



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:43 PM UTC

PDB ID : 7RD5 / pdb_00007rd5
Title : Crystal structure of Tspan15 large extracellular loop (Tspan15 LEL) in complex with 1C12 Fab
Authors : Lipper, C.H.; Gabriel, K.H.; Seegar, T.C.M.; Durr, K.L.; Tomlinson, M.G.; Blacklow, S.C.
Deposited on : 2021-07-09
Resolution : 3.60 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
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

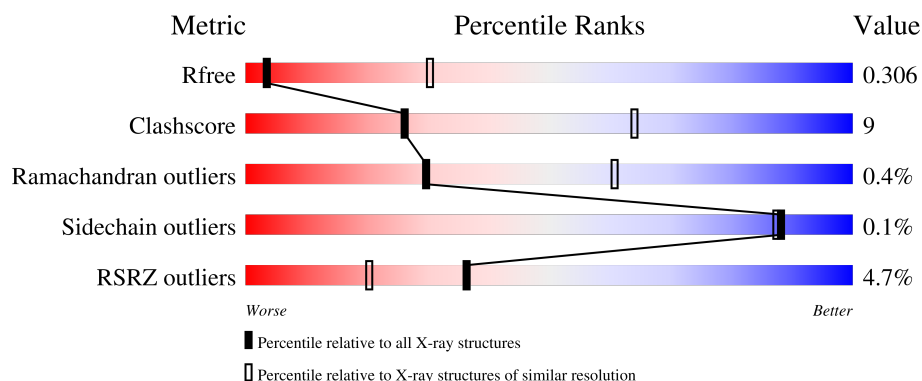
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	220	5% 80% 20%
1	C	220	2% 77% 23%
2	B	226	4% 77% 23%
2	D	226	2% 77% 23%
3	E	122	9% 81% 19%

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Mol	Chain	Length	Quality of chain
3	F	122	11% 83% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8279 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 1C12 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1593	996	262	328	7			
1	C	220	Total	C	N	O	S	0	0	0
			1584	992	261	324	7			

- Molecule 2 is a protein called 1C12 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	226	Total	C	N	O	S	0	0	0
			1614	1035	256	316	7			
2	D	226	Total	C	N	O	S	0	0	0
			1621	1037	258	319	7			

- Molecule 3 is a protein called Tetraspanin-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	122	Total	C	N	O	S	0	0	0
			937	589	154	183	11			
3	E	122	Total	C	N	O	S	0	0	0
			930	587	151	181	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	118	GLN	ASN	engineered mutation	UNP O95858
F	189	ASP	ASN	engineered mutation	UNP O95858
F	231	LEU	-	expression tag	UNP O95858
F	232	GLU	-	expression tag	UNP O95858
F	233	VAL	-	expression tag	UNP O95858
F	234	LEU	-	expression tag	UNP O95858
F	235	PHE	-	expression tag	UNP O95858
F	236	GLN	-	expression tag	UNP O95858

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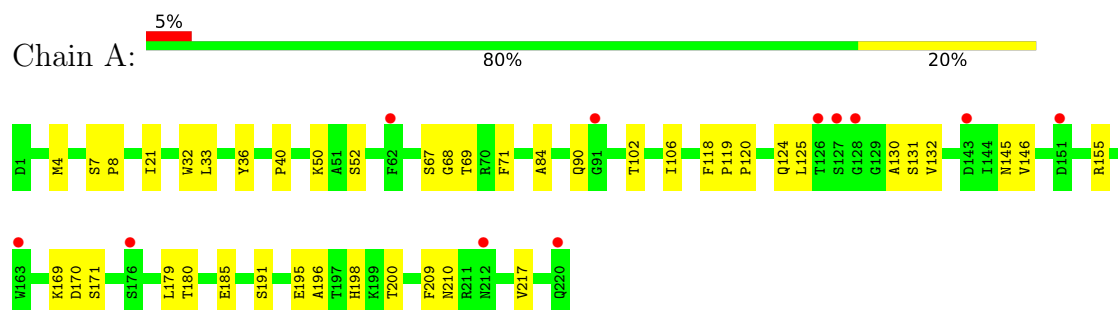
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Chain	Residue	Modelled	Actual	Comment	Reference
E	118	GLN	ASN	engineered mutation	UNP O95858
E	189	ASP	ASN	engineered mutation	UNP O95858
E	231	LEU	-	expression tag	UNP O95858
E	232	GLU	-	expression tag	UNP O95858
E	233	VAL	-	expression tag	UNP O95858
E	234	LEU	-	expression tag	UNP O95858
E	235	PHE	-	expression tag	UNP O95858
E	236	GLN	-	expression tag	UNP O95858

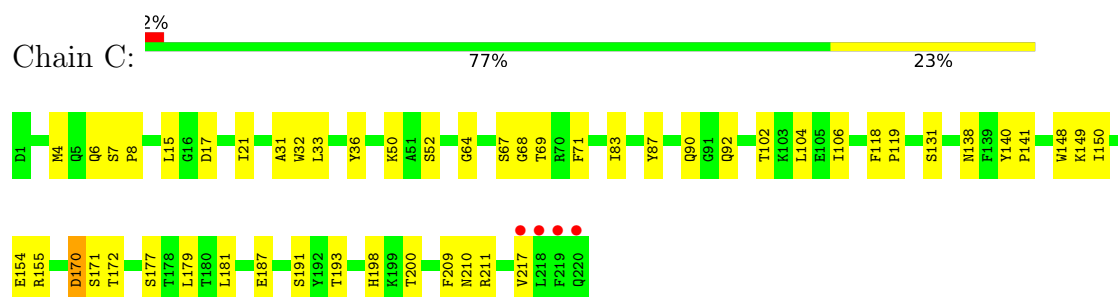
3 Residue-property plots [i](#)

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.

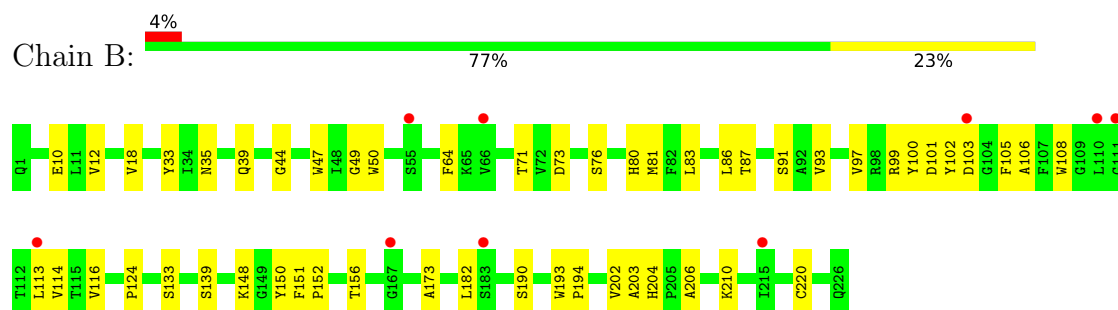
• Molecule 1: 1C12 Fab Light Chain



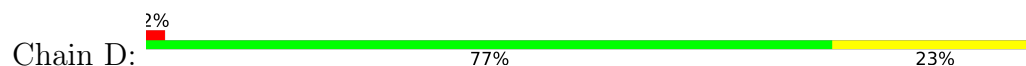
• Molecule 1: 1C12 Fab Light Chain

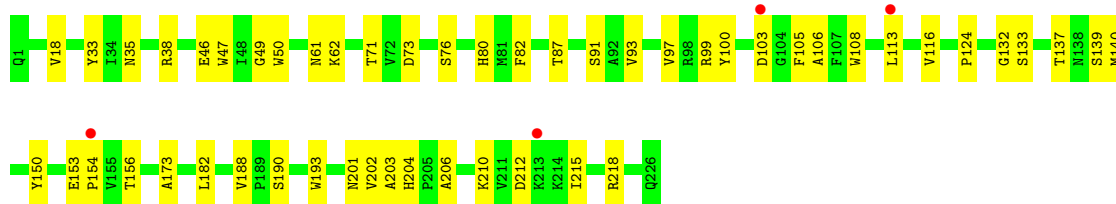


• Molecule 2: 1C12 Fab Heavy Chain

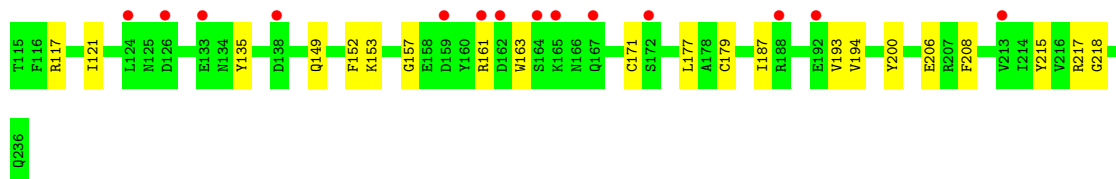
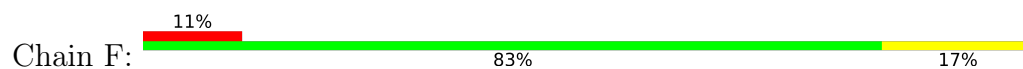


• Molecule 2: 1C12 Fab Heavy Chain

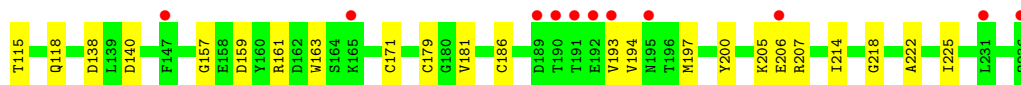
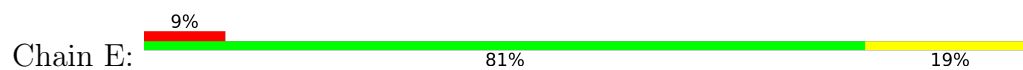




● Molecule 3: Tetraspanin-15



● Molecule 3: Tetraspanin-15



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	171.30Å 124.64Å 116.12Å 90.00° 98.17° 90.00°	Depositor
Resolution (Å)	47.50 – 3.60 47.50 – 3.60	Depositor EDS
% Data completeness (in resolution range)	95.6 (47.50-3.60) 95.8 (47.50-3.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, R_{free}	0.271 , 0.309 0.275 , 0.306	Depositor DCC
R_{free} test set	1983 reflections (7.01%)	wwPDB-VP
Wilson B-factor (Å ²)	121.6	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8279	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5014e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	A	0.17	0/1630	0.43	2/2236 (0.1%)
1	C	0.17	0/1621	0.44	0/2224
2	B	0.16	0/1663	0.41	0/2300
2	D	0.15	0/1669	0.40	0/2308
3	E	0.16	0/950	0.45	0/1294
3	F	0.16	0/957	0.42	0/1302
All	All	0.16	0/8490	0.42	2/11664 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	LYS	CA-C-N	5.04	131.17	121.54
1	A	169	LYS	C-N-CA	5.04	131.17	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	102	TYR	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	1593	0	1428	25	0
1	C	1584	0	1415	37	0
2	B	1614	0	1460	33	0
2	D	1621	0	1472	34	0
3	E	930	0	819	17	0
3	F	937	0	825	14	0
All	All	8279	0	7419	147	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 9.

All (147) 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:81:MET:HE2	2:B:83:LEU:HD11	1.51	0.89
2:D:132:GLY:HA2	2:D:218:ARG:HD2	1.56	0.87
1:C:149:LYS:HE2	1:C:154:GLU:HG3	1.60	0.84
1:C:106:ILE:HG21	1:C:171:SER:HB3	1.57	0.84
2:D:91:SER:HB2	2:D:116:VAL:HG22	1.61	0.83
1:C:155:ARG:HH12	1:C:181:LEU:HG	1.57	0.68
2:B:124:PRO:HB3	2:B:150:TYR:HB3	1.77	0.67
2:B:100:TYR:HB2	2:B:106:ALA:HB2	1.76	0.67
2:B:91:SER:HB2	2:B:116:VAL:HG22	1.76	0.67
3:F:149:GLN:HE22	3:F:163:TRP:HE1	1.43	0.67
1:C:217:VAL:HG21	2:D:133:SER:HB3	1.76	0.66
1:A:155:ARG:NH2	1:A:185:GLU:OE2	2.27	0.66
2:D:35:ASN:OD1	2:D:50:TRP:HB3	1.97	0.64
2:B:99:ARG:NH2	2:B:103:ASP:OD1	2.31	0.63
2:D:97:VAL:HG12	2:D:108:TRP:HA	1.81	0.62
2:D:100:TYR:HB2	2:D:106:ALA:HB2	1.80	0.62
1:A:180:THR:OG1	2:B:148:LYS:NZ	2.33	0.62
3:F:171:CYS:HA	3:F:179:CYS:HB2	1.82	0.61
2:D:87:THR:O	2:D:116:VAL:HG21	2.02	0.60
2:B:71:THR:HG23	2:B:80:HIS:HB2	1.84	0.60
1:A:106:ILE:HG21	1:A:171:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:152:PHE:O	3:F:217:ARG:NH2	2.34	0.60
1:C:198:HIS:O	1:C:200:THR:N	2.26	0.60
1:A:4:MET:HE3	1:A:90:GLN:HG2	1.84	0.59
2:B:173:ALA:HB2	2:B:182:LEU:HB2	1.83	0.59
1:A:7:SER:HB3	1:A:8:PRO:HD3	1.85	0.58
2:B:87:THR:O	2:B:116:VAL:HG21	2.03	0.58
2:D:173:ALA:HB2	2:D:182:LEU:HB2	1.84	0.58
1:A:198:HIS:O	1:A:200:THR:N	2.33	0.58
2:B:93:VAL:HG22	2:B:113:LEU:HD13	1.87	0.57
1:C:187:GLU:HG2	1:C:211:ARG:HD2	1.85	0.57
2:D:124:PRO:HB3	2:D:150:TYR:HB3	1.87	0.57
2:D:204:HIS:CE1	2:D:206:ALA:HB3	2.40	0.57
1:C:7:SER:HB3	1:C:8:PRO:HD3	1.87	0.57
3:E:186:CYS:HA	3:E:214:ILE:HG22	1.87	0.56
1:C:33:LEU:HD13	1:C:71:PHE:CD2	2.40	0.56
2:D:93:VAL:HG22	2:D:113:LEU:HD13	1.87	0.56
1:C:170:ASP:OD1	1:C:171:SER:N	2.39	0.55
1:A:8:PRO:HD2	1:A:21:ILE:HG23	1.90	0.54
2:B:204:HIS:CE1	2:B:206:ALA:HB3	2.42	0.54
1:C:32:TRP:CG	3:E:205:LYS:HZ3	2.26	0.54
2:D:38:ARG:NH2	2:D:46:GLU:OE1	2.40	0.54
2:D:204:HIS:HE1	2:D:206:ALA:HB3	1.73	0.53
3:E:159:ASP:HB3	3:E:207:ARG:HH21	1.71	0.53
1:C:119:PRO:HB3	1:C:209:PHE:CZ	2.44	0.52
1:C:50:LYS:O	1:C:52:SER:N	2.37	0.52
1:A:119:PRO:HB3	1:A:209:PHE:CZ	2.45	0.52
3:E:161:ARG:NH2	3:E:206:GLU:HA	2.24	0.52
1:C:32:TRP:CD1	3:E:205:LYS:HZ3	2.28	0.51
2:B:139:SER:O	2:B:190:SER:OG	2.24	0.51
3:F:117:ARG:O	3:F:121:ILE:HG12	2.11	0.51
1:A:191:SER:HA	1:A:210:ASN:HA	1.94	0.50
1:C:191:SER:HA	1:C:210:ASN:HA	1.94	0.50
2:D:156:THR:HB	2:D:203:ALA:HB3	1.92	0.50
2:B:12:VAL:HG11	2:B:18:VAL:HG12	1.94	0.50
2:D:47:TRP:CH2	2:D:49:GLY:HA2	2.46	0.50
1:C:21:ILE:HG21	1:C:102:THR:HG21	1.93	0.50
1:A:145:ASN:O	1:A:196:ALA:HA	2.12	0.50
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.47	0.48
3:F:193:VAL:HG22	3:F:194:VAL:H	1.77	0.48
1:A:33:LEU:HD13	1:A:71:PHE:CD1	2.47	0.48
1:A:50:LYS:O	1:A:52:SER:N	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:PRO:HD2	1:C:21:ILE:HG23	1.95	0.48
1:A:120:PRO:HG2	1:A:130:ALA:HB1	1.96	0.48
2:B:204:HIS:HE1	2:B:206:ALA:HB3	1.79	0.48
1:A:67:SER:O	1:A:69:THR:N	2.47	0.47
1:C:150:ILE:HD11	1:C:155:ARG:HH11	1.79	0.47
1:A:32:TRP:CE3	1:A:50:LYS:HE2	2.50	0.47
1:C:67:SER:O	1:C:69:THR:N	2.47	0.47
2:D:71:THR:CG2	2:D:80:HIS:HB2	2.45	0.47
2:B:18:VAL:HG22	2:B:83:LEU:HB2	1.97	0.47
2:B:73:ASP:OD2	2:B:76:SER:OG	2.26	0.47
3:E:171:CYS:HA	3:E:179:CYS:HB2	1.97	0.46
2:B:156:THR:HB	2:B:203:ALA:HB3	1.96	0.46
3:E:222:ALA:HA	3:E:225:ILE:HG12	1.96	0.46
2:D:99:ARG:NH2	2:D:103:ASP:OD1	2.43	0.46
3:E:197:MET:HA	3:E:200:TYR:CE1	2.50	0.46
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.97	0.46
1:A:217:VAL:HG21	2:B:133:SER:HB3	1.98	0.46
2:B:35:ASN:OD1	2:B:50:TRP:HB3	2.14	0.46
2:B:99:ARG:HB3	2:B:105:PHE:HD1	1.81	0.46
3:F:157:GLY:O	3:F:218:GLY:HA3	2.16	0.46
1:C:4:MET:HE3	1:C:90:GLN:HG2	1.98	0.46
1:C:118:PHE:HA	1:C:119:PRO:HD3	1.80	0.46
1:C:140:TYR:CD1	1:C:141:PRO:HA	2.51	0.45
1:A:124:GLN:HE22	1:A:131:SER:CB	2.29	0.45
2:B:10:GLU:HB2	2:B:114:VAL:HG22	1.98	0.45
3:E:115:THR:HB	3:E:118:GLN:HB3	1.98	0.45
3:F:161:ARG:NH2	3:F:206:GLU:HA	2.31	0.45
2:D:173:ALA:HB2	2:D:182:LEU:HD12	1.99	0.45
3:F:187:ILE:HA	3:F:215:TYR:CZ	2.52	0.45
2:D:139:SER:O	2:D:190:SER:OG	2.27	0.45
1:A:146:VAL:HA	1:A:195:GLU:O	2.17	0.44
1:C:148:TRP:HE1	1:C:177:SER:HB3	1.82	0.44
1:A:36:TYR:CE2	2:B:105:PHE:HB2	2.53	0.44
1:A:118:PHE:HA	1:A:119:PRO:HD3	1.84	0.44
2:B:39:GLN:HG3	2:B:44:GLY:O	2.17	0.44
1:C:6:GLN:HE22	1:C:87:TYR:HA	1.82	0.44
1:C:106:ILE:HG21	1:C:171:SER:CB	2.38	0.44
1:C:131:SER:HA	1:C:179:LEU:O	2.17	0.44
1:C:155:ARG:HH12	1:C:181:LEU:CG	2.27	0.44
2:B:97:VAL:HG12	2:B:108:TRP:HA	1.99	0.44
3:E:159:ASP:N	3:E:159:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:163:TRP:CD1	3:E:181:VAL:HG23	2.53	0.44
2:B:202:VAL:O	2:B:210:LYS:HA	2.17	0.44
2:B:151:PHE:HA	2:B:152:PRO:HA	1.84	0.43
2:B:86:LEU:HB3	2:B:116:VAL:HG11	2.01	0.43
1:C:104:LEU:HD12	1:C:104:LEU:HA	1.75	0.43
1:C:138:ASN:HA	1:C:172:THR:OG1	2.18	0.43
1:C:92:GLN:HA	3:E:205:LYS:HZ1	1.83	0.43
3:F:177:LEU:HD23	3:F:200:TYR:CE1	2.53	0.43
1:C:36:TYR:CE1	2:D:105:PHE:HB2	2.54	0.43
2:D:202:VAL:O	2:D:210:LYS:HA	2.19	0.43
2:B:33:TYR:N	3:F:206:GLU:OE2	2.45	0.43
3:E:193:VAL:HG22	3:E:194:VAL:N	2.34	0.43
3:F:135:TYR:CD1	3:F:163:TRP:HH2	2.36	0.43
2:B:101:ASP:O	3:F:208:PHE:HB2	2.19	0.42
2:B:193:TRP:HA	2:B:194:PRO:HA	1.77	0.42
1:C:154:GLU:H	1:C:154:GLU:CD	2.27	0.42
2:D:140:MET:HB3	2:D:188:VAL:O	2.19	0.42
3:E:138:ASP:OD1	3:E:140:ASP:HB2	2.19	0.42
1:C:149:LYS:HB2	1:C:193:THR:HB	2.00	0.42
2:D:18:VAL:O	2:D:82:PHE:HA	2.19	0.42
2:D:99:ARG:HA	2:D:105:PHE:HA	2.02	0.42
2:D:193:TRP:CH2	2:D:215:ILE:HG22	2.54	0.42
3:E:157:GLY:O	3:E:218:GLY:HA3	2.20	0.42
3:F:153:LYS:HG2	3:F:215:TYR:CZ	2.55	0.41
2:D:113:LEU:HD23	2:D:154:PRO:HD3	2.01	0.41
1:A:120:PRO:HB2	1:A:125:LEU:CD1	2.50	0.41
2:B:99:ARG:HG3	3:F:206:GLU:OE1	2.21	0.41
1:A:40:PRO:HD3	1:A:84:ALA:HA	2.02	0.41
2:D:71:THR:HG22	2:D:80:HIS:HB2	2.02	0.41
1:C:52:SER:HA	1:C:64:GLY:O	2.21	0.41
2:D:150:TYR:HE1	2:D:153:GLU:HA	1.84	0.41
1:C:31:ALA:O	1:C:50:LYS:HD3	2.21	0.41
3:E:193:VAL:HG22	3:E:194:VAL:H	1.85	0.41
1:C:83:ILE:HD11	1:C:106:ILE:HB	2.02	0.40
2:D:33:TYR:HE1	3:E:161:ARG:NH2	2.19	0.40
2:D:61:ASN:OD1	2:D:62:LYS:N	2.55	0.40
2:D:137:THR:O	2:D:139:SER:N	2.53	0.40
2:D:201:ASN:HD22	2:D:212:ASP:CG	2.29	0.40
2:D:73:ASP:HB3	2:D:76:SER:HB2	2.03	0.40
1:C:15:LEU:C	1:C:17:ASP:H	2.30	0.40
1:A:21:ILE:HG21	1:A:102:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:SER:HA	1:A:179:LEU:O	2.21	0.40
2:B:64:PHE:CD1	2:B:64:PHE:N	2.90	0.40
1:C:32:TRP:HE3	2:D:103:ASP:OD2	2.04	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	218/220 (99%)	203 (93%)	13 (6%)	2 (1%)	14	46
1	C	218/220 (99%)	202 (93%)	14 (6%)	2 (1%)	14	46
2	B	224/226 (99%)	219 (98%)	5 (2%)	0	100	100
2	D	224/226 (99%)	219 (98%)	5 (2%)	0	100	100
3	E	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
3	F	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
All	All	1124/1136 (99%)	1066 (95%)	54 (5%)	4 (0%)	30	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY
1	C	68	GLY
1	A	170	ASP
1	C	170	ASP

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	168/196 (86%)	168 (100%)	0	100	100
1	C	165/196 (84%)	165 (100%)	0	100	100
2	B	168/196 (86%)	167 (99%)	1 (1%)	78	79
2	D	170/196 (87%)	170 (100%)	0	100	100
3	E	96/112 (86%)	96 (100%)	0	100	100
3	F	97/112 (87%)	97 (100%)	0	100	100
All	All	864/1008 (86%)	863 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	220	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	138	ASN
2	B	80	HIS
2	B	169	HIS
3	F	230	ASN
1	C	6	GLN
1	C	37	GLN
1	C	138	ASN
1	C	161	ASN
1	C	190	ASN

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 [i](#)

There are no oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	220/220 (100%)	0.51	11 (5%) 34 19	103, 137, 180, 216	0
1	C	220/220 (100%)	0.40	4 (1%) 67 40	90, 119, 167, 213	0
2	B	226/226 (100%)	0.41	9 (3%) 42 24	105, 135, 165, 231	0
2	D	226/226 (100%)	0.34	4 (1%) 67 40	87, 121, 149, 201	0
3	E	122/122 (100%)	0.71	11 (9%) 15 11	82, 105, 191, 263	0
3	F	122/122 (100%)	0.74	14 (11%) 9 8	95, 117, 154, 222	0
All	All	1136/1136 (100%)	0.48	53 (4%) 36 20	82, 125, 172, 263	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	110	LEU	7.4
2	B	103	ASP	5.8
3	E	192	GLU	5.2
1	A	126	THR	5.0
1	A	128	GLY	5.0
3	F	133	GLU	4.4
3	F	188	ARG	4.3
3	E	147	PHE	4.1
1	C	220	GLN	4.1
2	B	111	GLY	4.0
2	D	154	PRO	3.6
1	A	143	ASP	3.4
2	D	113	LEU	3.4
3	F	162	ASP	3.4
2	B	113	LEU	3.3
1	A	91	GLY	3.2
2	D	213	LYS	3.2
3	E	190	THR	3.1
2	D	103	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASP	2.9
3	E	236	GLN	2.8
1	A	62	PHE	2.8
3	E	195	ASN	2.7
3	E	165	LYS	2.7
3	E	189	ASP	2.7
3	F	164	SER	2.6
3	F	172	SER	2.6
3	F	165	LYS	2.6
1	C	219	PHE	2.6
1	C	217	VAL	2.5
3	E	191	THR	2.5
3	F	159	ASP	2.4
3	E	193	VAL	2.4
3	E	206	GLU	2.4
1	A	220	GLN	2.4
2	B	66	VAL	2.4
3	F	192	GLU	2.4
3	F	167	GLN	2.3
3	F	161	ARG	2.3
3	F	138	ASP	2.3
2	B	55	SER	2.3
2	B	183	SER	2.3
1	A	163	TRP	2.2
3	F	124	LEU	2.2
1	A	176	SER	2.1
3	F	213	VAL	2.1
1	A	212	ASN	2.1
1	A	127	SER	2.1
2	B	215	ILE	2.1
3	E	231	LEU	2.1
2	B	167	GLY	2.1
3	F	126	ASP	2.0
1	C	218	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.