



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:01 PM UTC

PDB ID : 8F2V / pdb_00008f2v
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

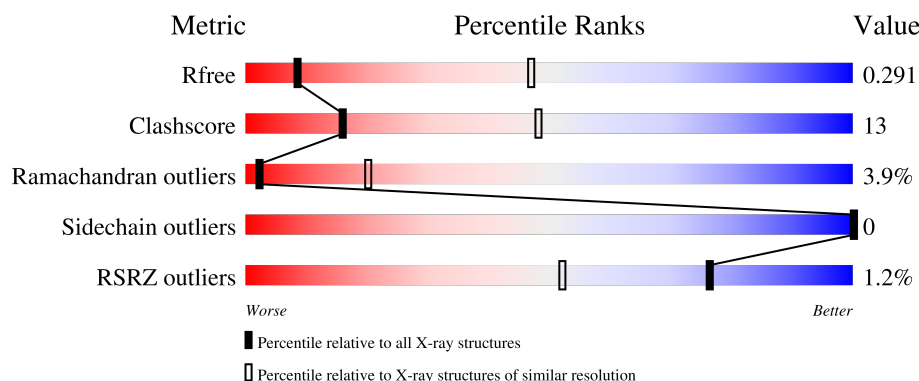
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	A	214	% 71% 25% ..
1	C	214	% 74% 23% .
1	E	214	% 71% 25% ..
2	B	223	% 71% 27% .
2	D	223	% 66% 33% .

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Mol	Chain	Length	Quality of chain
2	F	223	2% 63% 34%

2 Entry composition

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.

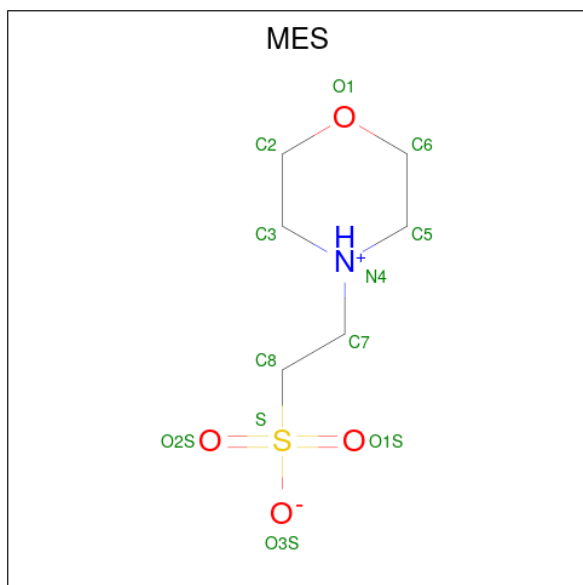
- Molecule 1 is a protein called Fab light chain.

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 (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).

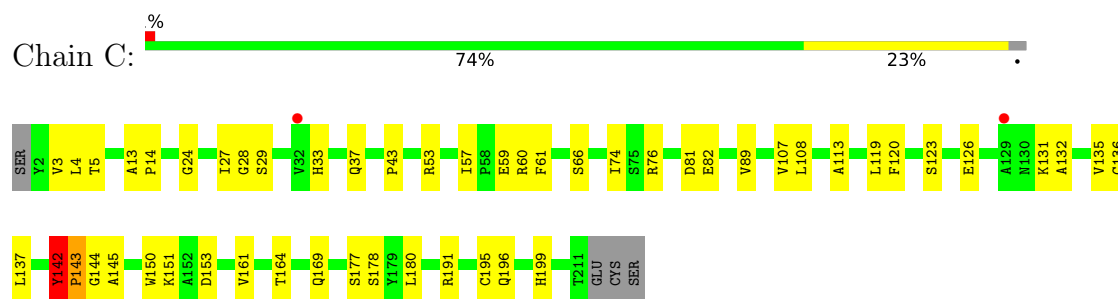


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

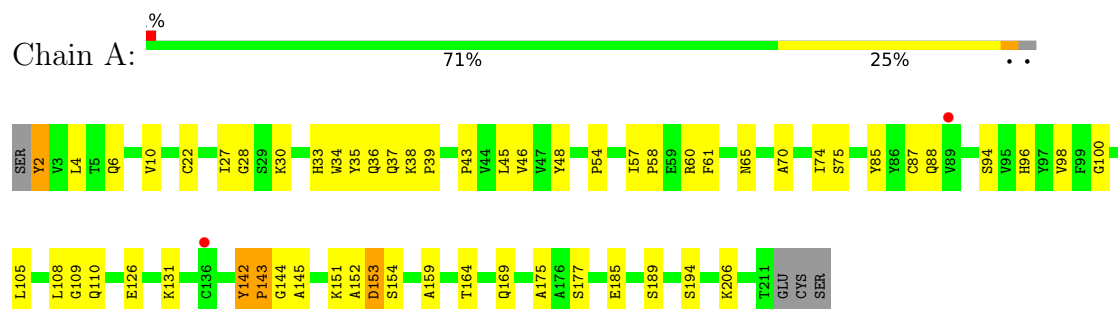
3 Residue-property plots [i](#)

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.

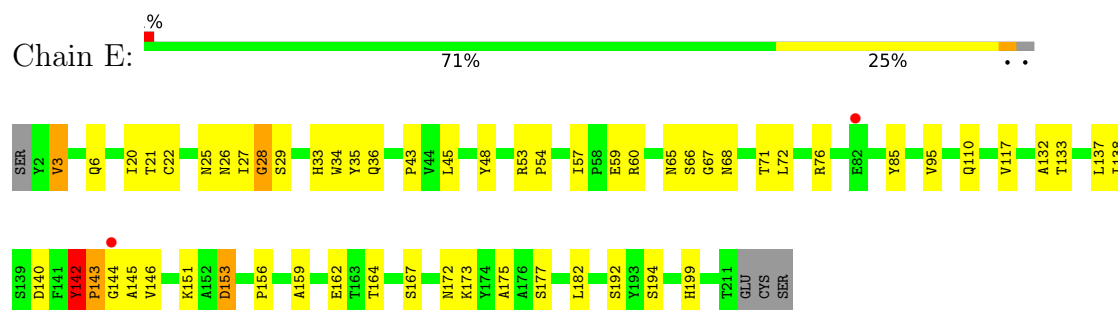
- Molecule 1: Fab light chain



- Molecule 1: Fab light chain



- Molecule 1: Fab light chain

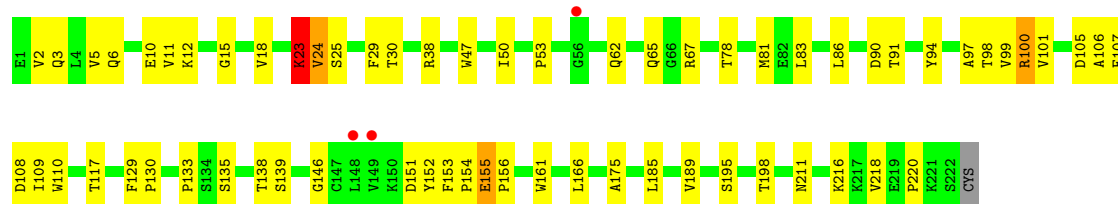


- Molecule 2: Fab heavy chain

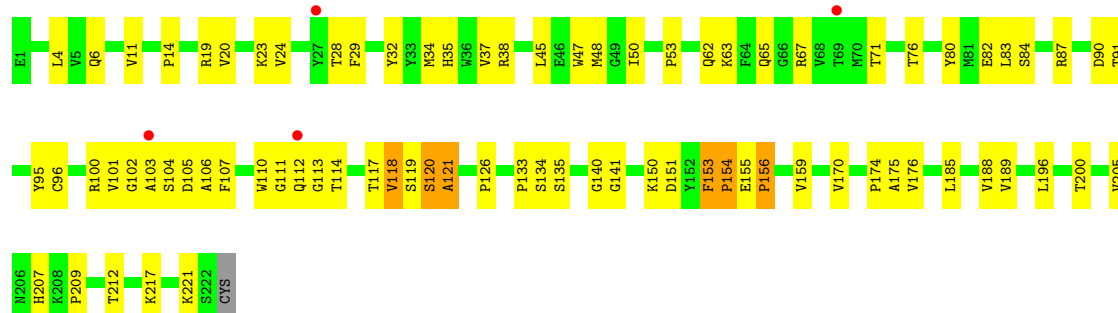




• Molecule 2: Fab heavy chain



• Molecule 2: Fab heavy chain



4 Data and refinement statistics

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 29.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.67-3.50) 94.5 (29.67-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.246 , 0.289 0.248 , 0.291	Depositor DCC
R_{free} test set	1346 reflections (3.92%)	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 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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	0.87	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.*

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

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	0.14	0/1620	0.40	0/2218
1	C	0.13	0/1620	0.37	0/2218
1	E	0.14	0/1620	0.40	0/2218
2	B	0.14	0/1687	0.47	4/2297 (0.2%)
2	D	0.13	0/1687	0.37	0/2297
2	F	0.15	0/1687	0.46	1/2297 (0.0%)
All	All	0.14	0/9921	0.41	5/13545 (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
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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	113	GLY	N-CA-C	6.53	120.07	111.52
2	B	23	LYS	CA-C-N	5.78	132.38	121.97
2	B	23	LYS	C-N-CA	5.78	132.38	121.97
2	B	100	ARG	CA-C-N	5.09	131.13	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	ARG	C-N-CA	5.09	131.13	121.97

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	TYR	Peptide
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

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	42	0
2	B	1649	0	1621	45	0
2	D	1649	0	1621	52	0
2	F	1649	0	1621	61	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	253	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 (253) 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
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
2:F:24:VAL:HG11	2:F:34:MET:HE1	1.75	0.68
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
2:B:152:TYR:OH	2:B:155:GLU:OE1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:103:ALA:O	2:F:105:ASP:N	2.35	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:F:120:SER:OG	2:F:121:ALA:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ARG:HD3	1:E:76:ARG:C	2.34	0.52
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
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
2:D:49:GLY:HA3	2:D:70:MET:HE1	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:C:13:ALA:HB3	2:F:62:GLN:CD	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:14:PRO:HD3	2:F:119:SER:C	2.43	0.43
2:F:29:PHE:CZ	2:F:53:PRO:HB3	2.53	0.43
2:F:35:HIS:HD1	2:F:47:TRP:HE1	1.65	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:HIS:ND1	2:D:50:ILE:HG23	2.34	0.42
2:D:55:GLY:C	2:D:57:SER:H	2.28	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
2:F:153:PHE:O	2:F:153:PHE:CG	2.71	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:E:142:TYR:O	1:E:143:PRO:C	2.63	0.42
1:C:151:LYS:HD3	1:C:196:GLN:OE1	2.20	0.42
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
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
2:F:150:LYS:HG2	2:F:151:ASP:CG	2.45	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:E:133:THR:HG1	2:F:150:LYS:HZ2	1.55	0.40
1:A:10:VAL:O	1:A:105:LEU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:81:MET:HE1	2:B:83:LEU:HG	2.03	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	23
1	C	208/214 (97%)	184 (88%)	17 (8%)	7 (3%)	3	23
1	E	208/214 (97%)	183 (88%)	17 (8%)	8 (4%)	2	20
2	B	220/223 (99%)	195 (89%)	18 (8%)	7 (3%)	3	24
2	D	220/223 (99%)	189 (86%)	23 (10%)	8 (4%)	2	22
2	F	220/223 (99%)	188 (86%)	19 (9%)	13 (6%)	1	12
All	All	1284/1311 (98%)	1118 (87%)	116 (9%)	50 (4%)	2	20

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	178 (100%)	0	100	100
1	C	178/182 (98%)	178 (100%)	0	100	100
1	E	178/182 (98%)	178 (100%)	0	100	100
2	B	188/189 (100%)	188 (100%)	0	100	100
2	D	188/189 (100%)	188 (100%)	0	100	100
2	F	188/189 (100%)	188 (100%)	0	100	100
All	All	1098/1113 (99%)	1098 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	26	ASN
2	D	65	GLN
2	D	211	ASN
1	A	6	GLN
1	A	190	HIS
2	B	65	GLN
1	E	37	GLN
2	F	39	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 oligosaccharides 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	F	301	-	12,12,12	2.34	1 (8%)	15,16,16	2.38	6 (40%)
3	MES	C	301	-	12,12,12	2.35	1 (8%)	15,16,16	2.40	6 (40%)
3	MES	A	301	-	12,12,12	2.34	1 (8%)	15,16,16	2.43	5 (33%)

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	F	301	-	-	4/6/14/14	0/1/1/1
3	MES	C	301	-	-	2/6/14/14	0/1/1/1
3	MES	A	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	-7.87	1.66	1.77
3	A	301	MES	C8-S	-7.84	1.66	1.77
3	F	301	MES	C8-S	-7.83	1.66	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	MES	C5-N4-C3	5.49	120.67	108.84
3	A	301	MES	C5-N4-C3	5.44	120.56	108.84
3	F	301	MES	C5-N4-C3	5.30	120.26	108.84
3	A	301	MES	C6-C5-N4	-3.86	104.25	110.12
3	F	301	MES	C6-C5-N4	-3.57	104.69	110.12
3	F	301	MES	C7-N4-C5	3.46	120.45	111.24
3	A	301	MES	C7-N4-C5	3.42	120.34	111.24
3	C	301	MES	C6-C5-N4	-3.37	105.00	110.12
3	C	301	MES	C7-N4-C5	3.06	119.39	111.24
3	C	301	MES	C7-N4-C3	3.03	119.32	111.24
3	A	301	MES	C7-N4-C3	2.95	119.10	111.24
3	F	301	MES	C7-N4-C3	2.94	119.06	111.24
3	C	301	MES	C2-C3-N4	-2.34	106.56	110.12
3	C	301	MES	O2S-S-C8	2.26	110.15	106.73
3	F	301	MES	O3S-S-C8	2.05	110.02	106.00
3	A	301	MES	O2S-S-C8	2.02	109.77	106.73
3	F	301	MES	C2-C3-N4	-2.00	107.08	110.12

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

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, 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	A	210/214 (98%)	0.18	2 (0%) 79 56	39, 105, 185, 225	0
1	C	210/214 (98%)	0.24	2 (0%) 79 56	55, 123, 204, 246	0
1	E	210/214 (98%)	0.14	2 (0%) 79 56	46, 87, 133, 158	0
2	B	222/223 (99%)	0.17	3 (1%) 73 48	44, 78, 195, 252	0
2	D	222/223 (99%)	0.29	2 (0%) 81 58	58, 105, 207, 257	0
2	F	222/223 (99%)	0.15	4 (1%) 67 42	40, 62, 139, 206	0
All	All	1296/1311 (98%)	0.20	15 (1%) 76 52	39, 89, 195, 257	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	103	ALA	3.2
1	C	129	ALA	3.1
2	F	112	GLN	2.7
1	A	136	CYS	2.5
2	B	56	GLY	2.3
1	A	89	VAL	2.3
2	F	27	TYR	2.2
2	B	149	VAL	2.2
1	E	144	GLY	2.2
2	B	148	LEU	2.1
1	E	82	GLU	2.1
2	D	206	ASN	2.1
1	C	32	VAL	2.1
2	F	69	THR	2.1
2	D	103	ALA	2.1

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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
3	MES	C	301	12/12	0.73	0.17	79,85,94,97	0
3	MES	F	301	12/12	0.75	0.19	75,85,89,93	0
3	MES	A	301	12/12	0.80	0.15	71,91,96,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.