEU	CA-CB-CG	9.82	137.89	115.30
1	F	440	ASP	CB-CG-OD2	9.70	127.03	118.30
1	D	27	LEU	CB-CG-CD2	-9.13	95.48	111.00
1	H	80	LEU	CA-CB-CG	8.70	135.31	115.30
1	C	463	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	D	27	LEU	CB-CG-CD1	8.09	124.75	111.00
1	C	463	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	F	143	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	E	519	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	E	519	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	267	ASN	CB-CA-C	-7.33	95.73	110.40
1	E	386	ILE	CG1-CB-CG2	-7.27	95.42	111.40
1	B	519	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	E	386	ILE	CB-CG1-CD1	7.11	133.79	113.90
1	B	519	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	310	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	D	27	LEU	CA-CB-CG	6.97	131.34	115.30
1	F	554	GLN	CA-CB-CG	6.92	128.62	113.40
1	H	578	ARG	CG-CD-NE	6.85	126.18	111.80
1	B	160	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	G	222	ASP	CB-CG-OD2	6.75	124.38	118.30
1	B	160	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	G	446	ARG	CA-CB-CG	6.63	127.99	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	522	LEU	CA-CB-CG	6.63	130.54	115.30
1	H	160	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	B	319	LEU	CB-CG-CD1	6.57	122.16	111.00
1	H	295	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	E	140	MET	CA-CB-CG	6.54	124.42	113.30
1	G	267	ASN	CB-CA-C	-6.54	97.33	110.40
1	A	267	ASN	N-CA-CB	-6.52	98.86	110.60
1	D	140	MET	CA-CB-CG	6.52	124.39	113.30
1	E	386	ILE	CA-CB-CG1	-6.42	98.80	111.00
1	C	463	ARG	CD-NE-CZ	6.36	132.51	123.60
1	E	45	SER	N-CA-CB	-6.36	100.96	110.50
1	G	160	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	H	140	MET	CA-CB-CG	6.26	123.95	113.30
1	G	267	ASN	N-CA-CB	-6.26	99.33	110.60
1	B	578	ARG	CG-CD-NE	6.24	124.91	111.80
1	A	160	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	F	119	GLU	N-CA-C	-6.21	94.24	111.00
1	F	571	LYS	CD-CE-NZ	-6.18	97.49	111.70
1	G	160	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	H	163	ASP	C-N-CA	-6.07	106.51	121.70
1	G	222	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	B	140	MET	CA-CB-CG	6.02	123.54	113.30
1	F	122	LEU	N-CA-CB	-5.99	98.42	110.40
1	B	578	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	F	295	ARG	CG-CD-NE	-5.92	99.36	111.80
1	H	160	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	H	578	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	160	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	384	ARG	CG-CD-NE	5.73	123.83	111.80
1	B	286	ARG	CB-CA-C	-5.68	99.05	110.40
1	B	522	LEU	CA-CB-CG	5.61	128.20	115.30
1	D	160	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	G	286	ARG	CB-CA-C	-5.60	99.20	110.40
1	G	384	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	286	ARG	CB-CA-C	-5.57	99.25	110.40
1	A	286	ARG	CB-CA-C	-5.51	99.38	110.40
1	B	203	ARG	CD-NE-CZ	5.49	131.29	123.60
1	H	286	ARG	CB-CA-C	-5.49	99.42	110.40
1	H	156	LEU	CA-CB-CG	5.48	127.90	115.30
1	F	156	LEU	CA-CB-CG	5.48	127.90	115.30
1	C	156	LEU	CA-CB-CG	5.47	127.89	115.30
1	H	500	ARG	CG-CD-NE	-5.47	100.31	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	THR	N-CA-CB	-5.45	99.94	110.30
1	D	286	ARG	CB-CA-C	-5.45	99.50	110.40
1	F	235	GLU	CB-CA-C	-5.44	99.51	110.40
1	G	289	THR	N-CA-CB	-5.44	99.97	110.30
1	E	300	LEU	CB-CG-CD1	5.39	120.16	111.00
1	F	293	GLN	CA-C-N	5.38	126.97	116.20
1	H	140	MET	CB-CA-C	-5.37	99.66	110.40
1	F	232	GLU	CG-CD-OE1	5.36	129.02	118.30
1	B	500	ARG	CG-CD-NE	-5.35	100.56	111.80
1	C	406	MET	N-CA-C	-5.35	96.55	111.00
1	F	116	ASP	CB-CG-OD1	5.35	123.11	118.30
1	F	286	ARG	CB-CA-C	5.33	121.06	110.40
1	C	104	PRO	C-N-CA	5.32	134.99	121.70
1	F	121	LEU	N-CA-C	5.31	125.35	111.00
1	A	289	THR	N-CA-CB	-5.31	100.20	110.30
1	B	519	ARG	CG-CD-NE	5.28	122.89	111.80
1	C	286	ARG	CB-CA-C	-5.27	99.86	110.40
1	B	519	ARG	CD-NE-CZ	5.21	130.90	123.60
1	D	160	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	G	360	MET	CG-SD-CE	5.17	108.47	100.20
1	H	397	GLU	OE1-CD-OE2	-5.15	117.11	123.30
1	B	505	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	F	298	LYS	CB-CA-C	-5.13	100.13	110.40
1	F	553	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	203	ARG	CG-CD-NE	-5.13	101.03	111.80
1	H	500	ARG	CD-NE-CZ	5.11	130.75	123.60
1	D	136	LEU	CB-CG-CD1	5.10	119.68	111.00
1	E	203	ARG	CG-CD-NE	-5.08	101.13	111.80
1	D	14	GLU	N-CA-CB	5.07	119.73	110.60
1	F	360	MET	CG-SD-CE	5.03	108.25	100.20
1	G	384	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	293	GLN	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	4599	0	4372	33	0
1	B	4613	0	4382	50	0
1	C	4508	0	4284	47	0
1	D	4599	0	4372	44	0
1	E	4567	0	4343	48	0
1	F	4534	0	4309	65	0
1	G	4541	0	4317	62	0
1	H	4613	0	4382	78	0
2	A	23	0	12	1	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	2	0
2	E	23	0	12	2	0
2	G	23	0	12	0	0
2	H	23	0	12	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
4	A	334	0	0	7	0
4	B	336	0	0	18	0
4	C	231	0	0	16	0
4	D	255	0	0	15	0
4	E	215	0	0	19	0
4	F	111	0	0	22	0
4	G	197	0	0	16	0
4	H	308	0	0	25	0
All	All	38743	0	34845	416	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 6.

All (416) 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:F:68:ALA:HB2	4:F:633:HOH:O	1.36	1.26
1:E:171:MET:SD	4:E:738:HOH:O	2.04	1.15
1:B:171:MET:SD	4:B:1021:HOH:O	2.02	1.15
1:H:136:LEU:HD12	1:H:140:MET:HE1	1.09	1.09
1:G:78:GLU:OE2	1:G:79:ARG:NH1	1.86	1.08
1:F:550:PHE:HB3	1:F:553:LEU:HD12	1.33	1.06
1:C:78:GLU:OE2	1:C:79:ARG:NH1	1.88	1.06
1:F:576:LEU:O	1:F:580:LYS:HG2	1.54	1.05
1:H:78:GLU:OE2	1:H:79:ARG:NH1	1.88	1.05
1:C:358:THR:HG22	4:C:878:HOH:O	1.61	0.98
1:H:231:VAL:HA	4:H:822:HOH:O	1.63	0.98
1:F:106:GLU:HG3	4:F:624:HOH:O	1.65	0.97
1:F:121:LEU:O	1:F:168:TYR:O	1.81	0.97
1:H:171:MET:HE1	4:H:715:HOH:O	1.63	0.96
1:H:171:MET:SD	4:H:972:HOH:O	2.22	0.95
1:F:103:TYR:HD1	1:F:580:LYS:HZ1	1.15	0.94
1:E:561:HIS:HA	1:E:567:GLN:OE1	1.67	0.93
1:E:171:MET:HE1	4:E:857:HOH:O	1.69	0.92
1:H:234:ILE:HB	4:H:822:HOH:O	1.71	0.90
1:H:467:LEU:HA	1:H:470:MET:HE2	1.54	0.90
1:B:312:GLU:HG2	4:B:948:HOH:O	1.70	0.90
1:H:423:GLU:HB2	4:H:813:HOH:O	1.71	0.88
1:H:136:LEU:HD12	1:H:140:MET:CE	2.00	0.88
1:E:487:TRP:HB2	4:E:753:HOH:O	1.72	0.88
1:G:581:ALA:HA	4:G:857:HOH:O	1.72	0.88
1:H:467:LEU:HA	1:H:470:MET:CE	2.04	0.87
1:B:500:ARG:NH1	4:B:705:HOH:O	2.05	0.87
1:H:136:LEU:CD1	1:H:140:MET:HE1	2.00	0.86
1:B:10:ASP:OD2	1:B:352:THR:HG21	1.76	0.85
1:C:560:LEU:HD13	1:C:566:HIS:CE1	2.12	0.85
1:C:70:ALA:HB2	4:C:893:HOH:O	1.76	0.84
1:B:171:MET:HE1	4:B:784:HOH:O	1.77	0.84
1:H:4:THR:CG2	1:H:14:GLU:OE2	2.26	0.84
1:E:557:ASP:CB	1:H:113:GLU:OE2	2.27	0.83
1:D:408:SER:HB2	4:D:937:HOH:O	1.79	0.82
1:D:171:MET:HE1	4:D:735:HOH:O	1.79	0.82
1:D:58:THR:HG21	1:D:72:ALA:O	1.79	0.82
1:G:560:LEU:HD13	1:G:566:HIS:CE1	2.15	0.82
1:H:560:LEU:HD13	1:H:566:HIS:CE1	2.14	0.82
2:D:601:AMP:N1	4:D:737:HOH:O	2.14	0.81
1:G:560:LEU:HD13	1:G:566:HIS:NE2	1.96	0.81
1:B:516:GLU:OE1	1:B:519:ARG:NH1	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ARG:NH1	4:C:885:HOH:O	2.14	0.79
1:H:258:ILE:CG2	4:H:950:HOH:O	2.30	0.79
1:H:258:ILE:HG23	4:H:950:HOH:O	1.81	0.79
1:E:171:MET:CE	4:E:857:HOH:O	2.27	0.78
1:H:171:MET:SD	4:H:913:HOH:O	2.42	0.77
1:E:516:GLU:OE1	1:E:519:ARG:NH1	2.18	0.77
1:D:72:ALA:HB1	4:D:939:HOH:O	1.83	0.77
1:F:517:GLU:N	1:F:517:GLU:OE1	2.18	0.77
1:B:489:MET:HE1	1:B:508:GLN:HB2	1.67	0.76
1:H:4:THR:HG23	1:H:14:GLU:OE2	1.86	0.76
1:F:554:GLN:HG2	4:F:636:HOH:O	1.86	0.76
1:D:163:ASP:OD2	4:D:909:HOH:O	2.02	0.76
1:E:557:ASP:HB3	1:H:113:GLU:OE2	1.86	0.76
1:F:383:CYS:HB2	4:F:629:HOH:O	1.85	0.76
1:A:311:GLU:OE1	4:A:790:HOH:O	2.04	0.76
2:D:601:AMP:C2	4:D:737:HOH:O	2.38	0.75
1:F:385:ILE:HG13	4:F:629:HOH:O	1.84	0.75
1:A:61:LYS:HD2	1:A:289:THR:HG22	1.69	0.75
1:D:61:LYS:HD2	1:D:289:THR:HG22	1.69	0.74
1:G:61:LYS:HD2	1:G:289:THR:HG22	1.69	0.74
1:C:317:THR:HG23	4:C:782:HOH:O	1.87	0.74
1:C:13:LEU:HD22	4:C:893:HOH:O	1.87	0.73
1:C:171:MET:HE1	4:C:806:HOH:O	1.87	0.73
1:F:108:TRP:CD1	4:F:624:HOH:O	2.40	0.73
1:B:102:HIS:ND1	1:B:171:MET:HE2	2.04	0.73
1:A:171:MET:HE3	1:A:174:ILE:HB	1.71	0.73
1:H:500:ARG:NH1	4:H:781:HOH:O	2.21	0.73
1:G:108:TRP:CE2	1:G:151:ARG:HD2	2.24	0.72
1:F:44:TRP:HB2	4:F:633:HOH:O	1.90	0.72
1:G:489:MET:HE1	1:G:508:GLN:HB2	1.71	0.72
1:E:32:GLU:OE2	1:E:49:ARG:CZ	2.37	0.72
1:F:103:TYR:CD1	1:F:580:LYS:NZ	2.55	0.71
1:C:70:ALA:CB	4:C:893:HOH:O	2.33	0.71
1:A:489:MET:HE1	1:A:508:GLN:HB2	1.72	0.71
1:E:243:PRO:O	4:E:897:HOH:O	2.08	0.70
1:H:219:ILE:CD1	4:H:950:HOH:O	2.38	0.70
1:D:48:ILE:HG12	4:D:939:HOH:O	1.91	0.70
1:B:322:HIS:O	4:B:1036:HOH:O	2.09	0.70
1:G:522:LEU:H	1:G:522:LEU:HD23	1.57	0.70
1:D:401:LEU:HD23	4:D:945:HOH:O	1.90	0.70
1:C:222:ASP:HB3	4:C:856:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:HIS:ND1	1:H:171:MET:HE2	2.07	0.69
1:G:31:ILE:CG2	1:G:48:ILE:HG22	2.21	0.69
1:B:522:LEU:HG	4:B:856:HOH:O	1.92	0.69
1:A:31:ILE:CG2	1:A:48:ILE:HG22	2.23	0.69
1:A:547:GLU:O	4:A:808:HOH:O	2.10	0.69
1:G:448:LEU:HD22	4:G:756:HOH:O	1.93	0.68
1:C:238:GLU:OE2	1:D:530:ARG:NH2	2.25	0.68
1:A:176:ASN:ND2	4:A:982:HOH:O	2.26	0.68
1:A:93:GLU:HG3	4:A:915:HOH:O	1.92	0.68
1:D:489:MET:HE1	1:D:508:GLN:HB2	1.76	0.68
1:B:102:HIS:ND1	1:B:171:MET:CE	2.57	0.67
1:H:102:HIS:ND1	1:H:171:MET:CE	2.57	0.67
1:H:219:ILE:HD11	4:H:950:HOH:O	1.92	0.67
1:F:100:PHE:CE1	1:F:577:GLN:HG3	2.30	0.67
1:E:557:ASP:HB2	1:H:113:GLU:OE2	1.94	0.67
1:F:103:TYR:HD1	1:F:580:LYS:NZ	1.89	0.66
1:G:310:ASP:OD2	4:G:890:HOH:O	2.12	0.66
1:F:195:GLN:HG3	4:F:652:HOH:O	1.95	0.66
1:G:31:ILE:CG2	1:G:48:ILE:CG2	2.74	0.65
1:D:102:HIS:CD2	1:D:171:MET:CE	2.79	0.65
1:E:6:ILE:HG23	1:E:7:PRO:HD2	1.79	0.65
1:G:171:MET:HE1	4:G:793:HOH:O	1.95	0.65
1:G:279:ASP:HA	4:G:832:HOH:O	1.97	0.65
1:C:560:LEU:HD13	1:C:566:HIS:NE2	2.11	0.65
1:E:174:ILE:CD1	1:E:386:ILE:HD13	2.27	0.64
1:H:466:GLU:OE2	1:H:500:ARG:NH1	2.29	0.64
1:B:384:ARG:NH1	4:B:1020:HOH:O	2.23	0.64
1:F:181:ASN:O	4:F:711:HOH:O	2.15	0.64
1:B:466:GLU:OE2	1:B:500:ARG:NH1	2.30	0.64
1:E:6:ILE:CG2	4:E:821:HOH:O	2.46	0.64
1:E:93:GLU:HG3	4:E:748:HOH:O	1.96	0.64
1:G:31:ILE:HG22	1:G:48:ILE:CG2	2.27	0.64
1:F:377:HIS:CD2	1:F:580:LYS:HD2	2.33	0.64
1:A:31:ILE:HG22	1:A:48:ILE:CG2	2.28	0.64
1:B:452:ALA:H	1:B:566:HIS:HD2	1.46	0.64
1:C:560:LEU:CD1	1:C:566:HIS:CE1	2.81	0.63
1:A:31:ILE:CG2	1:A:48:ILE:CG2	2.76	0.63
1:E:121:LEU:O	1:E:127:ARG:NH2	2.32	0.63
1:C:530:ARG:NH2	1:D:238:GLU:OE2	2.31	0.63
1:E:353:GLU:HB2	4:E:828:HOH:O	1.99	0.63
1:E:519:ARG:HD3	1:E:524:TYR:OH	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:452:ALA:H	1:H:566:HIS:HD2	1.48	0.61
1:C:121:LEU:O	1:C:127:ARG:NH2	2.33	0.61
1:B:519:ARG:HD3	1:B:524:TYR:OH	2.00	0.61
1:G:448:LEU:HB2	4:G:756:HOH:O	1.99	0.61
1:C:102:HIS:ND1	1:C:171:MET:CE	2.63	0.61
1:D:397:GLU:HB2	4:D:945:HOH:O	1.99	0.61
1:G:121:LEU:O	1:G:127:ARG:NH2	2.34	0.61
1:H:467:LEU:HD12	1:H:470:MET:HE3	1.82	0.61
1:F:102:HIS:CD2	1:F:171:MET:CE	2.83	0.61
1:E:136:LEU:HD13	1:E:400:TRP:CZ2	2.36	0.61
1:H:560:LEU:CD1	1:H:566:HIS:CE1	2.83	0.60
1:G:108:TRP:CD2	1:G:151:ARG:HD2	2.36	0.60
1:G:136:LEU:HD13	1:G:400:TRP:CZ2	2.36	0.60
1:E:45:SER:HB2	4:E:710:HOH:O	1.99	0.60
1:G:401:LEU:HD12	4:G:759:HOH:O	2.01	0.60
1:F:218:GLU:HG3	4:F:688:HOH:O	2.01	0.60
1:A:121:LEU:O	1:A:127:ARG:NH2	2.34	0.60
1:A:289:THR:HG21	4:A:862:HOH:O	2.02	0.60
1:G:108:TRP:CZ2	1:G:151:ARG:HD2	2.37	0.60
1:H:121:LEU:O	1:H:127:ARG:NH2	2.34	0.60
1:F:189:ARG:HD3	4:F:694:HOH:O	2.02	0.60
1:F:369:GLU:OE1	1:F:371:TYR:OH	2.20	0.59
1:B:485:THR:O	1:B:489:MET:HE2	2.02	0.59
1:H:33:GLU:HG2	1:H:48:ILE:HD11	1.84	0.59
1:D:102:HIS:CD2	1:D:171:MET:HE2	2.36	0.59
1:G:267:ASN:ND2	4:G:703:HOH:O	2.36	0.59
1:C:102:HIS:ND1	1:C:171:MET:HE2	2.18	0.59
1:G:560:LEU:HD13	1:G:566:HIS:CD2	2.36	0.59
1:E:499:GLU:HB2	4:E:850:HOH:O	2.03	0.59
1:H:560:LEU:HD13	1:H:566:HIS:NE2	2.18	0.59
1:D:289:THR:HG21	4:D:828:HOH:O	2.03	0.59
1:H:136:LEU:HD13	1:H:400:TRP:CZ2	2.38	0.58
1:H:234:ILE:HD12	4:H:822:HOH:O	2.02	0.58
1:F:136:LEU:HD13	1:F:400:TRP:CZ2	2.38	0.58
1:B:121:LEU:O	1:B:127:ARG:NH2	2.36	0.58
1:G:107:LYS:HD2	4:G:749:HOH:O	2.02	0.58
1:C:136:LEU:HD13	1:C:400:TRP:CZ2	2.39	0.58
1:D:351:THR:HG22	1:D:354:GLU:H	1.69	0.57
1:F:372:ILE:HG23	4:F:629:HOH:O	2.02	0.57
1:F:369:GLU:HG3	1:F:371:TYR:HE1	1.68	0.57
1:B:190:ASN:CB	1:B:352:THR:HG23	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:ALA:H	1:D:566:HIS:HD2	1.51	0.57
1:D:58:THR:CG2	1:D:72:ALA:O	2.52	0.57
1:D:61:LYS:HB2	1:D:289:THR:HG23	1.87	0.57
1:A:136:LEU:HD13	1:A:400:TRP:CZ2	2.39	0.57
1:G:97:ASN:HA	1:G:151:ARG:HH21	1.69	0.57
1:A:530:ARG:NH2	1:B:238:GLU:OE1	2.38	0.57
1:F:295:ARG:NH2	1:F:299:ASP:O	2.37	0.56
1:D:48:ILE:HG12	1:D:58:THR:HG22	1.87	0.56
1:H:33:GLU:HA	1:H:48:ILE:HG12	1.86	0.56
1:H:286:ARG:HG2	1:H:286:ARG:HH11	1.69	0.56
1:C:452:ALA:H	1:C:566:HIS:HD2	1.52	0.56
1:E:374:ASP:OD1	1:E:381:TYR:OH	2.19	0.56
1:B:102:HIS:CG	1:B:171:MET:HE2	2.41	0.56
1:H:156:LEU:CD2	4:H:913:HOH:O	2.54	0.56
1:F:374:ASP:OD1	1:F:381:TYR:OH	2.20	0.55
1:D:48:ILE:CG1	1:D:58:THR:HG22	2.36	0.55
1:G:560:LEU:CD1	1:G:566:HIS:NE2	2.68	0.55
1:E:6:ILE:HD12	1:E:13:LEU:HD11	1.88	0.55
1:F:102:HIS:CD2	1:F:171:MET:HE2	2.42	0.55
1:G:108:TRP:CE2	1:G:151:ARG:CD	2.89	0.55
1:H:80:LEU:HD13	1:H:85:PHE:HE2	1.71	0.55
1:C:374:ASP:OD1	1:C:381:TYR:OH	2.20	0.55
1:H:102:HIS:CG	1:H:171:MET:HE2	2.42	0.55
1:H:374:ASP:OD1	1:H:381:TYR:OH	2.20	0.55
1:H:4:THR:HG21	4:H:814:HOH:O	2.06	0.55
1:E:32:GLU:OE2	1:E:49:ARG:NH2	2.39	0.55
1:D:102:HIS:CG	1:D:171:MET:HE2	2.43	0.54
1:G:108:TRP:CD2	1:G:151:ARG:CD	2.90	0.54
1:F:295:ARG:HG2	1:F:295:ARG:NH2	2.22	0.54
1:D:2:THR:O	1:D:14:GLU:HG2	2.07	0.54
1:E:302:VAL:HB	4:E:824:HOH:O	2.07	0.54
1:H:102:HIS:CE1	1:H:171:MET:CE	2.90	0.54
1:H:500:ARG:NH2	1:H:551:TYR:O	2.40	0.54
1:C:286:ARG:HH11	1:C:286:ARG:HG2	1.73	0.54
1:D:27:LEU:HD21	1:D:378:LEU:HD22	1.88	0.54
1:E:425:GLU:O	1:E:429:ASN:HB2	2.07	0.54
1:F:518:ASP:HB2	4:F:680:HOH:O	2.08	0.54
1:F:19:ARG:HG2	4:F:666:HOH:O	2.07	0.54
1:F:440:ASP:OD2	1:F:442:PHE:HB2	2.08	0.53
1:H:31:ILE:CG2	1:H:48:ILE:HG23	2.38	0.53
1:G:374:ASP:OD1	1:G:381:TYR:OH	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:HB3	4:B:909:HOH:O	2.07	0.53
1:E:174:ILE:HD13	1:E:386:ILE:HD13	1.90	0.53
1:G:61:LYS:HB2	1:G:289:THR:HG23	1.88	0.53
1:B:374:ASP:OD1	1:B:381:TYR:OH	2.19	0.53
1:F:576:LEU:O	1:F:580:LYS:CG	2.43	0.53
1:F:561:HIS:HB2	4:F:619:HOH:O	2.07	0.53
1:F:206:LYS:HG3	1:F:274:PHE:CE2	2.44	0.53
1:D:102:HIS:CD2	1:D:171:MET:HE3	2.43	0.53
1:A:238:GLU:OE2	1:B:530:ARG:NH2	2.41	0.53
1:A:61:LYS:HB2	1:A:289:THR:HG23	1.91	0.52
1:D:2:THR:N	4:D:815:HOH:O	2.41	0.52
1:B:102:HIS:CE1	1:B:171:MET:CE	2.93	0.52
1:F:554:GLN:CG	4:F:636:HOH:O	2.53	0.52
1:G:446:ARG:NH1	4:G:876:HOH:O	2.33	0.52
1:G:286:ARG:HH11	1:G:286:ARG:HG2	1.74	0.52
1:B:286:ARG:HH11	1:B:286:ARG:HG2	1.74	0.52
1:B:500:ARG:NH2	1:B:551:TYR:O	2.43	0.52
1:G:351:THR:HG22	1:G:353:GLU:H	1.75	0.52
1:H:171:MET:CE	4:H:715:HOH:O	2.37	0.52
1:F:385:ILE:CG1	4:F:629:HOH:O	2.48	0.52
1:G:360:MET:HE1	1:G:370:VAL:HG11	1.91	0.52
1:D:286:ARG:HG2	1:D:286:ARG:HH11	1.75	0.52
1:B:125:ARG:HG3	4:B:982:HOH:O	2.09	0.52
1:H:327:SER:N	4:H:755:HOH:O	2.42	0.52
1:F:143:ASP:OD1	1:F:144:LEU:N	2.43	0.52
1:G:581:ALA:CA	4:G:857:HOH:O	2.41	0.52
1:E:238:GLU:OE2	1:F:530:ARG:NH2	2.43	0.52
1:A:545:SER:HB3	1:C:525:LEU:HD21	1.92	0.51
1:B:102:HIS:CE1	1:B:171:MET:HE2	2.46	0.51
1:B:190:ASN:HB2	1:B:352:THR:HG23	1.92	0.51
1:H:76:TYR:HD1	1:H:80:LEU:HD22	1.75	0.51
1:G:411:ARG:HG2	1:G:415:LEU:HD22	1.92	0.51
1:D:374:ASP:OD1	1:D:381:TYR:OH	2.20	0.51
1:H:102:HIS:CE1	1:H:171:MET:HE2	2.45	0.51
1:D:499:GLU:HB2	4:D:762:HOH:O	2.11	0.51
1:C:102:HIS:CE1	1:C:171:MET:HE3	2.45	0.51
1:F:102:HIS:CD2	1:F:171:MET:HE3	2.46	0.51
1:A:286:ARG:HH11	1:A:286:ARG:HG2	1.75	0.51
1:C:147:GLY:HA2	4:C:771:HOH:O	2.11	0.50
2:E:601:AMP:N1	4:E:795:HOH:O	2.33	0.50
1:E:9:LYS:HE3	2:E:601:AMP:N1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:ARG:HD3	1:D:524:TYR:OH	2.11	0.50
1:F:309:ASP:HA	4:F:610:HOH:O	2.11	0.50
1:G:519:ARG:HD3	1:G:524:TYR:OH	2.12	0.50
1:F:102:HIS:CG	1:F:171:MET:HE2	2.46	0.50
1:C:102:HIS:CE1	1:C:171:MET:CE	2.95	0.49
1:G:131:ASP:HB2	1:G:136:LEU:HD22	1.94	0.49
1:A:374:ASP:OD1	1:A:381:TYR:OH	2.20	0.49
1:C:317:THR:CG2	4:C:782:HOH:O	2.54	0.49
1:H:519:ARG:HD3	1:H:524:TYR:OH	2.13	0.49
1:C:351:THR:HG22	1:C:353:GLU:H	1.78	0.49
1:A:525:LEU:HD21	1:C:545:SER:HB3	1.95	0.49
1:E:286:ARG:HG2	1:E:286:ARG:HH11	1.78	0.49
1:A:131:ASP:HB2	1:A:136:LEU:HD22	1.95	0.49
1:H:2:THR:HG21	4:H:855:HOH:O	2.13	0.49
1:B:171:MET:CE	4:B:784:HOH:O	2.46	0.49
1:F:517:GLU:OE2	1:F:518:ASP:OD2	2.31	0.49
1:D:238:GLU:OE1	4:D:868:HOH:O	2.20	0.49
1:C:64:THR:HB	4:C:811:HOH:O	2.13	0.49
1:F:519:ARG:HD3	1:F:524:TYR:OH	2.13	0.48
1:B:316:HIS:HB3	4:B:934:HOH:O	2.13	0.48
1:G:485:THR:O	1:G:489:MET:HE2	2.13	0.48
1:H:284:LEU:HD13	4:H:950:HOH:O	2.13	0.48
1:G:274:PHE:HB2	4:G:768:HOH:O	2.12	0.48
1:F:425:GLU:OE1	1:F:425:GLU:N	2.47	0.48
1:E:5:PHE:HA	4:E:890:HOH:O	2.13	0.48
1:F:143:ASP:OD1	1:F:145:GLN:N	2.36	0.48
1:C:519:ARG:HD3	1:C:524:TYR:OH	2.14	0.48
1:H:510:LEU:HD23	4:H:960:HOH:O	2.13	0.48
1:G:415:LEU:HG	1:G:556:VAL:HB	1.96	0.48
1:H:36:TRP:CZ3	1:H:65:LYS:HG3	2.49	0.48
1:A:519:ARG:HD3	1:A:524:TYR:OH	2.13	0.48
1:B:325:ASP:OD2	4:B:785:HOH:O	2.20	0.48
1:H:317:THR:HB	4:H:894:HOH:O	2.15	0.47
1:F:567:GLN:HB2	4:F:639:HOH:O	2.14	0.47
1:G:238:GLU:OE2	1:H:530:ARG:NH2	2.47	0.47
1:H:4:THR:HG22	1:H:14:GLU:OE2	2.10	0.47
1:B:452:ALA:H	1:B:566:HIS:CD2	2.29	0.47
1:C:526:ASN:O	1:C:530:ARG:HG3	2.14	0.47
1:F:360:MET:HE1	1:F:370:VAL:HG11	1.96	0.47
1:E:526:ASN:O	1:E:530:ARG:HG3	2.15	0.47
1:G:522:LEU:H	1:G:522:LEU:CD2	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ASP:HB2	1:E:136:LEU:HD22	1.95	0.47
1:F:298:LYS:O	1:F:298:LYS:HG2	2.15	0.47
1:E:6:ILE:CD1	1:E:13:LEU:HD11	2.45	0.46
1:B:133:GLU:OE1	1:B:133:GLU:N	2.49	0.46
1:H:406:MET:HB2	4:H:857:HOH:O	2.14	0.46
1:E:446:ARG:NH1	1:E:460:TYR:O	2.48	0.46
1:B:134:ASN:ND2	4:B:1005:HOH:O	2.26	0.46
1:F:80:LEU:HD22	1:F:576:LEU:HD11	1.98	0.46
1:A:485:THR:O	1:A:489:MET:HE2	2.15	0.46
1:D:526:ASN:O	1:D:530:ARG:HG3	2.16	0.46
1:F:131:ASP:HB2	1:F:136:LEU:HD22	1.96	0.46
1:C:131:ASP:HB2	1:C:136:LEU:HD22	1.97	0.46
1:B:526:ASN:O	1:B:530:ARG:HG3	2.15	0.46
1:C:425:GLU:HG2	4:C:796:HOH:O	2.15	0.46
1:H:102:HIS:CE1	1:H:171:MET:HE3	2.50	0.46
1:F:526:ASN:O	1:F:530:ARG:HG3	2.16	0.46
1:B:134:ASN:HB2	1:H:133:GLU:HG3	1.96	0.46
1:H:470:MET:HE3	1:H:470:MET:HB2	1.75	0.46
1:G:443:THR:CG2	4:G:756:HOH:O	2.64	0.46
1:G:97:ASN:HA	1:G:151:ARG:NH2	2.31	0.46
1:F:286:ARG:HE	1:F:286:ARG:HB2	1.53	0.46
1:G:446:ARG:HG3	1:G:451:LEU:O	2.17	0.45
1:G:526:ASN:O	1:G:530:ARG:HG3	2.15	0.45
1:F:62:GLY:N	4:F:633:HOH:O	2.49	0.45
1:H:131:ASP:HB2	1:H:136:LEU:HD22	1.97	0.45
1:E:119:GLU:HA	4:E:840:HOH:O	2.16	0.45
1:F:143:ASP:C	1:F:143:ASP:OD1	2.53	0.45
1:E:116:ASP:C	1:E:116:ASP:OD1	2.55	0.45
1:G:160:ARG:HD2	1:G:163:ASP:OD1	2.16	0.45
1:H:526:ASN:O	1:H:530:ARG:HG3	2.17	0.45
1:D:165:GLN:HG2	4:D:941:HOH:O	2.17	0.45
1:D:36:TRP:CZ3	1:D:65:LYS:HG3	2.52	0.45
1:C:102:HIS:CG	1:C:171:MET:HE2	2.51	0.45
1:H:178:TYR:O	1:H:179:VAL:C	2.54	0.45
1:A:293:GLN:NE2	4:A:717:HOH:O	2.34	0.45
1:C:102:HIS:ND1	1:C:171:MET:HE3	2.31	0.45
1:H:509:THR:HG22	4:H:960:HOH:O	2.17	0.45
1:H:102:HIS:ND1	1:H:171:MET:HE3	2.33	0.44
1:G:581:ALA:C	4:G:857:HOH:O	2.55	0.44
1:C:13:LEU:CD2	4:C:893:HOH:O	2.54	0.44
1:H:327:SER:CA	4:H:755:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:TRP:CZ3	1:F:65:LYS:HG3	2.51	0.44
1:A:489:MET:CE	1:A:508:GLN:OE1	2.65	0.44
1:H:286:ARG:NH1	1:H:286:ARG:HG2	2.31	0.44
1:H:277:HIS:CG	1:H:278:PRO:HD2	2.52	0.44
1:H:510:LEU:N	4:H:960:HOH:O	2.50	0.44
1:H:160:ARG:HD2	1:H:163:ASP:OD1	2.17	0.44
1:A:277:HIS:CG	1:A:278:PRO:HD2	2.52	0.44
1:D:485:THR:O	1:D:489:MET:HE2	2.17	0.44
1:D:23:LYS:HE3	1:D:379:GLY:HA3	2.00	0.44
1:A:526:ASN:O	1:A:530:ARG:HG3	2.17	0.44
1:H:420:SER:O	1:H:421:GLU:HB2	2.17	0.44
1:G:36:TRP:CZ3	1:G:65:LYS:HG3	2.53	0.44
1:D:165:GLN:CD	4:D:941:HOH:O	2.55	0.43
1:A:31:ILE:HG22	1:A:48:ILE:HG22	1.94	0.43
1:C:560:LEU:HD13	1:C:566:HIS:CD2	2.54	0.43
1:C:277:HIS:CG	1:C:278:PRO:HD2	2.53	0.43
1:D:286:ARG:HG2	1:D:286:ARG:NH1	2.33	0.43
1:F:23:LYS:HE3	1:F:379:GLY:HA3	2.00	0.43
1:B:160:ARG:HD2	1:B:163:ASP:OD1	2.19	0.43
1:B:23:LYS:HE3	1:B:379:GLY:HA3	2.00	0.43
1:C:23:LYS:HE3	1:C:379:GLY:HA3	1.99	0.43
1:C:160:ARG:HH21	1:C:165:GLN:HB2	1.84	0.43
1:E:23:LYS:HE3	1:E:379:GLY:HA3	2.01	0.43
1:C:36:TRP:CZ3	1:C:65:LYS:HG3	2.53	0.43
1:G:519:ARG:NH1	1:H:333:ASP:OD2	2.52	0.43
1:F:178:TYR:HB3	4:F:693:HOH:O	2.17	0.43
1:F:29:PHE:N	1:F:29:PHE:HD1	2.17	0.43
1:D:160:ARG:HD2	1:D:163:ASP:OD1	2.18	0.43
1:B:286:ARG:HG2	1:B:286:ARG:NH1	2.33	0.43
1:E:36:TRP:CZ3	1:E:65:LYS:HG3	2.53	0.43
1:H:23:LYS:HE3	1:H:379:GLY:HA3	1.99	0.43
1:E:149:GLU:HB3	4:E:867:HOH:O	2.17	0.43
1:G:286:ARG:NH1	1:G:286:ARG:HG2	2.34	0.42
1:A:286:ARG:NH1	1:A:286:ARG:HG2	2.33	0.42
1:F:29:PHE:CD1	1:F:29:PHE:N	2.87	0.42
1:G:102:HIS:CE1	1:G:171:MET:HG2	2.54	0.42
1:E:286:ARG:HG2	1:E:286:ARG:NH1	2.35	0.42
1:H:140:MET:HE2	1:H:140:MET:HB2	1.62	0.42
1:H:174:ILE:HB	4:H:913:HOH:O	2.18	0.42
1:G:522:LEU:N	1:G:522:LEU:HD23	2.29	0.42
1:C:452:ALA:H	1:C:566:HIS:CD2	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:LYS:HD3	1:H:23:LYS:HA	1.97	0.42
1:C:351:THR:HG22	1:C:353:GLU:N	2.34	0.42
1:E:190:ASN:O	1:E:194:VAL:HG23	2.20	0.42
1:A:160:ARG:HD2	1:A:163:ASP:OD1	2.19	0.42
1:E:530:ARG:NH2	1:F:238:GLU:OE2	2.53	0.42
1:B:190:ASN:HB3	1:B:352:THR:HG23	2.00	0.42
1:B:14:GLU:HG2	4:B:702:HOH:O	2.19	0.42
1:E:329:LEU:HA	4:E:907:HOH:O	2.19	0.42
1:D:277:HIS:CG	1:D:278:PRO:HD2	2.55	0.42
1:B:102:HIS:CE1	1:B:171:MET:HE3	2.54	0.42
1:D:452:ALA:H	1:D:566:HIS:CD2	2.34	0.42
1:F:79:ARG:NH1	4:F:695:HOH:O	2.35	0.41
1:B:136:LEU:HA	1:B:136:LEU:HD23	1.85	0.41
1:G:446:ARG:NH1	1:G:460:TYR:O	2.51	0.41
1:B:518:ASP:HA	4:B:905:HOH:O	2.19	0.41
1:B:203:ARG:NH2	4:B:757:HOH:O	2.46	0.41
1:E:277:HIS:CG	1:E:278:PRO:HD2	2.55	0.41
1:F:277:HIS:CG	1:F:278:PRO:HD2	2.55	0.41
1:B:115:ASP:HA	4:B:737:HOH:O	2.20	0.41
1:C:359:LEU:HD23	4:C:878:HOH:O	2.21	0.41
1:F:29:PHE:HE2	1:F:80:LEU:HD21	1.85	0.41
1:D:485:THR:HG22	1:D:489:MET:HE2	2.02	0.41
1:G:127:ARG:NE	4:G:839:HOH:O	2.04	0.41
1:G:137:THR:OG1	1:G:140:MET:HG2	2.21	0.41
1:E:171:MET:HE1	4:E:745:HOH:O	2.20	0.41
1:E:171:MET:HE2	4:E:733:HOH:O	2.21	0.41
1:B:189:ARG:HA	1:B:381:TYR:CD2	2.55	0.41
1:A:9:LYS:HE3	2:A:601:AMP:N1	2.36	0.41
1:G:209:ILE:HA	1:G:214:ILE:HD12	2.03	0.41
1:G:97:ASN:HB3	4:G:853:HOH:O	2.21	0.41
1:C:286:ARG:HG2	1:C:286:ARG:NH1	2.34	0.41
1:D:190:ASN:O	1:D:194:VAL:HG23	2.21	0.41
1:D:2:THR:O	1:D:14:GLU:CG	2.69	0.40
1:H:80:LEU:HD13	1:H:85:PHE:CE2	2.55	0.40
1:C:514:ALA:HA	4:C:874:HOH:O	2.22	0.40
1:A:460:TYR:OH	4:A:1025:HOH:O	2.17	0.40
1:B:36:TRP:CZ3	1:B:65:LYS:HG3	2.56	0.40
1:C:59:ASN:ND2	4:C:880:HOH:O	2.54	0.40
1:G:108:TRP:CE3	1:G:151:ARG:HD2	2.57	0.40
1:E:127:ARG:NH2	4:E:840:HOH:O	2.54	0.40
1:G:351:THR:HG22	1:G:353:GLU:N	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:ASN:O	1:F:194:VAL:HG23	2.21	0.40
1:G:23:LYS:HE3	1:G:379:GLY:HA3	2.02	0.40
1:A:23:LYS:HE3	1:A:379:GLY:HA3	2.03	0.40
1:H:190:ASN:O	1:H:194:VAL:HG23	2.20	0.40
1:B:505:ARG:NH2	4:B:1003:HOH:O	2.54	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	580/586 (99%)	569 (98%)	10 (2%)	1 (0%)	52	61
1	B	581/586 (99%)	567 (98%)	13 (2%)	1 (0%)	52	61
1	C	568/586 (97%)	555 (98%)	12 (2%)	1 (0%)	52	61
1	D	580/586 (99%)	566 (98%)	13 (2%)	1 (0%)	52	61
1	E	576/586 (98%)	564 (98%)	11 (2%)	1 (0%)	52	61
1	F	572/586 (98%)	557 (97%)	14 (2%)	1 (0%)	52	61
1	G	573/586 (98%)	560 (98%)	12 (2%)	1 (0%)	52	61
1	H	581/586 (99%)	566 (97%)	14 (2%)	1 (0%)	52	61
All	All	4611/4688 (98%)	4504 (98%)	99 (2%)	8 (0%)	52	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	VAL
1	B	179	VAL
1	C	179	VAL
1	D	179	VAL
1	E	179	VAL

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Mol	Chain	Res	Type
1	F	179	VAL
1	G	179	VAL
1	H	179	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/487 (99%)	476 (98%)	8 (2%)	68	79
1	B	485/487 (100%)	475 (98%)	10 (2%)	61	71
1	C	475/487 (98%)	464 (98%)	11 (2%)	58	69
1	D	484/487 (99%)	473 (98%)	11 (2%)	58	69
1	E	481/487 (99%)	471 (98%)	10 (2%)	61	71
1	F	477/487 (98%)	455 (95%)	22 (5%)	33	37
1	G	478/487 (98%)	464 (97%)	14 (3%)	50	60
1	H	485/487 (100%)	471 (97%)	14 (3%)	50	60
All	All	3849/3896 (99%)	3749 (97%)	100 (3%)	54	65

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	113	GLU
1	A	136	LEU
1	A	195	GLN
1	A	203	ARG
1	A	479	GLU
1	A	517	GLU
1	A	560	LEU
1	B	113	GLU
1	B	203	ARG
1	B	292	LEU
1	B	319	LEU

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Mol	Chain	Res	Type
1	B	352	THR
1	B	384	ARG
1	B	437	GLU
1	B	522	LEU
1	B	560	LEU
1	B	584	TRP
1	C	119	GLU
1	C	134	ASN
1	C	136	LEU
1	C	156	LEU
1	C	195	GLN
1	C	203	ARG
1	C	298	LYS
1	C	436	GLU
1	C	455	SER
1	C	479	GLU
1	C	522	LEU
1	D	14	GLU
1	D	58	THR
1	D	134	ASN
1	D	195	GLN
1	D	203	ARG
1	D	351	THR
1	D	401	LEU
1	D	436	GLU
1	D	479	GLU
1	D	518	ASP
1	D	560	LEU
1	E	23	LYS
1	E	116	ASP
1	E	134	ASN
1	E	136	LEU
1	E	195	GLN
1	E	203	ARG
1	E	300	LEU
1	E	518	ASP
1	E	522	LEU
1	E	560	LEU
1	F	66	LYS
1	F	97	ASN
1	F	136	LEU
1	F	156	LEU

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Mol	Chain	Res	Type
1	F	164	ASN
1	F	195	GLN
1	F	203	ARG
1	F	286	ARG
1	F	292	LEU
1	F	293	GLN
1	F	317	THR
1	F	409	HIS
1	F	425	GLU
1	F	436	GLU
1	F	437	GLU
1	F	517	GLU
1	F	522	LEU
1	F	547	GLU
1	F	560	LEU
1	F	576	LEU
1	F	577	GLN
1	F	580	LYS
1	G	23	LYS
1	G	119	GLU
1	G	134	ASN
1	G	136	LEU
1	G	203	ARG
1	G	292	LEU
1	G	298	LYS
1	G	312	GLU
1	G	401	LEU
1	G	412	GLU
1	G	415	LEU
1	G	436	GLU
1	G	437	GLU
1	G	522	LEU
1	H	2	THR
1	H	4	THR
1	H	23	LYS
1	H	48	ILE
1	H	80	LEU
1	H	134	ASN
1	H	136	LEU
1	H	156	LEU
1	H	164	ASN
1	H	292	LEU

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Mol	Chain	Res	Type
1	H	312	GLU
1	H	401	LEU
1	H	455	SER
1	H	584	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	567	GLN
1	B	134	ASN
1	B	161	GLN
1	B	165	GLN
1	B	195	GLN
1	B	566	HIS
1	C	59	ASN
1	C	254	GLN
1	C	566	HIS
1	D	102	HIS
1	D	145	GLN
1	D	566	HIS
1	E	293	GLN
1	F	102	HIS
1	F	293	GLN
1	F	567	GLN
1	F	577	GLN
1	G	102	HIS
1	G	145	GLN
1	G	195	GLN
1	H	59	ASN
1	H	134	ASN
1	H	195	GLN
1	H	566	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 21 are monoatomic - leaving 7 for Mogul analysis.

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	AMP	A	601	-	20,25,25	1.46	4 (20%)	22,38,38	3.63	7 (31%)
2	AMP	B	601	-	20,25,25	1.34	3 (15%)	22,38,38	1.71	4 (18%)
2	AMP	C	601	-	20,25,25	1.25	2 (10%)	22,38,38	2.42	6 (27%)
2	AMP	D	601	-	20,25,25	1.53	4 (20%)	22,38,38	2.82	13 (59%)
2	AMP	E	601	-	20,25,25	1.35	2 (10%)	22,38,38	2.87	7 (31%)
2	AMP	G	601	-	20,25,25	1.42	2 (10%)	22,38,38	2.57	8 (36%)
2	AMP	H	601	-	20,25,25	1.55	2 (10%)	22,38,38	2.36	5 (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
2	AMP	A	601	-	-	0/6/26/26	0/3/3/3
2	AMP	B	601	-	-	0/6/26/26	0/3/3/3
2	AMP	C	601	-	-	0/6/26/26	0/3/3/3
2	AMP	D	601	-	-	0/6/26/26	0/3/3/3
2	AMP	E	601	-	-	0/6/26/26	0/3/3/3
2	AMP	G	601	-	-	0/6/26/26	0/3/3/3
2	AMP	H	601	-	-	0/6/26/26	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	AMP	C4-N3	-3.05	1.31	1.35
2	E	601	AMP	C4-N3	-2.86	1.31	1.35
2	A	601	AMP	C2-N3	-2.75	1.27	1.32
2	B	601	AMP	C5-N7	-2.35	1.31	1.39
2	D	601	AMP	C3'-C4'	-2.24	1.47	1.53
2	D	601	AMP	C4-N3	-2.18	1.32	1.35
2	A	601	AMP	O4'-C1'	2.09	1.43	1.41
2	B	601	AMP	C2-N3	2.26	1.36	1.32
2	D	601	AMP	O4'-C1'	2.31	1.44	1.41
2	H	601	AMP	C2-N3	2.60	1.36	1.32
2	G	601	AMP	C5-C4	2.91	1.47	1.40
2	C	601	AMP	C5-C4	3.11	1.47	1.40
2	E	601	AMP	C5-C4	3.32	1.48	1.40
2	A	601	AMP	C5-C4	3.36	1.48	1.40
2	C	601	AMP	O4'-C1'	3.48	1.45	1.41
2	G	601	AMP	O4'-C1'	3.53	1.45	1.41
2	B	601	AMP	C5-C4	3.93	1.49	1.40
2	D	601	AMP	C5-C4	4.31	1.50	1.40
2	H	601	AMP	O4'-C1'	5.17	1.47	1.41

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	AMP	N3-C2-N1	-10.93	120.53	128.89
2	E	601	AMP	N3-C2-N1	-8.71	122.22	128.89
2	H	601	AMP	N3-C2-N1	-8.37	122.49	128.89
2	D	601	AMP	N3-C2-N1	-8.19	122.62	128.89
2	C	601	AMP	N3-C2-N1	-8.18	122.63	128.89
2	G	601	AMP	N3-C2-N1	-8.00	122.77	128.89
2	A	601	AMP	C1'-N9-C4	-5.58	118.52	126.94
2	B	601	AMP	N3-C2-N1	-4.33	125.58	128.89
2	C	601	AMP	C4-C5-N7	-4.26	105.56	109.48
2	E	601	AMP	C1'-N9-C4	-4.17	120.65	126.94
2	G	601	AMP	C1'-N9-C4	-3.73	121.31	126.94
2	H	601	AMP	C4-C5-N7	-3.72	106.06	109.48
2	C	601	AMP	C1'-N9-C4	-3.69	121.37	126.94
2	B	601	AMP	O2P-P-O5'	-3.42	96.72	106.56
2	G	601	AMP	C2'-C1'-N9	-3.40	109.10	114.29
2	D	601	AMP	O2'-C2'-C3'	-3.05	101.90	111.83
2	H	601	AMP	C2'-C1'-N9	-2.86	109.92	114.29
2	D	601	AMP	O3'-C3'-C4'	-2.85	102.51	111.05
2	E	601	AMP	O2P-P-O5'	-2.78	98.56	106.56
2	B	601	AMP	C4-C5-N7	-2.57	107.11	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	AMP	O2P-P-O5'	-2.41	99.63	106.56
2	E	601	AMP	C4'-O4'-C1'	-2.28	107.21	109.72
2	D	601	AMP	C1'-N9-C4	-2.26	123.53	126.94
2	H	601	AMP	C4'-O4'-C1'	-2.26	107.23	109.72
2	D	601	AMP	C5'-C4'-C3'	-2.26	106.25	115.21
2	D	601	AMP	O3P-P-O5'	-2.19	100.27	106.56
2	C	601	AMP	O4'-C1'-N9	-2.07	103.77	108.10
2	G	601	AMP	O3P-P-O2P	2.01	115.03	107.38
2	A	601	AMP	O3P-P-O2P	2.01	115.04	107.38
2	D	601	AMP	N6-C6-N1	2.18	123.89	119.20
2	C	601	AMP	C2-N1-C6	2.22	122.73	118.77
2	G	601	AMP	C2-N1-C6	2.27	122.83	118.77
2	D	601	AMP	O3P-P-O1P	2.29	117.97	110.58
2	D	601	AMP	C4'-O4'-C1'	2.32	112.27	109.72
2	G	601	AMP	O4'-C1'-N9	2.35	113.03	108.10
2	C	601	AMP	O2P-P-O1P	2.49	118.61	110.58
2	B	601	AMP	C4'-O4'-C1'	2.52	112.48	109.72
2	E	601	AMP	O5'-P-O1P	2.74	114.11	107.14
2	A	601	AMP	N6-C6-N1	2.87	125.36	119.20
2	H	601	AMP	O3P-P-O2P	2.87	118.32	107.38
2	G	601	AMP	O5'-P-O1P	2.96	114.67	107.14
2	D	601	AMP	O4'-C4'-C5'	2.99	120.01	109.32
2	D	601	AMP	O4'-C1'-N9	3.05	114.49	108.10
2	E	601	AMP	C2'-C1'-N9	3.29	119.31	114.29
2	A	601	AMP	C4-C5-N7	3.37	112.58	109.48
2	D	601	AMP	C2'-C1'-N9	3.71	119.96	114.29
2	D	601	AMP	C2-N1-C6	4.34	126.52	118.77
2	E	601	AMP	C2-N1-C6	6.11	129.68	118.77
2	A	601	AMP	C2-N1-C6	6.70	130.75	118.77
2	A	601	AMP	C2'-C1'-N9	7.76	126.15	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	AMP	1	0
2	D	601	AMP	2	0
2	E	601	AMP	2	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	582/586 (99%)	-0.09	0 100 100	17, 28, 45, 64	0
1	B	583/586 (99%)	-0.05	2 (0%) 94 95	15, 27, 47, 82	0
1	C	570/586 (97%)	0.05	2 (0%) 93 93	22, 39, 57, 93	0
1	D	582/586 (99%)	0.01	3 (0%) 91 92	21, 36, 57, 86	0
1	E	578/586 (98%)	0.08	1 (0%) 95 96	24, 40, 63, 87	0
1	F	574/586 (97%)	1.01	94 (16%) 2 2	35, 66, 93, 111	0
1	G	575/586 (98%)	0.10	3 (0%) 91 92	23, 40, 60, 92	0
1	H	583/586 (99%)	-0.07	0 100 100	14, 30, 49, 74	0
All	All	4627/4688 (98%)	0.13	105 (2%) 64 68	14, 36, 71, 111	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	186	GLY	8.1
1	F	359	LEU	5.6
1	F	185	ALA	5.3
1	F	125	ARG	5.2
1	F	553	LEU	4.3
1	F	182	GLY	4.1
1	F	282	VAL	4.0
1	F	557	ASP	4.0
1	F	408	SER	3.9
1	F	414	ILE	3.8
1	F	221	ALA	3.8
1	F	560	LEU	3.7
1	F	91	LEU	3.7
1	F	284	LEU	3.6
1	F	283	ALA	3.6
1	F	556	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	297	LEU	3.5
1	F	280	PHE	3.5
1	F	101	VAL	3.5
1	F	34	ALA	3.4
1	F	85	PHE	3.4
1	F	209	ILE	3.4
1	F	117	VAL	3.4
1	C	113	GLU	3.4
1	F	103	TYR	3.4
1	F	419	GLY	3.3
1	C	406	MET	3.3
1	F	378	LEU	3.3
1	F	364	ASN	3.3
1	F	100	PHE	3.2
1	F	198	SER	3.1
1	F	48	ILE	3.1
1	F	573	TYR	2.9
1	F	104	PRO	2.9
1	F	126	LEU	2.9
1	F	113	GLU	2.9
1	F	390	MET	2.9
1	F	437	GLU	2.8
1	F	192	ALA	2.8
1	F	83	ASN	2.7
1	F	205	VAL	2.7
1	F	567	GLN	2.7
1	F	108	TRP	2.7
1	F	406	MET	2.6
1	F	187	ASN	2.6
1	F	95	ILE	2.6
1	F	167	VAL	2.6
1	F	410	LEU	2.6
1	F	156	LEU	2.6
1	F	275	GLY	2.5
1	D	125	ARG	2.5
1	F	346	TRP	2.5
1	F	121	LEU	2.5
1	F	197	LEU	2.5
1	F	363	PHE	2.5
1	F	158	PHE	2.5
1	F	381	TYR	2.4
1	F	341	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	231	VAL	2.4
1	F	102	HIS	2.4
1	F	194	VAL	2.4
1	F	249	GLY	2.4
1	F	409	HIS	2.4
1	F	72	ALA	2.4
1	F	569	LEU	2.4
1	F	255	TYR	2.4
1	F	169	ILE	2.4
1	F	412	GLU	2.3
1	F	281	GLY	2.3
1	F	522	LEU	2.3
1	G	433	GLN	2.3
1	F	74	GLY	2.3
1	F	86	PHE	2.3
1	E	422	TRP	2.3
1	F	438	GLY	2.2
1	F	387	VAL	2.2
1	F	520	GLN	2.2
1	F	37	LEU	2.2
1	F	449	LEU	2.2
1	F	141	LEU	2.2
1	F	349	SER	2.2
1	B	134	ASN	2.2
1	F	32	GLU	2.2
1	D	124	ASP	2.2
1	F	109	PHE	2.2
1	F	114	ASN	2.2
1	F	56	CYS	2.2
1	F	289	THR	2.2
1	F	383	CYS	2.1
1	B	132	PRO	2.1
1	F	384	ARG	2.1
1	F	135	GLU	2.1
1	D	326	SER	2.1
1	F	377	HIS	2.1
1	F	510	LEU	2.1
1	G	297	LEU	2.1
1	F	393	ILE	2.1
1	F	518	ASP	2.1
1	F	77	PHE	2.1
1	F	73	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	84	TYR	2.1
1	F	396	ALA	2.1
1	F	30	GLN	2.0
1	G	230	VAL	2.0
1	F	394	TYR	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(Å <sup>2</sup> )	Q<0.9
3	MG	D	602	1/1	0.96	0.20	4.01	15,15,15,15	0
3	MG	A	602	1/1	0.98	0.17	3.31	14,14,14,14	0
3	MG	B	602	1/1	0.99	0.18	3.26	7,7,7,7	0
3	MG	G	602	1/1	0.99	0.15	1.09	19,19,19,19	0
2	AMP	A	601	23/23	0.95	0.15	1.01	19,24,30,37	0
3	MG	C	602	1/1	0.99	0.15	0.70	17,17,17,17	0
2	AMP	D	601	23/23	0.95	0.16	0.61	18,25,44,57	0
2	AMP	E	601	23/23	0.96	0.14	0.01	23,31,35,40	0
3	MG	H	602	1/1	0.99	0.14	0.01	15,15,15,15	0
2	AMP	G	601	23/23	0.97	0.14	-0.13	28,36,42,45	0
2	AMP	C	601	23/23	0.97	0.14	-0.22	30,38,56,61	0
2	AMP	H	601	23/23	0.99	0.13	-0.31	16,19,23,25	0
2	AMP	B	601	23/23	0.99	0.12	-0.75	16,19,21,23	0
3	MG	E	602	1/1	0.96	0.11	-1.46	27,27,27,27	0
3	MG	A	603	1/1	0.99	0.09	-2.66	18,18,18,18	0
3	MG	B	603	1/1	0.97	0.07	-3.70	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	C	603	1/1	0.99	0.09	-3.86	26,26,26,26	0
3	MG	E	603	1/1	0.99	0.06	-4.13	34,34,34,34	0
3	MG	H	603	1/1	0.99	0.05	-4.20	20,20,20,20	0
3	MG	G	603	1/1	0.96	0.05	-4.92	34,34,34,34	0
3	MG	D	604	1/1	0.98	0.05	-5.29	34,34,34,34	0
3	MG	A	604	1/1	0.97	0.05	-	31,31,31,31	0
3	MG	B	604	1/1	0.99	0.06	-	24,24,24,24	0
3	MG	G	604	1/1	0.93	0.10	-	49,49,49,49	0
3	MG	H	604	1/1	0.97	0.05	-	29,29,29,29	0
3	MG	E	604	1/1	0.98	0.03	-	39,39,39,39	0
3	MG	D	603	1/1	0.97	0.07	-	28,28,28,28	0
3	MG	C	604	1/1	0.89	0.04	-	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.