



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:47 AM UTC

PDB ID : 2X9M / pdb_00002x9m
Title : Hendra virus attachment glycoprotein
Authors : Bowden, T.A.; Crispin, M.; Harvey, D.; Jones, E.Y.; Stuart, D.I.
Deposited on : 2010-03-23
Resolution : 2.90 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

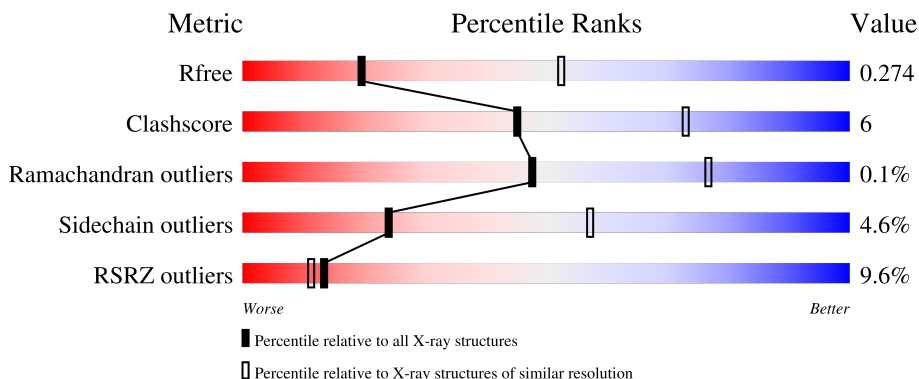
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	420	6% 84% 15% .
1	B	420	9% 83% 15% .
1	C	420	14% 84% 15% ..
1	D	420	9% 85% 13% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13464 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 GLYCOPROTEIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3311	2109	556	627	19			
1	B	418	Total	C	N	O	S	0	0	0
			3304	2104	555	626	19			
1	C	417	Total	C	N	O	S	0	0	0
			3296	2100	553	624	19			
1	D	417	Total	C	N	O	S	0	0	0
			3296	2100	553	624	19			

- 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		

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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	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	D	1	Total	C	N	O	0	0
			14	8	1	5		

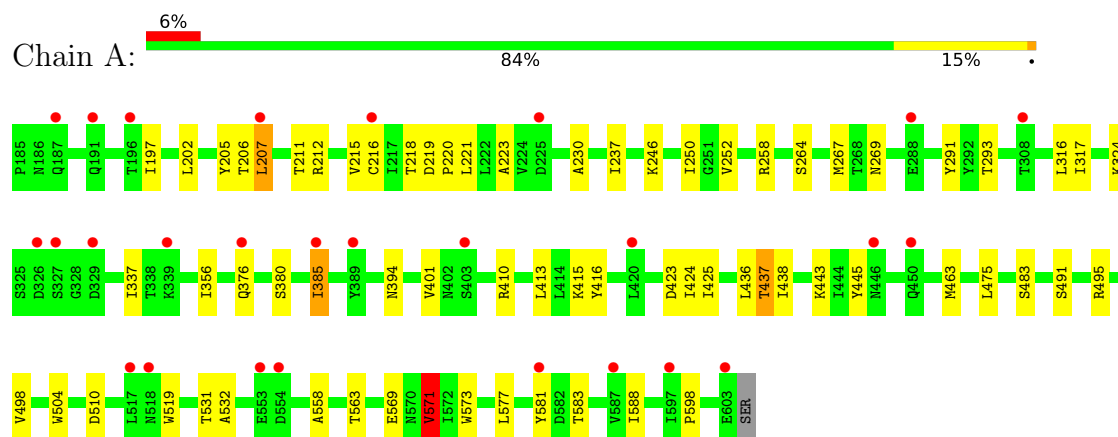
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	30	Total	O	0	0
			30	30		
3	C	34	Total	O	0	0
			34	34		
3	D	23	Total	O	0	0
			23	23		

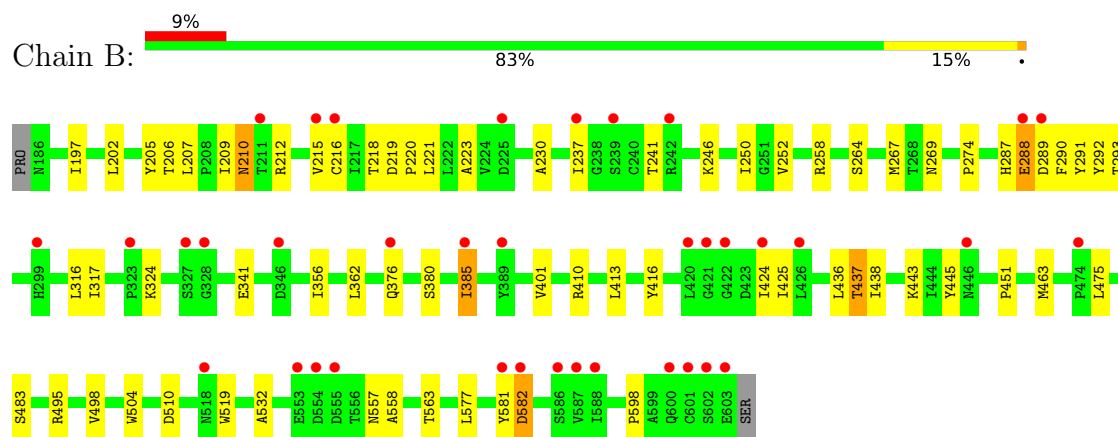
3 Residue-property plots [i](#)

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.

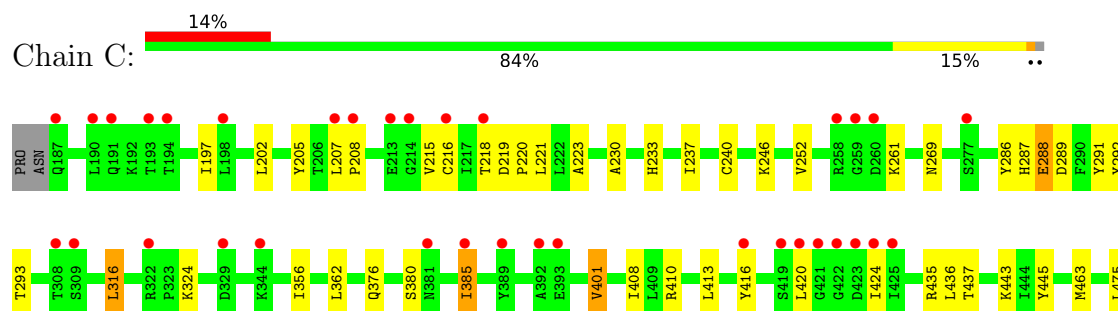
• Molecule 1: GLYCOPROTEIN G

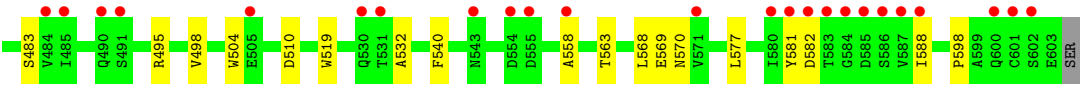


• Molecule 1: GLYCOPROTEIN G

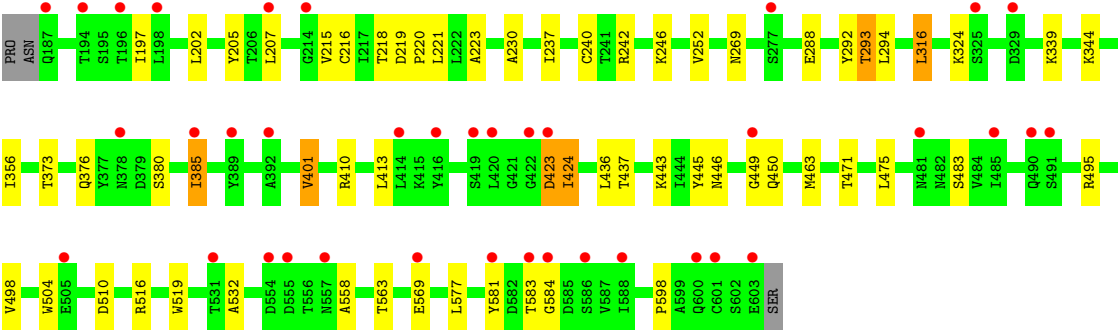
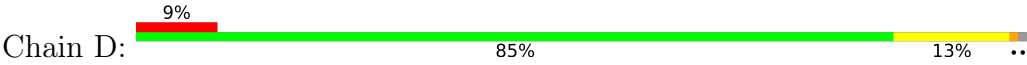


• Molecule 1: GLYCOPROTEIN G





● Molecule 1: GLYCOPROTEIN G



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.88Å 84.78Å 91.55Å 103.39° 99.63° 108.62°	Depositor
Resolution (Å)	44.20 – 2.90 44.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.20-2.90) 97.4 (44.20-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.233 , 0.273 0.236 , 0.274	Depositor DCC
R_{free} test set	1891 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13464	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8148e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.56	0/3392	0.74	2/4619 (0.0%)
1	B	0.55	0/3384	0.73	0/4608
1	C	0.55	0/3376	0.75	1/4597 (0.0%)
1	D	0.58	2/3376 (0.1%)	0.75	0/4597
All	All	0.56	2/13528 (0.0%)	0.74	3/18421 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	446	ASN	CG-ND2	-7.61	1.17	1.33
1	D	446	ASN	CG-OD1	-6.52	1.11	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	VAL	CG1-CB-CG2	5.99	123.99	110.80
1	C	540	PHE	N-CA-C	5.16	117.08	108.99
1	A	394	ASN	N-CA-C	5.06	116.80	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3311	0	3249	42	0
1	B	3304	0	3241	45	2
1	C	3296	0	3238	37	1
1	D	3296	0	3238	37	1
2	A	56	0	52	2	0
2	B	56	0	52	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	30	0	0	1	0
3	B	30	0	0	4	0
3	C	34	0	0	1	0
3	D	23	0	0	2	0
All	All	13464	0	13096	155	2

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 6.

All (155) 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:206:THR:O	1:A:207:LEU:HD22	1.77	0.83
1:D:344:LYS:HG2	3:D:2011:HOH:O	1.81	0.78
1:A:415:LYS:HE2	2:A:1604:NAG:H81	1.69	0.74
1:C:218:THR:HG21	1:C:240:CYS:HB3	1.69	0.74
1:B:212:ARG:NH2	1:B:246:LYS:HZ2	1.89	0.70
1:A:293:THR:HG22	1:A:317:ILE:O	1.92	0.69
1:B:209:ILE:HG13	1:D:207:LEU:HD13	1.76	0.67
1:A:416:TYR:CE2	1:A:424:ILE:HG13	2.31	0.66
1:D:293:THR:HG23	3:D:2008:HOH:O	1.96	0.66
1:C:401:VAL:HG22	1:C:504:TRP:CE2	2.31	0.65
1:D:401:VAL:HG22	1:D:504:TRP:CE2	2.32	0.64
1:A:571:VAL:HG22	1:A:573:TRP:CD1	2.32	0.64
1:D:218:THR:HG21	1:D:240:CYS:HB3	1.78	0.64
1:B:416:TYR:CE2	1:B:424:ILE:HG13	2.34	0.63
1:B:401:VAL:HG22	1:B:504:TRP:CE2	2.35	0.62
1:C:288:GLU:N	1:C:288:GLU:OE1	2.33	0.61
1:C:424:ILE:O	1:C:424:ILE:HG23	2.00	0.60
1:A:401:VAL:HG22	1:A:504:TRP:CE2	2.37	0.60
1:A:206:THR:C	1:A:207:LEU:HD22	2.26	0.60
1:A:385:ILE:HD13	1:A:385:ILE:N	2.18	0.59
1:D:450:GLN:HE21	1:D:516:ARG:CZ	2.16	0.58
1:A:218:THR:HG22	1:A:581:TYR:OH	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:THR:HG22	1:B:317:ILE:O	2.03	0.58
1:A:443:LYS:NZ	1:A:510:ASP:OD2	2.35	0.58
1:D:463:MET:HE2	1:D:483:SER:HA	1.86	0.58
1:C:385:ILE:N	1:C:385:ILE:HD13	2.19	0.58
1:C:463:MET:HE2	1:C:483:SER:HA	1.86	0.57
1:D:385:ILE:HD13	1:D:385:ILE:N	2.20	0.57
1:B:463:MET:HE2	1:B:483:SER:HA	1.87	0.57
1:B:385:ILE:N	1:B:385:ILE:HD13	2.19	0.57
1:C:292:TYR:HB3	1:C:316:LEU:HD11	1.86	0.56
1:A:581:TYR:O	1:A:583:THR:HG23	2.05	0.55
1:A:415:LYS:CE	2:A:1604:NAG:H81	2.36	0.55
1:A:463:MET:HE2	1:A:483:SER:HA	1.89	0.55
1:A:577:LEU:C	1:A:577:LEU:HD23	2.32	0.55
1:D:205:TYR:CE1	1:D:207:LEU:HD11	2.42	0.55
1:D:223:ALA:HB3	1:D:230:ALA:HB3	1.89	0.55
1:B:205:TYR:CE1	1:B:207:LEU:HD11	2.42	0.54
1:B:250:ILE:HG21	1:B:293:THR:HG21	1.89	0.54
1:B:212:ARG:CZ	1:B:246:LYS:NZ	2.71	0.54
1:C:223:ALA:HB3	1:C:230:ALA:HB3	1.88	0.54
1:C:205:TYR:CE1	1:C:207:LEU:HD11	2.42	0.54
1:D:216:CYS:SG	1:D:218:THR:HG23	2.47	0.54
1:B:401:VAL:HG13	1:B:504:TRP:CE3	2.43	0.54
1:C:410:ARG:HD2	1:C:436:LEU:HD11	1.89	0.54
1:B:288:GLU:O	1:B:289:ASP:HB2	2.08	0.53
1:B:498:VAL:O	1:B:498:VAL:HG12	2.09	0.53
1:D:532:ALA:HB1	1:D:558:ALA:O	2.08	0.53
1:C:532:ALA:HB1	1:C:558:ALA:O	2.08	0.53
1:D:205:TYR:CD1	1:D:207:LEU:HD11	2.43	0.53
1:A:250:ILE:HG21	1:A:293:THR:HG21	1.90	0.52
1:A:498:VAL:O	1:A:498:VAL:HG12	2.08	0.52
1:B:577:LEU:C	1:B:577:LEU:HD23	2.35	0.52
1:B:205:TYR:CD1	1:B:207:LEU:HD11	2.44	0.52
1:B:532:ALA:HB1	1:B:558:ALA:O	2.10	0.52
1:C:205:TYR:CD1	1:C:207:LEU:HD11	2.45	0.52
1:C:288:GLU:OE1	1:C:288:GLU:CA	2.58	0.52
1:B:410:ARG:HD2	1:B:436:LEU:HD11	1.92	0.51
1:D:443:LYS:NZ	1:D:563:THR:O	2.43	0.51
1:A:356:ILE:CG2	1:A:445:TYR:HA	2.41	0.51
1:D:577:LEU:C	1:D:577:LEU:HD23	2.36	0.51
1:C:216:CYS:SG	1:C:218:THR:HG23	2.50	0.51
1:A:531:THR:HG23	1:D:449:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:HIS:HB2	1:C:362:LEU:HD21	1.91	0.51
1:B:287:HIS:HB2	1:B:362:LEU:HD21	1.92	0.51
1:A:401:VAL:HG13	1:A:504:TRP:CE3	2.46	0.51
1:B:223:ALA:HB3	1:B:230:ALA:HB3	1.94	0.50
1:B:356:ILE:CG2	1:B:445:TYR:HA	2.42	0.50
1:D:356:ILE:CG2	1:D:445:TYR:HA	2.42	0.50
1:A:410:ARG:HD2	1:A:436:LEU:HD11	1.93	0.50
1:C:288:GLU:O	1:C:289:ASP:HB2	2.12	0.49
1:C:413:LEU:HG	1:C:475:LEU:HD22	1.94	0.49
1:A:532:ALA:HB1	1:A:558:ALA:O	2.13	0.49
1:C:356:ILE:CG2	1:C:445:TYR:HA	2.42	0.49
1:D:410:ARG:HD2	1:D:436:LEU:HD11	1.94	0.49
1:B:425:ILE:HG22	3:B:2021:HOH:O	2.12	0.49
1:C:443:LYS:NZ	1:C:563:THR:O	2.45	0.49
1:B:443:LYS:NZ	1:B:563:THR:O	2.46	0.49
1:A:223:ALA:HB3	1:A:230:ALA:HB3	1.95	0.49
1:D:498:VAL:HG12	1:D:498:VAL:O	2.14	0.48
1:A:337:ILE:CD1	1:A:424:ILE:HG12	2.43	0.48
1:D:583:THR:O	1:D:584:GLY:C	2.56	0.48
1:B:274:PRO:HD2	3:B:2008:HOH:O	2.13	0.48
1:A:337:ILE:HD12	1:A:424:ILE:HG12	1.95	0.48
1:B:293:THR:HG23	1:B:317:ILE:HB	1.96	0.48
1:D:413:LEU:HG	1:D:475:LEU:HD22	1.96	0.48
1:A:424:ILE:HG22	3:A:2019:HOH:O	2.14	0.47
1:C:577:LEU:HD23	1:C:577:LEU:C	2.39	0.47
1:B:252:VAL:HG22	1:B:269:ASN:HB3	1.97	0.47
1:B:443:LYS:NZ	1:B:510:ASP:OD2	2.42	0.47
1:C:581:TYR:CD1	1:C:588:ILE:HG21	2.50	0.47
1:A:413:LEU:HG	1:A:475:LEU:HD22	1.97	0.47
1:C:219:ASP:N	1:C:220:PRO:HD3	2.30	0.46
1:C:401:VAL:HG13	1:C:504:TRP:CE3	2.50	0.46
1:D:401:VAL:HG13	1:D:504:TRP:CE3	2.51	0.46
1:A:237:ILE:HD11	1:A:246:LYS:HD2	1.97	0.46
1:B:237:ILE:HD11	1:B:246:LYS:HD2	1.97	0.46
1:B:413:LEU:HG	1:B:475:LEU:HD22	1.97	0.46
1:C:498:VAL:HG12	1:C:498:VAL:O	2.14	0.46
1:A:216:CYS:SG	1:A:218:THR:HG23	2.55	0.46
1:A:219:ASP:N	1:A:220:PRO:HD3	2.30	0.46
1:D:443:LYS:NZ	1:D:510:ASP:OD2	2.47	0.46
1:B:219:ASP:N	1:B:220:PRO:HD3	2.30	0.46
1:A:443:LYS:NZ	1:A:563:THR:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:THR:CG2	1:B:317:ILE:O	2.64	0.45
1:C:435:ARG:HG3	3:C:2026:HOH:O	2.15	0.45
1:D:339:LYS:HD2	1:D:423:ASP:HB2	1.98	0.45
1:A:491:SER:OG	1:D:471:THR:HA	2.17	0.45
1:B:451:PRO:HD2	3:B:2026:HOH:O	2.16	0.45
1:D:219:ASP:N	1:D:220:PRO:HD3	2.32	0.45
1:A:252:VAL:HG22	1:A:269:ASN:HB3	1.98	0.45
1:B:557:ASN:ND2	1:B:582:ASP:OD2	2.48	0.45
1:B:206:THR:HA	1:D:207:LEU:O	2.17	0.44
1:A:197:ILE:HD12	1:A:598:PRO:HG2	1.98	0.44
1:B:197:ILE:HD12	1:B:598:PRO:HG2	1.99	0.44
1:C:237:ILE:HD11	1:C:246:LYS:HD2	2.00	0.44
1:A:581:TYR:HD1	1:A:588:ILE:HG21	1.81	0.44
1:A:211:THR:HG22	1:A:211:THR:O	2.17	0.44
1:C:197:ILE:HD12	1:C:598:PRO:HG2	1.99	0.44
1:C:408:ILE:C	1:C:408:ILE:HD12	2.42	0.44
1:D:424:ILE:HD12	1:D:424:ILE:H	1.83	0.44
1:D:294:LEU:HD13	1:D:316:LEU:HD23	2.00	0.44
1:B:212:ARG:CZ	1:B:246:LYS:HZ2	2.28	0.44
1:D:292:TYR:HB3	1:D:316:LEU:HD11	2.01	0.43
1:B:218:THR:HG22	1:B:581:TYR:OH	2.19	0.43
1:C:205:TYR:CE1	1:C:207:LEU:CD1	3.01	0.43
1:A:206:THR:HA	1:C:207:LEU:O	2.18	0.43
1:C:416:TYR:CE2	1:C:424:ILE:HG13	2.53	0.43
1:D:197:ILE:HD12	1:D:598:PRO:HG2	2.01	0.43
1:D:450:GLN:HE21	1:D:516:ARG:NH2	2.17	0.43
1:D:205:TYR:CE1	1:D:207:LEU:CD1	3.01	0.43
1:A:571:VAL:HG22	1:A:573:TRP:NE1	2.33	0.43
1:B:205:TYR:CE1	1:B:207:LEU:CD1	3.02	0.42
1:C:261:LYS:HE3	1:C:569:GLU:CG	2.48	0.42
1:C:252:VAL:HG22	1:C:269:ASN:HB3	2.00	0.42
1:B:216:CYS:SG	1:B:218:THR:HG23	2.60	0.42
1:D:581:TYR:CD2	1:D:581:TYR:N	2.87	0.42
1:A:267:MET:HE2	1:A:267:MET:HB2	1.95	0.42
1:D:237:ILE:HD11	1:D:246:LYS:HD2	2.02	0.42
1:B:267:MET:HE2	1:B:267:MET:HB2	1.97	0.41
1:D:252:VAL:HG22	1:D:269:ASN:HB3	2.02	0.41
1:B:437:THR:O	1:B:438:ILE:C	2.63	0.41
1:A:258:ARG:HB3	1:A:264:SER:OG	2.21	0.41
1:B:210:ASN:HD21	1:B:212:ARG:NE	2.19	0.41
1:B:510:ASP:OD1	1:B:510:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:O	1:A:438:ILE:C	2.64	0.41
1:D:216:CYS:SG	1:D:218:THR:CG2	3.09	0.41
1:A:581:TYR:CD1	1:A:588:ILE:HG21	2.56	0.41
1:B:258:ARG:HB3	1:B:264:SER:OG	2.21	0.40
1:C:286:TYR:CE2	1:C:288:GLU:OE1	2.74	0.40
1:A:205:TYR:O	1:C:208:PRO:HA	2.21	0.40
1:B:290:PHE:HB2	1:B:292:TYR:CE2	2.56	0.40
1:B:425:ILE:CG2	3:B:2021:HOH:O	2.69	0.40
1:C:233:HIS:CD2	1:C:233:HIS:C	2.99	0.40
1:C:510:ASP:OD1	1:C:510:ASP:C	2.64	0.40

All (2) 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:341:GLU:OE2	1:D:373:THR:OG1[1_556]	1.92	0.28
1:B:582:ASP:OD2	1:C:288:GLU:OE2[1_565]	2.13	0.07

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	417/420 (99%)	395 (95%)	21 (5%)	1 (0%)	43	72
1	B	416/420 (99%)	393 (94%)	23 (6%)	0	100	100
1	C	415/420 (99%)	392 (94%)	23 (6%)	0	100	100
1	D	415/420 (99%)	386 (93%)	28 (7%)	1 (0%)	43	72
All	All	1663/1680 (99%)	1566 (94%)	95 (6%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	GLU
1	D	288	GLU

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	376/377 (100%)	359 (96%)	17 (4%)	24	58
1	B	375/377 (100%)	359 (96%)	16 (4%)	26	60
1	C	374/377 (99%)	355 (95%)	19 (5%)	21	53
1	D	374/377 (99%)	357 (96%)	17 (4%)	24	58
All	All	1499/1508 (99%)	1430 (95%)	69 (5%)	24	57

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	LEU
1	A	207	LEU
1	A	212	ARG
1	A	215	VAL
1	A	221	LEU
1	A	291	TYR
1	A	316	LEU
1	A	324	LYS
1	A	376	GLN
1	A	380	SER
1	A	385	ILE
1	A	423	ASP
1	A	425	ILE
1	A	437	THR
1	A	495	ARG
1	A	519	TRP
1	A	571	VAL
1	B	202	LEU
1	B	210	ASN
1	B	215	VAL

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Mol	Chain	Res	Type
1	B	221	LEU
1	B	241	THR
1	B	288	GLU
1	B	291	TYR
1	B	316	LEU
1	B	324	LYS
1	B	376	GLN
1	B	380	SER
1	B	385	ILE
1	B	437	THR
1	B	495	ARG
1	B	519	TRP
1	B	582	ASP
1	C	202	LEU
1	C	215	VAL
1	C	221	LEU
1	C	288	GLU
1	C	291	TYR
1	C	293	THR
1	C	316	LEU
1	C	324	LYS
1	C	376	GLN
1	C	380	SER
1	C	385	ILE
1	C	401	VAL
1	C	420	LEU
1	C	437	THR
1	C	495	ARG
1	C	519	TRP
1	C	568	LEU
1	C	570	ASN
1	C	582	ASP
1	D	202	LEU
1	D	215	VAL
1	D	221	LEU
1	D	242	ARG
1	D	293	THR
1	D	316	LEU
1	D	324	LYS
1	D	376	GLN
1	D	380	SER
1	D	385	ILE

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Mol	Chain	Res	Type
1	D	401	VAL
1	D	423	ASP
1	D	424	ILE
1	D	437	THR
1	D	495	ARG
1	D	519	TRP
1	D	569	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	GLN
1	A	446	ASN
1	B	376	GLN
1	B	406	HIS
1	B	543	ASN
1	C	376	GLN
1	C	446	ASN
1	C	527	ASN
1	D	287	HIS
1	D	299	HIS
1	D	376	GLN
1	D	450	GLN
1	D	527	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 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	A	1604	1	14,14,15	0.65	0	17,19,21	1.75	3 (17%)
2	NAG	D	1604	1	14,14,15	0.50	0	17,19,21	0.92	0
2	NAG	B	1605	1	14,14,15	0.50	0	17,19,21	1.02	1 (5%)
2	NAG	A	1606	1	14,14,15	0.67	0	17,19,21	1.35	3 (17%)
2	NAG	B	1606	1	14,14,15	0.53	0	17,19,21	0.94	1 (5%)
2	NAG	A	1607	1	14,14,15	0.54	0	17,19,21	1.16	0
2	NAG	C	1604	1	14,14,15	0.45	0	17,19,21	1.48	3 (17%)
2	NAG	B	1604	1	14,14,15	0.42	0	17,19,21	0.94	0
2	NAG	A	1605	1	14,14,15	0.55	0	17,19,21	0.96	1 (5%)
2	NAG	B	1607	1	14,14,15	0.59	0	17,19,21	0.98	2 (11%)

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	A	1604	1	-	2/6/23/26	0/1/1/1
2	NAG	D	1604	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1605	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1606	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1606	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1607	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1604	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1604	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1605	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1607	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1604	NAG	C1-O5-C5	4.98	118.86	112.19
2	C	1604	NAG	C1-O5-C5	3.43	116.78	112.19
2	B	1605	NAG	C1-O5-C5	3.09	116.32	112.19
2	A	1605	NAG	C1-O5-C5	2.91	116.09	112.19
2	A	1604	NAG	O4-C4-C5	-2.81	102.40	109.32
2	A	1606	NAG	C1-O5-C5	-2.52	108.80	112.19
2	A	1606	NAG	C4-C3-C2	-2.50	107.35	111.02
2	B	1607	NAG	C1-O5-C5	2.45	115.47	112.19
2	C	1604	NAG	C3-C4-C5	2.39	114.56	110.23
2	A	1606	NAG	O3-C3-C4	2.38	115.98	110.38
2	B	1607	NAG	O5-C1-C2	-2.36	107.65	111.29
2	A	1604	NAG	C8-C7-N2	2.25	119.85	116.12
2	B	1606	NAG	C1-O5-C5	2.22	115.17	112.19
2	C	1604	NAG	C2-N2-C7	-2.14	120.03	122.90

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1604	NAG	C8-C7-N2-C2
2	C	1604	NAG	O7-C7-N2-C2
2	B	1604	NAG	O5-C5-C6-O6
2	A	1606	NAG	C8-C7-N2-C2
2	A	1606	NAG	O7-C7-N2-C2
2	B	1607	NAG	O5-C5-C6-O6
2	B	1604	NAG	C4-C5-C6-O6
2	A	1605	NAG	C4-C5-C6-O6
2	B	1607	NAG	C4-C5-C6-O6
2	A	1605	NAG	O5-C5-C6-O6
2	A	1604	NAG	C8-C7-N2-C2
2	A	1604	NAG	O7-C7-N2-C2
2	A	1605	NAG	C8-C7-N2-C2
2	B	1604	NAG	C8-C7-N2-C2
2	B	1606	NAG	C8-C7-N2-C2
2	B	1606	NAG	C4-C5-C6-O6
2	A	1605	NAG	O7-C7-N2-C2
2	B	1604	NAG	O7-C7-N2-C2
2	B	1606	NAG	O7-C7-N2-C2
2	B	1606	NAG	O5-C5-C6-O6
2	B	1605	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	B	1605	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1604	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	419/420 (99%)	0.81	27 (6%) 25 20	7, 25, 49, 91	0
1	B	418/420 (99%)	0.81	37 (8%) 15 13	8, 26, 52, 90	0
1	C	417/420 (99%)	1.00	58 (13%) 6 5	8, 27, 64, 94	0
1	D	417/420 (99%)	0.87	38 (9%) 15 12	8, 27, 55, 85	0
All	All	1671/1680 (99%)	0.87	160 (9%) 13 11	7, 26, 55, 94	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	LEU	5.6
1	C	581	TYR	5.1
1	D	583	THR	4.8
1	B	385	ILE	4.4
1	A	581	TYR	4.3
1	B	420	LEU	4.2
1	C	420	LEU	4.1
1	D	420	LEU	4.1
1	D	581	TYR	3.9
1	C	385	ILE	3.8
1	B	553	GLU	3.7
1	D	554	ASP	3.5
1	D	385	ILE	3.4
1	C	491	SER	3.4
1	D	419	SER	3.4
1	B	581	TYR	3.4
1	C	531	THR	3.3
1	B	424	ILE	3.3
1	C	601	CYS	3.3
1	C	424	ILE	3.3
1	C	586	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	191	GLN	3.2
1	C	425	ILE	3.2
1	C	490	GLN	3.2
1	A	327	SER	3.1
1	B	554	ASP	3.1
1	C	584	GLY	3.0
1	D	600	GLN	3.0
1	C	554	ASP	3.0
1	C	421	GLY	3.0
1	C	588	ILE	3.0
1	A	191	GLN	3.0
1	D	325	SER	3.0
1	A	385	ILE	2.9
1	C	416	TYR	2.9
1	C	214	GLY	2.9
1	B	446	ASN	2.9
1	A	288	GLU	2.8
1	C	602	SER	2.8
1	D	601	CYS	2.8
1	A	389	TYR	2.8
1	D	586	SER	2.8
1	A	216	CYS	2.8
1	C	600	GLN	2.8
1	B	582	ASP	2.8
1	D	584	GLY	2.8
1	A	376	GLN	2.7
1	C	198	LEU	2.7
1	A	329	ASP	2.7
1	C	194	THR	2.7
1	D	555	ASP	2.7
1	C	259	GLY	2.7
1	D	491	SER	2.7
1	A	518	ASN	2.7
1	D	423	ASP	2.7
1	C	580	ILE	2.7
1	B	555	ASP	2.7
1	C	555	ASP	2.7
1	D	187	GLN	2.7
1	C	309	SER	2.7
1	B	237	ILE	2.6
1	B	602	SER	2.6
1	C	423	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	450	GLN	2.6
1	A	553	GLU	2.6
1	B	518	ASN	2.6
1	B	327	SER	2.6
1	C	419	SER	2.6
1	D	569	GLU	2.6
1	C	187	GLN	2.5
1	C	216	CYS	2.5
1	A	446	ASN	2.5
1	A	403	SER	2.5
1	D	194	THR	2.5
1	D	196	THR	2.5
1	A	554	ASP	2.5
1	D	505	GLU	2.5
1	B	289	ASP	2.4
1	B	587	VAL	2.4
1	C	422	GLY	2.4
1	C	530	GLN	2.4
1	A	196	THR	2.4
1	D	531	THR	2.4
1	D	481	ASN	2.4
1	C	207	LEU	2.4
1	C	505	GLU	2.4
1	D	485	ILE	2.4
1	D	214	GLY	2.4
1	C	389	TYR	2.4
1	C	190	LEU	2.4
1	D	329	ASP	2.4
1	C	543	ASN	2.3
1	C	260	ASP	2.3
1	B	421	GLY	2.3
1	B	215	VAL	2.3
1	D	392	ALA	2.3
1	D	277	SER	2.3
1	D	389	TYR	2.3
1	D	603	GLU	2.3
1	B	600	GLN	2.3
1	C	308	THR	2.3
1	C	583	THR	2.3
1	B	389	TYR	2.3
1	B	474	PRO	2.3
1	D	422	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	603	GLU	2.2
1	C	558	ALA	2.2
1	D	378	ASN	2.2
1	B	376	GLN	2.2
1	A	326	ASP	2.2
1	B	225	ASP	2.2
1	B	346	ASP	2.2
1	B	299	HIS	2.2
1	B	216	CYS	2.2
1	B	239	SER	2.2
1	B	586	SER	2.2
1	A	517	LEU	2.2
1	C	322	ARG	2.2
1	C	582	ASP	2.2
1	C	585	ASP	2.2
1	A	187	GLN	2.2
1	C	485	ILE	2.2
1	C	218	THR	2.2
1	D	449	GLY	2.2
1	C	344	LYS	2.2
1	D	414	LEU	2.2
1	C	213	GLU	2.2
1	C	392	ALA	2.2
1	C	393	GLU	2.2
1	B	588	ILE	2.2
1	D	557	ASN	2.2
1	C	277	SER	2.2
1	B	603	GLU	2.2
1	C	381	ASN	2.1
1	A	308	THR	2.1
1	A	339	LYS	2.1
1	D	207	LEU	2.1
1	D	588	ILE	2.1
1	B	328	GLY	2.1
1	B	242	ARG	2.1
1	D	416	TYR	2.1
1	A	587	VAL	2.1
1	C	484	VAL	2.1
1	C	587	VAL	2.1
1	A	207	LEU	2.1
1	B	601	CYS	2.1
1	D	198	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	422	GLY	2.1
1	A	225	ASP	2.1
1	C	193	THR	2.1
1	C	258	ARG	2.1
1	C	329	ASP	2.1
1	B	288	GLU	2.1
1	D	490	GLN	2.0
1	C	571	VAL	2.0
1	B	323	PRO	2.0
1	B	426	LEU	2.0
1	B	211	THR	2.0
1	C	208	PRO	2.0
1	A	597	ILE	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	B	1606	14/15	0.77	0.14	20,23,24,25	0
2	NAG	A	1607	14/15	0.79	0.16	19,20,23,24	0
2	NAG	A	1606	14/15	0.84	0.14	18,20,21,22	0
2	NAG	B	1607	14/15	0.85	0.15	17,20,22,23	0
2	NAG	C	1604	14/15	0.85	0.15	16,18,20,21	0
2	NAG	D	1604	14/15	0.88	0.16	14,18,19,20	0
2	NAG	B	1605	14/15	0.89	0.13	7,14,15,17	0
2	NAG	A	1604	14/15	0.91	0.11	3,8,10,10	0
2	NAG	B	1604	14/15	0.93	0.09	9,13,14,14	0
2	NAG	A	1605	14/15	0.93	0.09	6,9,11,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.