Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:13 PM BST

PDB ID	:	6A76
Title	:	Crystal structure of the Fab fragment of B5209B, a murine monoclonal antibody specific for the fifth immunoglobulin domain (Ig5) of human ROBO1
Authors	:	Mizohata, E.; Nakayama, T.; Kado, Y.; Inoue, T.
Deposited on	:	2018-07-02
Resolution	:	1.50 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:

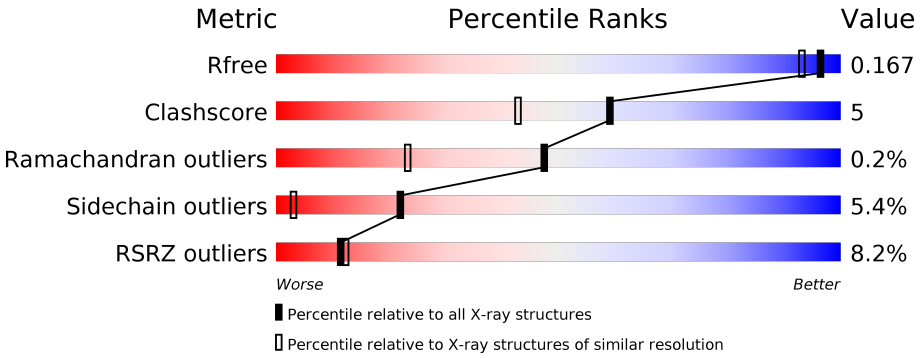
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	L	211	14% 80% 18%
2	H	221	3% 80% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	L	303	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3686 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.

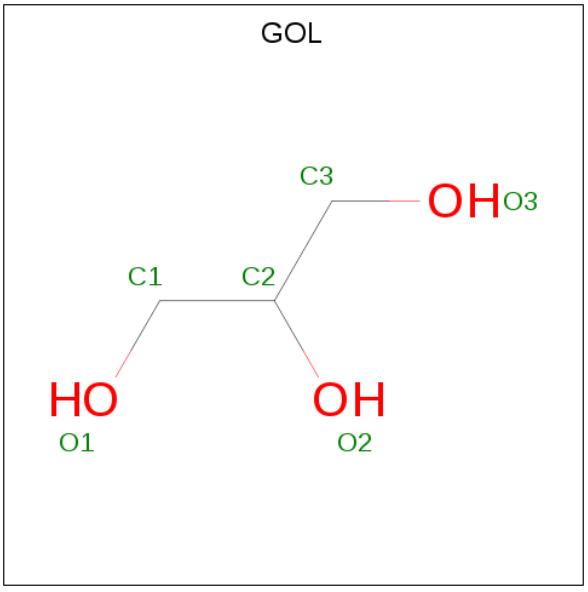
- Molecule 1 is a protein called Light chain of the anti-human Robo1 antibody B5209B Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	4	0
			1648	1022	278	341	7			

- Molecule 2 is a protein called Heavy chain of the anti-human Robo1 antibody B5209B Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	5	0
			1638	1032	265	332	9			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

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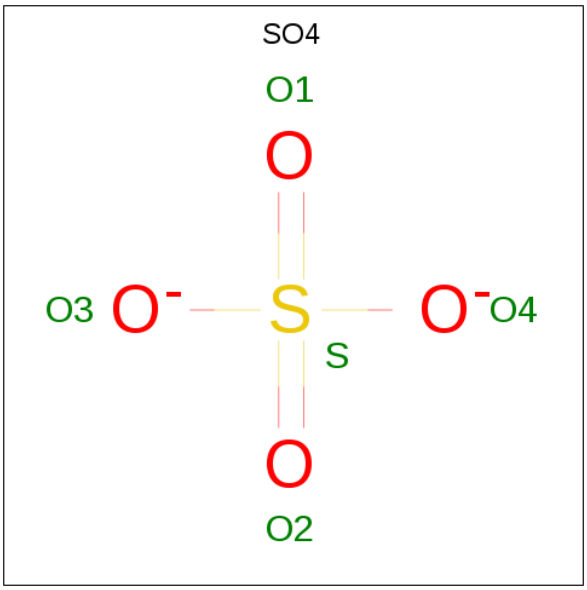
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

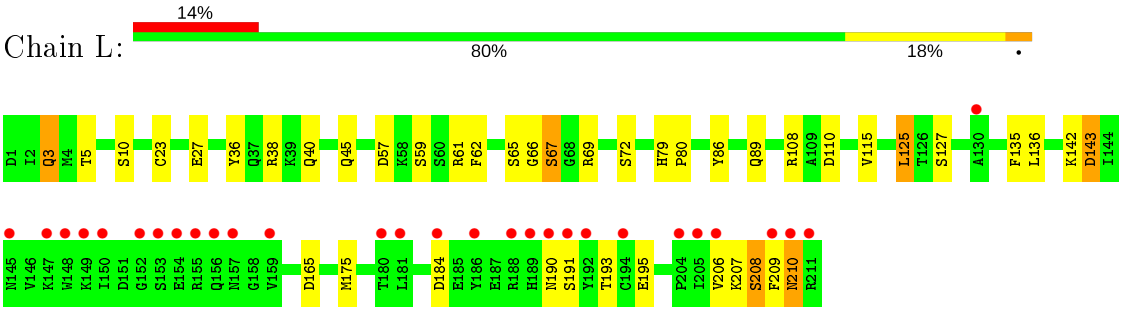
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	158	Total O 158 158	0	0
5	H	201	Total O 201 201	0	0

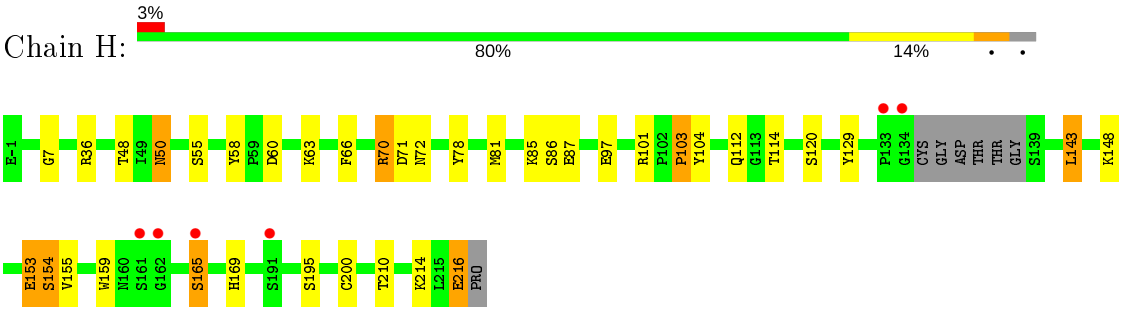
3 Residue-property plots (i)

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: Light chain of the anti-human Robo1 antibody B5209B Fab



- Molecule 2: Heavy chain of the anti-human Robo1 antibody B5209B Fab



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.43Å 83.95Å 129.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 41.97 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.50) 98.7 (41.97-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.129 , 0.165 0.131 , 0.167	Depositor DCC
R_{free} test set	3752 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3686	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: GOL, 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	1.56	16/1682 (1.0%)	1.37	21/2283 (0.9%)
2	H	1.58	12/1681 (0.7%)	1.36	16/2295 (0.7%)
All	All	1.57	28/3363 (0.8%)	1.36	37/4578 (0.8%)

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
2	H	2	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	153	GLU	CD-OE1	13.51	1.40	1.25
1	L	67[A]	SER	C-O	10.85	1.44	1.23
1	L	67[B]	SER	C-O	10.85	1.44	1.23
1	L	67[A]	SER	N-CA	-10.73	1.24	1.46
1	L	67[B]	SER	N-CA	-10.73	1.24	1.46
1	L	23	CYS	CB-SG	-10.42	1.64	1.82
2	H	120	SER	CB-OG	9.69	1.54	1.42
2	H	154[A]	SER	CB-OG	8.75	1.53	1.42
2	H	154[B]	SER	CB-OG	8.75	1.53	1.42
2	H	87	GLU	CG-CD	7.34	1.62	1.51
2	H	87	GLU	CB-CG	-6.65	1.39	1.52
1	L	65	SER	CB-OG	-6.57	1.33	1.42
1	L	27	GLU	CG-CD	6.47	1.61	1.51
1	L	10	SER	CB-OG	-6.31	1.34	1.42
2	H	86	SER	CB-OG	-6.30	1.34	1.42
1	L	143	ASP	CG-OD1	6.17	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	135	PHE	CG-CD2	-6.06	1.29	1.38
1	L	45	GLN	CG-CD	6.06	1.65	1.51
1	L	57	ASP	CB-CG	6.03	1.64	1.51
2	H	103	PRO	N-CA	-5.97	1.37	1.47
2	H	129	TYR	CE1-CZ	-5.96	1.30	1.38
2	H	87	GLU	CD-OE2	5.94	1.32	1.25
1	L	72	SER	CA-CB	5.93	1.61	1.52
1	L	143	ASP	CB-CG	5.71	1.63	1.51
2	H	78	TYR	CG-CD2	5.50	1.46	1.39
2	H	148	LYS	CE-NZ	-5.34	1.35	1.49
1	L	209	PHE	CG-CD2	-5.10	1.31	1.38
1	L	5	THR	CB-CG2	-5.05	1.35	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	101	ARG	NE-CZ-NH1	-14.14	113.23	120.30
2	H	81	MET	CG-SD-CE	-12.82	79.69	100.20
1	L	69	ARG	NE-CZ-NH1	-12.06	114.27	120.30
1	L	108	ARG	NE-CZ-NH2	-8.76	115.92	120.30
2	H	153	GLU	CG-CD-OE2	-8.53	101.24	118.30
2	H	101	ARG	CG-CD-NE	-8.24	94.49	111.80
2	H	216	GLU	CA-C-O	-8.14	103.00	120.10
1	L	67[A]	SER	CA-C-N	-7.91	100.38	116.20
1	L	67[B]	SER	CA-C-N	-7.91	100.38	116.20
2	H	36	ARG	NE-CZ-NH1	-7.83	116.38	120.30
1	L	57	ASP	CB-CG-OD1	7.64	125.17	118.30
2	H	153	GLU	OE1-CD-OE2	7.46	132.25	123.30
1	L	67[A]	SER	CA-C-O	6.91	134.60	120.10
1	L	67[B]	SER	CA-C-O	6.91	134.60	120.10
1	L	143	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	L	125	LEU	CB-CG-CD1	6.71	122.41	111.00
1	L	69	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	L	86	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	L	66	GLY	O-C-N	6.52	133.13	122.70
1	L	108	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	L	66	GLY	CA-C-N	-6.45	103.02	117.20
1	L	57	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	L	36	TYR	CG-CD2-CE2	6.09	126.17	121.30
2	H	71	ASP	CB-CG-OD1	5.93	123.64	118.30
2	H	60	ASP	CB-CG-OD1	5.83	123.55	118.30
1	L	62	PHE	CB-CG-CD1	5.82	124.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	67[A]	SER	N-CA-C	-5.66	95.72	111.00
1	L	67[B]	SER	N-CA-C	-5.66	95.72	111.00
2	H	70	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	L	175	MET	CG-SD-CE	-5.59	91.26	100.20
1	L	110	ASP	CB-CG-OD2	5.46	123.21	118.30
2	H	153	GLU	CB-CA-C	-5.39	99.61	110.40
2	H	66	PHE	CB-CG-CD1	5.13	124.39	120.80
2	H	58	TYR	CG-CD2-CE2	5.10	125.38	121.30
2	H	101	ARG	CD-NE-CZ	5.08	130.71	123.60
2	H	85	LYS	CD-CE-NZ	-5.07	100.05	111.70
2	H	143	LEU	CB-CG-CD2	-5.03	102.45	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	48	THR	CB
2	H	114	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	103	PRO	Mainchain

5.2 Too-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 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	1648	0	1581	16	0
2	H	1638	0	1591	15	0
3	H	18	0	24	0	0
3	L	18	0	24	6	0
4	H	5	0	0	0	0
5	H	201	0	0	3	1
5	L	158	0	0	7	1
All	All	3686	0	3220	31	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 5.

All (31) 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:H:210:THR:HG23	5:H:542:HOH:O	1.67	0.94
2:H:48:THR:HG23	2:H:97:GLU:OE2	1.75	0.87
2:H:114:THR:HG23	5:H:410:HOH:O	1.74	0.87
1:L:40:GLN:HG3	3:L:303:GOL:H2	1.60	0.83
2:H:70:ARG:HE	2:H:72:ASN:HD21	1.36	0.72
1:L:80:PRO:O	5:L:401:HOH:O	2.12	0.68
2:H:7:GLY:H	2:H:114:THR:HG21	1.68	0.59
5:L:517:HOH:O	2:H:169:HIS:HD2	1.85	0.58
2:H:70:ARG:NE	2:H:72:ASN:HD21	2.02	0.57
2:H:48:THR:CG2	2:H:97:GLU:OE2	2.50	0.54
1:L:79:HIS:HD2	5:L:471:HOH:O	1.90	0.53
2:H:50:ASN:HD22	2:H:50:ASN:H	1.59	0.50
2:H:104[B]:TYR:CD2	2:H:104[B]:TYR:C	2.85	0.50
2:H:7:GLY:HA3	2:H:114:THR:HG22	1.95	0.49
1:L:59:SER:OG	3:L:302:GOL:H11	2.12	0.49
2:H:63:LYS:HE3	5:H:586:HOH:O	2.14	0.48
2:H:50:ASN:ND2	2:H:55:SER:H	2.12	0.47
1:L:195:GLU:HG2	1:L:206:VAL:HG12	1.95	0.47
1:L:190:ASN:O	1:L:210:ASN:HA	2.14	0.47
2:H:159:TRP:CZ3	2:H:200:CYS:HB3	2.51	0.46
1:L:115:VAL:HG22	1:L:136:LEU:HD22	1.98	0.46
1:L:38:ARG:HH12	3:L:303:GOL:H12	1.83	0.44
1:L:165:ASP:OD2	3:L:303:GOL:H32	2.19	0.43
1:L:193:THR:HG23	1:L:208:SER:OG	2.18	0.43
1:L:67[B]:SER:HA	5:L:506:HOH:O	2.18	0.43
1:L:89:GLN:NE2	5:L:407:HOH:O	2.50	0.43
1:L:3:GLN:NE2	5:L:403:HOH:O	2.27	0.43
1:L:38:ARG:HH12	3:L:303:GOL:C1	2.33	0.41
1:L:79:HIS:HE1	5:L:543:HOH:O	2.04	0.41
2:H:50:ASN:HD22	2:H:50:ASN:N	2.18	0.41
1:L:61:ARG:HE	3:L:302:GOL:H2	1.87	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)
5:L:414:HOH:O	5:H:486:HOH:O[4_545]	1.88	0.32

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	L	213/211 (101%)	207 (97%)	6 (3%)	0	100 100
2	H	215/221 (97%)	207 (96%)	7 (3%)	1 (0%)	29 9
All	All	428/432 (99%)	414 (97%)	13 (3%)	1 (0%)	47 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	165	SER

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	L	189/185 (102%)	179 (95%)	10 (5%)	22 3
2	H	190/190 (100%)	179 (94%)	11 (6%)	20 2
All	All	379/375 (101%)	358 (94%)	21 (6%)	22 3

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	125	LEU
1	L	127	SER
1	L	142	LYS
1	L	143	ASP

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Mol	Chain	Res	Type
1	L	184	ASP
1	L	191	SER
1	L	207	LYS
1	L	208	SER
1	L	210	ASN
2	H	50	ASN
2	H	112	GLN
2	H	143	LEU
2	H	153	GLU
2	H	154[A]	SER
2	H	154[B]	SER
2	H	155	VAL
2	H	165	SER
2	H	195	SER
2	H	214	LYS
2	H	216	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	3	GLN
1	L	37	GLN
1	L	70	GLN
1	L	79	HIS
1	L	89	GLN
2	H	50	ASN
2	H	72	ASN
2	H	169	HIS

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 (i)

7 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	GOL	H	303	-	5,5,5	0.57	0	5,5,5	1.16	0
3	GOL	L	303	-	5,5,5	0.76	0	5,5,5	1.52	1 (20%)
3	GOL	H	301	-	5,5,5	0.99	0	5,5,5	0.68	0
3	GOL	L	301	-	5,5,5	0.94	0	5,5,5	1.41	1 (20%)
4	SO4	H	304	-	4,4,4	0.62	0	6,6,6	0.67	0
3	GOL	H	302	-	5,5,5	0.43	0	5,5,5	0.81	0
3	GOL	L	302	-	5,5,5	0.99	0	5,5,5	1.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	H	303	-	-	0/4/4/4	-
3	GOL	L	303	-	-	3/4/4/4	-
3	GOL	H	301	-	-	0/4/4/4	-
3	GOL	L	301	-	-	0/4/4/4	-
3	GOL	H	302	-	-	0/4/4/4	-
3	GOL	L	302	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	303	GOL	O3-C3-C2	2.58	122.57	110.20
3	L	301	GOL	O2-C2-C3	2.18	118.74	109.12

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	302	GOL	C1-C2-C3-O3
3	L	302	GOL	O2-C2-C3-O3
3	L	303	GOL	C1-C2-C3-O3
3	L	303	GOL	O2-C2-C3-O3
3	L	303	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	303	GOL	4	0
3	L	302	GOL	2	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, 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	L	211/211 (100%)	0.24	29 (13%) 3 3	13, 25, 61, 70	0
2	H	214/221 (96%)	-0.13	6 (2%) 53 57	13, 21, 60, 73	0
All	All	425/432 (98%)	0.05	35 (8%) 11 12	13, 23, 60, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	184	ASP	5.1
1	L	157	ASN	5.1
1	L	150	ILE	5.0
1	L	209	PHE	4.9
2	H	134	GLY	4.8
2	H	162	GLY	4.7
1	L	186	TYR	4.6
1	L	188	ARG	4.3
2	H	161	SER	4.1
1	L	181	LEU	3.6
1	L	210	ASN	3.6
1	L	205	ILE	3.5
1	L	156	GLN	3.5
1	L	192	TYR	3.3
1	L	155	ARG	2.9
1	L	153	SER	2.9
1	L	189	HIS	2.8
1	L	159	VAL	2.7
1	L	154	GLU	2.7
1	L	180	THR	2.7
1	L	145	ASN	2.6
1	L	190	ASN	2.6
1	L	204	PRO	2.3
1	L	191	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	130	ALA	2.3
2	H	165	SER	2.2
1	L	149	LYS	2.2
1	L	194[A]	CYS	2.1
1	L	147	LYS	2.1
2	H	133	PRO	2.1
1	L	148	TRP	2.1
2	H	191	SER	2.1
1	L	211	ARG	2.0
1	L	152	GLY	2.0
1	L	206	VAL	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
3	GOL	H	303	6/6	0.84	0.15	33,34,37,37	0
3	GOL	L	303	6/6	0.84	0.13	40,43,48,80	0
3	GOL	H	302	6/6	0.89	0.11	40,49,51,55	0
3	GOL	L	302	6/6	0.92	0.08	41,48,58,62	0
3	GOL	L	301	6/6	0.96	0.08	30,35,39,41	0
3	GOL	H	301	6/6	0.99	0.06	23,23,25,30	0
4	SO4	H	304	5/5	0.99	0.07	20,20,22,25	0

6.5 Other polymers (i)

There are no such residues in this entry.