



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:12 PM GMT

PDB ID : 2Z3B
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

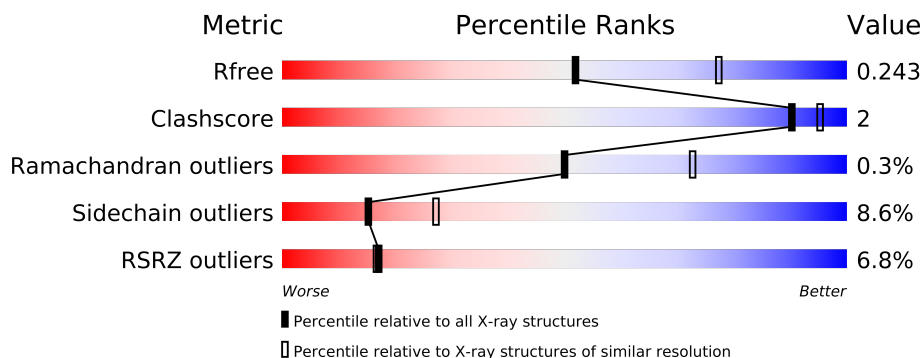
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	180	
1	B	180	
1	C	180	
1	D	180	
1	E	180	
1	F	180	
1	G	180	
1	H	180	
1	I	180	
1	J	180	
1	K	180	
1	L	180	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NA	A	1001	-	X
2	NA	B	1002	-	X
2	NA	D	1004	-	X
2	NA	E	1005	-	X
2	NA	F	1006	-	X
2	NA	J	1008	-	X
2	NA	K	1011	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16571 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Na 1	0	0
2	K	1	Total 1	Na 1	0	0
2	E	1	Total 1	Na 1	0	0
2	H	1	Total 1	Na 1	0	0
2	B	1	Total 1	Na 1	0	0
2	I	1	Total 1	Na 1	0	0
2	C	1	Total 1	Na 1	0	0
2	A	1	Total 1	Na 1	0	0
2	L	1	Total 1	Na 1	0	0
2	F	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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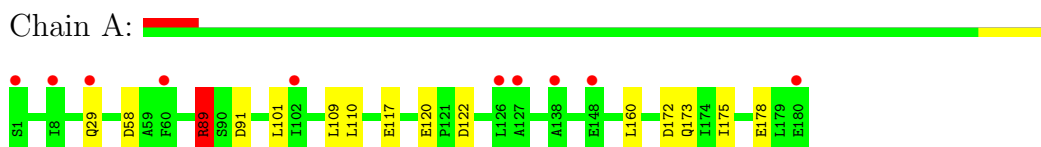
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	4	Total 4	O 4	0	0
3	K	4	Total 4	O 4	0	0
3	L	3	Total 3	O 3	0	0

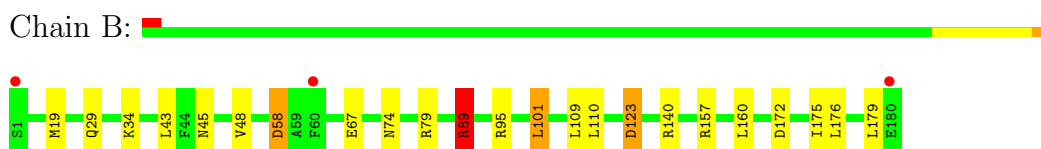
3 Residue-property plots

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

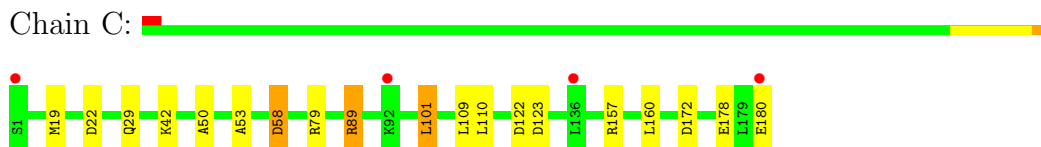
- Molecule 1: ATP-dependent protease hslV



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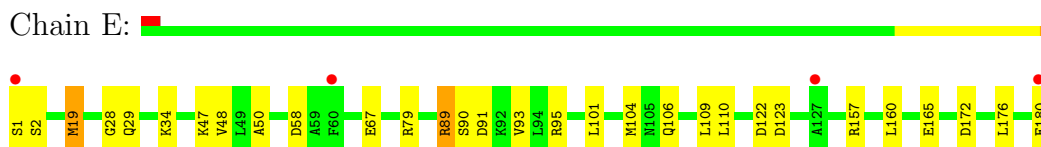
- Molecule 1: ATP-dependent protease hslV



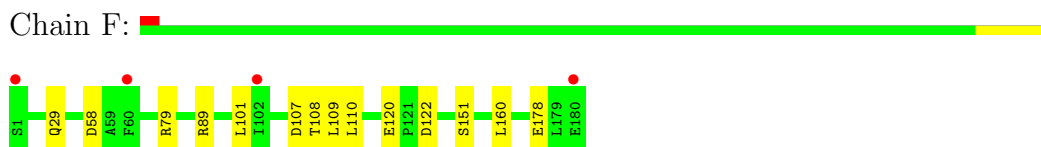
- Molecule 1: ATP-dependent protease hslV



- Molecule 1: ATP-dependent protease hslV

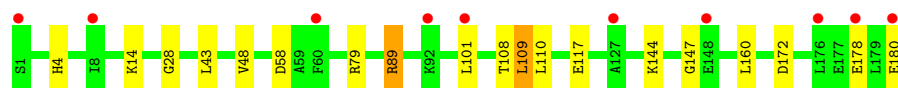


- Molecule 1: ATP-dependent protease hslV



- Molecule 1: ATP-dependent protease hslV

Chain G: 



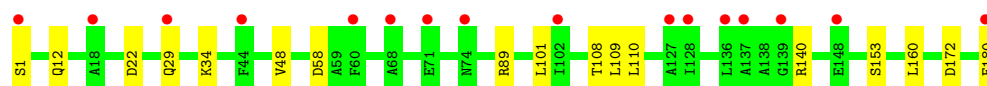
- Molecule 1: ATP-dependent protease hslV

Chain H: 



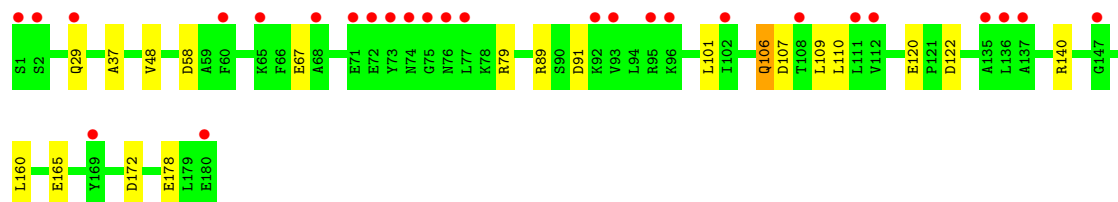
- Molecule 1: ATP-dependent protease hslV

Chain I: 



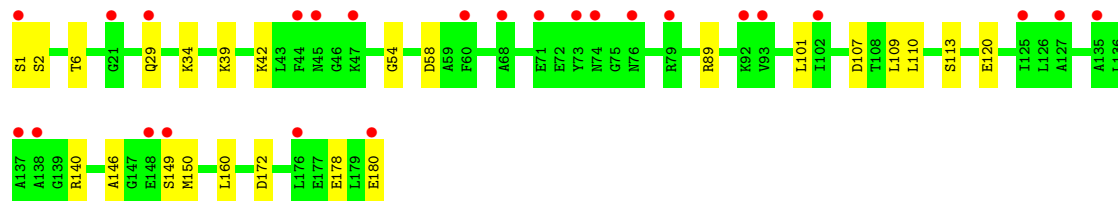
- Molecule 1: ATP-dependent protease hslV

Chain J: 



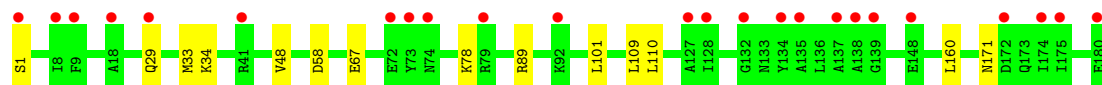
- Molecule 1: ATP-dependent protease hslV

Chain K: 



- Molecule 1: ATP-dependent protease hslV

Chain L: 



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 29.87 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (29.88-2.50) 95.4 (29.87-2.50)	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	REFMAC 5.1.24	Depositor
R, R_{free}	0.226 , 0.265 0.202 , 0.243	Depositor DCC
R_{free} test set	4576 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.8	EDS
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
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 90900 reflections	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.

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	0.76	0/1376	0.89	6/1847 (0.3%)
1	B	0.96	1/1376 (0.1%)	0.99	5/1847 (0.3%)
1	C	0.94	0/1376	1.01	8/1847 (0.4%)
1	D	0.97	3/1376 (0.2%)	0.95	5/1847 (0.3%)
1	E	1.04	1/1376 (0.1%)	1.00	6/1847 (0.3%)
1	F	0.86	0/1376	0.92	3/1847 (0.2%)
1	G	0.59	0/1376	0.81	3/1847 (0.2%)
1	H	0.61	0/1376	0.77	3/1847 (0.2%)
1	I	0.52	0/1376	0.77	3/1847 (0.2%)
1	J	0.55	0/1376	0.80	4/1847 (0.2%)
1	K	0.48	0/1376	0.73	3/1847 (0.2%)
1	L	0.55	0/1376	0.72	1/1847 (0.1%)
All	All	0.76	5/16512 (0.0%)	0.87	50/22164 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	180	GLU	CD-OE2	7.30	1.33	1.25
1	E	19	MET	SD-CE	-7.00	1.38	1.77
1	D	180	GLU	CD-OE1	6.16	1.32	1.25
1	B	19	MET	SD-CE	-5.54	1.46	1.77
1	D	19	MET	SD-CE	-5.33	1.48	1.77

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	ASP	CB-CG-OD2	8.83	126.25	118.30
1	C	172	ASP	CB-CG-OD2	8.42	125.88	118.30
1	G	58	ASP	CB-CG-OD2	8.36	125.82	118.30
1	D	58	ASP	CB-CG-OD2	7.96	125.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	172	ASP	CB-CG-OD2	7.88	125.39	118.30
1	B	123	ASP	CB-CG-OD1	7.68	125.22	118.30
1	B	58	ASP	CB-CG-OD2	7.53	125.07	118.30
1	F	107	ASP	CB-CG-OD2	7.30	124.87	118.30
1	H	172	ASP	CB-CG-OD2	7.29	124.86	118.30
1	E	172	ASP	CB-CG-OD2	7.13	124.72	118.30
1	D	107	ASP	CB-CG-OD2	7.13	124.72	118.30
1	E	58	ASP	CB-CG-OD2	7.08	124.67	118.30
1	B	172	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	122	ASP	CB-CG-OD2	6.72	124.35	118.30
1	I	58	ASP	CB-CG-OD2	6.69	124.33	118.30
1	D	172	ASP	CB-CG-OD2	6.61	124.25	118.30
1	C	22	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	172	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	89	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	58	ASP	CB-CG-OD2	6.34	124.01	118.30
1	I	22	ASP	CB-CG-OD2	6.03	123.72	118.30
1	J	122	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	89	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	G	172	ASP	CB-CG-OD2	5.85	123.56	118.30
1	F	122	ASP	CB-CG-OD2	5.81	123.53	118.30
1	G	89	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	I	172	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	123	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	101	LEU	CA-CB-CG	5.59	128.15	115.30
1	C	123	ASP	CB-CG-OD1	5.56	123.30	118.30
1	J	91	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	58	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	58	ASP	CB-CG-OD2	5.39	123.16	118.30
1	H	122	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	89	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	K	107	ASP	CB-CG-OD2	5.36	123.12	118.30
1	L	58	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	89	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	91	ASP	CB-CG-OD2	5.28	123.05	118.30
1	K	58	ASP	CB-CG-OD2	5.26	123.03	118.30
1	K	172	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	101	LEU	CA-CB-CG	5.20	127.26	115.30
1	E	122	ASP	CB-CG-OD2	5.18	122.97	118.30
1	E	123	ASP	CB-CG-OD1	5.18	122.97	118.30
1	J	58	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	89	ARG	NE-CZ-NH1	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	58	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	E	89	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	165	GLU	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1359	0	0	4	0
1	B	1359	0	0	4	0
1	C	1359	0	0	5	0
1	D	1359	0	0	6	0
1	E	1359	0	0	5	0
1	F	1359	0	0	1	0
1	G	1359	0	0	5	0
1	H	1359	0	0	3	0
1	I	1359	0	0	1	0
1	J	1359	0	0	2	1
1	K	1359	0	0	4	1
1	L	1359	0	0	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1	0	0	0	0
3	A	25	0	0	2	0
3	B	43	0	0	0	0
3	C	41	0	0	2	0
3	D	41	0	0	2	0
3	E	44	0	0	1	0
3	F	33	0	0	0	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	0	0
3	K	4	0	0	0	0
3	L	3	0	0	0	0
All	All	16571	0	0	35	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (35) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:117:GLU:OE1	3:G:1011:HOH:O	1.79	1.00
1:K:120:GLU:O	1:L:34:LYS:NZ	2.05	0.89
1:A:117:GLU:OE1	3:A:1020:HOH:O	1.93	0.85
1:K:39:LYS:NZ	1:K:54:GLY:O	2.20	0.73
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:F:108:THR:OG1	1:F:120:GLU:OE2	2.26	0.54
1:C:53:ALA:CB	3:C:1035:HOH:O	2.56	0.53
1:A:120:GLU:O	1:B:34:LYS:NZ	2.42	0.53
1:D:179:LEU:O	1:D:180:GLU:OXT	2.27	0.53
1:G:4:HIS:NE2	1:G:28:GLY:O	2.42	0.52
1:C:42:LYS:NZ	3:C:1025:HOH:O	2.43	0.52
1:E:2:SER:O	1:E:28:GLY:N	2.45	0.49
1:K:42:LYS:NZ	1:K:178:GLU:O	2.46	0.49
1:D:179:LEU:C	1:D:180:GLU:OXT	2.50	0.49
1:E:165:GLU:OE2	3:E:1030:HOH:O	2.20	0.49
1:D:120:GLU:O	1:E:34:LYS:NZ	2.47	0.48
1:A:89:ARG:NE	1:B:58:ASP:OD2	2.47	0.48
1:H:120:GLU:O	1:I:34:LYS:NZ	2.46	0.47
1:K:180:GLU:N	1:K:180:GLU:OE2	2.48	0.47
1:B:123:ASP:OD2	1:B:140:ARG:CD	2.63	0.46
1:H:180:GLU:N	1:H:180:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:19:MET:CE	1:C:50:ALA:C	2.84	0.46
1:B:89:ARG:NH1	1:C:58:ASP:OD2	2.49	0.46
1:J:106:GLN:NE2	1:J:107:ASP:OD1	2.49	0.46
1:G:144:LYS:NZ	1:J:165:GLU:OE2	2.50	0.45
1:D:108:THR:OG1	1:D:120:GLU:OE2	2.34	0.45
1:G:14:LYS:NZ	1:G:147:GLY:O	2.49	0.45
1:H:53:ALA:CB	3:H:1014:HOH:O	2.65	0.45
1:C:180:GLU:N	1:C:180:GLU:OE2	2.51	0.44
1:E:91:ASP:O	1:E:95:ARG:CB	2.67	0.42
1:L:171:ASN:C	1:L:171:ASN:OD1	2.57	0.42
1:G:108:THR:OG1	1:G:109:LEU:N	2.53	0.41
1:D:180:GLU:OE2	3:D:1044:HOH:O	2.22	0.40
1:E:19:MET:CE	1:E:50:ALA:C	2.90	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	Distance(Å)	Clash(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%)	33	55
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%)	21	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	178/180 (99%)	165 (93%)	13 (7%)	0	100	100
1	J	178/180 (99%)	170 (96%)	7 (4%)	1 (1%)	33	55
1	K	178/180 (99%)	166 (93%)	10 (6%)	2 (1%)	21	34
1	L	178/180 (99%)	169 (95%)	9 (5%)	0	100	100
All	All	2136/2160 (99%)	2038 (95%)	92 (4%)	6 (0%)	50	73

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%)	130 (94%)	8 (6%)	28	49
1	B	138/138 (100%)	121 (88%)	17 (12%)	7	12
1	C	138/138 (100%)	129 (94%)	9 (6%)	24	42
1	D	138/138 (100%)	126 (91%)	12 (9%)	15	27
1	E	138/138 (100%)	121 (88%)	17 (12%)	7	12
1	F	138/138 (100%)	129 (94%)	9 (6%)	24	42
1	G	138/138 (100%)	128 (93%)	10 (7%)	21	36
1	H	138/138 (100%)	125 (91%)	13 (9%)	13	23
1	I	138/138 (100%)	125 (91%)	13 (9%)	13	23
1	J	138/138 (100%)	126 (91%)	12 (9%)	15	27
1	K	138/138 (100%)	126 (91%)	12 (9%)	15	27
1	L	138/138 (100%)	127 (92%)	11 (8%)	17	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1656/1656 (100%)	1513 (91%)	143 (9%)	15	27

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
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	45	ASN
1	B	48	VAL
1	B	67	GLU
1	B	74	ASN
1	B	79	ARG
1	B	89	ARG
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	175	ILE
1	B	176	LEU
1	B	179	LEU
1	C	29	GLN
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	178	GLU
1	D	2	SER
1	D	33	MET
1	D	48	VAL

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Mol	Chain	Res	Type
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	157	ARG
1	D	160	LEU
1	D	180	GLU
1	E	1	SER
1	E	29	GLN
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	157	ARG
1	E	160	LEU
1	E	176	LEU
1	E	180	GLU
1	F	29	GLN
1	F	79	ARG
1	F	89	ARG
1	F	101	LEU
1	F	109	LEU
1	F	110	LEU
1	F	151	SER
1	F	160	LEU
1	F	178	GLU
1	G	43	LEU
1	G	48	VAL
1	G	79	ARG
1	G	89	ARG
1	G	101	LEU
1	G	109	LEU
1	G	110	LEU

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Mol	Chain	Res	Type
1	G	160	LEU
1	G	178	GLU
1	G	180	GLU
1	H	41	ARG
1	H	43	LEU
1	H	65	LYS
1	H	71	GLU
1	H	87	GLU
1	H	89	ARG
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	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	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	140	ARG
1	J	160	LEU
1	J	178	GLU
1	K	1	SER

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Mol	Chain	Res	Type
1	K	2	SER
1	K	29	GLN
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	67	GLU
1	L	78	LYS
1	L	89	ARG
1	L	101	LEU
1	L	109	LEU
1	L	110	LEU
1	L	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

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(Å ²)	Q<0.9
1	A	180/180 (100%)	0.18	10 (5%) 24 24	36, 58, 96, 116	0
1	B	180/180 (100%)	-0.11	3 (1%) 67 69	28, 45, 68, 82	0
1	C	180/180 (100%)	-0.07	4 (2%) 59 61	29, 46, 72, 85	0
1	D	180/180 (100%)	-0.07	5 (2%) 50 53	34, 50, 76, 90	0
1	E	180/180 (100%)	-0.05	4 (2%) 59 61	27, 43, 67, 78	0
1	F	180/180 (100%)	0.08	4 (2%) 59 61	29, 48, 83, 94	0
1	G	180/180 (100%)	0.37	10 (5%) 24 24	63, 81, 99, 110	0
1	H	180/180 (100%)	0.38	16 (8%) 10 9	60, 77, 104, 118	0
1	I	180/180 (100%)	0.52	16 (8%) 10 9	69, 87, 122, 138	0
1	J	180/180 (100%)	0.61	27 (15%) 3 3	67, 91, 125, 144	0
1	K	180/180 (100%)	0.70	25 (13%) 4 3	80, 104, 148, 167	0
1	L	180/180 (100%)	0.71	24 (13%) 4 3	72, 94, 133, 153	0
All	All	2160/2160 (100%)	0.27	148 (6%) 17 16	27, 72, 120, 167	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	92	LYS	6.6
1	H	180	GLU	5.2
1	K	47	LYS	4.7
1	C	1	SER	4.5
1	I	180	GLU	4.5
1	J	1	SER	4.4
1	H	138	ALA	4.3
1	B	1	SER	4.2
1	B	180	GLU	4.2
1	G	92	LYS	4.1
1	H	137	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	92	LYS	3.9
1	K	148	GLU	3.8
1	J	60	PHE	3.8
1	J	76	ASN	3.8
1	L	92	LYS	3.8
1	L	74	ASN	3.8
1	E	1	SER	3.7
1	D	1	SER	3.7
1	K	1	SER	3.7
1	J	180	GLU	3.7
1	L	73	TYR	3.6
1	K	180	GLU	3.6
1	G	60	PHE	3.6
1	L	127	ALA	3.6
1	A	180	GLU	3.6
1	J	71	GLU	3.6
1	I	127	ALA	3.5
1	I	71	GLU	3.5
1	K	127	ALA	3.5
1	K	60	PHE	3.5
1	J	136	LEU	3.4
1	K	74	ASN	3.4
1	I	1	SER	3.3
1	L	135	ALA	3.3
1	D	29	GLN	3.3
1	L	180	GLU	3.3
1	J	29	GLN	3.3
1	J	75	GLY	3.2
1	H	1	SER	3.2
1	L	1	SER	3.2
1	I	136	LEU	3.2
1	K	92	LYS	3.1
1	F	1	SER	3.1
1	J	93	VAL	3.1
1	K	93	VAL	3.1
1	K	137	ALA	3.1
1	K	138	ALA	3.1
1	H	60	PHE	3.1
1	K	21	GLY	3.1
1	G	1	SER	3.0
1	H	136	LEU	3.0
1	I	148	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	74	ASN	3.0
1	K	76	ASN	3.0
1	G	127	ALA	3.0
1	K	135	ALA	2.9
1	A	60	PHE	2.9
1	K	176	LEU	2.9
1	L	29	GLN	2.9
1	L	72	GLU	2.8
1	I	128	ILE	2.8
1	I	137	ALA	2.8
1	K	68	ALA	2.8
1	J	147	GLY	2.8
1	G	148	GLU	2.7
1	J	2	SER	2.7
1	A	102	ILE	2.6
1	A	148	GLU	2.6
1	J	102	ILE	2.6
1	L	132	GLY	2.6
1	E	180	GLU	2.6
1	L	9	PHE	2.6
1	K	71	GLU	2.6
1	F	102	ILE	2.6
1	I	139	GLY	2.6
1	H	29	GLN	2.6
1	J	73	TYR	2.6
1	K	44	PHE	2.6
1	H	4	HIS	2.5
1	I	74	ASN	2.5
1	D	135	ALA	2.5
1	F	180	GLU	2.5
1	H	139	GLY	2.5
1	G	101	LEU	2.5
1	A	126	LEU	2.5
1	E	60	PHE	2.5
1	E	127	ALA	2.5
1	I	102	ILE	2.5
1	J	95	ARG	2.4
1	A	1	SER	2.4
1	L	138	ALA	2.4
1	L	79	ARG	2.4
1	L	148	GLU	2.4
1	J	65	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	73	TYR	2.4
1	L	134	TYR	2.4
1	G	180	GLU	2.3
1	L	172	ASP	2.3
1	L	139	GLY	2.3
1	K	125	ILE	2.3
1	G	178	GLU	2.3
1	H	71	GLU	2.3
1	I	44	PHE	2.3
1	K	79	ARG	2.3
1	I	29	GLN	2.3
1	C	92	LYS	2.2
1	J	108	THR	2.2
1	H	127	ALA	2.2
1	B	60	PHE	2.2
1	H	133	ASN	2.2
1	I	60	PHE	2.2
1	L	174	ILE	2.2
1	G	8	ILE	2.2
1	L	175	ILE	2.2
1	A	127	ALA	2.2
1	D	101	LEU	2.2
1	A	138	ALA	2.2
1	I	18	ALA	2.2
1	J	135	ALA	2.2
1	K	149	SER	2.2
1	H	93	VAL	2.2
1	C	180	GLU	2.2
1	K	29	GLN	2.2
1	L	41	ARG	2.1
1	L	137	ALA	2.1
1	J	77	LEU	2.1
1	J	111	LEU	2.1
1	J	169	TYR	2.1
1	J	96	LYS	2.1
1	J	112	VAL	2.1
1	J	137	ALA	2.1
1	A	29	GLN	2.1
1	G	176	LEU	2.1
1	L	8	ILE	2.1
1	I	68	ALA	2.1
1	L	18	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	60	PHE	2.0
1	A	8	ILE	2.0
1	D	102	ILE	2.0
1	H	126	LEU	2.0
1	K	102	ILE	2.0
1	K	45	ASN	2.0
1	C	136	LEU	2.0
1	J	72	GLU	2.0
1	L	128	ILE	2.0
1	H	14	LYS	2.0
1	J	68	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NA	J	1008	1/1	0.24	6.55	79,79,79,79	0
2	NA	E	1005	1/1	0.31	6.55	47,47,47,47	0
2	NA	F	1006	1/1	0.24	4.94	44,44,44,44	0
2	NA	K	1011	1/1	0.30	3.79	96,96,96,96	0
2	NA	B	1002	1/1	0.20	3.36	44,44,44,44	0
2	NA	D	1004	1/1	0.25	3.34	58,58,58,58	0
2	NA	A	1001	1/1	0.25	3.05	49,49,49,49	0
2	NA	G	1007	1/1	0.26	1.81	87,87,87,87	0
2	NA	C	1003	1/1	0.14	1.07	43,43,43,43	0
2	NA	H	1010	1/1	0.18	1.00	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NA	L	1012	1/1	0.15	-0.30	84,84,84,84	0
2	NA	I	1009	1/1	0.10	-1.05	83,83,83,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.