



Full wwPDB X-ray Structure Validation Report

May 28, 2014 – 04:25 AM EDT

PDB ID : 4PY7
Title : Crystal Structure of Fab 3.1
Authors : Dreyfus, C.
Deposited on : 2014-03-26
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

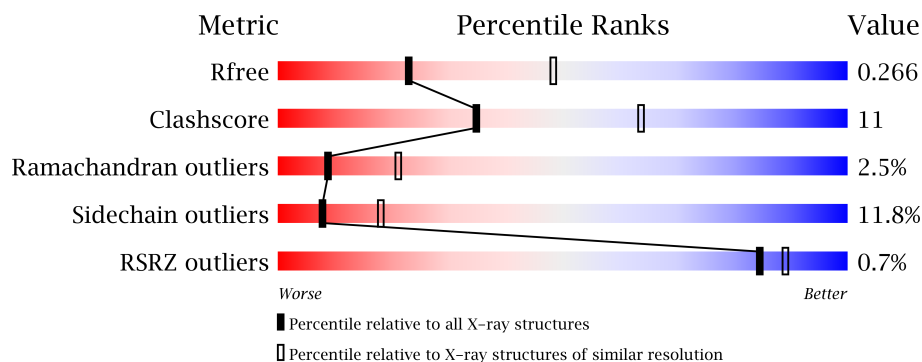
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	219	
1	I	219	
2	B	214	
2	J	214	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6498 atoms, of which 0 are hydrogen and 0 are deuterium.

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 antibody 3.1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	215	Total	C	N	O	S	0	0	0
			1635	1036	280	311	8			
1	A	216	Total	C	N	O	S	0	0	0
			1639	1038	280	313	8			

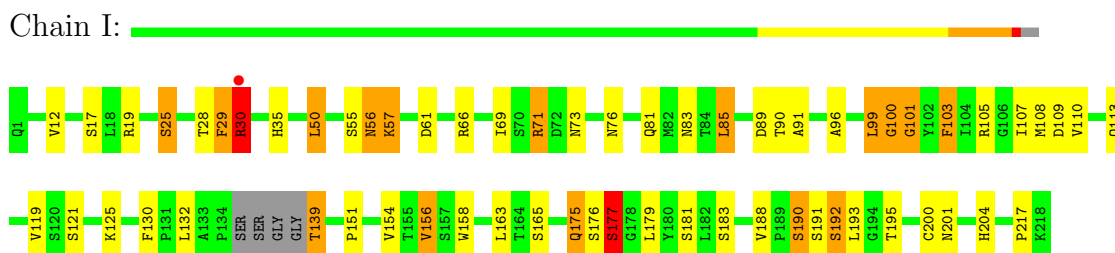
- Molecule 2 is a protein called antibody 3.1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	212	Total	C	N	O	S	0	0	0
			1612	1010	271	326	5			
2	B	212	Total	C	N	O	S	0	0	0
			1612	1010	271	326	5			

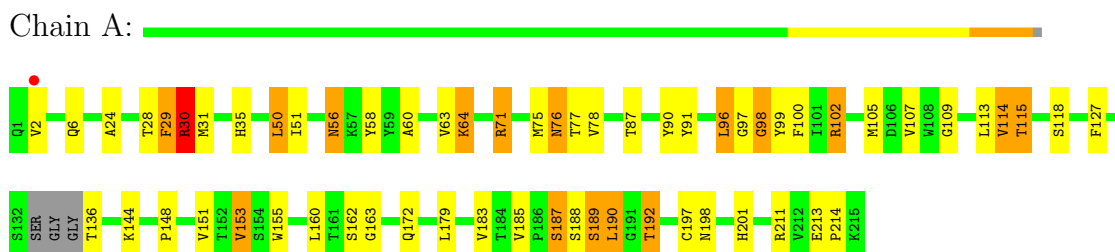
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

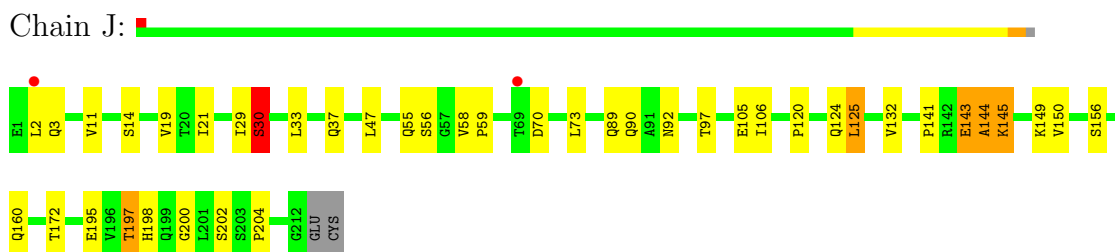
- Molecule 1: antibody 3.1 heavy chain



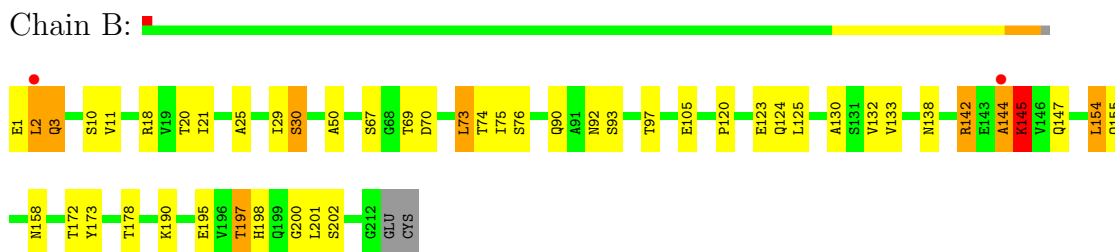
- Molecule 1: antibody 3.1 heavy chain



- Molecule 2: antibody 3.1 light chain



- Molecule 2: antibody 3.1 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	73.84Å 73.84Å 207.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 46.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.70) 98.3 (46.66-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.273 0.222 , 0.266	Depositor DCC
R_{free} test set	1521 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 5.1	EDS
Estimated twinning fraction	0.459 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 29944 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6498	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.59	0/1678	0.72	1/2287 (0.0%)
1	I	0.59	0/1674	0.73	0/2281
2	B	0.59	0/1647	0.69	0/2236
2	J	0.59	0/1647	0.69	0/2236
All	All	0.59	0/6646	0.71	1/9040 (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	I	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	98	GLY	N-CA-C	-5.26	99.95	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	25	SER	Peptide

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1639	0	1605	43	0
1	I	1635	0	1607	38	0
2	B	1612	0	1573	32	0
2	J	1612	0	1573	32	0
All	All	6498	0	6358	138	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (138) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:142:ARG:HH11	2:B:142:ARG:HG2	1.18	1.07
1:I:56:ASN:HA	1:I:57:LYS:HB2	1.35	1.03
2:B:144:ALA:HA	2:B:145:LYS:HB2	1.44	1.00
2:J:90:GLN:NE2	2:J:92:ASN:H	1.59	0.98
2:B:198:HIS:CD2	2:B:200:GLY:H	1.81	0.97
2:J:90:GLN:HE21	2:J:92:ASN:H	0.94	0.93
2:B:90:GLN:HE21	2:B:92:ASN:H	1.14	0.89
2:J:145:LYS:HG3	2:J:197:THR:HG23	1.56	0.87
2:B:90:GLN:NE2	2:B:92:ASN:H	1.75	0.83
2:J:198:HIS:CD2	2:J:200:GLY:H	1.96	0.83
1:I:151:PRO:O	1:I:204:HIS:HE1	1.60	0.83
2:B:198:HIS:HD2	2:B:200:GLY:H	1.27	0.80
1:A:188:SER:O	1:A:189:SER:HB3	1.83	0.77
1:A:148:PRO:O	1:A:201:HIS:HE1	1.67	0.76
2:B:142:ARG:HG2	2:B:142:ARG:NH1	1.87	0.76
2:J:90:GLN:HE21	2:J:92:ASN:N	1.78	0.74
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.70	0.74
1:A:63:VAL:O	1:A:64:LYS:CB	2.37	0.71
1:A:6:GLN:HE21	1:A:109:GLY:HA3	1.57	0.70
2:B:144:ALA:CA	2:B:145:LYS:HB2	2.21	0.70
2:B:144:ALA:HA	2:B:145:LYS:CB	2.22	0.68
1:I:56:ASN:N	1:I:56:ASN:HD22	1.90	0.68
1:I:176:SER:O	1:I:177:SER:HB3	1.94	0.68
1:I:28:THR:HA	1:I:76:ASN:HD21	1.60	0.67
2:J:144:ALA:HA	2:J:145:LYS:CB	2.24	0.67
1:I:17:SER:OG	1:I:83:ASN:ND2	2.26	0.67
1:A:144:LYS:HE2	1:A:172:GLN:HE22	1.59	0.66
2:J:141:PRO:HB2	1:A:30:ARG:HH21	1.60	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:175:GLN:HE22	1:I:181:SER:HB3	1.60	0.66
1:A:24:ALA:HB2	1:A:29:PHE:CD2	2.31	0.65
1:I:139:THR:N	1:I:190:SER:HG	1.95	0.65
2:J:11:VAL:HG23	1:A:75:MET:SD	2.37	0.65
2:B:142:ARG:HH11	2:B:142:ARG:CG	2.03	0.64
1:I:151:PRO:O	1:I:204:HIS:CE1	2.48	0.63
1:I:130:PHE:CE2	2:J:124:GLN:HG3	2.33	0.63
1:I:99:LEU:HD12	1:I:99:LEU:O	1.99	0.62
2:J:90:GLN:NE2	2:J:92:ASN:N	2.42	0.62
1:I:81:GLN:HE21	1:I:83:ASN:HD21	1.47	0.62
1:A:29:PHE:H	1:A:76:ASN:ND2	1.98	0.62
1:I:96:ALA:HB1	1:I:108:MET:HB3	1.80	0.62
1:I:29:PHE:H	1:I:76:ASN:ND2	1.98	0.61
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.84	0.60
1:I:56:ASN:CA	1:I:57:LYS:HB2	2.18	0.59
1:A:136:THR:HA	1:A:187:SER:OG	2.02	0.59
1:I:90:THR:O	1:I:91:ALA:HB2	2.03	0.58
1:I:30:ARG:O	1:I:30:ARG:HG3	2.04	0.57
2:J:198:HIS:HD2	2:J:200:GLY:H	1.48	0.57
1:A:50:LEU:HD23	1:A:58:TYR:HD2	1.68	0.57
2:J:145:LYS:HB3	2:J:197:THR:O	2.05	0.57
2:B:145:LYS:HB3	2:B:197:THR:O	2.05	0.57
1:A:63:VAL:O	1:A:64:LYS:HB2	2.04	0.56
1:I:175:GLN:NE2	1:I:181:SER:HB3	2.20	0.56
1:A:90:TYR:CD2	1:A:114:VAL:HG13	2.41	0.55
2:J:2:LEU:O	2:J:2:LEU:HD12	2.07	0.55
1:I:71:ARG:NE	1:I:73:ASN:HD21	2.04	0.55
1:A:28:THR:HG22	1:A:30:ARG:CG	2.37	0.55
2:J:144:ALA:HA	2:J:145:LYS:HB3	1.89	0.54
1:A:35:HIS:CE1	1:A:50:LEU:HD13	2.42	0.54
1:I:175:GLN:HG2	1:I:179:LEU:O	2.07	0.54
1:A:127:PHE:CE2	2:B:124:GLN:HG3	2.43	0.53
2:B:198:HIS:HD2	2:B:200:GLY:N	2.02	0.53
1:I:19:ARG:HD3	1:I:81:GLN:OE1	2.09	0.53
2:J:143:GLU:H	1:A:30:ARG:NH2	2.08	0.52
1:A:189:SER:HA	1:A:192:THR:HG22	1.91	0.51
1:A:51:ILE:HD13	1:A:71:ARG:HG3	1.93	0.51
2:B:105:GLU:OE2	2:B:173:TYR:OH	2.28	0.51
2:B:90:GLN:HE21	2:B:92:ASN:N	1.95	0.51
1:A:163:GLY:O	1:A:183:VAL:HA	2.11	0.51
2:B:147:GLN:HE22	2:B:154:LEU:HD21	1.75	0.51
1:A:60:ALA:O	1:A:63:VAL:O	2.27	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:142:ARG:O	2:B:142:ARG:NH1	2.43	0.50
2:B:2:LEU:HD12	2:B:2:LEU:O	2.11	0.50
1:I:66:ARG:NH2	1:I:89:ASP:OD2	2.45	0.49
2:J:149:LYS:NZ	2:J:195:GLU:OE1	2.45	0.49
2:B:18:ARG:HG3	2:B:76:SER:HA	1.94	0.48
1:I:71:ARG:HE	1:I:73:ASN:HD21	1.61	0.48
2:J:55:GLN:HG3	2:J:56:SER:N	2.28	0.48
2:J:197:THR:HB	2:J:204:PRO:HG3	1.95	0.48
1:A:100:PHE:HZ	1:A:102:ARG:HH11	1.61	0.48
1:I:101:GLY:N	1:I:103:PHE:O	2.45	0.48
1:A:179:LEU:C	1:A:179:LEU:HD12	2.34	0.47
1:I:191:SER:O	1:I:192:SER:HB3	2.14	0.47
1:I:56:ASN:ND2	1:I:56:ASN:N	2.61	0.47
1:I:99:LEU:O	1:I:100:GLY:O	2.32	0.47
1:A:213:GLU:HB2	1:A:214:PRO:HD2	1.97	0.47
2:B:29:ILE:O	2:B:29:ILE:HG22	2.15	0.47
1:A:6:GLN:HE22	1:A:91:TYR:HA	1.79	0.47
1:A:188:SER:O	1:A:189:SER:CB	2.58	0.47
2:J:143:GLU:O	2:J:144:ALA:CB	2.62	0.47
1:A:148:PRO:O	1:A:201:HIS:CE1	2.58	0.46
2:J:144:ALA:HA	2:J:145:LYS:HB2	1.94	0.46
1:A:28:THR:HG22	1:A:30:ARG:HG2	1.96	0.46
1:A:63:VAL:O	1:A:64:LYS:HB3	2.16	0.46
2:B:11:VAL:HG23	2:B:11:VAL:O	2.16	0.46
1:A:56:ASN:N	1:A:56:ASN:HD22	2.14	0.46
2:J:143:GLU:O	2:J:144:ALA:HB2	2.16	0.45
2:B:155:GLN:HE21	2:B:158:ASN:HD22	1.63	0.45
1:I:57:LYS:HE2	1:I:69:ILE:O	2.16	0.45
1:A:28:THR:HA	1:A:76:ASN:HD21	1.82	0.45
1:A:28:THR:HG22	1:A:30:ARG:HG3	1.97	0.45
1:A:77:THR:HG22	1:A:78:VAL:N	2.32	0.45
1:A:153:VAL:HA	1:A:198:ASN:O	2.16	0.44
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.99	0.44
1:A:96:LEU:HD12	1:A:97:GLY:N	2.32	0.44
2:J:55:GLN:HG3	2:J:56:SER:H	1.82	0.44
2:B:25:ALA:O	2:B:69:THR:HG23	2.18	0.44
1:I:99:LEU:HA	1:I:109:ASP:OD2	2.18	0.44
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.99	0.44
1:A:87:THR:HG23	1:A:115:THR:HA	1.98	0.44
2:J:145:LYS:HB2	1:A:99:TYR:CE1	2.53	0.44
1:I:35:HIS:CD2	1:I:108:MET:HG2	2.52	0.44
1:I:12:VAL:O	1:I:119:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:12:VAL:HG11	1:I:85:LEU:HD23	1.99	0.44
1:A:190:LEU:HD13	1:A:190:LEU:HA	1.68	0.43
1:I:109:ASP:OD1	1:I:110:VAL:HG23	2.18	0.43
2:J:29:ILE:O	2:J:30:SER:HB3	2.18	0.43
2:J:105:GLU:HG2	2:J:106:ILE:N	2.32	0.43
1:I:156:VAL:HA	1:I:201:ASN:O	2.19	0.43
1:A:155:TRP:CH2	1:A:197:CYS:HB3	2.55	0.42
2:B:29:ILE:O	2:B:30:SER:HB3	2.19	0.42
1:I:35:HIS:CE1	1:I:50:LEU:HD13	2.54	0.42
2:B:133:VAL:HG22	2:B:178:THR:HG23	2.01	0.42
2:J:125:LEU:HD12	2:J:125:LEU:HA	1.86	0.42
2:J:144:ALA:CA	2:J:145:LYS:CB	2.95	0.42
2:B:125:LEU:HA	2:B:125:LEU:HD23	1.84	0.42
2:B:144:ALA:CA	2:B:145:LYS:CB	2.91	0.42
1:A:31:MET:O	1:A:98:GLY:HA3	2.21	0.41
2:B:90:GLN:NE2	2:B:92:ASN:N	2.55	0.41
2:J:21:ILE:HD12	2:J:73:LEU:HD22	2.02	0.41
1:I:55:SER:C	1:I:56:ASN:HD22	2.24	0.41
2:J:58:VAL:HA	2:J:59:PRO:HD2	1.98	0.41
1:A:30:ARG:H	1:A:30:ARG:HG2	1.60	0.40
2:B:145:LYS:HG3	2:B:197:THR:HB	2.04	0.40
1:I:85:LEU:HD12	1:I:85:LEU:HA	1.89	0.40
1:A:2:VAL:HG12	1:A:107:VAL:HG11	2.04	0.40
1:I:158:TRP:CZ3	1:I:200:CYS:HB3	2.56	0.40
2:B:21:ILE:N	2:B:73:LEU:O	2.51	0.40
2:J:141:PRO:HB2	1:A:30:ARG:NH2	2.34	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	212/219 (97%)	199 (94%)	10 (5%)	3 (1%)	16	41
1	I	211/219 (96%)	194 (92%)	9 (4%)	8 (4%)	5	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	210/214 (98%)	191 (91%)	13 (6%)	6 (3%)	7	16
2	J	210/214 (98%)	195 (93%)	11 (5%)	4 (2%)	12	29
All	All	843/866 (97%)	779 (92%)	43 (5%)	21 (2%)	9	21

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	57	LYS
1	I	177	SER
1	I	192	SER
2	J	144	ALA
2	J	145	LYS
1	A	64	LYS
1	A	189	SER
2	B	145	LYS
1	I	100	GLY
1	I	101	GLY
2	J	3	GLN
2	B	50	ALA
2	B	144	ALA
1	I	25	SER
2	J	30	SER
2	B	30	SER
2	B	3	GLN
2	B	138	ASN
1	A	30	ARG
1	I	30	ARG
1	I	217	PRO

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	181/184 (98%)	159 (88%)	22 (12%)	7	17
1	I	181/184 (98%)	154 (85%)	27 (15%)	4	11
2	B	183/185 (99%)	161 (88%)	22 (12%)	7	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	183/185 (99%)	168 (92%)	15 (8%)	17	36
All	All	728/738 (99%)	642 (88%)	86 (12%)	8	18

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	29	PHE
1	I	30	ARG
1	I	50	LEU
1	I	56	ASN
1	I	61	ASP
1	I	71	ARG
1	I	85	LEU
1	I	99	LEU
1	I	103	PHE
1	I	105	ARG
1	I	107	ILE
1	I	113	GLN
1	I	121	SER
1	I	125	LYS
1	I	132	LEU
1	I	139	THR
1	I	154	VAL
1	I	156	VAL
1	I	163	LEU
1	I	165	SER
1	I	175	GLN
1	I	177	SER
1	I	183	SER
1	I	188	VAL
1	I	190	SER
1	I	193	LEU
1	I	195	THR
2	J	14	SER
2	J	19	VAL
2	J	30	SER
2	J	33	LEU
2	J	70	ASP
2	J	89	GLN
2	J	97	THR
2	J	125	LEU
2	J	143	GLU

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Mol	Chain	Res	Type
2	J	150	VAL
2	J	156	SER
2	J	160	GLN
2	J	172	THR
2	J	197	THR
2	J	202	SER
1	A	29	PHE
1	A	30	ARG
1	A	50	LEU
1	A	56	ASN
1	A	71	ARG
1	A	76	ASN
1	A	96	LEU
1	A	102	ARG
1	A	105	MET
1	A	113	LEU
1	A	114	VAL
1	A	115	THR
1	A	118	SER
1	A	151	VAL
1	A	153	VAL
1	A	160	LEU
1	A	162	SER
1	A	185	VAL
1	A	187	SER
1	A	190	LEU
1	A	192	THR
1	A	211	ARG
2	B	1	GLU
2	B	2	LEU
2	B	3	GLN
2	B	10	SER
2	B	20	THR
2	B	67	SER
2	B	70	ASP
2	B	73	LEU
2	B	74	THR
2	B	75	ILE
2	B	93	SER
2	B	97	THR
2	B	123	GLU
2	B	142	ARG

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Mol	Chain	Res	Type
2	B	145	LYS
2	B	154	LEU
2	B	172	THR
2	B	190	LYS
2	B	195	GLU
2	B	197	THR
2	B	201	LEU
2	B	202	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	56	ASN
1	I	73	ASN
1	I	76	ASN
1	I	83	ASN
1	I	175	GLN
1	I	204	HIS
2	J	90	GLN
2	J	124	GLN
2	J	138	ASN
2	J	160	GLN
2	J	198	HIS
1	A	6	GLN
1	A	56	ASN
1	A	76	ASN
1	A	172	GLN
1	A	201	HIS
2	B	90	GLN
2	B	138	ASN
2	B	147	GLN
2	B	155	GLN
2	B	198	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	216/219 (98%)	0.24	1 (0%) 88 92	20, 34, 54, 65	0
1	I	215/219 (98%)	0.21	1 (0%) 88 92	17, 33, 54, 67	0
2	B	212/214 (99%)	0.29	2 (0%) 81 85	28, 42, 55, 58	0
2	J	212/214 (99%)	0.34	2 (0%) 81 85	27, 42, 56, 60	0
All	All	855/866 (98%)	0.27	6 (0%) 84 89	17, 38, 56, 67	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	2	LEU	3.2
2	B	144	ALA	2.3
1	I	30	ARG	2.3
2	B	2	LEU	2.1
2	J	69	THR	2.0
1	A	2	VAL	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.