



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:45 PM UTC

PDB ID : 2Z3B / pdb_00002z3b
Title : Crystal Structure of Bacillus Subtilis CodW, a non-canonical HslV-like peptidase with an impaired catalytic apparatus
Authors : Rho, S.H.; Park, H.H.; Kang, G.B.; Lim, Y.J.; Kang, M.S.; Lim, B.K.; Seong, I.S.; Chung, C.H.; Wang, J.; Eom, S.H.
Deposited on : 2007-06-03
Resolution : 2.50 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

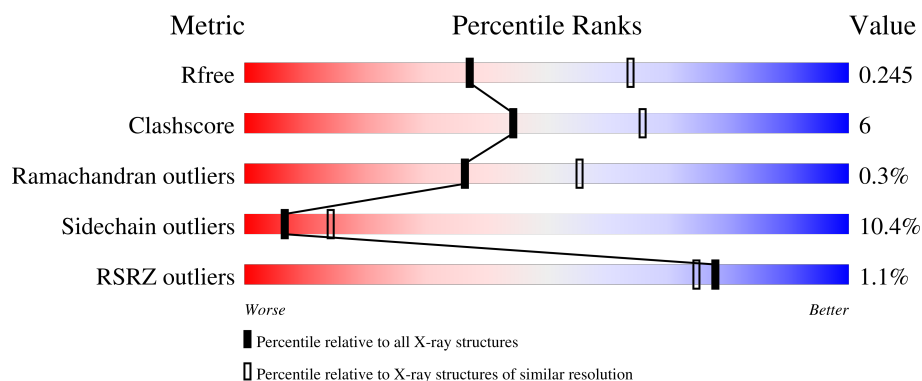
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	180	84%14%.
1	B	180	2% 79%16%5%
1	C	180	83%16%.
1	D	180	77%20%.
1	E	180	77%18%5%

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Mol	Chain	Length	Quality of chain
1	F	180	% 83% 15%
1	G	180	% 83% 13%
1	H	180	% 79% 19%
1	I	180	% 85% 13%
1	J	180	2% 78% 20%
1	K	180	2% 81% 17%
1	L	180	% 79% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16571 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 ATP-dependent protease hslV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	B	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	C	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	D	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	E	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	F	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	G	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	H	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	I	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	J	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	K	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			
1	L	180	Total	C	N	O	S	0	0	0
			1359	855	237	261	6			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Na 1	0	0
2	D	1	Total 1	Na 1	0	0
2	E	1	Total 1	Na 1	0	0
2	F	1	Total 1	Na 1	0	0
2	G	1	Total 1	Na 1	0	0
2	H	1	Total 1	Na 1	0	0
2	I	1	Total 1	Na 1	0	0
2	J	1	Total 1	Na 1	0	0
2	K	1	Total 1	Na 1	0	0
2	L	1	Total 1	Na 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total 25	O 25	0	0
3	B	43	Total 43	O 43	0	0
3	C	41	Total 41	O 41	0	0
3	D	41	Total 41	O 41	0	0
3	E	44	Total 44	O 44	0	0
3	F	33	Total 33	O 33	0	0
3	G	4	Total 4	O 4	0	0
3	H	4	Total 4	O 4	0	0
3	I	5	Total 5	O 5	0	0

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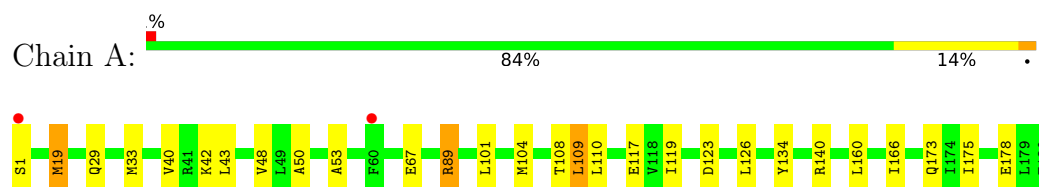
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	4	Total 4	O 4	0	0
3	K	4	Total 4	O 4	0	0
3	L	3	Total 3	O 3	0	0

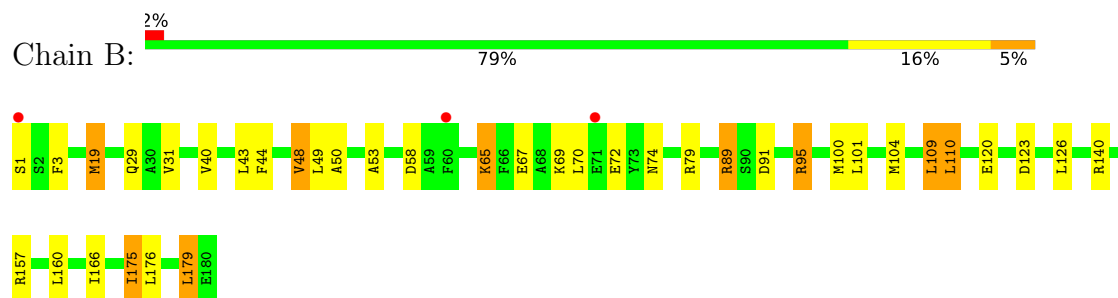
3 Residue-property plots

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.

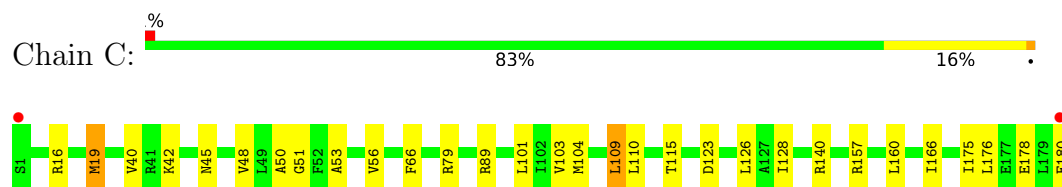
- Molecule 1: ATP-dependent protease hslV



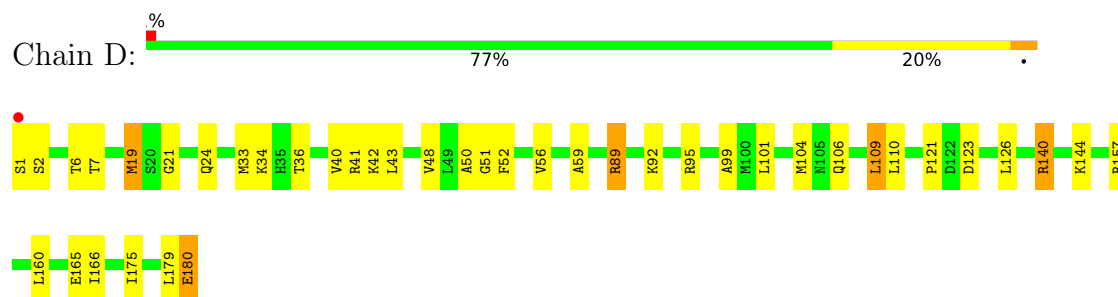
- Molecule 1: ATP-dependent protease hslV



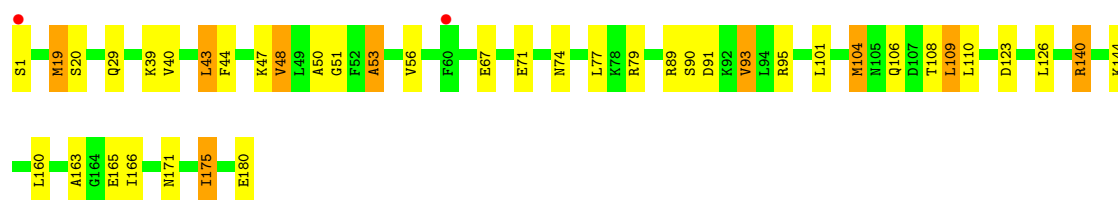
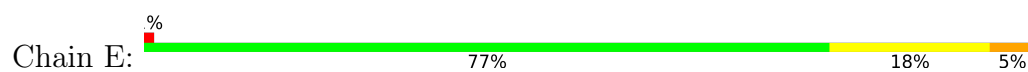
- Molecule 1: ATP-dependent protease hslV



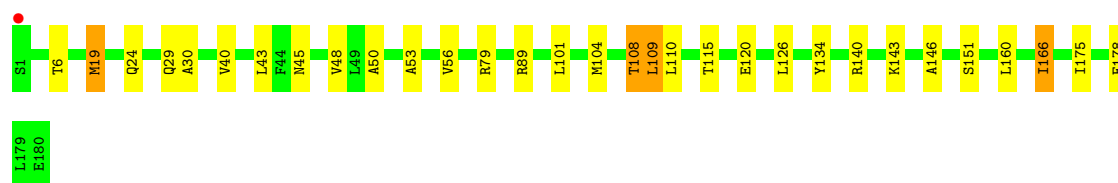
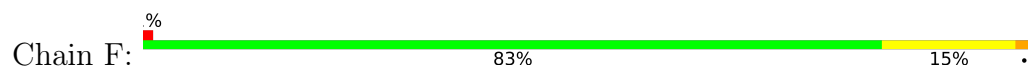
- Molecule 1: ATP-dependent protease hslV



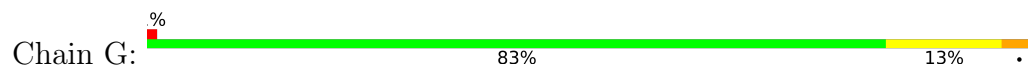
- Molecule 1: ATP-dependent protease hslV



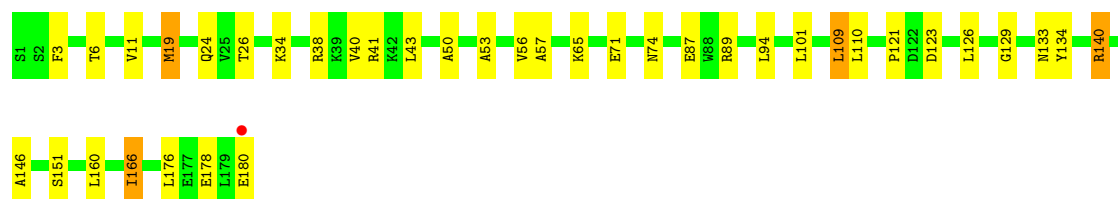
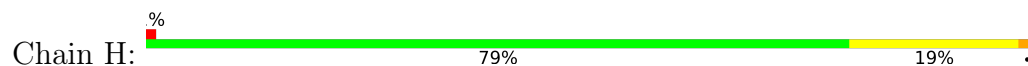
- Molecule 1: ATP-dependent protease hslV



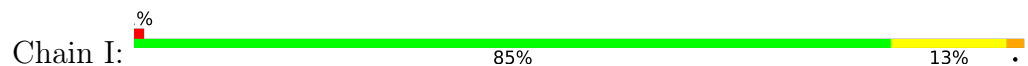
- Molecule 1: ATP-dependent protease hslV



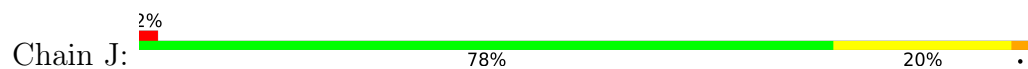
- Molecule 1: ATP-dependent protease hslV

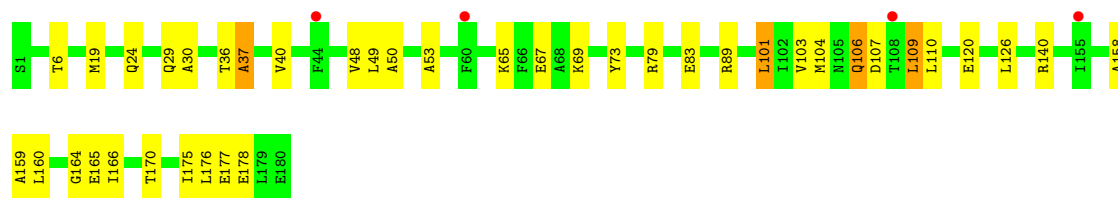


- Molecule 1: ATP-dependent protease hslV

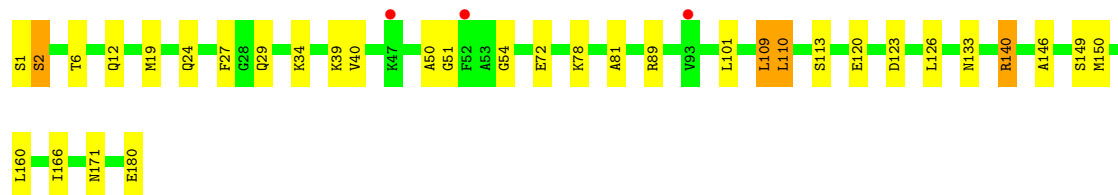
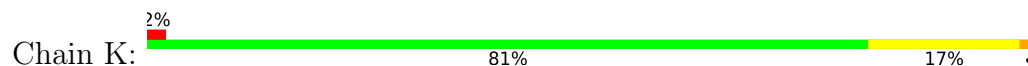


- Molecule 1: ATP-dependent protease hslV

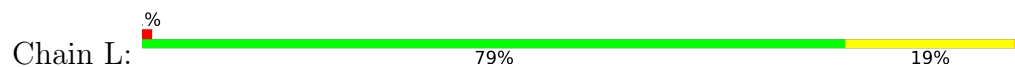




- Molecule 1: ATP-dependent protease hslV



- Molecule 1: ATP-dependent protease hslV



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.05Å 106.80Å 152.70Å 90.00° 112.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.50 29.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.88-2.50) 95.3 (29.88-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.51Å)	Xtriage
Refinement program	CNS, REFMAC 5.1.24	Depositor
R, R_{free}	0.226 , 0.265 0.206 , 0.245	Depositor DCC
R_{free} test set	4576 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.018 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16571	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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: NA

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	1.02	1/1376 (0.1%)	1.04	2/1847 (0.1%)
1	B	1.25	2/1376 (0.1%)	1.15	3/1847 (0.2%)
1	C	1.21	1/1376 (0.1%)	1.14	0/1847
1	D	1.24	3/1376 (0.2%)	1.16	1/1847 (0.1%)
1	E	1.37	4/1376 (0.3%)	1.14	1/1847 (0.1%)
1	F	1.13	3/1376 (0.2%)	1.07	2/1847 (0.1%)
1	G	0.79	1/1376 (0.1%)	0.95	1/1847 (0.1%)
1	H	0.78	1/1376 (0.1%)	0.96	2/1847 (0.1%)
1	I	0.70	0/1376	0.91	0/1847
1	J	0.74	0/1376	0.92	1/1847 (0.1%)
1	K	0.66	0/1376	0.89	0/1847
1	L	0.71	0/1376	0.89	2/1847 (0.1%)
All	All	1.00	16/16512 (0.1%)	1.02	15/22164 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	19	MET	SD-CE	-16.36	1.38	1.79
1	B	19	MET	SD-CE	-13.09	1.46	1.79
1	D	19	MET	SD-CE	-12.61	1.48	1.79
1	F	19	MET	SD-CE	-10.46	1.53	1.79
1	A	19	MET	SD-CE	-10.36	1.53	1.79
1	C	19	MET	SD-CE	-9.82	1.54	1.79
1	G	104	MET	SD-CE	-9.62	1.55	1.79
1	H	19	MET	SD-CE	-6.83	1.62	1.79
1	E	53	ALA	CA-CB	-6.17	1.42	1.53
1	E	163	ALA	CA-CB	-5.88	1.44	1.53
1	E	56	VAL	CA-CB	5.52	1.61	1.54
1	D	99	ALA	CA-CB	-5.50	1.45	1.53
1	B	100	MET	SD-CE	-5.31	1.66	1.79
1	D	36	THR	CA-CB	5.07	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	30	ALA	C-O	-5.02	1.18	1.23
1	F	146	ALA	CA-CB	-5.00	1.44	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	VAL	N-CA-C	6.71	117.79	107.99
1	H	166	ILE	N-CA-C	6.68	117.31	111.90
1	B	65	LYS	N-CA-C	-6.19	105.21	112.89
1	E	93	VAL	CB-CA-C	-6.18	104.50	111.80
1	F	108	THR	N-CA-C	6.11	118.36	109.07
1	G	108	THR	N-CA-C	6.08	117.44	108.86
1	F	166	ILE	CB-CA-C	-5.82	104.54	110.88
1	H	11	VAL	N-CA-C	5.73	116.12	108.27
1	J	30	ALA	N-CA-C	5.73	122.95	113.50
1	L	108	THR	N-CA-C	5.67	116.04	108.38
1	A	119	ILE	N-CA-C	5.32	115.56	108.11
1	A	108	THR	N-CA-C	5.21	116.75	108.79
1	L	31	VAL	N-CA-C	5.18	115.36	108.11
1	D	165	GLU	CA-CB-CG	5.16	124.42	114.10
1	B	175	ILE	N-CA-C	-5.15	100.89	108.11

There are no chirality outliers.

There are no planarity outliers.

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	1359	0	1377	15	0
1	B	1359	0	1377	21	0
1	C	1359	0	1377	17	0
1	D	1359	0	1377	22	0
1	E	1359	0	1377	21	0
1	F	1359	0	1377	13	0
1	G	1359	0	1377	21	0
1	H	1359	0	1377	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1359	0	1377	12	0
1	J	1359	0	1377	23	1
1	K	1359	0	1377	18	1
1	L	1359	0	1377	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	25	0	0	3	0
3	B	43	0	0	2	0
3	C	41	0	0	3	0
3	D	41	0	0	3	0
3	E	44	0	0	1	0
3	F	33	0	0	1	0
3	G	4	0	0	1	0
3	H	4	0	0	1	0
3	I	5	0	0	0	0
3	J	4	0	0	1	0
3	K	4	0	0	0	0
3	L	3	0	0	0	0
All	All	16571	0	16524	197	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 6.

All (197) 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:G:117:GLU:OE1	3:G:1011:HOH:O	1.79	1.00
1:B:123:ASP:OD2	1:B:140:ARG:HD3	1.69	0.92
1:J:19:MET:HE3	1:J:40:VAL:HG13	1.51	0.91
1:K:120:GLU:O	1:L:34:LYS:NZ	2.05	0.89
1:C:53:ALA:HB3	3:C:1035:HOH:O	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:MET:HE1	1:C:50:ALA:C	1.99	0.88
1:J:109:LEU:HD22	1:J:126:LEU:HD12	1.58	0.86
1:E:19:MET:HE1	1:E:50:ALA:C	2.00	0.86
1:A:117:GLU:OE1	3:A:1020:HOH:O	1.93	0.85
1:E:123:ASP:OD2	1:E:140:ARG:HD3	1.80	0.81
1:F:109:LEU:HD22	1:F:126:LEU:HD12	1.66	0.77
1:H:53:ALA:HB3	3:H:1014:HOH:O	1.85	0.76
1:B:19:MET:HE1	1:B:50:ALA:C	2.12	0.74
1:D:19:MET:HE1	1:D:50:ALA:C	2.12	0.74
1:F:19:MET:HE1	1:F:50:ALA:C	2.12	0.73
1:K:39:LYS:NZ	1:K:54:GLY:O	2.20	0.73
1:B:49:LEU:HG	1:B:179:LEU:HD13	1.70	0.73
1:C:19:MET:HE3	1:C:40:VAL:HG13	1.71	0.73
1:B:109:LEU:HD22	1:B:126:LEU:HD12	1.70	0.72
1:H:19:MET:HE1	1:H:50:ALA:C	2.15	0.71
1:A:19:MET:HE1	1:A:50:ALA:C	2.14	0.71
1:C:109:LEU:HD22	1:C:126:LEU:HD12	1.72	0.71
1:L:104:MET:HB3	1:L:109:LEU:HD23	1.71	0.71
1:H:19:MET:CE	1:H:40:VAL:HG13	2.21	0.71
1:C:19:MET:CE	1:C:40:VAL:HG13	2.24	0.68
1:D:123:ASP:OD2	1:D:140:ARG:HD3	1.93	0.68
1:E:91:ASP:O	1:E:95:ARG:HB2	1.93	0.68
1:G:19:MET:HE1	1:G:50:ALA:C	2.19	0.67
1:H:109:LEU:HD22	1:H:126:LEU:HD12	1.76	0.67
1:H:123:ASP:OD2	1:H:140:ARG:HD3	1.96	0.65
1:H:19:MET:HE2	1:H:40:VAL:HG13	1.79	0.65
1:A:173:GLN:O	3:A:1016:HOH:O	2.14	0.64
1:D:95:ARG:NH1	3:D:1045:HOH:O	2.30	0.64
1:J:53:ALA:HB3	3:J:1011:HOH:O	1.98	0.64
1:D:109:LEU:HD22	1:D:126:LEU:HD12	1.79	0.64
1:A:19:MET:HE3	1:A:40:VAL:HG13	1.80	0.64
1:I:123:ASP:OD2	1:I:140:ARG:HD3	1.99	0.63
1:J:19:MET:CE	1:J:40:VAL:HG13	2.28	0.63
1:K:109:LEU:HD22	1:K:126:LEU:HD12	1.80	0.62
1:J:19:MET:HE1	1:J:50:ALA:C	2.25	0.61
1:I:19:MET:HE1	1:I:50:ALA:C	2.26	0.61
1:L:19:MET:HE2	1:L:49:LEU:HB3	1.81	0.61
1:F:104:MET:HE3	1:F:109:LEU:HG	1.83	0.61
1:D:19:MET:CE	1:D:40:VAL:HG13	2.31	0.60
1:F:53:ALA:HB3	3:F:1030:HOH:O	2.01	0.60
1:K:19:MET:CE	1:K:40:VAL:HG13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:SER:HB2	3:B:1043:HOH:O	2.02	0.60
1:K:123:ASP:OD2	1:K:140:ARG:HD3	2.01	0.60
1:A:19:MET:CE	1:A:40:VAL:HG13	2.31	0.60
1:B:19:MET:CE	1:B:40:VAL:HG13	2.32	0.59
1:G:104:MET:HE3	1:G:109:LEU:HG	1.84	0.59
1:L:6:THR:O	1:L:129:GLY:HA3	2.01	0.59
1:C:176:LEU:C	1:C:176:LEU:HD23	2.27	0.59
1:E:19:MET:CE	1:E:40:VAL:HG13	2.32	0.59
1:J:104:MET:HE3	1:J:109:LEU:HG	1.84	0.58
1:L:66:PHE:CE1	1:L:103:VAL:HG11	2.38	0.58
1:B:89:ARG:HA	1:B:95:ARG:HB2	1.85	0.58
1:D:104:MET:HE3	1:D:109:LEU:HG	1.86	0.58
1:C:104:MET:HE3	1:C:109:LEU:HG	1.85	0.58
1:H:19:MET:HE3	1:H:40:VAL:HG22	1.86	0.58
1:C:128:ILE:HD12	3:C:1035:HOH:O	2.05	0.57
1:A:42:LYS:O	1:A:43:LEU:HD12	2.04	0.56
1:B:19:MET:HE3	1:B:40:VAL:HG13	1.86	0.56
1:D:42:LYS:C	1:D:43:LEU:HD12	2.31	0.56
1:E:109:LEU:HD22	1:E:126:LEU:HD12	1.87	0.56
1:G:166:ILE:CG2	1:J:140:ARG:HE	2.19	0.56
1:J:19:MET:HE2	1:J:49:LEU:HB3	1.88	0.55
1:D:19:MET:HE2	1:D:40:VAL:HG13	1.88	0.55
1:E:74:ASN:HD21	1:H:34:LYS:NZ	2.04	0.55
1:L:19:MET:HE3	1:L:40:VAL:HG13	1.89	0.55
1:K:81:ALA:HB2	1:K:110:LEU:HD23	1.88	0.55
1:G:140:ARG:HE	1:J:166:ILE:CG2	2.20	0.54
1:D:179:LEU:C	1:D:180:GLU:OXT	2.50	0.54
1:E:19:MET:HE3	1:E:40:VAL:HG13	1.90	0.54
1:K:19:MET:HE2	1:K:40:VAL:HG13	1.90	0.54
1:I:11:VAL:HG23	1:I:125:ILE:HG12	1.90	0.53
1:F:19:MET:HE3	1:F:40:VAL:HG13	1.91	0.53
1:D:179:LEU:O	1:D:180:GLU:OXT	2.27	0.53
1:G:43:LEU:HB2	1:G:48:VAL:HG22	1.89	0.53
1:G:166:ILE:HG22	1:J:140:ARG:HH21	1.73	0.53
1:H:121:PRO:HG3	1:H:126:LEU:HG	1.91	0.53
1:H:140:ARG:HH21	1:L:166:ILE:HG22	1.74	0.52
1:C:42:LYS:NZ	3:C:1025:HOH:O	2.43	0.52
1:E:104:MET:HE3	1:E:109:LEU:HG	1.92	0.51
1:K:81:ALA:CB	1:K:110:LEU:HD23	2.41	0.51
1:B:49:LEU:HB2	1:B:104:MET:HG2	1.91	0.51
1:H:19:MET:HE3	1:H:40:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:176:LEU:HD23	1:J:176:LEU:C	2.36	0.51
1:C:123:ASP:OD2	1:C:140:ARG:HD3	2.11	0.50
1:G:109:LEU:HD22	1:G:126:LEU:HD12	1.93	0.50
1:J:40:VAL:HG12	1:J:177:GLU:HG3	1.94	0.50
1:G:4:HIS:NE2	1:G:28:GLY:O	2.42	0.50
1:F:134:TYR:HB3	1:F:166:ILE:HD11	1.94	0.49
1:I:134:TYR:HE2	1:K:133:ASN:HB3	1.77	0.49
1:G:43:LEU:HD22	1:G:50:ALA:HB2	1.94	0.49
1:G:166:ILE:HG22	1:J:140:ARG:HE	1.77	0.49
1:B:19:MET:HE3	1:B:40:VAL:HG22	1.93	0.49
1:E:165:GLU:OE2	3:E:1030:HOH:O	2.20	0.49
1:H:134:TYR:HB3	1:H:166:ILE:HD11	1.95	0.48
1:A:89:ARG:NE	1:B:58:ASP:OD2	2.47	0.48
1:C:66:PHE:CE1	1:C:103:VAL:HG11	2.49	0.48
1:K:19:MET:HE3	1:K:40:VAL:HG13	1.95	0.48
1:F:19:MET:CE	1:F:40:VAL:HG13	2.44	0.48
1:E:19:MET:HE2	1:E:40:VAL:HG13	1.96	0.48
1:D:89:ARG:O	1:D:89:ARG:HD3	2.14	0.47
1:H:56:VAL:HG23	1:H:57:ALA:N	2.29	0.47
1:A:53:ALA:HB3	3:A:1022:HOH:O	2.14	0.47
1:B:70:LEU:C	1:B:72:GLU:H	2.23	0.47
1:K:19:MET:HE1	1:K:50:ALA:C	2.39	0.47
1:K:180:GLU:N	1:K:180:GLU:OE2	2.48	0.47
1:D:52:PHE:HD2	1:D:59:ALA:HB2	1.80	0.47
1:A:109:LEU:HD22	1:A:126:LEU:HD12	1.97	0.47
1:L:171:ASN:OD1	1:L:171:ASN:C	2.57	0.46
1:D:19:MET:HE3	1:D:40:VAL:HG13	1.97	0.46
1:H:180:GLU:N	1:H:180:GLU:OE2	2.48	0.46
1:D:42:LYS:O	1:D:43:LEU:HD12	2.15	0.46
1:B:104:MET:HE3	1:B:109:LEU:HG	1.98	0.46
1:K:2:SER:HB3	1:K:27:PHE:CE1	2.51	0.46
1:I:20:SER:OG	1:I:160:LEU:HD23	2.16	0.46
1:L:19:MET:HE1	1:L:50:ALA:C	2.41	0.46
1:L:43:LEU:HB2	1:L:48:VAL:HG22	1.96	0.46
1:D:121:PRO:HG3	1:D:126:LEU:HG	1.98	0.46
1:I:104:MET:HB3	1:I:109:LEU:HD23	1.98	0.46
1:J:106:GLN:NE2	1:J:107:ASP:OD1	2.49	0.46
1:A:123:ASP:OD2	1:A:140:ARG:HD3	2.16	0.45
1:E:166:ILE:HD13	1:E:166:ILE:HG21	1.63	0.45
1:L:127:ALA:HB3	1:L:136:LEU:HB2	1.97	0.45
1:E:74:ASN:HD21	1:H:34:LYS:HZ1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:LYS:NZ	1:J:165:GLU:OE2	2.50	0.45
1:I:104:MET:HE3	1:I:109:LEU:HG	1.99	0.45
1:J:6:THR:HG22	1:J:24:GLN:O	2.16	0.45
1:E:39:LYS:HD2	1:E:53:ALA:HA	1.99	0.45
1:H:6:THR:O	1:H:129:GLY:HA3	2.17	0.45
1:I:30:ALA:O	1:L:168:VAL:HG13	2.16	0.45
1:L:104:MET:CB	1:L:109:LEU:HD23	2.45	0.45
1:G:140:ARG:HE	1:J:166:ILE:HG21	1.81	0.45
1:B:53:ALA:HB3	3:B:1006:HOH:O	2.17	0.45
1:A:104:MET:HE3	1:A:109:LEU:HG	1.98	0.44
1:A:117:GLU:HG3	1:B:3:PHE:CD1	2.52	0.44
1:A:1:SER:HB3	1:F:115:THR:HG21	1.98	0.44
1:A:166:ILE:HG21	1:A:166:ILE:HD13	1.67	0.44
1:B:65:LYS:O	1:B:69:LYS:HG2	2.17	0.44
1:G:65:LYS:O	1:G:69:LYS:HG2	2.18	0.44
1:B:49:LEU:CG	1:B:179:LEU:HD13	2.46	0.44
1:C:180:GLU:N	1:C:180:GLU:OE2	2.51	0.44
1:C:45:ASN:N	1:C:45:ASN:HD22	2.16	0.44
1:L:111:LEU:HB2	1:L:126:LEU:HD13	2.00	0.43
1:J:164:GLY:HA2	1:J:170:THR:HB	1.99	0.43
1:L:104:MET:HE3	1:L:109:LEU:HG	2.00	0.43
1:E:43:LEU:HB2	1:E:48:VAL:HG22	2.00	0.43
1:C:104:MET:HB3	1:C:109:LEU:HD23	2.00	0.43
1:B:19:MET:HE2	1:B:40:VAL:HG13	2.01	0.43
1:F:43:LEU:HB2	1:F:48:VAL:CG2	2.48	0.43
1:K:24:GLN:OE1	1:K:171:ASN:HB3	2.18	0.43
1:G:9:PHE:CD2	1:G:9:PHE:C	2.96	0.43
1:G:13:HIS:O	1:G:14:LYS:HB2	2.19	0.43
1:J:65:LYS:O	1:J:69:LYS:HG2	2.19	0.43
1:B:110:LEU:HD12	1:B:120:GLU:HB2	2.01	0.42
1:J:101:LEU:HD22	1:J:103:VAL:HG13	2.01	0.42
1:H:6:THR:HG22	1:H:24:GLN:O	2.18	0.42
1:J:158:ALA:O	1:J:159:ALA:C	2.62	0.42
1:J:73:TYR:OH	1:J:83:GLU:HG3	2.20	0.42
1:E:77:LEU:HD23	1:E:108:THR:HG23	2.01	0.42
1:E:171:ASN:OD1	1:E:171:ASN:C	2.63	0.42
1:I:140:ARG:HH21	1:K:166:ILE:HG22	1.83	0.42
1:D:19:MET:HE1	1:D:51:GLY:N	2.34	0.42
1:C:166:ILE:HD13	1:C:166:ILE:HG21	1.85	0.42
1:D:7:THR:O	1:D:21:GLY:HA2	2.20	0.42
1:D:6:THR:HG22	1:D:24:GLN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ILE:HG21	1:D:166:ILE:HD13	1.79	0.42
1:F:108:THR:OG1	1:F:120:GLU:OE2	2.26	0.41
1:E:71:GLU:OE2	1:H:38:ARG:HD2	2.20	0.41
1:F:45:ASN:OD1	1:G:180:GLU:HB2	2.20	0.41
1:K:19:MET:HE1	1:K:51:GLY:N	2.35	0.41
1:G:5:ALA:HB1	1:G:53:ALA:HB1	2.01	0.41
1:G:101:LEU:HD22	1:G:102:ILE:N	2.35	0.41
1:I:19:MET:HE3	1:I:40:VAL:HG13	2.01	0.41
1:E:43:LEU:O	1:E:44:PHE:C	2.64	0.41
1:K:78:LYS:HA	1:K:110:LEU:HD21	2.03	0.41
1:G:108:THR:OG1	1:G:109:LEU:N	2.53	0.41
1:E:19:MET:HE1	1:E:51:GLY:N	2.34	0.41
1:C:19:MET:HE1	1:C:51:GLY:N	2.33	0.41
1:C:115:THR:HG21	1:D:1:SER:HB3	2.03	0.41
1:H:3:PHE:HA	1:H:26:THR:O	2.21	0.41
1:H:133:ASN:ND2	1:I:31:VAL:HG21	2.36	0.41
1:B:91:ASP:O	1:B:95:ARG:HB3	2.21	0.41
1:D:41:ARG:HD2	3:D:1041:HOH:O	2.20	0.41
1:F:6:THR:HG22	1:F:24:GLN:O	2.22	0.40
1:F:45:ASN:HD21	1:G:180:GLU:HG3	1.85	0.40
1:A:134:TYR:HB3	1:A:166:ILE:HD11	2.03	0.40
1:B:44:PHE:HB3	1:B:48:VAL:HG13	2.04	0.40
1:E:20:SER:HA	1:E:175:ILE:O	2.21	0.40
1:I:166:ILE:CG2	1:K:140:ARG:HE	2.34	0.40
1:J:36:THR:O	1:J:37:ALA:C	2.64	0.40
1:L:65:LYS:O	1:L:69:LYS:HG2	2.21	0.40
1:D:180:GLU:OE2	3:D:1044:HOH:O	2.22	0.40
1:E:91:ASP:O	1:E:95:ARG:CB	2.67	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:J:120:GLU:O	1:K:34:LYS:NZ[2_555]	2.07	0.13

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	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
1	B	178/180 (99%)	173 (97%)	5 (3%)	0	100	100
1	C	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
1	D	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
1	E	178/180 (99%)	173 (97%)	4 (2%)	1 (1%)	21	38
1	F	178/180 (99%)	170 (96%)	8 (4%)	0	100	100
1	G	178/180 (99%)	167 (94%)	11 (6%)	0	100	100
1	H	178/180 (99%)	169 (95%)	7 (4%)	2 (1%)	11	22
1	I	178/180 (99%)	165 (93%)	13 (7%)	0	100	100
1	J	178/180 (99%)	170 (96%)	7 (4%)	1 (1%)	21	38
1	K	178/180 (99%)	166 (93%)	10 (6%)	2 (1%)	11	22
1	L	178/180 (99%)	169 (95%)	9 (5%)	0	100	100
All	All	2136/2160 (99%)	2038 (95%)	92 (4%)	6 (0%)	36	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	106	GLN
1	H	74	ASN
1	J	37	ALA
1	H	146	ALA
1	K	6	THR
1	K	146	ALA

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	138/138 (100%)	127 (92%)	11 (8%)	11	24
1	B	138/138 (100%)	121 (88%)	17 (12%)	4	10
1	C	138/138 (100%)	126 (91%)	12 (9%)	9	21
1	D	138/138 (100%)	121 (88%)	17 (12%)	4	10
1	E	138/138 (100%)	119 (86%)	19 (14%)	3	7
1	F	138/138 (100%)	125 (91%)	13 (9%)	8	18
1	G	138/138 (100%)	126 (91%)	12 (9%)	9	21
1	H	138/138 (100%)	123 (89%)	15 (11%)	6	13
1	I	138/138 (100%)	123 (89%)	15 (11%)	6	13
1	J	138/138 (100%)	126 (91%)	12 (9%)	9	21
1	K	138/138 (100%)	124 (90%)	14 (10%)	7	15
1	L	138/138 (100%)	123 (89%)	15 (11%)	6	13
All	All	1656/1656 (100%)	1484 (90%)	172 (10%)	7	14

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	33	MET
1	A	48	VAL
1	A	67	GLU
1	A	89	ARG
1	A	101	LEU
1	A	109	LEU
1	A	110	LEU
1	A	160	LEU
1	A	175	ILE
1	A	178	GLU
1	B	29	GLN
1	B	43	LEU
1	B	48	VAL
1	B	67	GLU
1	B	74	ASN
1	B	79	ARG
1	B	89	ARG

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Mol	Chain	Res	Type
1	B	95	ARG
1	B	101	LEU
1	B	109	LEU
1	B	110	LEU
1	B	157	ARG
1	B	160	LEU
1	B	166	ILE
1	B	175	ILE
1	B	176	LEU
1	B	179	LEU
1	C	16	ARG
1	C	48	VAL
1	C	56	VAL
1	C	79	ARG
1	C	89	ARG
1	C	101	LEU
1	C	109	LEU
1	C	110	LEU
1	C	157	ARG
1	C	160	LEU
1	C	175	ILE
1	C	178	GLU
1	D	2	SER
1	D	33	MET
1	D	34	LYS
1	D	48	VAL
1	D	56	VAL
1	D	89	ARG
1	D	92	LYS
1	D	101	LEU
1	D	106	GLN
1	D	109	LEU
1	D	110	LEU
1	D	140	ARG
1	D	144	LYS
1	D	157	ARG
1	D	160	LEU
1	D	175	ILE
1	D	180	GLU
1	E	1	SER
1	E	29	GLN
1	E	43	LEU

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Mol	Chain	Res	Type
1	E	47	LYS
1	E	48	VAL
1	E	67	GLU
1	E	79	ARG
1	E	89	ARG
1	E	90	SER
1	E	93	VAL
1	E	101	LEU
1	E	104	MET
1	E	109	LEU
1	E	110	LEU
1	E	140	ARG
1	E	144	LYS
1	E	160	LEU
1	E	175	ILE
1	E	180	GLU
1	F	29	GLN
1	F	56	VAL
1	F	79	ARG
1	F	89	ARG
1	F	101	LEU
1	F	109	LEU
1	F	110	LEU
1	F	140	ARG
1	F	143	LYS
1	F	151	SER
1	F	160	LEU
1	F	175	ILE
1	F	178	GLU
1	G	43	LEU
1	G	48	VAL
1	G	79	ARG
1	G	82	VAL
1	G	89	ARG
1	G	101	LEU
1	G	109	LEU
1	G	110	LEU
1	G	160	LEU
1	G	175	ILE
1	G	178	GLU
1	G	180	GLU
1	H	41	ARG

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Mol	Chain	Res	Type
1	H	43	LEU
1	H	65	LYS
1	H	71	GLU
1	H	87	GLU
1	H	89	ARG
1	H	94	LEU
1	H	101	LEU
1	H	109	LEU
1	H	110	LEU
1	H	140	ARG
1	H	151	SER
1	H	160	LEU
1	H	176	LEU
1	H	178	GLU
1	I	1	SER
1	I	12	GLN
1	I	29	GLN
1	I	48	VAL
1	I	89	ARG
1	I	101	LEU
1	I	108	THR
1	I	109	LEU
1	I	110	LEU
1	I	140	ARG
1	I	153	SER
1	I	160	LEU
1	I	175	ILE
1	I	179	LEU
1	I	180	GLU
1	J	29	GLN
1	J	48	VAL
1	J	67	GLU
1	J	79	ARG
1	J	89	ARG
1	J	101	LEU
1	J	106	GLN
1	J	109	LEU
1	J	110	LEU
1	J	160	LEU
1	J	175	ILE
1	J	178	GLU
1	K	1	SER

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Mol	Chain	Res	Type
1	K	2	SER
1	K	12	GLN
1	K	29	GLN
1	K	72	GLU
1	K	89	ARG
1	K	101	LEU
1	K	109	LEU
1	K	110	LEU
1	K	113	SER
1	K	140	ARG
1	K	149	SER
1	K	150	MET
1	K	160	LEU
1	L	1	SER
1	L	29	GLN
1	L	33	MET
1	L	48	VAL
1	L	56	VAL
1	L	67	GLU
1	L	78	LYS
1	L	89	ARG
1	L	101	LEU
1	L	109	LEU
1	L	110	LEU
1	L	140	ARG
1	L	157	ARG
1	L	160	LEU
1	L	175	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	133	ASN
1	B	106	GLN
1	C	12	GLN
1	C	45	ASN
1	C	106	GLN
1	D	12	GLN
1	D	45	ASN
1	E	12	GLN
1	E	35	HIS

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Mol	Chain	Res	Type
1	E	74	ASN
1	E	106	GLN
1	E	145	HIS
1	F	12	GLN
1	F	29	GLN
1	F	35	HIS
1	F	76	ASN
1	G	106	GLN
1	H	106	GLN
1	I	12	GLN
1	I	106	GLN
1	J	12	GLN
1	J	35	HIS
1	J	106	GLN
1	K	12	GLN
1	K	106	GLN
1	L	12	GLN
1	L	29	GLN
1	L	106	GLN

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 12 ligands modelled in this entry, 12 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å ²)	Q<0.9
1	A	180/180 (100%)	-0.22	2 (1%) 78 75	36, 58, 96, 116	0
1	B	180/180 (100%)	-0.39	3 (1%) 69 65	28, 45, 68, 82	0
1	C	180/180 (100%)	-0.43	2 (1%) 78 75	29, 46, 72, 85	0
1	D	180/180 (100%)	-0.38	1 (0%) 85 83	34, 50, 76, 90	0
1	E	180/180 (100%)	-0.42	2 (1%) 78 75	27, 43, 67, 78	0
1	F	180/180 (100%)	-0.37	1 (0%) 85 83	29, 48, 83, 94	0
1	G	180/180 (100%)	0.08	2 (1%) 78 75	63, 81, 99, 110	0
1	H	180/180 (100%)	0.06	1 (0%) 85 83	60, 77, 104, 118	0
1	I	180/180 (100%)	0.31	1 (0%) 85 83	69, 87, 122, 138	0
1	J	180/180 (100%)	0.21	4 (2%) 62 58	67, 91, 125, 144	0
1	K	180/180 (100%)	0.48	3 (1%) 69 65	80, 104, 148, 167	0
1	L	180/180 (100%)	0.26	1 (0%) 85 83	72, 94, 133, 153	0
All	All	2160/2160 (100%)	-0.07	23 (1%) 78 75	27, 72, 120, 167	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	18	ALA	4.7
1	C	1	SER	4.6
1	E	1	SER	3.8
1	F	1	SER	3.7
1	D	1	SER	3.6
1	B	1	SER	3.1
1	G	92	LYS	2.9
1	A	1	SER	2.9
1	H	180	GLU	2.8
1	G	60	PHE	2.8
1	A	60	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	60	PHE	2.4
1	E	60	PHE	2.4
1	L	47	LYS	2.3
1	K	93	VAL	2.3
1	C	180	GLU	2.3
1	J	60	PHE	2.2
1	K	52	PHE	2.2
1	K	47	LYS	2.2
1	J	155	ILE	2.1
1	J	44	PHE	2.0
1	B	71	GLU	2.0
1	J	108	THR	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	NA	E	1005	1/1	0.42	0.21	47,47,47,47	0
2	NA	B	1002	1/1	0.55	0.19	44,44,44,44	0
2	NA	A	1001	1/1	0.58	0.19	49,49,49,49	0
2	NA	F	1006	1/1	0.64	0.19	44,44,44,44	0
2	NA	C	1003	1/1	0.68	0.14	43,43,43,43	0
2	NA	D	1004	1/1	0.70	0.19	58,58,58,58	0
2	NA	G	1007	1/1	0.75	0.25	87,87,87,87	0
2	NA	K	1011	1/1	0.81	0.21	96,96,96,96	0
2	NA	H	1010	1/1	0.83	0.28	82,82,82,82	0
2	NA	J	1008	1/1	0.84	0.31	79,79,79,79	0
2	NA	L	1012	1/1	0.84	0.28	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	I	1009	1/1	0.93	0.16	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.