Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2022 – 06:22 PM JST

PDB ID	:	7YRT
Title	:	Crystal structure of PAS like domain of FlrB, the histidine kinase involved in flagellar synthesis of Vibrio cholerae
Authors	:	Dasgupta, J.; Mukherjee, P.
Deposited on	:	2022-08-10
Resolution	:	2.27 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:

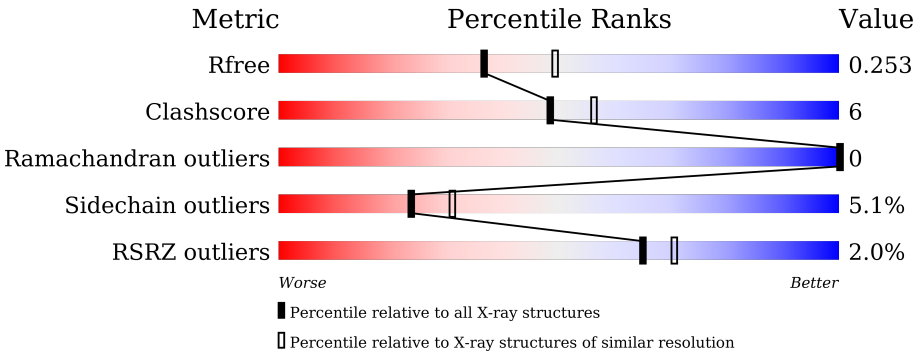
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	118	% 82% 14%
1	B	118	81% 14%
1	C	118	3% 86% 13%
1	D	118	4% 84% 12%
1	E	118	82% 15%
1	F	118	2% 83% 14%

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Mol	Chain	Length	Quality of chain
1	G	118	3% 74% 24%
1	H	118	2% 76% 18%
1	I	118	2% 80% 16%
1	J	118	% 80% 13% 8%
1	K	118	% 82% 14%
1	L	118	6% 77% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11031 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 FlrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			912	569	166	176	1			
1	B	115	Total	C	N	O	S	0	0	0
			912	569	166	176	1			
1	C	118	Total	C	N	O	S	0	0	0
			935	582	170	182	1			
1	D	117	Total	C	N	O	S	0	0	0
			927	576	169	181	1			
1	E	116	Total	C	N	O	S	0	0	0
			922	573	168	180	1			
1	F	116	Total	C	N	O	S	0	0	0
			921	574	167	179	1			
1	G	115	Total	C	N	O	S	0	0	0
			908	567	165	175	1			
1	H	115	Total	C	N	O	S	0	0	0
			912	569	166	176	1			
1	I	114	Total	C	N	O	S	0	0	0
			904	563	165	175	1			
1	J	109	Total	C	N	O	S	0	0	0
			858	536	155	166	1			
1	K	116	Total	C	N	O	S	0	0	0
			917	572	167	177	1			
1	L	116	Total	C	N	O	S	0	0	0
			918	571	167	179	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	initiating methionine	UNP A0A655ZU80
B	6	MET	-	initiating methionine	UNP A0A655ZU80
C	6	MET	-	initiating methionine	UNP A0A655ZU80
D	6	MET	-	initiating methionine	UNP A0A655ZU80
E	6	MET	-	initiating methionine	UNP A0A655ZU80

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Chain	Residue	Modelled	Actual	Comment	Reference
F	6	MET	-	initiating methionine	UNP A0A655ZU80
G	6	MET	-	initiating methionine	UNP A0A655ZU80
H	6	MET	-	initiating methionine	UNP A0A655ZU80
I	6	MET	-	initiating methionine	UNP A0A655ZU80
J	6	MET	-	initiating methionine	UNP A0A655ZU80
K	6	MET	-	initiating methionine	UNP A0A655ZU80
L	6	MET	-	initiating methionine	UNP A0A655ZU80

- Molecule 2 is water.

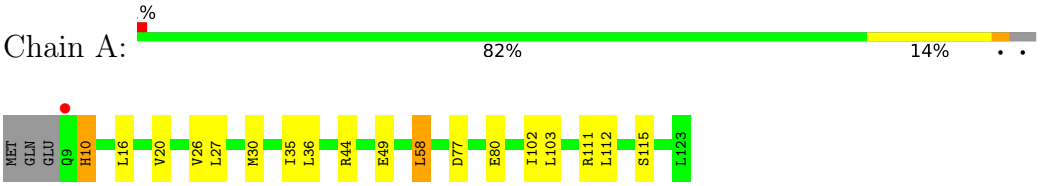
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total O 9 9	0	0
2	B	4	Total O 4 4	0	0
2	C	9	Total O 9 9	0	0
2	D	5	Total O 5 5	0	0
2	E	11	Total O 11 11	0	0
2	F	6	Total O 6 6	0	0
2	G	9	Total O 9 9	0	0
2	H	8	Total O 8 8	0	0
2	I	9	Total O 9 9	0	0
2	J	5	Total O 5 5	0	0
2	K	5	Total O 5 5	0	0
2	L	5	Total O 5 5	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.

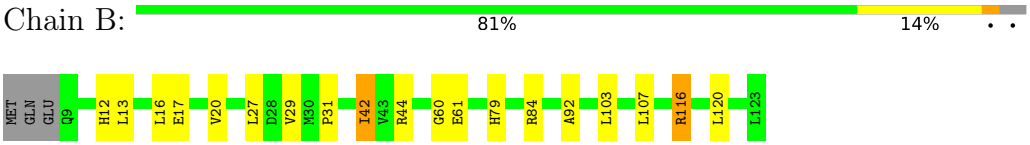
• Molecule 1: FlrB

Chain A:



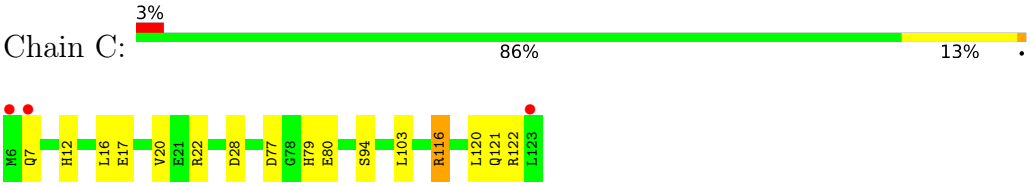
• Molecule 1: FlrB

Chain B:



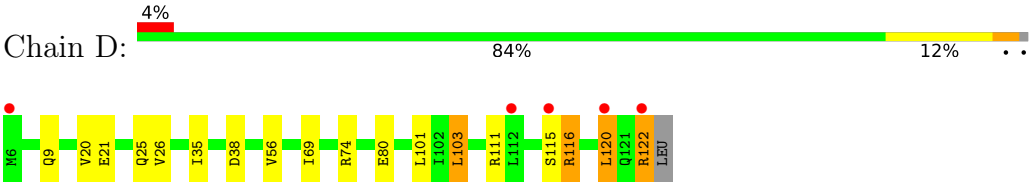
• Molecule 1: FlrB

Chain C:



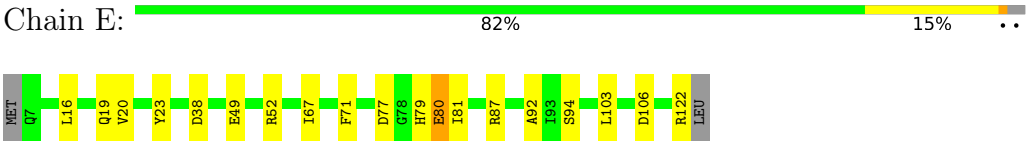
• Molecule 1: FlrB

Chain D:



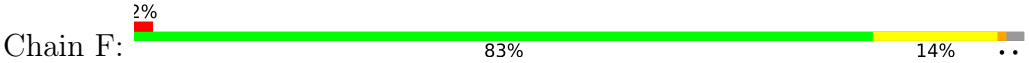
• Molecule 1: FlrB

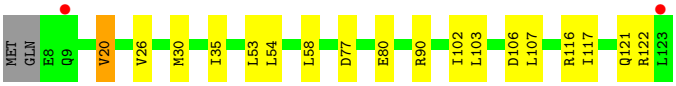
Chain E:



• Molecule 1: FlrB

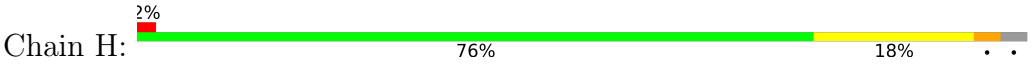
Chain F:

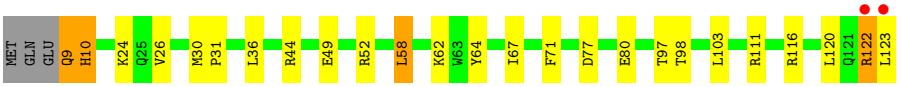




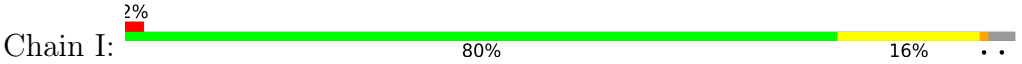
• Molecule 1: FlrB

• Molecule 1: FlrB

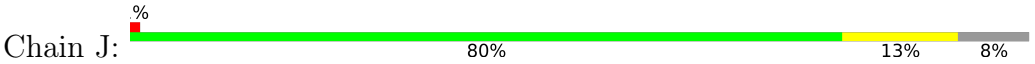


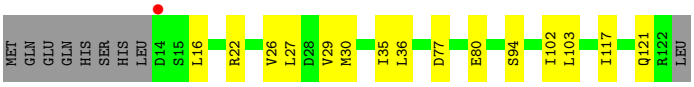


• Molecule 1: FlrB

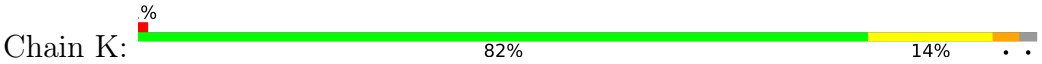


• Molecule 1: FlrB

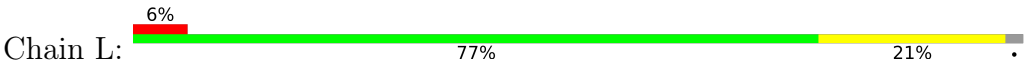


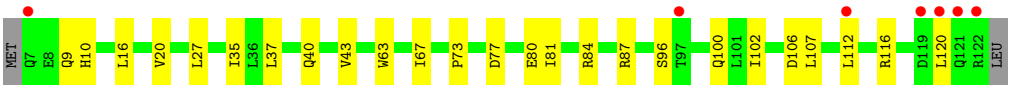


• Molecule 1: FlrB



• Molecule 1: FlrB





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	212.64Å 49.56Å 146.83Å 90.00° 92.53° 90.00°	Depositor
Resolution (Å)	48.26 – 2.27 48.26 – 2.27	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.26-2.27) 88.4 (48.26-2.27)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.185 , 0.251 0.195 , 0.253	Depositor DCC
R_{free} test set	3388 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	51.2	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11031	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1764e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.40	0/923	0.56	0/1251
1	B	0.40	0/923	0.57	0/1251
1	C	0.42	0/946	0.59	0/1282
1	D	0.38	0/938	0.52	0/1271
1	E	0.38	0/933	0.53	0/1264
1	F	0.38	0/932	0.57	0/1263
1	G	0.42	0/919	0.60	0/1246
1	H	0.39	0/923	0.57	0/1251
1	I	0.42	0/915	0.57	0/1240
1	J	0.36	0/867	0.54	0/1175
1	K	0.39	0/928	0.55	0/1258
1	L	0.35	0/929	0.50	0/1259
All	All	0.39	0/11076	0.56	0/15011

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	912	0	931	11	0
1	B	912	0	931	13	0
1	C	935	0	947	14	0
1	D	927	0	936	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	922	0	934	14	0
1	F	921	0	937	11	0
1	G	908	0	925	16	0
1	H	912	0	931	20	0
1	I	904	0	920	16	0
1	J	858	0	880	13	0
1	K	917	0	933	16	0
1	L	918	0	928	18	0
2	A	9	0	0	0	0
2	B	4	0	0	0	0
2	C	9	0	0	0	0
2	D	5	0	0	0	0
2	E	11	0	0	0	0
2	F	6	0	0	0	0
2	G	9	0	0	0	0
2	H	8	0	0	0	0
2	I	9	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
All	All	11031	0	11133	133	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 6.

All (133) 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:22:ARG:HH21	1:I:98:THR:HG23	1.45	0.79
1:I:59:VAL:O	1:L:116:ARG:NH1	2.17	0.78
1:B:16:LEU:HD11	1:F:20:VAL:HG21	1.68	0.76
1:C:16:LEU:HD11	1:K:20:VAL:HG21	1.68	0.76
1:H:36:LEU:HD22	1:J:22:ARG:HH11	1.52	0.75
1:G:49:GLU:OE2	1:G:52:ARG:NH2	2.22	0.72
1:A:20:VAL:HG22	1:E:20:VAL:HG22	1.74	0.70
1:B:20:VAL:HG22	1:F:20:VAL:HG13	1.74	0.69
1:B:29:VAL:HG23	1:F:103:LEU:HD11	1.75	0.69
1:C:22:ARG:HH11	1:K:98:THR:HG23	1.57	0.69
1:H:31:PRO:HD3	1:J:103:LEU:HD13	1.77	0.67
1:G:31:PRO:HD3	1:I:103:LEU:HD13	1.78	0.65
1:G:20:VAL:HG22	1:I:20:VAL:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:O	1:A:30:MET:HG3	1.97	0.64
1:H:98:THR:OG1	1:J:22:ARG:NH2	2.25	0.64
1:J:27:LEU:HA	1:J:30:MET:HE3	1.80	0.64
1:H:64:TYR:HA	1:H:67:ILE:HD12	1.80	0.63
1:H:116:ARG:HH11	1:H:120:LEU:HD11	1.63	0.62
1:C:22:ARG:NH1	1:K:98:THR:HG23	2.13	0.62
1:G:24:LYS:NZ	1:G:45:GLU:OE2	2.32	0.62
1:C:20:VAL:HG22	1:K:20:VAL:HG22	1.81	0.61
1:C:116:ARG:HH12	1:J:16:LEU:HD13	1.65	0.61
1:A:80:GLU:OE2	1:A:111:ARG:NH1	2.32	0.60
1:I:114:GLN:O	1:I:118:SER:OG	2.20	0.59
1:H:9:GLN:N	1:H:9:GLN:HE21	2.01	0.58
1:D:26:VAL:HG11	1:L:27:LEU:HD21	1.85	0.58
1:E:49:GLU:OE2	1:E:52:ARG:NH2	2.36	0.58
1:F:26:VAL:O	1:F:30:MET:HG3	2.03	0.57
1:I:80:GLU:OE1	1:I:111:ARG:NH1	2.36	0.57
1:L:16:LEU:O	1:L:20:VAL:HG23	2.06	0.55
1:K:36:LEU:HD23	1:K:45:GLU:HB3	1.89	0.55
1:H:103:LEU:HD11	1:J:29:VAL:HG23	1.89	0.54
1:L:87:ARG:NH1	1:L:106:ASP:OD2	2.40	0.54
1:G:72:ALA:HB1	1:G:74:ARG:HH21	1.71	0.54
1:D:56:VAL:HG11	1:D:69:ILE:HG22	1.89	0.54
1:B:42:ILE:HD11	1:B:60:GLY:HA2	1.88	0.54
1:C:77:ASP:HB3	1:C:80:GLU:O	2.08	0.53
1:I:26:VAL:O	1:I:30:MET:HG3	2.09	0.53
1:C:16:LEU:O	1:C:20:VAL:HG23	2.08	0.53
1:I:119:ASP:HA	1:I:122:ARG:NH1	2.24	0.53
1:E:87:ARG:HD3	1:E:106:ASP:OD2	2.08	0.53
1:H:36:LEU:HD22	1:J:22:ARG:NH1	2.22	0.52
1:H:49:GLU:OE2	1:H:52:ARG:NH2	2.41	0.52
1:L:116:ARG:O	1:L:120:LEU:HD13	2.09	0.52
1:D:116:ARG:O	1:D:120:LEU:HB2	2.10	0.51
1:G:72:ALA:HB1	1:G:74:ARG:NH2	2.25	0.51
1:A:35:ILE:HB	1:A:102:ILE:HB	1.91	0.51
1:L:73:PRO:HB3	1:L:81:ILE:HD11	1.93	0.51
1:G:29:VAL:HG23	1:I:103:LEU:HD11	1.93	0.51
1:A:16:LEU:HD11	1:E:20:VAL:HG21	1.92	0.51
1:K:111:ARG:NH1	1:K:114:GLN:OE1	2.43	0.51
1:K:38:ASP:OD2	1:K:44:ARG:NE	2.44	0.50
1:K:76:ASP:OD1	1:K:76:ASP:N	2.45	0.50
1:G:77:ASP:HB3	1:G:80:GLU:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:VAL:HG22	1:L:20:VAL:HG22	1.94	0.49
1:E:71:PHE:CD1	1:E:81:ILE:HD13	2.47	0.49
1:E:92:ALA:HB3	1:E:103:LEU:HB2	1.94	0.49
1:I:25:GLN:O	1:I:29:VAL:HG22	2.12	0.49
1:C:12:HIS:HB3	1:C:22:ARG:NH1	2.28	0.49
1:H:26:VAL:O	1:H:30:MET:HG3	2.13	0.48
1:D:80:GLU:OE2	1:D:111:ARG:NH1	2.45	0.48
1:J:26:VAL:HG12	1:J:30:MET:CE	2.43	0.48
1:L:112:LEU:O	1:L:116:ARG:HG3	2.14	0.48
1:A:16:LEU:O	1:A:20:VAL:HG23	2.14	0.47
1:D:9:GLN:NE2	1:L:40:GLN:HG2	2.30	0.47
1:B:16:LEU:O	1:B:20:VAL:HG23	2.14	0.47
1:L:63:TRP:O	1:L:67:ILE:HG13	2.13	0.47
1:K:16:LEU:O	1:K:20:VAL:HG23	2.14	0.47
1:G:16:LEU:HD11	1:I:20:VAL:HG21	1.96	0.47
1:F:53:LEU:HD21	1:F:106:ASP:HB2	1.97	0.47
1:B:42:ILE:HG12	1:B:61:GLU:O	2.15	0.46
1:J:26:VAL:HG12	1:J:30:MET:HE2	1.97	0.46
1:B:12:HIS:CE1	1:B:13:LEU:HG	2.50	0.46
1:I:16:LEU:O	1:I:20:VAL:HG23	2.15	0.46
1:H:67:ILE:HA	1:H:71:PHE:HD1	1.80	0.46
1:F:90:ARG:HB2	1:F:107:LEU:HD13	1.97	0.46
1:A:20:VAL:HG21	1:E:16:LEU:HD11	1.97	0.46
1:B:116:ARG:HD3	1:F:117:ILE:HD13	1.98	0.46
1:C:103:LEU:HD11	1:K:29:VAL:HG23	1.98	0.46
1:H:122:ARG:HB3	1:H:122:ARG:HH11	1.81	0.45
1:J:117:ILE:O	1:J:121:GLN:HG2	2.16	0.45
1:D:25:GLN:OE1	1:L:96:SER:HB3	2.16	0.45
1:L:77:ASP:HB3	1:L:80:GLU:O	2.16	0.45
1:L:107:LEU:HD13	1:L:107:LEU:HA	1.82	0.45
1:E:77:ASP:HB3	1:E:80:GLU:O	2.16	0.45
1:D:122:ARG:HA	1:D:122:ARG:HD2	1.69	0.44
1:I:30:MET:HA	1:I:31:PRO:HD2	1.81	0.44
1:H:44:ARG:HD3	1:H:44:ARG:HA	1.76	0.44
1:L:35:ILE:HB	1:L:102:ILE:HB	2.00	0.44
1:H:122:ARG:HB3	1:H:122:ARG:NH1	2.32	0.44
1:A:20:VAL:HG22	1:E:20:VAL:CG2	2.46	0.44
1:A:77:ASP:HB3	1:A:80:GLU:O	2.18	0.44
1:C:17:GLU:HG3	1:K:16:LEU:HD21	1.99	0.43
1:G:107:LEU:HD13	1:G:107:LEU:HA	1.89	0.43
1:H:58:LEU:HD12	1:H:58:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:PRO:HD3	1:F:103:LEU:HD13	1.99	0.43
1:C:120:LEU:HD23	1:K:120:LEU:HB2	2.00	0.43
1:I:113:LEU:O	1:I:117:ILE:HG13	2.18	0.43
1:B:84:ARG:HE	1:B:84:ARG:HB3	1.67	0.43
1:A:10:HIS:O	1:E:38:ASP:HB2	2.19	0.43
1:C:16:LEU:HA	1:C:16:LEU:HD12	1.75	0.42
1:F:54:LEU:HD12	1:F:58:LEU:HD11	2.01	0.42
1:G:22:ARG:NH2	1:I:98:THR:HG23	2.22	0.42
1:J:35:ILE:HB	1:J:102:ILE:HB	2.00	0.42
1:H:77:ASP:HB3	1:H:80:GLU:O	2.19	0.42
1:K:118:SER:HB2	1:K:122:ARG:HH12	1.85	0.42
1:C:121:GLN:O	1:D:74:ARG:NH1	2.53	0.42
1:F:77:ASP:HB3	1:F:80:GLU:O	2.19	0.42
1:H:67:ILE:HA	1:H:71:PHE:CD1	2.53	0.42
1:F:35:ILE:HB	1:F:102:ILE:HB	2.02	0.42
1:E:16:LEU:HD12	1:E:16:LEU:HA	1.82	0.42
1:A:58:LEU:HD12	1:A:58:LEU:HA	1.86	0.41
1:C:12:HIS:HB3	1:C:22:ARG:HH11	1.85	0.41
1:B:107:LEU:HD23	1:B:107:LEU:HA	1.83	0.41
1:H:9:GLN:C	1:H:10:HIS:HD1	2.24	0.41
1:K:103:LEU:HD12	1:K:103:LEU:HA	1.87	0.41
1:E:19:GLN:HG2	1:E:23:TYR:CE2	2.55	0.41
1:L:84:ARG:HE	1:L:84:ARG:HB3	1.71	0.41
1:G:35:ILE:HB	1:G:102:ILE:HB	2.03	0.41
1:H:24:LYS:HE2	1:K:121:GLN:O	2.21	0.41
1:G:38:ASP:HB3	1:G:44:ARG:HG3	2.02	0.41
1:B:42:ILE:HD12	1:B:44:ARG:CZ	2.51	0.41
1:D:38:ASP:HB2	1:L:10:HIS:O	2.21	0.41
1:L:37:LEU:HD23	1:L:43:VAL:HA	2.03	0.41
1:E:67:ILE:HA	1:E:71:PHE:HD2	1.86	0.41
1:L:27:LEU:HD23	1:L:27:LEU:HA	1.73	0.41
1:G:17:GLU:OE1	1:G:17:GLU:N	2.47	0.40
1:J:77:ASP:HB3	1:J:80:GLU:O	2.20	0.40
1:E:79:HIS:ND1	1:K:40:GLN:OE1	2.41	0.40
1:G:21:GLU:OE2	1:I:97:THR:HG21	2.21	0.40
1:H:103:LEU:CD1	1:J:29:VAL:HG23	2.52	0.40
1:D:101:LEU:HD11	1:D:103:LEU:HD13	2.02	0.40
1:B:92:ALA:HB3	1:B:103:LEU:HB2	2.03	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	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
1	B	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
1	C	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
1	D	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
1	E	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
1	F	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
1	G	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
1	H	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
1	I	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
1	J	107/118 (91%)	102 (95%)	5 (5%)	0	100	100
1	K	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
1	L	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
All	All	1358/1416 (96%)	1309 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	102/105 (97%)	93 (91%)	9 (9%)	10	11
1	B	102/105 (97%)	96 (94%)	6 (6%)	19	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	104/105 (99%)	98 (94%)	6 (6%)	20	25
1	D	103/105 (98%)	96 (93%)	7 (7%)	16	19
1	E	103/105 (98%)	100 (97%)	3 (3%)	42	56
1	F	103/105 (98%)	99 (96%)	4 (4%)	32	43
1	G	101/105 (96%)	93 (92%)	8 (8%)	12	14
1	H	102/105 (97%)	94 (92%)	8 (8%)	12	14
1	I	101/105 (96%)	99 (98%)	2 (2%)	55	70
1	J	95/105 (90%)	93 (98%)	2 (2%)	53	68
1	K	102/105 (97%)	97 (95%)	5 (5%)	25	33
1	L	102/105 (97%)	100 (98%)	2 (2%)	55	70
All	All	1220/1260 (97%)	1158 (95%)	62 (5%)	24	31

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	27	LEU
1	A	36	LEU
1	A	44	ARG
1	A	49	GLU
1	A	58	LEU
1	A	103	LEU
1	A	112	LEU
1	A	115	SER
1	B	17	GLU
1	B	27	LEU
1	B	42	ILE
1	B	79	HIS
1	B	116	ARG
1	B	120	LEU
1	C	7	GLN
1	C	28	ASP
1	C	79	HIS
1	C	94	SER
1	C	116	ARG
1	C	122	ARG
1	D	21	GLU
1	D	35	ILE

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Mol	Chain	Res	Type
1	D	103	LEU
1	D	115	SER
1	D	116	ARG
1	D	120	LEU
1	D	122	ARG
1	E	80	GLU
1	E	94	SER
1	E	122	ARG
1	F	20	VAL
1	F	116	ARG
1	F	121	GLN
1	F	122	ARG
1	G	27	LEU
1	G	51	GLN
1	G	96	SER
1	G	97	THR
1	G	103	LEU
1	G	111	ARG
1	G	122	ARG
1	G	123	LEU
1	H	9	GLN
1	H	10	HIS
1	H	58	LEU
1	H	62	LYS
1	H	97	THR
1	H	111	ARG
1	H	122	ARG
1	H	123	LEU
1	I	27	LEU
1	I	118	SER
1	J	36	LEU
1	J	94	SER
1	K	20	VAL
1	K	36	LEU
1	K	74	ARG
1	K	97	THR
1	K	103	LEU
1	L	9	GLN
1	L	100	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	121	GLN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	115/118 (97%)	-0.29	1 (0%) 84 87	49, 63, 88, 114	0
1	B	115/118 (97%)	-0.28	0 100 100	48, 65, 87, 107	0
1	C	118/118 (100%)	-0.13	3 (2%) 57 63	40, 60, 94, 110	0
1	D	117/118 (99%)	-0.01	5 (4%) 35 40	49, 67, 124, 137	0
1	E	116/118 (98%)	-0.22	0 100 100	49, 69, 102, 129	0
1	F	116/118 (98%)	-0.10	2 (1%) 70 75	52, 75, 108, 134	0
1	G	115/118 (97%)	-0.15	3 (2%) 56 62	40, 57, 88, 136	0
1	H	115/118 (97%)	-0.09	2 (1%) 70 75	47, 62, 102, 144	0
1	I	114/118 (96%)	-0.14	2 (1%) 68 74	47, 62, 102, 120	0
1	J	109/118 (92%)	-0.09	1 (0%) 84 87	48, 68, 111, 136	0
1	K	116/118 (98%)	-0.19	1 (0%) 84 87	46, 66, 100, 124	0
1	L	116/118 (98%)	0.18	7 (6%) 21 26	56, 80, 125, 150	0
All	All	1382/1416 (97%)	-0.12	27 (1%) 65 70	40, 66, 106, 150	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	123	LEU	7.9
1	L	122	ARG	5.8
1	L	120	LEU	5.3
1	H	123	LEU	5.1
1	C	123	LEU	4.8
1	G	123	LEU	4.1
1	L	121	GLN	3.8
1	D	122	ARG	3.7
1	L	119	ASP	3.6
1	C	7	GLN	3.6
1	D	112	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	7	GLN	2.9
1	D	120	LEU	2.8
1	K	84	ARG	2.7
1	D	6	MET	2.7
1	F	9	GLN	2.6
1	J	14	ASP	2.5
1	G	122	ARG	2.4
1	L	112	LEU	2.4
1	C	6	MET	2.4
1	D	115	SER	2.3
1	A	9	GLN	2.2
1	I	122	ARG	2.2
1	I	9	GLN	2.2
1	H	122	ARG	2.2
1	G	16	LEU	2.0
1	L	97	THR	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.