Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 03:01 AM EDT

PDB ID	:	2Q76
Title	:	Mouse anti-hen egg white lysozyme antibody F10.6.6 Fab fragment
Authors	:	Cauerhff, A.; Klinke, S.; Acierno, J.P.; Goldbaum, F.A.; Braden, B.C.
Deposited on	:	2007-06-06
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

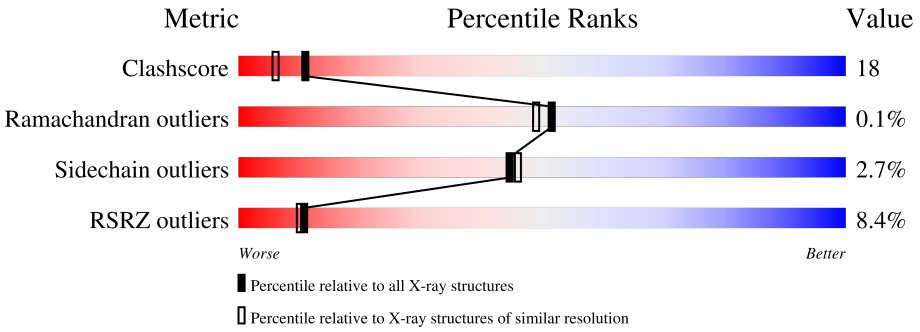
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	212	8% 69% 28% •
1	C	212	11% 67% 33% •
2	B	216	7% 71% 26% ••
2	D	216	6% 72% 25% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7001 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fab F10.6.6 fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	1639	1013	280	340	6	0	0	0
1	C	212	1639	1013	280	340	6	0	0	0

- Molecule 2 is a protein called Fab F10.6.6 fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	1613	1027	256	323	7	0	0	0
2	D	210	1593	1016	252	318	7	0	0	0

- Molecule 3 is water.

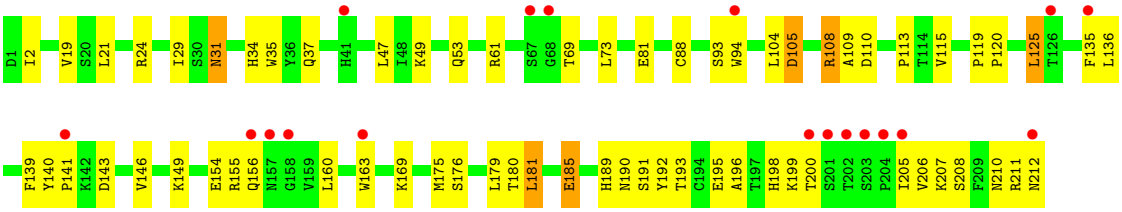
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	124	124	124	0	0
3	B	142	142	142	0	0
3	C	117	117	117	0	0
3	D	134	134	134	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

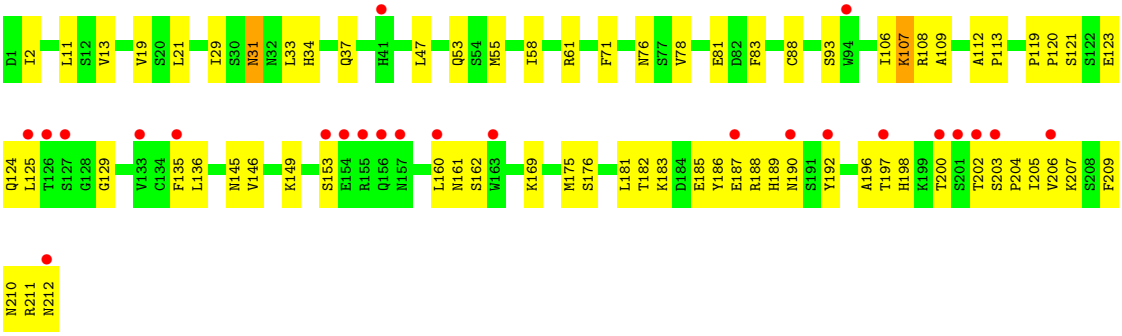
• Molecule 1: Fab F10.6.6 fragment Light Chain

Chain A:



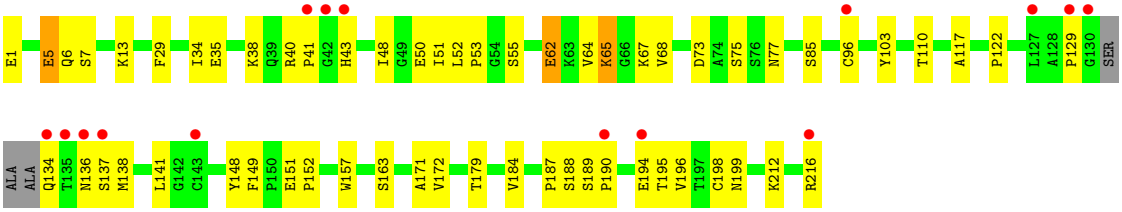
• Molecule 1: Fab F10.6.6 fragment Light Chain

Chain C:



• Molecule 2: Fab F10.6.6 fragment Heavy Chain

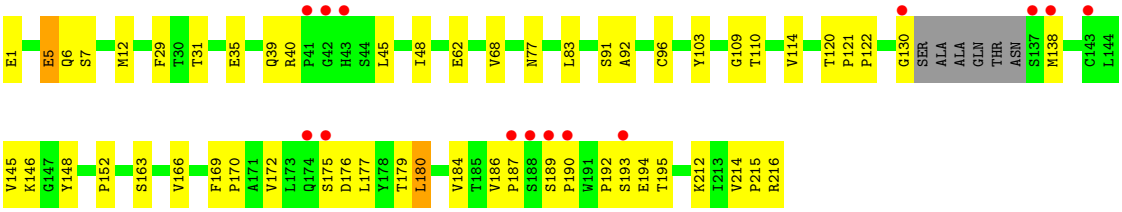
Chain B:



• Molecule 2: Fab F10.6.6 fragment Heavy Chain

Chain D:

6%
72%
25%


E1 E5 Q6 S7 M12 F29 T30 T31 E35 Q39 R40 P41 G42 H43 S44 L45 I48 E62 V68 N77 L83 S91 A92 C96 Y103 G109 T110 V114 T120 P121 P122 G130 SER ALA ALA GLN THR ASN S137 M138 C143 L144
V145 K146 G147 Y148 P152 S163 V166 F169 P170 A171 V172 L173 Q174 S175 D176 L177 Y178 T179 L180 V184 T185 V186 P187 S188 S189 P190 W191 P192 S193 E194 T195 K212 I213 V214 P215 R216

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.76Å 80.25Å 91.50Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 22.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 94.0 (22.87-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.233 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7001	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 27.94 % 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 2.0107e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/1676	0.63	0/2273
1	C	0.35	0/1676	0.62	0/2273
2	B	0.43	1/1658 (0.1%)	0.66	0/2269
2	D	0.42	1/1638 (0.1%)	0.69	0/2241
All	All	0.39	2/6648 (0.0%)	0.65	0/9056

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GLU	CD-OE2	6.98	1.33	1.25
2	D	5	GLU	CD-OE2	6.08	1.32	1.25

There are no bond angle outliers.

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	1639	0	1558	67	0
1	C	1639	0	1558	70	0
2	B	1613	0	1560	58	0
2	D	1593	0	1545	49	0
3	A	124	0	0	2	2
3	B	142	0	0	5	2
3	C	117	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	134	0	0	3	1
All	All	7001	0	6221	230	3

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 18.

All (230) 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:181:LEU:HD23	1:A:185:GLU:HG2	1.46	0.95
2:B:134:GLN:HA	2:B:188:SER:OG	1.67	0.94
2:D:187:PRO:O	2:D:190:PRO:HD2	1.69	0.93
2:B:6:GLN:HE21	2:B:110:THR:HG23	1.35	0.91
2:B:187:PRO:O	2:B:190:PRO:HD2	1.73	0.89
1:A:205:ILE:HD12	1:A:205:ILE:H	1.37	0.87
1:A:119:PRO:HG2	2:B:216:ARG:NH1	1.90	0.85
2:B:64:VAL:HG23	2:B:67:LYS:HG3	1.60	0.84
2:D:176:ASP:HB3	3:D:301:HOH:O	1.78	0.83
2:B:189:SER:OG	2:B:190:PRO:HD3	1.79	0.81
1:C:2:ILE:HD13	1:C:29:ILE:HG22	1.65	0.79
2:D:7:SER:O	2:D:110:THR:HG22	1.84	0.78
1:A:179:LEU:HG	1:A:181:LEU:HD11	1.64	0.77
2:B:6:GLN:NE2	2:B:110:THR:HG23	1.99	0.76
2:D:6:GLN:HE21	2:D:110:THR:HG23	1.50	0.75
1:C:31:ASN:HD22	1:C:31:ASN:H	1.33	0.75
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.67	0.75
1:A:31:ASN:H	1:A:31:ASN:HD22	1.35	0.73
1:C:113:PRO:HG2	1:C:205:ILE:HD12	1.70	0.72
2:B:187:PRO:C	2:B:190:PRO:HD2	2.09	0.72
2:B:122:PRO:HB3	2:B:148:TYR:HB3	1.72	0.72
2:D:187:PRO:HB2	2:D:190:PRO:CD	2.20	0.72
2:B:7:SER:O	2:B:110:THR:HG22	1.90	0.72
2:B:67:LYS:HD2	2:B:85:SER:HB2	1.71	0.72
1:A:154:GLU:HG2	1:A:156:GLN:OE1	1.90	0.71
2:B:40:ARG:HB3	2:B:41:PRO:HD2	1.73	0.71
2:B:187:PRO:HB2	2:B:190:PRO:CD	2.20	0.71
1:A:180:THR:C	1:A:181:LEU:HD12	2.12	0.69
1:A:160:LEU:HD11	2:B:172:VAL:HB	1.75	0.69
1:C:2:ILE:HD13	1:C:29:ILE:CG2	2.23	0.69
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.75	0.68
1:C:108:ARG:HG2	1:C:109:ALA:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLN:NE2	2:D:110:THR:HG23	2.09	0.66
1:A:2:ILE:HD13	1:A:29:ILE:HG22	1.76	0.66
2:B:62:GLU:HG2	2:B:68:VAL:CG2	2.25	0.66
2:D:189:SER:OG	2:D:190:PRO:HD3	1.94	0.66
1:C:107:LYS:HB2	1:C:107:LYS:NZ	2.11	0.66
2:B:13:LYS:HG2	3:B:253:HOH:O	1.95	0.65
2:B:187:PRO:HD2	2:B:190:PRO:HG2	1.78	0.65
1:C:2:ILE:HD12	1:C:93:SER:HB3	1.77	0.65
2:D:48:ILE:HG23	2:D:62:GLU:OE2	1.96	0.65
2:B:64:VAL:CG2	2:B:67:LYS:HE2	2.27	0.65
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.79	0.64
2:D:187:PRO:C	2:D:190:PRO:HD2	2.17	0.64
2:B:62:GLU:HG2	2:B:68:VAL:HB	1.78	0.64
1:C:182:THR:OG1	1:C:185:GLU:HB2	1.98	0.63
2:D:122:PRO:HB3	2:D:148:TYR:HB3	1.80	0.63
1:A:108:ARG:HG2	1:A:109:ALA:N	2.13	0.63
2:B:64:VAL:HG22	3:B:323:HOH:O	1.98	0.62
1:C:183:LYS:O	1:C:187:GLU:HG2	1.99	0.62
1:A:181:LEU:HD23	1:A:185:GLU:CG	2.27	0.62
1:C:211:ARG:HH11	1:C:211:ARG:HB3	1.66	0.61
2:D:1:GLU:OE2	2:D:1:GLU:HA	2.00	0.60
1:C:107:LYS:HB2	1:C:107:LYS:HZ3	1.66	0.60
1:A:155:ARG:HH22	1:A:185:GLU:CD	2.05	0.60
1:C:120:PRO:HB2	1:C:125:LEU:HD21	1.84	0.59
1:A:105:ASP:OD1	3:A:303:HOH:O	2.16	0.59
1:C:121:SER:O	1:C:125:LEU:HD23	2.03	0.59
1:A:31:ASN:HD22	1:A:31:ASN:N	1.97	0.59
2:B:137:SER:HA	3:B:333:HOH:O	2.02	0.59
1:C:160:LEU:HD11	2:D:172:VAL:HB	1.84	0.58
1:A:149:LYS:HD3	1:A:154:GLU:HA	1.86	0.58
1:A:205:ILE:HD11	3:A:320:HOH:O	2.02	0.58
2:D:195:THR:HG23	2:D:212:LYS:HE3	1.84	0.58
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.86	0.58
1:C:120:PRO:HB2	1:C:125:LEU:CD2	2.34	0.58
2:B:73:ASP:OD1	2:B:75:SER:HB3	2.03	0.57
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.86	0.57
1:C:83:PHE:HB3	1:C:106:ILE:HG12	1.85	0.57
2:D:138:MET:HB3	2:D:186:VAL:O	2.04	0.57
2:D:68:VAL:HG22	2:D:83:LEU:HD13	1.87	0.57
1:A:181:LEU:HD12	1:A:181:LEU:N	2.20	0.57
2:B:195:THR:HG23	2:B:212:LYS:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:GLU:HB3	3:B:319:HOH:O	2.05	0.56
1:A:169:LYS:HD3	3:C:314:HOH:O	2.04	0.56
1:A:179:LEU:HG	1:A:181:LEU:CD1	2.33	0.56
2:B:41:PRO:HA	3:B:345:HOH:O	2.04	0.56
1:C:161:ASN:HB3	1:C:175:MET:HE3	1.88	0.56
1:A:2:ILE:CD1	1:A:29:ILE:HG22	2.36	0.56
1:C:2:ILE:CD1	1:C:93:SER:HB3	2.36	0.56
2:B:5:GLU:HB2	2:D:5:GLU:HB2	1.88	0.56
1:C:149:LYS:HA	1:C:153:SER:O	2.06	0.56
1:A:198:HIS:CE1	1:A:200:THR:HG23	2.41	0.55
1:A:179:LEU:CG	1:A:181:LEU:HD11	2.35	0.55
2:B:29:PHE:CD1	2:B:77:ASN:HA	2.42	0.55
1:C:145:ASN:HB3	1:C:197:THR:HB	1.89	0.55
1:C:181:LEU:HD22	1:C:185:GLU:OE2	2.07	0.54
1:A:2:ILE:HD13	1:A:29:ILE:CG2	2.36	0.54
1:A:31:ASN:H	1:A:31:ASN:ND2	2.03	0.54
2:B:64:VAL:HG21	2:B:67:LYS:HE2	1.90	0.54
2:D:29:PHE:CD1	2:D:77:ASN:HA	2.42	0.53
2:B:62:GLU:HG2	2:B:68:VAL:CB	2.37	0.53
1:A:160:LEU:HG	2:B:172:VAL:HG11	1.90	0.53
1:A:120:PRO:HB2	1:A:125:LEU:HD13	1.91	0.53
1:A:49:LYS:HG3	1:A:53:GLN:HB2	1.89	0.53
1:C:186:TYR:CE1	1:C:211:ARG:HD3	2.44	0.53
1:C:136:LEU:HD12	1:C:136:LEU:N	2.24	0.52
1:C:211:ARG:HH11	1:C:211:ARG:CB	2.23	0.52
1:A:2:ILE:HD12	1:A:93:SER:HB3	1.90	0.52
2:B:1:GLU:OE1	2:D:109:GLY:O	2.28	0.52
1:C:129:GLY:HA2	3:C:261:HOH:O	2.09	0.52
2:D:187:PRO:HB2	2:D:190:PRO:HD3	1.92	0.52
1:C:162:SER:OG	2:D:170:PRO:HD2	2.11	0.51
1:A:61:ARG:NH2	1:C:81:GLU:OE1	2.40	0.51
1:A:205:ILE:HD12	1:A:205:ILE:N	2.17	0.51
1:C:190:ASN:O	1:C:210:ASN:HA	2.11	0.51
1:A:181:LEU:CD2	1:A:185:GLU:HG2	2.32	0.50
1:A:136:LEU:CD2	1:A:146:VAL:HG22	2.42	0.50
2:B:163:SER:OG	1:C:53:GLN:HB3	2.12	0.50
1:C:2:ILE:CD1	1:C:29:ILE:HG22	2.41	0.50
1:A:136:LEU:HD21	1:A:146:VAL:HG22	1.94	0.50
2:B:157:TRP:CZ3	2:B:198:CYS:HB3	2.47	0.50
2:B:122:PRO:CB	2:B:148:TYR:HB3	2.42	0.49
2:B:187:PRO:HB2	2:B:190:PRO:HD2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ASN:H	1:C:31:ASN:ND2	2.06	0.49
1:C:123:GLU:CD	1:C:123:GLU:H	2.15	0.49
1:A:53:GLN:HB3	2:D:163:SER:OG	2.11	0.49
1:A:149:LYS:HD3	1:A:154:GLU:CA	2.42	0.49
1:C:124:GLN:HG2	1:C:129:GLY:O	2.12	0.49
1:C:31:ASN:HD22	1:C:31:ASN:N	1.99	0.49
2:D:6:GLN:HB3	2:D:110:THR:CG2	2.43	0.49
1:A:160:LEU:CD1	2:B:172:VAL:HB	2.41	0.48
1:C:189:HIS:HB2	1:C:192:TYR:OH	2.14	0.48
2:D:190:PRO:O	2:D:194:GLU:HB2	2.13	0.48
1:C:113:PRO:CG	1:C:205:ILE:HD12	2.43	0.48
1:C:160:LEU:C	1:C:160:LEU:HD23	2.34	0.48
1:C:204:PRO:O	1:C:206:VAL:HG23	2.13	0.48
1:C:136:LEU:HD21	1:C:146:VAL:HG22	1.94	0.48
2:D:35:GLU:O	2:D:96:CYS:HA	2.13	0.48
1:A:24:ARG:HA	1:A:69:THR:O	2.14	0.48
1:A:210:ASN:O	1:A:212:ASN:N	2.46	0.48
2:B:117:ALA:HB3	2:B:149:PHE:CE2	2.49	0.48
2:D:172:VAL:HG23	3:D:236:HOH:O	2.14	0.47
2:D:180:LEU:C	2:D:180:LEU:HD23	2.34	0.47
1:C:124:GLN:HG2	1:C:129:GLY:C	2.34	0.47
1:C:108:ARG:HG2	1:C:109:ALA:H	1.77	0.47
1:C:211:ARG:CB	1:C:211:ARG:NH1	2.77	0.47
1:C:198:HIS:ND1	1:C:200:THR:HG23	2.29	0.47
2:D:91:SER:O	2:D:92:ALA:HB2	2.14	0.47
1:A:160:LEU:C	1:A:160:LEU:HD23	2.35	0.47
1:C:135:PHE:C	1:C:136:LEU:HD12	2.35	0.47
1:A:108:ARG:HG2	1:A:109:ALA:H	1.79	0.46
2:D:138:MET:SD	2:D:138:MET:N	2.89	0.46
1:C:185:GLU:HG3	1:C:188:ARG:NH2	2.29	0.46
1:C:176:SER:HB3	2:D:169:PHE:CD2	2.51	0.46
1:C:34:HIS:O	1:C:88:CYS:HA	2.16	0.46
2:D:187:PRO:HB2	2:D:190:PRO:HD2	1.96	0.46
2:B:141:LEU:HD12	2:B:196:VAL:HG11	1.98	0.46
1:A:19:VAL:HG12	1:A:21:LEU:HD13	1.96	0.45
2:B:6:GLN:HB3	2:B:110:THR:CG2	2.47	0.45
2:B:184:VAL:HG13	2:B:184:VAL:O	2.17	0.45
1:C:112:ALA:HB1	1:C:205:ILE:HD11	1.99	0.45
1:C:209:PHE:C	1:C:209:PHE:CD1	2.89	0.45
2:B:190:PRO:O	2:B:194:GLU:N	2.34	0.45
1:C:210:ASN:HB2	1:C:212:ASN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD12	1:A:136:LEU:N	2.31	0.45
2:B:35:GLU:HG3	2:B:103:TYR:CE2	2.52	0.45
2:B:52:LEU:HB3	2:B:55:SER:OG	2.16	0.45
2:B:190:PRO:O	2:B:194:GLU:HB2	2.17	0.45
2:D:122:PRO:CB	2:D:148:TYR:HB3	2.47	0.45
1:A:31:ASN:N	1:A:31:ASN:ND2	2.64	0.44
1:A:196:ALA:O	1:A:205:ILE:HD12	2.17	0.44
2:B:189:SER:N	2:B:190:PRO:CD	2.80	0.44
2:B:34:ILE:HG23	2:B:96:CYS:SG	2.57	0.44
2:D:122:PRO:HB2	2:D:145:VAL:HG13	1.99	0.44
1:C:210:ASN:C	1:C:212:ASN:H	2.21	0.44
2:D:35:GLU:HG3	2:D:103:TYR:CE2	2.53	0.44
1:A:149:LYS:HB2	1:A:193:THR:HB	1.99	0.44
1:A:192:TYR:O	1:A:208:SER:HB2	2.18	0.44
2:D:192:PRO:O	2:D:193:SER:C	2.55	0.44
1:A:104:LEU:C	1:A:104:LEU:HD23	2.38	0.44
1:C:210:ASN:C	1:C:212:ASN:N	2.71	0.44
1:C:206:VAL:HG12	1:C:207:LYS:N	2.32	0.43
1:A:34:HIS:O	1:A:88:CYS:HA	2.18	0.43
1:A:189:HIS:HB2	1:A:192:TYR:OH	2.17	0.43
1:C:19:VAL:HG12	1:C:21:LEU:HD13	2.00	0.43
2:D:68:VAL:HG22	2:D:83:LEU:CD1	2.48	0.43
1:A:169:LYS:HG3	3:C:233:HOH:O	2.17	0.43
2:B:136:ASN:C	2:B:138:MET:H	2.22	0.43
2:B:51:ILE:O	2:B:53:PRO:HD3	2.19	0.43
1:C:145:ASN:O	1:C:196:ALA:HA	2.18	0.43
2:D:176:ASP:O	2:D:177:LEU:HD23	2.19	0.43
2:B:64:VAL:HG23	2:B:64:VAL:O	2.17	0.43
2:B:35:GLU:OE2	2:B:50:GLU:OE2	2.37	0.43
1:A:35:TRP:CD2	1:A:73:LEU:HB2	2.54	0.42
1:A:156:GLN:OE1	1:A:156:GLN:N	2.52	0.42
2:B:151:GLU:OE1	2:B:171:ALA:HB3	2.18	0.42
2:D:12:MET:O	2:D:114:VAL:HA	2.18	0.42
2:D:175:SER:O	2:D:176:ASP:HB2	2.18	0.42
1:C:190:ASN:ND2	1:C:210:ASN:HB3	2.34	0.42
1:A:110:ASP:HB3	1:A:200:THR:HG22	2.01	0.42
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.01	0.42
1:C:136:LEU:CD2	1:C:146:VAL:HG22	2.49	0.42
2:D:40:ARG:HG2	2:D:92:ALA:HB2	2.01	0.42
1:C:121:SER:HB2	1:C:123:GLU:OE2	2.20	0.42
1:C:125:LEU:O	1:C:183:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:GLY:HA2	2:D:216:ARG:HD3	2.02	0.42
2:D:146:LYS:HB3	2:D:179:THR:HG23	2.00	0.42
2:D:1:GLU:HB3	3:D:279:HOH:O	2.19	0.42
2:D:166:VAL:HG22	2:D:184:VAL:HG23	2.01	0.42
1:A:190:ASN:O	1:A:210:ASN:HA	2.19	0.41
1:A:193:THR:HG23	1:A:208:SER:HB3	2.01	0.41
1:C:33:LEU:HG	1:C:71:PHE:CG	2.55	0.41
1:A:163:TRP:N	1:A:163:TRP:CE3	2.88	0.41
2:B:129:PRO:HD3	2:B:141:LEU:HD23	2.02	0.41
1:A:146:VAL:HG21	1:A:175:MET:HE2	2.02	0.41
2:B:41:PRO:O	2:B:43:HIS:CD2	2.73	0.41
1:C:55:MET:HB3	1:C:58:ILE:HG13	2.02	0.41
1:A:160:LEU:CD1	2:B:179:THR:HB	2.51	0.41
2:B:65:LYS:N	2:B:65:LYS:CD	2.83	0.41
1:C:120:PRO:CB	1:C:125:LEU:HD21	2.49	0.41
2:D:31:THR:HG22	2:D:31:THR:O	2.20	0.41
2:D:214:VAL:HA	2:D:215:PRO:HD3	1.95	0.41
1:C:13:VAL:HG21	1:C:78:VAL:HG11	2.01	0.41
2:B:64:VAL:HG23	2:B:67:LYS:CG	2.42	0.41
2:D:120:THR:HA	2:D:121:PRO:HD3	1.88	0.41
1:A:81:GLU:OE1	1:C:61:ARG:NH2	2.48	0.41
1:A:207:LYS:HA	1:A:207:LYS:HD3	1.88	0.41
1:C:119:PRO:HB3	1:C:209:PHE:CZ	2.56	0.41
2:D:6:GLN:HB3	2:D:110:THR:HG23	2.03	0.41
1:C:198:HIS:CE1	1:C:200:THR:HG23	2.57	0.40
1:C:202:THR:HG23	1:C:203:SER:N	2.36	0.40
2:D:146:LYS:HB2	2:D:179:THR:OG1	2.21	0.40
1:A:115:VAL:HA	1:A:135:PHE:O	2.22	0.40
2:B:6:GLN:HE21	2:B:110:THR:CG2	2.18	0.40
1:A:175:MET:HG2	1:A:176:SER:N	2.36	0.40
1:A:141:PRO:CD	1:A:199:LYS:HD3	2.51	0.40
1:C:31:ASN:ND2	1:C:31:ASN:N	2.67	0.40
1:A:140:TYR:CG	1:A:141:PRO:HA	2.57	0.40
1:C:206:VAL:CG1	1:C:207:LYS:N	2.84	0.40

All (3) 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)
3:C:311:HOH:O	3:D:290:HOH:O[4_547]	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:323:HOH:O	3:B:341:HOH:O[4_546]	2.02	0.18
3:A:302:HOH:O	3:B:263:HOH:O[4_546]	2.19	0.01

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	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	29	23
1	C	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
2	B	209/216 (97%)	198 (95%)	11 (5%)	0	100	100
2	D	206/216 (95%)	198 (96%)	8 (4%)	0	100	100
All	All	835/856 (98%)	799 (96%)	35 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ARG

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	191/191 (100%)	182 (95%)	9 (5%)	26	22
1	C	191/191 (100%)	186 (97%)	5 (3%)	46	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	183/185 (99%)	179 (98%)	4 (2%)	52 55
2	D	181/185 (98%)	179 (99%)	2 (1%)	73 78
All	All	746/752 (99%)	726 (97%)	20 (3%)	44 46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	94	TRP
1	A	105	ASP
1	A	108	ARG
1	A	125	LEU
1	A	143	ASP
1	A	181	LEU
1	A	185	GLU
1	A	191	SER
2	B	62	GLU
2	B	65	LYS
2	B	152	PRO
2	B	199	ASN
1	C	11	LEU
1	C	31	ASN
1	C	76	ASN
1	C	107	LYS
1	C	169	LYS
2	D	152	PRO
2	D	180	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	76	ASN
2	B	77	ASN
1	C	31	ASN
1	C	76	ASN
1	C	145	ASN
2	D	77	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 (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	212/212 (100%)	0.54	18 (8%)	10	10	9, 21, 39, 46	14 (6%)
1	C	212/212 (100%)	0.58	24 (11%)	5	4	9, 21, 45, 51	7 (3%)
2	B	213/216 (98%)	0.46	15 (7%)	16	15	10, 18, 33, 42	6 (2%)
2	D	210/216 (97%)	0.31	14 (6%)	17	17	8, 17, 32, 39	2 (0%)
All	All	847/856 (98%)	0.48	71 (8%)	11	10	8, 19, 41, 51	29 (3%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	130	GLY	7.8
1	C	212	ASN	7.3
2	D	137	SER	6.6
2	B	41	PRO	5.4
1	A	202	THR	5.0
1	A	204	PRO	4.8
1	A	163	TRP	4.7
1	A	201	SER	4.2
1	A	203	SER	4.2
1	C	202	THR	4.2
2	D	41	PRO	4.0
1	A	212	ASN	4.0
2	B	43	HIS	3.8
2	D	138	MET	3.8
2	B	96	CYS	3.7
2	B	42	GLY	3.7
1	A	157	ASN	3.7
2	D	190	PRO	3.5
1	C	163	TRP	3.5
2	B	137	SER	3.4
2	D	188	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	41	HIS	3.3
1	C	203	SER	3.3
2	B	190	PRO	3.2
1	A	205	ILE	3.2
1	C	41	HIS	3.2
2	D	130	GLY	3.1
1	A	67	SER	3.1
2	D	143	CYS	3.0
2	B	136	ASN	3.0
1	C	153	SER	3.0
1	C	201	SER	3.0
1	A	200	THR	2.9
1	A	94	TRP	2.9
2	D	42	GLY	2.9
2	B	143	CYS	2.9
2	B	135	THR	2.8
1	C	200	THR	2.8
1	C	127	SER	2.8
1	C	197	THR	2.8
1	C	160	LEU	2.7
1	A	141	PRO	2.7
2	B	127	LEU	2.7
1	C	154	GLU	2.7
2	D	174	GLN	2.7
1	C	157	ASN	2.6
1	C	94	TRP	2.6
2	B	134	GLN	2.6
1	A	68	GLY	2.5
2	B	129	PRO	2.4
1	A	135	PHE	2.3
1	C	133	VAL	2.3
1	C	190	ASN	2.3
1	C	187	GLU	2.3
2	B	194	GLU	2.3
2	B	216	ARG	2.2
1	C	126	THR	2.2
1	C	155	ARG	2.2
1	C	206	VAL	2.2
2	D	189	SER	2.2
2	D	193	SER	2.2
1	A	158	GLY	2.1
1	C	156	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	125	LEU	2.1
2	D	187	PRO	2.1
2	D	43	HIS	2.1
1	C	135	PHE	2.1
1	A	156	GLN	2.1
1	A	126	THR	2.0
1	C	192	TYR	2.0
2	D	175	SER	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.