



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2025 – 04:12 PM JST

PDB ID : 9LF8 / pdb_00009lf8
Title : Structure of MPXV M1R and mMM1-16 Fab complex
Authors : Zhang, Y.; Zhao, R.C.; Wu, L.L.; Wang, Q.H.
Deposited on : 2025-01-08
Resolution : 2.70 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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

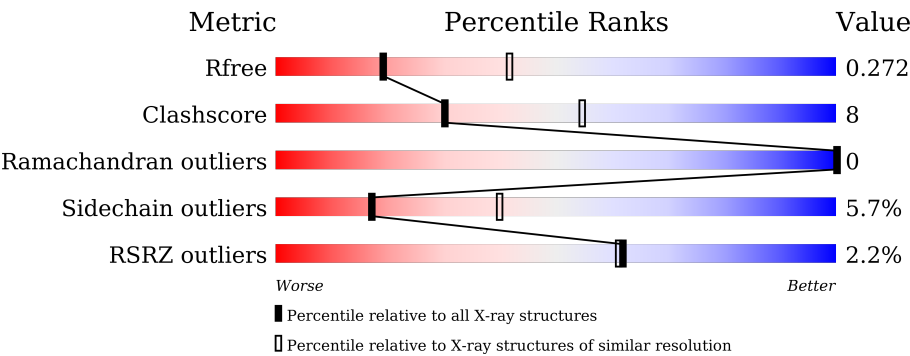
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	C	215	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>74%22%..</div></div>
1	E	215	<div><div>4%</div><div></div><div></div><div></div><div></div></div> <div>64%24%9%</div>
1	J	215	<div><div></div><div></div><div></div><div></div><div></div></div> <div>79%20%.</div>
1	L	215	<div><div></div><div></div><div></div><div></div><div></div></div> <div>87%12%.</div>
2	Q	181	<div><div></div><div></div><div></div><div></div><div></div></div> <div>80%12%7%</div>
2	R	181	<div><div>3%</div><div></div><div></div><div></div><div></div></div> <div>61%25%13%</div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	S	181	
2	T	181	
3	D	225	
3	F	225	
3	H	225	
3	O	225	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17006 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 mMM1-16 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	196	Total	C	N	O	S	0	0	0
			1496	933	254	304	5			
1	C	212	Total	C	N	O	S	0	0	0
			1628	1019	276	328	5			
1	L	212	Total	C	N	O	S	0	0	0
			1634	1022	279	328	5			
1	J	212	Total	C	N	O	S	0	0	0
			1634	1022	279	328	5			

- Molecule 2 is a protein called Entry-fusion complex associated protein OPG095.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	158	Total	C	N	O	S	0	0	0
			1192	736	198	249	9			
2	S	128	Total	C	N	O	S	0	0	0
			955	586	162	200	7			
2	Q	169	Total	C	N	O	S	0	0	0
			1263	776	215	263	9			
2	T	122	Total	C	N	O	S	0	0	0
			923	562	161	192	8			

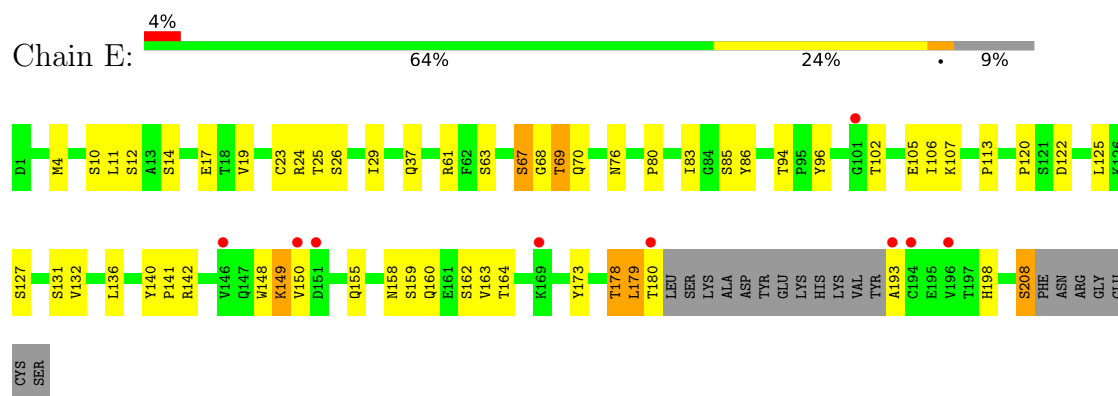
- Molecule 3 is a protein called mMM1-16 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	196	Total	C	N	O	S	0	0	0
			1475	939	242	288	6			
3	D	214	Total	C	N	O	S	0	0	0
			1602	1016	264	316	6			
3	H	214	Total	C	N	O	S	0	0	0
			1602	1016	264	316	6			
3	O	214	Total	C	N	O	S	0	0	0
			1602	1016	264	316	6			

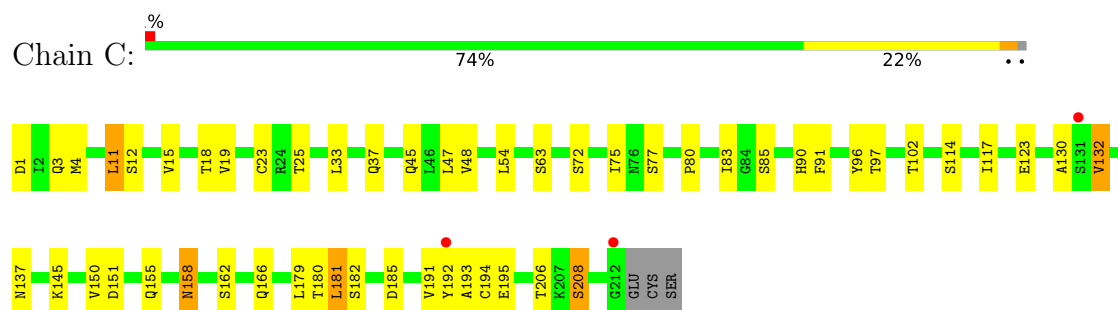
3 Residue-property plots

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.

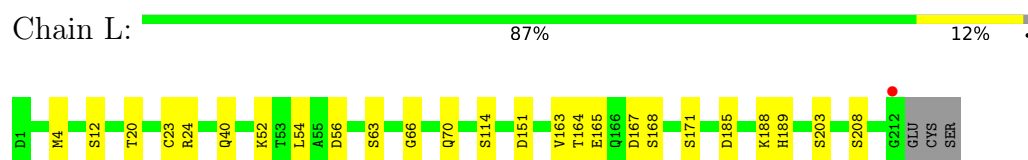
- Molecule 1: mMM1-16 Fab light chain



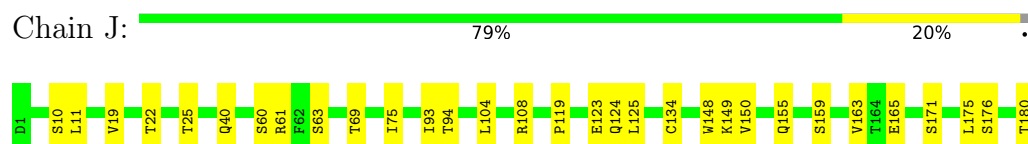
- Molecule 1: mMM1-16 Fab light chain



- Molecule 1: mMM1-16 Fab light chain



- Molecule 1: mMM1-16 Fab light chain

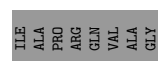
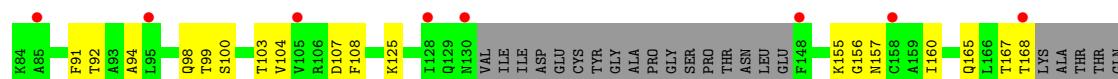
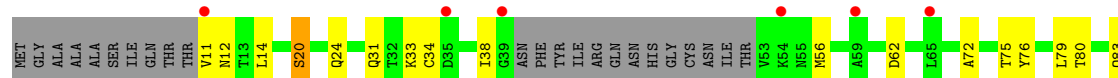




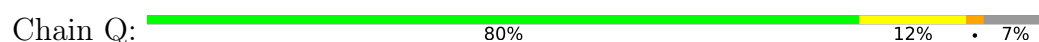
• Molecule 2: Entry-fusion complex associated protein OPG095



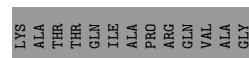
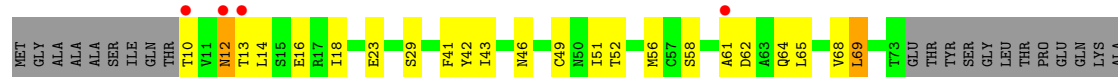
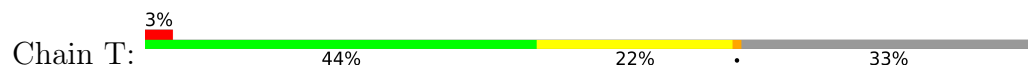
• Molecule 2: Entry-fusion complex associated protein OPG095



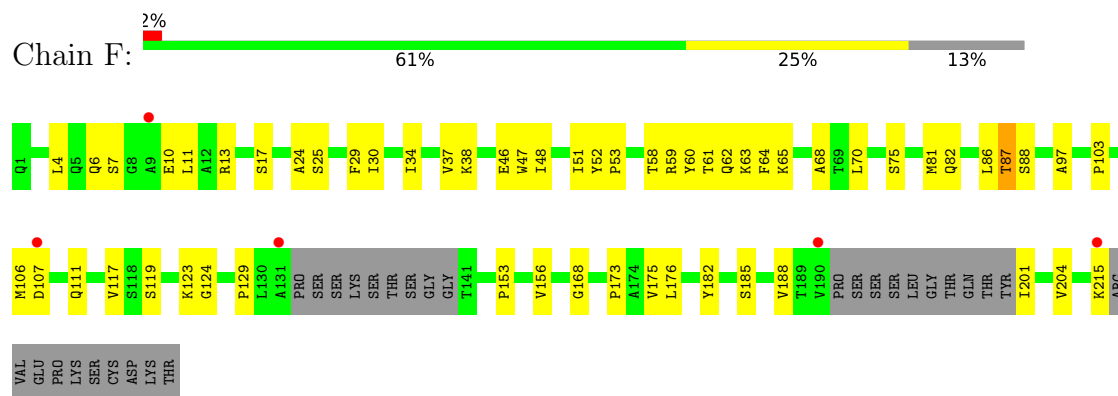
• Molecule 2: Entry-fusion complex associated protein OPG095



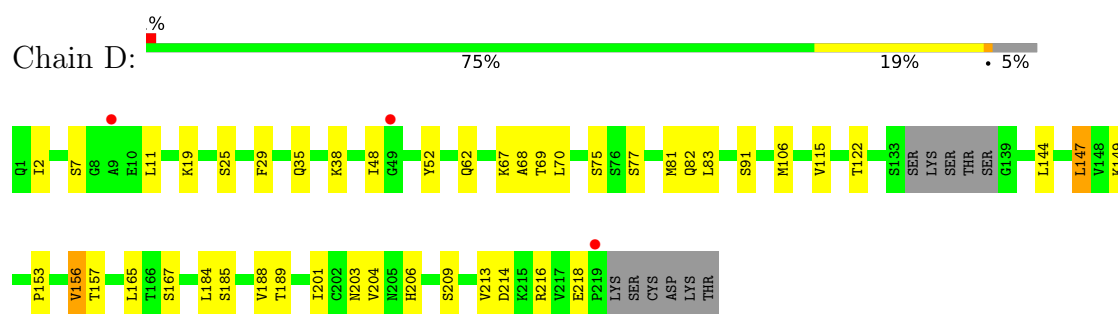
• Molecule 2: Entry-fusion complex associated protein OPG095



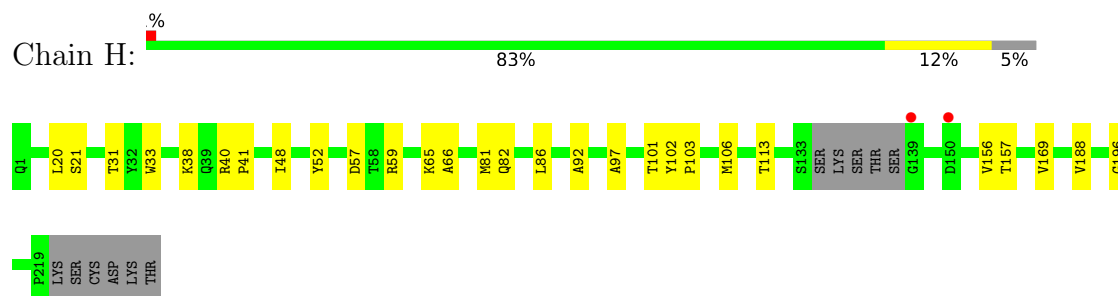
- Molecule 3: mMM1-16 Fab heavy chain



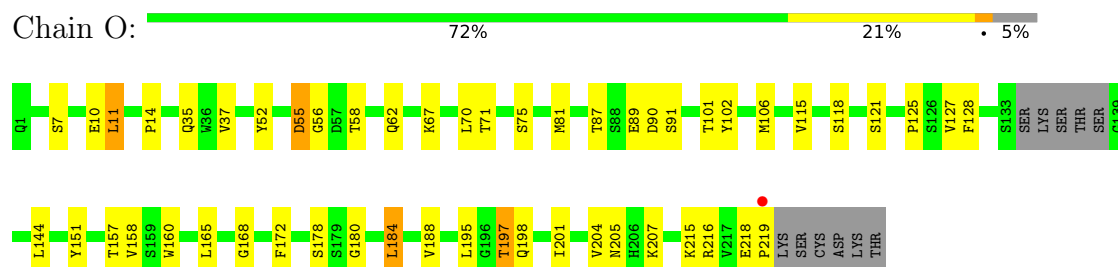
- Molecule 3: mMM1-16 Fab heavy chain



- Molecule 3: mMM1-16 Fab heavy chain



- Molecule 3: mMM1-16 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	177.38Å 177.38Å 90.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.34 – 2.70 44.34 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.34-2.70) 99.9 (44.34-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.202 , 0.274 0.201 , 0.272	Depositor DCC
R_{free} test set	3853 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17006	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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 [i](#)

5.1 Standard geometry [i](#)

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	C	0.44	0/1664	0.66	0/2261
1	E	0.38	0/1527	0.63	0/2076
1	J	0.50	0/1670	0.72	0/2268
1	L	0.51	0/1670	0.73	0/2268
2	Q	0.49	0/1276	0.69	0/1733
2	R	0.34	0/1201	0.53	0/1627
2	S	0.32	0/960	0.49	0/1297
2	T	0.50	0/926	0.72	0/1248
3	D	0.39	0/1642	0.55	0/2239
3	F	0.38	0/1510	0.57	0/2056
3	H	0.46	0/1642	0.74	3/2239 (0.1%)
3	O	0.46	0/1642	0.72	3/2239 (0.1%)
All	All	0.44	0/17330	0.66	6/23551 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	102	TYR	N-CA-C	-7.18	100.13	110.40
3	O	102	TYR	N-CA-C	-6.58	100.50	110.50
3	H	101	THR	N-CA-C	-5.96	104.91	111.82
3	H	102	TYR	CB-CA-C	5.61	117.27	108.63
3	O	101	THR	N-CA-C	-5.46	105.49	111.82
3	O	102	TYR	CB-CA-C	5.15	116.79	108.91

There are no chirality outliers.

There are no planarity outliers.

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	C	1628	0	1576	26	0
1	E	1496	0	1451	39	0
1	J	1634	0	1587	23	0
1	L	1634	0	1587	8	0
2	Q	1263	0	1245	19	0
2	R	1192	0	1180	34	0
2	S	955	0	949	20	0
2	T	923	0	909	24	0
3	D	1602	0	1569	21	0
3	F	1475	0	1448	37	0
3	H	1602	0	1569	15	0
3	O	1602	0	1569	28	0
All	All	17006	0	16639	280	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 8.

All (280) 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)
1:E:120:PRO:HD3	1:E:132:VAL:HG12	1.52	0.88
3:O:205:ASN:HD21	3:O:207:LYS:HD2	1.38	0.86
1:E:132:VAL:HG22	1:E:179:LEU:HB3	1.58	0.86
1:E:155:GLN:HB3	1:E:158:ASN:HD21	1.41	0.83
1:C:155:GLN:HB3	1:C:158:ASN:HD21	1.44	0.82
2:Q:17:ARG:HH21	2:Q:74:GLU:HB3	1.48	0.78
3:O:35:GLN:HB2	3:O:106:MET:HE3	1.67	0.75
2:T:41:PHE:HE1	2:T:133:ILE:HD11	1.51	0.75
2:Q:70:SER:O	2:Q:74:GLU:HG2	1.89	0.72
3:H:48:ILE:HD13	3:H:81:MET:HE1	1.71	0.71
2:T:133:ILE:HG22	2:T:134:ASP:H	1.56	0.70
2:Q:45:GLN:HB2	2:Q:135:GLU:HG2	1.73	0.70
1:C:4:MET:HE2	1:C:23:CYS:SG	2.30	0.70
2:Q:41:PHE:HD1	2:Q:131:VAL:HB	1.54	0.70
3:F:82:GLN:HE22	2:T:128:ILE:CD1	2.05	0.70
1:E:25:THR:HG21	1:E:29:ILE:HD13	1.74	0.70
3:F:38:LYS:HD3	3:F:46:GLU:OE2	1.92	0.69
3:H:169:VAL:HG22	3:H:188:VAL:HG22	1.75	0.68
1:J:11:LEU:HB3	1:J:104:LEU:HD12	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:48:ILE:HG21	3:H:81:MET:CE	2.24	0.68
1:C:11:LEU:HD11	1:C:19:VAL:HB	1.76	0.67
2:Q:41:PHE:CE2	2:Q:51:ILE:HB	2.30	0.67
1:C:151:ASP:HA	1:C:191:VAL:HB	1.78	0.66
3:F:82:GLN:NE2	2:T:128:ILE:HD11	2.10	0.66
1:E:193:ALA:HB2	1:E:208:SER:HB3	1.77	0.65
1:C:193:ALA:HB2	1:C:208:SER:HB2	1.79	0.65
2:R:105:VAL:O	2:R:109:GLU:HG3	1.95	0.65
2:Q:41:PHE:HE2	2:Q:51:ILE:HB	1.62	0.65
1:E:67:SER:OG	1:E:68:GLY:N	2.27	0.65
2:Q:41:PHE:CD1	2:Q:131:VAL:HB	2.32	0.63
3:D:204:VAL:HB	3:D:213:VAL:HG13	1.80	0.63
2:S:62:ASP:OD1	2:S:155:LYS:NZ	2.29	0.63
1:E:83:ILE:HD11	1:E:106:ILE:HG13	1.81	0.63
3:O:14:PRO:HD3	3:O:118:SER:O	1.99	0.63
3:O:160:TRP:HB3	3:O:165:LEU:HD23	1.80	0.63
2:T:69:LEU:HD21	2:T:112:VAL:HG11	1.81	0.63
1:E:80:PRO:HA	1:E:106:ILE:HD12	1.82	0.62
2:S:91:PHE:HZ	2:S:108:PHE:HB2	1.64	0.62
1:C:132:VAL:HG13	1:C:179:LEU:HB3	1.81	0.62
2:Q:51:ILE:HD12	2:Q:51:ILE:O	2.00	0.62
2:T:43:ILE:HG23	2:T:133:ILE:HB	1.81	0.61
3:H:48:ILE:HG21	3:H:81:MET:HE1	1.82	0.61
1:C:130:ALA:HB3	1:C:181:LEU:HD12	1.83	0.61
2:S:79:LEU:HD22	2:S:83:GLN:HB3	1.82	0.60
3:H:20:LEU:HD22	3:H:113:THR:HG21	1.83	0.60
3:D:216:ARG:NH1	3:D:218:GLU:OE2	2.34	0.60
1:E:122:ASP:HA	1:E:125:LEU:HD12	1.86	0.58
3:O:125:PRO:HB3	3:O:151:TYR:HB3	1.86	0.58
3:O:52:TYR:HD2	3:O:55:ASP:HB2	1.69	0.58
3:F:201:ILE:HD12	3:F:201:ILE:O	2.03	0.58
1:L:185:ASP:HA	1:L:188:LYS:HD3	1.84	0.58
3:D:201:ILE:HD12	3:D:214:ASP:HB3	1.86	0.57
3:O:37:VAL:HG23	3:O:106:MET:HE1	1.84	0.57
2:R:18:ILE:O	2:R:22:LEU:HB2	2.04	0.57
3:F:62:GLN:HA	3:F:65:LYS:HE3	1.86	0.57
2:T:14:LEU:HD11	2:T:163:LEU:HD22	1.87	0.57
3:O:67:LYS:NZ	3:O:90:ASP:OD1	2.30	0.57
3:F:70:LEU:CD2	3:F:81:MET:HG3	2.35	0.56
2:S:20:SER:C	2:S:24:GLN:HE21	2.13	0.56
2:Q:43:ILE:HD13	2:Q:51:ILE:HG12	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:12:ASN:O	2:Q:16:GLU:HG3	2.04	0.56
3:F:97:ALA:HB1	3:F:106:MET:HB3	1.87	0.56
1:C:123:GLU:OE1	1:C:123:GLU:N	2.33	0.56
3:F:82:GLN:NE2	2:T:128:ILE:CD1	2.69	0.56
1:J:149:LYS:NZ	1:J:195:GLU:OE1	2.37	0.56
2:S:100:SER:HG	2:S:103:THR:HG1	1.50	0.56
3:O:195:LEU:HD21	3:O:219:PRO:HD3	1.86	0.56
1:C:155:GLN:HB3	1:C:158:ASN:ND2	2.18	0.55
2:Q:17:ARG:HH21	2:Q:74:GLU:CB	2.18	0.55
3:O:216:ARG:HD2	3:O:218:GLU:HG3	1.87	0.55
1:J:123:GLU:OE1	1:J:123:GLU:N	2.23	0.55
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.87	0.55
2:R:8:GLN:O	2:R:12:ASN:ND2	2.39	0.55
1:C:90:HIS:CD2	1:C:97:THR:HG22	2.43	0.54
2:T:14:LEU:O	2:T:18:ILE:HG13	2.07	0.54
2:T:52:THR:HG23	2:T:147:GLU:HA	1.90	0.54
3:F:38:LYS:HB2	3:F:48:ILE:HD11	1.88	0.54
2:R:125:LYS:HD2	3:F:52:TYR:CD2	2.43	0.54
3:F:201:ILE:HG22	3:F:215:LYS:O	2.08	0.54
3:O:168:GLY:O	3:O:188:VAL:HA	2.07	0.54
3:F:13:ARG:HD2	2:T:51:ILE:HB	1.90	0.54
2:T:41:PHE:CE1	2:T:133:ILE:HD11	2.39	0.54
1:C:4:MET:HG2	1:C:25:THR:HG22	1.89	0.54
3:D:52:TYR:CD2	2:S:125:LYS:HG3	2.43	0.54
3:O:37:VAL:CG2	3:O:106:MET:HE1	2.39	0.53
3:H:57:ASP:CG	3:H:59:ARG:HH12	2.16	0.53
3:D:11:LEU:HB2	3:D:153:PRO:HG3	1.91	0.53
1:E:193:ALA:CB	1:E:208:SER:HB3	2.39	0.53
1:J:25:THR:O	1:J:69:THR:HB	2.09	0.53
3:O:127:VAL:O	3:O:215:LYS:HD3	2.08	0.53
3:F:70:LEU:HD23	3:F:81:MET:HG3	1.90	0.52
2:Q:43:ILE:CD1	2:Q:51:ILE:HG12	2.39	0.52
3:O:197:THR:OG1	3:O:198:GLN:N	2.41	0.52
1:E:141:PRO:HD2	1:E:198:HIS:CE1	2.45	0.52
1:E:11:LEU:HD23	1:E:19:VAL:HG13	1.92	0.52
3:O:158:VAL:HG22	3:O:204:VAL:HG22	1.92	0.52
3:H:65:LYS:O	3:H:66:ALA:HB3	2.09	0.52
1:E:155:GLN:HB3	1:E:158:ASN:ND2	2.19	0.51
1:C:15:VAL:HG22	1:C:80:PRO:HD3	1.92	0.51
2:R:95:LEU:HD22	2:R:111:TYR:CZ	2.45	0.51
2:R:7:ILE:O	2:R:11:VAL:HG23	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:76:TYR:CZ	2:R:104:VAL:HG11	2.46	0.51
1:C:1:ASP:OD1	1:C:1:ASP:N	2.41	0.51
1:L:4:MET:HE2	1:L:23:CYS:SG	2.52	0.50
2:R:65:LEU:HD11	2:R:112:VAL:CG1	2.42	0.50
1:C:150:VAL:HG22	1:C:192:TYR:CD1	2.46	0.50
1:E:132:VAL:HG23	1:E:148:TRP:CH2	2.47	0.50
2:R:36:ILE:HD12	2:R:153:SER:HA	1.93	0.50
2:R:43:ILE:HG23	2:R:133:ILE:HD11	1.94	0.50
3:D:29:PHE:CD2	3:D:77:SER:HA	2.47	0.50
3:D:38:LYS:HB2	3:D:48:ILE:HD11	1.93	0.50
1:E:113:PRO:HB3	1:E:136:LEU:HB3	1.93	0.49
2:R:60:ASP:O	2:R:64:GLN:HG3	2.12	0.49
3:H:196:GLY:HA3	2:T:42:TYR:CZ	2.47	0.49
1:E:120:PRO:CD	1:E:132:VAL:HG12	2.36	0.49
2:R:76:TYR:O	2:R:79:LEU:HB2	2.12	0.49
2:Q:95:LEU:O	2:Q:97:ILE:HD13	2.13	0.49
1:E:14:SER:HB2	1:E:17:GLU:OE2	2.13	0.49
2:R:8:GLN:HG3	2:R:12:ASN:HD21	1.77	0.49
3:D:68:ALA:HA	3:D:82:GLN:O	2.13	0.49
3:F:87:THR:OG1	3:F:88:SER:N	2.44	0.49
3:F:68:ALA:HA	3:F:82:GLN:O	2.13	0.49
1:C:137:ASN:ND2	3:D:189:THR:HG21	2.28	0.48
2:S:167:THR:OG1	2:S:168:THR:N	2.46	0.48
3:H:41:PRO:HD3	3:H:92:ALA:HA	1.95	0.48
2:T:161:LYS:O	2:T:165:GLN:N	2.44	0.48
2:S:99:THR:HB	2:S:107:ASP:OD2	2.12	0.48
2:T:10:THR:O	2:T:13:THR:HG22	2.14	0.48
1:E:25:THR:OG1	1:E:69:THR:HA	2.13	0.48
1:E:96:TYR:HB2	3:F:47:TRP:CD2	2.48	0.48
3:F:29:PHE:CE2	3:F:53:PRO:HB3	2.49	0.48
1:J:150:VAL:HG22	1:J:192:TYR:CD1	2.49	0.48
1:C:195:GLU:HG3	1:C:206:THR:OG1	2.14	0.48
2:S:33:LYS:HE3	2:S:34:CYS:O	2.14	0.48
1:J:119:PRO:HB3	1:J:209:PHE:CE2	2.49	0.48
2:T:23:GLU:HG3	2:T:56:MET:HE1	1.96	0.48
2:S:72:ALA:HA	2:S:75:THR:HG22	1.96	0.47
3:D:35:GLN:NE2	3:D:106:MET:HG2	2.29	0.47
1:J:176:SER:HB3	3:O:172:PHE:CE2	2.49	0.47
2:S:91:PHE:CE1	2:S:104:VAL:HG13	2.49	0.47
1:J:193:ALA:HB2	1:J:208:SER:HB3	1.95	0.47
1:E:37:GLN:HG3	1:E:86:TYR:CE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:30:ILE:H	3:F:30:ILE:HD12	1.80	0.47
1:E:132:VAL:CG2	1:E:179:LEU:HB3	2.38	0.47
1:E:163:VAL:HG12	1:E:164:THR:O	2.15	0.47
2:S:100:SER:O	2:S:104:VAL:HG23	2.15	0.47
3:H:33:TRP:CD2	3:H:103:PRO:HG3	2.50	0.47
1:J:40:GLN:H	1:J:40:GLN:NE2	2.13	0.47
3:O:70:LEU:CD2	3:O:81:MET:HG3	2.44	0.47
2:T:46:ASN:OD1	2:T:49:CYS:HB2	2.14	0.47
1:L:52:LYS:HE2	1:L:66:GLY:H	1.79	0.47
3:F:30:ILE:HD12	3:F:30:ILE:N	2.30	0.46
2:Q:16:GLU:O	2:Q:20:SER:OG	2.33	0.46
1:C:117:ILE:HD12	1:C:194:CYS:SG	2.56	0.46
2:S:92:THR:HG22	2:S:98:GLN:HA	1.97	0.46
1:C:85:SER:HA	1:C:102:THR:O	2.15	0.46
3:D:122:THR:HG22	3:D:209:SER:HB3	1.97	0.46
1:J:186:TYR:HA	1:J:192:TYR:OH	2.16	0.46
1:C:182:SER:OG	1:C:185:ASP:HB2	2.16	0.46
2:S:38:ILE:HD11	2:S:157:ASN:ND2	2.31	0.46
3:F:156:VAL:CG2	3:F:204:VAL:HG13	2.46	0.46
3:O:89:GLU:O	3:O:89:GLU:HG2	2.16	0.46
2:R:21:LYS:NZ	2:R:70:SER:HB2	2.30	0.46
1:J:163:VAL:HG22	1:J:175:LEU:HD12	1.98	0.46
3:F:168:GLY:O	3:F:188:VAL:HA	2.16	0.46
1:E:96:TYR:CE2	3:F:103:PRO:HB2	2.51	0.46
1:E:120:PRO:HB2	1:E:125:LEU:HD21	1.97	0.45
2:R:20:SER:O	2:R:23:GLU:HG2	2.17	0.45
3:H:38:LYS:HB2	3:H:48:ILE:HD11	1.98	0.45
1:J:61:ARG:O	1:J:75:ILE:HA	2.17	0.45
1:E:85:SER:HA	1:E:102:THR:O	2.16	0.45
1:J:181:LEU:HD23	1:J:181:LEU:HA	1.75	0.45
2:R:28:ALA:HB2	2:R:58:SER:HB3	1.98	0.45
2:R:133:ILE:HD13	2:R:168:THR:HG21	1.98	0.45
1:C:83:ILE:HD13	1:C:166:GLN:HB3	1.97	0.45
2:S:56:MET:HE3	2:S:56:MET:HB2	1.78	0.45
1:L:24:ARG:HE	1:L:70:GLN:NE2	2.15	0.45
2:R:169:LYS:O	2:R:172:THR:HG22	2.17	0.45
3:D:2:ILE:HD12	3:D:2:ILE:H	1.82	0.45
2:R:41:PHE:HD1	2:R:42:TYR:N	2.14	0.45
2:R:42:TYR:HD1	2:R:43:ILE:H	1.65	0.45
3:D:206:HIS:ND1	3:D:209:SER:OG	2.45	0.45
1:E:140:TYR:O	1:E:141:PRO:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:VAL:HG22	1:C:54:LEU:HD12	1.98	0.45
1:J:123:GLU:H	1:J:123:GLU:CD	2.15	0.45
3:O:178:SER:C	3:O:180:GLY:H	2.25	0.45
2:R:42:TYR:CD1	2:R:43:ILE:N	2.84	0.44
1:J:108:ARG:HD2	1:J:171:SER:HB2	1.99	0.44
1:E:24:ARG:NH2	1:E:70:GLN:HE22	2.15	0.44
1:E:142:ARG:HD2	1:E:173:TYR:CE2	2.52	0.44
2:S:94:ALA:HB1	2:S:165:GLN:HB3	1.99	0.44
2:T:168:THR:O	2:T:168:THR:OG1	2.29	0.44
1:E:105:GLU:OE1	1:E:173:TYR:OH	2.35	0.44
2:S:76:TYR:O	2:S:79:LEU:HB2	2.17	0.44
3:H:40:ARG:HG2	3:H:40:ARG:HH11	1.82	0.44
2:T:12:ASN:O	2:T:16:GLU:HG3	2.17	0.44
3:F:4:LEU:HD23	3:F:24:ALA:HA	1.99	0.44
2:Q:96:ASN:O	2:Q:97:ILE:HD12	2.18	0.44
3:D:67:LYS:O	3:D:83:LEU:HA	2.17	0.44
3:O:201:ILE:CD1	3:O:216:ARG:HA	2.46	0.44
1:E:83:ILE:CD1	1:E:106:ILE:HG13	2.47	0.44
1:J:40:GLN:HG2	1:J:165:GLU:HG3	2.00	0.43
3:O:201:ILE:HD12	3:O:216:ARG:HA	2.00	0.43
1:L:167:ASP:O	1:L:171:SER:N	2.45	0.43
1:E:162:SER:OG	3:F:173:PRO:O	2.29	0.43
2:R:8:GLN:HE21	2:R:12:ASN:ND2	2.15	0.43
3:F:176:LEU:HD13	3:F:182:TYR:CZ	2.53	0.43
1:E:25:THR:HG1	1:E:69:THR:HA	1.83	0.43
2:R:41:PHE:HE2	2:R:148:PHE:HB2	1.84	0.43
3:F:86:LEU:HD23	3:F:86:LEU:HA	1.88	0.43
1:C:158:ASN:OD1	1:C:158:ASN:N	2.51	0.43
3:D:156:VAL:HG12	3:D:184:LEU:HD13	2.00	0.43
3:F:123:LYS:HD3	3:F:124:GLY:O	2.19	0.43
3:D:70:LEU:HD23	3:D:81:MET:HG3	2.00	0.43
3:O:205:ASN:ND2	3:O:207:LYS:HD2	2.18	0.43
1:E:131:SER:HA	1:E:179:LEU:O	2.19	0.43
2:R:91:PHE:CE1	2:R:104:VAL:HG23	2.53	0.43
3:D:201:ILE:HD11	3:D:203:ASN:HD21	1.84	0.43
3:O:56:GLY:O	3:O:58:THR:HG23	2.19	0.43
3:F:11:LEU:HB2	3:F:153:PRO:HG3	2.00	0.43
3:D:91:SER:HA	3:D:115:VAL:O	2.19	0.43
3:F:6:GLN:H	3:F:111:GLN:HE22	1.65	0.43
1:E:12:SER:HB3	1:E:107:LYS:HG3	2.00	0.43
3:D:35:GLN:OE1	3:D:106:MET:HE2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:91:SER:HA	3:O:115:VAL:O	2.19	0.43
2:T:64:GLN:O	2:T:68:VAL:HG23	2.19	0.43
3:F:60:TYR:HH	3:F:70:LEU:H	1.62	0.42
1:E:4:MET:HE3	1:E:25:THR:CG2	2.49	0.42
3:F:51:ILE:HG13	3:F:58:THR:HG22	2.01	0.42
3:O:184:LEU:HD12	3:O:184:LEU:C	2.44	0.42
2:R:62:ASP:OD1	2:R:155:LYS:NZ	2.37	0.42
3:F:215:LYS:O	3:F:215:LYS:HD2	2.18	0.42
2:S:11:VAL:HG13	2:S:12:ASN:H	1.84	0.42
1:L:163:VAL:HG12	1:L:164:THR:O	2.18	0.42
2:R:51:ILE:HD13	2:R:146:LEU:HB2	2.02	0.42
1:J:150:VAL:HB	1:J:155:GLN:NE2	2.34	0.42
2:R:79:LEU:HD23	2:R:79:LEU:HA	1.86	0.42
1:C:3:GLN:HG2	3:O:62:GLN:HG3	2.02	0.42
2:T:146:LEU:HD23	2:T:146:LEU:HA	1.75	0.42
1:E:4:MET:HE2	1:E:23:CYS:SG	2.60	0.42
3:H:86:LEU:HD23	3:H:86:LEU:HA	1.87	0.42
1:J:190:LYS:HE2	1:J:210:ASN:HB3	2.02	0.42
2:S:14:LEU:HD22	2:S:75:THR:HG21	2.00	0.41
2:S:156:GLY:O	2:S:160:ILE:HG12	2.20	0.41
1:E:159:SER:HA	1:E:178:THR:O	2.20	0.41
1:J:125:LEU:HA	1:J:183:LYS:HZ1	1.85	0.41
2:T:149:ILE:O	2:T:160:ILE:HG21	2.20	0.41
2:R:167:THR:O	2:R:170:ALA:HB3	2.19	0.41
3:H:97:ALA:HB1	3:H:106:MET:HB3	2.02	0.41
3:F:7:SER:OG	3:F:10:GLU:OE2	2.38	0.41
1:L:151:ASP:OD2	1:L:189:HIS:HB3	2.21	0.41
1:C:18:THR:HA	1:C:75:ILE:O	2.20	0.41
3:F:63:LYS:HD2	3:F:64:PHE:CE2	2.56	0.41
2:T:61:ALA:HB1	2:T:155:LYS:HB3	2.01	0.41
2:R:8:GLN:HG3	2:R:12:ASN:ND2	2.36	0.41
3:H:31:THR:HA	3:H:52:TYR:OH	2.20	0.41
2:Q:101:VAL:HG23	2:Q:102:ASN:OD1	2.21	0.41
2:R:14:LEU:HD21	2:R:163:LEU:HD13	2.03	0.41
2:R:54:LYS:HD2	2:R:54:LYS:HA	1.93	0.41
2:R:137:TYR:HB2	2:R:171:THR:O	2.20	0.41
3:F:129:PRO:HB3	3:F:215:LYS:HE3	2.03	0.41
1:L:40:GLN:HE21	1:L:165:GLU:HB3	1.85	0.41
1:J:125:LEU:CA	1:J:183:LYS:HZ1	2.34	0.41
1:E:149:LYS:HE3	1:E:149:LYS:HB2	1.38	0.41
2:Q:38:ILE:HD13	2:Q:38:ILE:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:91:PHE:CZ	2:R:104:VAL:HG23	2.56	0.40
1:J:134:CYS:HB2	1:J:148:TRP:CH2	2.57	0.40
1:E:61:ARG:HB2	1:E:76:ASN:O	2.21	0.40
2:Q:61:ALA:O	2:Q:64:GLN:HB2	2.22	0.40
1:J:124:GLN:HG3	3:O:128:PHE:CE2	2.57	0.40
2:T:111:TYR:O	2:T:115:THR:OG1	2.35	0.40
3:F:37:VAL:HA	3:F:46:GLU:O	2.22	0.40
3:D:165:LEU:HD21	3:D:188:VAL:HG21	2.04	0.40
1:J:11:LEU:HD12	1:J:11:LEU:HA	1.92	0.40
3:O:11:LEU:HD21	3:O:118:SER:HB3	2.04	0.40
2:R:134:ASP:OD1	2:R:134:ASP:N	2.47	0.40
3:F:59:ARG:HG2	3:F:59:ARG:HH11	1.87	0.40
1:C:91:PHE:HA	1:C:96:TYR:CE1	2.57	0.40
3:D:147:LEU:CD1	3:D:149:LYS:HB2	2.52	0.40
2:Q:25:GLU:O	2:Q:25:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

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	C	210/215 (98%)	201 (96%)	9 (4%)	0	100	100
1	E	192/215 (89%)	181 (94%)	11 (6%)	0	100	100
1	J	210/215 (98%)	198 (94%)	12 (6%)	0	100	100
1	L	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
2	Q	167/181 (92%)	161 (96%)	6 (4%)	0	100	100
2	R	152/181 (84%)	140 (92%)	12 (8%)	0	100	100
2	S	122/181 (67%)	117 (96%)	5 (4%)	0	100	100
2	T	116/181 (64%)	100 (86%)	16 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	210/225 (93%)	195 (93%)	15 (7%)	0	100	100
3	F	190/225 (84%)	179 (94%)	11 (6%)	0	100	100
3	H	210/225 (93%)	197 (94%)	13 (6%)	0	100	100
3	O	210/225 (93%)	199 (95%)	11 (5%)	0	100	100
All	All	2199/2484 (88%)	2071 (94%)	128 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	C	184/188 (98%)	169 (92%)	15 (8%)	9	23
1	E	171/188 (91%)	157 (92%)	14 (8%)	9	23
1	J	185/188 (98%)	175 (95%)	10 (5%)	18	42
1	L	185/188 (98%)	176 (95%)	9 (5%)	21	47
2	Q	142/149 (95%)	135 (95%)	7 (5%)	21	47
2	R	136/149 (91%)	134 (98%)	2 (2%)	60	83
2	S	108/149 (72%)	105 (97%)	3 (3%)	38	68
2	T	106/149 (71%)	96 (91%)	10 (9%)	7	18
3	D	176/187 (94%)	164 (93%)	12 (7%)	13	32
3	F	161/187 (86%)	150 (93%)	11 (7%)	13	32
3	H	176/187 (94%)	172 (98%)	4 (2%)	45	74
3	O	176/187 (94%)	164 (93%)	12 (7%)	13	32
All	All	1906/2096 (91%)	1797 (94%)	109 (6%)	17	40

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	10	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	26	SER
1	E	63	SER
1	E	67	SER
1	E	69	THR
1	E	94	THR
1	E	127	SER
1	E	149	LYS
1	E	150	VAL
1	E	160	GLN
1	E	178	THR
1	E	179	LEU
1	E	180	THR
1	E	208	SER
2	R	7	ILE
2	R	8	GLN
3	F	17	SER
3	F	25	SER
3	F	34	ILE
3	F	61	THR
3	F	75	SER
3	F	87	THR
3	F	107	ASP
3	F	117	VAL
3	F	119	SER
3	F	175	VAL
3	F	185	SER
1	C	11	LEU
1	C	12	SER
1	C	33	LEU
1	C	45	GLN
1	C	63	SER
1	C	72	SER
1	C	77	SER
1	C	114	SER
1	C	132	VAL
1	C	145	LYS
1	C	158	ASN
1	C	162	SER
1	C	180	THR
1	C	181	LEU
1	C	208	SER
3	D	7	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	19	LYS
3	D	25	SER
3	D	62	GLN
3	D	69	THR
3	D	75	SER
3	D	144	LEU
3	D	147	LEU
3	D	156	VAL
3	D	157	THR
3	D	167	SER
3	D	185	SER
2	S	20	SER
2	S	31	GLN
2	S	80	THR
1	L	12	SER
1	L	20	THR
1	L	54	LEU
1	L	56	ASP
1	L	63	SER
1	L	114	SER
1	L	168	SER
1	L	203	SER
1	L	208	SER
3	H	21	SER
3	H	82	GLN
3	H	156	VAL
3	H	157	THR
2	Q	20	SER
2	Q	29	SER
2	Q	51	ILE
2	Q	74	GLU
2	Q	126	LEU
2	Q	149	ILE
2	Q	155	LYS
1	J	10	SER
1	J	19	VAL
1	J	22	THR
1	J	60	SER
1	J	63	SER
1	J	93	ILE
1	J	94	THR
1	J	159	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	180	THR
1	J	197	THR
3	O	7	SER
3	O	10	GLU
3	O	11	LEU
3	O	55	ASP
3	O	71	THR
3	O	75	SER
3	O	87	THR
3	O	121	SER
3	O	144	LEU
3	O	157	THR
3	O	184	LEU
3	O	197	THR
2	T	12	ASN
2	T	29	SER
2	T	58	SER
2	T	62	ASP
2	T	65	LEU
2	T	69	LEU
2	T	136	CYS
2	T	154	SER
2	T	158	CYS
2	T	167	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	45	GLN
1	E	70	GLN
1	E	79	GLN
1	E	158	ASN
1	E	199	GLN
2	R	12	ASN
2	R	64	GLN
3	F	82	GLN
1	C	30	HIS
1	C	137	ASN
3	D	205	ASN
2	S	24	GLN
2	S	27	ASN
1	L	31	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	70	GLN
1	L	79	GLN
1	L	199	GLN
2	Q	50	ASN
1	J	38	GLN
1	J	45	GLN
1	J	50	ASN
1	J	138	ASN
1	J	152	ASN
1	J	155	GLN
3	O	39	GLN
3	O	62	GLN
3	O	170	HIS
3	O	205	ASN
2	T	55	ASN
2	T	145	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 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 ⓘ

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	C	212/215 (98%)	-0.07	3 (1%) 73 73	34, 54, 90, 99	0
1	E	196/215 (91%)	0.29	9 (4%) 38 36	44, 66, 107, 120	0
1	J	212/215 (98%)	-0.37	0 100 100	30, 44, 79, 88	0
1	L	212/215 (98%)	-0.56	1 (0%) 87 86	31, 39, 56, 66	0
2	Q	169/181 (93%)	-0.37	0 100 100	31, 44, 64, 83	0
2	R	158/181 (87%)	0.50	6 (3%) 44 42	61, 80, 98, 104	0
2	S	128/181 (70%)	0.66	14 (10%) 12 11	59, 87, 101, 104	0
2	T	122/181 (67%)	0.67	6 (4%) 36 34	36, 80, 100, 107	0
3	D	214/225 (95%)	0.27	3 (1%) 73 73	45, 67, 86, 99	0
3	F	196/225 (87%)	0.21	5 (2%) 57 56	48, 69, 86, 93	0
3	H	214/225 (95%)	-0.33	2 (0%) 81 80	32, 49, 70, 94	0
3	O	214/225 (95%)	-0.18	1 (0%) 87 86	33, 51, 74, 86	0
All	All	2247/2484 (90%)	0.01	50 (2%) 62 61	30, 59, 94, 120	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	10	THR	4.8
1	E	150	VAL	4.2
2	S	11	VAL	4.2
1	E	193	ALA	3.7
2	T	105	VAL	3.7
2	S	39	GLY	3.6
2	R	43	ILE	3.5
2	R	48	GLY	3.1
2	S	95	LEU	3.0
2	R	143	PRO	2.9
2	S	168	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	41	PHE	2.8
3	D	9	ALA	2.8
2	T	13	THR	2.8
3	D	219	PRO	2.8
2	S	59	ALA	2.7
2	S	148	PHE	2.7
1	C	212	GLY	2.7
2	R	7	ILE	2.7
1	E	146	VAL	2.6
3	O	219	PRO	2.6
1	E	101	GLY	2.6
2	S	35	ASP	2.6
2	T	61	ALA	2.6
3	H	139	GLY	2.6
1	E	151	ASP	2.5
3	F	131	ALA	2.5
3	F	190	VAL	2.4
2	T	12	ASN	2.4
3	D	49	GLY	2.4
2	T	112	VAL	2.4
2	R	98	GLN	2.4
3	F	9	ALA	2.4
2	S	105	VAL	2.4
3	H	150	ASP	2.3
1	E	180	THR	2.3
2	S	130	ASN	2.2
3	F	215	LYS	2.2
1	C	192	TYR	2.2
1	E	196	VAL	2.2
1	E	194	CYS	2.2
1	L	212	GLY	2.2
1	C	131	SER	2.1
2	S	54	LYS	2.1
1	E	169	LYS	2.1
2	S	158	CYS	2.1
2	S	85	ALA	2.1
2	S	65	LEU	2.0
3	F	107	ASP	2.0
2	S	128	ILE	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 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.