



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2022 – 02:25 PM EDT

PDB ID : 7T0I
Title : Crystal structure of S25-39 Fab Unliganded 3
Authors : Legg, M.S.G.; Blackler, R.J.; Evans, S.V.
Deposited on : 2021-11-29
Resolution : 2.10 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
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)	:	2.27

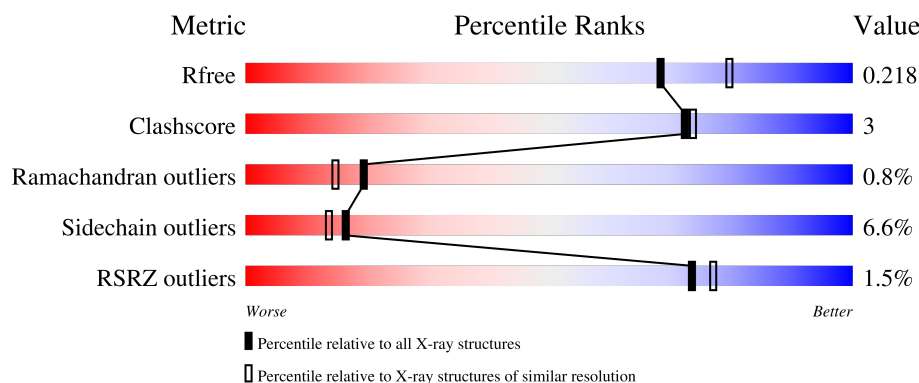
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. 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	B	222	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>
1	D	222	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	F	222	<div> <div></div> <div> <div></div> <div>86%</div> <div>8%</div> <div>• 5%</div> </div> </div>
1	H	222	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• •</div> </div> </div>
2	A	219	<div> <div></div> <div> <div></div> <div>86%</div> <div>13%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	C	219	<div><div></div><div>84%</div><div>15%</div><div></div></div>
2	E	219	<div><div>2%</div><div></div><div>78%</div><div>17%</div><div></div><div></div></div>
2	L	219	<div><div>3%</div><div></div><div>85%</div><div>13%</div><div></div><div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13498 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 S25-39 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	213	Total	C	N	O	S	0	0	0
			1616	1027	269	313	7			
1	B	214	Total	C	N	O	S	0	0	0
			1631	1037	271	316	7			
1	D	215	Total	C	N	O	S	0	0	0
			1632	1039	271	315	7			
1	F	210	Total	C	N	O	S	0	0	0
			1593	1012	266	308	7			

- Molecule 2 is a protein called S25-39 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	219	Total	C	N	O	S	0	0	0
			1698	1055	291	344	8			
2	A	219	Total	C	N	O	S	0	0	0
			1701	1056	291	346	8			
2	C	219	Total	C	N	O	S	0	0	0
			1697	1053	290	346	8			
2	E	219	Total	C	N	O	S	0	0	0
			1701	1056	291	346	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	32	Total	O	0	0
			32	32		
3	L	14	Total	O	0	0
			14	14		
3	B	48	Total	O	0	0
			48	48		
3	A	17	Total	O	0	0
			17	17		

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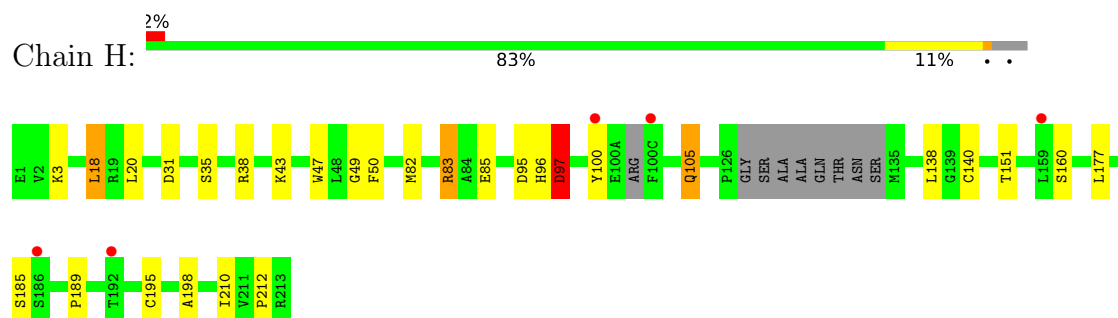
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	32	Total 32	O 32	0	0
3	C	43	Total 43	O 43	0	0
3	F	35	Total 35	O 35	0	0
3	E	8	Total 8	O 8	0	0

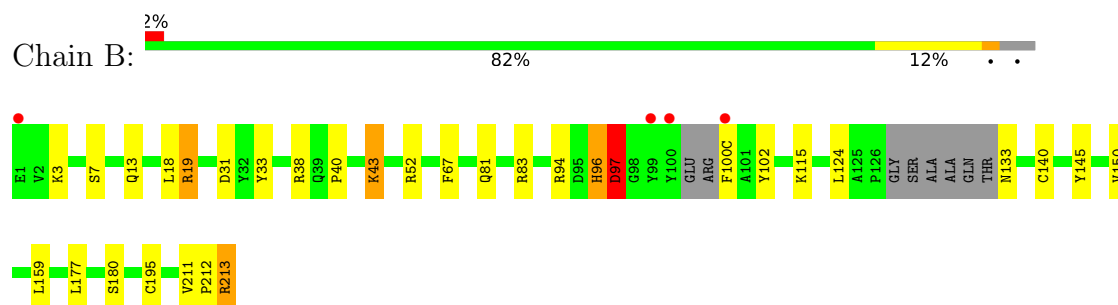
3 Residue-property plots

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.

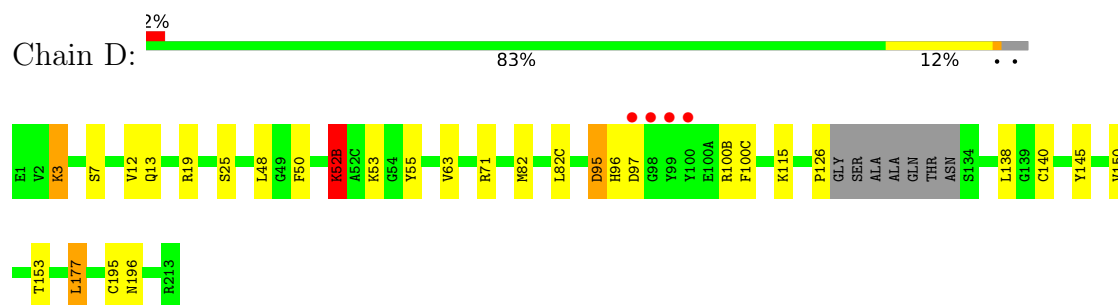
- Molecule 1: S25-39 Fab heavy chain



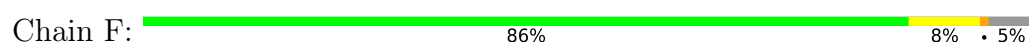
- Molecule 1: S25-39 Fab heavy chain

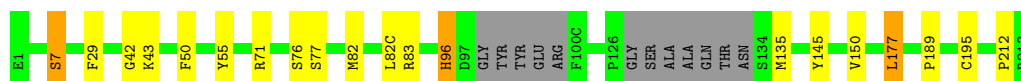


- Molecule 1: S25-39 Fab heavy chain

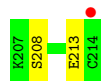
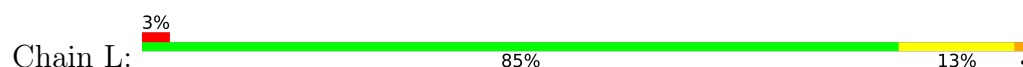


- Molecule 1: S25-39 Fab heavy chain

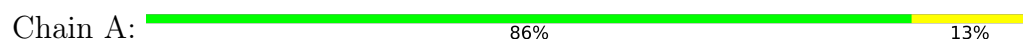




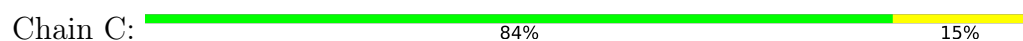
- Molecule 2: S25-39 Fab light chain



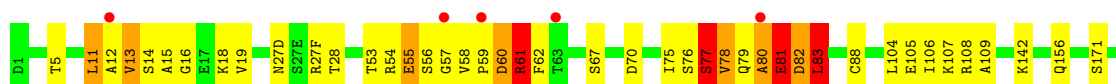
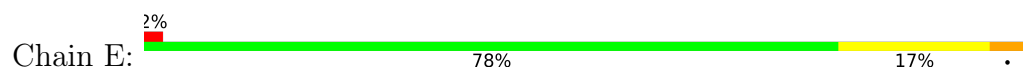
- Molecule 2: S25-39 Fab light chain



- Molecule 2: S25-39 Fab light chain



- Molecule 2: S25-39 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.56Å 111.75Å 154.70Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	29.89 – 2.10 29.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.89-2.10) 98.9 (29.89-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.180 , 0.225 0.174 , 0.218	Depositor DCC
R_{free} test set	4905 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.216 for -h,-k,l	Xtriage
Reported twinning fraction	0.760 for H, K, L 0.240 for h,-k,-l	Depositor
Outliers	0 of 99437 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13498	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	B	1.02	0/1674	1.05	6/2283 (0.3%)
1	D	1.00	0/1676	1.07	5/2289 (0.2%)
1	F	0.94	0/1634	0.99	1/2229 (0.0%)
1	H	1.05	1/1658 (0.1%)	1.04	5/2262 (0.2%)
2	A	0.88	0/1736	0.96	2/2351 (0.1%)
2	C	1.03	1/1732 (0.1%)	1.04	6/2347 (0.3%)
2	E	0.88	0/1736	1.00	4/2351 (0.2%)
2	L	0.78	0/1733	0.94	2/2347 (0.1%)
All	All	0.95	2/13579 (0.0%)	1.01	31/18459 (0.2%)

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
1	B	0	1
1	D	0	1
1	F	0	1
2	E	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	97	ASP	CB-CG	-5.44	1.40	1.51
2	C	86	TYR	CE1-CZ	-5.25	1.31	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52(B)	LYS	O-C-N	-12.31	103.00	122.70
1	B	19	ARG	NE-CZ-NH1	8.54	124.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	C	96	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	F	177	LEU	CA-CB-CG	7.94	133.56	115.30
2	C	181	LEU	CA-CB-CG	7.27	132.01	115.30
2	L	181	LEU	CA-CB-CG	6.77	130.88	115.30
2	E	88	CYS	CA-CB-SG	6.55	125.79	114.00
2	A	181	LEU	CA-CB-CG	6.52	130.29	115.30
1	B	38	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	H	177	LEU	CA-CB-CG	6.30	129.80	115.30
2	C	155	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	19	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	D	82	MET	CG-SD-CE	-6.00	90.59	100.20
1	H	38	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	H	31	ASP	CB-CG-OD1	5.87	123.58	118.30
1	H	18	LEU	CB-CG-CD1	5.79	120.84	111.00
2	E	11	LEU	CA-CB-CG	5.76	128.54	115.30
2	E	181	LEU	CA-CB-CG	5.74	128.50	115.30
1	H	95	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	C	188	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	D	177	LEU	CA-CB-CG	5.57	128.10	115.30
2	A	96	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	C	21	MET	CG-SD-CE	5.29	108.67	100.20
2	L	11	LEU	CA-CB-CG	5.28	127.43	115.30
1	B	31	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	95	ASP	CB-CG-OD2	5.16	122.95	118.30
2	E	83	LEU	CB-CG-CD1	5.12	119.70	111.00
2	C	155	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	31	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	124	LEU	CB-CG-CD1	5.01	119.52	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	96	HIS	Peptide
1	D	52(B)	LYS	Mainchain
2	E	80	ALA	Peptide
1	F	96	HIS	Peptide

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	B	1631	0	1588	12	0
1	D	1632	0	1587	9	0
1	F	1593	0	1559	8	0
1	H	1616	0	1572	10	0
2	A	1701	0	1648	10	0
2	C	1697	0	1637	11	0
2	E	1701	0	1648	22	0
2	L	1698	0	1646	9	1
3	A	17	0	0	0	0
3	B	48	0	0	2	0
3	C	43	0	0	0	0
3	D	32	0	0	0	0
3	E	8	0	0	0	0
3	F	35	0	0	1	0
3	H	32	0	0	1	0
3	L	14	0	0	0	0
All	All	13498	0	12885	90	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 3.

All (90) 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)
2:E:108:ARG:NH1	2:E:109:ALA:O	2.02	0.92
2:C:123:GLU:O	2:C:126:THR:HG22	1.89	0.72
2:C:189:HIS:O	2:C:211:ARG:NH1	2.23	0.71
2:E:77:SER:O	2:E:78:VAL:HG23	1.90	0.71
2:A:18:LYS:HG3	2:A:76:SER:HA	1.80	0.63
2:E:78:VAL:HG22	2:E:82:ASP:OD2	1.98	0.63
2:E:108:ARG:HD2	2:E:171:SER:HB2	1.82	0.62
1:H:105:GLN:HE21	1:H:105:GLN:H	1.48	0.61
2:C:183:LYS:HE2	2:C:187:GLU:OE1	2.02	0.60
2:C:186:TYR:CE2	2:C:211:ARG:HD2	2.37	0.59
1:B:212:PRO:O	1:B:213:ARG:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:GLU:O	2:E:83:LEU:N	2.37	0.58
2:L:150:ILE:HD12	2:L:155:ARG:HG3	1.86	0.57
1:H:83:ARG:NH1	1:H:85:GLU:OE2	2.38	0.57
2:L:11:LEU:HD23	2:L:104:LEU:HD12	1.87	0.56
2:L:108:ARG:NH1	2:L:109:ALA:O	2.40	0.54
1:B:19:ARG:HD3	3:B:334:HOH:O	2.06	0.54
1:D:3:LYS:HG3	1:D:25:SER:OG	2.08	0.53
2:E:19:VAL:HG13	2:E:75:ILE:HG23	1.91	0.53
2:L:192:TYR:O	2:L:208:SER:HA	2.09	0.53
2:A:13:VAL:HG13	2:A:17:GLU:HB2	1.92	0.52
2:C:61:ARG:NH1	2:C:82:ASP:OD1	2.43	0.51
2:E:82:ASP:O	2:E:104:LEU:HD23	2.10	0.51
1:D:48:LEU:HD22	1:D:63:VAL:HG11	1.92	0.51
1:B:83:ARG:NH1	3:B:302:HOH:O	2.29	0.50
2:L:13:VAL:HG13	2:L:17:GLU:HB2	1.94	0.50
1:H:96:HIS:O	1:H:97:ASP:HB2	2.12	0.50
2:E:53:THR:HG22	2:E:54:ARG:O	2.12	0.50
2:E:59:PRO:O	2:E:60:ASP:HB3	2.12	0.50
1:F:55:TYR:CD1	1:F:71:ARG:HD3	2.47	0.49
1:F:29:PHE:CD2	1:F:76:SER:HA	2.48	0.49
1:D:145:TYR:CE2	1:D:150:VAL:HG13	2.47	0.49
1:F:189:PRO:HB3	1:F:212:PRO:HG3	1.95	0.49
1:H:105:GLN:HG3	3:H:331:HOH:O	2.12	0.49
1:D:95:ASP:OD1	1:D:96:HIS:N	2.47	0.48
2:A:186:TYR:CE2	2:A:211:ARG:HD2	2.48	0.48
2:C:54:ARG:HD3	2:C:58:VAL:O	2.14	0.47
1:F:145:TYR:CE2	1:F:150:VAL:HG13	2.48	0.47
2:E:27(D):ASN:OD1	2:E:28:THR:N	2.45	0.47
2:E:56:SER:HA	2:E:57:GLY:C	2.35	0.47
2:L:83:LEU:HD21	2:L:166:GLN:HB3	1.96	0.47
1:F:42:GLY:O	1:F:43:LYS:HG2	2.14	0.47
2:E:62:PHE:CE1	2:E:75:ILE:HD13	2.50	0.47
2:L:90:GLN:O	2:L:96:ARG:HA	2.14	0.47
2:A:120:PRO:HD3	2:A:132:VAL:HG22	1.97	0.47
2:E:80:ALA:HB2	2:E:106:ILE:HD13	1.96	0.46
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.50	0.46
1:D:126:PRO:HD3	1:D:138:LEU:HD23	1.97	0.46
1:H:189:PRO:HB3	1:H:212:PRO:HG3	1.96	0.46
1:B:94:ARG:NH2	1:B:100(C):PHE:O	2.49	0.46
2:C:192:TYR:O	2:C:208:SER:HA	2.16	0.45
1:B:145:TYR:CE2	1:B:150:VAL:HG13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:GLU:O	1:H:85:GLU:HG2	2.16	0.45
2:C:11:LEU:HD23	2:C:104:LEU:HA	1.99	0.45
1:B:211:VAL:HG22	1:B:212:PRO:HD2	1.97	0.45
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.99	0.45
1:B:40:PRO:HB2	1:B:43:LYS:HG3	1.98	0.45
2:E:55:GLU:O	2:E:58:VAL:HB	2.17	0.45
2:E:77:SER:OG	2:E:78:VAL:N	2.49	0.45
2:C:136:LEU:HD21	2:C:146:VAL:HG22	1.99	0.45
1:B:96:HIS:O	1:B:97:ASP:HB2	2.17	0.45
2:E:60:ASP:HA	2:E:61:ARG:HB3	1.99	0.45
1:D:55:TYR:CD1	1:D:71:ARG:HD3	2.52	0.44
2:E:192:TYR:O	2:E:208:SER:HA	2.17	0.44
2:A:39:LYS:NZ	2:A:81:GLU:O	2.31	0.44
2:A:161:ASN:HB3	2:A:175:MET:HE2	1.99	0.43
2:L:140:TYR:CG	2:L:141:PRO:HA	2.53	0.43
1:D:153:THR:OG1	1:D:196:ASN:HB2	2.18	0.43
2:L:193:THR:HG23	2:L:206:VAL:HG13	2.00	0.43
1:F:7:SER:HB2	3:F:322:HOH:O	2.17	0.43
2:E:56:SER:HA	2:E:57:GLY:O	2.18	0.43
2:E:12:ALA:HA	2:E:105:GLU:O	2.19	0.43
2:E:12:ALA:O	2:E:13:VAL:HG23	2.18	0.43
2:A:93:ASN:O	2:A:94:LEU:HB2	2.19	0.43
1:H:138:LEU:HD22	1:H:210:ILE:HG21	2.01	0.43
2:E:18:LYS:HA	2:E:76:SER:HA	2.01	0.42
2:E:189:HIS:O	2:E:211:ARG:NH1	2.49	0.42
1:B:67:PHE:HA	1:B:81:GLN:O	2.20	0.42
1:F:83:ARG:HA	1:F:83:ARG:HD2	1.96	0.42
2:C:90:GLN:O	2:C:96:ARG:HA	2.20	0.41
1:F:82:MET:HB3	1:F:82(C):LEU:HD21	2.02	0.41
1:H:151:THR:OG1	1:H:198:ALA:HB3	2.20	0.41
1:D:52(B):LYS:O	1:D:53:LYS:N	2.53	0.41
1:H:20:LEU:HG	1:H:82:MET:HE2	2.02	0.41
1:B:33:TYR:CE2	1:B:52:ARG:HG2	2.55	0.41
1:B:180:SER:HB3	2:A:135:PHE:CE2	2.55	0.41
1:B:100(C):PHE:HB3	1:B:102:TYR:CE1	2.56	0.41
2:A:192:TYR:O	2:A:208:SER:HA	2.21	0.41
2:A:54:ARG:HD3	2:A:58:VAL:O	2.22	0.40
1:D:12:VAL:HG11	1:D:82(C):LEU:HD13	2.03	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)
2:L:27(E):SER:OG	2:L:213:GLU:OE2[3_445]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	B	208/222 (94%)	202 (97%)	5 (2%)	1 (0%)	29	26
1	D	211/222 (95%)	207 (98%)	3 (1%)	1 (0%)	29	26
1	F	204/222 (92%)	201 (98%)	3 (2%)	0	100	100
1	H	207/222 (93%)	202 (98%)	3 (1%)	2 (1%)	15	11
2	A	217/219 (99%)	208 (96%)	9 (4%)	0	100	100
2	C	217/219 (99%)	206 (95%)	11 (5%)	0	100	100
2	E	217/219 (99%)	196 (90%)	13 (6%)	8 (4%)	3	1
2	L	217/219 (99%)	203 (94%)	13 (6%)	1 (0%)	29	26
All	All	1698/1764 (96%)	1625 (96%)	60 (4%)	13 (1%)	19	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	97	ASP
1	H	100	TYR
1	B	97	ASP
2	E	60	ASP
2	E	78	VAL
2	E	77	SER
2	E	81	GLU
2	E	82	ASP
1	D	97	ASP
2	E	15	ALA
2	E	61	ARG
2	L	200	THR

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Mol	Chain	Res	Type
2	E	16	GLY

5.3.2 Protein sidechains ⓘ

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	B	181/187 (97%)	168 (93%)	13 (7%)	14	11
1	D	180/187 (96%)	170 (94%)	10 (6%)	21	18
1	F	177/187 (95%)	170 (96%)	7 (4%)	31	32
1	H	178/187 (95%)	167 (94%)	11 (6%)	18	15
2	A	194/194 (100%)	182 (94%)	12 (6%)	18	15
2	C	193/194 (100%)	182 (94%)	11 (6%)	20	18
2	E	194/194 (100%)	176 (91%)	18 (9%)	9	6
2	L	193/194 (100%)	177 (92%)	16 (8%)	11	7
All	All	1490/1524 (98%)	1392 (93%)	98 (7%)	16	14

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	LYS
1	H	18	LEU
1	H	35	SER
1	H	43	LYS
1	H	50	PHE
1	H	83	ARG
1	H	105	GLN
1	H	140	CYS
1	H	160	SER
1	H	185	SER
1	H	195	CYS
2	L	10	SER
2	L	11	LEU
2	L	13	VAL

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Mol	Chain	Res	Type
2	L	19	VAL
2	L	60	ASP
2	L	67	SER
2	L	81	GLU
2	L	83	LEU
2	L	107	LYS
2	L	126	THR
2	L	142	LYS
2	L	143	ASP
2	L	155	ARG
2	L	169	LYS
2	L	181	LEU
2	L	194	CYS
1	B	3	LYS
1	B	7	SER
1	B	13	GLN
1	B	18	LEU
1	B	43	LYS
1	B	97	ASP
1	B	115	LYS
1	B	133	ASN
1	B	140	CYS
1	B	159	LEU
1	B	177	LEU
1	B	195	CYS
1	B	213	ARG
2	A	5	THR
2	A	7	SER
2	A	11	LEU
2	A	13	VAL
2	A	56	SER
2	A	83	LEU
2	A	107	LYS
2	A	127	SER
2	A	142	LYS
2	A	181	LEU
2	A	203	SER
2	A	212	ASN
1	D	3	LYS
1	D	7	SER
1	D	13	GLN
1	D	50	PHE

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Mol	Chain	Res	Type
1	D	100(B)	ARG
1	D	100(C)	PHE
1	D	115	LYS
1	D	140	CYS
1	D	177	LEU
1	D	195	CYS
2	C	5	THR
2	C	7	SER
2	C	11	LEU
2	C	19	VAL
2	C	83	LEU
2	C	107	LYS
2	C	127	SER
2	C	142	LYS
2	C	156	GLN
2	C	181	LEU
2	C	185	GLU
1	F	7	SER
1	F	50	PHE
1	F	77	SER
1	F	96	HIS
1	F	135	MET
1	F	177	LEU
1	F	195	CYS
2	E	5	THR
2	E	11	LEU
2	E	13	VAL
2	E	14	SER
2	E	27(F)	ARG
2	E	55	GLU
2	E	61	ARG
2	E	67	SER
2	E	70	ASP
2	E	77	SER
2	E	79	GLN
2	E	81	GLU
2	E	83	LEU
2	E	107	LYS
2	E	142	LYS
2	E	156	GLN
2	E	181	LEU
2	E	199	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	75	GLN
1	H	105	GLN
2	L	190	ASN
2	L	212	ASN
1	B	133	ASN
2	A	42	GLN
2	A	212	ASN
2	C	42	GLN
2	C	79	GLN
2	C	93	ASN
2	C	190	ASN
2	C	212	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	B	214/222 (96%)	-0.33	4 (1%) 66 71	22, 36, 56, 74	0
1	D	215/222 (96%)	-0.29	4 (1%) 66 71	22, 37, 63, 80	0
1	F	210/222 (94%)	-0.25	0 100 100	24, 38, 68, 86	0
1	H	213/222 (95%)	-0.21	5 (2%) 60 65	21, 35, 73, 97	0
2	A	219/219 (100%)	-0.21	1 (0%) 91 92	26, 45, 69, 85	0
2	C	219/219 (100%)	-0.29	1 (0%) 91 92	23, 37, 57, 73	0
2	E	219/219 (100%)	0.11	5 (2%) 60 65	28, 52, 75, 97	0
2	L	219/219 (100%)	0.08	6 (2%) 54 60	29, 52, 74, 88	0
All	All	1728/1764 (97%)	-0.17	26 (1%) 73 77	21, 41, 69, 97	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	99	TYR	4.9
2	E	59	PRO	4.6
1	B	100	TYR	3.6
2	E	80	ALA	3.5
2	E	63	THR	3.4
1	B	99	TYR	3.0
1	B	100(C)	PHE	2.8
2	C	214	CYS	2.8
2	L	62	PHE	2.7
2	L	169	LYS	2.6
1	H	100(C)	PHE	2.5
1	D	97	ASP	2.5
1	H	159	LEU	2.5
1	D	98	GLY	2.3
2	E	12	ALA	2.3
1	H	192	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	197	THR	2.2
2	L	200	THR	2.2
2	A	80	ALA	2.2
1	H	186	SER	2.1
2	E	57	GLY	2.1
1	B	1	GLU	2.1
2	L	214	CYS	2.0
2	L	16	GLY	2.0
1	H	100	TYR	2.0
1	D	100	TYR	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.