Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 05:44 PM BST

PDB ID	:	6JKW
Title	:	Seleno-methionine PNGM-1 from deep-sea sediment metagenome
Authors	:	Hong, M.K.; Park, K.S.; Jeon, J.H.; Lee, J.H.; Park, Y.S.; Lee, S.H.; Kang, L.W.
Deposited on	:	2019-03-02
Resolution	:	2.29 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

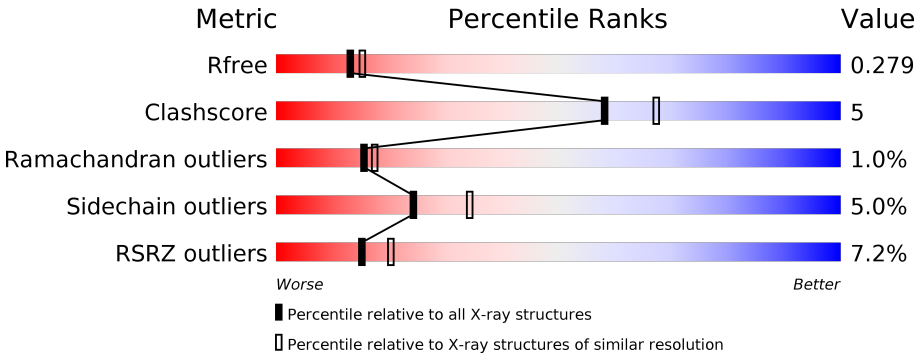
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.29 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_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	372	5% 86% 13%
1	B	372	5% 87% 11%
1	C	372	8% 86% 12%
1	D	372	7% 89% 9%
1	E	372	7% 85% 13%
1	F	372	7% 84% 15%

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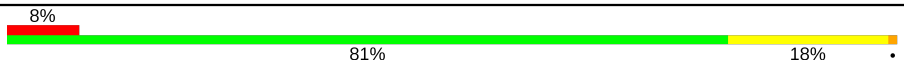
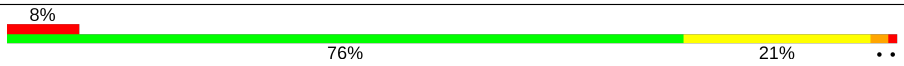
Mol	Chain	Length	Quality of chain
1	G	372	
1	H	372	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23910 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 Metallo-beta-lactamases PNGM-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	Se	0	0	0
			2933	1853	506	554	3	17			
1	B	372	Total	C	N	O	S	Se	0	0	0
			2933	1853	506	554	3	17			
1	C	372	Total	C	N	O	S	Se	0	0	0
			2933	1853	506	554	3	17			
1	D	372	Total	C	N	O	S	Se	0	0	0
			2933	1853	506	554	3	17			
1	E	372	Total	C	N	O	S	Se	0	0	0
			2933	1853	506	554	3	17			
1	F	372	Total	C	N	O	S	Se	0	0	0
			2933	1853	506	554	3	17			
1	G	372	Total	C	N	O	S	Se	0	0	0
			2933	1853	506	554	3	17			
1	H	372	Total	C	N	O	S	Se	0	0	0
			2933	1853	506	554	3	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	H	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is water.

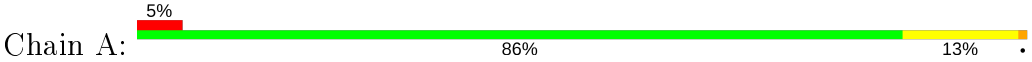
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	79	Total O 79 79	0	0
3	B	81	Total O 81 81	0	0
3	C	46	Total O 46 46	0	0
3	D	63	Total O 63 63	0	0
3	E	53	Total O 53 53	0	0
3	F	43	Total O 43 43	0	0
3	G	39	Total O 39 39	0	0
3	H	26	Total O 26 26	0	0

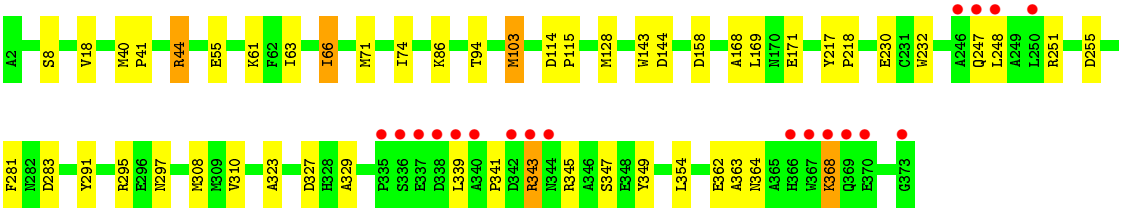
3 Residue-property plots (i)

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

- Molecule 1: Metallo-beta-lactamases PNGM-1

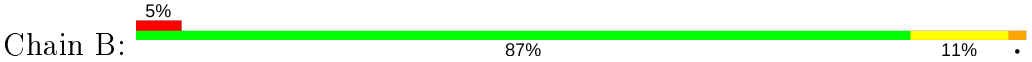
Chain A:

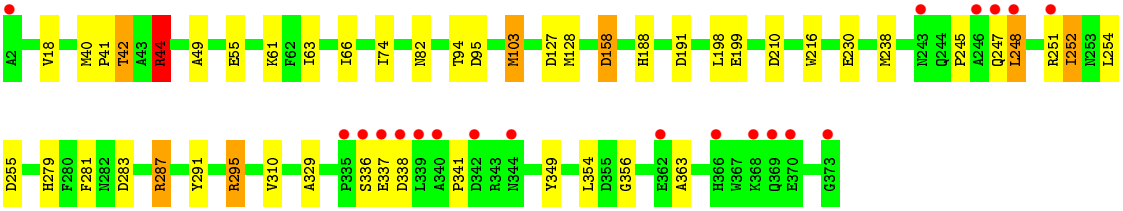




- Molecule 1: Metallo-beta-lactamases PNGM-1

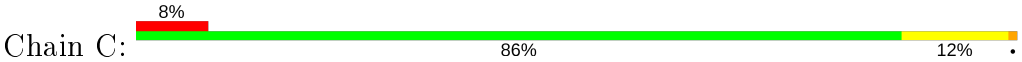
Chain B:

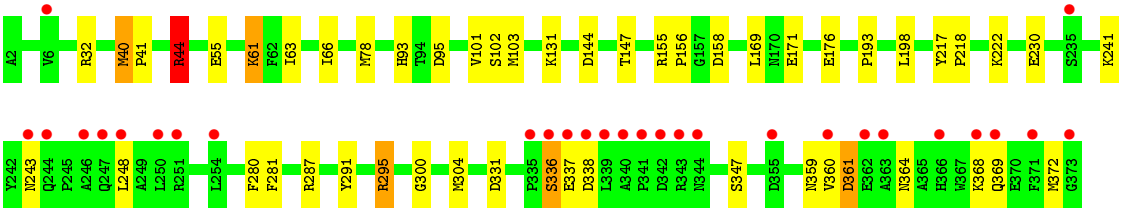




- Molecule 1: Metallo-beta-lactamases PNGM-1

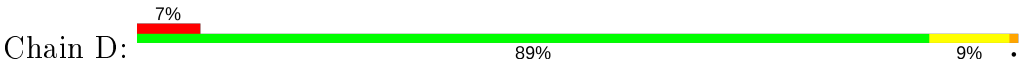
Chain C:

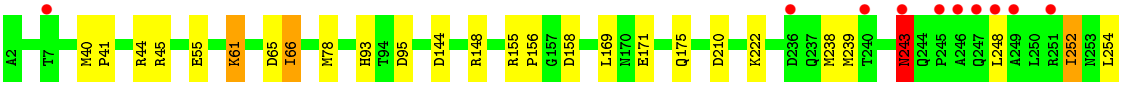


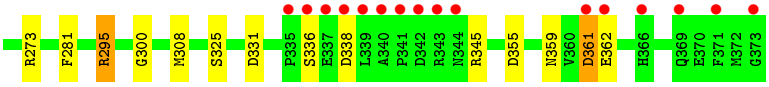


- Molecule 1: Metallo-beta-lactamases PNGM-1

Chain D:

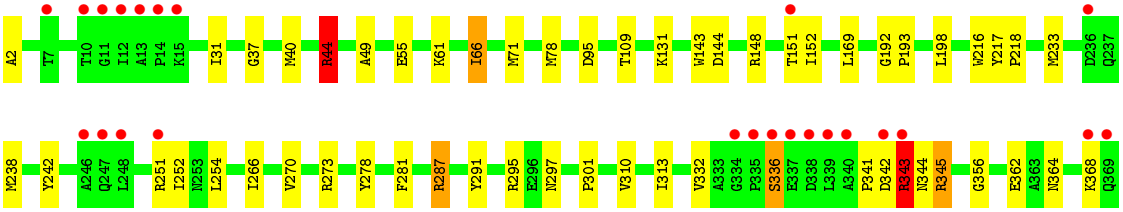






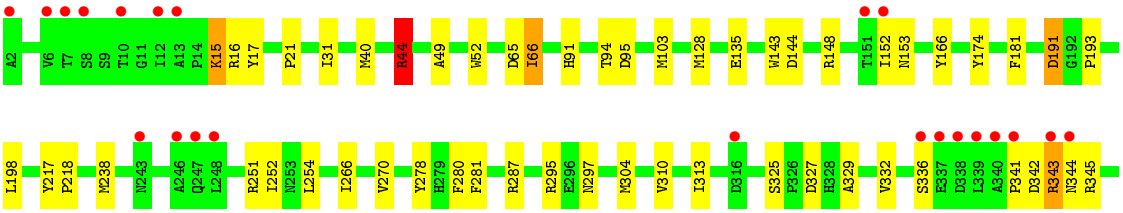
• Molecule 1: Metallo-beta-lactamases PNGM-1

Chain E:



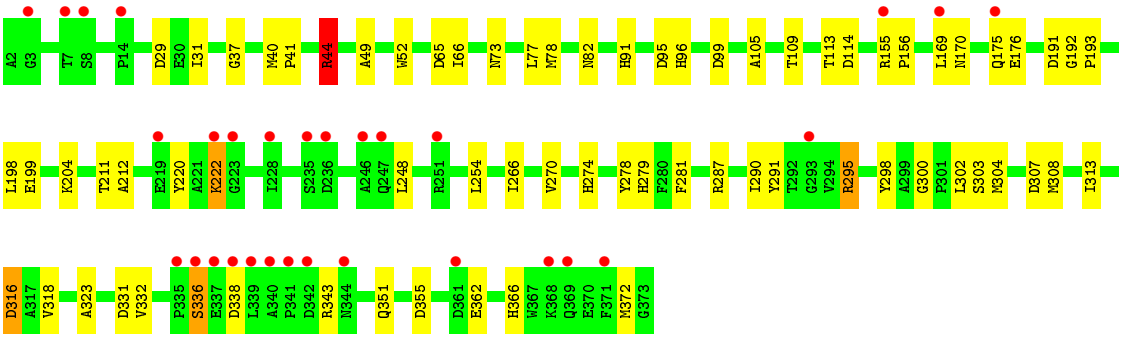
• Molecule 1: Metallo-beta-lactamases PNGM-1

Chain F:



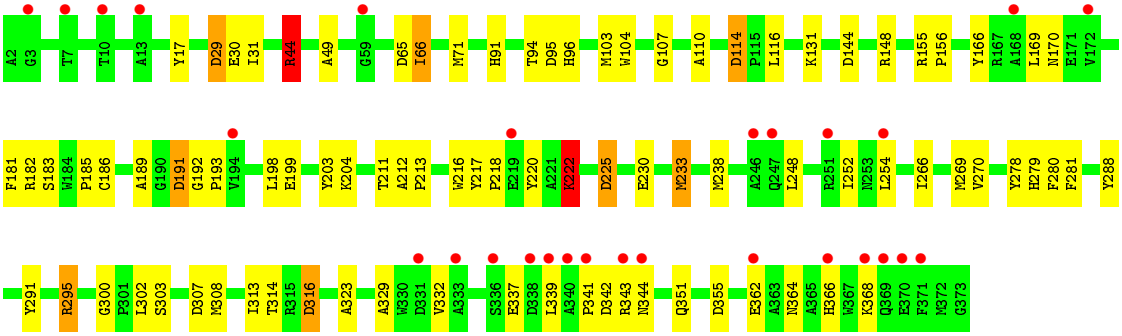
• Molecule 1: Metallo-beta-lactamases PNGM-1

Chain G:



• Molecule 1: Metallo-beta-lactamases PNGM-1

Chain H:


A2 G3 T7 T10 A13 Y17 D29 E30 I31 R44 A49 G59 D65 I66 M71 H91 T94 D95 H96 M103 W104 G107 A110 D114 P115 L116 K131 D144 R148 R155 P156 Y166 R167 A168 L169 N170 E171 V172
F181 R182 S183 W184 P185 C186 A189 G190 D191 G192 P193 V194 L198 E199 Y203 K204 T211 A212 P213 W216 Y217 P218 E219 Y220 A221 K222 D225 E230 M233 M238 A246 Q247 L248 R251 I252 M253 L254 I266 M269 V270 Y278 H279 F280 P281 Y288
Y291 R296 G300 P301 L302 S303 D307 M308 I313 T314 R315 D316 A323 A329 W330 D331 V332 A333 S336 E337 D338 L339 A340 P341 D342 R343 N344 Q351 D355 E362 A363 N364 A365 H366 W367 K368 Q369 E370 F371 M372 G373

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.86Å 83.12Å 162.83Å 90.00° 110.18° 90.00°	Depositor
Resolution (Å)	34.93 – 2.29 34.93 – 2.28	Depositor EDS
% Data completeness (in resolution range)	97.4 (34.93-2.29) 97.5 (34.93-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.47 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.211 , 0.274 0.217 , 0.279	Depositor DCC
R_{free} test set	6795 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23910	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 89.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9735e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN

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	0.87	0/3002	0.90	4/4064 (0.1%)
1	B	0.89	0/3002	0.92	7/4064 (0.2%)
1	C	0.80	0/3002	0.89	5/4064 (0.1%)
1	D	0.83	0/3002	0.91	7/4064 (0.2%)
1	E	0.79	0/3002	0.89	5/4064 (0.1%)
1	F	0.80	1/3002 (0.0%)	0.91	9/4064 (0.2%)
1	G	0.80	1/3002 (0.0%)	0.88	4/4064 (0.1%)
1	H	0.76	0/3002	0.87	4/4064 (0.1%)
All	All	0.82	2/24016 (0.0%)	0.90	45/32512 (0.1%)

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	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	52	TRP	CB-CG	-6.76	1.38	1.50
1	F	52	TRP	CB-CG	-5.16	1.41	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	295	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	F	44	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	E	44	ARG	NE-CZ-NH2	-8.61	115.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	345	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	C	295	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	E	345	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	D	345	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	H	44	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	44	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	295	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	G	44	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	G	295	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	C	61	LYS	CD-CE-NZ	-6.62	96.47	111.70
1	B	295	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	F	345	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	D	273	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	D	61	LYS	CD-CE-NZ	-6.50	96.75	111.70
1	H	65	ASP	CB-CG-OD2	6.43	124.08	118.30
1	B	103	MSE	CA-CB-CG	6.38	124.14	113.30
1	A	345	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	158	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	E	345	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	287	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	295	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	355	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	D	210	ASP	CB-CG-OD1	5.75	123.48	118.30
1	D	295	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	F	287	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	G	287	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	H	44	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	F	327	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	E	44	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	F	191	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	G	99	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	44	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	F	44	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	287	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	H	295	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	127	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	327	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	F	16	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	103	MSE	CA-CB-CG	5.07	121.91	113.30
1	F	295	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	345	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	32	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	E	151	THR	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	2933	0	2754	31	1
1	B	2933	0	2754	30	0
1	C	2933	0	2754	28	0
1	D	2933	0	2754	16	0
1	E	2933	0	2754	31	0
1	F	2933	0	2754	30	1
1	G	2933	0	2754	32	0
1	H	2933	0	2754	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	79	0	0	1	0
3	B	81	0	0	0	0
3	C	46	0	0	0	0
3	D	63	0	0	0	0
3	E	53	0	0	0	0
3	F	43	0	0	3	0
3	G	39	0	0	0	0
3	H	26	0	0	0	0
All	All	23910	0	22032	218	1

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 5.

All (218) 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:E:66:ILE:HD11	1:E:71:MSE:HE1	1.36	1.02
1:A:66:ILE:HD11	1:A:71:MSE:HE1	1.64	0.80
1:D:359:ASN:ND2	1:D:361:ASP:OD1	2.16	0.79
1:F:342:ASP:O	1:F:344:ASN:N	2.17	0.77
1:G:295:ARG:NH2	1:G:300:GLY:O	2.15	0.76
1:E:342:ASP:O	1:E:344:ASN:N	2.18	0.76
1:D:295:ARG:NH2	1:D:300:GLY:O	2.21	0.74
1:H:295:ARG:NH2	1:H:300:GLY:O	2.22	0.73
1:B:44:ARG:NH2	1:B:283:ASP:OD1	2.22	0.73
1:F:40:MSE:HG3	3:F:539:HOH:O	1.90	0.71
1:B:55:GLU:OE1	1:B:61:LYS:HE2	1.92	0.69
1:H:211:THR:OG1	1:H:212:ALA:O	2.11	0.68
1:H:185:PRO:HG2	1:H:216:TRP:CE3	2.31	0.66
1:G:113:THR:O	1:G:155:ARG:NH2	2.29	0.66
1:E:291:TYR:CZ	1:E:295:ARG:HD2	2.31	0.65
1:C:359:ASN:ND2	1:C:361:ASP:OD2	2.29	0.65
1:C:364:ASN:O	1:C:368:LYS:HB2	1.97	0.65
1:D:238:MSE:HE2	1:D:252:ILE:HD13	1.79	0.65
1:A:55:GLU:OE1	1:A:61:LYS:HE2	1.97	0.64
1:C:44:ARG:HD2	1:H:329:ALA:O	1.99	0.63
1:B:238:MSE:HE2	1:B:252:ILE:HD13	1.81	0.63
1:H:364:ASN:O	1:H:368:LYS:HB2	1.99	0.62
1:C:44:ARG:HD3	1:C:281:PHE:CZ	2.34	0.62
1:A:297:ASN:ND2	1:F:363:ALA:HB1	2.15	0.62
1:B:94:THR:HG23	1:E:144:ASP:OD2	1.99	0.62
1:A:63:ILE:CD1	1:A:103:MSE:HE3	2.29	0.62
1:G:31:ILE:HB	1:G:313:ILE:HB	1.83	0.61
1:F:198:LEU:C	1:F:198:LEU:HD23	2.23	0.59
1:A:329:ALA:O	1:F:44:ARG:HD2	2.03	0.58
1:H:181:PHE:CZ	1:H:198:LEU:HD12	2.38	0.58
1:H:66:ILE:HD12	1:H:103:MSE:HE3	1.85	0.58
1:E:238:MSE:HE2	1:E:252:ILE:HD13	1.86	0.58
1:F:17:TYR:CE2	1:G:78:MSE:HE2	2.39	0.58
1:F:174:TYR:HB3	1:F:181:PHE:HB2	1.86	0.57
1:F:40:MSE:SE	3:F:539:HOH:O	2.73	0.57
1:B:63:ILE:CD1	1:B:103:MSE:HE3	2.35	0.57
1:D:155:ARG:N	1:D:156:PRO:HD2	2.20	0.57
1:B:251:ARG:HD3	1:B:255:ASP:OD2	2.05	0.56
1:C:155:ARG:N	1:C:156:PRO:HD2	2.20	0.56
1:E:266:ILE:O	1:E:270:VAL:HG23	2.05	0.56
1:C:40:MSE:HB3	1:C:41:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:HE	1:A:343:ARG:HA	1.71	0.55
1:C:40:MSE:HB3	1:C:41:PRO:CD	2.37	0.55
1:G:291:TYR:HB2	1:G:304:MSE:HE2	1.88	0.55
1:H:29:ASP:O	1:H:203:TYR:OH	2.18	0.55
1:B:329:ALA:O	1:E:44:ARG:HD2	2.07	0.55
1:F:44:ARG:HD3	1:F:281:PHE:CE1	2.42	0.54
1:H:218:PRO:HB3	1:H:269:MSE:HE2	1.88	0.54
1:C:55:GLU:OE1	1:C:61:LYS:HE2	2.08	0.54
1:G:198:LEU:HD23	1:G:199:GLU:N	2.23	0.54
1:G:351:GLN:NE2	1:G:355:ASP:OD1	2.32	0.54
1:H:170:ASN:O	1:H:182:ARG:NH1	2.40	0.54
1:H:192:GLY:N	1:H:193:PRO:CD	2.71	0.54
1:G:308:MSE:HE3	1:G:323:ALA:HB3	1.89	0.54
1:D:144:ASP:OD1	1:D:148:ARG:NH1	2.41	0.54
1:F:40:MSE:CG	3:F:539:HOH:O	2.50	0.54
1:H:316:ASP:N	1:H:316:ASP:OD1	2.31	0.53
1:A:349:TYR:CG	1:A:354:LEU:HD21	2.43	0.53
1:E:364:ASN:O	1:E:368:LYS:HB2	2.09	0.53
1:H:49:ALA:HB1	1:H:95:ASP:HB2	1.90	0.53
1:A:86:LYS:NZ	3:A:502:HOH:O	2.35	0.53
1:E:233:MSE:HE1	1:E:242:TYR:HE2	1.74	0.52
1:D:239:MSE:O	1:D:243:ASN:HA	2.09	0.52
1:B:188:HIS:CE1	1:B:210:ASP:HB3	2.45	0.52
1:F:364:ASN:O	1:F:368:LYS:HB2	2.07	0.52
1:A:128:MSE:HE3	1:F:143:TRP:CD1	2.44	0.51
1:H:238:MSE:HE2	1:H:252:ILE:HD13	1.93	0.51
1:C:280:PHE:CZ	1:C:304:MSE:HE3	2.46	0.51
1:C:291:TYR:CZ	1:C:295:ARG:HD2	2.45	0.51
1:H:44:ARG:HD3	1:H:281:PHE:CE1	2.46	0.50
1:H:213:PRO:HB3	1:H:266:ILE:HD11	1.93	0.50
1:G:204:LYS:NZ	1:G:222:LYS:O	2.40	0.50
1:B:74:ILE:HG21	1:B:103:MSE:HE1	1.94	0.50
1:G:170:ASN:ND2	1:G:220:TYR:CD1	2.79	0.50
1:H:31:ILE:HB	1:H:313:ILE:HB	1.92	0.50
1:E:198:LEU:C	1:E:198:LEU:HD23	2.31	0.50
1:E:217:TYR:HB3	1:E:218:PRO:HD3	1.94	0.50
1:G:40:MSE:HB3	1:G:41:PRO:HD2	1.93	0.50
1:F:44:ARG:HD3	1:F:281:PHE:CZ	2.46	0.49
1:C:368:LYS:HG2	1:C:372:MSE:HE2	1.93	0.49
1:G:290:ILE:HG22	1:G:304:MSE:HE1	1.93	0.49
1:C:241:LYS:O	1:E:2:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:MSE:CB	1:C:41:PRO:CD	2.90	0.49
1:F:31:ILE:HB	1:F:313:ILE:HB	1.94	0.49
1:H:114:ASP:HA	1:H:155:ARG:NH2	2.28	0.49
1:A:364:ASN:O	1:A:368:LYS:HB2	2.12	0.49
1:C:63:ILE:CD1	1:C:103:MSE:HE3	2.42	0.49
1:G:291:TYR:CE1	1:G:302:LEU:HD23	2.47	0.49
1:H:170:ASN:ND2	1:H:220:TYR:CD1	2.80	0.49
1:G:49:ALA:HB1	1:G:95:ASP:HB2	1.94	0.48
1:G:44:ARG:HD3	1:G:281:PHE:CE1	2.48	0.48
1:A:74:ILE:HG21	1:A:103:MSE:HE1	1.95	0.48
1:H:91:HIS:CE1	1:H:96:HIS:CD2	3.01	0.48
1:H:71:MSE:SE	1:H:103:MSE:HE2	2.63	0.48
1:G:37:GLY:HA3	1:G:49:ALA:O	2.13	0.48
1:B:329:ALA:H	1:E:44:ARG:HG2	1.77	0.48
1:A:168:ALA:HB1	1:A:171:GLU:CG	2.44	0.48
1:B:40:MSE:HB3	1:B:41:PRO:HD2	1.94	0.48
1:G:266:ILE:O	1:G:270:VAL:HG23	2.14	0.48
1:G:274:HIS:CB	1:G:318:VAL:HG11	2.44	0.48
1:C:217:TYR:HB3	1:C:218:PRO:HD3	1.95	0.47
1:E:109:THR:CG2	1:E:148:ARG:HH21	2.27	0.47
1:H:144:ASP:OD1	1:H:148:ARG:NH1	2.48	0.47
1:F:266:ILE:O	1:F:270:VAL:HG23	2.15	0.47
1:H:198:LEU:HD23	1:H:199:GLU:N	2.29	0.47
1:H:217:TYR:HB3	1:H:218:PRO:HD3	1.96	0.47
1:B:356:GLY:HA3	1:E:216:TRP:CH2	2.49	0.47
1:E:44:ARG:HD3	1:E:281:PHE:CE1	2.49	0.47
1:F:217:TYR:HB3	1:F:218:PRO:HD3	1.97	0.47
1:A:217:TYR:HB3	1:A:218:PRO:HD3	1.97	0.47
1:B:40:MSE:HE3	1:B:41:PRO:HD2	1.96	0.47
1:A:44:ARG:HD3	1:A:281:PHE:CE1	2.50	0.47
1:B:198:LEU:HD23	1:B:199:GLU:N	2.29	0.47
1:F:166:TYR:OH	1:F:191:ASP:OD2	2.14	0.47
1:A:44:ARG:NH2	1:A:283:ASP:OD1	2.44	0.46
1:A:40:MSE:HE3	1:A:41:PRO:HD2	1.97	0.46
1:B:49:ALA:HB1	1:B:95:ASP:HB2	1.97	0.46
1:G:211:THR:OG1	1:G:212:ALA:O	2.21	0.46
1:B:44:ARG:HH22	1:B:283:ASP:CG	2.16	0.46
1:B:349:TYR:CG	1:B:354:LEU:HD21	2.50	0.46
1:E:40:MSE:HE1	1:E:233:MSE:HE2	1.98	0.46
1:G:82:ASN:ND2	1:G:336:SER:OG	2.48	0.46
1:B:363:ALA:HB1	1:E:297:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:TYR:HD2	1:H:225:ASP:OD2	1.98	0.46
1:C:44:ARG:HD3	1:C:281:PHE:CE1	2.51	0.46
1:A:251:ARG:HD3	1:A:255:ASP:OD2	2.16	0.46
1:B:245:PRO:HG2	1:B:248:LEU:HD22	1.97	0.45
1:D:55:GLU:OE1	1:D:61:LYS:HE2	2.15	0.45
1:A:18:VAL:HG22	1:D:78:MSE:HE1	1.97	0.45
1:D:40:MSE:HG3	1:D:281:PHE:CE1	2.51	0.45
1:H:186:CYS:HB3	1:H:211:THR:HB	1.97	0.45
1:H:233:MSE:HE2	1:H:280:PHE:HB2	1.97	0.45
1:B:42:THR:HG22	1:B:281:PHE:HZ	1.82	0.45
1:D:45:ARG:HD3	1:G:73:ASN:OD1	2.16	0.45
1:H:351:GLN:NE2	1:H:355:ASP:OD1	2.36	0.45
1:A:44:ARG:HD2	1:F:329:ALA:O	2.16	0.45
1:F:91:HIS:HB3	1:F:193:PRO:HB3	1.98	0.45
1:H:307:ASP:O	1:H:308:MSE:HB2	2.15	0.45
1:B:63:ILE:HD13	1:B:103:MSE:HE3	1.98	0.45
1:E:273:ARG:O	1:E:301:PRO:HG2	2.17	0.44
1:A:144:ASP:OD2	1:F:94:THR:HG23	2.16	0.44
1:F:152:ILE:HG22	1:F:153:ASN:N	2.33	0.44
1:A:18:VAL:HG22	1:D:78:MSE:CE	2.47	0.44
1:B:128:MSE:HE3	1:E:143:TRP:CD1	2.53	0.44
1:B:198:LEU:C	1:B:198:LEU:HD23	2.38	0.44
1:G:78:MSE:HA	1:G:332:VAL:HG11	1.98	0.44
1:A:66:ILE:O	1:A:66:ILE:HG23	2.18	0.44
1:D:40:MSE:HB3	1:D:41:PRO:HD2	1.99	0.44
1:D:93:HIS:HB3	1:D:95:ASP:OD2	2.17	0.44
1:H:204:LYS:NZ	1:H:222:LYS:O	2.50	0.44
1:E:55:GLU:HG2	1:E:61:LYS:HE2	1.99	0.44
1:F:144:ASP:OD1	1:F:148:ARG:NH1	2.51	0.43
1:H:104:TRP:HA	1:H:116:LEU:HD11	2.00	0.43
1:H:266:ILE:O	1:H:270:VAL:HG23	2.18	0.43
1:C:295:ARG:NH2	1:C:300:GLY:O	2.33	0.43
1:A:94:THR:HG23	1:F:144:ASP:OD2	2.19	0.43
1:A:40:MSE:HE1	1:A:232:TRP:CZ2	2.54	0.43
1:G:155:ARG:N	1:G:156:PRO:HD2	2.33	0.43
1:H:291:TYR:CE1	1:H:302:LEU:HD23	2.54	0.43
1:H:170:ASN:OD1	1:H:182:ARG:HD3	2.18	0.43
1:E:343:ARG:O	1:E:344:ASN:ND2	2.51	0.43
1:E:49:ALA:HB1	1:E:95:ASP:HB2	2.00	0.43
1:F:49:ALA:HB1	1:F:95:ASP:HB2	2.00	0.43
1:D:66:ILE:HG23	1:D:66:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:ASP:N	1:G:316:ASP:OD1	2.46	0.42
1:D:308:MSE:HE2	1:D:325:SER:OG	2.19	0.42
1:F:238:MSE:HE2	1:F:252:ILE:HD13	2.01	0.42
1:B:18:VAL:HG22	1:C:78:MSE:HE1	2.00	0.42
1:C:40:MSE:HG3	1:C:281:PHE:CE1	2.54	0.42
1:A:71:MSE:HE1	1:A:103:MSE:HB2	2.02	0.42
1:D:44:ARG:HD2	1:D:281:PHE:CE1	2.55	0.42
1:H:91:HIS:HB3	1:H:193:PRO:HB3	2.02	0.42
1:B:216:TRP:CH2	1:E:356:GLY:HA3	2.54	0.42
1:B:287:ARG:HD3	1:H:288:TYR:OH	2.19	0.42
1:E:144:ASP:OD1	1:E:148:ARG:NH1	2.52	0.42
1:G:192:GLY:N	1:G:193:PRO:CD	2.83	0.42
1:F:66:ILE:HD11	1:F:103:MSE:HE2	2.02	0.42
1:G:105:ALA:O	1:G:109:THR:HG23	2.20	0.42
1:A:308:MSE:HE3	1:A:323:ALA:HB3	2.02	0.42
1:F:21:PRO:HG2	1:F:325:SER:HB3	2.01	0.42
1:H:308:MSE:HE3	1:H:323:ALA:HB3	2.01	0.42
1:E:44:ARG:HD3	1:E:281:PHE:CZ	2.55	0.42
1:G:91:HIS:HE1	1:G:96:HIS:CE1	2.37	0.42
1:B:82:ASN:HD22	1:B:336:SER:HB3	1.85	0.42
1:C:101:VAL:HG13	1:C:102:SER:N	2.35	0.42
1:H:30:GLU:HG3	1:H:314:THR:HG22	2.02	0.42
1:C:93:HIS:HB3	1:C:95:ASP:OD2	2.20	0.42
1:E:31:ILE:HB	1:E:313:ILE:HB	2.02	0.42
1:G:198:LEU:HD23	1:G:198:LEU:C	2.40	0.42
1:H:155:ARG:N	1:H:156:PRO:CD	2.83	0.41
1:H:212:ALA:HB1	1:H:213:PRO:CD	2.50	0.41
1:B:44:ARG:HD3	1:B:281:PHE:CE1	2.54	0.41
1:E:78:MSE:HE2	1:H:17:TYR:CE2	2.56	0.41
1:E:192:GLY:N	1:E:193:PRO:CD	2.83	0.41
1:H:166:TYR:OH	1:H:191:ASP:OD2	2.18	0.41
1:A:168:ALA:HB1	1:A:171:GLU:HG3	2.01	0.41
1:F:280:PHE:CZ	1:F:304:MSE:HE3	2.55	0.41
1:G:307:ASP:O	1:G:308:MSE:HB2	2.21	0.41
1:B:18:VAL:HG22	1:C:78:MSE:CE	2.51	0.41
1:B:291:TYR:CZ	1:B:295:ARG:HD2	2.55	0.41
1:H:66:ILE:CD1	1:H:103:MSE:HE3	2.50	0.41
1:H:332:VAL:HG13	1:H:332:VAL:O	2.21	0.41
1:C:155:ARG:N	1:C:156:PRO:CD	2.83	0.41
1:G:295:ARG:HA	1:G:298:TYR:O	2.20	0.41
1:A:143:TRP:CD1	1:F:128:MSE:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASP:OD2	1:H:94:THR:HG23	2.21	0.41
1:C:198:LEU:C	1:C:198:LEU:HD23	2.41	0.41
1:C:147:THR:HB	1:H:189:ALA:HB1	2.03	0.40
1:C:287:ARG:HD3	1:E:287:ARG:HD2	2.02	0.40
1:E:37:GLY:HA3	1:E:49:ALA:O	2.22	0.40
1:H:29:ASP:O	1:H:203:TYR:CE1	2.73	0.40
1:A:291:TYR:CZ	1:A:295:ARG:HD2	2.56	0.40
1:A:363:ALA:HB1	1:F:297:ASN:ND2	2.36	0.40
1:G:77:LEU:HD23	1:G:77:LEU:HA	1.84	0.40
1:C:368:LYS:CG	1:C:372:MSE:HE2	2.52	0.40
1:G:91:HIS:CE1	1:G:96:HIS:CD2	3.09	0.40
1:H:107:GLY:O	1:H:110:ALA:HB3	2.20	0.40
1:A:114:ASP:HB3	1:A:115:PRO:HD2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:SER:O	1:F:344:ASN:ND2[2_455]	2.19	0.01

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	370/372 (100%)	350 (95%)	18 (5%)	2 (0%)	29	35
1	B	370/372 (100%)	353 (95%)	14 (4%)	3 (1%)	19	23
1	C	370/372 (100%)	344 (93%)	23 (6%)	3 (1%)	19	23
1	D	370/372 (100%)	354 (96%)	13 (4%)	3 (1%)	19	23
1	E	370/372 (100%)	343 (93%)	23 (6%)	4 (1%)	14	15
1	F	370/372 (100%)	340 (92%)	24 (6%)	6 (2%)	9	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	370/372 (100%)	351 (95%)	14 (4%)	5 (1%)	11	11
1	H	370/372 (100%)	346 (94%)	19 (5%)	5 (1%)	11	11
All	All	2960/2976 (100%)	2781 (94%)	148 (5%)	31 (1%)	15	17

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	341	PRO
1	E	343	ARG
1	F	343	ARG
1	C	336	SER
1	D	243	ASN
1	E	336	SER
1	G	222	LYS
1	H	222	LYS
1	H	279	HIS
1	D	65	ASP
1	F	66	ILE
1	F	336	SER
1	G	65	ASP
1	G	279	HIS
1	H	342	ASP
1	B	279	HIS
1	B	341	PRO
1	C	360	VAL
1	F	15	LYS
1	F	65	ASP
1	G	336	SER
1	A	341	PRO
1	B	66	ILE
1	E	66	ILE
1	A	66	ILE
1	D	66	ILE
1	F	341	PRO
1	G	66	ILE
1	H	341	PRO
1	H	66	ILE
1	C	66	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/285 (106%)	290 (96%)	12 (4%)	31	44
1	B	302/285 (106%)	290 (96%)	12 (4%)	31	44
1	C	302/285 (106%)	283 (94%)	19 (6%)	18	24
1	D	302/285 (106%)	288 (95%)	14 (5%)	27	38
1	E	302/285 (106%)	289 (96%)	13 (4%)	29	40
1	F	302/285 (106%)	291 (96%)	11 (4%)	35	49
1	G	302/285 (106%)	284 (94%)	18 (6%)	19	26
1	H	302/285 (106%)	280 (93%)	22 (7%)	14	18
All	All	2416/2280 (106%)	2295 (95%)	121 (5%)	24	34

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	44	ARG
1	A	158	ASP
1	A	169	LEU
1	A	230	GLU
1	A	247	GLN
1	A	248	LEU
1	A	310	VAL
1	A	339	LEU
1	A	343	ARG
1	A	362	GLU
1	A	368	LYS
1	B	42	THR
1	B	44	ARG
1	B	158	ASP
1	B	191	ASP
1	B	230	GLU
1	B	247	GLN
1	B	248	LEU

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Mol	Chain	Res	Type
1	B	252	ILE
1	B	254	LEU
1	B	310	VAL
1	B	337	GLU
1	B	338	ASP
1	C	40	MSE
1	C	44	ARG
1	C	131	LYS
1	C	158	ASP
1	C	169	LEU
1	C	171	GLU
1	C	176	GLU
1	C	193	PRO
1	C	222	LYS
1	C	230	GLU
1	C	243	ASN
1	C	248	LEU
1	C	331	ASP
1	C	336	SER
1	C	337	GLU
1	C	338	ASP
1	C	347	SER
1	C	361	ASP
1	C	369	GLN
1	D	158	ASP
1	D	169	LEU
1	D	171	GLU
1	D	175	GLN
1	D	222	LYS
1	D	243	ASN
1	D	248	LEU
1	D	252	ILE
1	D	254	LEU
1	D	331	ASP
1	D	336	SER
1	D	338	ASP
1	D	361	ASP
1	D	362	GLU
1	E	44	ARG
1	E	131	LYS
1	E	152	ILE
1	E	169	LEU

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Mol	Chain	Res	Type
1	E	251	ARG
1	E	254	LEU
1	E	278	TYR
1	E	310	VAL
1	E	332	VAL
1	E	336	SER
1	E	343	ARG
1	E	345	ARG
1	E	362	GLU
1	F	15	LYS
1	F	44	ARG
1	F	135	GLU
1	F	251	ARG
1	F	254	LEU
1	F	278	TYR
1	F	310	VAL
1	F	332	VAL
1	F	343	ARG
1	F	362	GLU
1	F	372	MSE
1	G	29	ASP
1	G	44	ARG
1	G	114	ASP
1	G	169	LEU
1	G	175	GLN
1	G	176	GLU
1	G	191	ASP
1	G	248	LEU
1	G	254	LEU
1	G	278	TYR
1	G	303	SER
1	G	316	ASP
1	G	331	ASP
1	G	338	ASP
1	G	343	ARG
1	G	362	GLU
1	G	366	HIS
1	G	372	MSE
1	H	29	ASP
1	H	44	ARG
1	H	114	ASP
1	H	131	LYS

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Mol	Chain	Res	Type
1	H	169	LEU
1	H	183	SER
1	H	191	ASP
1	H	222	LYS
1	H	225	ASP
1	H	230	GLU
1	H	233	MSE
1	H	248	LEU
1	H	254	LEU
1	H	278	TYR
1	H	303	SER
1	H	316	ASP
1	H	337	GLU
1	H	339	LEU
1	H	343	ARG
1	H	344	ASN
1	H	362	GLU
1	H	366	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	297	ASN
1	A	369	GLN
1	B	175	GLN
1	B	344	ASN
1	C	351	GLN
1	D	359	ASN
1	E	75	GLN
1	E	344	ASN
1	F	82	ASN
1	F	344	ASN
1	F	369	GLN
1	G	82	ASN
1	G	243	ASN
1	G	344	ASN
1	H	243	ASN
1	H	344	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	355/372 (95%)	0.10	19 (5%)	25	32	9, 20, 58, 103	0
1	B	355/372 (95%)	0.12	20 (5%)	24	30	9, 19, 56, 109	0
1	C	355/372 (95%)	0.26	29 (8%)	11	15	13, 27, 70, 122	0
1	D	355/372 (95%)	0.23	26 (7%)	15	20	13, 26, 62, 114	0
1	E	355/372 (95%)	0.32	26 (7%)	15	20	12, 29, 59, 108	0
1	F	355/372 (95%)	0.33	26 (7%)	15	20	13, 31, 62, 100	0
1	G	355/372 (95%)	0.55	30 (8%)	10	14	15, 35, 61, 114	0
1	H	355/372 (95%)	0.66	28 (7%)	12	17	18, 39, 67, 88	0
All	All	2840/2976 (95%)	0.32	204 (7%)	15	20	9, 29, 64, 122	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	340	ALA	8.2
1	C	340	ALA	7.7
1	E	338	ASP	6.9
1	D	340	ALA	6.5
1	C	338	ASP	6.4
1	H	341	PRO	6.2
1	F	343	ARG	6.0
1	A	338	ASP	5.9
1	E	343	ARG	5.9
1	B	338	ASP	5.7
1	D	343	ARG	5.7
1	D	338	ASP	5.6
1	F	338	ASP	5.5
1	B	373	GLY	5.4
1	E	339	LEU	5.2
1	C	343	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	248	LEU	4.9
1	E	7	THR	4.9
1	F	151	THR	4.9
1	G	246	ALA	4.8
1	C	339	LEU	4.7
1	G	339	LEU	4.6
1	G	341	PRO	4.5
1	G	7	THR	4.4
1	H	371	PHE	4.4
1	H	333	ALA	4.4
1	A	246	ALA	4.3
1	F	339	LEU	4.3
1	D	369	GLN	4.3
1	A	344	ASN	4.2
1	D	335	PRO	4.2
1	B	344	ASN	4.2
1	H	339	LEU	4.2
1	A	337	GLU	4.1
1	F	369	GLN	4.1
1	G	247	GLN	4.1
1	F	10	THR	4.0
1	G	371	PHE	4.0
1	B	335	PRO	4.0
1	D	339	LEU	4.0
1	A	373	GLY	3.9
1	E	369	GLN	3.9
1	A	247	GLN	3.9
1	C	369	GLN	3.9
1	H	168	ALA	3.9
1	B	369	GLN	3.8
1	H	10	THR	3.8
1	F	337	GLU	3.7
1	A	250	LEU	3.7
1	E	337	GLU	3.7
1	G	169	LEU	3.7
1	F	7	THR	3.6
1	C	371	PHE	3.6
1	A	339	LEU	3.6
1	A	342	ASP	3.6
1	E	247	GLN	3.6
1	F	336	SER	3.5
1	G	335	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	3.5
1	H	340	ALA	3.5
1	D	366	HIS	3.5
1	B	248	LEU	3.4
1	D	373	GLY	3.4
1	E	14	PRO	3.4
1	A	336	SER	3.4
1	H	344	ASN	3.4
1	B	247	GLN	3.3
1	C	373	GLY	3.3
1	B	340	ALA	3.3
1	E	371	PHE	3.3
1	A	248	LEU	3.3
1	D	341	PRO	3.3
1	G	344	ASN	3.3
1	H	338	ASP	3.3
1	C	247	GLN	3.2
1	B	366	HIS	3.2
1	F	13	ALA	3.2
1	G	368	LYS	3.2
1	B	337	GLU	3.1
1	F	366	HIS	3.1
1	F	247	GLN	3.1
1	B	336	SER	3.1
1	D	371	PHE	3.1
1	H	247	GLN	3.1
1	A	335	PRO	3.1
1	C	341	PRO	3.1
1	F	371	PHE	3.1
1	C	360	VAL	3.1
1	C	335	PRO	3.1
1	B	339	LEU	3.0
1	E	246	ALA	3.0
1	C	248	LEU	3.0
1	C	243	ASN	3.0
1	D	251	ARG	3.0
1	E	335	PRO	3.0
1	H	219	GLU	2.9
1	E	336	SER	2.9
1	G	8	SER	2.9
1	E	251	ARG	2.9
1	D	337	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	293	GLY	2.9
1	C	342	ASP	2.9
1	A	366	HIS	2.9
1	D	243	ASN	2.8
1	C	344	ASN	2.8
1	H	343	ARG	2.8
1	A	340	ALA	2.8
1	H	366	HIS	2.8
1	A	343	ARG	2.8
1	C	337	GLU	2.8
1	C	363	ALA	2.8
1	D	336	SER	2.8
1	D	247	GLN	2.8
1	D	249	ALA	2.7
1	D	342	ASP	2.7
1	H	251	ARG	2.7
1	B	243	ASN	2.7
1	D	344	ASN	2.7
1	A	369	GLN	2.7
1	C	250	LEU	2.7
1	H	3	GLY	2.7
1	F	152	ILE	2.7
1	G	336	SER	2.7
1	G	155	ARG	2.7
1	C	366	HIS	2.7
1	B	342	ASP	2.7
1	H	331	ASP	2.6
1	C	246	ALA	2.6
1	F	12	ILE	2.6
1	G	219	GLU	2.6
1	H	362	GLU	2.6
1	A	367	TRP	2.6
1	H	7	THR	2.6
1	G	251	ARG	2.6
1	H	369	GLN	2.6
1	C	254	LEU	2.5
1	H	336	SER	2.5
1	E	151	THR	2.5
1	F	341	PRO	2.5
1	G	14	PRO	2.5
1	H	370	GLU	2.5
1	B	362	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	373	GLY	2.5
1	B	370	GLU	2.5
1	H	254	LEU	2.5
1	F	340	ALA	2.5
1	E	10	THR	2.5
1	D	245	PRO	2.4
1	C	336	SER	2.4
1	D	240	THR	2.4
1	G	3	GLY	2.4
1	G	338	ASP	2.4
1	E	340	ALA	2.4
1	F	6	VAL	2.4
1	C	362	GLU	2.4
1	F	246	ALA	2.4
1	G	222	LYS	2.4
1	C	235	SER	2.4
1	G	228	ILE	2.4
1	E	248	LEU	2.4
1	H	13	ALA	2.4
1	H	246	ALA	2.3
1	G	337	GLU	2.3
1	G	236	ASP	2.3
1	F	248	LEU	2.3
1	C	244	GLN	2.3
1	H	59	GLY	2.2
1	C	251	ARG	2.2
1	D	7	THR	2.2
1	A	368	LYS	2.2
1	E	15	LYS	2.2
1	G	223	GLY	2.2
1	F	316	ASP	2.2
1	F	2	ALA	2.2
1	D	236	ASP	2.2
1	H	172	VAL	2.2
1	G	361	ASP	2.2
1	G	369	GLN	2.2
1	D	246	ALA	2.1
1	D	362	GLU	2.1
1	E	342	ASP	2.1
1	E	368	LYS	2.1
1	F	370	GLU	2.1
1	B	368	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	334	GLY	2.1
1	G	235	SER	2.1
1	E	11	GLY	2.1
1	H	368	LYS	2.1
1	E	12	ILE	2.1
1	D	361	ASP	2.1
1	E	13	ALA	2.1
1	G	342	ASP	2.0
1	F	344	ASN	2.0
1	B	246	ALA	2.0
1	A	370	GLU	2.0
1	F	8	SER	2.0
1	C	355	ASP	2.0
1	E	236	ASP	2.0
1	F	243	ASN	2.0
1	G	175	GLN	2.0
1	B	251	ARG	2.0
1	C	6	VAL	2.0
1	H	194	VAL	2.0
1	C	368	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	G	401	1/1	0.98	0.06	41,41,41,41	0
2	ZN	H	401	1/1	0.98	0.11	45,45,45,45	0
2	ZN	F	401	1/1	0.98	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	401	1/1	0.98	0.08	33,33,33,33	0
2	ZN	C	402	1/1	0.99	0.10	28,28,28,28	0
2	ZN	E	401	1/1	0.99	0.07	33,33,33,33	0
2	ZN	A	401	1/1	0.99	0.07	30,30,30,30	0
2	ZN	H	402	1/1	0.99	0.09	33,33,33,33	0
2	ZN	C	401	1/1	0.99	0.05	39,39,39,39	0
2	ZN	G	402	1/1	0.99	0.10	26,26,26,26	0
2	ZN	B	402	1/1	0.99	0.12	19,19,19,19	0
2	ZN	D	401	1/1	0.99	0.05	37,37,37,37	0
2	ZN	A	402	1/1	0.99	0.09	21,21,21,21	0
2	ZN	F	402	1/1	0.99	0.09	24,24,24,24	0
2	ZN	E	402	1/1	0.99	0.10	24,24,24,24	0
2	ZN	D	402	1/1	1.00	0.08	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.