



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 AM UTC

PDB ID : 8X29 / pdb_00008x29
Title : Crystal structure of H5 hemagglutinin from swan-infecting H5N8 influenza virus in complex with LSTa
Authors : Jin, X.Y.; Han, P.; Song, H.; Qi, J.X.
Deposited on : 2023-11-09
Resolution : 2.61 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

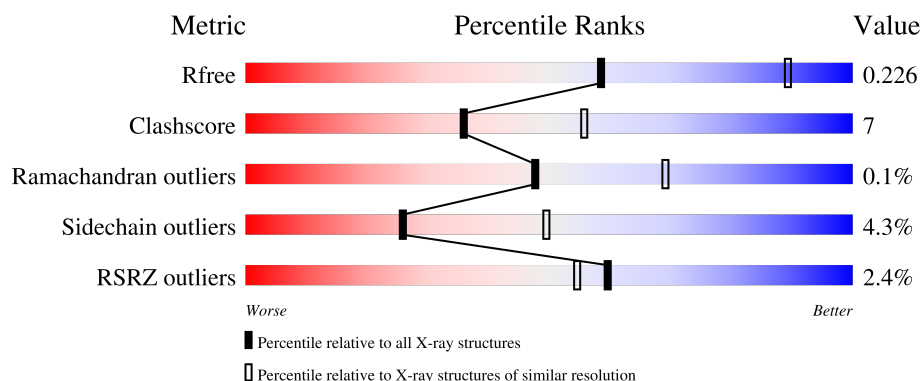
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	506	6% 78% 17% ..
1	B	506	81% 15% ..
1	C	506	6% 76% 19% ..

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
2	NAG	A	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12385 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	491	Total	C	N	O	S	0	0	0
			3928	2475	681	750	22			
1	B	491	Total	C	N	O	S	0	0	0
			3928	2475	681	750	22			
1	C	491	Total	C	N	O	S	0	0	0
			3928	2475	681	750	22			

There are 9 discrepancies between the modelled and reference sequences:

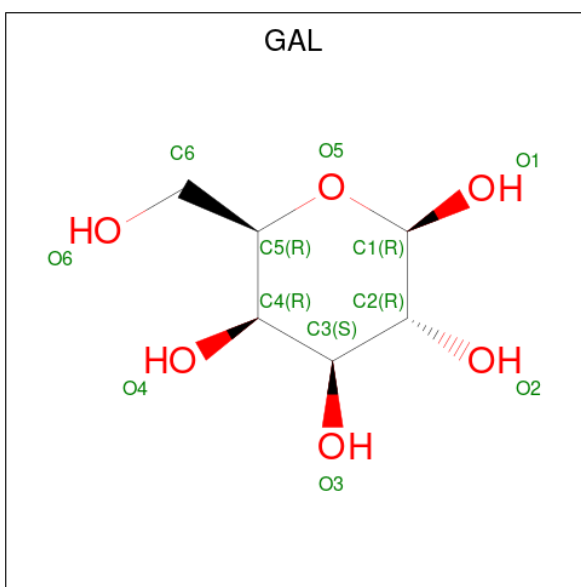
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
A	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
A	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5
B	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
B	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
B	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5
C	86	VAL	ALA	engineered mutation	UNP A0A8E4ZAK5
C	188	ILE	THR	engineered mutation	UNP A0A8E4ZAK5
C	273	ASN	HIS	engineered mutation	UNP A0A8E4ZAK5

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



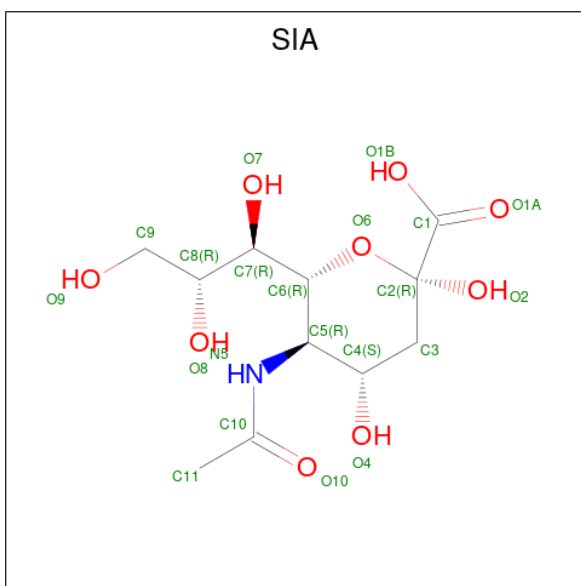
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			20	11	1	8		

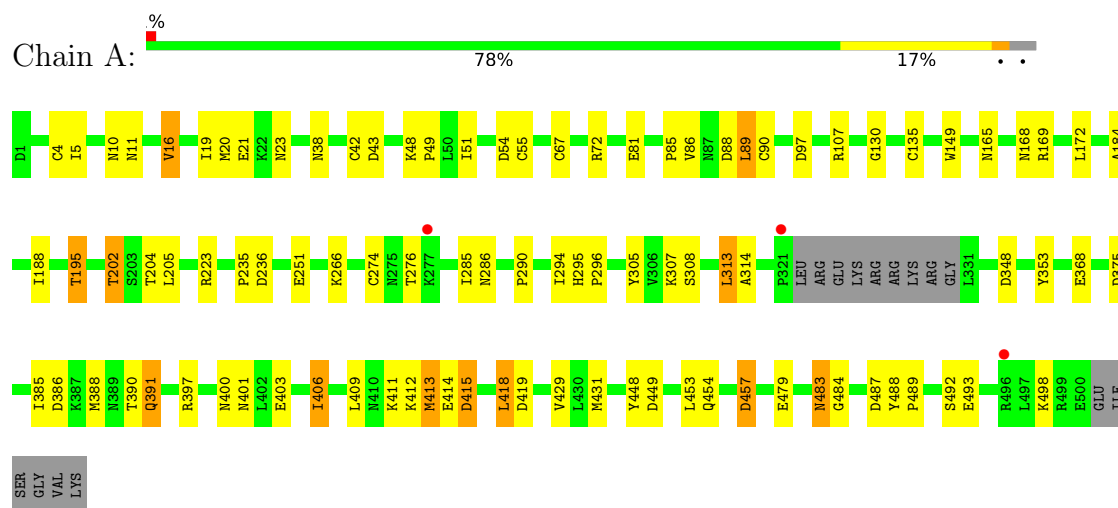
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total 179	O 179	0	0
5	B	131	Total 131	O 131	0	0
5	C	91	Total 91	O 91	0	0

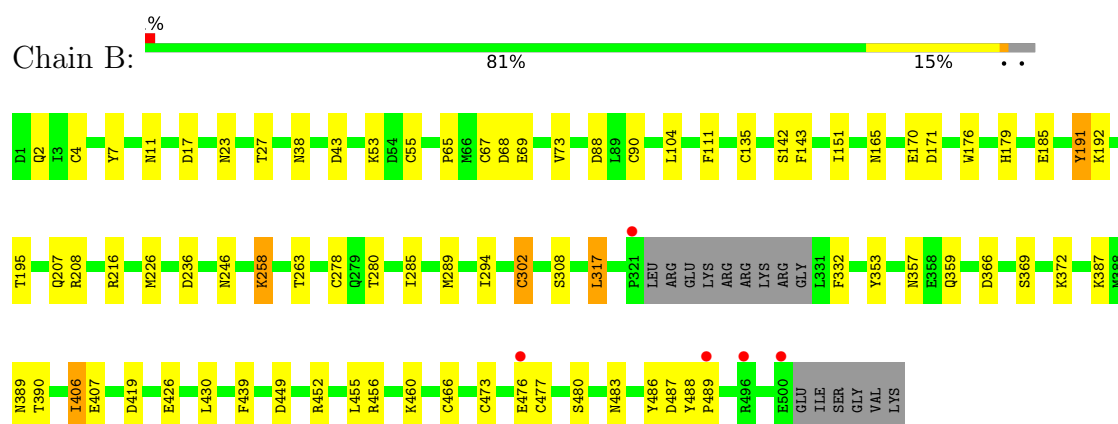
3 Residue-property plots [i](#)

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.

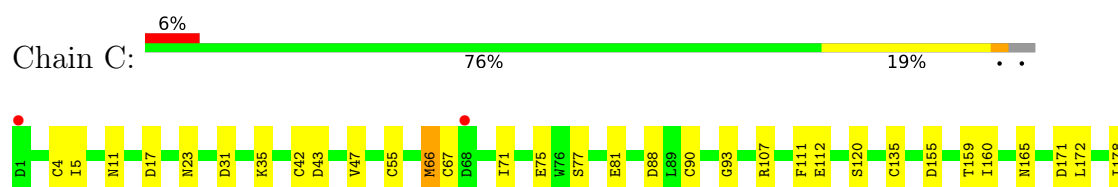
• Molecule 1: Hemagglutinin

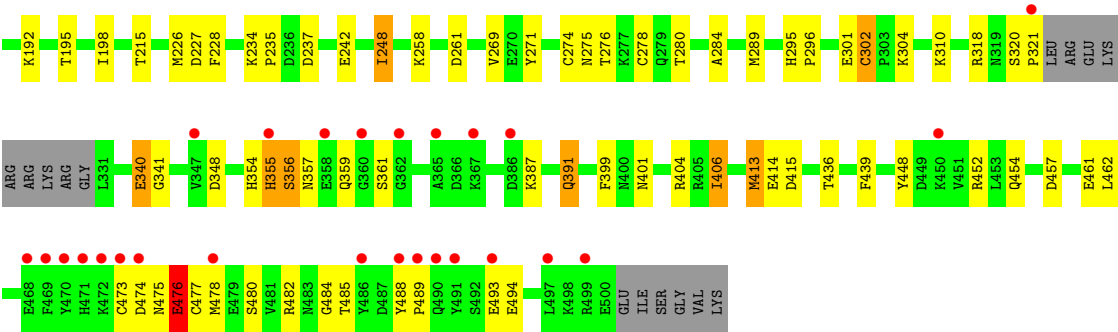


• Molecule 1: Hemagglutinin



• 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	80.15Å 108.50Å 133.19Å 90.00° 99.79° 90.00°	Depositor
Resolution (Å)	26.33 – 2.61 26.33 – 2.61	Depositor EDS
% Data completeness (in resolution range)	92.7 (26.33-2.61) 92.7 (26.33-2.61)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.184 , 0.231 0.189 , 0.226	Depositor DCC
R_{free} test set	2000 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12385	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 4.48% 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: GAL, NAG, SIA

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	0.70	0/4018	1.23	18/5443 (0.3%)
1	B	0.69	0/4018	1.23	22/5443 (0.4%)
1	C	0.66	0/4018	1.22	23/5443 (0.4%)
All	All	0.68	0/12054	1.23	63/16329 (0.4%)

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	A	0	3
1	B	0	2
1	C	0	1
All	All	0	6

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	THR	CA-CB-OG1	-7.57	98.25	109.60
1	B	487	ASP	CA-CB-CG	7.20	119.80	112.60
1	C	155	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	251	GLU	CB-CG-CD	6.80	124.16	112.60
1	C	302	CYS	CB-CA-C	-6.79	98.70	109.08
1	B	195	THR	CA-CB-OG1	-6.76	99.46	109.60
1	C	159	THR	CA-CB-OG1	-6.58	99.72	109.60
1	B	185	GLU	CB-CG-CD	6.50	123.66	112.60
1	A	457	ASP	CA-CB-CG	6.49	119.09	112.60
1	C	195	THR	CA-CB-OG1	-6.30	100.14	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	PRO	N-CA-C	-6.25	101.45	111.38
1	A	479	GLU	CB-CG-CD	6.22	123.18	112.60
1	C	171	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	391	GLN	CB-CA-C	-6.08	98.33	110.42
1	C	31	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	191	TYR	CA-C-N	-6.04	111.13	120.31
1	B	191	TYR	C-N-CA	-6.04	111.13	120.31
1	B	111	PHE	CB-CA-C	-6.03	98.85	109.71
1	A	97	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	386	ASP	CB-CA-C	6.01	121.07	110.85
1	B	88	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	88	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	236	ASP	CB-CA-C	5.96	115.73	109.83
1	B	332	PHE	CA-CB-CG	-5.96	107.84	113.80
1	B	419	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	17	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	390	THR	CA-CB-OG1	-5.88	100.77	109.60
1	A	348	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	449	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	81	GLU	N-CA-CB	-5.83	101.31	110.69
1	A	375	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	215	THR	CA-CB-OG1	-5.75	100.97	109.60
1	C	81	GLU	CB-CA-C	5.74	119.70	109.38
1	C	227	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	17	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	43	ASP	CA-CB-CG	5.65	118.25	112.60
1	C	476	GLU	CB-CG-CD	5.65	122.20	112.60
1	A	21	GLU	CB-CG-CD	5.62	122.16	112.60
1	B	302	CYS	CB-CA-C	-5.56	100.77	109.22
1	B	390	THR	CA-CB-OG1	-5.53	101.31	109.60
1	B	68	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	263	THR	CA-CB-OG1	-5.47	101.40	109.60
1	C	457	ASP	CA-CB-CG	5.45	118.05	112.60
1	C	391	GLN	CB-CA-C	-5.42	99.63	111.71
1	C	111	PHE	CB-CA-C	-5.40	99.49	109.37
1	A	386	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	419	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	348	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	258	LYS	CB-CA-C	5.33	118.35	110.14
1	B	372	LYS	N-CA-CB	5.30	118.01	110.06
1	A	168	ASN	N-CA-C	-5.30	103.04	110.35
1	B	236	ASP	CA-CB-CG	5.23	117.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	271	TYR	CB-CA-C	5.23	120.17	109.76
1	A	172	LEU	N-CA-CB	-5.22	102.57	110.77
1	B	73	VAL	N-CA-CB	-5.21	106.84	112.37
1	C	192	LYS	N-CA-C	-5.16	106.14	112.90
1	C	43	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	251	GLU	N-CA-C	-5.11	105.28	112.12
1	C	237	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	171	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	261	ASP	CB-CA-C	5.07	118.89	110.78
1	B	460	LYS	N-CA-CB	-5.04	102.65	110.57
1	C	340	GLU	CB-CG-CD	5.03	121.16	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	223	ARG	Sidechain
1	A	397	ARG	Sidechain
1	B	216	ARG	Sidechain
1	B	452	ARG	Sidechain
1	C	318	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	3928	0	3809	59	0
1	B	3928	0	3809	42	0
1	C	3928	0	3809	52	0
2	A	56	0	52	14	0
2	B	56	0	52	7	0
2	C	57	0	54	9	0
3	C	11	0	10	3	0
4	C	20	0	17	2	0
5	A	179	0	0	6	0
5	B	131	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	91	0	0	2	0
All	All	12385	0	11612	157	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 7.

All (157) 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:A:165:ASN:HD21	2:A:601:NAG:C1	1.33	1.38
1:B:165:ASN:HD21	2:B:601:NAG:C1	1.54	1.20
1:A:165:ASN:ND2	2:A:601:NAG:C1	2.15	1.09
3:C:605:GAL:O3	4:C:606:SIA:C2	2.05	1.04
1:A:23:ASN:HD21	2:A:603:NAG:C1	1.77	0.97
2:A:601:NAG:O4	2:C:601:NAG:C1	2.16	0.94
1:B:278:CYS:HG	1:B:302:CYS:HG	0.94	0.94
1:A:90:CYS:HG	1:A:135:CYS:HG	1.12	0.94
3:C:605:GAL:HO3	4:C:606:SIA:C2	1.82	0.90
1:C:90:CYS:HG	1:C:135:CYS:HG	0.88	0.88
1:C:42:CYS:HG	1:C:274:CYS:HG	0.88	0.88
1:C:165:ASN:HD21	2:C:602:NAG:C1	1.88	0.87
1:B:165:ASN:ND2	2:B:601:NAG:C1	2.40	0.81
1:B:90:CYS:HG	1:B:135:CYS:HG	1.24	0.80
1:A:11:ASN:HD21	2:A:602:NAG:C1	1.96	0.79
1:A:202:THR:HG22	1:A:204:THR:H	1.48	0.78
1:B:23:ASN:ND2	2:B:603:NAG:C1	2.47	0.77
1:B:4:CYS:HG	1:B:466:CYS:HG	0.78	0.77
1:A:202:THR:HB	1:A:205:LEU:HB3	1.66	0.76
1:A:42:CYS:HG	1:A:274:CYS:HG	1.32	0.76
1:B:473:CYS:HG	1:B:477:CYS:HG	0.77	0.75
1:C:23:ASN:HD21	2:C:603:NAG:C1	2.00	0.73
1:C:278:CYS:HG	1:C:302:CYS:HG	1.34	0.73
1:B:55:CYS:HG	1:B:67:CYS:HG	0.74	0.72
1:B:11:ASN:HD21	2:B:602:NAG:C1	2.03	0.72
1:C:120:SER:HB2	5:C:771:HOH:O	1.91	0.70
1:B:406:ILE:H	1:B:406:ILE:HD12	1.55	0.70
2:C:604:NAG:O4	3:C:605:GAL:C1	2.40	0.70
1:A:406:ILE:H	1:A:406:ILE:HD12	1.55	0.69
1:A:88:ASP:O	1:A:89:LEU:HB2	1.92	0.68
1:A:55:CYS:CB	1:A:67:CYS:HG	2.07	0.67
1:C:165:ASN:HD21	2:C:602:NAG:C2	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASN:HD21	2:B:603:NAG:C1	2.08	0.64
1:B:38:ASN:OD1	1:B:38:ASN:C	2.42	0.62
1:B:477:CYS:O	1:B:480:SER:HB2	2.02	0.60
1:A:81:GLU:OE1	1:A:266:LYS:NZ	2.27	0.60
1:A:23:ASN:ND2	2:A:603:NAG:C1	2.59	0.59
1:B:406:ILE:HD12	1:B:406:ILE:N	2.18	0.59
1:C:454:GLN:NE2	1:C:484:GLY:O	2.36	0.59
1:C:355:HIS:O	1:C:356:SER:HB2	2.03	0.59
1:A:19:ILE:HD11	1:A:431:MET:HA	1.85	0.59
1:A:388:MET:HE3	1:A:391:GLN:HE21	1.68	0.58
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.67	0.57
1:A:313:LEU:HD13	1:A:429:VAL:HG22	1.86	0.57
1:B:55:CYS:CB	1:B:67:CYS:HG	2.16	0.57
1:C:413:MET:HG3	1:C:414:GLU:N	2.20	0.57
1:A:290:PRO:HG3	1:A:385:ILE:HD12	1.87	0.57
1:A:409:LEU:C	1:A:409:LEU:HD23	2.30	0.57
1:A:406:ILE:HD12	1:A:406:ILE:N	2.20	0.56
1:B:278:CYS:HG	1:B:302:CYS:CB	2.17	0.56
1:B:308:SER:HB3	1:B:426:GLU:OE2	2.05	0.56
1:A:454:GLN:NE2	1:A:484:GLY:HA2	2.21	0.56
1:C:355:HIS:HB3	1:C:478:MET:HE1	1.89	0.55
1:A:5:ILE:HG13	1:A:448:TYR:HA	1.89	0.55
1:A:406:ILE:H	1:A:406:ILE:CD1	2.20	0.55
1:C:75:GLU:OE1	1:C:258:LYS:NZ	2.37	0.54
1:C:23:ASN:HD21	2:C:603:NAG:C2	2.21	0.54
1:B:285:ILE:HD11	1:B:294:ILE:HG13	1.90	0.53
1:C:295:HIS:ND1	1:C:296:PRO:HD2	2.23	0.53
1:C:359:GLN:N	1:C:359:GLN:OE1	2.41	0.52
1:B:476:GLU:OE2	1:B:476:GLU:HA	2.09	0.52
1:C:340:GLU:CG	1:C:341:GLY:N	2.73	0.52
1:A:403:GLU:HA	1:A:406:ILE:HD13	1.91	0.52
1:C:304:LYS:HB3	1:C:391:GLN:NE2	2.25	0.51
1:B:473:CYS:HG	1:B:477:CYS:CB	2.21	0.51
1:B:176:TRP:HE1	1:B:207:GLN:HE22	1.57	0.51
1:A:483:ASN:OD1	2:A:604:NAG:C1	2.59	0.51
1:C:11:ASN:OD1	1:C:11:ASN:N	2.44	0.51
1:C:276:THR:HG21	1:C:284:ALA:HB1	1.93	0.51
1:A:72:ARG:N	5:A:704:HOH:O	2.31	0.51
1:C:35:LYS:HD3	5:C:770:HOH:O	2.11	0.51
1:A:454:GLN:HE22	1:A:484:GLY:HA2	1.75	0.50
1:B:4:CYS:CB	1:B:466:CYS:HG	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASN:C	1:A:483:ASN:HD22	2.20	0.50
1:C:66:MET:HA	1:C:66:MET:HE2	1.93	0.50
1:A:235:PRO:HD2	5:A:833:HOH:O	2.11	0.50
1:A:295:HIS:CG	1:A:296:PRO:HD2	2.47	0.50
1:B:480:SER:HB3	1:B:486:TYR:HA	1.94	0.50
1:A:16:VAL:HG11	1:A:314:ALA:HB2	1.94	0.49
1:C:401:ASN:ND2	1:C:404:ARG:HH22	2.10	0.49
1:C:473:CYS:SG	1:C:477:CYS:SG	3.10	0.49
1:A:4:CYS:O	1:A:353:TYR:HA	2.13	0.49
1:C:47:VAL:HB	1:C:77:SER:HB3	1.94	0.49
1:C:165:ASN:ND2	2:C:602:NAG:C1	2.69	0.49
1:B:353:TYR:OH	1:B:366:ASP:OD1	2.26	0.48
2:A:601:NAG:O4	2:C:601:NAG:O5	2.16	0.48
1:C:93:GLY:HA3	1:C:226:MET:O	2.14	0.48
1:A:23:ASN:HD21	2:A:603:NAG:C2	2.24	0.48
1:A:11:ASN:HD21	2:A:602:NAG:C2	2.27	0.48
1:C:160:ILE:O	1:C:242:GLU:HA	2.13	0.48
1:A:38:ASN:OD1	1:A:38:ASN:C	2.56	0.47
1:A:488:TYR:N	1:A:489:PRO:HD2	2.29	0.47
1:B:53:LYS:NZ	1:B:69:GLU:OE1	2.32	0.47
1:B:289:MET:HA	1:B:289:MET:HE2	1.96	0.47
1:C:401:ASN:ND2	1:C:404:ARG:NH2	2.62	0.47
1:A:285:ILE:HD11	1:A:294:ILE:HG13	1.96	0.47
1:C:42:CYS:CB	1:C:274:CYS:HG	2.27	0.47
1:C:399:PHE:CE1	1:C:406:ILE:HG22	2.50	0.47
1:C:480:SER:HB2	1:C:485:THR:O	2.14	0.47
1:B:165:ASN:HD21	2:B:601:NAG:C2	2.19	0.47
1:B:357:ASN:OD1	1:B:357:ASN:C	2.56	0.47
1:C:452:ARG:HD2	1:C:461:GLU:OE2	2.14	0.47
1:A:165:ASN:HD21	2:A:601:NAG:C2	2.18	0.46
1:C:55:CYS:HG	1:C:67:CYS:CB	2.24	0.46
1:B:27:THR:HG23	1:B:317:LEU:O	2.15	0.46
1:A:19:ILE:HD12	1:A:19:ILE:H	1.81	0.46
1:A:48:LYS:HG3	1:A:49:PRO:HD2	1.98	0.46
1:B:135:CYS:O	1:B:142:SER:HB3	2.16	0.45
1:C:493:GLU:HG2	1:C:494:GLU:N	2.32	0.45
1:B:406:ILE:H	1:B:406:ILE:CD1	2.26	0.45
1:B:55:CYS:HB3	1:B:67:CYS:SG	2.57	0.45
1:A:413:MET:SD	1:C:413:MET:HB3	2.57	0.45
1:A:307:LYS:HG3	1:A:418:LEU:HD23	1.99	0.45
1:C:320:SER:O	1:C:321:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:CYS:CB	1:B:67:CYS:SG	3.05	0.44
1:A:184:ALA:O	1:A:188:ILE:HD12	2.17	0.44
1:A:305:TYR:HE2	1:A:418:LEU:HD21	1.82	0.44
1:A:449:ASP:OD1	5:A:701:HOH:O	2.21	0.44
5:A:719:HOH:O	1:C:406:ILE:HD13	2.18	0.44
1:C:340:GLU:HG3	1:C:341:GLY:N	2.32	0.44
1:A:165:ASN:CG	2:A:601:NAG:C1	2.88	0.43
1:A:487:ASP:OD1	1:A:489:PRO:HG2	2.18	0.43
1:C:357:ASN:HD21	1:C:475:ASN:ND2	2.16	0.43
1:B:488:TYR:N	1:B:489:PRO:HD2	2.33	0.43
1:C:477:CYS:O	1:C:480:SER:N	2.47	0.43
1:B:179:HIS:O	1:B:246:ASN:HB3	2.19	0.43
1:A:10:ASN:OD1	1:A:10:ASN:C	2.63	0.42
1:B:455:LEU:O	1:B:456:ARG:C	2.61	0.42
1:A:400:ASN:OD1	1:A:400:ASN:C	2.62	0.42
1:A:488:TYR:N	1:A:489:PRO:CD	2.83	0.42
1:B:7:TYR:CD2	1:B:317:LEU:HD12	2.55	0.42
1:B:406:ILE:O	1:B:407:GLU:C	2.63	0.42
1:C:178:ILE:HB	1:C:198:ILE:HD12	2.02	0.42
1:C:234:LYS:HB3	1:C:235:PRO:CD	2.50	0.42
1:C:355:HIS:CE1	1:C:482:ARG:NH2	2.88	0.42
1:A:43:ASP:O	1:A:276:THR:HG22	2.19	0.42
1:A:55:CYS:HB3	1:A:67:CYS:HG	1.85	0.41
1:B:483:ASN:ND2	2:B:604:NAG:C1	2.83	0.41
1:C:228:PHE:HE1	1:C:248:ILE:HG21	1.85	0.41
1:C:278:CYS:HG	1:C:302:CYS:CB	2.34	0.41
1:C:488:TYR:HB3	1:C:489:PRO:HD3	2.02	0.41
1:C:4:CYS:HB2	1:C:354:HIS:HB3	2.01	0.41
1:C:5:ILE:HD13	1:C:448:TYR:HA	2.03	0.41
1:A:20:MET:HE1	1:B:439:PHE:CD2	2.55	0.41
1:A:130:GLY:HA3	1:A:149:TRP:HB3	2.03	0.41
1:A:11:ASN:ND2	2:A:602:NAG:C1	2.75	0.41
1:A:415:ASP:HB3	5:A:858:HOH:O	2.21	0.41
1:A:403:GLU:CA	1:A:406:ILE:HD13	2.50	0.40
2:A:601:NAG:O3	2:C:601:NAG:H82	2.21	0.40
1:B:65:PRO:HG3	1:B:143:PHE:O	2.21	0.40
1:B:191:TYR:O	1:B:192:LYS:C	2.59	0.40
1:C:474:ASP:HB3	1:C:476:GLU:HG3	2.03	0.40
1:C:474:ASP:O	1:C:477:CYS:N	2.51	0.40
1:A:286:ASN:ND2	5:A:730:HOH:O	2.54	0.40
1:A:413:MET:CE	1:A:414:GLU:HG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:HIS:HB2	1:C:361:SER:HA	2.04	0.40
1:C:436:THR:O	1:C:439:PHE:HB3	2.22	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	487/506 (96%)	467 (96%)	19 (4%)	1 (0%)	43	64
1	B	487/506 (96%)	469 (96%)	18 (4%)	0	100	100
1	C	487/506 (96%)	457 (94%)	29 (6%)	1 (0%)	43	64
All	All	1461/1518 (96%)	1393 (95%)	66 (4%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	356	SER
1	A	89	LEU

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	433/446 (97%)	411 (95%)	22 (5%)	21	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	433/446 (97%)	418 (96%)	15 (4%)	32 57
1	C	433/446 (97%)	414 (96%)	19 (4%)	25 48
All	All	1299/1338 (97%)	1243 (96%)	56 (4%)	26 49

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	51	ILE
1	A	54	ASP
1	A	86	VAL
1	A	195	THR
1	A	202	THR
1	A	308	SER
1	A	313	LEU
1	A	368	GLU
1	A	401	ASN
1	A	406	ILE
1	A	411	LYS
1	A	412	LYS
1	A	413	MET
1	A	415	ASP
1	A	418	LEU
1	A	453	LEU
1	A	457	ASP
1	A	483	ASN
1	A	492	SER
1	A	493	GLU
1	A	498	LYS
1	B	2	GLN
1	B	104	LEU
1	B	151	ILE
1	B	170	GLU
1	B	208	ARG
1	B	226	MET
1	B	258	LYS
1	B	280	THR
1	B	317	LEU
1	B	359	GLN
1	B	369	SER
1	B	387	LYS

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Mol	Chain	Res	Type
1	B	389	ASN
1	B	406	ILE
1	B	430	LEU
1	C	66	MET
1	C	71	ILE
1	C	107	ARG
1	C	112	GLU
1	C	172	LEU
1	C	248	ILE
1	C	269	VAL
1	C	275	ASN
1	C	280	THR
1	C	289	MET
1	C	301	GLU
1	C	310	LYS
1	C	355	HIS
1	C	387	LYS
1	C	406	ILE
1	C	413	MET
1	C	415	ASP
1	C	462	LEU
1	C	476	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	109	ASN
1	A	138	GLN
1	A	146	ASN
1	A	154	ASN
1	A	165	ASN
1	A	193	ASN
1	A	218	GLN
1	A	220	ASN
1	A	391	GLN
1	A	408	ASN
1	A	454	GLN
1	A	483	ASN
1	B	11	ASN
1	B	15	GLN
1	B	23	ASN

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Mol	Chain	Res	Type
1	B	87	ASN
1	B	165	ASN
1	B	189	ASN
1	B	207	GLN
1	B	389	ASN
1	B	391	GLN
1	B	401	ASN
1	B	483	ASN
1	C	2	GLN
1	C	23	ASN
1	C	165	ASN
1	C	168	ASN
1	C	355	HIS
1	C	391	GLN
1	C	401	ASN
1	C	454	GLN
1	C	475	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](#)

14 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	-	14,14,15	0.65	0	17,19,21	1.49	1 (5%)
2	NAG	C	602	-	14,14,15	0.55	0	17,19,21	1.50	3 (17%)
2	NAG	B	602	-	14,14,15	0.47	0	17,19,21	1.60	4 (23%)
2	NAG	B	603	-	14,14,15	0.53	0	17,19,21	2.44	3 (17%)
3	GAL	C	605	-	11,11,12	0.69	0	15,15,17	1.37	2 (13%)
2	NAG	A	602	-	14,14,15	0.56	0	17,19,21	0.83	1 (5%)
2	NAG	A	601	-	14,14,15	0.57	0	17,19,21	1.44	2 (11%)
2	NAG	A	604	-	14,14,15	0.43	0	17,19,21	0.86	0
2	NAG	C	603	-	14,14,15	0.44	0	17,19,21	1.40	1 (5%)
2	NAG	C	604	-	15,15,15	0.23	0	21,21,21	1.22	3 (14%)
2	NAG	C	601	-	14,14,15	0.39	0	17,19,21	2.07	5 (29%)
4	SIA	C	606	-	20,20,21	0.82	1 (5%)	21,28,31	0.92	1 (4%)
2	NAG	A	603	-	14,14,15	0.42	0	17,19,21	1.67	4 (23%)
2	NAG	B	604	-	14,14,15	0.45	0	17,19,21	2.42	3 (17%)

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	-	-	0/6/23/26	0/1/1/1
2	NAG	C	602	-	-	4/6/23/26	0/1/1/1
2	NAG	B	602	-	-	4/6/23/26	0/1/1/1
2	NAG	B	603	-	-	0/6/23/26	0/1/1/1
3	GAL	C	605	-	-	2/2/19/22	0/1/1/1
2	NAG	A	602	-	-	3/6/23/26	0/1/1/1
2	NAG	A	601	-	-	2/6/23/26	0/1/1/1
2	NAG	A	604	-	-	4/6/23/26	0/1/1/1
2	NAG	C	603	-	-	2/6/23/26	0/1/1/1
2	NAG	C	604	-	-	4/6/26/26	0/1/1/1
2	NAG	C	601	-	-	4/6/23/26	0/1/1/1
4	SIA	C	606	-	-	0/18/34/38	0/1/1/1
2	NAG	A	603	-	-	4/6/23/26	0/1/1/1
2	NAG	B	604	-	-	6/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	606	SIA	O1B-C1	-2.35	1.23	1.30

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604	NAG	O5-C1-C2	8.41	124.31	111.29
2	B	603	NAG	O5-C1-C2	8.38	124.25	111.29
2	C	601	NAG	O5-C1-C2	-6.50	101.23	111.29
2	B	602	NAG	O5-C1-C2	-4.77	103.91	111.29
2	C	603	NAG	C1-C2-N2	4.18	117.02	110.43
2	A	603	NAG	O5-C1-C2	-4.17	104.84	111.29
2	B	604	NAG	C1-O5-C5	4.15	117.75	112.19
2	B	601	NAG	O5-C1-C2	-4.00	105.10	111.29
2	C	602	NAG	C2-N2-C7	3.63	127.77	122.90
3	C	605	GAL	C1-C2-C3	3.61	114.91	109.64
2	A	601	NAG	C1-O5-C5	-3.31	107.75	112.19
2	B	603	NAG	C1-O5-C5	3.21	116.49	112.19
2	C	604	NAG	C1-C2-N2	3.07	114.28	110.73
2	A	603	NAG	C4-C3-C2	-2.94	106.70	111.02
2	B	603	NAG	C1-C2-N2	2.94	115.06	110.43
2	A	603	NAG	O3-C3-C2	2.90	115.44	109.40
2	A	601	NAG	O5-C1-C2	-2.88	106.84	111.29
2	C	601	NAG	C1-C2-N2	2.66	114.63	110.43
2	A	603	NAG	C1-C2-N2	2.51	114.39	110.43
2	C	602	NAG	C1-O5-C5	2.50	115.54	112.19
2	B	604	NAG	C1-C2-N2	2.49	114.36	110.43
3	C	605	GAL	C2-C3-C4	2.48	115.22	110.86
4	C	606	SIA	O1B-C1-C2	2.44	119.06	112.71
2	C	601	NAG	O3-C3-C2	2.44	114.47	109.40
2	C	602	NAG	O5-C1-C2	-2.34	107.67	111.29
2	B	602	NAG	C1-C2-N2	2.31	114.07	110.43
2	C	601	NAG	C1-O5-C5	2.29	115.26	112.19
2	A	602	NAG	C1-C2-N2	2.25	113.98	110.43
2	B	602	NAG	O3-C3-C2	2.21	113.99	109.40
2	C	601	NAG	C4-C3-C2	-2.17	107.84	111.02
2	C	604	NAG	C1-C2-C3	-2.14	107.63	110.54
2	B	602	NAG	C4-C3-C2	-2.12	107.91	111.02
2	C	604	NAG	O1-C1-C2	2.10	113.58	109.22

There are no chirality outliers.

All (39) torsion outliers are listed below:

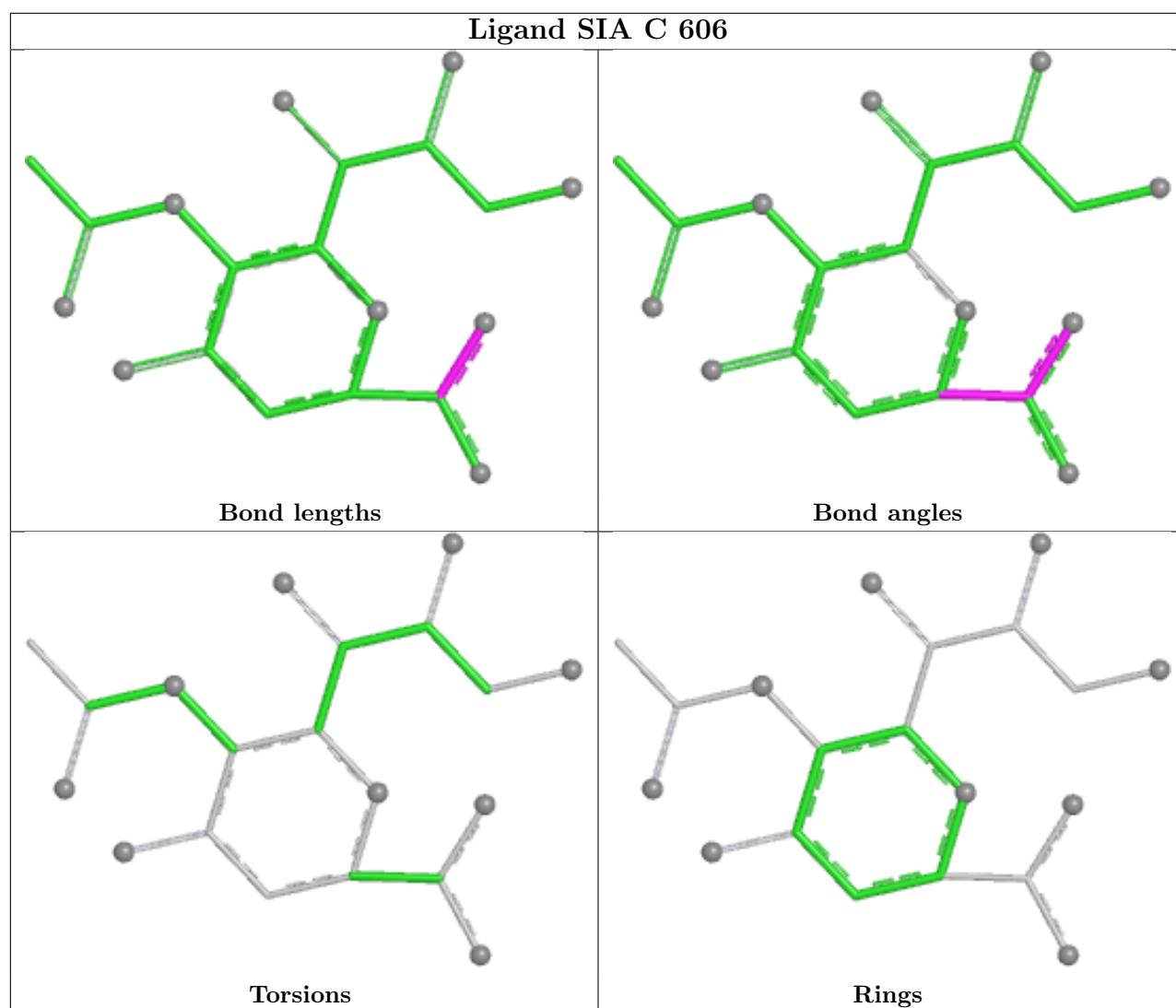
Mol	Chain	Res	Type	Atoms
2	A	604	NAG	C8-C7-N2-C2
2	A	604	NAG	O7-C7-N2-C2
2	C	601	NAG	C8-C7-N2-C2
2	C	601	NAG	O7-C7-N2-C2
2	C	602	NAG	C8-C7-N2-C2
2	C	602	NAG	O7-C7-N2-C2
2	C	604	NAG	C8-C7-N2-C2
2	C	604	NAG	O7-C7-N2-C2
2	A	603	NAG	C4-C5-C6-O6
2	A	601	NAG	O5-C5-C6-O6
2	C	604	NAG	O5-C5-C6-O6
3	C	605	GAL	O5-C5-C6-O6
2	A	604	NAG	O5-C5-C6-O6
2	A	603	NAG	O5-C5-C6-O6
2	B	602	NAG	C4-C5-C6-O6
2	B	604	NAG	C4-C5-C6-O6
2	A	604	NAG	C4-C5-C6-O6
2	C	604	NAG	C4-C5-C6-O6
2	C	603	NAG	O5-C5-C6-O6
2	A	601	NAG	C4-C5-C6-O6
2	A	603	NAG	C8-C7-N2-C2
2	A	603	NAG	O7-C7-N2-C2
2	B	604	NAG	C8-C7-N2-C2
2	B	602	NAG	O5-C5-C6-O6
2	B	604	NAG	O5-C5-C6-O6
2	A	602	NAG	O5-C5-C6-O6
2	C	602	NAG	O5-C5-C6-O6
2	B	604	NAG	O7-C7-N2-C2
3	C	605	GAL	C4-C5-C6-O6
2	A	602	NAG	C8-C7-N2-C2
2	C	603	NAG	C4-C5-C6-O6
2	B	602	NAG	C8-C7-N2-C2
2	B	604	NAG	C1-C2-N2-C7
2	B	602	NAG	O7-C7-N2-C2
2	C	602	NAG	C4-C5-C6-O6
2	A	602	NAG	O7-C7-N2-C2
2	C	601	NAG	O5-C5-C6-O6
2	C	601	NAG	C1-C2-N2-C7
2	B	604	NAG	C3-C2-N2-C7

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAG	3	0
2	C	602	NAG	3	0
2	B	602	NAG	1	0
2	B	603	NAG	2	0
3	C	605	GAL	3	0
2	A	602	NAG	3	0
2	A	601	NAG	7	0
2	A	604	NAG	1	0
2	C	603	NAG	2	0
2	C	604	NAG	1	0
2	C	601	NAG	3	0
4	C	606	SIA	2	0
2	A	603	NAG	3	0
2	B	604	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 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	491/506 (97%)	-0.33	3 (0%) 85 83	10, 28, 60, 99	0
1	B	491/506 (97%)	-0.27	5 (1%) 79 76	12, 32, 62, 90	0
1	C	491/506 (97%)	0.07	28 (5%) 29 24	13, 39, 99, 140	0
All	All	1473/1518 (97%)	-0.18	36 (2%) 59 54	10, 33, 75, 140	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	PRO	4.6
1	C	473	CYS	4.3
1	C	497	LEU	3.5
1	C	489	PRO	3.5
1	C	491	TYR	3.4
1	C	471	HIS	3.1
1	A	321	PRO	3.0
1	C	469	PHE	3.0
1	B	489	PRO	2.9
1	C	362	GLY	2.9
1	C	358	GLU	2.8
1	C	1	ASP	2.8
1	C	355	HIS	2.8
1	C	347	VAL	2.7
1	C	470	TYR	2.4
1	C	360	GLY	2.4
1	A	496	ARG	2.4
1	C	478	MET	2.3
1	C	365	ALA	2.3
1	C	499	ARG	2.3
1	C	490	GLN	2.3
1	B	476	GLU	2.2
1	C	386	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	500	GLU	2.2
1	C	486	TYR	2.2
1	C	468	GLU	2.2
1	C	321	PRO	2.2
1	C	367	LYS	2.2
1	C	450	LYS	2.2
1	C	493	GLU	2.1
1	C	488	TYR	2.1
1	C	68	ASP	2.1
1	B	496	ARG	2.1
1	C	474	ASP	2.0
1	A	277	LYS	2.0
1	C	472	LYS	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	C	604	15/15	0.54	0.20	90,115,139,140	0
2	NAG	C	601	14/15	0.71	0.16	72,107,118,120	0
2	NAG	B	604	14/15	0.73	0.18	76,91,102,105	0
2	NAG	A	604	14/15	0.74	0.22	82,112,127,132	0
2	NAG	C	603	14/15	0.74	0.16	72,86,101,109	0
2	NAG	A	603	14/15	0.74	0.15	61,86,90,94	0
2	NAG	A	602	14/15	0.76	0.15	68,75,85,87	0
2	NAG	B	602	14/15	0.76	0.17	81,88,98,98	0
2	NAG	B	603	14/15	0.82	0.12	59,73,86,101	0
2	NAG	C	602	14/15	0.82	0.13	42,58,74,78	0

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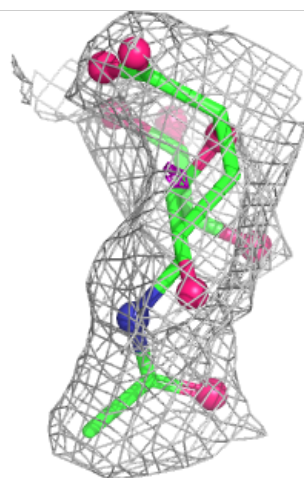
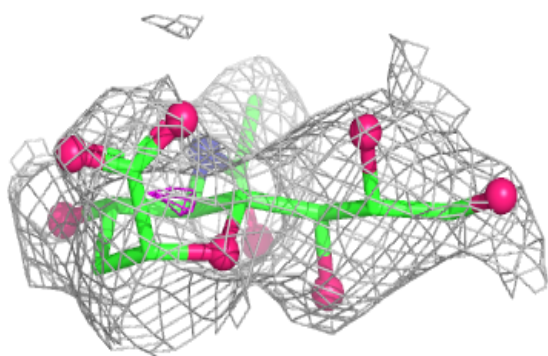
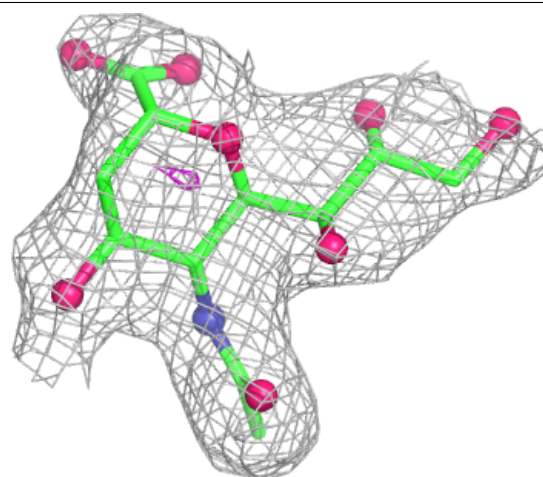
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	601	14/15	0.86	0.13	44,48,58,63	0
3	GAL	C	605	11/12	0.86	0.12	50,64,69,73	0
2	NAG	A	601	14/15	0.91	0.10	37,42,51,53	0
4	SIA	C	606	20/21	0.92	0.09	32,40,53,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SIA C 606:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.