Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2024 – 02:04 PM EDT

PDB ID	:	8V34
Title	:	Crystal structure of S. aureus TarK N-terminal domain
Authors	:	Li, F.K.K.; Strynadka, N.C.J.
Deposited on	:	2023-11-26
Resolution	:	3.00 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:

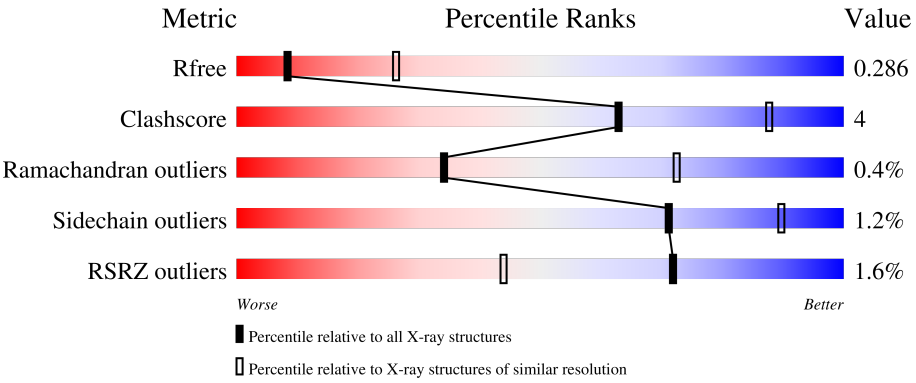
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	178	82% 9% 9%
1	B	178	86% 7% 7%
1	C	178	83% 10% 6%
1	D	178	80% 12% 8%
1	E	178	79% 10% 11%

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Mol	Chain	Length	Quality of chain
1	F	178	4% 74% 13% 13%
1	G	178	79% 11% 8%
1	H	178	2% 81% 10% 10%
1	I	178	2% 78% 12% 10%
1	J	178	4% 69% 13% 17%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13127 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 CDP-glycerol glycerophosphotransferase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	165	Total	C	N	O	S	0	0	0
			1349	863	215	268	3			
1	A	162	Total	C	N	O	S	0	0	0
			1324	849	212	260	3			
1	C	167	Total	C	N	O	S	0	0	0
			1365	873	218	271	3			
1	D	164	Total	C	N	O	S	0	0	0
			1340	858	214	265	3			
1	E	159	Total	C	N	O	S	0	0	0
			1305	836	209	257	3			
1	F	155	Total	C	N	O	S	0	0	0
			1274	818	202	251	3			
1	G	163	Total	C	N	O	S	0	0	0
			1331	852	212	264	3			
1	H	161	Total	C	N	O	S	0	0	0
			1318	844	210	261	3			
1	I	161	Total	C	N	O	S	0	0	0
			1318	844	210	261	3			
1	J	147	Total	C	N	O	S	0	0	0
			1203	775	193	231	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	GLY	-	expression tag	UNP A0A6B5GWD3
B	174	SER	-	expression tag	UNP A0A6B5GWD3
B	175	LEU	-	expression tag	UNP A0A6B5GWD3
B	176	VAL	-	expression tag	UNP A0A6B5GWD3
B	177	PRO	-	expression tag	UNP A0A6B5GWD3
B	178	ARG	-	expression tag	UNP A0A6B5GWD3
A	173	GLY	-	expression tag	UNP A0A6B5GWD3
A	174	SER	-	expression tag	UNP A0A6B5GWD3
A	175	LEU	-	expression tag	UNP A0A6B5GWD3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	176	VAL	-	expression tag	UNP A0A6B5GWD3
A	177	PRO	-	expression tag	UNP A0A6B5GWD3
A	178	ARG	-	expression tag	UNP A0A6B5GWD3
C	173	GLY	-	expression tag	UNP A0A6B5GWD3
C	174	SER	-	expression tag	UNP A0A6B5GWD3
C	175	LEU	-	expression tag	UNP A0A6B5GWD3
C	176	VAL	-	expression tag	UNP A0A6B5GWD3
C	177	PRO	-	expression tag	UNP A0A6B5GWD3
C	178	ARG	-	expression tag	UNP A0A6B5GWD3
D	173	GLY	-	expression tag	UNP A0A6B5GWD3
D	174	SER	-	expression tag	UNP A0A6B5GWD3
D	175	LEU	-	expression tag	UNP A0A6B5GWD3
D	176	VAL	-	expression tag	UNP A0A6B5GWD3
D	177	PRO	-	expression tag	UNP A0A6B5GWD3
D	178	ARG	-	expression tag	UNP A0A6B5GWD3
E	173	GLY	-	expression tag	UNP A0A6B5GWD3
E	174	SER	-	expression tag	UNP A0A6B5GWD3
E	175	LEU	-	expression tag	UNP A0A6B5GWD3
E	176	VAL	-	expression tag	UNP A0A6B5GWD3
E	177	PRO	-	expression tag	UNP A0A6B5GWD3
E	178	ARG	-	expression tag	UNP A0A6B5GWD3
F	173	GLY	-	expression tag	UNP A0A6B5GWD3
F	174	SER	-	expression tag	UNP A0A6B5GWD3
F	175	LEU	-	expression tag	UNP A0A6B5GWD3
F	176	VAL	-	expression tag	UNP A0A6B5GWD3
F	177	PRO	-	expression tag	UNP A0A6B5GWD3
F	178	ARG	-	expression tag	UNP A0A6B5GWD3
G	173	GLY	-	expression tag	UNP A0A6B5GWD3
G	174	SER	-	expression tag	UNP A0A6B5GWD3
G	175	LEU	-	expression tag	UNP A0A6B5GWD3
G	176	VAL	-	expression tag	UNP A0A6B5GWD3
G	177	PRO	-	expression tag	UNP A0A6B5GWD3
G	178	ARG	-	expression tag	UNP A0A6B5GWD3
H	173	GLY	-	expression tag	UNP A0A6B5GWD3
H	174	SER	-	expression tag	UNP A0A6B5GWD3
H	175	LEU	-	expression tag	UNP A0A6B5GWD3
H	176	VAL	-	expression tag	UNP A0A6B5GWD3
H	177	PRO	-	expression tag	UNP A0A6B5GWD3
H	178	ARG	-	expression tag	UNP A0A6B5GWD3
I	173	GLY	-	expression tag	UNP A0A6B5GWD3
I	174	SER	-	expression tag	UNP A0A6B5GWD3
I	175	LEU	-	expression tag	UNP A0A6B5GWD3

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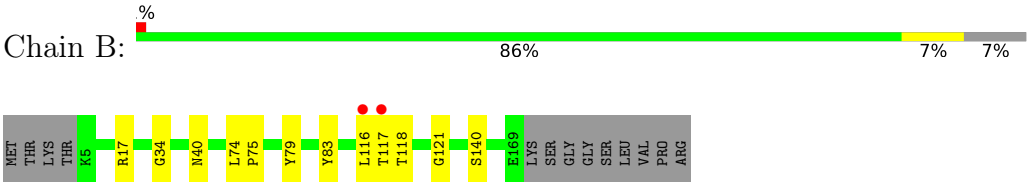
Chain	Residue	Modelled	Actual	Comment	Reference
I	176	VAL	-	expression tag	UNP A0A6B5GWD3
I	177	PRO	-	expression tag	UNP A0A6B5GWD3
I	178	ARG	-	expression tag	UNP A0A6B5GWD3
J	173	GLY	-	expression tag	UNP A0A6B5GWD3
J	174	SER	-	expression tag	UNP A0A6B5GWD3
J	175	LEU	-	expression tag	UNP A0A6B5GWD3
J	176	VAL	-	expression tag	UNP A0A6B5GWD3
J	177	PRO	-	expression tag	UNP A0A6B5GWD3
J	178	ARG	-	expression tag	UNP A0A6B5GWD3

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.

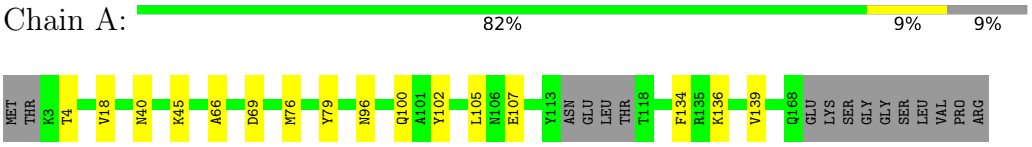
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain B:



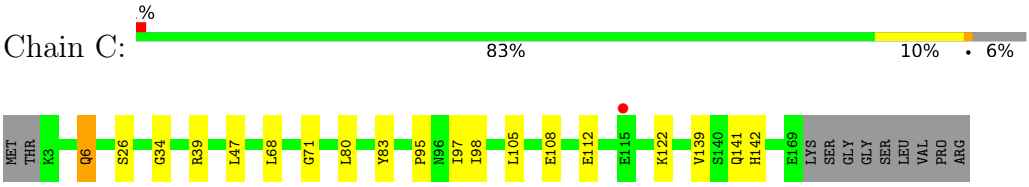
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain A:



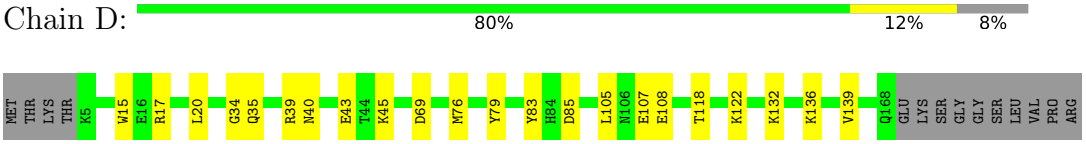
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain C:



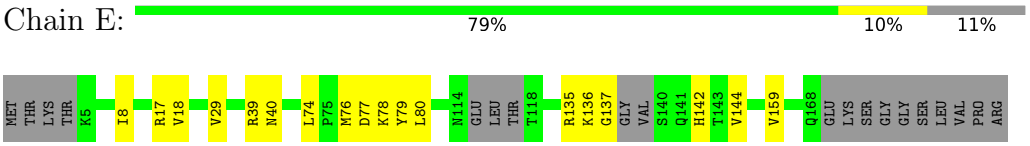
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain D:



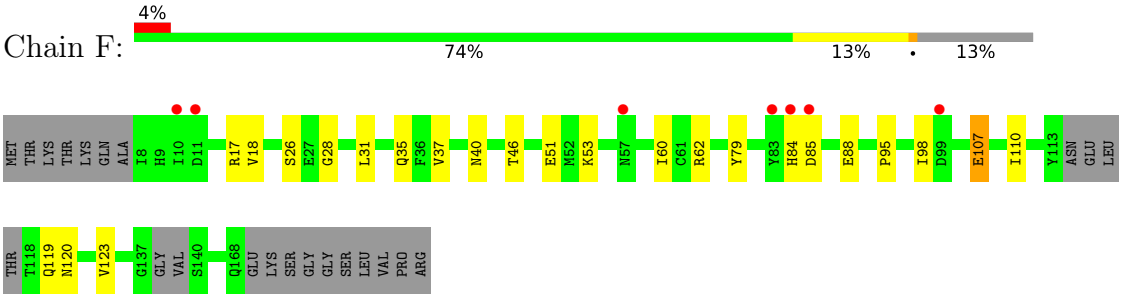
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain E:



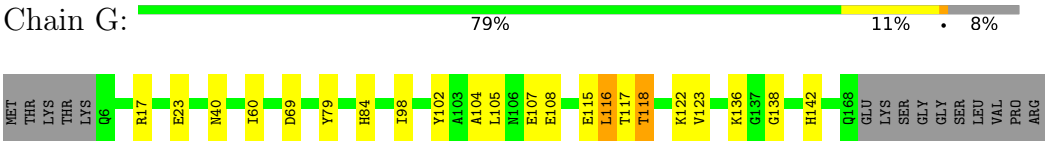
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain F:



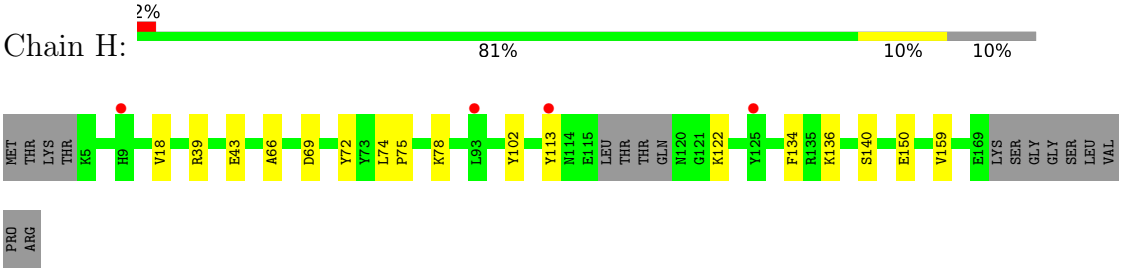
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain G:



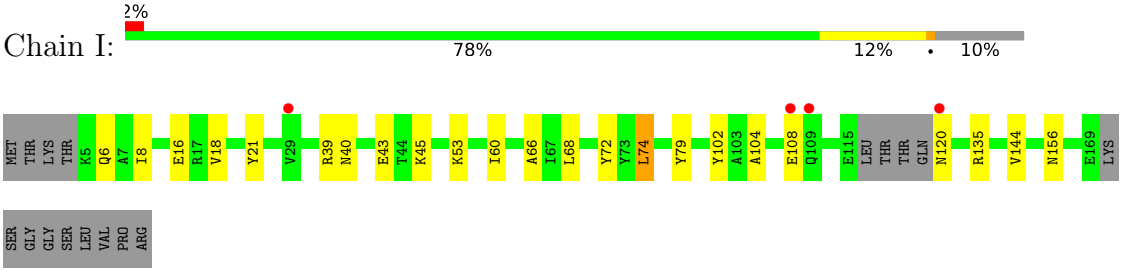
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain H:



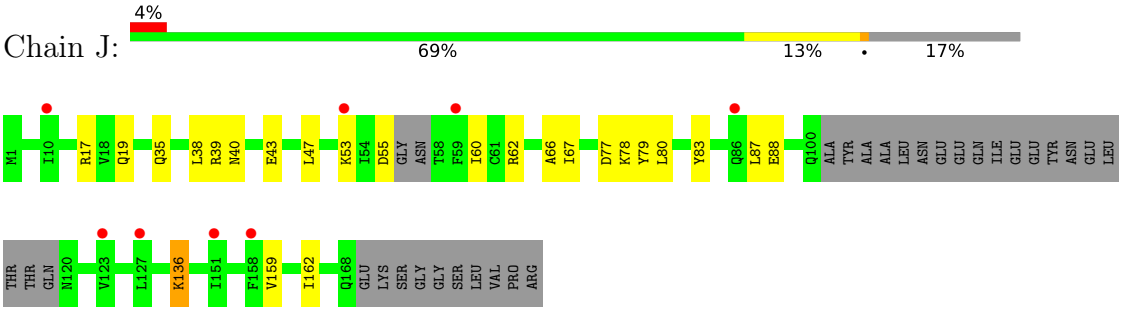
• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain I:



• Molecule 1: CDP-glycerol glycerophosphotransferase family protein

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.89Å 93.67Å 136.76Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	47.49 – 3.00 47.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.49-3.00) 94.0 (47.49-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.236 , 0.288 0.235 , 0.286	Depositor DCC
R_{free} test set	2280 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l 0.009 for k,h,-l 0.023 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13127	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.24	0/1351	0.47	0/1834
1	B	0.25	0/1377	0.48	0/1872
1	C	0.25	0/1393	0.48	0/1893
1	D	0.26	0/1368	0.49	0/1860
1	E	0.25	0/1331	0.48	0/1806
1	F	0.25	0/1300	0.49	0/1765
1	G	0.26	0/1359	0.49	0/1849
1	H	0.24	0/1345	0.46	0/1826
1	I	0.25	0/1345	0.47	0/1826
1	J	0.25	0/1227	0.50	0/1663
All	All	0.25	0/13396	0.48	0/18194

There are no bond length outliers.

There are no bond angle outliers.

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	1324	0	1275	9	0
1	B	1349	0	1292	6	0
1	C	1365	0	1312	12	0
1	D	1340	0	1286	14	0
1	E	1305	0	1248	12	0
1	F	1274	0	1216	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1331	0	1273	13	0
1	H	1318	0	1258	10	0
1	I	1318	0	1258	13	0
1	J	1203	0	1176	15	0
All	All	13127	0	12594	111	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 4.

All (111) 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:B:118:THR:HG23	1:B:121:GLY:H	1.48	0.77
1:D:39:ARG:HD2	1:D:43:GLU:HG3	1.68	0.75
1:H:78:LYS:HB3	1:H:159:VAL:HG21	1.69	0.73
1:G:17:ARG:HG3	1:I:74:LEU:HD11	1.74	0.69
1:J:39:ARG:HD2	1:J:43:GLU:HG3	1.77	0.66
1:E:78:LYS:HB3	1:E:159:VAL:HG21	1.78	0.65
1:C:112:GLU:HG2	1:C:122:LYS:HD2	1.79	0.65
1:H:69:ASP:OD1	1:H:136:LYS:NZ	2.28	0.64
1:G:69:ASP:OD1	1:G:136:LYS:NZ	2.25	0.64
1:C:105:LEU:HB2	1:C:108:GLU:HB2	1.81	0.63
1:E:8:ILE:HD11	1:E:29:VAL:HG21	1.82	0.61
1:J:78:LYS:HB3	1:J:159:VAL:HG21	1.82	0.61
1:D:105:LEU:HG	1:D:108:GLU:HG3	1.83	0.60
1:H:78:LYS:NZ	1:H:150:GLU:OE2	2.32	0.59
1:J:87:LEU:HD12	1:J:88:GLU:H	1.66	0.59
1:G:117:THR:HG22	1:G:118:THR:HG23	1.84	0.59
1:E:135:ARG:HG2	1:E:144:VAL:HG22	1.85	0.58
1:A:105:LEU:HD12	1:A:107:GLU:H	1.70	0.57
1:E:74:LEU:HD23	1:E:76:MET:H	1.71	0.56
1:I:16:GLU:HB2	1:I:21:TYR:HE1	1.72	0.55
1:C:6:GLN:H	1:C:6:GLN:CD	2.09	0.55
1:J:53:LYS:HB3	1:J:60:ILE:HG12	1.89	0.55
1:H:39:ARG:HD2	1:H:43:GLU:HG2	1.91	0.53
1:C:71:GLY:O	1:E:137:GLY:N	2.36	0.52
1:J:38:LEU:HB3	1:J:47:LEU:HB2	1.91	0.52
1:F:51:GLU:HB2	1:F:62:ARG:HB3	1.92	0.52
1:F:53:LYS:HB2	1:F:60:ILE:HG22	1.91	0.52
1:J:66:ALA:HB1	1:J:136:LYS:HD3	1.91	0.52
1:I:53:LYS:HD2	1:I:60:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:40:ASN:HB3	1:J:79:TYR:CD2	2.45	0.51
1:G:105:LEU:HD23	1:G:107:GLU:HB2	1.91	0.51
1:H:74:LEU:HD12	1:H:75:PRO:HD2	1.93	0.51
1:A:69:ASP:OD1	1:A:136:LYS:NZ	2.38	0.51
1:E:40:ASN:HA	1:E:79:TYR:HA	1.93	0.50
1:I:120:ASN:OD1	1:I:156:ASN:ND2	2.42	0.50
1:H:122:LYS:H	1:H:122:LYS:HD2	1.76	0.50
1:F:119:GLN:HG3	1:F:120:ASN:H	1.76	0.50
1:B:17:ARG:NH2	1:H:72:TYR:O	2.45	0.50
1:A:96:ASN:O	1:A:100:GLN:HG2	2.12	0.49
1:G:23:GLU:HG2	1:G:60:ILE:HG23	1.94	0.49
1:G:136:LYS:O	1:G:142:HIS:HA	2.13	0.49
1:I:40:ASN:HA	1:I:79:TYR:HA	1.94	0.48
1:B:140:SER:HA	1:H:140:SER:HB2	1.95	0.48
1:J:40:ASN:HA	1:J:79:TYR:HA	1.96	0.48
1:A:45:LYS:HD3	1:D:17:ARG:HH12	1.78	0.48
1:J:77:ASP:O	1:J:162:ILE:HG13	2.13	0.47
1:F:40:ASN:HA	1:F:79:TYR:HA	1.97	0.47
1:F:95:PRO:O	1:F:98:ILE:HG12	2.14	0.47
1:E:78:LYS:HB3	1:E:159:VAL:CG2	2.45	0.47
1:I:39:ARG:HH11	1:I:43:GLU:HG2	1.80	0.47
1:I:135:ARG:HG2	1:I:144:VAL:HG22	1.98	0.46
1:C:112:GLU:HG2	1:C:122:LYS:CD	2.43	0.46
1:D:45:LYS:HA	1:D:45:LYS:HD2	1.74	0.46
1:I:45:LYS:NZ	1:I:68:LEU:O	2.49	0.46
1:B:34:GLY:HA3	1:B:83:TYR:CZ	2.50	0.45
1:D:35:GLN:O	1:D:35:GLN:HG3	2.17	0.45
1:F:120:ASN:HA	1:F:123:VAL:HG12	1.96	0.45
1:D:69:ASP:OD1	1:D:136:LYS:NZ	2.43	0.45
1:J:47:LEU:HD22	1:J:67:ILE:HD11	1.99	0.45
1:F:26:SER:HB2	1:F:31:LEU:HD21	1.99	0.45
1:D:118:THR:O	1:D:122:LYS:HG3	2.17	0.45
1:J:17:ARG:HD3	1:J:17:ARG:HA	1.78	0.45
1:J:39:ARG:O	1:J:80:LEU:N	2.46	0.45
1:H:18:VAL:HG13	1:H:134:PHE:CZ	2.52	0.44
1:D:105:LEU:HD12	1:D:107:GLU:H	1.83	0.44
1:F:37:VAL:CG1	1:F:46:THR:HG23	2.47	0.44
1:D:17:ARG:O	1:D:132:LYS:HE2	2.18	0.43
1:F:35:GLN:HB3	1:F:84:HIS:NE2	2.34	0.43
1:F:84:HIS:O	1:F:85:ASP:HB2	2.18	0.43
1:F:37:VAL:HG11	1:F:46:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:ASN:HA	1:G:79:TYR:HA	2.01	0.43
1:F:17:ARG:HB2	1:F:18:VAL:H	1.62	0.43
1:A:18:VAL:HG21	1:A:66:ALA:HB2	1.99	0.43
1:D:40:ASN:HA	1:D:79:TYR:HA	2.01	0.42
1:G:116:LEU:O	1:G:122:LYS:HE2	2.19	0.42
1:E:39:ARG:O	1:E:80:LEU:N	2.44	0.42
1:E:136:LYS:O	1:E:142:HIS:HA	2.19	0.42
1:F:53:LYS:HE3	1:F:53:LYS:HB3	1.70	0.42
1:A:139:VAL:HG12	1:D:139:VAL:HG12	2.01	0.42
1:A:4:THR:OG1	1:G:23:GLU:OE1	2.25	0.42
1:E:137:GLY:HA3	1:E:142:HIS:CE1	2.54	0.42
1:F:119:GLN:HG3	1:F:120:ASN:N	2.33	0.42
1:J:35:GLN:H	1:J:83:TYR:HE1	1.67	0.42
1:C:34:GLY:HA3	1:C:83:TYR:CZ	2.54	0.42
1:I:53:LYS:HB2	1:I:60:ILE:HG12	2.01	0.42
1:J:19:GLN:HE21	1:J:62:ARG:HG2	1.85	0.42
1:I:18:VAL:HG21	1:I:66:ALA:HB2	2.01	0.42
1:B:40:ASN:HA	1:B:79:TYR:HA	2.02	0.41
1:G:17:ARG:NH1	1:I:72:TYR:O	2.52	0.41
1:I:8:ILE:HD12	1:I:8:ILE:N	2.34	0.41
1:H:18:VAL:HG11	1:H:66:ALA:HB2	2.02	0.41
1:F:107:GLU:HA	1:F:110:ILE:HB	2.03	0.41
1:G:104:ALA:HB1	1:G:108:GLU:OE1	2.20	0.41
1:C:139:VAL:HG13	1:C:141:GLN:O	2.20	0.41
1:C:141:GLN:HG2	1:E:142:HIS:HD2	1.86	0.41
1:C:39:ARG:O	1:C:80:LEU:N	2.43	0.41
1:D:15:TRP:CZ2	1:D:20:LEU:HD13	2.56	0.41
1:I:104:ALA:HB1	1:I:108:GLU:OE1	2.20	0.41
1:C:97:ILE:HD12	1:C:97:ILE:HA	1.85	0.41
1:A:40:ASN:HA	1:A:79:TYR:HA	2.02	0.41
1:C:95:PRO:O	1:C:98:ILE:HG12	2.21	0.41
1:F:51:GLU:HG3	1:F:62:ARG:HD3	2.02	0.41
1:G:115:GLU:O	1:G:117:THR:N	2.54	0.41
1:J:78:LYS:HB3	1:J:159:VAL:CG2	2.48	0.41
1:D:34:GLY:HA3	1:D:83:TYR:CZ	2.56	0.40
1:D:83:TYR:CE2	1:D:85:ASP:HB2	2.55	0.40
1:A:18:VAL:HG23	1:A:134:PHE:CZ	2.56	0.40
1:E:17:ARG:HB3	1:E:18:VAL:H	1.66	0.40
1:C:47:LEU:HB2	1:C:68:LEU:HD21	2.02	0.40
1:G:98:ILE:HG21	1:G:123:VAL:HG23	2.03	0.40
1:B:74:LEU:HD23	1:B:75:PRO:HD2	2.02	0.40

There are no symmetry-related clashes.

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	158/178 (89%)	150 (95%)	8 (5%)	0	100 100
1	B	163/178 (92%)	153 (94%)	8 (5%)	2 (1%)	13 48
1	C	165/178 (93%)	153 (93%)	12 (7%)	0	100 100
1	D	162/178 (91%)	157 (97%)	5 (3%)	0	100 100
1	E	153/178 (86%)	147 (96%)	6 (4%)	0	100 100
1	F	149/178 (84%)	137 (92%)	11 (7%)	1 (1%)	22 60
1	G	161/178 (90%)	151 (94%)	7 (4%)	3 (2%)	8 36
1	H	157/178 (88%)	150 (96%)	7 (4%)	0	100 100
1	I	157/178 (88%)	151 (96%)	5 (3%)	1 (1%)	25 64
1	J	141/178 (79%)	129 (92%)	12 (8%)	0	100 100
All	All	1566/1780 (88%)	1478 (94%)	81 (5%)	7 (0%)	34 72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	116	LEU
1	B	116	LEU
1	B	117	THR
1	I	6	GLN
1	G	118	THR
1	F	28	GLY
1	G	138	GLY

5.3.2 Protein sidechains (i)

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	144/158 (91%)	142 (99%)	2 (1%)	67 88
1	B	147/158 (93%)	147 (100%)	0	100 100
1	C	149/158 (94%)	146 (98%)	3 (2%)	55 83
1	D	146/158 (92%)	145 (99%)	1 (1%)	84 94
1	E	142/158 (90%)	141 (99%)	1 (1%)	84 94
1	F	139/158 (88%)	137 (99%)	2 (1%)	67 88
1	G	145/158 (92%)	143 (99%)	2 (1%)	67 88
1	H	143/158 (90%)	141 (99%)	2 (1%)	67 88
1	I	143/158 (90%)	141 (99%)	2 (1%)	67 88
1	J	133/158 (84%)	131 (98%)	2 (2%)	65 87
All	All	1431/1580 (91%)	1414 (99%)	17 (1%)	71 90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	MET
1	A	102	TYR
1	C	6	GLN
1	C	26	SER
1	C	142	HIS
1	D	76	MET
1	E	77	ASP
1	F	88	GLU
1	F	107	GLU
1	G	84	HIS
1	G	102	TYR
1	H	102	TYR
1	H	113	TYR
1	I	74	LEU
1	I	102	TYR
1	J	55	ASP

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Mol	Chain	Res	Type
1	J	136	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	114	ASN
1	C	141	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	162/178 (91%)	-0.16	0 100 100	47, 76, 148, 188	0
1	B	165/178 (92%)	-0.14	2 (1%) 79 54	54, 84, 140, 188	0
1	C	167/178 (93%)	-0.10	1 (0%) 89 72	53, 90, 150, 205	0
1	D	164/178 (92%)	-0.10	0 100 100	58, 89, 160, 188	0
1	E	159/178 (89%)	-0.02	0 100 100	65, 94, 150, 219	0
1	F	155/178 (87%)	0.10	7 (4%) 33 12	68, 114, 181, 236	0
1	G	163/178 (91%)	-0.11	0 100 100	53, 86, 137, 163	0
1	H	161/178 (90%)	-0.03	4 (2%) 57 29	65, 97, 165, 206	0
1	I	161/178 (90%)	0.12	4 (2%) 57 29	64, 109, 174, 208	0
1	J	147/178 (82%)	0.26	8 (5%) 25 9	65, 117, 162, 185	0
All	All	1604/1780 (90%)	-0.02	26 (1%) 72 44	47, 96, 162, 236	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	99	ASP	3.4
1	J	151	ILE	3.3
1	H	9	HIS	2.9
1	C	115	GLU	2.8
1	F	10	ILE	2.8
1	J	158	PHE	2.7
1	H	125	TYR	2.7
1	J	59	PHE	2.7
1	B	116	LEU	2.6
1	I	108	GLU	2.5
1	I	109	GLN	2.5
1	B	117	THR	2.5
1	H	113	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	10	ILE	2.4
1	J	123	VAL	2.3
1	H	93	LEU	2.3
1	F	57	ASN	2.3
1	J	86	GLN	2.3
1	F	11	ASP	2.2
1	F	85	ASP	2.2
1	F	83	TYR	2.2
1	J	53	LYS	2.1
1	I	29	VAL	2.1
1	F	84	HIS	2.1
1	I	120	ASN	2.0
1	J	127	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.