



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:11 am BST

PDB ID : 1GPO
Title : CRYSTAL STRUCTURE OF THE RATIONALLY DESIGNED ANTIBODY
M41 AS A FAB FRAGMENT
Authors : Schiweck, W.; Skerra, A.
Deposited on : 1997-03-27
Resolution : 1.95 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 ⓘ](#)) 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

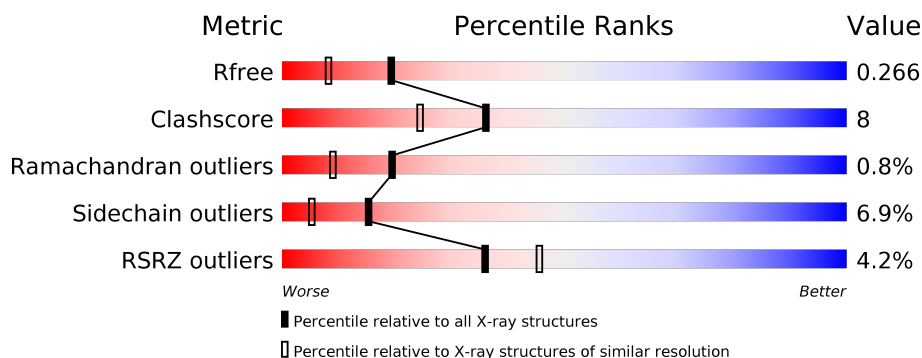
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 $\leq 5\%$. 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	L	219	<div> <div></div> <div>75% 22% ..</div> </div>
1	M	219	<div> <div>9%</div> <div>74% 25% .</div> </div>
2	H	221	<div> <div>3%</div> <div>76% 18% . .</div> </div>
2	I	221	<div> <div>4%</div> <div>74% 20% . .</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7281 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 ANTIBODY M41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	2	0	0
			1676	1046	279	346	5			
1	M	218	Total	C	N	O	S	78	0	0
			1693	1055	282	351	5			

- Molecule 2 is a protein called ANTIBODY M41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	2	0	0
			1636	1033	266	331	6			
2	I	212	Total	C	N	O	S	3	0	0
			1617	1023	261	327	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	3	LYS	GLN	CONFLICT	EMBL AJ303449
H	32	ASP	GLY	CONFLICT	EMBL AJ303449
H	33	PHE	TYR	CONFLICT	EMBL AJ303449
H	35	SER	ASN	CONFLICT	EMBL AJ303449
H	39	GLN	LYS	CONFLICT	EMBL AJ303449
H	44	ARG	LYS	CONFLICT	EMBL AJ303449
H	50	PHE	TYR	CONFLICT	EMBL AJ303449
H	51	VAL	ILE	CONFLICT	EMBL AJ303449
H	52	GLN	SER	CONFLICT	EMBL AJ303449
H	54	SER	GLY	CONFLICT	EMBL AJ303449
H	56	GLU	SER	CONFLICT	EMBL AJ303449
H	58	ALA	TYR	CONFLICT	EMBL AJ303449
H	64	LYS	GLU	CONFLICT	EMBL AJ303449
H	81	ASP	GLN	CONFLICT	EMBL AJ303449
H	92	VAL	THR	CONFLICT	EMBL AJ303449
H	94	TYR	PHE	CONFLICT	EMBL AJ303449

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Chain	Residue	Modelled	Actual	Comment	Reference
H	97	ASN	ARG	CONFLICT	EMBL AJ303449
H	98	TRP	LEU	CONFLICT	EMBL AJ303449
H	99	HIS	PHE	CONFLICT	EMBL AJ303449
H	?	-	SER	DELETION	EMBL AJ303449
H	?	-	TYR	DELETION	EMBL AJ303449
H	?	-	TYR	DELETION	EMBL AJ303449
H	?	-	PHE	DELETION	EMBL AJ303449
H	109	VAL	LEU	CONFLICT	EMBL AJ303449
I	3	LYS	GLN	CONFLICT	EMBL AJ303449
I	32	ASP	GLY	CONFLICT	EMBL AJ303449
I	33	PHE	TYR	CONFLICT	EMBL AJ303449
I	35	SER	ASN	CONFLICT	EMBL AJ303449
I	39	GLN	LYS	CONFLICT	EMBL AJ303449
I	44	ARG	LYS	CONFLICT	EMBL AJ303449
I	50	PHE	TYR	CONFLICT	EMBL AJ303449
I	51	VAL	ILE	CONFLICT	EMBL AJ303449
I	52	GLN	SER	CONFLICT	EMBL AJ303449
I	54	SER	GLY	CONFLICT	EMBL AJ303449
I	56	GLU	SER	CONFLICT	EMBL AJ303449
I	58	ALA	TYR	CONFLICT	EMBL AJ303449
I	64	LYS	GLU	CONFLICT	EMBL AJ303449
I	81	ASP	GLN	CONFLICT	EMBL AJ303449
I	92	VAL	THR	CONFLICT	EMBL AJ303449
I	94	TYR	PHE	CONFLICT	EMBL AJ303449
I	97	ASN	ARG	CONFLICT	EMBL AJ303449
I	98	TRP	LEU	CONFLICT	EMBL AJ303449
I	99	HIS	PHE	CONFLICT	EMBL AJ303449
I	?	-	SER	DELETION	EMBL AJ303449
I	?	-	TYR	DELETION	EMBL AJ303449
I	?	-	TYR	DELETION	EMBL AJ303449
I	?	-	PHE	DELETION	EMBL AJ303449
I	109	VAL	LEU	CONFLICT	EMBL AJ303449

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

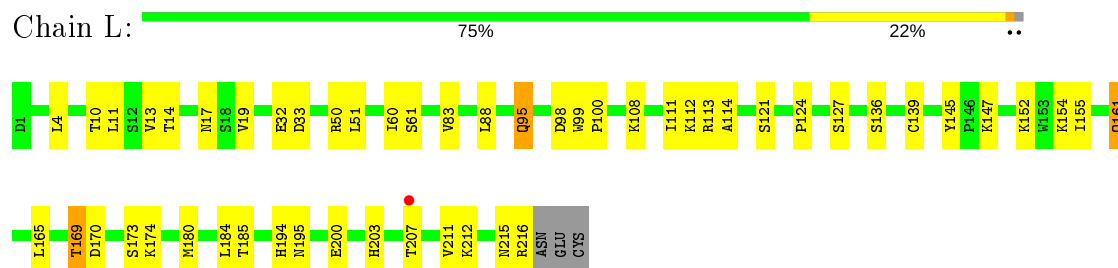
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	174	Total	O	0	0
			174	174		
4	H	185	Total	O	0	0
			185	185		
4	M	134	Total	O	0	0
			134	134		
4	I	156	Total	O	0	0
			156	156		

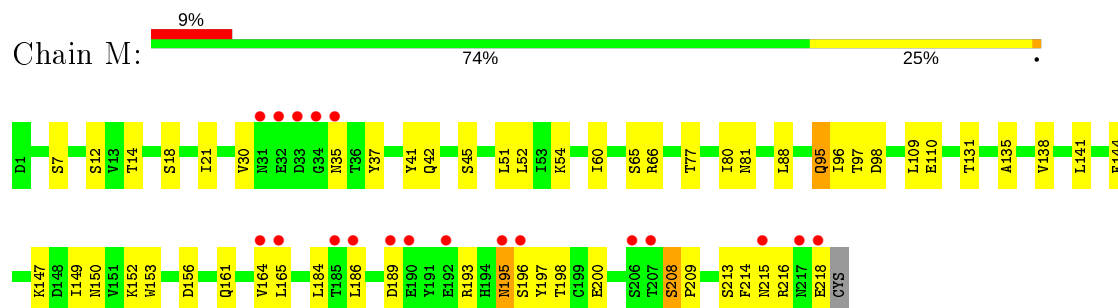
3 Residue-property plots [i](#)

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: ANTIBODY M41



• Molecule 1: ANTIBODY M41





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.47Å 103.51Å 113.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.95 8.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	81.3 (8.00-1.95) 83.8 (8.00-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.96Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , 0.283 0.206 , 0.266	Depositor DCC
R_{free} test set	6871 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 133.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7281	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 25.07 % 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 3.3991e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	L	0.53	0/1714	0.77	0/2330
1	M	0.56	0/1731	0.76	0/2353
2	H	0.58	0/1681	0.84	1/2307 (0.0%)
2	I	0.57	0/1662	0.81	1/2282 (0.0%)
All	All	0.56	0/6788	0.80	2/9272 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	131	GLN	N-CA-C	7.63	131.60	111.00
2	I	177	LEU	CA-CB-CG	5.66	128.32	115.30

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	L	1676	0	1600	25	0
1	M	1693	0	1612	33	0
2	H	1636	0	1578	23	0
2	I	1617	0	1561	24	0
3	H	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	5	0	0	1	0
4	H	185	0	0	2	0
4	I	156	0	0	2	0
4	L	174	0	0	2	0
4	M	134	0	0	2	0
All	All	7281	0	6351	103	0

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 8.

All (103) 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)
2:I:153:THR:HG22	2:I:196:ASN:HD22	1.34	0.91
1:M:195:ASN:HA	1:M:216:ARG:HG3	1.56	0.88
2:H:156:SER:H	2:H:196:ASN:HD21	1.30	0.79
1:L:95:GLN:HE22	1:L:98:ASP:H	1.33	0.77
1:M:95:GLN:HE22	1:M:98:ASP:H	1.35	0.72
1:L:136:SER:OG	1:L:185:THR:HG22	1.91	0.69
2:I:188:TRP:CH2	2:I:212:PRO:HG3	2.29	0.68
1:L:88:LEU:HD21	1:L:173:SER:HA	1.76	0.67
2:I:156:SER:H	2:I:196:ASN:HD21	1.43	0.65
1:M:135:ALA:O	1:M:186:LEU:HD23	1.97	0.64
2:H:156:SER:H	2:H:196:ASN:ND2	1.96	0.63
1:M:42:GLN:HB2	1:M:52:LEU:HD11	1.82	0.60
1:M:12:SER:HA	1:M:110:GLU:O	2.01	0.60
2:I:34:TRP:HB3	2:I:78:TYR:CZ	2.37	0.59
2:I:42:GLY:O	2:I:43:ASN:HB2	2.03	0.57
1:M:95:GLN:NE2	1:M:97:THR:H	2.00	0.57
1:M:35:ASN:HB2	1:M:37:TYR:CE2	2.40	0.57
1:M:141:LEU:HD23	1:M:149:ILE:HD13	1.86	0.57
1:L:169:THR:HG23	1:L:170:ASP:O	2.04	0.57
2:I:156:SER:H	2:I:196:ASN:ND2	2.03	0.56
2:I:119:PRO:HB3	2:I:145:TYR:HB3	1.86	0.56
1:M:95:GLN:HE21	1:M:97:THR:H	1.54	0.56
1:L:200:GLU:HG2	1:L:211:VAL:HG22	1.88	0.55
2:I:8:GLY:HA3	2:I:20:LEU:HD23	1.88	0.55
2:I:199:HIS:HB3	2:I:204:THR:HG23	1.89	0.55
2:I:71:ARG:HG3	3:I:651:SO4:O2	2.07	0.54
2:H:129:ALA:O	2:H:130:ALA:HB2	2.08	0.53
2:H:177:LEU:HA	4:H:723:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:PRO:HG2	2:H:213:ARG:CZ	2.40	0.52
1:L:165:LEU:HD11	2:H:171:GLN:HB2	1.92	0.52
2:H:40:PHE:HB3	2:H:41:PRO:HD2	1.92	0.52
2:I:202:SER:OG	2:I:204:THR:HG22	2.09	0.52
1:L:195:ASN:O	1:L:215:ASN:HA	2.09	0.51
1:M:141:LEU:O	1:M:144:PHE:HE2	1.94	0.51
2:I:154:TRP:CZ3	2:I:195:CYS:HB3	2.46	0.51
1:M:189:ASP:O	1:M:193:ARG:HB2	2.11	0.51
2:H:34:TRP:HB3	2:H:78:TYR:CZ	2.46	0.51
1:M:197:TYR:HB2	1:M:214:PHE:CE2	2.46	0.50
2:H:65:SER:HA	4:H:806:HOH:O	2.13	0.49
1:M:35:ASN:HB2	1:M:37:TYR:HE2	1.78	0.49
2:I:170:LEU:HD11	2:I:173:ASP:HA	1.96	0.48
1:M:66:ARG:O	1:M:80:ILE:HA	2.13	0.48
1:M:215:ASN:HD22	1:M:218:GLU:HB2	1.79	0.47
1:M:141:LEU:HD23	1:M:149:ILE:CD1	2.45	0.47
1:M:21:ILE:O	1:M:77:THR:HA	2.15	0.47
2:H:1:GLU:HB3	2:H:2:VAL:H	1.61	0.47
2:H:19:SER:HA	2:H:80:LEU:O	2.15	0.47
2:H:199:HIS:HB3	2:H:204:THR:HB	1.96	0.47
1:M:216:ARG:HB3	1:M:216:ARG:HH11	1.79	0.46
2:I:14:PRO:O	2:I:15:SER:HB2	2.15	0.46
1:L:121:SER:O	1:L:139:CYS:HA	2.15	0.46
1:L:33:ASP:HB2	4:L:363:HOH:O	2.16	0.46
1:L:113:ARG:HG2	1:L:114:ALA:N	2.31	0.46
2:H:36:TRP:O	2:H:48:MET:HB2	2.15	0.46
1:L:145:TYR:O	1:L:203:HIS:HE1	1.99	0.46
1:M:195:ASN:O	1:M:215:ASN:HA	2.15	0.46
1:M:153:TRP:HA	1:M:198:THR:O	2.16	0.45
2:I:39:GLN:HB2	2:I:45:LEU:HD23	1.97	0.45
1:L:17:ASN:O	1:L:83:VAL:HG23	2.16	0.45
2:H:4:LEU:N	2:H:4:LEU:HD12	2.32	0.45
1:M:54:LYS:HB2	1:M:60:ILE:HD11	1.99	0.45
1:M:37:TYR:HB3	1:M:96:ILE:HG12	1.99	0.44
1:M:41:TYR:CE1	1:M:51:LEU:HD13	2.53	0.44
1:L:99:TRP:CD2	1:L:100:PRO:HA	2.51	0.44
1:M:88:LEU:HD12	1:M:109:LEU:O	2.18	0.44
2:H:51:VAL:HG23	2:H:57:THR:HG22	1.99	0.44
1:L:51:LEU:HG	1:L:60:ILE:HD11	1.99	0.44
1:M:152:LYS:HD3	1:M:152:LYS:HA	1.82	0.44
2:H:33:PHE:HB2	2:H:98:TRP:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:33:PHE:HB2	2:I:98:TRP:CG	2.52	0.43
1:L:174:LYS:HD3	1:L:174:LYS:HA	1.90	0.43
1:L:147:LYS:HG2	4:L:353:HOH:O	2.17	0.43
1:M:195:ASN:CA	1:M:216:ARG:HG3	2.36	0.43
1:M:164:VAL:O	1:M:165:LEU:HD23	2.18	0.43
2:I:52:GLN:NE2	4:I:575:HOH:O	2.51	0.43
2:H:13:LYS:NZ	2:H:13:LYS:HB3	2.34	0.43
1:L:152:LYS:NZ	1:L:161:GLN:HE21	2.16	0.43
1:M:208:SER:HA	1:M:209:PRO:HD3	1.89	0.43
2:I:12:VAL:O	2:I:111:VAL:HA	2.19	0.42
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.01	0.42
2:H:56:GLU:HG2	2:H:57:THR:N	2.34	0.42
1:M:81:ASN:HB3	4:M:224:HOH:O	2.19	0.42
1:L:111:ILE:CG2	1:L:112:LYS:N	2.82	0.42
2:H:145:TYR:CE2	2:H:150:VAL:HG13	2.55	0.42
2:H:166:PHE:HA	2:H:167:PRO:HD3	1.88	0.42
2:I:87:THR:HG23	4:I:622:HOH:O	2.19	0.42
1:L:155:ILE:HD11	1:L:184:LEU:HD21	2.02	0.42
1:M:197:TYR:O	1:M:213:SER:HA	2.19	0.42
1:M:198:THR:HG22	1:M:200:GLU:HG3	2.02	0.42
2:H:71:ARG:HG3	3:H:650:SO4:O2	2.19	0.41
2:I:6:GLU:HA	2:I:21:THR:O	2.19	0.41
1:M:150:ASN:HA	4:M:303:HOH:O	2.20	0.41
2:H:150:VAL:HA	2:H:198:ALA:O	2.21	0.41
1:L:212:LYS:HA	1:L:212:LYS:HD2	1.73	0.41
1:L:194:HIS:O	1:L:216:ARG:HD3	2.21	0.41
1:M:195:ASN:HA	1:M:216:ARG:CG	2.37	0.41
1:L:10:THR:HG22	1:L:108:LYS:HB3	2.03	0.41
2:I:52:GLN:HG3	2:I:56:GLU:O	2.21	0.41
1:L:154:LYS:HE3	1:L:200:GLU:OE2	2.21	0.41
2:I:127:GLY:O	2:I:129:ALA:N	2.54	0.40
1:L:13:VAL:HG22	1:L:14:THR:N	2.35	0.40
2:I:170:LEU:HB2	2:I:175:TYR:CE1	2.57	0.40
2:I:211:VAL:HA	2:I:212:PRO:HD3	1.86	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	L	214/219 (98%)	202 (94%)	12 (6%)	0	100	100
1	M	216/219 (99%)	201 (93%)	14 (6%)	1 (0%)	29	17
2	H	212/221 (96%)	197 (93%)	11 (5%)	4 (2%)	8	2
2	I	210/221 (95%)	195 (93%)	13 (6%)	2 (1%)	15	6
All	All	852/880 (97%)	795 (93%)	50 (6%)	7 (1%)	19	9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	64	LYS
2	H	130	ALA
2	H	128	SER
1	M	195	ASN
2	I	128	SER
2	I	2	VAL
2	H	84	SER

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	L	194/197 (98%)	182 (94%)	12 (6%)	18	7
1	M	196/197 (100%)	181 (92%)	15 (8%)	13	4
2	H	191/198 (96%)	176 (92%)	15 (8%)	12	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	189/198 (96%)	178 (94%)	11 (6%)	20 8
All	All	770/790 (98%)	717 (93%)	53 (7%)	15 5

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	LEU
1	L	11	LEU
1	L	19	VAL
1	L	32	GLU
1	L	50	ARG
1	L	61	SER
1	L	95	GLN
1	L	127	SER
1	L	161	GLN
1	L	169	THR
1	L	180	MET
1	L	207	THR
2	H	1	GLU
2	H	12	VAL
2	H	43	ASN
2	H	53	TYR
2	H	71	ARG
2	H	84	SER
2	H	98	TRP
2	H	131	GLN
2	H	149	PRO
2	H	161	SER
2	H	170	LEU
2	H	172	SER
2	H	177	LEU
2	H	190	SER
2	H	191	GLU
1	M	7	SER
1	M	14	THR
1	M	18	SER
1	M	30	VAL
1	M	45	SER
1	M	65	SER
1	M	95	GLN
1	M	131	THR
1	M	138	VAL

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Mol	Chain	Res	Type
1	M	147	LYS
1	M	156	ASP
1	M	161	GLN
1	M	184	LEU
1	M	196	SER
1	M	208	SER
2	I	53	TYR
2	I	71	ARG
2	I	74	SER
2	I	98	TRP
2	I	105	GLN
2	I	149	PRO
2	I	150	VAL
2	I	153	THR
2	I	169	VAL
2	I	177	LEU
2	I	192	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	17	ASN
1	L	42	GLN
1	L	95	GLN
1	L	129	GLN
1	L	142	ASN
1	L	143	ASN
1	L	161	GLN
1	L	162	ASN
1	L	166	ASN
1	L	171	GLN
2	H	5	GLN
2	H	43	ASN
2	H	164	HIS
2	H	196	ASN
1	M	17	ASN
1	M	35	ASN
1	M	95	GLN
1	M	129	GLN
1	M	142	ASN
1	M	143	ASN
1	M	150	ASN

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Mol	Chain	Res	Type
1	M	194	HIS
2	I	43	ASN
2	I	171	GLN
2	I	196	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z > 2$
3	SO4	H	650	-	4,4,4	0.68	0	6,6,6	0.31	0
3	SO4	I	651	-	4,4,4	0.85	0	6,6,6	0.32	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	650	SO4	1	0
3	I	651	SO4	1	0

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	L	216/219 (98%)	-0.22	1 (0%) 91 94	9, 24, 42, 64	1 (0%)
1	M	208/219 (94%)	0.28	19 (9%) 9 15	10, 29, 67, 87	2 (0%)
2	H	214/221 (96%)	-0.25	7 (3%) 46 56	8, 20, 42, 75	2 (0%)
2	I	212/221 (95%)	-0.08	9 (4%) 36 45	9, 24, 46, 81	3 (1%)
All	All	850/880 (96%)	-0.07	36 (4%) 36 45	8, 24, 57, 87	8 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1	GLU	6.2
2	H	132	THR	5.6
2	H	130	ALA	5.4
1	M	32	GLU	5.3
1	M	217	ASN	5.0
1	M	33	ASP	4.8
1	M	206	SER	4.6
1	M	31	ASN	4.3
2	I	130	ALA	4.1
2	I	132	THR	4.1
1	M	164	VAL	4.1
2	H	128	SER	3.7
2	I	128	SER	3.3
2	I	129	ALA	3.3
2	I	127	GLY	3.2
2	H	129	ALA	3.2
2	H	131	GLN	3.1
1	M	218	GLU	3.0
1	L	207	THR	2.9
1	M	207	THR	2.9
2	H	214	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	215	ASN	2.8
1	M	35	ASN	2.7
1	M	165	LEU	2.6
2	I	131	GLN	2.6
1	M	195	ASN	2.6
1	M	34	GLY	2.6
1	M	185	THR	2.4
1	M	186	LEU	2.3
1	M	189	ASP	2.2
2	I	2	VAL	2.2
1	M	192	GLU	2.1
1	M	196	SER	2.1
1	M	190	GLU	2.1
2	H	1	GLU	2.0
2	I	133	ASN	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(\AA^2)	Q<0.9
3	SO4	H	650	5/5	0.99	0.08	27,31,35,36	0
3	SO4	I	651	5/5	0.99	0.05	21,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.