



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:23 PM UTC

PDB ID : 6J4N / pdb_00006j4n
Title : Structure of papua new guinea MBL-1(PNGM-1) native
Authors : Hong, M.K.; Park, K.S.; Jeon, J.H.; Lee, J.H.; Park, Y.S.; Lee, S.H.; Kang, L.W.
Deposited on : 2019-01-10
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

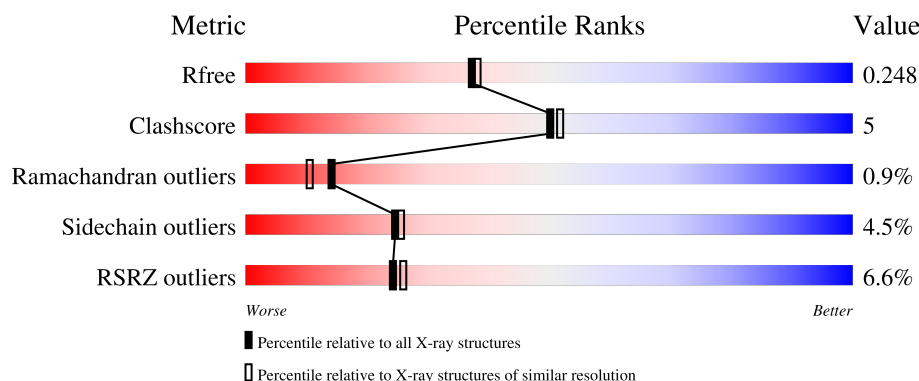
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



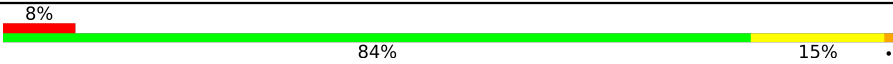
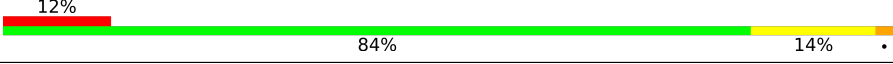
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	372	4% 86% 13% .
1	B	372	4% 86% 13% .
1	C	372	8% 85% 13% .
1	D	372	5% 89% 9% .
1	E	372	5% 83% 15% ..

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Mol	Chain	Length	Quality of chain
1	F	372	 8% 84% 15% •
1	G	372	 8% 85% 14% •
1	H	372	 12% 84% 14% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24786 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	0	0	0
			2933	1853	506	554	20			
1	B	372	Total	C	N	O	S	0	0	0
			2933	1853	506	554	20			
1	C	372	Total	C	N	O	S	0	0	0
			2933	1853	506	554	20			
1	D	372	Total	C	N	O	S	0	0	0
			2933	1853	506	554	20			
1	E	372	Total	C	N	O	S	0	0	0
			2933	1853	506	554	20			
1	F	372	Total	C	N	O	S	0	0	0
			2933	1853	506	554	20			
1	G	372	Total	C	N	O	S	0	0	0
			2933	1853	506	554	20			
1	H	372	Total	C	N	O	S	0	0	0
			2933	1853	506	554	20			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0

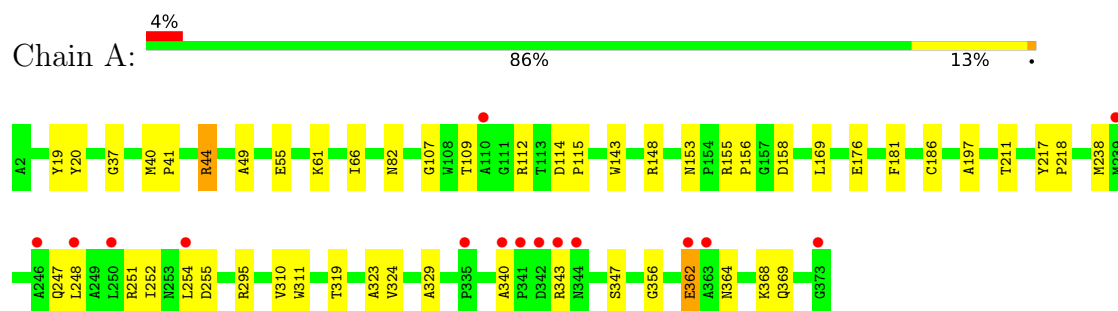
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	186	Total 186	O 186	0	0
3	B	205	Total 205	O 205	0	0
3	C	165	Total 165	O 165	0	0
3	D	181	Total 181	O 181	0	0
3	E	173	Total 173	O 173	0	0
3	F	132	Total 132	O 132	0	0
3	G	137	Total 137	O 137	0	0
3	H	127	Total 127	O 127	0	0

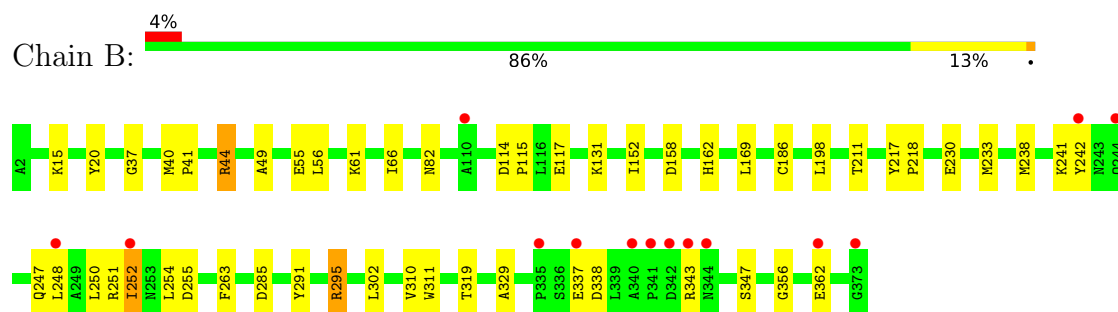
3 Residue-property plots

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.

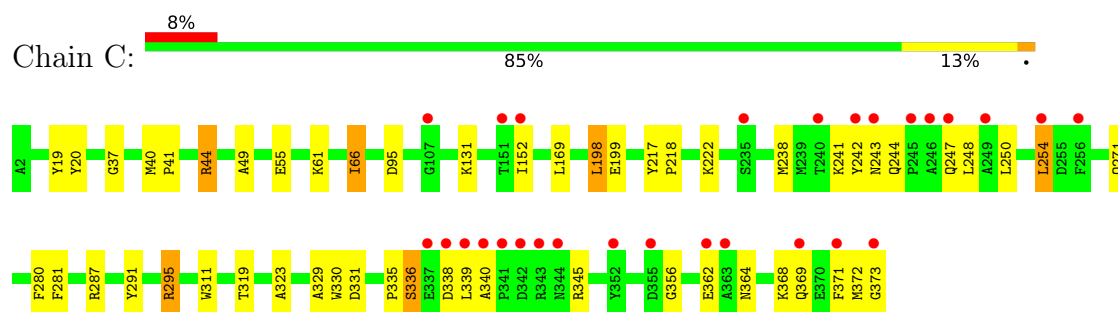
• Molecule 1: Metallo-beta-lactamases PNGM-1



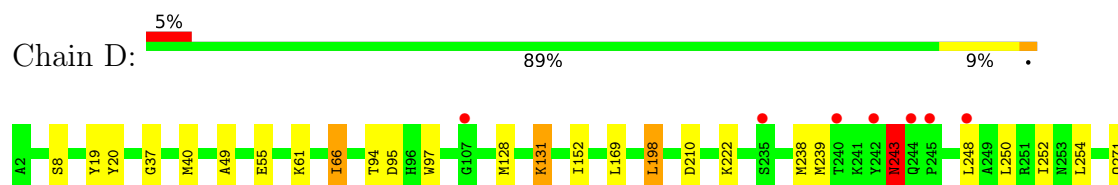
• Molecule 1: Metallo-beta-lactamases PNGM-1

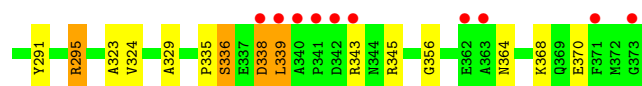


• Molecule 1: Metallo-beta-lactamases PNGM-1

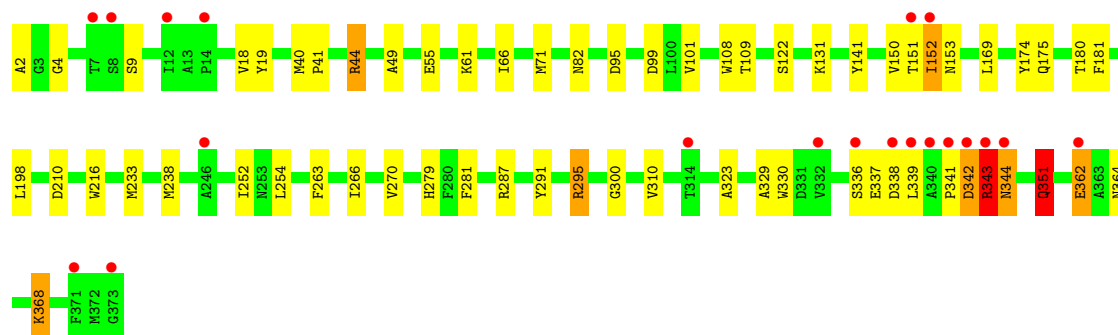
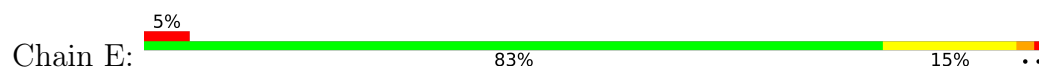


• Molecule 1: Metallo-beta-lactamases PNGM-1

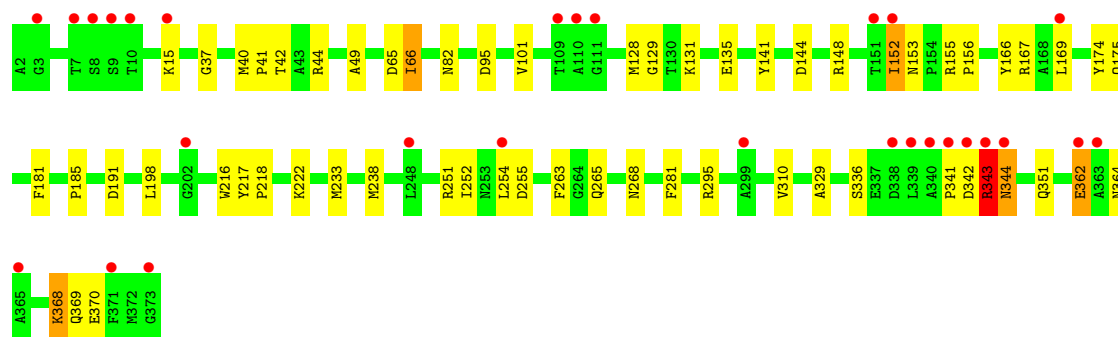
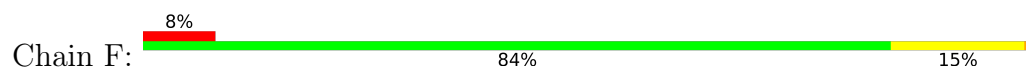




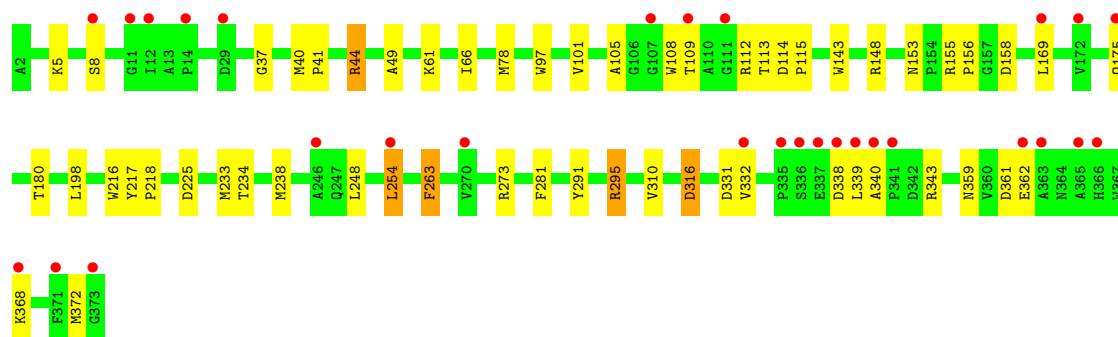
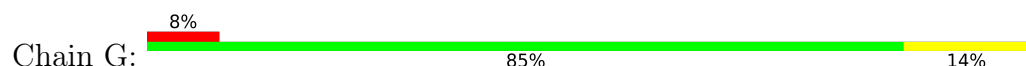
• Molecule 1: Metallo-beta-lactamases PNGM-1



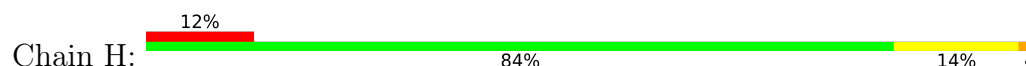
• Molecule 1: Metallo-beta-lactamases PNGM-1

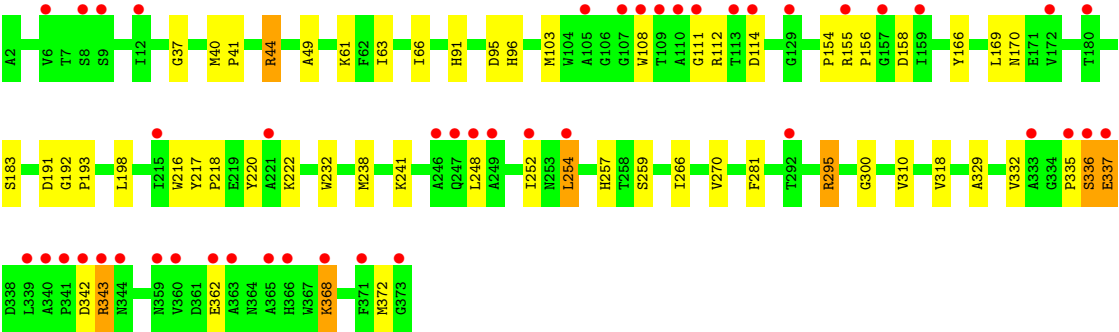


• Molecule 1: Metallo-beta-lactamases PNGM-1



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.27Å 83.02Å 163.47Å 90.00° 110.55° 90.00°	Depositor
Resolution (Å)	45.39 – 2.10 45.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.39-2.10) 98.1 (45.39-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.82 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.190 , 0.244 0.198 , 0.248	Depositor DCC
R_{free} test set	8773 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24786	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 84.26 % 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 1.7453e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.09	0/3019	1.21	2/4115 (0.0%)
1	B	1.10	2/3019 (0.1%)	1.19	1/4115 (0.0%)
1	C	1.06	1/3019 (0.0%)	1.21	2/4115 (0.0%)
1	D	1.10	2/3019 (0.1%)	1.25	5/4115 (0.1%)
1	E	1.08	1/3019 (0.0%)	1.25	7/4115 (0.2%)
1	F	1.08	0/3019	1.27	9/4115 (0.2%)
1	G	1.10	1/3019 (0.0%)	1.22	0/4115
1	H	1.10	0/3019	1.27	1/4115 (0.0%)
All	All	1.09	7/24152 (0.0%)	1.23	27/32920 (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
1	F	0	1
1	H	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	271	GLN	N-CA	6.69	1.51	1.46
1	C	271	GLN	N-CA	5.63	1.50	1.46
1	D	40	MET	N-CA	5.39	1.49	1.46
1	E	4	GLY	C-O	5.25	1.29	1.23
1	B	56	LEU	C-O	5.16	1.29	1.23
1	G	97	TRP	N-CA	5.08	1.50	1.46
1	B	198	LEU	C-O	5.03	1.30	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	ILE	CA-C-N	7.39	127.36	120.34
1	D	66	ILE	C-N-CA	7.39	127.36	120.34
1	C	66	ILE	CA-C-N	7.04	127.03	120.34
1	C	66	ILE	C-N-CA	7.04	127.03	120.34
1	F	344	ASN	CA-C-O	-6.47	115.65	121.67
1	H	154	PRO	N-CA-C	6.38	121.83	113.86
1	F	362	GLU	CB-CG-CD	5.92	122.67	112.60
1	A	362	GLU	CB-CG-CD	5.74	122.36	112.60
1	E	44	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	D	97	TRP	CA-C-N	5.64	126.35	120.03
1	D	97	TRP	C-N-CA	5.64	126.35	120.03
1	F	42	THR	CB-CA-C	5.64	118.72	110.26
1	F	129	GLY	CA-C-N	5.58	127.69	120.44
1	F	129	GLY	C-N-CA	5.58	127.69	120.44
1	E	342	ASP	CA-C-N	5.54	132.11	121.54
1	E	342	ASP	C-N-CA	5.54	132.11	121.54
1	E	210	ASP	CA-CB-CG	5.49	118.09	112.60
1	F	66	ILE	CA-C-N	5.42	125.49	120.34
1	F	66	ILE	C-N-CA	5.42	125.49	120.34
1	E	122	SER	N-CA-C	-5.39	103.58	110.53
1	D	210	ASP	CA-CB-CG	5.32	117.92	112.60
1	F	185	PRO	N-CA-C	5.29	119.61	111.57
1	B	285	ASP	CA-CB-CG	5.17	117.77	112.60
1	E	362	GLU	CB-CG-CD	5.17	121.38	112.60
1	A	362	GLU	N-CA-CB	5.15	117.48	110.01
1	E	351	GLN	CB-CG-CD	5.13	121.32	112.60
1	F	175	GLN	CB-CA-C	5.12	118.13	111.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	343	ARG	Peptide
1	F	152	ILE	Peptide
1	H	337	GLU	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	2933	0	2754	36	1
1	B	2933	0	2754	33	1
1	C	2933	0	2754	34	0
1	D	2933	0	2754	24	0
1	E	2933	0	2754	43	1
1	F	2933	0	2754	43	1
1	G	2933	0	2754	33	0
1	H	2933	0	2754	42	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	186	0	0	2	0
3	B	205	0	0	4	0
3	C	165	0	0	1	0
3	D	181	0	0	2	0
3	E	173	0	0	3	0
3	F	132	0	0	3	0
3	G	137	0	0	1	0
3	H	127	0	0	2	0
All	All	24786	0	22032	241	2

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 (241) 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:44:ARG:HD2	1:F:329:ALA:O	1.53	1.05
1:C:44:ARG:HD2	1:H:329:ALA:O	1.58	1.03
1:C:329:ALA:O	1:H:44:ARG:HD2	1.61	0.99
1:B:329:ALA:O	1:E:44:ARG:HD2	1.65	0.96
1:A:329:ALA:O	1:F:44:ARG:HD2	1.67	0.95
1:D:329:ALA:O	1:G:44:ARG:HD2	1.68	0.93
1:B:44:ARG:HD2	1:E:329:ALA:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LYS:HE2	3:D:665:HOH:O	1.89	0.70
1:G:113:THR:O	1:G:155:ARG:NH2	2.24	0.70
1:G:225:ASP:OD2	1:G:273:ARG:NH1	2.23	0.70
1:E:342:ASP:O	1:E:344:ASN:HB2	1.92	0.69
1:E:40:MET:HB3	1:E:41:PRO:HD2	1.77	0.66
1:A:364:ASN:O	1:A:368:LYS:HB2	1.95	0.66
1:D:335:PRO:O	1:D:336:SER:O	2.13	0.66
1:H:266:ILE:O	1:H:270:VAL:HG23	1.96	0.66
1:H:318:VAL:O	3:H:501:HOH:O	2.14	0.65
1:D:364:ASN:O	1:D:368:LYS:HB2	1.97	0.64
1:C:44:ARG:HD3	1:C:281:PHE:CZ	2.33	0.64
1:E:44:ARG:HD3	1:E:281:PHE:CZ	2.33	0.63
1:A:40:MET:HB3	1:A:41:PRO:HD2	1.80	0.63
1:B:329:ALA:H	1:E:44:ARG:HG2	1.64	0.63
1:A:329:ALA:H	1:F:44:ARG:HG2	1.64	0.62
1:D:345:ARG:HD3	3:D:603:HOH:O	1.99	0.62
1:F:40:MET:HE1	1:F:233:MET:HE2	1.82	0.62
1:A:44:ARG:HG2	1:F:329:ALA:H	1.65	0.61
1:C:254:LEU:HD21	1:H:368:LYS:HD2	1.83	0.61
1:F:40:MET:HB3	1:F:41:PRO:HD2	1.83	0.61
1:F:152:ILE:HG22	1:F:153:ASN:O	2.01	0.61
1:A:238:MET:HE2	1:A:252:ILE:HD13	1.81	0.61
1:H:368:LYS:O	1:H:372:MET:HG3	2.00	0.61
1:F:342:ASP:O	1:F:344:ASN:N	2.34	0.60
1:G:40:MET:CE	1:G:233:MET:HE2	2.32	0.60
1:E:40:MET:HE1	1:E:233:MET:HE2	1.82	0.60
1:D:49:ALA:HB1	1:D:95:ASP:HB2	1.82	0.60
1:B:251:ARG:HD3	1:B:255:ASP:OD2	2.01	0.60
1:F:44:ARG:HD3	1:F:281:PHE:CZ	2.37	0.60
1:F:152:ILE:HG22	1:F:153:ASN:N	2.17	0.60
1:E:175:GLN:NE2	1:E:180:THR:OG1	2.35	0.60
1:B:55:GLU:OE1	1:B:61:LYS:HE2	2.01	0.59
1:A:55:GLU:OE1	1:A:61:LYS:HE2	2.01	0.59
1:A:356:GLY:HA3	1:F:216:TRP:CH2	2.38	0.59
1:C:364:ASN:O	1:C:368:LYS:HB2	2.03	0.58
1:D:239:MET:O	1:D:243:ASN:HA	2.05	0.57
1:F:364:ASN:O	1:F:368:LYS:HB2	2.03	0.57
1:H:170:ASN:ND2	1:H:220:TYR:CD1	2.73	0.57
1:H:49:ALA:HB1	1:H:95:ASP:HB2	1.87	0.57
1:C:44:ARG:CD	1:H:329:ALA:O	2.46	0.56
1:E:61:LYS:NZ	3:E:503:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:C	1:C:198:LEU:HD23	2.30	0.56
1:D:329:ALA:H	1:G:44:ARG:HG2	1.70	0.56
1:G:198:LEU:HD23	1:G:198:LEU:C	2.31	0.55
1:E:238:MET:HE2	1:E:252:ILE:HD13	1.88	0.55
1:H:238:MET:HE2	1:H:252:ILE:HG21	1.88	0.55
1:G:109:THR:HG22	1:G:148:ARG:NE	2.22	0.55
1:B:238:MET:HE2	1:B:252:ILE:HD13	1.89	0.54
1:G:105:ALA:O	1:G:109:THR:HG23	2.08	0.54
1:H:217:TYR:HB3	1:H:218:PRO:HD3	1.90	0.54
1:B:329:ALA:N	1:E:44:ARG:HG2	2.23	0.53
1:C:329:ALA:H	1:H:44:ARG:HG2	1.73	0.53
1:E:198:LEU:C	1:E:198:LEU:HD23	2.34	0.53
1:A:107:GLY:O	1:A:112:ARG:CB	2.56	0.53
1:G:175:GLN:NE2	1:G:180:THR:OG1	2.43	0.52
1:C:217:TYR:HB3	1:C:218:PRO:HD3	1.90	0.52
1:D:238:MET:HE2	1:D:252:ILE:HD13	1.91	0.52
1:C:40:MET:HB3	1:C:41:PRO:HD2	1.90	0.52
1:E:152:ILE:CG2	1:E:153:ASN:O	2.57	0.52
1:F:238:MET:HE2	1:F:252:ILE:HD13	1.91	0.52
1:B:61:LYS:HE3	3:B:524:HOH:O	2.10	0.52
1:A:44:ARG:CD	1:F:329:ALA:O	2.42	0.52
1:E:266:ILE:O	1:E:270:VAL:HG23	2.10	0.51
1:A:82:ASN:HB2	3:A:562:HOH:O	2.10	0.51
1:H:44:ARG:HD3	1:H:281:PHE:CZ	2.45	0.51
1:A:44:ARG:HG2	1:F:329:ALA:N	2.26	0.51
1:D:19:TYR:O	1:D:323:ALA:HA	2.11	0.51
1:H:295:ARG:NH2	1:H:300:GLY:O	2.36	0.51
1:B:40:MET:CE	1:B:233:MET:HE2	2.41	0.50
1:G:263:PHE:CD1	1:G:263:PHE:C	2.89	0.50
1:H:114:ASP:HA	1:H:155:ARG:NH2	2.27	0.50
1:B:114:ASP:HB3	1:B:115:PRO:HD2	1.93	0.50
1:B:250:LEU:O	1:B:254:LEU:HD23	2.11	0.50
1:F:40:MET:HB3	1:F:41:PRO:CD	2.41	0.50
1:D:250:LEU:CD2	1:G:372:MET:HE3	2.42	0.50
1:F:101:VAL:HG21	1:F:141:TYR:CE2	2.47	0.50
1:D:329:ALA:H	1:G:44:ARG:CG	2.25	0.49
1:B:356:GLY:HA3	1:E:216:TRP:CH2	2.47	0.49
1:G:40:MET:HE2	1:G:233:MET:HE2	1.94	0.49
1:D:94:THR:HG21	1:G:101:VAL:HG22	1.95	0.49
1:E:49:ALA:HB1	1:E:95:ASP:HB2	1.95	0.49
1:D:198:LEU:C	1:D:198:LEU:HD23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:TYR:CZ	1:C:295:ARG:HD2	2.47	0.49
1:E:152:ILE:HG22	1:E:153:ASN:C	2.36	0.49
1:H:91:HIS:CE1	1:H:96:HIS:CD2	3.00	0.49
1:F:49:ALA:HB1	1:F:95:ASP:HB2	1.94	0.49
1:A:40:MET:HB3	1:A:41:PRO:CD	2.42	0.49
1:D:356:GLY:HA3	1:G:216:TRP:CH2	2.47	0.49
1:C:55:GLU:OE1	1:C:61:LYS:HE2	2.13	0.49
1:H:155:ARG:N	1:H:156:PRO:HD2	2.28	0.48
1:C:238:MET:O	1:C:242:TYR:HB2	2.12	0.48
1:B:343:ARG:O	1:B:343:ARG:HD3	2.13	0.48
1:D:128:MET:HE3	1:G:143:TRP:CD1	2.49	0.48
1:F:343:ARG:O	1:F:343:ARG:HD3	2.14	0.48
1:A:44:ARG:CG	1:F:329:ALA:N	2.77	0.48
1:C:49:ALA:HB1	1:C:95:ASP:HB2	1.96	0.47
1:H:335:PRO:O	1:H:336:SER:O	2.32	0.47
1:A:329:ALA:N	1:F:44:ARG:HG2	2.28	0.47
1:C:250:LEU:HD11	1:H:368:LYS:HG3	1.96	0.47
1:F:144:ASP:OD1	1:F:148:ARG:NH1	2.48	0.47
1:G:112:ARG:CD	1:G:114:ASP:O	2.61	0.47
1:H:108:TRP:CD1	1:H:156:PRO:HG2	2.49	0.47
1:B:250:LEU:O	1:B:254:LEU:CD2	2.63	0.47
1:E:351:GLN:NE2	3:E:510:HOH:O	2.48	0.47
1:A:251:ARG:HD3	1:A:255:ASP:OD2	2.15	0.47
1:B:217:TYR:HB3	1:B:218:PRO:HD3	1.97	0.47
1:C:335:PRO:O	1:C:336:SER:O	2.33	0.47
1:C:345:ARG:HD3	3:C:615:HOH:O	2.14	0.47
1:E:152:ILE:HG22	1:E:153:ASN:O	2.14	0.47
1:F:82:ASN:HD22	1:F:336:SER:CB	2.27	0.47
1:C:40:MET:HE2	1:C:280:PHE:HA	1.97	0.47
1:F:342:ASP:OD1	1:F:344:ASN:HB2	2.14	0.47
1:C:19:TYR:O	1:C:323:ALA:HA	2.15	0.47
1:C:44:ARG:HG2	1:H:329:ALA:H	1.79	0.47
1:C:329:ALA:HB3	1:H:44:ARG:HG3	1.96	0.47
1:F:198:LEU:C	1:F:198:LEU:HD23	2.40	0.47
1:B:40:MET:HB3	1:B:41:PRO:HD2	1.96	0.47
1:F:251:ARG:HD3	1:F:255:ASP:OD2	2.15	0.47
1:H:111:GLY:O	1:H:112:ARG:C	2.56	0.47
1:A:176:GLU:OE1	1:B:162:HIS:ND1	2.47	0.46
1:A:311:TRP:HA	1:A:319:THR:O	2.15	0.46
1:C:241:LYS:O	1:E:2:ALA:N	2.48	0.46
1:F:174:TYR:HB3	1:F:181:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:359:ASN:ND2	1:G:361:ASP:H	2.13	0.46
1:B:37:GLY:HA3	1:B:49:ALA:O	2.15	0.46
1:B:291:TYR:CE1	1:B:302:LEU:HD23	2.50	0.46
1:E:82:ASN:HD22	1:E:336:SER:HB2	1.80	0.46
1:B:186:CYS:HB3	1:B:211:THR:HB	1.97	0.46
1:E:55:GLU:OE1	1:E:61:LYS:HE2	2.16	0.46
1:G:112:ARG:HD2	1:G:114:ASP:O	2.15	0.46
1:A:324:VAL:HG12	1:D:324:VAL:HG12	1.97	0.46
1:D:335:PRO:C	1:D:336:SER:O	2.58	0.46
1:A:343:ARG:HE	1:A:343:ARG:HA	1.81	0.45
1:E:174:TYR:HB3	1:E:181:PHE:HB2	1.99	0.45
1:G:44:ARG:HD3	1:G:281:PHE:CZ	2.51	0.45
1:A:155:ARG:N	1:A:156:PRO:HD2	2.31	0.45
1:C:44:ARG:HG2	1:H:329:ALA:N	2.32	0.45
1:D:291:TYR:CZ	1:D:295:ARG:HD2	2.51	0.45
1:E:151:THR:O	1:E:152:ILE:HG13	2.15	0.45
1:A:44:ARG:CG	1:F:329:ALA:H	2.28	0.45
1:A:109:THR:HG22	1:A:148:ARG:NE	2.31	0.45
1:B:40:MET:HB3	1:B:41:PRO:CD	2.47	0.45
1:A:153:ASN:ND2	1:A:340:ALA:O	2.42	0.45
1:C:287:ARG:HD3	1:E:287:ARG:HD2	1.99	0.45
1:H:40:MET:HB3	1:H:41:PRO:HD2	1.99	0.45
1:C:311:TRP:HA	1:C:319:THR:O	2.18	0.44
1:B:343:ARG:O	1:B:343:ARG:CG	2.65	0.44
1:A:217:TYR:HB3	1:A:218:PRO:HD3	2.00	0.44
1:D:37:GLY:HA3	1:D:49:ALA:O	2.18	0.44
1:H:343:ARG:O	1:H:343:ARG:HD3	2.17	0.44
1:A:186:CYS:HB3	1:A:211:THR:HB	2.00	0.44
1:E:44:ARG:HD3	1:E:281:PHE:CE1	2.51	0.44
1:G:114:ASP:HB3	1:G:115:PRO:HD2	2.00	0.44
1:H:332:VAL:HG13	1:H:332:VAL:O	2.18	0.44
1:G:37:GLY:HA3	1:G:49:ALA:O	2.18	0.44
1:C:198:LEU:HD23	1:C:199:GLU:N	2.33	0.44
1:G:254:LEU:HD13	1:G:254:LEU:HA	1.85	0.44
1:B:82:ASN:HB2	3:B:653:HOH:O	2.17	0.44
1:C:330:TRP:CZ2	1:H:241:LYS:HE3	2.53	0.44
1:F:37:GLY:HA3	1:F:49:ALA:O	2.17	0.44
1:B:291:TYR:CZ	1:B:295:ARG:HD2	2.53	0.44
1:C:37:GLY:HA3	1:C:49:ALA:O	2.17	0.43
1:F:351:GLN:NE2	3:F:513:HOH:O	2.51	0.43
1:G:316:ASP:OD1	1:G:316:ASP:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:254:LEU:HD13	1:H:254:LEU:HA	1.86	0.43
1:A:44:ARG:HG3	1:F:329:ALA:HB3	2.00	0.43
1:A:343:ARG:O	1:A:343:ARG:HD3	2.18	0.43
1:H:232:TRP:CH2	1:H:257:HIS:CE1	3.06	0.43
1:A:61:LYS:HE3	3:A:548:HOH:O	2.17	0.43
1:D:339:LEU:HD12	1:D:339:LEU:HA	1.84	0.43
1:E:364:ASN:O	1:E:368:LYS:HB2	2.19	0.43
1:F:181:PHE:CZ	1:F:198:LEU:HD12	2.53	0.43
1:F:370:GLU:HB3	3:F:508:HOH:O	2.17	0.43
1:H:166:TYR:OH	1:H:191:ASP:OD2	2.21	0.43
1:H:37:GLY:HA3	1:H:49:ALA:O	2.19	0.43
1:C:356:GLY:HA3	1:H:216:TRP:CH2	2.53	0.43
1:E:71:MET:HB2	1:E:99:ASP:OD2	2.19	0.43
1:H:112:ARG:HG2	1:H:114:ASP:O	2.19	0.43
1:G:153:ASN:HB2	1:G:340:ALA:O	2.19	0.43
1:C:329:ALA:O	1:H:44:ARG:CD	2.49	0.42
1:C:242:TYR:HB2	1:C:244:GLN:HG3	2.01	0.42
1:G:217:TYR:N	1:G:218:PRO:CD	2.82	0.42
1:H:108:TRP:HB2	1:H:112:ARG:NH2	2.35	0.42
1:A:114:ASP:HB3	1:A:115:PRO:HD2	2.01	0.42
1:B:238:MET:O	1:B:242:TYR:HB2	2.20	0.42
1:D:55:GLU:OE1	1:D:61:LYS:HE2	2.19	0.42
1:B:117:GLU:HG3	3:B:678:HOH:O	2.19	0.42
1:G:40:MET:HB3	1:G:41:PRO:HD2	2.01	0.42
1:B:329:ALA:O	1:E:44:ARG:CD	2.54	0.42
1:F:343:ARG:NE	1:F:343:ARG:HA	2.34	0.42
1:A:19:TYR:O	1:A:323:ALA:HA	2.20	0.42
1:D:343:ARG:HD3	1:D:343:ARG:O	2.20	0.42
1:E:291:TYR:CZ	1:E:295:ARG:HD2	2.55	0.42
1:E:82:ASN:HD22	1:E:336:SER:CB	2.32	0.42
1:H:63:ILE:CD1	1:H:103:MET:CE	2.98	0.42
1:A:143:TRP:CD1	1:F:128:MET:HE3	2.55	0.42
1:B:15:LYS:NZ	3:B:512:HOH:O	2.52	0.42
1:H:192:GLY:N	1:H:193:PRO:CD	2.83	0.42
1:E:40:MET:CE	1:E:233:MET:HE2	2.47	0.42
1:G:234:THR:O	1:G:238:MET:HG2	2.20	0.42
1:E:19:TYR:O	1:E:323:ALA:HA	2.20	0.41
1:F:167:ARG:NH1	3:F:504:HOH:O	2.47	0.41
1:G:78:MET:C	1:G:332:VAL:HG11	2.45	0.41
1:A:20:TYR:CD2	1:D:20:TYR:HB3	2.56	0.41
1:C:371:PHE:O	1:C:373:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:TRP:CZ2	1:E:152:ILE:HG21	2.56	0.41
1:F:155:ARG:N	1:F:156:PRO:HD2	2.35	0.41
1:F:265:GLN:O	1:F:268:ASN:HB3	2.20	0.41
1:E:82:ASN:HB2	3:E:555:HOH:O	2.19	0.41
1:A:37:GLY:HA3	1:A:49:ALA:O	2.21	0.41
1:F:263:PHE:CD1	1:F:263:PHE:C	2.99	0.41
1:E:263:PHE:CD1	1:E:263:PHE:C	2.98	0.41
1:B:20:TYR:CD2	1:C:20:TYR:HB3	2.55	0.41
1:B:241:LYS:HE3	1:E:330:TRP:CZ2	2.56	0.41
1:B:311:TRP:HA	1:B:319:THR:O	2.21	0.41
1:G:175:GLN:HG2	3:G:537:HOH:O	2.21	0.41
1:G:217:TYR:HB3	1:G:218:PRO:HD3	2.03	0.41
1:H:198:LEU:C	1:H:198:LEU:HD23	2.45	0.41
1:B:44:ARG:CG	1:E:329:ALA:H	2.34	0.40
1:E:9:SER:OG	1:H:61:LYS:HE3	2.22	0.40
1:E:108:TRP:HZ2	1:E:152:ILE:HG21	1.86	0.40
1:B:263:PHE:CD1	1:B:263:PHE:C	2.99	0.40
1:E:40:MET:HG3	1:E:281:PHE:CE1	2.56	0.40
1:E:101:VAL:HG21	1:E:141:TYR:CE2	2.56	0.40
1:F:166:TYR:OH	1:F:191:ASP:OD2	2.17	0.40
1:G:291:TYR:CZ	1:G:295:ARG:HD2	2.56	0.40
1:A:181:PHE:HA	1:A:197:ALA:O	2.22	0.40
1:C:329:ALA:H	1:H:44:ARG:CG	2.33	0.40
1:F:152:ILE:CG2	1:F:153:ASN:N	2.83	0.40
1:F:217:TYR:N	1:F:218:PRO:CD	2.84	0.40
1:G:108:TRP:CD1	1:G:156:PRO:HG2	2.57	0.40
1:H:96:HIS:CD2	3:H:503:HOH:O	2.73	0.40
1:E:295:ARG:NH2	1:E:300:GLY:O	2.42	0.40
1:F:217:TYR:HB3	1:F:218:PRO:HD3	2.04	0.40

All (2) 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]	2.02	0.18
1:B:347:SER:O	1:E:344:ASN:ND2[2_555]	2.16	0.04

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	370/372 (100%)	354 (96%)	15 (4%)	1 (0%)	36	36
1	B	370/372 (100%)	356 (96%)	12 (3%)	2 (0%)	24	22
1	C	370/372 (100%)	348 (94%)	17 (5%)	5 (1%)	9	5
1	D	370/372 (100%)	349 (94%)	17 (5%)	4 (1%)	11	8
1	E	370/372 (100%)	349 (94%)	16 (4%)	5 (1%)	9	5
1	F	370/372 (100%)	353 (95%)	13 (4%)	4 (1%)	11	8
1	G	370/372 (100%)	357 (96%)	11 (3%)	2 (0%)	24	22
1	H	370/372 (100%)	352 (95%)	14 (4%)	4 (1%)	11	8
All	All	2960/2976 (100%)	2818 (95%)	115 (4%)	27 (1%)	14	10

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	336	SER
1	D	336	SER
1	E	338	ASP
1	E	341	PRO
1	E	343	ARG
1	F	343	ARG
1	H	336	SER
1	C	372	MET
1	D	243	ASN
1	G	66	ILE
1	G	338	ASP
1	B	338	ASP
1	C	338	ASP
1	F	341	PRO
1	H	222	LYS
1	H	259	SER
1	C	66	ILE

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Mol	Chain	Res	Type
1	C	340	ALA
1	D	66	ILE
1	F	65	ASP
1	E	66	ILE
1	E	279	HIS
1	A	66	ILE
1	B	66	ILE
1	D	338	ASP
1	F	66	ILE
1	H	66	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	302/302 (100%)	292 (97%)	10 (3%)	33	37
1	B	302/302 (100%)	289 (96%)	13 (4%)	26	27
1	C	302/302 (100%)	287 (95%)	15 (5%)	22	22
1	D	302/302 (100%)	289 (96%)	13 (4%)	26	27
1	E	302/302 (100%)	286 (95%)	16 (5%)	20	19
1	F	302/302 (100%)	290 (96%)	12 (4%)	28	29
1	G	302/302 (100%)	285 (94%)	17 (6%)	19	18
1	H	302/302 (100%)	289 (96%)	13 (4%)	26	27
All	All	2416/2416 (100%)	2307 (96%)	109 (4%)	24	25

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	158	ASP
1	A	169	LEU
1	A	247	GLN
1	A	248	LEU

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Mol	Chain	Res	Type
1	A	254	LEU
1	A	295	ARG
1	A	310	VAL
1	A	362	GLU
1	A	369	GLN
1	B	44	ARG
1	B	131	LYS
1	B	152	ILE
1	B	158	ASP
1	B	169	LEU
1	B	230	GLU
1	B	247	GLN
1	B	248	LEU
1	B	252	ILE
1	B	295	ARG
1	B	310	VAL
1	B	337	GLU
1	B	362	GLU
1	C	44	ARG
1	C	131	LYS
1	C	152	ILE
1	C	169	LEU
1	C	198	LEU
1	C	222	LYS
1	C	243	ASN
1	C	247	GLN
1	C	248	LEU
1	C	254	LEU
1	C	295	ARG
1	C	331	ASP
1	C	339	LEU
1	C	362	GLU
1	C	369	GLN
1	D	8	SER
1	D	131	LYS
1	D	152	ILE
1	D	169	LEU
1	D	198	LEU
1	D	222	LYS
1	D	243	ASN
1	D	248	LEU
1	D	254	LEU

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Mol	Chain	Res	Type
1	D	295	ARG
1	D	338	ASP
1	D	339	LEU
1	D	370	GLU
1	E	18	VAL
1	E	109	THR
1	E	131	LYS
1	E	150	VAL
1	E	152	ILE
1	E	169	LEU
1	E	254	LEU
1	E	295	ARG
1	E	310	VAL
1	E	337	GLU
1	E	339	LEU
1	E	343	ARG
1	E	344	ASN
1	E	351	GLN
1	E	362	GLU
1	E	368	LYS
1	F	15	LYS
1	F	131	LYS
1	F	135	GLU
1	F	169	LEU
1	F	222	LYS
1	F	254	LEU
1	F	295	ARG
1	F	310	VAL
1	F	343	ARG
1	F	362	GLU
1	F	368	LYS
1	F	369	GLN
1	G	5	LYS
1	G	8	SER
1	G	44	ARG
1	G	61	LYS
1	G	158	ASP
1	G	169	LEU
1	G	248	LEU
1	G	254	LEU
1	G	263	PHE
1	G	295	ARG

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Mol	Chain	Res	Type
1	G	310	VAL
1	G	316	ASP
1	G	331	ASP
1	G	339	LEU
1	G	343	ARG
1	G	362	GLU
1	G	368	LYS
1	H	44	ARG
1	H	158	ASP
1	H	169	LEU
1	H	183	SER
1	H	248	LEU
1	H	254	LEU
1	H	295	ARG
1	H	310	VAL
1	H	337	GLU
1	H	342	ASP
1	H	343	ARG
1	H	362	GLU
1	H	368	LYS

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

Mol	Chain	Res	Type
1	A	244	GLN
1	A	297	ASN
1	A	344	ASN
1	B	344	ASN
1	D	170	ASN
1	D	359	ASN
1	E	82	ASN
1	E	175	GLN
1	E	344	ASN
1	E	351	GLN
1	F	82	ASN
1	F	170	ASN
1	F	244	GLN
1	F	344	ASN
1	F	369	GLN
1	G	170	ASN
1	G	175	GLN
1	G	243	ASN

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Mol	Chain	Res	Type
1	G	257	HIS
1	G	344	ASN
1	G	359	ASN
1	G	369	GLN
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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	372/372 (100%)	0.07	15 (4%)	42	44	9, 18, 49, 87	0
1	B	372/372 (100%)	0.02	14 (3%)	44	46	7, 15, 48, 81	0
1	C	372/372 (100%)	0.28	28 (7%)	20	21	10, 22, 57, 101	0
1	D	372/372 (100%)	0.15	17 (4%)	37	39	10, 19, 50, 92	0
1	E	372/372 (100%)	0.33	20 (5%)	31	33	10, 22, 45, 100	0
1	F	372/372 (100%)	0.60	28 (7%)	20	21	12, 27, 50, 92	0
1	G	372/372 (100%)	0.66	29 (7%)	19	20	12, 27, 47, 88	0
1	H	372/372 (100%)	0.86	46 (12%)	8	8	13, 28, 54, 90	0
All	All	2976/2976 (100%)	0.37	197 (6%)	24	26	7, 23, 50, 101	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	339	LEU	7.3
1	C	341	PRO	6.4
1	D	373	GLY	6.3
1	C	373	GLY	6.2
1	D	341	PRO	6.2
1	D	340	ALA	6.0
1	B	373	GLY	5.8
1	G	339	LEU	5.8
1	C	340	ALA	5.8
1	A	373	GLY	5.7
1	F	339	LEU	5.4
1	F	152	ILE	5.3
1	C	339	LEU	5.2
1	F	373	GLY	5.1
1	F	344	ASN	5.0
1	E	152	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	343	ARG	4.8
1	E	151	THR	4.7
1	E	343	ARG	4.4
1	C	344	ASN	4.4
1	C	343	ARG	4.3
1	E	373	GLY	4.3
1	H	337	GLU	4.1
1	F	151	THR	4.1
1	G	8	SER	3.9
1	F	110	ALA	3.9
1	D	362	GLU	3.8
1	A	340	ALA	3.7
1	C	362	GLU	3.7
1	C	342	ASP	3.7
1	F	340	ALA	3.6
1	D	339	LEU	3.6
1	A	246	ALA	3.5
1	G	373	GLY	3.5
1	H	363	ALA	3.4
1	F	111	GLY	3.4
1	C	363	ALA	3.4
1	D	343	ARG	3.4
1	A	344	ASN	3.3
1	E	344	ASN	3.3
1	H	111	GLY	3.3
1	H	343	ARG	3.3
1	F	341	PRO	3.3
1	D	342	ASP	3.3
1	A	341	PRO	3.2
1	F	371	PHE	3.2
1	B	362	GLU	3.2
1	B	248	LEU	3.2
1	H	254	LEU	3.2
1	G	338	ASP	3.2
1	A	343	ARG	3.2
1	H	157	GLY	3.1
1	D	371	PHE	3.1
1	H	109	THR	3.1
1	E	341	PRO	3.1
1	F	362	GLU	3.1
1	H	344	ASN	3.0
1	H	340	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	365	ALA	3.0
1	D	248	LEU	3.0
1	H	362	GLU	3.0
1	A	342	ASP	3.0
1	H	371	PHE	3.0
1	G	337	GLU	3.0
1	F	169	LEU	2.9
1	E	342	ASP	2.9
1	B	344	ASN	2.9
1	D	242	TYR	2.9
1	G	371	PHE	2.9
1	B	335	PRO	2.9
1	C	247	GLN	2.8
1	H	366	HIS	2.8
1	C	245	PRO	2.8
1	H	159	ILE	2.8
1	G	336	SER	2.8
1	F	342	ASP	2.8
1	G	111	GLY	2.8
1	H	339	LEU	2.8
1	A	335	PRO	2.8
1	H	341	PRO	2.7
1	D	338	ASP	2.7
1	E	246	ALA	2.7
1	C	256	PHE	2.7
1	G	254	LEU	2.7
1	G	29	ASP	2.7
1	H	373	GLY	2.7
1	C	371	PHE	2.6
1	B	341	PRO	2.6
1	C	152	ILE	2.6
1	G	246	ALA	2.6
1	H	221	ALA	2.6
1	H	252	ILE	2.6
1	H	107	GLY	2.6
1	F	109	THR	2.6
1	G	365	ALA	2.6
1	H	248	LEU	2.6
1	G	362	GLU	2.6
1	B	343	ARG	2.6
1	E	338	ASP	2.6
1	F	254	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLU	2.5
1	C	338	ASP	2.5
1	A	363	ALA	2.5
1	D	363	ALA	2.5
1	H	110	ALA	2.5
1	H	180	THR	2.5
1	E	8	SER	2.5
1	F	9	SER	2.5
1	H	8	SER	2.5
1	G	169	LEU	2.5
1	B	252	ILE	2.5
1	G	172	VAL	2.5
1	F	10	THR	2.5
1	D	245	PRO	2.5
1	G	107	GLY	2.5
1	E	12	ILE	2.5
1	E	7	THR	2.5
1	C	242	TYR	2.4
1	F	8	SER	2.4
1	H	9	SER	2.4
1	G	335	PRO	2.4
1	G	341	PRO	2.4
1	A	110	ALA	2.4
1	E	340	ALA	2.4
1	H	342	ASP	2.4
1	H	335	PRO	2.4
1	C	337	GLU	2.4
1	E	371	PHE	2.4
1	G	175	GLN	2.4
1	H	6	VAL	2.4
1	C	369	GLN	2.4
1	G	11	GLY	2.4
1	H	12	ILE	2.4
1	H	215	ILE	2.4
1	H	292	THR	2.4
1	H	246	ALA	2.3
1	B	342	ASP	2.3
1	C	235	SER	2.3
1	G	340	ALA	2.3
1	H	249	ALA	2.3
1	B	244	GLN	2.3
1	H	113	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	254	LEU	2.3
1	D	235	SER	2.2
1	H	247	GLN	2.2
1	E	332	VAL	2.2
1	H	360	VAL	2.2
1	B	340	ALA	2.2
1	F	363	ALA	2.2
1	H	336	SER	2.2
1	D	240	THR	2.2
1	G	332	VAL	2.2
1	D	244	GLN	2.2
1	H	108	TRP	2.2
1	F	15	LYS	2.2
1	A	239	MET	2.2
1	C	249	ALA	2.2
1	H	333	ALA	2.2
1	A	248	LEU	2.2
1	A	254	LEU	2.2
1	H	368	LYS	2.2
1	C	240	THR	2.2
1	E	362	GLU	2.1
1	F	202	GLY	2.1
1	B	110	ALA	2.1
1	C	246	ALA	2.1
1	F	299	ALA	2.1
1	A	250	LEU	2.1
1	B	242	TYR	2.1
1	G	109	THR	2.1
1	G	12	ILE	2.1
1	H	129	GLY	2.1
1	F	365	ALA	2.1
1	G	368	LYS	2.1
1	C	355	ASP	2.1
1	C	352	TYR	2.1
1	E	314	THR	2.1
1	C	107	GLY	2.1
1	H	172	VAL	2.1
1	G	363	ALA	2.1
1	E	336	SER	2.1
1	F	7	THR	2.1
1	H	155	ARG	2.1
1	D	107	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	270	VAL	2.1
1	H	359	ASN	2.0
1	H	114	ASP	2.0
1	E	14	PRO	2.0
1	F	3	GLY	2.0
1	B	337	GLU	2.0
1	H	105	ALA	2.0
1	C	243	ASN	2.0
1	F	248	LEU	2.0
1	F	338	ASP	2.0
1	G	366	HIS	2.0
1	C	151	THR	2.0
1	G	14	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	H	402	1/1	0.98	0.03	23,23,23,23	0
2	ZN	D	401	1/1	0.99	0.07	29,29,29,29	0
2	ZN	E	401	1/1	0.99	0.04	27,27,27,27	0
2	ZN	E	402	1/1	0.99	0.02	18,18,18,18	0
2	ZN	F	401	1/1	0.99	0.03	31,31,31,31	0
2	ZN	G	401	1/1	0.99	0.07	28,28,28,28	0
2	ZN	G	402	1/1	0.99	0.02	19,19,19,19	0
2	ZN	H	401	1/1	0.99	0.05	31,31,31,31	0
2	ZN	C	402	1/1	0.99	0.02	24,24,24,24	0
2	ZN	B	402	1/1	1.00	0.01	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	401	1/1	1.00	0.05	30,30,30,30	0
2	ZN	F	402	1/1	1.00	0.03	21,21,21,21	0
2	ZN	A	401	1/1	1.00	0.05	25,25,25,25	0
2	ZN	A	402	1/1	1.00	0.01	20,20,20,20	0
2	ZN	D	402	1/1	1.00	0.01	19,19,19,19	0
2	ZN	B	401	1/1	1.00	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.