



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 08:38 AM EDT

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 : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

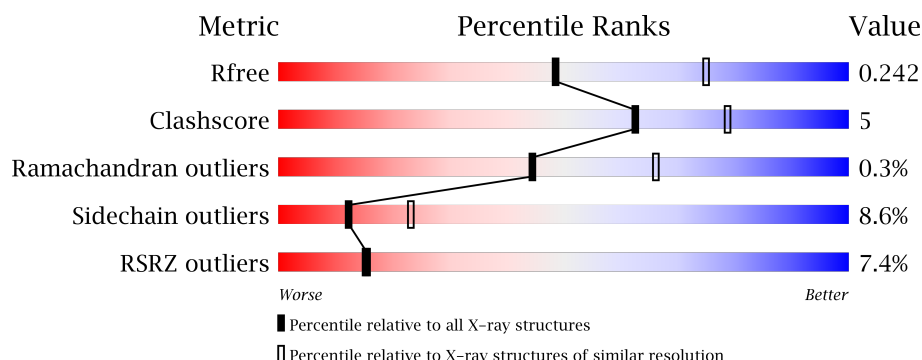
1 Overall quality at a glance

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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. 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	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	180	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	180	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	180	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div> </div>
1	E	180	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 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 (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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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

- Molecule 1: ATP-dependent protease hslV

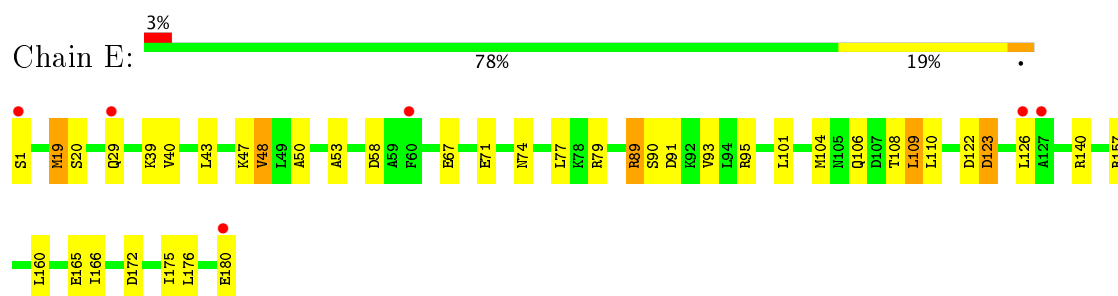


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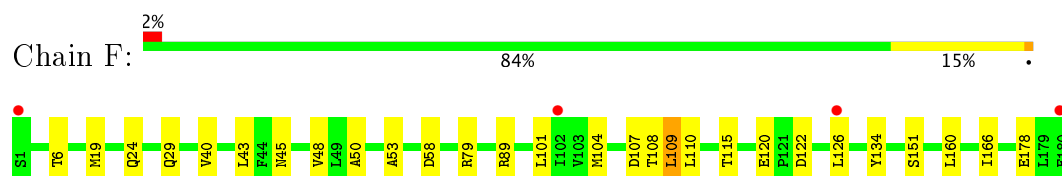
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- The chart displays the distribution of 180 samples across 30 categories. The categories are labeled on the x-axis: S1, M19, D22, Q29, V40, K42, M45, A50, A53, D58, F66, R79, R89, K92, L101, I102, V103, M104, L109, L110, T115, D122, D123, L126, A127, I128, L136, R140, R157, L160, I166, D172, L176, R177, and E180. The y-axis represents the number of samples, ranging from 0 to 180. The bars are color-coded: green for categories with 10 or more samples, orange for categories with 5 to 9 samples, and yellow for categories with 1 to 4 samples. Red dots are placed above the bars for categories S1, K92, and L136, indicating their total sample counts.
- | Category | Sample Count |
|----------|--------------|
| S1 | 10 |
| M19 | 1 |
| D22 | 1 |
| Q29 | 1 |
| V40 | 1 |
| K42 | 1 |
| M45 | 1 |
| A50 | 1 |
| A53 | 1 |
| D58 | 1 |
| F66 | 1 |
| R79 | 1 |
| R89 | 5 |
| K92 | 10 |
| L101 | 10 |
| I102 | 10 |
| V103 | 1 |
| M104 | 1 |
| L109 | 5 |
| L110 | 5 |
| T115 | 1 |
| D122 | 1 |
| D123 | 5 |
| L126 | 10 |
| A127 | 10 |
| I128 | 1 |
| L136 | 10 |
| R140 | 1 |
| R157 | 1 |
| L160 | 1 |
| I166 | 1 |
| D172 | 1 |
| L176 | 1 |
| R177 | 1 |
| E180 | 1 |

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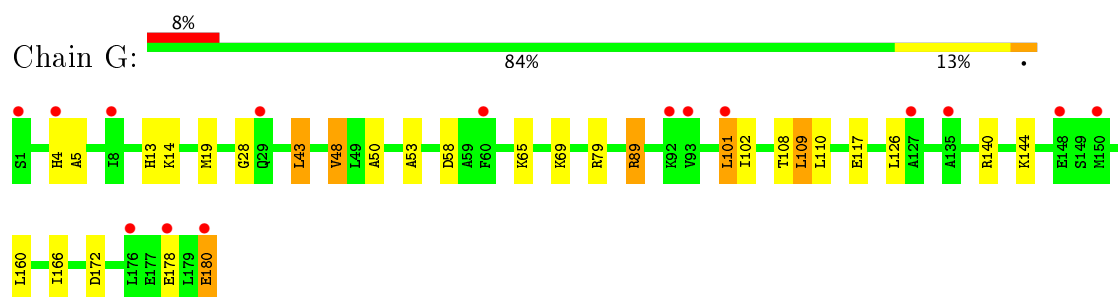
- Molecule 1: ATP-dependent protease hslV



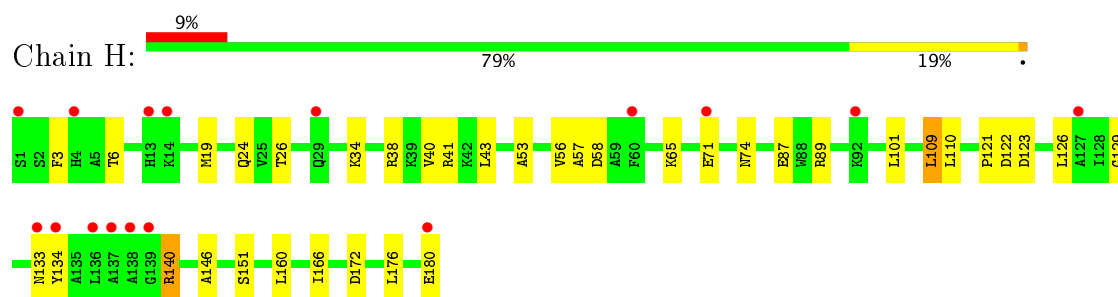
- Molecule 1: ATP-dependent protease hslV



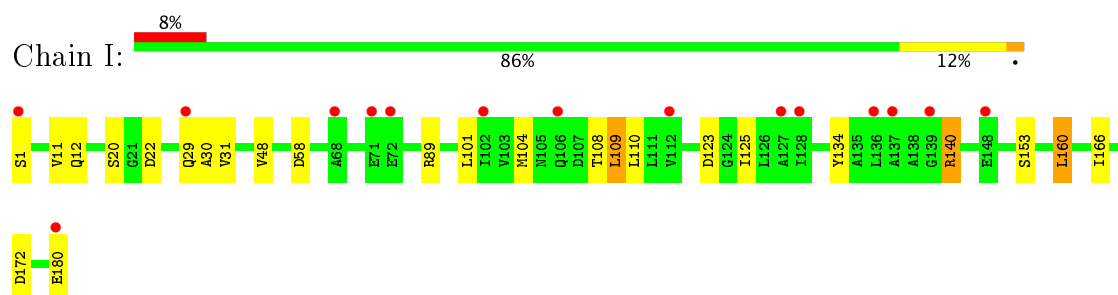
- Molecule 1: ATP-dependent protease hslV



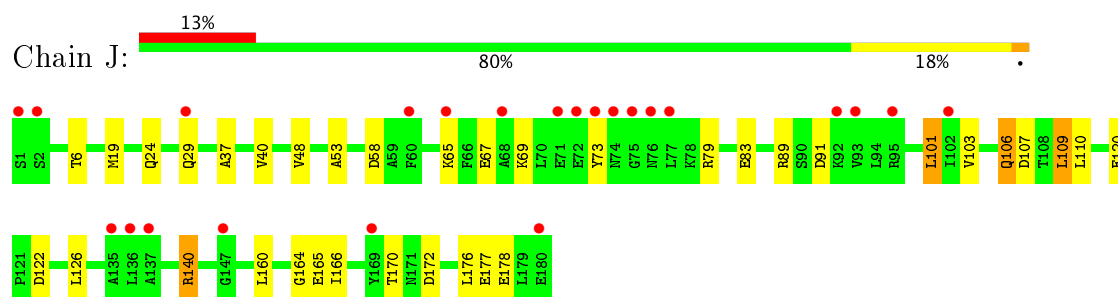
- Molecule 1: ATP-dependent protease hslV



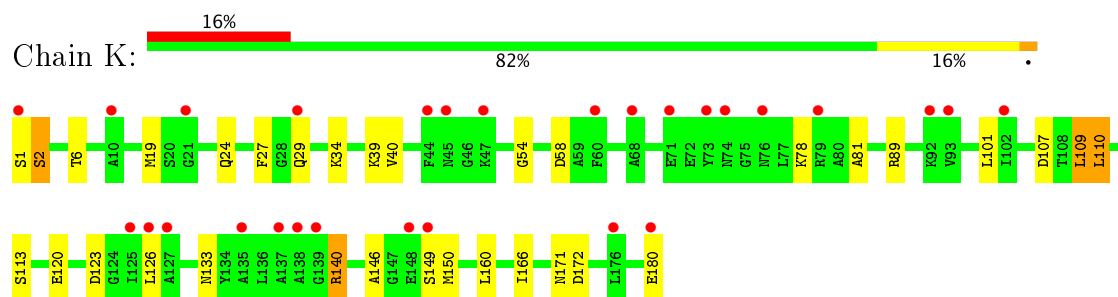
- Molecule 1: ATP-dependent protease hslV



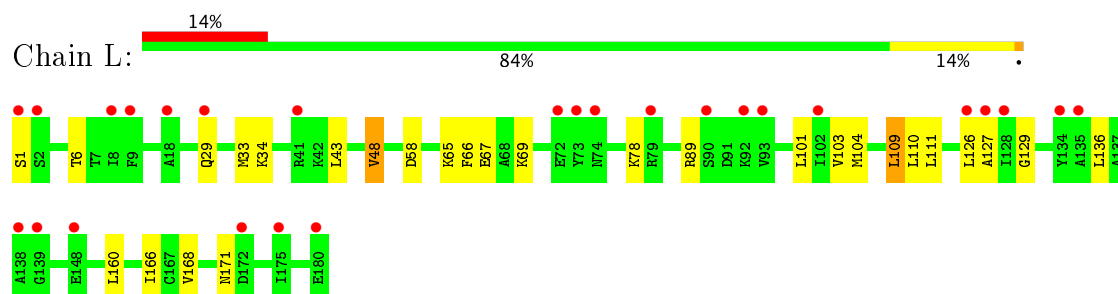
- Molecule 1: ATP-dependent protease hslV



- 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 29.87 – 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	CNS, REFMAC 5.1.24	Depositor
R, R_{free}	0.226 , 0.265 0.202 , 0.242	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 , 49.0	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	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 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	13	0
1	B	1359	0	1377	17	0
1	C	1359	0	1377	17	0
1	D	1359	0	1377	20	0
1	E	1359	0	1377	16	0
1	F	1359	0	1377	13	0
1	G	1359	0	1377	19	0
1	H	1359	0	1377	17	0
1	I	1359	0	1377	9	0
1	J	1359	0	1377	19	1
1	K	1359	0	1377	15	1
1	L	1359	0	1377	12	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	165	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (165) 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:H:19:MET:HE2	1:H:40:VAL:HG13	1.52	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
1:J:109:LEU:HD22	1:J:126:LEU:HD12	1.58	0.86
1:A:117:GLU:OE1	3:A:1020:HOH:O	1.93	0.85
1:B:19:MET:HE2	1:B:40:VAL:HG13	1.59	0.84
1:D:19:MET:HE2	1:D:40:VAL:HG13	1.62	0.82
1:E:123:ASP:OD2	1:E:140:ARG:HD3	1.80	0.81
1:K:19:MET:HE2	1:K:40:VAL:HG13	1.65	0.79
1:E:19:MET:HE2	1:E:40:VAL:HG13	1.66	0.77
1:C:19:MET:HE2	1:C:40:VAL:HG13	1.65	0.77
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: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:B:109:LEU:HD22	1:B:126:LEU:HD12	1.70	0.72
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:A:19:MET:HE2	1:A:40:VAL:HG13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:J:19:MET:CE	1:J:40:VAL:HG13	2.28	0.63
1:I:123:ASP:OD2	1:I:140:ARG:HD3	1.99	0.63
1:K:109:LEU:HD22	1:K:126:LEU:HD12	1.80	0.62
1:E:19:MET:HE1	1:E:50:ALA:C	2.20	0.61
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
1:J:19:MET:HE2	1:J:40:VAL:HG13	1.82	0.60
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:D:19:MET:CE	1:D:40:VAL:HG13	2.31	0.60
1:L:6:THR:O	1:L:129:GLY:HA3	2.01	0.59
1:C:19:MET:HE1	1:C:50:ALA:C	2.23	0.59
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:E:19:MET:CE	1:E:40:VAL:HG13	2.32	0.58
1:F:104:MET:HE3	1:F:109:LEU:HG	1.86	0.58
1:F:19:MET:HE2	1:F:40:VAL:HG13	1.85	0.57
1:B:19:MET:CE	1:B:40:VAL:HG13	2.32	0.57
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: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:E:74:ASN:HD21	1:H:34:LYS:NZ	2.04	0.55
1:K:81:ALA:HB2	1:K:110:LEU:HD23	1.88	0.55
1:C:176:LEU:C	1:C:176:LEU:HD23	2.27	0.54
1:G:140:ARG:HE	1:J:166:ILE:CG2	2.20	0.54
1:D:104:MET:HE3	1:D:109:LEU:HG	1.90	0.53
1:I:11:VAL:HG23	1:I:125:ILE:HG12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:PRO:HG3	1:H:126:LEU:HG	1.91	0.53
1:E:74:ASN:HD21	1:H:34:LYS:HZ1	1.57	0.53
1:H:140:ARG:HH21	1:L:166:ILE:HG22	1.74	0.52
1:D:42:LYS:C	1:D:43:LEU:HD12	2.31	0.52
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:D:19:MET:HE1	1:D:50:ALA:C	2.30	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:D:179:LEU:C	1:D:180:GLU:OXT	2.50	0.49
1:G:166:ILE:HG22	1:J:140:ARG:HE	1.77	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:D:89:ARG:HD3	1:D:89:ARG:O	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:K:180:GLU:OE2	1:K:180:GLU:N	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:C:42:LYS:NZ	3:C:1025:HOH:O	2.43	0.46
1:F:19:MET:CE	1:F:40:VAL:HG13	2.44	0.46
1:H:180:GLU:OE2	1:H:180:GLU:N	2.48	0.46
1:J:176:LEU:C	1:J:176:LEU:HD23	2.36	0.46
1:D:42:LYS:O	1:D:43:LEU:HD12	2.15	0.46
1:C:19:MET:CE	1:C:50:ALA:C	2.84	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:J:19:MET:HE3	1:J:40:VAL:HG13	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:127:ALA:HB3	1:L:136:LEU:HB2	1.97	0.45
1:G:144:LYS:NZ	1:J:165:GLU:OE2	2.50	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:L:104:MET:CB	1:L:109:LEU:HD23	2.45	0.45
1:I:30:ALA:O	1:L:168:VAL:HG13	2.16	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:C:104:MET:HE3	1:C:109:LEU:HG	1.97	0.44
1:A:117:GLU:HG3	1:B:3:PHE:CD1	2.52	0.44
1:A:166:ILE:HD13	1:A:166:ILE:HG21	1.67	0.44
1:B:65:LYS:O	1:B:69:LYS:HG2	2.17	0.44
1:A:1:SER:HB3	1:F:115:THR:HG21	1.98	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:G:19:MET:HE1	1:G:50:ALA:C	2.38	0.43
1:J:164:GLY:HA2	1:J:170:THR:HB	1.99	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: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: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:B:70:LEU:C	1:B:72:GLU:H	2.23	0.42
1:J:101:LEU:HD22	1:J:103:VAL:HG13	2.01	0.42
1:F:19:MET:HE1	1:F:50:ALA:C	2.39	0.42
1:H:6:THR:HG22	1:H:24:GLN:O	2.18	0.42
1:L:171:ASN:OD1	1:L:171:ASN:C	2.57	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:I:140:ARG:HH21	1:K:166:ILE:HG22	1.83	0.42
1:C:166:ILE:HG21	1:C:166:ILE:HD13	1.85	0.42
1:D:7:THR:O	1:D:21:GLY:HA2	2.20	0.42
1:D:166:ILE:HD13	1:D:166:ILE:HG21	1.79	0.42
1:D:6:THR:HG22	1:D:24:GLN:O	2.20	0.42
1:F:108:THR:OG1	1:F:120:GLU:OE2	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:101:LEU:HD22	1:G:102:ILE:N	2.35	0.41
1:G:5:ALA:HB1	1:G:53:ALA:HB1	2.01	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:C:115:THR:HG21	1:D:1:SER:HB3	2.03	0.41
1:H:133:ASN:ND2	1:I:31:VAL:HG21	2.36	0.41
1:H:3:PHE:HA	1:H:26:THR:O	2.21	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: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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	178/180 (99%)	172 (97%)	6 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	28	48
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%)	17	29
1	I	178/180 (99%)	165 (93%)	13 (7%)	0	100	100
1	J	178/180 (99%)	170 (96%)	7 (4%)	1 (1%)	28	48
1	K	178/180 (99%)	166 (93%)	10 (6%)	2 (1%)	17	29
1	L	178/180 (99%)	169 (95%)	9 (5%)	0	100	100
All	All	2136/2160 (99%)	2038 (95%)	92 (4%)	6 (0%)	44	66

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%)	23	43
1	B	138/138 (100%)	121 (88%)	17 (12%)	5	10
1	C	138/138 (100%)	129 (94%)	9 (6%)	20	37
1	D	138/138 (100%)	126 (91%)	12 (9%)	12	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	138/138 (100%)	121 (88%)	17 (12%)	5	10
1	F	138/138 (100%)	129 (94%)	9 (6%)	20	37
1	G	138/138 (100%)	128 (93%)	10 (7%)	17	31
1	H	138/138 (100%)	125 (91%)	13 (9%)	10	19
1	I	138/138 (100%)	125 (91%)	13 (9%)	10	19
1	J	138/138 (100%)	126 (91%)	12 (9%)	12	23
1	K	138/138 (100%)	126 (91%)	12 (9%)	12	23
1	L	138/138 (100%)	127 (92%)	11 (8%)	14	27
All	All	1656/1656 (100%)	1513 (91%)	143 (9%)	12	23

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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. All (18) such sidechains are listed below:

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.10	10 (5%) 25 26	36, 58, 96, 116	0
1	B	180/180 (100%)	-0.14	8 (4%) 35 37	28, 45, 68, 82	0
1	C	180/180 (100%)	-0.12	4 (2%) 62 64	29, 46, 72, 85	0
1	D	180/180 (100%)	-0.15	5 (2%) 53 56	34, 50, 76, 90	0
1	E	180/180 (100%)	-0.12	6 (3%) 47 50	27, 43, 67, 78	0
1	F	180/180 (100%)	0.01	4 (2%) 62 64	29, 48, 83, 94	0
1	G	180/180 (100%)	0.33	15 (8%) 12 12	63, 81, 99, 110	0
1	H	180/180 (100%)	0.33	16 (8%) 10 10	60, 77, 104, 118	0
1	I	180/180 (100%)	0.48	15 (8%) 12 12	69, 87, 122, 138	0
1	J	180/180 (100%)	0.58	23 (12%) 4 3	67, 91, 125, 144	0
1	K	180/180 (100%)	0.72	28 (15%) 2 2	80, 104, 148, 167	0
1	L	180/180 (100%)	0.71	26 (14%) 3 2	72, 94, 133, 153	0
All	All	2160/2160 (100%)	0.23	160 (7%) 15 15	27, 72, 120, 167	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	92	LYS	6.8
1	I	180	GLU	5.1
1	H	180	GLU	5.0
1	B	1	SER	5.0
1	K	47	LYS	4.9
1	C	1	SER	4.8
1	K	148	GLU	4.7
1	J	1	SER	4.6
1	J	71	GLU	4.5
1	H	138	ALA	4.3
1	K	180	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	92	LYS	4.3
1	G	92	LYS	4.2
1	H	92	LYS	4.1
1	B	180	GLU	4.1
1	H	137	ALA	4.1
1	E	1	SER	3.9
1	D	1	SER	3.8
1	K	138	ALA	3.8
1	J	180	GLU	3.8
1	I	127	ALA	3.7
1	K	135	ALA	3.7
1	J	136	LEU	3.6
1	J	75	GLY	3.6
1	J	29	GLN	3.5
1	K	76	ASN	3.5
1	K	1	SER	3.5
1	A	180	GLU	3.5
1	G	1	SER	3.4
1	J	76	ASN	3.4
1	L	127	ALA	3.3
1	L	135	ALA	3.3
1	K	21	GLY	3.3
1	K	93	VAL	3.3
1	J	60	PHE	3.3
1	F	1	SER	3.3
1	L	180	GLU	3.2
1	G	127	ALA	3.2
1	J	74	ASN	3.2
1	K	137	ALA	3.2
1	H	1	SER	3.2
1	K	74	ASN	3.2
1	I	1	SER	3.1
1	J	2	SER	3.1
1	K	60	PHE	3.1
1	I	71	GLU	3.1
1	G	60	PHE	3.1
1	I	148	GLU	3.0
1	J	102	ILE	3.0
1	J	147	GLY	3.0
1	K	92	LYS	3.0
1	I	128	ILE	3.0
1	H	136	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	102	ILE	2.9
1	L	148	GLU	2.9
1	L	9	PHE	2.9
1	D	29	GLN	2.9
1	A	102	ILE	2.9
1	A	126	LEU	2.8
1	K	127	ALA	2.8
1	I	137	ALA	2.8
1	I	136	LEU	2.8
1	I	102	ILE	2.8
1	G	180	GLU	2.8
1	H	4	HIS	2.7
1	K	149	SER	2.7
1	K	176	LEU	2.7
1	G	148	GLU	2.7
1	K	68	ALA	2.7
1	K	125	ILE	2.7
1	L	29	GLN	2.7
1	H	139	GLY	2.7
1	I	139	GLY	2.7
1	H	14	LYS	2.6
1	K	139	GLY	2.6
1	J	93	VAL	2.6
1	A	148	GLU	2.6
1	H	71	GLU	2.6
1	J	169	TYR	2.6
1	L	41	ARG	2.5
1	C	92	LYS	2.5
1	L	74	ASN	2.5
1	E	127	ALA	2.5
1	A	60	PHE	2.5
1	K	79	ARG	2.5
1	K	71	GLU	2.4
1	K	73	TYR	2.4
1	J	68	ALA	2.4
1	L	1	SER	2.4
1	J	73	TYR	2.4
1	D	135	ALA	2.4
1	K	45	ASN	2.4
1	J	95	ARG	2.4
1	B	60	PHE	2.4
1	G	176	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	8	ILE	2.3
1	L	8	ILE	2.3
1	J	135	ALA	2.3
1	C	136	LEU	2.3
1	E	180	GLU	2.3
1	F	180	GLU	2.3
1	J	137	ALA	2.3
1	L	18	ALA	2.3
1	K	44	PHE	2.3
1	L	90	SER	2.3
1	L	93	VAL	2.3
1	A	1	SER	2.3
1	I	68	ALA	2.3
1	K	10	ALA	2.3
1	A	135	ALA	2.3
1	B	127	ALA	2.3
1	I	106	GLN	2.3
1	G	178	GLU	2.3
1	H	134	TYR	2.3
1	J	72	GLU	2.3
1	H	133	ASN	2.2
1	L	73	TYR	2.2
1	L	72	GLU	2.2
1	L	138	ALA	2.2
1	H	29	GLN	2.2
1	K	29	GLN	2.2
1	L	134	TYR	2.2
1	J	65	LYS	2.2
1	G	4	HIS	2.2
1	L	139	GLY	2.2
1	G	93	VAL	2.2
1	G	150	MET	2.2
1	B	135	ALA	2.2
1	I	72	GLU	2.2
1	F	126	LEU	2.2
1	H	13	HIS	2.2
1	I	29	GLN	2.2
1	B	102	ILE	2.2
1	L	175	ILE	2.2
1	E	60	PHE	2.2
1	G	135	ALA	2.1
1	C	180	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	126	LEU	2.1
1	L	172	ASP	2.1
1	D	102	ILE	2.1
1	B	136	LEU	2.1
1	H	60	PHE	2.1
1	A	138	ALA	2.1
1	B	128	ILE	2.1
1	K	102	ILE	2.1
1	G	101	LEU	2.1
1	K	126	LEU	2.1
1	L	79	ARG	2.1
1	L	2	SER	2.1
1	E	29	GLN	2.1
1	L	102	ILE	2.0
1	L	128	ILE	2.0
1	A	51	GLY	2.0
1	A	127	ALA	2.0
1	H	127	ALA	2.0
1	I	112	VAL	2.0
1	D	101	LEU	2.0
1	G	29	GLN	2.0
1	J	77	LEU	2.0
1	L	126	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NA	E	1005	1/1	0.75	0.31	8.20	47,47,47,47	0
2	NA	F	1006	1/1	0.61	0.27	6.70	44,44,44,44	0
2	NA	D	1004	1/1	0.59	0.26	3.72	58,58,58,58	0
2	NA	J	1008	1/1	0.93	0.19	3.24	79,79,79,79	0
2	NA	B	1002	1/1	0.85	0.19	3.22	44,44,44,44	0
2	NA	A	1001	1/1	0.51	0.25	3.08	49,49,49,49	0
2	NA	K	1011	1/1	0.82	0.22	1.90	96,96,96,96	0
2	NA	C	1003	1/1	0.68	0.16	1.50	43,43,43,43	0
2	NA	G	1007	1/1	0.84	0.22	1.06	87,87,87,87	0
2	NA	H	1010	1/1	0.90	0.17	0.59	82,82,82,82	0
2	NA	L	1012	1/1	0.83	0.14	-0.55	84,84,84,84	0
2	NA	I	1009	1/1	0.85	0.10	-1.79	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.