Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 06:01 AM EDT

PDB ID	:	7T0K
Title	:	Crystal structure of S25-2 Fab Unliganded 4
Authors	:	Legg, M.S.G.; Blackler, R.J.; Evans, S.V.
Deposited on	:	2021-11-29
Resolution	:	2.00 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:

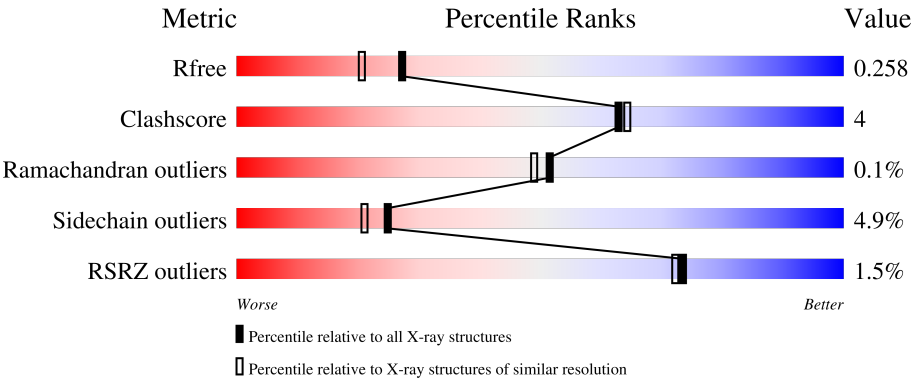
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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.



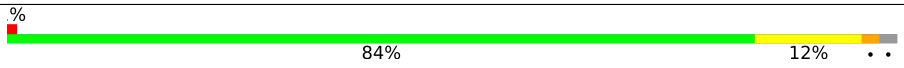
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	219	3% 88% 11% ·
1	C	219	4% 89% 10% ·
1	E	219	87% 12% ·
1	L	219	% 88% 10% ·
2	B	223	% 88% 11% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	223	
2	F	223	
2	H	223	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	B	305	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13900 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 S25-2 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	218	Total	C	N	O	S	0	0	0
			1694	1053	289	345	7			
1	A	219	Total	C	N	O	S	0	0	0
			1700	1056	290	346	8			
1	C	218	Total	C	N	O	S	0	0	0
			1694	1053	289	345	7			
1	E	219	Total	C	N	O	S	0	0	0
			1701	1056	290	347	8			

- Molecule 2 is a protein called S25-2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1654	1047	276	324	7			
2	B	223	Total	C	N	O	S	0	0	0
			1693	1074	282	330	7			
2	D	222	Total	C	N	O	S	0	0	0
			1692	1073	282	330	7			
2	F	215	Total	C	N	O	S	0	0	0
			1649	1049	274	319	7			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	5	Total	I	0	0
			5	5		
3	H	5	Total	I	0	0
			5	5		
3	A	1	Total	I	0	0
			1	1		
3	B	5	Total	I	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total I 2 2	0	0
3	D	7	Total I 7 7	0	0
3	E	4	Total I 4 4	0	0
3	F	5	Total I 5 5	0	0

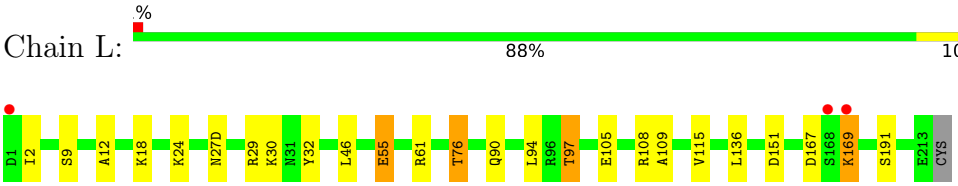
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	40	Total O 40 40	0	0
4	H	71	Total O 71 71	0	0
4	A	38	Total O 38 38	0	0
4	B	62	Total O 62 62	0	0
4	C	23	Total O 23 23	0	0
4	D	57	Total O 57 57	0	0
4	E	52	Total O 52 52	0	0
4	F	46	Total O 46 46	0	0

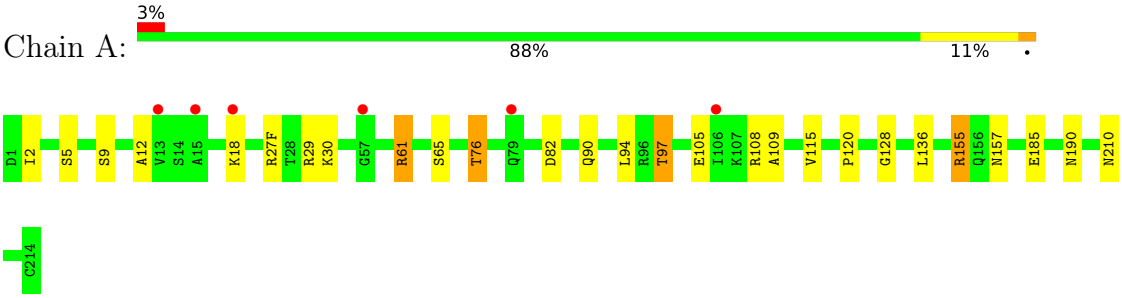
3 Residue-property plots (i)

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.

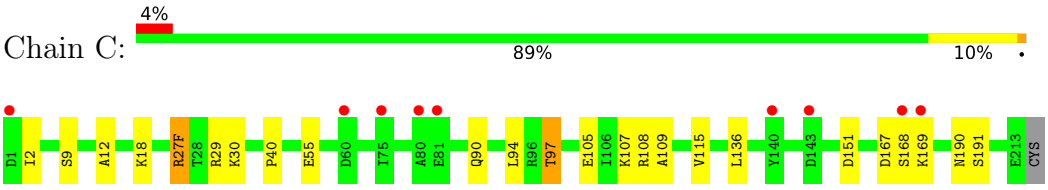
• Molecule 1: S25-2 Fab light chain



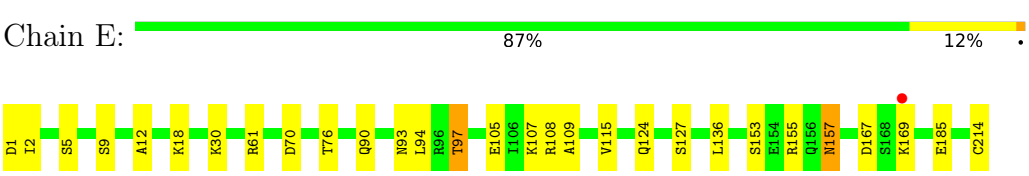
• Molecule 1: S25-2 Fab light chain



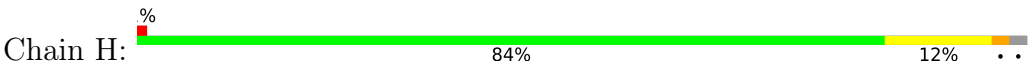
• Molecule 1: S25-2 Fab light chain

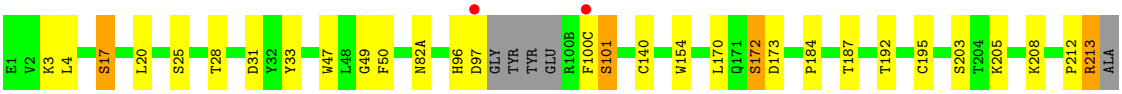


• Molecule 1: S25-2 Fab light chain



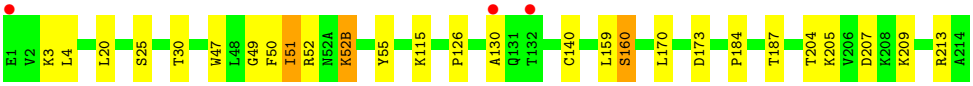
• Molecule 2: S25-2 Fab heavy chain





• Molecule 2: S25-2 Fab heavy chain

Chain B:

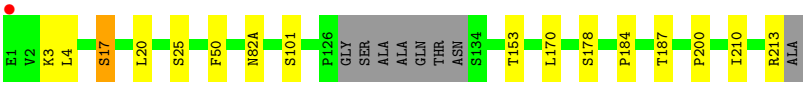


• Molecule 2: S25-2 Fab heavy chain

Chain D:

• Molecule 2: S25-2 Fab heavy chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.56Å 135.50Å 73.98Å 90.00° 94.26° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 38.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.00) 99.6 (38.17-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.222 , 0.255 0.226 , 0.258	Depositor DCC
R_{free} test set	6137 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 25.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13900	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 5.59% 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

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

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	0.50	0/1735	0.72	0/2351
1	C	0.47	0/1729	0.70	0/2343
1	E	0.54	0/1736	0.71	0/2351
1	L	0.50	0/1729	0.72	0/2343
2	B	0.57	0/1739	0.73	0/2376
2	D	0.51	0/1738	0.73	0/2374
2	F	0.56	0/1694	0.75	1/2313 (0.0%)
2	H	0.54	0/1697	0.74	0/2318
All	All	0.52	0/13797	0.72	1/18769 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	210	ILE	CA-CB-CG1	-5.65	100.27	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	ALA	Peptide
2	D	130	ALA	Peptide

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	1700	0	1649	16	0
1	C	1694	0	1644	11	1
1	E	1701	0	1649	15	0
1	L	1694	0	1644	13	0
2	B	1693	0	1638	23	0
2	D	1692	0	1639	13	0
2	F	1649	0	1604	6	0
2	H	1654	0	1609	20	0
3	A	1	0	0	0	0
3	B	5	0	0	4	0
3	C	2	0	0	1	0
3	D	7	0	0	2	0
3	E	4	0	0	1	0
3	F	5	0	0	2	0
3	H	5	0	0	1	0
3	L	5	0	0	1	0
4	A	38	0	0	1	0
4	B	62	0	0	2	0
4	C	23	0	0	0	0
4	D	57	0	0	3	0
4	E	52	0	0	1	0
4	F	46	0	0	0	0
4	H	71	0	0	3	0
4	L	40	0	0	4	0
All	All	13900	0	13076	115	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 4.

All (115) 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)
3:B:302:IOD:I	4:B:449:HOH:O	2.58	0.91
2:D:130:ALA:HB1	2:D:131:GLN:HB2	1.56	0.87
1:A:155:ARG:NH2	1:A:185:GLU:OE2	2.23	0.71
1:A:128:GLY:O	4:A:401:HOH:O	2.09	0.71
3:D:307:IOD:I	4:D:457:HOH:O	2.80	0.70
2:B:184:PRO:O	2:B:187:THR:HG22	1.95	0.66
2:D:129:ALA:HB3	4:D:443:HOH:O	1.96	0.65
2:D:184:PRO:O	2:D:187:THR:HG22	1.96	0.65
2:F:184:PRO:O	2:F:187:THR:HG22	1.96	0.65
1:E:5:SER:O	3:E:304:IOD:I	2.85	0.65
2:H:184:PRO:O	2:H:187:THR:HG22	1.96	0.65
1:A:90:GLN:HE21	1:A:97:THR:CG2	2.10	0.64
1:C:90:GLN:HE21	1:C:97:THR:CG2	2.09	0.64
1:E:90:GLN:HE21	1:E:97:THR:CG2	2.11	0.63
1:E:61:ARG:HB2	1:E:76:THR:HG22	1.81	0.63
1:L:90:GLN:HE21	1:L:97:THR:CG2	2.12	0.63
1:A:190:ASN:ND2	1:A:210:ASN:OD1	2.31	0.62
1:A:61:ARG:HB2	1:A:76:THR:HG22	1.81	0.61
2:H:172:SER:OG	2:H:173:ASP:N	2.32	0.60
3:L:302:IOD:I	4:L:422:HOH:O	2.85	0.60
1:C:90:GLN:HE21	1:C:97:THR:HG22	1.67	0.59
1:E:124:GLN:O	1:E:127:SER:OG	2.10	0.59
1:L:61:ARG:HB2	1:L:76:THR:HG22	1.83	0.59
1:E:90:GLN:HE21	1:E:97:THR:HG22	1.67	0.59
2:H:96:HIS:CE1	4:H:401:HOH:O	2.54	0.59
4:L:420:HOH:O	2:H:101:SER:HB3	2.02	0.59
2:D:30:THR:HG23	2:D:52(B):LYS:HB3	1.84	0.58
1:E:185:GLU:HG2	4:E:439:HOH:O	2.03	0.57
1:L:90:GLN:HE21	1:L:97:THR:HG22	1.68	0.57
1:A:90:GLN:HE21	1:A:97:THR:HG22	1.70	0.56
2:H:33:TYR:HB2	2:H:96:HIS:H	1.71	0.56
1:E:108:ARG:NH1	1:E:109:ALA:O	2.39	0.55
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.40	0.55
1:C:108:ARG:NH1	1:C:109:ALA:O	2.38	0.55
1:A:108:ARG:NH1	1:A:109:ALA:O	2.39	0.55
1:L:108:ARG:NH1	1:L:109:ALA:O	2.39	0.55
4:L:439:HOH:O	2:B:115:LYS:HD3	2.06	0.54
2:H:96:HIS:CD2	2:H:97:ASP:H	2.26	0.54
1:A:12:ALA:HA	1:A:105:GLU:O	2.09	0.53
2:B:51:ILE:HD13	2:B:52:ARG:N	2.23	0.53
1:C:40:PRO:HD3	3:C:302:IOD:I	2.80	0.52
1:L:12:ALA:HA	1:L:105:GLU:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LEU:O	3:B:305:IOD:I	2.97	0.52
2:B:213:ARG:HG2	4:B:407:HOH:O	2.09	0.51
1:C:12:ALA:HA	1:C:105:GLU:O	2.11	0.50
2:H:192:THR:HG22	4:H:410:HOH:O	2.12	0.50
1:E:12:ALA:HA	1:E:105:GLU:O	2.11	0.50
2:H:17:SER:OG	2:H:82(A):ASN:ND2	2.42	0.49
1:L:24:LYS:HG3	4:L:418:HOH:O	2.12	0.49
2:B:126:PRO:O	2:B:213:ARG:HD3	2.13	0.48
1:L:27(D):ASN:HB2	1:L:32:TYR:CE2	2.49	0.48
2:H:96:HIS:ND1	4:H:401:HOH:O	2.34	0.48
1:A:61:ARG:HH22	1:A:82:ASP:CG	2.17	0.48
2:D:200:PRO:HA	3:D:305:IOD:I	2.85	0.47
2:B:51:ILE:C	2:B:51:ILE:CD1	2.82	0.47
2:H:212:PRO:O	2:H:213:ARG:CB	2.62	0.47
2:B:52(B):LYS:O	2:B:52(B):LYS:HG3	2.15	0.46
2:B:160:SER:OG	3:B:305:IOD:I	2.93	0.46
1:A:2:ILE:O	1:A:97:THR:HG21	2.17	0.45
1:A:155:ARG:NH1	1:A:157:ASN:O	2.50	0.45
1:C:2:ILE:O	1:C:97:THR:HG21	2.16	0.45
1:E:2:ILE:O	1:E:97:THR:HG21	2.17	0.45
2:D:83:ARG:HB3	4:D:446:HOH:O	2.17	0.44
2:F:17:SER:OG	2:F:82(A):ASN:OD1	2.36	0.44
2:D:17:SER:OG	2:D:82(A):ASN:ND2	2.43	0.44
2:H:154:TRP:CZ3	2:H:195:CYS:HB3	2.53	0.44
2:B:51:ILE:CD1	2:B:52:ARG:N	2.81	0.44
2:F:3:LYS:O	2:F:4:LEU:HD23	2.18	0.44
1:L:115:VAL:HG13	1:L:136:LEU:HD13	2.00	0.44
1:L:90:GLN:HE21	1:L:97:THR:HG23	1.83	0.44
2:H:28:THR:OG1	2:H:31:ASP:OD2	2.35	0.44
2:H:205:LYS:HB2	2:B:207:ASP:HB2	2.00	0.44
1:L:2:ILE:O	1:L:97:THR:HG21	2.18	0.43
1:C:90:GLN:HE21	1:C:97:THR:HG23	1.80	0.43
1:C:115:VAL:HG13	1:C:136:LEU:HD13	2.00	0.43
2:D:34:MET:HB3	2:D:78:LEU:HD22	1.99	0.43
1:E:136:LEU:N	1:E:136:LEU:HD22	2.34	0.43
1:A:90:GLN:HE21	1:A:97:THR:HG23	1.80	0.43
1:E:155:ARG:NE	1:E:157:ASN:OD1	2.48	0.43
1:C:136:LEU:HD22	1:C:136:LEU:N	2.34	0.43
2:B:3:LYS:HG2	2:B:25:SER:OG	2.19	0.43
2:B:51:ILE:HD11	2:B:55:TYR:HB3	2.01	0.43
2:H:3:LYS:O	2:H:4:LEU:HD23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:LYS:HG2	2:F:25:SER:OG	2.18	0.43
2:H:3:LYS:HG2	2:H:25:SER:OG	2.19	0.42
2:H:154:TRP:CH2	2:H:195:CYS:HB3	2.55	0.42
2:B:3:LYS:O	2:B:4:LEU:HD23	2.19	0.42
2:D:3:LYS:O	2:D:4:LEU:HD23	2.19	0.42
1:A:136:LEU:N	1:A:136:LEU:HD22	2.35	0.42
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.54	0.42
2:B:205:LYS:HE3	3:B:303:IOD:I	2.89	0.42
1:E:115:VAL:HG13	1:E:136:LEU:HD13	2.02	0.42
2:D:3:LYS:HG2	2:D:25:SER:OG	2.20	0.42
2:B:51:ILE:HD12	2:B:52:ARG:O	2.20	0.42
1:L:151:ASP:HA	1:L:191:SER:OG	2.20	0.41
2:B:126:PRO:O	2:B:213:ARG:CG	2.68	0.41
2:F:200:PRO:HA	3:F:304:IOD:I	2.90	0.41
2:D:47:TRP:CH2	2:D:49:GLY:HA2	2.54	0.41
2:H:208:LYS:NZ	2:B:204:THR:OG1	2.39	0.41
1:A:115:VAL:HG13	1:A:136:LEU:HD13	2.01	0.41
2:F:153:THR:HA	3:F:302:IOD:I	2.90	0.41
2:H:100(C):PHE:O	3:H:303:IOD:I	3.08	0.41
1:A:120:PRO:O	2:B:213:ARG:NH2	2.46	0.41
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.56	0.41
1:C:151:ASP:HA	1:C:191:SER:OG	2.21	0.41
2:B:126:PRO:O	2:B:213:ARG:CD	2.69	0.41
2:B:173:ASP:OD2	1:E:153:SER:HA	2.21	0.41
1:E:90:GLN:HE21	1:E:97:THR:HG23	1.83	0.41
2:H:203:SER:HB3	2:B:209:LYS:HB3	2.03	0.41
2:D:17:SER:HG	2:D:82(A):ASN:HD22	1.68	0.41
1:L:46:LEU:HD23	1:L:55:GLU:HG3	2.03	0.40
1:L:167:ASP:OD1	1:L:169:LYS:N	2.54	0.40
1:C:167:ASP:OD1	1:C:169:LYS:N	2.55	0.40
1:E:167:ASP:OD1	1:E:169:LYS:N	2.54	0.40
2:D:28:THR:OG1	2:D:31:ASP:OD2	2.36	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:27(F):ARG:NH1	1:C:190:ASN:OD1[2_445]	2.02	0.18

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	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
1	C	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	E	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
1	L	216/219 (99%)	211 (98%)	5 (2%)	0	100	100
2	B	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
2	D	220/223 (99%)	214 (97%)	5 (2%)	1 (0%)	29	23
2	F	211/223 (95%)	208 (99%)	3 (1%)	0	100	100
2	H	214/223 (96%)	208 (97%)	6 (3%)	0	100	100
All	All	1732/1768 (98%)	1688 (98%)	43 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	128	SER

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	195/195 (100%)	183 (94%)	12 (6%)	18	13
1	C	194/195 (100%)	184 (95%)	10 (5%)	23	19
1	E	195/195 (100%)	184 (94%)	11 (6%)	21	17
1	L	194/195 (100%)	185 (95%)	9 (5%)	27	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	187/190 (98%)	179 (96%)	8 (4%)	29	26
2	D	188/190 (99%)	179 (95%)	9 (5%)	25	22
2	F	185/190 (97%)	178 (96%)	7 (4%)	33	31
2	H	186/190 (98%)	178 (96%)	8 (4%)	29	26
All	All	1524/1540 (99%)	1450 (95%)	74 (5%)	25	21

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	9	SER
1	L	18	LYS
1	L	29	ARG
1	L	30	LYS
1	L	55	GLU
1	L	76	THR
1	L	94	LEU
1	L	97	THR
1	L	169	LYS
2	H	17	SER
2	H	20	LEU
2	H	50	PHE
2	H	101	SER
2	H	140	CYS
2	H	170	LEU
2	H	172	SER
2	H	213	ARG
1	A	5	SER
1	A	9	SER
1	A	18	LYS
1	A	27(F)	ARG
1	A	29	ARG
1	A	30	LYS
1	A	61	ARG
1	A	65	SER
1	A	76	THR
1	A	94	LEU
1	A	97	THR
1	A	155	ARG
2	B	20	LEU
2	B	30	THR
2	B	50	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	51	ILE
2	B	52(B)	LYS
2	B	140	CYS
2	B	160	SER
2	B	170	LEU
1	C	9	SER
1	C	18	LYS
1	C	27(F)	ARG
1	C	29	ARG
1	C	30	LYS
1	C	55	GLU
1	C	94	LEU
1	C	97	THR
1	C	107	LYS
1	C	168	SER
2	D	17	SER
2	D	20	LEU
2	D	30	THR
2	D	50	PHE
2	D	52(B)	LYS
2	D	101	SER
2	D	138	LEU
2	D	170	LEU
2	D	213	ARG
1	E	1	ASP
1	E	9	SER
1	E	18	LYS
1	E	30	LYS
1	E	70	ASP
1	E	93	ASN
1	E	94	LEU
1	E	97	THR
1	E	107	LYS
1	E	157	ASN
1	E	214	CYS
2	F	17	SER
2	F	20	LEU
2	F	50	PHE
2	F	101	SER
2	F	170	LEU
2	F	178	SER
2	F	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	42	GLN
1	L	156	GLN
1	L	190	ASN
1	L	212	ASN
2	H	96	HIS
1	A	42	GLN
1	C	42	GLN
1	C	156	GLN
1	C	190	ASN
1	C	212	ASN
1	E	42	GLN
1	E	93	ASN
1	E	190	ASN
1	E	212	ASN
2	F	164	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 34 ligands modelled in this entry, 34 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 (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	219/219 (100%)	-0.04	6 (2%)	54	53	29, 48, 75, 89	0
1	C	218/219 (99%)	0.18	9 (4%)	37	36	33, 53, 83, 94	0
1	E	219/219 (100%)	-0.23	1 (0%)	91	90	25, 39, 63, 85	0
1	L	218/219 (99%)	-0.19	3 (1%)	75	74	27, 44, 65, 90	0
2	B	223/223 (100%)	-0.31	3 (1%)	77	76	25, 37, 56, 80	0
2	D	222/223 (99%)	-0.29	1 (0%)	91	90	27, 40, 61, 83	0
2	F	215/223 (96%)	-0.16	1 (0%)	91	90	25, 40, 80, 100	0
2	H	218/223 (97%)	-0.26	2 (0%)	84	83	25, 37, 60, 86	0
All	All	1752/1768 (99%)	-0.16	26 (1%)	73	72	25, 42, 72, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	168	SER	5.1
1	E	169	LYS	4.1
1	C	1	ASP	3.9
1	C	169	LYS	3.7
1	L	169	LYS	3.6
2	H	97	ASP	3.1
1	A	79	GLN	3.1
1	C	140	TYR	2.9
1	C	60	ASP	2.5
2	H	100(C)	PHE	2.5
2	F	1	GLU	2.4
1	L	168	SER	2.3
2	D	132	THR	2.3
2	B	1	GLU	2.3
1	C	143	ASP	2.3
1	A	18	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	2.3
1	A	15	ALA	2.2
1	A	106	ILE	2.2
1	C	81	GLU	2.1
2	B	132	THR	2.1
1	C	80	ALA	2.1
1	C	75	ILE	2.1
2	B	130	ALA	2.0
1	A	57	GLY	2.0
1	L	1	ASP	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)

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	IOD	H	302	1/1	0.86	0.10	54,54,54,54	1
3	IOD	F	302	1/1	0.89	0.07	68,68,68,68	1
3	IOD	D	306	1/1	0.95	0.04	59,59,59,59	1
3	IOD	D	307	1/1	0.95	0.05	58,58,58,58	1
3	IOD	E	303	1/1	0.95	0.08	45,45,45,45	1
3	IOD	L	305	1/1	0.95	0.05	80,80,80,80	1
3	IOD	L	304	1/1	0.96	0.03	71,71,71,71	1
3	IOD	E	304	1/1	0.97	0.05	57,57,57,57	1
3	IOD	B	303	1/1	0.97	0.07	46,46,46,46	1
3	IOD	F	304	1/1	0.97	0.04	73,73,73,73	1
3	IOD	L	302	1/1	0.98	0.10	40,40,40,40	1
3	IOD	H	303	1/1	0.98	0.07	52,52,52,52	1
3	IOD	H	305	1/1	0.98	0.04	53,53,53,53	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IOD	L	303	1/1	0.98	0.08	46,46,46,46	1
3	IOD	B	304	1/1	0.98	0.06	54,54,54,54	1
3	IOD	C	302	1/1	0.98	0.03	70,70,70,70	1
3	IOD	D	302	1/1	0.99	0.10	36,36,36,36	1
3	IOD	D	303	1/1	0.99	0.09	43,43,43,43	1
3	IOD	D	304	1/1	0.99	0.05	50,50,50,50	1
3	IOD	D	305	1/1	0.99	0.03	59,59,59,59	1
3	IOD	B	301	1/1	0.99	0.10	38,38,38,38	0
3	IOD	H	301	1/1	0.99	0.10	32,32,32,32	0
3	IOD	H	304	1/1	0.99	0.09	43,43,43,43	1
3	IOD	B	305	1/1	0.99	0.06	43,43,43,43	1
3	IOD	L	301	1/1	0.99	0.11	41,41,41,41	0
3	IOD	F	303	1/1	0.99	0.06	37,37,37,37	1
3	IOD	D	301	1/1	0.99	0.10	34,34,34,34	1
3	IOD	F	305	1/1	0.99	0.06	47,47,47,47	1
3	IOD	B	302	1/1	1.00	0.09	40,40,40,40	1
3	IOD	F	301	1/1	1.00	0.10	28,28,28,28	1
3	IOD	A	301	1/1	1.00	0.10	36,36,36,36	0
3	IOD	E	301	1/1	1.00	0.11	27,27,27,27	0
3	IOD	E	302	1/1	1.00	0.10	29,29,29,29	0
3	IOD	C	301	1/1	1.00	0.11	35,35,35,35	1

6.5 Other polymers (i)

There are no such residues in this entry.