



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:22 AM EDT

PDB ID : 3T5P / pdb_00003t5p
Title : Crystal structure of a putative diacylglycerol kinase from Bacillus anthracis str. Sterne
Authors : Hou, J.; Zheng, H.; Chruszcz, M.; Cooper, D.R.; Onopriyenko, O.; Grimshaw, S.; Savchenko, A.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-07-27
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
Mogul	:	2022.3.0, CSD as543be (2022)
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

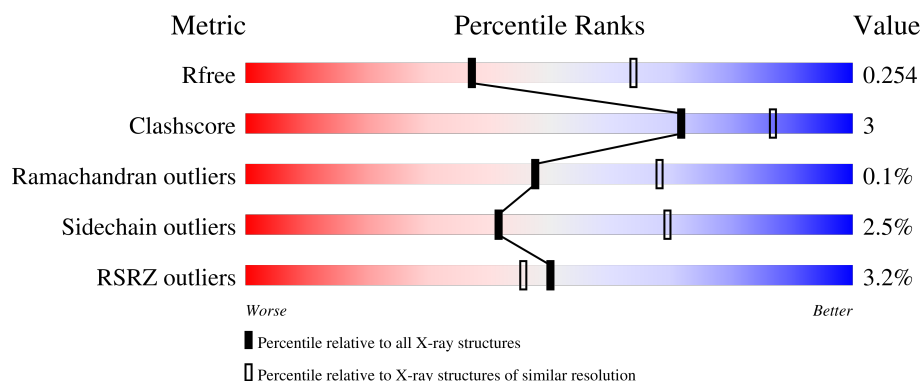
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

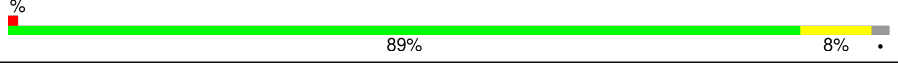
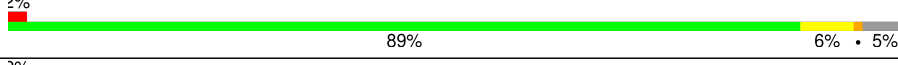
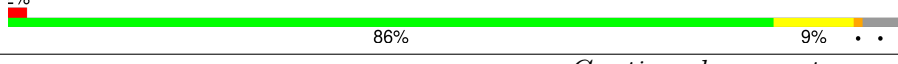
The reported resolution of this entry is 2.50 Å.

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	306	
1	B	306	
1	C	306	
1	D	306	

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Mol	Chain	Length	Quality of chain
1	E	306	
1	F	306	
1	G	306	
1	H	306	
1	I	306	
1	J	306	
1	K	306	
1	L	306	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26322 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 BmrU protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	Se	0	0	0
			2159	1389	353	410	5	2			
1	B	299	Total	C	N	O	S	Se	0	0	0
			2267	1453	368	439	5	2			
1	C	292	Total	C	N	O	S	Se	0	0	0
			2173	1397	355	413	5	3			
1	D	293	Total	C	N	O	S	Se	0	0	0
			2216	1425	359	425	5	2			
1	E	295	Total	C	N	O	S	Se	0	0	0
			2202	1411	362	422	5	2			
1	F	273	Total	C	N	O	S	Se	0	0	0
			2036	1315	330	384	5	2			
1	G	291	Total	C	N	O	S	Se	0	0	0
			2179	1403	354	415	5	2			
1	H	272	Total	C	N	O	S	Se	0	0	0
			1970	1267	323	373	5	2			
1	I	277	Total	C	N	O	S	Se	0	0	0
			2078	1338	338	395	5	2			
1	J	278	Total	C	N	O	S	Se	0	0	0
			2070	1336	336	391	5	2			
1	K	289	Total	C	N	O	S	Se	0	0	0
			2169	1393	349	420	5	2			
1	L	302	Total	C	N	O	S	Se	0	0	0
			2286	1469	371	439	5	2			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	TYR	-	expression tag	UNP Q81KC6
A	-4	PHE	-	expression tag	UNP Q81KC6
A	-3	GLN	-	expression tag	UNP Q81KC6
A	-2	ASN	-	expression tag	UNP Q81KC6
A	-1	SER	-	expression tag	UNP Q81KC6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP Q81KC6
B	-5	TYR	-	expression tag	UNP Q81KC6
B	-4	PHE	-	expression tag	UNP Q81KC6
B	-3	GLN	-	expression tag	UNP Q81KC6
B	-2	ASN	-	expression tag	UNP Q81KC6
B	-1	SER	-	expression tag	UNP Q81KC6
B	0	ALA	-	expression tag	UNP Q81KC6
C	-5	TYR	-	expression tag	UNP Q81KC6
C	-4	PHE	-	expression tag	UNP Q81KC6
C	-3	GLN	-	expression tag	UNP Q81KC6
C	-2	ASN	-	expression tag	UNP Q81KC6
C	-1	SER	-	expression tag	UNP Q81KC6
C	0	ALA	-	expression tag	UNP Q81KC6
D	-5	TYR	-	expression tag	UNP Q81KC6
D	-4	PHE	-	expression tag	UNP Q81KC6
D	-3	GLN	-	expression tag	UNP Q81KC6
D	-2	ASN	-	expression tag	UNP Q81KC6
D	-1	SER	-	expression tag	UNP Q81KC6
D	0	ALA	-	expression tag	UNP Q81KC6
E	-5	TYR	-	expression tag	UNP Q81KC6
E	-4	PHE	-	expression tag	UNP Q81KC6
E	-3	GLN	-	expression tag	UNP Q81KC6
E	-2	ASN	-	expression tag	UNP Q81KC6
E	-1	SER	-	expression tag	UNP Q81KC6
E	0	ALA	-	expression tag	UNP Q81KC6
F	-5	TYR	-	expression tag	UNP Q81KC6
F	-4	PHE	-	expression tag	UNP Q81KC6
F	-3	GLN	-	expression tag	UNP Q81KC6
F	-2	ASN	-	expression tag	UNP Q81KC6
F	-1	SER	-	expression tag	UNP Q81KC6
F	0	ALA	-	expression tag	UNP Q81KC6
G	-5	TYR	-	expression tag	UNP Q81KC6
G	-4	PHE	-	expression tag	UNP Q81KC6
G	-3	GLN	-	expression tag	UNP Q81KC6
G	-2	ASN	-	expression tag	UNP Q81KC6
G	-1	SER	-	expression tag	UNP Q81KC6
G	0	ALA	-	expression tag	UNP Q81KC6
H	-5	TYR	-	expression tag	UNP Q81KC6
H	-4	PHE	-	expression tag	UNP Q81KC6
H	-3	GLN	-	expression tag	UNP Q81KC6
H	-2	ASN	-	expression tag	UNP Q81KC6
H	-1	SER	-	expression tag	UNP Q81KC6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ALA	-	expression tag	UNP Q81KC6
I	-5	TYR	-	expression tag	UNP Q81KC6
I	-4	PHE	-	expression tag	UNP Q81KC6
I	-3	GLN	-	expression tag	UNP Q81KC6
I	-2	ASN	-	expression tag	UNP Q81KC6
I	-1	SER	-	expression tag	UNP Q81KC6
I	0	ALA	-	expression tag	UNP Q81KC6
J	-5	TYR	-	expression tag	UNP Q81KC6
J	-4	PHE	-	expression tag	UNP Q81KC6
J	-3	GLN	-	expression tag	UNP Q81KC6
J	-2	ASN	-	expression tag	UNP Q81KC6
J	-1	SER	-	expression tag	UNP Q81KC6
J	0	ALA	-	expression tag	UNP Q81KC6
K	-5	TYR	-	expression tag	UNP Q81KC6
K	-4	PHE	-	expression tag	UNP Q81KC6
K	-3	GLN	-	expression tag	UNP Q81KC6
K	-2	ASN	-	expression tag	UNP Q81KC6
K	-1	SER	-	expression tag	UNP Q81KC6
K	0	ALA	-	expression tag	UNP Q81KC6
L	-5	TYR	-	expression tag	UNP Q81KC6
L	-4	PHE	-	expression tag	UNP Q81KC6
L	-3	GLN	-	expression tag	UNP Q81KC6
L	-2	ASN	-	expression tag	UNP Q81KC6
L	-1	SER	-	expression tag	UNP Q81KC6
L	0	ALA	-	expression tag	UNP Q81KC6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total 1	Mg 1	0	0
2	I	1	Total 1	Mg 1	0	0
2	J	1	Total 1	Mg 1	0	0
2	K	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0

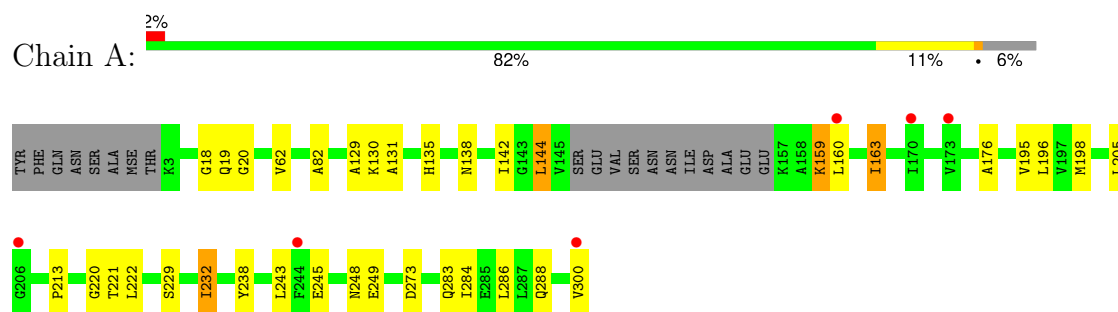
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	66	Total 66	O 66	0	0
3	C	43	Total 43	O 43	0	0
3	D	61	Total 61	O 61	0	0
3	E	32	Total 32	O 32	0	0
3	F	36	Total 36	O 36	0	0
3	G	45	Total 45	O 45	0	0
3	H	10	Total 10	O 10	0	0
3	I	38	Total 38	O 38	0	0
3	J	35	Total 35	O 35	0	0
3	K	49	Total 49	O 49	0	0
3	L	62	Total 62	O 62	0	0

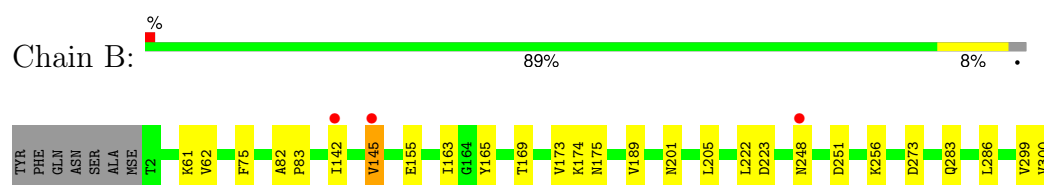
3 Residue-property plots [i](#)

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

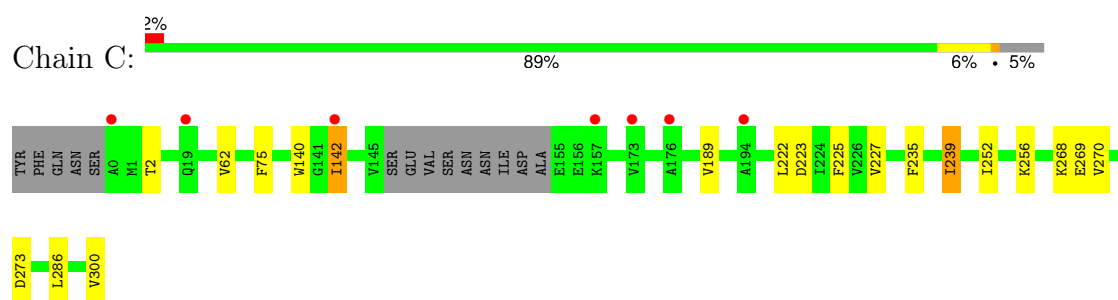
- Molecule 1: BmrU protein



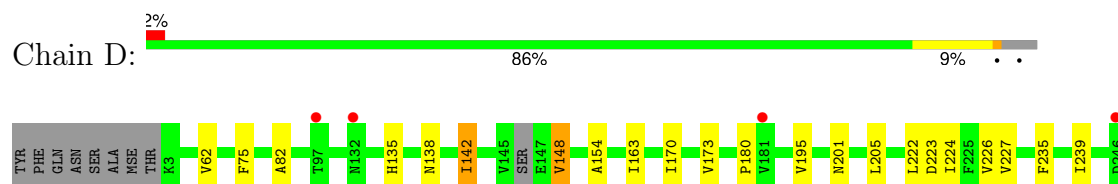
- Molecule 1: BmrU protein



- Molecule 1: BmrU protein

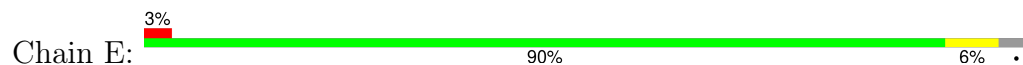


- Molecule 1: BmrU protein

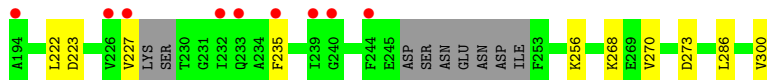
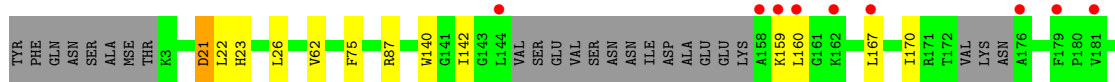
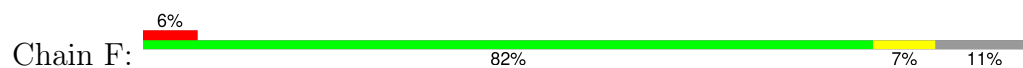




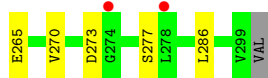
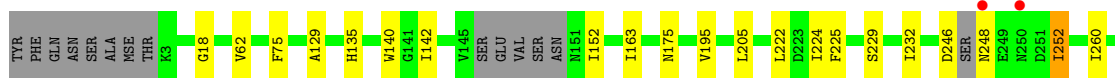
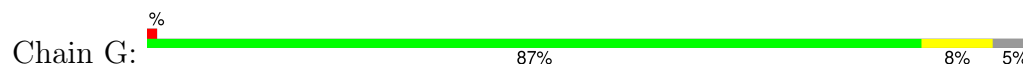
● Molecule 1: BmrU protein



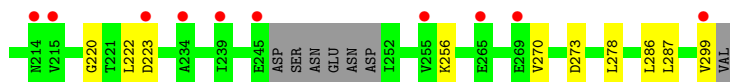
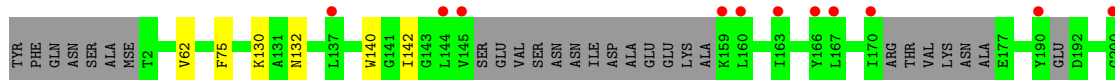
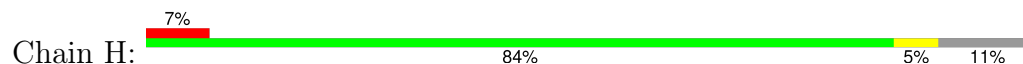
● Molecule 1: BmrU protein



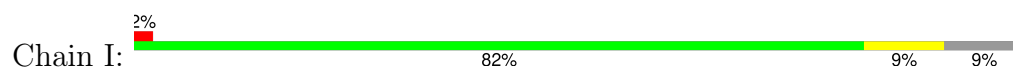
● Molecule 1: BmrU protein

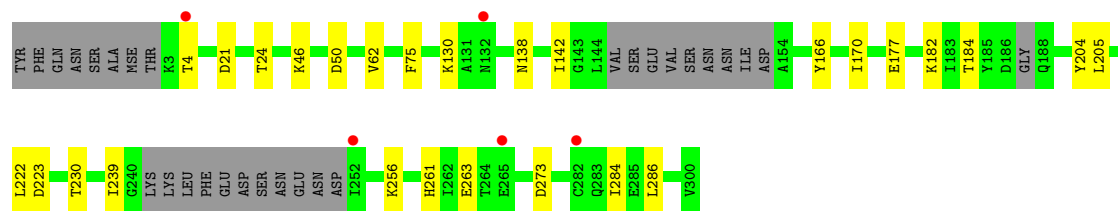


● Molecule 1: BmrU protein

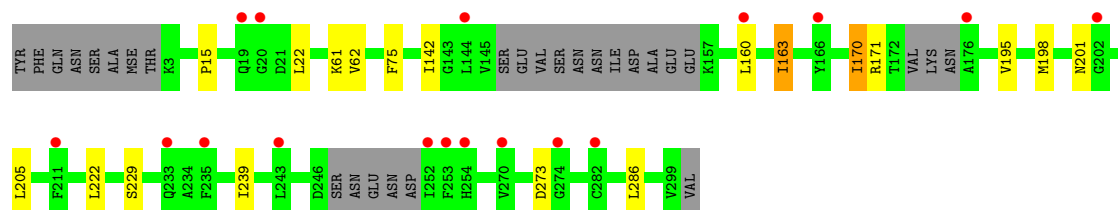
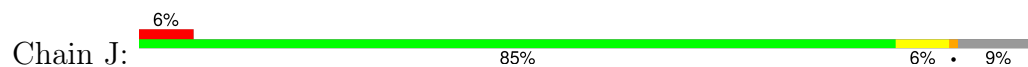


● Molecule 1: BmrU protein

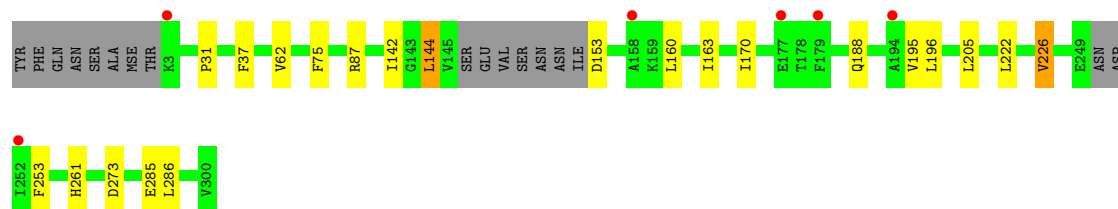
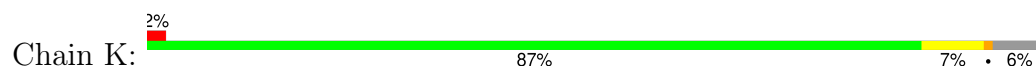




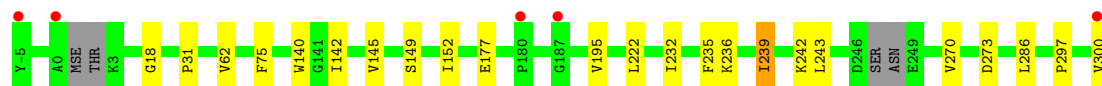
• Molecule 1: BmrU protein



• Molecule 1: BmrU protein



• Molecule 1: BmrU protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.02Å 115.10Å 208.02Å 90.00° 92.34° 90.00°	Depositor
Resolution (Å)	29.56 – 2.50 29.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.56-2.50) 98.6 (29.56-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.241 0.216 , 0.254	Depositor DCC
R_{free} test set	6264 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26322	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.37% 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: MG

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	0.74	2/2203 (0.1%)	0.88	3/2994 (0.1%)
1	B	0.81	0/2312	0.86	0/3142
1	C	0.72	0/2215	0.83	0/3011
1	D	0.77	0/2259	0.82	0/3066
1	E	0.73	0/2246	0.81	0/3056
1	F	0.74	1/2077 (0.0%)	0.81	0/2823
1	G	0.78	0/2222	0.85	2/3021 (0.1%)
1	H	0.66	0/2008	0.79	0/2736
1	I	0.72	0/2119	0.84	2/2878 (0.1%)
1	J	0.72	0/2111	0.80	0/2869
1	K	0.76	2/2212 (0.1%)	0.82	1/3007 (0.0%)
1	L	0.78	0/2331	0.84	4/3166 (0.1%)
All	All	0.75	5/26315 (0.0%)	0.83	12/35769 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	LEU	N-CA	5.64	1.53	1.46
1	A	159	LYS	CA-C	5.53	1.60	1.52
1	F	87	ARG	C-O	-5.53	1.19	1.24
1	K	37	PHE	C-O	-5.42	1.20	1.25
1	K	87	ARG	C-O	-5.34	1.19	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	4	THR	N-CA-C	10.41	124.34	108.52
1	A	159	LYS	N-CA-C	8.00	121.88	108.20
1	A	159	LYS	CA-C-N	7.54	135.94	121.54
1	A	159	LYS	C-N-CA	7.54	135.94	121.54
1	L	18	GLY	O-C-N	-6.74	116.32	122.86
1	I	4	THR	N-CA-CB	-5.99	101.72	111.24
1	L	18	GLY	CA-C-N	-5.51	113.68	122.66
1	L	18	GLY	C-N-CA	-5.51	113.68	122.66
1	L	31	PRO	N-CA-C	5.42	117.32	110.70
1	G	18	GLY	CA-C-N	-5.11	113.13	122.38
1	G	18	GLY	C-N-CA	-5.11	113.13	122.38
1	K	31	PRO	N-CA-C	5.03	116.83	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	LYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2159	0	2094	24	0
1	B	2267	0	2226	15	0
1	C	2173	0	2110	13	0
1	D	2216	0	2171	28	0
1	E	2202	0	2122	10	0
1	F	2036	0	1966	12	0
1	G	2179	0	2114	12	0
1	H	1970	0	1841	8	0
1	I	2078	0	2022	12	0
1	J	2070	0	2011	10	0
1	K	2169	0	2087	11	0
1	L	2286	0	2228	14	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	28	0	0	2	0
3	B	66	0	0	1	0
3	C	43	0	0	0	0
3	D	61	0	0	4	0
3	E	32	0	0	0	0
3	F	36	0	0	0	0
3	G	45	0	0	0	0
3	H	10	0	0	0	0
3	I	38	0	0	0	0
3	J	35	0	0	1	0
3	K	49	0	0	1	0
3	L	62	0	0	0	0
All	All	26322	0	24992	166	0

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 3.

All (166) 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:I:222:LEU:HG	1:I:286:LEU:HD13	1.49	0.94
1:L:297:PRO:HA	1:L:300:VAL:HG23	1.57	0.86
1:D:222:LEU:HG	1:D:286:LEU:HD13	1.56	0.85
1:H:222:LEU:HG	1:H:286:LEU:HD13	1.62	0.82
1:D:226:VAL:O	1:D:252:ILE:HG22	1.84	0.77
1:A:222:LEU:HG	1:A:286:LEU:HD13	1.67	0.76
1:E:222:LEU:HG	1:E:286:LEU:HD13	1.68	0.75
1:K:226:VAL:HG22	1:K:253:PHE:HB3	1.68	0.75
1:D:148:VAL:HG21	1:D:154:ALA:HB2	1.69	0.74
1:K:222:LEU:HG	1:K:286:LEU:HD13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:LEU:HG	1:L:286:LEU:HD13	1.71	0.72
1:A:163:ILE:HD11	1:A:198:MSE:HE1	1.72	0.70
1:A:176:ALA:HB3	1:A:232:ILE:HD11	1.74	0.68
1:B:222:LEU:HG	1:B:286:LEU:HD13	1.76	0.68
1:C:222:LEU:HG	1:C:286:LEU:HD13	1.77	0.67
1:I:222:LEU:CG	1:I:286:LEU:HD13	2.24	0.66
1:G:163:ILE:HD13	1:G:205:LEU:HB3	1.78	0.66
1:D:226:VAL:O	1:D:252:ILE:CG2	2.44	0.65
1:J:163:ILE:HD11	1:J:198:MSE:HE1	1.79	0.65
1:J:222:LEU:HG	1:J:286:LEU:HD13	1.78	0.65
1:C:235:PHE:CE1	1:C:239:ILE:HD11	2.32	0.65
1:F:222:LEU:HG	1:F:286:LEU:HD13	1.78	0.65
1:G:222:LEU:HG	1:G:286:LEU:HD13	1.79	0.64
1:J:163:ILE:HD12	1:J:205:LEU:HB3	1.79	0.63
1:B:299:VAL:HG12	1:B:300:VAL:HG13	1.78	0.63
1:I:21:ASP:HB3	1:I:24:THR:H	1.64	0.63
1:G:246:ASP:O	1:G:248:ASN:N	2.32	0.63
1:F:21:ASP:OD1	1:F:23:HIS:N	2.32	0.62
1:A:144:LEU:HD13	1:A:196:LEU:HD11	1.81	0.62
1:C:235:PHE:CE1	1:C:239:ILE:CD1	2.82	0.62
1:F:21:ASP:OD1	1:F:21:ASP:C	2.43	0.61
1:F:159:LYS:O	1:F:160:LEU:CB	2.48	0.61
1:D:75:PHE:CD1	1:D:273:ASP:HB2	2.37	0.60
1:L:75:PHE:CD1	1:L:273:ASP:HB2	2.36	0.59
1:A:18:GLY:C	1:A:20:GLY:N	2.58	0.59
1:A:144:LEU:HD13	1:A:196:LEU:CD1	2.33	0.59
1:L:235:PHE:CZ	1:L:239:ILE:HD11	2.37	0.59
1:F:75:PHE:CD1	1:F:273:ASP:HB2	2.38	0.58
1:C:75:PHE:CD1	1:C:273:ASP:HB2	2.39	0.57
1:A:243:LEU:O	1:A:245:GLU:N	2.37	0.57
1:K:75:PHE:CD1	1:K:273:ASP:HB2	2.38	0.57
1:L:300:VAL:CG1	1:L:300:VAL:O	2.53	0.56
1:I:75:PHE:CD1	1:I:273:ASP:HB2	2.40	0.56
1:K:153:ASP:N	3:K:565:HOH:O	2.38	0.55
1:E:75:PHE:CD1	1:E:273:ASP:HB2	2.41	0.55
1:A:18:GLY:C	1:A:20:GLY:H	2.13	0.55
1:H:75:PHE:CD1	1:H:273:ASP:HB2	2.41	0.55
1:B:169:THR:O	1:B:173:VAL:HG23	2.07	0.55
1:B:248:ASN:O	1:B:251:ASP:N	2.39	0.55
1:K:144:LEU:HD13	1:K:196:LEU:HD11	1.88	0.55
1:A:213:PRO:HG3	1:A:238:TYR:OH	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:TRP:NE1	1:H:270:VAL:HG11	2.23	0.54
1:D:223:ASP:OD1	1:D:256:LYS:NZ	2.41	0.53
1:D:163:ILE:HG21	1:D:205:LEU:HB3	1.90	0.53
1:L:145:VAL:O	1:L:145:VAL:HG13	2.08	0.53
1:A:138:ASN:HB2	1:A:273:ASP:OD1	2.07	0.53
1:A:220:GLY:C	1:A:286:LEU:CD2	2.81	0.53
1:A:82:ALA:HB1	1:A:135:HIS:ND1	2.23	0.53
1:D:222:LEU:CG	1:D:286:LEU:HD13	2.33	0.53
1:D:180:PRO:HG2	1:D:265:GLU:CG	2.39	0.53
1:F:167:LEU:O	1:F:170:ILE:HG22	2.08	0.53
1:L:297:PRO:HA	1:L:300:VAL:CG2	2.35	0.52
1:A:195:VAL:HG23	1:A:229:SER:HA	1.91	0.52
1:L:300:VAL:O	1:L:300:VAL:HG12	2.10	0.51
1:B:283:GLN:OE1	1:D:281:PRO:HG2	2.10	0.51
1:C:142:ILE:HG21	1:C:268:LYS:HG2	1.92	0.51
1:J:75:PHE:CD1	1:J:273:ASP:HB2	2.45	0.51
1:K:144:LEU:HD13	1:K:196:LEU:CD1	2.41	0.51
1:C:225:PHE:CZ	1:C:252:ILE:HG21	2.46	0.50
1:G:75:PHE:CD1	1:G:273:ASP:HB2	2.48	0.49
1:K:222:LEU:CG	1:K:286:LEU:HD13	2.39	0.49
1:L:232:ILE:HG22	1:L:236:LYS:HE3	1.94	0.49
1:B:75:PHE:CD1	1:B:273:ASP:HB2	2.48	0.48
1:H:222:LEU:CG	1:H:286:LEU:HD13	2.38	0.48
1:E:222:LEU:CG	1:E:286:LEU:HD13	2.42	0.47
1:L:222:LEU:CG	1:L:286:LEU:HD13	2.43	0.47
1:B:61:LYS:HG2	3:D:515:HOH:O	2.15	0.47
1:I:223:ASP:OD1	1:I:256:LYS:NZ	2.47	0.47
1:B:165:TYR:CZ	1:B:169:THR:HG21	2.49	0.47
1:C:227:VAL:HG21	1:C:235:PHE:CD2	2.50	0.47
1:D:135:HIS:HD2	3:D:467:HOH:O	1.98	0.47
1:J:195:VAL:HG23	1:J:229:SER:HA	1.97	0.47
1:A:288:GLN:HG3	3:A:345:HOH:O	2.14	0.47
1:I:130:LYS:O	1:I:284:ILE:HA	2.15	0.47
1:D:235:PHE:CE1	1:D:239:ILE:HD11	2.50	0.47
1:I:184:THR:HB	1:I:261:HIS:HB3	1.97	0.46
1:A:82:ALA:CB	1:A:135:HIS:CG	2.99	0.46
1:A:144:LEU:CD1	1:A:196:LEU:HD11	2.44	0.46
1:G:175:ASN:HD21	1:G:232:ILE:HD12	1.80	0.46
1:F:22:LEU:HD11	1:F:26:LEU:HD11	1.98	0.46
1:D:82:ALA:HB1	1:D:135:HIS:CG	2.50	0.46
1:G:75:PHE:CE1	1:G:273:ASP:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:ILE:CG1	1:G:260:ILE:HD13	2.46	0.46
1:A:131:ALA:HA	1:A:283:GLN:O	2.16	0.45
1:G:163:ILE:HG21	1:G:205:LEU:HB3	1.97	0.45
1:D:82:ALA:CB	1:D:135:HIS:CG	2.99	0.45
1:D:170:ILE:CD1	1:D:235:PHE:CE2	2.98	0.45
1:A:129:ALA:HB2	1:A:222:LEU:HD21	1.99	0.45
1:A:130:LYS:O	1:A:284:ILE:HA	2.16	0.45
1:E:223:ASP:OD1	1:E:256:LYS:NZ	2.46	0.45
1:D:148:VAL:HG11	1:D:154:ALA:HA	1.99	0.45
1:G:195:VAL:HG23	1:G:229:SER:HA	1.99	0.45
1:I:46:LYS:HG3	1:I:50:ASP:OD2	2.17	0.45
1:I:182:LYS:HB3	1:I:263:GLU:HB2	1.99	0.45
1:L:235:PHE:O	1:L:239:ILE:HD12	2.16	0.45
1:A:163:ILE:HD13	1:A:205:LEU:HB3	1.98	0.45
1:E:195:VAL:HG12	1:E:227:VAL:O	2.17	0.45
1:J:170:ILE:HD12	1:J:171:ARG:N	2.32	0.45
1:C:225:PHE:CE1	1:C:252:ILE:HG21	2.51	0.45
1:C:142:ILE:CG2	1:C:268:LYS:HG2	2.47	0.44
1:A:82:ALA:HB1	1:A:135:HIS:CE1	2.53	0.44
1:D:170:ILE:HD11	1:D:235:PHE:CD2	2.51	0.44
1:B:163:ILE:HG21	1:B:205:LEU:HB3	2.00	0.44
1:D:195:VAL:HG12	1:D:227:VAL:O	2.17	0.44
1:I:166:TYR:CZ	1:I:170:ILE:HD13	2.52	0.44
1:I:204:TYR:O	1:I:205:LEU:HD23	2.18	0.44
1:C:222:LEU:CG	1:C:286:LEU:HD13	2.47	0.44
1:J:201:ASN:HA	3:J:324:HOH:O	2.17	0.44
1:D:201:ASN:HA	3:D:303:HOH:O	2.17	0.44
1:G:129:ALA:O	1:G:135:HIS:HA	2.18	0.44
1:H:223:ASP:OD1	1:H:256:LYS:NZ	2.50	0.44
1:D:82:ALA:HB1	1:D:135:HIS:ND1	2.33	0.44
1:H:130:LYS:HE3	1:H:287:LEU:HD11	2.00	0.43
1:H:132:ASN:HB2	1:H:278:LEU:HD11	1.99	0.43
1:A:18:GLY:O	1:A:20:GLY:N	2.52	0.43
1:B:174:LYS:O	1:B:175:ASN:C	2.61	0.43
1:J:170:ILE:HD12	1:J:171:ARG:H	1.82	0.43
1:E:281:PRO:HG2	1:K:261:HIS:CD2	2.54	0.43
1:F:21:ASP:OD1	1:F:22:LEU:N	2.52	0.43
1:B:201:ASN:HA	3:B:302:HOH:O	2.18	0.43
1:E:175:ASN:O	1:E:176:ALA:C	2.62	0.43
1:L:243:LEU:HD12	1:L:243:LEU:HA	1.83	0.42
1:D:180:PRO:HG2	1:D:265:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:GLY:C	1:H:286:LEU:CD2	2.92	0.42
1:L:140:TRP:NE1	1:L:270:VAL:HG11	2.34	0.42
1:D:135:HIS:HE1	3:D:315:HOH:O	2.01	0.42
1:D:170:ILE:HD11	1:D:235:PHE:CE2	2.54	0.42
1:D:235:PHE:CZ	1:D:239:ILE:HD11	2.55	0.42
1:C:227:VAL:HG21	1:C:235:PHE:CE2	2.55	0.42
1:E:166:TYR:CZ	1:E:170:ILE:CD1	3.02	0.42
1:B:223:ASP:OD1	1:B:256:LYS:NZ	2.52	0.42
1:F:227:VAL:HG21	1:F:235:PHE:CD1	2.55	0.42
1:B:82:ALA:N	1:B:83:PRO:CD	2.83	0.42
1:D:138:ASN:HB2	1:D:273:ASP:OD1	2.19	0.42
1:D:224:ILE:O	1:D:254:HIS:HD2	2.03	0.42
1:B:145:VAL:HG12	1:B:145:VAL:O	2.19	0.41
1:I:138:ASN:HB2	1:I:273:ASP:OD1	2.20	0.41
1:K:144:LEU:CD1	1:K:196:LEU:HD11	2.50	0.41
1:K:163:ILE:HG21	1:K:205:LEU:HB3	2.03	0.41
1:F:223:ASP:OD1	1:F:256:LYS:NZ	2.52	0.41
1:G:140:TRP:NE1	1:G:270:VAL:HG11	2.35	0.41
1:J:15:PRO:HA	1:J:22:LEU:HD13	2.01	0.41
1:E:170:ILE:HD12	1:E:170:ILE:HA	1.95	0.41
1:A:221:THR:N	1:A:286:LEU:HD22	2.35	0.41
1:C:140:TRP:NE1	1:C:270:VAL:HG11	2.34	0.41
1:F:140:TRP:NE1	1:F:270:VAL:HG11	2.35	0.41
1:G:225:PHE:CE1	1:G:252:ILE:HG21	2.55	0.41
1:A:163:ILE:HG21	1:A:205:LEU:HB3	2.02	0.41
1:B:222:LEU:CG	1:B:286:LEU:HD13	2.49	0.41
1:D:224:ILE:HD12	1:D:255:VAL:HG13	2.03	0.41
3:A:311:HOH:O	1:J:61:LYS:HG2	2.21	0.41
1:L:149:SER:HA	1:L:152:ILE:HD11	2.03	0.40
1:C:223:ASP:OD1	1:C:256:LYS:NZ	2.54	0.40
1:F:140:TRP:CD1	1:F:270:VAL:HG11	2.55	0.40
1:D:142:ILE:HG21	1:D:268:LYS:HD3	2.03	0.40
1:E:261:HIS:HE2	1:K:261:HIS:CE1	2.39	0.40

There are no symmetry-related clashes.

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	283/306 (92%)	270 (95%)	12 (4%)	1 (0%)	30	49
1	B	297/306 (97%)	288 (97%)	9 (3%)	0	100	100
1	C	288/306 (94%)	277 (96%)	11 (4%)	0	100	100
1	D	287/306 (94%)	278 (97%)	8 (3%)	1 (0%)	36	55
1	E	291/306 (95%)	280 (96%)	11 (4%)	0	100	100
1	F	263/306 (86%)	257 (98%)	6 (2%)	0	100	100
1	G	285/306 (93%)	276 (97%)	8 (3%)	1 (0%)	30	49
1	H	262/306 (86%)	256 (98%)	6 (2%)	0	100	100
1	I	269/306 (88%)	259 (96%)	10 (4%)	0	100	100
1	J	270/306 (88%)	262 (97%)	8 (3%)	0	100	100
1	K	283/306 (92%)	274 (97%)	9 (3%)	0	100	100
1	L	296/306 (97%)	284 (96%)	12 (4%)	0	100	100
All	All	3374/3672 (92%)	3261 (97%)	110 (3%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	G	152	ILE
1	D	173	VAL

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	224/257 (87%)	216 (96%)	8 (4%)	31	58
1	B	244/257 (95%)	239 (98%)	5 (2%)	48	75
1	C	225/257 (88%)	218 (97%)	7 (3%)	35	62
1	D	235/257 (91%)	232 (99%)	3 (1%)	61	82
1	E	229/257 (89%)	224 (98%)	5 (2%)	45	73
1	F	210/257 (82%)	205 (98%)	5 (2%)	43	70
1	G	227/257 (88%)	222 (98%)	5 (2%)	45	73
1	H	194/257 (76%)	191 (98%)	3 (2%)	57	80
1	I	217/257 (84%)	212 (98%)	5 (2%)	44	72
1	J	215/257 (84%)	209 (97%)	6 (3%)	38	66
1	K	226/257 (88%)	217 (96%)	9 (4%)	28	54
1	L	242/257 (94%)	236 (98%)	6 (2%)	42	69
All	All	2688/3084 (87%)	2621 (98%)	67 (2%)	42	69

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	142	ILE
1	A	144	LEU
1	A	163	ILE
1	A	232	ILE
1	A	248	ASN
1	A	249	GLU
1	A	300	VAL
1	B	62	VAL
1	B	142	ILE
1	B	145	VAL
1	B	155	GLU
1	B	189	VAL
1	C	2	THR
1	C	62	VAL
1	C	142	ILE
1	C	189	VAL
1	C	239	ILE
1	C	269	GLU
1	C	300	VAL
1	D	62	VAL
1	D	142	ILE

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Mol	Chain	Res	Type
1	D	148	VAL
1	E	19	GLN
1	E	62	VAL
1	E	142	ILE
1	E	178	THR
1	E	239	ILE
1	F	21	ASP
1	F	62	VAL
1	F	142	ILE
1	F	268	LYS
1	F	300	VAL
1	G	62	VAL
1	G	142	ILE
1	G	252	ILE
1	G	265	GLU
1	G	277	SER
1	H	62	VAL
1	H	142	ILE
1	H	299	VAL
1	I	62	VAL
1	I	142	ILE
1	I	177	GLU
1	I	230	THR
1	I	239	ILE
1	J	62	VAL
1	J	142	ILE
1	J	160	LEU
1	J	163	ILE
1	J	170	ILE
1	J	239	ILE
1	K	62	VAL
1	K	142	ILE
1	K	144	LEU
1	K	160	LEU
1	K	170	ILE
1	K	188	GLN
1	K	195	VAL
1	K	226	VAL
1	K	285	GLU
1	L	62	VAL
1	L	142	ILE
1	L	177	GLU

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Mol	Chain	Res	Type
1	L	195	VAL
1	L	239	ILE
1	L	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	248	ASN
1	A	288	GLN
1	C	23	HIS
1	C	201	ASN
1	D	135	HIS
1	D	138	ASN
1	D	175	ASN
1	D	201	ASN
1	D	233	GLN
1	E	188	GLN
1	F	44	HIS
1	F	48	GLN
1	F	138	ASN
1	F	201	ASN
1	G	134	GLN
1	G	138	ASN
1	G	201	ASN
1	G	233	GLN
1	G	261	HIS
1	H	134	GLN
1	I	201	ASN
1	J	134	GLN
1	K	23	HIS
1	K	134	GLN
1	K	138	ASN
1	K	201	ASN
1	L	122	HIS
1	L	138	ASN
1	L	150	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	285/306 (93%)	0.27	6 (2%) 63 59	38, 63, 97, 125	0
1	B	297/306 (97%)	0.04	3 (1%) 79 76	30, 53, 98, 109	0
1	C	289/306 (94%)	0.19	7 (2%) 59 55	38, 64, 111, 126	0
1	D	291/306 (95%)	0.18	7 (2%) 59 55	33, 57, 109, 130	0
1	E	293/306 (95%)	0.17	9 (3%) 51 47	37, 62, 103, 112	0
1	F	271/306 (88%)	0.52	18 (6%) 24 21	35, 66, 133, 166	0
1	G	289/306 (94%)	0.25	4 (1%) 73 70	34, 59, 102, 139	0
1	H	270/306 (88%)	0.51	21 (7%) 19 17	44, 78, 127, 139	0
1	I	275/306 (89%)	0.21	5 (1%) 67 64	36, 62, 109, 130	0
1	J	276/306 (90%)	0.56	17 (6%) 26 23	36, 72, 115, 141	2 (0%)
1	K	287/306 (93%)	0.04	6 (2%) 63 59	33, 56, 106, 124	0
1	L	300/306 (98%)	0.16	5 (1%) 69 65	34, 58, 100, 111	0
All	All	3423/3672 (93%)	0.25	108 (3%) 50 46	30, 63, 110, 166	2 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	252	ILE	9.6
1	J	253	PHE	6.7
1	D	250	ASN	3.8
1	L	187	GLY	3.7
1	G	274	GLY	3.5
1	J	254	HIS	3.5
1	J	282	CYS	3.5
1	K	194	ALA	3.4
1	I	252	ILE	3.3
1	J	19	GLN	3.3
1	F	176	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	160	LEU	3.2
1	K	3	LYS	3.2
1	A	160	LEU	3.2
1	F	232	ILE	3.2
1	L	-5	TYR	3.1
1	D	299	VAL	3.1
1	F	181	VAL	3.1
1	I	265	GLU	3.1
1	D	246	ASP	3.1
1	E	177	GLU	3.0
1	F	244	PHE	3.0
1	F	144	LEU	2.9
1	J	235	PHE	2.9
1	E	265	GLU	2.9
1	C	0	ALA	2.8
1	F	233	GLN	2.8
1	F	239	ILE	2.8
1	E	163	ILE	2.8
1	F	160	LEU	2.8
1	J	270	VAL	2.7
1	H	170	ILE	2.7
1	F	240	GLY	2.7
1	A	300	VAL	2.7
1	E	173	VAL	2.7
1	J	274	GLY	2.7
1	K	252	ILE	2.7
1	C	173	VAL	2.7
1	F	167	LEU	2.7
1	H	265	GLU	2.7
1	J	166	TYR	2.7
1	F	194	ALA	2.6
1	L	0	ALA	2.6
1	F	226	VAL	2.6
1	I	4	THR	2.6
1	H	200	GLY	2.5
1	C	142	ILE	2.5
1	A	244	PHE	2.5
1	I	282	CYS	2.5
1	H	166	TYR	2.5
1	A	173	VAL	2.5
1	F	158	ALA	2.5
1	B	145	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	194	ALA	2.4
1	H	239	ILE	2.4
1	H	144	LEU	2.4
1	H	190	TYR	2.4
1	F	235	PHE	2.4
1	H	159	LYS	2.4
1	H	214	ASN	2.4
1	D	97	THR	2.4
1	F	227	VAL	2.3
1	J	233	GLN	2.3
1	F	159	LYS	2.3
1	E	267	GLU	2.3
1	J	144	LEU	2.3
1	H	145	VAL	2.3
1	G	248	ASN	2.3
1	K	158	ALA	2.3
1	E	189	VAL	2.3
1	I	132	ASN	2.2
1	J	176	ALA	2.2
1	F	179	PHE	2.2
1	J	211	PHE	2.2
1	E	300	VAL	2.2
1	H	215	VAL	2.2
1	J	243	LEU	2.2
1	H	255	VAL	2.2
1	G	250	ASN	2.2
1	J	160	LEU	2.2
1	H	269	GLU	2.2
1	D	132	ASN	2.2
1	H	234	ALA	2.2
1	J	20	GLY	2.2
1	H	163	ILE	2.2
1	H	245	GLU	2.2
1	D	253	PHE	2.2
1	E	250	ASN	2.1
1	K	177	GLU	2.1
1	L	300	VAL	2.1
1	L	180	PRO	2.1
1	C	19	GLN	2.1
1	A	206	GLY	2.1
1	H	167	LEU	2.1
1	H	299	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	179	PHE	2.1
1	C	157	LYS	2.1
1	D	181	VAL	2.0
1	G	278	LEU	2.0
1	H	137	LEU	2.0
1	E	266	GLU	2.0
1	A	170	ILE	2.0
1	F	162	LYS	2.0
1	H	223	ASP	2.0
1	C	176	ALA	2.0
1	B	248	ASN	2.0
1	J	202	GLY	2.0
1	B	142	ILE	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	MG	H	301	1/1	0.88	0.10	73,73,73,73	0
2	MG	F	301	1/1	0.95	0.06	58,58,58,58	0
2	MG	I	301	1/1	0.96	0.06	59,59,59,59	0
2	MG	J	301	1/1	0.96	0.06	69,69,69,69	0
2	MG	G	301	1/1	0.98	0.04	43,43,43,43	0
2	MG	C	301	1/1	0.98	0.04	56,56,56,56	0
2	MG	D	301	1/1	0.98	0.03	39,39,39,39	0
2	MG	A	301	1/1	0.98	0.03	48,48,48,48	0
2	MG	L	301	1/1	0.98	0.04	44,44,44,44	0
2	MG	B	301	1/1	0.99	0.03	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	E	301	1/1	0.99	0.04	59,59,59,59	0
2	MG	K	301	1/1	1.00	0.02	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.