



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:13 PM UTC

PDB ID : 1HXK / pdb_00001hxx
Title : GOLGI ALPHA-MANNOSIDASE II IN COMPLEX WITH DEOXYMAN-
NOJIRIMICIN
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Deposited on : 2001-01-16
Resolution : 1.50 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

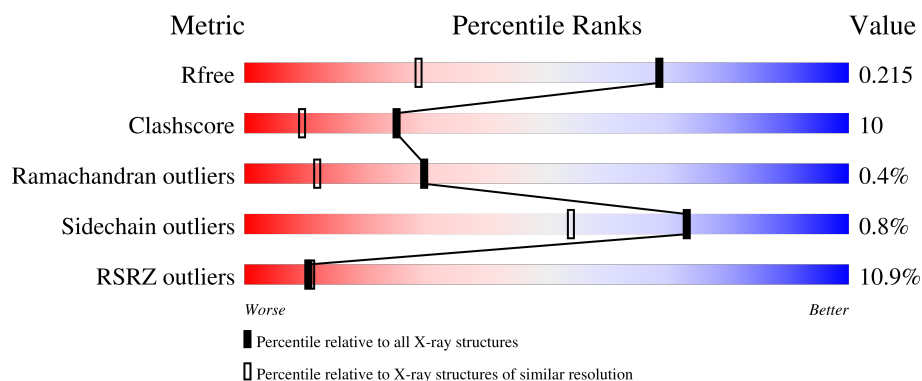
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	1015	11% 79% 20%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9198 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 ALPHA-MANNOSIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1014	Total	C	N	O	S	0	0	0
			8181	5202	1434	1506	39			

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

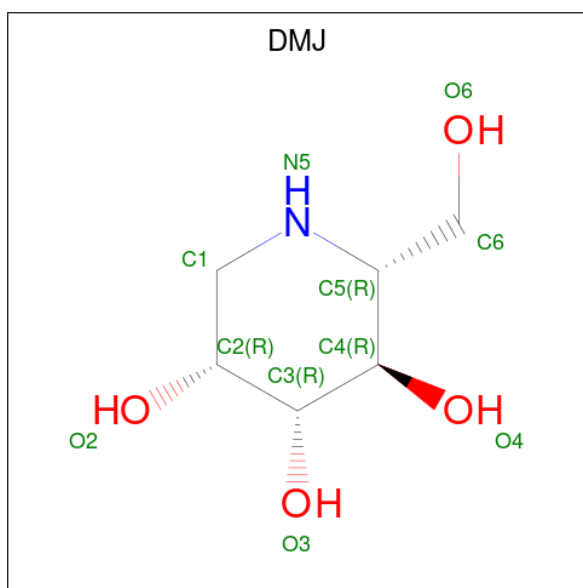


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

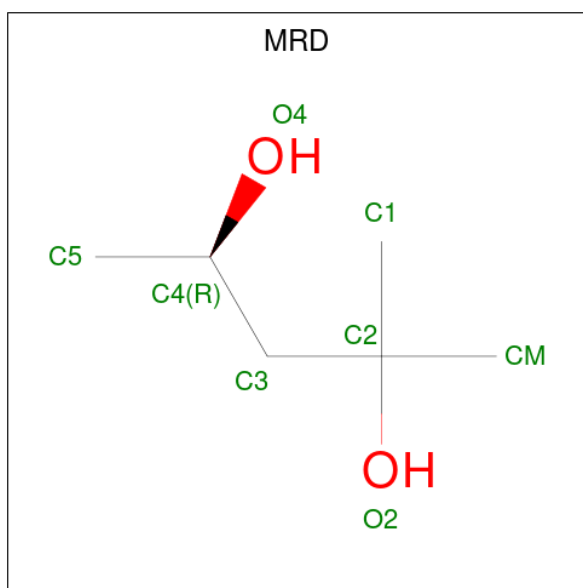
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 1-DEOXYMANNOJIRIMYCIN (CCD ID: DMJ) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



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

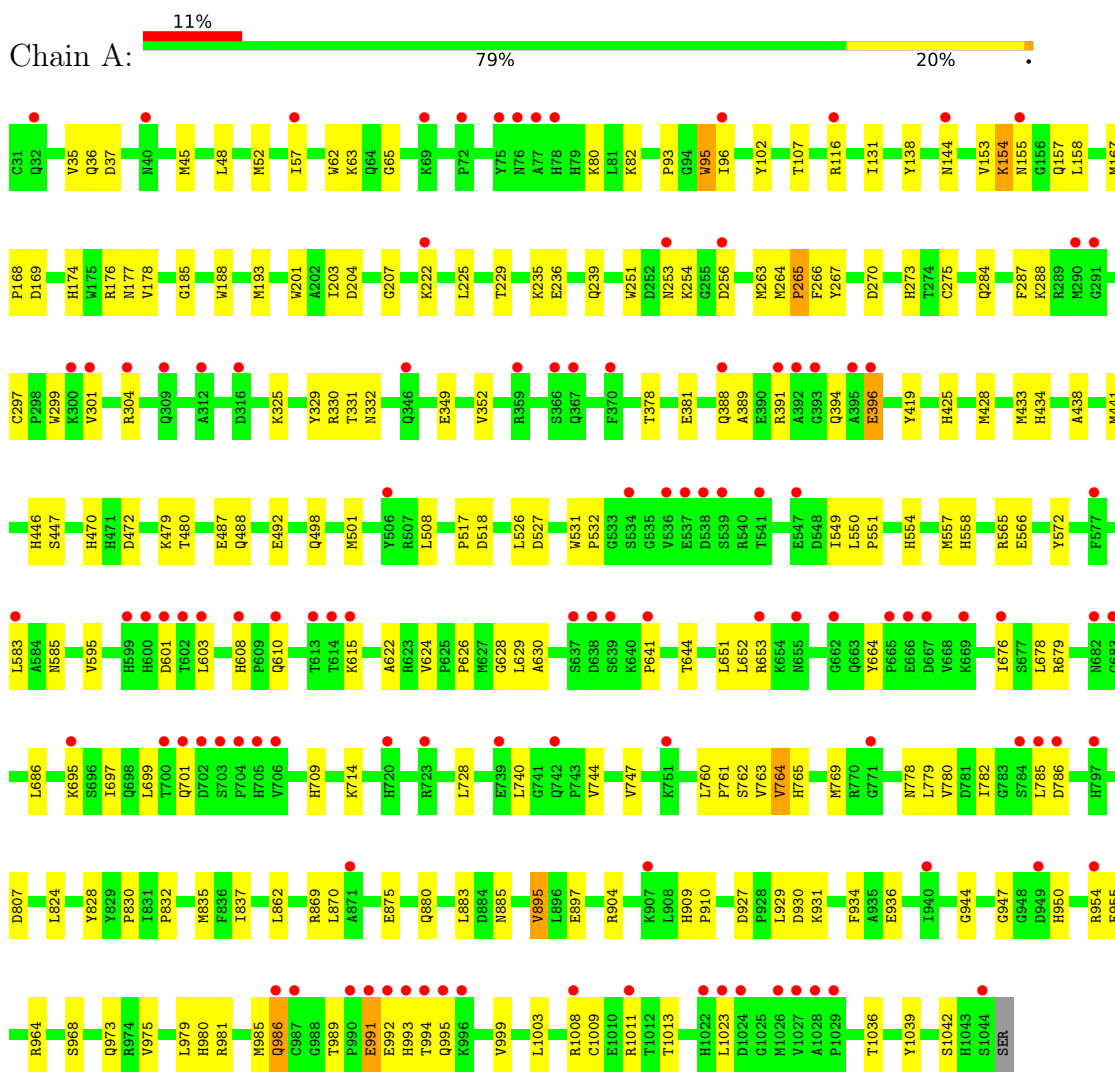
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	983	Total 983	O 983	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: ALPHA-MANNOSIDASE II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.81Å 109.62Å 138.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.90 – 1.50 85.90 – 1.50	Depositor EDS
% Data completeness (in resolution range)	87.0 (85.90-1.50) 87.0 (85.90-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.216 0.197 , 0.215	Depositor DCC
R_{free} test set	6888 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MRD, DMJ, ZN

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	0.34	0/8406	0.88	27/11416 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLY	N-CA-C	-8.99	103.41	111.95
1	A	664	TYR	CA-C-N	8.32	127.90	119.24
1	A	664	TYR	C-N-CA	8.32	127.90	119.24
1	A	169	ASP	N-CA-C	-6.97	100.87	110.35
1	A	45	MET	N-CA-C	6.68	119.39	111.71
1	A	107	THR	N-CA-C	6.62	119.34	111.33
1	A	168	PRO	N-CA-C	6.57	121.82	111.38
1	A	266	PHE	N-CA-C	6.56	119.39	109.95
1	A	35	VAL	N-CA-C	6.53	116.78	111.62
1	A	330	ARG	N-CA-C	6.24	120.96	113.23
1	A	447	SER	N-CA-C	-6.14	99.68	109.76
1	A	763	VAL	N-CA-C	6.13	116.66	108.27
1	A	517	PRO	N-CA-C	5.95	120.53	111.19
1	A	1013	THR	N-CA-C	-5.84	102.82	110.53
1	A	178	VAL	N-CA-C	-5.81	104.86	110.72
1	A	167	MET	N-CA-C	-5.69	96.36	108.66
1	A	36	GLN	N-CA-C	5.53	120.02	113.28
1	A	63	LYS	N-CA-C	5.50	117.99	111.33
1	A	267	TYR	N-CA-C	5.42	117.95	111.71
1	A	518	ASP	N-CA-C	-5.37	96.91	107.69
1	A	728	LEU	N-CA-C	5.30	118.86	109.96
1	A	955	GLU	N-CA-C	5.28	118.51	111.75
1	A	968	SER	N-CA-C	5.28	117.78	111.71
1	A	895	VAL	N-CA-C	5.18	115.04	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	764	VAL	N-CA-C	-5.16	99.83	107.51
1	A	875	GLU	N-CA-C	5.08	118.45	111.54
1	A	780	VAL	N-CA-C	5.03	115.34	107.99

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	8181	0	7971	156	0
2	A	14	0	13	0	0
3	A	1	0	0	0	0
4	A	11	0	12	2	0
5	A	8	0	14	3	0
6	A	983	0	0	51	0
All	All	9198	0	8010	158	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 10.

All (158) 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:297:CYS:HB3	6:A:1770:HOH:O	1.66	0.95
1:A:979:LEU:HD21	1:A:999:VAL:HG11	1.58	0.86
1:A:441:MET:HB3	6:A:1761:HOH:O	1.74	0.85
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.63	0.80
1:A:883:LEU:HD23	6:A:1615:HOH:O	1.83	0.77
1:A:824:LEU:HB2	6:A:2082:HOH:O	1.83	0.77
1:A:185:GLY:HA2	6:A:1631:HOH:O	1.85	0.76
1:A:904:ARG:HG2	1:A:985:MET:SD	2.26	0.75
1:A:641:PRO:HG2	1:A:644:THR:HB	1.67	0.74
1:A:630:ALA:HB3	6:A:1583:HOH:O	1.89	0.72
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:ARG:HG2	1:A:1042:SER:HB2	1.72	0.71
1:A:653:ARG:HD3	1:A:744:VAL:HG22	1.71	0.70
1:A:740:LEU:HD22	1:A:760:LEU:HD22	1.76	0.68
1:A:498:GLN:HE21	1:A:526:LEU:H	1.42	0.67
1:A:986:GLN:HG2	6:A:1267:HOH:O	1.93	0.67
1:A:954:ARG:HH12	1:A:981:ARG:HH21	1.43	0.66
1:A:155:ASN:HD21	1:A:157:GLN:HE21	1.41	0.66
1:A:284:GLN:HA	6:A:1688:HOH:O	1.95	0.66
1:A:869:ARG:HG2	6:A:1615:HOH:O	1.97	0.65
1:A:480:THR:H	1:A:880:GLN:HE22	1.45	0.65
1:A:572:TYR:CD2	1:A:615:LYS:HD3	2.33	0.64
1:A:947:GLY:HA3	6:A:1729:HOH:O	1.98	0.63
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.83	0.62
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.48	0.62
1:A:235:LYS:O	1:A:239:GLN:HG3	1.99	0.62
1:A:583:LEU:HD22	1:A:944:GLY:N	2.15	0.61
1:A:80:LYS:HE2	6:A:2001:HOH:O	2.00	0.60
1:A:203:ILE:HG12	6:A:1713:HOH:O	2.01	0.59
1:A:96:ILE:HA	1:A:479:LYS:HG3	1.82	0.59
1:A:153:VAL:HG22	1:A:158:LEU:HD12	1.83	0.59
1:A:765:HIS:HE1	6:A:1783:HOH:O	1.85	0.59
1:A:870:LEU:N	6:A:1615:HOH:O	2.35	0.58
1:A:628:GLY:HA2	6:A:1729:HOH:O	2.03	0.58
1:A:954:ARG:NH1	1:A:981:ARG:HH21	2.01	0.58
1:A:203:ILE:N	6:A:1713:HOH:O	2.28	0.57
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.87	0.57
1:A:201:TRP:CD1	6:A:1713:HOH:O	2.57	0.57
1:A:299:TRP:HB2	6:A:1770:HOH:O	2.03	0.57
1:A:699:LEU:HG	6:A:1646:HOH:O	2.05	0.56
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.88	0.55
1:A:551:PRO:HG2	6:A:1375:HOH:O	2.06	0.55
1:A:950:HIS:HE1	6:A:1788:HOH:O	1.89	0.55
1:A:679:ARG:HH12	1:A:701:GLN:CD	2.14	0.55
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.88	0.54
1:A:254:LYS:HD3	1:A:256:ASP:OD2	2.07	0.54
1:A:229:THR:HG21	1:A:263:MET:HE2	1.89	0.54
1:A:929:LEU:HD11	6:A:1542:HOH:O	2.08	0.54
1:A:154:LYS:HB3	1:A:154:LYS:NZ	2.22	0.54
1:A:678:LEU:HD12	1:A:769:MET:HE1	1.90	0.54
1:A:287:PHE:HB3	1:A:352:VAL:HG22	1.90	0.54
5:A:1104:MRD:H1C3	6:A:1871:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:GLN:HG3	6:A:1726:HOH:O	2.09	0.53
1:A:96:ILE:HG12	1:A:102:TYR:OH	2.08	0.53
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.92	0.53
1:A:116:ARG:HG3	6:A:1326:HOH:O	2.09	0.53
1:A:158:LEU:C	1:A:158:LEU:HD13	2.33	0.53
1:A:565:ARG:HG2	6:A:1542:HOH:O	2.09	0.53
1:A:325:LYS:HE2	6:A:1334:HOH:O	2.07	0.53
1:A:1009:CYS:SG	1:A:1023:LEU:HD12	2.49	0.53
1:A:378:THR:OG1	1:A:381:GLU:HG3	2.09	0.52
1:A:601:ASP:HB2	1:A:608:HIS:HE1	1.74	0.52
1:A:301:VAL:HG23	1:A:301:VAL:O	2.09	0.52
1:A:57:ILE:HD11	6:A:1586:HOH:O	2.10	0.52
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.92	0.52
1:A:470:HIS:CE1	1:A:472:ASP:HB2	2.45	0.52
1:A:624:VAL:HG22	6:A:1583:HOH:O	2.09	0.52
1:A:438:ALA:HA	6:A:1761:HOH:O	2.10	0.51
1:A:980:HIS:HE1	6:A:1184:HOH:O	1.92	0.51
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.41	0.51
1:A:299:TRP:HE3	6:A:1770:HOH:O	1.93	0.50
1:A:480:THR:HG23	6:A:1738:HOH:O	2.12	0.50
1:A:678:LEU:CD1	1:A:769:MET:HE1	2.42	0.50
1:A:992:GLU:O	1:A:994:THR:HG23	2.11	0.50
1:A:273:HIS:HE1	5:A:1104:MRD:O4	1.95	0.49
1:A:835:MET:HE2	1:A:862:LEU:HD22	1.93	0.49
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.42	0.49
1:A:583:LEU:HD22	1:A:944:GLY:CA	2.42	0.49
1:A:95:TRP:CZ3	4:A:1103:DMJ:H11	2.47	0.49
1:A:154:LYS:HB3	1:A:154:LYS:HZ3	1.76	0.49
1:A:441:MET:HE3	6:A:1715:HOH:O	2.12	0.48
1:A:695:LYS:HG3	1:A:709:HIS:CE1	2.48	0.48
1:A:531:TRP:HA	1:A:532:PRO:C	2.38	0.48
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.49	0.48
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.48	0.48
1:A:626:PRO:O	1:A:950:HIS:HD2	1.97	0.48
1:A:419:TYR:CE2	1:A:830:PRO:HG3	2.48	0.48
1:A:595:VAL:HG21	1:A:615:LYS:HG2	1.96	0.47
1:A:934:PHE:CE2	1:A:936:GLU:HB2	2.48	0.47
1:A:989:THR:HG22	1:A:991:GLU:HG3	1.95	0.47
1:A:807:ASP:CG	1:A:832:PRO:HG2	2.39	0.47
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.49	0.47
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLN:HG2	6:A:1637:HOH:O	2.15	0.47
1:A:425:HIS:HA	1:A:428:MET:HE3	1.96	0.46
1:A:472:ASP:OD2	4:A:1103:DMJ:O3	2.33	0.46
1:A:1008:ARG:CG	1:A:1042:SER:HB2	2.42	0.46
1:A:138:TYR:CE1	1:A:193:MET:HE1	2.51	0.46
1:A:488:GLN:O	1:A:492:GLU:HG3	2.16	0.46
1:A:601:ASP:HB2	1:A:608:HIS:CE1	2.49	0.46
1:A:48:LEU:HG	1:A:52:MET:SD	2.56	0.46
1:A:225:LEU:C	1:A:225:LEU:HD23	2.41	0.46
1:A:652:LEU:O	1:A:653:ARG:HB3	2.15	0.46
1:A:270:ASP:OD1	1:A:273:HIS:HD2	1.99	0.45
1:A:603:LEU:N	1:A:603:LEU:HD22	2.31	0.45
1:A:188:TRP:HB3	6:A:1631:HOH:O	2.16	0.45
1:A:653:ARG:HD3	1:A:744:VAL:CG2	2.42	0.45
1:A:761:PRO:O	1:A:762:SER:HB2	2.16	0.45
1:A:714:LYS:HD2	6:A:1630:HOH:O	2.17	0.45
1:A:389:ALA:O	1:A:394:GLN:HG2	2.17	0.45
1:A:869:ARG:HG3	1:A:885:ASN:ND2	2.32	0.45
1:A:782:ILE:O	1:A:785:LEU:HD13	2.17	0.45
1:A:144:ASN:HB3	6:A:1686:HOH:O	2.17	0.44
1:A:222:LYS:HD2	6:A:2066:HOH:O	2.16	0.44
1:A:764:VAL:HB	1:A:779:LEU:HB3	1.98	0.44
1:A:909:HIS:HA	1:A:910:PRO:HD3	1.87	0.44
1:A:264:MET:HE3	6:A:1532:HOH:O	2.17	0.44
1:A:558:HIS:CE1	6:A:1761:HOH:O	2.70	0.44
1:A:527:ASP:O	1:A:931:LYS:HE3	2.18	0.44
1:A:869:ARG:HG3	1:A:885:ASN:HD21	1.83	0.44
1:A:883:LEU:CD2	6:A:1615:HOH:O	2.53	0.44
1:A:251:TRP:C	1:A:251:TRP:CD1	2.95	0.44
1:A:554:HIS:HE1	6:A:2004:HOH:O	2.01	0.44
1:A:396:GLU:OE1	1:A:396:GLU:N	2.47	0.43
1:A:155:ASN:C	1:A:155:ASN:OD1	2.60	0.43
1:A:786:ASP:HB3	6:A:2065:HOH:O	2.18	0.43
1:A:425:HIS:ND1	1:A:428:MET:HE1	2.33	0.43
1:A:1011:ARG:NH2	6:A:1744:HOH:O	2.52	0.43
1:A:331:THR:HA	1:A:394:GLN:HE21	1.83	0.43
1:A:549:ILE:HG23	1:A:550:LEU:N	2.34	0.43
1:A:389:ALA:HB1	1:A:394:GLN:CD	2.43	0.43
1:A:446:HIS:HE1	1:A:508:LEU:HD23	1.84	0.43
1:A:837:ILE:HG23	1:A:862:LEU:HD21	2.01	0.43
1:A:82:LYS:HG3	6:A:1771:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:MET:HE1	1:A:487:GLU:HG3	2.01	0.42
1:A:188:TRP:CB	6:A:1631:HOH:O	2.67	0.42
1:A:332:ASN:H	1:A:394:GLN:HE22	1.68	0.42
1:A:301:VAL:CG2	6:A:1220:HOH:O	2.68	0.42
1:A:1039:TYR:HE2	6:A:1744:HOH:O	2.02	0.42
1:A:558:HIS:HA	1:A:629:LEU:HD23	2.01	0.41
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.85	0.41
1:A:48:LEU:HD11	1:A:236:GLU:HG2	2.02	0.41
5:A:1104:MRD:H1C1	6:A:2049:HOH:O	2.20	0.41
1:A:37:ASP:HB3	1:A:253:ASN:ND2	2.35	0.41
1:A:177:ASN:HD21	1:A:433:MET:HB2	1.84	0.41
1:A:434:HIS:CD2	1:A:927:ASP:HA	2.55	0.41
1:A:498:GLN:NE2	1:A:526:LEU:H	2.14	0.41
1:A:807:ASP:OD1	1:A:832:PRO:HG2	2.20	0.41
1:A:954:ARG:NH1	1:A:981:ARG:NH2	2.69	0.41
1:A:566:GLU:HA	1:A:622:ALA:O	2.21	0.41
1:A:676:ILE:HD13	1:A:747:VAL:HG21	2.02	0.41
1:A:438:ALA:HB1	1:A:501:MET:HE3	2.03	0.41
1:A:824:LEU:C	1:A:824:LEU:HD23	2.45	0.41
1:A:557:MET:HA	1:A:930:ASP:O	2.20	0.40
1:A:288:LYS:HD2	1:A:349:GLU:CD	2.46	0.40
1:A:131:ILE:HD11	6:A:1722:HOH:O	2.21	0.40
1:A:388:GLN:CG	1:A:391:ARG:HH21	2.34	0.40
1:A:265:PRO:HD3	1:A:329:TYR:OH	2.21	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	1012/1015 (100%)	975 (96%)	33 (3%)	4 (0%)	30 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	993	HIS
1	A	991	GLU
1	A	204	ASP

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	901/902 (100%)	894 (99%)	7 (1%)	73	54

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	A	265	PRO
1	A	275	CYS
1	A	396	GLU
1	A	585	ASN
1	A	828	TYR
1	A	986	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	79	HIS
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	240	GLN
1	A	273	HIS
1	A	309	GLN
1	A	346	GLN

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Mol	Chain	Res	Type
1	A	347	ASN
1	A	367	GLN
1	A	394	GLN
1	A	434	HIS
1	A	460	GLN
1	A	470	HIS
1	A	488	GLN
1	A	498	GLN
1	A	554	HIS
1	A	599	HIS
1	A	608	HIS
1	A	682	ASN
1	A	698	GLN
1	A	720	HIS
1	A	765	HIS
1	A	778	ASN
1	A	812	GLN
1	A	866	GLN
1	A	880	GLN
1	A	885	ASN
1	A	919	HIS
1	A	923	GLN
1	A	937	ASN
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	986	GLN
1	A	993	HIS
1	A	995	GLN
1	A	1018	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	DMJ	A	1103	3	11,11,11	1.72	2 (18%)	13,15,15	1.38	2 (15%)
2	NAG	A	1101	1	14,14,15	0.51	0	17,19,21	0.69	1 (5%)
5	MRD	A	1104	-	7,7,7	0.47	0	9,10,10	0.33	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
4	DMJ	A	1103	3	-	1/2/19/19	0/1/1/1
2	NAG	A	1101	1	-	2/6/23/26	0/1/1/1
5	MRD	A	1104	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	DMJ	C2-C3	4.50	1.59	1.52
4	A	1103	DMJ	C1-N5	2.50	1.50	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	DMJ	C1-N5-C5	2.85	115.96	109.71
4	A	1103	DMJ	O6-C6-C5	2.79	117.85	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	NAG	C8-C7-N2-C2
2	A	1101	NAG	O7-C7-N2-C2
4	A	1103	DMJ	N5-C5-C6-O6
5	A	1104	MRD	C2-C3-C4-O4
5	A	1104	MRD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	DMJ	2	0
5	A	1104	MRD	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1014/1015 (99%)	0.54	111 (10%)	10 11	6, 14, 27, 47	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	7.3
1	A	290	MET	6.3
1	A	583	LEU	5.9
1	A	682	ASN	5.2
1	A	991	GLU	5.0
1	A	720	HIS	5.0
1	A	702	ASP	4.4
1	A	301	VAL	4.4
1	A	75	TYR	4.2
1	A	994	THR	4.2
1	A	600	HIS	4.2
1	A	1024	ASP	4.1
1	A	990	PRO	4.1
1	A	986	GLN	4.0
1	A	638	ASP	3.9
1	A	601	ASP	3.8
1	A	1026	MET	3.8
1	A	1008	ARG	3.8
1	A	538	ASP	3.7
1	A	701	GLN	3.6
1	A	537	GLU	3.6
1	A	116	ARG	3.6
1	A	992	GLU	3.6
1	A	76	ASN	3.5
1	A	785	LEU	3.4
1	A	704	PRO	3.4
1	A	703	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLY	3.3
1	A	534	SER	3.3
1	A	602	THR	3.2
1	A	396	GLU	3.2
1	A	641	PRO	3.1
1	A	653	ARG	3.1
1	A	1023	LEU	3.0
1	A	547	GLU	3.0
1	A	614	THR	3.0
1	A	1027	VAL	3.0
1	A	78	HIS	3.0
1	A	669	LYS	3.0
1	A	1044	SER	2.9
1	A	393	GLY	2.9
1	A	599	HIS	2.9
1	A	676	ILE	2.9
1	A	536	VAL	2.9
1	A	665	PRO	2.8
1	A	723	ARG	2.8
1	A	155	ASN	2.8
1	A	655	ASN	2.7
1	A	706	VAL	2.7
1	A	615	LYS	2.7
1	A	797	HIS	2.7
1	A	637	SER	2.7
1	A	253	ASN	2.6
1	A	1022	HIS	2.6
1	A	739	GLU	2.6
1	A	954	ARG	2.6
1	A	144	ASN	2.6
1	A	995	GLN	2.6
1	A	784	SER	2.6
1	A	1028	ALA	2.6
1	A	700	THR	2.6
1	A	603	LEU	2.6
1	A	667	ASP	2.5
1	A	300	LYS	2.5
1	A	32	GLN	2.5
1	A	541	THR	2.5
1	A	639	SER	2.5
1	A	695	LYS	2.5
1	A	304	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	256	ASP	2.5
1	A	395	ALA	2.4
1	A	666	GLU	2.4
1	A	392	ALA	2.4
1	A	367	GLN	2.4
1	A	388	GLN	2.3
1	A	40	ASN	2.3
1	A	786	ASP	2.3
1	A	742	GLN	2.3
1	A	346	GLN	2.3
1	A	610	GLN	2.3
1	A	987	CYS	2.3
1	A	309	GLN	2.3
1	A	57	ILE	2.3
1	A	871	ALA	2.2
1	A	949	ASP	2.2
1	A	608	HIS	2.2
1	A	662	GLY	2.2
1	A	996	LYS	2.2
1	A	391	ARG	2.2
1	A	69	LYS	2.2
1	A	683	GLY	2.2
1	A	1011	ARG	2.2
1	A	539	SER	2.1
1	A	771	GLY	2.1
1	A	613	THR	2.1
1	A	907	LYS	2.1
1	A	370	PHE	2.1
1	A	577	PHE	2.1
1	A	72	PRO	2.1
1	A	312	ALA	2.1
1	A	940	ILE	2.1
1	A	705	HIS	2.1
1	A	359	ARG	2.1
1	A	366	SER	2.1
1	A	1029	PRO	2.1
1	A	751	LYS	2.0
1	A	77	ALA	2.0
1	A	96	ILE	2.0
1	A	316	ASP	2.0
1	A	222	LYS	2.0
1	A	506	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	1101	14/15	0.69	0.19	45,50,53,55	0
4	DMJ	A	1103	11/11	0.87	0.13	15,17,18,18	0
5	MRD	A	1104	8/8	0.88	0.11	17,18,19,19	0
3	ZN	A	1102	1/1	1.00	0.02	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.