Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:21 PM GMT

PDB ID	:	4XJR
Title	:	The catalytic mechanism of human parainfluenza virus type 3 haemagglutinin-neuraminidase revealed
Authors	:	Dirr, L.; El-Deeb, I.; Guillon, P.; Carroux, C.; Chavas, L.; von Itzstein, M.
Deposited on	:	2015-01-09
Resolution	:	3.00 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 (i) symbol.

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

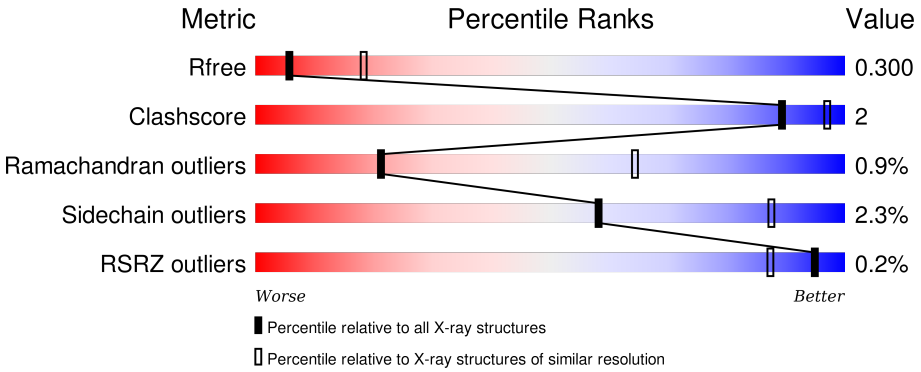
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	454	86% 8% 6%
1	B	454	84% 10% 6%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6869 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	429	Total	C	N	O	S	0	1	0
			3369	2129	583	637	20			
1	B	426	Total	C	N	O	S	0	1	0
			3339	2112	574	633	20			

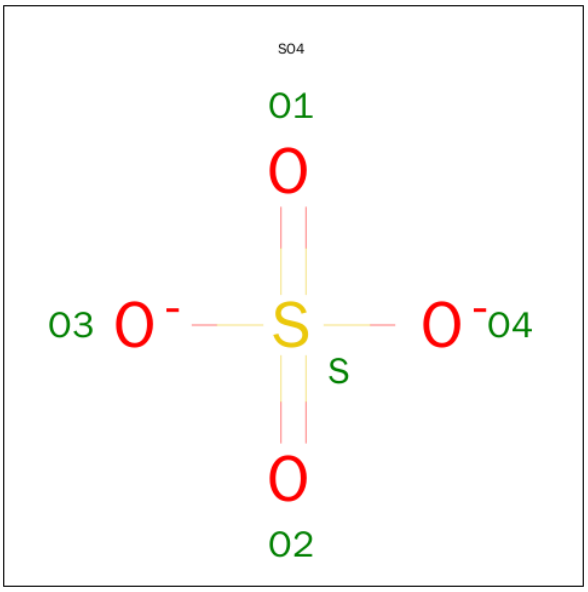
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	HIS	-	expression tag	UNP G8G134
A	574	HIS	-	expression tag	UNP G8G134
A	575	HIS	-	expression tag	UNP G8G134
A	576	HIS	-	expression tag	UNP G8G134
A	577	HIS	-	expression tag	UNP G8G134
A	578	HIS	-	expression tag	UNP G8G134
B	573	HIS	-	expression tag	UNP G8G134
B	574	HIS	-	expression tag	UNP G8G134
B	575	HIS	-	expression tag	UNP G8G134
B	576	HIS	-	expression tag	UNP G8G134
B	577	HIS	-	expression tag	UNP G8G134
B	578	HIS	-	expression tag	UNP G8G134

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

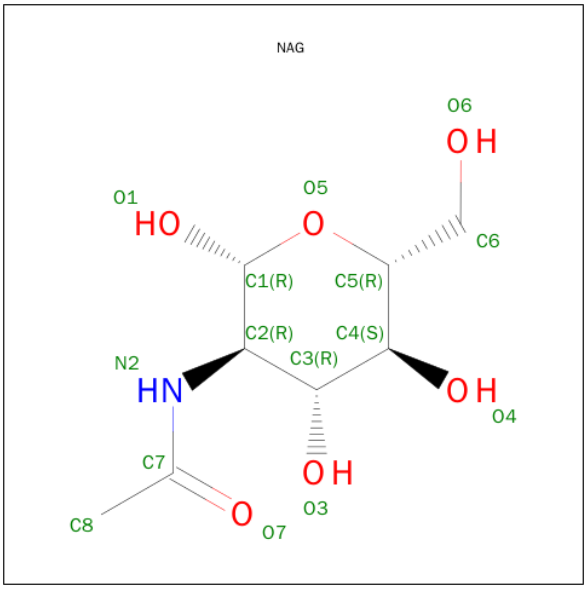


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is a polymer of unknown type called SUGAR (N-ACETYL-D-GLUCOSAMINE).

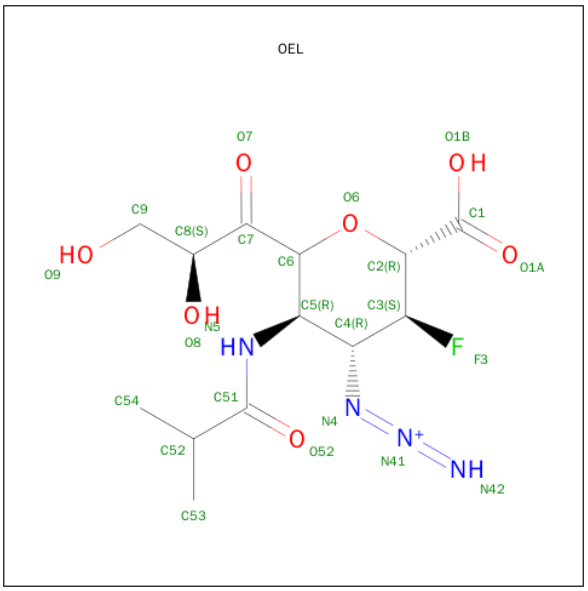
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is (6R)-2,6-anhydro-3,4,5-trideoxy-6-[(2S)-2,3-dihydroxypropanoyl]-3-fluoro-5-[(2-methylpropanoyl)amino]-4-triaza-1,2-dien-2-ium-1-yl-L-gulonic acid (three-letter code: OEL) (formula: $C_{13}H_{20}FN_4O_7$).

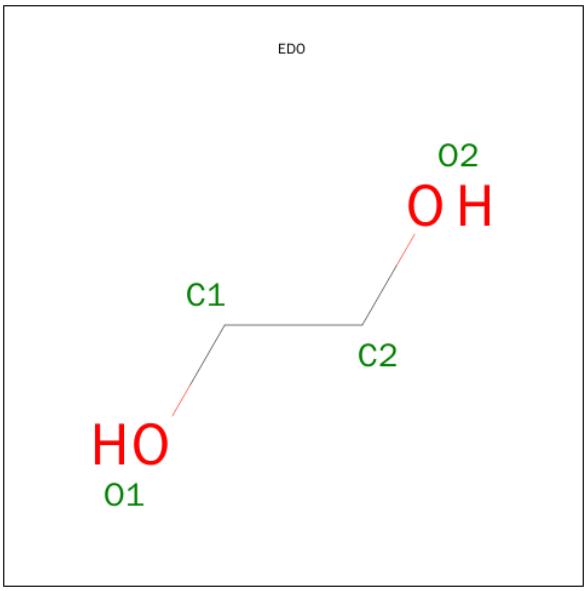


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C F N O 25 13 1 4 7	0	0
6	B	1	Total C F N O 25 13 1 4 7	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is water.

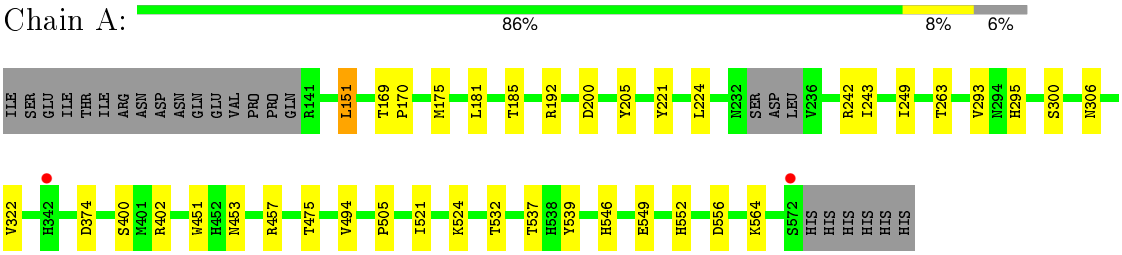
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total O 3 3	0	0
9	B	2	Total O 2 2	0	0

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.

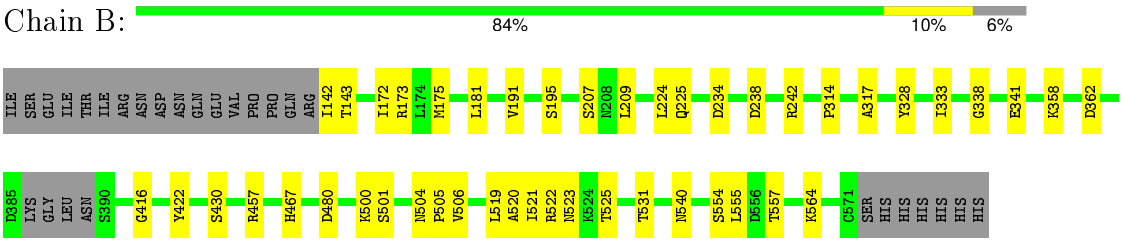
- Molecule 1: Hemagglutinin-neuraminidase

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	81.85Å 98.30Å 103.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 45.71 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.00) 99.9 (45.71-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.190 , 0.298 0.194 , 0.300	Depositor DCC
R_{free} test set	873 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.9	EDS
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	2 of 17298 reflections (0.012%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6869	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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, CA, EDO, SO4, OEL

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	0.48	0/3449	0.72	1/4698 (0.0%)
1	B	0.47	0/3419	0.70	0/4660
All	All	0.48	0/6868	0.71	1/9358 (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	151	LEU	CA-CB-CG	5.19	127.24	115.30

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	3369	0	3329	14	0
1	B	3339	0	3294	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
4	A	28	0	25	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	25	0	17	1	0
6	B	25	0	17	0	0
7	B	39	0	34	1	0
8	B	4	0	6	0	0
9	A	3	0	0	0	0
9	B	2	0	0	0	0
All	All	6869	0	6748	32	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 2.

All (32) 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)
7:B:603:NAG:O4	7:B:604:BMA:O5	2.16	0.59
1:B:172:ILE:O	1:B:519:LEU:HD13	2.06	0.55
1:A:451:TRP:CH2	1:A:453:ASN:HB2	2.42	0.55
1:A:242:ARG:NH1	1:B:242:ARG:O	2.40	0.54
1:A:263:THR:OG1	1:A:295:HIS:HB3	2.08	0.54
1:B:191:VAL:HG22	1:B:209:LEU:HG	1.90	0.53
1:A:505:PRO:HB2	1:A:521:ILE:HD12	1.91	0.52
1:B:505:PRO:HB2	1:B:521:ILE:HD12	1.93	0.51
1:B:142:ILE:HG23	1:B:143:THR:HG23	1.93	0.51
1:A:224:LEU:HD23	1:A:293:VAL:HG21	1.93	0.50
1:B:314:PRO:HB2	1:B:341[A]:GLU:HB3	1.95	0.49
1:A:221:TYR:HD1	1:A:249:ILE:HD13	1.79	0.48
1:B:555:LEU:HB2	1:B:557:THR:HG22	1.95	0.47
1:A:192:ARG:NH2	6:A:606:OEL:F3	2.35	0.47
1:B:181:LEU:HA	1:B:225:GLN:HE22	1.80	0.46
1:A:494:VAL:HG21	1:A:546:HIS:HB3	1.97	0.46
1:A:175:MET:HE2	1:A:564:LYS:HB3	1.96	0.46
1:B:506:VAL:HG22	1:B:520:ALA:HA	1.98	0.46
1:A:181:LEU:HD22	1:A:205:TYR:CZ	2.51	0.45
1:B:504:ASN:O	1:B:506:VAL:HG23	2.17	0.45
1:B:358:LYS:HA	1:B:362:ASP:OD2	2.16	0.45
1:B:317:ALA:O	1:B:338:GLY:HA3	2.17	0.45
1:A:169:THR:HA	1:A:170:PRO:C	2.38	0.44
1:B:238:ASP:OD1	1:B:564:LYS:NZ	2.51	0.44
1:A:552:HIS:O	1:A:556:ASP:N	2.51	0.44
1:B:224:LEU:HD12	1:B:225:GLN:N	2.34	0.43
1:B:523:ASN:OD1	1:B:525:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HG21	1:B:175:MET:O	2.19	0.43
1:B:328:TYR:HB3	1:B:333:ILE:HD12	2.02	0.42
1:A:400:SER:OG	1:A:402:ARG:HB2	2.20	0.41
1:B:422:TYR:CZ	1:B:480:ASP:HA	2.56	0.40
1:B:430:SER:OG	1:B:467:HIS:N	2.55	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	426/454 (94%)	394 (92%)	26 (6%)	6 (1%)	14	51
1	B	422/454 (93%)	385 (91%)	35 (8%)	2 (0%)	34	76
All	All	848/908 (93%)	779 (92%)	61 (7%)	8 (1%)	21	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	ASP
1	A	524	LYS
1	A	539	TYR
1	A	322	VAL
1	B	522	ARG
1	A	475	THR
1	A	549	GLU
1	B	416	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	388/412 (94%)	380 (98%)	8 (2%)	61 89
1	B	385/412 (93%)	375 (97%)	10 (3%)	54 85
All	All	773/824 (94%)	755 (98%)	18 (2%)	58 87

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	LEU
1	A	200	ASP
1	A	243	ILE
1	A	300	SER
1	A	306	ASN
1	A	457	ARG
1	A	532	THR
1	A	537	THR
1	B	173	ARG
1	B	195	SER
1	B	207	SER
1	B	234	ASP
1	B	457	ARG
1	B	500	LYS
1	B	501	SER
1	B	531	THR
1	B	540	ASN
1	B	554	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	GLN
1	B	295	HIS
1	B	313	GLN
1	B	417	ASN

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Mol	Chain	Res	Type
1	B	453	ASN
1	B	540	ASN

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)

5 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	$\#\|Z\|>2$
4	NAG	A	603	1,4	14,14,15	0.54	0	15,19,21	2.12	6 (40%)
4	NAG	A	604	4	14,14,15	0.43	0	15,19,21	1.11	1 (6%)
7	NAG	B	602	1,7	14,14,15	0.37	0	15,19,21	1.50	3 (20%)
7	NAG	B	603	7	14,14,15	0.61	0	15,19,21	1.45	2 (13%)
7	BMA	B	604	7	11,11,12	0.62	0	14,15,17	1.91	2 (14%)

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
4	NAG	A	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	604	4	-	0/6/23/26	0/1/1/1
7	NAG	B	602	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	603	7	-	0/6/23/26	0/1/1/1
7	BMA	B	604	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	NAG	O4-C4-C3	-2.92	103.75	110.34
7	B	603	NAG	C4-C3-C2	-2.87	106.77	111.23
4	A	603	NAG	C3-C4-C5	-2.50	105.83	110.20
7	B	604	BMA	C2-C3-C4	-2.43	106.92	111.04
7	B	602	NAG	O7-C7-N2	-2.12	117.53	121.86
4	A	603	NAG	C6-C5-C4	2.06	118.09	113.02
4	A	603	NAG	O4-C4-C5	2.10	114.81	109.24
7	B	603	NAG	O4-C4-C3	2.33	115.57	110.34
7	B	602	NAG	C2-N2-C7	2.65	126.44	123.04
7	B	602	NAG	C8-C7-N2	3.28	122.39	116.11
4	A	603	NAG	C8-C7-N2	3.39	122.60	116.11
4	A	604	NAG	C1-O5-C5	3.65	116.88	112.25
4	A	603	NAG	C2-N2-C7	4.27	128.53	123.04
7	B	604	BMA	C1-O5-C5	5.68	119.45	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	603	NAG	1	0
7	B	604	BMA	1	0

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	SO4	A	602	-	4,4,4	0.38	0	6,6,6	0.24	0
5	NAG	A	605	1	14,14,15	0.54	0	15,19,21	1.59	3 (20%)
6	OEL	A	606	1	19,25,25	3.03	2 (10%)	14,35,35	1.87	1 (7%)
5	NAG	B	605	1	14,14,15	0.30	0	15,19,21	0.96	1 (6%)
6	OEL	B	606	1	19,25,25	3.14	2 (10%)	14,35,35	1.57	2 (14%)
8	EDO	B	607	-	3,3,3	0.45	0	2,2,2	0.52	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
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
5	NAG	A	605	1	-	0/6/23/26	0/1/1/1
6	OEL	A	606	1	-	0/19/45/45	0/1/1/1
5	NAG	B	605	1	-	0/6/23/26	0/1/1/1
6	OEL	B	606	1	-	1/19/45/45	0/1/1/1
8	EDO	B	607	-	-	0/1/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	606	OEL	N41-N4	5.37	1.38	1.23
6	B	606	OEL	N41-N4	5.90	1.39	1.23
6	A	606	OEL	O7-C7	11.78	1.42	1.21
6	B	606	OEL	O7-C7	12.06	1.42	1.21

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	606	OEL	O52-C51-C52	-6.04	114.32	122.63
6	B	606	OEL	O52-C51-C52	-3.74	117.48	122.63
5	A	605	NAG	C4-C3-C2	-2.11	107.95	111.23
5	A	605	NAG	C3-C2-N2	2.36	116.22	110.56
6	B	606	OEL	C4-N4-N41	2.56	122.10	115.50
5	B	605	NAG	C1-O5-C5	3.19	116.29	112.25
5	A	605	NAG	C1-O5-C5	4.69	118.20	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	606	OEL	C4-N4-N41-N42

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	OEL	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.

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	429/454 (94%)	-0.32	2 (0%) 91 76	23, 41, 75, 104	0
1	B	426/454 (93%)	-0.32	0 100 100	27, 44, 73, 97	0
All	All	855/908 (94%)	-0.32	2 (0%) 95 87	23, 43, 73, 104	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	SER	3.0
1	A	342	HIS	2.3

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
7	NAG	B	603	14/15	0.89	0.24	0.17	49,59,65,66	0
7	NAG	B	602	14/15	0.92	0.15	-1.05	47,50,53,54	0
7	BMA	B	604	11/12	0.81	0.28	-	48,58,64,67	0
4	NAG	A	604	14/15	0.85	0.20	-	45,55,60,60	0
4	NAG	A	603	14/15	0.91	0.20	-	50,55,61,63	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
6	OEL	A	606	25/25	0.93	0.19	0.99	42,48,52,57	0
6	OEL	B	606	25/25	0.91	0.23	0.85	41,47,57,63	0
3	SO4	A	602	5/5	0.97	0.12	-1.87	53,58,60,64	0
2	CA	B	601	1/1	0.97	0.05	-3.22	55,55,55,55	0
2	CA	A	601	1/1	0.98	0.06	-3.30	35,35,35,35	0
5	NAG	B	605	14/15	0.86	0.19	-	62,64,65,65	0
5	NAG	A	605	14/15	0.80	0.34	-	61,66,73,74	0
8	EDO	B	607	4/4	0.96	0.16	-	31,32,34,35	0

6.5 Other polymers

There are no such residues in this entry.