Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:51 PM GMT

PDB ID	:	4MZE
Title	:	Crystal structure of hPIV3 hemagglutinin-neuraminidase, H552Q/Q559R mutant
Authors	:	Xu, R.; Wilson, I.A.
Deposited on	:	2013-09-30
Resolution	:	1.80 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 ①) were used in the production of this report:

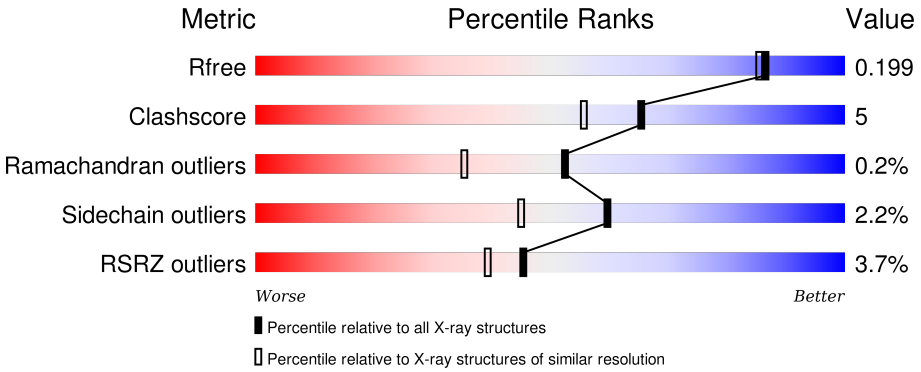
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	437	4% 89% 9%
1	B	437	3% 89% 9%

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
10	MAN	B	605	-	-	-	X
2	NAG	A	601	-	-	-	X
5	PO4	B	610[A]	-	-	-	X
5	PO4	B	610[B]	-	-	-	X
7	EDO	A	618	-	-	-	X
7	EDO	A	619	-	-	-	X
7	EDO	B	616	-	-	-	X
8	PEG	A	622	-	-	X	X
8	PEG	A	623	-	-	X	X
8	PEG	B	621	-	-	X	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7803 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.

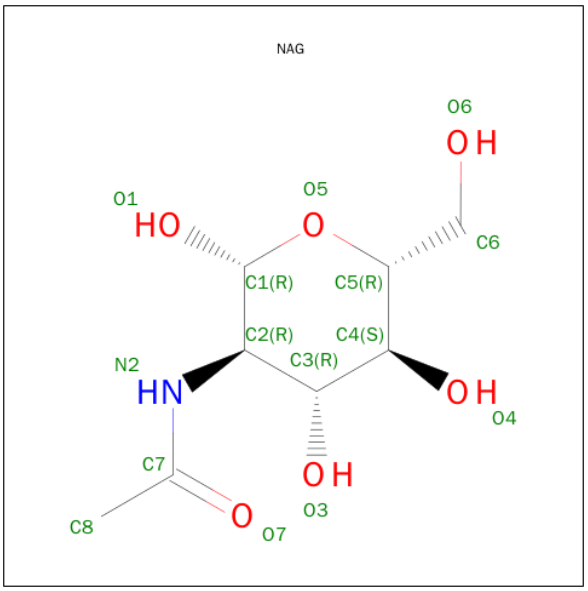
- Molecule 1 is a protein called Hemagglutinin-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	6	0
			3409	2155	586	647	21			
1	B	432	Total	C	N	O	S	0	2	0
			3395	2145	586	644	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLN	HIS	ENGINEERED MUTATION	UNP P08492
A	559	ARG	GLN	ENGINEERED MUTATION	UNP P08492
B	552	GLN	HIS	ENGINEERED MUTATION	UNP P08492
B	559	ARG	GLN	ENGINEERED MUTATION	UNP P08492

- 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 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0

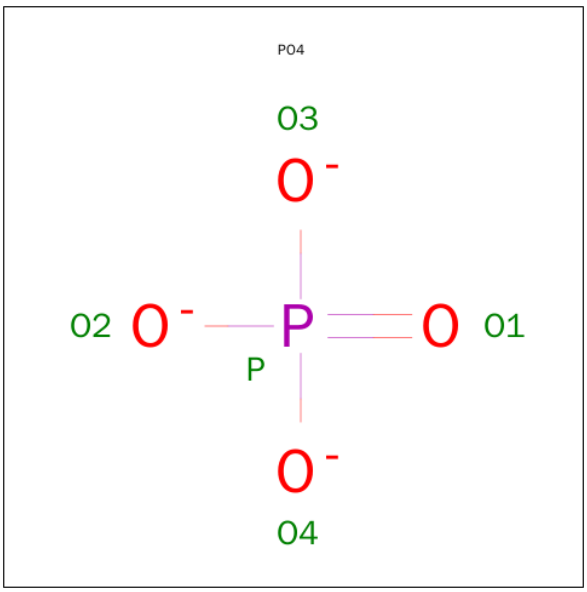
- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total C N O 94 52 2 40	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total C N O 24 14 1 9	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

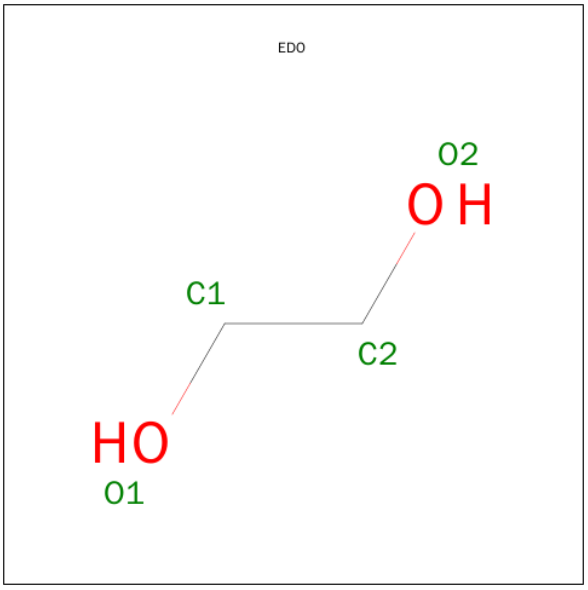


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 10 8 2	0	1
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	A	1	Total Ca 1 1	0	0

- 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	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

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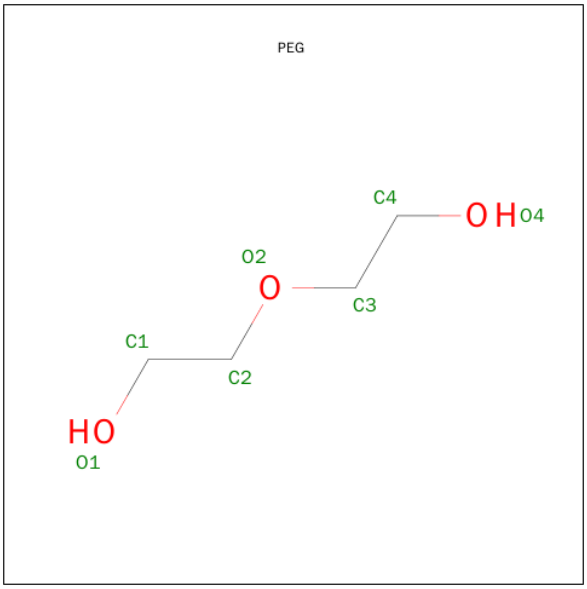
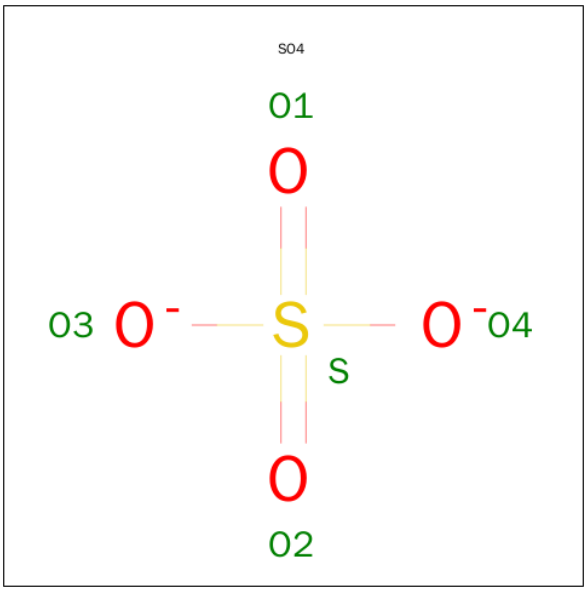
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 7 4 3	0	0
8	A	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0
8	B	1	Total C O 7 4 3	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0

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

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

- Molecule 11 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 12 is water.

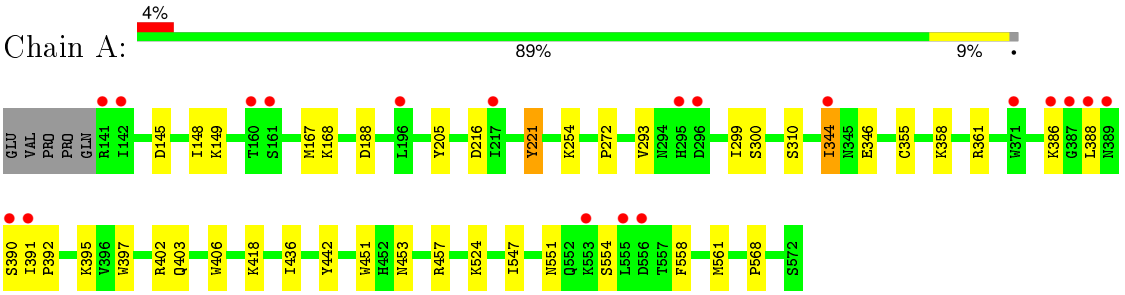
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	336	Total O 336 336	0	0
12	B	302	Total O 302 302	0	0

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.

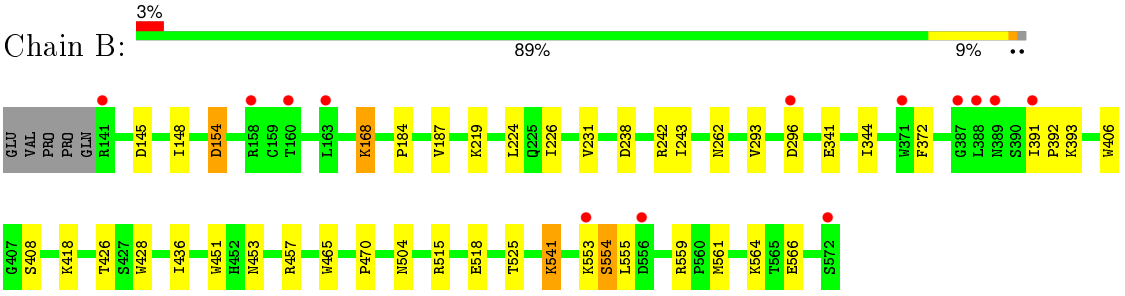
- Molecule 1: Hemagglutinin-neuraminidase

Chain A:



- Molecule 1: Hemagglutinin-neuraminidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.03Å 96.64Å 105.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.92 – 1.80 28.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.92-1.80) 99.6 (28.92-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.161 , 0.196 0.165 , 0.199	Depositor DCC
R_{free} test set	4010 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 79888 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7803	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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, PO4, EDO, SO4, FUL, PEG, CA, 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	0.68	0/3507	0.75	0/4775
1	B	0.67	0/3481	0.76	1/4741 (0.0%)
All	All	0.67	0/6988	0.75	1/9516 (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	B	561	MET	CG-SD-CE	-5.63	91.19	100.20

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	3409	0	3390	33	0
1	B	3395	0	3366	30	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	94	0	79	0	0
4	A	24	0	22	0	0
5	A	5	0	0	0	0
5	B	15	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	32	0	48	10	0
7	B	28	0	42	3	0
8	A	14	0	20	9	0
8	B	14	0	20	8	0
9	A	5	0	0	0	0
10	B	61	0	52	0	0
11	B	39	0	34	0	0
12	A	336	0	0	5	0
12	B	302	0	0	4	0
All	All	7803	0	7099	71	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 5.

All (71) 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:238:ASP:OD1	1:B:564:LYS:NZ	2.11	0.84
1:A:216:ASP:HB2	8:A:622:PEG:H32	1.62	0.80
1:B:148:ILE:HD11	1:B:231:VAL:HG23	1.66	0.77
5:B:610[B]:PO4:O1	12:B:963:HOH:O	2.03	0.76
1:B:541:LYS:NZ	1:B:566:GLU:OE2	2.19	0.75
1:B:393:LYS:NZ	12:B:920:HOH:O	2.25	0.70
1:B:154:ASP:OD2	1:B:418:LYS:NZ	2.27	0.67
1:A:524:LYS:HE3	8:A:623:PEG:H12	1.76	0.67
1:A:386:LYS:HE2	1:A:392:PRO:HD3	1.82	0.60
1:A:402:ARG:HH11	7:A:616:EDO:H11	1.68	0.59
1:B:372:PHE:CZ	8:B:621:PEG:H42	2.37	0.58
1:B:408[B]:SER:HA	8:B:621:PEG:H22	1.85	0.58
1:A:168:LYS:H	7:A:619:EDO:H22	1.69	0.57
1:B:262:ASN:HB2	7:B:616:EDO:H11	1.85	0.57
1:A:293:VAL:HG22	1:A:299:ILE:HG12	1.88	0.56
8:B:620:PEG:H32	12:B:839:HOH:O	2.05	0.56
1:A:344:ILE:HD12	1:A:346:GLU:HG3	1.87	0.55
1:B:408[A]:SER:HA	8:B:621:PEG:H22	1.88	0.55
1:B:426:THR:OG1	8:B:621:PEG:H12	2.06	0.55
1:B:406:TRP:HE1	8:B:621:PEG:C3	2.21	0.54
1:B:451:TRP:CZ2	1:B:453:ASN:HB2	2.46	0.51
1:A:205:TYR:HE1	1:A:547:ILE:HD13	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASP:HB2	1:A:148:ILE:HD12	1.93	0.51
1:B:145:ASP:HB2	1:B:148:ILE:HD12	1.93	0.50
1:B:504:ASN:OD1	7:B:619:EDO:H11	2.10	0.50
1:B:418:LYS:HD3	1:B:436:ILE:HD13	1.92	0.50
1:A:221:TYR:HB3	7:A:617:EDO:H12	1.94	0.50
1:A:167[B]:MET:HG2	1:A:568:PRO:HB2	1.94	0.49
1:A:524:LYS:HG3	12:A:1024:HOH:O	2.13	0.49
1:B:406:TRP:HE1	8:B:621:PEG:H32	1.78	0.48
1:B:451:TRP:CH2	1:B:453:ASN:HB2	2.48	0.48
8:A:622:PEG:H22	12:A:864:HOH:O	2.13	0.47
8:A:623:PEG:H32	8:A:623:PEG:H12	1.61	0.47
8:B:620:PEG:H41	8:B:620:PEG:H21	1.56	0.47
1:A:344:ILE:HD13	12:A:928:HOH:O	2.13	0.47
1:B:391:ILE:HD12	1:B:392:PRO:HD2	1.96	0.47
7:A:618:EDO:H12	12:A:1030:HOH:O	2.13	0.47
1:A:205:TYR:CE1	1:A:547:ILE:HD13	2.50	0.47
1:B:184:PRO:HD2	1:B:559:ARG:NH1	2.28	0.47
8:A:623:PEG:H21	12:A:793:HOH:O	2.16	0.46
1:A:451:TRP:CZ2	1:A:453:ASN:HB2	2.51	0.46
1:B:168:LYS:NZ	1:B:168:LYS:HB3	2.31	0.46
1:A:272:PRO:HG3	8:A:622:PEG:H42	1.99	0.45
1:B:554:SER:OG	5:B:611:PO4:O2	2.28	0.45
1:A:388:LEU:H	1:A:388:LEU:HD12	1.81	0.45
1:B:341:GLU:OE2	12:B:974:HOH:O	2.21	0.44
1:B:525:THR:O	1:B:553:LYS:NZ	2.42	0.44
1:B:553:LYS:C	1:B:555:LEU:H	2.19	0.43
1:A:403:GLN:HE21	7:A:616:EDO:H12	1.83	0.43
1:B:515:ARG:NE	1:B:518:GLU:OE1	2.35	0.43
7:A:620:EDO:H21	8:A:622:PEG:H41	1.99	0.43
1:A:149:LYS:HA	1:A:149:LYS:HD3	1.92	0.43
1:A:310[B]:SER:HB2	1:A:395:LYS:HG2	2.00	0.43
1:B:465:TRP:CE2	7:B:615:EDO:H21	2.54	0.43
1:A:254:LYS:HD2	8:A:622:PEG:H31	2.01	0.43
1:A:167[B]:MET:HA	7:A:619:EDO:H22	2.01	0.42
1:A:167[A]:MET:HA	7:A:619:EDO:H22	2.01	0.42
1:B:428:TRP:CG	1:B:470:PRO:HA	2.54	0.42
1:A:188:ASP:N	1:A:188:ASP:OD1	2.31	0.42
1:A:551:ASN:HB2	1:A:558:PHE:CE1	2.55	0.42
1:A:451:TRP:CH2	1:A:453:ASN:HB2	2.55	0.41
1:A:397:TRP:CD2	1:A:442:TYR:HB3	2.54	0.41
1:A:355:CYS:HB3	1:A:358:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ARG:NH1	7:A:616:EDO:H11	2.35	0.41
1:A:406:TRP:HE1	7:A:618:EDO:H11	1.86	0.41
1:B:428:TRP:CD2	1:B:470:PRO:HA	2.55	0.41
1:B:224:LEU:HD23	1:B:293:VAL:HG21	2.01	0.41
1:B:226:ILE:HD12	1:B:243:ILE:HD11	2.03	0.40
1:A:310[A]:SER:HB3	1:A:395:LYS:HG2	2.02	0.40
1:A:418:LYS:HD3	1:A:436:ILE:HD13	2.02	0.40
1:A:524:LYS:HE3	8:A:623:PEG:H32	2.02	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	436/437 (100%)	412 (94%)	23 (5%)	1 (0%)	52 35
1	B	432/437 (99%)	408 (94%)	23 (5%)	1 (0%)	52 35
All	All	868/874 (99%)	820 (94%)	46 (5%)	2 (0%)	52 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	554	SER
1	B	554	SER

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	397/396 (100%)	389 (98%)	8 (2%)	63 49
1	B	393/396 (99%)	384 (98%)	9 (2%)	58 42
All	All	790/792 (100%)	773 (98%)	17 (2%)	60 45

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	TYR
1	A	300	SER
1	A	344	ILE
1	A	361	ARG
1	A	390	SER
1	A	391	ILE
1	A	457	ARG
1	A	561	MET
1	B	154	ASP
1	B	168	LYS
1	B	187	VAL
1	B	219	LYS
1	B	242	ARG
1	B	296	ASP
1	B	344	ILE
1	B	457	ARG
1	B	541	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

18 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	602	1,3	14,14,15	1.03	1 (7%)	15,19,21	0.50	0
3	NAG	A	603	3	14,14,15	0.49	0	15,19,21	0.63	1 (6%)
3	BMA	A	604	3	11,11,12	1.06	1 (9%)	14,15,17	0.74	0
3	MAN	A	605	3	11,11,12	1.53	3 (27%)	14,15,17	1.69	3 (21%)
3	MAN	A	606	3	11,11,12	1.45	2 (18%)	14,15,17	1.21	1 (7%)
3	MAN	A	607	3	11,11,12	1.21	2 (18%)	14,15,17	1.06	1 (7%)
3	MAN	A	608	3	11,11,12	0.92	0	14,15,17	1.28	2 (14%)
3	MAN	A	609	3	11,11,12	1.03	0	14,15,17	1.37	3 (21%)
4	NAG	A	610	1,4	14,14,15	0.51	0	15,19,21	0.63	1 (6%)
4	FUL	A	611	4	10,10,11	1.02	1 (10%)	14,14,16	2.17	4 (28%)
10	NAG	B	601	1,10	14,14,15	0.63	0	15,19,21	0.32	0
10	NAG	B	602	10	14,14,15	0.31	0	15,19,21	0.38	0
10	BMA	B	603	10	11,11,12	0.87	0	14,15,17	1.31	2 (14%)
10	MAN	B	604	10	11,11,12	1.82	3 (27%)	14,15,17	0.96	1 (7%)
10	MAN	B	605	10	11,11,12	1.86	3 (27%)	14,15,17	1.15	1 (7%)
11	NAG	B	606	11,1	14,14,15	0.63	0	15,19,21	0.48	0
11	NAG	B	607	11	14,14,15	0.72	1 (7%)	15,19,21	0.52	0
11	BMA	B	608	11	11,11,12	1.23	1 (9%)	14,15,17	1.77	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	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1
3	BMA	A	604	3	-	0/2/19/22	0/1/1/1
3	MAN	A	605	3	-	0/2/19/22	0/1/1/1
3	MAN	A	606	3	-	0/2/19/22	0/1/1/1
3	MAN	A	607	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	A	608	3	-	0/2/19/22	0/1/1/1
3	MAN	A	609	3	-	0/2/19/22	0/1/1/1
4	NAG	A	610	1,4	-	0/6/23/26	0/1/1/1
4	FUL	A	611	4	-	0/0/17/20	0/1/1/1
10	NAG	B	601	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	602	10	-	0/6/23/26	0/1/1/1
10	BMA	B	603	10	-	0/2/19/22	0/1/1/1
10	MAN	B	604	10	-	0/2/19/22	0/1/1/1
10	MAN	B	605	10	-	0/2/19/22	0/1/1/1
11	NAG	B	606	11,1	-	0/6/23/26	0/1/1/1
11	NAG	B	607	11	-	0/6/23/26	0/1/1/1
11	BMA	B	608	11	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAG	O5-C1	-3.78	1.37	1.43
3	A	607	MAN	O5-C1	-2.84	1.39	1.43
11	B	607	NAG	O5-C1	-2.41	1.39	1.43
3	A	604	BMA	O5-C1	-2.23	1.40	1.43
3	A	606	MAN	O5-C1	-2.20	1.40	1.43
3	A	605	MAN	C2-C3	2.00	1.55	1.52
3	A	605	MAN	O4-C4	2.02	1.47	1.43
3	A	607	MAN	C1-C2	2.03	1.57	1.52
4	A	611	FUL	C4-C3	2.12	1.58	1.52
10	B	604	MAN	O5-C5	2.22	1.48	1.43
10	B	604	MAN	C4-C5	2.36	1.58	1.53
10	B	605	MAN	C4-C3	2.40	1.58	1.52
11	B	608	BMA	O5-C5	2.75	1.49	1.43
3	A	605	MAN	O5-C5	3.09	1.50	1.43
10	B	605	MAN	C2-C3	3.26	1.57	1.52
3	A	606	MAN	C2-C3	3.32	1.57	1.52
10	B	605	MAN	O5-C5	3.89	1.52	1.43
10	B	604	MAN	C2-C3	4.33	1.58	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	608	BMA	C1-C2-C3	-4.92	103.72	109.54
3	A	607	MAN	O2-C2-C3	-2.62	104.85	110.12
11	B	608	BMA	O2-C2-C3	-2.60	104.90	110.12
3	A	608	MAN	C1-C2-C3	-2.52	106.56	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	603	BMA	O2-C2-C3	-2.15	105.79	110.12
3	A	603	NAG	O4-C4-C3	-2.01	105.81	110.34
10	B	604	MAN	O2-C2-C1	2.03	113.28	109.21
3	A	609	MAN	O5-C1-C2	2.12	114.29	110.86
4	A	610	NAG	C1-O5-C5	2.12	114.94	112.25
3	A	605	MAN	O5-C1-C2	2.13	114.32	110.86
3	A	605	MAN	O3-C3-C2	2.16	113.90	110.00
11	B	608	BMA	C1-O5-C5	2.28	115.14	112.25
10	B	605	MAN	C3-C4-C5	2.33	114.26	110.20
3	A	609	MAN	O3-C3-C2	2.34	114.23	110.00
3	A	609	MAN	C1-O5-C5	2.54	115.47	112.25
4	A	611	FUL	O2-C2-C1	2.72	114.65	109.21
3	A	608	MAN	C1-O5-C5	2.86	115.88	112.25
3	A	606	MAN	C1-O5-C5	3.30	116.44	112.25
10	B	603	BMA	C1-O5-C5	3.34	116.48	112.25
4	A	611	FUL	C3-C4-C5	3.67	115.91	109.72
4	A	611	FUL	O5-C5-C4	4.27	116.93	109.53
4	A	611	FUL	C1-O5-C5	4.45	119.26	112.38
3	A	605	MAN	C1-O5-C5	5.17	118.81	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
2	NAG	A	601	1	14,14,15	0.61	0	15,19,21	0.99	1 (6%)
5	PO4	A	612	-	4,4,4	0.36	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	A	614	-	3,3,3	0.81	0	2,2,2	0.34	0
7	EDO	A	615	-	3,3,3	0.58	0	2,2,2	0.73	0
7	EDO	A	616	-	3,3,3	0.47	0	2,2,2	0.45	0
7	EDO	A	617	-	3,3,3	0.58	0	2,2,2	0.61	0
7	EDO	A	618	-	3,3,3	0.51	0	2,2,2	0.78	0
7	EDO	A	619	-	3,3,3	0.57	0	2,2,2	0.42	0
7	EDO	A	620	-	3,3,3	0.51	0	2,2,2	0.58	0
7	EDO	A	621	-	3,3,3	0.35	0	2,2,2	0.85	0
8	PEG	A	622	-	6,6,6	0.45	0	5,5,5	1.94	3 (60%)
8	PEG	A	623	-	6,6,6	0.54	0	5,5,5	1.53	0
9	SO4	A	624	-	4,4,4	0.07	0	6,6,6	0.15	0
2	NAG	B	609	1	14,14,15	0.87	1 (7%)	15,19,21	1.06	1 (6%)
5	PO4	B	610[A]	-	4,4,4	0.45	0	6,6,6	0.28	0
5	PO4	B	610[B]	-	4,4,4	0.58	0	6,6,6	0.27	0
5	PO4	B	611	-	4,4,4	0.29	0	6,6,6	0.27	0
7	EDO	B	613	-	3,3,3	0.97	0	2,2,2	0.51	0
7	EDO	B	614	-	3,3,3	0.61	0	2,2,2	0.39	0
7	EDO	B	615	-	3,3,3	0.46	0	2,2,2	0.56	0
7	EDO	B	616	-	3,3,3	0.58	0	2,2,2	0.35	0
7	EDO	B	617	-	3,3,3	0.52	0	2,2,2	0.55	0
7	EDO	B	618	-	3,3,3	0.60	0	2,2,2	0.44	0
7	EDO	B	619	-	3,3,3	0.59	0	2,2,2	0.19	0
8	PEG	B	620	-	6,6,6	0.59	0	5,5,5	1.27	0
8	PEG	B	621	-	6,6,6	0.50	0	5,5,5	1.75	2 (40%)

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	601	1	-	0/6/23/26	0/1/1/1
5	PO4	A	612	-	-	0/0/0/0	0/0/0/0
7	EDO	A	614	-	-	0/1/1/1	0/0/0/0
7	EDO	A	615	-	-	0/1/1/1	0/0/0/0
7	EDO	A	616	-	-	0/1/1/1	0/0/0/0
7	EDO	A	617	-	-	0/1/1/1	0/0/0/0
7	EDO	A	618	-	-	0/1/1/1	0/0/0/0
7	EDO	A	619	-	-	0/1/1/1	0/0/0/0
7	EDO	A	620	-	-	0/1/1/1	0/0/0/0
7	EDO	A	621	-	-	0/1/1/1	0/0/0/0
8	PEG	A	622	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	A	623	-	-	0/4/4/4	0/0/0/0
9	SO4	A	624	-	-	0/0/0/0	0/0/0/0
2	NAG	B	609	1	-	0/6/23/26	0/1/1/1
5	PO4	B	610[A]	-	-	0/0/0/0	0/0/0/0
5	PO4	B	610[B]	-	-	0/0/0/0	0/0/0/0
5	PO4	B	611	-	-	0/0/0/0	0/0/0/0
7	EDO	B	613	-	-	0/1/1/1	0/0/0/0
7	EDO	B	614	-	-	0/1/1/1	0/0/0/0
7	EDO	B	615	-	-	0/1/1/1	0/0/0/0
7	EDO	B	616	-	-	0/1/1/1	0/0/0/0
7	EDO	B	617	-	-	0/1/1/1	0/0/0/0
7	EDO	B	618	-	-	0/1/1/1	0/0/0/0
7	EDO	B	619	-	-	0/1/1/1	0/0/0/0
8	PEG	B	620	-	-	0/4/4/4	0/0/0/0
8	PEG	B	621	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	609	NAG	O5-C1	2.95	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	621	PEG	O1-C1-C2	2.07	124.79	112.03
8	A	622	PEG	O2-C2-C1	2.18	120.46	110.43
8	A	622	PEG	C3-O2-C2	2.27	123.07	113.31
8	A	622	PEG	O2-C3-C4	2.29	120.98	110.43
8	B	621	PEG	O2-C2-C1	2.67	122.74	110.43
2	B	609	NAG	C1-O5-C5	3.29	116.42	112.25
2	A	601	NAG	C1-O5-C5	3.64	116.87	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	616	EDO	3	0
7	A	617	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	618	EDO	2	0
7	A	619	EDO	3	0
7	A	620	EDO	1	0
8	A	622	PEG	5	0
8	A	623	PEG	4	0
5	B	610[B]	PO4	1	0
5	B	611	PO4	1	0
7	B	615	EDO	1	0
7	B	616	EDO	1	0
7	B	619	EDO	1	0
8	B	620	PEG	2	0
8	B	621	PEG	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	432/437 (98%)	-0.12	19 (4%)	38	32	14, 25, 48, 96	0
1	B	432/437 (98%)	-0.16	13 (3%)	54	48	14, 25, 52, 75	0
All	All	864/874 (98%)	-0.14	32 (3%)	45	39	14, 25, 51, 96	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	13.2
1	A	389	ASN	7.3
1	A	387	GLY	7.1
1	B	388	LEU	5.7
1	A	391	ILE	4.7
1	B	387	GLY	4.7
1	A	371	TRP	4.4
1	B	371	TRP	4.0
1	A	556	ASP	4.0
1	A	555	LEU	3.9
1	B	572	SER	3.8
1	A	553	LYS	3.7
1	B	163	LEU	3.5
1	B	389	ASN	3.5
1	A	141	ARG	3.4
1	A	390	SER	3.3
1	B	141	ARG	3.2
1	A	160	THR	3.0
1	B	160	THR	3.0
1	B	391	ILE	2.9
1	B	296	ASP	2.6
1	B	556	ASP	2.4
1	A	142	ILE	2.4
1	B	158	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	386	LYS	2.2
1	B	553	LYS	2.2
1	A	217	ILE	2.1
1	A	196	LEU	2.1
1	A	296	ASP	2.1
1	A	344	ILE	2.1
1	A	161	SER	2.0
1	A	295	HIS	2.0

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, 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
10	MAN	B	605	11/12	0.87	0.18	5.92	23,42,50,52	0
10	NAG	B	601	14/15	0.93	0.14	0.61	32,41,53,55	0
11	NAG	B	607	14/15	0.94	0.15	-	45,49,66,76	0
3	NAG	A	602	14/15	0.90	0.12	-	38,49,54,58	0
3	MAN	A	608	11/12	0.86	0.29	-	80,95,105,108	0
4	FUL	A	611	10/11	0.82	0.29	-	59,82,92,102	0
11	BMA	B	608	11/12	0.75	0.26	-	79,89,96,99	0
3	MAN	A	605	11/12	0.89	0.20	-	40,47,55,67	0
11	NAG	B	606	14/15	0.93	0.11	-	32,45,50,54	0
3	MAN	A	609	11/12	0.81	0.25	-	60,72,85,87	0
3	NAG	A	603	14/15	0.92	0.10	-	36,41,51,54	0
10	BMA	B	603	11/12	0.86	0.23	-	40,45,51,55	0
10	NAG	B	602	14/15	0.87	0.24	-	45,56,65,70	0
3	MAN	A	606	11/12	0.78	0.18	-	58,68,83,84	0
3	BMA	A	604	11/12	0.81	0.12	-	35,53,59,63	0
3	MAN	A	607	11/12	0.78	0.33	-	85,94,100,113	0
10	MAN	B	604	11/12	0.83	0.27	-	40,47,56,60	0
4	NAG	A	610	14/15	0.83	0.27	-	46,66,72,79	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, 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
8	PEG	A	622	7/7	0.70	0.39	10.92	44,48,59,65	0
8	PEG	B	621	7/7	0.86	0.24	9.23	23,32,51,57	0
5	PO4	B	610[B]	5/5	0.96	0.18	4.72	26,27,32,32	5
5	PO4	B	610[A]	5/5	0.96	0.18	3.80	20,21,23,25	5
7	EDO	A	619	4/4	0.88	0.17	3.52	34,37,37,48	0
8	PEG	A	623	7/7	0.81	0.19	2.39	39,42,49,59	0
2	NAG	A	601	14/15	0.79	0.33	2.36	48,65,76,76	0
7	EDO	A	618	4/4	0.91	0.15	2.29	29,38,38,48	0
7	EDO	B	616	4/4	0.91	0.21	2.15	40,48,49,56	0
7	EDO	A	617	4/4	0.88	0.14	1.67	41,42,46,60	0
8	PEG	B	620	7/7	0.86	0.13	1.62	34,45,57,58	0
7	EDO	A	620	4/4	0.90	0.10	0.44	42,42,47,48	0
7	EDO	B	613	4/4	0.94	0.10	0.18	19,23,27,30	0
7	EDO	B	614	4/4	0.96	0.09	-0.09	23,28,37,45	0
7	EDO	A	614	4/4	0.96	0.11	-0.20	20,21,26,29	0
5	PO4	B	611	5/5	0.95	0.18	-0.85	50,64,79,84	0
6	CA	B	612	1/1	0.99	0.04	-1.70	24,24,24,24	0
6	CA	A	613	1/1	0.99	0.05	-1.90	24,24,24,24	0
5	PO4	A	612	5/5	0.99	0.05	-2.30	26,27,29,33	0
7	EDO	A	616	4/4	0.90	0.12	-	43,50,53,60	0
7	EDO	B	618	4/4	0.84	0.20	-	31,44,52,61	0
7	EDO	B	617	4/4	0.85	0.23	-	35,46,57,61	0
7	EDO	B	619	4/4	0.83	0.34	-	45,48,53,64	0
7	EDO	A	621	4/4	0.95	0.35	-	37,42,47,58	0
7	EDO	B	615	4/4	0.94	0.12	-	34,38,40,44	0
2	NAG	B	609	14/15	0.74	0.23	-	53,66,74,78	0
9	SO4	A	624	5/5	0.93	0.42	-	80,86,107,110	0
7	EDO	A	615	4/4	0.97	0.11	-	27,30,33,35	0

6.5 Other polymers

There are no such residues in this entry.