



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 AM GMT

PDB ID : 2OW6  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

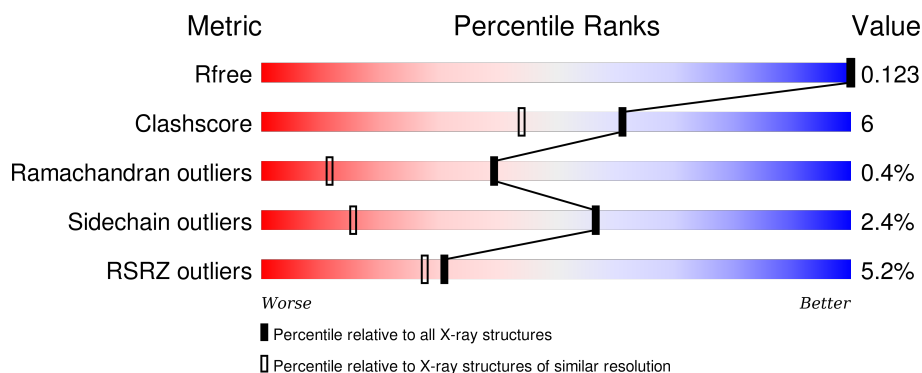
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1495 (1.26-1.14)
Clashscore	102246	1607 (1.26-1.14)
Ramachandran outliers	100387	1540 (1.26-1.14)
Sidechain outliers	100360	1538 (1.26-1.14)
RSRZ outliers	91569	1500 (1.26-1.14)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	2002	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	2003	-	-	-	X
5	NK1	A	4001	-	-	-	X

## 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.

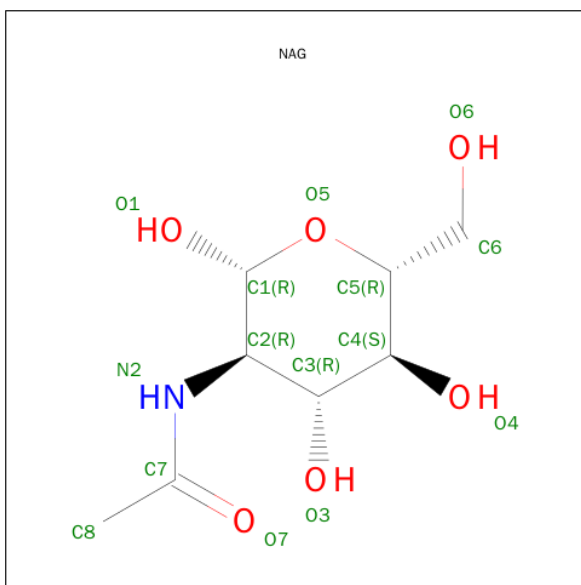
- Molecule 1 is a protein called Alpha-mannosidase 2.

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

There are 13 discrepancies between the modelled and reference sequences:

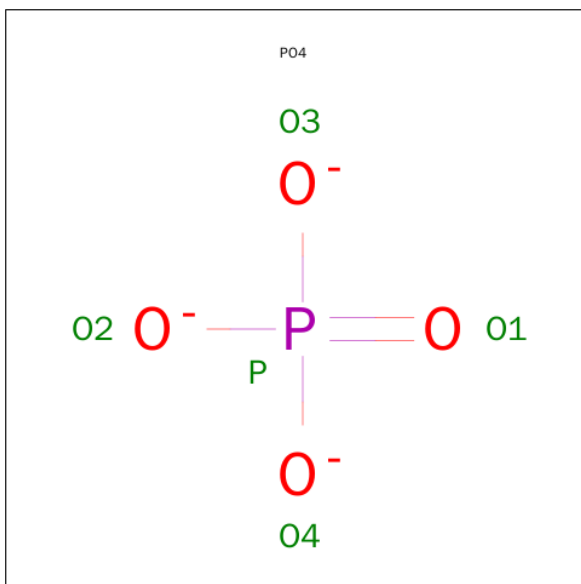
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	EXPRESSION TAG	UNP Q24451
A	2	SER	-	EXPRESSION TAG	UNP Q24451
A	3	SER	-	EXPRESSION TAG	UNP Q24451
A	4	HIS	-	EXPRESSION TAG	UNP Q24451
A	5	HIS	-	EXPRESSION TAG	UNP Q24451
A	6	HIS	-	EXPRESSION TAG	UNP Q24451
A	7	HIS	-	EXPRESSION TAG	UNP Q24451
A	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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

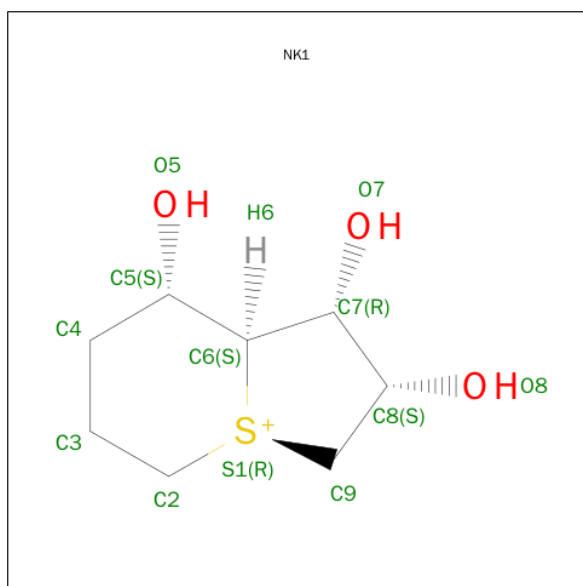


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

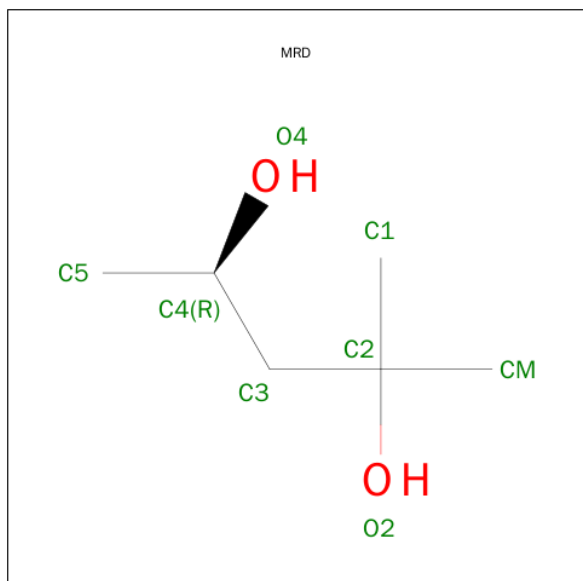
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (1R,5S,6S,7R,8S)-1-THIONIABICYCLO[4.3.0]NONAN-5,7,8-TRIOL (three-letter code: NK1) (formula: C<sub>8</sub>H<sub>15</sub>O<sub>3</sub>S).



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 (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

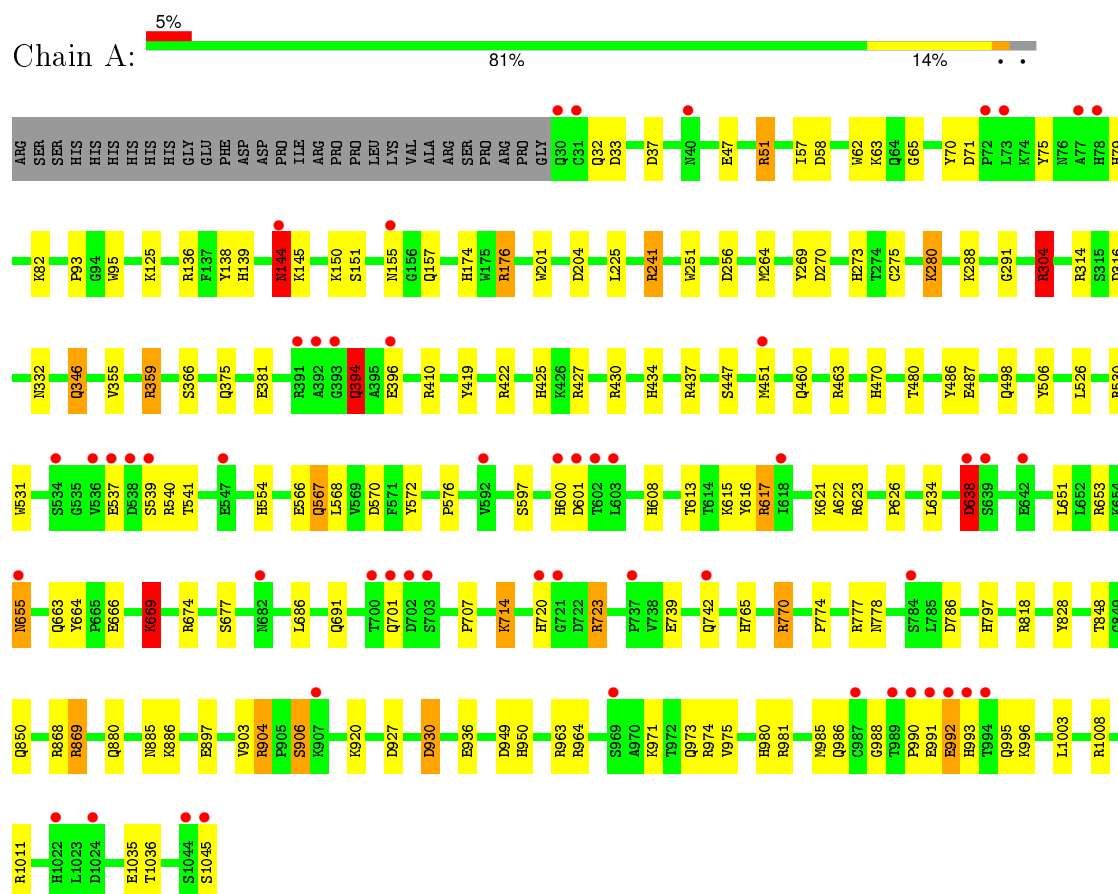
- Molecule 7 is water.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	69.01Å 109.62Å 138.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.19 20.01 – 1.19	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-1.19) 93.7 (20.01-1.19)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.19Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.118 , 0.150 0.122 , 0.123	Depositor DCC
$R_{free}$ test set	5006 reflections (1.62%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.9	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 330560 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	9888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, NK1, ZN, NAG, 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	0.77	3/8680 (0.0%)	1.32	90/11781 (0.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	SER	CB-OG	-6.12	1.34	1.42
1	A	251	TRP	CD1-NE1	-5.34	1.28	1.38
1	A	597	SER	CB-OG	-5.31	1.35	1.42

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ARG	NE-CZ-NH2	-19.71	110.44	120.30
1	A	437	ARG	NE-CZ-NH1	-16.10	112.25	120.30
1	A	974	ARG	NE-CZ-NH2	-14.39	113.10	120.30
1	A	75	TYR	CB-CG-CD1	-11.32	114.20	121.00
1	A	314	ARG	NE-CZ-NH2	-10.80	114.90	120.30
1	A	818[A]	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	A	818[B]	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	A	304	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	359[A]	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	359[B]	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	A	316[A]	ASP	CB-CG-OD1	-8.79	110.39	118.30
1	A	316[B]	ASP	CB-CG-OD1	-8.79	110.39	118.30
1	A	410	ARG	NH1-CZ-NH2	8.55	128.81	119.40
1	A	904	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	A	786	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	949	ASP	CB-CG-OD1	8.03	125.53	118.30
1	A	674	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	A	531	TRP	CE3-CZ3-CH2	7.64	129.60	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	963	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	241	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	1035	GLU	OE1-CD-OE2	-7.38	114.44	123.30
1	A	936	GLU	OE1-CD-OE2	-7.38	114.45	123.30
1	A	136	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	540	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	869	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	572	TYR	CB-CG-CD1	7.19	125.31	121.00
1	A	314	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	664	TYR	CG-CD1-CE1	-7.08	115.63	121.30
1	A	291	GLY	O-C-N	-7.05	111.41	122.70
1	A	201	TRP	CA-CB-CG	7.04	127.08	113.70
1	A	531	TRP	CZ3-CH2-CZ2	-7.02	113.17	121.60
1	A	930	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	A	600	HIS	N-CA-CB	6.90	123.02	110.60
1	A	251	TRP	NE1-CE2-CZ2	-6.83	122.88	130.40
1	A	269	TYR	CB-CG-CD1	6.65	124.99	121.00
1	A	669	LYS	CA-CB-CG	6.62	127.95	113.40
1	A	304	ARG	CD-NE-CZ	6.59	132.83	123.60
1	A	463	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	381	GLU	OE1-CD-OE2	-6.53	115.46	123.30
1	A	530	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	576	PRO	O-C-N	-6.33	112.58	122.70
1	A	437	ARG	CD-NE-CZ	6.23	132.32	123.60
1	A	1008	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	A	427	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	51	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	437	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	A	974	ARG	NH1-CZ-NH2	6.07	126.08	119.40
1	A	981	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	674	ARG	CD-NE-CZ	6.07	132.09	123.60
1	A	1008	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	A	974	ARG	CD-NE-CZ	6.02	132.03	123.60
1	A	616	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	A	777	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	A	58	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	430	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	992	GLU	O-C-N	5.87	132.09	122.70
1	A	570	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	930	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	151	SER	N-CA-CB	5.80	119.20	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	TYR	CB-CG-CD1	-5.66	117.60	121.00
1	A	486	TYR	CB-CG-CD2	5.65	124.39	121.00
1	A	691	GLN	OE1-CD-NE2	5.65	134.90	121.90
1	A	430	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	617	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	381	GLU	CG-CD-OE2	5.55	129.40	118.30
1	A	664	TYR	CD1-CE1-CZ	5.54	124.79	119.80
1	A	638	ASP	CA-CB-CG	-5.53	101.24	113.40
1	A	394	GLN	CB-CA-C	5.48	121.37	110.40
1	A	634	LEU	CB-CG-CD2	5.45	120.26	111.00
1	A	576	PRO	C-N-CA	5.43	135.28	121.70
1	A	897	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	A	1011	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	617	ARG	CA-CB-CG	5.32	125.11	113.40
1	A	868	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	33	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	613	THR	O-C-N	-5.24	114.31	122.70
1	A	144	ASN	CA-CB-CG	5.21	124.86	113.40
1	A	770[A]	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	770[B]	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	638	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	394	GLN	CG-CD-NE2	-5.15	104.33	116.70
1	A	176	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	251	TRP	CD2-CE2-CZ2	5.13	128.46	122.30
1	A	419	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	567	GLN	CA-CB-CG	5.11	124.64	113.40
1	A	623	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	70	TYR	CG-CD2-CE2	5.08	125.36	121.30
1	A	981	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	422	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	8377	0	8225	90	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	48	0
All	All	9888	0	8266	92	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 6.

All (92) 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
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:H	1:A:346:GLN:HE21	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:988:GLY:O	1:A:990:PRO:HD3	2.02	0.59
1:A:138:TYR:OH	1:A:150:LYS:HE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:TRP:CD2	1:A:65:GLY:HA3	2.43	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:125:LYS:HE2	7:A:5050: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
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:720:HIS:C	1:A:723:ARG:HH21	2.16	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:NZ	1:A:971:LYS:HB2	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: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:903:VAL:O	1:A:985[B]:MET:HE1	2.16	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:LYS:NZ	7:A:6117:HOH:O	2.48	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: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:615:LYS:NZ	7:A:5422:HOH:O	2.50	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
1:A:638:ASP:OD1	1:A:638:ASP:N	2.50	0.41
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
1:A:714:LYS:NZ	7:A:5219:HOH:O	2.51	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%)	39	11

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 ⓘ

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%)	910 (98%)	23 (2%)	55 13

All (23) 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	396	GLU
1	A	451	MET
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	723	ARG
1	A	828	TYR

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Mol	Chain	Res	Type
1	A	906	SER
1	A	1045	SER

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

Mol	Chain	Res	Type
1	A	91	ASN
1	A	119	HIS
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	240	GLN
1	A	249	GLN
1	A	273	HIS
1	A	346	GLN
1	A	347	ASN
1	A	388	GLN
1	A	394	GLN
1	A	425	HIS
1	A	434	HIS
1	A	460	GLN
1	A	469	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	655	ASN
1	A	698	GLN
1	A	701	GLN
1	A	765	HIS
1	A	880	GLN
1	A	885	ASN
1	A	919	HIS
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	993	HIS
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 ⓘ

There are no carbohydrates 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	0.77	0	15,19,21	1.57	2 (13%)
3	PO4	A	2002	-	4,4,4	1.71	1 (25%)	6,6,6	0.27	0
3	PO4	A	2003	-	4,4,4	1.57	2 (50%)	6,6,6	0.27	0
5	NK1	A	4001	4	10,13,13	0.87	0	8,19,19	1.14	1 (12%)
6	MRD	A	5001	-	6,7,7	0.74	0	7,10,10	1.08	1 (14%)

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	2001	1	-	0/6/23/26	0/1/1/1
3	PO4	A	2002	-	-	0/0/0/0	0/0/0/0
3	PO4	A	2003	-	-	0/0/0/0	0/0/0/0
5	NK1	A	4001	4	-	0/0/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MRD	A	5001	-	-	0/5/5/5	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2003	PO4	P-O2	2.05	1.60	1.53
3	A	2003	PO4	P-O3	2.11	1.61	1.53
3	A	2002	PO4	P-O3	2.73	1.63	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NAG	C3-C2-N2	-3.81	101.44	110.56
6	A	5001	MRD	CM-C2-C1	-2.46	104.89	110.24
5	A	4001	NK1	C4-C5-C6	2.14	114.83	110.60
2	A	2001	NAG	C4-C3-C2	2.97	115.84	111.23

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1016/1045 (97%)	0.41	53 (5%) 31 28	9, 17, 37, 84	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	990	PRO	9.2
1	A	30	GLN	8.0
1	A	701	GLN	7.9
1	A	702	ASP	7.7
1	A	993	HIS	7.2
1	A	720	HIS	7.1
1	A	992	GLU	6.8
1	A	602	THR	6.7
1	A	991	GLU	6.5
1	A	603	LEU	6.1
1	A	538	ASP	6.0
1	A	638	ASP	5.4
1	A	78	HIS	5.1
1	A	534	SER	4.4
1	A	703	SER	4.1
1	A	600	HIS	4.0
1	A	989	THR	4.0
1	A	144	ASN	4.0
1	A	721	GLY	3.9
1	A	536	VAL	3.7
1	A	682	ASN	3.7
1	A	392	ALA	3.6
1	A	655	ASN	3.5
1	A	1024	ASP	3.5
1	A	537	GLU	3.2
1	A	784	SER	3.2
1	A	539	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1045	SER	3.1
1	A	391	ARG	3.0
1	A	987	CYS	2.9
1	A	994	THR	2.8
1	A	31	CYS	2.8
1	A	547	GLU	2.7
1	A	393	GLY	2.7
1	A	700	THR	2.6
1	A	1022	HIS	2.6
1	A	592	VAL	2.6
1	A	601	ASP	2.5
1	A	639	SER	2.5
1	A	1044	SER	2.5
1	A	742[A]	GLN	2.4
1	A	737	PRO	2.4
1	A	618	ILE	2.3
1	A	72	PRO	2.3
1	A	77	ALA	2.2
1	A	396	GLU	2.2
1	A	73	LEU	2.2
1	A	40	ASN	2.2
1	A	642	GLU	2.1
1	A	907	LYS	2.1
1	A	969	SER	2.1
1	A	451	MET	2.1
1	A	155	ASN	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	2003	5/5	0.63	0.55	30.98	9,16,23,54	0
3	PO4	A	2002	5/5	0.95	0.18	4.51	25,33,41,43	0
5	NK1	A	4001	12/12	0.97	0.09	2.17	11,15,19,21	0
6	MRD	A	5001	8/8	0.93	0.10	0.91	16,17,24,25	0
4	ZN	A	3001	1/1	1.00	0.05	-2.38	12,12,12,12	0
2	NAG	A	2001	14/15	0.53	0.44	-	47,67,85,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.