Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 12:39 PM EST

PDB ID	:	8F2V
Title	:	Antibody Fab directed against SARS-CoV-2 Spike Protein Receptor Binding Domain (RBD)
Authors	:	Chen, J.C.-H.
Deposited on	:	2022-11-08
Resolution	:	3.50 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:

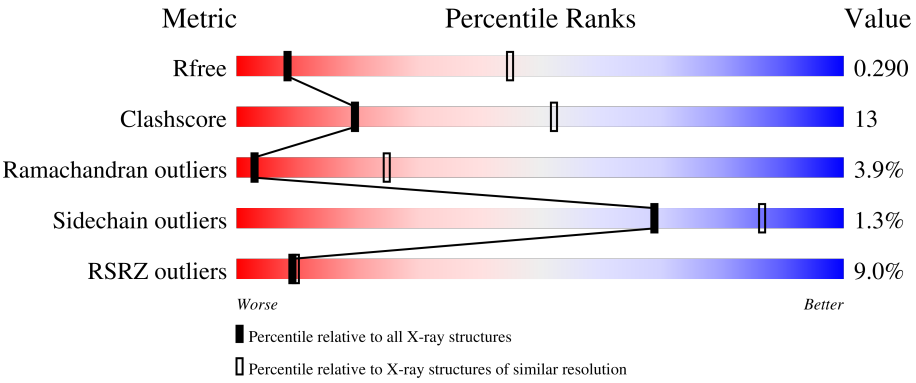
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	214	10% 71% 26%
1	C	214	12% 72% 25%
1	E	214	71% 25%
2	B	223	18% 70% 28%
2	D	223	12% 66% 31%

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Mol	Chain	Length	Quality of chain
2	F	223	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9720 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.

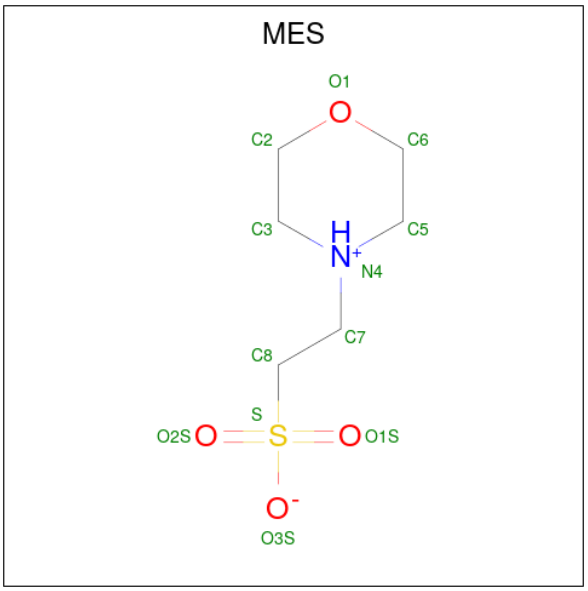
- Molecule 1 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	210	Total	C	N	O	S	0	0	0
			1579	990	266	319	4			
1	A	210	Total	C	N	O	S	0	0	0
			1579	990	266	319	4			
1	E	210	Total	C	N	O	S	0	0	0
			1579	990	266	319	4			

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	222	Total	C	N	O	S	0	0	0
			1649	1035	276	329	9			
2	B	222	Total	C	N	O	S	0	0	0
			1649	1035	276	329	9			
2	F	222	Total	C	N	O	S	0	0	0
			1649	1035	276	329	9			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

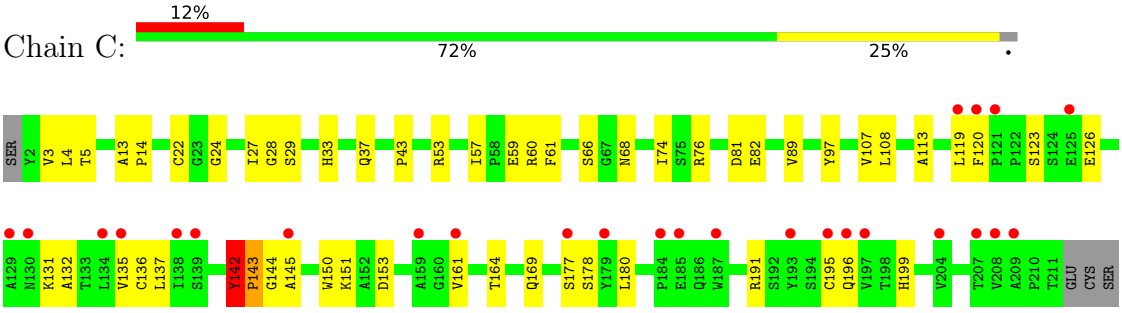


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

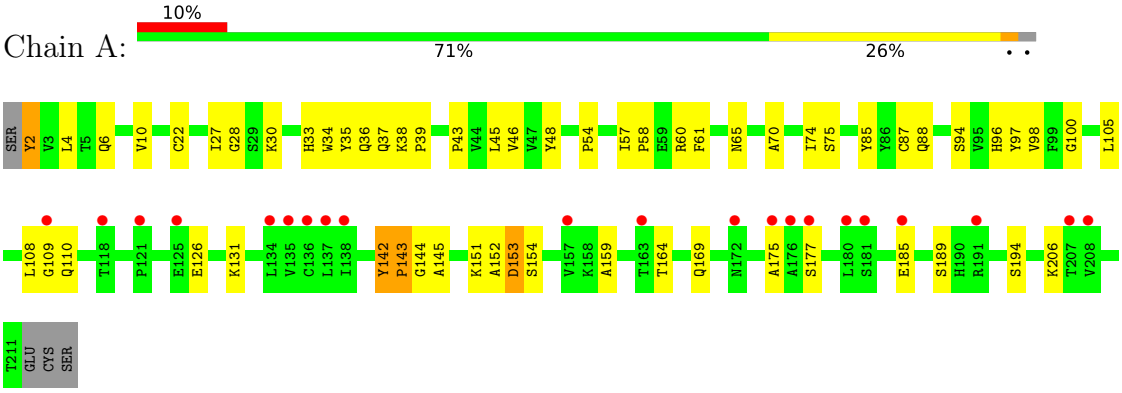
3 Residue-property plots (i)

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.

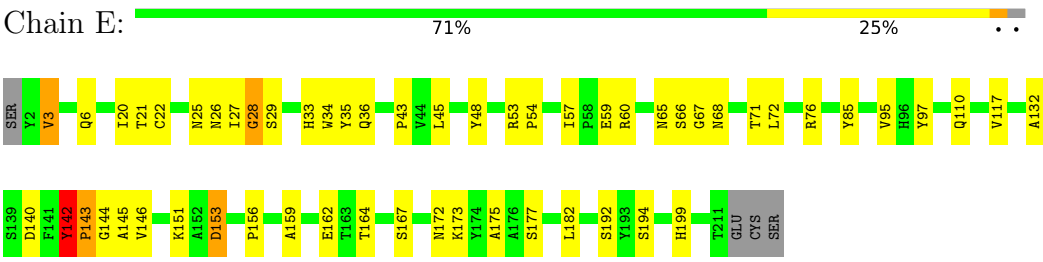
• Molecule 1: Fab light chain



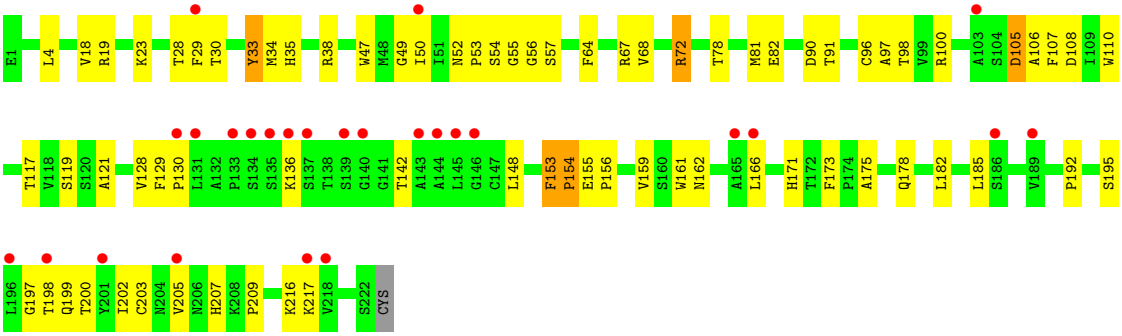
• Molecule 1: Fab light chain



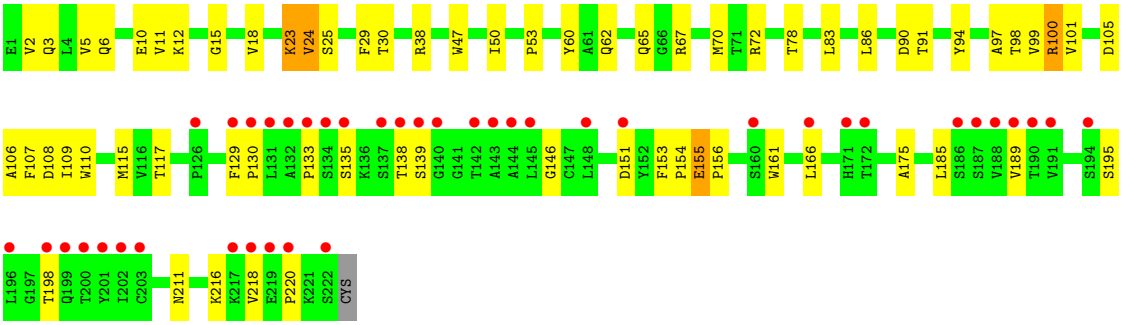
• Molecule 1: Fab light chain



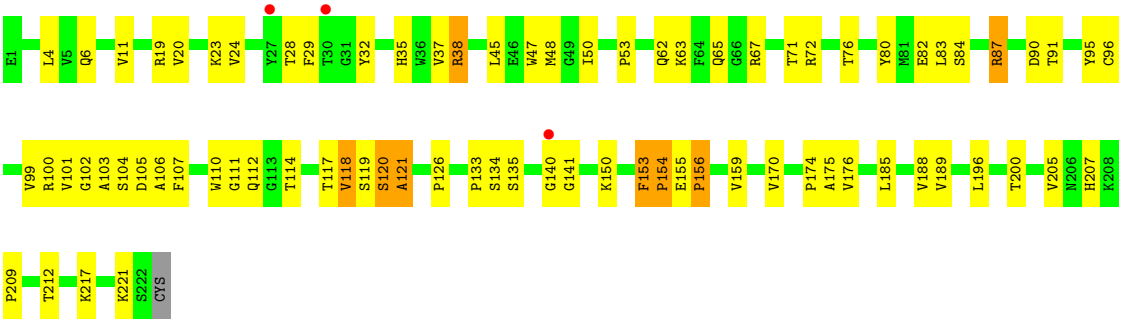
• Molecule 2: Fab heavy chain



• Molecule 2: Fab heavy chain



• Molecule 2: Fab heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.01Å 184.18Å 181.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.67 – 3.50 90.53 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.67-3.50) 94.7 (90.53-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.246 , 0.289 0.246 , 0.290	Depositor DCC
R_{free} test set	1189 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å^2)	83.9	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.032 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	9720	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: MES

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	0.26	0/1620	0.52	0/2218
1	C	0.25	0/1620	0.49	0/2218
1	E	0.26	0/1620	0.52	0/2218
2	B	0.26	0/1687	0.57	0/2297
2	D	0.26	0/1687	0.53	0/2297
2	F	0.27	0/1687	0.55	0/2297
All	All	0.26	0/9921	0.53	0/13545

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	A	0	2
1	C	0	1
1	E	0	1
2	B	0	2
2	D	0	1
2	F	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	2	TYR	Peptide
2	B	153	PHE	Peptide
2	B	155	GLU	Peptide
1	C	142	TYR	Peptide
2	D	153	PHE	Peptide
1	E	142	TYR	Peptide
2	F	153	PHE	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	1579	0	1524	40	0
1	C	1579	0	1526	35	0
1	E	1579	0	1524	41	0
2	B	1649	0	1621	44	0
2	D	1649	0	1621	50	0
2	F	1649	0	1621	58	0
3	A	12	0	12	0	0
3	C	12	0	12	1	0
3	F	12	0	12	0	0
All	All	9720	0	9473	246	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 13.

All (246) 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:B:100:ARG:HB2	2:B:108:ASP:HB3	1.59	0.84
1:A:153:ASP:OD1	1:A:154:SER:N	2.10	0.83
2:B:98:THR:HG22	2:B:109:ILE:HG22	1.60	0.81
1:E:33:HIS:HB3	1:E:48:TYR:HA	1.65	0.78
1:A:54:PRO:HG2	1:A:57:ILE:HD12	1.67	0.76
1:A:94:SER:O	1:A:96:HIS:ND1	2.19	0.76
2:F:32:TYR:HB3	2:F:100:ARG:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:TRP:HZ2	2:D:50:ILE:HG13	1.50	0.74
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.21	0.72
1:A:6:GLN:NE2	1:A:87:CYS:SG	2.57	0.72
2:B:138:THR:OG1	2:B:139:SER:OG	2.07	0.72
1:E:137:LEU:HD13	2:F:188:VAL:HG21	1.72	0.71
1:A:108:LEU:O	1:A:110:GLN:N	2.23	0.70
1:E:117:VAL:HG22	1:E:138:ILE:HG23	1.72	0.70
1:A:28:GLY:O	1:A:65:ASN:ND2	2.26	0.69
1:A:6:GLN:HE22	1:A:87:CYS:H	1.41	0.69
1:C:33:HIS:HE2	2:D:105:ASP:HB3	1.58	0.68
2:F:32:TYR:HD1	2:F:101:VAL:HG22	1.58	0.68
1:C:136:CYS:HB3	1:C:178:SER:HB3	1.75	0.68
1:C:131:LYS:HE3	1:C:132:ALA:H	1.57	0.67
2:F:38:ARG:NH2	2:F:90:ASP:OD1	2.28	0.67
2:D:30:THR:HA	2:D:53:PRO:HB2	1.79	0.65
1:C:143:PRO:O	1:C:145:ALA:N	2.29	0.65
1:A:126:GLU:HG2	1:A:131:LYS:HB2	1.79	0.65
1:C:24:GLY:H	1:C:27:ILE:HD11	1.61	0.65
1:A:4:LEU:HD21	1:A:27:ILE:HD11	1.80	0.64
1:E:151:LYS:HE3	1:E:156:PRO:HG3	1.78	0.64
2:F:19:ARG:HG3	2:F:82:GLU:HG3	1.78	0.63
2:D:38:ARG:HE	2:D:64:PHE:HZ	1.47	0.63
1:E:53:ARG:NH2	1:E:59:GLU:O	2.29	0.63
2:D:175:ALA:HB2	2:D:185:LEU:HD23	1.80	0.63
2:B:195:SER:HA	2:B:198:THR:HB	1.80	0.62
2:F:87:ARG:HB3	2:F:90:ASP:HB2	1.80	0.62
2:D:200:THR:HG23	2:D:217:LYS:HE3	1.80	0.61
1:E:45:LEU:HD11	2:F:106:ALA:HB1	1.82	0.61
2:F:175:ALA:HB2	2:F:185:LEU:HD23	1.83	0.61
2:D:100:ARG:NH1	2:D:108:ASP:OD2	2.33	0.61
2:F:11:VAL:HG12	2:F:117:THR:HB	1.83	0.61
2:B:166:LEU:HD21	2:B:189:VAL:HG21	1.84	0.60
2:B:6:GLN:NE2	2:B:94:TYR:O	2.32	0.60
1:E:33:HIS:CB	1:E:48:TYR:HA	2.32	0.60
2:F:4:LEU:HB2	2:F:111:GLY:HA2	1.84	0.60
1:A:151:LYS:HB2	1:A:194:SER:HB2	1.84	0.59
2:D:35:HIS:HD2	2:D:107:PHE:CE1	2.20	0.59
2:B:62:GLN:HA	2:B:65:GLN:HB2	1.82	0.59
1:A:143:PRO:O	1:A:145:ALA:N	2.36	0.59
2:B:130:PRO:HB2	2:B:218:VAL:HG13	1.85	0.59
1:E:143:PRO:O	1:E:145:ALA:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:103:ALA:O	2:F:105:ASP:N	2.35	0.59
2:F:120:SER:OG	2:F:121:ALA:N	2.36	0.59
1:E:45:LEU:HD21	1:E:48:TYR:HB3	1.84	0.59
2:D:91:THR:HG23	2:D:117:THR:HA	1.84	0.58
1:E:35:TYR:HE1	1:E:45:LEU:HD12	1.69	0.57
1:E:21:THR:HG22	1:E:71:THR:HG22	1.86	0.57
2:F:200:THR:HG23	2:F:217:LYS:HE2	1.86	0.57
2:D:129:PHE:HD2	2:D:148:LEU:HD23	1.70	0.57
1:C:14:PRO:HG2	1:E:95:VAL:HB	1.87	0.56
1:C:60:ARG:NH1	1:C:81:ASP:OD2	2.33	0.56
2:D:119:SER:HB3	2:D:153:PHE:CZ	2.41	0.56
2:B:24:VAL:HG21	2:B:29:PHE:HD1	1.70	0.56
2:F:37:VAL:HG22	2:F:47:TRP:HA	1.87	0.56
2:F:170:VAL:HG22	2:F:189:VAL:HG22	1.88	0.56
1:A:94:SER:O	1:A:94:SER:OG	2.24	0.55
2:F:4:LEU:HD22	2:F:24:VAL:HG12	1.87	0.55
2:B:133:PRO:HD2	2:B:220:PRO:HA	1.88	0.55
1:E:133:THR:OG1	2:F:150:LYS:NZ	2.26	0.55
2:D:154:PRO:HD2	2:D:207:HIS:NE2	2.20	0.55
2:F:35:HIS:CE1	2:F:50:ILE:HD13	2.42	0.55
1:E:6:GLN:HG2	1:E:22:CYS:HB2	1.90	0.54
1:C:33:HIS:CG	2:D:106:ALA:HB2	2.42	0.54
2:D:29:PHE:CE2	2:D:53:PRO:HB3	2.43	0.53
1:C:33:HIS:NE2	2:D:105:ASP:HB3	2.23	0.53
2:D:175:ALA:HA	2:D:185:LEU:HB3	1.91	0.53
2:F:154:PRO:HB2	2:F:156:PRO:HD2	1.91	0.53
2:F:37:VAL:O	2:F:95:TYR:N	2.42	0.53
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.28	0.53
2:F:133:PRO:HG3	2:F:196:LEU:HD22	1.91	0.53
2:F:175:ALA:HA	2:F:185:LEU:HB3	1.91	0.53
1:E:27:ILE:HG22	1:E:65:ASN:HD21	1.74	0.53
2:B:47:TRP:HZ2	2:B:50:ILE:HG23	1.74	0.53
1:E:20:ILE:HB	1:E:72:LEU:HB3	1.91	0.53
2:F:67:ARG:NH1	2:F:84:SER:O	2.42	0.52
1:C:27:ILE:O	1:C:29:SER:N	2.43	0.52
1:C:120:PHE:HB2	1:C:135:VAL:HB	1.89	0.52
2:D:97:ALA:HB1	2:D:107:PHE:HB3	1.90	0.52
1:A:6:GLN:NE2	1:A:87:CYS:H	2.06	0.52
1:C:164:THR:HG22	1:C:177:SER:H	1.75	0.51
1:C:137:LEU:HB3	2:D:173:PHE:CZ	2.45	0.51
1:C:153:ASP:OD1	1:C:191:ARG:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:OH	1:A:88:GLN:OE1	2.15	0.51
2:D:198:THR:HG23	2:D:199:GLN:OE1	2.11	0.51
2:B:175:ALA:HB2	2:B:185:LEU:HD23	1.93	0.51
1:E:146:VAL:HG23	1:E:199:HIS:HB2	1.93	0.51
2:D:178:GLN:HG2	2:D:182:LEU:O	2.11	0.50
2:D:202:ILE:HG12	2:D:217:LYS:HG3	1.93	0.50
2:D:47:TRP:CZ2	2:D:50:ILE:HG13	2.40	0.50
1:A:43:PRO:HG2	2:B:110:TRP:CD2	2.47	0.50
2:D:142:THR:HG22	2:D:192:PRO:HA	1.92	0.50
2:F:154:PRO:HD2	2:F:207:HIS:CE1	2.47	0.50
2:F:91:THR:OG1	2:F:118:VAL:HG12	2.11	0.49
2:F:154:PRO:HD2	2:F:207:HIS:NE2	2.27	0.49
1:C:37:GLN:HG3	1:C:43:PRO:HG3	1.94	0.49
2:D:55:GLY:O	2:D:57:SER:N	2.46	0.49
1:E:27:ILE:H	1:E:68:ASN:HA	1.77	0.49
2:F:159:VAL:HG13	2:F:205:VAL:HG22	1.94	0.49
1:C:61:PHE:CD1	1:C:74:ILE:HG12	2.48	0.49
2:F:118:VAL:HG22	2:F:119:SER:H	1.77	0.49
1:A:38:LYS:HB3	1:A:39:PRO:HD2	1.94	0.49
1:A:152:ALA:O	1:A:154:SER:N	2.46	0.49
1:A:164:THR:HB	1:A:177:SER:H	1.78	0.49
2:B:23:LYS:HA	2:B:78:THR:HG22	1.95	0.49
2:D:130:PRO:HD3	2:D:216:LYS:HE2	1.94	0.49
1:E:27:ILE:O	1:E:29:SER:N	2.45	0.49
1:A:22:CYS:N	1:A:70:ALA:O	2.43	0.48
2:D:33:TYR:HB3	2:D:53:PRO:HD2	1.96	0.48
2:B:67:ARG:HH21	2:B:83:LEU:HD22	1.78	0.48
2:B:146:GLY:HA2	2:B:161:TRP:CZ2	2.48	0.48
1:E:25:ASN:O	1:E:27:ILE:N	2.46	0.48
2:D:52:ASN:HB3	2:D:55:GLY:O	2.13	0.48
1:A:27:ILE:HG22	1:A:65:ASN:HD21	1.78	0.48
1:E:110:GLN:NE2	1:E:172:ASN:HB2	2.29	0.48
1:C:24:GLY:N	1:C:27:ILE:HD11	2.28	0.48
1:E:162:GLU:HB3	2:F:176:VAL:HG21	1.95	0.48
2:D:153:PHE:CG	2:D:153:PHE:O	2.65	0.48
2:B:161:TRP:HB3	2:B:166:LEU:HD23	1.96	0.48
1:E:60:ARG:HD3	1:E:76:ARG:C	2.34	0.48
2:F:96:CYS:O	2:F:111:GLY:N	2.47	0.48
2:B:10:GLU:HB3	2:B:12:LYS:HE2	1.95	0.47
2:B:138:THR:HA	2:B:139:SER:HA	1.57	0.47
2:D:53:PRO:HA	2:D:72:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:GLN:OE1	2:F:96:CYS:HB3	2.14	0.47
1:A:6:GLN:NE2	1:A:100:GLY:HA3	2.29	0.47
2:B:155:GLU:O	2:B:155:GLU:HG3	2.14	0.47
1:A:36:GLN:HB2	1:A:85:TYR:CE2	2.49	0.47
2:B:130:PRO:HD3	2:B:216:LYS:HE2	1.95	0.47
1:E:54:PRO:HD2	1:E:57:ILE:HG13	1.96	0.47
2:F:35:HIS:HE2	2:F:99:VAL:HG11	1.80	0.47
2:B:99:VAL:HB	2:B:105:ASP:HB3	1.97	0.47
1:C:123:SER:HB3	1:C:126:GLU:HB2	1.96	0.46
1:C:53:ARG:CZ	1:C:59:GLU:HA	2.45	0.46
2:F:118:VAL:HG13	2:F:119:SER:N	2.30	0.46
2:B:11:VAL:HG22	2:B:117:THR:HB	1.97	0.46
1:E:43:PRO:HG2	2:F:110:TRP:CD2	2.51	0.46
2:D:33:TYR:HB3	2:D:52:ASN:HA	1.98	0.46
2:D:34:MET:HB3	2:D:98:THR:HA	1.97	0.46
1:E:151:LYS:HB2	1:E:194:SER:HB2	1.98	0.46
2:F:154:PRO:HG2	2:F:209:PRO:CB	2.46	0.46
1:E:34:TRP:CE2	1:E:72:LEU:HB2	2.51	0.46
2:F:6:GLN:HB3	2:F:114:THR:OG1	2.16	0.46
2:D:159:VAL:HG22	2:D:205:VAL:HG22	1.98	0.46
2:D:195:SER:HB2	2:D:199:GLN:OE1	2.15	0.46
1:E:142:TYR:HB3	1:E:143:PRO:HD3	1.97	0.45
1:A:4:LEU:HD23	1:A:4:LEU:HA	1.78	0.45
1:C:82:GLU:HG3	1:C:107:VAL:H	1.81	0.45
2:D:35:HIS:CD2	2:D:107:PHE:CE1	3.04	0.45
1:A:4:LEU:CD2	1:A:27:ILE:HD11	2.45	0.45
1:C:136:CYS:HB2	1:C:150:TRP:CZ2	2.51	0.45
1:A:6:GLN:HE22	1:A:87:CYS:N	2.10	0.45
1:C:5:THR:HB	2:B:5:VAL:HG21	1.98	0.45
2:D:161:TRP:CZ3	2:D:203:CYS:HB3	2.52	0.45
2:B:3:GLN:O	2:B:24:VAL:HA	2.17	0.45
2:B:97:ALA:HB1	2:B:107:PHE:HB3	1.97	0.45
2:B:30:THR:HA	2:B:53:PRO:HB2	1.99	0.45
2:D:35:HIS:HB3	2:D:49:GLY:O	2.17	0.44
1:C:113:ALA:HB3	1:C:142:TYR:H	1.82	0.44
1:C:169:GLN:HE21	1:C:169:GLN:HB2	1.62	0.44
3:C:301:MES:H51	3:C:301:MES:H81	1.69	0.44
1:A:46:VAL:HA	1:A:57:ILE:HD13	1.98	0.44
1:E:28:GLY:N	1:E:67:GLY:O	2.48	0.44
1:E:45:LEU:CD1	2:F:106:ALA:HB1	2.47	0.44
1:E:133:THR:HG1	2:F:150:LYS:HZ2	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ALA:O	1:C:199:HIS:NE2	2.50	0.44
1:E:164:THR:HG23	2:F:174:PRO:HG2	2.00	0.44
1:A:33:HIS:ND1	2:B:106:ALA:HB2	2.32	0.44
1:A:2:TYR:N	1:A:98:VAL:HG11	2.32	0.44
2:F:20:VAL:HG13	2:F:114:THR:HG21	1.99	0.44
2:D:128:VAL:HG23	2:D:216:LYS:NZ	2.33	0.43
1:A:169:GLN:OE1	1:A:175:ALA:HB2	2.18	0.43
1:E:43:PRO:HG3	2:F:45:LEU:HD21	2.00	0.43
2:F:71:THR:O	2:F:80:TYR:N	2.44	0.43
1:C:5:THR:HG22	2:B:23:LYS:HG2	2.00	0.43
2:B:23:LYS:O	2:B:24:VAL:HG22	2.17	0.43
2:F:29:PHE:CZ	2:F:53:PRO:HB3	2.53	0.43
2:F:153:PHE:O	2:F:153:PHE:CG	2.71	0.43
1:A:60:ARG:HB3	1:A:75:SER:O	2.19	0.43
1:A:61:PHE:CD2	1:A:74:ILE:HG12	2.53	0.43
2:B:23:LYS:HD2	2:B:78:THR:HG22	2.00	0.43
2:F:6:GLN:HB3	2:F:6:GLN:HE21	1.65	0.43
1:C:13:ALA:HB3	2:F:62:GLN:CD	2.39	0.43
2:B:2:VAL:HA	2:B:25:SER:HB2	2.01	0.43
2:D:154:PRO:HG2	2:D:209:PRO:CG	2.49	0.43
2:F:107:PHE:HD2	2:F:110:TRP:CZ2	2.37	0.43
1:C:76:ARG:NE	2:B:211:ASN:OD1	2.52	0.42
1:A:45:LEU:HD21	1:A:48:TYR:HB3	2.01	0.42
1:C:60:ARG:HG2	1:C:76:ARG:HH21	1.84	0.42
2:B:91:THR:HG23	2:B:117:THR:HA	2.01	0.42
2:F:83:LEU:HD21	2:F:90:ASP:OD2	2.19	0.42
1:E:132:ALA:O	1:E:182:LEU:N	2.49	0.42
2:F:126:PRO:HD2	2:F:212:THR:HG21	2.01	0.42
1:C:169:GLN:HG2	2:D:171:HIS:NE2	2.34	0.42
2:D:19:ARG:HA	2:D:81:MET:O	2.19	0.42
2:F:32:TYR:CD1	2:F:101:VAL:HG22	2.47	0.42
1:A:126:GLU:HG3	2:B:129:PHE:CD2	2.55	0.42
2:B:38:ARG:HH21	2:B:90:ASP:HA	1.84	0.42
2:D:35:HIS:ND1	2:D:50:ILE:HG23	2.34	0.42
2:D:119:SER:HB3	2:D:153:PHE:CE1	2.54	0.42
2:F:38:ARG:HB3	2:F:48:MET:SD	2.60	0.42
1:E:164:THR:HB	1:E:177:SER:H	1.84	0.42
2:D:4:LEU:HD23	2:D:96:CYS:SG	2.59	0.42
2:D:107:PHE:HD2	2:D:110:TRP:CZ2	2.37	0.42
2:B:12:LYS:HG3	2:B:18:VAL:HB	2.00	0.42
1:C:151:LYS:HD3	1:C:196:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:134:SER:HA	2:F:221:LYS:HD3	2.02	0.41
2:B:130:PRO:HB3	2:B:218:VAL:HG22	2.01	0.41
2:F:87:ARG:O	2:F:118:VAL:HG11	2.20	0.41
1:A:206:LYS:HD2	1:A:206:LYS:HA	1.85	0.41
2:F:63:LYS:H	2:F:63:LYS:HG3	1.43	0.41
1:C:4:LEU:HD21	1:C:89:VAL:HG22	2.01	0.41
1:C:161:VAL:HG22	1:C:180:LEU:HB2	2.02	0.41
2:D:23:LYS:HG3	2:D:78:THR:HG22	2.02	0.41
1:A:96:HIS:HA	2:B:47:TRP:CZ3	2.56	0.41
2:F:67:ARG:HB2	2:F:84:SER:O	2.20	0.41
2:D:18:VAL:O	2:D:82:GLU:HA	2.20	0.41
1:A:34:TRP:O	1:A:45:LEU:HD12	2.20	0.41
2:B:107:PHE:N	2:B:107:PHE:CD1	2.88	0.41
1:E:3:VAL:HG23	1:E:3:VAL:O	2.21	0.41
2:F:62:GLN:HA	2:F:65:GLN:HB2	2.01	0.41
2:B:175:ALA:HA	2:B:185:LEU:HB3	2.02	0.41
1:E:140:ASP:HA	1:E:173:LYS:HB3	2.01	0.41
2:B:60:TYR:HD1	2:B:70:MET:HE3	1.85	0.41
1:E:167:SER:N	1:E:175:ALA:O	2.44	0.41
2:D:68:VAL:HA	2:D:82:GLU:O	2.20	0.41
1:A:37:GLN:HB2	1:A:43:PRO:HA	2.03	0.41
1:A:185:GLU:O	1:A:189:SER:HB3	2.21	0.41
1:E:36:GLN:NE2	1:E:85:TYR:OH	2.45	0.41
1:C:57:ILE:HD13	1:C:57:ILE:HA	1.85	0.40
2:D:121:ALA:HB3	2:D:153:PHE:CG	2.56	0.40
1:C:119:LEU:HD12	1:C:195:CYS:SG	2.60	0.40
2:D:162:ASN:HB2	2:D:166:LEU:HD13	2.03	0.40
1:E:28:GLY:HA2	1:E:66:SER:O	2.21	0.40
1:A:10:VAL:O	1:A:105:LEU:HA	2.22	0.40
1:A:57:ILE:HA	1:A:58:PRO:HD3	1.94	0.40
2:B:15:GLY:N	2:B:86:LEU:O	2.52	0.40
1:E:153:ASP:N	1:E:192:SER:O	2.48	0.40
2:F:118:VAL:HG13	2:F:119:SER:H	1.87	0.40
2:F:23:LYS:HE2	2:F:76:THR:O	2.21	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	208/214 (97%)	179 (86%)	22 (11%)	7 (3%)	3	28
1	C	208/214 (97%)	184 (88%)	17 (8%)	7 (3%)	3	28
1	E	208/214 (97%)	183 (88%)	17 (8%)	8 (4%)	3	25
2	B	220/223 (99%)	195 (89%)	18 (8%)	7 (3%)	4	29
2	D	220/223 (99%)	189 (86%)	23 (10%)	8 (4%)	3	26
2	F	220/223 (99%)	188 (86%)	19 (9%)	13 (6%)	1	15
All	All	1284/1311 (98%)	1118 (87%)	116 (9%)	50 (4%)	3	25

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	28	GLY
1	C	142	TYR
1	C	143	PRO
2	D	136	LYS
2	D	154	PRO
2	D	156	PRO
1	A	142	TYR
1	A	143	PRO
1	A	153	ASP
2	B	24	VAL
2	B	101	VAL
2	B	154	PRO
2	B	156	PRO
1	E	3	VAL
1	E	26	ASN
1	E	142	TYR
1	E	143	PRO
2	F	104	SER
2	F	120	SER
2	F	154	PRO

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Mol	Chain	Res	Type
2	F	156	PRO
1	C	144	GLY
2	D	54	SER
2	D	56	GLY
2	D	155	GLU
1	A	30	LYS
1	A	109	GLY
1	A	144	GLY
2	B	23	LYS
2	B	135	SER
1	E	28	GLY
1	E	144	GLY
2	F	112	GLN
2	F	135	SER
1	C	3	VAL
1	C	66	SER
1	C	108	LEU
1	A	159	ALA
2	F	121	ALA
2	F	141	GLY
2	D	28	THR
1	E	153	ASP
1	E	159	ALA
2	F	28	THR
2	D	197	GLY
2	B	151	ASP
2	F	140	GLY
2	F	155	GLU
2	F	118	VAL
2	F	102	GLY

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	178/182 (98%)	177 (99%)	1 (1%)	86 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	178/182 (98%)	175 (98%)	3 (2%)	60 82
1	E	178/182 (98%)	177 (99%)	1 (1%)	86 94
2	B	188/189 (100%)	185 (98%)	3 (2%)	62 83
2	D	188/189 (100%)	185 (98%)	3 (2%)	62 83
2	F	188/189 (100%)	185 (98%)	3 (2%)	62 83
All	All	1098/1113 (99%)	1084 (99%)	14 (1%)	69 86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	22	CYS
1	C	68	ASN
1	C	97	TYR
2	D	33	TYR
2	D	72	ARG
2	D	105	ASP
1	A	97	TYR
2	B	72	ARG
2	B	100	ARG
2	B	115	MET
1	E	97	TYR
2	F	38	ARG
2	F	72	ARG
2	F	87	ARG

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

Mol	Chain	Res	Type
1	A	6	GLN

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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MES	A	301	-	12,12,12	2.29	1 (8%)	14,16,16	2.52	6 (42%)
3	MES	F	301	-	12,12,12	2.29	1 (8%)	14,16,16	2.47	5 (35%)
3	MES	C	301	-	12,12,12	2.30	1 (8%)	14,16,16	2.47	7 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	301	-	-	2/6/14/14	0/1/1/1
3	MES	F	301	-	-	4/6/14/14	0/1/1/1
3	MES	C	301	-	-	2/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	MES	C8-S	-7.71	1.66	1.77
3	A	301	MES	C8-S	-7.67	1.66	1.77
3	F	301	MES	C8-S	-7.66	1.66	1.77

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	MES	C5-N4-C3	5.26	120.67	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	MES	C5-N4-C3	5.21	120.56	108.83
3	F	301	MES	C5-N4-C3	5.08	120.26	108.83
3	A	301	MES	C6-C5-N4	-3.86	104.25	110.10
3	F	301	MES	C7-N4-C5	3.60	120.45	111.23
3	F	301	MES	C6-C5-N4	-3.57	104.69	110.10
3	A	301	MES	C7-N4-C5	3.56	120.34	111.23
3	C	301	MES	C6-C5-N4	-3.37	105.00	110.10
3	C	301	MES	C7-N4-C5	3.19	119.39	111.23
3	C	301	MES	C7-N4-C3	3.16	119.32	111.23
3	A	301	MES	C7-N4-C3	3.07	119.10	111.23
3	F	301	MES	C7-N4-C3	3.06	119.06	111.23
3	C	301	MES	O2S-S-C8	2.69	110.15	106.92
3	F	301	MES	O3S-S-C8	2.63	110.02	105.77
3	A	301	MES	O2S-S-C8	2.37	109.77	106.92
3	A	301	MES	O3S-S-C8	2.34	109.56	105.77
3	C	301	MES	C2-C3-N4	-2.34	106.56	110.10
3	C	301	MES	O3S-S-C8	2.06	109.10	105.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	MES	C8-C7-N4-C5
3	F	301	MES	C8-C7-N4-C5
3	F	301	MES	C7-C8-S-O2S
3	F	301	MES	C7-C8-S-O3S
3	C	301	MES	C8-C7-N4-C3
3	C	301	MES	C8-C7-N4-C5
3	F	301	MES	C7-C8-S-O1S
3	A	301	MES	C8-C7-N4-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	MES	1	0

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	210/214 (98%)	0.61	21 (10%) 7 8	39, 105, 185, 225	0
1	C	210/214 (98%)	0.69	26 (12%) 4 5	55, 123, 204, 246	0
1	E	210/214 (98%)	0.18	0 100 100	46, 87, 133, 158	0
2	B	222/223 (99%)	0.90	41 (18%) 1 1	44, 78, 195, 252	0
2	D	222/223 (99%)	0.86	26 (11%) 4 5	58, 105, 207, 257	0
2	F	222/223 (99%)	0.21	3 (1%) 75 69	40, 62, 139, 206	0
All	All	1296/1311 (98%)	0.58	117 (9%) 9 10	39, 89, 195, 257	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	134	SER	9.8
1	C	195	CYS	8.4
2	B	135	SER	7.9
2	D	137	SER	7.5
2	D	218	VAL	6.6
2	B	138	THR	6.3
2	D	131	LEU	6.0
2	D	144	ALA	5.8
2	D	140	GLY	5.4
1	A	191	ARG	5.3
1	C	159	ALA	5.0
2	D	143	ALA	4.9
1	A	207	THR	4.9
2	D	146	GLY	4.8
1	A	176	ALA	4.7
2	B	143	ALA	4.7
2	D	145	LEU	4.6
2	B	201	TYR	4.4
2	D	189	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	148	LEU	4.2
2	D	165	ALA	4.2
2	B	137	SER	4.1
1	A	137	LEU	3.9
2	D	130	PRO	3.9
1	C	119	LEU	3.8
2	B	188	VAL	3.8
2	B	194	SER	3.8
2	B	200	THR	3.8
2	B	171	HIS	3.7
2	D	201	TYR	3.7
2	B	191	VAL	3.7
2	B	222	SER	3.6
2	B	219	GLU	3.6
2	D	103	ALA	3.6
2	B	145	LEU	3.5
1	A	208	VAL	3.5
2	B	218	VAL	3.3
2	B	133	PRO	3.3
2	B	220	PRO	3.3
1	A	118	THR	3.3
2	D	135	SER	3.3
1	C	207	THR	3.3
2	B	187	SER	3.2
2	D	217	LYS	3.2
2	B	203	CYS	3.2
2	B	130	PRO	3.2
2	B	190	THR	3.2
2	D	136	LYS	3.2
2	B	196	LEU	3.2
2	D	186	SER	3.1
1	C	130	ASN	3.1
2	F	30	THR	3.1
2	B	139	SER	3.1
2	B	142	THR	3.1
1	C	129	ALA	3.1
1	A	138	ILE	3.1
2	B	144	ALA	3.1
2	D	205	VAL	3.0
1	C	187	TRP	3.0
1	A	109	GLY	3.0
2	B	172	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	166	LEU	2.9
2	F	27	TYR	2.9
1	C	184	PRO	2.9
1	A	125	GLU	2.9
1	A	136	CYS	2.9
1	A	181	SER	2.9
1	C	204	VAL	2.8
2	B	198	THR	2.8
2	B	132	ALA	2.7
1	C	208	VAL	2.7
1	A	177	SER	2.7
1	A	175	ALA	2.7
2	B	202	ILE	2.7
1	A	135	VAL	2.7
1	C	121	PRO	2.6
2	D	196	LEU	2.6
2	B	189	VAL	2.6
2	B	199	GLN	2.6
1	A	134	LEU	2.6
2	B	140	GLY	2.6
2	D	139	SER	2.6
1	C	196	GLN	2.6
1	A	163	THR	2.6
2	B	160	SER	2.4
2	B	151	ASP	2.4
1	A	172	ASN	2.4
2	B	129	PHE	2.4
1	C	179	TYR	2.4
2	B	186	SER	2.4
2	B	217	LYS	2.4
1	C	135	VAL	2.3
2	D	50	ILE	2.3
1	A	157	VAL	2.3
2	D	198	THR	2.3
1	C	125	GLU	2.3
1	C	197	VAL	2.3
1	C	139	SER	2.3
1	C	193	TYR	2.3
2	B	126	PRO	2.3
1	C	134	LEU	2.3
2	D	134	SER	2.3
2	D	133	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	120	PHE	2.2
1	C	138	ILE	2.2
1	C	145	ALA	2.2
1	A	185	GLU	2.2
2	B	166	LEU	2.2
1	A	121	PRO	2.2
1	C	209	ALA	2.2
1	C	177	SER	2.1
1	A	180	LEU	2.1
1	C	161	VAL	2.1
2	B	131	LEU	2.1
2	D	29	PHE	2.1
1	C	185	GLU	2.1
2	F	140	GLY	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	MES	A	301	12/12	0.81	0.37	71,91,96,98	0
3	MES	F	301	12/12	0.81	0.36	75,85,89,93	0
3	MES	C	301	12/12	0.86	0.29	79,85,94,97	0

6.5 Other polymers (i)

There are no such residues in this entry.