Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 05:48 PM BST

PDB ID	:	6O9H
Title	:	Mouse ECD with Fab1
Authors	:	Min, X.; Wang, Z.
Deposited on	:	2019-03-13
Resolution	:	2.10 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 following versions of software and data (see references ①) were used in the production of this report:

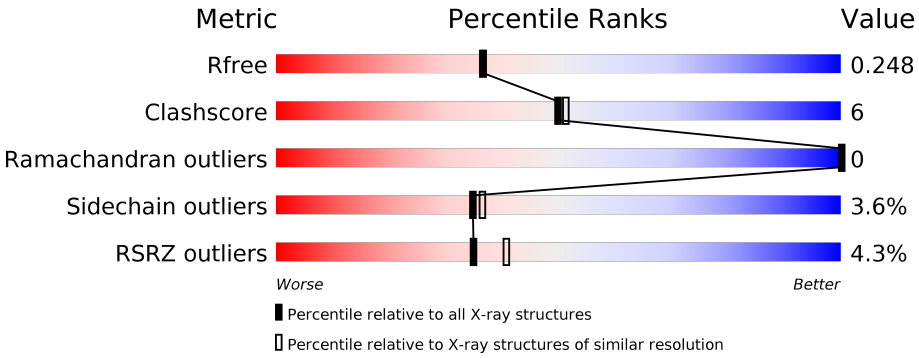
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	225	4% 80% 12% • 7%
1	H	225	5% 78% 14% • 5%
2	B	220	2% 85% 14% •
2	L	220	2% 85% 12% •
3	C	137	7% 60% 5% • 34%
3	D	137	3% 62% • 34%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8673 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 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	213	Total	C	N	O	S	0	1	0
			1615	1030	266	311	8			
1	A	210	Total	C	N	O	S	0	0	0
			1594	1019	263	304	8			

- Molecule 2 is a protein called Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1654	1031	275	341	7			
2	B	217	Total	C	N	O	S	0	0	0
			1676	1044	279	346	7			

- Molecule 3 is a protein called Gastric inhibitory polypeptide receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	90	Total	C	N	O	S	0	0	0
			734	461	127	138	8			
3	C	90	Total	C	N	O	S	0	0	0
			734	461	127	138	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	MET	-	expression tag	UNP Q0P543
D	-26	GLY	-	expression tag	UNP Q0P543
D	-25	SER	-	expression tag	UNP Q0P543
D	-24	SER	-	expression tag	UNP Q0P543
D	-23	HIS	-	expression tag	UNP Q0P543
D	-22	HIS	-	expression tag	UNP Q0P543
D	-21	HIS	-	expression tag	UNP Q0P543
D	-20	HIS	-	expression tag	UNP Q0P543

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	HIS	-	expression tag	UNP Q0P543
D	-18	HIS	-	expression tag	UNP Q0P543
D	-17	SER	-	expression tag	UNP Q0P543
D	-16	SER	-	expression tag	UNP Q0P543
D	-15	GLY	-	expression tag	UNP Q0P543
D	-14	LEU	-	expression tag	UNP Q0P543
D	-13	VAL	-	expression tag	UNP Q0P543
D	-12	PRO	-	expression tag	UNP Q0P543
D	-11	ARG	-	expression tag	UNP Q0P543
D	-10	GLY	-	expression tag	UNP Q0P543
D	-9	SER	-	expression tag	UNP Q0P543
D	-8	HIS	-	expression tag	UNP Q0P543
D	-7	MET	-	expression tag	UNP Q0P543
C	-27	MET	-	expression tag	UNP Q0P543
C	-26	GLY	-	expression tag	UNP Q0P543
C	-25	SER	-	expression tag	UNP Q0P543
C	-24	SER	-	expression tag	UNP Q0P543
C	-23	HIS	-	expression tag	UNP Q0P543
C	-22	HIS	-	expression tag	UNP Q0P543
C	-21	HIS	-	expression tag	UNP Q0P543
C	-20	HIS	-	expression tag	UNP Q0P543
C	-19	HIS	-	expression tag	UNP Q0P543
C	-18	HIS	-	expression tag	UNP Q0P543
C	-17	SER	-	expression tag	UNP Q0P543
C	-16	SER	-	expression tag	UNP Q0P543
C	-15	GLY	-	expression tag	UNP Q0P543
C	-14	LEU	-	expression tag	UNP Q0P543
C	-13	VAL	-	expression tag	UNP Q0P543
C	-12	PRO	-	expression tag	UNP Q0P543
C	-11	ARG	-	expression tag	UNP Q0P543
C	-10	GLY	-	expression tag	UNP Q0P543
C	-9	SER	-	expression tag	UNP Q0P543
C	-8	HIS	-	expression tag	UNP Q0P543
C	-7	MET	-	expression tag	UNP Q0P543

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

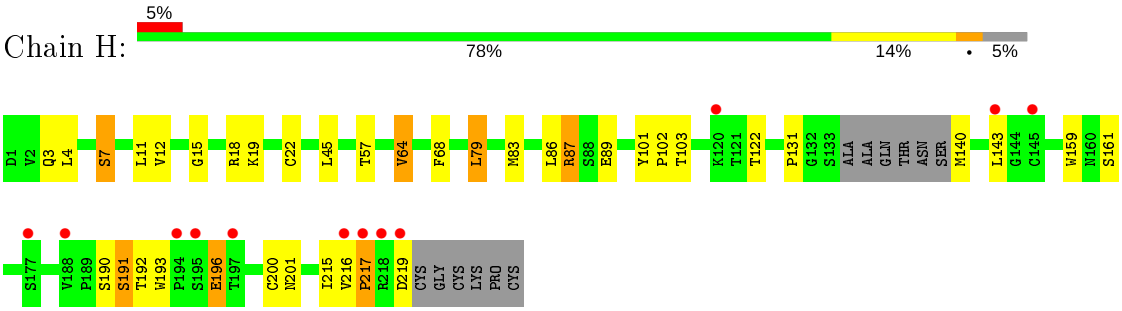
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	130	Total O 130 130	0	0
5	L	134	Total O 134 134	0	0
5	A	126	Total O 126 126	0	0
5	B	131	Total O 131 131	0	0
5	D	67	Total O 67 67	0	0
5	C	76	Total O 76 76	0	0

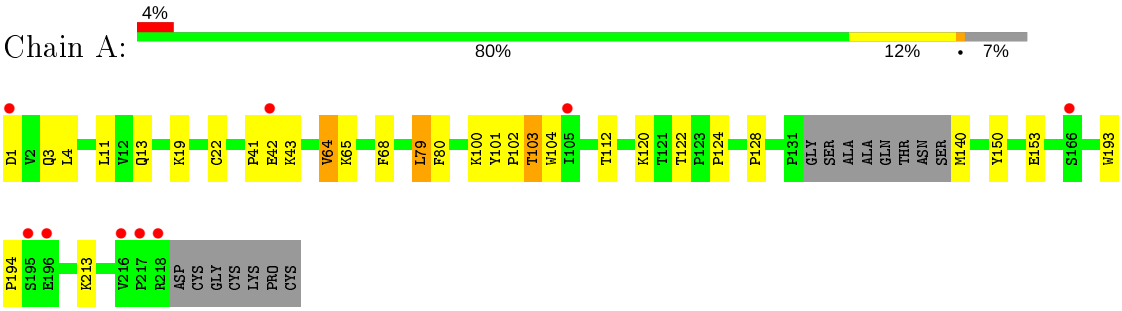
3 Residue-property plots (i)

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.

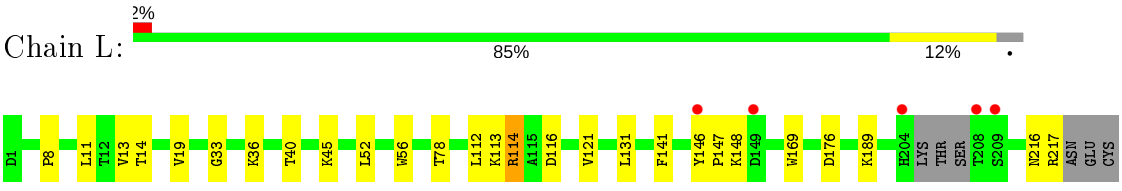
- Molecule 1: Heavy chain



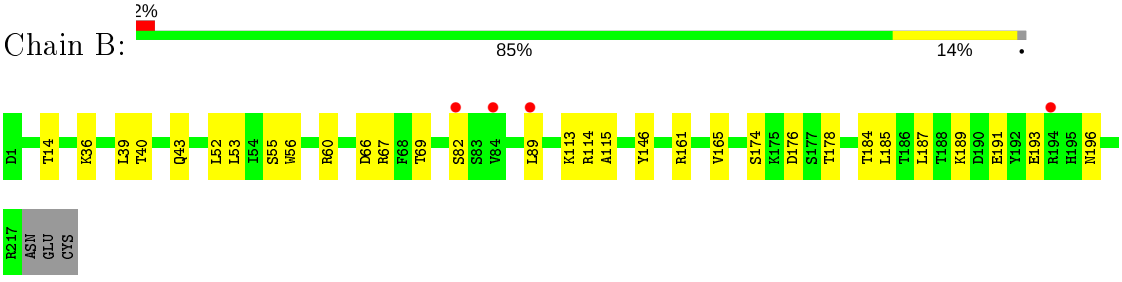
- Molecule 1: Heavy chain



- Molecule 2: Light chain

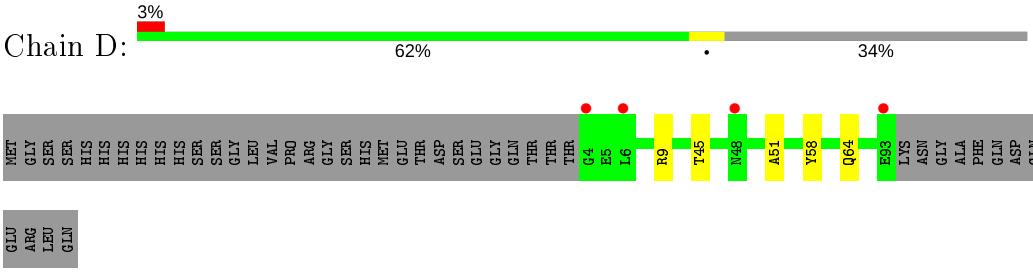


- Molecule 2: Light chain



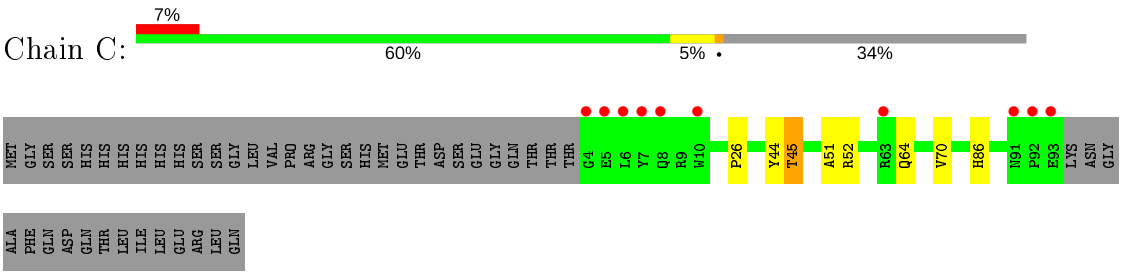
• Molecule 3: Gastric inhibitory polypeptide receptor

Chain D:



• Molecule 3: Gastric inhibitory polypeptide receptor

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.08Å 48.97Å 150.91Å 90.00° 101.08° 90.00°	Depositor
Resolution (Å)	19.93 – 2.10 29.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.93-2.10) 98.4 (29.53-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.203 , 0.248 0.204 , 0.248	Depositor DCC
R_{free} test set	3071 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8673	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.26	0/1639	0.51	0/2240
1	H	0.26	0/1663	0.52	0/2272
2	B	0.26	0/1713	0.49	0/2329
2	L	0.25	0/1690	0.47	0/2297
3	C	0.25	0/761	0.42	0/1037
3	D	0.27	0/761	0.44	0/1037
All	All	0.26	0/8227	0.49	0/11212

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	216	VAL	Peptide
1	H	217	PRO	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	1594	0	1568	25	0
1	H	1615	0	1585	27	0
2	B	1676	0	1614	21	0
2	L	1654	0	1588	16	0
3	C	734	0	639	4	0
3	D	734	0	639	5	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	126	0	0	8	1
5	B	131	0	0	1	1
5	C	76	0	0	1	1
5	D	67	0	0	0	1
5	H	130	0	0	12	1
5	L	134	0	0	3	1
All	All	8673	0	7633	91	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 6.

All (91) 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:1:ASP:O	5:A:401:HOH:O	1.97	0.81
3:D:9:ARG:HD3	3:D:58:TYR:HA	1.65	0.79
2:B:60:ARG:HH11	2:B:69:THR:HG22	1.46	0.78
1:A:140:MET:N	5:A:404:HOH:O	2.16	0.76
2:B:14:THR:HG22	2:B:113:LYS:HB2	1.68	0.76
1:A:103:THR:CG2	2:B:40:THR:HG21	2.17	0.73
2:B:114:ARG:NH2	5:B:303:HOH:O	2.22	0.72
1:H:217:PRO:O	5:H:302:HOH:O	2.10	0.69
1:A:13:GLN:NE2	5:A:403:HOH:O	2.14	0.68
1:H:193:TRP:O	5:H:301:HOH:O	2.09	0.68
1:H:161:SER:H	1:H:201:ASN:HD21	1.42	0.68
1:A:153:GLU:OE1	5:A:402:HOH:O	2.11	0.67
1:A:103:THR:HG21	2:B:40:THR:HG21	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:PRO:O	5:H:302:HOH:O	2.15	0.64
1:A:64:VAL:HG13	1:A:68:PHE:HB2	1.80	0.64
1:H:190:SER:N	5:H:304:HOH:O	2.31	0.63
2:L:113:LYS:O	5:L:301:HOH:O	2.15	0.62
1:H:57:THR:HG23	5:H:307:HOH:O	1.99	0.62
1:H:140:MET:N	5:H:303:HOH:O	2.34	0.60
1:A:103:THR:HG21	2:B:40:THR:CG2	2.31	0.59
2:B:165:VAL:HG12	2:B:185:LEU:HD23	1.85	0.59
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.83	0.59
1:A:103:THR:HG22	2:B:40:THR:HG21	1.84	0.59
1:H:3:GLN:NE2	5:H:308:HOH:O	2.36	0.58
1:A:103:THR:CG2	2:B:40:THR:CG2	2.81	0.57
1:H:12:VAL:HG11	1:H:86:LEU:HD12	1.85	0.57
1:H:64:VAL:HG13	1:H:68:PHE:HB2	1.85	0.56
1:A:3:GLN:HB3	5:A:407:HOH:O	2.06	0.56
1:A:100:LYS:NZ	5:A:405:HOH:O	2.24	0.55
1:H:143:LEU:HD22	1:H:215:ILE:HG21	1.88	0.55
2:L:11:LEU:HD11	2:L:19:VAL:HG11	1.89	0.55
3:C:70:VAL:HG13	3:C:86:HIS:HB3	1.89	0.54
1:A:41:PRO:O	1:A:42:GLU:HG2	2.08	0.53
2:B:89:LEU:HD12	2:B:174:SER:HA	1.91	0.53
2:L:216:ASN:O	2:L:217:ARG:HB2	2.09	0.53
1:A:22:CYS:HB3	1:A:79:LEU:HB3	1.90	0.53
2:B:187:LEU:HB3	2:B:191:GLU:HG3	1.90	0.53
1:H:7:SER:HB2	5:H:334:HOH:O	2.09	0.53
1:A:128:PRO:HD3	1:A:213:LYS:HE2	1.92	0.52
1:H:161:SER:H	1:H:201:ASN:ND2	2.07	0.52
3:D:45:THR:HG21	3:D:51:ALA:HB2	1.93	0.50
1:H:19:LYS:NZ	5:H:312:HOH:O	2.44	0.50
2:B:36:LYS:HG2	2:B:56:TRP:CD2	2.47	0.49
1:A:103:THR:HG23	2:B:55:SER:HB2	1.95	0.48
2:L:13:VAL:HA	2:L:113:LYS:HZ1	1.77	0.48
1:H:191:SER:N	5:H:304:HOH:O	2.22	0.48
2:L:36:LYS:HG2	2:L:56:TRP:CE3	2.49	0.48
1:A:101:TYR:CD1	1:A:102:PRO:HA	2.49	0.47
1:A:120:LYS:NZ	5:A:403:HOH:O	2.45	0.47
2:B:67:ARG:HB2	2:B:82:SER:O	2.15	0.47
3:C:45:THR:HG21	3:C:51:ALA:HB2	1.97	0.46
2:L:45:LYS:HD2	5:L:321:HOH:O	2.15	0.46
2:B:114:ARG:HG2	2:B:115:ALA:N	2.30	0.46
1:H:159:TRP:CZ3	1:H:200:CYS:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:13:VAL:HA	2:L:113:LYS:NZ	2.32	0.45
3:C:26:PRO:HB3	3:C:44:TYR:CG	2.51	0.45
2:L:8:PRO:HG3	2:L:11:LEU:HD23	1.99	0.45
1:H:45:LEU:N	5:H:315:HOH:O	2.46	0.45
1:H:101:TYR:CG	1:H:102:PRO:HA	2.52	0.45
2:B:165:VAL:HA	2:B:184:THR:O	2.16	0.45
1:H:15:GLY:N	1:H:86:LEU:O	2.44	0.44
2:B:176:ASP:HB3	2:B:178:THR:HG23	1.99	0.44
1:H:101:TYR:CD1	1:H:102:PRO:HA	2.52	0.44
1:A:65:LYS:HE3	1:A:65:LYS:HB2	1.71	0.44
1:H:12:VAL:HG21	1:H:18:ARG:HB2	1.99	0.44
2:B:189:LYS:O	2:B:193:GLU:HG2	2.18	0.44
3:D:64:GLN:H	3:D:64:GLN:HG2	1.68	0.44
2:L:148:LYS:HE3	2:L:169:TRP:CG	2.53	0.44
3:D:9:ARG:CD	3:D:58:TYR:HA	2.41	0.44
2:B:113:LYS:HA	2:B:146:TYR:OH	2.17	0.44
3:C:64:GLN:NE2	5:C:202:HOH:O	2.26	0.43
1:H:193:TRP:CH2	1:H:217:PRO:HA	2.53	0.43
2:L:114:ARG:HD2	2:L:176:ASP:O	2.18	0.43
1:H:190:SER:OG	5:H:303:HOH:O	2.21	0.43
1:A:101:TYR:CG	1:A:102:PRO:HA	2.54	0.43
1:H:83:MET:HB3	1:H:86:LEU:HD21	2.00	0.43
2:L:116:ASP:O	5:L:302:HOH:O	2.21	0.43
1:H:87:ARG:HG3	1:H:89:GLU:HG2	2.01	0.42
1:A:43:LYS:HB3	1:A:43:LYS:HE2	1.90	0.42
1:H:192:THR:O	1:H:196:GLU:HG3	2.19	0.42
1:A:104:TRP:HE3	5:A:417:HOH:O	2.02	0.42
2:L:146:TYR:CG	2:L:147:PRO:HA	2.55	0.42
2:L:113:LYS:HA	2:L:146:TYR:OH	2.20	0.42
2:L:121:VAL:HA	2:L:141:PHE:O	2.20	0.42
2:L:189:LYS:HB3	2:L:189:LYS:HE2	1.85	0.41
2:B:43:GLN:HB2	2:B:53:LEU:HD11	2.03	0.41
2:B:36:LYS:HG2	2:B:56:TRP:CE3	2.55	0.41
2:L:33:GLY:HA2	3:D:9:ARG:HE	1.86	0.40
1:A:193:TRP:CG	1:A:194:PRO:HA	2.56	0.40
1:H:22:CYS:HB3	1:H:79:LEU:HB3	2.02	0.40
1:A:19:LYS:HE2	1:A:80:PHE:CD1	2.56	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)
5:H:406:HOH:O	5:B:403:HOH:O[2_544]	2.01	0.19
5:D:342:HOH:O	5:C:264:HOH:O[2_655]	2.05	0.15
5:L:323:HOH:O	5:A:502:HOH:O[2_544]	2.10	0.10

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	206/225 (92%)	202 (98%)	4 (2%)	0	100	100
1	H	210/225 (93%)	205 (98%)	5 (2%)	0	100	100
2	B	215/220 (98%)	208 (97%)	7 (3%)	0	100	100
2	L	210/220 (96%)	203 (97%)	7 (3%)	0	100	100
3	C	88/137 (64%)	86 (98%)	2 (2%)	0	100	100
3	D	88/137 (64%)	84 (96%)	4 (4%)	0	100	100
All	All	1017/1164 (87%)	988 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	179/190 (94%)	172 (96%)	7 (4%)	32	33
1	H	182/190 (96%)	171 (94%)	11 (6%)	19	16
2	B	194/197 (98%)	189 (97%)	5 (3%)	46	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	191/197 (97%)	184 (96%)	7 (4%)	34 35
3	C	76/117 (65%)	74 (97%)	2 (3%)	46 50
3	D	76/117 (65%)	76 (100%)	0	100 100
All	All	898/1008 (89%)	866 (96%)	32 (4%)	35 36

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	4	LEU
1	H	7	SER
1	H	11	LEU
1	H	64	VAL
1	H	79	LEU
1	H	87	ARG
1	H	103	THR
1	H	122	THR
1	H	191	SER
1	H	196	GLU
1	H	219	ASP
2	L	14	THR
2	L	40	THR
2	L	52	LEU
2	L	78	THR
2	L	112	LEU
2	L	114	ARG
2	L	131	LEU
1	A	4	LEU
1	A	11	LEU
1	A	64	VAL
1	A	79	LEU
1	A	103	THR
1	A	112	THR
1	A	122	THR
2	B	39	LEU
2	B	52	LEU
2	B	66	ASP
2	B	161	ARG
2	B	196	ASN
3	C	45	THR
3	C	52	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	201	ASN
3	D	33	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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, 95^{th} 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	210/225 (93%)	0.27	9 (4%) 35 41	20, 33, 55, 68	0
1	H	213/225 (94%)	0.37	12 (5%) 24 29	18, 31, 56, 69	0
2	B	217/220 (98%)	0.30	4 (1%) 68 72	21, 34, 49, 56	0
2	L	214/220 (97%)	0.32	5 (2%) 60 65	23, 36, 48, 69	0
3	C	90/137 (65%)	0.44	10 (11%) 5 7	22, 33, 56, 64	0
3	D	90/137 (65%)	0.27	4 (4%) 34 40	18, 32, 52, 71	0
All	All	1034/1164 (88%)	0.32	44 (4%) 35 41	18, 33, 52, 71	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	PRO	4.5
3	C	63	ARG	3.8
2	L	208	THR	3.8
1	H	216	VAL	3.6
3	C	8	GLN	3.6
3	C	7	TYR	3.6
1	H	195	SER	3.6
3	D	6	LEU	3.5
2	L	204	HIS	3.5
3	C	4	GLY	3.5
1	H	197	THR	3.3
3	C	6	LEU	3.2
1	H	194	PRO	3.1
3	D	48	ASN	3.1
3	C	10	TRP	3.0
3	C	92	PRO	3.0
2	L	209	SER	2.9
2	B	194	ARG	2.8
1	H	145	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	4	GLY	2.8
3	C	93	GLU	2.8
3	C	91	ASN	2.7
1	A	105	ILE	2.7
2	L	146	TYR	2.6
3	D	93	GLU	2.6
1	H	219	ASP	2.6
1	H	217	PRO	2.6
2	B	89	LEU	2.4
1	A	42	GLU	2.4
1	H	218	ARG	2.4
1	A	218	ARG	2.3
1	A	196	GLU	2.3
1	H	120	LYS	2.3
1	A	1	ASP	2.2
2	L	149	ASP	2.2
1	A	216	VAL	2.2
3	C	5	GLU	2.2
1	A	195	SER	2.2
2	B	84	VAL	2.2
1	H	177	SER	2.2
1	H	143	LEU	2.1
1	A	166	SER	2.1
1	H	188	VAL	2.0
2	B	82	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)

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, 95^{th} 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
4	NA	A	301	1/1	0.89	0.11	29,29,29,29	0
4	NA	D	201	1/1	0.95	0.10	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.