



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:44 AM UTC

PDB ID : 8ELE / pdb_00008ele
Title : Co-crystal structure of Chaetomium glucosidase with compound 16
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2022-09-23
Resolution : 2.60 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

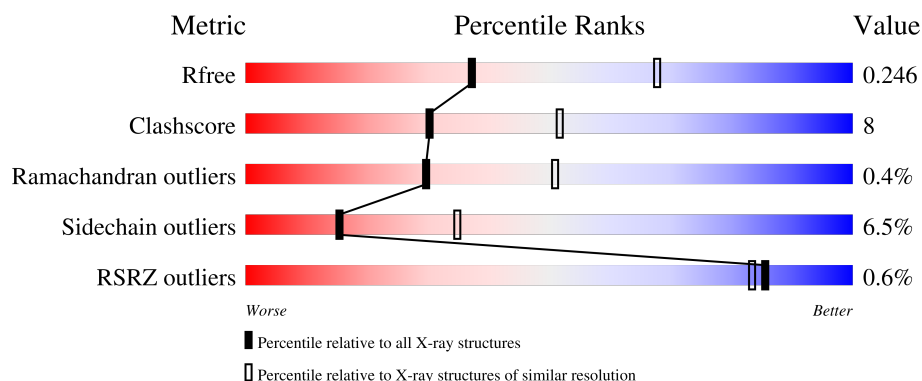
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	819	 73% 18% • 7%
1	B	819	 74% 17% • 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12325 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 Chaetomium alpha glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			6067	3899	1024	1131	13			
1	B	763	Total	C	N	O	S	0	0	0
			6067	3895	1020	1139	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP G0SFD1
A	0	GLY	-	expression tag	UNP G0SFD1
A	1	ILE	-	expression tag	UNP G0SFD1
A	2	LEU	-	expression tag	UNP G0SFD1
A	3	PRO	-	expression tag	UNP G0SFD1
A	4	SER	-	expression tag	UNP G0SFD1
A	5	PRO	-	expression tag	UNP G0SFD1
A	6	GLY	-	expression tag	UNP G0SFD1
A	7	MET	-	expression tag	UNP G0SFD1
A	8	PRO	-	expression tag	UNP G0SFD1
A	9	ALA	-	expression tag	UNP G0SFD1
A	10	LEU	-	expression tag	UNP G0SFD1
A	11	LEU	-	expression tag	UNP G0SFD1
A	12	SER	-	expression tag	UNP G0SFD1
A	13	LEU	-	expression tag	UNP G0SFD1
A	14	VAL	-	expression tag	UNP G0SFD1
A	15	SER	-	expression tag	UNP G0SFD1
A	16	LEU	-	expression tag	UNP G0SFD1
A	17	LEU	-	expression tag	UNP G0SFD1
A	18	SER	-	expression tag	UNP G0SFD1
A	19	VAL	-	expression tag	UNP G0SFD1
A	20	LEU	-	expression tag	UNP G0SFD1
A	21	LEU	-	expression tag	UNP G0SFD1
A	22	MET	-	expression tag	UNP G0SFD1
A	23	GLY	-	expression tag	UNP G0SFD1

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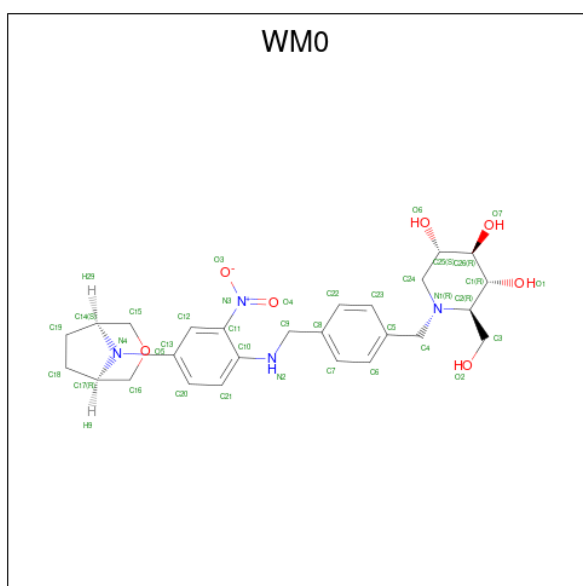
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	CYS	-	expression tag	UNP G0SFD1
A	25	VAL	-	expression tag	UNP G0SFD1
A	26	ALA	-	expression tag	UNP G0SFD1
A	27	GLU	-	expression tag	UNP G0SFD1
A	28	THR	-	expression tag	UNP G0SFD1
A	29	GLY	-	expression tag	UNP G0SFD1
A	810	SER	-	expression tag	UNP G0SFD1
A	811	GLY	-	expression tag	UNP G0SFD1
A	812	HIS	-	expression tag	UNP G0SFD1
A	813	HIS	-	expression tag	UNP G0SFD1
A	814	HIS	-	expression tag	UNP G0SFD1
A	815	HIS	-	expression tag	UNP G0SFD1
A	816	HIS	-	expression tag	UNP G0SFD1
A	817	HIS	-	expression tag	UNP G0SFD1
B	-1	MET	-	initiating methionine	UNP G0SFD1
B	0	GLY	-	expression tag	UNP G0SFD1
B	1	ILE	-	expression tag	UNP G0SFD1
B	2	LEU	-	expression tag	UNP G0SFD1
B	3	PRO	-	expression tag	UNP G0SFD1
B	4	SER	-	expression tag	UNP G0SFD1
B	5	PRO	-	expression tag	UNP G0SFD1
B	6	GLY	-	expression tag	UNP G0SFD1
B	7	MET	-	expression tag	UNP G0SFD1
B	8	PRO	-	expression tag	UNP G0SFD1
B	9	ALA	-	expression tag	UNP G0SFD1
B	10	LEU	-	expression tag	UNP G0SFD1
B	11	LEU	-	expression tag	UNP G0SFD1
B	12	SER	-	expression tag	UNP G0SFD1
B	13	LEU	-	expression tag	UNP G0SFD1
B	14	VAL	-	expression tag	UNP G0SFD1
B	15	SER	-	expression tag	UNP G0SFD1
B	16	LEU	-	expression tag	UNP G0SFD1
B	17	LEU	-	expression tag	UNP G0SFD1
B	18	SER	-	expression tag	UNP G0SFD1
B	19	VAL	-	expression tag	UNP G0SFD1
B	20	LEU	-	expression tag	UNP G0SFD1
B	21	LEU	-	expression tag	UNP G0SFD1
B	22	MET	-	expression tag	UNP G0SFD1
B	23	GLY	-	expression tag	UNP G0SFD1
B	24	CYS	-	expression tag	UNP G0SFD1
B	25	VAL	-	expression tag	UNP G0SFD1
B	26	ALA	-	expression tag	UNP G0SFD1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLU	-	expression tag	UNP G0SFD1
B	28	THR	-	expression tag	UNP G0SFD1
B	29	GLY	-	expression tag	UNP G0SFD1
B	810	SER	-	expression tag	UNP G0SFD1
B	811	GLY	-	expression tag	UNP G0SFD1
B	812	HIS	-	expression tag	UNP G0SFD1
B	813	HIS	-	expression tag	UNP G0SFD1
B	814	HIS	-	expression tag	UNP G0SFD1
B	815	HIS	-	expression tag	UNP G0SFD1
B	816	HIS	-	expression tag	UNP G0SFD1
B	817	HIS	-	expression tag	UNP G0SFD1

- Molecule 2 is (2R,3R,4R,5S)-2-(hydroxymethyl)-1-{{4-({2-nitro-4-[(1R,5S)-3-oxa-8-azabicyclo[3.2.1]octan-8-yl]anilino}methyl)phenyl}methyl}piperidine-3,4,5-triol (CCD ID: WM0) (formula: C₂₆H₃₄N₄O₇) (labeled as "Ligand of Interest" by depositor).



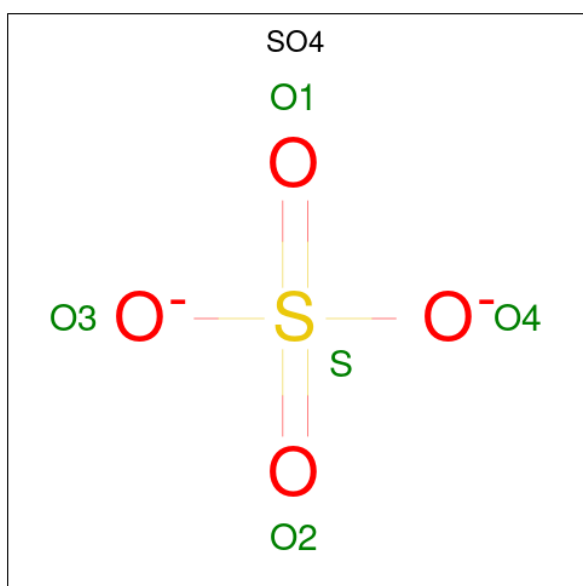
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	26	4	7		
2	B	1	Total	C	N	O	0	0
			37	26	4	7		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



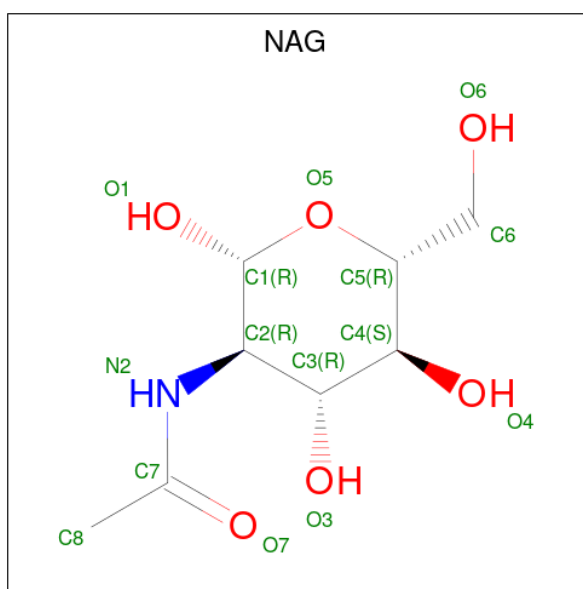
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

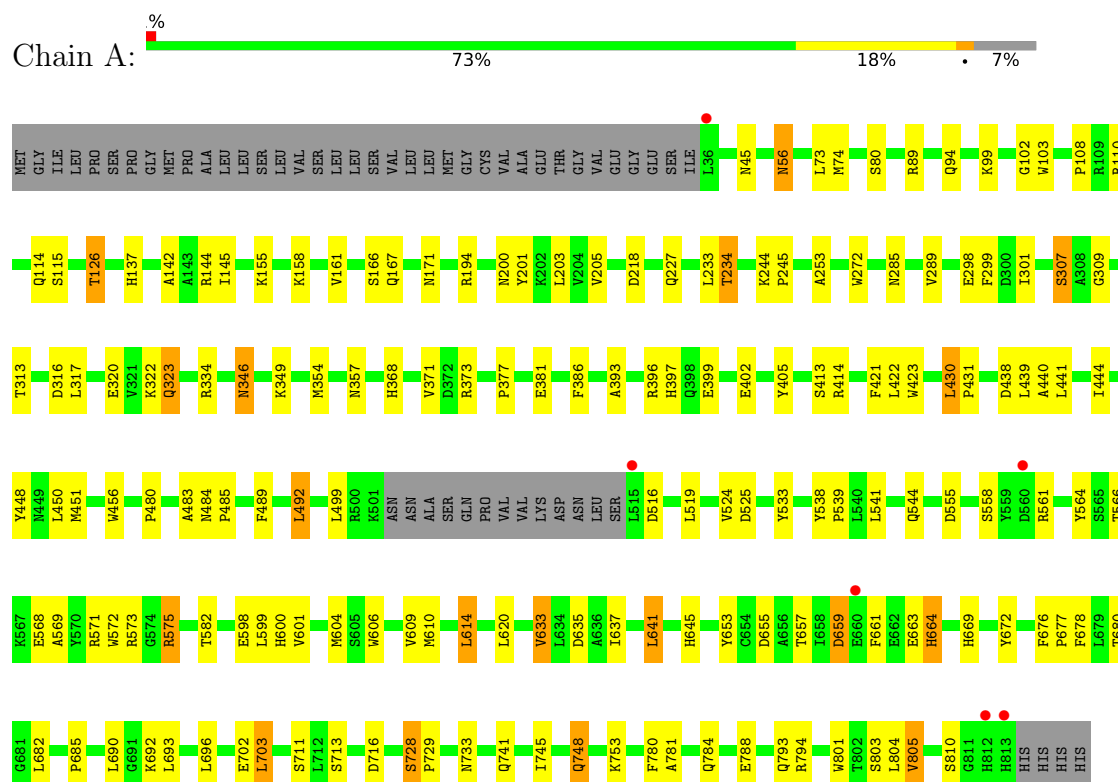
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total 14	O 14	0	0
6	B	27	Total 27	O 27	0	0

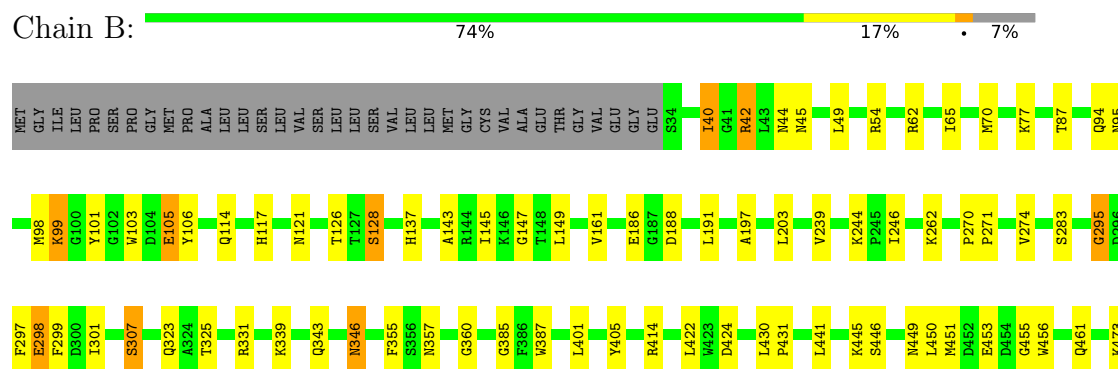
3 Residue-property plots

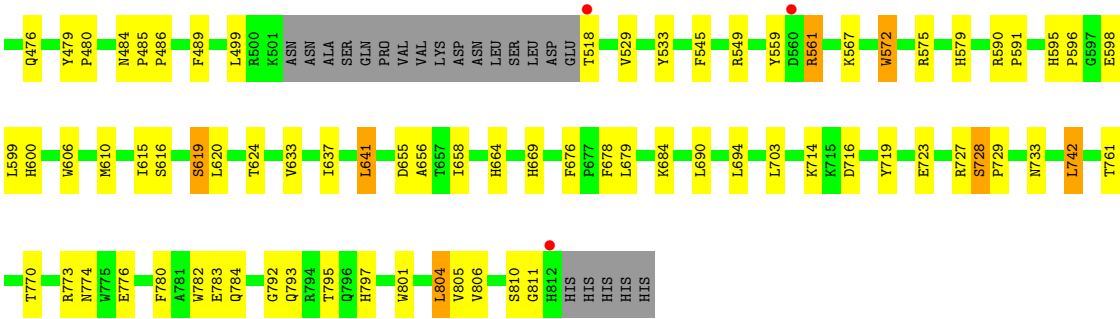
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chaetomium alpha glucosidase



• Molecule 1: Chaetomium alpha glucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.82Å 178.73Å 180.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.03 – 2.60 47.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.03-2.60) 98.4 (47.03-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.248 0.195 , 0.246	Depositor DCC
R_{free} test set	3447 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12325	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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, SO4, GOL, WM0

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	1.05	0/6243	1.44	6/8499 (0.1%)
1	B	1.04	0/6243	1.45	11/8497 (0.1%)
All	All	1.04	0/12486	1.45	17/16996 (0.1%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ARG	CB-CA-C	6.66	120.66	109.48
1	B	684	LYS	CB-CA-C	5.82	117.84	109.11
1	B	343	GLN	CA-C-N	5.74	125.55	120.10
1	B	343	GLN	C-N-CA	5.74	125.55	120.10
1	B	773	ARG	N-CA-C	-5.50	105.28	111.28
1	A	373	ARG	CA-C-N	5.49	128.19	120.28
1	A	373	ARG	C-N-CA	5.49	128.19	120.28
1	A	126	THR	CA-CB-OG1	-5.44	101.43	109.60
1	B	811	GLY	CA-C-O	-5.25	117.79	121.88
1	B	188	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	295	GLY	CA-C-N	5.12	128.15	120.87
1	B	295	GLY	C-N-CA	5.12	128.15	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	690	LEU	CA-C-N	5.07	125.61	119.98
1	B	690	LEU	C-N-CA	5.07	125.61	119.98
1	A	368	HIS	CA-C-N	5.02	128.33	120.75
1	A	368	HIS	C-N-CA	5.02	128.33	120.75
1	B	95	ASN	CA-C-O	-5.01	116.07	121.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	780	PHE	Peptide
1	B	780	PHE	Peptide

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	6067	0	5738	106	0
1	B	6067	0	5731	89	0
2	A	37	0	0	4	0
2	B	37	0	0	4	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	30	0	0	2	0
4	B	20	0	0	0	0
5	B	14	0	13	0	0
6	A	14	0	0	0	0
6	B	27	0	0	3	0
All	All	12325	0	11498	199	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 8.

All (199) 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)
2:B:1003:WM0:C15	2:B:1003:WM0:O5	1.86	1.24
2:A:901:WM0:C15	2:A:901:WM0:O5	1.86	1.22
1:A:659:ASP:OD1	1:A:663:GLU:O	1.57	1.20
1:A:568:GLU:OE2	1:A:633:VAL:HG13	1.85	0.77
1:A:598:GLU:OE2	1:A:600:HIS:HE1	1.68	0.76
1:A:685:PRO:HG3	1:A:748:GLN:HE22	1.50	0.75
1:B:784:GLN:HE21	1:B:793:GLN:HE21	1.35	0.75
1:B:103:TRP:H	1:B:357:ASN:ND2	1.85	0.74
1:B:137:HIS:HD2	1:B:307:SER:OG	1.73	0.71
1:B:346:ASN:HD22	1:B:346:ASN:H	1.38	0.71
1:B:559:TYR:CE1	1:B:658:ILE:HG13	2.26	0.71
1:A:598:GLU:OE2	1:A:600:HIS:CE1	2.44	0.71
1:B:572:TRP:H	1:B:600:HIS:HD2	1.37	0.71
1:B:385:GLY:HA2	1:B:387:TRP:CZ3	2.27	0.70
1:B:103:TRP:H	1:B:357:ASN:HD21	1.39	0.67
1:B:128:SER:O	1:B:143:ALA:HA	1.95	0.67
1:A:102:GLY:HA3	1:A:357:ASN:HD21	1.60	0.66
1:A:664:HIS:HD1	1:A:664:HIS:C	2.04	0.66
1:B:54:ARG:NE	1:B:70:MET:HE2	2.12	0.65
1:A:110:ARG:HH22	1:A:323:GLN:HG3	1.61	0.65
1:A:659:ASP:OD1	1:A:663:GLU:C	2.39	0.65
1:A:664:HIS:C	1:A:664:HIS:ND1	2.57	0.63
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.33	0.62
2:B:1003:WM0:N2	2:B:1003:WM0:O4	2.32	0.62
1:A:690:LEU:HD11	1:A:745:ILE:HD11	1.81	0.61
1:B:561:ARG:HE	1:B:664:HIS:HD2	1.49	0.60
1:A:569:ALA:HB1	1:A:599:LEU:HD22	1.82	0.60
1:A:234:THR:HA	1:A:285:ASN:OD1	2.01	0.60
1:B:784:GLN:NE2	1:B:793:GLN:HE21	2.00	0.59
1:B:42:ARG:NH2	6:B:1101:HOH:O	2.36	0.59
1:A:371:VAL:O	1:A:399:GLU:HA	2.02	0.59
1:A:561:ARG:NH2	1:A:657:THR:O	2.36	0.58
1:B:87:THR:HB	1:B:121:ASN:HD21	1.67	0.58
1:A:393:ALA:O	1:A:396:ARG:HB2	2.03	0.57
1:A:659:ASP:OD1	1:A:659:ASP:N	2.36	0.57
1:B:114:GLN:HE22	1:B:414:ARG:HH22	1.52	0.56
1:B:561:ARG:HA	6:B:1110:HOH:O	2.05	0.56
1:A:685:PRO:CG	1:A:748:GLN:HE22	2.18	0.56
1:A:489:PHE:CE1	1:A:610:MET:HE3	2.41	0.56
1:B:595:HIS:ND1	1:B:596:PRO:HD2	2.20	0.56
1:B:572:TRP:H	1:B:600:HIS:CD2	2.22	0.55
1:B:783:GLU:OE1	1:B:795:THR:HG23	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:MET:HE2	1:B:101:TYR:HD1	1.72	0.54
1:A:114:GLN:NE2	1:A:414:ARG:HH12	2.05	0.54
1:A:171:ASN:N	4:A:903:SO4:O4	2.38	0.54
2:A:901:WM0:C15	2:A:901:WM0:C16	2.52	0.53
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.43	0.53
1:B:137:HIS:CD2	1:B:307:SER:OG	2.59	0.53
1:B:149:LEU:HD11	1:B:295:GLY:HA2	1.91	0.53
1:B:203:LEU:HD11	1:B:301:ILE:HG23	1.90	0.53
1:B:590:ARG:HB3	1:B:591:PRO:CD	2.38	0.53
1:A:103:TRP:H	1:A:357:ASN:ND2	2.06	0.53
1:B:430:LEU:HB2	1:B:431:PRO:HD3	1.90	0.53
1:B:77:LYS:H	1:B:121:ASN:ND2	2.07	0.53
1:A:114:GLN:HE22	1:A:414:ARG:HH22	1.55	0.53
1:A:748:GLN:O	1:A:753:LYS:HD2	2.09	0.53
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.44	0.52
1:B:62:ARG:HD2	1:B:70:MET:HE3	1.91	0.52
1:B:801:TRP:O	1:B:804:LEU:HB2	2.09	0.52
1:B:106:TYR:CD2	1:B:360:GLY:HA2	2.45	0.52
1:A:672:TYR:CE2	1:A:711:SER:HA	2.45	0.52
1:B:203:LEU:HD11	1:B:301:ILE:CG2	2.40	0.51
1:B:579:HIS:NE2	1:B:723:GLU:OE1	2.34	0.51
1:A:73:LEU:HD22	1:A:145:ILE:HD12	1.91	0.51
1:B:572:TRP:N	1:B:600:HIS:HD2	2.07	0.51
1:B:65:ILE:HD13	1:B:197:ALA:HB1	1.93	0.51
1:B:669:HIS:ND1	1:B:716:ASP:OD1	2.36	0.51
1:A:421:PHE:CD2	2:A:901:WM0:C3	2.93	0.50
1:A:56:ASN:H	1:A:56:ASN:HD22	1.60	0.50
1:A:158:LYS:HD3	1:A:272:TRP:CD1	2.47	0.49
1:A:564:TYR:OH	1:A:635:ASP:OD2	2.20	0.49
1:A:572:TRP:H	1:A:600:HIS:HD2	1.59	0.49
1:A:678:PHE:O	1:A:741:GLN:HG3	2.12	0.49
1:A:728:SER:OG	1:A:729:PRO:HD3	2.13	0.49
1:A:244:LYS:HB3	1:A:245:PRO:HD3	1.94	0.49
1:B:98:MET:HE2	1:B:101:TYR:CD1	2.47	0.49
1:B:567:LYS:O	1:B:567:LYS:HD3	2.13	0.49
1:A:803:SER:C	1:A:805:VAL:H	2.19	0.49
2:B:1003:WM0:C6	2:B:1003:WM0:C24	2.91	0.49
1:A:696:LEU:HG	1:A:703:LEU:HD22	1.95	0.48
1:A:397:HIS:HA	1:A:399:GLU:OE1	2.14	0.48
1:A:728:SER:N	1:A:729:PRO:CD	2.76	0.48
1:A:346:ASN:H	1:A:346:ASN:HD22	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HH22	1:A:323:GLN:CG	2.26	0.48
1:A:456:TRP:CD2	1:A:480:PRO:HA	2.49	0.48
1:B:145:ILE:O	1:B:298:GLU:HA	2.13	0.48
1:A:669:HIS:HA	1:A:716:ASP:OD2	2.14	0.48
1:A:166:SER:HA	1:A:285:ASN:O	2.14	0.47
1:B:473:LYS:HA	1:B:476:GLN:HG3	1.96	0.47
1:A:167:GLN:NE2	1:A:201:TYR:OH	2.48	0.47
1:A:137:HIS:HD2	1:A:307:SER:HB3	1.80	0.47
1:B:784:GLN:HE21	1:B:793:GLN:HG3	1.78	0.47
1:A:784:GLN:NE2	1:A:793:GLN:HE21	2.12	0.47
1:B:114:GLN:O	1:B:126:THR:HA	2.14	0.47
1:A:430:LEU:HB2	1:A:431:PRO:HD3	1.97	0.47
1:A:485:PRO:HB3	1:A:606:TRP:CE2	2.50	0.47
1:B:600:HIS:HA	1:B:655:ASP:OD1	2.15	0.47
1:B:782:TRP:CG	1:B:792:GLY:HA3	2.50	0.46
1:A:448:TYR:OH	1:A:544:GLN:NE2	2.48	0.46
1:A:114:GLN:HE21	1:A:414:ARG:HH12	1.63	0.46
1:B:422:LEU:HB3	1:B:484:ASN:HD22	1.81	0.46
1:A:227:GLN:N	1:A:227:GLN:CD	2.74	0.46
1:B:40:ILE:HD13	1:B:529:VAL:HG21	1.97	0.46
1:B:161:VAL:HG11	1:B:299:PHE:HE1	1.80	0.45
1:A:161:VAL:HG11	1:A:299:PHE:HE2	1.81	0.45
1:A:538:TYR:HB3	1:A:539:PRO:HD3	1.99	0.45
1:B:456:TRP:CD2	1:B:480:PRO:HA	2.51	0.45
1:A:253:ALA:HA	1:B:262:LYS:HE3	1.99	0.45
1:A:313:THR:O	1:A:316:ASP:HB2	2.16	0.45
1:A:609:VAL:HG23	1:A:680:THR:HB	1.98	0.45
1:B:103:TRP:N	1:B:357:ASN:HD21	2.11	0.45
1:B:575:ARG:NH1	1:B:598:GLU:OE2	2.49	0.45
1:B:239:VAL:HG12	1:B:246:ILE:HD11	1.97	0.45
1:B:451:MET:SD	1:B:455:GLY:HA2	2.56	0.45
1:A:803:SER:C	1:A:805:VAL:N	2.74	0.45
1:B:678:PHE:HZ	1:B:742:LEU:HD13	1.82	0.45
1:B:728:SER:N	1:B:729:PRO:CD	2.80	0.45
1:A:74:MET:HA	1:A:89:ARG:O	2.16	0.45
1:B:590:ARG:HB3	1:B:591:PRO:HD2	1.99	0.45
1:A:784:GLN:HE21	1:A:793:GLN:HE21	1.65	0.44
1:A:555:ASP:OD1	1:A:558:SER:HB3	2.17	0.44
1:A:110:ARG:NH2	1:A:323:GLN:HG3	2.31	0.44
1:A:483:ALA:O	1:A:582:THR:HB	2.18	0.44
1:A:561:ARG:HE	1:A:664:HIS:CD2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:O	1:A:645:HIS:HB2	2.17	0.44
1:A:741:GLN:NE2	1:A:741:GLN:HA	2.33	0.44
1:A:441:LEU:HD22	1:A:533:TYR:CE2	2.52	0.44
1:B:637:ILE:O	1:B:641:LEU:HB2	2.17	0.44
1:B:479:TYR:HA	1:B:480:PRO:HD3	1.88	0.43
1:A:423:TRP:H	1:A:484:ASN:ND2	2.16	0.43
1:A:702:GLU:HA	1:A:713:SER:OG	2.19	0.43
2:A:901:WM0:C6	2:A:901:WM0:C24	2.96	0.43
1:A:203:LEU:HD11	1:A:301:ILE:HG23	2.00	0.43
1:B:559:TYR:CD1	1:B:658:ILE:HG13	2.53	0.43
1:A:499:LEU:HD12	1:A:499:LEU:HA	1.87	0.43
1:A:672:TYR:CZ	1:A:711:SER:HA	2.53	0.43
1:B:99:LYS:HB3	1:B:117:HIS:O	2.18	0.43
1:A:161:VAL:HG11	1:A:299:PHE:CE2	2.54	0.43
1:A:194:ARG:HG3	1:A:200:ASN:OD1	2.18	0.43
1:B:346:ASN:H	1:B:346:ASN:ND2	2.13	0.43
1:B:615:ILE:O	1:B:619:SER:HB3	2.19	0.43
1:A:604:MET:HE3	1:A:604:MET:HB2	1.85	0.43
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.82	0.43
1:B:533:TYR:C	1:B:533:TYR:CD1	2.97	0.43
1:B:545:PHE:CZ	1:B:549:ARG:HD2	2.53	0.43
1:B:94:GLN:OE1	1:B:797:HIS:HE1	2.02	0.43
1:B:385:GLY:HA2	1:B:387:TRP:CE3	2.53	0.43
1:B:499:LEU:HD12	1:B:499:LEU:HA	1.87	0.43
1:A:690:LEU:HD11	1:A:745:ILE:CD1	2.47	0.43
1:B:489:PHE:CE1	1:B:610:MET:HE3	2.53	0.42
1:A:144:ARG:HB2	1:A:317:LEU:HD21	1.99	0.42
1:A:402:GLU:OE2	1:A:405:TYR:OH	2.37	0.42
1:A:205:VAL:HG11	1:A:289:VAL:HG11	1.99	0.42
1:B:323:GLN:HE21	1:B:323:GLN:HA	1.83	0.42
1:B:405:TYR:CE2	3:B:1001:GOL:H32	2.55	0.42
1:B:147:GLY:HA3	1:B:297:PHE:CZ	2.55	0.42
1:B:804:LEU:HD12	1:B:804:LEU:HA	1.86	0.42
1:A:346:ASN:HD22	1:A:346:ASN:N	2.17	0.42
1:B:106:TYR:CE2	1:B:360:GLY:HA2	2.55	0.42
1:B:270:PRO:HA	1:B:271:PRO:HD3	1.96	0.42
1:B:355:PHE:HB2	1:B:806:VAL:HG21	2.02	0.42
1:B:484:ASN:O	1:B:485:PRO:C	2.63	0.42
1:A:492:LEU:HD12	1:A:492:LEU:HA	1.79	0.41
1:B:770:THR:O	1:B:774:ASN:ND2	2.43	0.41
1:A:609:VAL:CG2	1:A:680:THR:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ARG:O	1:B:728:SER:HB3	2.20	0.41
1:A:56:ASN:H	1:A:56:ASN:ND2	2.17	0.41
1:A:450:LEU:O	4:A:906:SO4:O3	2.37	0.41
1:A:685:PRO:HG3	1:A:748:GLN:NE2	2.25	0.41
1:B:450:LEU:HD13	1:B:461:GLN:OE1	2.21	0.41
1:A:108:PRO:HG2	1:A:439:LEU:HD22	2.03	0.41
1:A:422:LEU:HB3	1:A:484:ASN:HD22	1.85	0.41
1:A:653:TYR:CG	1:A:677:PRO:HG2	2.56	0.41
1:B:518:THR:N	6:B:1105:HOH:O	2.53	0.41
1:A:728:SER:H	1:A:729:PRO:CD	2.32	0.41
1:B:599:LEU:HB2	1:B:656:ALA:HB3	2.01	0.41
1:A:145:ILE:O	1:A:298:GLU:HA	2.20	0.41
1:A:489:PHE:CZ	1:A:610:MET:HE3	2.56	0.41
1:A:571:ARG:O	1:A:573:ARG:NH1	2.54	0.41
1:A:653:TYR:CD2	1:A:677:PRO:HG2	2.55	0.41
1:B:346:ASN:HD22	1:B:346:ASN:N	2.12	0.41
1:B:486:PRO:HD2	1:B:606:TRP:HB3	2.02	0.41
1:A:377:PRO:HG3	1:B:401:LEU:HG	2.03	0.41
1:A:614:LEU:HD12	1:A:614:LEU:HA	1.88	0.41
1:B:424:ASP:OD2	2:B:1003:WM0:O2	2.39	0.41
1:B:105:GLU:OE2	1:B:325:THR:HG23	2.22	0.40
1:B:620:LEU:HD12	1:B:620:LEU:HA	1.98	0.40
1:A:110:ARG:HD3	1:A:516:ASP:OD2	2.21	0.40
1:A:381:GLU:HA	1:A:386:PHE:HB2	2.03	0.40
1:A:440:ALA:O	1:A:444:ILE:HG13	2.21	0.40
1:B:714:LYS:HA	1:B:719:TYR:CD1	2.56	0.40
1:A:354:MET:HE1	1:A:781:ALA:HB2	2.03	0.40
1:A:524:VAL:HG23	1:A:525:ASP:OD1	2.20	0.40
1:A:430:LEU:CB	1:A:431:PRO:HD3	2.51	0.40
1:A:142:ALA:HA	1:A:301:ILE:O	2.22	0.40
1:A:451:MET:HE1	1:A:544:GLN:HB2	2.04	0.40
1:A:601:VAL:HG12	1:A:655:ASP:OD1	2.21	0.40
1:B:561:ARG:HE	1:B:664:HIS:CD2	2.34	0.40
1:B:633:VAL:HG12	1:B:637:ILE:HD12	2.04	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	761/819 (93%)	722 (95%)	36 (5%)	3 (0%)	30	51
1	B	759/819 (93%)	713 (94%)	43 (6%)	3 (0%)	30	51
All	All	1520/1638 (93%)	1435 (94%)	79 (5%)	6 (0%)	30	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	728	SER
1	B	728	SER
1	B	733	ASN
1	A	309	GLY
1	A	804	LEU
1	B	572	TRP

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	627/707 (89%)	583 (93%)	44 (7%)	14	31
1	B	630/707 (89%)	592 (94%)	38 (6%)	17	37
All	All	1257/1414 (89%)	1175 (94%)	82 (6%)	15	35

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	56	ASN
1	A	80	SER
1	A	94	GLN
1	A	99	LYS
1	A	115	SER
1	A	126	THR
1	A	155	LYS
1	A	218	ASP
1	A	233	LEU
1	A	234	THR
1	A	307	SER
1	A	320	GLU
1	A	322	LYS
1	A	323	GLN
1	A	334	ARG
1	A	346	ASN
1	A	349	LYS
1	A	413	SER
1	A	430	LEU
1	A	438	ASP
1	A	492	LEU
1	A	519	LEU
1	A	541	LEU
1	A	566	THR
1	A	575	ARG
1	A	614	LEU
1	A	620	LEU
1	A	633	VAL
1	A	637	ILE
1	A	641	LEU
1	A	659	ASP
1	A	661	PHE
1	A	664	HIS
1	A	676	PHE
1	A	682	LEU
1	A	692	LYS
1	A	693	LEU
1	A	703	LEU
1	A	748	GLN
1	A	788	GLU
1	A	794	ARG
1	A	805	VAL

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Mol	Chain	Res	Type
1	A	810	SER
1	B	40	ILE
1	B	42	ARG
1	B	44	ASN
1	B	45	ASN
1	B	49	LEU
1	B	99	LYS
1	B	105	GLU
1	B	128	SER
1	B	186	GLU
1	B	191	LEU
1	B	244	LYS
1	B	274	VAL
1	B	283	SER
1	B	298	GLU
1	B	307	SER
1	B	331	ARG
1	B	339	LYS
1	B	346	ASN
1	B	441	LEU
1	B	445	LYS
1	B	446	SER
1	B	449	ASN
1	B	453	GLU
1	B	561	ARG
1	B	616	SER
1	B	619	SER
1	B	624	THR
1	B	641	LEU
1	B	676	PHE
1	B	679	LEU
1	B	694	LEU
1	B	703	LEU
1	B	742	LEU
1	B	761	THR
1	B	776	GLU
1	B	804	LEU
1	B	805	VAL
1	B	810	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	56	ASN
1	A	86	HIS
1	A	114	GLN
1	A	137	HIS
1	A	157	GLN
1	A	167	GLN
1	A	242	GLN
1	A	249	GLN
1	A	287	HIS
1	A	343	GLN
1	A	346	ASN
1	A	357	ASN
1	A	383	ASN
1	A	398	GLN
1	A	484	ASN
1	A	544	GLN
1	A	600	HIS
1	A	741	GLN
1	A	748	GLN
1	A	784	GLN
1	A	797	HIS
1	A	813	HIS
1	B	44	ASN
1	B	85	GLN
1	B	114	GLN
1	B	121	ASN
1	B	137	HIS
1	B	157	GLN
1	B	167	GLN
1	B	287	HIS
1	B	323	GLN
1	B	346	ASN
1	B	357	ASN
1	B	398	GLN
1	B	476	GLN
1	B	481	HIS
1	B	484	ASN
1	B	600	HIS
1	B	639	HIS
1	B	664	HIS
1	B	733	ASN
1	B	748	GLN

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Mol	Chain	Res	Type
1	B	784	GLN
1	B	797	HIS
1	B	812	HIS

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](#)

15 ligands are modelled in this entry.

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	NAG	B	1002	1	14,14,15	0.83	0	17,19,21	1.89	2 (11%)
4	SO4	A	908	-	4,4,4	0.30	0	6,6,6	0.15	0
4	SO4	A	907	-	4,4,4	0.30	0	6,6,6	0.09	0
4	SO4	B	1007	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	A	903	-	4,4,4	0.35	0	6,6,6	0.17	0
4	SO4	B	1004	-	4,4,4	0.36	0	6,6,6	0.25	0
4	SO4	B	1005	-	4,4,4	0.26	0	6,6,6	0.15	0
3	GOL	B	1001	-	5,5,5	0.21	0	5,5,5	0.38	0
2	WM0	B	1003	-	41,41,41	9.29	19 (46%)	51,59,59	2.64	15 (29%)
3	GOL	A	902	-	5,5,5	0.14	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	WM0	A	901	-	41,41,41	9.24	17 (41%)	51,59,59	3.13	18 (35%)
4	SO4	A	905	-	4,4,4	0.34	0	6,6,6	0.22	0
4	SO4	A	906	-	4,4,4	0.25	0	6,6,6	0.17	0
4	SO4	A	904	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	B	1006	-	4,4,4	0.34	0	6,6,6	0.14	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
5	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
3	GOL	B	1001	-	-	2/4/4/4	-
2	WM0	B	1003	-	-	0/17/58/58	0/6/5/5
3	GOL	A	902	-	-	2/4/4/4	-
2	WM0	A	901	-	-	5/17/58/58	0/6/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	WM0	C15-C14	-37.37	0.89	1.51
2	B	1003	WM0	C15-C14	-37.29	0.89	1.51
2	A	901	WM0	O5-C15	23.03	1.86	1.43
2	B	1003	WM0	O5-C15	23.00	1.86	1.43
2	A	901	WM0	C14-N4	-21.47	1.27	1.47
2	B	1003	WM0	C14-N4	-21.45	1.27	1.47
2	B	1003	WM0	C4-N1	-16.44	1.19	1.47
2	A	901	WM0	C4-N1	-15.48	1.21	1.47
2	A	901	WM0	C19-C14	-13.81	1.19	1.53
2	B	1003	WM0	C19-C14	-13.78	1.19	1.53
2	B	1003	WM0	C18-C17	-13.11	1.21	1.53
2	A	901	WM0	C18-C17	-13.09	1.21	1.53
2	B	1003	WM0	C16-C17	-12.14	1.31	1.51
2	A	901	WM0	O5-C16	-12.13	1.19	1.43
2	A	901	WM0	C16-C17	-12.13	1.31	1.51
2	B	1003	WM0	O5-C16	-12.08	1.20	1.43
2	A	901	WM0	O4-N3	10.52	1.40	1.22
2	B	1003	WM0	O4-N3	10.46	1.40	1.22
2	B	1003	WM0	C25-C26	-4.70	1.45	1.52
2	A	901	WM0	C10-N2	3.97	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	WM0	C17-N4	-3.91	1.43	1.47
2	A	901	WM0	C1-C26	-3.88	1.42	1.52
2	B	1003	WM0	C17-N4	-3.74	1.44	1.47
2	B	1003	WM0	C10-N2	3.72	1.47	1.37
2	B	1003	WM0	C1-C26	-3.64	1.42	1.52
2	A	901	WM0	C25-C26	-3.33	1.47	1.52
2	B	1003	WM0	C10-C11	-3.32	1.35	1.40
2	B	1003	WM0	C13-N4	3.06	1.47	1.40
2	A	901	WM0	C13-N4	3.00	1.47	1.40
2	B	1003	WM0	C24-N1	-2.87	1.42	1.47
2	A	901	WM0	C4-C5	2.78	1.56	1.51
2	A	901	WM0	O7-C26	2.59	1.49	1.43
2	B	1003	WM0	C19-C18	-2.58	1.47	1.54
2	A	901	WM0	C19-C18	-2.57	1.47	1.54
2	B	1003	WM0	C4-C5	2.41	1.55	1.51
2	B	1003	WM0	C9-C8	2.05	1.56	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	WM0	C18-C17-N4	-12.83	93.64	102.03
2	B	1003	WM0	C18-C17-N4	-12.60	93.80	102.03
2	A	901	WM0	O1-C1-C26	-6.74	94.50	110.38
2	A	901	WM0	O5-C16-C17	6.46	120.01	111.16
2	B	1003	WM0	O5-C16-C17	6.41	119.93	111.16
5	B	1002	NAG	C1-O5-C5	6.22	120.52	112.19
2	A	901	WM0	C18-C17-C16	-5.41	106.80	111.64
2	A	901	WM0	C13-N4-C14	5.28	126.83	121.18
2	B	1003	WM0	C18-C17-C16	-5.24	106.95	111.64
2	A	901	WM0	C13-N4-C17	5.20	126.75	121.18
2	A	901	WM0	C21-C10-N2	-5.16	113.22	121.75
2	A	901	WM0	C26-C1-C2	-4.56	103.67	111.37
2	A	901	WM0	O1-C1-C2	-4.49	101.64	109.87
2	A	901	WM0	C19-C14-N4	-4.33	99.20	102.03
2	B	1003	WM0	C13-N4-C14	4.11	125.58	121.18
2	B	1003	WM0	C19-C14-N4	-4.04	99.39	102.03
2	B	1003	WM0	C13-N4-C17	4.02	125.49	121.18
5	B	1002	NAG	C4-C3-C2	3.78	116.55	111.02
2	B	1003	WM0	C11-C10-N2	-3.42	117.52	123.38
2	B	1003	WM0	O6-C25-C26	-2.81	104.33	110.15
2	B	1003	WM0	O1-C1-C26	-2.73	103.94	110.38
2	A	901	WM0	C18-C19-C14	2.53	107.86	104.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1003	WM0	C18-C19-C14	2.49	107.79	104.08
2	A	901	WM0	C12-C11-C10	-2.47	119.30	121.55
2	A	901	WM0	C4-N1-C24	2.28	114.88	110.33
2	A	901	WM0	C25-C26-C1	-2.25	106.90	110.86
2	B	1003	WM0	C3-C2-N1	-2.24	107.95	112.51
2	A	901	WM0	C9-C8-C7	-2.17	116.51	120.94
2	A	901	WM0	C23-C5-C6	2.17	121.45	118.23
2	B	1003	WM0	O7-C26-C25	-2.16	105.64	110.05
2	A	901	WM0	C22-C8-C7	2.15	121.44	118.23
2	B	1003	WM0	C5-C4-N1	2.13	116.19	112.73
2	B	1003	WM0	O2-C3-C2	-2.10	106.92	111.55
2	A	901	WM0	C24-C25-C26	2.02	112.57	110.17
2	B	1003	WM0	C3-C2-C1	-2.01	109.91	112.93

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	WM0	C11-C10-N2-C9
2	A	901	WM0	C1-C2-C3-O2
3	A	902	GOL	C1-C2-C3-O3
2	A	901	WM0	C21-C10-N2-C9
2	A	901	WM0	C5-C4-N1-C24
3	B	1001	GOL	O1-C1-C2-C3
3	A	902	GOL	O2-C2-C3-O3
3	B	1001	GOL	O1-C1-C2-O2
2	A	901	WM0	C5-C4-N1-C2

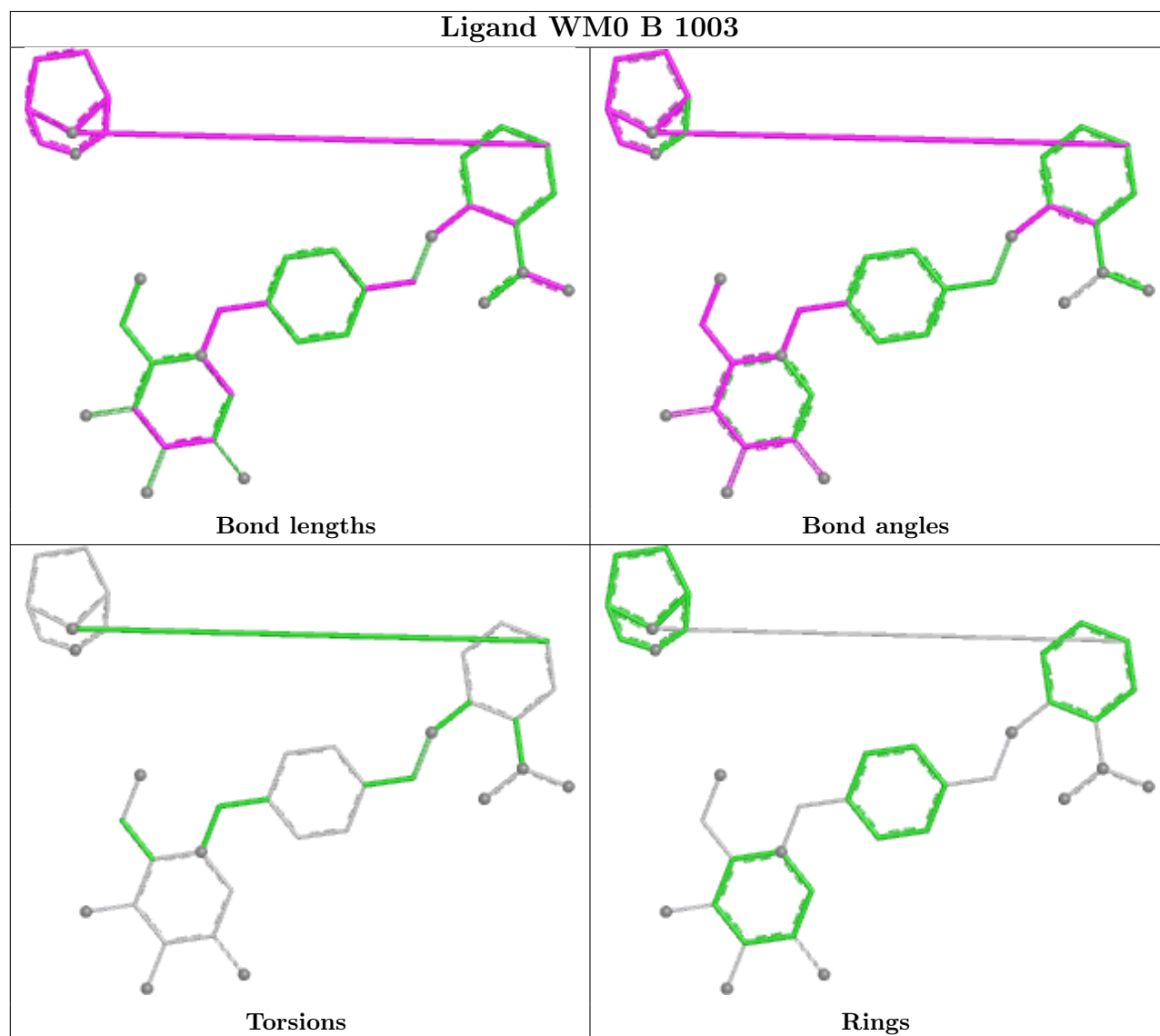
There are no ring outliers.

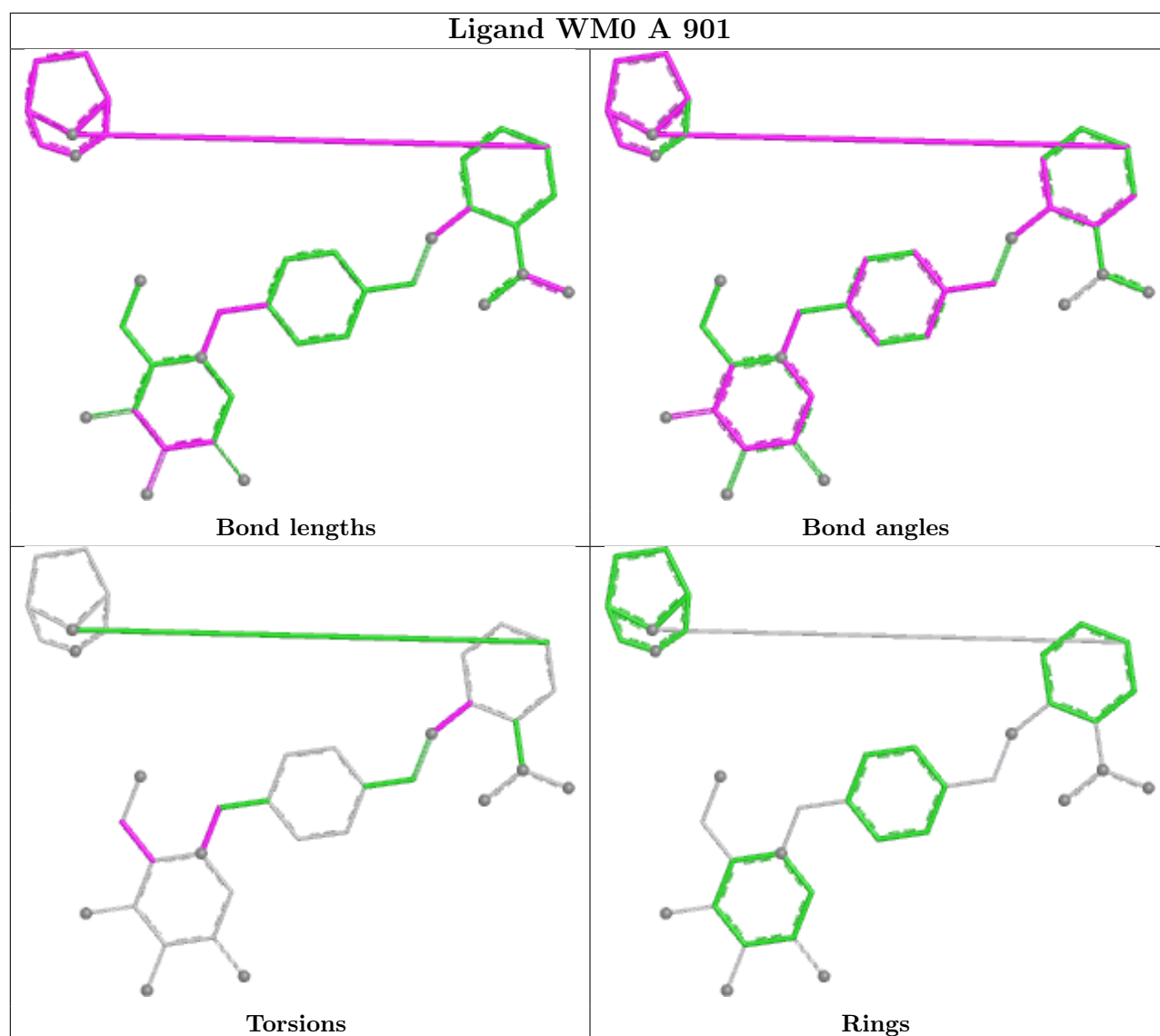
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	SO4	1	0
3	B	1001	GOL	1	0
2	B	1003	WM0	4	0
2	A	901	WM0	4	0
4	A	906	SO4	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 [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 [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	765/819 (93%)	-0.19	6 (0%)	82 80	42, 63, 93, 116	0
1	B	763/819 (93%)	-0.27	3 (0%)	88 86	42, 62, 90, 127	0
All	All	1528/1638 (93%)	-0.23	9 (0%)	85 83	42, 63, 91, 127	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	518	THR	3.5
1	A	515	LEU	3.3
1	A	812	HIS	3.2
1	B	812	HIS	3.2
1	B	560	ASP	3.0
1	A	660	GLU	2.6
1	A	813	HIS	2.6
1	A	560	ASP	2.3
1	A	36	LEU	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.

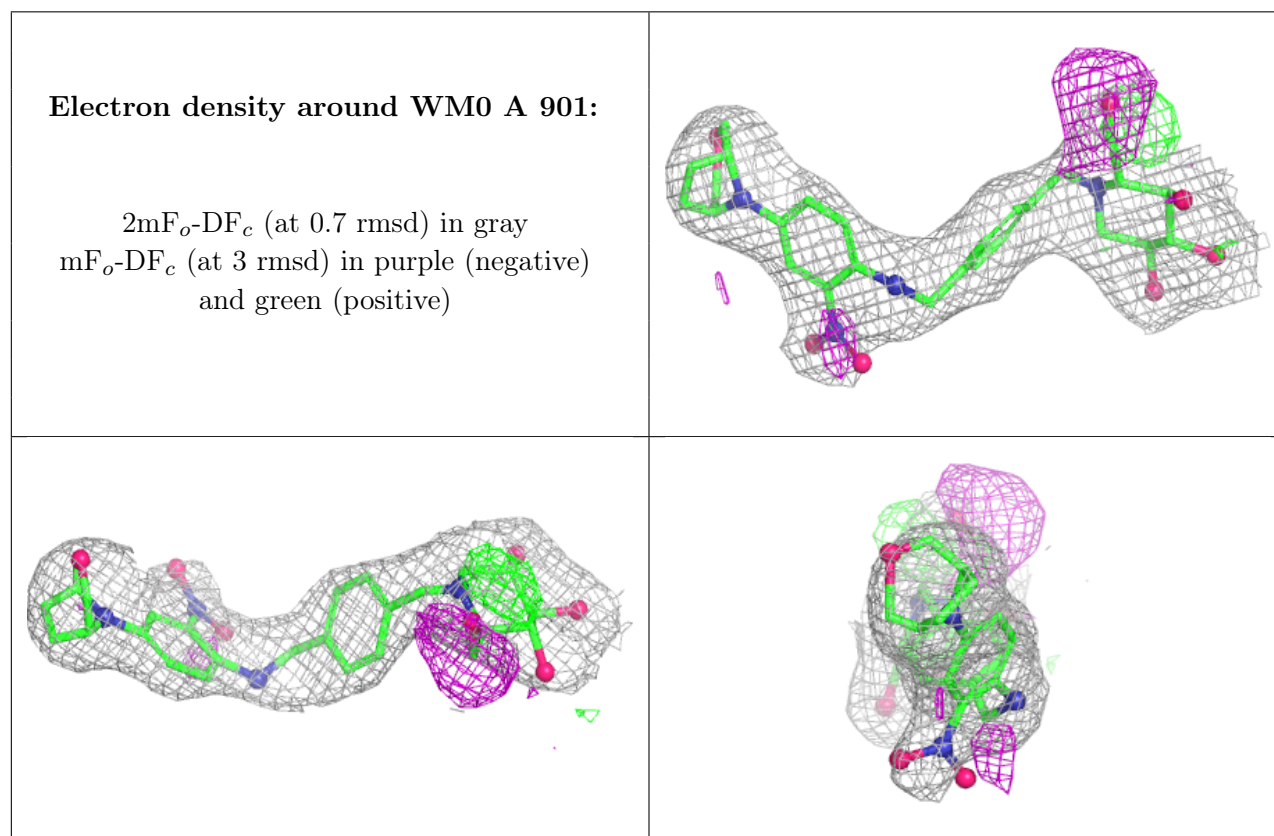
6.4 Ligands [i](#)

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.

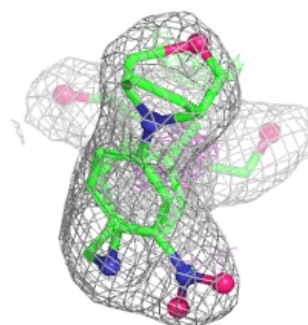
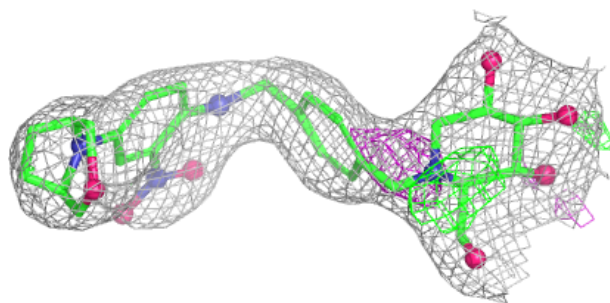
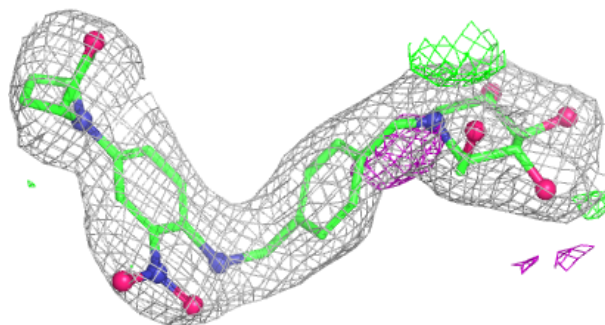
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	1002	14/15	0.78	0.12	81,96,102,103	0
4	SO4	A	904	5/5	0.82	0.10	91,98,108,134	0
4	SO4	A	903	5/5	0.83	0.09	108,113,127,132	0
4	SO4	B	1005	5/5	0.87	0.12	77,80,105,112	0
4	SO4	A	908	5/5	0.87	0.07	99,121,128,131	0
4	SO4	A	907	5/5	0.88	0.07	85,96,103,109	0
2	WM0	A	901	37/37	0.88	0.15	34,54,135,139	0
3	GOL	A	902	6/6	0.90	0.12	73,82,100,103	0
4	SO4	B	1006	5/5	0.92	0.15	79,84,93,98	0
4	SO4	A	906	5/5	0.92	0.12	84,86,116,125	0
3	GOL	B	1001	6/6	0.93	0.12	50,65,74,88	0
4	SO4	B	1007	5/5	0.94	0.10	69,79,93,101	0
2	WM0	B	1003	37/37	0.94	0.12	34,54,135,139	0
4	SO4	A	905	5/5	0.98	0.05	51,55,61,64	0
4	SO4	B	1004	5/5	0.98	0.06	49,56,65,80	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 WM0 B 1003:

$2mF_o-DF_c$ (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.