



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:54 PM BST

PDB ID : 3J9F
EMDB ID: : EMD-6243
Title : Poliovirus complexed with soluble, deglycosylated poliovirus receptor (Pvr) at 4 degrees C
Authors : Strauss, M.; Filman, D.J.; Belnap, D.M.; Cheng, N.; Noel, R.T.; Hogle, J.M.
Deposited on : 2015-01-15
Resolution : 9.00 Å(reported)
Based on PDB ID : 1HXS

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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) : trunk27241

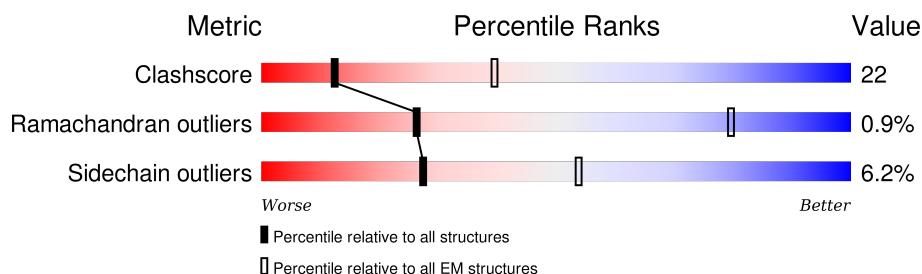
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	302	71% 22% • 6%
2	2	272	77% 19% ••
3	3	238	70% 26% •••
4	4	69	55% 38% 7%
5	7	116	56% 33% 11%
6	8	102	56% 34% 10%
7	9	92	68% 26% 5%

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
12	NAG	9	401	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 9313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	283	Total	C	N	O	S	0	0
			2221	1416	378	422	5		

- Molecule 2 is a protein called Protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	267	Total	C	N	O	S	0	0
			2075	1312	357	392	14		

- Molecule 3 is a protein called Protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	235	Total	C	N	O	S	0	0
			1834	1169	299	349	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	CONFLICT	UNP P03300

- Molecule 4 is a protein called Protein VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	69	Total	C	N	O	S	0	0
			534	333	91	109	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	MYR	-	MYRISTOYLATION	UNP P03300

- Molecule 5 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	116	Total	C	N	O	S	2	0
			904	572	159	168	5		

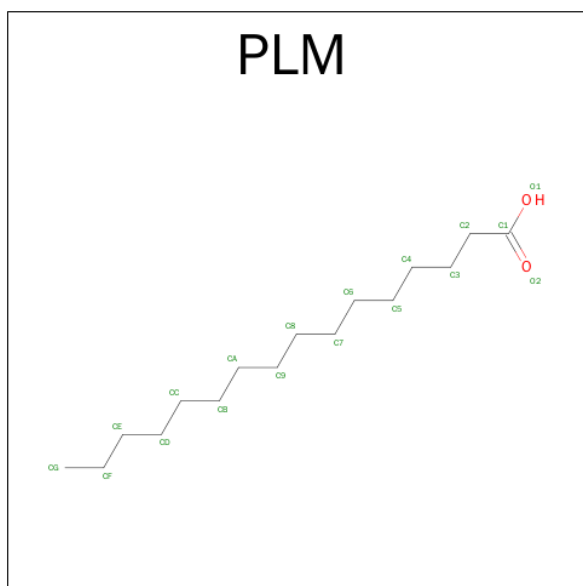
- Molecule 6 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	102	Total	C	N	O	S	4	0
			771	489	130	148	4		

- Molecule 7 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	92	Total	C	N	O	S	2	0
			699	440	118	138	3		

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
8	1	1	Total	C	O	0
			18	16	2	

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				AltConf
9	7	3	Total	C	N	O	0
			39	22	2	15	

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Mol	Chain	Residues	Atoms				AltConf
9	8	3	Total	C	N	O	0
			39	22	2	15	

- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				AltConf
10	7	5	Total	C	N	O	0
			60	34	2	24	

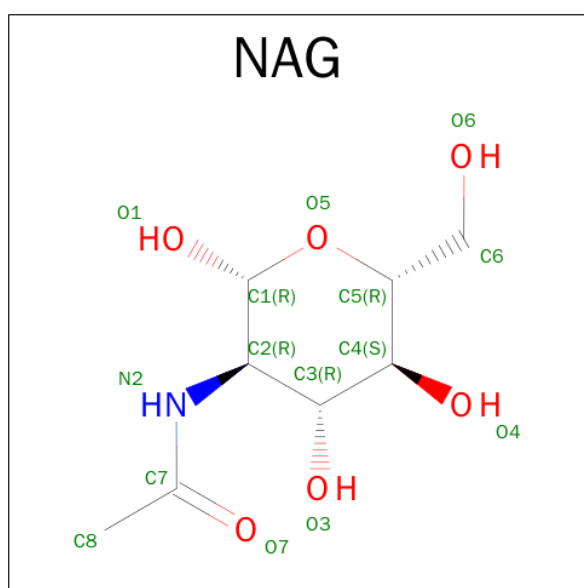
- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				AltConf
11	8	2	Total	C	N	O	0
			56	32	4	20	
11	8	2	Total	C	N	O	0
			56	32	4	20	

- Molecule 12 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				AltConf
12	9	4	Total	C	N	O	0
			49	28	2	19	

- Molecule 13 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

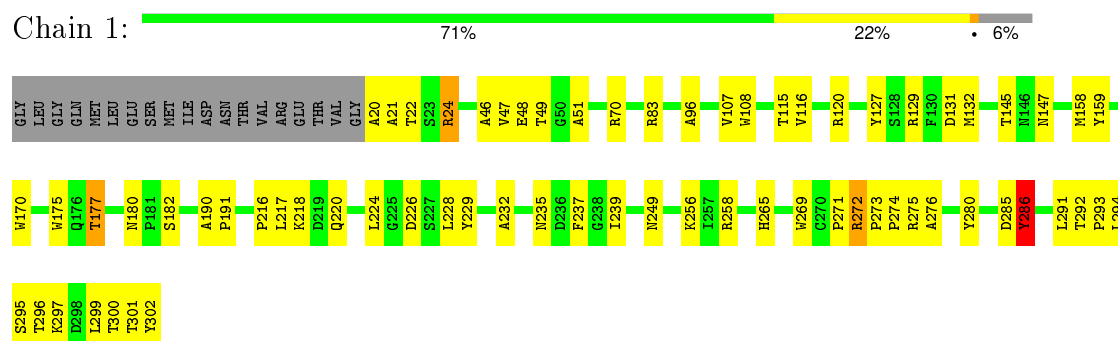


Mol	Chain	Residues	Atoms				AltConf
13	9	1	Total	C	N	O	0
			14	8	1	5	

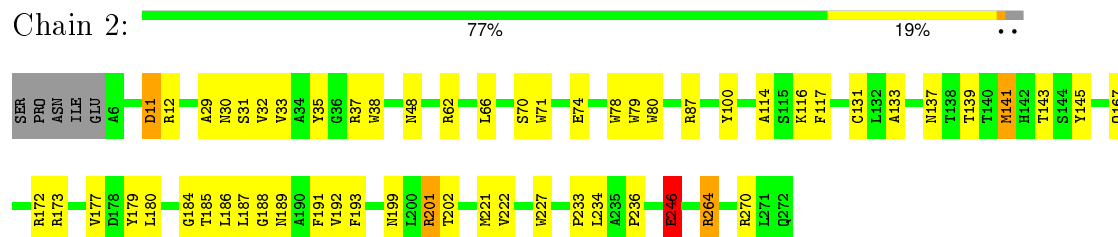
3 Residue-property plots

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. 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. 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.

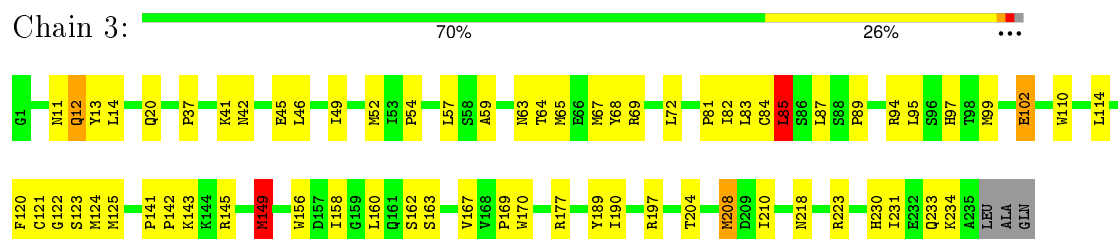
• Molecule 1: Protein VP1



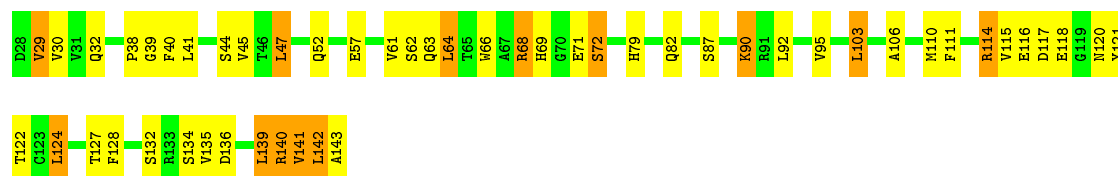
• Molecule 2: Protein VP2



• Molecule 3: Protein VP3

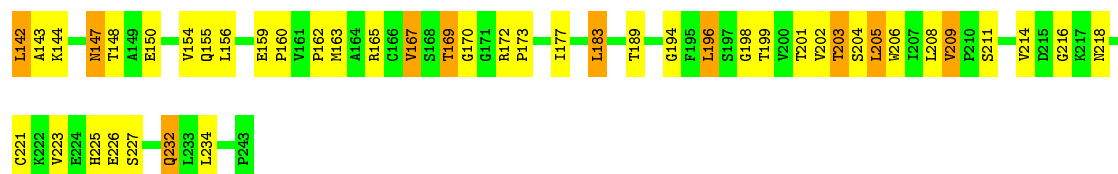


Chain 7:  56% 33% 11%



• Molecule 6: Poliovirus receptor

Chain 8:  56% 34% 10%



• Molecule 7: Poliovirus receptor

Chain 9:  68% 26% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	3822	Depositor
Resolution determination method	FSC 0.5	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Kodak SO-163 film	Depositor

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, MYR, FUC, PLM, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.78	0/2284	1.49	26/3124 (0.8%)
2	2	0.79	0/2132	1.46	29/2916 (1.0%)
3	3	0.85	3/1881 (0.2%)	1.53	21/2562 (0.8%)
4	4	0.91	0/528	1.57	7/714 (1.0%)
5	7	0.69	0/925	0.61	0/1258
6	8	0.67	0/790	0.56	0/1083
7	9	0.56	0/717	0.51	0/987
All	All	0.78	3/9257 (0.0%)	1.32	83/12644 (0.7%)

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
2	2	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	42	ASN	C-N	9.49	1.55	1.34
3	3	102	GLU	CB-CG	8.28	1.67	1.52
3	3	102	GLU	CD-OE2	6.35	1.32	1.25

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	12	GLN	O-C-N	25.53	163.54	122.70
3	3	12	GLN	CA-C-N	-22.88	66.87	117.20
1	1	83	ARG	NE-CZ-NH2	-20.79	109.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	12	GLN	C-N-CA	-18.74	74.85	121.70
1	1	83	ARG	NE-CZ-NH1	18.22	129.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	11	ASP	Mainchain

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	1	2221	0	2173	133	0
2	2	2075	0	1994	109	0
3	3	1834	0	1816	128	0
4	4	534	0	524	45	0
5	7	904	0	877	132	0
6	8	771	0	766	106	0
7	9	699	0	674	20	0
8	1	18	0	31	5	0
9	7	39	0	34	1	0
9	8	39	0	34	2	0
10	7	60	0	52	2	0
11	8	56	0	50	3	0
12	9	49	0	43	8	0
13	9	14	0	13	1	0
All	All	9313	0	9081	406	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 22.

The worst 5 of 406 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)
5:7:140:ARG:HG2	6:8:142[B]:LEU:CD2	1.39	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:7:115:VAL:CG1	6:8:198:GLY:HA3	1.07	1.51
5:7:115:VAL:HG11	6:8:198:GLY:CA	1.01	1.46
5:7:140:ARG:CG	6:8:142[B]:LEU:HD23	1.46	1.43
5:7:41:LEU:CG	6:8:143[B]:ALA:HB2	1.51	1.37

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 PDB entries followed by that with respect to all EM entries.

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	1	281/302 (93%)	272 (97%)	8 (3%)	1 (0%)	39	80
2	2	265/272 (97%)	252 (95%)	11 (4%)	2 (1%)	24	69
3	3	233/238 (98%)	223 (96%)	10 (4%)	0	100	100
4	4	66/69 (96%)	54 (82%)	6 (9%)	6 (9%)	1	17
5	7	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
6	8	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
7	9	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	17	63
All	All	1149/1191 (96%)	1085 (94%)	54 (5%)	10 (1%)	26	67

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	15	ASN
4	4	23	SER
4	4	24	THR
4	4	19	ALA
4	4	21	GLY

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 PDB entries followed by that with respect to all EM entries.

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	1	245/261 (94%)	241 (98%)	4 (2%)	70	88
2	2	227/232 (98%)	221 (97%)	6 (3%)	54	80
3	3	210/212 (99%)	205 (98%)	5 (2%)	57	82
4	4	57/57 (100%)	54 (95%)	3 (5%)	28	64
5	7	99/99 (100%)	80 (81%)	19 (19%)	2	13
6	8	90/90 (100%)	75 (83%)	15 (17%)	3	19
7	9	77/77 (100%)	67 (87%)	10 (13%)	5	28
All	All	1005/1028 (98%)	943 (94%)	62 (6%)	27	60

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	7	103	LEU
5	7	140	ARG
7	9	302	VAL
5	7	124	LEU
5	7	142[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	218	ASN
7	9	322	GLN
5	7	52	GLN
2	2	272	GLN
4	4	31	ASN

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 ⓘ

19 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$
9	NAG	7	401	9,5	14,14,15	0.94	0	15,19,21	0.98	1 (6%)
9	NAG	7	402	9	14,14,15	0.52	0	15,19,21	0.90	0
9	BMA	7	403	9	11,11,12	0.63	0	15,15,17	1.04	0
10	NAG	7	404	10,5	14,14,15	1.04	1 (7%)	15,19,21	1.83	4 (26%)
10	NAG	7	405	10	14,14,15	0.73	0	15,19,21	1.32	2 (13%)
10	FUC	7	406	10	10,10,11	0.90	0	13,14,16	1.66	3 (23%)
10	BMA	7	407	10	11,11,12	0.27	0	15,15,17	0.60	0
10	MAN	7	408	10	11,11,12	0.65	0	15,15,17	0.58	0
11	NAG	8	301	11,6	14,14,15	0.77	0	15,19,21	1.53	3 (20%)
11	NAG	8	302	11	14,14,15	0.68	0	15,19,21	0.96	1 (6%)
11	NAG	8	303	11,6	14,14,15	0.72	0	15,19,21	0.79	0
11	NAG	8	304	11	14,14,15	0.66	0	15,19,21	0.96	0
9	NAG	8	305	9,6	14,14,15	0.71	0	15,19,21	1.14	3 (20%)
9	NAG	8	306	9	14,14,15	0.45	0	15,19,21	1.23	1 (6%)
9	BMA	8	307	9	11,11,12	0.27	0	15,15,17	0.58	0
12	NAG	9	401	12,7	14,14,15	0.55	0	15,19,21	0.59	0
12	FUC	9	402	12	10,10,11	0.76	0	13,14,16	1.24	2 (15%)
12	NAG	9	403	12	14,14,15	0.55	0	15,19,21	1.18	1 (6%)
12	BMA	9	404	12	11,11,12	0.25	0	15,15,17	0.59	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
9	NAG	7	401	9,5	-	0/6/23/26	0/1/1/1
9	NAG	7	402	9	-	0/6/23/26	0/1/1/1
9	BMA	7	403	9	-	0/2/19/22	1/1/1/1
10	NAG	7	404	10,5	-	0/6/23/26	0/1/1/1
10	NAG	7	405	10	-	0/6/23/26	0/1/1/1
10	FUC	7	406	10	-	0/0/17/20	0/1/1/1
10	BMA	7	407	10	-	0/2/19/22	0/1/1/1
10	MAN	7	408	10	-	0/2/19/22	0/1/1/1
11	NAG	8	301	11,6	-	0/6/23/26	0/1/1/1
11	NAG	8	302	11	-	0/6/23/26	0/1/1/1
11	NAG	8	303	11,6	-	0/6/23/26	0/1/1/1
11	NAG	8	304	11	-	0/6/23/26	0/1/1/1
9	NAG	8	305	9,6	-	0/6/23/26	0/1/1/1
9	NAG	8	306	9	-	0/6/23/26	0/1/1/1
9	BMA	8	307	9	-	0/2/19/22	0/1/1/1
12	NAG	9	401	12,7	-	0/6/23/26	0/1/1/1
12	FUC	9	402	12	-	0/0/17/20	0/1/1/1
12	NAG	9	403	12	-	0/6/23/26	0/1/1/1
12	BMA	9	404	12	-	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)
10	7	404	NAG	C1-C2	-2.17	1.49	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	7	406	FUC	O5-C1-C2	-3.68	105.02	110.89
10	7	404	NAG	O4-C4-C3	-3.59	102.27	110.36
10	7	405	NAG	O5-C5-C4	-2.92	105.30	110.13
11	8	301	NAG	O5-C5-C4	-2.61	105.82	110.13
11	8	302	NAG	O5-C5-C4	-2.46	106.06	110.13

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	7	403	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	7	401	NAG	1	0
10	7	404	NAG	1	0
10	7	406	FUC	2	0
11	8	303	NAG	3	0
9	8	305	NAG	2	0
12	9	401	NAG	8	0
12	9	402	FUC	3	0
12	9	403	NAG	4	0

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
8	PLM	1	901	-	14,17,17	0.61	0	14,17,17	0.78	0
13	NAG	9	405	7	14,14,15	1.31	1 (7%)	15,19,21	1.47	1 (6%)

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
8	PLM	1	901	-	-	0/13/15/15	0/0/0/0
13	NAG	9	405	7	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	9	405	NAG	C1-C2	3.58	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
13	9	405	NAG	C1-O5-C5	4.10	118.17	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	1	901	PLM	5	0
13	9	405	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.