Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2023 – 02:27 PM EDT

PDB ID	:	8CWK
Title	:	Fab arm of antibodies 4G1-C2 and 10G4 bound to CoV-2 receptor binding domain (RBD)
Authors	:	Langley, D.B.; Christ, D.
Deposited on	:	2022-05-19
Resolution	:	2.37 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

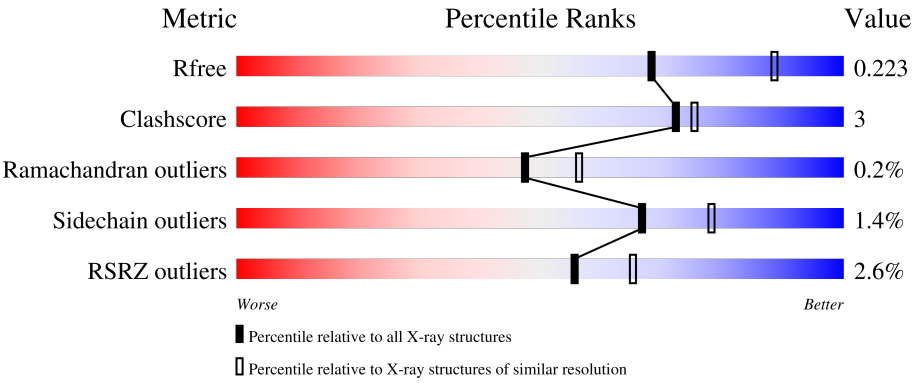
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.37 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 of 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	H	228	86% 9% ·
2	L	215	2% 91% 7% ·
3	A	232	3% 89% 7% ·
4	B	215	% 90% 9% ·
5	C	204	6% 83% 15% ·

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8339 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 of Fab arm of antibody 10G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	218	1625	1026	275	318	6	0	0	0

- Molecule 2 is a protein called Light chain of Fab arm of antibody 10G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	213	1634	1023	276	329	6	0	1	0

- Molecule 3 is a protein called Heavy chain of Fab arm of antibody 4G1-C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	223	1659	1043	276	334	6	0	1	0

- Molecule 4 is a protein called Light chain of Fab arm of antibody 4G1-C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	213	1636	1026	273	332	5	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	TYR	ASN	conflict	UNP Q6GMX0
B	30	TYR	ASN	conflict	UNP Q6GMX0
B	31	ASP	ASN	conflict	UNP Q6GMX0
B	32	ASP	TYR	conflict	UNP Q6GMX0
B	38	GLN	LEU	conflict	UNP Q6GMX0
B	45	LYS	ASN	conflict	UNP Q6GMX0
B	50	SER	ALA	conflict	UNP Q6GMX0
B	79	GLN	ARG	conflict	UNP Q6GMX0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	81	GLU	ASP	conflict	UNP Q6GMX0
B	91	ALA	SER	conflict	UNP Q6GMX0
B	92	TRP	TYR	conflict	UNP Q6GMX0
B	93	PRO	ASN	conflict	UNP Q6GMX0
B	94	TYR	ILE	conflict	UNP Q6GMX0
B	100	GLN	GLY	conflict	UNP Q6GMX0
B	103	LYS	ASN	conflict	UNP Q6GMX0
B	215	SER	-	expression tag	UNP Q6GMX0

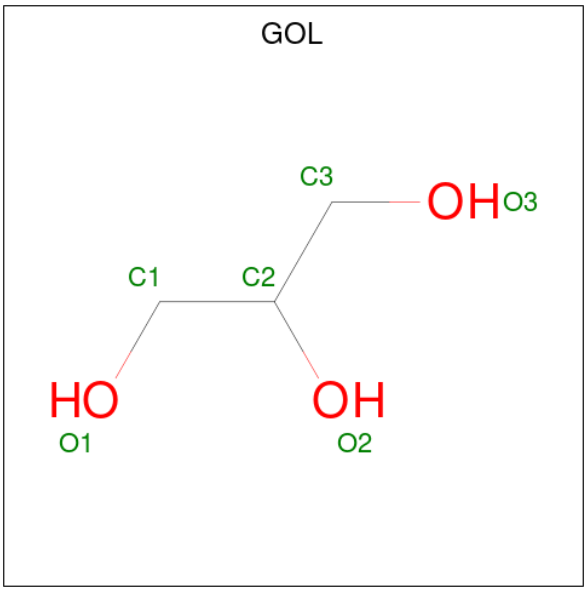
- Molecule 5 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1544	990	258	288	8			

There are 8 discrepancies between the modelled and reference sequences:

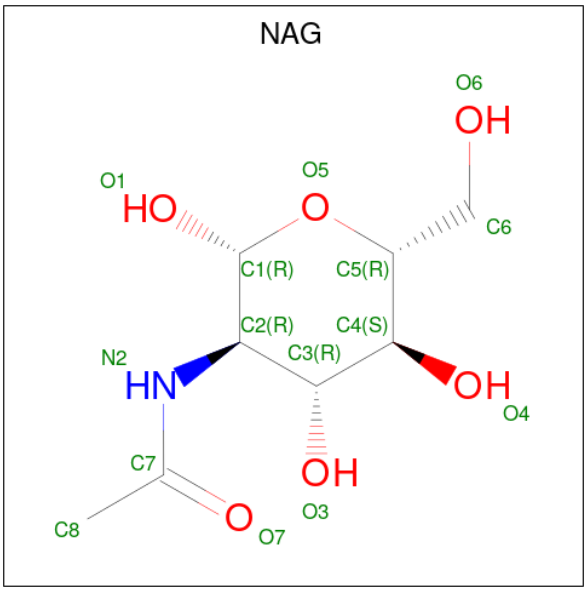
Chain	Residue	Modelled	Actual	Comment	Reference
C	529	GLY	-	expression tag	UNP P0DTC2
C	530	SER	-	expression tag	UNP P0DTC2
C	531	HIS	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
C	536	HIS	-	expression tag	UNP P0DTC2

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0

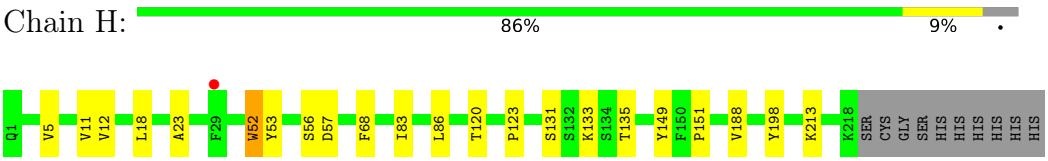
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	16	Total O 16 16	0	0
8	L	32	Total O 32 32	0	0
8	A	54	Total O 54 54	0	0
8	B	39	Total O 39 39	0	0
8	C	36	Total O 36 36	0	0

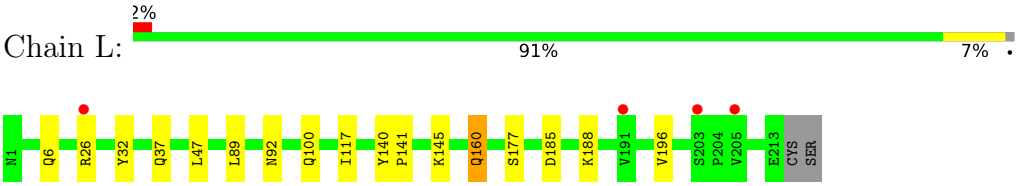
3 Residue-property plots (i)

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.

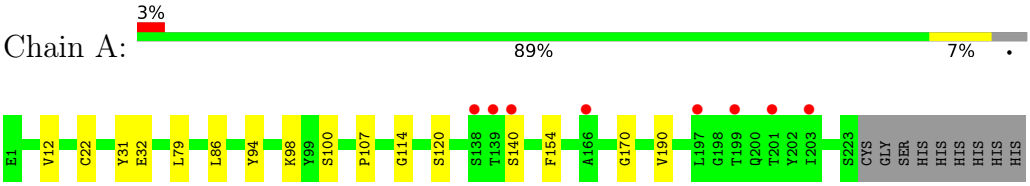
• Molecule 1: Heavy chain of Fab arm of antibody 10G4



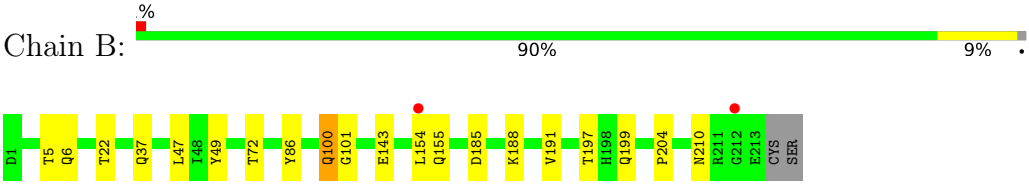
• Molecule 2: Light chain of Fab arm of antibody 10G4



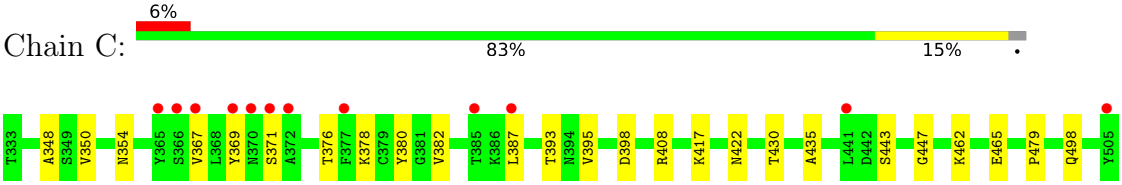
• Molecule 3: Heavy chain of Fab arm of antibody 4G1-C2

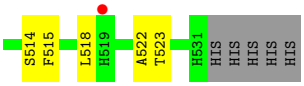


• Molecule 4: Light chain of Fab arm of antibody 4G1-C2



• Molecule 5: Spike protein S1




S514
F515
L518
H519
A522
T523
H531
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	133.16Å 99.34Å 124.96Å 90.00° 108.63° 90.00°	Depositor
Resolution (Å)	43.23 – 2.37 45.80 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.23-2.37) 99.2 (45.80-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.186 , 0.223 0.186 , 0.223	Depositor DCC
R_{free} test set	3116 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8339	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: NAG, GOL

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	H	0.32	0/1666	0.54	0/2273
2	L	0.36	0/1671	0.54	0/2274
3	A	0.35	0/1701	0.55	0/2321
4	B	0.35	0/1674	0.56	0/2281
5	C	0.32	0/1589	0.50	0/2167
All	All	0.34	0/8301	0.54	0/11316

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	H	1625	0	1564	13	0
2	L	1634	0	1560	8	0
3	A	1659	0	1574	10	0
4	B	1636	0	1556	13	0
5	C	1544	0	1432	13	0
6	A	6	0	8	3	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	6	0	8	0	0
6	L	12	0	16	0	0
7	C	14	0	13	0	0
7	L	14	0	13	0	0
8	A	54	0	0	0	0
8	B	39	0	0	2	0
8	C	36	0	0	0	0
8	H	16	0	0	0	0
8	L	32	0	0	0	0
All	All	8339	0	7760	54	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 3.

All (54) 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)
4:B:199:GLN:OE1	8:B:401:HOH:O	2.07	0.72
4:B:6:GLN:H	4:B:100:GLN:HE21	1.41	0.69
4:B:6:GLN:H	4:B:100:GLN:NE2	1.93	0.67
4:B:37:GLN:HB2	4:B:47:LEU:HD11	1.78	0.65
4:B:22:THR:HG22	4:B:72:THR:HG22	1.79	0.65
1:H:11:VAL:HG22	1:H:151:PRO:HG3	1.79	0.64
6:A:301:GOL:H32	5:C:348:ALA:HB2	1.80	0.64
3:A:31:TYR:HD1	6:A:301:GOL:H31	1.65	0.61
3:A:12:VAL:HG11	3:A:86:LEU:HD13	1.82	0.60
2:L:32:TYR:HD2	2:L:92:ASN:HD22	1.48	0.59
4:B:143:GLU:O	8:B:401:HOH:O	2.17	0.58
2:L:185:ASP:HA	2:L:188:LYS:HD3	1.86	0.57
2:L:6:GLN:O	2:L:100:GLN:NE2	2.38	0.57
4:B:197:THR:HG22	4:B:204:PRO:HB3	1.87	0.57
5:C:367:VAL:O	5:C:371:SER:HB3	2.06	0.56
1:H:68:PHE:CE1	1:H:83:ILE:HG23	2.41	0.56
4:B:185:ASP:HA	4:B:188:LYS:HE2	1.90	0.54
1:H:131:SER:O	1:H:135:THR:HG23	2.09	0.52
5:C:350:VAL:HG22	5:C:422:ASN:HB3	1.94	0.50
1:H:52:TRP:CD2	1:H:57:ASP:HB2	2.46	0.50
3:A:107:PRO:HG3	4:B:49:TYR:HB3	1.94	0.50
3:A:22:CYS:HB3	3:A:79:LEU:HB3	1.93	0.49
3:A:94:TYR:O	3:A:114:GLY:HA2	2.13	0.49
5:C:518:LEU:HD21	5:C:522:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:380:TYR:O	5:C:430:THR:HA	2.13	0.49
3:A:31:TYR:CD1	6:A:301:GOL:H31	2.48	0.48
2:L:160:GLN:O	2:L:177:SER:HA	2.13	0.48
5:C:447:GLY:HA2	5:C:498:GLN:HG2	1.96	0.48
1:H:53:TYR:CD1	5:C:479:PRO:HD3	2.49	0.47
3:A:170:GLY:O	3:A:190:VAL:HA	2.14	0.47
5:C:354:ASN:O	5:C:398:ASP:HA	2.14	0.47
5:C:382:VAL:HG21	5:C:387:LEU:HD21	1.96	0.47
3:A:32:GLU:HG3	3:A:98:LYS:HD2	1.98	0.46
3:A:100:SER:OG	3:A:107:PRO:HD2	2.16	0.46
1:H:5:VAL:HG23	1:H:23:ALA:HB3	1.98	0.45
1:H:123:PRO:HB3	1:H:149:TYR:HB3	1.99	0.45
5:C:462:LYS:HB2	5:C:465:GLU:OE1	2.17	0.45
1:H:18:LEU:HD12	1:H:18:LEU:HA	1.74	0.45
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.98	0.44
4:B:191:VAL:HG22	4:B:210:ASN:OD1	2.18	0.44
4:B:154:LEU:HD12	4:B:155:GLN:N	2.32	0.43
2:L:140:TYR:CG	2:L:141:PRO:HA	2.53	0.43
4:B:5:THR:HA	4:B:100:GLN:HE22	1.83	0.43
1:H:12:VAL:HG11	1:H:18:LEU:HD22	2.01	0.43
1:H:11:VAL:HG21	1:H:120:THR:HG22	2.00	0.42
2:L:145:LYS:O	2:L:196:VAL:HA	2.18	0.42
4:B:86:TYR:O	4:B:101:GLY:HA2	2.19	0.42
3:A:120:SER:HB3	3:A:154:PHE:HZ	1.84	0.42
1:H:133:LYS:HB3	2:L:117:ILE:HG22	2.02	0.42
5:C:376:THR:HB	5:C:435:ALA:HB3	2.01	0.42
1:H:12:VAL:HG21	1:H:86:LEU:HD13	2.01	0.41
5:C:395:VAL:HA	5:C:514:SER:O	2.20	0.41
5:C:393:THR:HA	5:C:523:THR:OG1	2.21	0.41
1:H:188:VAL:HG11	1:H:198:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

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	H	216/228 (95%)	213 (99%)	2 (1%)	1 (0%)	29 32
2	L	212/215 (99%)	203 (96%)	9 (4%)	0	100 100
3	A	222/232 (96%)	214 (96%)	7 (3%)	1 (0%)	29 32
4	B	212/215 (99%)	204 (96%)	8 (4%)	0	100 100
5	C	197/204 (97%)	189 (96%)	8 (4%)	0	100 100
All	All	1059/1094 (97%)	1023 (97%)	34 (3%)	2 (0%)	47 56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	56	SER
3	A	140	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	H	177/190 (93%)	175 (99%)	2 (1%)	73 84
2	L	183/189 (97%)	180 (98%)	3 (2%)	62 75
3	A	183/195 (94%)	183 (100%)	0	100 100
4	B	183/190 (96%)	182 (100%)	1 (0%)	88 94
5	C	163/176 (93%)	157 (96%)	6 (4%)	34 42
All	All	889/940 (95%)	877 (99%)	12 (1%)	67 80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	52	TRP
1	H	213	LYS
2	L	26	ARG

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Mol	Chain	Res	Type
2	L	89	LEU
2	L	160	GLN
4	B	100	GLN
5	C	369	TYR
5	C	378	LYS
5	C	408	ARG
5	C	417	LYS
5	C	443	SER
5	C	515	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	203	ASN
3	A	113	GLN
4	B	100	GLN
5	C	334	ASN
5	C	531	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
6	GOL	H	301	-	5,5,5	0.37	0	5,5,5	0.27	0
6	GOL	C	602	-	5,5,5	0.39	0	5,5,5	0.34	0
7	NAG	C	601	5	14,14,15	0.70	1 (7%)	17,19,21	0.81	1 (5%)
7	NAG	L	301	2	14,14,15	0.62	0	17,19,21	0.47	0
6	GOL	A	301	-	5,5,5	0.41	0	5,5,5	0.37	0
6	GOL	L	302	-	5,5,5	0.41	0	5,5,5	0.51	0
6	GOL	B	300	-	5,5,5	0.36	0	5,5,5	0.32	0
6	GOL	L	303	-	5,5,5	0.32	0	5,5,5	0.56	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
6	GOL	H	301	-	-	0/4/4/4	-
6	GOL	C	602	-	-	0/4/4/4	-
7	NAG	C	601	5	-	0/6/23/26	0/1/1/1
7	NAG	L	301	2	-	2/6/23/26	0/1/1/1
6	GOL	A	301	-	-	4/4/4/4	-
6	GOL	L	302	-	-	0/4/4/4	-
6	GOL	B	300	-	-	2/4/4/4	-
6	GOL	L	303	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	601	NAG	O5-C1	2.45	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	601	NAG	C1-O5-C5	2.94	116.18	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	303	GOL	C1-C2-C3-O3
6	A	301	GOL	C1-C2-C3-O3
6	B	300	GOL	O1-C1-C2-C3
7	L	301	NAG	O5-C5-C6-O6
7	L	301	NAG	C4-C5-C6-O6
6	A	301	GOL	O1-C1-C2-C3
6	L	303	GOL	O2-C2-C3-O3
6	B	300	GOL	O1-C1-C2-O2
6	A	301	GOL	O2-C2-C3-O3
6	A	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	GOL	3	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	H	218/228 (95%)	0.33	1 (0%)	91	95	42, 58, 83, 95	0
2	L	213/215 (99%)	0.38	4 (1%)	66	76	37, 54, 78, 95	0
3	A	223/232 (96%)	0.45	8 (3%)	42	55	34, 55, 91, 128	0
4	B	213/215 (99%)	0.28	2 (0%)	84	90	37, 52, 76, 91	0
5	C	199/204 (97%)	0.58	13 (6%)	18	27	40, 63, 98, 135	0
All	All	1066/1094 (97%)	0.40	28 (2%)	56	65	34, 56, 85, 135	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	C	372	ALA	7.9
5	C	369	TYR	6.2
5	C	371	SER	5.5
5	C	370	ASN	5.1
3	A	140	SER	4.1
3	A	139	THR	3.8
3	A	166	ALA	3.4
3	A	138	SER	3.3
5	C	377	PHE	3.0
5	C	385	THR	3.0
4	B	212	GLY	3.0
3	A	197	LEU	2.9
5	C	505	TYR	2.8
3	A	199	THR	2.7
5	C	365	TYR	2.5
5	C	367	VAL	2.4
2	L	203	SER	2.4
4	B	154	LEU	2.4
2	L	26	ARG	2.4
1	H	29	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	191	VAL	2.3
2	L	205	VAL	2.3
5	C	366	SER	2.2
5	C	519	HIS	2.1
3	A	201	THR	2.1
5	C	441	LEU	2.0
3	A	203	ILE	2.0
5	C	387	LEU	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
6	GOL	H	301	6/6	0.71	0.36	91,96,97,97	0
7	NAG	C	601	14/15	0.76	0.17	81,97,104,106	0
7	NAG	L	301	14/15	0.84	0.20	89,97,104,107	0
6	GOL	C	602	6/6	0.86	0.28	92,93,93,94	0
6	GOL	L	303	6/6	0.86	0.19	75,79,80,81	0
6	GOL	A	301	6/6	0.86	0.34	76,78,80,80	0
6	GOL	B	300	6/6	0.90	0.21	64,73,74,75	0
6	GOL	L	302	6/6	0.94	0.24	53,66,67,68	0

6.5 Other polymers (i)

There are no such residues in this entry.