wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:18 PM GMT

PDB ID	:	4C53
Title	:	Crystal Structure of Guanarito virus GP2 in the post-fusion conformation
Authors	:	Parsy, M.; Huiskonen, J.T.; Harlos, K.; Bowden, T.A.
Deposited on	:	2013-09-10
Resolution	:	4.14 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

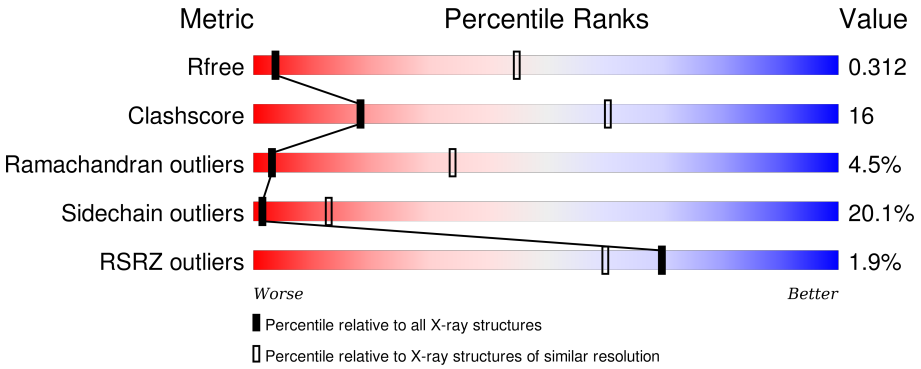
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.14 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	1023 (4.68-3.60)
Clashscore	102246	1122 (4.68-3.60)
Ramachandran outliers	100387	1068 (4.68-3.60)
Sidechain outliers	100360	1054 (4.68-3.60)
RSRZ outliers	91569	1027 (4.68-3.60)

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 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.

Mol	Chain	Length	Quality of chain
1	A	138	3% 38% 26% 8% • 27%
1	B	138	43% 30% 9% • 17%
1	C	138	% 43% 26% • 26%

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
3	NAG	A	1407	-	-	-	X
3	NAG	B	1417	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3007 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 PRE-GLYCOPROTEIN POLYPROTEIN GP COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			837	533	143	154	7			
1	B	115	Total	C	N	O	S	0	0	0
			959	607	164	181	7			
1	C	102	Total	C	N	O	S	0	0	0
			853	547	142	157	7			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	THR	-	EXPRESSION TAG	UNP A1A3Z2
A	291	GLY	-	EXPRESSION TAG	UNP A1A3Z2
A	419	GLY	-	EXPRESSION TAG	UNP A1A3Z2
A	420	THR	-	EXPRESSION TAG	UNP A1A3Z2
A	421	LYS	-	EXPRESSION TAG	UNP A1A3Z2
A	422	HIS	-	EXPRESSION TAG	UNP A1A3Z2
A	423	HIS	-	EXPRESSION TAG	UNP A1A3Z2
A	424	HIS	-	EXPRESSION TAG	UNP A1A3Z2
A	425	HIS	-	EXPRESSION TAG	UNP A1A3Z2
A	426	HIS	-	EXPRESSION TAG	UNP A1A3Z2
A	427	HIS	-	EXPRESSION TAG	UNP A1A3Z2
B	290	THR	-	EXPRESSION TAG	UNP A1A3Z2
B	291	GLY	-	EXPRESSION TAG	UNP A1A3Z2
B	419	GLY	-	EXPRESSION TAG	UNP A1A3Z2
B	420	THR	-	EXPRESSION TAG	UNP A1A3Z2
B	421	LYS	-	EXPRESSION TAG	UNP A1A3Z2
B	422	HIS	-	EXPRESSION TAG	UNP A1A3Z2
B	423	HIS	-	EXPRESSION TAG	UNP A1A3Z2
B	424	HIS	-	EXPRESSION TAG	UNP A1A3Z2
B	425	HIS	-	EXPRESSION TAG	UNP A1A3Z2
B	426	HIS	-	EXPRESSION TAG	UNP A1A3Z2
B	427	HIS	-	EXPRESSION TAG	UNP A1A3Z2
C	290	THR	-	EXPRESSION TAG	UNP A1A3Z2

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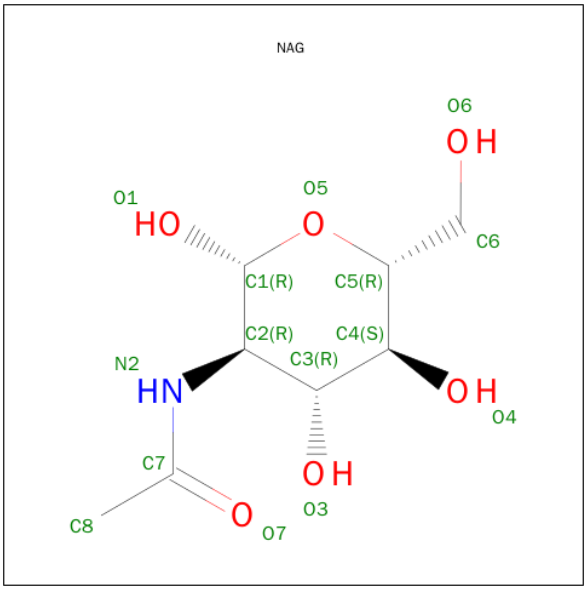
Chain	Residue	Modelled	Actual	Comment	Reference
C	291	GLY	-	EXPRESSION TAG	UNP A1A3Z2
C	419	GLY	-	EXPRESSION TAG	UNP A1A3Z2
C	420	THR	-	EXPRESSION TAG	UNP A1A3Z2
C	421	LYS	-	EXPRESSION TAG	UNP A1A3Z2
C	422	HIS	-	EXPRESSION TAG	UNP A1A3Z2
C	423	HIS	-	EXPRESSION TAG	UNP A1A3Z2
C	424	HIS	-	EXPRESSION TAG	UNP A1A3Z2
C	425	HIS	-	EXPRESSION TAG	UNP A1A3Z2
C	426	HIS	-	EXPRESSION TAG	UNP A1A3Z2
C	427	HIS	-	EXPRESSION TAG	UNP A1A3Z2

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

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

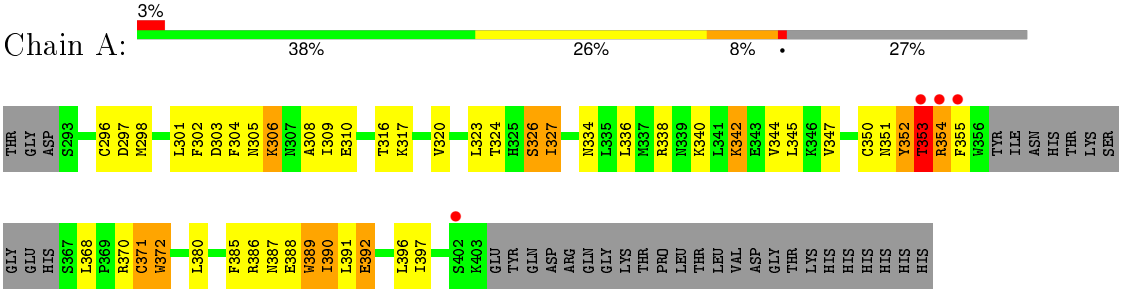
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	7	Total	C	N	O	0	0
			83	46	2	35		
5	C	7	Total	C	N	O	0	0
			83	46	2	35		
5	C	7	Total	C	N	O	0	0
			83	46	2	35		

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.

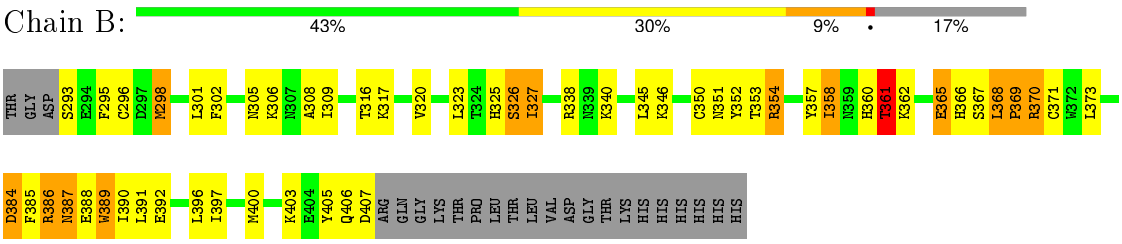
- Molecule 1: PRE-GLYCOPROTEIN POLYPROTEIN GP COMPLEX

Chain A:



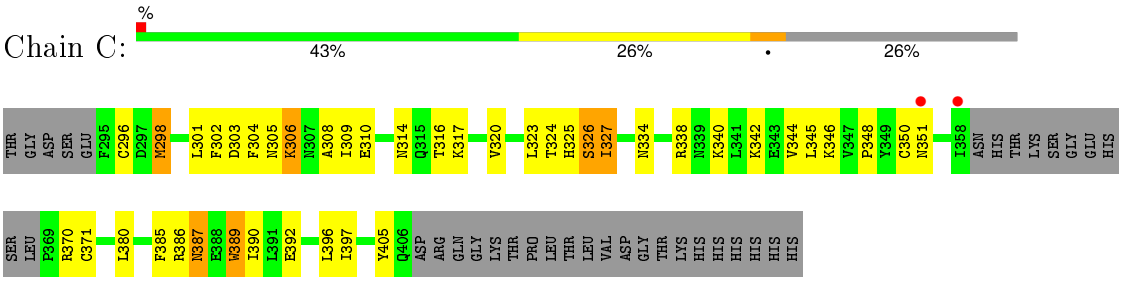
- Molecule 1: PRE-GLYCOPROTEIN POLYPROTEIN GP COMPLEX

Chain B:



- Molecule 1: PRE-GLYCOPROTEIN POLYPROTEIN GP COMPLEX

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	98.50Å 98.50Å 78.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.44 – 4.14 38.44 – 4.14	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.44-4.14) 99.6 (38.44-4.14)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 4.13Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.255 , 0.276 0.293 , 0.312	Depositor DCC
R_{free} test set	259 reflections (4.45%)	DCC
Wilson B-factor (Å^2)	192.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 179.7	EDS
Estimated twinning fraction	0.061 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 5822 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	3007	wwPDB-VP
Average B, all atoms (Å^2)	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: BMA, NAG, 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	0.50	0/853	0.81	1/1150 (0.1%)
1	B	0.53	0/980	0.85	0/1323
1	C	0.50	0/871	0.77	0/1175
All	All	0.51	0/2704	0.81	1/3648 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	351	ASN	C-N-CA	5.12	134.50	121.70

There are no chirality outliers.

There are no planarity outliers.

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	837	0	823	35	0
1	B	959	0	928	36	0
1	C	853	0	833	34	0
2	A	39	0	34	0	0
3	A	28	0	26	0	0
3	B	14	0	13	0	0
4	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	83	0	70	2	0
5	C	166	0	140	10	0
All	All	3007	0	2892	90	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 16.

The worst 5 of 90 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:B:323:LEU:O	1:B:327:ILE:HG22	1.75	0.86
1:C:323:LEU:O	1:C:327:ILE:HG22	1.79	0.82
1:A:323:LEU:O	1:A:327:ILE:HG22	1.79	0.80
1:C:350:CYS:HG	1:C:371:CYS:HG	0.81	0.80
1:A:303:ASP:HA	1:A:306:LYS:HG2	1.69	0.74

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	97/138 (70%)	91 (94%)	3 (3%)	3 (3%)	5 44
1	B	113/138 (82%)	98 (87%)	5 (4%)	10 (9%)	1 17
1	C	98/138 (71%)	92 (94%)	5 (5%)	1 (1%)	19 65
All	All	308/414 (74%)	281 (91%)	13 (4%)	14 (4%)	3 34

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	THR

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Mol	Chain	Res	Type
1	A	371	CYS
1	B	352	TYR
1	B	365	GLU
1	B	367	SER

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	96/130 (74%)	75 (78%)	21 (22%)	1	10
1	B	110/130 (85%)	86 (78%)	24 (22%)	1	10
1	C	97/130 (75%)	81 (84%)	16 (16%)	3	21
All	All	303/390 (78%)	242 (80%)	61 (20%)	1	13

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	340	LYS
1	B	366	HIS
1	C	386	ARG
1	B	346	LYS
1	B	358	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	C	339	ASN

5.3.3 RNA

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)

26 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	$\#\|Z\|>2$
2	NAG	A	1404	1,2	14,14,15	0.65	0	15,19,21	1.09	1 (6%)
2	NAG	A	1405	2	14,14,15	0.83	0	15,19,21	1.04	2 (13%)
2	BMA	A	1406	2	11,11,12	0.71	0	14,15,17	0.82	1 (7%)
4	NAG	B	1408	1,4	14,14,15	0.77	0	15,19,21	1.30	3 (20%)
4	NAG	B	1409	4	14,14,15	0.64	0	15,19,21	1.08	1 (6%)
5	NAG	B	1410	1,5	14,14,15	0.66	0	15,19,21	1.33	3 (20%)
5	NAG	B	1411	5	14,14,15	0.71	0	15,19,21	1.12	0
5	BMA	B	1412	5	11,11,12	0.53	0	14,15,17	0.80	0
5	MAN	B	1413	5	11,11,12	0.70	0	14,15,17	0.81	0
5	MAN	B	1414	5	11,11,12	0.64	0	14,15,17	0.74	0
5	MAN	B	1415	5	11,11,12	0.59	0	14,15,17	0.81	0
5	MAN	B	1416	5	11,11,12	0.50	0	14,15,17	0.82	0
5	NAG	C	1407	1,5	14,14,15	0.73	0	15,19,21	1.37	3 (20%)
5	NAG	C	1408	5	14,14,15	0.75	0	15,19,21	1.16	0
5	BMA	C	1409	5	11,11,12	0.52	0	14,15,17	0.87	0
5	MAN	C	1410	5	11,11,12	0.63	0	14,15,17	0.94	1 (7%)
5	MAN	C	1411	5	11,11,12	0.66	0	14,15,17	0.76	0
5	MAN	C	1412	5	11,11,12	0.60	0	14,15,17	0.81	0
5	MAN	C	1413	5	11,11,12	0.49	0	14,15,17	0.81	0
5	NAG	C	1414	1,5	14,14,15	0.73	0	15,19,21	1.35	2 (13%)
5	NAG	C	1415	5	14,14,15	0.59	0	15,19,21	1.16	2 (13%)
5	BMA	C	1416	5	11,11,12	0.75	0	14,15,17	0.72	0
5	MAN	C	1417	5	11,11,12	0.72	0	14,15,17	0.91	0
5	MAN	C	1418	5	11,11,12	0.72	0	14,15,17	0.70	0
5	MAN	C	1419	5	11,11,12	0.71	0	14,15,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	C	1420	5	11,11,12	0.54	0	14,15,17	0.73	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	1404	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1405	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1406	2	-	0/2/19/22	0/1/1/1
4	NAG	B	1408	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1409	4	-	0/6/23/26	0/1/1/1
5	NAG	B	1410	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1411	5	-	0/6/23/26	0/1/1/1
5	BMA	B	1412	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1413	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1414	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1415	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1416	5	-	0/2/19/22	0/1/1/1
5	NAG	C	1407	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1408	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1409	5	-	0/2/19/22	0/1/1/1
5	MAN	C	1410	5	-	0/2/19/22	0/1/1/1
5	MAN	C	1411	5	-	0/2/19/22	0/1/1/1
5	MAN	C	1412	5	-	0/2/19/22	0/1/1/1
5	MAN	C	1413	5	-	0/2/19/22	0/1/1/1
5	NAG	C	1414	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1415	5	-	0/6/23/26	0/1/1/1
5	BMA	C	1416	5	-	0/2/19/22	0/1/1/1
5	MAN	C	1417	5	-	0/2/19/22	0/1/1/1
5	MAN	C	1418	5	-	0/2/19/22	0/1/1/1
5	MAN	C	1419	5	-	0/2/19/22	0/1/1/1
5	MAN	C	1420	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1414	NAG	C4-C3-C2	-2.70	107.02	111.23
4	B	1408	NAG	C1-O5-C5	-2.65	108.89	112.25
5	B	1410	NAG	C4-C3-C2	-2.54	107.29	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1415	NAG	C4-C3-C2	-2.36	107.56	111.23
5	C	1407	NAG	C4-C3-C2	-2.31	107.64	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1411	NAG	2	0
5	B	1412	BMA	2	0
5	C	1408	NAG	2	0
5	C	1409	BMA	2	0
5	C	1414	NAG	2	0
5	C	1415	NAG	1	0
5	C	1416	BMA	2	0
5	C	1417	MAN	4	0
5	C	1418	MAN	2	0
5	C	1419	MAN	3	0
5	C	1420	MAN	1	0

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
3	NAG	A	1407	1	14,14,15	0.76	0	15,19,21	1.20	2 (13%)
3	NAG	A	1408	1	14,14,15	0.65	0	15,19,21	1.39	3 (20%)
3	NAG	B	1417	1	14,14,15	0.75	0	15,19,21	1.20	2 (13%)

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	1407	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1417	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1408	NAG	C2-N2-C7	-2.44	119.90	123.04
3	A	1408	NAG	C4-C3-C2	-2.41	107.49	111.23
3	B	1417	NAG	C4-C3-C2	-2.37	107.55	111.23
3	A	1407	NAG	C4-C3-C2	-2.34	107.58	111.23
3	A	1407	NAG	C8-C7-N2	2.48	120.85	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	101/138 (73%)	0.03	4 (3%) 42 32	131, 220, 273, 279	0
1	B	115/138 (83%)	-0.15	0 100 100	124, 215, 260, 270	0
1	C	102/138 (73%)	-0.11	2 (1%) 68 58	132, 213, 276, 293	0
All	All	318/414 (76%)	-0.08	6 (1%) 70 60	124, 216, 273, 293	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	ARG	5.3
1	A	353	THR	3.7
1	A	355	PHE	2.8
1	C	351	ASN	2.6
1	C	358	ILE	2.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	MAN	C	1411	11/12	0.17	0.72	-	300,300,300,300	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BMA	B	1412	11/12	0.31	0.51	-	297,297,297,297	0
2	NAG	A	1404	14/15	0.47	0.63	-	283,289,293,293	0
5	MAN	C	1412	11/12	0.60	0.43	-	300,300,300,300	0
5	MAN	C	1420	11/12	0.76	0.29	-	296,296,296,296	0
5	NAG	C	1414	14/15	0.87	0.30	-	275,278,284,287	0
5	MAN	B	1414	11/12	0.57	0.89	-	300,300,300,300	0
5	MAN	C	1410	11/12	0.41	0.58	-	300,300,300,300	0
4	NAG	B	1408	14/15	0.82	0.35	-	259,262,268,274	0
5	MAN	B	1416	11/12	0.60	0.59	-	300,300,300,300	0
4	NAG	B	1409	14/15	0.74	0.55	-	278,278,278,278	0
5	MAN	B	1415	11/12	0.48	0.70	-	300,300,300,300	0
5	MAN	C	1418	11/12	0.89	0.24	-	300,300,300,300	0
5	MAN	C	1419	11/12	0.78	0.38	-	300,300,300,300	0
5	MAN	B	1413	11/12	0.47	0.77	-	300,300,300,300	0
5	NAG	C	1407	14/15	0.81	0.52	-	275,282,284,284	0
5	NAG	C	1408	14/15	0.84	0.52	-	294,294,294,294	0
5	BMA	C	1416	11/12	0.56	0.40	-	299,299,299,299	0
5	BMA	C	1409	11/12	0.69	0.39	-	298,298,298,298	0
2	NAG	A	1405	14/15	0.86	0.65	-	292,292,292,292	0
5	NAG	B	1410	14/15	0.85	0.21	-	269,274,274,274	0
5	MAN	C	1413	11/12	0.70	0.35	-	297,297,297,297	0
5	MAN	C	1417	11/12	0.79	0.39	-	300,300,300,300	0
2	BMA	A	1406	11/12	0.57	0.40	-	293,293,293,293	0
5	NAG	C	1415	14/15	0.72	0.40	-	293,293,293,293	0
5	NAG	B	1411	14/15	0.72	0.23	-	288,288,288,288	0

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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	1407	14/15	0.63	1.20	7.87	262,263,265,265	0
3	NAG	B	1417	14/15	0.82	0.93	4.98	260,267,269,270	0
3	NAG	A	1408	14/15	0.66	0.61	-	279,279,279,279	0

6.5 Other polymers (i)

There are no such residues in this entry.