



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:07 PM UTC

PDB ID : 5XL8 / pdb_00005xl8
Title : The structure of hemagglutinin G228S mutant from a avian-origin H4N6 influenza virus (A/duck/Czech/1956)
Authors : Song, H.; Qi, J.; Gao, G.F.
Deposited on : 2017-05-10
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

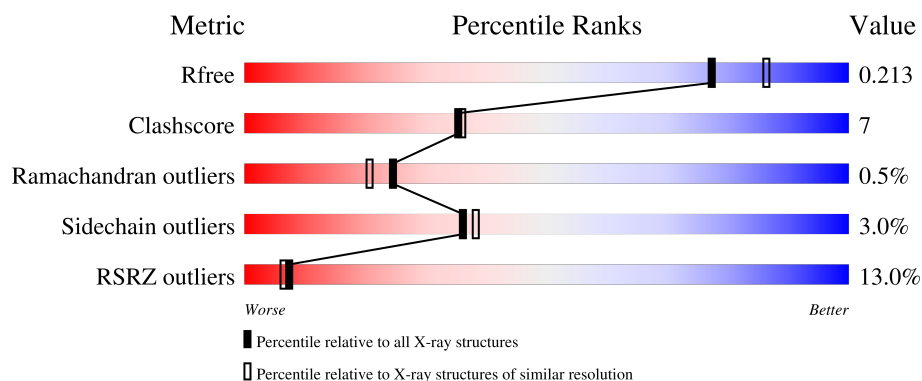
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	503	11% 82% 12% ..
1	B	503	16% 82% 12% ...
1	C	503	11% 84% 12% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12745 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.

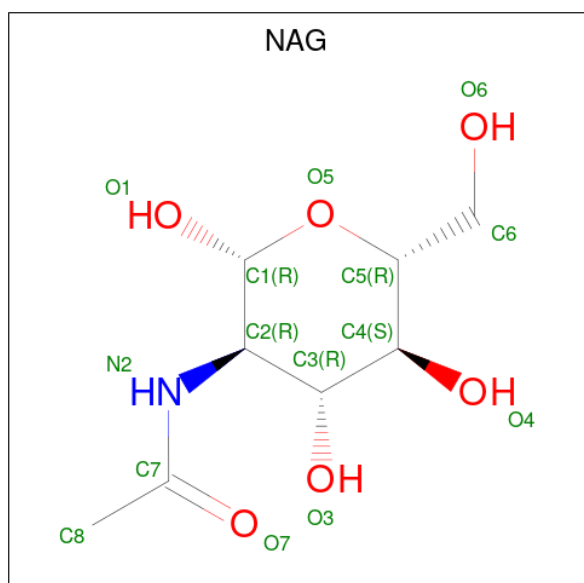
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3833	2390	682	745	16			
1	B	486	Total	C	N	O	S	0	0	0
			3833	2390	682	745	16			
1	C	486	Total	C	N	O	S	0	0	0
			3833	2390	682	745	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	SER	GLY	engineered mutation	UNP A3KF09
B	225	SER	GLY	engineered mutation	UNP A3KF09
C	225	SER	GLY	engineered mutation	UNP A3KF09

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	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		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

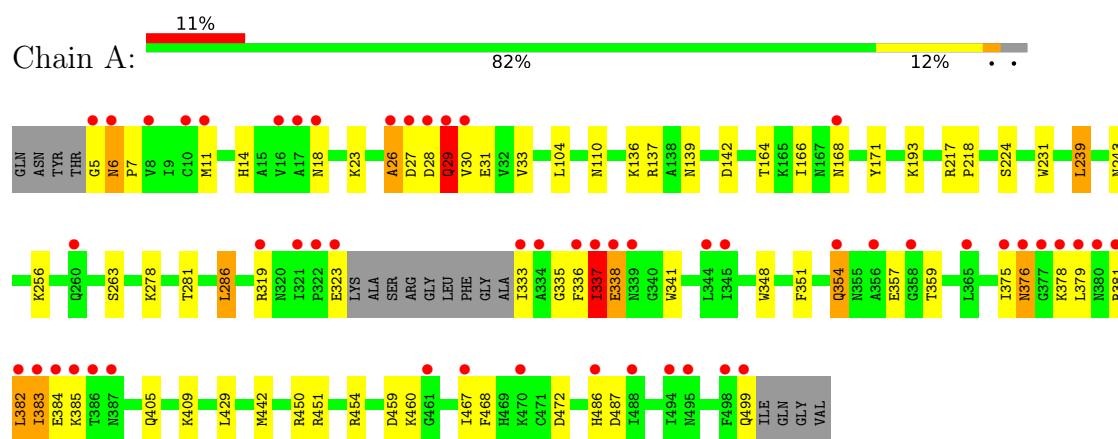
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	382	Total	O	0	0
			382	382		
3	B	388	Total	O	0	0
			388	388		
3	C	392	Total	O	0	0
			392	392		

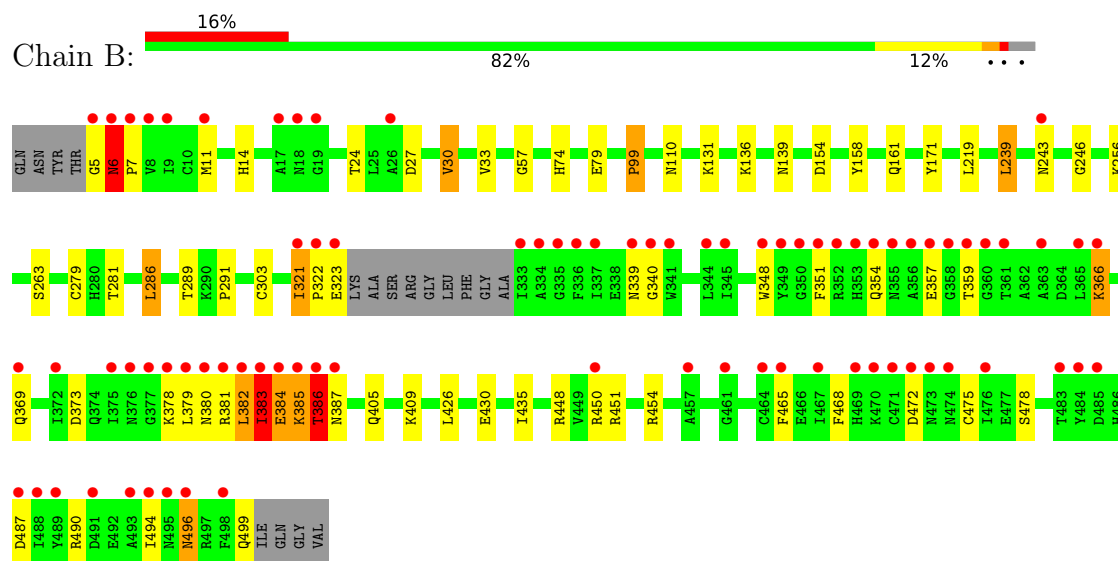
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

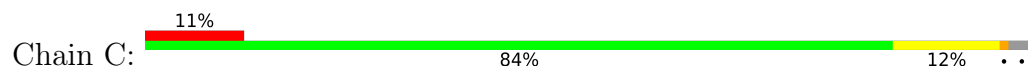
• Molecule 1: Hemagglutinin

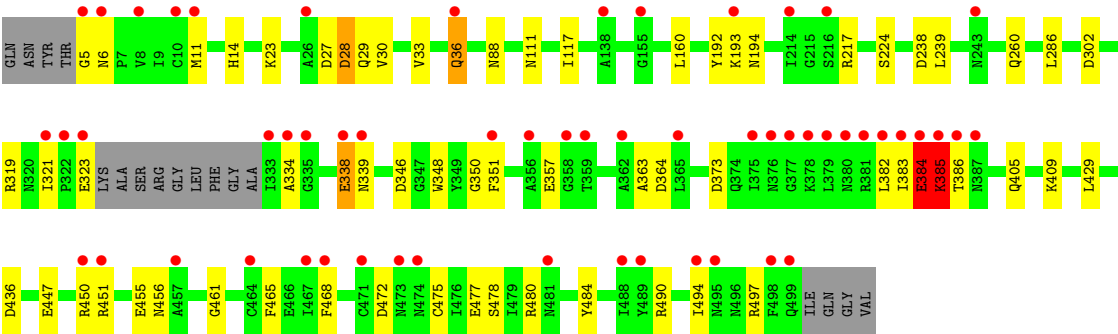


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 115.97Å 132.34Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	43.16 – 2.00 43.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.16-2.00) 99.6 (43.16-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.186 , 0.214 0.189 , 0.213	Depositor DCC
R_{free} test set	6484 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12745	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NAG

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	0.46	0/3910	0.81	1/5302 (0.0%)
1	B	0.49	0/3910	0.85	6/5302 (0.1%)
1	C	0.48	1/3910 (0.0%)	0.79	4/5302 (0.1%)
All	All	0.48	1/11730 (0.0%)	0.82	11/15906 (0.1%)

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
1	B	0	1
1	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	GLU	CA-C	7.18	1.62	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	ILE	CA-C-N	8.67	129.33	120.14
1	B	321	ILE	C-N-CA	8.67	129.33	120.14
1	C	385	LYS	N-CA-C	-8.66	96.25	109.41
1	B	6	ASN	CA-C-N	-6.59	113.50	120.03
1	B	6	ASN	C-N-CA	-6.59	113.50	120.03
1	B	454	ARG	CB-CA-C	-6.24	109.39	116.63
1	A	29	GLN	CA-CB-CG	5.66	125.42	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	382	LEU	CA-C-N	-5.49	115.91	122.22
1	C	382	LEU	C-N-CA	-5.49	115.91	122.22
1	B	382	LEU	N-CA-C	-5.46	105.41	111.36
1	C	350	GLY	N-CA-C	5.08	118.10	110.18

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	383	ILE	Peptide
1	C	338	GLU	Peptide
1	C	385	LYS	Peptide

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	3833	0	3700	65	0
1	B	3833	0	3700	61	1
1	C	3833	0	3700	48	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	28	0	26	1	0
3	A	382	0	0	10	1
3	B	388	0	0	12	0
3	C	392	0	0	11	0
All	All	12745	0	11178	169	1

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 7.

All (169) 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:386:THR:HG23	3:B:979:HOH:O	1.19	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:GLU:OE2	3:B:701:HOH:O	1.81	0.97
1:C:484:TYR:O	3:C:702:HOH:O	1.83	0.96
1:B:386:THR:CG2	3:B:979:HOH:O	1.80	0.96
1:C:373:ASP:OD1	3:C:701:HOH:O	1.83	0.95
1:A:14:HIS:HD2	1:A:348:TRP:HA	1.33	0.94
1:B:14:HIS:HD2	1:B:348:TRP:HA	1.34	0.90
1:C:384:GLU:HG3	1:C:385:LYS:HG2	1.55	0.87
1:C:456:ASN:OD1	3:C:703:HOH:O	1.92	0.86
1:C:384:GLU:HG2	1:C:385:LYS:H	1.41	0.85
1:A:454:ARG:HD3	1:A:486:HIS:CE1	2.13	0.82
1:C:14:HIS:HD2	1:C:348:TRP:HA	1.44	0.81
1:B:14:HIS:CD2	1:B:348:TRP:HA	2.17	0.80
1:B:99:PRO:O	3:B:703:HOH:O	1.99	0.79
1:B:366:LYS:O	3:B:704:HOH:O	2.01	0.79
1:B:5:GLY:HA2	1:B:468:PHE:HA	1.63	0.79
1:C:14:HIS:CD2	1:C:348:TRP:HA	2.18	0.78
1:A:14:HIS:CD2	1:A:348:TRP:HA	2.20	0.76
1:B:384:GLU:HB2	1:B:385:LYS:HD2	1.68	0.76
1:B:339:ASN:ND2	1:B:340:GLY:O	2.20	0.75
1:B:496:ASN:HD22	1:B:496:ASN:N	1.86	0.73
1:C:323:GLU:HG3	1:C:339:ASN:HD22	1.54	0.72
1:A:281:THR:HG23	1:A:286:LEU:HD11	1.73	0.71
1:C:319:ARG:HG3	3:C:763:HOH:O	1.90	0.71
1:A:23:LYS:HD2	1:B:381:ARG:NH1	2.07	0.70
1:C:88:ASN:OD1	3:C:704:HOH:O	2.10	0.69
1:A:323:GLU:O	3:A:701:HOH:O	2.10	0.69
1:C:36:GLN:HA	1:C:36:GLN:OE1	1.92	0.69
1:C:447:GLU:OE1	1:C:450:ARG:NH1	2.26	0.68
1:B:27:ASP:OD1	3:B:706:HOH:O	2.11	0.68
1:A:354:GLN:HG2	1:A:359:THR:HG22	1.76	0.68
1:A:486:HIS:HD2	1:A:487:ASP:N	1.92	0.68
1:C:477:GLU:HG2	1:C:480:ARG:HH21	1.59	0.68
1:A:451:ARG:NH1	3:A:705:HOH:O	2.24	0.67
1:A:26:ALA:O	3:A:702:HOH:O	2.12	0.67
1:B:378:LYS:NZ	1:B:430:GLU:O	2.28	0.67
1:A:11:MET:HB2	1:A:336:PHE:HE2	1.60	0.66
1:C:436:ASP:OD2	3:C:705:HOH:O	2.13	0.66
1:B:379:LEU:HA	1:B:382:LEU:CB	2.27	0.65
1:A:31:GLU:OE1	3:A:703:HOH:O	2.15	0.64
1:C:384:GLU:CG	1:C:385:LYS:H	2.08	0.64
1:B:279:CYS:SG	1:B:286:LEU:HD23	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:GLU:CG	1:C:385:LYS:HG2	2.27	0.64
1:C:302:ASP:OD1	1:C:386:THR:HB	1.99	0.63
1:B:382:LEU:HD11	1:B:426:LEU:HD21	1.80	0.63
1:A:454:ARG:HD3	1:A:486:HIS:HE1	1.62	0.62
1:C:5:GLY:HA2	1:C:468:PHE:HA	1.80	0.62
1:B:340:GLY:HA2	3:B:714:HOH:O	1.99	0.62
1:B:322:PRO:O	1:B:323:GLU:HB2	1.99	0.61
1:B:448:ARG:HA	1:B:451:ARG:HH21	1.65	0.61
1:B:291:PRO:HD3	1:B:383:ILE:HD12	1.82	0.60
1:C:384:GLU:CG	1:C:385:LYS:N	2.65	0.60
1:C:334:ALA:HB1	1:C:338:GLU:HG3	1.83	0.60
1:A:381:ARG:CZ	1:C:23:LYS:HD3	2.32	0.59
1:A:11:MET:HE1	1:A:351:PHE:CE2	2.37	0.59
1:B:475:CYS:O	1:B:478:SER:OG	2.17	0.58
1:A:451:ARG:HD2	1:C:461:GLY:HA2	1.85	0.58
1:B:79:GLU:OE1	3:B:708:HOH:O	2.17	0.58
1:A:29:GLN:HE21	1:A:29:GLN:HA	1.68	0.58
1:A:376:ASN:HA	1:A:379:LEU:HG	1.87	0.57
1:B:385:LYS:HD2	1:B:385:LYS:N	2.19	0.57
1:B:384:GLU:HB2	1:B:385:LYS:CD	2.34	0.57
1:A:11:MET:HB2	1:A:336:PHE:CE2	2.37	0.57
1:A:499:GLN:NE2	3:A:711:HOH:O	2.35	0.57
1:A:337:ILE:O	1:A:338:GLU:HG3	2.05	0.56
1:A:14:HIS:CE1	1:A:33:VAL:HG21	2.41	0.56
1:A:379:LEU:HA	1:A:382:LEU:HD12	1.86	0.56
1:B:171:TYR:CZ	1:B:256:LYS:HD2	2.41	0.56
1:B:11:MET:HE1	1:B:351:PHE:CD2	2.40	0.56
1:C:27:ASP:HB2	1:C:30:VAL:HG22	1.88	0.56
1:B:369:GLN:NE2	1:B:373:ASP:OD1	2.37	0.55
1:A:136:LYS:NZ	3:A:717:HOH:O	2.39	0.55
1:A:405:GLN:HG2	1:A:409:LYS:HD3	1.89	0.55
1:C:405:GLN:HG2	1:C:409:LYS:HD3	1.89	0.55
1:B:303:CYS:O	1:B:387:ASN:HB3	2.08	0.54
1:A:171:TYR:CZ	1:A:256:LYS:HD2	2.42	0.54
1:A:335:GLY:HA2	1:A:341:TRP:HZ2	1.73	0.54
1:A:137:ARG:NE	1:A:142:ASP:OD2	2.36	0.54
1:A:486:HIS:CD2	1:A:487:ASP:N	2.73	0.53
1:C:384:GLU:HG2	1:C:385:LYS:N	2.18	0.53
1:A:11:MET:HE1	1:A:351:PHE:CD2	2.43	0.53
1:A:375:ILE:O	1:A:378:LYS:HG2	2.10	0.52
1:A:29:GLN:HA	1:A:29:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:GLU:O	1:C:497:ARG:NH1	2.41	0.51
1:C:323:GLU:HG3	1:C:339:ASN:ND2	2.24	0.51
1:B:256:LYS:NZ	3:B:718:HOH:O	2.40	0.51
1:A:383:ILE:HG12	1:A:383:ILE:O	2.11	0.51
1:C:238:ASP:OD2	3:C:706:HOH:O	2.17	0.51
1:A:381:ARG:NH2	1:C:23:LYS:HD3	2.26	0.51
1:B:405:GLN:HG2	1:B:409:LYS:HD3	1.93	0.50
1:B:487:ASP:HA	1:B:490:ARG:HB2	1.91	0.50
1:A:450:ARG:NH2	1:A:459:ASP:OD2	2.45	0.50
1:B:14:HIS:CE1	1:B:33:VAL:HG11	2.47	0.50
1:B:291:PRO:CD	1:B:383:ILE:HD12	2.42	0.49
1:B:6:ASN:H	1:B:7:PRO:CD	2.26	0.49
1:B:379:LEU:HA	1:B:382:LEU:HB3	1.93	0.49
1:B:490:ARG:O	1:B:494:ILE:HG12	2.13	0.48
1:C:475:CYS:O	1:C:478:SER:OG	2.27	0.48
1:A:335:GLY:HA2	1:A:341:TRP:CZ2	2.47	0.48
1:A:281:THR:HG23	1:A:286:LEU:CD1	2.42	0.48
1:C:357:GLU:OE2	1:C:472:ASP:HB2	2.13	0.48
1:A:28:ASP:OD2	3:A:704:HOH:O	2.19	0.48
1:C:346:ASP:OD2	1:C:363:ALA:HB2	2.13	0.47
1:C:351:PHE:CD2	1:C:480:ARG:HG2	2.48	0.47
1:A:14:HIS:HE1	1:A:33:VAL:HG21	1.78	0.47
1:A:384:GLU:OE1	1:A:384:GLU:N	2.46	0.47
1:B:131:LYS:HE3	1:B:131:LYS:HB2	1.78	0.47
1:C:217:ARG:HB2	1:C:224:SER:O	2.14	0.47
1:C:477:GLU:HG2	1:C:480:ARG:NH2	2.28	0.47
1:A:429:LEU:HD13	1:C:429:LEU:HD21	1.96	0.47
1:A:166:ILE:HG22	1:A:168:ASN:OD1	2.15	0.46
1:B:379:LEU:HA	1:B:382:LEU:HB2	1.96	0.46
1:A:376:ASN:CA	1:A:379:LEU:HG	2.45	0.46
1:C:11:MET:HE1	1:C:351:PHE:CD2	2.50	0.46
1:A:7:PRO:HD2	1:A:467:ILE:O	2.16	0.46
1:A:217:ARG:HB2	1:A:224:SER:O	2.16	0.46
1:A:286:LEU:HD12	1:A:286:LEU:N	2.31	0.46
1:B:14:HIS:CE1	1:B:33:VAL:HG21	2.50	0.46
1:B:366:LYS:HG3	3:B:704:HOH:O	2.15	0.46
1:B:496:ASN:N	1:B:496:ASN:ND2	2.60	0.46
1:A:376:ASN:HB2	1:A:379:LEU:HG	1.97	0.46
1:B:24:THR:HG21	1:B:435:ILE:HD12	1.97	0.46
1:C:11:MET:HE1	1:C:351:PHE:CG	2.52	0.45
2:C:602:NAG:H83	3:C:824:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:THR:O	1:B:383:ILE:HG21	2.17	0.45
1:B:11:MET:HE1	1:B:351:PHE:CE2	2.52	0.45
1:A:136:LYS:HD3	1:A:139:ASN:HA	1.99	0.44
1:C:28:ASP:N	1:C:28:ASP:OD1	2.46	0.44
1:A:27:ASP:HB2	1:A:30:VAL:HG22	1.99	0.44
1:A:164:THR:HG23	1:A:239:LEU:HD23	1.98	0.44
1:B:27:ASP:HB2	1:B:30:VAL:HG22	1.99	0.44
1:A:11:MET:HE3	1:A:11:MET:HB3	1.73	0.44
1:B:450:ARG:HB2	1:B:465:PHE:HZ	1.83	0.44
1:C:14:HIS:CE1	1:C:33:VAL:HG11	2.53	0.44
1:A:486:HIS:CD2	1:A:486:HIS:C	2.96	0.44
1:B:339:ASN:CG	1:B:340:GLY:N	2.76	0.44
1:C:192:TYR:O	1:C:194:ASN:N	2.48	0.43
1:B:136:LYS:HE2	3:B:729:HOH:O	2.17	0.43
1:B:139:ASN:ND2	3:B:702:HOH:O	1.98	0.43
1:B:158:TYR:CZ	1:B:246:GLY:HA2	2.53	0.43
1:A:5:GLY:HA2	1:A:468:PHE:HA	2.01	0.43
1:B:291:PRO:CG	1:B:383:ILE:HD12	2.48	0.43
1:A:193:LYS:HD2	3:A:810:HOH:O	2.19	0.43
1:B:219:LEU:HD23	3:C:1019:HOH:O	2.19	0.43
1:B:110:ASN:HA	1:B:263:SER:O	2.18	0.42
1:A:442:MET:HE3	1:A:442:MET:HA	2.02	0.42
1:C:14:HIS:CE1	1:C:33:VAL:HG21	2.54	0.42
1:B:357:GLU:OE2	1:B:472:ASP:HB2	2.20	0.42
1:C:383:ILE:HD12	1:C:383:ILE:HA	1.88	0.42
1:B:379:LEU:HD12	1:B:382:LEU:HB3	2.01	0.42
1:A:357:GLU:OE2	1:A:472:ASP:HB2	2.20	0.41
1:A:460:LYS:HE2	1:A:460:LYS:HB3	1.86	0.41
1:C:111:ASN:HB3	3:C:813:HOH:O	2.19	0.41
1:C:351:PHE:CE1	1:C:364:ASP:HB2	2.55	0.41
1:A:454:ARG:HD3	1:A:486:HIS:ND1	2.33	0.41
1:B:161:GLN:O	1:B:243:ASN:HA	2.20	0.41
1:B:281:THR:HG23	1:B:286:LEU:HD21	2.02	0.41
1:C:323:GLU:O	3:C:707:HOH:O	2.21	0.41
1:A:27:ASP:HB2	1:A:30:VAL:CG2	2.51	0.41
1:A:278:LYS:NZ	3:A:728:HOH:O	2.49	0.41
1:B:57:GLY:O	1:B:74:HIS:HE1	2.02	0.41
1:C:450:ARG:HB2	1:C:465:PHE:HZ	1.85	0.41
1:A:378:LYS:HE2	1:A:378:LYS:HB3	1.82	0.41
1:B:354:GLN:HG3	1:B:359:THR:HG22	2.03	0.40
1:C:490:ARG:O	1:C:494:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HB2	1:A:231:TRP:CZ3	2.56	0.40
1:A:218:PRO:HG3	1:B:239:LEU:HD22	2.03	0.40
1:A:6:ASN:ND2	3:A:733:HOH:O	2.54	0.40
1:A:110:ASN:HA	1:A:263:SER:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASP:O	3:A:756:HOH:O[1_454]	2.12	0.08

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	482/503 (96%)	462 (96%)	16 (3%)	4 (1%)	16	11
1	B	482/503 (96%)	462 (96%)	18 (4%)	2 (0%)	30	27
1	C	482/503 (96%)	462 (96%)	19 (4%)	1 (0%)	43	42
All	All	1446/1509 (96%)	1386 (96%)	53 (4%)	7 (0%)	24	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ILE
1	B	6	ASN
1	A	338	GLU
1	A	6	ASN
1	A	26	ALA
1	C	6	ASN
1	B	386	THR

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	421/433 (97%)	408 (97%)	13 (3%)	35	37
1	B	421/433 (97%)	408 (97%)	13 (3%)	35	37
1	C	421/433 (97%)	409 (97%)	12 (3%)	37	40
All	All	1263/1299 (97%)	1225 (97%)	38 (3%)	36	38

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	29	GLN
1	A	239	LEU
1	A	243	ASN
1	A	286	LEU
1	A	319	ARG
1	A	333	ILE
1	A	337	ILE
1	A	354	GLN
1	A	376	ASN
1	A	382	LEU
1	A	383	ILE
1	A	385	LYS
1	B	30	VAL
1	B	99	PRO
1	B	239	LEU
1	B	286	LEU
1	B	321	ILE
1	B	366	LYS
1	B	380	ASN
1	B	383	ILE
1	B	384	GLU
1	B	385	LYS
1	B	386	THR
1	B	496	ASN
1	B	499	GLN

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Mol	Chain	Res	Type
1	C	28	ASP
1	C	29	GLN
1	C	36	GLN
1	C	117	ILE
1	C	160	LEU
1	C	193	LYS
1	C	239	LEU
1	C	260	GLN
1	C	286	LEU
1	C	321	ILE
1	C	384	GLU
1	C	451	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	29	GLN
1	A	64	ASN
1	A	124	ASN
1	A	243	ASN
1	A	260	GLN
1	A	387	ASN
1	A	443	ASN
1	A	452	GLN
1	A	486	HIS
1	B	14	HIS
1	B	43	ASN
1	B	64	ASN
1	B	74	HIS
1	B	258	ASN
1	B	342	GLN
1	B	380	ASN
1	B	496	ASN
1	C	14	HIS
1	C	64	ASN
1	C	207	GLN
1	C	342	GLN
1	C	353	HIS
1	C	387	ASN
1	C	432	GLN
1	C	443	ASN

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Mol	Chain	Res	Type
1	C	496	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
2	NAG	B	601	1	14,14,15	0.40	0	17,19,21	0.40	0
2	NAG	A	602	1	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
2	NAG	C	601	1	14,14,15	0.37	0	17,19,21	0.41	0
2	NAG	A	601	1	14,14,15	0.29	0	17,19,21	0.36	0
2	NAG	B	602	1	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
2	NAG	C	602	1	14,14,15	0.34	0	17,19,21	0.75	1 (5%)

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	B	601	1	-	2/6/23/26	0/1/1/1
2	NAG	A	602	1	-	2/6/23/26	0/1/1/1
2	NAG	C	601	1	-	2/6/23/26	0/1/1/1
2	NAG	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	-	2/6/23/26	0/1/1/1
2	NAG	C	602	1	-	2/6/23/26	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(°)
2	C	602	NAG	C1-O5-C5	2.69	115.78	112.19
2	B	602	NAG	C1-O5-C5	2.36	115.35	112.19
2	A	602	NAG	C1-O5-C5	2.07	114.95	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	NAG	O5-C5-C6-O6
2	C	601	NAG	C4-C5-C6-O6
2	B	601	NAG	O5-C5-C6-O6
2	A	602	NAG	C8-C7-N2-C2
2	A	602	NAG	O7-C7-N2-C2
2	B	602	NAG	C8-C7-N2-C2
2	B	602	NAG	O7-C7-N2-C2
2	C	602	NAG	C8-C7-N2-C2
2	C	602	NAG	O7-C7-N2-C2
2	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	NAG	1	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, 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	486/503 (96%)	0.36	53 (10%) 10 9	14, 30, 75, 166	0
1	B	486/503 (96%)	0.51	81 (16%) 4 4	12, 28, 89, 158	0
1	C	486/503 (96%)	0.47	56 (11%) 9 8	12, 30, 78, 148	0
All	All	1458/1509 (96%)	0.45	190 (13%) 7 6	12, 29, 82, 166	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	LEU	9.1
1	B	383	ILE	9.0
1	A	336	PHE	8.9
1	C	382	LEU	8.7
1	C	383	ILE	8.6
1	C	386	THR	8.2
1	A	379	LEU	7.7
1	B	379	LEU	7.7
1	B	322	PRO	7.4
1	B	336	PHE	7.4
1	A	377	GLY	7.0
1	B	382	LEU	6.4
1	C	26	ALA	6.4
1	A	17	ALA	6.1
1	B	386	THR	6.1
1	B	498	PHE	6.0
1	A	381	ARG	6.0
1	A	26	ALA	6.0
1	C	379	LEU	6.0
1	B	377	GLY	5.8
1	B	333	ILE	5.7
1	A	383	ILE	5.6
1	A	376	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	381	ARG	5.5
1	B	384	GLU	5.4
1	B	5	GLY	5.4
1	B	356	ALA	5.3
1	C	384	GLU	5.3
1	A	337	ILE	5.3
1	B	385	LYS	5.2
1	B	380	ASN	5.0
1	B	335	GLY	4.9
1	C	5	GLY	4.8
1	A	386	THR	4.8
1	B	334	ALA	4.8
1	A	385	LYS	4.7
1	A	333	ILE	4.7
1	C	333	ILE	4.6
1	C	11	MET	4.5
1	C	498	PHE	4.5
1	B	387	ASN	4.5
1	C	138	ALA	4.4
1	C	385	LYS	4.4
1	B	339	ASN	4.3
1	B	474	ASN	4.3
1	C	377	GLY	4.3
1	A	322	PRO	4.2
1	B	471	CYS	4.2
1	B	488	ILE	4.2
1	B	473	ASN	4.2
1	A	354	GLN	4.0
1	B	489	TYR	4.0
1	A	356	ALA	3.9
1	A	339	ASN	3.9
1	C	380	ASN	3.9
1	C	356	ALA	3.9
1	B	381	ARG	3.9
1	B	358	GLY	3.8
1	A	18	ASN	3.8
1	B	361	THR	3.7
1	B	26	ALA	3.7
1	A	5	GLY	3.6
1	C	494	ILE	3.6
1	A	375	ILE	3.6
1	B	321	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	468	PHE	3.6
1	A	486	HIS	3.5
1	A	321	ILE	3.5
1	B	469	HIS	3.5
1	B	359	THR	3.5
1	A	11	MET	3.3
1	A	384	GLU	3.3
1	B	470	LYS	3.3
1	C	351	PHE	3.3
1	C	387	ASN	3.2
1	C	365	LEU	3.2
1	A	498	PHE	3.2
1	C	321	ILE	3.1
1	C	464	CYS	3.1
1	B	8	VAL	3.1
1	B	11	MET	3.1
1	A	380	ASN	3.1
1	B	341	TRP	3.0
1	B	17	ALA	3.0
1	B	476	ILE	3.0
1	C	334	ALA	3.0
1	A	6	ASN	3.0
1	A	168	ASN	3.0
1	B	376	ASN	3.0
1	B	496	ASN	3.0
1	B	9	ILE	3.0
1	A	378	LYS	3.0
1	C	322	PRO	3.0
1	C	8	VAL	2.9
1	B	467	ILE	2.9
1	C	499	GLN	2.9
1	B	355	ASN	2.9
1	A	28	ASP	2.9
1	C	323	GLU	2.9
1	B	353	HIS	2.8
1	B	323	GLU	2.8
1	A	8	VAL	2.8
1	C	488	ILE	2.8
1	B	378	LYS	2.8
1	C	378	LYS	2.8
1	B	487	ASP	2.8
1	B	352	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	354	GLN	2.7
1	C	338	GLU	2.7
1	A	344	LEU	2.7
1	A	358	GLY	2.7
1	B	366	LYS	2.7
1	B	345	ILE	2.7
1	B	351	PHE	2.7
1	B	465	PHE	2.7
1	C	495	ASN	2.7
1	C	155	GLY	2.7
1	C	193	LYS	2.6
1	A	345	ILE	2.6
1	B	7	PRO	2.6
1	B	491	ASP	2.6
1	B	349	TYR	2.6
1	B	372	ILE	2.6
1	C	467	ILE	2.6
1	C	481	ASN	2.6
1	B	494	ILE	2.6
1	C	375	ILE	2.5
1	A	387	ASN	2.5
1	A	27	ASP	2.5
1	A	334	ALA	2.5
1	B	19	GLY	2.5
1	B	375	ILE	2.5
1	A	461	GLY	2.5
1	C	335	GLY	2.5
1	B	484	TYR	2.5
1	B	450	ARG	2.5
1	B	18	ASN	2.5
1	B	348	TRP	2.5
1	C	243	ASN	2.5
1	B	363	ALA	2.4
1	B	344	LEU	2.4
1	B	350	GLY	2.4
1	C	358	GLY	2.4
1	C	6	ASN	2.4
1	A	495	ASN	2.4
1	A	16	VAL	2.4
1	C	471	CYS	2.4
1	B	340	GLY	2.3
1	C	214	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	30	VAL	2.3
1	B	357	GLU	2.3
1	C	36	GLN	2.3
1	A	467	ILE	2.3
1	B	472	ASP	2.3
1	B	6	ASN	2.3
1	C	376	ASN	2.3
1	C	473	ASN	2.3
1	A	338	GLU	2.2
1	A	488	ILE	2.2
1	A	494	ILE	2.2
1	B	337	ILE	2.2
1	A	470	LYS	2.2
1	B	360	GLY	2.2
1	B	461	GLY	2.2
1	A	29	GLN	2.2
1	A	499	GLN	2.2
1	A	323	GLU	2.1
1	C	10	CYS	2.1
1	B	243	ASN	2.1
1	B	485	ASP	2.1
1	C	450	ARG	2.1
1	B	457	ALA	2.1
1	C	362	ALA	2.1
1	B	365	LEU	2.1
1	B	464	CYS	2.1
1	C	474	ASN	2.1
1	B	483	THR	2.1
1	A	319	ARG	2.1
1	C	451	ARG	2.1
1	C	457	ALA	2.1
1	C	359	THR	2.1
1	B	493	ALA	2.1
1	C	216	SER	2.1
1	A	365	LEU	2.0
1	B	369	GLN	2.0
1	C	489	TYR	2.0
1	B	495	ASN	2.0
1	C	339	ASN	2.0
1	A	260	GLN	2.0
1	A	10	CYS	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	601	14/15	0.57	0.24	66,83,89,91	0
2	NAG	B	601	14/15	0.66	0.21	72,82,89,91	0
2	NAG	C	601	14/15	0.69	0.20	77,85,89,89	0
2	NAG	A	602	14/15	0.88	0.10	30,33,39,42	0
2	NAG	C	602	14/15	0.88	0.09	23,29,33,41	0
2	NAG	B	602	14/15	0.91	0.09	27,34,38,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.