



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:45 AM GMT

PDB ID : 1V3C
Title : Structure of the hemagglutinin-neuraminidase from human parainfluenza virus type III: complex with NEU5AC
Authors : Lawrence, M.C.; Borg, N.A.; Streltsov, V.A.; Pilling, P.A.; Epa, V.C.; Varghese, J.N.; McKimm-Breschkin, J.L.; Colman, P.M.
Deposited on : 2003-10-30
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

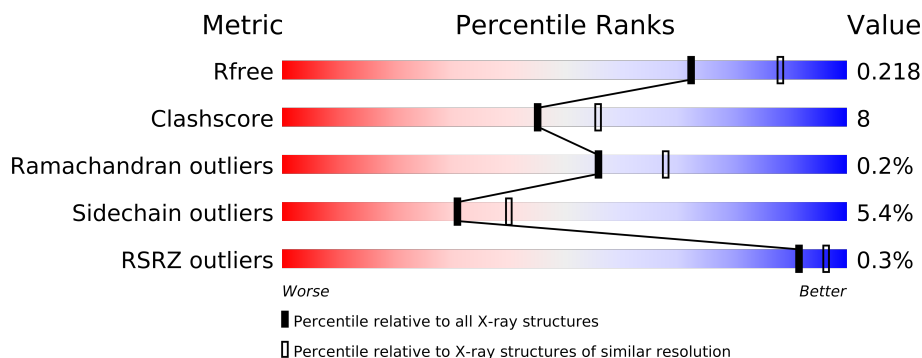
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	431	<div><div></div><div></div><div></div><div></div><div></div></div>
1	B	431	<div><div></div><div></div><div></div><div></div><div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	3081	-	X
2	NAG	B	5231	-	X
7	SO4	A	3002	-	X
7	SO4	B	3001	-	X
7	SO4	B	3003	-	X

2 Entry composition i

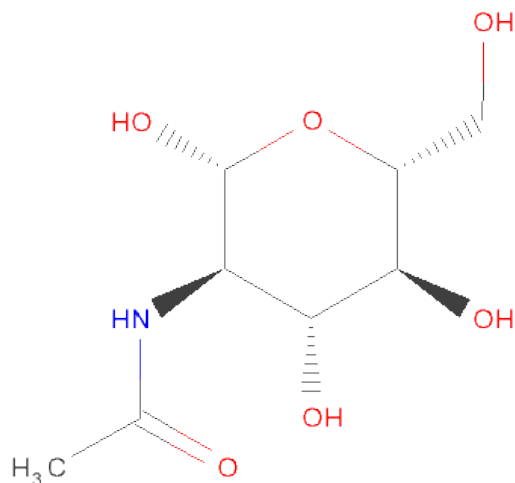
There are 8 unique types of molecules in this entry. The entry contains 7762 atoms, of which 0 are hydrogen and 0 are deuterium.

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-neuraminidaseglycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	1	0
			3383	2142	581	640	20			
1	B	431	Total	C	N	O	S	0	1	0
			3383	2142	581	640	20			

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



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

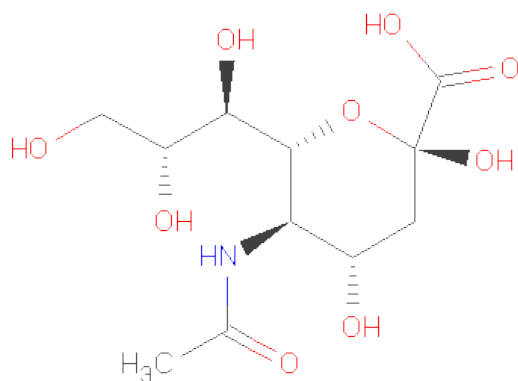
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- 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 SUGAR (5-N-ACETYL-BETA-D-NEURAMINICACID) (three-letter code: SLB) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	11	1	9		
5	B	1	Total	C	N	O	0	0
			21	11	1	9		

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

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is water.

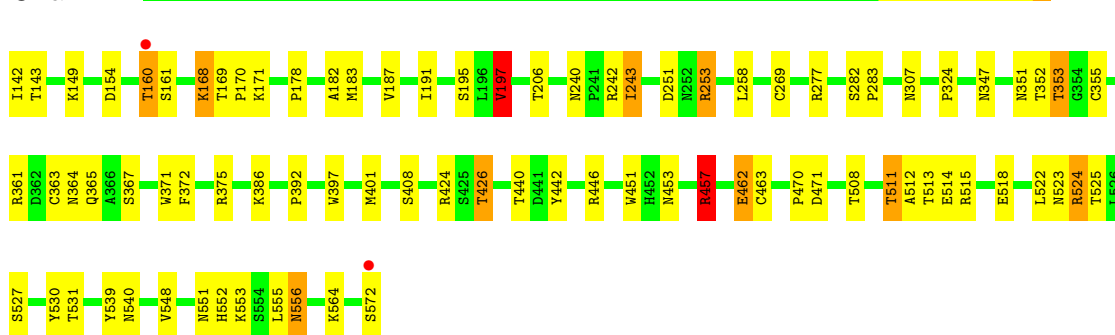
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	395	Total	O	0	0
			395	395		
8	B	439	Total	O	0	0
			439	439		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

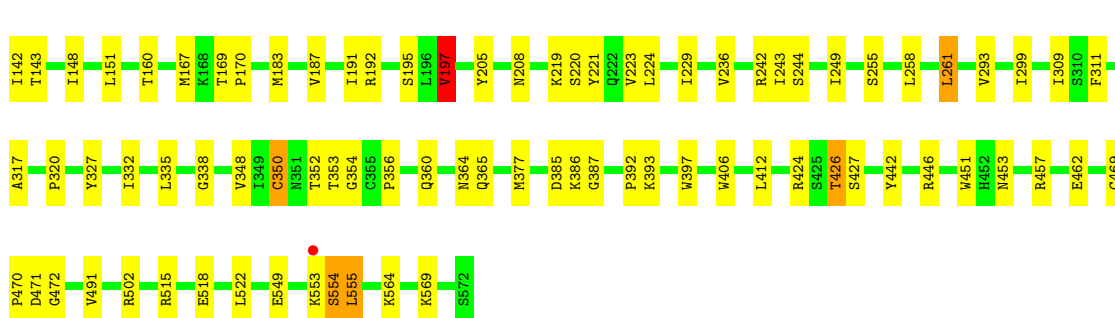
- Molecule 1: hemagglutinin-neuraminidaseglycoprotein

Chain A:



- Molecule 1: hemagglutinin-neuraminidaseglycoprotein

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.62Å 218.62Å 109.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.50 – 2.30 7.50 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.3 (7.50-2.30) 92.3 (7.50-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.176 , 0.222 0.175 , 0.218	Depositor DCC
R_{free} test set	3106 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 66519 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7762	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SLB, CA, NAG, NDG, SO4

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	0.55	0/3469	0.84	5/4730 (0.1%)
1	B	0.54	0/3469	0.83	2/4730 (0.0%)
All	All	0.55	0/6938	0.83	7/9460 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	197	VAL	CB-CA-C	-5.90	100.18	111.40
1	A	197	VAL	CB-CA-C	-5.65	100.66	111.40
1	A	457	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	350	CYS	CA-CB-SG	5.23	123.42	114.00
1	A	243	ILE	CB-CA-C	-5.22	101.15	111.60
1	A	253	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3383	0	3350	65	0
1	B	3383	0	3348	50	0
2	A	14	0	13	0	0
2	B	28	0	26	0	0
3	A	28	0	25	3	0
4	B	28	0	25	1	0
5	A	21	0	18	0	0
5	B	21	0	18	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	10	0	0	0	0
7	B	10	0	0	0	0
8	A	395	0	0	10	0
8	B	439	0	0	7	0
All	All	7762	0	6823	116	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (116) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:524:ARG:H	1:A:524:ARG:HD2	1.18	1.06
1:A:424:ARG:HG2	1:A:426:THR:HG22	1.51	0.90
1:B:187:VAL:HG22	1:B:555:LEU:HD23	1.57	0.86
1:A:347:ASN:HD22	1:A:364:ASN:HD21	1.25	0.80
1:B:386:LYS:HG3	1:B:392:PRO:HB3	1.63	0.79
1:A:511:THR:HG22	1:A:513:THR:H	1.48	0.76
1:A:195:SER:OG	8:A:3521:HOH:O	2.04	0.74
1:B:424:ARG:HG2	1:B:426:THR:HG22	1.67	0.74
1:A:168:LYS:HE3	8:A:3840:HOH:O	1.90	0.72
1:A:524:ARG:CD	1:A:524:ARG:H	1.92	0.71
1:B:554:SER:HB2	1:B:555:LEU:HD12	1.71	0.71
1:A:347:ASN:ND2	1:A:364:ASN:HD21	1.88	0.70
1:A:171:LYS:HE2	1:A:518:GLU:O	1.92	0.70
1:A:530:TYR:HB3	8:A:3623:HOH:O	1.93	0.69
1:B:549:GLU:OE2	8:B:5667:HOH:O	2.11	0.68
1:A:277:ARG:HD2	1:A:371:TRP:CZ2	2.28	0.68
1:A:511:THR:CG2	1:A:513:THR:H	2.07	0.67
1:B:187:VAL:HG22	1:B:555:LEU:CD2	2.26	0.64
1:A:457:ARG:NH2	1:A:463:CYS:O	2.30	0.64
1:A:527:SER:HB2	1:A:551:ASN:HB3	1.80	0.64
1:A:524:ARG:N	1:A:524:ARG:HD2	2.01	0.64
1:A:142:ILE:HG23	1:A:143:THR:HG23	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:251:ASP:OD2	1:A:253:ARG:NH2	2.31	0.63
1:A:511:THR:HG22	1:A:514:GLU:H	1.63	0.63
1:A:169:THR:HG23	1:A:170:PRO:HA	1.81	0.62
1:A:511:THR:HG22	1:A:513:THR:N	2.16	0.61
1:A:553:LYS:HD3	8:A:3761:HOH:O	2.00	0.60
1:B:515:ARG:HD2	1:B:518:GLU:OE1	2.02	0.59
1:A:361:ARG:O	1:A:365:GLN:HG3	2.02	0.59
1:B:293:VAL:HG22	1:B:299:ILE:HG12	1.85	0.59
1:B:151:LEU:HD23	1:B:151:LEU:C	2.23	0.58
1:B:261:LEU:HB2	1:B:332:ILE:HD11	1.85	0.58
1:A:160:THR:HG23	1:A:161:SER:H	1.68	0.57
1:A:277:ARG:HD2	1:A:371:TRP:CE2	2.41	0.55
1:A:352:THR:O	1:A:355:CYS:HB2	2.06	0.55
1:B:554:SER:HB2	1:B:555:LEU:CD1	2.36	0.54
1:B:348:VAL:HG22	1:B:364:ASN:HD22	1.73	0.53
1:B:353:THR:OG1	4:B:3511:NDG:H6C2	2.09	0.53
1:B:169:THR:HG23	1:B:170:PRO:HA	1.91	0.53
1:B:192:ARG:NE	8:B:5667:HOH:O	2.38	0.52
1:B:224:LEU:O	1:B:244:SER:HA	2.09	0.52
1:A:462:GLU:HG3	8:A:3825:HOH:O	2.09	0.52
1:A:524:ARG:CD	1:A:524:ARG:N	2.69	0.52
1:B:354:GLY:O	1:B:356:PRO:HD3	2.08	0.52
1:A:178:PRO:HB3	1:B:223:VAL:HG21	1.92	0.51
1:B:502:ARG:NH2	8:B:5668:HOH:O	2.34	0.51
1:A:408:SER:OG	1:A:426:THR:HG23	2.11	0.49
1:A:183:MET:SD	1:B:183:MET:HE3	2.52	0.49
1:B:386:LYS:HE3	1:B:387:GLY:O	2.13	0.49
1:A:197:VAL:HG13	1:A:324:PRO:CB	2.43	0.49
1:A:397:TRP:CD2	1:A:442:TYR:HB3	2.47	0.48
1:A:511:THR:HG23	1:A:512:ALA:N	2.28	0.48
1:B:142:ILE:HG22	8:B:5442:HOH:O	2.13	0.48
1:A:367:SER:HB2	1:A:401:MET:CE	2.42	0.48
1:B:554:SER:C	1:B:555:LEU:HD12	2.33	0.48
1:A:511:THR:HG22	1:A:514:GLU:N	2.28	0.48
1:B:397:TRP:CD2	1:B:442:TYR:HB3	2.49	0.48
1:B:221:TYR:CE1	1:B:249:ILE:HD12	2.49	0.48
1:B:555:LEU:HD12	1:B:555:LEU:N	2.28	0.48
1:B:148:ILE:HD13	1:B:229:ILE:HG22	1.96	0.48
1:A:351:ASN:OD1	1:A:353:THR:HG23	2.14	0.48
1:A:372:PHE:O	1:A:375:ARG:HG2	2.13	0.47
1:A:511:THR:CG2	1:A:512:ALA:N	2.78	0.47
1:A:142:ILE:HG23	1:A:143:THR:N	2.28	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:352:THR:HG22	1:A:470:PRO:HG2	1.97	0.47
1:A:386:LYS:HB3	1:A:392:PRO:HA	1.95	0.47
1:B:451:TRP:CH2	1:B:453:ASN:HB2	2.49	0.47
1:A:451:TRP:CH2	1:A:453:ASN:HB2	2.50	0.47
1:B:317:ALA:O	1:B:338:GLY:HA3	2.15	0.46
1:B:427:SER:HB3	8:B:5503:HOH:O	2.16	0.45
1:A:195:SER:HB2	8:A:3520:HOH:O	2.15	0.45
1:A:197:VAL:HG22	1:A:258:LEU:HB2	1.98	0.45
1:B:142:ILE:HG23	1:B:143:THR:HG23	1.99	0.45
1:B:377:MET:HG3	1:B:406:TRP:CZ2	2.51	0.45
1:A:197:VAL:HG13	1:A:324:PRO:HB3	1.99	0.44
1:B:261:LEU:HD13	1:B:327:TYR:CE2	2.53	0.44
1:B:219:LYS:O	1:B:220:SER:HB3	2.17	0.44
1:A:527:SER:HB2	1:A:551:ASN:CB	2.46	0.44
1:B:191:ILE:HA	1:B:208:ASN:O	2.18	0.44
1:B:471:ASP:OD1	1:B:472:GLY:N	2.50	0.44
1:A:555:LEU:O	1:A:556:ASN:HB3	2.17	0.43
1:B:187:VAL:HG12	8:B:5254:HOH:O	2.18	0.43
1:B:192:ARG:HA	1:B:549:GLU:OE2	2.18	0.43
1:B:309:ILE:HB	1:B:311:PHE:CE1	2.53	0.43
1:A:195:SER:HB3	1:A:206:THR:HG22	2.00	0.43
1:A:253:ARG:HG2	1:A:269:CYS:CB	2.48	0.43
1:B:197:VAL:HG22	1:B:258:LEU:HB2	2.01	0.43
1:A:523:ASN:OD1	1:A:525:THR:HG23	2.17	0.43
1:B:187:VAL:CG2	1:B:555:LEU:CD2	2.94	0.43
1:A:515:ARG:CD	1:A:518:GLU:OE1	2.67	0.42
1:A:253:ARG:HG2	1:A:269:CYS:HB2	2.00	0.42
1:B:469:CYS:HA	1:B:470:PRO:HD3	1.93	0.42
1:B:255:SER:O	1:B:320:PRO:HB2	2.20	0.42
1:A:168:LYS:HE2	1:A:168:LYS:HB3	1.90	0.42
1:A:515:ARG:HD2	1:A:518:GLU:OE1	2.18	0.42
1:B:335:LEU:HB2	1:B:412:LEU:HG	2.02	0.42
1:A:552:HIS:HE1	8:A:3873:HOH:O	2.03	0.42
1:A:142:ILE:CG2	1:A:143:THR:N	2.83	0.42
3:A:3511:NAG:H61	3:A:3512:NAG:H82	2.01	0.42
1:B:195:SER:O	1:B:205:TYR:HA	2.19	0.41
1:A:142:ILE:HD12	8:A:3850:HOH:O	2.20	0.41
1:A:182:ALA:O	1:A:191:ILE:HD12	2.20	0.41
1:B:426:THR:HG21	8:B:5260:HOH:O	2.21	0.41
1:B:220:SER:O	1:B:249:ILE:HA	2.21	0.41
1:A:307:ASN:ND2	8:A:3815:HOH:O	2.54	0.41
1:A:282:SER:HA	1:A:283:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:261:LEU:HD13	1:B:327:TYR:CZ	2.56	0.41
3:A:3511:NAG:H61	3:A:3512:NAG:C8	2.51	0.41
1:B:350:CYS:HB3	1:B:360:GLN:NE2	2.35	0.41
1:A:539:TYR:O	1:A:540:ASN:HB2	2.21	0.41
1:A:363:CYS:SG	1:A:470:PRO:HG3	2.60	0.40
1:B:569:LYS:C	1:B:569:LYS:HD3	2.40	0.40
1:A:462:GLU:H	1:A:462:GLU:CD	2.24	0.40
1:A:531:THR:HG22	1:A:548:VAL:HG13	2.03	0.40
3:A:3511:NAG:H83	3:A:3511:NAG:O3	2.21	0.40
1:A:553:LYS:HA	8:A:3761:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/431 (100%)	406 (94%)	23 (5%)	1 (0%)	56	68
1	B	430/431 (100%)	404 (94%)	25 (6%)	1 (0%)	56	68
All	All	860/862 (100%)	810 (94%)	48 (6%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	522	LEU
1	A	522	LEU

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	391/390 (100%)	369 (94%)	22 (6%)	30	38
1	B	391/390 (100%)	371 (95%)	20 (5%)	33	43
All	All	782/780 (100%)	740 (95%)	42 (5%)	31	40

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	154	ASP
1	A	160	THR
1	A	168	LYS
1	A	187	VAL
1	A	197	VAL
1	A	240	ASN
1	A	242	ARG
1	A	243	ILE
1	A	353	THR
1	A	426	THR
1	A	440	THR
1	A	446	ARG
1	A	457	ARG
1	A	462	GLU
1	A	471	ASP
1	A	508	THR
1	A	511	THR
1	A	524	ARG
1	A	556	ASN
1	A	564	LYS
1	A	572	SER
1	B	160	THR
1	B	167	MET
1	B	197	VAL
1	B	236	VAL
1	B	242	ARG
1	B	243	ILE
1	B	261	LEU
1	B	352	THR
1	B	365	GLN
1	B	385	ASP
1	B	393	LYS
1	B	426	THR
1	B	446	ARG

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Mol	Chain	Res	Type
1	B	457	ARG
1	B	462	GLU
1	B	491	VAL
1	B	553	LYS
1	B	554	SER
1	B	555	LEU
1	B	564	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	A	262	ASN
1	A	345	ASN
1	A	347	ASN
1	A	360	GLN
1	A	504	ASN
1	A	556	ASN
1	B	240	ASN
1	B	250	ASN
1	B	262	ASN
1	B	294	ASN
1	B	347	ASN
1	B	360	GLN
1	B	364	ASN
1	B	365	GLN
1	B	499	GLN
1	B	504	ASN
1	B	556	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	3511	1,3	12,14,15	0.55	0	15,19,21	0.95	1 (6%)
3	NAG	A	3512	3	12,14,15	0.45	0	15,19,21	0.72	0
4	NDG	B	3511	1,4	12,14,15	0.51	0	15,19,21	1.01	1 (6%)
4	NAG	B	3512	4	12,14,15	0.44	0	15,19,21	0.86	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
3	NAG	A	3511	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3512	3	-	0/6/23/26	0/1/1/1
4	NDG	B	3511	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	3512	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3511	NDG	C3-C2-N2	-2.69	107.66	111.76
3	A	3511	NAG	C2-N2-C7	-2.55	118.80	123.09
4	B	3512	NAG	C2-N2-C7	-2.07	119.62	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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$
7	SO4	A	3002	-	4,4,4	0.36	0	6,6,6	0.16	0
7	SO4	A	3004	-	4,4,4	0.35	0	6,6,6	0.16	0
2	NAG	A	3081	1	12,14,15	0.44	0	15,19,21	0.72	0
5	SLB	A	3215	-	21,21,21	1.25	2 (9%)	31,31,31	1.68	10 (32%)
7	SO4	B	3001	-	4,4,4	0.32	0	6,6,6	0.19	0
7	SO4	B	3003	-	4,4,4	0.46	0	6,6,6	0.27	0
2	NAG	B	3081	1	12,14,15	0.51	0	15,19,21	0.79	1 (6%)
5	SLB	B	4215	-	21,21,21	1.93	3 (14%)	31,31,31	1.78	9 (29%)
2	NAG	B	5231	1	12,14,15	0.56	0	15,19,21	0.85	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
7	SO4	A	3002	-	-	0/0/0/0	0/0/0/0
7	SO4	A	3004	-	-	0/0/0/0	0/0/0/0
2	NAG	A	3081	1	-	0/6/23/26	0/1/1/1
5	SLB	A	3215	-	-	0/20/38/38	0/1/1/1
7	SO4	B	3001	-	-	0/0/0/0	0/0/0/0
7	SO4	B	3003	-	-	0/0/0/0	0/0/0/0
2	NAG	B	3081	1	-	0/6/23/26	0/1/1/1
5	SLB	B	4215	-	-	0/20/38/38	0/1/1/1
2	NAG	B	5231	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4215	SLB	C2-C1	-6.74	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4215	SLB	C3-C2	3.31	1.56	1.51
5	B	4215	SLB	C5-N5	3.12	1.51	1.45
5	A	3215	SLB	C2-C1	-2.70	1.51	1.53
5	A	3215	SLB	C6-C5	2.10	1.56	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	4215	SLB	O2-C2-C1	-4.16	102.81	109.86
5	A	3215	SLB	O2-C2-C1	-3.31	104.25	109.86
5	B	4215	SLB	C6-C5-N5	-2.87	105.97	110.99
5	B	4215	SLB	C8-C7-C6	-2.78	107.60	112.99
5	B	4215	SLB	O1A-C1-C2	-2.72	119.70	123.48
5	A	3215	SLB	C2-O6-C6	2.69	118.02	113.93
5	B	4215	SLB	C7-C6-C5	-2.66	110.33	114.24
5	A	3215	SLB	O8-C8-C9	-2.62	103.09	109.20
5	A	3215	SLB	O4-C4-C3	-2.62	103.72	109.92
5	A	3215	SLB	C6-C5-N5	-2.39	106.81	110.99
5	B	4215	SLB	C4-C5-N5	2.31	115.22	110.12
2	B	5231	NAG	C3-C2-N2	-2.29	108.27	111.76
5	A	3215	SLB	C5-N5-C10	-2.29	116.91	123.02
5	B	4215	SLB	O8-C8-C9	-2.23	104.00	109.20
2	B	3081	NAG	C2-N2-C7	-2.20	119.39	123.09
5	B	4215	SLB	O4-C4-C3	-2.14	104.84	109.92
5	A	3215	SLB	O6-C2-C3	2.13	111.47	110.22
5	A	3215	SLB	O8-C8-C7	2.11	114.30	109.05
5	A	3215	SLB	C4-C5-N5	2.08	114.72	110.12
5	B	4215	SLB	O6-C6-C7	2.05	108.97	106.34
5	A	3215	SLB	O1A-C1-C2	-2.04	120.65	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/431 (100%)	-0.80	2 (0%) 88 94	15, 27, 52, 84	0
1	B	431/431 (100%)	-0.84	1 (0%) 93 97	16, 27, 50, 76	0
All	All	862/862 (100%)	-0.82	3 (0%) 91 96	15, 27, 51, 84	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	553	LYS	2.4
1	A	572	SER	2.3
1	A	160	THR	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	3511	14/15	0.23	4.47	69,74,79,80	0
3	NAG	A	3512	14/15	0.19	1.91	74,76,79,79	0
4	NDG	B	3511	14/15	0.16	0.69	59,63,65,67	0
4	NAG	B	3512	14/15	0.17	-	53,65,70,74	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	SO4	B	3003	5/5	0.17	5.94	50,53,65,66	0
7	SO4	B	3001	5/5	0.15	5.78	60,61,67,68	0
2	NAG	A	3081	14/15	0.21	5.22	70,75,77,78	0
7	SO4	A	3002	5/5	0.14	4.09	83,84,86,88	0
2	NAG	B	5231	14/15	0.24	2.77	53,64,69,70	0
2	NAG	B	3081	14/15	0.16	1.62	48,58,63,64	0
5	SLB	A	3215	21/21	0.09	1.53	25,28,36,46	0
5	SLB	B	4215	21/21	0.09	0.99	23,28,38,45	0
7	SO4	A	3004	5/5	0.13	0.54	66,66,69,70	0
6	CA	A	1001	1/1	0.05	-1.34	39,39,39,39	0
6	CA	B	2001	1/1	0.04	-3.15	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.