



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:44 PM GMT

PDB ID : 1M6B
Title : Structure of the HER3 (ERBB3) Extracellular Domain
Authors : Leahy, D.J.; Cho, H.-S.
Deposited on : 2002-07-15
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

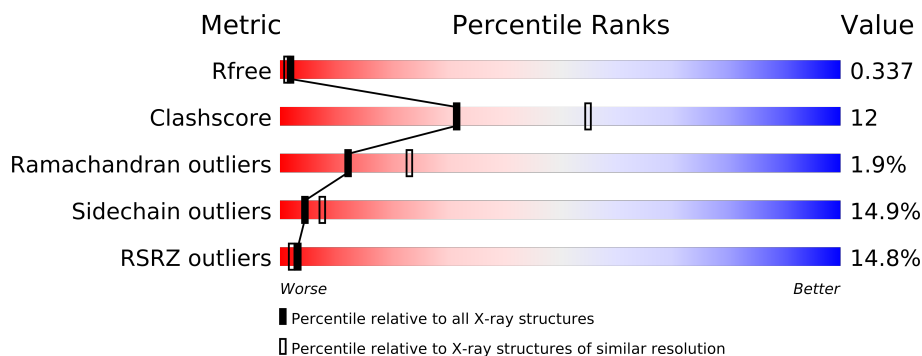
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 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	621	
1	B	621	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	627	-	X
2	NAG	A	630	-	X
2	NAG	B	622	-	X
5	SO4	B	5001	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9012 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.

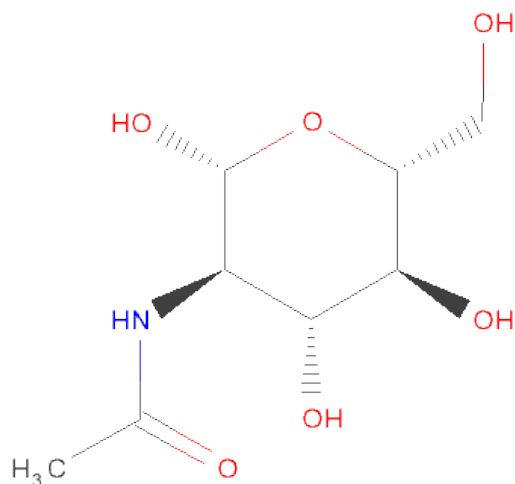
- Molecule 1 is a protein called Receptor protein-tyrosine kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4206	2603	765	784	54			
1	B	584	Total	C	N	O	S	0	0	0
			4478	2766	813	840	59			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	VAL	ILE	ENGINEERED	UNP P21860
B	61	VAL	ILE	ENGINEERED	UNP P21860

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



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

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

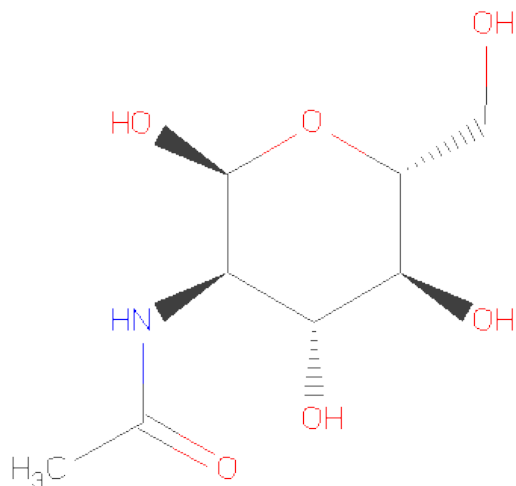
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	VAL	ILE	ENGINEERED	UNP P21860
B	61	VAL	ILE	ENGINEERED	UNP P21860

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

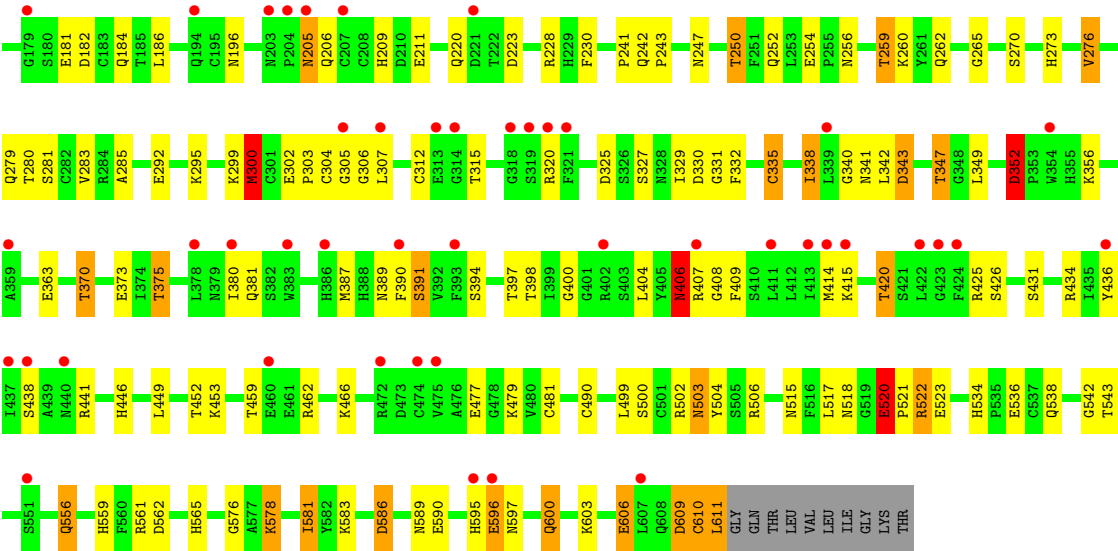
- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total 20	O 20	0	0
6	B	65	Total 65	O 65	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.26Å 49.62Å 190.86Å 90.00° 125.56° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 28.74 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.60) 90.7 (28.74-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.235 , 0.294 0.299 , 0.337	Depositor DCC
R_{free} test set	2610 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 1.4	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 54360 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9012	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: NAG, NDG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/4308	0.84	15/5845 (0.3%)
1	B	0.62	1/4586 (0.0%)	0.86	8/6222 (0.1%)
All	All	0.59	1/8894 (0.0%)	0.85	23/12067 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	MET	SD-CE	5.39	2.08	1.77

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ASP	CB-CG-OD2	8.78	126.20	118.30
1	A	221	ASP	CB-CG-OD2	6.58	124.22	118.30
1	B	146	ASP	CB-CG-OD2	6.36	124.02	118.30
1	B	143	ASP	CB-CG-OD2	6.24	123.91	118.30
1	B	325	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	232	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	609	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	143	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	325	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	146	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	352	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	343	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	93	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	134	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	210	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	289	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	159	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	152	ASP	CB-CG-OD2	5.31	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	343	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	159	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	278	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	562	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4206	0	3996	79	0
1	B	4478	0	4242	123	0
2	A	98	0	91	0	0
2	B	70	0	65	2	0
3	A	28	0	25	1	0
3	B	28	0	25	1	0
4	B	14	0	13	0	0
5	B	5	0	0	4	0
6	A	20	0	0	3	0
6	B	65	0	0	7	0
All	All	9012	0	8457	202	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (202) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:300:MET:SD	1:B:300:MET:CE	2.08	1.42
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.11	1.11
1:B:335:CYS:O	1:B:370:THR:HG22	1.56	1.03
1:B:452:THR:HG22	1:B:459:THR:HG21	1.42	1.00
1:B:578:LYS:H	1:B:578:LYS:HE2	1.31	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:247:ASN:ND2	6:B:1072:HOH:O	2.01	0.91
1:B:520:GLU:HB2	1:B:521:PRO:CD	2.00	0.90
1:B:452:THR:CG2	1:B:459:THR:HG21	2.03	0.87
1:B:168:HIS:HD2	1:B:170:VAL:HB	1.41	0.86
1:B:250:THR:HG21	1:B:254:GLU:OE2	1.75	0.86
1:B:534:HIS:HD2	1:B:536:GLU:H	1.26	0.84
1:A:330:ASP:O	1:A:333:VAL:HG23	1.77	0.83
1:A:145:ARG:HE	1:A:155:ILE:HD13	1.44	0.83
1:B:335:CYS:O	1:B:370:THR:CG2	2.28	0.82
1:B:436:TYR:CE2	1:B:438:SER:HB2	2.18	0.79
1:A:315:THR:HG21	1:A:343:ASP:HB2	1.65	0.79
1:B:452:THR:HG22	1:B:459:THR:CG2	2.12	0.78
1:A:469:ARG:NH2	1:A:477:GLU:OE2	2.16	0.76
1:A:551:SER:HB2	1:A:566:CYS:H	1.51	0.75
1:B:36:ARG:HD3	1:B:37:CYS:H	1.50	0.75
1:B:520:GLU:HB2	1:B:521:PRO:HD3	1.68	0.75
1:B:434:ARG:HG2	1:B:462:ARG:HB2	1.69	0.75
1:B:116:ARG:NH1	1:B:116:ARG:HG3	1.92	0.75
1:B:559:HIS:NE2	5:B:5001:SO4:O2	2.21	0.74
1:B:565:HIS:HD2	6:B:1058:HOH:O	1.72	0.73
1:A:87:ARG:HG2	1:A:124:LEU:HD12	1.69	0.73
1:A:456:ARG:HH11	1:A:456:ARG:HB2	1.54	0.72
1:B:534:HIS:CD2	1:B:536:GLU:H	2.08	0.72
1:B:420:THR:HG22	1:B:479:LYS:NZ	2.04	0.72
1:B:559:HIS:NE2	5:B:5001:SO4:O4	2.25	0.70
1:B:247:ASN:CG	6:B:1072:HOH:O	2.27	0.69
1:A:73:ASN:ND2	1:A:103:ASN:OD1	2.25	0.69
1:B:414:MET:O	1:B:415:LYS:HG2	1.92	0.68
1:B:243:PRO:HA	1:B:259:THR:HG23	1.77	0.67
1:B:315:THR:HG22	1:B:343:ASP:OD2	1.94	0.67
1:A:150:ASP:HB3	1:A:153:ALA:HB2	1.77	0.67
1:B:381:GLN:HG2	1:B:415:LYS:HE2	1.77	0.67
1:B:116:ARG:HH11	1:B:116:ARG:CG	1.97	0.66
1:B:586:ASP:HB2	1:B:590:GLU:H	1.60	0.66
1:B:534:HIS:CD2	1:B:536:GLU:HB2	2.32	0.65
1:B:209:HIS:HD2	1:B:211:GLU:H	1.41	0.65
1:A:375:THR:HA	1:A:402:ARG:HH11	1.61	0.65
1:B:520:GLU:CB	1:B:521:PRO:CD	2.74	0.64
1:B:520:GLU:HB2	1:B:521:PRO:HD2	1.77	0.64
1:B:150:ASP:HB3	1:B:153:ALA:HB2	1.80	0.64
1:B:420:THR:HG22	1:B:479:LYS:HZ3	1.63	0.63
1:A:552:ASP:HA	1:A:564:PRO:O	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:ARG:CB	1:B:36:ARG:HH11	2.12	0.62
1:B:559:HIS:NE2	5:B:5001:SO4:S	2.69	0.62
1:B:220:GLN:HB2	1:B:223:ASP:OD2	2.00	0.62
1:A:551:SER:HB2	1:A:566:CYS:N	2.15	0.61
1:A:70:VAL:HB	1:A:100:VAL:HG22	1.83	0.60
3:A:624:NAG:H81	6:A:1045:HOH:O	2.00	0.60
1:A:117:LEU:HD13	1:A:120:LEU:HD22	1.83	0.60
1:A:440:ASN:HD22	1:A:468:ASN:ND2	1.99	0.60
1:B:243:PRO:HA	1:B:259:THR:CG2	2.33	0.59
1:B:302:GLU:HG3	1:B:303:PRO:HD2	1.84	0.58
1:A:315:THR:CG2	1:A:343:ASP:HB2	2.34	0.58
1:A:440:ASN:H	1:A:468:ASN:HD22	1.52	0.58
1:B:578:LYS:N	1:B:578:LYS:HE2	2.11	0.58
1:A:436:TYR:CE2	1:A:438:SER:HB2	2.40	0.57
1:B:586:ASP:HB2	1:B:590:GLU:N	2.19	0.57
1:A:341:ASN:HD22	1:A:377:TYR:H	1.52	0.57
1:B:283:VAL:HG12	1:B:285:ALA:H	1.69	0.56
1:B:36:ARG:HD3	1:B:37:CYS:HB2	1.87	0.56
1:A:332:PHE:O	1:A:335:CYS:HB2	2.06	0.56
1:B:373:GLU:HG3	1:B:398:THR:HB	1.87	0.56
1:B:304:CYS:O	1:B:306:GLY:N	2.38	0.56
1:B:129:TYR:CE2	1:B:131:GLU:HB2	2.41	0.55
1:A:72:MET:HE1	1:A:102:LEU:HB2	1.87	0.55
1:B:114:GLN:OE1	1:B:116:ARG:HD3	2.07	0.55
1:B:606:GLU:HB2	1:B:609:ASP:OD2	2.06	0.55
1:B:241:PRO:HG2	1:B:260:LYS:HG3	1.89	0.55
1:A:256:ASN:HD21	1:A:258:HIS:HB2	1.72	0.55
1:B:565:HIS:CD2	6:B:1058:HOH:O	2.55	0.55
1:A:84:ARG:HD3	1:A:119:GLN:HG3	1.88	0.54
1:A:574:VAL:O	1:A:580:PRO:HA	2.07	0.54
1:A:466:LYS:HG3	1:A:467:HIS:CD2	2.42	0.54
1:B:520:GLU:CB	1:B:521:PRO:HD3	2.34	0.54
1:B:610:CYS:O	1:B:611:LEU:O	2.25	0.54
1:A:456:ARG:HB2	1:A:456:ARG:NH1	2.20	0.54
1:B:534:HIS:HD2	1:B:536:GLU:HB2	1.73	0.54
1:B:438:SER:OG	1:B:466:LYS:HG3	2.08	0.54
1:B:36:ARG:CD	1:B:37:CYS:H	2.19	0.53
1:B:36:ARG:HH11	1:B:36:ARG:HB2	1.73	0.53
1:A:397:THR:HG22	1:A:398:THR:OG1	2.09	0.53
1:A:87:ARG:NH2	1:A:227:CYS:O	2.27	0.53
1:A:425:ARG:NH1	6:A:1025:HOH:O	2.41	0.52
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:415:LYS:HA	1:A:439:ALA:O	2.10	0.52
1:B:262:GLN:HB2	1:B:281:SER:CB	2.40	0.52
1:B:400:GLY:O	1:B:431:SER:HB2	2.09	0.52
1:A:449:LEU:HD12	1:A:499:LEU:HD12	1.92	0.51
1:A:349:LEU:HD12	1:A:382:SER:OG	2.10	0.51
1:A:341:ASN:HD22	1:A:376:GLY:HA3	1.75	0.51
1:A:201:GLY:HA3	1:A:206:GLN:OE1	2.11	0.51
1:B:80:LEU:HD13	1:B:83:LEU:HD22	1.92	0.50
1:B:518:ASN:HA	1:B:522:ARG:CZ	2.40	0.50
1:B:146:ASP:OD1	1:B:186:LEU:HA	2.11	0.50
1:B:209:HIS:CD2	1:B:211:GLU:H	2.25	0.50
1:A:440:ASN:H	1:A:468:ASN:ND2	2.09	0.50
1:B:47:VAL:HA	1:B:71:ALA:O	2.12	0.50
1:A:519:GLY:O	1:A:522:ARG:HD3	2.12	0.50
1:A:222:THR:HG22	1:A:222:THR:O	2.12	0.50
1:B:168:HIS:CD2	1:B:170:VAL:HB	2.32	0.50
1:B:609:ASP:O	1:B:610:CYS:SG	2.70	0.50
1:A:54:ASP:OD1	1:A:56:SER:HB3	2.12	0.49
1:B:247:ASN:OD1	1:B:247:ASN:C	2.50	0.49
1:A:469:ARG:HD3	6:A:1022:HOH:O	2.11	0.49
1:B:330:ASP:C	1:B:332:PHE:H	2.16	0.49
1:B:243:PRO:HD2	6:B:1065:HOH:O	2.13	0.48
1:B:446:HIS:HA	6:B:1042:HOH:O	2.14	0.48
1:A:520:GLU:HB2	1:A:521:PRO:HD3	1.96	0.48
1:A:279:GLN:CG	1:A:280:THR:H	2.25	0.48
1:A:127:GLY:HA3	1:A:154:GLU:O	2.14	0.48
1:B:143:ASP:H	1:B:184:GLN:HE22	1.61	0.48
1:B:409:PHE:CE2	1:B:436:TYR:HB2	2.49	0.48
1:A:341:ASN:ND2	1:A:376:GLY:HA3	2.28	0.48
1:A:409:PHE:CD2	1:A:436:TYR:HB2	2.49	0.47
1:A:174:ARG:HB3	1:A:184:GLN:HB3	1.96	0.47
1:A:38:GLU:OE1	1:A:62:ARG:NH1	2.47	0.47
1:B:404:LEU:HD13	1:B:408:GLY:HA2	1.96	0.47
1:B:515:ASN:HB3	1:B:518:ASN:O	2.14	0.47
1:B:583:LYS:NZ	6:B:1069:HOH:O	2.47	0.47
1:A:450:ASN:ND2	1:A:453:LYS:HD2	2.29	0.47
1:B:409:PHE:CD2	1:B:436:TYR:HB2	2.49	0.47
1:B:397:THR:HA	1:B:426:SER:O	2.13	0.47
1:B:205:ASN:ND2	1:B:206:GLN:HG3	2.29	0.47
1:B:499:LEU:HA	1:B:499:LEU:HD23	1.78	0.46
1:B:78:LEU:HD23	1:B:115:LEU:HD22	1.98	0.46
1:A:373:GLU:HG3	1:A:398:THR:HB	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:ASN:HD21	1:A:381:GLN:HG3	1.81	0.46
1:A:394:SER:HB2	1:A:425:ARG:HD3	1.97	0.46
1:B:453:LYS:HE2	2:B:627:NAG:O6	2.15	0.46
1:A:72:MET:CE	1:A:102:LEU:HB2	2.46	0.46
1:B:406:ASN:HB3	1:B:407:ARG:H	1.49	0.46
1:A:449:LEU:CD1	1:A:499:LEU:HD12	2.46	0.45
1:B:506:ARG:HD3	1:B:523:GLU:OE1	2.16	0.45
1:A:368:PHE:HB2	1:A:392:VAL:CG1	2.46	0.45
1:B:595:HIS:C	1:B:597:ASN:H	2.19	0.45
1:A:376:GLY:HA2	1:A:403:SER:H	1.81	0.45
1:B:576:GLY:HA3	1:B:581:ILE:CD1	2.47	0.45
1:B:262:GLN:HB2	1:B:281:SER:HB3	1.99	0.45
1:B:205:ASN:HD22	1:B:206:GLN:HG3	1.81	0.45
1:B:380:ILE:HG21	1:B:390:PHE:CE2	2.51	0.45
1:B:420:THR:HG22	1:B:479:LYS:HZ1	1.81	0.45
1:A:309:PRO:HA	1:A:336:THR:OG1	2.17	0.45
1:B:230:PHE:HA	1:B:265:GLY:O	2.17	0.45
1:B:559:HIS:CD2	5:B:5001:SO4:O2	2.70	0.45
1:B:243:PRO:CA	1:B:259:THR:HG23	2.46	0.45
1:A:514:CYS:HB2	1:A:516:PHE:CE1	2.52	0.45
1:A:417:LEU:HD22	1:A:441:ARG:HG3	1.98	0.44
1:B:72:MET:CE	1:B:102:LEU:HB2	2.47	0.44
1:A:356:LYS:O	1:A:358:PRO:HD3	2.17	0.44
1:A:375:THR:HA	1:A:402:ARG:NH1	2.27	0.44
1:A:222:THR:CG2	1:A:222:THR:O	2.65	0.44
1:A:349:LEU:HD23	1:A:360:LEU:HD12	1.99	0.44
1:A:96:PHE:CD2	1:A:129:TYR:HB2	2.52	0.44
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.76	0.44
1:A:74:GLU:HB3	1:A:110:HIS:HB3	2.00	0.44
1:B:59:GLN:O	1:B:82:ASN:ND2	2.39	0.44
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.65	0.43
1:A:440:ASN:HD22	1:A:468:ASN:HD21	1.62	0.43
1:B:340:GLY:H	1:B:375:THR:HB	1.83	0.43
1:B:242:GLN:O	1:B:259:THR:HG23	2.17	0.43
1:B:128:VAL:HG21	1:B:144:TRP:CE3	2.54	0.43
1:A:400:GLY:HA3	1:A:402:ARG:CZ	2.48	0.43
1:B:589:ASN:HA	1:B:589:ASN:HD22	1.62	0.43
1:B:148:VAL:HG21	1:B:155:ILE:HD11	2.00	0.43
1:A:315:THR:CG2	1:A:316:GLY:N	2.82	0.43
1:A:71:ALA:C	1:A:72:MET:HG2	2.39	0.43
1:A:91:VAL:O	1:A:91:VAL:CG1	2.66	0.43
1:B:503:ASN:HB2	1:B:504:TYR:H	1.62	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:452:THR:OG1	2:B:627:NAG:H5	2.19	0.43
1:B:347:THR:HG22	1:B:352:ASP:HB2	2.00	0.43
1:A:45:GLU:HG2	1:A:69:LEU:HD23	2.00	0.42
1:A:169:GLU:OE2	1:B:62:ARG:NH2	2.53	0.42
1:A:47:VAL:HA	1:A:71:ALA:O	2.18	0.42
1:B:70:VAL:HG21	1:B:78:LEU:HD22	2.01	0.42
1:B:115:LEU:HA	1:B:115:LEU:HD23	1.81	0.42
1:A:579:GLY:HA2	1:A:580:PRO:HD2	1.87	0.42
1:B:262:GLN:HB2	1:B:281:SER:HB2	2.02	0.42
1:B:506:ARG:NH1	1:B:523:GLU:OE2	2.53	0.42
1:B:338:ILE:HD13	1:B:342:LEU:HD11	2.00	0.42
1:B:375:THR:O	1:B:400:GLY:HA3	2.20	0.42
1:B:143:ASP:N	1:B:184:GLN:HE22	2.17	0.41
1:B:538:GLN:HB3	1:B:556:GLN:HB3	2.01	0.41
1:B:256:ASN:O	1:B:259:THR:OG1	2.38	0.41
1:A:177:GLY:HA3	1:A:182:ASP:CB	2.51	0.41
1:B:517:LEU:HD13	1:B:542:GLY:O	2.20	0.41
1:B:389:ASN:OD1	1:B:391:SER:HB3	2.21	0.41
1:B:142:ILE:HG22	1:B:142:ILE:O	2.20	0.41
1:A:561:ARG:HG2	1:A:562:ASP:N	2.36	0.41
1:A:101:MET:CE	1:A:102:LEU:HD12	2.51	0.41
1:B:481:CYS:SG	1:B:490:CYS:N	2.93	0.41
1:B:387:MET:HA	3:B:624:NAG:O6	2.20	0.41
1:A:78:LEU:O	1:A:116:ARG:HB2	2.21	0.40
1:A:203:ASN:HB2	1:A:206:GLN:HG3	2.02	0.40
1:A:521:PRO:O	1:A:523:GLU:HG3	2.21	0.40
1:B:276:VAL:HG21	1:B:292:GLU:HG3	2.02	0.40
1:B:86:VAL:O	1:B:123:ILE:HA	2.21	0.40
1:B:84:ARG:NH2	1:B:119:GLN:HG3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	545/621 (88%)	482 (88%)	52 (10%)	11 (2%)	11	21
1	B	580/621 (93%)	525 (90%)	45 (8%)	10 (2%)	14	26
All	All	1125/1242 (91%)	1007 (90%)	97 (9%)	21 (2%)	12	23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	460	GLU
1	B	520	GLU
1	B	586	ASP
1	A	296	ASN
1	B	305	GLY
1	B	596	GLU
1	B	600	GLN
1	B	610	CYS
1	A	279	GLN
1	A	577	ALA
1	A	120	LEU
1	A	193	PRO
1	A	288	PRO
1	B	279	GLN
1	B	406	ASN
1	A	306	GLY
1	A	571	PRO
1	B	331	GLY
1	A	574	VAL
1	B	79	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	474/537 (88%)	398 (84%)	76 (16%)	3	6
1	B	506/537 (94%)	436 (86%)	70 (14%)	5	9
All	All	980/1074 (91%)	834 (85%)	146 (15%)	4	7

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	36	ARG
1	A	49	THR
1	A	56	SER
1	A	59	GLN
1	A	73	ASN
1	A	77	THR
1	A	87	ARG
1	A	89	THR
1	A	91	VAL
1	A	98	ILE
1	A	105	ASN
1	A	109	SER
1	A	114	GLN
1	A	116	ARG
1	A	118	THR
1	A	142	ILE
1	A	145	ARG
1	A	151	ARG
1	A	152	ASP
1	A	154	GLU
1	A	181	GLU
1	A	189	THR
1	A	190	ILE
1	A	205	ASN
1	A	210	ASP
1	A	220	GLN
1	A	233	SER
1	A	239	ARG
1	A	247	ASN
1	A	249	LEU
1	A	273	HIS
1	A	276	VAL
1	A	280	THR
1	A	294	ASP
1	A	295	LYS
1	A	298	LEU
1	A	299	LYS
1	A	310	LYS
1	A	312	CYS
1	A	315	THR
1	A	319	SER

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Mol	Chain	Res	Type
1	A	324	VAL
1	A	326	SER
1	A	329	ILE
1	A	341	ASN
1	A	352	ASP
1	A	357	ILE
1	A	367	VAL
1	A	375	THR
1	A	379	ASN
1	A	389	ASN
1	A	397	THR
1	A	402	ARG
1	A	407	ARG
1	A	410	SER
1	A	419	VAL
1	A	431	SER
1	A	441	ARG
1	A	448	SER
1	A	452	THR
1	A	456	ARG
1	A	469	ARG
1	A	499	LEU
1	A	517	LEU
1	A	527	GLU
1	A	529	GLU
1	A	532	SER
1	A	536	GLU
1	A	541	GLU
1	A	549	SER
1	A	551	SER
1	A	561	ARG
1	A	562	ASP
1	A	570	CYS
1	A	575	LEU
1	B	9	VAL
1	B	10	CYS
1	B	13	THR
1	B	36	ARG
1	B	37	CYS
1	B	38	GLU
1	B	49	THR
1	B	74	GLU

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Mol	Chain	Res	Type
1	B	84	ARG
1	B	87	ARG
1	B	95	LYS
1	B	106	THR
1	B	108	SER
1	B	116	ARG
1	B	131	GLU
1	B	142	ILE
1	B	158	LYS
1	B	169	GLU
1	B	181	GLU
1	B	182	ASP
1	B	196	ASN
1	B	205	ASN
1	B	250	THR
1	B	252	GLN
1	B	259	THR
1	B	270	SER
1	B	273	HIS
1	B	276	VAL
1	B	280	THR
1	B	295	LYS
1	B	299	LYS
1	B	300	MET
1	B	307	LEU
1	B	312	CYS
1	B	320	ARG
1	B	327	SER
1	B	329	ILE
1	B	335	CYS
1	B	338	ILE
1	B	341	ASN
1	B	347	THR
1	B	349	LEU
1	B	352	ASP
1	B	356	LYS
1	B	363	GLU
1	B	370	THR
1	B	375	THR
1	B	391	SER
1	B	394	SER
1	B	406	ASN

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Mol	Chain	Res	Type
1	B	420	THR
1	B	425	ARG
1	B	441	ARG
1	B	449	LEU
1	B	477	GLU
1	B	500	SER
1	B	502	ARG
1	B	503	ASN
1	B	520	GLU
1	B	522	ARG
1	B	543	THR
1	B	556	GLN
1	B	561	ARG
1	B	578	LYS
1	B	581	ILE
1	B	596	GLU
1	B	600	GLN
1	B	603	LYS
1	B	606	GLU
1	B	611	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	198	HIS
1	A	247	ASN
1	A	256	ASN
1	A	341	ASN
1	A	379	ASN
1	A	381	GLN
1	A	386	HIS
1	A	467	HIS
1	A	468	ASN
1	A	538	GLN
1	A	565	HIS
1	B	138	HIS
1	B	168	HIS
1	B	184	GLN
1	B	205	ASN
1	B	209	HIS
1	B	229	HIS

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Mol	Chain	Res	Type
1	B	467	HIS
1	B	534	HIS
1	B	589	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

4 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	624	1,3	12,14,15	0.98	1 (8%)	15,19,21	2.16	4 (26%)
3	NAG	A	625	3	12,14,15	0.49	0	15,19,21	1.52	2 (13%)
3	NAG	B	624	1,3	12,14,15	0.58	0	15,19,21	1.39	2 (13%)
3	NAG	B	625	3	12,14,15	0.67	0	15,19,21	1.15	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	624	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	625	3	-	0/6/23/26	0/1/1/1
3	NAG	B	624	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	625	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	624	NAG	C2-N2	-2.21	1.43	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	624	NAG	C3-C2-N2	-4.88	104.33	111.76
3	A	625	NAG	O5-C5-C6	3.74	110.91	106.98
3	A	624	NAG	O5-C5-C4	-3.45	106.27	110.65
3	B	624	NAG	O5-C5-C6	3.45	110.60	106.98
3	B	625	NAG	O5-C5-C6	3.29	110.43	106.98
3	A	624	NAG	O5-C5-C6	2.97	110.09	106.98
3	A	624	NAG	C2-N2-C7	-2.60	118.73	123.09
3	B	624	NAG	C3-C2-N2	-2.42	108.08	111.76
3	A	625	NAG	C3-C4-C5	-2.18	106.31	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

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	A	622	1	12,14,15	0.59	0	15,19,21	1.27	2 (13%)
2	NAG	A	623	1	12,14,15	0.63	0	15,19,21	1.27	1 (6%)
2	NAG	A	626	1	12,14,15	0.68	0	15,19,21	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	627	1	12,14,15	0.59	0	15,19,21	1.36	1 (6%)
2	NAG	A	628	1	12,14,15	0.61	0	15,19,21	1.33	1 (6%)
2	NAG	A	629	1	12,14,15	0.62	0	15,19,21	1.56	3 (20%)
2	NAG	A	630	1	12,14,15	0.54	0	15,19,21	1.47	3 (20%)
5	SO4	B	5001	-	4,4,4	0.35	0	6,6,6	0.28	0
2	NAG	B	622	1	12,14,15	0.75	0	15,19,21	2.54	6 (40%)
2	NAG	B	623	1	12,14,15	0.64	0	15,19,21	1.65	4 (26%)
4	NDG	B	626	1	12,14,15	0.53	0	15,19,21	2.03	3 (20%)
2	NAG	B	627	1	12,14,15	0.68	0	15,19,21	0.92	0
2	NAG	B	628	1	12,14,15	0.82	1 (8%)	15,19,21	1.87	3 (20%)
2	NAG	B	629	1	12,14,15	0.73	0	15,19,21	1.25	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
2	NAG	A	622	1	-	0/6/23/26	0/1/1/1
2	NAG	A	623	1	-	0/6/23/26	0/1/1/1
2	NAG	A	626	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	627	1	-	0/6/23/26	0/1/1/1
2	NAG	A	628	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	629	1	-	0/6/23/26	0/1/1/1
2	NAG	A	630	1	-	0/6/23/26	0/1/1/1
5	SO4	B	5001	-	-	0/0/0/0	0/0/0/0
2	NAG	B	622	1	-	0/6/23/26	0/1/1/1
2	NAG	B	623	1	-	0/6/23/26	0/1/1/1
4	NDG	B	626	1	-	0/6/23/26	0/1/1/1
2	NAG	B	627	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	628	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	629	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	628	NAG	C2-N2	-2.07	1.43	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	622	NAG	C2-N2-C7	-7.10	111.17	123.09
4	B	626	NDG	O-C5-C6	6.04	113.32	106.98
2	B	628	NAG	C2-N2-C7	-4.28	115.91	123.09
2	A	630	NAG	O5-C5-C4	4.01	115.74	110.65
2	B	628	NAG	C3-C2-N2	-3.92	105.79	111.76
2	A	628	NAG	O5-C5-C6	3.83	111.00	106.98
2	A	623	NAG	O5-C5-C6	3.71	110.87	106.98
2	A	629	NAG	O5-C5-C6	3.42	110.57	106.98
2	A	627	NAG	O5-C5-C6	3.27	110.41	106.98
2	B	623	NAG	O5-C5-C6	3.12	110.26	106.98
2	B	622	NAG	O7-C7-N2	-2.99	115.66	121.90
2	B	622	NAG	C3-C4-C5	2.86	115.31	110.20
4	B	626	NDG	C3-C4-C5	-2.72	105.34	110.20
2	B	628	NAG	O5-C5-C6	2.72	109.84	106.98
2	A	630	NAG	O5-C5-C6	2.72	109.83	106.98
2	A	629	NAG	C2-N2-C7	-2.63	118.67	123.09
2	B	623	NAG	O5-C5-C4	2.62	113.98	110.65
2	B	622	NAG	O5-C5-C6	-2.52	104.33	106.98
2	A	626	NAG	C3-C4-C5	2.49	114.66	110.20
4	B	626	NDG	O3-C3-C2	2.40	114.14	109.09
2	A	622	NAG	C3-C2-N2	-2.39	108.12	111.76
2	B	623	NAG	C3-C4-C5	2.38	114.45	110.20
2	A	629	NAG	C3-C4-C5	-2.35	106.01	110.20
2	B	629	NAG	O5-C5-C4	2.31	113.58	110.65
2	A	630	NAG	C3-C4-C5	2.30	114.31	110.20
2	B	622	NAG	C4-C3-C2	2.23	116.77	111.32
2	B	622	NAG	C6-C5-C4	-2.17	107.75	113.00
2	A	622	NAG	O4-C4-C5	2.14	114.93	109.28
2	B	623	NAG	C4-C3-C2	2.02	116.26	111.32

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	626	NAG	C1
2	B	627	NAG	C1
2	B	628	NAG	C1
2	A	628	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	629	NAG	O7-C7-N2-C2

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	549/621 (88%)	1.07	105 (19%) 2 1	4, 13, 23, 57	0
1	B	584/621 (94%)	0.82	65 (11%) 6 4	6, 17, 28, 66	0
All	All	1133/1242 (91%)	0.94	170 (15%) 3 2	4, 15, 26, 66	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	SER	6.6
1	A	574	VAL	6.4
1	A	248	LYS	6.4
1	A	560	PHE	6.0
1	A	578	LYS	6.0
1	A	297	GLY	6.0
1	A	296	ASN	5.7
1	B	320	ARG	5.5
1	A	580	PRO	5.2
1	A	561	ARG	5.1
1	A	193	PRO	5.1
1	A	108	SER	5.0
1	A	298	LEU	5.0
1	A	413	ILE	4.9
1	A	572	HIS	4.8
1	B	204	PRO	4.8
1	A	557	CYS	4.4
1	A	577	ALA	4.3
1	B	194	GLN	4.2
1	A	293	VAL	4.2
1	A	294	ASP	4.2
1	B	607	LEU	4.2
1	B	52	ASN	4.1
1	A	245	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	569	SER	4.1
1	A	246	TYR	4.0
1	B	162	ARG	4.0
1	A	36	ARG	3.9
1	A	305	GLY	3.9
1	A	555	ALA	3.9
1	A	194	GLN	3.9
1	A	380	ILE	3.8
1	A	540	MET	3.8
1	B	390	PHE	3.8
1	A	520	GLU	3.8
1	A	291	MET	3.8
1	A	411	LEU	3.7
1	A	461	GLU	3.7
1	B	422	LEU	3.6
1	A	573	GLY	3.6
1	B	380	ILE	3.5
1	B	407	ARG	3.5
1	A	402	ARG	3.5
1	B	318	GLY	3.5
1	A	304	CYS	3.5
1	B	305	GLY	3.5
1	B	424	PHE	3.4
1	B	475	VAL	3.4
1	A	273	HIS	3.4
1	A	196	ASN	3.4
1	A	568	SER	3.4
1	A	321	PHE	3.4
1	A	303	PRO	3.4
1	B	120	LEU	3.4
1	B	307	LEU	3.4
1	A	289	ASP	3.4
1	A	107	ASN	3.3
1	B	321	PHE	3.3
1	A	244	LEU	3.3
1	A	412	LEU	3.3
1	A	563	GLY	3.2
1	A	249	LEU	3.2
1	B	107	ASN	3.2
1	A	11	PRO	3.1
1	B	205	ASN	3.1
1	A	526	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	354	TRP	3.1
1	A	252	GLN	3.1
1	A	422	LEU	3.1
1	A	535	PRO	3.1
1	A	414	MET	3.1
1	A	507	GLY	3.0
1	A	381	GLN	3.0
1	B	437	ILE	2.9
1	A	306	GLY	2.9
1	B	68	VAL	2.9
1	B	413	ILE	2.9
1	A	295	LYS	2.9
1	B	314	GLY	2.8
1	B	203	ASN	2.8
1	A	579	GLY	2.8
1	A	437	ILE	2.8
1	A	571	PRO	2.8
1	B	64	VAL	2.8
1	B	86	VAL	2.8
1	A	313	GLU	2.8
1	A	378	LEU	2.8
1	A	556	GLN	2.8
1	B	359	ALA	2.8
1	A	570	CYS	2.8
1	B	123	ILE	2.7
1	B	121	THR	2.7
1	B	423	GLY	2.7
1	A	308	CYS	2.7
1	A	339	LEU	2.7
1	B	85	VAL	2.7
1	B	460	GLU	2.7
1	A	320	ARG	2.6
1	B	596	GLU	2.6
1	A	416	ASN	2.6
1	A	251	PHE	2.6
1	B	378	LEU	2.6
1	B	109	SER	2.6
1	A	110	HIS	2.6
1	A	562	ASP	2.6
1	A	292	GLU	2.6
1	B	9	VAL	2.6
1	A	390	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	438	SER	2.6
1	A	204	PRO	2.6
1	B	313	GLU	2.6
1	A	299	LYS	2.5
1	A	290	LYS	2.5
1	A	551	SER	2.5
1	B	66	GLY	2.5
1	B	411	LEU	2.5
1	A	443	LEU	2.5
1	B	98	ILE	2.5
1	A	254	GLU	2.4
1	A	541	GLU	2.4
1	A	575	LEU	2.4
1	A	382	SER	2.4
1	A	211	GLU	2.4
1	A	301	CYS	2.4
1	B	402	ARG	2.4
1	A	379	ASN	2.4
1	A	154	GLU	2.3
1	A	300	MET	2.3
1	B	383	TRP	2.3
1	A	527	GLU	2.3
1	A	237	VAL	2.3
1	B	179	GLY	2.3
1	B	71	ALA	2.3
1	A	274	ASN	2.3
1	A	344	PHE	2.3
1	A	286	CYS	2.3
1	A	151	ARG	2.3
1	B	595	HIS	2.3
1	B	386	HIS	2.2
1	B	438	SER	2.2
1	B	339	LEU	2.2
1	A	559	HIS	2.2
1	B	83	LEU	2.2
1	B	167	CYS	2.2
1	B	393	PHE	2.2
1	A	424	PHE	2.2
1	B	221	ASP	2.2
1	B	62	ARG	2.1
1	B	436	TYR	2.1
1	B	319	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	243	PRO	2.1
1	A	260	LYS	2.1
1	B	472	ARG	2.1
1	B	474	CYS	2.1
1	B	551	SER	2.1
1	A	253	LEU	2.1
1	A	269	ALA	2.1
1	A	134	ASP	2.1
1	A	307	LEU	2.1
1	A	488	GLY	2.1
1	B	440	ASN	2.1
1	B	415	LYS	2.0
1	A	195	CYS	2.0
1	B	110	HIS	2.0
1	A	439	ALA	2.0
1	B	414	MET	2.0
1	A	302	GLU	2.0
1	A	210	ASP	2.0
1	B	65	THR	2.0
1	B	207	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	624	14/15	0.23	0.57	44,55,62,66	0
3	NAG	B	624	14/15	0.19	-0.56	53,65,68,75	0
3	NAG	B	625	14/15	0.33	-	82,87,89,90	0
3	NAG	A	625	14/15	0.28	-	73,78,80,81	0

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	627	14/15	0.32	3.05	58,68,70,72	0
2	NAG	A	630	14/15	0.35	2.88	67,76,79,80	0
5	SO4	B	5001	5/5	0.26	2.41	86,87,88,89	0
2	NAG	B	622	14/15	0.37	2.28	46,59,64,64	0
2	NAG	B	628	14/15	0.25	0.96	53,62,65,65	0
2	NAG	A	622	14/15	0.22	0.65	42,49,52,54	0
2	NAG	A	629	14/15	0.19	0.39	58,70,74,74	0
2	NAG	A	628	14/15	0.22	0.21	63,71,75,76	0
2	NAG	B	629	14/15	0.21	0.17	63,72,75,77	0
4	NDG	B	626	14/15	0.26	-0.01	64,73,80,81	0
2	NAG	A	626	14/15	0.22	-0.13	62,74,79,81	0
2	NAG	B	627	14/15	0.23	-0.28	59,69,73,74	0
2	NAG	B	623	14/15	0.21	-0.30	65,76,78,79	0
2	NAG	A	623	14/15	0.17	-1.34	65,75,77,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.