



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 07:56 PM BST

PDB ID : 3GBN
Title : Crystal Structure of Fab CR6261 in Complex with the 1918 H1N1 influenza virus hemagglutinin
Authors : Ekiert, D.C.; Elsliger, M.A.; Wilson, I.A.
Deposited on : 2009-02-20
Resolution : 2.20 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 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

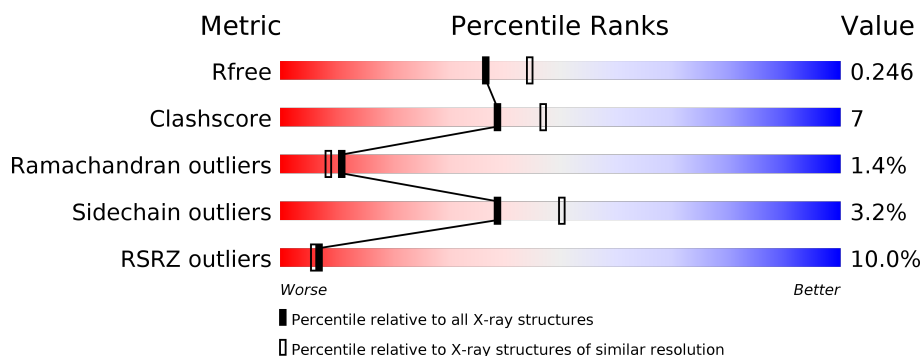
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	A	331	
2	B	179	
3	H	226	
4	L	221	
5	C	4	

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
5	NAG	C	1	-	-	-	X
6	NAG	B	180	X	-	-	-
7	EDO	B	185	-	-	X	-
8	GOL	A	332	-	-	X	-
9	ETX	A	333	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6618 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	2	0
			2501	1577	427	486	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q9WFX3
A	8	ASP	-	expression tag	UNP Q9WFX3
A	9	PRO	-	expression tag	UNP Q9WFX3
A	10	GLY	-	expression tag	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	2	0
			1399	873	240	280	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP Q9WFX3
B	178	GLY	-	expression tag	UNP Q9WFX3
B	179	ARG	-	expression tag	UNP Q9WFX3

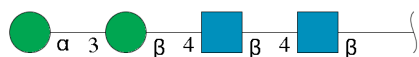
- Molecule 3 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	160	Total	C	N	O	S	0	0	0
			1209	774	196	231	8			

- Molecule 4 is a protein called Fab Lambda Light Chain.

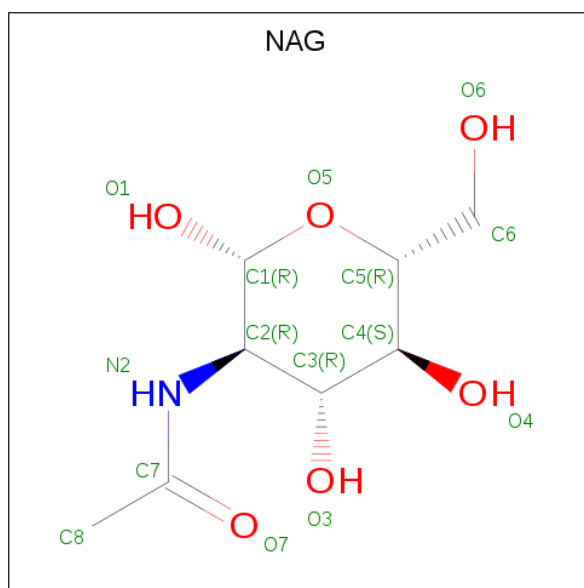
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	151	Total	C	N	O	S	0	0	0
			1085	677	180	224	4			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	4	Total	C	N	O		0	0	0
			50	28	2	20				

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



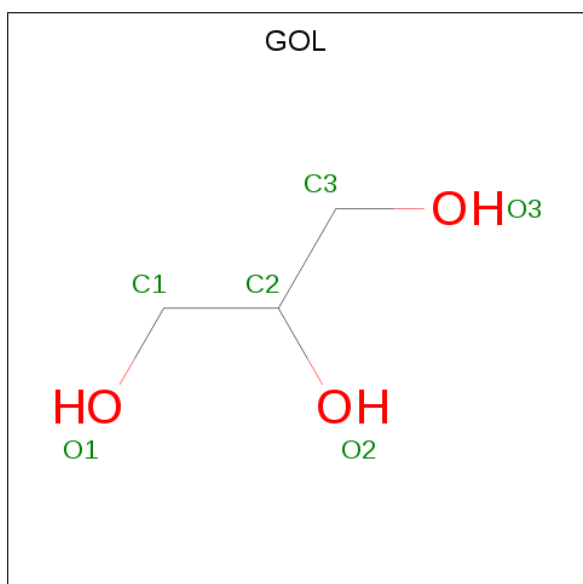
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O		0	0
			14	8	1	5			
6	B	1	Total	C	N	O		0	0
			14	8	1	5			

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



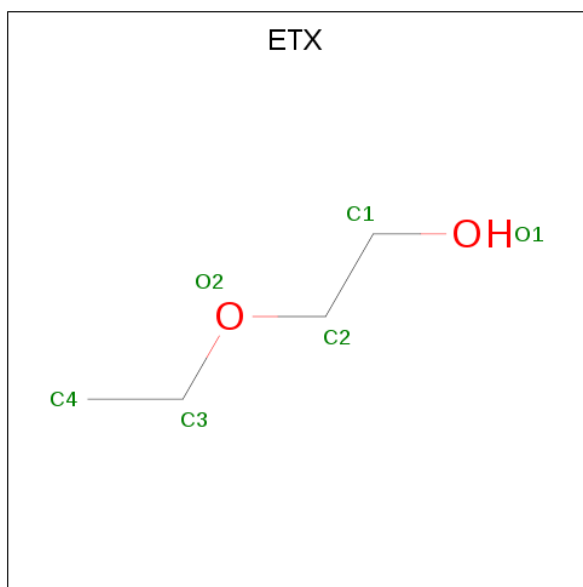
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

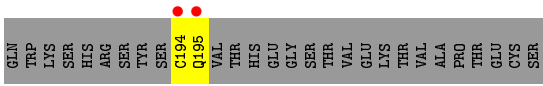
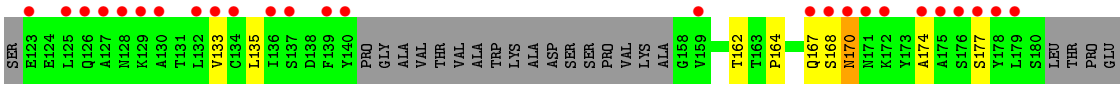
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Cl	0	0
			1	1		

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

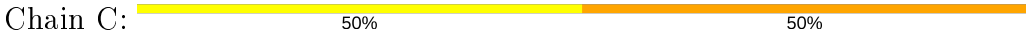
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	O	0	0
			14	14		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	82	Total 82	O 82	0	0
12	B	124	Total 124	O 124	0	0
12	H	79	Total 79	O 79	0	0
12	L	8	Total 8	O 8	0	0



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	201.92Å 202.25Å 202.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.72 – 2.20 39.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (39.72-2.20) 94.8 (39.72-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.205 , 0.241 0.206 , 0.246	Depositor DCC
R_{free} test set	3391 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6618	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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, BMA, NAG, CL, ETX, EDO, UNL, MAN

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	0.73	0/2565	0.71	1/3505 (0.0%)
2	B	1.04	2/1432 (0.1%)	0.89	3/1929 (0.2%)
3	H	0.93	1/1238 (0.1%)	0.85	1/1676 (0.1%)
4	L	0.70	0/1103	0.73	0/1503
All	All	0.85	3/6338 (0.0%)	0.79	5/8613 (0.1%)

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	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	92	CYS	CB-SG	-6.96	1.70	1.82
2	B	1	GLY	N-CA	5.59	1.54	1.46
2	B	78	GLU	CD-OE2	-5.13	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	ARG	NE-CZ-NH2	-11.40	114.60	120.30
2	B	153	ARG	NE-CZ-NH1	8.43	124.52	120.30
3	H	42	GLY	N-CA-C	-6.63	96.51	113.10
1	A	315	ARG	NE-CZ-NH2	-6.53	117.03	120.30
2	B	19	ASP	CB-CG-OD2	5.38	123.14	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	150	GLU	Peptide

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	A	2501	0	2365	41	0
2	B	1399	0	1305	13	0
3	H	1209	0	1191	13	0
4	L	1085	0	1005	27	0
5	C	50	0	43	1	0
6	A	14	0	13	1	0
6	B	14	0	13	0	0
7	A	4	0	6	2	0
7	B	12	0	18	6	0
7	H	4	0	6	0	0
8	A	6	0	8	7	0
8	B	6	0	8	0	0
9	A	6	0	10	7	0
10	B	1	0	0	0	0
11	B	14	0	0	0	0
12	A	82	0	0	1	0
12	B	124	0	0	1	0
12	H	79	0	0	1	0
12	L	8	0	0	0	0
All	All	6618	0	5991	92	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 7.

The worst 5 of 92 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:L:9:SER:C	4:L:11:VAL:N	2.12	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HE	8:A:332:GOL:H31	1.23	1.01
1:A:321:ARG:HE	8:A:332:GOL:C3	1.77	0.96
1:A:321:ARG:NE	8:A:332:GOL:H31	1.83	0.93
3:H:174:PHE:CE2	4:L:135:LEU:HD23	2.06	0.89

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	328/331 (99%)	308 (94%)	13 (4%)	7 (2%)	7	4
2	B	173/179 (97%)	169 (98%)	4 (2%)	0	100	100
3	H	152/226 (67%)	146 (96%)	4 (3%)	2 (1%)	12	9
4	L	139/221 (63%)	129 (93%)	8 (6%)	2 (1%)	11	8
All	All	792/957 (83%)	752 (95%)	29 (4%)	11 (1%)	11	8

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
3	H	152	VAL
4	L	94	ARG
1	A	187	THR
3	H	151	PRO

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	270/285 (95%)	264 (98%)	6 (2%)	52	65
2	B	148/152 (97%)	147 (99%)	1 (1%)	84	91
3	H	132/189 (70%)	126 (96%)	6 (4%)	27	34
4	L	115/182 (63%)	107 (93%)	8 (7%)	15	16
All	All	665/808 (82%)	644 (97%)	21 (3%)	39	50

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	142	CYS
3	H	180	SER
4	L	103	LYS
3	H	120	SER
4	L	162	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
4	L	170	ASN
4	L	195	GLN

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](#)

4 monosaccharides 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
5	NAG	C	1	1,5	14,14,15	0.72	0	17,19,21	2.59	6 (35%)
5	NAG	C	2	5	14,14,15	0.49	0	17,19,21	1.95	5 (29%)
5	BMA	C	3	5	11,11,12	0.47	0	15,15,17	1.54	2 (13%)
5	MAN	C	4	5	11,11,12	1.19	1 (9%)	15,15,17	1.38	3 (20%)

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
5	NAG	C	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	4	MAN	C2-C3	-2.02	1.49	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C4-C3-C2	-7.31	100.31	111.02
5	C	1	NAG	C2-N2-C7	-4.62	116.33	122.90
5	C	2	NAG	O5-C5-C6	4.51	114.28	107.20
5	C	3	BMA	C2-C3-C4	-4.37	103.33	110.89
5	C	2	NAG	C6-C5-C4	-3.80	104.11	113.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2	NAG	1	0
5	C	3	BMA	1	0

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is unknown and 1 is monoatomic - leaving 10 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	$\# Z > 2$
7	EDO	B	184	-	3,3,3	0.60	0	2,2,2	0.07	0
7	EDO	H	228	-	3,3,3	0.30	0	2,2,2	0.34	0
9	ETX	A	333	-	5,5,5	0.46	0	4,4,4	1.51	1 (25%)
7	EDO	B	185	-	3,3,3	0.33	0	2,2,2	0.95	0
6	NAG	A	330	1	14,14,15	0.72	1 (7%)	17,19,21	1.40	1 (5%)
6	NAG	B	180	2	14,14,15	0.81	1 (7%)	17,19,21	1.64	2 (11%)
8	GOL	B	181	-	5,5,5	0.49	0	5,5,5	1.34	0
7	EDO	A	331	-	3,3,3	0.92	0	2,2,2	0.70	0
8	GOL	A	332	-	5,5,5	1.10	1 (20%)	5,5,5	1.32	1 (20%)
7	EDO	B	183	-	3,3,3	0.61	0	2,2,2	0.52	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
7	EDO	B	184	-	-	0/1/1/1	-
7	EDO	H	228	-	-	1/1/1/1	-
9	ETX	A	333	-	-	1/3/3/3	-
7	EDO	B	185	-	-	1/1/1/1	-
6	NAG	A	330	1	-	2/6/23/26	0/1/1/1
6	NAG	B	180	2	1/1/5/7	0/6/23/26	0/1/1/1
8	GOL	B	181	-	-	1/4/4/4	-
7	EDO	A	331	-	-	1/1/1/1	-
8	GOL	A	332	-	-	2/4/4/4	-
7	EDO	B	183	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	180	NAG	C1-C2	2.34	1.55	1.52
6	A	330	NAG	C1-C2	2.12	1.55	1.52
8	A	332	GOL	O2-C2	-2.10	1.37	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	180	NAG	C1-O5-C5	4.77	118.66	112.19
6	A	330	NAG	C1-O5-C5	4.40	118.15	112.19
9	A	333	ETX	C3-O2-C2	-2.89	102.53	112.90
6	B	180	NAG	C1-C2-N2	-2.49	106.23	110.49
8	A	332	GOL	C3-C2-C1	2.35	120.84	111.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	180	NAG	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	330	NAG	O5-C5-C6-O6
6	A	330	NAG	C4-C5-C6-O6
7	H	228	EDO	O1-C1-C2-O2
7	B	185	EDO	O1-C1-C2-O2
7	A	331	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	184	EDO	1	0
9	A	333	ETX	7	0
7	B	185	EDO	5	0
6	A	330	NAG	1	0
7	A	331	EDO	2	0
8	A	332	GOL	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	L	2
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	168:SER	C	170:ASN	N	2.74
1	H	180:SER	C	182:SER	N	2.31
1	L	9:SER	C	11:VAL	N	2.12

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	A	328/331 (99%)	0.30	33 (10%) 7 6	15, 37, 55, 60	0
2	B	173/179 (96%)	0.22	5 (2%) 51 49	19, 26, 39, 59	0
3	H	160/226 (70%)	0.44	13 (8%) 12 10	17, 30, 47, 59	0
4	L	151/221 (68%)	0.83	30 (19%) 1 1	25, 40, 61, 97	0
All	All	812/957 (84%)	0.41	81 (9%) 7 6	15, 34, 55, 97	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	142	CYS	9.7
3	H	143	LEU	6.9
4	L	136	ILE	6.5
4	L	125	LEU	6.2
4	L	139	PHE	5.9

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](#)

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
5	NAG	C	1	14/15	0.79	0.44	28,49,62,66	14
5	BMA	C	3	11/12	0.86	0.18	40,46,56,57	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	C	2	14/15	0.87	0.28	24,47,61,62	14
5	MAN	C	4	11/12	0.91	0.18	23,27,36,48	11

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
8	GOL	A	332	6/6	0.82	0.23	36,57,59,61	0
11	UNL	B	186	14/-	0.83	0.18	66,84,91,97	0
6	NAG	B	180	14/15	0.86	0.22	53,74,80,81	0
7	EDO	A	331	4/4	0.89	0.18	32,59,63,65	0
7	EDO	B	183	4/4	0.89	0.18	36,48,51,56	0
6	NAG	A	330	14/15	0.90	0.21	73,81,86,89	0
9	ETX	A	333	6/6	0.92	0.26	21,40,51,62	0
7	EDO	B	184	4/4	0.93	0.26	41,54,62,67	0
8	GOL	B	181	6/6	0.94	0.20	33,55,57,63	0
7	EDO	B	185	4/4	0.95	0.21	46,53,54,57	0
7	EDO	H	228	4/4	0.97	0.18	39,48,52,55	0
10	CL	B	182	1/1	0.99	0.14	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.