



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 02:59 PM GMT

PDB ID : 3T5P
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 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>

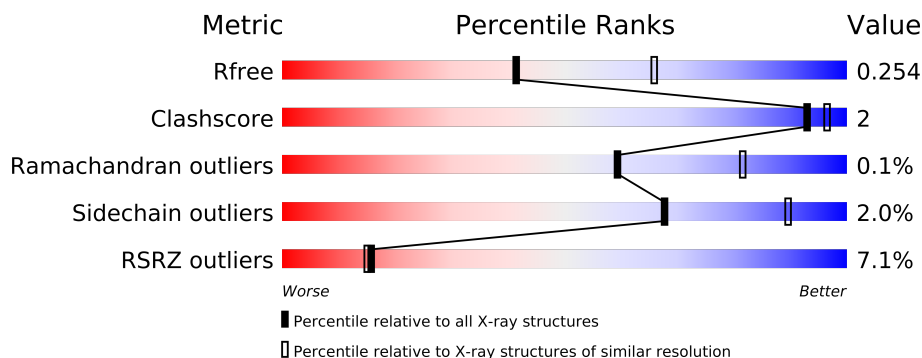
The following versions of software and data (see [references](#)) were used in the production of this report:

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	306	
1	B	306	
1	C	306	
1	D	306	
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 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 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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0

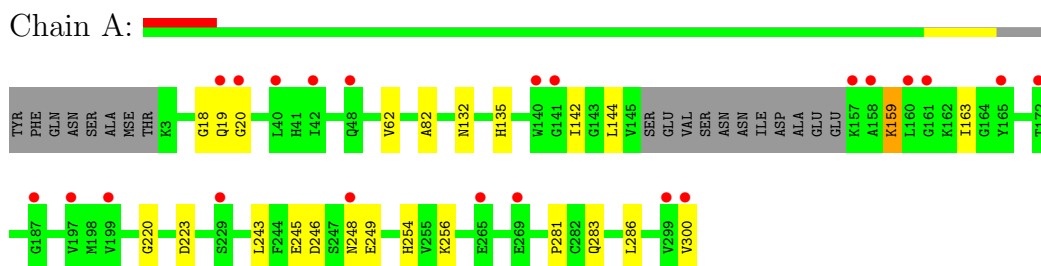
- Molecule 3 is water.

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

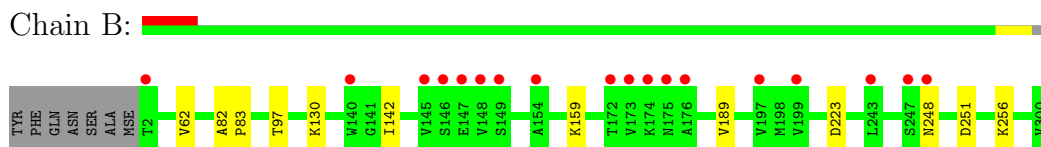
3 Residue-property plots

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.

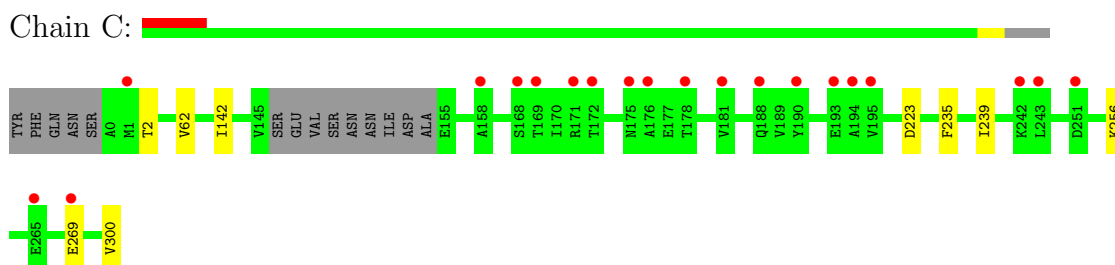
- Molecule 1: BmrU protein



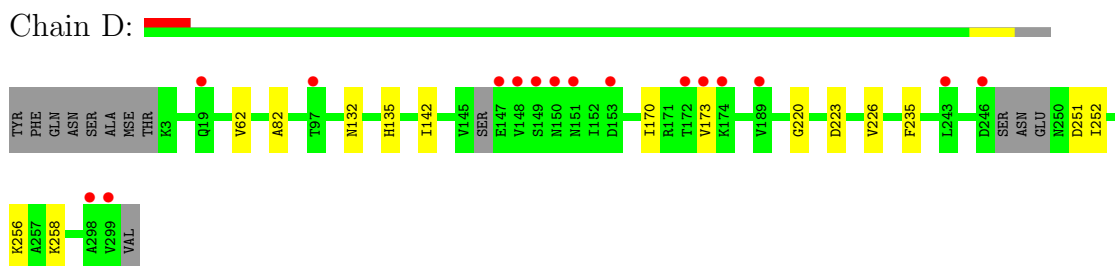
- Molecule 1: BmrU protein



- Molecule 1: BmrU protein

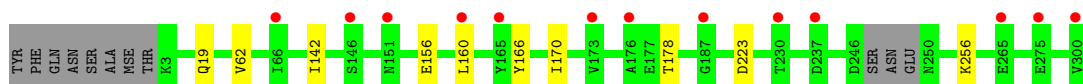


- Molecule 1: BmrU protein



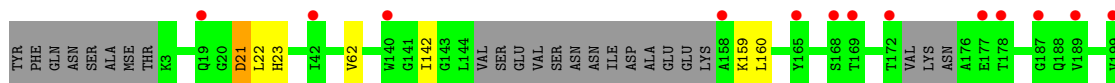
- Molecule 1: BmrU protein





• Molecule 1: BmrU protein

Chain F:



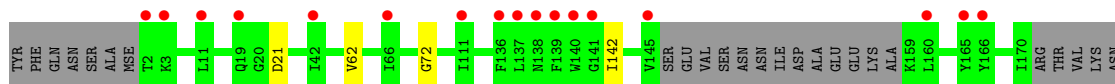
• Molecule 1: BmrU protein

Chain G:



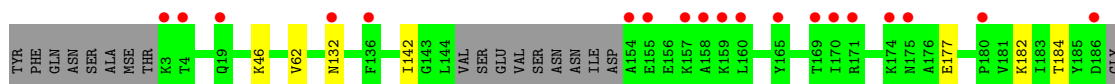
• Molecule 1: BmrU protein

Chain H:



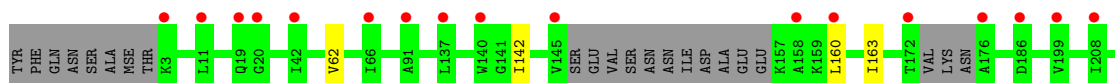
• Molecule 1: BmrU protein

Chain I:

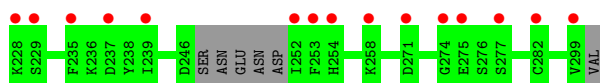


• Molecule 1: BmrU protein

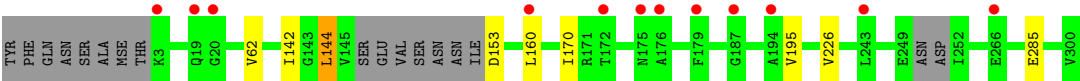
Chain J:



• Molecule 1: BmrU protein

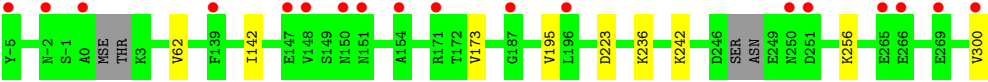


Chain K: 



● Molecule 1: BmrU protein

Chain L: 



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 5.5.0109	Depositor
R, R_{free}	0.205 , 0.241 0.216 , 0.254	Depositor DCC
R_{free} test set	6264 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 28.2	EDS
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 124704 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	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.

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	0.57	0/2203	0.67	2/2994 (0.1%)
1	B	0.63	0/2312	0.65	0/3142
1	C	0.56	0/2215	0.62	0/3011
1	D	0.60	0/2259	0.63	0/3066
1	E	0.56	0/2246	0.60	0/3056
1	F	0.55	0/2077	0.61	0/2823
1	G	0.59	0/2222	0.65	0/3021
1	H	0.48	0/2008	0.60	0/2736
1	I	0.55	0/2119	0.62	0/2878
1	J	0.54	0/2111	0.60	0/2869
1	K	0.57	0/2212	0.63	1/3007 (0.0%)
1	L	0.59	0/2331	0.62	0/3166
All	All	0.57	0/26315	0.63	3/35769 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	LYS	C-N-CA	5.70	135.94	121.70
1	A	144	LEU	CB-CG-CD1	5.68	120.66	111.00
1	K	144	LEU	CB-CG-CD1	5.35	120.09	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	LYS	Peptide

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	2159	0	0	9	0
1	B	2267	0	0	5	0
1	C	2173	0	0	2	0
1	D	2216	0	0	6	0
1	E	2202	0	0	3	0
1	F	2036	0	1	5	0
1	G	2179	0	0	2	0
1	H	1970	0	0	2	0
1	I	2078	0	0	7	0
1	J	2070	0	0	0	0
1	K	2169	0	0	1	0
1	L	2286	0	44	3	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	28	0	0	0	0
3	B	66	0	0	0	0
3	C	43	0	0	0	0
3	D	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
3	I	38	0	0	0	0
3	J	35	0	0	0	0
3	K	49	0	0	1	0
3	L	62	0	0	0	0
All	All	26322	0	45	44	0

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:226:VAL:O	1:D:252:ILE:CG2	2.44	0.65
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:C:235:PHE:CE1	1:C:239:ILE:CD1	2.82	0.62
1:F:159:LYS:O	1:F:160:LEU:CB	2.48	0.61
1:A:243:LEU:O	1:A:245:GLU:N	2.37	0.57
1:F:21:ASP:C	1:F:21:ASP:OD1	2.43	0.56
1:L:300:VAL:O	1:L:300:VAL:CG1	2.53	0.56
1:K:153:ASP:N	3:K:565:HOH:O	2.38	0.55
1:A:18:GLY:C	1:A:20:GLY:N	2.58	0.55
1:B:248:ASN:O	1:B:251:ASP:N	2.39	0.55
1:D:223:ASP:OD1	1:D:256:LYS:NZ	2.41	0.54
1:I:182:LYS:N	1:I:263:GLU:O	2.40	0.54
1:E:223:ASP:OD1	1:E:256:LYS:NZ	2.46	0.49
1:I:132:ASN:OD1	1:I:283:GLN:N	2.45	0.49
1:I:184:THR:N	1:I:261:HIS:O	2.46	0.48
1:B:97:THR:OG1	1:B:159:LYS:O	2.32	0.48
1:A:220:GLY:C	1:A:286:LEU:CD2	2.81	0.48
1:A:132:ASN:ND2	1:A:281:PRO:O	2.46	0.48
1:I:223:ASP:OD1	1:I:256:LYS:NZ	2.47	0.47
1:I:182:LYS:O	1:I:263:GLU:N	2.48	0.47
1:A:82:ALA:CB	1:A:135:HIS:CG	2.99	0.46
1:D:170:ILE:CD1	1:D:235:PHE:CE2	2.98	0.45
1:D:82:ALA:CB	1:D:135:HIS:CG	2.99	0.45
1:D:220:GLY:O	1:D:258:LYS:NZ	2.49	0.45
1:L:173:VAL:O	1:L:236:LYS:NZ	2.50	0.44
1:H:72:GLY:N	3:H:491:HOH:O	2.49	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:223:ASP:OD1	1:H:256:LYS:NZ	2.50	0.44
1:E:156:GLU:O	1:E:160:LEU:N	2.51	0.44
1:G:214:ASN:O	1:G:256:LYS:NZ	2.51	0.43
1:A:223:ASP:OD1	1:A:256:LYS:NZ	2.51	0.43
1:A:18:GLY:O	1:A:20:GLY:N	2.52	0.43
1:L:223:ASP:OD1	1:L:256:LYS:NZ	2.51	0.43
1:B:223:ASP:OD1	1:B:256:LYS:NZ	2.52	0.43
1:B:130:LYS:NZ	1:D:132:ASN:O	2.52	0.43
1:F:21:ASP:OD1	1:F:22:LEU:N	2.52	0.43
1:F:223:ASP:OD1	1:F:256:LYS:NZ	2.52	0.42
1:E:166:TYR:CZ	1:E:170:ILE:CD1	3.02	0.42
1:B:82:ALA:N	1:B:83:PRO:CD	2.83	0.42
1:A:246:ASP:OD2	1:A:254:HIS:ND1	2.53	0.41
1:I:184:THR:O	1:I:261:HIS:N	2.53	0.41
1:A:132:ASN:OD1	1:A:283:GLN:N	2.53	0.41
1:I:132:ASN:ND2	1:I:281:PRO:O	2.54	0.41
1:C:223:ASP:OD1	1:C:256:LYS:NZ	2.54	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%)	43	66
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%)	50	73
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%)	43	66
1	H	262/306 (86%)	256 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	59	81

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%)	218 (97%)	6 (3%)	57	83
1	B	244/257 (95%)	241 (99%)	3 (1%)	82	95
1	C	225/257 (88%)	220 (98%)	5 (2%)	64	88
1	D	235/257 (91%)	232 (99%)	3 (1%)	80	94
1	E	229/257 (89%)	225 (98%)	4 (2%)	73	92
1	F	210/257 (82%)	206 (98%)	4 (2%)	69	90
1	G	227/257 (88%)	222 (98%)	5 (2%)	64	88
1	H	194/257 (76%)	191 (98%)	3 (2%)	76	93
1	I	217/257 (84%)	212 (98%)	5 (2%)	63	87
1	J	215/257 (84%)	211 (98%)	4 (2%)	69	90
1	K	226/257 (88%)	218 (96%)	8 (4%)	48	74
1	L	242/257 (94%)	238 (98%)	4 (2%)	73	92
All	All	2688/3084 (87%)	2634 (98%)	54 (2%)	68	89

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	142	ILE
1	A	163	ILE
1	A	248	ASN
1	A	249	GLU
1	A	300	VAL
1	B	62	VAL
1	B	142	ILE
1	B	189	VAL
1	C	2	THR
1	C	62	VAL
1	C	142	ILE
1	C	269	GLU
1	C	300	VAL
1	D	62	VAL
1	D	142	ILE
1	D	251	ASP
1	E	19	GLN
1	E	62	VAL
1	E	142	ILE
1	E	178	THR
1	F	21	ASP
1	F	62	VAL
1	F	142	ILE
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	21	ASP
1	H	62	VAL
1	H	142	ILE
1	I	46	LYS
1	I	62	VAL
1	I	142	ILE
1	I	177	GLU
1	I	230	THR
1	J	62	VAL
1	J	142	ILE
1	J	160	LEU
1	J	163	ILE
1	K	62	VAL

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Mol	Chain	Res	Type
1	K	142	ILE
1	K	144	LEU
1	K	160	LEU
1	K	170	ILE
1	K	195	VAL
1	K	226	VAL
1	K	285	GLU
1	L	62	VAL
1	L	142	ILE
1	L	195	VAL
1	L	242	LYS

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	287/306 (93%)	0.38	25 (8%)	10 9	38, 63, 97, 125	0
1	B	299/306 (97%)	0.24	18 (6%)	21 21	30, 53, 98, 109	0
1	C	292/306 (95%)	0.22	20 (6%)	17 17	38, 64, 111, 126	0
1	D	293/306 (95%)	0.31	16 (5%)	24 24	33, 57, 109, 130	0
1	E	295/306 (96%)	0.13	13 (4%)	33 34	37, 62, 103, 112	0
1	F	273/306 (89%)	0.50	23 (8%)	11 10	35, 66, 133, 166	0
1	G	291/306 (95%)	0.35	14 (4%)	29 30	34, 59, 102, 139	0
1	H	272/306 (88%)	0.51	29 (10%)	6 6	44, 78, 127, 139	0
1	I	277/306 (90%)	0.35	26 (9%)	9 8	36, 62, 109, 130	0
1	J	278/306 (90%)	0.62	32 (11%)	5 5	36, 73, 115, 141	2 (0%)
1	K	289/306 (94%)	0.09	12 (4%)	35 36	33, 56, 106, 124	0
1	L	302/306 (98%)	0.28	18 (5%)	21 21	34, 58, 99, 111	0
All	All	3448/3672 (93%)	0.33	246 (7%)	16 15	30, 63, 110, 166	2 (0%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	232	ILE	7.0
1	I	154	ALA	6.8
1	H	299	VAL	6.3
1	L	-5	TYR	5.6
1	J	253	PHE	5.1
1	H	2	THR	5.0
1	H	165	TYR	5.0
1	G	153	ASP	4.9
1	J	145	VAL	4.8
1	I	169	THR	4.7
1	J	176	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	299	VAL	4.6
1	J	252	ILE	4.6
1	D	149	SER	4.5
1	B	148	VAL	4.5
1	H	160	LEU	4.5
1	F	169	THR	4.5
1	G	299	VAL	4.5
1	G	151	ASN	4.4
1	L	187	GLY	4.3
1	G	152	ILE	4.3
1	L	0	ALA	4.3
1	F	172	THR	4.3
1	I	171	ARG	4.2
1	C	172	THR	4.1
1	L	148	VAL	4.1
1	F	165	TYR	4.0
1	I	165	TYR	3.9
1	F	235	PHE	3.9
1	A	160	LEU	3.9
1	I	174	LYS	3.8
1	A	248	ASN	3.8
1	F	233	GLN	3.8
1	C	158	ALA	3.7
1	A	172	THR	3.7
1	D	148	VAL	3.6
1	I	170	ILE	3.6
1	B	149	SER	3.6
1	F	237	ASP	3.6
1	H	234	ALA	3.6
1	A	199	VAL	3.5
1	H	145	VAL	3.5
1	D	174	LYS	3.4
1	B	2	THR	3.4
1	D	172	THR	3.3
1	F	178	THR	3.3
1	J	199	VAL	3.3
1	J	237	ASP	3.3
1	A	174	LYS	3.3
1	J	254	HIS	3.2
1	J	158	ALA	3.2
1	H	235	PHE	3.2
1	G	265	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	175	ASN	3.2
1	D	97	THR	3.2
1	B	199	VAL	3.1
1	E	173	VAL	3.1
1	J	208	ILE	3.1
1	F	177	GLU	3.1
1	F	158	ALA	3.1
1	A	300	VAL	3.1
1	E	300	VAL	3.1
1	H	139	PHE	3.1
1	A	19	GLN	3.1
1	H	19	GLN	3.0
1	F	189	VAL	3.0
1	B	197	VAL	3.0
1	K	243	LEU	3.0
1	A	229	SER	3.0
1	H	11	LEU	3.0
1	F	187	GLY	3.0
1	A	157	LYS	3.0
1	K	3	LYS	3.0
1	L	250	ASN	3.0
1	G	168	SER	3.0
1	J	299	VAL	2.9
1	J	160	LEU	2.9
1	I	238	TYR	2.9
1	A	299	VAL	2.9
1	K	160	LEU	2.9
1	I	160	LEU	2.9
1	I	240	GLY	2.9
1	F	244	PHE	2.9
1	D	150	ASN	2.9
1	D	151	ASN	2.9
1	H	187	GLY	2.9
1	I	237	ASP	2.9
1	A	175	ASN	2.8
1	F	168	SER	2.8
1	I	155	GLU	2.8
1	D	173	VAL	2.8
1	D	153	ASP	2.8
1	F	199	VAL	2.8
1	L	150	ASN	2.8
1	L	251	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	175	ASN	2.8
1	A	265	GLU	2.8
1	A	140	TRP	2.8
1	K	175	ASN	2.8
1	L	151	ASN	2.8
1	K	194	ALA	2.7
1	E	187	GLY	2.7
1	F	19	GLN	2.7
1	F	240	GLY	2.7
1	C	171	ARG	2.7
1	I	157	LYS	2.7
1	L	300	VAL	2.7
1	L	154	ALA	2.7
1	B	147	GLU	2.7
1	E	151	ASN	2.7
1	H	265	GLU	2.7
1	C	243	LEU	2.7
1	D	243	LEU	2.7
1	L	171	ARG	2.7
1	I	277	SER	2.6
1	E	265	GLU	2.6
1	K	176	ALA	2.6
1	B	140	TRP	2.6
1	I	3	LYS	2.6
1	J	186	ASP	2.6
1	J	235	PHE	2.6
1	E	230	THR	2.6
1	A	269	GLU	2.6
1	G	3	LYS	2.6
1	L	147	GLU	2.6
1	J	3	LYS	2.6
1	I	239	ILE	2.6
1	A	158	ALA	2.5
1	C	176	ALA	2.5
1	D	19	GLN	2.5
1	J	275	GLU	2.5
1	J	277	SER	2.5
1	L	269	GLU	2.5
1	A	197	VAL	2.5
1	C	181	VAL	2.5
1	I	186	ASP	2.5
1	I	159	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	228	LYS	2.5
1	A	48	GLN	2.5
1	A	187	GLY	2.5
1	B	146	SER	2.5
1	H	136	PHE	2.5
1	J	229	SER	2.5
1	I	189	VAL	2.5
1	J	140	TRP	2.5
1	L	266	GLU	2.5
1	B	247	SER	2.5
1	A	176	ALA	2.4
1	C	242	LYS	2.4
1	F	272	THR	2.4
1	B	175	ASN	2.4
1	A	165	TYR	2.4
1	B	174	LYS	2.4
1	H	243	LEU	2.4
1	C	1	MSE	2.4
1	D	246	ASP	2.4
1	A	20	GLY	2.4
1	C	193	GLU	2.4
1	E	275	GLU	2.4
1	J	137	LEU	2.4
1	B	145	VAL	2.4
1	B	172	THR	2.4
1	K	266	GLU	2.4
1	C	269	GLU	2.3
1	H	199	VAL	2.3
1	F	42	ILE	2.3
1	H	66	ILE	2.3
1	G	248	ASN	2.3
1	C	195	VAL	2.3
1	D	189	VAL	2.3
1	K	187	GLY	2.3
1	F	268	LYS	2.3
1	H	232	ILE	2.3
1	C	169	THR	2.3
1	H	141	GLY	2.3
1	H	266	GLU	2.3
1	G	160	LEU	2.3
1	H	137	LEU	2.3
1	I	4	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	172	THR	2.3
1	J	19	GLN	2.3
1	J	20	GLY	2.2
1	B	243	LEU	2.2
1	B	176	ALA	2.2
1	C	265	GLU	2.2
1	A	141	GLY	2.2
1	C	251	ASP	2.2
1	L	196	LEU	2.2
1	I	158	ALA	2.2
1	A	42	ILE	2.2
1	G	172	THR	2.2
1	L	139	PHE	2.2
1	G	199	VAL	2.2
1	H	138	ASN	2.2
1	C	190	TYR	2.2
1	D	147	GLU	2.2
1	L	265	GLU	2.2
1	H	204	TYR	2.2
1	A	40	LEU	2.2
1	C	194	ALA	2.2
1	I	19	GLN	2.2
1	K	179	PHE	2.2
1	F	140	TRP	2.2
1	B	154	ALA	2.2
1	D	298	ALA	2.2
1	H	166	TYR	2.2
1	H	182	LYS	2.1
1	I	188	GLN	2.1
1	J	258	LYS	2.1
1	H	42	ILE	2.1
1	L	-2	ASN	2.1
1	F	282	CYS	2.1
1	J	239	ILE	2.1
1	H	180	PRO	2.1
1	J	66	ILE	2.1
1	E	160	LEU	2.1
1	G	274	GLY	2.1
1	H	140	TRP	2.1
1	G	74	VAL	2.1
1	F	263	GLU	2.1
1	I	136	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	3	LYS	2.1
1	E	165	TYR	2.1
1	B	173	VAL	2.1
1	J	91	ALA	2.1
1	K	19	GLN	2.1
1	I	132	ASN	2.1
1	J	42	ILE	2.1
1	I	180	PRO	2.1
1	A	161	GLY	2.1
1	E	66	ILE	2.1
1	J	11	LEU	2.1
1	J	274	GLY	2.0
1	K	20	GLY	2.0
1	E	237	ASP	2.0
1	K	172	THR	2.0
1	E	176	ALA	2.0
1	B	248	ASN	2.0
1	C	168	SER	2.0
1	G	277	SER	2.0
1	J	271	ASP	2.0
1	J	282	CYS	2.0
1	C	188	GLN	2.0
1	C	178	THR	2.0
1	E	146	SER	2.0
1	H	111	ILE	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(\AA^2)	Q<0.9
2	MG	H	301	1/1	0.16	-0.43	73,73,73,73	0
2	MG	D	301	1/1	0.13	-0.63	39,39,39,39	0
2	MG	L	301	1/1	0.10	-0.80	44,44,44,44	0
2	MG	F	301	1/1	0.12	-0.90	58,58,58,58	0
2	MG	B	301	1/1	0.10	-0.97	36,36,36,36	0
2	MG	K	301	1/1	0.08	-1.40	53,53,53,53	0
2	MG	G	301	1/1	0.10	-1.47	43,43,43,43	0
2	MG	J	301	1/1	0.08	-1.50	69,69,69,69	0
2	MG	C	301	1/1	0.09	-1.61	56,56,56,56	0
2	MG	A	301	1/1	0.09	-1.61	48,48,48,48	0
2	MG	I	301	1/1	0.05	-3.02	59,59,59,59	0
2	MG	E	301	1/1	0.04	-3.61	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.