



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:12 PM GMT

PDB ID : 4HJ1
Title : Crystal structure of glycoprotein C from Rift Valley Fever Virus (glycosylated)
Authors : Dessau, M.; Modis, Y.
Deposited on : 2012-10-12
Resolution : 1.90 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
<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 : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

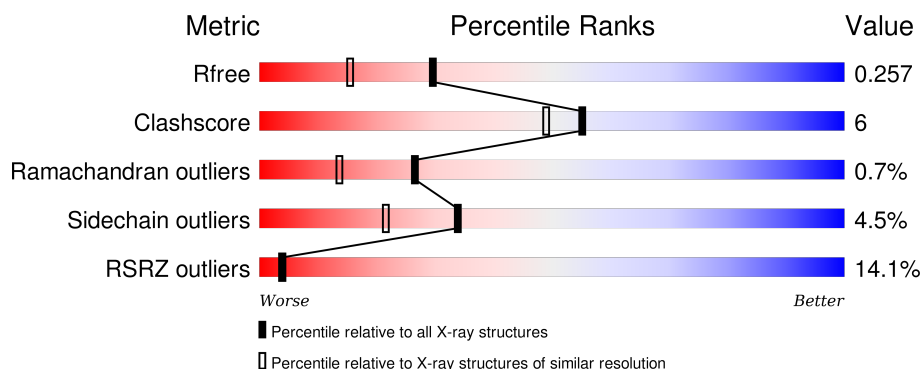
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 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 $\leq 5\%$. 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	432	<div> <div>6%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	B	432	<div> <div>27%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	C	432	<div> <div>15%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	432	<div> <div>9%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	D	1210	-	-	X	X
7	BMA	D	1205	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14382 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 ENVELOPE GLYCOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	2	0
			3279	2036	561	653	29			
1	B	427	Total	C	N	O	S	0	0	0
			3242	2011	557	645	29			
1	C	430	Total	C	N	O	S	0	1	0
			3271	2031	561	649	30			
1	D	431	Total	C	N	O	S	0	5	0
			3296	2046	562	658	30			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	688	ASP	-	EXPRESSION TAG	UNP A2T075
A	689	PRO	-	EXPRESSION TAG	UNP A2T075
A	690	GLY	-	EXPRESSION TAG	UNP A2T075
B	688	ASP	-	EXPRESSION TAG	UNP A2T075
B	689	PRO	-	EXPRESSION TAG	UNP A2T075
B	690	GLY	-	EXPRESSION TAG	UNP A2T075
C	688	ASP	-	EXPRESSION TAG	UNP A2T075
C	689	PRO	-	EXPRESSION TAG	UNP A2T075
C	690	GLY	-	EXPRESSION TAG	UNP A2T075
D	688	ASP	-	EXPRESSION TAG	UNP A2T075
D	689	PRO	-	EXPRESSION TAG	UNP A2T075
D	690	GLY	-	EXPRESSION TAG	UNP A2T075

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

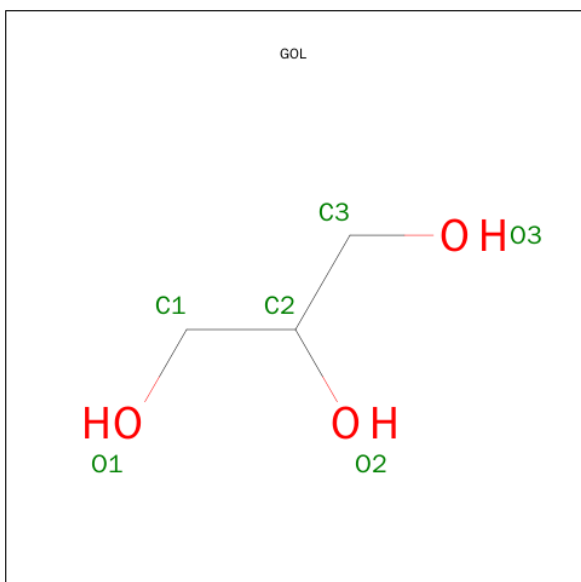
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total C N O 39 22 2 15	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	5	Total C N O 61 34 2 25	0	0
7	D	5	Total C N O 61 34 2 25	0	0

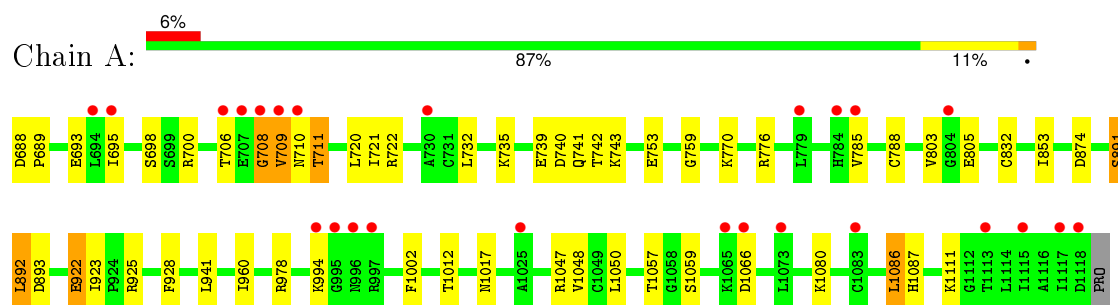
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	332	Total O 332 332	0	0
8	B	111	Total O 111 111	0	0
8	C	170	Total O 170 170	0	0
8	D	324	Total O 324 324	0	0

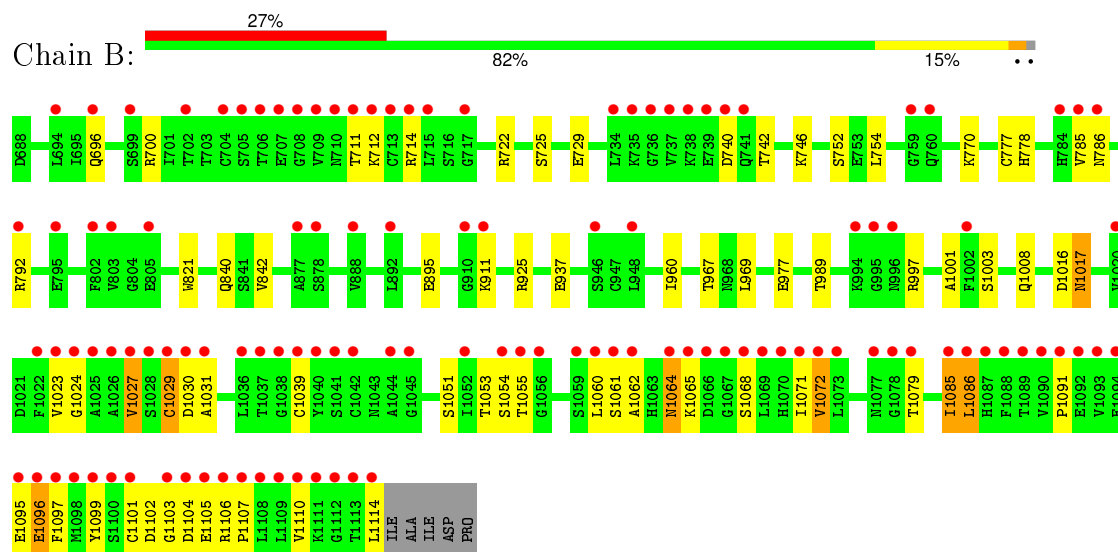
3 Residue-property plots

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.

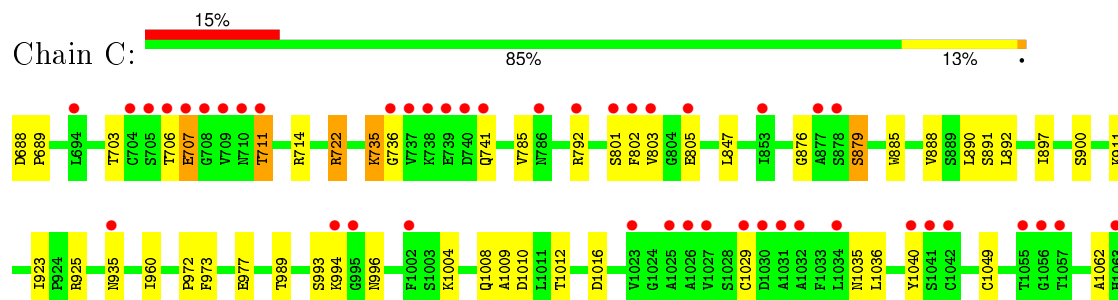
• Molecule 1: ENVELOPE GLYCOPROTEIN

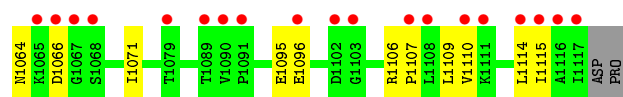


• Molecule 1: ENVELOPE GLYCOPROTEIN

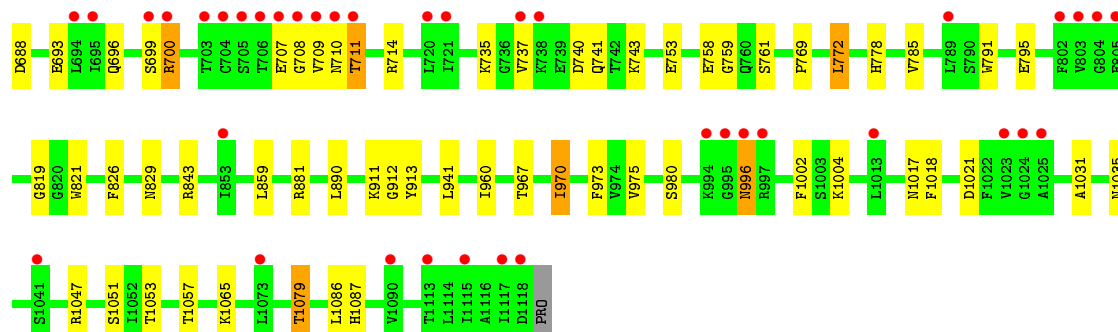
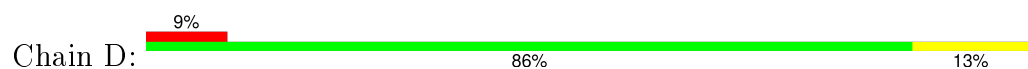


• Molecule 1: ENVELOPE GLYCOPROTEIN





• Molecule 1: ENVELOPE GLYCOPROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.68Å 56.37Å 140.19Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	29.76 – 1.90 29.75 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.76-1.90) 97.4 (29.75-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.214 , 0.255 0.215 , 0.257	Depositor DCC
R_{free} test set	7722 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 154031 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14382	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.67 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.9715e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, MES

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	0.51	0/3345	0.69	1/4523 (0.0%)
1	B	0.39	1/3302 (0.0%)	0.56	0/4463
1	C	0.40	0/3331	0.59	0/4502
1	D	0.51	0/3368	0.66	2/4553 (0.0%)
All	All	0.45	1/13346 (0.0%)	0.63	3/18041 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1097	PHE	CG-CD2	-6.11	1.29	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1047	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	D	772	LEU	CA-CB-CG	5.33	127.55	115.30
1	D	881	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3279	0	3155	39	0
1	B	3242	0	3111	39	0
1	C	3271	0	3145	36	0
1	D	3296	0	3168	52	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	50	0	43	1	0
4	A	12	0	13	1	0
4	B	12	0	13	0	0
4	C	12	0	13	0	0
4	D	24	0	26	3	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	12	0	16	10	0
6	B	39	0	34	0	0
7	C	61	0	52	0	0
7	D	61	0	52	3	0
8	A	332	0	0	12	0
8	B	111	0	0	1	0
8	C	170	0	0	7	0
8	D	324	0	0	11	0
All	All	14382	0	12917	166	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 6.

The worst 5 of 166 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:D:912:GLY:HA3	5:D:1210:GOL:H11	1.41	1.02
1:B:1060:LEU:HA	1:B:1101:CYS:HB3	1.53	0.89
1:B:1104:ASP:HB3	1:B:1105:GLU:HA	1.53	0.89
1:B:1102:ASP:HB3	1:B:1104:ASP:N	1.90	0.83
1:A:753:GLU:HG2	1:A:1002:PHE:CE1	2.13	0.82

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	431/432 (100%)	417 (97%)	10 (2%)	4 (1%)	21	9
1	B	425/432 (98%)	404 (95%)	17 (4%)	4 (1%)	21	9
1	C	429/432 (99%)	413 (96%)	13 (3%)	3 (1%)	26	14
1	D	434/432 (100%)	422 (97%)	11 (2%)	1 (0%)	52	42
All	All	1719/1728 (100%)	1656 (96%)	51 (3%)	12 (1%)	26	14

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	ILE
1	B	960	ILE
1	C	785	VAL
1	C	960	ILE
1	D	960	ILE

5.3.2 Protein sidechains

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	373/372 (100%)	356 (95%)	17 (5%)	33	21
1	B	368/372 (99%)	345 (94%)	23 (6%)	22	10
1	C	371/372 (100%)	359 (97%)	12 (3%)	46	35
1	D	376/372 (101%)	361 (96%)	15 (4%)	38	26
All	All	1488/1488 (100%)	1421 (96%)	67 (4%)	34	21

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	997	ARG
1	B	1085	ILE
1	D	1017	ASN
1	B	1016	ASP
1	B	1030	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	741	GLN
1	C	1008	GLN
1	D	829	ASN
1	B	1064	ASN
1	D	784	HIS

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 ⓘ

17 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	$\# Z > 2$
3	NAG	A	1202	1,3	14,14,15	0.61	0	15,19,21	1.21	1 (6%)
3	NAG	A	1203	3	14,14,15	0.71	0	15,19,21	1.11	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	A	1204	3	11,11,12	0.79	0	14,15,17	1.29	3 (21%)
3	BMA	A	1205	3	11,11,12	0.74	0	14,15,17	1.91	3 (21%)
6	NAG	B	1202	1,6	14,14,15	0.56	0	15,19,21	1.10	0
6	NAG	B	1203	6	14,14,15	0.41	0	15,19,21	1.62	3 (20%)
6	BMA	B	1204	6	11,11,12	1.05	1 (9%)	14,15,17	1.24	1 (7%)
7	NAG	C	1202	1,7	14,14,15	0.47	0	15,19,21	1.33	3 (20%)
7	NAG	C	1203	7	14,14,15	0.55	0	15,19,21	1.17	1 (6%)
7	BMA	C	1204	7	11,11,12	0.49	0	14,15,17	0.98	1 (7%)
7	BMA	C	1205	7	11,11,12	0.48	0	14,15,17	1.44	2 (14%)
7	BMA	C	1206	7	11,11,12	0.50	0	14,15,17	2.09	2 (14%)
7	NAG	D	1202	1,7	14,14,15	0.51	0	15,19,21	1.14	2 (13%)
7	NAG	D	1203	7	14,14,15	0.76	0	15,19,21	1.31	1 (6%)
7	BMA	D	1204	7	11,11,12	0.89	1 (9%)	14,15,17	3.32	6 (42%)
7	BMA	D	1205	7	11,11,12	0.67	0	14,15,17	2.79	5 (35%)
7	BMA	D	1206	7	11,11,12	0.49	0	14,15,17	2.04	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
3	NAG	A	1202	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1203	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1204	3	-	0/2/19/22	0/1/1/1
3	BMA	A	1205	3	-	0/2/19/22	0/1/1/1
6	NAG	B	1202	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1203	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1204	6	-	0/2/19/22	0/1/1/1
7	NAG	C	1202	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1203	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1204	7	-	0/2/19/22	0/1/1/1
7	BMA	C	1205	7	-	0/2/19/22	1/1/1/1
7	BMA	C	1206	7	-	0/2/19/22	0/1/1/1
7	NAG	D	1202	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	1203	7	-	0/6/23/26	0/1/1/1
7	BMA	D	1204	7	-	0/2/19/22	0/1/1/1
7	BMA	D	1205	7	-	0/2/19/22	0/1/1/1
7	BMA	D	1206	7	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1204	BMA	O5-C1	2.21	1.47	1.43
6	B	1204	BMA	O5-C1	3.02	1.48	1.43

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1206	BMA	C1-O5-C5	-6.17	104.42	112.25
7	D	1204	BMA	C3-C4-C5	-5.73	100.21	110.20
7	D	1203	NAG	O4-C4-C5	-3.60	99.70	109.24
7	C	1202	NAG	C4-C3-C2	-3.29	106.12	111.23
7	D	1204	BMA	C1-C2-C3	-3.12	105.85	109.54

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1205	BMA	C1-C2-C3-C4-C5-O5

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1205	BMA	1	0
7	D	1202	NAG	1	0
7	D	1206	BMA	2	0

5.6 Ligand geometry [i](#)

14 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
2	NAG	A	1201	1	14,14,15	0.50	0	15,19,21	1.17	2 (13%)
4	MES	A	1206	-	11,12,12	0.68	0	14,16,16	7.45	8 (57%)
5	GOL	A	1207	-	5,5,5	0.16	0	5,5,5	0.58	0
2	NAG	B	1201	1	14,14,15	0.47	0	15,19,21	1.07	0
4	MES	B	1205	-	11,12,12	0.67	0	14,16,16	1.15	0
5	GOL	B	1206	-	5,5,5	0.28	0	5,5,5	0.31	0
2	NAG	C	1201	1	14,14,15	0.51	0	15,19,21	1.17	2 (13%)
4	MES	C	1207	-	11,12,12	0.52	0	14,16,16	7.33	5 (35%)
5	GOL	C	1208	-	5,5,5	0.17	0	5,5,5	0.41	0
2	NAG	D	1201	1	14,14,15	0.45	0	15,19,21	0.87	0
4	MES	D	1207	-	11,12,12	0.65	0	14,16,16	6.97	7 (50%)
4	MES	D	1208	-	11,12,12	0.63	0	14,16,16	7.74	4 (28%)
5	GOL	D	1209	-	5,5,5	0.33	0	5,5,5	0.48	0
5	GOL	D	1210	-	5,5,5	0.11	0	5,5,5	0.49	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
2	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
4	MES	A	1206	-	-	0/6/14/14	0/1/1/1
5	GOL	A	1207	-	-	0/4/4/4	0/0/0/0
2	NAG	B	1201	1	-	0/6/23/26	0/1/1/1
4	MES	B	1205	-	-	0/6/14/14	0/1/1/1
5	GOL	B	1206	-	-	0/4/4/4	0/0/0/0
2	NAG	C	1201	1	-	0/6/23/26	0/1/1/1
4	MES	C	1207	-	-	0/6/14/14	0/1/1/1
5	GOL	C	1208	-	-	0/4/4/4	0/0/0/0
2	NAG	D	1201	1	-	0/6/23/26	0/1/1/1
4	MES	D	1207	-	-	0/6/14/14	0/1/1/1
4	MES	D	1208	-	-	0/6/14/14	0/1/1/1
5	GOL	D	1209	-	-	0/4/4/4	0/0/0/0
5	GOL	D	1210	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1207	MES	O3S-S-O1S	-12.74	81.97	111.61
4	D	1208	MES	O3S-S-O2S	-12.61	82.26	111.61
4	A	1206	MES	O3S-S-O2S	-11.79	84.17	111.61
4	D	1207	MES	O3S-S-O2S	-11.00	86.00	111.61
4	A	1206	MES	O3S-S-O1S	-10.97	86.08	111.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1206	MES	1	0
4	D	1208	MES	3	0
5	D	1210	GOL	10	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	A	431/432 (99%)	0.37	25 (5%) 26 29	22, 37, 68, 100	0
1	B	427/432 (98%)	1.62	117 (27%) 1 1	35, 70, 169, 214	0
1	C	430/432 (99%)	0.71	63 (14%) 3 3	28, 52, 110, 139	0
1	D	431/432 (99%)	0.49	38 (8%) 12 14	21, 39, 71, 128	0
All	All	1719/1728 (99%)	0.80	243 (14%) 4 4	21, 49, 120, 214	0

The worst 5 of 243 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	706	THR	13.8
1	B	709	VAL	13.4
1	B	1023	VAL	12.4
1	B	1067	GLY	10.8
1	B	737	VAL	10.5

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
7	BMA	D	1205	11/12	0.66	0.21	6.57	64,73,76,76	0
7	NAG	C	1202	14/15	0.83	0.17	0.63	75,78,90,93	0
7	NAG	C	1203	14/15	0.80	0.14	0.39	69,78,84,92	0
6	NAG	B	1203	14/15	0.87	0.12	-0.09	75,81,83,88	0
6	NAG	B	1202	14/15	0.80	0.13	-0.40	79,83,91,92	0
3	NAG	A	1202	14/15	0.95	0.10	-0.70	37,39,52,57	0
7	NAG	D	1202	14/15	0.94	0.10	-0.84	37,38,48,53	0
7	NAG	D	1203	14/15	0.94	0.10	-0.86	35,36,44,44	0
3	NAG	A	1203	14/15	0.92	0.11	-1.75	34,38,46,51	0
6	BMA	B	1204	11/12	0.59	0.14	-	88,93,96,99	0
7	BMA	D	1206	11/12	0.79	0.35	-	94,103,107,109	0
7	BMA	C	1206	11/12	0.64	0.44	-	108,113,115,116	0
3	BMA	A	1204	11/12	0.79	0.20	-	101,104,105,106	0
3	BMA	A	1205	11/12	0.83	0.18	-	102,103,104,104	0
7	BMA	C	1205	11/12	0.64	0.29	-	105,110,113,115	0
7	BMA	D	1204	11/12	0.81	0.17	-	51,64,73,84	0
7	BMA	C	1204	11/12	0.81	0.27	-	98,102,107,109	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	D	1210	6/6	0.79	0.33	2.90	33,39,47,47	0
4	MES	A	1206	12/12	0.91	0.18	1.84	52,57,60,60	12
4	MES	D	1208	12/12	0.93	0.19	1.78	55,63,70,71	12
5	GOL	B	1206	6/6	0.90	0.13	1.27	69,70,71,71	0
4	MES	C	1207	12/12	0.94	0.15	0.98	33,40,49,49	12
4	MES	B	1205	12/12	0.96	0.17	0.77	59,67,74,75	0
4	MES	D	1207	12/12	0.95	0.12	-0.12	69,76,81,81	0
5	GOL	C	1208	6/6	0.96	0.08	-0.23	47,54,57,62	0
5	GOL	D	1209	6/6	0.94	0.09	-0.81	35,39,40,43	0
5	GOL	A	1207	6/6	0.94	0.08	-0.84	35,36,39,41	0
2	NAG	D	1201	14/15	0.81	0.29	-	79,89,94,95	0
2	NAG	B	1201	14/15	0.64	0.34	-	129,141,158,160	0
2	NAG	C	1201	14/15	0.71	0.37	-	103,110,114,115	0
2	NAG	A	1201	14/15	0.83	0.31	-	82,96,99,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.