



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 05:19 PM GMT

PDB ID : 3HTQ
Title : the hemagglutinin structure of an avian H1N1 influenza A virus in complex with LSTc
Authors : Wang, G.; Li, A.; Zhang, Q.; Wu, C.; Zhang, R.; Cai, Q.; Song, W.; Yuen, K.-Y.
Deposited on : 2009-06-12
Resolution : 2.96 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>

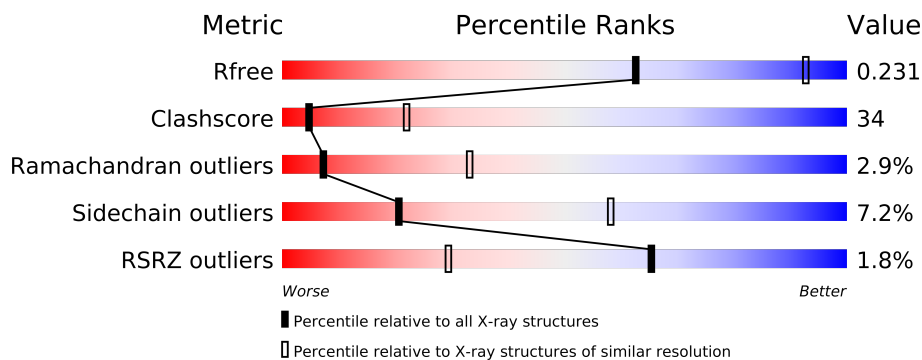
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
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) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.96 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	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

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	324	
2	B	160	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	632	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4098 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2530	1596	432	491	11			

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1286	803	220	256	7			

- 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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			32	17	1	14		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	74	Total	O	0	0
			74	74		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	198.44Å 198.44Å 198.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 2.96 49.61 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.61-2.96) 99.9 (49.61-2.95)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.96Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.218 , 0.261 0.222 , 0.231	Depositor DCC
R_{free} test set	1368 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
Estimated twinning fraction	0.022 for -l,-k,-h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27293 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4098	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: SIA, GAL, NAG, NDG

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	0.36	0/2594	0.63	0/3534
2	B	0.42	0/1312	0.64	0/1766
All	All	0.38	0/3906	0.64	0/5300

There are no bond length outliers.

There are no bond angle outliers.

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	2530	0	2443	203	0
2	B	1286	0	1197	86	0
3	A	28	0	25	1	0
4	A	28	0	26	5	0
5	A	32	0	28	5	0
6	A	120	0	0	27	0
6	B	74	0	0	12	1
All	All	4098	0	3719	263	1

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 34.

All (263) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:628:ASN:HB2	6:B:119:HOH:O	1.70	0.90
2:B:635:ASN:HD21	2:B:637:CYS:HB2	1.39	0.86
1:A:289:ILE:HD11	1:A:298:VAL:HG11	1.62	0.80
1:A:126:SER:HB2	6:A:406:HOH:O	1.83	0.79
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.65	0.78
1:A:96:PRO:HB2	1:A:229:ARG:HD2	1.64	0.78
1:A:299:HIS:HD2	1:A:301:ILE:H	1.32	0.77
2:B:616:ARG:HH11	2:B:616:ARG:HG2	1.50	0.76
1:A:48:LEU:HD11	2:B:563:PHE:HE1	1.51	0.76
1:A:86:THR:HG22	1:A:87:SER:N	2.02	0.75
1:A:9:ILE:HD13	1:A:10:GLY:N	2.01	0.75
2:B:585:ASP:O	2:B:589:LEU:HG	1.88	0.73
1:A:226:GLN:HB3	6:A:409:HOH:O	1.87	0.72
1:A:131:GLU:OE1	1:A:132(A):THR:HG22	1.89	0.72
1:A:289:ILE:HG21	6:A:338:HOH:O	1.90	0.72
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.55	0.72
2:B:631:LYS:HE2	6:B:115:HOH:O	1.91	0.71
1:A:27:ASN:OD1	4:A:632:NAG:H61	1.91	0.70
2:B:568:LYS:O	2:B:569:GLU:HB2	1.90	0.70
1:A:217:ILE:HD13	1:A:217:ILE:H	1.57	0.70
2:B:627:ARG:HD2	2:B:660:PRO:HG2	1.72	0.69
1:A:75:LEU:HD22	1:A:117:ARG:NH1	2.07	0.69
1:A:201:TYR:CE2	1:A:248:THR:HG23	2.29	0.68
1:A:289:ILE:HD12	1:A:298:VAL:HG21	1.76	0.68
2:B:553:ASN:O	2:B:557:GLU:HG2	1.94	0.68
2:B:633:ILE:O	2:B:635:ASN:N	2.28	0.67
1:A:94:CYS:O	1:A:224:ARG:HD3	1.96	0.66
1:A:166:LYS:HE2	6:A:367:HOH:O	1.95	0.66
1:A:296:GLN:HG2	1:A:298:VAL:H	1.60	0.66
2:B:503:PHE:O	2:B:616:ARG:HD3	1.95	0.66
1:A:169:THR:HG22	1:A:242:THR:OG1	1.97	0.65
1:A:171:ASN:HB2	6:A:345:HOH:O	1.95	0.64
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.77	0.64
1:A:317:MET:HE3	2:B:552:VAL:HG22	1.79	0.64
1:A:131:GLU:CD	1:A:132(A):THR:HG22	2.17	0.64
2:B:647:GLU:HG2	6:B:141:HOH:O	1.98	0.63
1:A:97:GLY:HA2	1:A:229:ARG:HG3	1.79	0.63
1:A:289:ILE:HG22	1:A:290:ASN:N	2.13	0.63
1:A:175:GLU:HG2	6:A:348:HOH:O	1.97	0.63
1:A:42:ASN:HD21	1:A:288:ALA:H	1.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:299:HIS:HE1	6:A:347:HOH:O	1.81	0.62
1:A:95:TYR:CE1	1:A:226:GLN:HG3	2.34	0.62
1:A:304:GLY:HA2	2:B:563:PHE:CE1	2.34	0.62
1:A:156:LYS:HB3	6:A:395:HOH:O	1.99	0.61
1:A:138:ALA:O	1:A:224:ARG:NH1	2.33	0.61
1:A:309:TYR:HD2	2:B:589:LEU:HD13	1.65	0.61
2:B:644:CYS:HA	6:B:73:HOH:O	2.02	0.60
1:A:156:LYS:HG3	1:A:161:TYR:HB2	1.83	0.59
1:A:25:GLU:OE2	1:A:322:ARG:NH2	2.35	0.59
1:A:217:ILE:HD13	1:A:217:ILE:N	2.16	0.59
2:B:530:GLN:NE2	2:B:530:GLN:HA	2.17	0.59
2:B:635:ASN:C	2:B:635:ASN:HD22	2.06	0.59
1:A:134:GLY:CA	1:A:153:TRP:HB3	2.31	0.59
1:A:309:TYR:CD2	2:B:589:LEU:HD13	2.37	0.59
1:A:42:ASN:O	1:A:44:LYS:HG3	2.03	0.59
1:A:156:LYS:HB2	1:A:194:LEU:O	2.02	0.59
1:A:299:HIS:HD2	1:A:301:ILE:N	2.01	0.59
1:A:211:ARG:HG3	6:A:404:HOH:O	2.01	0.59
1:A:86:THR:CG2	1:A:87:SER:N	2.66	0.59
1:A:5:ASP:N	6:A:427:HOH:O	2.36	0.58
1:A:296:GLN:HG3	6:A:338:HOH:O	2.03	0.58
1:A:217:ILE:HB	6:A:364:HOH:O	2.03	0.58
6:A:418:HOH:O	2:B:589:LEU:HB3	2.02	0.58
1:A:32:HIS:CD2	2:B:521:TRP:HE1	2.21	0.58
1:A:289:ILE:CD1	1:A:298:VAL:HG21	2.33	0.57
1:A:9:ILE:C	1:A:9:ILE:HD13	2.24	0.57
1:A:180:TRP:HZ3	1:A:235:THR:HG22	1.70	0.57
1:A:201:TYR:HE2	1:A:248:THR:HG23	1.70	0.57
1:A:131:GLU:HB3	1:A:155:THR:HB	1.86	0.57
1:A:185:PRO:HG2	1:A:191:GLN:HE21	1.70	0.57
1:A:48:LEU:HD11	2:B:563:PHE:CE1	2.36	0.56
1:A:23:VAL:CG2	2:B:602:LEU:HD23	2.35	0.56
1:A:9:ILE:HG21	2:B:619:TYR:HA	1.87	0.56
2:B:530:GLN:HE21	2:B:530:GLN:HA	1.71	0.55
1:A:36:LEU:HA	1:A:293:LEU:HD22	1.87	0.55
4:A:632:NAG:H2	6:A:388:HOH:O	2.06	0.55
1:A:86:THR:HG22	1:A:87:SER:H	1.69	0.55
2:B:526:HIS:HB2	2:B:649:MET:CE	2.36	0.55
1:A:190:GLU:HA	1:A:193:THR:CG2	2.36	0.55
1:A:122:PRO:O	1:A:126:SER:HB2	2.06	0.55
1:A:180:TRP:HB3	1:A:254:PRO:HG3	1.88	0.55
2:B:616:ARG:NH1	2:B:616:ARG:HG2	2.16	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:TYR:CD1	1:A:212:ARG:NH2	2.75	0.55
1:A:126:SER:C	1:A:128:PRO:HD3	2.27	0.54
1:A:149:ARG:HG2	1:A:149:ARG:NH1	2.21	0.54
1:A:43:GLY:HA2	1:A:286:HIS:O	2.07	0.54
2:B:551:LYS:HE3	2:B:603:GLU:OE2	2.07	0.54
2:B:632:GLU:HG2	2:B:638:PHE:CE2	2.42	0.54
1:A:299:HIS:CD2	1:A:301:ILE:H	2.20	0.54
1:A:86:THR:C	1:A:88:ASN:H	2.11	0.54
1:A:317:MET:CE	2:B:552:VAL:HG22	2.38	0.54
1:A:311:LYS:NZ	2:B:589:LEU:CB	2.71	0.53
1:A:119:GLU:HG3	1:A:256:TYR:CZ	2.43	0.53
2:B:629:ASN:ND2	2:B:660:PRO:HA	2.23	0.53
1:A:112:VAL:HG11	1:A:115:PHE:HB2	1.90	0.53
1:A:217:ILE:H	1:A:217:ILE:CD1	2.20	0.53
1:A:311:LYS:HD2	6:A:418:HOH:O	2.09	0.53
2:B:567:GLY:HA2	6:B:46:HOH:O	2.08	0.53
1:A:38:GLU:OE2	1:A:290:ASN:HB3	2.09	0.53
1:A:155:THR:O	1:A:161:TYR:CE1	2.62	0.53
1:A:300:PRO:HG3	1:A:309:TYR:CZ	2.43	0.53
1:A:100:ILE:HG13	1:A:233:TYR:CE2	2.44	0.53
1:A:169:THR:HG22	1:A:242:THR:HG23	1.91	0.52
1:A:52:ALA:O	1:A:80:TRP:HA	2.09	0.52
2:B:530:GLN:HE21	2:B:530:GLN:CA	2.22	0.52
2:B:589:LEU:C	6:B:201:HOH:O	2.47	0.52
2:B:603:GLU:OE1	2:B:603:GLU:HA	2.09	0.52
1:A:104:GLU:O	1:A:108:GLN:HG3	2.09	0.52
1:A:23:VAL:HG21	2:B:602:LEU:HD23	1.91	0.52
1:A:67:GLY:O	1:A:148:TYR:HA	2.09	0.52
1:A:63:GLY:CA	1:A:92:GLY:HA2	2.40	0.52
1:A:68:ASN:HB3	1:A:71:CYS:SG	2.51	0.51
1:A:38:GLU:HG2	1:A:293:LEU:HD12	1.93	0.51
1:A:86:THR:CG2	1:A:87:SER:H	2.23	0.51
1:A:103:GLU:HB2	6:A:328:HOH:O	2.10	0.51
1:A:66:LEU:HD22	1:A:151:LEU:HD11	1.92	0.51
1:A:192:GLN:HG3	1:A:193:THR:N	2.26	0.50
1:A:48:LEU:O	1:A:49:ASN:HB2	2.11	0.50
1:A:83:ILE:HB	1:A:268:ILE:HG12	1.92	0.50
1:A:169:THR:HG22	1:A:242:THR:CG2	2.42	0.50
1:A:170:ASN:ND2	1:A:239:GLN:HA	2.27	0.50
1:A:155:THR:O	1:A:161:TYR:HE1	1.95	0.50
1:A:311:LYS:NZ	2:B:589:LEU:HB3	2.26	0.50
2:B:631:LYS:HD2	6:B:161:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:653:LYS:NZ	6:B:4:HOH:O	2.45	0.50
1:A:127:TRP:N	1:A:128:PRO:HD3	2.28	0.49
1:A:32:HIS:HD2	2:B:521:TRP:HE1	1.58	0.49
1:A:15:ASN:ND2	4:A:631:NAG:C7	2.75	0.49
1:A:113:SER:HB2	6:A:397:HOH:O	2.12	0.49
1:A:72:ASP:CG	1:A:149:ARG:HE	2.15	0.49
1:A:128:PRO:O	1:A:129:ASN:CG	2.51	0.49
1:A:97:GLY:HA3	1:A:230:MET:O	2.12	0.49
1:A:164:LEU:C	1:A:164:LEU:HD12	2.33	0.49
2:B:541:THR:O	2:B:545:ILE:HG12	2.12	0.49
2:B:635:ASN:ND2	2:B:637:CYS:H	2.10	0.49
1:A:190:GLU:CD	5:A:801:SIA:H92	2.33	0.48
1:A:127:TRP:HB2	1:A:132:THR:HG21	1.95	0.48
2:B:619:TYR:CE1	2:B:636:GLY:HA2	2.48	0.48
1:A:296:GLN:HB3	1:A:307:PRO:HB2	1.94	0.48
1:A:220:ARG:HB2	1:A:221:PRO:HD2	1.94	0.48
1:A:70:GLU:HB2	1:A:91:ASN:OD1	2.12	0.48
1:A:120:ILE:HG13	1:A:168:TYR:CD1	2.48	0.48
1:A:200:ALA:HB3	1:A:250:ASN:ND2	2.29	0.48
1:A:294:PRO:HG2	1:A:295:PHE:CD1	2.48	0.48
2:B:592:TRP:N	6:B:201:HOH:O	2.46	0.48
2:B:635:ASN:C	2:B:635:ASN:ND2	2.66	0.48
1:A:192:GLN:HB3	1:A:198:THR:CG2	2.44	0.48
1:A:289:ILE:CG2	1:A:290:ASN:N	2.75	0.48
1:A:29:THR:HG22	1:A:323:ASN:HB3	1.96	0.48
1:A:190:GLU:HG3	6:A:373:HOH:O	2.14	0.47
1:A:94:CYS:HB3	3:A:626:NDG:O7	2.14	0.47
2:B:635:ASN:HD22	2:B:637:CYS:H	1.60	0.47
1:A:45:LEU:HD13	1:A:84:ILE:HD13	1.96	0.47
1:A:55:GLN:NE2	1:A:275:VAL:HG21	2.29	0.47
1:A:300:PRO:HG3	1:A:309:TYR:CE2	2.49	0.47
1:A:161:TYR:CE2	1:A:249:GLY:HA2	2.50	0.47
2:B:647:GLU:O	2:B:650:GLU:HB3	2.14	0.47
1:A:190:GLU:HA	1:A:193:THR:HG22	1.95	0.47
1:A:317:MET:HE1	2:B:552:VAL:HA	1.97	0.47
1:A:91:ASN:ND2	6:A:366:HOH:O	2.48	0.47
2:B:562:GLN:HB3	6:B:129:HOH:O	2.13	0.47
1:A:187:THR:HA	6:A:364:HOH:O	2.14	0.47
1:A:27:ASN:CG	4:A:632:NAG:H61	2.36	0.47
1:A:189:SER:O	1:A:193:THR:HG22	2.14	0.46
1:A:304:GLY:HA2	2:B:563:PHE:CD1	2.51	0.46
1:A:9:ILE:HG13	2:B:618:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:5:ASP:HB2	6:A:434:HOH:O	2.16	0.46
2:B:653:LYS:C	2:B:655:GLY:H	2.19	0.46
2:B:593:THR:O	2:B:597:GLU:HB2	2.15	0.46
2:B:572:ASN:HD22	2:B:572:ASN:N	2.13	0.46
1:A:96:PRO:HB3	1:A:223:VAL:HB	1.96	0.46
2:B:627:ARG:HD2	2:B:660:PRO:CG	2.44	0.46
1:A:201:TYR:CE2	1:A:248:THR:CG2	2.99	0.46
2:B:647:GLU:HA	2:B:647:GLU:OE2	2.16	0.46
2:B:635:ASN:HD21	2:B:637:CYS:CB	2.18	0.46
1:A:122:PRO:HD2	6:A:406:HOH:O	2.16	0.46
2:B:627:ARG:HG2	2:B:627:ARG:HH11	1.81	0.46
1:A:269:ILE:HG12	1:A:303:ILE:HD12	1.98	0.46
1:A:131:GLU:OE2	1:A:132(A):THR:HG22	2.16	0.45
1:A:311:LYS:HZ1	2:B:589:LEU:CB	2.29	0.45
1:A:58:LYS:HB2	6:A:366:HOH:O	2.15	0.45
1:A:119:GLU:HB3	1:A:122:PRO:HG3	1.97	0.45
1:A:20:VAL:HB	2:B:604:ASN:ND2	2.31	0.45
2:B:562:GLN:OE1	2:B:562:GLN:N	2.49	0.45
2:B:506:MET:CE	2:B:612:ASP:HA	2.47	0.45
2:B:530:GLN:NE2	2:B:530:GLN:CA	2.78	0.45
1:A:190:GLU:OE1	5:A:801:SIA:H92	2.17	0.45
1:A:217:ILE:O	1:A:217:ILE:HG12	2.17	0.45
1:A:47:LYS:O	1:A:280:THR:HG22	2.17	0.45
1:A:294:PRO:HD3	2:B:556:ILE:HG12	1.99	0.45
2:B:627:ARG:CD	2:B:660:PRO:HG2	2.44	0.45
1:A:194:LEU:HD21	5:A:801:SIA:H111	1.99	0.45
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.51	0.44
1:A:326:SER:HA	6:A:407:HOH:O	2.17	0.44
1:A:201:TYR:HE2	1:A:248:THR:CG2	2.29	0.44
1:A:133:LYS:O	1:A:135:VAL:N	2.43	0.44
1:A:95:TYR:HA	1:A:96:PRO:HD2	1.85	0.44
2:B:548:ILE:O	2:B:552:VAL:HG23	2.18	0.44
1:A:51:ILE:HB	1:A:81:SER:HB3	1.99	0.44
2:B:520:GLY:HA3	2:B:536:ALA:HB1	2.00	0.44
1:A:46:CYS:HB3	1:A:278:CYS:O	2.17	0.44
2:B:625:GLN:HE22	2:B:655:GLY:C	2.21	0.43
2:B:633:ILE:O	2:B:635:ASN:ND2	2.51	0.43
1:A:78:ASN:O	1:A:79:SER:HB2	2.17	0.43
1:A:295:PHE:CE2	2:B:596:ALA:HB2	2.53	0.43
1:A:75:LEU:HD22	1:A:117:ARG:HH11	1.81	0.43
2:B:553:ASN:C	2:B:557:GLU:HG2	2.39	0.43
1:A:113:SER:HB3	1:A:261:ASN:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:623:LYS:NZ	6:B:56:HOH:O	2.51	0.43
1:A:126:SER:HA	6:A:411:HOH:O	2.17	0.43
1:A:86:THR:C	1:A:88:ASN:N	2.72	0.43
1:A:311:LYS:NZ	2:B:589:LEU:HB2	2.34	0.43
1:A:170:ASN:HB2	1:A:237:LEU:HD23	2.00	0.42
1:A:70:GLU:HG3	1:A:91:ASN:OD1	2.20	0.42
1:A:102:TYR:CE2	1:A:106:ARG:HD2	2.55	0.42
1:A:127:TRP:HB2	1:A:132:THR:CG2	2.49	0.42
1:A:156:LYS:NZ	1:A:192:GLN:O	2.50	0.42
1:A:63:GLY:HA3	1:A:92:GLY:HA2	2.01	0.42
1:A:156:LYS:CG	1:A:161:TYR:HB2	2.47	0.42
1:A:79:SER:O	1:A:112:VAL:O	2.37	0.42
1:A:194:LEU:CD2	5:A:801:SIA:H111	2.48	0.42
1:A:136:THR:HG23	1:A:139:CYS:H	1.84	0.42
2:B:625:GLN:NE2	2:B:657:TYR:H	2.17	0.42
2:B:573:LEU:HD23	2:B:573:LEU:HA	1.91	0.42
1:A:114:SER:OG	1:A:261:ASN:HB2	2.20	0.42
1:A:261:ASN:HA	1:A:261:ASN:HD22	1.62	0.42
1:A:223:VAL:O	1:A:224:ARG:C	2.58	0.42
1:A:223:VAL:HG23	1:A:229:ARG:NH1	2.34	0.42
1:A:65:LEU:CD1	1:A:105:LEU:HD21	2.49	0.42
1:A:161:TYR:N	6:A:387:HOH:O	2.39	0.41
1:A:53:PRO:HB3	1:A:82:TYR:CZ	2.55	0.41
2:B:509:PHE:O	2:B:635:ASN:HA	2.20	0.41
1:A:99:PHE:O	1:A:102:TYR:HB2	2.20	0.41
1:A:15:ASN:HD22	4:A:631:NAG:C7	2.34	0.41
1:A:8:CYS:O	2:B:514:TRP:HH2	2.03	0.41
1:A:308:LYS:HD3	1:A:308:LYS:HA	1.88	0.41
1:A:269:ILE:HD13	1:A:269:ILE:HA	1.97	0.41
1:A:5:ASP:HA	2:B:527:GLN:O	2.21	0.41
1:A:104:GLU:HG3	1:A:108:GLN:HE21	1.86	0.41
1:A:66:LEU:CD1	1:A:93:THR:HG22	2.50	0.41
1:A:155:THR:HG22	1:A:156:LYS:H	1.85	0.41
1:A:226:GLN:NE2	5:A:801:SIA:O1B	2.54	0.41
1:A:159:THR:O	1:A:196:GLN:NE2	2.53	0.41
1:A:209:TYR:O	1:A:210:ASN:HB2	2.21	0.41
1:A:119:GLU:HG3	1:A:256:TYR:CE2	2.55	0.41
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.55	0.41
1:A:185:PRO:HD2	1:A:217:ILE:HG22	2.03	0.41
1:A:23:VAL:HG22	2:B:602:LEU:HD23	2.01	0.41
1:A:6:THR:O	2:B:649:MET:HE1	2.20	0.41
1:A:284:THR:HG22	1:A:302:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:570:PHE:N	6:B:60:HOH:O	2.53	0.41
1:A:222:LYS:HG2	1:A:227:ALA:HB2	2.02	0.41
1:A:193:THR:HG21	6:A:361:HOH:O	2.20	0.41
2:B:626:LEU:HA	2:B:657:TYR:CE2	2.56	0.40
1:A:22:THR:HG22	2:B:604:ASN:HB3	2.02	0.40
2:B:564:THR:HG22	2:B:565:ALA:N	2.37	0.40
1:A:35:ASN:HD22	1:A:36:LEU:H	1.69	0.40
1:A:45:LEU:HD21	1:A:271:SER:OG	2.22	0.40
1:A:119:GLU:OE2	1:A:122:PRO:HA	2.22	0.40
1:A:187:THR:O	1:A:217:ILE:HB	2.21	0.40
1:A:212:ARG:HG2	1:A:213:PHE:N	2.37	0.40
2:B:572:ASN:ND2	2:B:572:ASN:N	2.69	0.40
1:A:65:LEU:HD11	1:A:109:LEU:CD1	2.51	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	Distance(Å)	Clash(Å)
6:B:41:HOH:O	6:B:41:HOH:O[5_555]	1.64	0.56

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	322/324 (99%)	275 (85%)	36 (11%)	11 (3%)	6	28
2	B	158/160 (99%)	139 (88%)	16 (10%)	3 (2%)	12	49
All	All	480/484 (99%)	414 (86%)	52 (11%)	14 (3%)	7	33

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	TRP
1	A	197	ASN
1	A	199	ASP

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Mol	Chain	Res	Type
2	B	634	GLY
1	A	210	ASN
1	A	325	PRO
1	A	79	SER
1	A	134	GLY
1	A	224	ARG
1	A	200	ALA
2	B	511	GLU
2	B	572	ASN
1	A	69	PRO
1	A	96	PRO

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	282/282 (100%)	260 (92%)	22 (8%)	18	53
2	B	136/136 (100%)	128 (94%)	8 (6%)	28	68
All	All	418/418 (100%)	388 (93%)	30 (7%)	21	58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	17	THR
1	A	35	ASN
1	A	38	GLU
1	A	39	ASP
1	A	42	ASN
1	A	72	ASP
1	A	80	TRP
1	A	91	ASN
1	A	99	PHE
1	A	107	GLU
1	A	163	LYS
1	A	193	THR
1	A	214	THR

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Mol	Chain	Res	Type
1	A	217	ILE
1	A	229	ARG
1	A	238	ASP
1	A	261	ASN
1	A	270	THR
1	A	272	ASP
1	A	296	GLN
1	A	321	LEU
2	B	515	THR
2	B	562	GLN
2	B	572	ASN
2	B	580	LEU
2	B	616	ARG
2	B	623	LYS
2	B	635	ASN
2	B	658	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	35	ASN
1	A	42	ASN
1	A	49	ASN
1	A	55	GLN
1	A	129	ASN
1	A	191	GLN
1	A	250	ASN
1	A	261	ASN
1	A	276	HIS
1	A	299	HIS
2	B	530	GLN
2	B	553	ASN
2	B	560	ASN
2	B	572	ASN
2	B	625	GLN
2	B	628	ASN
2	B	635	ASN
2	B	642	HIS

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	NDG	A	626	1,3	12,14,15	0.58	0	15,19,21	1.17	2 (13%)
3	NDG	A	627	3	12,14,15	0.59	0	15,19,21	0.78	1 (6%)
5	SIA	A	801	5	20,20,21	3.98	1 (5%)	23,28,31	2.47	3 (13%)
5	GAL	A	802	5	12,12,12	0.46	0	17,17,17	0.68	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	NDG	A	626	1,3	-	0/6/23/26	0/1/1/1
3	NDG	A	627	3	-	1/6/23/26	0/1/1/1
5	SIA	A	801	5	-	0/15/34/38	0/1/1/1
5	GAL	A	802	5	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	801	SIA	O6-C2	17.54	1.44	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	SIA	O6-C2-C3	-10.81	110.78	124.91
5	A	801	SIA	C7-C6-C5	-3.12	109.73	114.25
3	A	626	NDG	C2-N2-C7	-2.76	120.06	123.39
3	A	627	NDG	C2-N2-C7	-2.31	120.60	123.39
5	A	801	SIA	C3-C2-C1	-2.09	109.40	121.08
3	A	626	NDG	C3-C2-N2	-2.00	108.62	111.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	627	NDG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
4	NAG	A	631	1	12,14,15	0.55	0	15,19,21	0.86	1 (6%)
4	NAG	A	632	1	12,14,15	0.60	0	15,19,21	1.12	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
4	NAG	A	631	1	-	0/6/23/26	0/1/1/1
4	NAG	A	632	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	632	NAG	C2-N2-C7	-2.78	120.03	123.39
4	A	631	NAG	C2-N2-C7	-2.56	120.30	123.39

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	324/324 (100%)	-0.00	7 (2%) 59 26	38, 64, 89, 102	0
2	B	160/160 (100%)	-0.16	1 (0%) 86 47	38, 54, 72, 90	0
All	All	484/484 (100%)	-0.06	8 (1%) 65 31	38, 60, 88, 102	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	263	GLY	3.5
1	A	142	PHE	3.3
1	A	327	ILE	3.1
1	A	158	GLY	2.6
1	A	141	TYR	2.4
1	A	133	LYS	2.2
2	B	660	PRO	2.2
1	A	277	ASN	2.2

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(\AA^2)	Q<0.9
5	GAL	A	802	12/12	0.77	10.85	141,147,148,149	0
5	SIA	A	801	20/21	0.37	2.39	130,134,139,139	0
3	NDG	A	626	14/15	0.23	1.29	85,91,95,100	0
3	NDG	A	627	14/15	0.33	-	105,108,111,112	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(\AA^2)	Q<0.9
4	NAG	A	632	14/15	0.31	2.98	92,94,98,98	0
4	NAG	A	631	14/15	0.40	-	95,99,101,102	0

6.5 Other polymers

There are no such residues in this entry.