



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:54 AM UTC

PDB ID : 2F7P / pdb_00002f7p
Title : Golgi alpha-mannosidase II complex with benzyl-mannostatin A
Authors : Kuntz, D.A.; Rose, D.R.
Deposited on : 2005-12-01
Resolution : 1.28 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

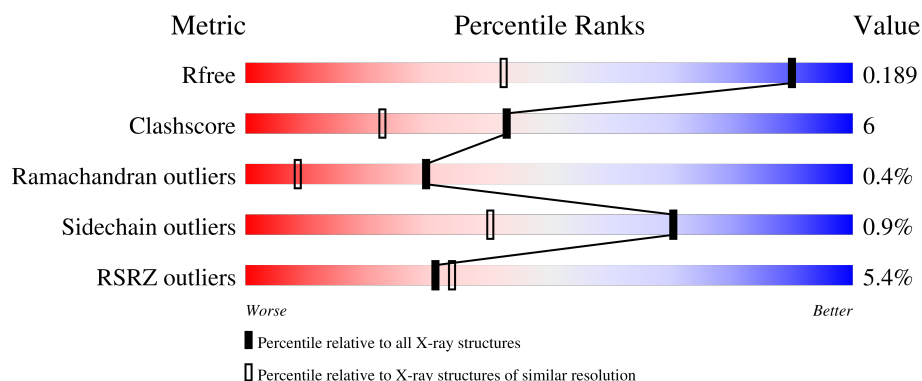
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.28 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	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (1.30-1.26)

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	5% 84% 12% ..

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 9645 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.

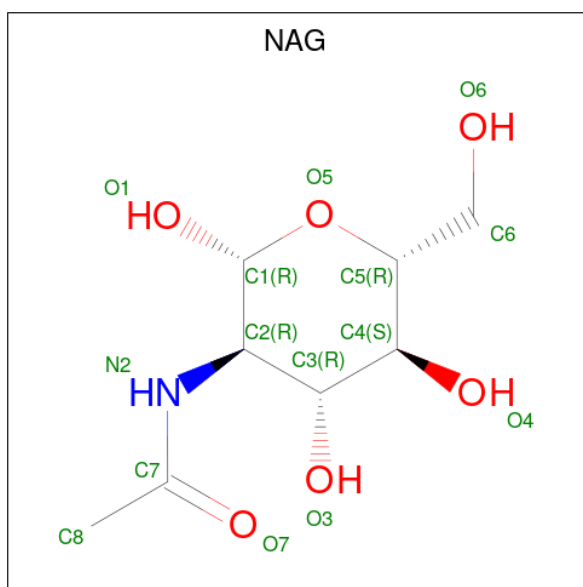
- Molecule 1 is a protein called alpha-mannosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1014	Total	C	N	O	S	0	36	0
			8377	5327	1457	1549	44			

There are 12 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

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

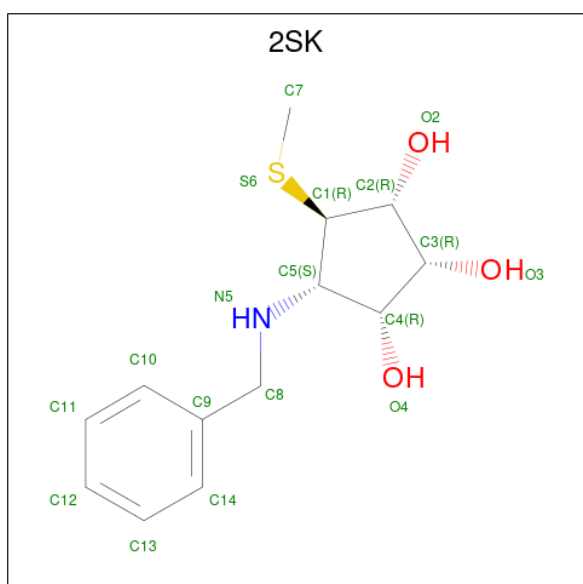


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

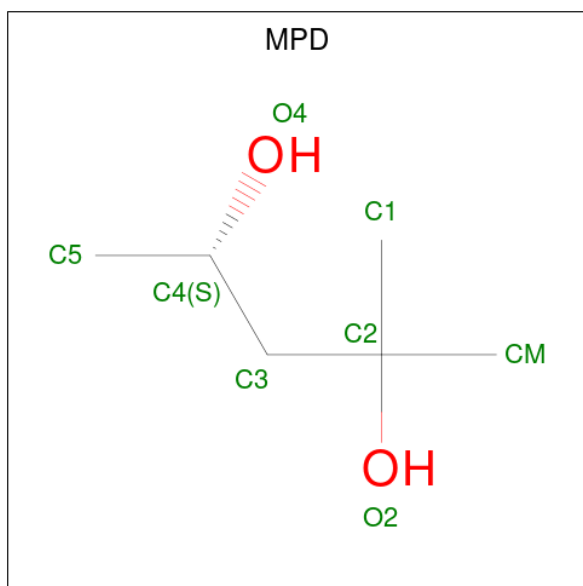
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (1R,2R,3R,4S,5R)-4-(BENZYLAMINO)-5-(METHYLTHIO)CYCLOPENTANE-1,2,3-TRIOL (CCD ID: 2SK) (formula: C₁₃H₁₉NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			19	14	1	3	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		

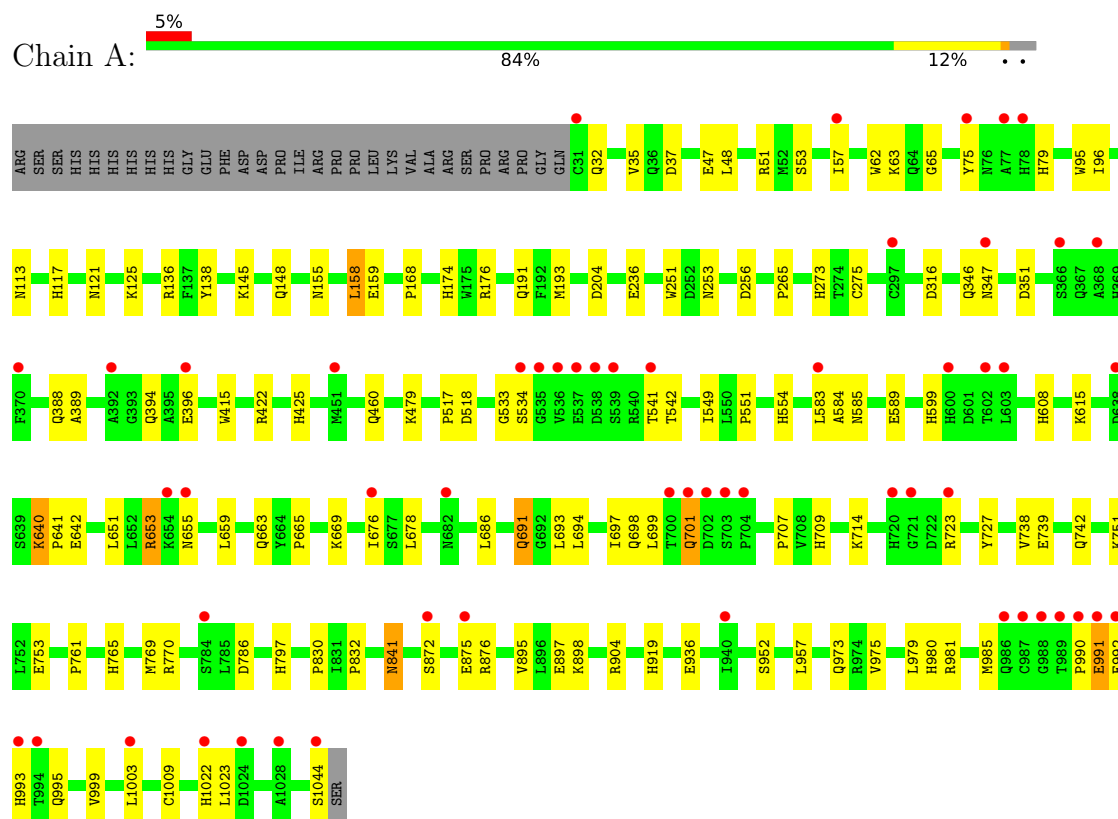
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1226	Total	O	0	0
			1226	1226		

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	68.95Å 109.87Å 139.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.33 – 1.28 29.33 – 1.28	Depositor EDS
% Data completeness (in resolution range)	94.5 (29.33-1.28) 94.8 (29.33-1.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.28Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.166 , 0.180 0.174 , 0.189	Depositor DCC
R_{free} test set	5190 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	9.0	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9645	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: 2SK, MPD, ZN, NAG

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	1.04	21/8703 (0.2%)	1.06	24/11815 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	ARG	C-O	7.01	1.27	1.23
1	A	655	ASN	CG-OD1	5.83	1.34	1.23
1	A	191	GLN	CD-OE1	5.77	1.34	1.23
1	A	422	ARG	N-CA	5.75	1.50	1.46
1	A	121	ASN	CG-OD1	5.72	1.34	1.23
1	A	973	GLN	CD-OE1	5.68	1.34	1.23
1	A	701	GLN	CD-OE1	5.64	1.34	1.23
1	A	549	ILE	CA-CB	5.61	1.62	1.54
1	A	765	HIS	ND1-CE1	5.61	1.38	1.32
1	A	273	HIS	ND1-CE1	5.55	1.38	1.32
1	A	608	HIS	ND1-CE1	5.53	1.38	1.32
1	A	460	GLN	CD-OE1	5.43	1.33	1.23
1	A	79	HIS	ND1-CE1	5.39	1.38	1.32
1	A	761	PRO	CA-C	5.35	1.58	1.52
1	A	599	HIS	ND1-CE1	5.34	1.37	1.32
1	A	148	GLN	CD-OE1	5.33	1.33	1.23
1	A	980	HIS	ND1-CE1	5.24	1.37	1.32
1	A	554	HIS	ND1-CE1	5.10	1.37	1.32
1	A	388	GLN	CD-OE1	5.10	1.33	1.23
1	A	425	HIS	ND1-CE1	5.08	1.37	1.32
1	A	698	GLN	CD-OE1	5.02	1.33	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	PRO	N-CA-C	9.08	126.52	114.27
1	A	35	VAL	N-CA-C	7.24	117.79	111.56
1	A	599	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	A	517	PRO	N-CA-C	6.56	121.49	111.19
1	A	168	PRO	N-CA-C	6.43	121.61	111.38
1	A	640	LYS	CA-C-N	6.22	126.13	119.85
1	A	640	LYS	C-N-CA	6.22	126.13	119.85
1	A	79	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	A	265	PRO	N-CA-C	6.17	125.19	112.47
1	A	841	ASN	N-CA-C	6.14	121.43	113.88
1	A	699	LEU	N-CA-C	6.14	117.97	111.28
1	A	518	ASP	N-CA-C	-6.07	97.24	107.99
1	A	761	PRO	N-CA-C	-5.81	102.02	110.80
1	A	608	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	599	HIS	CB-CG-ND1	5.70	131.25	122.70
1	A	79	HIS	CB-CG-ND1	5.33	130.69	122.70
1	A	642	GLU	N-CA-C	5.28	117.04	111.28
1	A	396	GLU	N-CA-C	-5.21	101.26	109.50
1	A	1022	HIS	N-CA-C	-5.20	100.82	109.46
1	A	554	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	A	35	VAL	CB-CA-C	-5.10	106.60	111.44
1	A	425	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	608	HIS	CB-CG-ND1	5.08	130.32	122.70
1	A	875	GLU	N-CA-C	5.08	118.60	111.74

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	8172	100	0
2	A	14	0	13	3	0
3	A	1	0	0	0	0
4	A	19	0	6	6	0
5	A	8	0	14	0	0
6	A	1226	0	0	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9645	0	8205	103	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 (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:663:GLN:HG3	6:A:5567:HOH:O	1.73	0.87
1:A:739:GLU:HG3	6:A:5814:HOH:O	1.78	0.83
1:A:96:ILE:HG22	6:A:5837:HOH:O	1.81	0.80
1:A:678:LEU:HD12	1:A:769[B]:MET:HE1	1.66	0.77
1:A:96:ILE:CG2	6:A:5837:HOH:O	2.33	0.77
1:A:990:PRO:O	1:A:992:GLU:HG2	1.86	0.76
1:A:651[B]:LEU:HD22	1:A:659:LEU:HD11	1.68	0.75
1:A:678:LEU:CD1	1:A:769[B]:MET:HE1	2.16	0.75
1:A:75[B]:TYR:HD2	6:A:5130:HOH:O	1.70	0.73
1:A:145:LYS:HE3	6:A:5312:HOH:O	1.87	0.73
1:A:136:ARG:HD3	6:A:5742:HOH:O	1.89	0.72
1:A:742:GLN:HG3	6:A:5483:HOH:O	1.93	0.69
1:A:53[B]:SER:HB2	6:A:5160:HOH:O	1.91	0.69
1:A:533:GLY:C	6:A:5604:HOH:O	2.38	0.66
1:A:63:LYS:HE2	6:A:5229:HOH:O	1.95	0.65
1:A:541:THR:HG23	6:A:5522:HOH:O	1.96	0.64
1:A:693:LEU:HD13	6:A:5477:HOH:O	1.97	0.64
1:A:753:GLU:OE2	1:A:770[B]:ARG:NH2	2.33	0.62
1:A:346[A]:GLN:CD	6:A:5379:HOH:O	2.43	0.61
1:A:47:GLU:OE2	1:A:51:ARG:HD3	2.00	0.61
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.31	0.60
1:A:701:GLN:HG2	6:A:5459:HOH:O	2.01	0.59
1:A:876:ARG:O	4:A:5009[A]:2SK:C7	2.50	0.59
1:A:346[A]:GLN:NE2	6:A:5379:HOH:O	2.35	0.59
1:A:653:ARG:NH1	6:A:5487:HOH:O	2.34	0.59
1:A:651[A]:LEU:CD1	1:A:653:ARG:HG2	2.33	0.57
1:A:37:ASP:HB2	1:A:253[B]:ASN:ND2	2.19	0.57
1:A:37:ASP:HB2	6:A:6222:HOH:O	2.05	0.56
1:A:876:ARG:O	4:A:5009[A]:2SK:H71	2.06	0.56
1:A:651[A]:LEU:HD12	1:A:653:ARG:HG2	1.88	0.55
1:A:904:ARG:HG2	1:A:985:MET:SD	2.47	0.55
1:A:979[B]:LEU:HD21	1:A:999:VAL:HG11	1.87	0.54
1:A:542:THR:OG1	1:A:615:LYS:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:957:LEU:HD11	1:A:979[A]:LEU:HG	1.89	0.54
1:A:723:ARG:HG2	1:A:723:ARG:HH11	1.73	0.54
1:A:841:ASN:O	1:A:898:LYS:HE2	2.09	0.53
1:A:155[A]:ASN:ND2	6:A:5343:HOH:O	2.42	0.52
1:A:584:ALA:HA	6:A:6048:HOH:O	2.09	0.52
1:A:739:GLU:CG	6:A:5814:HOH:O	2.48	0.52
1:A:251:TRP:C	1:A:251:TRP:CD1	2.87	0.52
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.92	0.52
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.45	0.51
2:A:5002:NAG:H82	2:A:5002:NAG:C3	2.40	0.51
1:A:256:ASP:HB2	6:A:6227:HOH:O	2.10	0.51
1:A:714:LYS:HE3	1:A:738:VAL:HG22	1.92	0.50
1:A:75[B]:TYR:CD2	6:A:5130:HOH:O	2.55	0.50
1:A:158[A]:LEU:C	1:A:158[A]:LEU:HD23	2.36	0.50
1:A:534:SER:N	6:A:5604:HOH:O	2.44	0.50
1:A:138:TYR:CE1	1:A:193[A]:MET:CE	2.95	0.50
1:A:786:ASP:CB	6:A:5412:HOH:O	2.60	0.50
1:A:47:GLU:OE1	1:A:51:ARG:NH1	2.45	0.49
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.46	0.49
1:A:678:LEU:HD13	1:A:769[B]:MET:HE1	1.91	0.49
1:A:694:LEU:O	1:A:709[B]:HIS:HD2	1.96	0.48
1:A:990:PRO:O	1:A:991:GLU:C	2.56	0.48
2:A:5002:NAG:H82	2:A:5002:NAG:H3	1.96	0.48
1:A:727:TYR:CE2	4:A:5009[B]:2SK:H73	2.48	0.48
1:A:872:SER:HB2	6:A:5413:HOH:O	2.13	0.48
1:A:415:TRP:CH2	4:A:5009[B]:2SK:H71	2.48	0.47
1:A:952:SER:HB3	1:A:995:GLN:HE22	1.78	0.47
1:A:534:SER:O	6:A:5604:HOH:O	2.20	0.47
1:A:316:ASP:CG	6:A:5254:HOH:O	2.57	0.47
1:A:57[A]:ILE:HD11	6:A:5148:HOH:O	2.14	0.47
1:A:113[B]:ASN:OD1	1:A:347:ASN:OD1	2.33	0.47
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.97	0.46
1:A:158[A]:LEU:HD23	1:A:159:GLU:N	2.29	0.46
1:A:117[B]:HIS:HE1	1:A:351:ASP:OD1	1.99	0.46
1:A:415:TRP:HH2	4:A:5009[B]:2SK:H71	1.81	0.46
1:A:53[B]:SER:CB	6:A:5160:HOH:O	2.54	0.46
1:A:723:ARG:HD2	1:A:872:SER:CB	2.46	0.45
1:A:551:PRO:HG2	6:A:5554:HOH:O	2.17	0.45
1:A:981[A]:ARG:NE	6:A:5659:HOH:O	2.50	0.44
1:A:786:ASP:HA	6:A:5412:HOH:O	2.17	0.44
1:A:125:LYS:HE3	6:A:5108:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:PRO:HG2	1:A:797[B]:HIS:ND1	2.33	0.44
1:A:389:ALA:HB1	1:A:394:GLN:CG	2.47	0.44
1:A:389:ALA:O	1:A:394:GLN:HG2	2.18	0.44
1:A:541:THR:CG2	6:A:5522:HOH:O	2.57	0.44
1:A:691:GLN:NE2	6:A:5475:HOH:O	2.48	0.44
1:A:57[B]:ILE:HG23	6:A:5150:HOH:O	2.17	0.43
1:A:96:ILE:HD12	1:A:479:LYS:HE2	2.00	0.43
1:A:479:LYS:NZ	6:A:5392:HOH:O	2.50	0.43
1:A:876:ARG:HB3	4:A:5009[A]:2SK:H71	1.99	0.43
1:A:952:SER:HB3	1:A:995:GLN:NE2	2.34	0.43
1:A:1009:CYS:SG	1:A:1023:LEU:HD12	2.59	0.43
2:A:5002:NAG:H82	2:A:5002:NAG:O3	2.19	0.43
1:A:589:GLU:OE2	1:A:751:LYS:HD3	2.20	0.42
1:A:898:LYS:HE2	1:A:898:LYS:HA	2.01	0.42
1:A:651[A]:LEU:C	1:A:651[A]:LEU:HD13	2.45	0.42
1:A:981[B]:ARG:NE	6:A:5659:HOH:O	2.53	0.42
1:A:640:LYS:HA	1:A:641:PRO:HD3	1.86	0.42
1:A:995:GLN:CG	6:A:6013:HOH:O	2.68	0.41
1:A:753:GLU:OE2	1:A:770[B]:ARG:CZ	2.68	0.41
1:A:786:ASP:CG	6:A:5412:HOH:O	2.63	0.41
1:A:389:ALA:HB1	1:A:394:GLN:CD	2.45	0.41
1:A:919:HIS:HE1	6:A:5697:HOH:O	2.04	0.41
1:A:936:GLU:HG3	6:A:6024:HOH:O	2.19	0.41
1:A:583:LEU:HD12	1:A:583:LEU:HA	1.91	0.41
1:A:32:GLN:NE2	6:A:6227:HOH:O	2.53	0.41
1:A:96:ILE:HG23	1:A:479:LYS:HE2	2.03	0.41
1:A:830:PRO:HB2	1:A:832:PRO:HD3	2.03	0.41
1:A:48:LEU:HD11	1:A:236:GLU:HG2	2.02	0.41
1:A:158[A]:LEU:C	1:A:158[A]:LEU:CD2	2.94	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	1048/1045 (100%)	1022 (98%)	22 (2%)	4 (0%)	30 8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	991	GLU
1	A	95	TRP
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	937/929 (101%)	928 (99%)	9 (1%)	68 35

All (9) 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	669	LYS
1	A	676	ILE
1	A	691	GLN
1	A	1044	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	367	GLN
1	A	371	ASN

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Mol	Chain	Res	Type
1	A	742	GLN
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 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	2SK	A	5009[B]	-	17,19,19	1.06	1 (5%)	19,26,26	1.95	5 (26%)
2	NAG	A	5002	1	14,14,15	0.66	0	17,19,21	0.83	1 (5%)
4	2SK	A	5009[A]	-	17,19,19	1.06	1 (5%)	19,26,26	1.95	5 (26%)
5	MPD	A	5003	-	7,7,7	0.44	0	9,10,10	0.71	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	2SK	A	5009[B]	-	-	0/7/27/27	0/2/2/2
2	NAG	A	5002	1	-	3/6/23/26	0/1/1/1
4	2SK	A	5009[A]	-	-	1/7/27/27	0/2/2/2
5	MPD	A	5003	-	1/1/2/2	3/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5009[A]	2SK	C1-S6	-2.86	1.78	1.82
4	A	5009[B]	2SK	C1-S6	-2.86	1.78	1.82

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5009[A]	2SK	C3-C2-C1	-3.94	102.48	106.34
4	A	5009[B]	2SK	C3-C2-C1	-3.94	102.48	106.34
4	A	5009[A]	2SK	C8-N5-C5	3.87	121.43	114.07
4	A	5009[B]	2SK	C8-N5-C5	3.87	121.43	114.07
4	A	5009[A]	2SK	C3-C4-C5	3.72	107.83	102.70
4	A	5009[B]	2SK	C3-C4-C5	3.72	107.83	102.70
4	A	5009[A]	2SK	C12-C13-C14	2.46	123.27	120.24
4	A	5009[B]	2SK	C12-C13-C14	2.46	123.27	120.24
4	A	5009[A]	2SK	C13-C14-C9	-2.06	117.72	120.61
4	A	5009[B]	2SK	C13-C14-C9	-2.06	117.72	120.61
2	A	5002	NAG	C2-N2-C7	-2.02	120.19	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	5003	MPD	C4

All (7) torsion outliers are listed below:

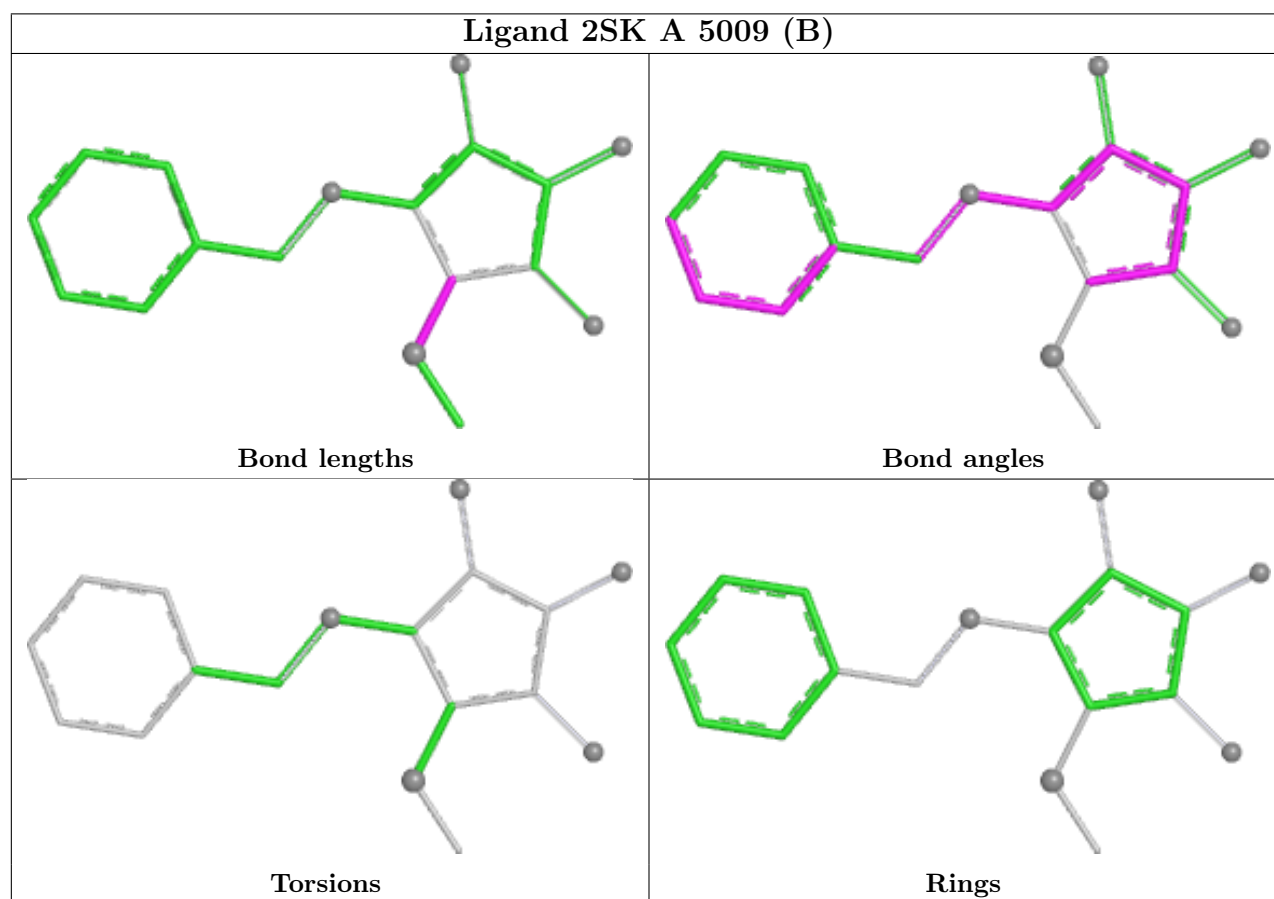
Mol	Chain	Res	Type	Atoms
2	A	5002	NAG	C8-C7-N2-C2
2	A	5002	NAG	O7-C7-N2-C2
4	A	5009[A]	2SK	C2-C1-S6-C7
5	A	5003	MPD	C2-C3-C4-O4
5	A	5003	MPD	C2-C3-C4-C5
2	A	5002	NAG	C3-C2-N2-C7
5	A	5003	MPD	O2-C2-C3-C4

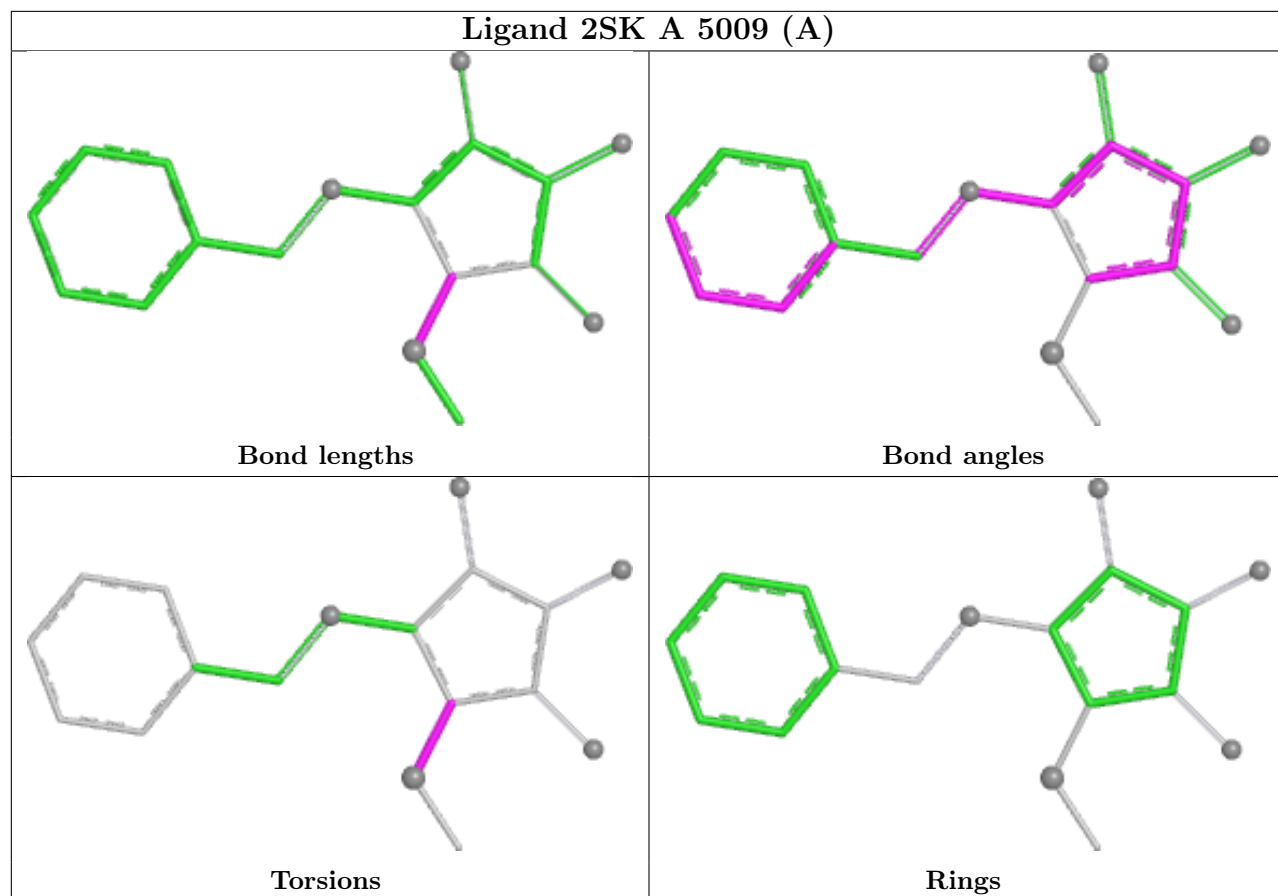
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5009[B]	2SK	3	0
2	A	5002	NAG	3	0
4	A	5009[A]	2SK	3	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 [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%)	0.13	55 (5%) 31 34	3, 10, 23, 67	36 (3%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	7.6
1	A	991	GLU	4.5
1	A	539	SER	4.3
1	A	992	GLU	4.3
1	A	534	SER	4.1
1	A	538	ASP	4.1
1	A	703	SER	3.9
1	A	701	GLN	3.9
1	A	784	SER	3.7
1	A	720	HIS	3.5
1	A	990	PRO	3.5
1	A	1024	ASP	3.5
1	A	583	LEU	3.3
1	A	655	ASN	3.3
1	A	537	GLU	3.2
1	A	78	HIS	3.2
1	A	603	LEU	3.2
1	A	536	VAL	3.2
1	A	704	PRO	3.2
1	A	989	THR	3.1
1	A	366	SER	3.1
1	A	1028	ALA	3.0
1	A	638	ASP	3.0
1	A	994	THR	3.0
1	A	682	ASN	2.9
1	A	702	ASP	2.9
1	A	535	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	986	GLN	2.9
1	A	600	HIS	2.8
1	A	987	CYS	2.7
1	A	396	GLU	2.7
1	A	77	ALA	2.6
1	A	1044	SER	2.6
1	A	1022	HIS	2.6
1	A	872	SER	2.6
1	A	370	PHE	2.6
1	A	297	CYS	2.5
1	A	988	GLY	2.5
1	A	723	ARG	2.4
1	A	721	GLY	2.4
1	A	451	MET	2.4
1	A	31	CYS	2.4
1	A	940	ILE	2.3
1	A	602	THR	2.3
1	A	392	ALA	2.3
1	A	541	THR	2.3
1	A	347	ASN	2.3
1	A	676	ILE	2.2
1	A	875	GLU	2.1
1	A	57[A]	ILE	2.1
1	A	700	THR	2.1
1	A	368	ALA	2.1
1	A	1003	LEU	2.1
1	A	654	LYS	2.0
1	A	75[A]	TYR	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,

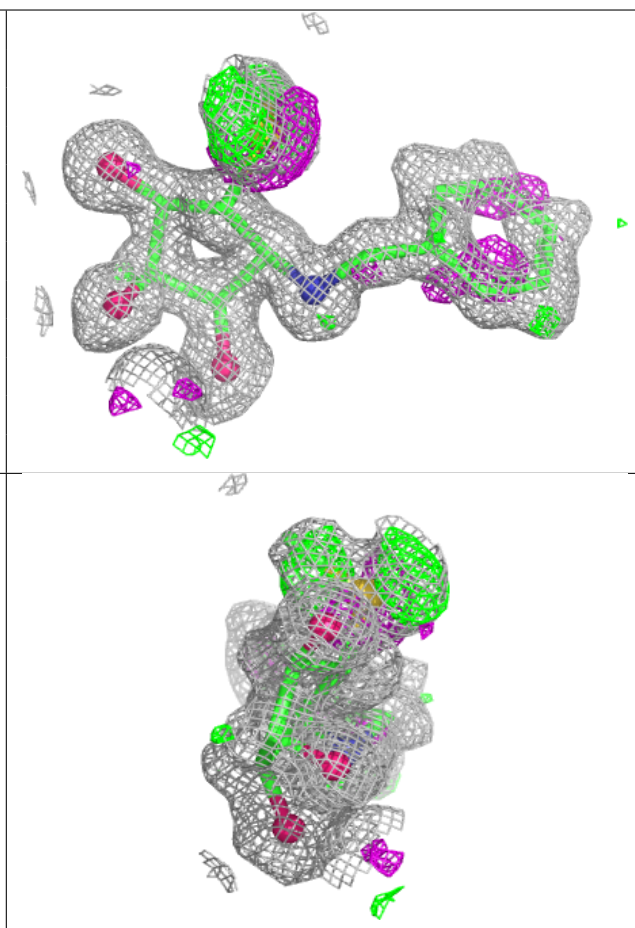
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	5002	14/15	0.66	0.19	33,40,44,44	0
4	2SK	A	5009[A]	18/18	0.95	0.09	6,7,19,19	1
4	2SK	A	5009[B]	18/18	0.95	0.09	6,7,19,19	1
5	MPD	A	5003	8/8	0.96	0.07	10,13,15,17	0
3	ZN	A	5001	1/1	1.00	0.01	5,5,5,5	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.

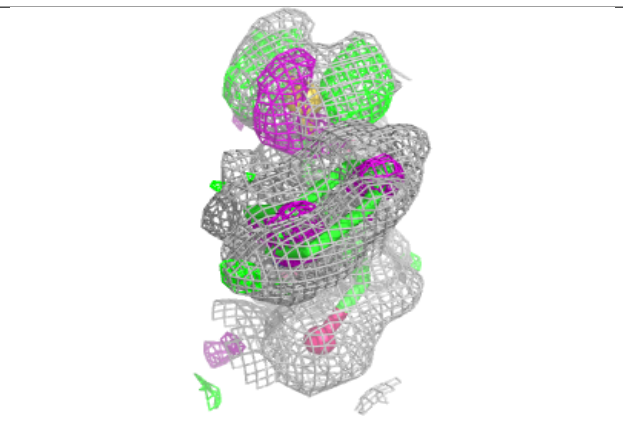
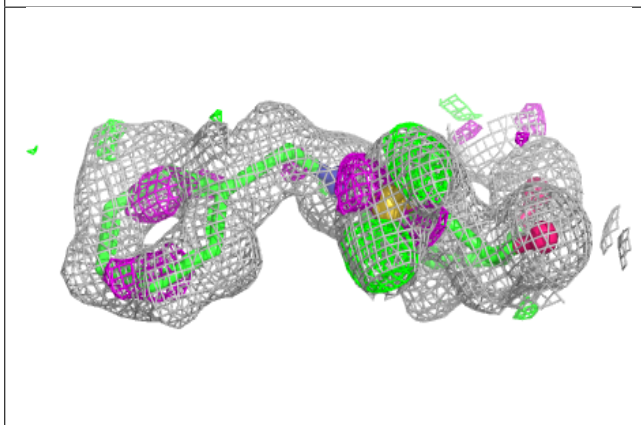
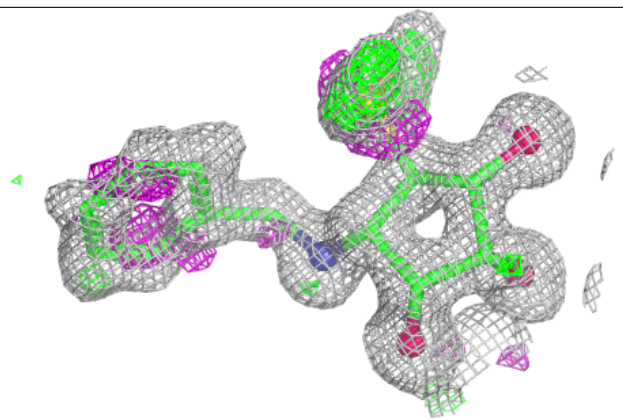
Electron density around 2SK A 5009 (A):

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2SK A 5009 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.