



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:20 PM UTC

PDB ID : 2F7R / pdb_00002f7r
Title : Golgi alpha-mannosidase II complex with benzyl-aminocyclopentitol
Authors : Kuntz, D.A.; Rose, D.R.
Deposited on : 2005-12-01
Resolution : 1.35 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

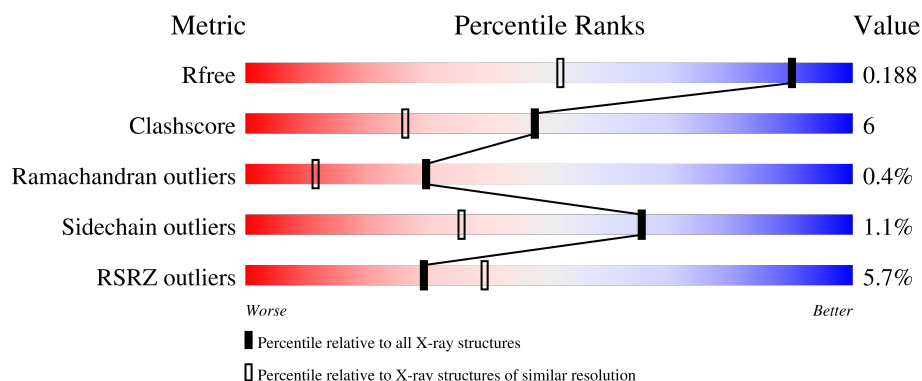
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

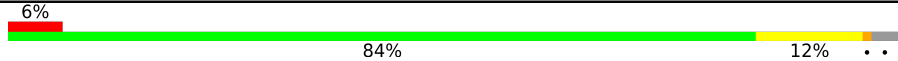
The reported resolution of this entry is 1.35 Å.

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 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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
5	MPD	A	5003	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9511 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	18	0
			8242	5238	1440	1522	42			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	cloning artifact	GB 517481
A	2	SER	-	cloning artifact	GB 517481
A	3	SER	-	cloning artifact	GB 517481
A	4	HIS	-	expression tag	GB 517481
A	5	HIS	-	expression tag	GB 517481
A	6	HIS	-	expression tag	GB 517481
A	7	HIS	-	expression tag	GB 517481
A	8	HIS	-	expression tag	GB 517481
A	9	HIS	-	expression tag	GB 517481
A	10	GLY	-	cloning artifact	GB 517481
A	11	GLU	-	cloning artifact	GB 517481
A	12	PHE	-	cloning artifact	GB 517481

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

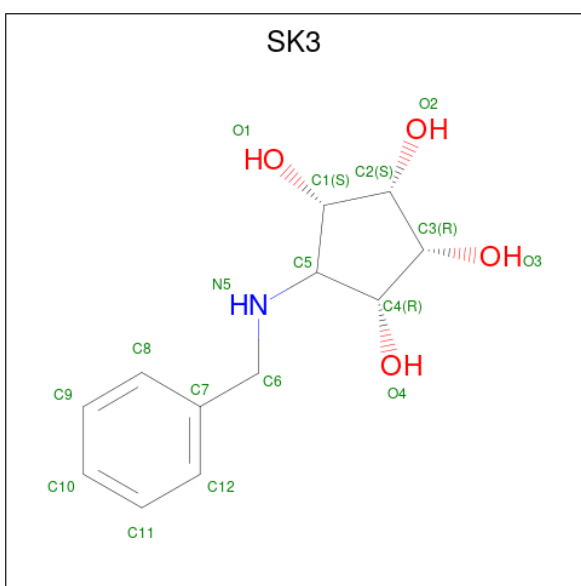


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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 (1R,2R,3S,4S,5R)-5-(BENZYLAMINO)CYCLOPENTANE-1,2,3,4-TETROL (CCD ID: SK3) (formula: C₁₂H₁₇NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	12	1	4		

- 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		

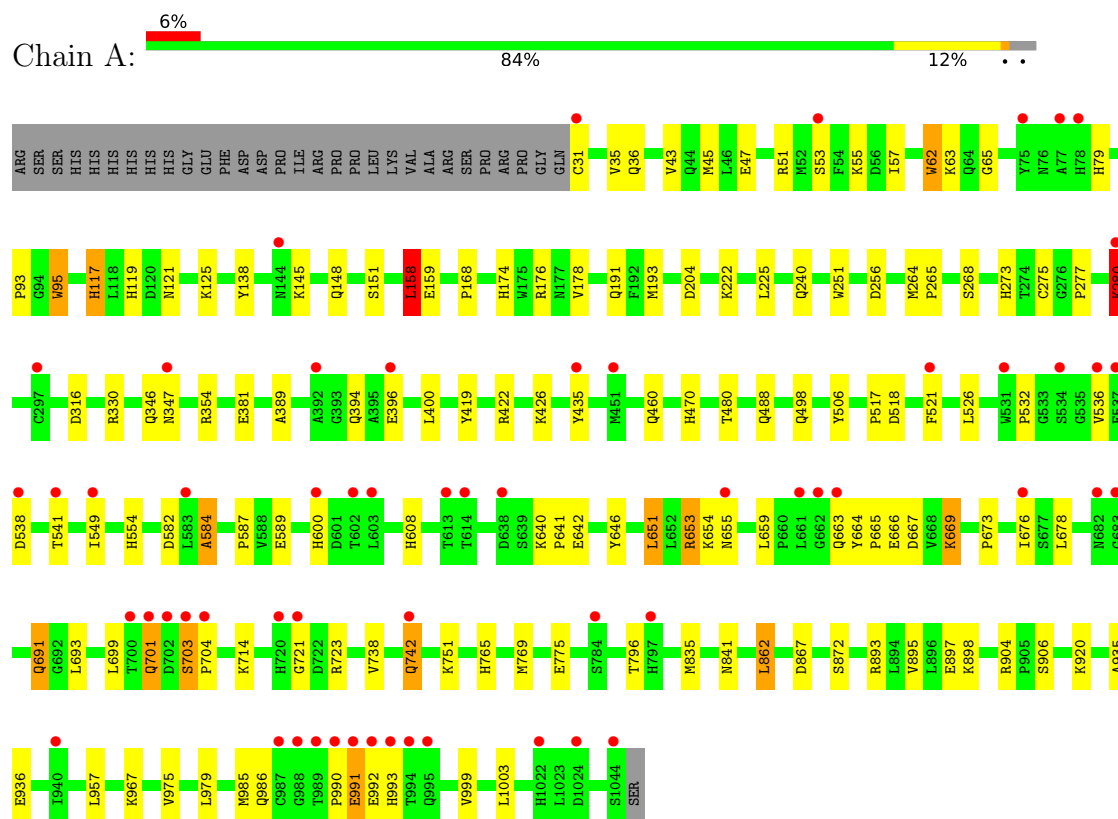
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1229	Total	O	0	0
			1229	1229		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: alpha-mannosidase II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.68Å 109.14Å 138.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.21 – 1.35 29.21 – 1.35	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.21-1.35) 91.2 (29.21-1.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.164 , 0.186 0.167 , 0.188	Depositor DCC
R_{free} test set	5680 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9511	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: SK3, ZN, NAG, MPD

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	1.22	23/8545 (0.3%)	1.22	38/11603 (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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	ARG	C-O	8.65	1.28	1.23
1	A	280	LYS	C-N	7.49	1.43	1.33
1	A	347	ASN	CG-OD1	7.09	1.37	1.23
1	A	422	ARG	N-CA	6.72	1.51	1.46
1	A	742	GLN	CD-OE1	6.67	1.36	1.23
1	A	191	GLN	CD-OE1	6.52	1.35	1.23
1	A	273	HIS	ND1-CE1	6.14	1.38	1.32
1	A	655	ASN	CG-OD1	5.86	1.34	1.23
1	A	119	HIS	ND1-CE1	5.86	1.38	1.32
1	A	765	HIS	ND1-CE1	5.85	1.38	1.32
1	A	549	ILE	CA-CB	5.75	1.62	1.54
1	A	148	GLN	CD-OE1	5.73	1.34	1.23
1	A	498	GLN	CD-OE1	5.57	1.34	1.23
1	A	79	HIS	ND1-CE1	5.54	1.38	1.32
1	A	121	ASN	CG-OD1	5.52	1.34	1.23
1	A	488	GLN	CD-OE1	5.45	1.33	1.23
1	A	608	HIS	ND1-CE1	5.43	1.38	1.32
1	A	701	GLN	CD-OE1	5.43	1.33	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	554	HIS	ND1-CE1	5.42	1.38	1.32
1	A	867	ASP	C-O	5.29	1.29	1.23
1	A	347	ASN	CG-ND2	-5.21	1.22	1.33
1	A	240	GLN	CD-OE1	5.11	1.33	1.23
1	A	460	GLN	CD-NE2	-5.07	1.22	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	PRO	N-CA-C	7.96	123.75	114.20
1	A	584	ALA	N-CA-C	-7.40	103.33	112.88
1	A	35	VAL	N-CA-C	7.25	117.77	111.90
1	A	119	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	A	518	ASP	N-CA-C	-6.65	96.22	107.99
1	A	79	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	A	178	VAL	N-CA-C	-6.42	104.23	110.72
1	A	536	VAL	N-CA-C	-6.34	106.10	111.56
1	A	517	PRO	N-CA-C	6.34	122.16	111.32
1	A	841	ASN	N-CA-C	6.24	121.55	113.88
1	A	608	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	A	396	GLU	N-CA-C	-5.89	100.20	109.50
1	A	168	PRO	N-CA-C	5.86	120.70	111.38
1	A	316	ASP	CB-CA-C	-5.84	101.47	110.81
1	A	45	MET	N-CA-C	5.80	118.39	111.71
1	A	280	LYS	O-C-N	5.79	128.12	122.09
1	A	265	PRO	N-CA-C	5.75	124.31	112.47
1	A	277	PRO	N-CA-C	5.74	121.04	113.86
1	A	119	HIS	CB-CG-ND1	5.66	131.18	122.70
1	A	935	ALA	N-CA-C	5.63	120.15	113.28
1	A	642	GLU	N-CA-C	5.63	118.18	111.71
1	A	79	HIS	CB-CG-ND1	5.55	131.03	122.70
1	A	582	ASP	CA-C-N	-5.53	111.25	122.31
1	A	582	ASP	C-N-CA	-5.53	111.25	122.31
1	A	703	SER	N-CA-C	5.47	117.94	110.01
1	A	608	HIS	CB-CG-ND1	5.41	130.81	122.70
1	A	381	GLU	CB-CG-CD	-5.39	103.44	112.60
1	A	699	LEU	N-CA-C	5.39	117.23	111.36
1	A	862	LEU	N-CA-C	-5.39	100.99	109.50
1	A	600	HIS	N-CA-C	-5.38	99.74	108.41
1	A	36	GLN	N-CA-C	5.38	119.99	113.38
1	A	62	TRP	N-CA-C	-5.33	98.61	107.99
1	A	691	GLN	CB-CG-CD	-5.20	103.75	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	554	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	796	THR	CA-C-N	-5.10	114.64	122.60
1	A	796	THR	C-N-CA	-5.10	114.64	122.60
1	A	330	ARG	N-CA-C	5.08	119.48	113.28
1	A	538	ASP	N-CA-C	-5.08	98.42	107.98

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117[B]	HIS	Mainchain
1	A	158[B]	LEU	Mainchain
1	A	506	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	8242	0	8026	90	0
2	A	14	0	13	2	0
3	A	1	0	0	0	0
4	A	17	0	15	2	0
5	A	8	0	14	0	0
6	A	1229	0	0	33	0
All	All	9511	0	8068	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:663:GLN:HG3	6:A:5696:HOH:O	1.52	1.09
1:A:117[B]:HIS:CE1	1:A:354:ARG:HE	1.83	0.95
1:A:117[B]:HIS:HE1	1:A:354:ARG:HE	1.20	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:5002:NAG:H2	6:A:6086:HOH:O	1.78	0.82
1:A:990:PRO:O	1:A:992:GLU:HG2	1.80	0.81
1:A:678:LEU:HD12	1:A:769[A]:MET:HE1	1.65	0.79
1:A:225:LEU:HD21	1:A:264[B]:MET:HE2	1.67	0.75
1:A:723:ARG:HG2	1:A:723:ARG:HH11	1.51	0.74
1:A:63:LYS:HE2	6:A:5232:HOH:O	1.87	0.74
1:A:693:LEU:HD13	6:A:5730:HOH:O	1.88	0.74
1:A:651[B]:LEU:HD22	1:A:659:LEU:HD11	1.71	0.73
1:A:117[B]:HIS:HE1	1:A:354:ARG:NE	1.90	0.70
1:A:280:LYS:NZ	6:A:6131:HOH:O	2.24	0.68
1:A:541:THR:HG23	6:A:5608:HOH:O	1.92	0.68
1:A:47:GLU:OE2	1:A:51:ARG:HD3	1.93	0.68
1:A:47:GLU:OE1	1:A:51:ARG:NH1	2.31	0.64
1:A:906:SER:HB3	6:A:5070:HOH:O	1.97	0.63
1:A:957:LEU:HD11	1:A:979[A]:LEU:HG	1.81	0.63
1:A:723:ARG:HD2	1:A:872:SER:CB	2.29	0.62
1:A:678:LEU:CD1	1:A:769[A]:MET:HE1	2.29	0.61
1:A:742:GLN:HG3	6:A:5724:HOH:O	2.01	0.60
1:A:256:ASP:HB2	6:A:5354:HOH:O	2.01	0.60
1:A:904:ARG:HG2	1:A:985:MET:SD	2.42	0.60
1:A:389:ALA:HB1	1:A:394:GLN:CG	2.33	0.59
1:A:125:LYS:HE3	6:A:5398:HOH:O	2.02	0.59
1:A:640:LYS:HD2	1:A:646:TYR:CE1	2.37	0.59
1:A:117[B]:HIS:CE1	1:A:354:ARG:NE	2.63	0.59
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.39	0.57
1:A:521:PHE:HZ	1:A:936:GLU:OE2	1.88	0.56
1:A:723:ARG:HH11	1:A:723:ARG:CG	2.17	0.56
1:A:31:CYS:N	6:A:5370:HOH:O	2.39	0.56
1:A:979[B]:LEU:HD21	1:A:999:VAL:HG11	1.88	0.56
1:A:651[A]:LEU:CD1	1:A:653:ARG:HG2	2.36	0.55
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.42	0.54
1:A:346:GLN:NE2	6:A:5293:HOH:O	2.40	0.54
1:A:222:LYS:HD3	6:A:6171:HOH:O	2.09	0.53
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.38	0.53
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.92	0.52
1:A:268:SER:OG	4:A:5009:SK3:H10	2.10	0.52
1:A:589:GLU:OE2	1:A:751:LYS:HD3	2.11	0.51
1:A:435:TYR:CE2	1:A:526:LEU:HD13	2.45	0.50
1:A:158[A]:LEU:HD23	1:A:159:GLU:N	2.26	0.50
1:A:251:TRP:C	1:A:251:TRP:CD1	2.89	0.49
1:A:967:LYS:NZ	6:A:5498:HOH:O	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:HE3	6:A:6075:HOH:O	2.11	0.49
1:A:990:PRO:O	1:A:991:GLU:C	2.55	0.49
1:A:53:SER:OG	1:A:55:LYS:HG2	2.13	0.49
1:A:389:ALA:HB1	1:A:394:GLN:HG2	1.93	0.49
1:A:587:PRO:HG3	6:A:5812:HOH:O	2.12	0.48
1:A:138:TYR:CE1	1:A:193[A]:MET:CE	2.96	0.48
1:A:701:GLN:HG2	6:A:5817:HOH:O	2.14	0.48
2:A:5002:NAG:H82	2:A:5002:NAG:O3	2.13	0.48
1:A:703:SER:HB2	1:A:704:PRO:HD2	1.95	0.47
1:A:480:THR:HG23	6:A:5882:HOH:O	2.14	0.47
1:A:47:GLU:OE2	1:A:51:ARG:NH1	2.48	0.47
1:A:47:GLU:CD	1:A:51:ARG:NH1	2.73	0.47
1:A:389:ALA:HB1	1:A:394:GLN:CD	2.40	0.47
1:A:669:LYS:N	1:A:669:LYS:HD2	2.30	0.46
1:A:666:GLU:HB2	6:A:5685:HOH:O	2.16	0.46
1:A:95:TRP:CE2	4:A:5009:SK3:H2	2.51	0.46
1:A:151[A]:SER:OG	6:A:6102:HOH:O	2.21	0.46
1:A:714:LYS:HE3	1:A:738:VAL:HG22	1.98	0.45
1:A:986:GLN:NE2	6:A:5363:HOH:O	2.50	0.45
1:A:222:LYS:HE2	6:A:6176:HOH:O	2.15	0.45
1:A:57[A]:ILE:HD11	6:A:5990:HOH:O	2.17	0.45
1:A:667:ASP:O	1:A:669:LYS:HD2	2.17	0.45
1:A:723:ARG:HD2	1:A:872:SER:OG	2.17	0.45
1:A:584:ALA:HA	6:A:5661:HOH:O	2.16	0.44
1:A:920:LYS:HG3	6:A:5555:HOH:O	2.17	0.44
1:A:651[A]:LEU:HD12	1:A:653:ARG:HG2	1.99	0.44
1:A:653:ARG:HD2	1:A:654:LYS:O	2.18	0.44
1:A:897:GLU:OE2	6:A:6014:HOH:O	2.21	0.44
1:A:57[B]:ILE:HG23	6:A:5147:HOH:O	2.18	0.43
1:A:663:GLN:O	1:A:664:TYR:C	2.62	0.43
1:A:721:GLY:HA3	6:A:5923:HOH:O	2.19	0.43
1:A:723:ARG:CG	1:A:723:ARG:NH1	2.80	0.43
1:A:714:LYS:HD2	6:A:5918:HOH:O	2.17	0.43
1:A:57[A]:ILE:HG12	6:A:5147:HOH:O	2.19	0.42
1:A:640:LYS:HA	1:A:641:PRO:HD3	1.83	0.42
1:A:653:ARG:NH1	6:A:5715:HOH:O	2.52	0.42
1:A:280:LYS:NZ	1:A:280:LYS:CB	2.82	0.42
1:A:346:GLN:CD	6:A:5293:HOH:O	2.63	0.42
1:A:389:ALA:O	1:A:394:GLN:HG2	2.20	0.41
1:A:419:TYR:C	1:A:426:LYS:HE2	2.46	0.41
1:A:775:GLU:HA	1:A:893:ARG:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PRO:HD2	1:A:470:HIS:CE1	2.55	0.41
1:A:225:LEU:C	1:A:225:LEU:HD23	2.46	0.41
1:A:669:LYS:HD3	6:A:5746:HOH:O	2.21	0.41
1:A:835:MET:HE2	1:A:862:LEU:HD22	2.01	0.40
1:A:43:VAL:O	1:A:400:LEU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1030/1045 (99%)	1004 (98%)	22 (2%)	4 (0%)	30 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	991	GLU
1	A	993	HIS
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	919/929 (99%)	907 (99%)	12 (1%)	61 30

All (12) 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	280	LYS
1	A	651[A]	LEU
1	A	651[B]	LEU
1	A	653	ARG
1	A	669	LYS
1	A	673	PRO
1	A	676	ILE
1	A	691	GLN
1	A	898	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	249	GLN
1	A	367	GLN
1	A	812	GLN
1	A	993	HIS

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 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
5	MPD	A	5003	-	7,7,7	0.68	0	9,10,10	0.77	0
2	NAG	A	5002	1	14,14,15	0.58	0	17,19,21	0.84	0
4	SK3	A	5009	3	18,18,18	0.81	0	24,25,25	3.46	8 (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
5	MPD	A	5003	-	1/1/2/2	3/5/5/5	-
2	NAG	A	5002	1	-	3/6/23/26	0/1/1/1
4	SK3	A	5009	3	-	0/5/25/25	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5009	SK3	C8-C7-C12	10.22	133.43	118.23
4	A	5009	SK3	C9-C8-C7	-6.74	111.13	120.61
4	A	5009	SK3	C6-C7-C8	-6.15	108.38	120.94
4	A	5009	SK3	C11-C12-C7	-5.72	112.57	120.61
4	A	5009	SK3	C9-C10-C11	4.64	126.22	119.87
4	A	5009	SK3	C1-C2-C3	3.12	107.50	102.53
4	A	5009	SK3	C3-C4-C5	2.88	106.68	102.70
4	A	5009	SK3	C2-C1-C5	-2.59	99.12	102.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	5003	MPD	C4

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5002	NAG	C3-C2-N2-C7
2	A	5002	NAG	C8-C7-N2-C2
2	A	5002	NAG	O7-C7-N2-C2
5	A	5003	MPD	C2-C3-C4-O4
5	A	5003	MPD	C2-C3-C4-C5
5	A	5003	MPD	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5002	NAG	2	0
4	A	5009	SK3	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%)	0.18	58 (5%) 29 39	6, 12, 25, 68	18 (1%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	6.4
1	A	703	SER	5.2
1	A	613	THR	5.1
1	A	614	THR	4.7
1	A	720	HIS	4.3
1	A	990	PRO	4.0
1	A	992	GLU	3.9
1	A	662	GLY	3.9
1	A	991	GLU	3.7
1	A	682	ASN	3.6
1	A	602	THR	3.4
1	A	534	SER	3.3
1	A	994	THR	3.2
1	A	987	CYS	3.1
1	A	1044	SER	3.1
1	A	583	LEU	3.0
1	A	144	ASN	3.0
1	A	77	ALA	2.9
1	A	53	SER	2.9
1	A	541	THR	2.8
1	A	538	ASP	2.8
1	A	638	ASP	2.8
1	A	940	ILE	2.8
1	A	701	GLN	2.8
1	A	702	ASP	2.8
1	A	995	GLN	2.7
1	A	661	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	683	GLY	2.6
1	A	600	HIS	2.6
1	A	704	PRO	2.5
1	A	396	GLU	2.5
1	A	549	ILE	2.5
1	A	603	LEU	2.5
1	A	78	HIS	2.4
1	A	784	SER	2.4
1	A	655	ASN	2.4
1	A	1022	HIS	2.4
1	A	280	LYS	2.4
1	A	1024	ASP	2.3
1	A	537[A]	GLU	2.3
1	A	297	CYS	2.3
1	A	721	GLY	2.2
1	A	988	GLY	2.2
1	A	521	PHE	2.2
1	A	75	TYR	2.2
1	A	451	MET	2.2
1	A	392	ALA	2.2
1	A	347	ASN	2.2
1	A	663	GLN	2.1
1	A	536	VAL	2.1
1	A	531	TRP	2.1
1	A	435	TYR	2.1
1	A	742	GLN	2.1
1	A	700	THR	2.1
1	A	989	THR	2.1
1	A	797	HIS	2.0
1	A	31	CYS	2.0
1	A	676	ILE	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	5002	14/15	0.75	0.16	36,43,46,46	0
5	MPD	A	5003	8/8	0.95	0.08	13,16,19,20	0
4	SK3	A	5009	17/17	0.97	0.07	7,9,25,25	0
3	ZN	A	5001	1/1	1.00	0.01	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.