



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:00 PM UTC

PDB ID : 1R34 / pdb_00001r34
Title : Golgi alpha-mannosidase II complex with 5-thio-D-mannopyranosylamidinium salt
Authors : Kuntz, D.A.; Xin, W.; Kavelekar, L.M.; Rose, D.R.; Pinto, B.M.
Deposited on : 2003-09-30
Resolution : 1.95 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

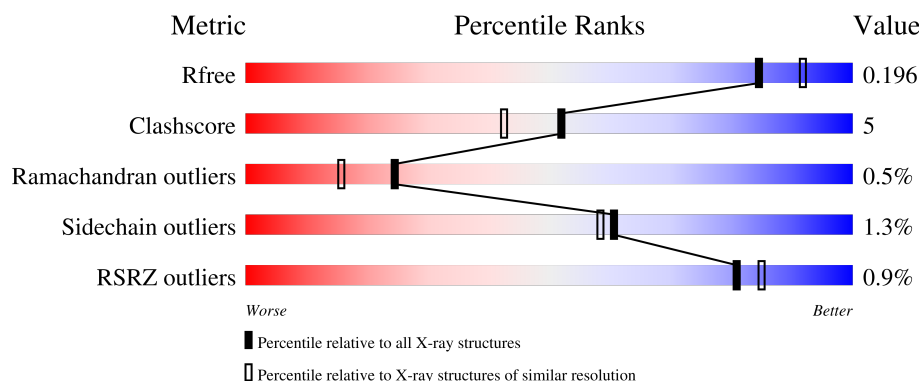
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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
2	NAG	A	1066	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	1067	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9283 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.

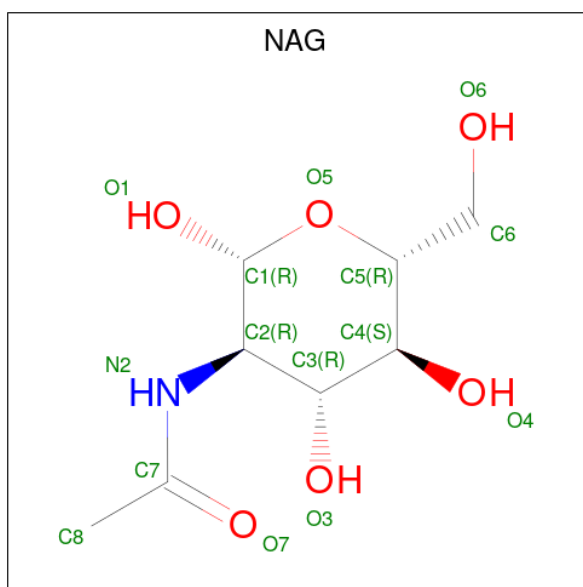
- Molecule 1 is a protein called putative golgi alpha-mannosidase II.

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

There are 12 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

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

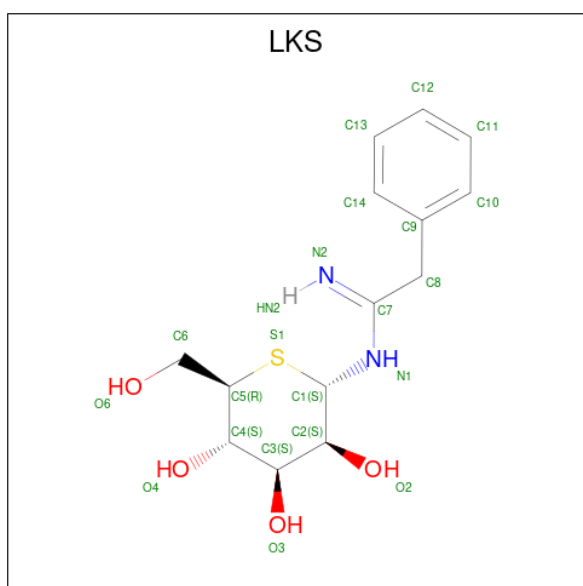


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

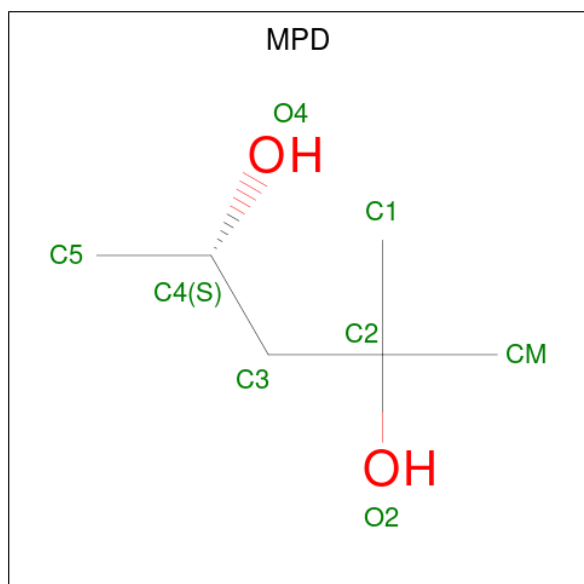
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-[(1Z)-2-phenylethanimidoyl]-5-thio-alpha-D-mannopyranosylamine (CCD ID: LKS) (formula: C₁₄H₂₀N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			21	14	2	4	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

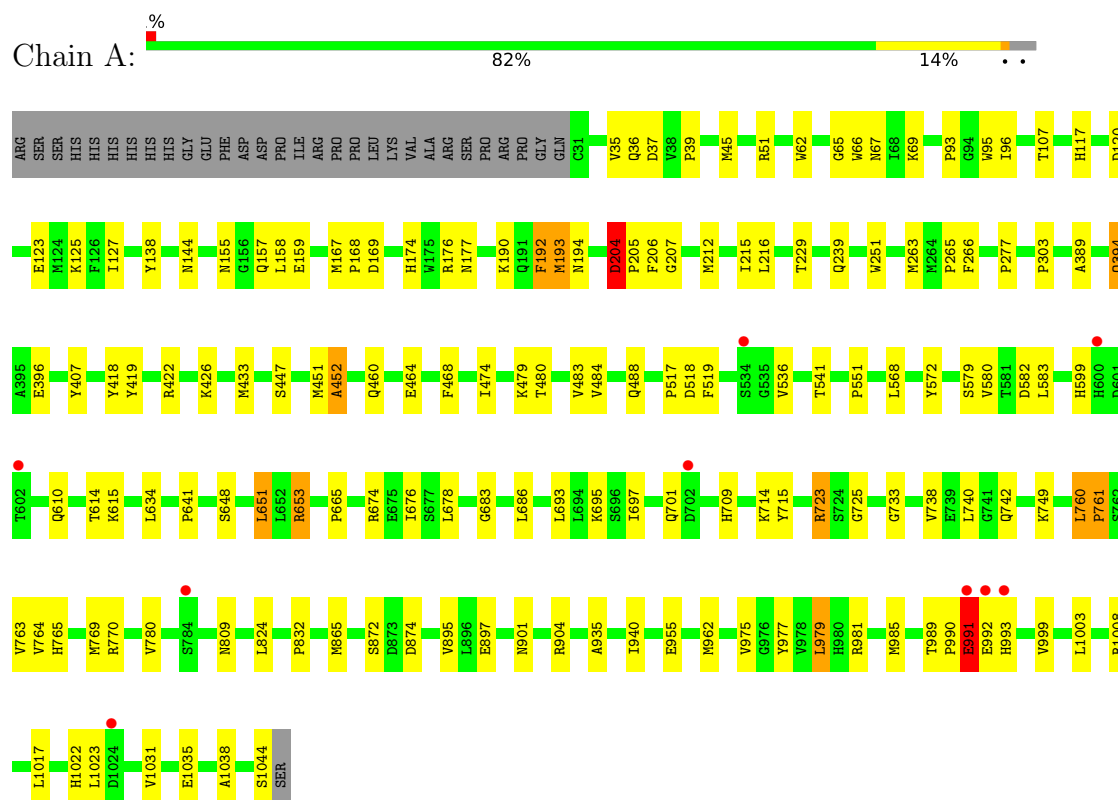
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1058	Total	O	0	0
			1058	1058		

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: putative golgi 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	68.77Å 109.57Å 138.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.25 – 1.95 29.25 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.25-1.95) 92.0 (29.25-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.151 , 0.196 0.151 , 0.196	Depositor DCC
R_{free} test set	2308 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.6	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	0.96	EDS
Total number of atoms	9283	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 4.51% 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: ZN, MPD, NAG, LKS

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	1.07	4/8406 (0.0%)	1.17	38/11416 (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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	761	PRO	C-O	9.47	1.33	1.23
1	A	422	ARG	C-O	9.35	1.28	1.23
1	A	483	VAL	CA-CB	5.44	1.61	1.54
1	A	215	ILE	CA-CB	5.22	1.60	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ALA	N-CA-C	-14.41	95.70	113.28
1	A	168	PRO	N-CA-C	8.66	124.40	111.41
1	A	36	GLN	N-CA-C	8.10	123.28	113.23
1	A	207	GLY	N-CA-C	-8.02	103.30	112.29
1	A	665	PRO	N-CA-C	7.75	123.56	114.03
1	A	1023	LEU	N-CA-C	6.95	120.57	109.24
1	A	167	MET	N-CA-C	-6.87	94.78	109.01
1	A	45	MET	N-CA-C	6.55	119.24	111.71
1	A	760	LEU	CA-C-N	-6.42	112.87	120.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	760	LEU	C-N-CA	-6.42	112.87	120.13
1	A	764	VAL	N-CA-C	-6.26	98.19	107.51
1	A	780	VAL	N-CA-C	6.21	117.06	107.99
1	A	517	PRO	N-CA-C	6.12	121.78	111.32
1	A	536	VAL	N-CA-C	-6.11	106.56	111.81
1	A	193	MET	CG-SD-CE	-5.96	87.80	100.90
1	A	518	ASP	N-CA-C	-5.92	97.51	107.99
1	A	169	ASP	N-CA-C	-5.79	102.47	110.35
1	A	962	MET	N-CA-C	-5.74	98.92	108.34
1	A	265	PRO	N-CA-C	5.73	124.28	112.47
1	A	396	GLU	N-CA-C	-5.69	99.73	109.24
1	A	763	VAL	N-CA-C	5.58	115.91	108.27
1	A	761	PRO	N-CA-C	-5.57	101.47	110.55
1	A	935	ALA	N-CA-C	5.54	118.50	111.69
1	A	35	VAL	CB-CA-C	-5.48	106.23	111.44
1	A	266	PHE	N-CA-C	5.48	118.44	110.17
1	A	204	ASP	N-CA-C	5.45	121.86	109.81
1	A	120	ASP	N-CA-C	5.43	119.75	113.18
1	A	277	PRO	N-CA-C	5.42	120.63	113.86
1	A	648	SER	N-CA-C	-5.36	102.58	110.52
1	A	447	SER	N-CA-C	-5.25	101.15	109.76
1	A	192	PHE	N-CA-C	5.22	119.92	113.50
1	A	701	GLN	N-CA-C	5.22	116.97	111.28
1	A	117	HIS	N-CA-C	5.15	116.89	111.28
1	A	955	GLU	N-CA-C	5.14	118.65	112.38
1	A	107	THR	N-CA-C	5.08	116.82	111.28
1	A	51	ARG	N-CA-C	5.04	117.88	111.69
1	A	303	PRO	N-CA-C	-5.03	103.87	111.41
1	A	93	PRO	N-CA-C	-5.01	105.72	112.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	TYR	Sidechain

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	82	0
2	A	14	0	13	1	0
3	A	1	0	0	0	0
4	A	21	0	16	0	0
5	A	8	0	14	0	0
6	A	1058	0	0	22	0
All	All	9283	0	8014	82	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 (82) 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:678:LEU:HD12	1:A:769:MET:HE1	1.49	0.93
1:A:723:ARG:HH11	1:A:723:ARG:HG3	1.43	0.84
1:A:568:LEU:HD12	1:A:770:ARG:HD3	1.67	0.76
1:A:940:ILE:HD12	6:A:1740:HOH:O	1.85	0.75
1:A:709:HIS:HB3	6:A:1909:HOH:O	1.84	0.75
1:A:989:THR:HG22	1:A:991:GLU:HG2	1.68	0.74
1:A:678:LEU:CD1	1:A:769:MET:HE1	2.18	0.73
1:A:599:HIS:HD2	1:A:610:GLN:HG3	1.54	0.71
1:A:714:LYS:HE3	1:A:738:VAL:HG22	1.74	0.68
1:A:981:ARG:CZ	6:A:1811:HOH:O	2.42	0.68
1:A:484:VAL:O	1:A:488:GLN:HG3	1.96	0.66
1:A:599:HIS:CD2	1:A:610:GLN:HG3	2.33	0.64
1:A:979:LEU:HD21	1:A:999:VAL:HG11	1.79	0.63
1:A:541:THR:HG23	6:A:1877:HOH:O	1.97	0.62
1:A:599:HIS:HD2	1:A:610:GLN:CG	2.13	0.60
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.83	0.60
1:A:138:TYR:CE1	1:A:193:MET:HE1	2.37	0.60
1:A:69:LYS:HE2	6:A:1173:HOH:O	2.02	0.59
1:A:651:LEU:HD13	1:A:653:ARG:HG2	1.85	0.58
1:A:1031:VAL:HB	1:A:1035:GLU:HG2	1.86	0.57
1:A:194:ASN:ND2	2:A:1066:NAG:C7	2.68	0.55
1:A:155:ASN:HB3	6:A:1316:HOH:O	2.05	0.55
1:A:177:ASN:HD21	1:A:433:MET:HB2	1.73	0.54
1:A:989:THR:CG2	1:A:991:GLU:HG2	2.36	0.53
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.38	0.53
1:A:723:ARG:HD3	1:A:872:SER:OG	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:ARG:HG2	1:A:985:MET:SD	2.49	0.53
1:A:541:THR:CG2	6:A:1877:HOH:O	2.57	0.52
1:A:192:PHE:O	1:A:193:MET:HE2	2.10	0.52
1:A:723:ARG:HG3	1:A:723:ARG:NH1	2.22	0.51
1:A:1008:ARG:CZ	1:A:1022:HIS:CD2	2.93	0.51
1:A:580:VAL:HG22	1:A:634:LEU:HD22	1.93	0.49
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.95	0.49
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.47	0.49
1:A:190:LYS:HD3	1:A:1017:LEU:HD22	1.93	0.49
1:A:144:ASN:HB3	6:A:1631:HOH:O	2.12	0.49
1:A:480:THR:HG23	6:A:1242:HOH:O	2.12	0.49
1:A:651:LEU:CD1	1:A:653:ARG:HG2	2.44	0.47
1:A:809:ASN:H	1:A:832:PRO:HG3	1.81	0.46
1:A:451:MET:HA	1:A:451:MET:HE2	1.98	0.46
1:A:897:GLU:OE2	6:A:1403:HOH:O	2.21	0.46
1:A:96:ILE:HD12	1:A:479:LYS:HE2	1.98	0.45
1:A:975:VAL:HG21	1:A:1003:LEU:HD13	1.98	0.45
1:A:251:TRP:CD1	1:A:251:TRP:C	2.94	0.45
1:A:614:THR:HB	6:A:1871:HOH:O	2.16	0.45
1:A:740:LEU:HD22	1:A:760:LEU:HD22	1.98	0.45
1:A:990:PRO:O	1:A:991:GLU:C	2.59	0.45
1:A:125:LYS:HD3	1:A:157:GLN:HA	2.00	0.44
1:A:460:GLN:O	1:A:464:GLU:HG2	2.18	0.44
1:A:551:PRO:HG2	6:A:1945:HOH:O	2.18	0.44
1:A:715:TYR:CD1	1:A:865:MET:HE1	2.53	0.44
1:A:206:PHE:HB2	1:A:418:TYR:CE2	2.52	0.44
1:A:452:ALA:HA	1:A:519:PHE:CG	2.53	0.44
1:A:1008:ARG:NH1	1:A:1022:HIS:NE2	2.66	0.44
1:A:725:GLY:HA3	1:A:874:ASP:CG	2.44	0.43
1:A:204:ASP:H	1:A:205:PRO:HD3	1.83	0.43
1:A:579:SER:HB3	1:A:641:PRO:HB3	2.01	0.43
1:A:749:LYS:HE2	6:A:1959:HOH:O	2.17	0.43
1:A:583:LEU:HD12	1:A:583:LEU:HA	1.88	0.43
1:A:572:TYR:CD2	1:A:615:LYS:HE3	2.54	0.42
1:A:468:PHE:CZ	1:A:474:ILE:HA	2.55	0.42
1:A:977:TYR:O	1:A:1038:ALA:HA	2.19	0.42
1:A:761:PRO:HA	6:A:1891:HOH:O	2.18	0.42
1:A:229:THR:HG21	1:A:263:MET:HE2	2.01	0.42
1:A:582:ASP:HB2	6:A:1950:HOH:O	2.19	0.42
1:A:733:GLY:HA2	6:A:1148:HOH:O	2.19	0.42
1:A:66:TRP:CZ3	1:A:239:GLN:HG3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PHE:CD1	1:A:206:PHE:N	2.84	0.42
1:A:981:ARG:NH2	6:A:1811:HOH:O	2.52	0.42
1:A:67:ASN:HB3	6:A:1175:HOH:O	2.19	0.42
1:A:127:ILE:HA	1:A:159:GLU:O	2.20	0.42
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.54	0.42
1:A:824:LEU:C	1:A:824:LEU:HD23	2.44	0.41
1:A:389:ALA:O	1:A:394:GLN:HB2	2.20	0.41
1:A:674:ARG:HD3	6:A:1967:HOH:O	2.19	0.41
1:A:614:THR:CB	6:A:1871:HOH:O	2.68	0.41
1:A:901:ASN:HB2	6:A:2049:HOH:O	2.20	0.41
1:A:419:TYR:C	1:A:426:LYS:HE2	2.46	0.41
1:A:742:GLN:HA	6:A:1903:HOH:O	2.20	0.41
1:A:37:ASP:O	1:A:39:PRO:HD3	2.20	0.41
1:A:693:LEU:HD23	1:A:765:HIS:CD2	2.56	0.40
1:A:212:MET:O	1:A:216:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1012/1045 (97%)	980 (97%)	27 (3%)	5 (0%)	24 16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	991	GLU
1	A	95	TRP
1	A	683	GLY
1	A	993	HIS
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	901/929 (97%)	889 (99%)	12 (1%)	61	58

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	158	LEU
1	A	394	GLN
1	A	651	LEU
1	A	653	ARG
1	A	676	ILE
1	A	695	LYS
1	A	723	ARG
1	A	979	LEU
1	A	991	GLU
1	A	992	GLU
1	A	1044	SER

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	121	ASN
1	A	144	ASN
1	A	253	ASN
1	A	491	GLN
1	A	585	ASN
1	A	599	HIS
1	A	610	GLN
1	A	709	HIS
1	A	919	HIS
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 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	LKS	A	1102	3	21,22,22	5.86	15 (71%)	18,30,30	3.40	5 (27%)
5	MPD	A	1067	-	7,7,7	0.46	0	9,10,10	0.67	0
2	NAG	A	1066	1	14,14,15	0.82	0	17,19,21	0.74	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	LKS	A	1102	3	-	0/7/30/30	1/2/2/2
5	MPD	A	1067	-	1/1/2/2	3/5/5/5	-
2	NAG	A	1066	1	1/1/5/7	5/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	LKS	C1-C2	18.10	1.69	1.52
4	A	1102	LKS	C1-S1	-9.27	1.59	1.82
4	A	1102	LKS	C14-C9	6.76	1.52	1.38
4	A	1102	LKS	C12-C11	6.28	1.52	1.38
4	A	1102	LKS	C5-S1	-6.00	1.73	1.82
4	A	1102	LKS	C10-C9	5.29	1.49	1.38
4	A	1102	LKS	C11-C10	5.28	1.47	1.38
4	A	1102	LKS	C13-C14	5.07	1.47	1.38
4	A	1102	LKS	C12-C13	4.80	1.48	1.38
4	A	1102	LKS	C8-C7	4.49	1.54	1.51
4	A	1102	LKS	C7-N2	-3.70	1.19	1.27
4	A	1102	LKS	C3-C2	3.59	1.61	1.52
4	A	1102	LKS	C6-C5	-3.39	1.48	1.52
4	A	1102	LKS	O2-C2	-3.11	1.35	1.43
4	A	1102	LKS	C4-C5	2.45	1.55	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	LKS	C2-C1-N1	-12.44	95.22	111.25
4	A	1102	LKS	O2-C2-C3	5.24	122.73	110.38
4	A	1102	LKS	C4-C3-C2	2.63	115.45	110.83
4	A	1102	LKS	C9-C8-C7	-2.25	108.96	113.62
4	A	1102	LKS	O3-C3-C4	-2.09	105.45	110.38

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1066	NAG	C1
5	A	1067	MPD	C4

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1066	NAG	C1-C2-N2-C7
2	A	1066	NAG	C8-C7-N2-C2
2	A	1066	NAG	O7-C7-N2-C2
5	A	1067	MPD	C2-C3-C4-O4
5	A	1067	MPD	C2-C3-C4-C5
2	A	1066	NAG	C4-C5-C6-O6
2	A	1066	NAG	O5-C5-C6-O6
5	A	1067	MPD	O2-C2-C3-C4

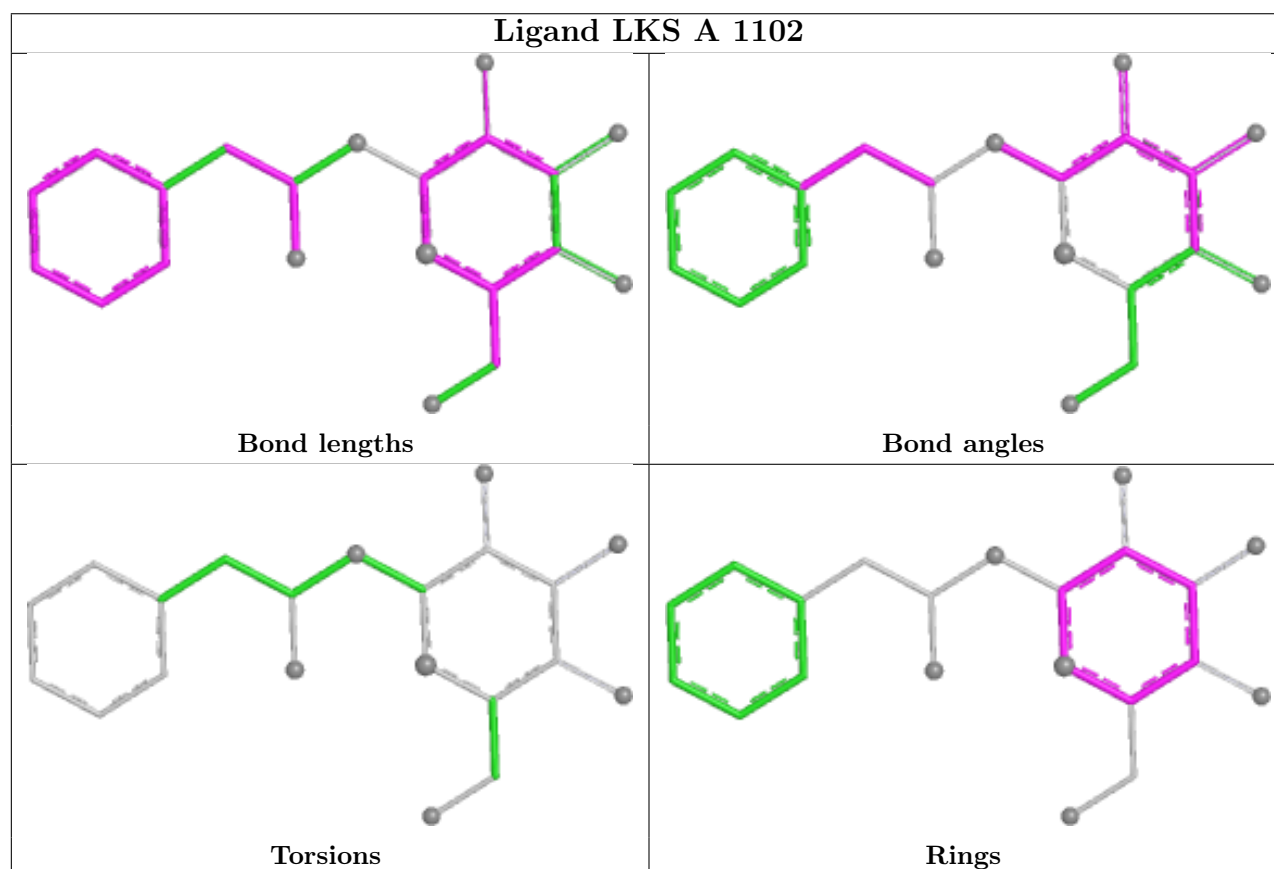
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	LKS	C1-C2-C3-C4-C5-S1

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1066	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	1014/1045 (97%)	-0.56	9 (0%)	81 85	4, 12, 28, 63	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	3.5
1	A	991	GLU	3.2
1	A	702	ASP	2.6
1	A	784	SER	2.5
1	A	992	GLU	2.5
1	A	602	THR	2.3
1	A	534	SER	2.1
1	A	600	HIS	2.0
1	A	1024	ASP	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](#)

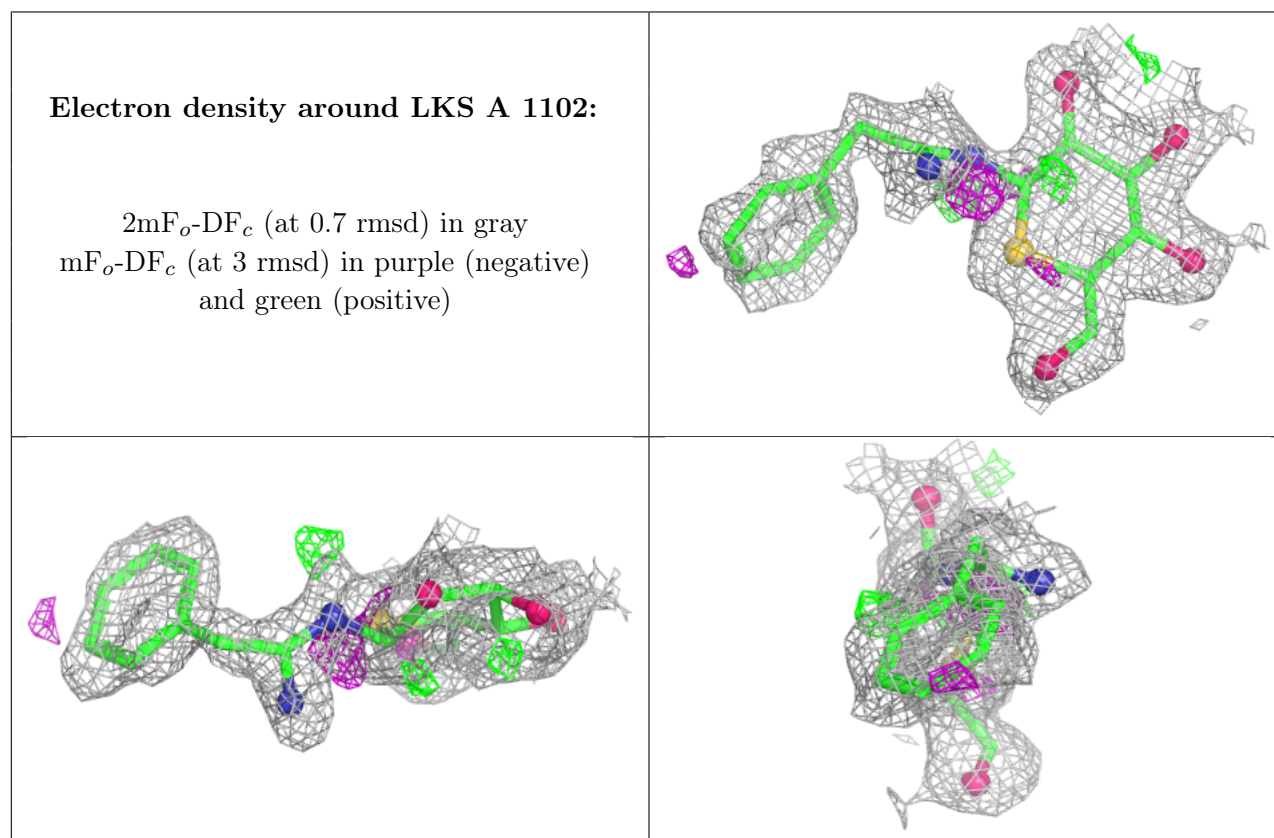
There are no oligosaccharides in this entry.

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	1066	14/15	0.66	0.16	42,50,52,55	0
4	LKS	A	1102	21/21	0.92	0.11	15,24,34,35	0
5	MPD	A	1067	8/8	0.92	0.09	17,21,26,26	0
3	ZN	A	1101	1/1	1.00	0.04	12,12,12,12	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.