Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:45 am BST

PDB ID	:	4CYB
Title	:	DpsC from Streptomyces coelicolor
Authors	:	Townsend, P.D.; Hitchings, M.D.; Del Sol, R.; Pohl, E.
Deposited on	:	2014-04-10
Resolution	:	1.78 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 following versions of software and data (see references ①) were used in the production of this report:

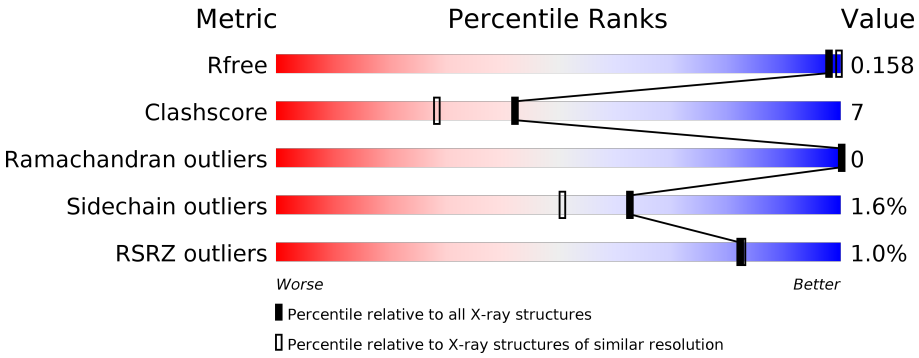
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 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	173	84% 15%
1	B	173	83% 17%
1	C	173	85% 13%
1	D	173	87% 12%
1	E	173	87% 11%
1	F	173	86% 13%

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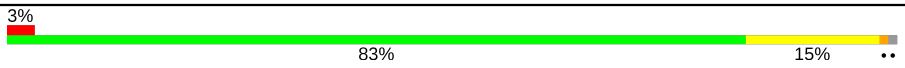
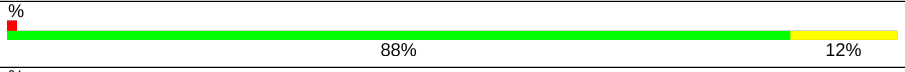
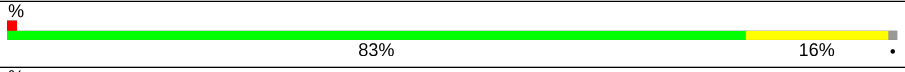
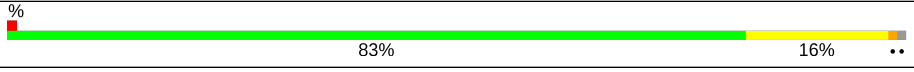
Mol	Chain	Length	Quality of chain
1	G	173	
1	H	173	
1	I	173	
1	J	173	
1	K	173	
1	L	173	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18131 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 PUTATIVE DNA PROTECTION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	2	0
			1373	869	238	260	6			
1	B	172	Total	C	N	O	S	0	4	0
			1394	883	245	260	6			
1	C	172	Total	C	N	O	S	0	2	0
			1374	871	238	259	6			
1	D	171	Total	C	N	O	S	0	3	0
			1375	872	237	260	6			
1	E	171	Total	C	N	O	S	0	1	0
			1368	866	238	259	5			
1	F	172	Total	C	N	O	S	0	2	0
			1375	873	238	259	5			
1	G	172	Total	C	N	O	S	0	2	0
			1385	876	242	262	5			
1	H	172	Total	C	N	O	S	0	2	0
			1376	871	239	261	5			
1	I	172	Total	C	N	O	S	0	6	0
			1400	888	243	262	7			
1	J	173	Total	C	N	O	S	0	1	0
			1378	872	240	261	5			
1	K	171	Total	C	N	O	S	0	6	0
			1388	882	238	262	6			
1	L	172	Total	C	N	O	S	0	5	0
			1388	882	239	262	5			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Na 1 1	0	0
3	L	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	K	1	Total Na 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	145	Total O 145 145	0	0
4	B	130	Total O 130 130	0	0
4	C	166	Total O 166 166	0	0

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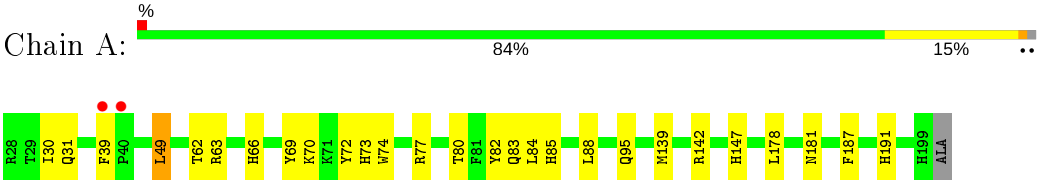
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	126	Total O 126 126	0	0
4	E	136	Total O 136 136	0	0
4	F	89	Total O 89 89	0	0
4	G	136	Total O 136 136	0	0
4	H	101	Total O 101 101	0	0
4	I	157	Total O 157 157	0	0
4	J	113	Total O 113 113	0	0
4	K	140	Total O 140 140	0	0
4	L	102	Total O 102 102	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

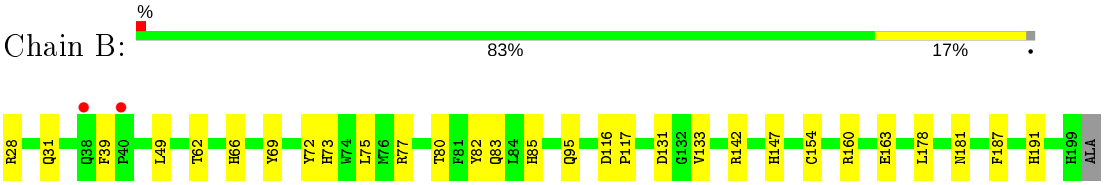
- Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain A:



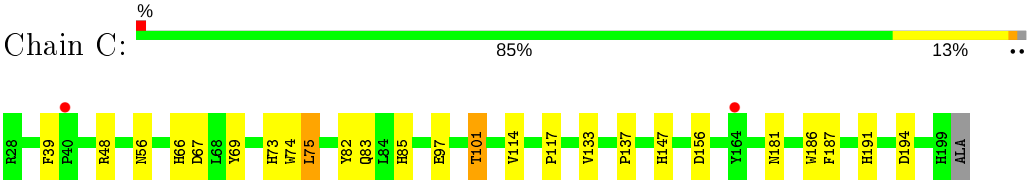
- Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain B:



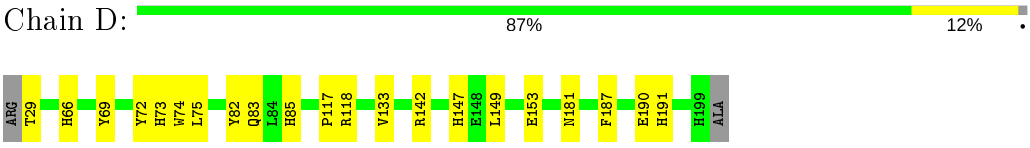
- Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain C:



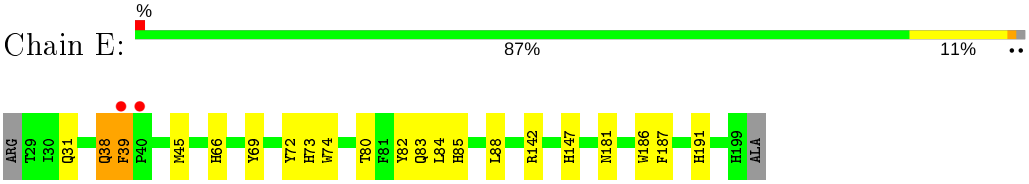
- Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain D:



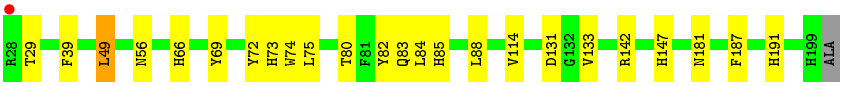
- Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain E:



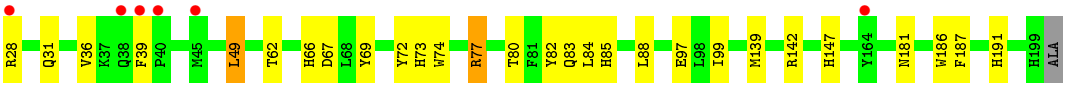
- Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain F:



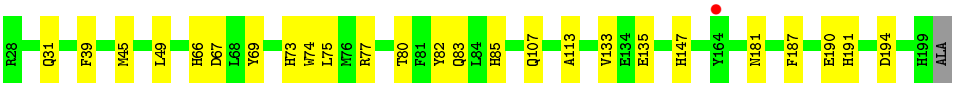
• Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain G:



• Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain H:

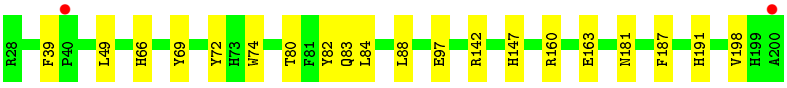


• Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain I:

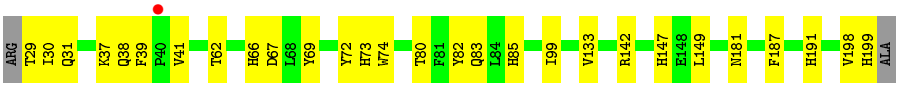
• Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain J:



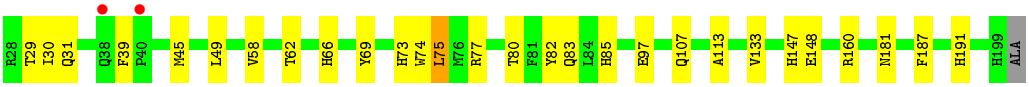
• Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain K:



• Molecule 1: PUTATIVE DNA PROTECTION PROTEIN

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.22Å 153.12Å 170.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.12 – 1.78 76.56 – 1.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.12-1.78) 100.0 (76.56-1.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.159 , 0.194 0.160 , 0.158	Depositor DCC
R_{free} test set	11455 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18131	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, FE

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	0.92	1/1407 (0.1%)	0.89	3/1917 (0.2%)
1	B	0.93	0/1434	0.88	3/1952 (0.2%)
1	C	0.92	2/1408 (0.1%)	0.88	3/1919 (0.2%)
1	D	0.93	1/1412 (0.1%)	0.84	1/1924 (0.1%)
1	E	0.93	2/1399 (0.1%)	0.86	0/1906
1	F	0.93	1/1409 (0.1%)	0.85	1/1921 (0.1%)
1	G	0.95	2/1419 (0.1%)	0.86	1/1932 (0.1%)
1	H	0.87	1/1410 (0.1%)	0.84	1/1921 (0.1%)
1	I	0.89	1/1446 (0.1%)	0.86	1/1968 (0.1%)
1	J	0.93	1/1409 (0.1%)	0.83	0/1920
1	K	0.99	1/1434 (0.1%)	0.93	0/1954
1	L	0.98	2/1431 (0.1%)	0.88	2/1951 (0.1%)
All	All	0.93	15/17018 (0.1%)	0.87	16/23185 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	74	TRP	CD2-CE2	7.58	1.50	1.41
1	J	74	TRP	CD2-CE2	6.70	1.49	1.41
1	E	186	TRP	CD2-CE2	6.58	1.49	1.41
1	D	74	TRP	CD2-CE2	6.52	1.49	1.41
1	G	74	TRP	CD2-CE2	6.51	1.49	1.41
1	H	74	TRP	CD2-CE2	6.40	1.49	1.41
1	L	74	TRP	CD2-CE2	5.98	1.48	1.41
1	A	74	TRP	CD2-CE2	5.91	1.48	1.41
1	L	97	GLU	CD-OE1	5.70	1.31	1.25
1	K	74	TRP	CD2-CE2	5.69	1.48	1.41
1	C	74	TRP	CD2-CE2	5.63	1.48	1.41
1	C	186	TRP	CD2-CE2	5.58	1.48	1.41
1	G	186	TRP	CD2-CE2	5.11	1.47	1.41
1	E	74	TRP	CD2-CE2	5.09	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	186	TRP	CD2-CE2	5.01	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	LEU	CA-CB-CG	6.35	129.91	115.30
1	C	48	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	L	75	LEU	CB-CG-CD2	5.78	120.82	111.00
1	B	131	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	49	LEU	CA-CB-CG	5.58	128.14	115.30
1	I	49	LEU	CA-CB-CG	5.58	128.12	115.30
1	C	156	ASP	CB-CG-OD2	5.45	123.20	118.30
1	L	77	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	75	LEU	CB-CG-CD2	5.24	119.91	111.00
1	G	77	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	F	131	ASP	CB-CG-OD1	5.17	122.95	118.30
1	H	45	MET	CG-SD-CE	-5.16	91.95	100.20
1	B	75	LEU	CB-CG-CD2	5.10	119.67	111.00
1	A	63	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	77	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	D	118	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1373	0	1361	29	0
1	B	1394	0	1397	30	0
1	C	1374	0	1365	21	0
1	D	1375	0	1369	18	0
1	E	1368	0	1357	27	0
1	F	1375	0	1369	20	0
1	G	1385	0	1376	26	0
1	H	1376	0	1364	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1400	0	1406	29	0
1	J	1378	0	1364	20	0
1	K	1388	0	1391	33	0
1	L	1388	0	1389	30	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	C	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	145	0	0	1	0
4	B	130	0	0	4	0
4	C	166	0	0	3	0
4	D	126	0	0	1	0
4	E	136	0	0	3	0
4	F	89	0	0	1	0
4	G	136	0	0	2	0
4	H	101	0	0	2	0
4	I	157	0	0	3	0
4	J	113	0	0	2	0
4	K	140	0	0	5	0
4	L	102	0	0	3	0
All	All	18131	0	16508	228	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 7.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:VAL:HG23	1:I:45[A]:MET:SD	1.93	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ASP:HB2	1:K:198:VAL:HG11	1.45	0.94
1:I:36:VAL:CG2	1:I:45[A]:MET:SD	2.68	0.81
4:B:2117:HOH:O	1:K:41:VAL:HG11	1.80	0.81
1:K:31:GLN:HB3	1:L:133[A]:VAL:HG12	1.69	0.74
1:E:69:TYR:OH	1:E:147:HIS:HE1	1.71	0.74
1:E:31:GLN:HB3	1:F:133[A]:VAL:CG1	2.18	0.74
1:B:160[B]:ARG:HD2	4:B:2100:HOH:O	1.87	0.73
1:D:69:TYR:OH	1:D:147:HIS:HE1	1.74	0.71
1:I:69:TYR:OH	1:I:147:HIS:HE1	1.76	0.68
1:K:133[A]:VAL:HG12	1:L:31:GLN:HB3	1.76	0.68
1:A:69:TYR:OH	1:A:147:HIS:HE1	1.77	0.68
1:E:45:MET:HE3	4:E:2007:HOH:O	1.93	0.67
1:J:97:GLU:HG3	4:J:2055:HOH:O	1.94	0.67
1:K:31:GLN:HB3	1:L:133[A]:VAL:CG1	2.24	0.67
1:L:69:TYR:OH	1:L:147:HIS:HE1	1.77	0.67
1:J:69:TYR:OH	1:J:147:HIS:HE1	1.77	0.67
1:E:83[A]:GLN:CB	1:H:83[A]:GLN:HE21	2.07	0.67
4:H:2096:HOH:O	1:J:198:VAL:HG13	1.94	0.66
1:K:69:TYR:OH	1:K:147:HIS:HE1	1.78	0.66
1:A:83:GLN:H	1:D:83:GLN:HE21	1.43	0.66
1:C:194:ASP:HB2	1:K:198:VAL:CG1	2.21	0.66
1:K:133[A]:VAL:CG1	1:L:31:GLN:HB3	2.27	0.64
1:H:147:HIS:HD2	1:H:181:ASN:OD1	1.80	0.64
1:C:194:ASP:CB	1:K:198:VAL:HG11	2.26	0.64
1:A:147:HIS:HD2	1:A:181:ASN:OD1	1.80	0.64
1:L:62[A]:THR:HG22	4:L:2027:HOH:O	1.98	0.64
1:G:97[A]:GLU:HG3	4:G:2072:HOH:O	1.97	0.63
1:B:147:HIS:HD2	1:B:181:ASN:OD1	1.82	0.63
1:F:69:TYR:OH	1:F:147:HIS:HE1	1.82	0.63
1:C:69:TYR:OH	1:C:147:HIS:HE1	1.80	0.63
1:F:147:HIS:HD2	1:F:181:ASN:OD1	1.82	0.63
1:H:107:GLN:NE2	1:H:113:ALA:H	1.97	0.62
1:B:69:TYR:OH	1:B:147:HIS:HE1	1.81	0.62
1:I:147:HIS:HD2	1:I:181:ASN:OD1	1.83	0.62
1:L:107:GLN:NE2	1:L:113:ALA:H	1.98	0.61
1:G:69:TYR:OH	1:G:147:HIS:HE1	1.84	0.61
1:A:31:GLN:HB3	1:B:133[A]:VAL:HG12	1.81	0.61
1:E:31:GLN:HB3	1:F:133[A]:VAL:HG12	1.83	0.60
1:G:83:GLN:HE22	1:K:80:THR:HA	1.66	0.60
1:I:153:GLU:HG3	4:I:2043:HOH:O	2.01	0.60
1:B:28:ARG:N	4:B:2001:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:HIS:HD2	1:G:181:ASN:OD1	1.85	0.59
1:H:69:TYR:OH	1:H:147:HIS:HE1	1.85	0.59
1:E:147:HIS:HD2	1:E:181:ASN:OD1	1.85	0.59
1:J:160:ARG:NH2	1:J:163:GLU:OE2	2.29	0.59
1:A:73:HIS:CE1	1:A:85:HIS:CE1	2.91	0.59
1:C:147:HIS:HD2	1:C:181:ASN:OD1	1.86	0.58
1:A:83:GLN:H	1:D:83:GLN:NE2	2.01	0.58
1:D:147:HIS:HD2	1:D:181:ASN:OD1	1.86	0.58
1:A:191:HIS:CE1	1:F:82:TYR:H	2.22	0.58
1:G:77:ARG:HH12	1:H:31:GLN:HE21	1.50	0.57
1:E:83[A]:GLN:HB2	1:H:83[A]:GLN:HE21	1.69	0.57
1:J:147:HIS:HD2	1:J:181:ASN:OD1	1.87	0.57
1:L:147:HIS:HD2	1:L:181:ASN:OD1	1.87	0.57
1:L:187:PHE:O	1:L:191:HIS:HD2	1.88	0.57
1:I:83[A]:GLN:H	1:L:83[A]:GLN:HE21	1.52	0.57
1:E:83[B]:GLN:H	1:H:83[B]:GLN:NE2	2.03	0.57
1:K:72:TYR:OH	1:K:142:ARG:HD2	2.05	0.57
1:C:83:GLN:HE22	1:G:80:THR:HA	1.69	0.56
1:E:83[B]:GLN:HE21	1:E:191:HIS:HE1	1.54	0.55
1:A:30:ILE:HG13	1:B:133[A]:VAL:HG13	1.88	0.55
1:G:36:VAL:HG13	1:G:49:LEU:HD23	1.89	0.55
1:H:80:THR:HA	1:J:83[A]:GLN:HE22	1.71	0.55
1:K:187:PHE:O	1:K:191:HIS:HD2	1.90	0.55
1:B:187:PHE:O	1:B:191:HIS:HD2	1.89	0.55
1:F:73:HIS:CE1	1:F:85:HIS:CE1	2.94	0.55
1:L:75:LEU:HD13	1:L:133[B]:VAL:HG22	1.89	0.54
1:A:84:LEU:O	1:A:88:LEU:HG	2.07	0.54
1:B:83[B]:GLN:OE1	1:L:83[B]:GLN:OE1	2.26	0.54
1:D:75:LEU:HD13	1:D:133:VAL:HG22	1.89	0.54
1:E:83[A]:GLN:H	1:H:83[A]:GLN:NE2	2.05	0.54
1:A:31:GLN:HB3	1:B:133[A]:VAL:CG1	2.38	0.54
1:E:31:GLN:HB3	1:F:133[A]:VAL:HG11	1.86	0.54
1:B:80:THR:HA	1:I:83[A]:GLN:HE22	1.72	0.54
1:I:160:ARG:NH1	4:I:2143:HOH:O	2.24	0.53
1:K:147:HIS:HD2	1:K:181:ASN:OD1	1.91	0.53
1:H:107:GLN:HE22	1:H:113:ALA:H	1.55	0.53
1:G:77:ARG:HH12	1:H:31:GLN:NE2	2.06	0.53
1:J:187:PHE:O	1:J:191:HIS:HD2	1.92	0.53
1:E:191:HIS:CE1	1:J:82:TYR:H	2.26	0.53
1:B:191:HIS:CE1	1:L:82:TYR:H	2.26	0.53
1:A:66:HIS:HE1	4:A:2020:HOH:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83[A]:GLN:H	1:H:83[A]:GLN:HE21	1.57	0.53
1:H:194:ASP:HB2	1:J:198:VAL:HG11	1.89	0.53
1:C:56:ASN:OD1	1:C:114[A]:VAL:HG23	2.08	0.53
1:C:97:GLU:O	1:C:101:THR:HG23	2.09	0.53
1:K:38:GLN:CG	4:K:2008:HOH:O	2.56	0.53
1:D:73:HIS:CE1	1:D:85:HIS:CE1	2.97	0.52
1:F:66:HIS:HE1	4:F:2015:HOH:O	1.92	0.52
1:G:187:PHE:O	1:G:191:HIS:HD2	1.92	0.52
1:H:66:HIS:HE1	4:H:2016:HOH:O	1.92	0.52
1:H:187:PHE:O	1:H:191:HIS:HD2	1.92	0.52
1:A:72:TYR:OH	1:A:142:ARG:HD2	2.09	0.52
1:K:66:HIS:HE1	4:K:2022:HOH:O	1.92	0.52
1:I:83[A]:GLN:H	1:L:83[A]:GLN:NE2	2.07	0.52
1:A:82:TYR:H	1:D:191:HIS:CE1	2.29	0.51
1:D:187:PHE:O	1:D:191:HIS:HD2	1.92	0.51
1:H:83[B]:GLN:H	1:J:83[B]:GLN:NE2	2.08	0.51
1:A:80:THR:HA	1:D:83:GLN:HE22	1.74	0.51
1:C:66:HIS:HE1	4:C:2017:HOH:O	1.92	0.51
1:I:80:THR:HA	1:L:83[A]:GLN:HE22	1.76	0.51
1:L:66:HIS:HE1	4:L:2020:HOH:O	1.93	0.51
1:A:62:THR:HG23	1:A:95:GLN:NE2	2.26	0.51
1:F:187:PHE:O	1:F:191:HIS:HD2	1.94	0.51
1:G:73:HIS:CE1	1:G:85:HIS:CE1	2.99	0.51
1:L:58:VAL:O	1:L:62[A]:THR:HG23	2.11	0.51
1:G:66:HIS:HE1	4:G:2019:HOH:O	1.94	0.51
1:A:83:GLN:HE22	1:F:80:THR:HA	1.76	0.51
1:I:187:PHE:O	1:I:191:HIS:HD2	1.93	0.51
1:F:56:ASN:OD1	1:F:114[A]:VAL:HG23	2.11	0.51
1:C:137:PRO:HB2	1:K:199:HIS:CE1	2.46	0.51
1:E:66:HIS:HE1	4:E:2017:HOH:O	1.94	0.50
1:C:73:HIS:CE1	1:C:85:HIS:CE1	2.99	0.50
1:G:84:LEU:O	1:G:88:LEU:HG	2.10	0.50
1:H:66:HIS:HD2	1:H:67:ASP:OD1	1.94	0.50
1:F:72:TYR:OH	1:F:142:ARG:HD2	2.12	0.50
1:G:191:HIS:CE1	1:K:82:TYR:H	2.30	0.49
1:A:62:THR:HG23	1:A:95:GLN:HE21	1.77	0.49
1:I:66:HIS:HE1	4:I:2028:HOH:O	1.95	0.49
1:L:73:HIS:CE1	1:L:85:HIS:CE1	3.00	0.49
1:C:187:PHE:O	1:C:191:HIS:HD2	1.96	0.49
1:K:73:HIS:CE1	1:K:85:HIS:CE1	3.01	0.49
1:D:82:TYR:H	1:F:191:HIS:CE1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:THR:HA	1:I:83[B]:GLN:HE22	1.76	0.49
1:I:82:TYR:H	1:L:191:HIS:CE1	2.30	0.49
1:E:83[B]:GLN:HE22	1:J:80:THR:HA	1.78	0.48
1:K:30:ILE:HG12	1:L:133[A]:VAL:HG13	1.94	0.48
1:B:72:TYR:OH	1:B:142:ARG:HD2	2.13	0.48
1:G:28:ARG:NH1	1:H:135:GLU:OE2	2.46	0.48
1:E:187:PHE:O	1:E:191:HIS:HD2	1.97	0.48
1:B:160[B]:ARG:NH2	1:B:163:GLU:OE2	2.47	0.48
1:I:73:HIS:CE1	1:I:85:HIS:CE1	3.02	0.47
1:H:82:TYR:H	1:J:191:HIS:CE1	2.33	0.47
1:K:38:GLN:HG3	4:K:2008:HOH:O	2.13	0.47
1:B:73:HIS:CE1	1:B:85:HIS:CE1	3.02	0.47
1:E:72:TYR:OH	1:E:142:ARG:HD2	2.14	0.47
1:E:80:THR:HA	1:H:83[A]:GLN:HE22	1.80	0.47
1:A:83:GLN:HB3	1:D:83:GLN:HE21	1.79	0.47
1:B:83[B]:GLN:HE22	1:L:80:THR:HA	1.78	0.47
1:A:69:TYR:OH	1:A:147:HIS:CE1	2.65	0.47
1:C:101:THR:HG22	4:C:2085:HOH:O	2.14	0.47
1:F:49:LEU:O	1:F:49:LEU:HD13	2.15	0.47
1:K:149:LEU:HD23	1:K:149:LEU:C	2.35	0.47
1:K:198:VAL:HG12	4:K:2138:HOH:O	2.15	0.46
1:I:83[A]:GLN:HB3	1:L:83[A]:GLN:HE21	1.79	0.46
1:K:62:THR:HG22	1:K:99:ILE:HG13	1.98	0.46
1:C:83:GLN:HE21	1:G:83:GLN:HB2	1.79	0.46
1:J:66:HIS:HE1	4:J:2019:HOH:O	1.97	0.46
1:B:83[B]:GLN:H	1:I:83[B]:GLN:NE2	2.14	0.46
1:F:75:LEU:HD13	1:F:133[B]:VAL:HG22	1.98	0.46
1:J:69:TYR:OH	1:J:147:HIS:CE1	2.64	0.46
1:J:84:LEU:O	1:J:88:LEU:HG	2.16	0.46
1:A:83:GLN:NE2	1:F:83:GLN:H	2.14	0.46
1:I:75:LEU:HD13	1:I:133:VAL:HG22	1.98	0.46
1:C:83:GLN:HE21	1:G:83:GLN:H	1.64	0.45
1:A:83:GLN:HE21	1:F:83:GLN:H	1.65	0.45
1:E:80:THR:C	1:H:83[B]:GLN:HE22	2.18	0.45
1:K:30:ILE:CG1	1:L:133[A]:VAL:HG13	2.47	0.45
1:B:116:ASP:CG	1:B:117:PRO:HD2	2.37	0.45
1:A:83:GLN:CB	1:D:83:GLN:HE21	2.30	0.45
1:G:72:TYR:CE1	1:G:139:MET:HG2	2.52	0.45
1:L:160:ARG:HB3	1:L:160:ARG:NH1	2.32	0.45
1:E:82:TYR:H	1:H:191:HIS:CE1	2.35	0.45
1:D:66:HIS:HE1	4:D:2031:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:29:THR:HB	4:K:2001:HOH:O	2.17	0.44
1:B:62:THR:HG23	1:B:95:GLN:OE1	2.17	0.44
1:E:84:LEU:O	1:E:88:LEU:HG	2.18	0.44
1:C:191:HIS:CE1	1:G:82:TYR:H	2.34	0.44
1:A:77:ARG:HH12	1:B:31:GLN:HE21	1.66	0.44
1:D:72:TYR:OH	1:D:142:ARG:HD2	2.18	0.44
1:I:49:LEU:HD13	1:I:53[A]:GLN:OE1	2.17	0.44
1:E:73:HIS:CE1	1:E:85:HIS:CE1	3.05	0.44
1:J:72:TYR:OH	1:J:142:ARG:HD2	2.17	0.44
1:E:38:GLN:HE21	1:E:39:PHE:H	1.66	0.44
4:C:2161:HOH:O	1:K:198:VAL:HG13	2.17	0.44
1:B:66:HIS:HE1	4:B:2019:HOH:O	2.00	0.43
1:C:66:HIS:HD2	1:C:67:ASP:OD1	1.99	0.43
1:B:82:TYR:HB3	1:I:83[A]:GLN:HG3	2.01	0.43
1:B:83[A]:GLN:H	1:I:83[A]:GLN:NE2	2.15	0.43
1:A:187:PHE:O	1:A:191:HIS:HD2	2.00	0.43
1:F:84:LEU:O	1:F:88:LEU:HG	2.19	0.43
1:C:117:PRO:HB2	1:D:117:PRO:HB2	1.99	0.43
1:A:30:ILE:CG1	1:B:133[A]:VAL:HG13	2.49	0.43
1:D:149:LEU:O	1:D:153[A]:GLU:HG2	2.18	0.43
1:A:83:GLN:HE21	1:F:83:GLN:CB	2.32	0.43
1:H:80:THR:C	1:J:83[B]:GLN:HE22	2.22	0.43
1:I:69:TYR:OH	1:I:147:HIS:CE1	2.64	0.43
1:C:82:TYR:H	1:K:191:HIS:CE1	2.37	0.43
1:E:83[A]:GLN:CB	1:H:83[A]:GLN:NE2	2.80	0.43
1:K:133[A]:VAL:HG12	1:L:31:GLN:CB	2.47	0.43
1:A:72:TYR:CE1	1:A:139:MET:HG2	2.54	0.42
1:D:190:GLU:HA	1:D:190:GLU:OE1	2.19	0.42
1:E:147:HIS:CD2	1:E:181:ASN:OD1	2.69	0.42
1:H:83[A]:GLN:HB3	1:J:83[A]:GLN:HE21	1.83	0.42
1:H:190:GLU:HA	1:H:190:GLU:OE1	2.19	0.42
1:I:56:ASN:OD1	1:I:114[A]:VAL:HG23	2.20	0.42
1:B:80:THR:C	1:I:83[B]:GLN:HE22	2.22	0.42
1:B:83[A]:GLN:H	1:I:83[A]:GLN:HE21	1.66	0.42
1:H:73:HIS:CE1	1:H:85:HIS:CE1	3.07	0.42
1:B:82:TYR:H	1:I:191:HIS:CE1	2.38	0.42
1:L:107:GLN:HE22	1:L:113:ALA:H	1.65	0.42
1:G:66:HIS:HD2	1:G:67:ASP:OD1	2.02	0.42
1:H:82:TYR:H	1:J:83[B]:GLN:HE21	1.67	0.42
1:E:45:MET:HB2	4:E:2007:HOH:O	2.19	0.42
1:H:83[A]:GLN:H	1:J:83[A]:GLN:HE21	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154[B]:CYS:HB3	1:B:178:LEU:HD13	2.00	0.41
1:B:83[A]:GLN:CB	1:I:83[A]:GLN:HE21	2.32	0.41
1:H:75:LEU:HD13	1:H:133:VAL:HG22	2.02	0.41
1:A:82:TYR:H	1:D:191:HIS:HE1	1.66	0.41
1:G:31:GLN:NE2	1:H:77:ARG:HH12	2.17	0.41
1:G:83:GLN:HE21	1:K:83:GLN:CB	2.34	0.41
1:G:83:GLN:NE2	1:K:83:GLN:H	2.19	0.41
1:B:80:THR:CA	1:I:83[B]:GLN:HE22	2.34	0.41
1:L:62[A]:THR:CG2	4:L:2027:HOH:O	2.63	0.41
1:C:75:LEU:HD13	1:C:133:VAL:HG22	2.03	0.41
1:K:133[A]:VAL:HG13	1:L:30:ILE:HG13	2.03	0.41
1:K:31:GLN:CB	1:L:133[A]:VAL:HG12	2.47	0.41
1:G:62:THR:HG22	1:G:99:ILE:HG13	2.03	0.41
1:E:69:TYR:OH	1:E:147:HIS:CE1	2.62	0.41
1:A:70:LYS:HD2	1:A:70:LYS:HA	1.94	0.41
1:I:62:THR:HG23	1:I:95:GLN:OE1	2.21	0.41
1:G:72:TYR:OH	1:G:142:ARG:HD2	2.21	0.40
1:F:147:HIS:CD2	1:F:181:ASN:OD1	2.68	0.40
1:C:83:GLN:HE21	1:G:83:GLN:CB	2.33	0.40
1:G:31:GLN:HE21	1:H:77:ARG:HH12	1.67	0.40
1:K:66:HIS:HD2	1:K:67:ASP:OD1	2.04	0.40
1:L:69:TYR:OH	1:L:147:HIS:CE1	2.66	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	172/173 (99%)	170 (99%)	2 (1%)	0	100	100
1	B	174/173 (101%)	171 (98%)	3 (2%)	0	100	100
1	C	172/173 (99%)	171 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	172/173 (99%)	171 (99%)	1 (1%)	0	100	100
1	E	170/173 (98%)	167 (98%)	3 (2%)	0	100	100
1	F	172/173 (99%)	167 (97%)	5 (3%)	0	100	100
1	G	172/173 (99%)	169 (98%)	3 (2%)	0	100	100
1	H	172/173 (99%)	170 (99%)	2 (1%)	0	100	100
1	I	176/173 (102%)	175 (99%)	1 (1%)	0	100	100
1	J	172/173 (99%)	171 (99%)	1 (1%)	0	100	100
1	K	175/173 (101%)	171 (98%)	4 (2%)	0	100	100
1	L	175/173 (101%)	171 (98%)	4 (2%)	0	100	100
All	All	2074/2076 (100%)	2044 (99%)	30 (1%)	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	151/150 (101%)	149 (99%)	2 (1%)	69	59
1	B	154/150 (103%)	152 (99%)	2 (1%)	69	59
1	C	151/150 (101%)	149 (99%)	2 (1%)	69	59
1	D	152/150 (101%)	151 (99%)	1 (1%)	84	79
1	E	150/150 (100%)	148 (99%)	2 (1%)	69	59
1	F	151/150 (101%)	148 (98%)	3 (2%)	55	40
1	G	152/150 (101%)	150 (99%)	2 (1%)	69	59
1	H	151/150 (101%)	149 (99%)	2 (1%)	69	59
1	I	156/150 (104%)	152 (97%)	4 (3%)	46	29
1	J	150/150 (100%)	148 (99%)	2 (1%)	69	59
1	K	155/150 (103%)	153 (99%)	2 (1%)	69	59
1	L	154/150 (103%)	149 (97%)	5 (3%)	39	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1827/1800 (102%)	1798 (98%)	29 (2%)	62 51

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	PHE
1	A	49	LEU
1	B	39	PHE
1	B	49	LEU
1	C	39	PHE
1	C	101	THR
1	D	29	THR
1	E	38	GLN
1	E	39	PHE
1	F	29	THR
1	F	39	PHE
1	F	49	LEU
1	G	39	PHE
1	G	49	LEU
1	H	39	PHE
1	H	49	LEU
1	I	39	PHE
1	I	49	LEU
1	I	175[A]	SER
1	I	175[B]	SER
1	J	39	PHE
1	J	49	LEU
1	K	37	LYS
1	K	39	PHE
1	L	29	THR
1	L	39	PHE
1	L	45	MET
1	L	49	LEU
1	L	148	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	83	GLN
1	A	95	GLN

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Mol	Chain	Res	Type
1	A	147	HIS
1	A	170	ASN
1	A	191	HIS
1	B	31	GLN
1	B	66	HIS
1	B	147	HIS
1	B	170	ASN
1	B	191	HIS
1	C	53	GLN
1	C	66	HIS
1	C	83	GLN
1	C	147	HIS
1	C	170	ASN
1	C	191	HIS
1	D	53	GLN
1	D	66	HIS
1	D	83	GLN
1	D	147	HIS
1	D	170	ASN
1	D	191	HIS
1	E	38	GLN
1	E	53	GLN
1	E	66	HIS
1	E	147	HIS
1	E	191	HIS
1	F	66	HIS
1	F	147	HIS
1	F	170	ASN
1	F	191	HIS
1	G	31	GLN
1	G	66	HIS
1	G	83	GLN
1	G	147	HIS
1	G	170	ASN
1	G	191	HIS
1	H	31	GLN
1	H	66	HIS
1	H	107	GLN
1	H	147	HIS
1	H	170	ASN
1	H	191	HIS
1	I	66	HIS

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Mol	Chain	Res	Type
1	I	147	HIS
1	I	170	ASN
1	I	191	HIS
1	J	53	GLN
1	J	66	HIS
1	J	147	HIS
1	J	170	ASN
1	J	191	HIS
1	K	38	GLN
1	K	66	HIS
1	K	147	HIS
1	K	162	GLN
1	K	170	ASN
1	K	191	HIS
1	L	53	GLN
1	L	66	HIS
1	L	107	GLN
1	L	147	HIS
1	L	170	ASN
1	L	191	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	172/173 (99%)	-0.44	2 (1%) 79 79	19, 27, 45, 65	0
1	B	172/173 (99%)	-0.41	2 (1%) 79 79	18, 25, 41, 68	0
1	C	172/173 (99%)	-0.31	2 (1%) 79 79	18, 26, 48, 70	0
1	D	171/173 (98%)	-0.54	0 100 100	17, 25, 39, 55	0
1	E	171/173 (98%)	-0.32	2 (1%) 79 79	20, 27, 45, 65	0
1	F	172/173 (99%)	-0.31	1 (0%) 89 89	23, 30, 50, 81	0
1	G	172/173 (99%)	-0.27	6 (3%) 44 42	19, 26, 45, 70	0
1	H	172/173 (99%)	-0.38	1 (0%) 89 89	19, 27, 44, 60	0
1	I	172/173 (99%)	-0.61	0 100 100	18, 24, 37, 67	0
1	J	173/173 (100%)	-0.50	2 (1%) 79 79	19, 24, 42, 60	0
1	K	171/173 (98%)	-0.25	1 (0%) 89 89	18, 23, 39, 78	0
1	L	172/173 (99%)	-0.23	2 (1%) 79 79	18, 25, 42, 67	0
All	All	2062/2076 (99%)	-0.38	21 (1%) 82 82	17, 26, 45, 81	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	40	PRO	6.7
1	K	40	PRO	6.2
1	J	200	ALA	4.6
1	E	40	PRO	3.9
1	G	39	PHE	3.8
1	B	40	PRO	3.4
1	L	38	GLN	3.2
1	G	38	GLN	3.1
1	A	40	PRO	3.0
1	J	40	PRO	3.0
1	A	39	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	39	PHE	2.8
1	L	40	PRO	2.6
1	F	28	ARG	2.5
1	G	28	ARG	2.4
1	G	164	TYR	2.4
1	C	40	PRO	2.2
1	H	164	TYR	2.2
1	C	164	TYR	2.1
1	G	45	MET	2.1
1	B	38	GLN	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	J	1300	1/1	0.97	0.09	28,28,28,28	0
3	NA	K	1300	1/1	0.97	0.11	23,23,23,23	0
3	NA	L	1300	1/1	0.98	0.04	27,27,27,27	0
2	FE	H	1200	1/1	0.99	0.15	15,15,15,15	1
2	FE	B	1200	1/1	0.99	0.13	17,17,17,17	1
3	NA	C	1300	1/1	0.99	0.10	27,27,27,27	0
2	FE	C	1200	1/1	0.99	0.12	18,18,18,18	1
2	FE	I	1200	1/1	1.00	0.13	14,14,14,14	1
2	FE	A	1200	1/1	1.00	0.14	15,15,15,15	1
2	FE	G	1200	1/1	1.00	0.11	16,16,16,16	1
2	FE	E	1200	1/1	1.00	0.11	18,18,18,18	1
2	FE	J	1201	1/1	1.00	0.15	14,14,14,14	1
2	FE	F	1200	1/1	1.00	0.12	17,17,17,17	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	K	1200	1/1	1.00	0.13	14,14,14,14	1
2	FE	L	1200	1/1	1.00	0.16	13,13,13,13	1
2	FE	D	1200	1/1	1.00	0.17	13,13,13,13	1

6.5 Other polymers (i)

There are no such residues in this entry.