Full wwPDB X-ray Structure Validation Report (i)

Jan 10, 2023 – 12:11 PM JST

PDB ID	:	7XSG
Title	:	Crystal structure of ClAgl29B
Authors	:	Shishiuchi, R.; Kang, H.; Tagami, T.; Okuyama, M.
Deposited on	:	2022-05-14
Resolution	:	1.61 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 (i) 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 (1)) were used in the production of this report:

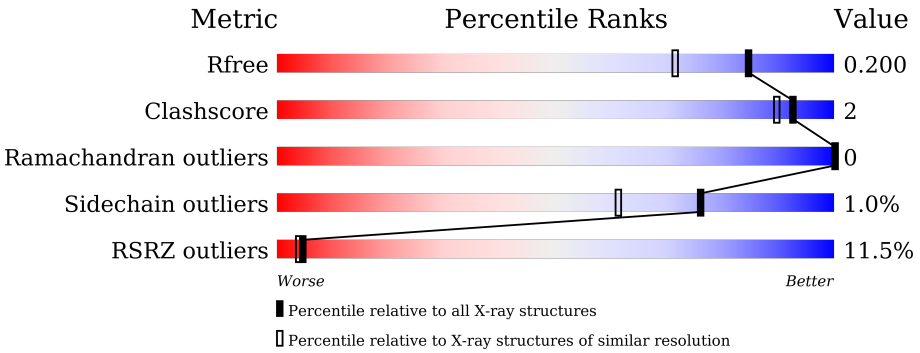
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 1.61 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	A	587	16% 87% 5% 7%
1	B	587	5% 89% · 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10033 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 Alpha-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	8	0
			4481	2882	727	855	17			
1	B	545	Total	C	N	O	S	0	12	0
			4504	2893	731	863	17			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP K1KV82
A	1	GLY	-	expression tag	UNP K1KV82
A	2	SER	-	expression tag	UNP K1KV82
A	3	SER	-	expression tag	UNP K1KV82
A	4	HIS	-	expression tag	UNP K1KV82
A	5	HIS	-	expression tag	UNP K1KV82
A	6	HIS	-	expression tag	UNP K1KV82
A	7	HIS	-	expression tag	UNP K1KV82
A	8	HIS	-	expression tag	UNP K1KV82
A	9	HIS	-	expression tag	UNP K1KV82
A	10	SER	-	expression tag	UNP K1KV82
A	11	SER	-	expression tag	UNP K1KV82
A	12	GLY	-	expression tag	UNP K1KV82
A	13	LEU	-	expression tag	UNP K1KV82
A	14	VAL	-	expression tag	UNP K1KV82
A	15	PRO	-	expression tag	UNP K1KV82
A	16	ARG	-	expression tag	UNP K1KV82
A	17	GLY	-	expression tag	UNP K1KV82
A	18	SER	-	expression tag	UNP K1KV82
A	19	HIS	-	expression tag	UNP K1KV82
A	20	MET	-	expression tag	UNP K1KV82
B	0	MET	-	initiating methionine	UNP K1KV82
B	1	GLY	-	expression tag	UNP K1KV82
B	2	SER	-	expression tag	UNP K1KV82
B	3	SER	-	expression tag	UNP K1KV82

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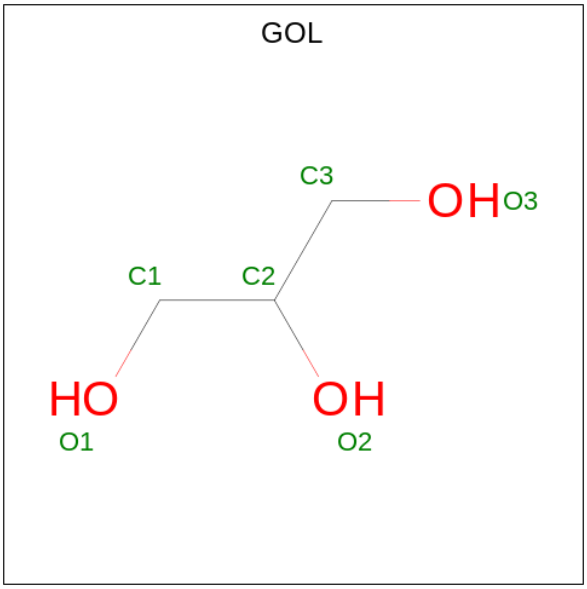
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP K1KV82
B	5	HIS	-	expression tag	UNP K1KV82
B	6	HIS	-	expression tag	UNP K1KV82
B	7	HIS	-	expression tag	UNP K1KV82
B	8	HIS	-	expression tag	UNP K1KV82
B	9	HIS	-	expression tag	UNP K1KV82
B	10	SER	-	expression tag	UNP K1KV82
B	11	SER	-	expression tag	UNP K1KV82
B	12	GLY	-	expression tag	UNP K1KV82
B	13	LEU	-	expression tag	UNP K1KV82
B	14	VAL	-	expression tag	UNP K1KV82
B	15	PRO	-	expression tag	UNP K1KV82
B	16	ARG	-	expression tag	UNP K1KV82
B	17	GLY	-	expression tag	UNP K1KV82
B	18	SER	-	expression tag	UNP K1KV82
B	19	HIS	-	expression tag	UNP K1KV82
B	20	MET	-	expression tag	UNP K1KV82

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

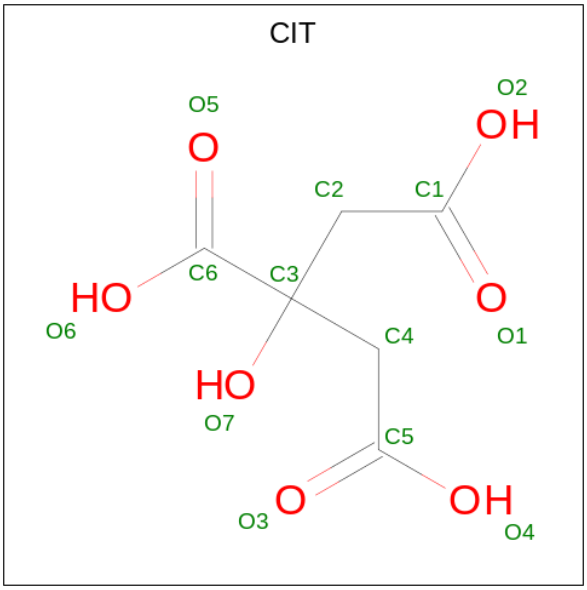
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0

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



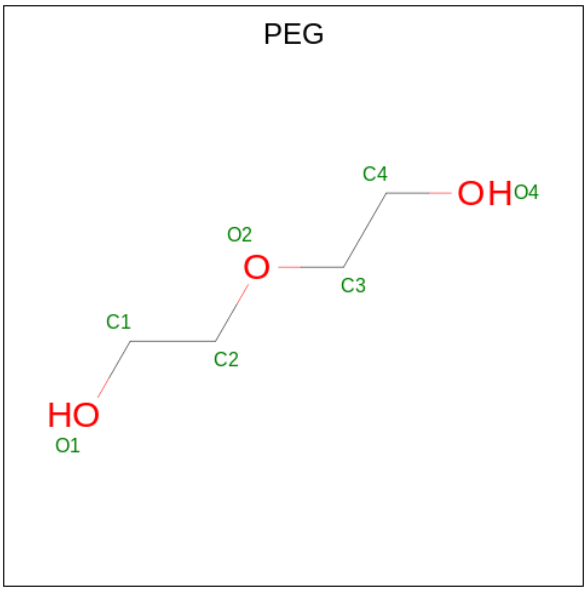
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

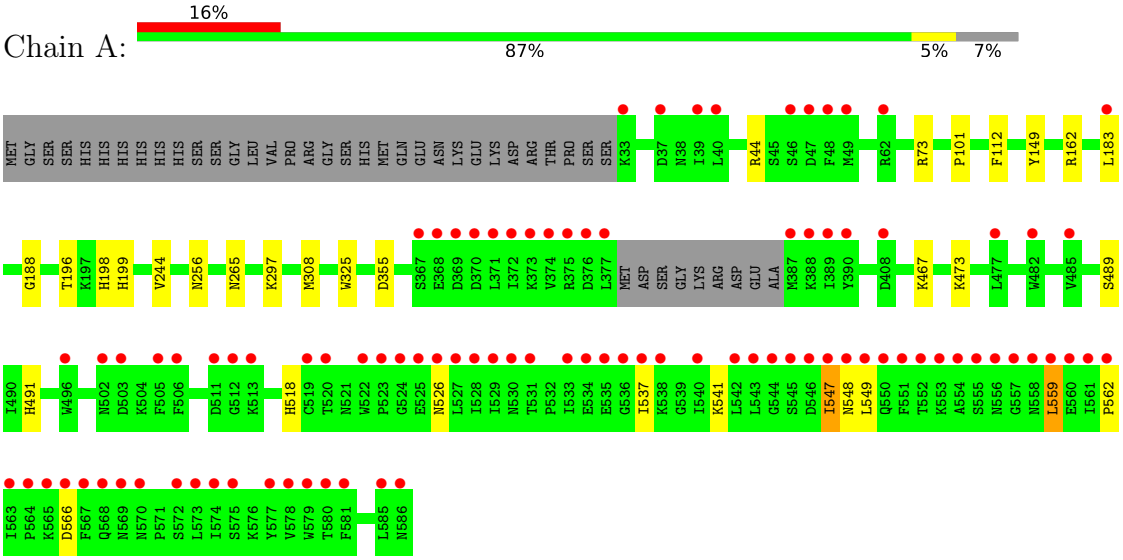
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	393	Total O 393 393	0	0
6	B	615	Total O 615 615	0	0

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.

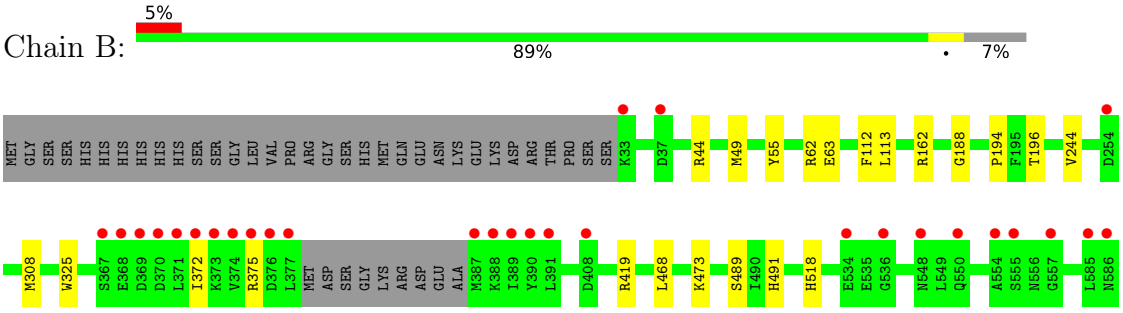
• Molecule 1: Alpha-L-fucosidase

Chain A:



• Molecule 1: Alpha-L-fucosidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.13Å 123.41Å 166.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.42 – 1.61 45.38 – 1.61	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.42-1.61) 99.5 (45.38-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.8.0349	Depositor
R, R_{free}	0.172 , 0.188 0.185 , 0.200	Depositor DCC
R_{free} test set	9719 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	14.5	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10033	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: PEG, GOL, CIT, 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	0.41	0/4604	0.71	1/6237 (0.0%)
1	B	0.45	0/4627	0.71	1/6268 (0.0%)
All	All	0.43	0/9231	0.71	2/12505 (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
1	A	0	2
1	B	0	2
All	All	0	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})
1	B	419	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	149	TYR	CB-CG-CD1	5.16	124.10	121.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162[A]	ARG	Sidechain
1	A	44	ARG	Sidechain
1	B	162[A]	ARG	Sidechain
1	B	44	ARG	Sidechain

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	4481	0	4316	16	0
1	B	4504	0	4330	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	16	1	0
3	B	6	0	8	0	0
4	A	13	0	5	0	0
5	B	7	0	10	0	0
6	A	393	0	0	2	0
6	B	615	0	0	3	0
All	All	10033	0	8685	27	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 2.

All (27) 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:256:ASN:HD21	1:A:265:ASN:H	1.19	0.86
1:A:541:LYS:HA	1:A:549:LEU:HD13	1.83	0.61
1:A:547:ILE:HD12	1:A:548:ASN:O	2.02	0.59
1:A:73:ARG:HG3	6:A:701:HOH:O	2.05	0.56
1:B:55:TYR:HE1	1:B:63:GLU:OE1	1.89	0.56
1:B:62:ARG:HD2	6:B:702:HOH:O	2.06	0.55
1:B:188:GLY:O	1:B:491:HIS:HE1	1.88	0.55
1:A:183:LEU:HD21	1:A:473[A]:LYS:HE3	1.94	0.50
1:B:372:ILE:HG23	1:B:375:ARG:HH21	1.78	0.48
1:B:244:VAL:HG13	1:B:308[B]:MET:SD	2.55	0.47
1:A:244:VAL:HG13	1:A:308[B]:MET:SD	2.54	0.47
1:A:526:ASN:HD22	1:A:562:PRO:HA	1.80	0.46
1:B:489:SER:OG	1:B:518:HIS:HE1	1.98	0.46
1:B:491:HIS:HD2	6:B:1201:HOH:O	1.97	0.46
1:A:537:ILE:HD13	1:A:559:LEU:HD21	1.98	0.45
1:A:467:LYS:HA	3:A:604:GOL:H12	1.98	0.45
1:B:55:TYR:CE1	1:B:63:GLU:OE1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HD12	1:A:549:LEU:N	2.33	0.44
1:A:549:LEU:N	1:A:549:LEU:CD1	2.81	0.43
1:B:468:LEU:O	1:B:473:LYS:HE3	2.18	0.43
1:A:489:SER:OG	1:A:518:HIS:HE1	2.02	0.42
1:A:188:GLY:O	1:A:491:HIS:HE1	2.02	0.42
1:A:101:PRO:HB3	1:A:355:ASP:HB3	2.01	0.42
1:B:62:ARG:NH1	6:B:702:HOH:O	2.46	0.41
1:A:198:HIS:CG	1:A:199:HIS:H	2.38	0.41
1:A:297:LYS:HE3	6:A:775:HOH:O	2.21	0.40
1:B:113:LEU:HB3	1:B:194:PRO:HA	2.04	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	A	549/587 (94%)	534 (97%)	15 (3%)	0	100	100
1	B	553/587 (94%)	538 (97%)	15 (3%)	0	100	100
All	All	1102/1174 (94%)	1072 (97%)	30 (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	488/517 (94%)	482 (99%)	6 (1%)	71 54
1	B	492/517 (95%)	488 (99%)	4 (1%)	81 70
All	All	980/1034 (95%)	970 (99%)	10 (1%)	76 61

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	PHE
1	A	196	THR
1	A	325	TRP
1	A	547	ILE
1	A	559	LEU
1	A	566	ASP
1	B	49	MET
1	B	112	PHE
1	B	196	THR
1	B	325	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	518	HIS
1	A	526	ASN
1	A	550	GLN
1	B	186	ASN
1	B	255	GLN
1	B	259	GLN
1	B	275	GLN
1	B	491	HIS
1	B	518	HIS
1	B	586	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	GOL	A	602	-	5,5,5	0.09	0	5,5,5	0.17	0
4	CIT	A	603	-	12,12,12	1.36	1 (8%)	17,17,17	1.41	2 (11%)
3	GOL	B	602	-	5,5,5	0.17	0	5,5,5	0.44	0
3	GOL	A	604	-	5,5,5	0.02	0	5,5,5	0.25	0
5	PEG	B	603	-	6,6,6	0.33	0	5,5,5	0.29	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	A	602	-	-	0/4/4/4	-
4	CIT	A	603	-	-	0/16/16/16	-
3	GOL	B	602	-	-	0/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
5	PEG	B	603	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	CIT	C3-C6	2.41	1.55	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	CIT	O5-C6-C3	-3.77	116.91	122.25
4	A	603	CIT	O6-C6-C3	2.62	117.59	113.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-O2
3	A	604	GOL	O2-C2-C3-O3
5	B	603	PEG	O2-C3-C4-O4
3	A	604	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	GOL	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, 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	545/587 (92%)	0.82	96 (17%) 1 1	10, 20, 51, 100	0
1	B	545/587 (92%)	0.13	29 (5%) 26 24	8, 12, 34, 67	0
All	All	1090/1174 (92%)	0.47	125 (11%) 4 4	8, 15, 47, 100	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	SER	8.5
1	A	549	LEU	7.6
1	A	522	TRP	7.5
1	A	573	LEU	7.2
1	A	567	PHE	7.1
1	A	527	LEU	6.6
1	A	564	PRO	6.4
1	A	528	ILE	6.3
1	A	559	LEU	6.3
1	A	561	ILE	6.2
1	A	554	ALA	6.0
1	A	557	GLY	5.9
1	B	377	LEU	5.9
1	A	372	ILE	5.8
1	B	375	ARG	5.5
1	A	39	ILE	5.3
1	A	374	VAL	5.3
1	A	376	ASP	5.3
1	B	389	ILE	5.3
1	A	569	ASN	5.2
1	A	546	ASP	4.9
1	A	586	ASN	4.8
1	A	377	LEU	4.8
1	B	586	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	388	LYS	4.6
1	A	563	ILE	4.6
1	A	529	ILE	4.5
1	B	374	VAL	4.5
1	A	389	ILE	4.5
1	A	547	ILE	4.5
1	A	581	PHE	4.4
1	A	47	ASP	4.4
1	A	368	GLU	4.3
1	B	33	LYS	4.3
1	A	553	LYS	4.3
1	A	524	GLY	4.2
1	A	375	ARG	4.1
1	A	579	TRP	4.1
1	A	369	ASP	4.0
1	A	534	GLU	4.0
1	B	557	GLY	4.0
1	A	558	ASN	4.0
1	A	556	ASN	3.9
1	A	371	LEU	3.9
1	B	369	ASP	3.9
1	A	574	ILE	3.8
1	B	372	ILE	3.8
1	A	572	SER	3.8
1	A	578	VAL	3.8
1	A	526	ASN	3.8
1	A	373	LYS	3.7
1	A	388	LYS	3.7
1	A	535	GLU	3.7
1	B	534	GLU	3.6
1	B	555	SER	3.6
1	A	536	GLY	3.6
1	A	525	GLU	3.6
1	A	552	THR	3.5
1	A	550	GLN	3.5
1	A	390	TYR	3.4
1	A	387	MET	3.4
1	B	373	LYS	3.4
1	B	376	ASP	3.4
1	B	536	GLY	3.3
1	A	542	LEU	3.3
1	A	545	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	48	PHE	3.3
1	A	37	ASP	3.2
1	A	566	ASP	3.2
1	A	520	THR	3.2
1	B	408	ASP	3.2
1	A	531	THR	3.2
1	B	387	MET	3.2
1	A	367	SER	3.2
1	A	548	ASN	3.0
1	A	519	CYS	3.0
1	A	40	LEU	2.9
1	A	565	LYS	2.9
1	A	585	LEU	2.8
1	B	391	LEU	2.8
1	B	371	LEU	2.8
1	A	530	ASN	2.8
1	B	37	ASP	2.7
1	B	390	TYR	2.7
1	A	537	ILE	2.7
1	A	523	PRO	2.7
1	A	551	PHE	2.7
1	A	575	SER	2.6
1	A	543	LEU	2.6
1	A	49[A]	MET	2.6
1	A	503	ASP	2.5
1	A	544	GLY	2.5
1	A	485	VAL	2.5
1	B	368	GLU	2.4
1	A	496	TRP	2.4
1	A	512	GLY	2.4
1	A	511	ASP	2.4
1	A	580	THR	2.4
1	B	548	ASN	2.3
1	A	513	LYS	2.3
1	A	577	TYR	2.3
1	A	408	ASP	2.3
1	A	533	ILE	2.3
1	A	568	GLN	2.3
1	A	33	LYS	2.3
1	A	538	LYS	2.3
1	A	502	ASN	2.3
1	A	46	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	562	PRO	2.2
1	A	62	ARG	2.2
1	A	370	ASP	2.2
1	B	254[A]	ASP	2.2
1	B	370	ASP	2.2
1	B	367	SER	2.2
1	A	506	PHE	2.2
1	A	560	GLU	2.2
1	B	554	ALA	2.2
1	A	570	ASN	2.1
1	A	183	LEU	2.1
1	A	482	TRP	2.1
1	A	540	ILE	2.1
1	B	550	GLN	2.1
1	A	477	LEU	2.1
1	A	505	PHE	2.0
1	B	585	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
5	PEG	B	603	7/7	0.62	0.21	36,41,47,48	0
3	GOL	A	604	6/6	0.80	0.22	37,43,46,48	0
4	CIT	A	603	13/13	0.81	0.20	22,25,28,29	0
3	GOL	B	602	6/6	0.88	0.13	19,21,25,27	0
2	NA	A	601	1/1	0.91	0.28	33,33,33,33	0
3	GOL	A	602	6/6	0.96	0.07	19,21,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	B	601	1/1	0.99	0.08	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.