Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 03:05 AM EST

PDB ID	:	1ORJ
Title	:	FLAGELLAR EXPORT CHAPERONE
Authors	:	Evdokimov, A.G.; Phan, J.; Tropea, J.E.; Routzahn, K.M.; Peters III, H.K.; Pokross, M.; Waugh, D.S.
Deposited on	:	2003-03-13
Resolution	:	2.25 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:

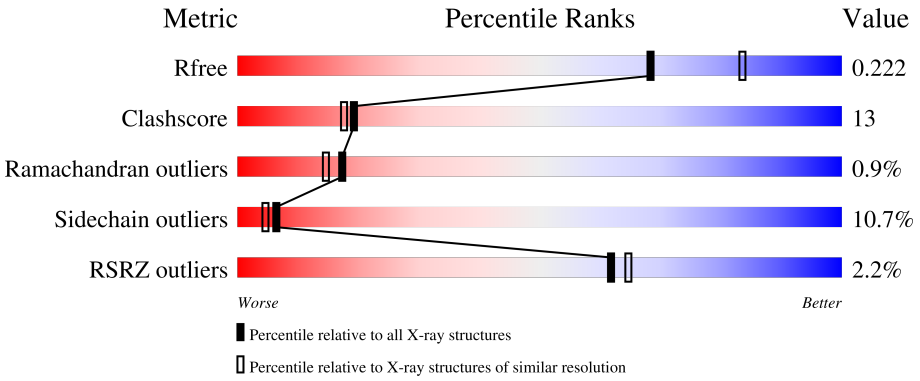
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	130	3% 66% 23% 7%
1	B	130	2% 62% 14% 5% 19%
1	C	130	2% 55% 20% 5% 20%
1	D	130	2% 63% 27% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4130 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 flagellar protein FliS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1054	676	175	201	2			
1	B	105	Total	C	N	O	S	0	0	0
			879	567	141	170	1			
1	C	104	Total	C	N	O	S	0	0	0
			870	561	139	169	1			
1	D	125	Total	C	N	O	S	0	0	0
			1044	670	172	200	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1125	HIS	-	expression tag	UNP O67806
A	1126	HIS	-	expression tag	UNP O67806
A	1127	HIS	-	expression tag	UNP O67806
A	1128	HIS	-	expression tag	UNP O67806
A	1129	HIS	-	expression tag	UNP O67806
A	1130	HIS	-	expression tag	UNP O67806
B	2125	HIS	-	expression tag	UNP O67806
B	2126	HIS	-	expression tag	UNP O67806
B	2127	HIS	-	expression tag	UNP O67806
B	2128	HIS	-	expression tag	UNP O67806
B	2129	HIS	-	expression tag	UNP O67806
B	2130	HIS	-	expression tag	UNP O67806
C	3125	HIS	-	expression tag	UNP O67806
C	3126	HIS	-	expression tag	UNP O67806
C	3127	HIS	-	expression tag	UNP O67806
C	3128	HIS	-	expression tag	UNP O67806
C	3129	HIS	-	expression tag	UNP O67806
C	3130	HIS	-	expression tag	UNP O67806
D	4125	HIS	-	expression tag	UNP O67806
D	4126	HIS	-	expression tag	UNP O67806
D	4127	HIS	-	expression tag	UNP O67806

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4128	HIS	-	expression tag	UNP O67806
D	4129	HIS	-	expression tag	UNP O67806
D	4130	HIS	-	expression tag	UNP O67806

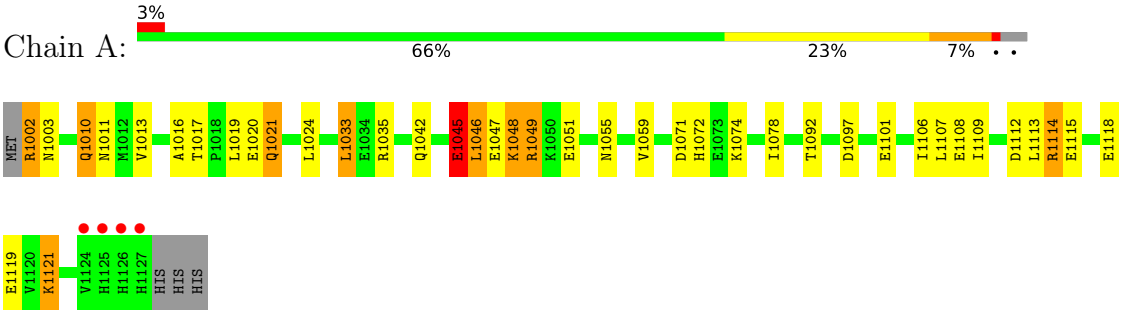
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	77	Total O 77 77	0	0
2	B	69	Total O 69 69	0	0
2	C	56	Total O 56 56	0	0
2	D	81	Total O 81 81	0	0

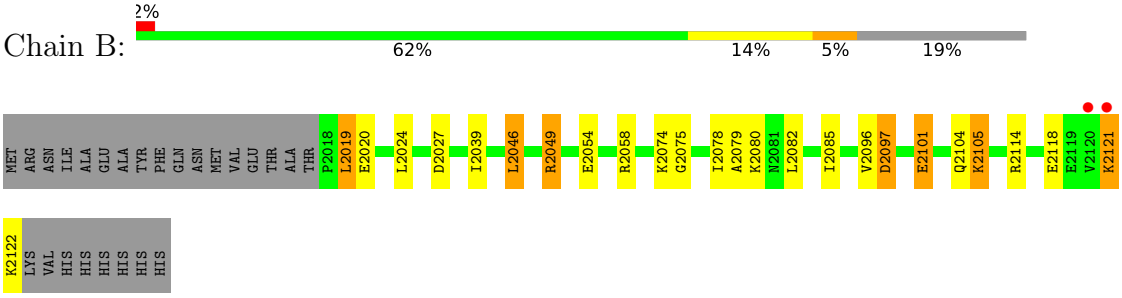
3 Residue-property plots (i)

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.

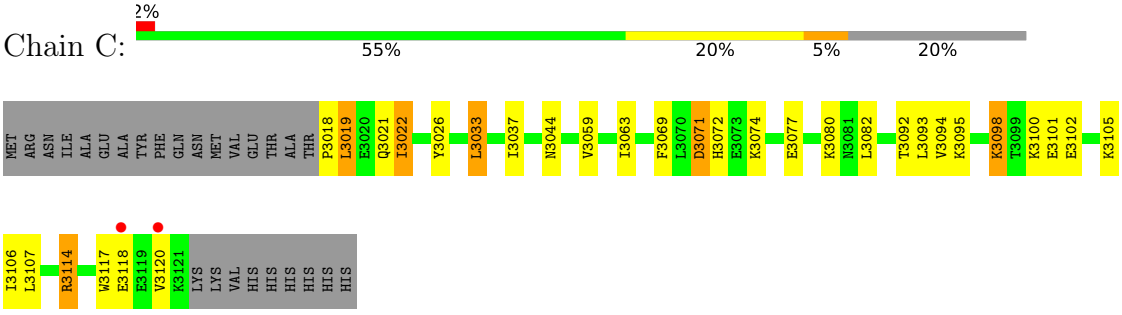
• Molecule 1: flagellar protein FliS



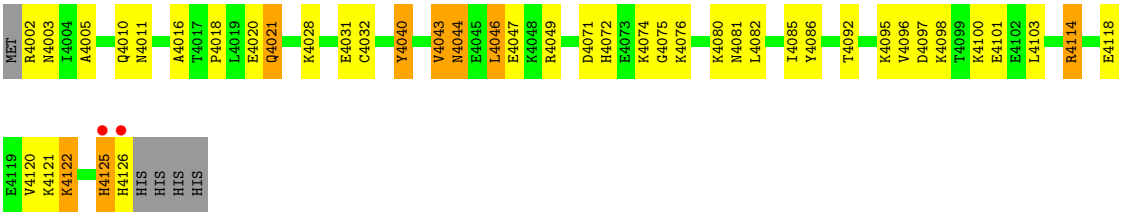
• Molecule 1: flagellar protein FliS



• Molecule 1: flagellar protein FliS



• Molecule 1: flagellar protein FliS


MET
B4002
N4003
I4004
A4005
Q4010
N4011
A4016
T4017
P4018
L4019
E4020
Q4021
K4028
E4031
C4032
Y4040
V4043
N4044
E4045
L4046
E4047
K4048
R4049
D4071
H4072
E4073
K4074
G4075
K4076
K4080
N4081
L4082
I4085
Y4086
T4092
K4095
V4096
D4097
K4098
T4099
K4100
E4101
E4102
L4103
R4114
E4118
E4119
V4120
K4121
K4122
H4125
H4126
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.07Å 131.76Å 74.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.00 – 2.25 43.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (43.00-2.25) 95.0 (43.01-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.19, SHELXL	Depositor
R, R_{free}	0.189 , 0.247 0.203 , 0.222	Depositor DCC
R_{free} test set	2120 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.634	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 101.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4130	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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	0.36	0/1068	0.85	0/1437
1	B	0.35	0/888	0.99	4/1192 (0.3%)
1	C	0.36	0/879	0.92	2/1181 (0.2%)
1	D	0.33	0/1057	0.88	2/1422 (0.1%)
All	All	0.35	0/3892	0.91	8/5232 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2049	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	B	2049	ARG	CD-NE-CZ	7.31	133.83	123.60
1	B	2049	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	3074	LYS	C-N-CA	-5.86	109.99	122.30
1	D	4040	TYR	CB-CG-CD1	5.75	124.45	121.00
1	D	4086	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	B	2074	LYS	C-N-CA	-5.57	110.60	122.30
1	C	3071	ASP	CB-CG-OD1	5.35	123.12	118.30

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	1054	0	1084	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	879	0	921	17	0
1	C	870	0	908	22	1
1	D	1044	0	1077	36	0
2	A	77	0	0	4	0
2	B	69	0	0	3	1
2	C	56	0	0	3	0
2	D	81	0	0	9	0
All	All	4130	0	3990	101	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (101) 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:A:1114:ARG:HD3	1:A:1118:GLU:OE2	1.80	0.81
1:D:4016:ALA:O	1:D:4020:GLU:HG3	1.85	0.78
1:B:2049:ARG:HD3	2:B:5059:HOH:O	1.84	0.76
1:D:4044:ASN:HD22	1:D:4044:ASN:H	1.35	0.75
1:A:1109:ILE:O	1:A:1112:ASP:OD1	2.04	0.74
1:B:2054:GLU:O	1:B:2058:ARG:HG3	1.88	0.73
1:A:1016:ALA:O	1:A:1020:GLU:HG3	1.90	0.72
1:C:3037:ILE:HG23	1:C:3100:LYS:HE3	1.73	0.71
1:A:1017:THR:O	1:A:1021:GLN:HG2	1.91	0.70
1:B:2101:GLU:O	1:B:2105:LYS:HG2	1.91	0.70
1:D:4043:VAL:HG13	1:D:4049:ARG:NH2	2.07	0.70
1:C:3018:PRO:O	1:C:3022:ILE:HG23	1.94	0.68
1:A:1020:GLU:HG2	1:A:1121:LYS:NZ	2.09	0.68
1:A:1042:GLN:O	1:A:1045:GLU:HB2	1.94	0.68
1:A:1020:GLU:HG2	1:A:1121:LYS:HZ1	1.58	0.66
1:D:4081:ASN:O	1:D:4085:ILE:HD12	1.95	0.66
1:C:3101:GLU:HG2	1:C:3105:LYS:HE3	1.78	0.66
1:B:2118:GLU:O	1:B:2121:LYS:HB3	1.98	0.64
1:A:1033:LEU:HD13	1:A:1107:LEU:HB2	1.79	0.63
1:D:4043:VAL:HG13	1:D:4049:ARG:CZ	2.28	0.63
1:D:4121:LYS:HG2	1:D:4125:HIS:CE1	2.34	0.62
1:B:2121:LYS:O	1:B:2121:LYS:HG3	1.98	0.62
1:D:4098:LYS:HD2	1:D:4103:LEU:HD21	1.83	0.60
1:C:3019:LEU:HD21	1:C:3120:VAL:CG1	2.30	0.60
1:D:4071:ASP:HB2	2:D:5137:HOH:O	2.01	0.59
1:D:4018:PRO:O	1:D:4021:GLN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3019:LEU:HD21	1:C:3120:VAL:HG12	1.85	0.58
1:A:1042:GLN:OE1	1:A:1048:LYS:HD2	2.04	0.58
1:A:1046:LEU:O	1:A:1046:LEU:HG	2.03	0.57
1:A:1114:ARG:O	1:A:1118:GLU:HG2	2.04	0.56
1:A:1072:HIS:HD2	2:A:5034:HOH:O	1.89	0.55
1:A:1035:ARG:NE	1:A:1051:GLU:OE2	2.39	0.55
1:C:3072:HIS:HD2	2:C:5168:HOH:O	1.89	0.55
1:D:4043:VAL:HG22	1:D:4049:ARG:HA	1.88	0.55
1:C:3101:GLU:O	1:C:3105:LYS:HG3	2.06	0.54
1:C:3095:LYS:O	1:C:3098:LYS:HG2	2.08	0.53
1:D:4044:ASN:H	1:D:4044:ASN:ND2	2.03	0.53
1:A:1010:GLN:HB2	2:A:5062:HOH:O	2.08	0.53
1:C:3033:LEU:HD13	1:C:3107:LEU:HB2	1.89	0.53
1:C:3095:LYS:O	1:C:3098:LYS:NZ	2.39	0.53
1:D:4118:GLU:O	1:D:4122:LYS:HE2	2.09	0.52
1:D:4011:ASN:HA	2:D:5043:HOH:O	2.10	0.52
1:C:3022:ILE:HD12	1:C:3026:TYR:CD2	2.45	0.52
1:D:4046:LEU:HD13	1:D:4047:GLU:OE2	2.11	0.51
1:C:3098:LYS:HA	1:C:3102:GLU:OE1	2.11	0.51
1:B:2020:GLU:HG3	2:B:5180:HOH:O	2.11	0.50
1:D:4002:ARG:N	2:D:5222:HOH:O	2.45	0.49
1:C:3092:THR:HG21	1:C:3106:ILE:HD11	1.94	0.49
1:A:1010:GLN:HG2	1:A:1013:VAL:CG2	2.42	0.49
1:D:4075:GLY:O	1:D:4076:LYS:HB2	2.13	0.49
1:C:3018:PRO:HG2	1:C:3069:PHE:CE2	2.48	0.49
1:A:1092:THR:HB	1:A:1106:ILE:HD11	1.94	0.49
1:D:4071:ASP:OD2	1:D:4074:LYS:HB2	2.13	0.48
1:D:4121:LYS:O	1:D:4125:HIS:ND1	2.47	0.48
1:C:3022:ILE:HD11	1:C:3117:TRP:CG	2.49	0.47
1:D:4092:THR:O	1:D:4095:LYS:HG2	2.14	0.47
1:D:4043:VAL:CG2	1:D:4049:ARG:HA	2.43	0.47
1:D:4010:GLN:NE2	2:D:5224:HOH:O	2.48	0.47
1:A:1019:LEU:HD12	1:A:1019:LEU:O	2.15	0.47
1:A:1055:ASN:O	1:A:1059:VAL:HG23	2.15	0.46
1:C:3114:ARG:HD2	2:C:5147:HOH:O	2.15	0.46
1:D:4097:ASP:O	2:D:5167:HOH:O	2.20	0.46
1:D:4010:GLN:NE2	1:D:4010:GLN:HA	2.31	0.46
1:A:1049:ARG:HH11	1:A:1049:ARG:HB2	1.81	0.46
1:A:1112:ASP:OD2	1:C:3021:GLN:NE2	2.50	0.45
1:D:4040:TYR:CD1	1:D:4100:LYS:HB2	2.52	0.45
1:A:1002:ARG:HG3	1:A:1078:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2121:LYS:NZ	2:B:5180:HOH:O	2.49	0.45
1:A:1002:ARG:N	2:A:5129:HOH:O	2.50	0.45
1:C:3059:VAL:O	1:C:3063:ILE:HG12	2.17	0.45
1:B:2097:ASP:OD1	1:B:2097:ASP:N	2.50	0.44
1:B:2027:ASP:OD1	1:B:2114:ARG:NH2	2.50	0.44
1:A:1010:GLN:HG2	1:A:1013:VAL:HG23	2.00	0.44
1:B:2046:LEU:HD23	1:B:2046:LEU:HA	1.90	0.44
1:B:2101:GLU:HA	1:B:2104:GLN:HB2	1.99	0.44
1:C:3022:ILE:HD12	1:C:3026:TYR:HD2	1.82	0.44
1:A:1112:ASP:OD1	1:A:1113:LEU:N	2.50	0.44
1:A:1097:ASP:OD1	1:A:1097:ASP:N	2.46	0.43
1:A:1071:ASP:OD2	1:A:1074:LYS:HB2	2.19	0.43
1:D:4114:ARG:HD3	1:D:4118:GLU:OE2	2.17	0.43
1:B:2082:LEU:O	1:B:2085:ILE:HB	2.18	0.43
1:C:3092:THR:CG2	1:C:3106:ILE:HD11	2.49	0.42
1:D:4100:LYS:NZ	2:D:5265:HOH:O	2.50	0.42
1:D:4072:HIS:HD2	2:D:5045:HOH:O	2.00	0.42
1:D:4082:LEU:HD23	1:D:4082:LEU:HA	1.86	0.42
1:D:4092:THR:HA	1:D:4095:LYS:NZ	2.35	0.42
1:B:2027:ASP:OD1	1:B:2114:ARG:NE	2.50	0.42
1:C:3071:ASP:HA	2:C:5237:HOH:O	2.19	0.42
1:B:2075:GLY:H	1:B:2080:LYS:CE	2.33	0.42
1:B:2019:LEU:HD13	1:B:2019:LEU:HA	1.78	0.41
1:C:3093:LEU:O	1:C:3098:LYS:HE3	2.20	0.41
1:D:4005:ALA:HB2	1:D:4120:VAL:HG11	2.02	0.41
1:D:4028:LYS:HA	1:D:4028:LYS:HD2	1.88	0.41
1:D:4040:TYR:CE1	1:D:4100:LYS:HB2	2.56	0.41
1:D:4114:ARG:HD2	2:D:5070:HOH:O	2.21	0.41
1:D:4028:LYS:HE3	1:D:4032:CYS:SG	2.61	0.41
1:A:1046:LEU:HD12	2:A:5264:HOH:O	2.21	0.41
1:B:2024:LEU:O	1:B:2027:ASP:HB2	2.20	0.41
1:B:2078:ILE:HG23	1:B:2079:ALA:N	2.36	0.41
1:D:4125:HIS:ND1	1:D:4125:HIS:N	2.69	0.41
1:D:4080:LYS:NZ	2:D:5009:HOH:O	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3077:GLU:OE2	2:B:5174:HOH:O[2_554]	2.17	0.03

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	124/130 (95%)	118 (95%)	3 (2%)	3 (2%)	6 3
1	B	103/130 (79%)	100 (97%)	3 (3%)	0	100 100
1	C	102/130 (78%)	99 (97%)	3 (3%)	0	100 100
1	D	123/130 (95%)	119 (97%)	3 (2%)	1 (1%)	19 17
All	All	452/520 (87%)	436 (96%)	12 (3%)	4 (1%)	17 14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1003	ASN
1	A	1011	ASN
1	A	1045	GLU
1	D	4003	ASN

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	117/121 (97%)	101 (86%)	16 (14%)	3 2
1	B	99/121 (82%)	90 (91%)	9 (9%)	9 7
1	C	98/121 (81%)	88 (90%)	10 (10%)	7 5
1	D	116/121 (96%)	105 (90%)	11 (10%)	8 6
All	All	430/484 (89%)	384 (89%)	46 (11%)	6 4

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	ARG
1	A	1010	GLN
1	A	1021	GLN
1	A	1024	LEU
1	A	1033	LEU
1	A	1045	GLU
1	A	1046	LEU
1	A	1047	GLU
1	A	1048	LYS
1	A	1049	ARG
1	A	1101	GLU
1	A	1108	GLU
1	A	1114	ARG
1	A	1115	GLU
1	A	1119	GLU
1	A	1121	LYS
1	B	2019	LEU
1	B	2039	ILE
1	B	2046	LEU
1	B	2096	VAL
1	B	2097	ASP
1	B	2101	GLU
1	B	2105	LYS
1	B	2121	LYS
1	B	2122	LYS
1	C	3019	LEU
1	C	3022	ILE
1	C	3033	LEU
1	C	3044	ASN
1	C	3080	LYS
1	C	3082	LEU
1	C	3094	VAL
1	C	3098	LYS
1	C	3114	ARG
1	C	3118	GLU
1	D	4021	GLN
1	D	4031	GLU
1	D	4043	VAL
1	D	4044	ASN
1	D	4046	LEU
1	D	4096	VAL
1	D	4101	GLU

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Mol	Chain	Res	Type
1	D	4114	ARG
1	D	4122	LYS
1	D	4125	HIS
1	D	4126	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1010	GLN
1	A	1072	HIS
1	B	2042	GLN
1	D	4010	GLN
1	D	4044	ASN
1	D	4072	HIS
1	D	4081	ASN

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 (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	126/130 (96%)	0.06	4 (3%)	47	50	20, 42, 77, 117	0
1	B	105/130 (80%)	-0.17	2 (1%)	66	69	22, 38, 72, 108	0
1	C	104/130 (80%)	-0.19	2 (1%)	66	69	20, 41, 73, 89	0
1	D	125/130 (96%)	-0.04	2 (1%)	72	74	21, 38, 63, 110	0
All	All	460/520 (88%)	-0.08	10 (2%)	62	65	20, 40, 73, 117	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2121	LYS	4.4
1	A	1126	HIS	4.0
1	B	2120	VAL	3.5
1	D	4126	HIS	3.3
1	A	1125	HIS	3.2
1	A	1127	HIS	3.2
1	C	3120	VAL	3.1
1	A	1124	VAL	2.8
1	D	4125	HIS	2.6
1	C	3118	GLU	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.