



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 04:30 AM EDT

PDB ID : 2Z91
Title : Crystal structure of the Fab fragment of anti-ciguatoxin antibody 10C9
Authors : Ui, M.; Tanaka, Y.; Tsumoto, K.
Deposited on : 2007-09-14
Resolution : 2.60 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

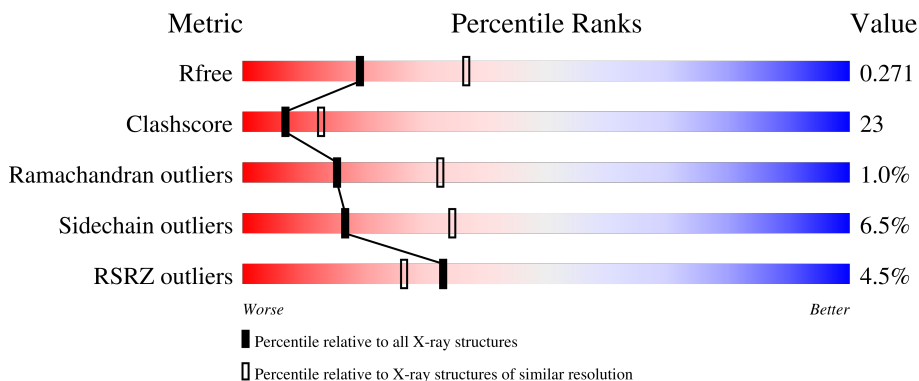
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	218	 3% (poor fit), 62% (0 outliers), 29% (1 outlier), 5% (2 outliers)
1	C	218	 6% (poor fit), 56% (0 outliers), 33% (1 outlier), 7% (2 outliers)
2	B	213	 5% (poor fit), 60% (0 outliers), 35% (1 outlier), 2% (2 outliers)
2	D	213	 2% (poor fit), 58% (0 outliers), 36% (1 outlier), 4% (2 outliers)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6477 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 Anti-ciguatoxin antibody 10C9 FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	Total	C	N	O	S	0	0	0
			1598	1018	257	316	7			
1	C	203	Total	C	N	O	S	0	0	0
			1573	1005	253	308	7			

- Molecule 2 is a protein called Anti-ciguatoxin antibody 10C9 FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	211	Total	C	N	O	S	0	0	0
			1611	998	270	334	9			
2	D	208	Total	C	N	O	S	0	0	0
			1592	988	267	328	9			

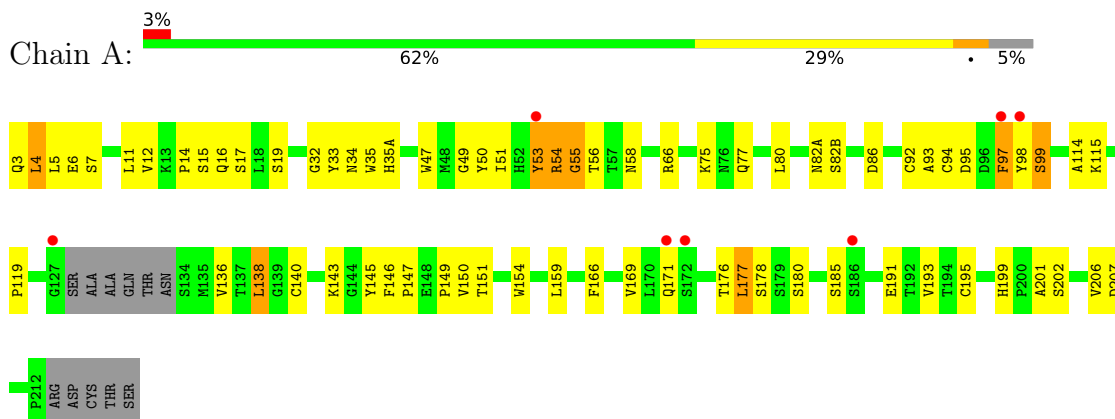
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	27	Total	O	0	0
			27	27		
3	C	27	Total	O	0	0
			27	27		
3	D	26	Total	O	0	0
			26	26		

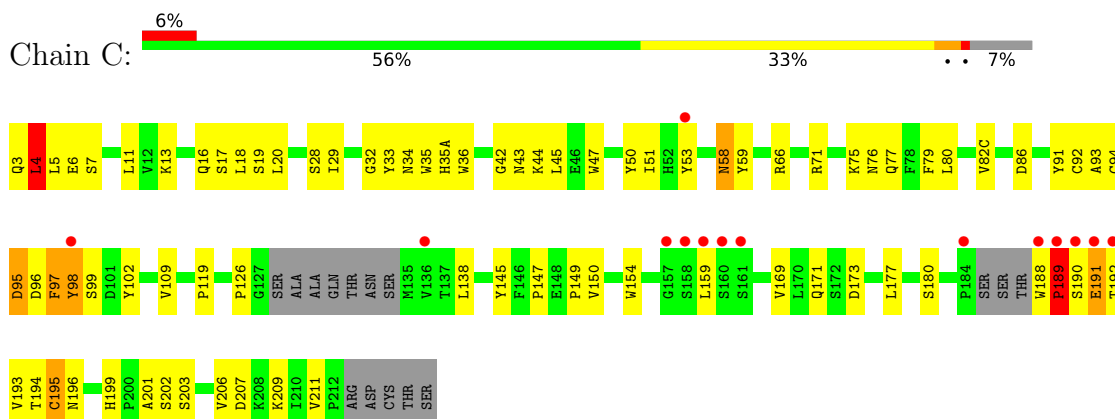
3 Residue-property plots

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.

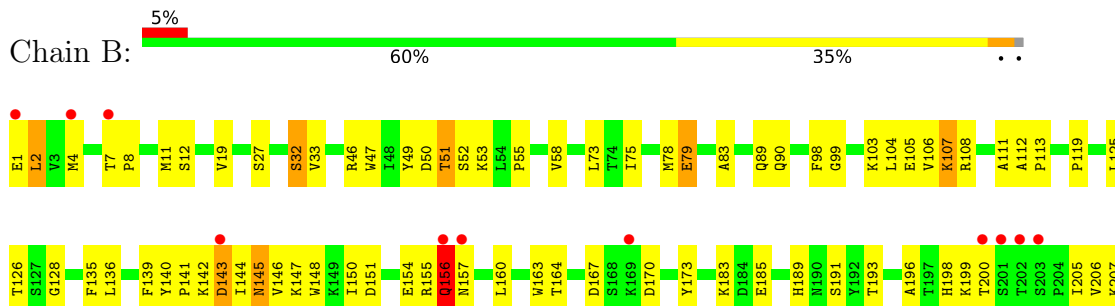
- Molecule 1: Anti-ciguatoxin antibody 10C9 FAB heavy chain



- Molecule 1: Anti-ciguatoxin antibody 10C9 FAB heavy chain



- Molecule 2: Anti-ciguatoxin antibody 10C9 FAB light chain



S208
F209
N210
R211
N212
GLU
CYS

- Molecule 2: Anti-ciguatoxin antibody 10C9 FAB light chain

Chain D: 2%
58% 36%

E1 L2 V3 M4 P8 M1 P15 V19 A25 S26 S27 S32 V33 S43 R46 W47 I48 Y49 D50 T51 S52 L54 V58 F62 S67 I75 M78 E79 A80 E81 D82 A83 Q89 Q90 N94 P95 V106 K107 D110 F118 P119

P120 E123 Q124 L125 T126 G129 V133 C134 F135 L136 N137 Y140 P141 K142 D143 I144 N145 V146 K147 W148 D151 G152 S153 R155 Q156 N157 G158 V159 L160 N161 Y173 S174 M175 S176 L179 T182 K183 D184 E185 Y186 F187 R188 H189 N190 T193 C194 E195 H198 K199

THR SER T202 S203 P204 T205 V206 F209 N210 R211 N212 E213 CYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.84Å 78.26Å 89.04Å 90.00° 99.25° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 38.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-2.60) 100.0 (38.32-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.270 0.220 , 0.271	Depositor DCC
R_{free} test set	2829 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtrriage
Anisotropy	0.540	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6477	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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 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	A	0.42	0/1644	0.73	1/2254 (0.0%)
1	C	0.40	0/1618	0.75	1/2217 (0.0%)
2	B	0.44	0/1650	0.70	1/2243 (0.0%)
2	D	0.40	0/1629	0.70	1/2211 (0.0%)
All	All	0.42	0/6541	0.72	4/8925 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	156	GLN	N-CA-C	7.69	131.77	111.00
2	B	156	GLN	N-CA-C	6.82	129.42	111.00
1	C	4	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	140	CYS	CA-CB-SG	5.21	123.38	114.00

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	A	1598	0	1541	64	1
1	C	1573	0	1518	85	0
2	B	1611	0	1536	83	1
2	D	1592	0	1517	83	0
3	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	0	0	0
3	C	27	0	0	0	0
3	D	26	0	0	0	0
All	All	6477	0	6112	285	1

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 23.

All (285) 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:C:18:LEU:HD21	1:C:109:VAL:HG11	1.32	1.10
1:C:188:TRP:CG	1:C:189:PRO:HD2	1.87	1.10
2:D:155:ARG:O	2:D:156:GLN:HB2	1.53	1.04
2:D:189:HIS:O	2:D:211:ARG:HD3	1.62	0.99
2:B:78:MET:HE3	2:B:104:LEU:HD21	1.49	0.94
1:C:18:LEU:CD2	1:C:109:VAL:HG11	1.99	0.91
2:D:32:SER:O	2:D:33:VAL:HG23	1.75	0.85
2:B:156:GLN:HG3	2:B:157:ASN:ND2	1.92	0.85
2:D:79:GLU:HB3	2:D:81:GLU:HG2	1.57	0.84
1:C:188:TRP:O	1:C:190:SER:N	2.14	0.81
2:B:7:THR:HG23	2:B:8:PRO:HA	1.63	0.81
2:B:185:GLU:OE2	2:B:189:HIS:NE2	2.12	0.81
1:A:75:LYS:HE2	1:C:5:LEU:HD11	1.64	0.79
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.66	0.78
2:D:202:THR:HG22	2:D:203:SER:H	1.51	0.76
1:C:188:TRP:CB	1:C:189:PRO:HD2	2.15	0.76
1:A:77:GLN:HE22	1:C:7:SER:HB2	1.51	0.75
2:B:156:GLN:HG3	2:B:157:ASN:HD22	1.51	0.75
1:C:188:TRP:CD2	1:C:189:PRO:HD2	2.20	0.75
1:C:194:THR:HG22	1:C:209:LYS:HA	1.69	0.75
2:B:50:ASP:HB3	2:B:53:LYS:HD3	1.69	0.74
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.70	0.74
2:D:195:GLU:HG3	2:D:206:VAL:HG22	1.68	0.74
1:C:126:PRO:HD2	1:C:188:TRP:CH2	2.23	0.74
2:D:188:ARG:NH2	2:D:189:HIS:NE2	2.36	0.73
2:D:2:LEU:HD21	2:D:27:SER:HB2	1.70	0.71
1:A:98:TYR:O	1:A:99:SER:HB3	1.89	0.70
1:C:191:GLU:CD	1:C:192:THR:H	1.93	0.70
1:A:3:GLN:C	1:A:4:LEU:HD23	2.12	0.70
2:D:161:ASN:HB3	2:D:175:MET:HE3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:HIS:ND1	2:D:199:LYS:N	2.42	0.68
2:D:159:VAL:HG22	2:D:179:LEU:HD13	1.75	0.68
1:C:171:GLN:O	1:C:171:GLN:HG3	1.92	0.68
2:B:7:THR:CG2	2:B:8:PRO:HA	2.24	0.67
2:D:156:GLN:HG2	2:D:157:ASN:O	1.94	0.67
2:D:147:LYS:HG3	2:D:155:ARG:NH2	2.10	0.67
1:C:188:TRP:C	1:C:190:SER:H	1.99	0.67
2:B:12:SER:HA	2:B:105:GLU:O	1.95	0.66
2:B:193:THR:HA	2:B:208:SER:HB3	1.78	0.66
1:A:55:GLY:HA3	1:C:203:SER:OG	1.97	0.65
2:D:4:MET:HE1	2:D:25:ALA:HA	1.78	0.65
2:B:83:ALA:HB2	2:B:106:VAL:HG23	1.78	0.65
1:C:188:TRP:CG	1:C:189:PRO:CD	2.73	0.65
2:D:120:PRO:HD2	2:D:186:TYR:CZ	2.32	0.64
2:B:83:ALA:HB2	2:B:106:VAL:CG2	2.27	0.64
2:D:202:THR:HG22	2:D:203:SER:N	2.12	0.64
2:B:112:ALA:N	2:B:200:THR:HG21	2.13	0.64
2:B:198:HIS:CG	2:B:199:LYS:H	2.15	0.63
2:D:147:LYS:HG3	2:D:155:ARG:HH21	1.63	0.63
1:A:199:HIS:HD2	1:A:202:SER:OG	1.82	0.63
2:D:211:ARG:C	2:D:213:GLU:H	2.01	0.63
2:D:198:HIS:CG	2:D:199:LYS:H	2.10	0.63
1:C:35(A):HIS:NE2	1:C:95:ASP:OD2	2.32	0.63
1:C:199:HIS:HD2	1:C:202:SER:OG	1.81	0.62
1:C:32:GLY:O	1:C:33:TYR:HB2	1.98	0.62
2:D:198:HIS:CG	2:D:199:LYS:N	2.66	0.61
1:A:82(B):SER:H	1:C:16:GLN:NE2	1.99	0.61
1:A:54:ARG:O	1:A:56:THR:N	2.34	0.61
1:C:169:VAL:HG11	2:D:160:LEU:HD22	1.83	0.61
2:B:143:ASP:OD2	2:B:143:ASP:N	2.33	0.61
2:B:142:LYS:HB2	2:B:173:TYR:CE2	2.36	0.60
1:C:97:PHE:O	1:C:98:TYR:HD1	1.84	0.60
1:C:29:ILE:HA	1:C:35:TRP:CZ2	2.36	0.60
1:C:147:PRO:O	1:C:199:HIS:HE1	1.85	0.60
1:A:98:TYR:HD1	2:B:49:TYR:HH	1.47	0.59
2:B:32:SER:O	2:B:33:VAL:HG23	2.02	0.59
1:C:51:ILE:CD1	1:C:71:ARG:HD3	2.32	0.59
2:D:78:MET:HG3	2:D:79:GLU:N	2.18	0.59
2:D:210:ASN:C	2:D:210:ASN:HD22	2.07	0.58
1:C:35:TRP:CE3	1:C:94:CYS:HB3	2.39	0.58
2:B:2:LEU:HD21	2:B:27:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:O	1:A:33:TYR:HB2	2.03	0.57
2:D:202:THR:CG2	2:D:203:SER:H	2.11	0.57
2:B:151:ASP:HA	2:B:191:SER:HB2	1.87	0.57
1:A:54:ARG:CD	1:A:55:GLY:N	2.68	0.57
2:B:111:ALA:C	2:B:200:THR:HG21	2.25	0.57
1:C:194:THR:HG22	1:C:209:LYS:CA	2.35	0.56
2:D:89:GLN:HG2	2:D:90:GLN:N	2.20	0.56
2:B:211:ARG:O	2:B:212:ASN:HB2	2.03	0.56
2:D:148:TRP:O	2:D:155:ARG:N	2.38	0.56
1:A:98:TYR:CE1	2:B:55:PRO:HA	2.41	0.56
1:A:6:GLU:HG3	1:A:92:CYS:SG	2.45	0.56
1:C:34:ASN:O	1:C:94:CYS:HA	2.06	0.56
1:C:97:PHE:O	1:C:98:TYR:CD1	2.58	0.56
2:D:151:ASP:OD2	2:D:189:HIS:ND1	2.39	0.56
2:B:126:THR:O	2:B:126:THR:HG22	2.06	0.55
1:A:169:VAL:HG11	2:B:160:LEU:HD22	1.87	0.55
2:B:150:ILE:HA	2:B:191:SER:O	2.05	0.55
2:D:188:ARG:HE	2:D:189:HIS:CD2	2.24	0.55
1:A:98:TYR:O	1:A:99:SER:CB	2.54	0.55
1:C:193:VAL:HG23	1:C:193:VAL:O	2.05	0.55
1:A:34:ASN:O	1:A:94:CYS:HA	2.06	0.55
1:A:54:ARG:HD3	1:A:55:GLY:N	2.22	0.55
1:C:6:GLU:HG3	1:C:92:CYS:SG	2.47	0.54
2:D:2:LEU:CD2	2:D:27:SER:HB2	2.38	0.54
1:C:99:SER:H	2:D:46:ARG:NH2	2.06	0.54
2:D:144:ILE:HG13	2:D:198:HIS:HB2	1.88	0.54
2:D:136:LEU:HD21	2:D:146:VAL:HG12	1.90	0.54
1:A:3:GLN:O	1:A:4:LEU:HD23	2.07	0.54
1:A:51:ILE:HD11	1:A:55:GLY:HA2	1.89	0.54
2:D:15:PRO:HA	2:D:78:MET:HG2	1.90	0.54
2:D:8:PRO:HG3	2:D:11:MET:HB3	1.90	0.53
2:B:198:HIS:CG	2:B:199:LYS:N	2.77	0.53
2:D:83:ALA:HB2	2:D:106:VAL:HG23	1.91	0.53
2:B:46:ARG:HD3	2:B:49:TYR:HB3	1.91	0.53
1:A:7:SER:HB2	1:C:77:GLN:HE22	1.73	0.52
2:D:50:ASP:O	2:D:51:THR:HG23	2.09	0.52
1:A:53:TYR:CD1	1:A:53:TYR:C	2.82	0.52
2:D:124:GLN:HG2	2:D:129:GLY:O	2.10	0.52
2:B:78:MET:HE3	2:B:104:LEU:CD2	2.33	0.52
1:A:5:LEU:HD11	1:C:75:LYS:HE2	1.92	0.52
1:A:143:LYS:HB3	1:A:176:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:GLN:HB3	1:C:4:LEU:CD2	2.40	0.52
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.92	0.51
2:B:210:ASN:ND2	2:B:212:ASN:HA	2.25	0.51
1:C:53:TYR:HD1	1:C:53:TYR:O	1.93	0.51
1:A:82(B):SER:H	1:C:16:GLN:HE22	1.58	0.51
1:A:98:TYR:HD1	2:B:49:TYR:OH	1.92	0.51
2:B:2:LEU:CD2	2:B:27:SER:HB2	2.40	0.51
1:C:44:LYS:HD3	1:C:45:LEU:N	2.24	0.51
2:D:204:PRO:O	2:D:206:VAL:HG23	2.10	0.51
1:C:196:ASN:N	1:C:196:ASN:ND2	2.59	0.51
2:B:155:ARG:HG3	2:B:155:ARG:O	2.11	0.51
2:B:144:ILE:HG12	2:B:145:ASN:N	2.26	0.50
1:A:75:LYS:CE	1:C:5:LEU:HD11	2.38	0.50
1:A:147:PRO:O	1:A:199:HIS:HE1	1.94	0.50
1:A:98:TYR:CD1	2:B:49:TYR:OH	2.63	0.50
1:A:5:LEU:HG	1:C:75:LYS:NZ	2.25	0.50
2:D:133:VAL:HG12	2:D:134:CYS:N	2.26	0.50
1:A:54:ARG:C	1:A:56:THR:H	2.14	0.50
1:C:28:SER:HA	1:C:76:ASN:HD21	1.76	0.50
1:A:77:GLN:NE2	1:C:7:SER:HB2	2.24	0.50
2:D:147:LYS:HE2	2:D:155:ARG:NH2	2.26	0.50
1:A:82(A):ASN:ND2	1:C:13:LYS:HD3	2.27	0.50
2:D:210:ASN:HD22	2:D:211:ARG:N	2.10	0.50
1:A:7:SER:CB	1:C:77:GLN:HE22	2.25	0.49
2:B:78:MET:CE	2:B:104:LEU:HD21	2.31	0.49
1:C:96:ASP:OD2	1:C:99:SER:HB2	2.11	0.49
2:D:110:ASP:OD1	2:D:141:PRO:HD3	2.12	0.49
2:D:140:TYR:O	2:D:198:HIS:HE1	1.95	0.49
2:B:156:GLN:CA	2:B:156:GLN:HE21	2.25	0.49
2:D:8:PRO:CG	2:D:11:MET:HB3	2.41	0.49
2:B:4:MET:HE1	2:B:90:GLN:HG3	1.93	0.49
2:B:126:THR:O	2:B:126:THR:CG2	2.60	0.49
1:C:138:LEU:HD21	1:C:188:TRP:CD1	2.48	0.49
1:C:19:SER:O	1:C:20:LEU:HD23	2.13	0.49
2:B:89:GLN:NE2	2:B:98:PHE:CZ	2.81	0.49
1:C:4:LEU:HD23	1:C:4:LEU:N	2.28	0.49
1:C:53:TYR:O	1:C:53:TYR:CD1	2.65	0.49
1:A:97:PHE:CE1	1:A:98:TYR:HB2	2.48	0.48
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.48	0.48
1:C:47:TRP:HZ2	1:C:50:TYR:CD2	2.32	0.48
2:B:140:TYR:O	2:B:198:HIS:HE1	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:ASN:HA	2:D:211:ARG:HG2	1.95	0.48
2:B:136:LEU:N	2:B:136:LEU:HD12	2.29	0.48
1:A:14:PRO:O	1:A:15:SER:OG	2.30	0.48
1:A:180:SER:HB3	2:B:135:PHE:CE2	2.49	0.48
2:B:19:VAL:HB	2:B:75:ILE:HB	1.96	0.48
2:B:156:GLN:HE21	2:B:156:GLN:HA	1.79	0.48
2:D:62:PHE:CE1	2:D:75:ILE:HG12	2.48	0.48
1:C:51:ILE:HD13	1:C:71:ARG:HD3	1.95	0.47
2:D:185:GLU:OE1	2:D:188:ARG:NH2	2.48	0.47
2:B:144:ILE:HG12	2:B:145:ASN:H	1.78	0.47
1:C:180:SER:HB3	2:D:135:PHE:CE2	2.50	0.47
1:A:138:LEU:HD23	1:A:193:VAL:HG11	1.96	0.47
1:A:150:VAL:CG1	1:A:177:LEU:HD13	2.45	0.47
1:C:51:ILE:HD11	1:C:71:ARG:HD3	1.95	0.47
2:B:141:PRO:HB2	2:B:143:ASP:OD2	2.15	0.47
2:D:125:LEU:O	2:D:183:LYS:HD2	2.14	0.47
2:D:155:ARG:HE	2:D:155:ARG:HA	1.80	0.47
2:D:136:LEU:HD23	2:D:144:ILE:HD13	1.96	0.46
1:C:66:ARG:NH2	1:C:86:ASP:OD2	2.48	0.46
1:A:16:GLN:HB3	1:C:17:SER:HB2	1.96	0.46
2:D:135:PHE:HB3	2:D:137:ASN:HD21	1.80	0.46
2:D:188:ARG:NE	2:D:189:HIS:NE2	2.64	0.46
2:B:196:ALA:HB3	2:B:205:ILE:CG2	2.46	0.46
1:C:19:SER:HA	1:C:80:LEU:O	2.15	0.46
1:C:99:SER:N	2:D:46:ARG:NH2	2.64	0.46
1:C:138:LEU:HD21	1:C:188:TRP:NE1	2.31	0.46
2:B:107:LYS:HB2	2:B:107:LYS:NZ	2.30	0.46
2:B:148:TRP:O	2:B:154:GLU:HA	2.15	0.46
1:C:96:ASP:OD2	1:C:96:ASP:C	2.53	0.46
2:D:188:ARG:HH21	2:D:189:HIS:CD2	2.31	0.46
1:A:53:TYR:C	1:A:53:TYR:HD1	2.19	0.46
2:B:136:LEU:HD21	2:B:146:VAL:HG12	1.98	0.46
2:B:157:ASN:HD22	2:B:157:ASN:N	2.13	0.46
2:D:32:SER:O	2:D:33:VAL:CG2	2.58	0.45
1:A:54:ARG:C	1:A:54:ARG:HD2	2.36	0.45
1:C:93:ALA:HB1	1:C:102:TYR:O	2.17	0.45
2:B:205:ILE:O	2:B:205:ILE:HG23	2.15	0.45
2:D:123:GLU:O	2:D:126:THR:HB	2.15	0.45
1:C:98:TYR:HB3	2:D:49:TYR:CZ	2.51	0.45
1:A:119:PRO:CB	1:A:145:TYR:HB3	2.43	0.45
1:A:136:VAL:HG23	1:A:185:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:MET:HB3	2:B:99:GLY:HA2	1.98	0.45
2:B:55:PRO:HG2	2:B:58:VAL:CG2	2.47	0.45
2:D:211:ARG:C	2:D:213:GLU:N	2.70	0.45
1:A:35:TRP:CE3	1:A:94:CYS:HB3	2.52	0.45
2:B:55:PRO:HG2	2:B:58:VAL:HG23	1.98	0.45
1:A:177:LEU:HD23	1:A:178:SER:N	2.31	0.45
2:B:147:LYS:HE3	2:B:154:GLU:OE1	2.16	0.45
2:B:107:LYS:HG3	2:B:108:ARG:N	2.32	0.44
1:C:42:GLY:O	1:C:43:ASN:HB2	2.17	0.44
1:C:206:VAL:HG12	1:C:207:ASP:N	2.32	0.44
2:D:19:VAL:HB	2:D:75:ILE:HB	1.99	0.44
2:B:142:LYS:HE3	2:B:163:TRP:CD1	2.53	0.44
2:B:147:LYS:HE3	2:B:154:GLU:CD	2.37	0.44
1:A:17:SER:HB3	1:C:17:SER:H	1.81	0.44
1:C:119:PRO:CB	1:C:145:TYR:HB3	2.40	0.44
1:C:154:TRP:CZ3	1:C:195:CYS:HB3	2.52	0.44
1:C:147:PRO:HD2	1:C:201:ALA:CB	2.48	0.44
2:B:119:PRO:HG3	2:B:209:PHE:CG	2.52	0.44
2:D:142:LYS:HB3	2:D:173:TYR:CD2	2.53	0.44
2:D:195:GLU:HG2	2:D:204:PRO:HB2	1.99	0.44
1:C:5:LEU:HD13	1:C:6:GLU:N	2.33	0.44
2:D:133:VAL:CG1	2:D:134:CYS:N	2.80	0.44
2:D:188:ARG:O	2:D:188:ARG:HG2	2.18	0.44
1:A:19:SER:HA	1:A:80:LEU:O	2.17	0.44
1:A:6:GLU:OE1	1:A:6:GLU:N	2.49	0.43
2:D:156:GLN:CG	2:D:157:ASN:N	2.81	0.43
2:B:103:LYS:HB2	2:B:103:LYS:HE3	1.78	0.43
2:B:196:ALA:HB3	2:B:205:ILE:HG23	1.99	0.43
1:C:98:TYR:CG	1:C:98:TYR:O	2.72	0.43
1:C:188:TRP:C	1:C:190:SER:N	2.66	0.43
2:D:185:GLU:OE1	2:D:188:ARG:CZ	2.67	0.43
2:B:50:ASP:O	2:B:52:SER:N	2.49	0.43
2:B:128:GLY:HA2	2:B:183:LYS:HB2	2.00	0.43
1:C:18:LEU:HB2	1:C:82(C):VAL:HG11	2.00	0.43
1:C:190:SER:OG	1:C:191:GLU:N	2.52	0.43
1:A:77:GLN:HE22	1:C:7:SER:CB	2.27	0.43
2:B:7:THR:CG2	2:B:8:PRO:CA	2.94	0.43
2:B:156:GLN:HA	2:B:156:GLN:NE2	2.33	0.43
2:B:196:ALA:O	2:B:205:ILE:HG22	2.19	0.43
1:A:147:PRO:HD2	1:A:201:ALA:CB	2.49	0.43
2:B:11:MET:O	2:B:105:GLU:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:PHE:CD1	2:D:118:PHE:N	2.87	0.43
2:B:206:VAL:HG12	2:B:207:LYS:N	2.34	0.43
2:D:182:THR:O	2:D:183:LYS:C	2.56	0.43
2:D:48:ILE:HG12	2:D:54:LEU:HD23	2.01	0.42
2:D:119:PRO:HG3	2:D:209:PHE:CG	2.54	0.42
1:C:91:TYR:CE2	2:D:43:SER:HB2	2.54	0.42
1:A:66:ARG:HH22	1:A:86:ASP:CG	2.23	0.42
2:B:156:GLN:CA	2:B:156:GLN:NE2	2.82	0.42
1:C:192:THR:HG22	1:C:194:THR:HG23	2.02	0.42
1:A:14:PRO:O	1:A:15:SER:CB	2.67	0.42
2:B:167:ASP:HB3	2:B:170:ASP:OD1	2.19	0.42
1:C:188:TRP:HB3	1:C:189:PRO:HD2	1.98	0.42
1:C:3:GLN:HB3	1:C:4:LEU:HD23	2.01	0.42
2:D:193:THR:HG23	2:D:206:VAL:HG13	2.00	0.42
1:A:4:LEU:HD12	1:A:93:ALA:HA	2.02	0.42
2:B:89:GLN:HG2	2:B:90:GLN:N	2.34	0.42
2:B:8:PRO:HG2	2:B:11:MET:HB3	2.02	0.42
2:B:53:LYS:N	2:B:53:LYS:HD2	2.35	0.42
1:A:50:TYR:CD1	1:A:50:TYR:C	2.93	0.41
1:C:99:SER:H	2:D:46:ARG:HH22	1.67	0.41
2:D:175:MET:CG	2:D:176:SER:N	2.82	0.41
2:B:128:GLY:C	2:B:183:LYS:HB2	2.41	0.41
2:D:185:GLU:OE2	2:D:188:ARG:NH1	2.53	0.41
2:D:50:ASP:C	2:D:51:THR:CG2	2.88	0.41
1:C:58:ASN:HD22	1:C:59:TYR:N	2.17	0.41
2:B:142:LYS:HB2	2:B:173:TYR:CZ	2.55	0.41
2:D:187:GLU:HA	2:D:211:ARG:NE	2.35	0.41
1:A:98:TYR:HD1	2:B:49:TYR:CZ	2.38	0.41
2:D:47:TRP:O	2:D:48:ILE:HG13	2.20	0.41
1:C:191:GLU:CD	1:C:192:THR:N	2.68	0.41
1:A:54:ARG:HD2	1:A:55:GLY:N	2.35	0.41
1:A:166:PHE:CD1	2:B:164:THR:HG23	2.55	0.41
1:C:18:LEU:HD23	1:C:109:VAL:HG11	1.97	0.41
1:A:35(A):HIS:NE2	1:A:95:ASP:OD1	2.53	0.41
2:B:107:LYS:HG3	2:B:108:ARG:H	1.86	0.41
1:C:4:LEU:CD2	1:C:4:LEU:N	2.84	0.41
1:C:35:TRP:CD1	1:C:35:TRP:N	2.89	0.41
2:D:47:TRP:CE2	2:D:58:VAL:HG13	2.55	0.41
2:D:50:ASP:O	2:D:52:SER:N	2.51	0.41
1:A:53:TYR:CD1	1:A:54:ARG:N	2.89	0.41
1:A:154:TRP:CZ3	1:A:195:CYS:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TRP:CZ3	1:C:92:CYS:HB3	2.56	0.41
2:B:125:LEU:O	2:B:183:LYS:HE2	2.22	0.40
2:B:119:PRO:HG3	2:B:209:PHE:CD2	2.57	0.40
2:D:94:ASN:HA	2:D:95:PRO:HA	1.92	0.40
2:D:161:ASN:HB3	2:D:175:MET:CE	2.45	0.40
1:A:114:ALA:HB3	1:A:146:PHE:CE2	2.55	0.40
2:D:118:PHE:HA	2:D:119:PRO:HD3	1.93	0.40
1:A:206:VAL:CG1	1:A:207:ASP:N	2.84	0.40
2:B:78:MET:HG3	2:B:79:GLU:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLU:OE2	2:B:185:GLU:OE2[2_554]	2.08	0.12

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	203/218 (93%)	184 (91%)	17 (8%)	2 (1%)	15 32
1	C	197/218 (90%)	180 (91%)	16 (8%)	1 (0%)	29 52
2	B	209/213 (98%)	195 (93%)	12 (6%)	2 (1%)	15 32
2	D	202/213 (95%)	186 (92%)	13 (6%)	3 (2%)	10 21
All	All	811/862 (94%)	745 (92%)	58 (7%)	8 (1%)	15 32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLY

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Mol	Chain	Res	Type
1	A	99	SER
1	C	189	PRO
2	B	51	THR
2	B	156	GLN
2	D	51	THR
2	D	156	GLN
2	D	33	VAL

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	187/196 (95%)	173 (92%)	14 (8%)	13	27
1	C	183/196 (93%)	167 (91%)	16 (9%)	10	20
2	B	186/188 (99%)	176 (95%)	10 (5%)	22	44
2	D	183/188 (97%)	175 (96%)	8 (4%)	28	53
All	All	739/768 (96%)	691 (94%)	48 (6%)	17	34

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	11	LEU
1	A	12	VAL
1	A	53	TYR
1	A	54	ARG
1	A	58	ASN
1	A	97	PHE
1	A	115	LYS
1	A	138	LEU
1	A	149	PRO
1	A	151	THR
1	A	159	LEU
1	A	171	GLN
1	A	177	LEU

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Mol	Chain	Res	Type
2	B	1	GLU
2	B	2	LEU
2	B	32	SER
2	B	47	TRP
2	B	51	THR
2	B	73	LEU
2	B	79	GLU
2	B	107	LYS
2	B	143	ASP
2	B	145	ASN
1	C	4	LEU
1	C	11	LEU
1	C	58	ASN
1	C	79	PHE
1	C	95	ASP
1	C	97	PHE
1	C	98	TYR
1	C	149	PRO
1	C	150	VAL
1	C	159	LEU
1	C	173	ASP
1	C	177	LEU
1	C	189	PRO
1	C	191	GLU
1	C	195	CYS
1	C	211	VAL
2	D	50	ASP
2	D	51	THR
2	D	78	MET
2	D	79	GLU
2	D	81	GLU
2	D	107	LYS
2	D	184	ASP
2	D	210	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	58	ASN
1	A	77	GLN
1	A	199	HIS

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Mol	Chain	Res	Type
2	B	37	GLN
2	B	156	GLN
2	B	157	ASN
2	B	210	ASN
2	B	212	ASN
1	C	16	GLN
1	C	58	ASN
1	C	76	ASN
1	C	77	GLN
1	C	199	HIS
2	D	34	HIS
2	D	137	ASN
2	D	156	GLN
2	D	157	ASN
2	D	210	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 monosaccharides 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

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	207/218 (94%)	0.03	7 (3%) 45 38	14, 30, 49, 67	0
1	C	203/218 (93%)	0.28	14 (6%) 16 12	13, 31, 54, 79	0
2	B	211/213 (99%)	0.22	11 (5%) 27 21	17, 34, 51, 65	0
2	D	208/213 (97%)	0.14	5 (2%) 59 53	13, 36, 55, 76	0
All	All	829/862 (96%)	0.17	37 (4%) 33 26	13, 33, 53, 79	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	TYR	6.2
1	C	192	THR	4.6
1	A	98	TYR	4.6
1	C	160	SER	4.3
2	B	202	THR	4.2
1	C	189	PRO	4.2
1	C	157	GLY	4.0
2	D	155	ARG	4.0
2	D	157	ASN	3.8
1	C	53	TYR	3.6
1	C	191	GLU	3.4
1	A	171	GLN	3.3
2	B	1	GLU	3.1
2	D	156	GLN	3.0
2	B	157	ASN	2.9
1	C	159	LEU	2.8
1	C	190	SER	2.8
2	B	200	THR	2.8
2	B	7	THR	2.7
2	B	169	LYS	2.7
1	A	127	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	136	VAL	2.6
1	A	186	SER	2.5
2	B	201	SER	2.5
1	C	188	TRP	2.5
2	D	129	GLY	2.4
1	A	53	TYR	2.2
2	D	67	SER	2.2
1	C	184	PRO	2.1
1	A	172	SER	2.1
2	B	143	ASP	2.1
1	C	158	SER	2.1
2	B	4	MET	2.1
1	C	161	SER	2.0
2	B	203	SER	2.0
2	B	156	GLN	2.0
1	A	97	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.