Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 04:39 am BST

PDB ID	:	5JO4
Title	:	Antibody Fab Fragment Complex
Authors	:	Zhang, Z.; Prachanronarong, K.P.; Marasco, W.A.; Schiffer, C.A.S.
Deposited on	:	2016-05-01
Resolution	:	2.53 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 following versions of software and data (see references (i)) were used in the production of this report:

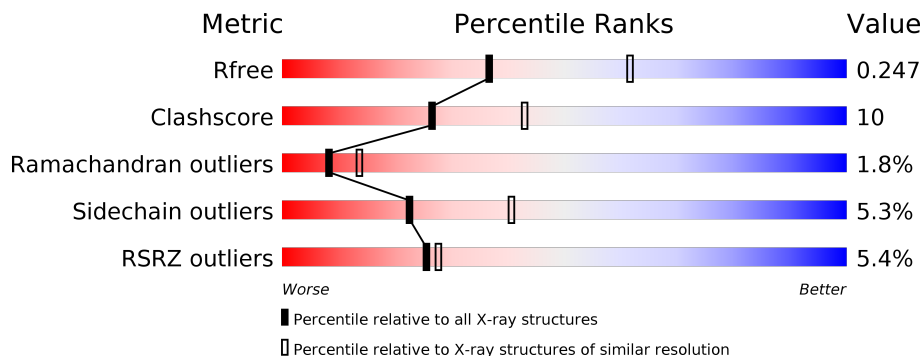|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.53 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		10
Ramachandran outliers		1.8%
Sidechain outliers		5.3%
RSRZ outliers		5.4%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 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	228	75% ... 21%
2	B	215	85% ... 13%
3	C	222	71% ... 25%
4	D	214	70% ... 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6757 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 D80 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1644	1039	270	327	8			

- Molecule 2 is a protein called D80 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1645	1025	281	334	5			

- Molecule 3 is a protein called G6 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	221	Total	C	N	O	S	0	0	0
			1645	1034	274	330	7			

- Molecule 4 is a protein called G6 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	209	Total	C	N	O	S	0	0	0
			1596	1001	265	326	4			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 5	O 4	S 1	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	86	Total 86	O 86	0	0
6	B	74	Total 74	O 74	0	0
6	C	29	Total 29	O 29	0	0
6	D	33	Total 33	O 33	0	0

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 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.
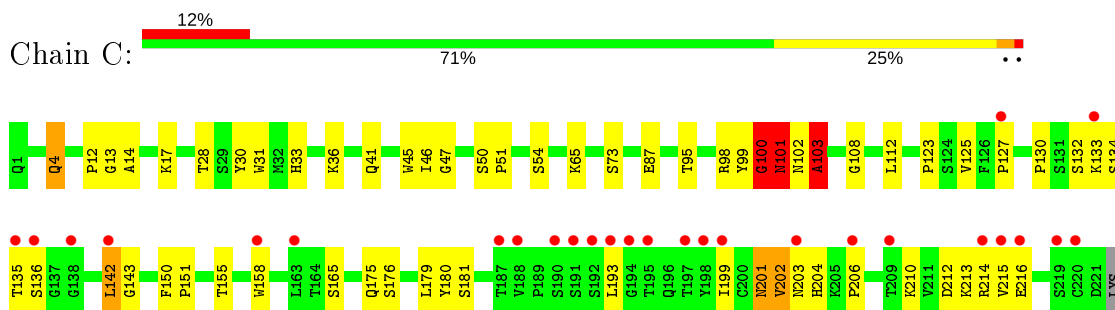
- Molecule 1: D80 Fab Heavy Chain
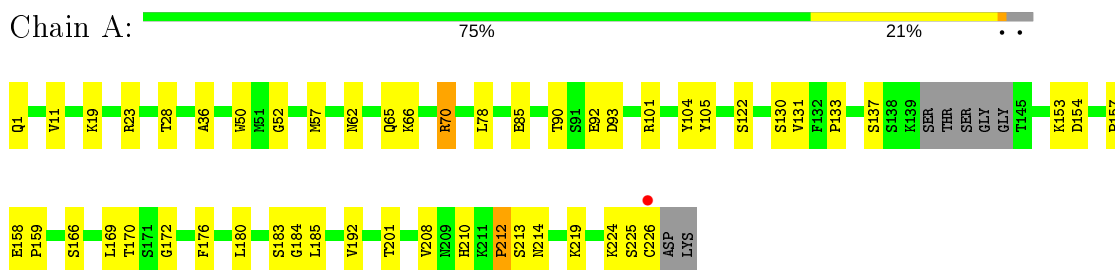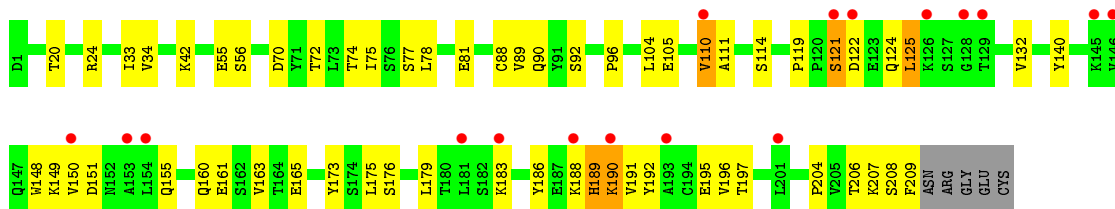
Chain A:

- Molecule 2: D80 Fab Light Chain
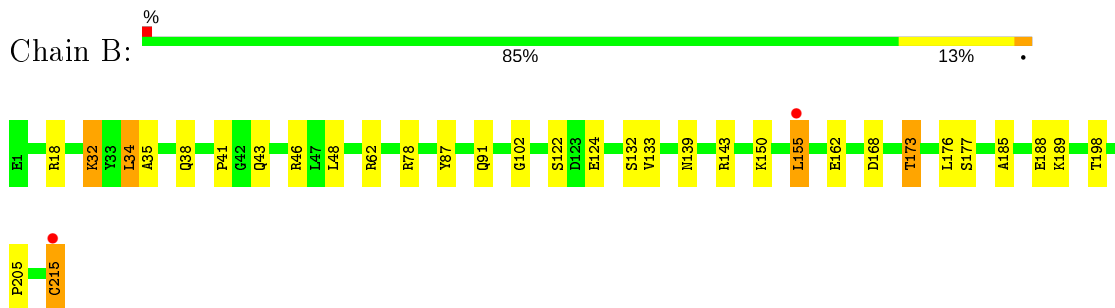
Chain B:

- Molecule 3: G6 Fab Heavy Chain

Chain C:

- Molecule 4: G6 Fab Light Chain

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.16Å 50.78Å 139.74Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	50.39 – 2.53 63.30 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.39-2.53) 96.4 (63.30-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.29 (at 2.55Å)	Xtriage
Refinement program	PHENIX dev_2037	Depositor
R, R_{free}	0.197 , 0.248 0.197 , 0.247	Depositor DCC
R_{free} test set	2015 reflections (5.93%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.7	EDS
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6757	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.55	0/1682	0.68	0/2290
2	B	0.54	0/1679	0.65	0/2279
3	C	0.44	0/1685	0.64	0/2297
4	D	0.43	0/1631	0.63	0/2217
All	All	0.49	0/6677	0.65	0/9083

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
3	C	0	2
4	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	100	GLY	Peptide
3	C	103	ALA	Peptide
4	D	189	HIS	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	1644	0	1606	31	0
2	B	1645	0	1603	23	0
3	C	1645	0	1607	47	0
4	D	1596	0	1556	41	0
5	B	5	0	0	0	0
6	A	86	0	0	7	0
6	B	74	0	0	5	1
6	C	29	0	0	2	1
6	D	33	0	0	2	0
All	All	6757	0	6372	133	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 10.

All (133) 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)
3:C:102:ASN:HB2	3:C:103:ALA:HB2	1.48	0.95
4:D:188:LYS:H	4:D:189:HIS:HB3	1.35	0.91
1:A:1:GLN:N	1:A:1:GLN:OE1	2.07	0.87
3:C:175:GLN:NE2	3:C:181:SER:OG	2.09	0.85
4:D:33:ILE:HD11	4:D:88:CYS:HB2	1.58	0.84
4:D:208:SER:O	6:D:301:HOH:O	1.98	0.82
2:B:78:ARG:NH1	6:B:404:HOH:O	2.12	0.81
3:C:203:ASN:HB3	3:C:210:LYS:HG2	1.62	0.81
4:D:175:LEU:HD12	4:D:176:SER:H	1.51	0.74
1:A:122:SER:OG	6:A:301:HOH:O	2.07	0.73
3:C:130:PRO:HG3	3:C:142:LEU:HB3	1.72	0.71
4:D:175:LEU:HD12	4:D:176:SER:N	2.07	0.69
2:B:18:ARG:NE	6:B:402:HOH:O	2.06	0.69
4:D:24:ARG:NH1	4:D:70:ASP:OD1	2.26	0.69
4:D:161:GLU:HG2	4:D:175:LEU:HD11	1.75	0.68
4:D:165:GLU:OE2	6:D:302:HOH:O	2.10	0.68
1:A:225:SER:HB2	1:A:226:CYS:HB2	1.76	0.68
3:C:175:GLN:HA	4:D:160:GLN:HE22	1.58	0.67

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:O	6:A:304:HOH:O	2.12	0.67
3:C:102:ASN:CB	3:C:103:ALA:HB2	2.22	0.66
3:C:214:ARG:NH2	3:C:216:GLU:OE2	2.29	0.65
1:A:131:VAL:HG21	1:A:208:VAL:HG21	1.76	0.65
1:A:90:THR:HG22	1:A:92:GLU:H	1.60	0.65
1:A:23:ARG:NH1	6:A:310:HOH:O	2.30	0.64
3:C:199:ILE:O	3:C:201:ASN:ND2	2.31	0.64
1:A:70:ARG:HH22	1:A:93:ASP:CG	2.02	0.63
4:D:186:TYR:O	4:D:192:TYR:OH	2.18	0.62
4:D:188:LYS:N	4:D:189:HIS:HB3	2.11	0.62
1:A:1:GLN:N	1:A:28:THR:OG1	2.33	0.62
1:A:36:ALA:HB2	1:A:105:TYR:O	2.02	0.60
3:C:41:GLN:HB2	6:C:308:HOH:O	2.01	0.60
4:D:148:TRP:HB2	4:D:155:GLN:NE2	2.17	0.60
4:D:161:GLU:CG	4:D:175:LEU:HD11	2.32	0.59
3:C:135:THR:OG1	3:C:136:SER:N	2.36	0.58
4:D:121:SER:HB3	4:D:124:GLN:HE21	1.67	0.58
4:D:188:LYS:HB2	4:D:188:LYS:NZ	2.20	0.56
2:B:143:ARG:HH11	2:B:143:ARG:HG2	1.70	0.56
3:C:150:PHE:HB2	3:C:179:LEU:HD11	1.88	0.56
1:A:169:LEU:HD21	1:A:192:VAL:HG21	1.88	0.55
3:C:100:GLY:HA3	3:C:101:ASN:OD1	2.07	0.54
2:B:185:ALA:O	2:B:189:LYS:HG3	2.07	0.54
4:D:163:VAL:HG22	4:D:175:LEU:HD13	1.90	0.54
1:A:225:SER:H	1:A:226:CYS:C	2.09	0.54
2:B:38:GLN:OE1	2:B:46:ARG:NH1	2.39	0.54
2:B:38:GLN:HB2	2:B:48:LEU:HD11	1.90	0.54
3:C:134:SER:H	3:C:135:THR:HA	1.73	0.53
2:B:18:ARG:NH2	6:B:411:HOH:O	2.39	0.53
3:C:100:GLY:HA3	3:C:101:ASN:HB2	1.90	0.53
3:C:143:GLY:HA2	3:C:158:TRP:CH2	2.44	0.53
3:C:150:PHE:HB2	3:C:179:LEU:CD1	2.39	0.53
1:A:224:LYS:NZ	2:B:215:CYS:SG	2.72	0.52
1:A:158:GLU:HB2	1:A:159:PRO:HA	1.91	0.52
3:C:33:HIS:HB2	3:C:95:THR:HG23	1.91	0.51
4:D:34:VAL:HB	4:D:89:VAL:HG13	1.90	0.51
1:A:50:TRP:CZ2	1:A:52:GLY:HA2	2.45	0.51
1:A:219:LYS:NZ	2:B:124:GLU:OE1	2.23	0.51
4:D:188:LYS:HB3	4:D:189:HIS:HA	1.92	0.51
2:B:150:LYS:HE3	2:B:155:LEU:HD12	1.93	0.51
2:B:41:PRO:O	2:B:43:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:VAL:O	4:D:140:TYR:HB3	2.11	0.50
3:C:201:ASN:N	3:C:201:ASN:HD22	2.09	0.50
4:D:192:TYR:HD2	4:D:209:PHE:CZ	2.30	0.50
4:D:132:VAL:HG13	4:D:179:LEU:HB3	1.94	0.49
3:C:100:GLY:CA	3:C:101:ASN:HB2	2.42	0.49
3:C:28:THR:HA	3:C:51:PRO:HG2	1.95	0.49
1:A:166:SER:O	6:A:306:HOH:O	2.20	0.48
2:B:139:ASN:ND2	2:B:173:THR:HG21	2.28	0.48
3:C:127:PRO:HD3	3:C:213:LYS:HD3	1.96	0.48
3:C:125:VAL:HG21	3:C:202:VAL:HG11	1.96	0.48
4:D:20:THR:HG22	4:D:74:THR:OG1	2.13	0.48
1:A:62:ASN:OD1	4:D:92:SER:OG	2.25	0.48
4:D:151:ASP:HA	4:D:191:VAL:HG13	1.96	0.48
2:B:132:SER:O	6:B:405:HOH:O	2.19	0.48
1:A:131:VAL:CG2	1:A:208:VAL:HG21	2.44	0.47
1:A:176:PHE:CE2	2:B:177:SER:HB3	2.49	0.47
4:D:105:GLU:OE2	4:D:173:TYR:OH	2.31	0.47
4:D:155:GLN:CD	4:D:155:GLN:H	2.17	0.47
3:C:101:ASN:HB3	3:C:102:ASN:H	1.34	0.47
3:C:133:LYS:HA	3:C:134:SER:HA	1.66	0.47
3:C:100:GLY:HA3	3:C:101:ASN:CB	2.44	0.47
1:A:65:GLN:NE2	6:A:313:HOH:O	2.46	0.47
4:D:190:LYS:HG3	4:D:190:LYS:O	2.15	0.47
3:C:199:ILE:HG23	3:C:213:LYS:H	1.79	0.47
3:C:103:ALA:HB1	4:D:55:GLU:OE2	2.15	0.46
3:C:204:HIS:CE1	3:C:206:PRO:HB2	2.51	0.46
4:D:150:VAL:HG12	4:D:192:TYR:CD1	2.50	0.46
1:A:1:GLN:NE2	6:A:305:HOH:O	2.14	0.45
2:B:32:LYS:NZ	6:B:403:HOH:O	2.07	0.45
4:D:78:LEU:HD11	4:D:104:LEU:HD21	1.97	0.45
3:C:30:TYR:CE2	3:C:98:ARG:HB2	2.51	0.45
4:D:125:LEU:O	4:D:183:LYS:HD2	2.16	0.45
1:A:172:GLY:O	1:A:192:VAL:HA	2.17	0.45
3:C:87:GLU:OE2	3:C:87:GLU:N	2.48	0.45
3:C:45:TRP:CD2	4:D:96:PRO:HD2	2.51	0.45
3:C:214:ARG:HH12	3:C:216:GLU:CD	2.20	0.45
3:C:36:LYS:HB2	3:C:46:ILE:HD11	1.98	0.45
4:D:189:HIS:O	4:D:191:VAL:N	2.50	0.45
2:B:162:GLU:OE1	2:B:176:LEU:HD11	2.17	0.44
2:B:168:ASP:HB3	2:B:173:THR:H	1.82	0.44
3:C:127:PRO:HG2	4:D:121:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:ARG:NH1	3:C:216:GLU:OE2	2.51	0.44
3:C:99:TYR:O	3:C:100:GLY:C	2.56	0.44
2:B:198:THR:HG22	2:B:205:PRO:HG3	2.00	0.43
3:C:180:TYR:OH	6:C:301:HOH:O	2.21	0.43
3:C:150:PHE:HA	3:C:151:PRO:HA	1.75	0.43
2:B:34:LEU:HG	2:B:35:ALA:N	2.32	0.43
1:A:157:PRO:HD2	1:A:212:PRO:CB	2.49	0.43
3:C:65:LYS:HE2	3:C:65:LYS:HB2	1.74	0.43
4:D:77:SER:O	4:D:77:SER:OG	2.37	0.43
1:A:104:TYR:OH	6:A:302:HOH:O	2.07	0.42
2:B:62:ARG:HD2	2:B:78:ARG:O	2.19	0.42
4:D:206:THR:O	4:D:207:LYS:HD3	2.20	0.42
3:C:31:TRP:CE2	3:C:50:SER:HB2	2.55	0.42
4:D:149:LYS:NZ	4:D:195:GLU:CD	2.73	0.41
4:D:192:TYR:O	4:D:208:SER:HA	2.20	0.41
3:C:130:PRO:HD3	3:C:215:VAL:HG12	2.02	0.41
3:C:4:GLN:OE1	3:C:108:GLY:HA3	2.20	0.41
2:B:143:ARG:NH1	2:B:143:ARG:HG2	2.33	0.41
3:C:210:LYS:NZ	3:C:212:ASP:OD1	2.44	0.41
3:C:31:TRP:CZ2	3:C:50:SER:HB2	2.56	0.41
4:D:148:TRP:HB2	4:D:155:GLN:CD	2.41	0.41
1:A:19:LYS:HG3	1:A:85:GLU:HB2	2.02	0.41
4:D:122:ASP:HA	4:D:125:LEU:HD12	2.03	0.41
1:A:210:HIS:ND1	1:A:213:SER:HB3	2.36	0.41
2:B:87:TYR:O	2:B:102:GLY:HA2	2.20	0.41
1:A:183:SER:O	1:A:185:LEU:N	2.54	0.41
3:C:130:PRO:HB2	3:C:193:LEU:HD21	2.02	0.41
1:A:133:PRO:HD2	2:B:122:SER:HB3	2.03	0.40
4:D:119:PRO:HB3	4:D:209:PHE:CE1	2.57	0.40
1:A:153:LYS:HG3	1:A:154:ASP:N	2.37	0.40
1:A:66:LYS:HE3	1:A:66:LYS:HB2	1.63	0.40
3:C:155:THR:O	3:C:202:VAL:HA	2.22	0.40
3:C:45:TRP:CH2	3:C:47:GLY:HA2	2.56	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)
6:B:455:HOH:O	6:C:329:HOH:O[4_747]	2.15	0.05

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	217/228 (95%)	195 (90%)	19 (9%)	3 (1%)	11	19
2	B	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	29	47
3	C	219/222 (99%)	186 (85%)	26 (12%)	7 (3%)	4	5
4	D	207/214 (97%)	195 (94%)	8 (4%)	4 (2%)	8	12
All	All	856/879 (97%)	781 (91%)	60 (7%)	15 (2%)	8	14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	12	PRO
3	C	101	ASN
4	D	190	LYS
3	C	100	GLY
3	C	103	ALA
4	D	110	VAL
1	A	57	MET
1	A	184	GLY
2	B	32	LYS
3	C	13	GLY
4	D	111	ALA
3	C	14	ALA
4	D	204	PRO
3	C	123	PRO
1	A	212	PRO

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	182/187 (97%)	173 (95%)	9 (5%)	25	45
2	B	186/186 (100%)	179 (96%)	7 (4%)	33	56
3	C	186/187 (100%)	174 (94%)	12 (6%)	17	31
4	D	184/188 (98%)	173 (94%)	11 (6%)	19	34
All	All	738/748 (99%)	699 (95%)	39 (5%)	22	40

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	70	ARG
1	A	78	LEU
1	A	101	ARG
1	A	130	SER
1	A	137	SER
1	A	170	THR
1	A	201	THR
1	A	214	ASN
2	B	34	LEU
2	B	91	GLN
2	B	133	VAL
2	B	155	LEU
2	B	173	THR
2	B	188	GLU
2	B	215	CYS
3	C	4	GLN
3	C	17	LYS
3	C	54	SER
3	C	73	SER
3	C	101	ASN
3	C	112	LEU
3	C	132	SER
3	C	142	LEU
3	C	165	SER
3	C	176	SER
3	C	201	ASN
3	C	202	VAL
4	D	42	LYS
4	D	56	SER
4	D	72	THR

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Mol	Chain	Res	Type
4	D	75	ILE
4	D	81	GLU
4	D	90	GLN
4	D	114	SER
4	D	121	SER
4	D	125	LEU
4	D	196	VAL
4	D	197	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	175	GLN
3	C	201	ASN
4	D	124	GLN
4	D	160	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	SO4	B	301	-	4,4,4	0.21	0	6,6,6	0.17	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	221/228 (96%)	-0.03	1 (0%)	91	92	21, 43, 77, 112	0
2	B	215/215 (100%)	-0.20	2 (0%)	84	86	21, 40, 77, 111	0
3	C	221/222 (99%)	0.57	27 (12%)	4	4	31, 68, 126, 138	0
4	D	209/214 (97%)	0.26	17 (8%)	12	12	28, 57, 108, 121	0
All	All	866/879 (98%)	0.15	47 (5%)	25	28	21, 50, 111, 138	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	197	THR	6.6
3	C	215	VAL	5.6
3	C	195	THR	5.4
1	A	226	CYS	5.3
3	C	198	TYR	4.6
2	B	215	CYS	4.4
3	C	188	VAL	4.1
4	D	121	SER	4.0
4	D	154	LEU	3.9
3	C	216	GLU	3.8
4	D	128	GLY	3.6
3	C	135	THR	3.4
3	C	220	CYS	3.4
3	C	192	SER	3.4
3	C	142	LEU	3.3
3	C	163	LEU	3.3
4	D	129	THR	3.2
3	C	199	ILE	3.2
3	C	206	PRO	3.2
3	C	194	GLY	3.0
3	C	190	SER	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	136	SER	2.9
4	D	145	LYS	2.8
3	C	193	LEU	2.7
3	C	203	ASN	2.7
4	D	110	VAL	2.6
4	D	181	LEU	2.6
3	C	191	SER	2.6
3	C	138	GLY	2.6
4	D	122	ASP	2.5
3	C	187	THR	2.5
3	C	209	THR	2.5
3	C	158	TRP	2.5
2	B	155	LEU	2.4
3	C	133	LYS	2.3
4	D	183	LYS	2.3
4	D	201	LEU	2.3
4	D	146	VAL	2.3
4	D	188	LYS	2.3
4	D	153	ALA	2.2
4	D	190	LYS	2.2
3	C	219	SER	2.2
3	C	127	PRO	2.2
4	D	150	VAL	2.1
4	D	193	ALA	2.1
3	C	214	ARG	2.1
4	D	126	LYS	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	301	5/5	0.96	0.17	56,58,66,70	0

6.5 Other polymers (i)

There are no such residues in this entry.