



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:55 PM UTC

PDB ID : 1QWN / pdb_00001qwn
Title : GOLGI ALPHA-MANNOSIDASE II Covalent Intermediate Complex with 5-fluoro-gulosyl-fluoride
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Deposited on : 2003-09-02
Resolution : 1.20 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

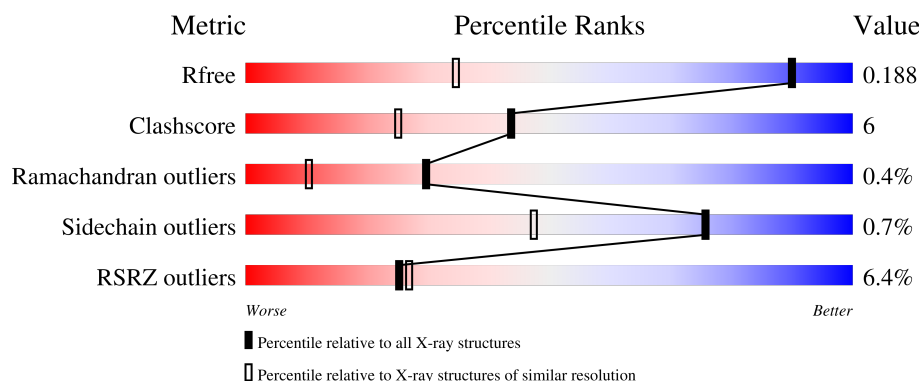
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	

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
6	MPD	A	2002	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9601 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.

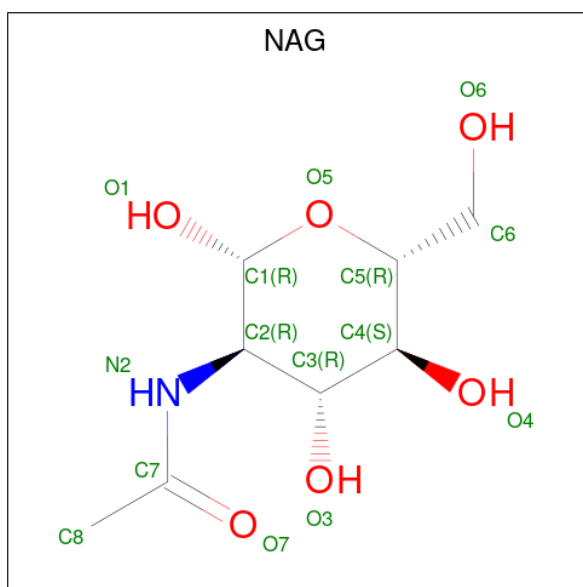
- Molecule 1 is a protein called Alpha-mannosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1014	Total	C	N	O	S	0	40	0
			8524	5414	1500	1565	45			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	cloning artifact	UNP Q24451
A	2	SER	-	cloning artifact	UNP Q24451
A	3	SER	-	cloning artifact	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	-	cloning artifact	UNP Q24451
A	11	GLU	-	cloning artifact	UNP Q24451
A	12	PHE	-	cloning artifact	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

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

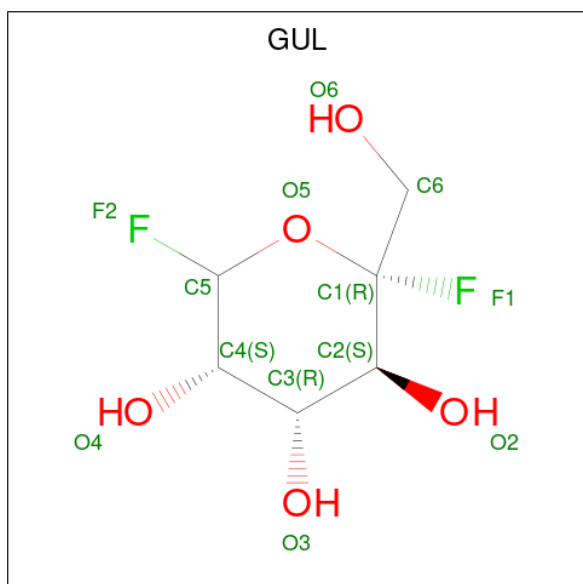


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

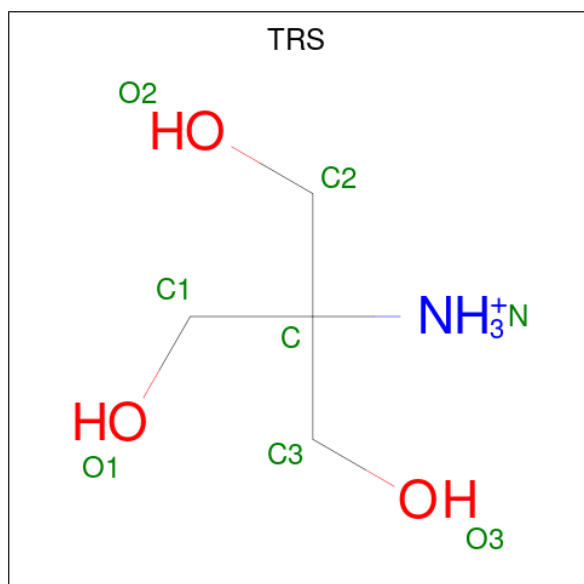
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2R,3S,4R,5S)-2,6-difluoro-2-(hydroxymethyl)oxane-3,4,5-triol (CCD ID: GUL) (formula: C₆H₁₀F₂O₅).



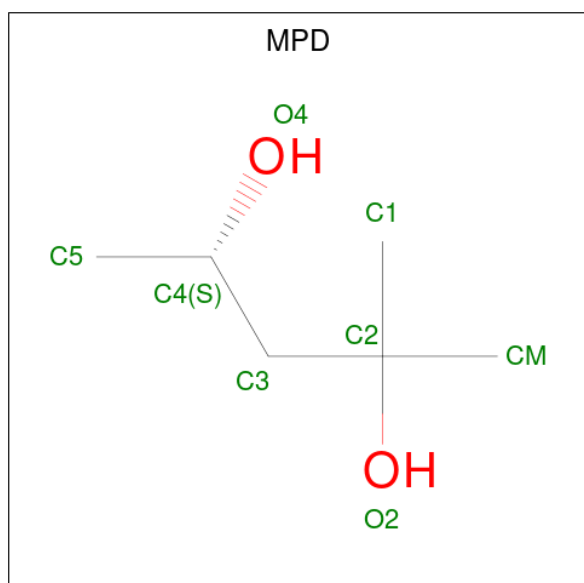
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

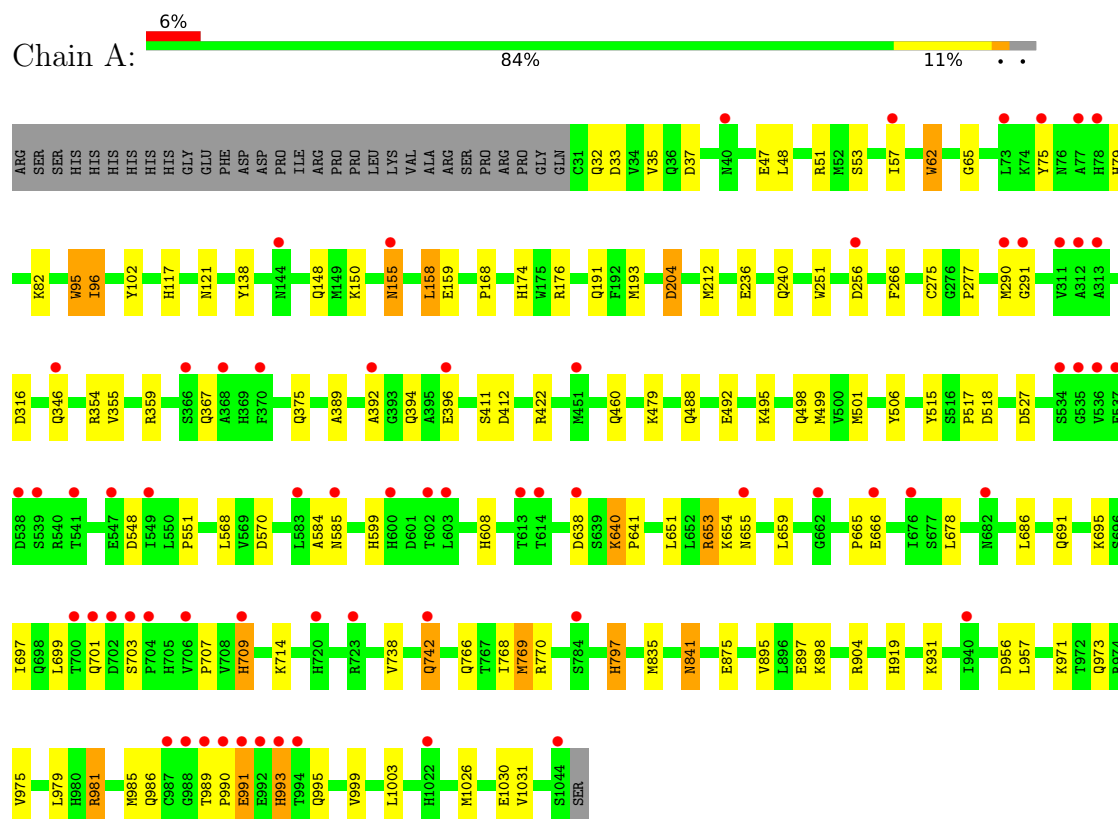
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1034	Total	O	0	0
			1034	1034		

3 Residue-property plots

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	69.02Å 110.02Å 138.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.20 30.00 – 1.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-1.20) 96.7 (30.00-1.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.15Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.175 , 0.192 0.171 , 0.188	Depositor DCC
R_{free} test set	2529 reflections (0.70%)	wwPDB-VP
Wilson B-factor (Å ²)	8.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.1	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	0.97	EDS
Total number of atoms	9601	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, TRS, MPD, ZN, GUL

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	1.09	30/8756 (0.3%)	1.08	33/11880 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	MET	SD-CE	-15.43	1.41	1.79
1	A	212	MET	SD-CE	-9.12	1.56	1.79
1	A	499	MET	SD-CE	-9.06	1.56	1.79
1	A	769[A]	MET	SD-CE	8.15	2.00	1.79
1	A	769[B]	MET	SD-CE	8.15	2.00	1.79
1	A	96	ILE	CG1-CD1	-7.64	1.22	1.51
1	A	742	GLN	CD-OE1	7.28	1.37	1.23
1	A	422	ARG	C-O	7.23	1.27	1.23
1	A	835	MET	SD-CE	-6.63	1.62	1.79
1	A	919	HIS	ND1-CE1	6.41	1.39	1.32
1	A	986	GLN	CD-OE1	6.00	1.34	1.23
1	A	655	ASN	CG-OD1	5.88	1.34	1.23
1	A	498	GLN	CD-OE1	5.80	1.34	1.23
1	A	148	GLN	CD-OE1	5.79	1.34	1.23
1	A	993	HIS	ND1-CE1	5.76	1.38	1.32
1	A	973	GLN	CD-OE1	5.69	1.34	1.23
1	A	460	GLN	CD-OE1	5.43	1.33	1.23
1	A	191	GLN	CD-OE1	5.42	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	599	HIS	ND1-CE1	5.37	1.38	1.32
1	A	608	HIS	ND1-CE1	5.37	1.38	1.32
1	A	367	GLN	CD-OE1	5.37	1.33	1.23
1	A	701	GLN	CD-OE1	5.36	1.33	1.23
1	A	121	ASN	CG-OD1	5.32	1.33	1.23
1	A	96	ILE	CA-CB	5.30	1.61	1.54
1	A	79	HIS	ND1-CE1	5.26	1.37	1.32
1	A	240	GLN	CD-OE1	5.22	1.33	1.23
1	A	367	GLN	CD-NE2	-5.16	1.22	1.33
1	A	488	GLN	CD-OE1	5.13	1.33	1.23
1	A	709[A]	HIS	ND1-CE1	5.02	1.37	1.32
1	A	709[B]	HIS	ND1-CE1	5.02	1.37	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	PRO	N-CA-C	9.02	125.12	114.03
1	A	35	VAL	N-CA-C	7.32	117.83	111.90
1	A	699	LEU	N-CA-C	6.89	118.87	111.36
1	A	599	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	A	993	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	A	709[A]	HIS	CB-CG-CD2	-6.45	122.81	131.20
1	A	709[B]	HIS	CB-CG-CD2	-6.45	122.81	131.20
1	A	79	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	A	517	PRO	N-CA-C	6.42	122.30	111.32
1	A	277	PRO	N-CA-C	6.04	121.41	113.86
1	A	841	ASN	N-CA-C	5.99	121.25	113.88
1	A	919	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	A	703	SER	N-CA-C	5.82	118.44	110.01
1	A	608	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	A	875	GLU	N-CA-C	5.76	119.61	112.24
1	A	993	HIS	CB-CG-ND1	5.66	131.19	122.70
1	A	518	ASP	N-CA-C	-5.63	98.03	107.99
1	A	599	HIS	CB-CG-ND1	5.56	131.03	122.70
1	A	79	HIS	CB-CG-ND1	5.53	131.00	122.70
1	A	501	MET	CG-SD-CE	-5.53	88.73	100.90
1	A	709[A]	HIS	CB-CG-ND1	5.47	130.91	122.70
1	A	709[B]	HIS	CB-CG-ND1	5.47	130.91	122.70
1	A	392	ALA	N-CA-C	-5.26	106.84	113.20
1	A	396	GLU	N-CA-C	-5.24	101.23	109.50
1	A	168	PRO	N-CA-C	5.20	119.65	111.38
1	A	204	ASP	N-CA-C	5.20	121.30	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	993	HIS	N-CA-C	5.16	121.78	110.80
1	A	608	HIS	CB-CG-ND1	5.12	130.37	122.70
1	A	266	PHE	N-CA-C	5.08	117.26	109.95
1	A	640	LYS	CA-C-N	5.06	124.96	119.85
1	A	640	LYS	C-N-CA	5.06	124.96	119.85
1	A	62	TRP	N-CA-C	-5.03	99.13	107.99
1	A	584	ALA	N-CA-C	-5.02	107.18	113.15

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	TYR	Sidechain
1	A	155[B]	ASN	Mainchain
1	A	797[B]	HIS	Mainchain

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	8524	0	8282	101	2
2	A	14	0	13	0	0
3	A	1	0	0	0	0
4	A	12	0	6	1	0
5	A	8	0	12	0	0
6	A	8	0	14	2	0
7	A	1034	0	0	31	1
All	All	9601	0	8327	103	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (103) 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:971[B]:LYS:HB2	1:A:971[B]:LYS:NZ	1.22	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971[B]:LYS:NZ	1:A:971[B]:LYS:CB	2.09	1.15
1:A:971[B]:LYS:CB	1:A:971[B]:LYS:HZ3	1.59	1.15
1:A:651[B]:LEU:HD22	1:A:659:LEU:HD11	1.22	1.14
1:A:75[B]:TYR:HD1	7:A:2788:HOH:O	1.31	1.09
1:A:506[B]:TYR:OH	7:A:2904:HOH:O	1.70	1.04
1:A:971[B]:LYS:HB2	1:A:971[B]:LYS:HZ2	1.22	1.00
1:A:651[B]:LEU:CD2	1:A:659:LEU:HD11	1.93	0.97
1:A:117[B]:HIS:CE1	1:A:354:ARG:HE	1.84	0.95
1:A:651[B]:LEU:HD22	1:A:659:LEU:CD1	1.98	0.92
1:A:37:ASP:HB2	7:A:3030:HOH:O	1.70	0.91
1:A:82:LYS:HD2	1:A:375:GLN:HE22	1.36	0.90
1:A:138[B]:TYR:OH	7:A:2347:HOH:O	1.85	0.90
1:A:117[B]:HIS:HE1	1:A:354:ARG:HE	0.92	0.90
1:A:981[A]:ARG:HH11	1:A:981[A]:ARG:HB2	1.41	0.86
1:A:117[B]:HIS:HE1	1:A:354:ARG:NE	1.74	0.84
1:A:75[B]:TYR:CE1	7:A:2944:HOH:O	2.29	0.83
1:A:75[B]:TYR:HE1	7:A:2944:HOH:O	1.60	0.83
1:A:256:ASP:HB2	7:A:3032:HOH:O	1.77	0.82
1:A:75[B]:TYR:OH	7:A:3037:HOH:O	2.01	0.78
1:A:709[A]:HIS:ND1	7:A:3031:HOH:O	2.20	0.74
6:A:2002:MPD:H11	7:A:2845:HOH:O	1.90	0.70
1:A:957:LEU:HD13	1:A:981[A]:ARG:NH1	2.07	0.70
1:A:37:ASP:N	7:A:3030:HOH:O	2.13	0.70
1:A:678:LEU:HD12	1:A:769[B]:MET:HE1	1.73	0.69
1:A:971[B]:LYS:HB2	1:A:971[B]:LYS:HZ3	0.85	0.68
1:A:695:LYS:HG3	1:A:709[A]:HIS:NE2	2.09	0.67
1:A:678:LEU:CD1	1:A:769[B]:MET:HE1	2.25	0.67
1:A:138[A]:TYR:OH	1:A:150:LYS:HE3	1.97	0.65
1:A:651[A]:LEU:CD1	1:A:653:ARG:HG2	2.28	0.63
1:A:707:PRO:HG2	1:A:797[B]:HIS:CE1	2.34	0.62
1:A:742:GLN:HG3	7:A:2692:HOH:O	1.99	0.62
1:A:989:THR:CG2	1:A:991:GLU:HG3	2.29	0.62
1:A:904:ARG:HG2	1:A:985:MET:SD	2.40	0.62
1:A:841:ASN:O	1:A:898:LYS:HE2	2.01	0.60
1:A:981[A]:ARG:HH11	1:A:981[A]:ARG:CB	2.14	0.59
1:A:82:LYS:HD2	1:A:375:GLN:NE2	2.13	0.59
1:A:37:ASP:CB	7:A:3030:HOH:O	2.40	0.58
1:A:714:LYS:HD2	7:A:2510:HOH:O	2.02	0.58
1:A:47:GLU:OE2	1:A:51:ARG:CD	2.52	0.57
1:A:979[A]:LEU:HD21	1:A:999:VAL:HG11	1.87	0.56
1:A:981[A]:ARG:CZ	1:A:1031:VAL:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.36	0.55
1:A:989:THR:HG22	1:A:991:GLU:HG3	1.87	0.55
6:A:2002:MPD:H13	7:A:2702:HOH:O	2.07	0.54
1:A:251:TRP:C	1:A:251:TRP:CD1	2.85	0.54
1:A:57[A]:ILE:HD11	7:A:2474:HOH:O	2.09	0.53
1:A:981[A]:ARG:NH1	1:A:1031:VAL:O	2.42	0.53
1:A:316[B]:ASP:CG	7:A:2850:HOH:O	2.52	0.52
1:A:956:ASP:OD1	1:A:981[B]:ARG:NH1	2.43	0.52
1:A:96:ILE:HG23	1:A:479:LYS:CE	2.39	0.52
1:A:32:GLN:NE2	7:A:3032:HOH:O	2.43	0.51
1:A:389:ALA:HB1	1:A:394:GLN:CG	2.40	0.51
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.93	0.51
1:A:47:GLU:OE2	1:A:51:ARG:HD2	2.11	0.50
1:A:33:ASP:O	7:A:3030:HOH:O	2.19	0.50
1:A:990:PRO:O	1:A:991:GLU:C	2.54	0.50
1:A:981[B]:ARG:HB2	1:A:1031:VAL:HG23	1.93	0.49
1:A:96:ILE:HG23	1:A:479:LYS:HE2	1.93	0.49
1:A:638:ASP:HA	7:A:3025:HOH:O	2.13	0.49
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.48	0.49
1:A:47:GLU:OE2	1:A:51:ARG:HD3	2.11	0.49
1:A:653:ARG:HD3	1:A:654:LYS:O	2.13	0.48
1:A:981[B]:ARG:NH2	1:A:1030:GLU:OE1	2.47	0.48
1:A:158[A]:LEU:C	1:A:158[A]:LEU:HD23	2.39	0.47
1:A:389:ALA:HB1	1:A:394:GLN:HG2	1.96	0.47
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.48	0.47
1:A:51:ARG:HG3	7:A:2963:HOH:O	2.14	0.47
1:A:290:MET:HE1	7:A:2909:HOH:O	2.15	0.47
1:A:506[B]:TYR:CE2	1:A:515:TYR:CD1	3.04	0.46
1:A:158[A]:LEU:HD23	1:A:159:GLU:N	2.31	0.46
1:A:1026[B]:MET:HE2	7:A:2729:HOH:O	2.16	0.46
1:A:714:LYS:HE3	1:A:738:VAL:HG22	1.97	0.46
1:A:95:TRP:CZ2	4:A:2003:GUL:H62	2.51	0.46
1:A:411[B]:SER:OG	1:A:412:ASP:N	2.48	0.46
1:A:48:LEU:HD11	1:A:236:GLU:HG2	1.99	0.45
1:A:714:LYS:HE2	1:A:714:LYS:HB3	1.70	0.45
1:A:316[B]:ASP:OD2	7:A:2850:HOH:O	2.21	0.45
1:A:981[A]:ARG:HH22	1:A:1030:GLU:HB3	1.81	0.45
1:A:492:GLU:OE1	1:A:495:LYS:NZ	2.44	0.45
1:A:1026[A]:MET:HE3	7:A:2729:HOH:O	2.15	0.45
1:A:551:PRO:HG2	7:A:2274:HOH:O	2.17	0.45
1:A:766[B]:GLN:HG2	1:A:768:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138[A]:TYR:CE1	1:A:193[A]:MET:CE	3.01	0.44
1:A:355:VAL:HG12	1:A:359[B]:ARG:CZ	2.47	0.44
1:A:995:GLN:HG3	7:A:2578:HOH:O	2.18	0.44
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.99	0.44
1:A:990:PRO:O	1:A:991:GLU:O	2.36	0.44
1:A:568:LEU:HD12	1:A:770[B]:ARG:HD3	2.00	0.43
1:A:568:LEU:HD12	1:A:770[A]:ARG:HD3	2.00	0.43
1:A:666:GLU:HB2	7:A:2657:HOH:O	2.18	0.43
1:A:155[A]:ASN:OD1	1:A:155[A]:ASN:C	2.61	0.42
1:A:291:GLY:N	7:A:2376:HOH:O	2.29	0.42
1:A:678:LEU:HD13	1:A:769[B]:MET:HE1	2.00	0.42
1:A:389:ALA:O	1:A:394:GLN:HG2	2.19	0.42
1:A:158[A]:LEU:C	1:A:158[A]:LEU:CD2	2.93	0.42
1:A:570[B]:ASP:OD2	1:A:570[B]:ASP:C	2.64	0.41
1:A:389:ALA:HB1	1:A:394:GLN:CD	2.45	0.41
1:A:640:LYS:HA	1:A:641:PRO:HD3	1.89	0.41
1:A:359[A]:ARG:NE	7:A:2572:HOH:O	2.52	0.41
1:A:256:ASP:CB	7:A:3032:HOH:O	2.52	0.41
1:A:527:ASP:O	1:A:931:LYS:HE3	2.22	0.40
1:A:506[B]:TYR:CE2	1:A:515:TYR:CE1	3.09	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346[B]:GLN:NE2	1:A:548:ASP:O[4_465]	2.07	0.13
1:A:53[B]:SER:OG	7:A:2447:HOH:O[1_455]	2.16	0.04

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	1052/1045 (101%)	1024 (97%)	24 (2%)	4 (0%)	30	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	991	GLU
1	A	993	HIS
1	A	95	TRP
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	941/929 (101%)	933 (99%)	8 (1%)	70	40

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158[A]	LEU
1	A	158[B]	LEU
1	A	275	CYS
1	A	585	ASN
1	A	653	ARG
1	A	691	GLN
1	A	981[A]	ARG
1	A	981[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	91	ASN
1	A	249	GLN
1	A	253	ASN

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Mol	Chain	Res	Type
1	A	347	ASN
1	A	367	GLN
1	A	380	GLN
1	A	643	HIS
1	A	812	GLN
1	A	923	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	GUL	A	2003	3,1	9,12,13	2.17	2 (22%)	14,18,20	2.14	4 (28%)
2	NAG	A	2001	1	14,14,15	0.65	0	17,19,21	0.67	0
6	MPD	A	2002	-	7,7,7	0.67	0	9,10,10	0.61	0
5	TRS	A	2004	-	7,7,7	1.69	2 (28%)	9,9,9	1.40	3 (33%)

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	GUL	A	2003	3,1	-	0/2/23/26	0/1/1/1
2	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
6	MPD	A	2002	-	1/1/2/2	2/5/5/5	-
5	TRS	A	2004	-	-	1/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2003	GUL	C4-C3	4.85	1.59	1.52
4	A	2003	GUL	O5-C1	3.65	1.44	1.37
5	A	2004	TRS	C2-C	-3.36	1.44	1.53
5	A	2004	TRS	O3-C3	2.62	1.50	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	GUL	C5-O5-C1	5.07	122.46	113.70
4	A	2003	GUL	C1-C2-C3	3.51	114.57	110.71
4	A	2003	GUL	C5-C4-C3	2.81	113.74	109.64
5	A	2004	TRS	O2-C2-C	2.30	117.28	110.88
4	A	2003	GUL	O3-C3-C4	-2.09	105.80	110.05
5	A	2004	TRS	C3-C-N	-2.05	102.94	108.17
5	A	2004	TRS	C3-C-C2	2.01	116.00	110.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	2002	MPD	C4

All (5) 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	2002	MPD	C2-C3-C4-O4
6	A	2002	MPD	C2-C3-C4-C5
5	A	2004	TRS	C1-C-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2003	GUL	1	0
6	A	2002	MPD	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1014/1045 (97%)	0.28	65 (6%)	25 27	3, 10, 21, 39	40 (3%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	7.2
1	A	534	SER	5.2
1	A	991	GLU	4.3
1	A	535	GLY	4.1
1	A	536	VAL	4.1
1	A	290	MET	4.1
1	A	583	LEU	4.0
1	A	720[A]	HIS	3.9
1	A	539	SER	3.8
1	A	682	ASN	3.8
1	A	702	ASP	3.7
1	A	990	PRO	3.7
1	A	701	GLN	3.7
1	A	638	ASP	3.6
1	A	600	HIS	3.5
1	A	992	GLU	3.5
1	A	451[A]	MET	3.4
1	A	704	PRO	3.3
1	A	703	SER	3.3
1	A	784	SER	3.2
1	A	75[A]	TYR	3.2
1	A	78	HIS	3.2
1	A	57[A]	ILE	3.2
1	A	538	ASP	3.2
1	A	655	ASN	3.1
1	A	614	THR	3.1
1	A	676	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	613	THR	2.9
1	A	392	ALA	2.9
1	A	366	SER	2.9
1	A	346[A]	GLN	2.8
1	A	602	THR	2.8
1	A	940	ILE	2.8
1	A	994	THR	2.7
1	A	541	THR	2.7
1	A	709[A]	HIS	2.7
1	A	396	GLU	2.6
1	A	537	GLU	2.6
1	A	662	GLY	2.6
1	A	291	GLY	2.5
1	A	700	THR	2.5
1	A	368	ALA	2.5
1	A	1022	HIS	2.5
1	A	77	ALA	2.5
1	A	603	LEU	2.5
1	A	313	ALA	2.4
1	A	989	THR	2.4
1	A	370	PHE	2.4
1	A	1044	SER	2.3
1	A	144	ASN	2.3
1	A	155[A]	ASN	2.3
1	A	988	GLY	2.3
1	A	547	GLU	2.3
1	A	40	ASN	2.2
1	A	585	ASN	2.2
1	A	723	ARG	2.2
1	A	312	ALA	2.1
1	A	311	VAL	2.1
1	A	987	CYS	2.1
1	A	666	GLU	2.1
1	A	742	GLN	2.1
1	A	256	ASP	2.1
1	A	73	LEU	2.0
1	A	549	ILE	2.0
1	A	706	VAL	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 [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	2001	14/15	0.44	0.31	31,58,59,59	0
5	TRS	A	2004	8/8	0.94	0.08	11,13,14,14	0
6	MPD	A	2002	8/8	0.95	0.08	10,12,16,18	0
4	GUL	A	2003	12/13	0.98	0.04	6,7,8,9	0
3	ZN	A	2005	1/1	1.00	0.01	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.