Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:52 AM GMT

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 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
http://wwpdb.org/validation/2016/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:

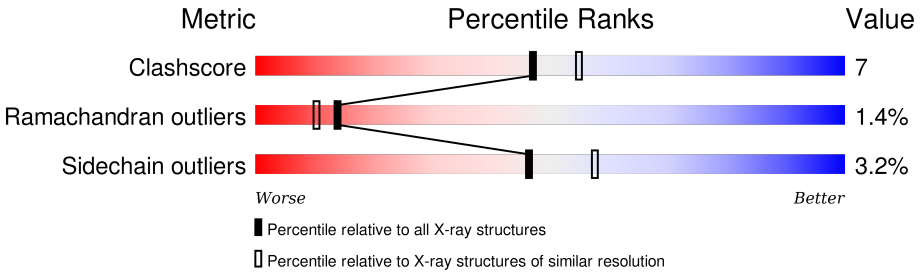
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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. 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	331	85% 12%
2	B	179	88% 7%
3	H	226	60% 9% 29%
4	L	221	52% 14% 32%

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
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			

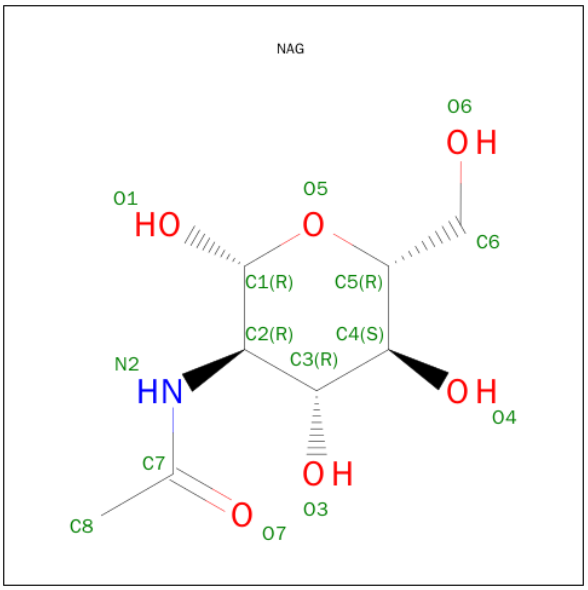
- Molecule 4 is a protein called Fab Lambda Light Chain.

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 a polymer of unknown type called SUGAR (4-MER).

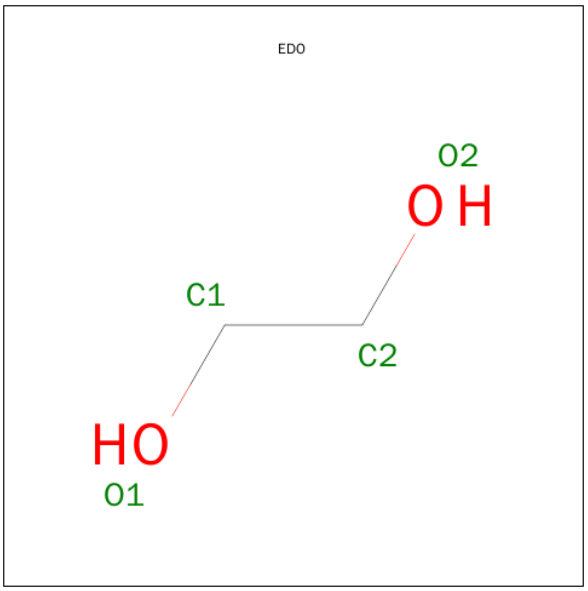
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



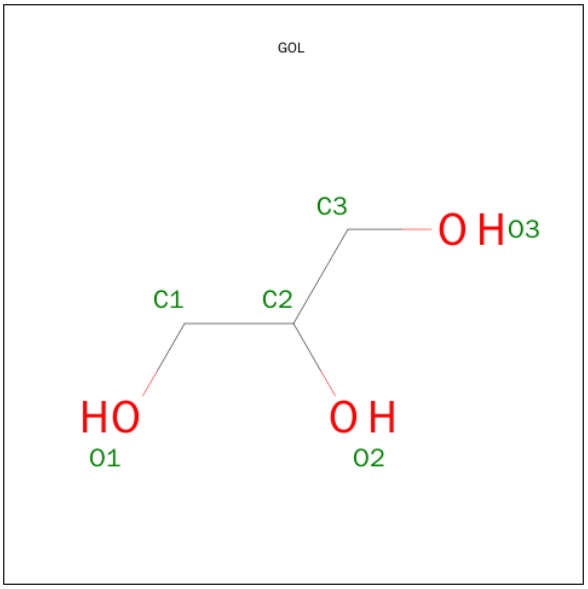
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



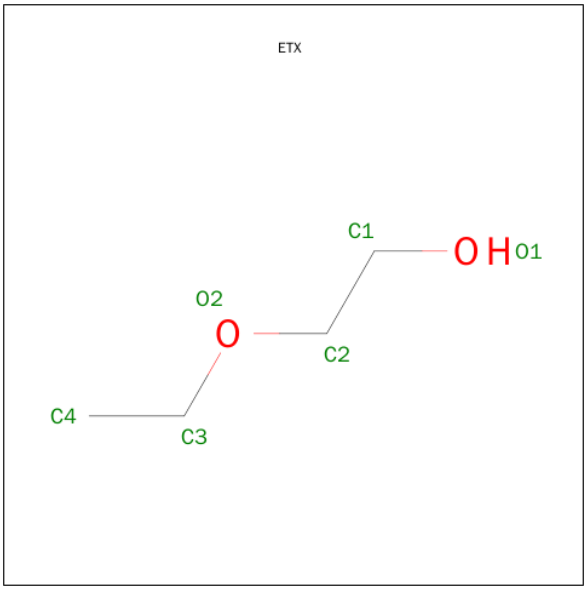
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0

- 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 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0

- Molecule 9 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: $C_4H_{10}O_2$).



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

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

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

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

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

- Molecule 12 is water.

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

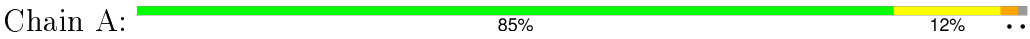
3 Residue-property plots (i)

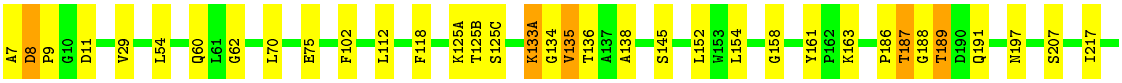
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS failed to run properly.

- Molecule 1: Hemagglutinin

Chain A:



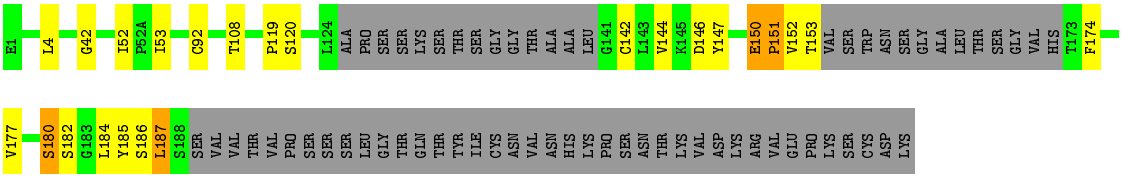


- Molecule 2: Hemagglutinin

Chain B:

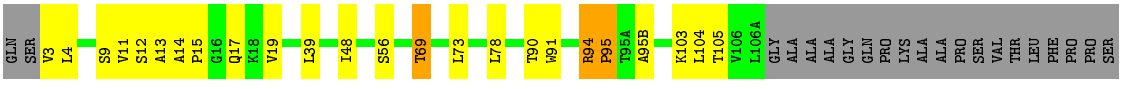
- Molecule 3: Fab Heavy Chain

Chain H:



- Molecule 4: Fab Lambda Light Chain

Chain L:



SER
THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

4 Data and refinement statistics (i)

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	95.1 (39.72-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.205 , 0.241	Depositor
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.000	Xtriage
Estimated twinning fraction	0.017 for -l,-k,-h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 66142 reflections	Xtriage
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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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(^{o})	Ideal(^{o})
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 (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	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	A	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.

All (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
2:B:29:GLU:H	7:B:185:EDO:H12	1.38	0.88
3:H:177:VAL:HG12	3:H:186:SER:O	1.77	0.84
3:H:180:SER:C	3:H:182:SER:N	2.31	0.83
1:A:70:LEU:HD11	1:A:112:LEU:HD11	1.67	0.76
1:A:134:GLY:CA	1:A:135:VAL:O	2.35	0.74
1:A:134:GLY:HA2	1:A:135:VAL:O	1.87	0.73
1:A:29:VAL:HB	9:A:333:ETX:H22	1.70	0.72
4:L:133:VAL:HG12	4:L:135:LEU:HD12	1.71	0.72
2:B:29:GLU:N	7:B:185:EDO:H12	2.08	0.67
3:H:147:TYR:CD2	3:H:185:TYR:O	2.47	0.67
3:H:147:TYR:CE2	3:H:185:TYR:O	2.48	0.67
4:L:91:TRP:CZ2	4:L:95(B):ALA:HB1	2.30	0.67
4:L:9:SER:O	4:L:11:VAL:N	2.27	0.66
1:A:321:ARG:NE	8:A:332:GOL:C3	2.49	0.64
2:B:19:ASP:N	2:B:19:ASP:OD1	2.28	0.64
1:A:188:GLY:CA	1:A:217:ILE:HD11	2.28	0.64
1:A:54:LEU:HD23	1:A:279:THR:O	1.98	0.63
4:L:13:ALA:HB1	4:L:17:GLN:HG2	1.82	0.62
1:A:60[A]:GLN:HE21	1:A:62:GLY:H	1.47	0.61
4:L:133:VAL:HG12	4:L:135:LEU:CD1	2.32	0.60
1:A:186:PRO:O	1:A:187:THR:C	2.41	0.59
1:A:188:GLY:HA3	1:A:217:ILE:HD11	1.85	0.59
4:L:104:LEU:HD23	4:L:104:LEU:C	2.24	0.58
3:H:52:ILE:HD13	3:H:52:ILE:N	2.18	0.58
1:A:310:ARG:NH1	2:B:90:ASP:OD1	2.32	0.57
1:A:188:GLY:HA2	1:A:189:THR:HB	1.88	0.56
1:A:321:ARG:HE	8:A:332:GOL:H32	1.63	0.56
4:L:167:GLN:HE21	4:L:174:ALA:HB2	1.71	0.55
2:B:143:LYS:NZ	7:B:185:EDO:H11	2.23	0.54
3:H:146:ASP:HB3	3:H:184:LEU:HD13	1.89	0.54
4:L:15:PRO:HA	4:L:78:LEU:O	2.06	0.54
1:A:134:GLY:HA3	1:A:135:VAL:O	2.05	0.54
2:B:145:ASP:HA	7:B:185:EDO:H21	1.88	0.53
4:L:13:ALA:HB1	4:L:17:GLN:CG	2.37	0.53
1:A:29:VAL:CB	9:A:333:ETX:H22	2.37	0.53
4:L:4:LEU:HD11	4:L:90:THR:HG22	1.91	0.52
1:A:125(A):LYS:HG2	1:A:125(B):THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:HG2	6:A:330:NAG:H82	1.92	0.52
1:A:29:VAL:HB	9:A:333:ETX:C2	2.40	0.52
1:A:321:ARG:CD	8:A:332:GOL:H31	2.40	0.51
1:A:29:VAL:CG1	9:A:333:ETX:H22	2.39	0.51
4:L:94:ARG:CB	4:L:95:PRO:CD	2.87	0.51
1:A:238:GLU:HG3	1:A:239:PRO:HD2	1.93	0.50
3:H:108:THR:HG22	12:H:261:HOH:O	2.10	0.49
1:A:138:ALA:O	1:A:224:ARG:NH1	2.44	0.49
2:B:9:PHE:O	2:B:135:ASN:HA	2.13	0.49
1:A:8:ASP:N	1:A:9:PRO:CD	2.75	0.49
3:H:119:PRO:HB2	3:H:144:VAL:HG13	1.94	0.49
1:A:152:LEU:HD23	1:A:154:LEU:HD21	1.94	0.49
1:A:313:LYS:HE2	7:A:331:EDO:H12	1.95	0.48
1:A:161:TYR:HB3	1:A:197:ASN:ND2	2.28	0.48
3:H:150:GLU:HG2	3:H:151:PRO:HD3	1.95	0.48
4:L:39:LEU:N	4:L:39:LEU:HD23	2.29	0.48
1:A:152:LEU:HD23	1:A:154:LEU:CD2	2.44	0.48
4:L:69:THR:CG2	4:L:69:THR:O	2.62	0.47
9:A:333:ETX:C1	2:B:105:GLU:HG2	2.46	0.46
4:L:164:PRO:HA	4:L:174:ALA:O	2.16	0.46
1:A:301:THR:HB	1:A:305:CYS:SG	2.56	0.45
4:L:69:THR:HG23	4:L:69:THR:O	2.17	0.45
1:A:321:ARG:CZ	8:A:332:GOL:H12	2.47	0.45
1:A:60[A]:GLN:NE2	1:A:62:GLY:H	2.13	0.45
9:A:333:ETX:H11	2:B:105:GLU:HG2	1.99	0.45
4:L:9:SER:CA	4:L:11:VAL:N	2.78	0.45
4:L:48:ILE:HD13	4:L:73:LEU:HD13	1.98	0.45
1:A:11:ASP:OD1	7:B:185:EDO:O1	2.35	0.45
2:B:1:GLY:H2	7:B:184:EDO:C2	2.31	0.44
4:L:167:GLN:NE2	4:L:174:ALA:HB2	2.33	0.44
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.99	0.44
3:H:187:LEU:HD12	3:H:187:LEU:C	2.38	0.44
9:A:333:ETX:H32	12:B:226:HOH:O	2.18	0.44
1:A:7:ALA:N	2:B:139:GLU:OE1	2.52	0.43
1:A:186:PRO:O	1:A:188:GLY:N	2.52	0.43
4:L:3:VAL:HG12	4:L:4:LEU:N	2.33	0.43
2:B:21:TRP:CZ2	3:H:53:ILE:HG21	2.54	0.42
4:L:104:LEU:CD2	4:L:104:LEU:C	2.88	0.42
4:L:94:ARG:O	4:L:95:PRO:C	2.57	0.42
1:A:191:GLN:HB2	1:A:217:ILE:HD12	2.01	0.42
4:L:168:SER:C	4:L:170:ASN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:150:GLU:CB	3:H:151:PRO:HD3	2.49	0.41
1:A:60[B]:GLN:NE2	12:A:369:HOH:O	2.46	0.41
1:A:135:VAL:HG13	1:A:145:SER:C	2.40	0.41
1:A:313:LYS:HE2	7:A:331:EDO:C1	2.50	0.41
4:L:194:CYS:O	4:L:195:GLN:C	2.59	0.41
1:A:133(A):LYS:HA	1:A:134:GLY:HA2	1.96	0.41
5:A:2:NAG:H61	5:A:3:BMA:C1	2.50	0.41
4:L:104:LEU:HD23	4:L:105:THR:N	2.37	0.40
4:L:14:ALA:O	4:L:17:GLN:HB3	2.21	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	328/331 (99%)	308 (94%)	13 (4%)	7 (2%)	9 5
2	B	173/179 (97%)	169 (98%)	4 (2%)	0	100 100
3	H	152/226 (67%)	146 (96%)	4 (3%)	2 (1%)	15 11
4	L	139/221 (63%)	129 (93%)	8 (6%)	2 (1%)	14 10
All	All	792/957 (83%)	752 (95%)	29 (4%)	11 (1%)	14 10

All (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
1	A	125(C)	SER

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Mol	Chain	Res	Type
1	A	163	LYS
1	A	189	THR
1	A	133(A)	LYS
4	L	95	PRO
1	A	158	GLY

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%)	60 72
2	B	148/152 (97%)	147 (99%)	1 (1%)	88 94
3	H	132/189 (70%)	126 (96%)	6 (4%)	34 41
4	L	115/182 (63%)	107 (93%)	8 (7%)	19 19
All	All	665/808 (82%)	644 (97%)	21 (3%)	46 57

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

Mol	Chain	Res	Type
1	A	8	ASP
1	A	102	PHE
1	A	118	PHE
1	A	136	THR
1	A	207	SER
1	A	320	LEU
2	B	19	ASP
3	H	4	LEU
3	H	120	SER
3	H	142	CYS
3	H	153	THR
3	H	180	SER
3	H	187	LEU
4	L	12	SER
4	L	19	VAL
4	L	56	SER

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Mol	Chain	Res	Type
4	L	69	THR
4	L	103	LYS
4	L	162	THR
4	L	170	ASN
4	L	177	SER

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

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

4 carbohydrates 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	A	1	1,5	14,14,15	0.69	0	15,19,21	2.93	5 (33%)
5	NAG	A	2	5	14,14,15	0.48	0	15,19,21	1.67	3 (20%)
5	BMA	A	3	5	11,11,12	0.46	0	14,15,17	1.61	2 (14%)
5	MAN	A	4	5	11,11,12	1.19	1 (9%)	14,15,17	1.39	3 (21%)

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	A	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2	5	-	0/6/23/26	0/1/1/1
5	BMA	A	3	5	-	0/2/19/22	0/1/1/1
5	MAN	A	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	A	4	MAN	C2-C3	-2.17	1.49	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	NAG	C4-C3-C2	-7.02	100.31	111.23
5	A	1	NAG	C2-N2-C7	-5.22	116.33	123.04
5	A	3	BMA	C2-C3-C4	-4.54	103.33	111.04
5	A	2	NAG	C6-C5-C4	-3.61	104.11	113.02
5	A	4	MAN	O2-C2-C3	-2.44	105.21	110.12
5	A	2	NAG	O7-C7-C8	-2.30	117.85	122.06
5	A	4	MAN	O4-C4-C3	-2.06	105.70	110.34
5	A	4	MAN	O4-C4-C5	2.08	114.75	109.24
5	A	3	BMA	C1-O5-C5	2.58	115.52	112.25
5	A	1	NAG	O3-C3-C4	2.79	116.62	110.34
5	A	1	NAG	O4-C4-C3	3.11	117.33	110.34
5	A	2	NAG	O5-C5-C6	3.20	114.28	107.35
5	A	1	NAG	C3-C2-N2	4.60	121.58	110.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	NAG	1	0
5	A	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	$\#\|Z\| > 2$
6	NAG	A	330	1	14,14,15	0.72	1 (7%)	15,19,21	1.47	1 (6%)
7	EDO	A	331	-	3,3,3	0.90	0	2,2,2	0.68	0
8	GOL	A	332	-	5,5,5	1.08	1 (20%)	5,5,5	1.33	1 (20%)
9	ETX	A	333	-	5,5,5	0.45	0	4,4,4	1.40	1 (25%)
6	NAG	B	180	2	14,14,15	0.81	1 (7%)	15,19,21	1.65	2 (13%)
8	GOL	B	181	-	5,5,5	0.45	0	5,5,5	1.32	1 (20%)
7	EDO	B	183	-	3,3,3	0.61	0	2,2,2	0.54	0
7	EDO	B	184	-	3,3,3	0.61	0	2,2,2	0.16	0
7	EDO	B	185	-	3,3,3	0.34	0	2,2,2	0.99	0
7	EDO	H	228	-	3,3,3	0.31	0	2,2,2	0.43	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	NAG	A	330	1	-	0/6/23/26	0/1/1/1
7	EDO	A	331	-	-	0/1/1/1	0/0/0/0
8	GOL	A	332	-	-	0/4/4/4	0/0/0/0
9	ETX	A	333	-	-	0/3/3/3	0/0/0/0
6	NAG	B	180	2	1/1/5/7	0/6/23/26	0/1/1/1
8	GOL	B	181	-	-	0/4/4/4	0/0/0/0
7	EDO	B	183	-	-	0/1/1/1	0/0/0/0
7	EDO	B	184	-	-	0/1/1/1	0/0/0/0
7	EDO	B	185	-	-	0/1/1/1	0/0/0/0
7	EDO	H	228	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	332	GOL	O2-C2	-2.13	1.37	1.43
6	A	330	NAG	C1-C2	2.20	1.55	1.52
6	B	180	NAG	C1-C2	2.44	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	333	ETX	C3-O2-C2	-2.68	102.53	112.80
6	B	180	NAG	C2-N2-C7	-2.07	120.39	123.04
8	B	181	GOL	O2-C2-C3	2.01	117.85	108.65
8	A	332	GOL	C3-C2-C1	2.48	120.84	111.12
6	A	330	NAG	C1-O5-C5	4.65	118.15	112.25
6	B	180	NAG	C1-O5-C5	5.05	118.66	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	180	NAG	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:

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

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers

EDS failed to run properly - this section will therefore be empty.