



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:49 AM UTC

PDB ID : 2OW6 / pdb_00002ow6
Title : Golgi alpha-mannosidase II complex with (1r,5s,6s,7r,8s)-1-thioniabicyclo[4.3.0]nonan-5,7,8-triol chloride
Authors : Kuntz, D.A.
Deposited on : 2007-02-15
Resolution : 1.19 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

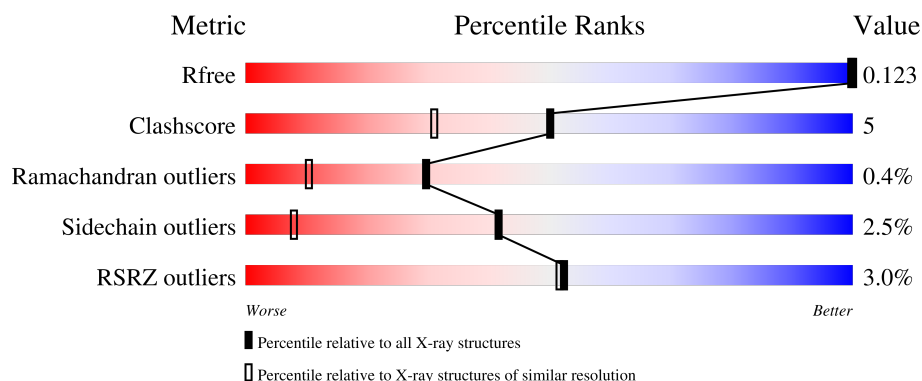
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

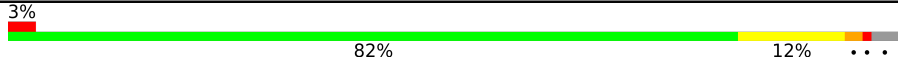
The reported resolution of this entry is 1.19 Å.

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	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	1045	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9888 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.

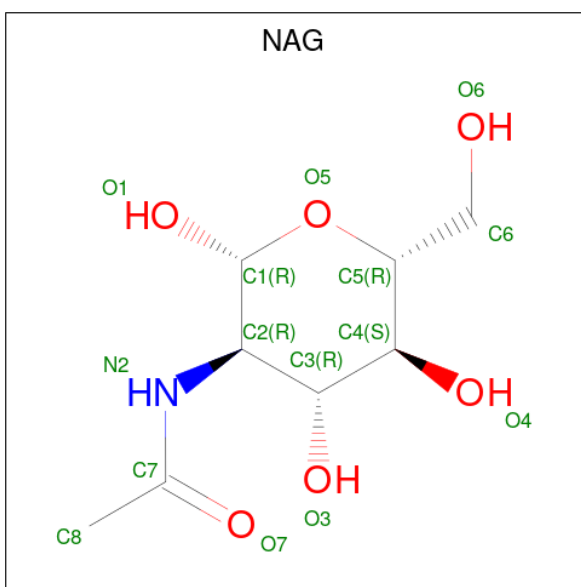
- Molecule 1 is a protein called Alpha-mannosidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	0	31	0
			8377	5336	1461	1536	44			

There are 13 discrepancies between the modelled and reference sequences:

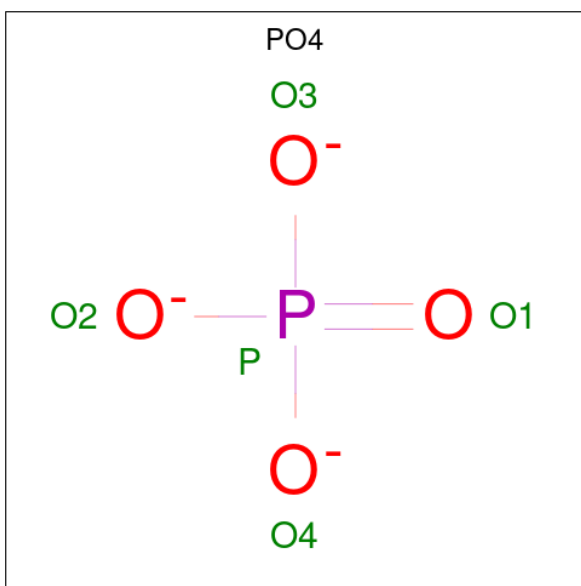
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	expression tag	UNP Q24451
A	2	SER	-	expression tag	UNP Q24451
A	3	SER	-	expression tag	UNP Q24451
A	4	HIS	-	expression tag	UNP Q24451
A	5	HIS	-	expression tag	UNP Q24451
A	6	HIS	-	expression tag	UNP Q24451
A	7	HIS	-	expression tag	UNP Q24451
A	8	HIS	-	expression tag	UNP Q24451
A	9	HIS	-	expression tag	UNP Q24451
A	10	GLY	-	expression tag	UNP Q24451
A	11	GLU	-	expression tag	UNP Q24451
A	12	PHE	-	expression tag	UNP Q24451
A	907	LYS	GLU	conflict	UNP Q24451

- 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 PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

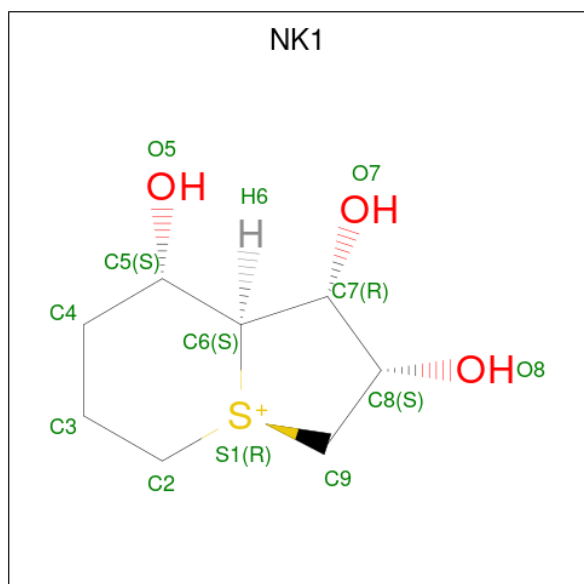


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

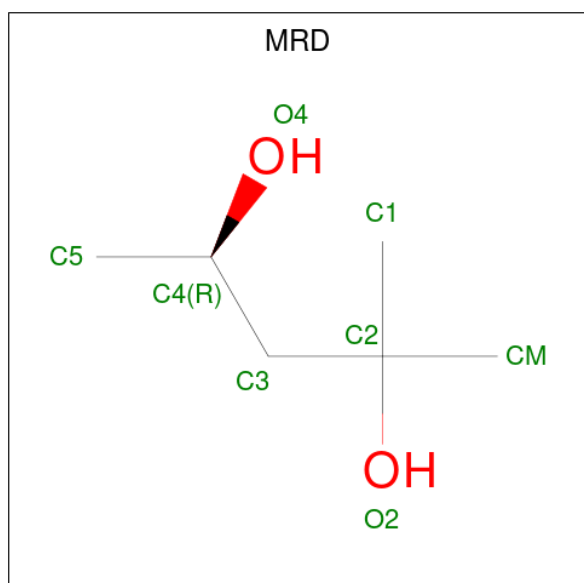
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (1R,5S,6S,7R,8S)-1-THIONIABICYCLO[4.3.0]NONAN-5,7,8-TRIOL (CCD ID: NK1) (formula: $C_8H_{15}O_3S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			12	8	3	1		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



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

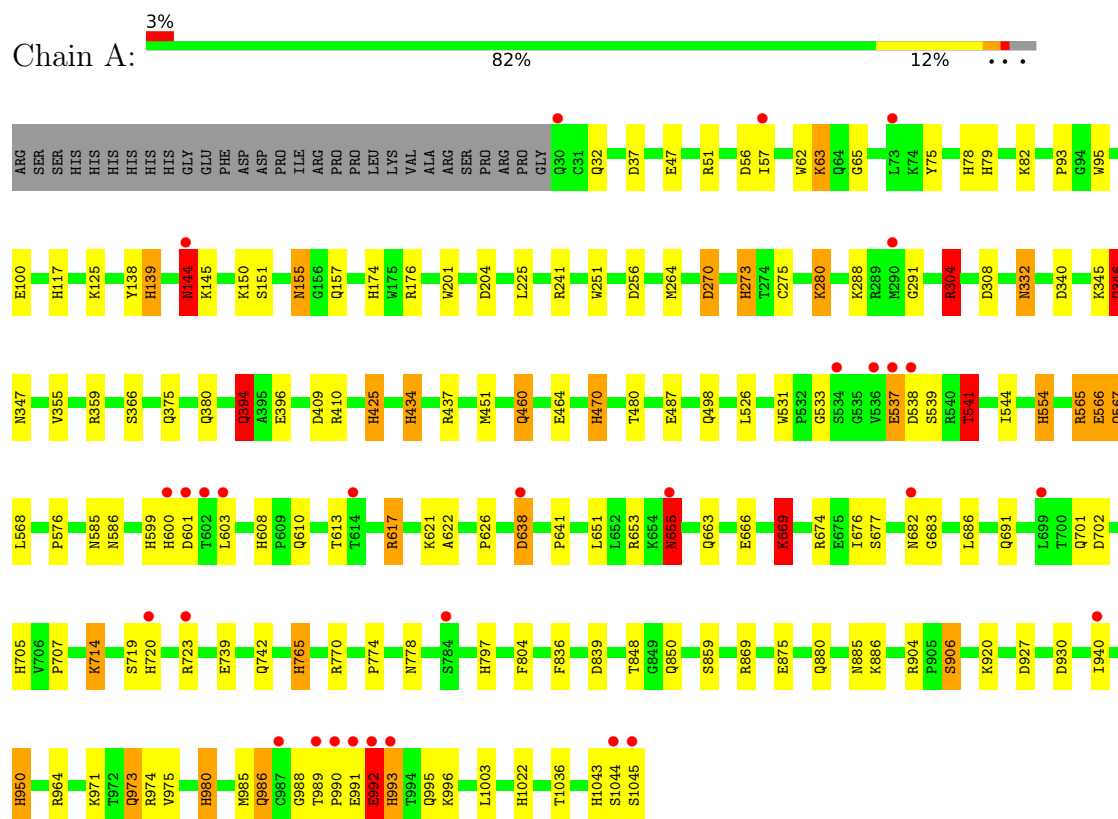
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1462	Total	O	0	4
			1466	1466		

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 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.01Å 109.62Å 138.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.19 30.00 – 1.19	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-1.19) 93.6 (30.00-1.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.19Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.118 , 0.150 0.122 , 0.123	Depositor DCC
R_{free} test set	5008 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 66.7	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	0.98	EDS
Total number of atoms	9888	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAG, NK1, ZN, MRD

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	0.94	3/8680 (0.0%)	1.40	114/11781 (1.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	LYS	C-O	-6.28	1.18	1.23
1	A	974	ARG	N-CA	-6.13	1.38	1.46
1	A	139	HIS	CD2-NE2	5.14	1.43	1.37

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	691	GLN	OE1-CD-NE2	12.29	134.90	122.60
1	A	144	ASN	CA-CB-CG	12.26	124.86	112.60
1	A	638	ASP	CA-CB-CG	-11.36	101.24	112.60
1	A	410	ARG	NE-CZ-NH2	-9.73	110.44	119.20
1	A	437	ARG	NE-CZ-NH1	-9.25	112.25	121.50
1	A	576	PRO	CA-C-N	8.94	135.28	122.05
1	A	576	PRO	C-N-CA	8.94	135.28	122.05
1	A	291	GLY	O-C-N	-8.68	111.41	122.70
1	A	600	HIS	N-CA-CB	8.50	123.02	110.35
1	A	78	HIS	CA-CB-CG	-8.46	105.34	113.80
1	A	155	ASN	OD1-CG-ND2	-8.14	114.46	122.60
1	A	533	GLY	O-C-N	8.11	129.46	122.64
1	A	394	GLN	CG-CD-NE2	-8.04	104.33	116.40
1	A	836	PHE	CA-CB-CG	7.83	121.63	113.80
1	A	691	GLN	CB-CG-CD	-7.39	100.04	112.60
1	A	980	HIS	CB-CG-CD2	-7.33	121.67	131.20
1	A	410	ARG	NH1-CZ-NH2	7.32	128.81	119.30
1	A	993	HIS	CA-CB-CG	7.15	120.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	PRO	O-C-N	-7.15	112.58	122.37
1	A	992	GLU	O-C-N	7.14	132.09	122.59
1	A	201	TRP	CA-CB-CG	7.09	127.08	113.60
1	A	347	ASN	OD1-CG-ND2	7.09	129.69	122.60
1	A	986	GLN	CA-C-O	-7.06	112.62	120.60
1	A	585	ASN	OD1-CG-ND2	7.05	129.65	122.60
1	A	669	LYS	CA-CB-CG	6.93	127.95	114.10
1	A	683	GLY	O-C-N	6.91	128.68	121.77
1	A	973	GLN	CA-C-N	6.80	133.75	122.33
1	A	973	GLN	C-N-CA	6.80	133.75	122.33
1	A	974	ARG	NE-CZ-NH2	-6.77	113.10	119.20
1	A	839	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	340	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	613	THR	O-C-N	-6.69	114.31	122.34
1	A	470	HIS	CB-CG-CD2	-6.64	122.56	131.20
1	A	538	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	425	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	531	TRP	CE3-CZ3-CH2	6.54	129.60	121.10
1	A	980	HIS	CB-CG-ND1	6.53	132.50	122.70
1	A	655	ASN	CB-CA-C	-6.50	104.60	110.71
1	A	682	ASN	O-C-N	6.45	130.28	122.35
1	A	464	GLU	CB-CG-CD	6.42	123.52	112.60
1	A	531	TRP	CZ3-CH2-CZ2	-6.40	113.17	121.50
1	A	409	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	973	GLN	O-C-N	-6.37	115.76	122.96
1	A	875	GLU	CB-CG-CD	6.26	123.23	112.60
1	A	993	HIS	CA-C-N	-6.24	112.34	122.82
1	A	993	HIS	C-N-CA	-6.24	112.34	122.82
1	A	989	THR	O-C-N	6.22	126.27	121.23
1	A	308	ASP	CA-C-N	6.15	129.66	120.31
1	A	308	ASP	C-N-CA	6.15	129.66	120.31
1	A	151	SER	N-CA-CB	6.11	119.20	110.16
1	A	100	GLU	CA-C-N	6.10	128.37	120.44
1	A	100	GLU	C-N-CA	6.10	128.37	120.44
1	A	586	ASN	CA-CB-CG	6.10	118.70	112.60
1	A	394	GLN	CB-CA-C	6.07	121.37	109.72
1	A	251	TRP	CD2-CE2-CZ2	6.06	128.46	122.40
1	A	460	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	A	304	ARG	CD-NE-CZ	6.02	132.83	124.40
1	A	63	LYS	CG-CD-CE	5.98	125.05	111.30
1	A	56	ASP	CA-C-N	-5.91	113.95	122.45
1	A	56	ASP	C-N-CA	-5.91	113.95	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	GLY	CA-C-O	-5.87	113.13	121.52
1	A	950	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	A	273	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	155	ASN	CB-CG-ND2	5.75	125.03	116.40
1	A	950	HIS	CA-CB-CG	5.72	119.52	113.80
1	A	676	ILE	CA-CB-CG2	5.71	120.22	110.50
1	A	765	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	A	380	GLN	OE1-CD-NE2	5.68	128.28	122.60
1	A	437	ARG	CD-NE-CZ	5.66	132.32	124.40
1	A	566	GLU	CB-CG-CD	-5.63	103.03	112.60
1	A	75	TYR	O-C-N	5.57	130.18	123.16
1	A	702	ASP	CA-CB-CG	-5.57	107.03	112.60
1	A	567	GLN	CB-CG-CD	5.57	122.06	112.60
1	A	669	LYS	CB-CG-CD	5.56	124.08	111.30
1	A	950	HIS	CB-CG-ND1	5.55	131.03	122.70
1	A	613	THR	CA-C-N	5.55	131.57	121.41
1	A	613	THR	C-N-CA	5.55	131.57	121.41
1	A	682	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	617	ARG	CA-CB-CG	5.50	125.11	114.10
1	A	674	ARG	CD-NE-CZ	5.50	132.09	124.40
1	A	610	GLN	CB-CG-CD	5.46	121.88	112.60
1	A	396	GLU	CB-CG-CD	5.46	121.87	112.60
1	A	974	ARG	CD-NE-CZ	5.45	132.03	124.40
1	A	554	HIS	CB-CG-ND1	5.41	130.81	122.70
1	A	565	ARG	CB-CG-CD	5.41	123.73	111.30
1	A	682	ASN	OD1-CG-ND2	5.40	128.00	122.60
1	A	100	GLU	O-C-N	-5.34	116.07	122.15
1	A	1043	HIS	CA-CB-CG	-5.34	108.46	113.80
1	A	554	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	567	GLN	CA-CB-CG	5.27	124.64	114.10
1	A	117	HIS	ND1-CE1-NE2	5.24	113.64	108.40
1	A	719	SER	CA-C-O	-5.23	113.23	119.35
1	A	537	GLU	CA-C-N	-5.22	115.05	122.41
1	A	537	GLU	C-N-CA	-5.22	115.05	122.41
1	A	332	ASN	CA-C-N	5.22	130.04	123.10
1	A	332	ASN	C-N-CA	5.22	130.04	123.10
1	A	974	ARG	NH1-CZ-NH2	5.22	126.08	119.30
1	A	859	SER	O-C-N	-5.21	116.80	123.06
1	A	600	HIS	O-C-N	5.20	129.28	122.68
1	A	641	PRO	CB-CA-C	-5.20	104.14	110.95
1	A	544	ILE	CB-CG1-CD1	5.17	124.65	113.80
1	A	541	THR	CA-CB-CG2	5.15	119.26	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	705	HIS	CB-CG-CD2	5.14	137.88	131.20
1	A	610	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	394	GLN	CB-CG-CD	5.12	121.30	112.60
1	A	1022	HIS	CA-CB-CG	5.11	118.91	113.80
1	A	434	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	600	HIS	CA-CB-CG	-5.09	108.71	113.80
1	A	804	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	1044	SER	O-C-N	5.05	129.04	122.42
1	A	599	HIS	CA-CB-CG	-5.03	108.77	113.80
1	A	346	GLN	CG-CD-NE2	5.03	123.94	116.40
1	A	603	LEU	O-C-N	-5.02	114.90	122.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8377	0	8225	87	0
2	A	14	0	13	0	0
3	A	10	0	0	0	0
4	A	1	0	0	0	0
5	A	12	0	14	0	0
6	A	8	0	14	3	0
7	A	1466	0	0	47	0
All	All	9888	0	8266	89	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 5.

All (89) 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:155:ASN:HD21	1:A:157:GLN:HE21	1.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.33	0.77
6:A:5001:MRD:H1C1	7:A:5645:HOH:O	1.85	0.75
1:A:742[A]:GLN:HG3	7:A:5205:HOH:O	1.89	0.72
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.73	0.71
1:A:655:ASN:HB2	7:A:6243:HOH:O	1.90	0.71
1:A:47:GLU:OE2	1:A:51:ARG:HD3	1.93	0.68
1:A:375:GLN:HG3	7:A:6433:HOH:O	1.93	0.68
1:A:82:LYS:HG3	7:A:6181:HOH:O	1.95	0.67
1:A:79:HIS:HE1	7:A:5673:HOH:O	1.79	0.66
6:A:5001:MRD:H1C3	7:A:5646:HOH:O	1.97	0.65
1:A:57:ILE:HD11	7:A:6056:HOH:O	1.96	0.64
1:A:498:GLN:HE21	1:A:526:LEU:H	1.44	0.64
1:A:225:LEU:HD21	1:A:264[B]:MET:SD	2.38	0.64
1:A:346:GLN:HE21	1:A:346:GLN:H	1.46	0.64
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.81	0.62
1:A:241:ARG:HD3	7:A:6438:HOH:O	1.99	0.62
1:A:950:HIS:HE1	7:A:5329:HOH:O	1.83	0.61
1:A:332:ASN:H	1:A:394:GLN:HE22	1.48	0.60
1:A:273:HIS:HE1	6:A:5001:MRD:O4	1.84	0.60
1:A:980:HIS:HE1	7:A:5799:HOH:O	1.84	0.60
1:A:537:GLU:OE2	1:A:539:SER:HB3	2.00	0.60
1:A:904:ARG:HG2	1:A:985[A]:MET:SD	2.42	0.60
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.85	0.59
1:A:990:PRO:O	1:A:992:GLU:HG2	2.02	0.59
1:A:138:TYR:OH	1:A:150:LYS:HE2	2.02	0.59
1:A:988:GLY:O	1:A:990:PRO:HD3	2.02	0.59
1:A:669:LYS:HE2	7:A:6180:HOH:O	2.03	0.58
1:A:739:GLU:HG2	7:A:6337:HOH:O	2.04	0.58
1:A:765:HIS:HE1	7:A:5398:HOH:O	1.87	0.57
1:A:480:THR:H	1:A:880:GLN:HE22	1.53	0.57
1:A:986:GLN:HG3	7:A:5089:HOH:O	2.06	0.55
1:A:567:GLN:HB2	7:A:6383:HOH:O	2.06	0.55
1:A:626:PRO:O	1:A:950:HIS:HD2	1.90	0.54
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.90	0.54
1:A:720:HIS:C	1:A:723:ARG:HH21	2.16	0.54
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.43	0.53
1:A:125:LYS:HE2	7:A:5050:HOH:O	2.09	0.53
1:A:707:PRO:HG2	1:A:797[A]:HIS:CE1	2.44	0.53
1:A:995:GLN:HG3	7:A:5347:HOH:O	2.09	0.53
1:A:270:ASP:OD1	1:A:273:HIS:HD2	1.91	0.53
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:THR:HG23	7:A:5235:HOH:O	2.08	0.52
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.40	0.52
1:A:150:LYS:HD3	7:A:5552:HOH:O	2.09	0.52
1:A:568:LEU:HD12	1:A:770[A]:ARG:HD3	1.93	0.51
1:A:366:SER:HB3	7:A:6458:HOH:O	2.10	0.51
1:A:139:HIS:CD2	7:A:6202:HOH:O	2.65	0.50
1:A:139:HIS:HD2	7:A:6202:HOH:O	1.94	0.50
1:A:992:GLU:OE1	1:A:992:GLU:HA	2.13	0.49
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.47	0.49
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.48	0.48
1:A:155:ASN:ND2	1:A:157:GLN:HE21	2.00	0.48
1:A:332:ASN:H	1:A:394:GLN:NE2	2.11	0.48
1:A:971:LYS:HB2	1:A:971:LYS:NZ	2.28	0.48
1:A:617:ARG:HD2	7:A:5408:HOH:O	2.13	0.48
1:A:686:LEU:HD11	1:A:774:PRO:HG3	1.97	0.47
1:A:886:LYS:NZ	7:A:6117:HOH:O	2.48	0.46
1:A:288:LYS:NZ	7:A:6424:HOH:O	2.47	0.46
1:A:82:LYS:HE3	7:A:6181:HOH:O	2.15	0.46
1:A:567:GLN:HB2	7:A:6437:HOH:O	2.16	0.46
1:A:37:ASP:HB2	7:A:6259:HOH:O	2.15	0.46
1:A:304:ARG:NH2	7:A:5765:HOH:O	2.49	0.46
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.98	0.46
1:A:770[A]:ARG:NH2	7:A:5385:HOH:O	2.50	0.45
1:A:996:LYS:HE3	7:A:6318:HOH:O	2.16	0.45
1:A:256:ASP:HB2	7:A:5156:HOH:O	2.16	0.45
1:A:460:GLN:NE2	7:A:6406:HOH:O	2.50	0.45
1:A:280:LYS:HD2	7:A:6170:HOH:O	2.16	0.45
1:A:498:GLN:NE2	1:A:526:LEU:H	2.11	0.45
1:A:621:LYS:NZ	7:A:6177:HOH:O	2.50	0.44
1:A:714:LYS:NZ	7:A:5218:HOH:O	2.50	0.44
1:A:920:LYS:HG3	7:A:5374:HOH:O	2.17	0.44
1:A:848[B]:THR:HG22	1:A:850:GLN:H	1.83	0.43
1:A:714:LYS:NZ	7:A:5219:HOH:O	2.51	0.43
1:A:32:GLN:NE2	7:A:5156:HOH:O	2.51	0.43
1:A:885:ASN:ND2	1:A:885:ASN:H	2.17	0.43
1:A:601:ASP:HB2	1:A:608:HIS:CE1	2.55	0.42
1:A:355:VAL:O	1:A:359[B]:ARG:HG3	2.20	0.42
1:A:655:ASN:HB2	7:A:6141:HOH:O	2.19	0.42
1:A:663[A]:GLN:NE2	7:A:6105:HOH:O	2.49	0.42
1:A:720:HIS:CE1	7:A:5990:HOH:O	2.72	0.42
1:A:990:PRO:O	1:A:992:GLU:OE2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:OD1	1:A:145:LYS:HG2	2.21	0.41
1:A:554:HIS:HE1	7:A:5266:HOH:O	2.03	0.41
1:A:145:LYS:HE2	7:A:5875:HOH:O	2.19	0.41
1:A:554:HIS:HD2	7:A:5271:HOH:O	2.04	0.40
1:A:566:GLU:HA	1:A:622:ALA:O	2.21	0.40
1:A:906:SER:HB3	7:A:6238:HOH:O	2.20	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	1045/1045 (100%)	1017 (97%)	24 (2%)	4 (0%)	30	10

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	933/929 (100%)	909 (97%)	24 (3%)	40 7

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	144	ASN
1	A	275	CYS
1	A	280	LYS
1	A	304	ARG
1	A	346	GLN
1	A	394	GLN
1	A	451	MET
1	A	541	THR
1	A	565	ARG
1	A	638	ASP
1	A	651	LEU
1	A	653	ARG
1	A	655	ASN
1	A	666[A]	GLU
1	A	666[B]	GLU
1	A	669	LYS
1	A	677	SER
1	A	701	GLN
1	A	714	LYS
1	A	906	SER
1	A	940	ILE
1	A	992	GLU
1	A	1045	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	240	GLN
1	A	273	HIS
1	A	346	GLN
1	A	347	ASN
1	A	367	GLN

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Mol	Chain	Res	Type
1	A	371	ASN
1	A	394	GLN
1	A	425	HIS
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	600	HIS
1	A	608	HIS
1	A	610	GLN
1	A	655	ASN
1	A	701	GLN
1	A	765	HIS
1	A	812	GLN
1	A	880	GLN
1	A	885	ASN
1	A	919	HIS
1	A	923	GLN
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	993	HIS
1	A	1005	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

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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
2	NAG	A	2001	1	14,14,15	0.81	0	17,19,21	1.54	2 (11%)
3	PO4	A	2003	-	4,4,4	1.73	2 (50%)	6,6,6	0.64	0
5	NK1	A	4001	4	10,13,13	0.80	0	10,19,19	1.49	2 (20%)
6	MRD	A	5001	-	7,7,7	0.81	0	9,10,10	1.41	2 (22%)
3	PO4	A	2002	-	4,4,4	2.06	2 (50%)	6,6,6	0.58	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
6	MRD	A	5001	-	-	2/5/5/5	-
2	NAG	A	2001	1	-	4/6/23/26	0/1/1/1
5	NK1	A	4001	4	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002	PO4	P-O3	2.95	1.63	1.54
3	A	2002	PO4	P-O4	-2.63	1.47	1.54
3	A	2003	PO4	P-O3	2.18	1.61	1.54
3	A	2003	PO4	P-O2	2.11	1.60	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NAG	C1-C2-N2	-3.70	104.60	110.43
5	A	4001	NK1	C4-C5-C6	3.39	114.83	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NAG	C4-C3-C2	3.29	115.84	111.02
6	A	5001	MRD	CM-C2-C1	-2.56	104.89	110.63
5	A	4001	NK1	C2-S1-C9	2.33	105.14	100.28
6	A	5001	MRD	O2-C2-C3	2.26	117.74	109.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	NAG	C8-C7-N2-C2
2	A	2001	NAG	O7-C7-N2-C2
6	A	5001	MRD	C2-C3-C4-O4
6	A	5001	MRD	C2-C3-C4-C5
2	A	2001	NAG	O5-C5-C6-O6
2	A	2001	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5001	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

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	1016/1045 (97%)	0.03	30 (2%) 52 52	8, 17, 37, 84	31 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	603	LEU	4.8
1	A	990	PRO	4.8
1	A	720	HIS	3.7
1	A	987	CYS	3.7
1	A	993	HIS	3.5
1	A	991	GLU	3.3
1	A	655	ASN	3.1
1	A	602	THR	3.1
1	A	638	ASP	2.9
1	A	784	SER	2.9
1	A	992	GLU	2.9
1	A	536	VAL	2.8
1	A	600	HIS	2.8
1	A	989	THR	2.7
1	A	30	GLN	2.7
1	A	73	LEU	2.6
1	A	534	SER	2.6
1	A	538	ASP	2.6
1	A	1045	SER	2.5
1	A	144	ASN	2.5
1	A	57	ILE	2.4
1	A	682	ASN	2.3
1	A	290	MET	2.3
1	A	537	GLU	2.2
1	A	614	THR	2.2
1	A	699	LEU	2.2
1	A	723	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	2.1
1	A	940	ILE	2.1
1	A	601	ASP	2.1

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(Å ²)	Q<0.9
3	PO4	A	2003	5/5	0.48	0.20	9,16,23,54	0
2	NAG	A	2001	14/15	0.60	0.19	47,67,85,86	0
3	PO4	A	2002	5/5	0.95	0.10	25,33,41,43	0
6	MRD	A	5001	8/8	0.96	0.07	16,17,24,25	0
5	NK1	A	4001	12/12	0.99	0.06	11,15,19,21	0
4	ZN	A	3001	1/1	1.00	0.01	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.