



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2023 – 12:08 PM EDT

PDB ID : 8EL2
Title : SARS-CoV-2 RBD bound to neutralizing antibody Fab ICO-hu23
Authors : Besaw, J.E.; Kuo, A.; Morizumi, T.; Ernst, O.P.
Deposited on : 2022-09-22
Resolution : 2.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.35
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) : 2.35

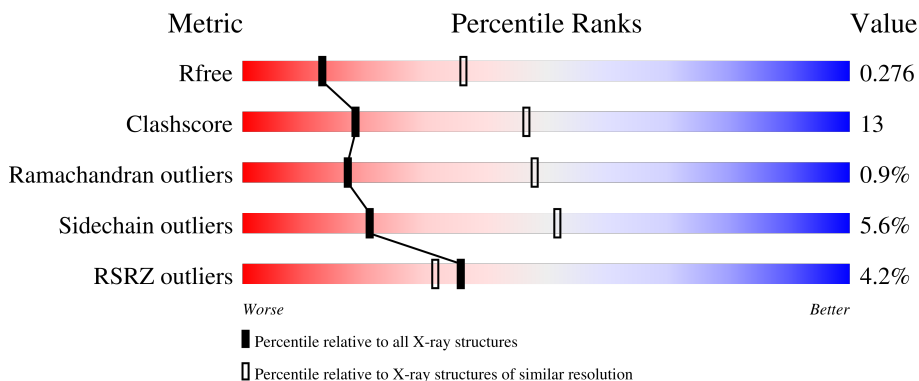
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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.



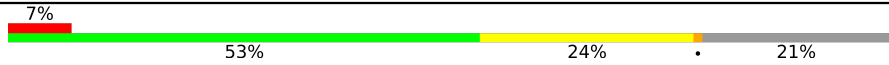
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. 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	H	234	 70% 22% 6%
1	I	234	 73% 19% 6%
2	K	216	 72% 25% ..
2	L	216	 72% 25% ..
3	A	231	 58% 20% .. 16%

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Mol	Chain	Length	Quality of chain
3	B	231	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (7%), a large green segment (53%), a yellow segment (24%), and a grey segment (16%). The percentages are labeled below the bar.</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9548 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 Fab ICO-hu23 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	219	Total 1670	C 1066	N 277	O 319	S 8	0	0	0
1	I	219	Total 1672	C 1067	N 278	O 319	S 8	0	0	0

- Molecule 2 is a protein called Fab ICO-hu23 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	213	Total 1580	C 987	N 260	O 328	S 5	0	0	0
2	K	213	Total 1573	C 984	N 256	O 328	S 5	0	0	0

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	194	Total 1545	C 990	N 257	O 290	S 8	6	2	0
3	B	183	Total 1466	C 942	N 241	O 275	S 8	6	2	0

There are 16 discrepancies between the modelled and reference sequences:

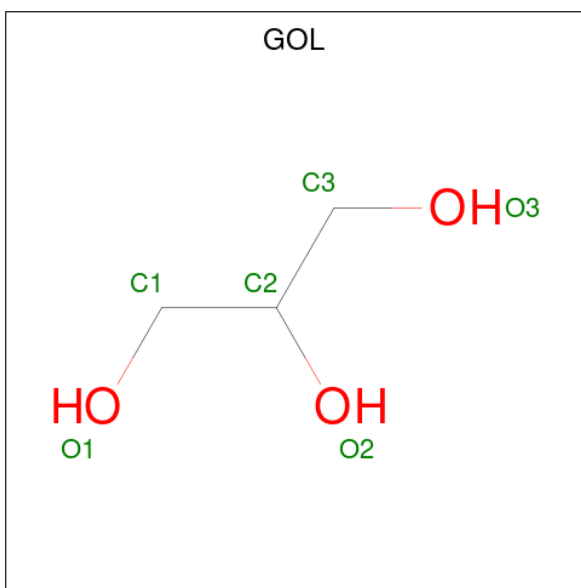
Chain	Residue	Modelled	Actual	Comment	Reference
A	317	ALA	-	expression tag	UNP P0DTC2
A	318	SER	-	expression tag	UNP P0DTC2
A	542	HIS	-	expression tag	UNP P0DTC2
A	543	HIS	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	317	ALA	-	expression tag	UNP P0DTC2
B	318	SER	-	expression tag	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



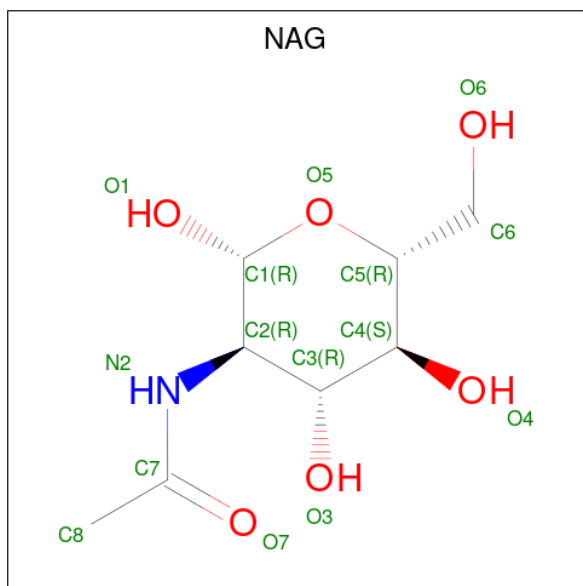
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total Zn 1 1	0	0
5	K	1	Total Zn 1 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



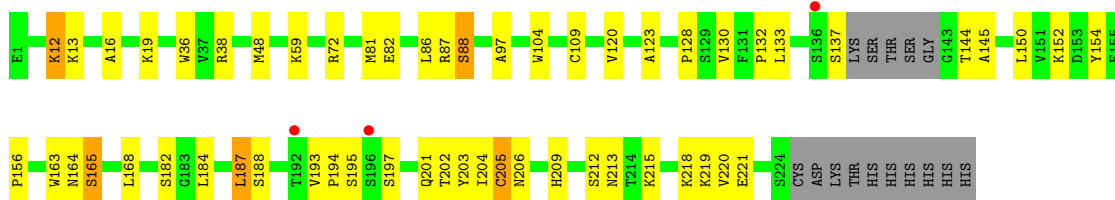
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0

3 Residue-property plots

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.

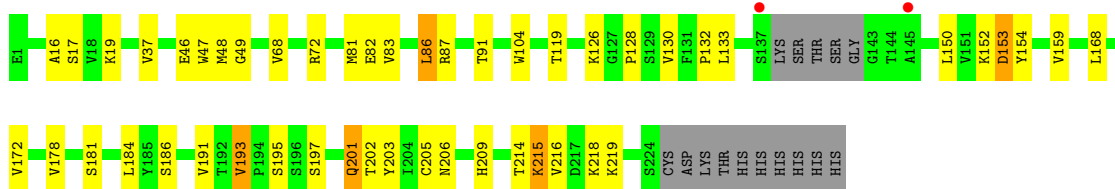
- Molecule 1: Fab ICO-hu23 Heavy Chain

Chain H: 



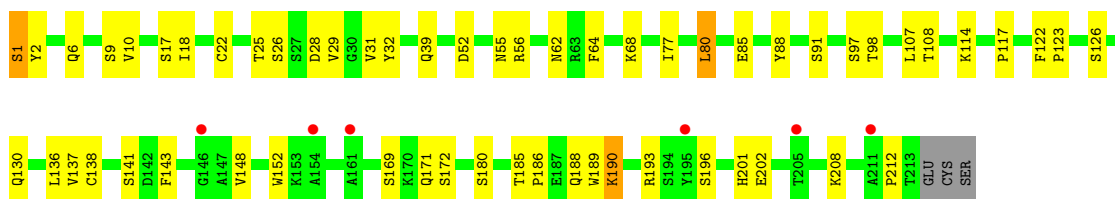
- Molecule 1: Fab ICO-hu23 Heavy Chain

Chain I: 



- Molecule 2: Fab ICO-hu23 Light Chain

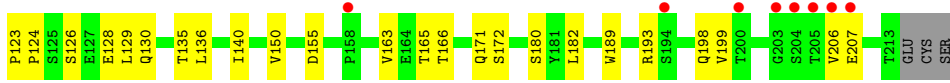
Chain L: 



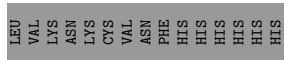
- Molecule 2: Fab ICO-hu23 Light Chain

Chain K: 

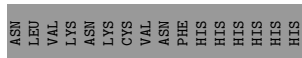
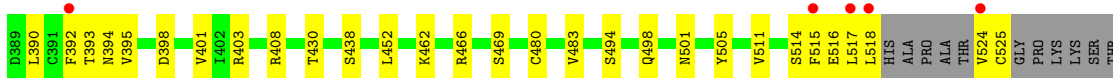
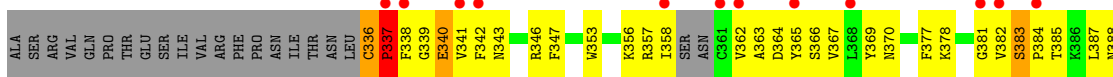




• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.30Å 140.30Å 202.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.78 – 2.89 46.78 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.78-2.89) 90.3 (46.78-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.239 , 0.281 0.235 , 0.276	Depositor DCC
R_{free} test set	2012 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	75.6	Xtrriage
Anisotropy	0.145	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9548	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GOL, NAG, ZN

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	0.41	1/1718 (0.1%)	0.55	1/2345 (0.0%)
1	I	0.34	0/1720	0.56	0/2347
2	K	0.33	0/1611	0.55	0/2202
2	L	0.32	0/1618	0.57	0/2210
3	A	0.39	0/1592	0.70	3/2167 (0.1%)
3	B	0.34	0/1508	0.61	1/2048 (0.0%)
All	All	0.36	1/9767 (0.0%)	0.59	5/13319 (0.0%)

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	A	0	1
3	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	165	SER	CB-OG	-9.84	1.29	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	335	LEU	CA-CB-CG	8.69	135.28	115.30
3	A	387	LEU	CA-CB-CG	7.99	133.67	115.30
3	B	337	PRO	N-CA-CB	-5.37	96.69	102.60
3	A	378	LYS	CD-CE-NZ	5.26	123.81	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	187	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	340	GLU	Peptide
3	B	383	SER	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	H	1670	0	1615	35	1
1	I	1672	0	1622	36	1
2	K	1573	0	1513	38	0
2	L	1580	0	1529	32	0
3	A	1545	0	1463	56	5
3	B	1466	0	1380	55	1
4	B	6	0	8	0	0
4	L	6	0	8	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	14	0	13	0	0
6	B	14	0	13	3	0
All	All	9548	0	9164	246	6

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 13.

The worst 5 of 246 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:K:155:ASP:CG	2:K:193:ARG:CD	1.79	1.46
3:B:336:CYS:HB3	3:B:337:PRO:CD	1.44	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:336:CYS:CB	3:B:337:PRO:HD3	1.61	1.26
3:A:523:THR:CG2	3:A:524:VAL:H	1.43	1.26
2:K:155:ASP:OD2	2:K:193:ARG:CG	1.86	1.22

The worst 5 of 6 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)
3:A:519:HIS:CE1	3:A:519:HIS:NE2[4_465]	1.32	0.88
3:A:519:HIS:ND1	3:A:519:HIS:CE1[4_465]	1.32	0.88
3:A:519:HIS:NE2	3:A:519:HIS:NE2[4_465]	1.50	0.70
1:I:201:GLN:OE1	3:B:378:LYS:NZ[6_554]	1.80	0.40
3:A:519:HIS:ND1	3:A:519:HIS:ND1[4_465]	1.83	0.37

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	215/234 (92%)	203 (94%)	11 (5%)	1 (0%)	29	61
1	I	215/234 (92%)	205 (95%)	8 (4%)	2 (1%)	17	48
2	K	211/216 (98%)	196 (93%)	14 (7%)	1 (0%)	29	61
2	L	211/216 (98%)	200 (95%)	10 (5%)	1 (0%)	29	61
3	A	194/231 (84%)	181 (93%)	9 (5%)	4 (2%)	7	26
3	B	179/231 (78%)	163 (91%)	14 (8%)	2 (1%)	14	42
All	All	1225/1362 (90%)	1148 (94%)	66 (5%)	11 (1%)	17	48

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	195	SER

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Mol	Chain	Res	Type
3	A	371	SER
3	A	520	ALA
3	B	337	PRO
1	I	197	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	183/198 (92%)	174 (95%)	9 (5%)	25	57
1	I	184/198 (93%)	173 (94%)	11 (6%)	19	49
2	K	179/184 (97%)	169 (94%)	10 (6%)	21	52
2	L	181/184 (98%)	170 (94%)	11 (6%)	18	48
3	A	169/203 (83%)	158 (94%)	11 (6%)	17	45
3	B	160/203 (79%)	153 (96%)	7 (4%)	28	61
All	All	1056/1170 (90%)	997 (94%)	59 (6%)	21	52

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	205	CYS
3	B	357	ARG
2	K	75	LEU
3	B	346	ARG
3	A	403	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	164	ASN
1	I	201	GLN
3	A	394	ASN
2	K	55	ASN

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Mol	Chain	Res	Type
2	L	192	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
4	GOL	L	301	-	5,5,5	0.54	0	5,5,5	0.27	0
6	NAG	A	601	3	14,14,15	0.22	0	17,19,21	0.43	0
4	GOL	B	602	-	5,5,5	0.53	0	5,5,5	0.30	0
6	NAG	B	601	-	14,14,15	0.20	0	17,19,21	0.47	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	L	301	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	601	3	-	2/6/23/26	0/1/1/1
4	GOL	B	602	-	-	0/4/4/4	-
6	NAG	B	601	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	GOL	C1-C2-C3-O3
4	L	301	GOL	O2-C2-C3-O3
6	B	601	NAG	C4-C5-C6-O6
6	B	601	NAG	O5-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	NAG	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 [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	H	219/234 (93%)	0.01	3 (1%) 75 75	57, 80, 168, 190	0
1	I	219/234 (93%)	-0.06	2 (0%) 84 84	59, 87, 149, 162	0
2	K	213/216 (98%)	0.27	9 (4%) 36 32	54, 95, 140, 155	0
2	L	213/216 (98%)	0.23	6 (2%) 53 49	53, 92, 141, 160	0
3	A	194/231 (83%)	0.41	15 (7%) 13 10	66, 103, 169, 222	0
3	B	183/231 (79%)	0.35	17 (9%) 8 6	62, 101, 168, 186	0
All	All	1241/1362 (91%)	0.19	52 (4%) 36 32	53, 95, 158, 222	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	518	LEU	6.0
3	A	515	PHE	5.7
3	A	390	LEU	5.4
3	B	338	PHE	4.7
2	K	205	THR	4.4

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, 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
4	GOL	L	301	6/6	0.62	0.23	140,140,140,140	0
4	GOL	B	602	6/6	0.73	0.14	113,113,113,113	0
5	ZN	L	302	1/1	0.82	0.19	147,147,147,147	0
6	NAG	A	601	14/15	0.83	0.14	127,132,139,144	0
6	NAG	B	601	14/15	0.86	0.19	134,148,153,156	0
5	ZN	K	301	1/1	0.95	0.16	144,144,144,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.