



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:43 AM UTC

PDB ID : 9C24 / pdb_00009c24
Title : Fab F946 in complex with OspCB
Authors : Rudolph, M.J.; Mantis, N.
Deposited on : 2024-05-30
Resolution : 2.80 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:

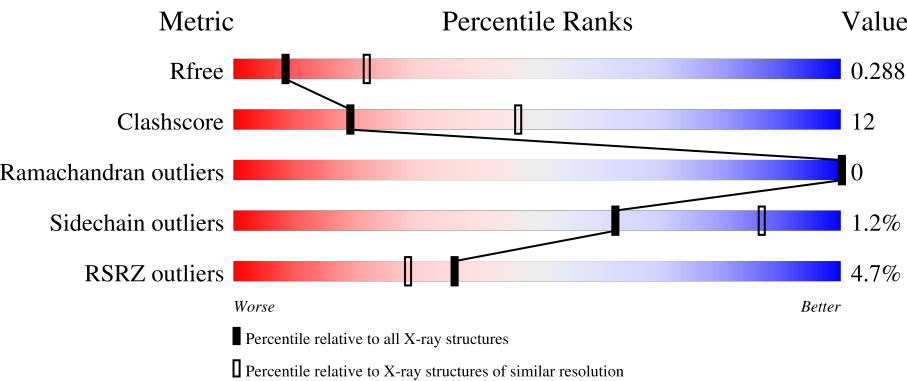
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	230	<div><div>2%</div><div><div></div><div>73%</div><div>17%</div><div>10%</div></div></div>
1	H	230	<div><div>3%</div><div><div></div><div>72%</div><div>17%</div><div>10%</div></div></div>
2	B	214	<div><div>7%</div><div><div></div><div>72%</div><div>25%</div><div></div></div></div>
2	L	214	<div><div>9%</div><div><div></div><div>68%</div><div>27%</div><div></div></div></div>
3	C	165	<div><div>2%</div><div><div></div><div>65%</div><div>28%</div><div>5%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	165	<div><div></div><div>3%</div><div>69%</div><div>26%</div><div>• •</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8726 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 F946 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	207	Total	C	N	O	S	0	0	0
			1563	1004	254	301	4			
1	A	207	Total	C	N	O	S	0	0	0
			1566	1005	254	303	4			

- Molecule 2 is a protein called F946 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	205	Total	C	N	O	S	0	0	0
			1579	998	259	318	4			
2	B	208	Total	C	N	O	S	0	0	0
			1603	1011	266	322	4			

- Molecule 3 is a protein called Outer surface protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	157	Total	C	N	O	S	0	0	0
			1169	728	197	242	2			
3	D	158	Total	C	N	O	S	0	0	0
			1174	731	198	243	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	19	Total	O	0	0
			19	19		
4	L	7	Total	O	0	0
			7	7		
4	A	21	Total	O	0	0
			21	21		
4	B	8	Total	O	0	0
			8	8		

Continued on next page...

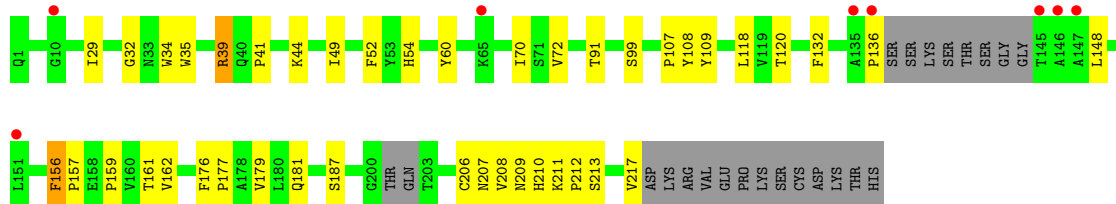
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	6	Total	O	0	0
			6	6		
4	D	11	Total	O	0	0
			11	11		

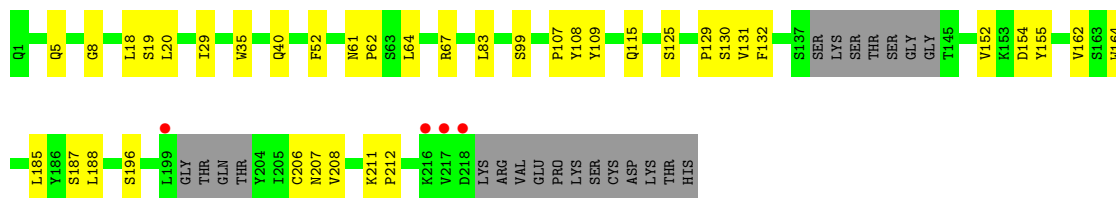
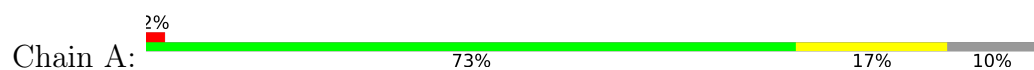
3 Residue-property plots [i](#)

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.

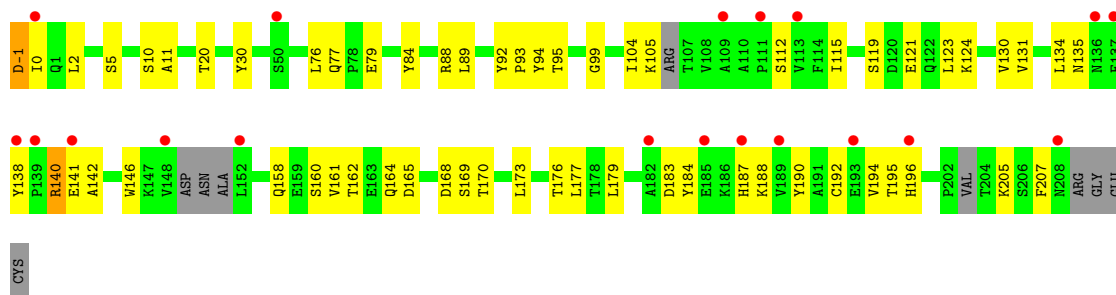
- Molecule 1: F946 Fab Heavy Chain



- Molecule 1: F946 Fab Heavy Chain

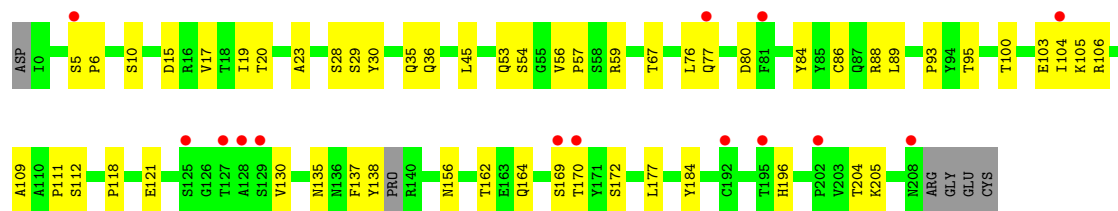


- Molecule 2: F946 Fab Light Chain

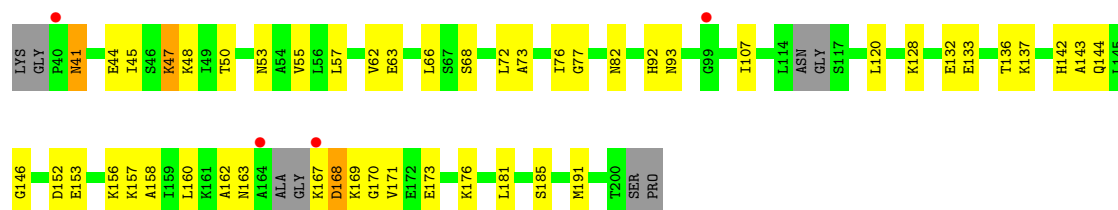


- Molecule 2: F946 Fab Light Chain

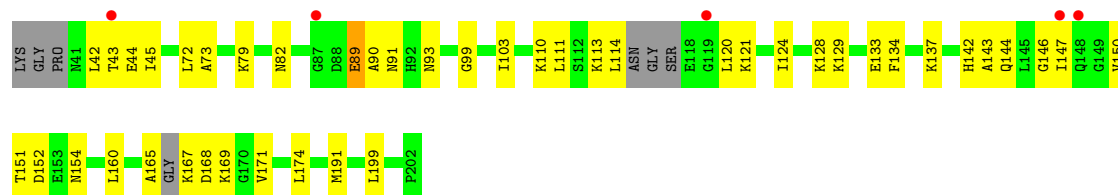




• Molecule 3: Outer surface protein C



• Molecule 3: Outer surface protein C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.79Å 96.46Å 188.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.80 48.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.91-2.80) 98.4 (48.91-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.234 , 0.288 0.234 , 0.288	Depositor DCC
R_{free} test set	1689 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8726	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/1610	0.37	0/2202
1	H	0.13	0/1607	0.42	0/2198
2	B	0.13	0/1637	0.41	0/2221
2	L	0.18	0/1612	0.59	4/2185 (0.2%)
3	C	0.10	0/1171	0.33	0/1562
3	D	0.09	0/1176	0.30	0/1570
All	All	0.13	0/8813	0.42	4/11938 (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	H	0	1
3	C	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	140	ARG	CA-C-N	9.28	138.40	121.70
2	L	140	ARG	C-N-CA	9.28	138.40	121.70
2	L	-1	ASP	CA-C-N	9.03	137.96	121.70
2	L	-1	ASP	C-N-CA	9.03	137.96	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	168	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	47	LYS	Peptide
1	H	156	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	1566	0	1532	23	0
1	H	1563	0	1533	30	0
2	B	1603	0	1570	39	0
2	L	1579	0	1542	51	0
3	C	1169	0	1235	41	0
3	D	1174	0	1239	37	0
4	A	21	0	0	1	0
4	B	8	0	0	0	0
4	C	6	0	0	2	0
4	D	11	0	0	1	0
4	H	19	0	0	0	0
4	L	7	0	0	0	0
All	All	8726	0	8651	202	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 12.

All (202) 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:A:5:GLN:HG3	1:A:115:GLN:HE22	1.41	0.85
1:A:152:VAL:HB	1:A:188:LEU:HB3	1.63	0.79
1:H:181:GLN:OE1	1:H:187:SER:OG	2.01	0.77
1:H:118:LEU:HD23	1:H:159:PRO:HD3	1.67	0.75
1:H:41:PRO:HB2	1:H:44:LYS:HG3	1.69	0.75
2:B:112:SER:HB2	2:B:135:ASN:HB2	1.69	0.73
1:A:18:LEU:HB3	1:A:83:LEU:HB3	1.70	0.73
1:H:177:PRO:HD2	2:L:160:SER:HB3	1.70	0.72
3:C:120:LEU:HD11	3:C:191:MET:HE2	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:134:LEU:HD22	2:L:173:LEU:HD13	1.72	0.72
3:C:173:GLU:OE2	3:C:173:GLU:N	2.18	0.71
3:C:66:LEU:HD22	3:C:181:LEU:HD12	1.74	0.70
2:L:79:GLU:N	2:L:79:GLU:OE2	2.24	0.69
2:B:17:VAL:HG23	2:B:76:LEU:HD11	1.75	0.68
2:B:35:GLN:HB3	2:B:45:LEU:HD11	1.75	0.68
3:D:167:LYS:HA	3:D:171:VAL:HB	1.74	0.67
2:L:112:SER:HB2	2:L:135:ASN:HB3	1.77	0.66
2:L:183:ASP:O	2:L:190:TYR:OH	2.12	0.66
3:C:132:GLU:O	3:C:136:THR:OG1	2.14	0.64
2:L:131:VAL:HG22	2:L:176:THR:HG22	1.81	0.63
2:L:194:VAL:HG12	2:L:195:THR:H	1.63	0.63
1:A:40:GLN:HE22	2:B:36:GLN:HE22	1.47	0.62
3:C:158:ALA:HA	3:C:170:GLY:H	1.65	0.62
2:B:19:ILE:HG21	2:B:100:THR:HG21	1.81	0.62
2:B:57:PRO:HB2	2:B:59:ARG:HD3	1.81	0.61
3:D:79:LYS:HD3	3:D:89:GLU:HG2	1.83	0.61
2:L:121:GLU:OE1	2:L:121:GLU:N	2.31	0.60
3:D:90:ALA:HB1	3:D:91:ASN:HD22	1.65	0.60
3:D:110:LYS:NZ	4:D:302:HOH:O	2.34	0.60
1:H:34:TRP:HB2	1:H:99:SER:HB2	1.84	0.60
1:A:29:ILE:HG22	1:A:35:TRP:CE2	2.36	0.60
1:A:99:SER:HB3	1:A:108:TYR:HB3	1.84	0.60
1:H:39:ARG:HB3	1:H:49:ILE:HD11	1.84	0.59
2:L:140:ARG:HG3	2:L:196:HIS:ND1	2.17	0.59
2:B:53:GLN:O	2:B:56:VAL:HG12	2.03	0.58
3:D:144:GLN:OE1	3:D:144:GLN:N	2.36	0.58
1:A:40:GLN:NE2	4:A:301:HOH:O	2.32	0.57
1:H:99:SER:HB3	1:H:108:TYR:HB3	1.85	0.57
2:L:142:ALA:HB2	2:L:196:HIS:CE1	2.39	0.57
3:D:73:ALA:HB1	3:D:160:LEU:HD12	1.87	0.57
2:B:15:ASP:O	2:B:76:LEU:HD13	2.04	0.57
3:C:142:HIS:CD2	3:C:143:ALA:H	2.23	0.57
3:C:72:LEU:HD11	3:D:72:LEU:HD11	1.86	0.56
1:H:179:VAL:HG11	2:L:158:GLN:HG3	1.87	0.56
3:C:168:ASP:HA	3:C:171:VAL:HG12	1.88	0.56
3:D:143:ALA:O	3:D:147:ILE:HD11	2.06	0.56
1:A:62:PRO:HD2	2:B:93:PRO:HG3	1.88	0.56
3:C:144:GLN:OE1	3:C:144:GLN:N	2.39	0.56
3:D:151:THR:OG1	3:D:154:ASN:OD1	2.24	0.55
2:B:5:SER:HB3	2:B:6:PRO:HD3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:190:TYR:HB2	2:L:207:PHE:CE1	2.42	0.55
3:C:47:LYS:HA	3:C:50:THR:HB	1.88	0.55
3:C:142:HIS:CE1	3:D:82:ASN:HB3	2.42	0.55
3:C:128:LYS:O	3:C:132:GLU:HG3	2.07	0.55
3:D:93:ASN:ND2	3:D:152:ASP:OD1	2.28	0.55
2:L:2:LEU:HD11	2:L:88:ARG:HB3	1.89	0.54
3:D:129:LYS:O	3:D:133:GLU:HG3	2.07	0.54
1:A:129:PRO:HB3	1:A:155:TYR:HB3	1.88	0.54
2:L:10:SER:HB3	2:L:105:LYS:HD2	1.90	0.54
2:L:177:LEU:HD22	2:L:179:LEU:HG	1.88	0.54
3:C:44:GLU:OE1	4:C:301:HOH:O	2.19	0.53
2:L:190:TYR:HB2	2:L:207:PHE:HE1	1.73	0.53
2:L:121:GLU:HA	2:L:124:LYS:HD3	1.90	0.53
2:L:-1:ASP:HA	2:L:0:ILE:HG22	1.90	0.53
2:L:194:VAL:HG12	2:L:195:THR:N	2.24	0.52
1:H:60:TYR:HE1	1:H:70:ILE:HG13	1.74	0.52
3:D:142:HIS:HD2	3:D:143:ALA:H	1.58	0.52
1:H:210:HIS:ND1	1:H:213:SER:OG	2.39	0.52
3:C:72:LEU:HD21	3:D:72:LEU:HD21	1.92	0.52
3:C:142:HIS:O	3:C:146:GLY:N	2.37	0.52
3:C:73:ALA:O	3:C:76:ILE:HG13	2.09	0.52
3:C:133:GLU:OE2	3:C:176:LYS:NZ	2.35	0.52
1:H:29:ILE:HG22	1:H:35:TRP:CE2	2.44	0.52
1:H:162:VAL:HG22	1:H:208:VAL:HG22	1.92	0.51
1:A:164:TRP:CZ3	1:A:206:CYS:HB3	2.45	0.51
2:B:88:ARG:NH2	2:B:95:THR:OG1	2.43	0.51
3:C:157:LYS:HG2	3:C:163:ASN:HD22	1.75	0.51
2:L:146:TRP:CZ3	2:L:192:CYS:HB3	2.46	0.51
1:H:109:TYR:CD2	2:L:89:LEU:HD13	2.46	0.51
2:L:165:ASP:OD1	2:L:168:ASP:N	2.27	0.51
1:A:162:VAL:HG22	1:A:208:VAL:HG22	1.93	0.51
2:B:109:ALA:H	2:B:138:TYR:HB3	1.74	0.51
2:B:111:PRO:HD3	2:B:196:HIS:HD2	1.76	0.51
3:C:41:ASN:ND2	4:C:304:HOH:O	2.34	0.51
3:D:144:GLN:HG2	3:D:169:LYS:NZ	2.26	0.51
2:B:59:ARG:NH2	2:B:80:ASP:OD2	2.44	0.51
3:C:153:GLU:O	3:C:157:LYS:HG3	2.11	0.50
3:D:144:GLN:HG2	3:D:169:LYS:HZ2	1.76	0.50
2:B:204:THR:O	2:B:205:LYS:HD2	2.12	0.50
3:C:62:VAL:HG23	3:C:107:ILE:HG12	1.92	0.50
3:D:142:HIS:HD2	3:D:143:ALA:N	2.08	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:88:ARG:NH2	2:L:95:THR:OG1	2.42	0.50
3:D:142:HIS:CD2	3:D:143:ALA:H	2.30	0.50
3:C:68:SER:HB2	3:D:103:ILE:HD13	1.94	0.50
2:B:17:VAL:HG23	2:B:76:LEU:CD1	2.42	0.49
3:C:173:GLU:H	3:C:173:GLU:CD	2.15	0.49
3:C:137:LYS:HG2	3:C:173:GLU:OE1	2.12	0.49
3:C:157:LYS:HB3	3:C:167:LYS:O	2.12	0.49
2:L:76:LEU:C	2:L:77:GLN:HG2	2.38	0.49
3:C:82:ASN:HB3	3:D:142:HIS:CE1	2.48	0.49
3:C:45:ILE:O	3:C:48:LYS:HB2	2.12	0.49
1:H:210:HIS:CD2	1:H:212:PRO:HD2	2.49	0.48
1:H:136:PRO:HB3	1:H:148:LEU:HD21	1.94	0.48
2:B:118:PRO:HG2	2:B:184:TYR:CE1	2.48	0.48
3:D:111:LEU:HD13	3:D:128:LYS:HA	1.96	0.48
2:L:165:ASP:HB3	2:L:170:THR:H	1.78	0.48
2:B:5:SER:HB2	2:B:20:THR:HB	1.95	0.48
1:H:91:THR:HG23	1:H:120:THR:HA	1.95	0.48
2:L:134:LEU:HB2	2:L:173:LEU:HB3	1.95	0.48
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.96	0.47
1:H:162:VAL:HA	1:H:207:ASN:O	2.14	0.47
3:D:142:HIS:CD2	3:D:143:ALA:N	2.82	0.47
3:C:142:HIS:HD2	3:C:143:ALA:H	1.60	0.47
1:H:161:THR:HB	1:H:209:ASN:HB3	1.95	0.47
2:B:156:ASN:HB2	2:B:177:LEU:HD12	1.96	0.47
1:A:107:PRO:HD3	2:B:30:TYR:CD1	2.49	0.47
2:B:103:GLU:HG2	2:B:104:ILE:N	2.30	0.47
3:C:142:HIS:ND1	3:D:82:ASN:HB3	2.29	0.47
3:D:142:HIS:O	3:D:146:GLY:N	2.38	0.47
3:D:165:ALA:O	3:D:167:LYS:N	2.48	0.47
3:C:152:ASP:O	3:C:156:LYS:HG3	2.14	0.47
1:A:40:GLN:HE22	2:B:36:GLN:NE2	2.12	0.46
2:B:121:GLU:OE1	2:B:121:GLU:N	2.48	0.46
2:B:19:ILE:HD13	2:B:100:THR:HG21	1.98	0.46
3:D:90:ALA:HB1	3:D:91:ASN:ND2	2.31	0.46
2:B:137:PHE:HB2	2:B:196:HIS:HE2	1.82	0.45
2:L:11:ALA:O	2:L:105:LYS:N	2.44	0.45
2:L:30:TYR:OH	3:C:47:LYS:HB2	2.16	0.45
1:A:131:VAL:HG22	1:A:152:VAL:HG13	1.97	0.45
1:A:211:LYS:HB2	1:A:212:PRO:HD3	1.99	0.45
3:C:157:LYS:HG2	3:C:163:ASN:ND2	2.31	0.45
3:D:120:LEU:HD11	3:D:191:MET:HE2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:PHE:O	2:B:170:THR:OG1	2.33	0.45
3:D:113:LYS:N	3:D:113:LYS:HD2	2.31	0.45
2:L:104:ILE:HB	2:L:164:GLN:NE2	2.32	0.45
2:L:123:LEU:HD11	2:L:184:TYR:CE2	2.52	0.45
2:L:140:ARG:HA	2:L:140:ARG:HD2	1.86	0.45
3:D:114:LEU:HB3	3:D:124:ILE:HD13	1.98	0.45
3:C:53:ASN:O	3:C:57:LEU:HD23	2.17	0.45
3:C:92:HIS:C	3:C:93:ASN:HD22	2.25	0.44
3:D:121:LYS:HB3	3:D:121:LYS:HE3	1.63	0.44
1:H:206:CYS:O	1:H:217:VAL:HB	2.17	0.44
2:L:-1:ASP:CA	2:L:0:ILE:HG22	2.47	0.44
1:H:35:TRP:HB2	1:H:52:PHE:CE1	2.53	0.44
3:C:142:HIS:CD2	3:C:143:ALA:N	2.85	0.44
2:L:92:TYR:HB2	2:L:93:PRO:HA	1.99	0.44
3:C:146:GLY:O	3:D:79:LYS:HD2	2.18	0.44
1:H:132:PHE:HB3	2:L:119:SER:OG	2.17	0.44
2:B:59:ARG:CZ	2:B:77:GLN:HG3	2.48	0.44
3:D:43:THR:OG1	3:D:44:GLU:N	2.50	0.44
1:H:156:PHE:HD1	1:H:156:PHE:HA	1.66	0.43
2:L:92:TYR:HA	2:L:94:TYR:H	1.83	0.43
2:L:140:ARG:NE	2:L:141:GLU:O	2.51	0.43
2:L:205:LYS:HD3	2:L:205:LYS:HA	1.90	0.43
1:A:154:ASP:HA	1:A:185:LEU:HB3	1.99	0.43
3:C:77:GLY:H	3:C:93:ASN:HD21	1.65	0.43
1:H:157:PRO:C	1:H:159:PRO:HD2	2.43	0.43
2:L:164:GLN:NE2	2:L:169:SER:HB3	2.33	0.43
1:A:35:TRP:HB2	1:A:52:PHE:CE1	2.53	0.43
2:L:130:VAL:HG22	2:L:177:LEU:HB3	2.00	0.43
2:B:10:SER:HB2	2:B:105:LYS:HB2	2.01	0.43
2:B:130:VAL:CG1	2:B:177:LEU:HB3	2.47	0.43
1:H:211:LYS:HD2	1:H:211:LYS:HA	1.82	0.43
2:L:138:TYR:CD1	2:L:170:THR:HG22	2.54	0.43
1:H:107:PRO:HD3	2:L:30:TYR:CD1	2.53	0.43
1:H:176:PHE:N	1:H:176:PHE:CD1	2.87	0.43
1:A:40:GLN:NE2	2:B:36:GLN:HE22	2.15	0.43
2:L:161:VAL:HG22	2:L:162:THR:O	2.19	0.43
2:B:23:ALA:HB3	2:B:67:THR:HA	2.01	0.43
3:C:160:LEU:HD23	3:C:162:ALA:H	1.83	0.43
2:L:187:HIS:HB2	2:L:190:TYR:CZ	2.54	0.43
1:H:156:PHE:O	1:H:210:HIS:NE2	2.51	0.42
2:L:146:TRP:CE3	2:L:177:LEU:HD12	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:LEU:HD23	1:H:148:LEU:HA	1.88	0.42
2:L:88:ARG:O	2:L:94:TYR:HA	2.19	0.42
3:C:55:VAL:HG11	3:C:120:LEU:CD1	2.50	0.42
3:D:137:LYS:NZ	3:D:168:ASP:O	2.53	0.42
1:A:109:TYR:CD2	2:B:89:LEU:HD13	2.55	0.42
1:A:130:SER:HB3	1:A:132:PHE:CZ	2.55	0.42
2:B:28:SER:OG	2:B:29:SER:N	2.52	0.42
3:D:134:PHE:CE1	3:D:174:LEU:HB2	2.55	0.42
2:B:162:THR:HG22	2:B:172:SER:H	1.83	0.42
3:C:63:GLU:OE1	3:C:185:SER:OG	2.33	0.42
1:H:32:GLY:HA2	1:H:54:HIS:HD2	1.85	0.41
3:D:45:ILE:HG21	3:D:199:LEU:HD22	2.02	0.41
3:D:99:GLY:O	3:D:103:ILE:HG13	2.21	0.41
2:L:188:LYS:HD2	2:L:188:LYS:H	1.85	0.41
2:B:138:TYR:CD1	2:B:196:HIS:HE1	2.38	0.41
3:D:147:ILE:O	3:D:150:VAL:HG23	2.21	0.41
2:B:164:GLN:HE21	2:B:169:SER:HB3	1.85	0.41
2:L:134:LEU:CD2	2:L:196:HIS:HE2	2.34	0.41
2:L:134:LEU:HD23	2:L:196:HIS:HE2	1.86	0.41
2:L:187:HIS:HB2	2:L:190:TYR:OH	2.21	0.41
1:A:207:ASN:OD1	1:A:207:ASN:N	2.54	0.41
2:B:53:GLN:HG3	2:B:54:SER:N	2.37	0.40
3:C:157:LYS:O	3:C:169:LYS:N	2.41	0.40
2:L:5:SER:HB2	2:L:20:THR:HB	2.03	0.40
2:L:84:TYR:O	2:L:99:GLY:HA2	2.21	0.40
2:B:84:TYR:HB2	2:B:100:THR:HG23	2.03	0.40
1:H:176:PHE:N	1:H:176:PHE:HD1	2.19	0.40
1:A:61:ASN:HB3	1:A:64:LEU:HD12	2.03	0.40
2:B:106:ARG:NH2	2:B:109:ALA:HB2	2.36	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	A	201/230 (87%)	197 (98%)	4 (2%)	0	100	100
1	H	201/230 (87%)	196 (98%)	5 (2%)	0	100	100
2	B	204/214 (95%)	200 (98%)	4 (2%)	0	100	100
2	L	197/214 (92%)	190 (96%)	7 (4%)	0	100	100
3	C	151/165 (92%)	151 (100%)	0	0	100	100
3	D	152/165 (92%)	152 (100%)	0	0	100	100
All	All	1106/1218 (91%)	1086 (98%)	20 (2%)	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	A	179/199 (90%)	174 (97%)	5 (3%)	38	73
1	H	178/199 (89%)	176 (99%)	2 (1%)	65	87
2	B	182/187 (97%)	181 (100%)	1 (0%)	81	93
2	L	180/187 (96%)	179 (99%)	1 (1%)	78	92
3	C	129/133 (97%)	128 (99%)	1 (1%)	73	90
3	D	129/133 (97%)	127 (98%)	2 (2%)	55	83
All	All	977/1038 (94%)	965 (99%)	12 (1%)	63	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	39	ARG
1	H	72	VAL
2	L	115	ILE
1	A	19	SER
1	A	67	ARG
1	A	125	SER
1	A	187	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	SER
2	B	86	CYS
3	C	41	ASN
3	D	42	LEU
3	D	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	40	GLN
1	H	78	GLN
2	L	36	GLN
2	L	98	GLN
2	L	158	GLN
1	A	40	GLN
1	A	115	GLN
1	A	174	HIS
2	B	156	ASN
2	B	196	HIS
3	C	93	ASN
3	C	141	ASN
3	C	142	HIS
3	C	163	ASN
3	D	142	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	207/230 (90%)	0.16	4 (1%) 66 57	34, 70, 146, 166	0
1	H	207/230 (90%)	0.23	8 (3%) 43 34	30, 66, 169, 215	0
2	B	208/214 (97%)	0.58	14 (6%) 24 17	47, 109, 157, 194	0
2	L	205/214 (95%)	0.64	19 (9%) 14 10	40, 109, 155, 199	0
3	C	157/165 (95%)	0.17	4 (2%) 58 48	42, 72, 112, 136	0
3	D	158/165 (95%)	0.24	5 (3%) 50 40	42, 83, 117, 143	0
All	All	1142/1218 (93%)	0.35	54 (4%) 36 29	30, 83, 152, 215	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	ALA	3.6
2	B	81	PHE	3.4
2	L	111	PRO	3.4
1	H	136	PRO	3.2
2	B	125	SER	3.1
2	L	196	HIS	3.1
1	A	217	VAL	3.1
2	L	148	VAL	3.0
3	C	167	LYS	3.0
2	L	138	TYR	2.9
2	B	127	THR	2.9
2	L	50	SER	2.8
1	A	199	LEU	2.8
3	D	87	GLY	2.8
3	D	147	ILE	2.7
1	H	147	ALA	2.6
2	B	77	GLN	2.6
2	B	104	ILE	2.6
2	L	139	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	109	ALA	2.6
2	B	129	SER	2.5
2	L	152	LEU	2.5
2	L	137	PHE	2.5
2	L	193	GLU	2.5
3	D	43	THR	2.5
1	H	65	LYS	2.5
2	B	208	ASN	2.4
2	L	141	GLU	2.4
1	H	135	ALA	2.4
2	L	136	ASN	2.4
2	L	185	GLU	2.4
3	C	164	ALA	2.3
3	D	119	GLY	2.3
2	L	0	ILE	2.3
2	B	170	THR	2.3
2	L	182	ALA	2.3
1	H	145	THR	2.3
2	B	5	SER	2.2
3	C	40	PRO	2.2
2	L	187	HIS	2.2
2	B	192	CYS	2.2
1	A	216	LYS	2.2
2	L	208	ASN	2.2
1	A	218	ASP	2.1
1	H	151	LEU	2.1
1	H	10	GLY	2.1
2	B	195	THR	2.1
3	C	99	GLY	2.1
2	B	169	SER	2.1
2	L	189	VAL	2.1
2	L	113	VAL	2.0
3	D	148	GLN	2.0
2	B	202	PRO	2.0
1	H	146	ALA	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.