



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:40 PM UTC

PDB ID : 8EQ7 / pdb_00008eq7
Title : Co-crystal structure of Chaetomium glucosidase with compound 20
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2022-10-07
Resolution : 2.21 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

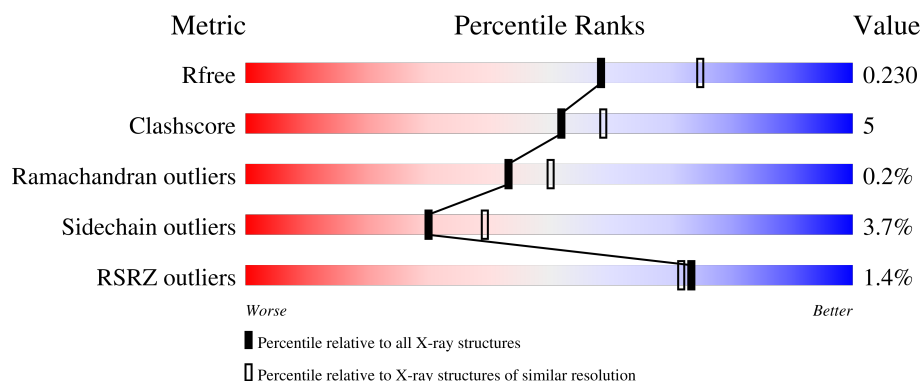
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	819	
1	B	819	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12713 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	2	0
			6063	3896	1024	1130	13			
1	B	766	Total	C	N	O	S	0	0	0
			6085	3905	1022	1145	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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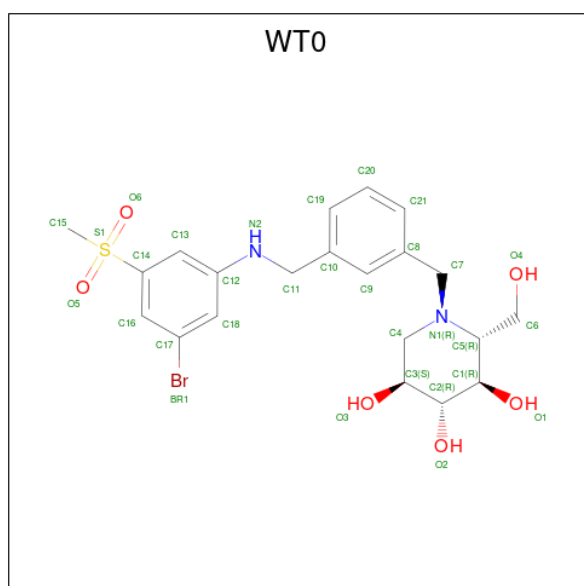
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	CYS	-	expression tag	UNP G0SFD1
A	25	VAL	-	expression tag	UNP G0SFD1
A	26	ALA	-	expression tag	UNP G0SFD1
A	27	GLU	-	expression tag	UNP G0SFD1
A	28	THR	-	expression tag	UNP G0SFD1
A	29	GLY	-	expression tag	UNP G0SFD1
A	810	SER	-	expression tag	UNP 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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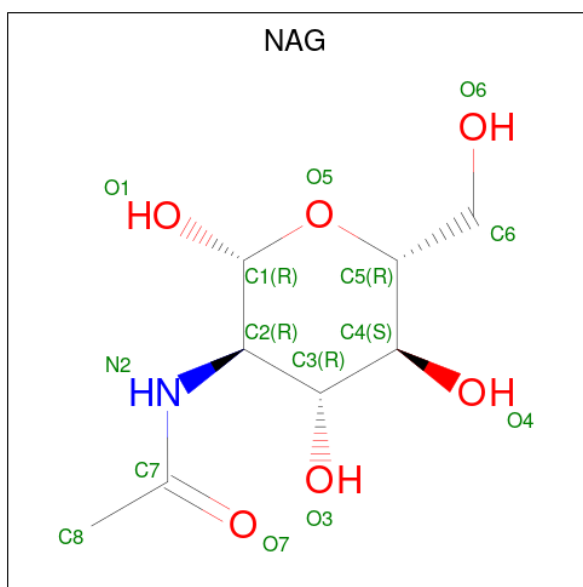
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLU	-	expression tag	UNP G0SFD1
B	28	THR	-	expression tag	UNP G0SFD1
B	29	GLY	-	expression tag	UNP G0SFD1
B	810	SER	-	expression tag	UNP G0SFD1
B	811	GLY	-	expression tag	UNP G0SFD1
B	812	HIS	-	expression tag	UNP G0SFD1
B	813	HIS	-	expression tag	UNP 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)-1-[(3-{[3-bromo-5-(methanesulfonyl)anilino]methyl}phenyl)methyl]-2-(hydroxymethyl)piperidine-3,4,5-triol (CCD ID: WT0) (formula: $C_{21}H_{27}BrN_2O_6S$) (labeled as "Ligand of Interest" by depositor).



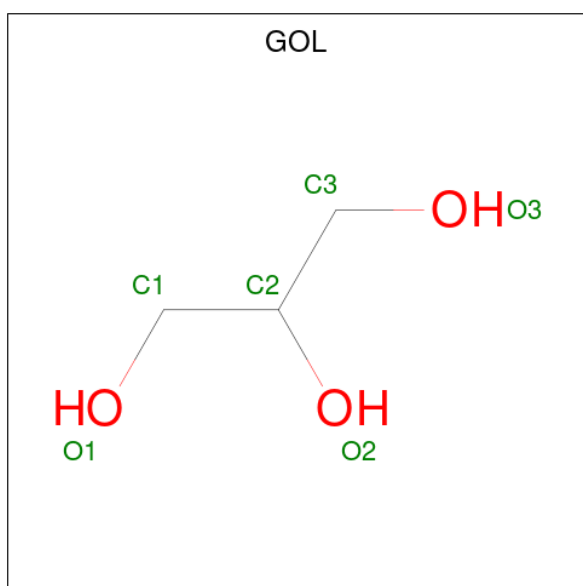
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	1
			62	2	42	4	12	2		
2	B	1	Total	Br	C	N	O	S	0	0
			31	1	21	2	6	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



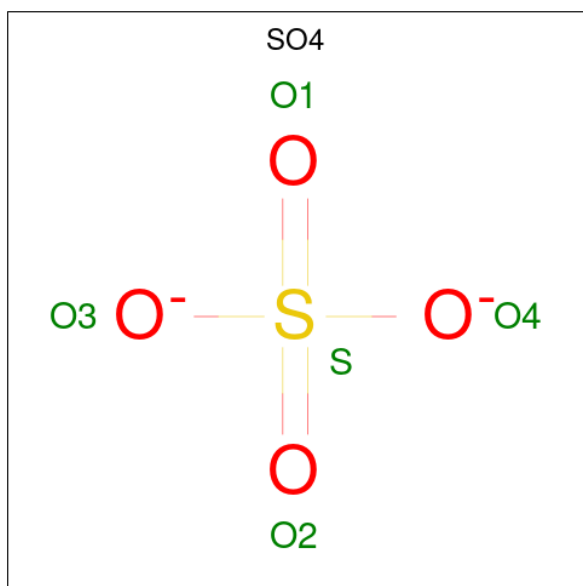
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



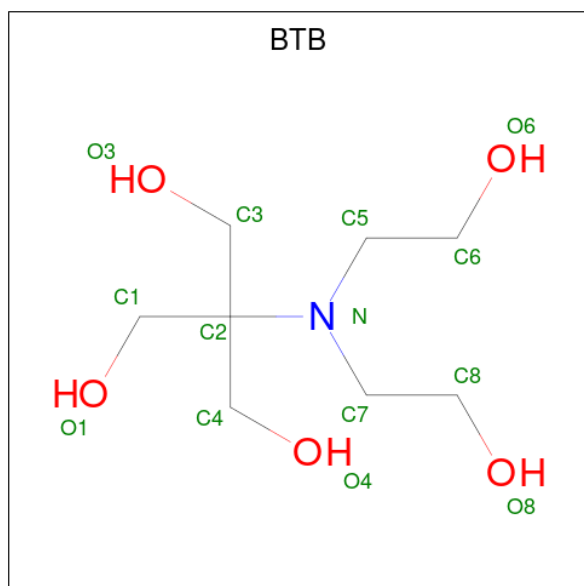
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



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

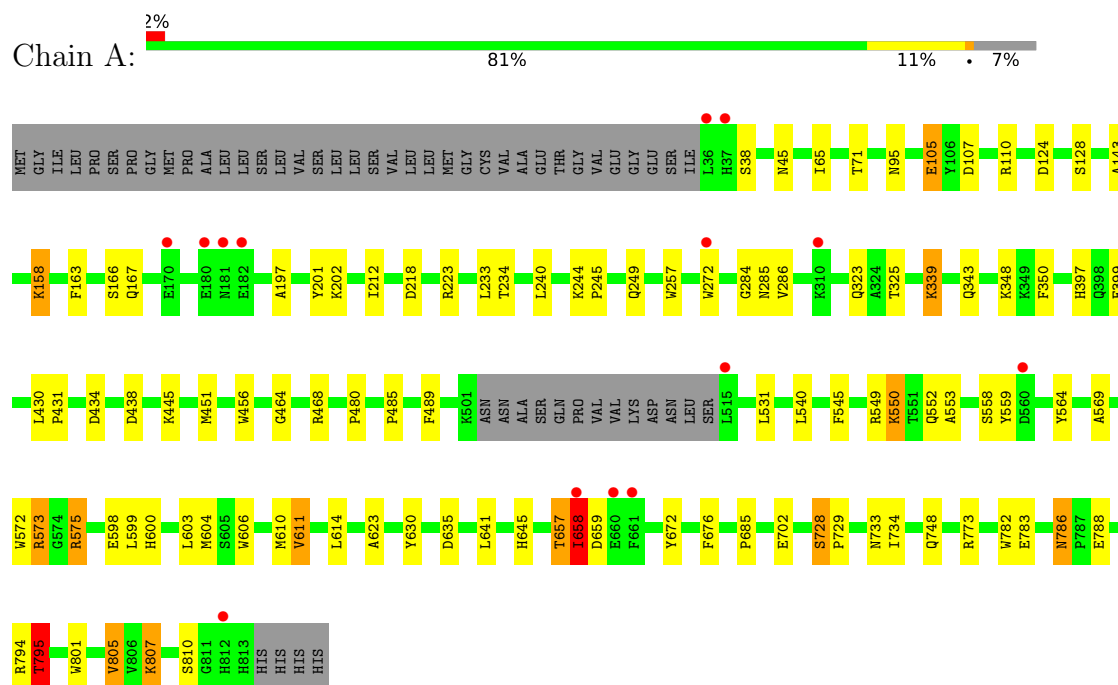
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	161	Total	O	0	0
			161	161		
7	B	176	Total	O	0	0
			176	176		

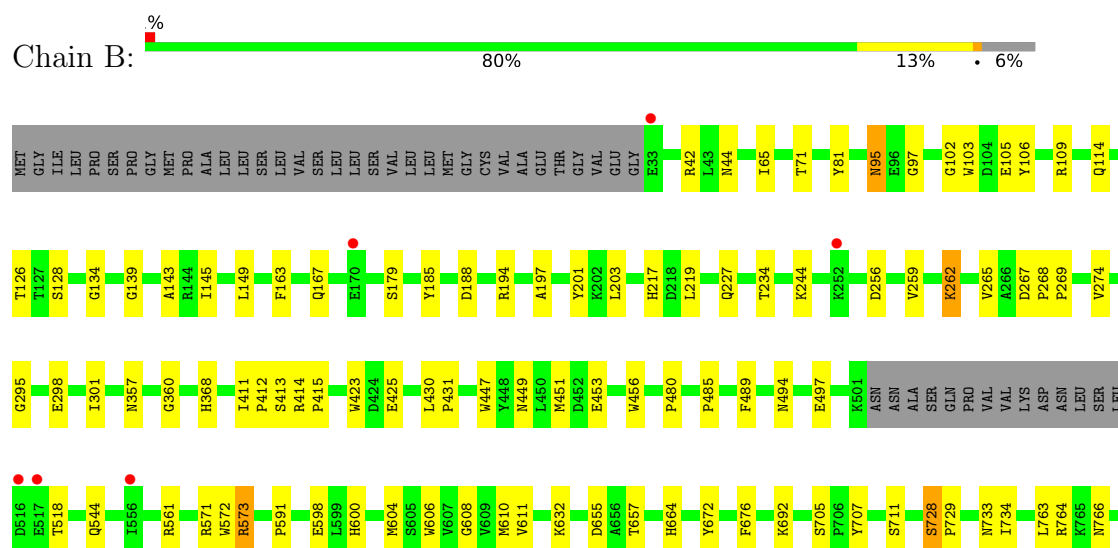
3 Residue-property plots

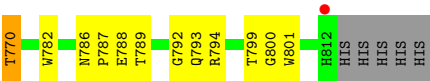
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	135.94Å 178.85Å 179.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.81 – 2.21 46.81 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.81-2.21) 100.0 (46.81-2.21)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.185 , 0.230 0.190 , 0.230	Depositor DCC
R_{free} test set	5422 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12713	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: GOL, NAG, WT0, SO4, BTB

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	2/6245 (0.0%)	1.38	16/8506 (0.2%)
1	B	1.01	0/6261	1.37	1/8522 (0.0%)
All	All	1.02	2/12506 (0.0%)	1.38	17/17028 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	ASP	C-N	12.92	1.49	1.33
1	A	702	GLU	CA-C	5.37	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASP	CA-C-N	12.11	131.91	119.56
1	A	107	ASP	C-N-CA	12.11	131.91	119.56
1	A	575	ARG	CB-CA-C	8.77	124.51	109.51
1	A	795	THR	CA-CB-OG1	-6.40	100.00	109.60
1	A	464	GLY	CA-C-O	-5.68	118.31	122.23
1	A	782	TRP	CA-C-N	5.55	128.17	120.29
1	A	782	TRP	C-N-CA	5.55	128.17	120.29
1	A	158	LYS	CB-CA-C	5.54	118.88	109.80
1	A	657	THR	CB-CA-C	-5.38	100.99	114.11
1	A	658	ILE	CA-C-N	5.35	131.76	121.54
1	A	658	ILE	C-N-CA	5.35	131.76	121.54
1	A	95	ASN	CA-C-O	-5.19	115.76	121.31
1	B	188	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	611	VAL	N-CA-CB	5.10	116.52	110.55
1	A	623	ALA	CA-C-N	5.06	127.02	120.44
1	A	623	ALA	C-N-CA	5.06	127.02	120.44
1	A	124	ASP	CB-CA-C	5.02	118.32	110.19

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	6063	0	5720	56	0
1	B	6085	0	5737	70	0
2	A	62	0	0	1	0
2	B	31	0	0	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
5	A	50	0	0	1	0
5	B	25	0	0	1	0
6	B	14	0	19	1	0
7	A	161	0	0	1	0
7	B	176	0	0	1	0
All	All	12713	0	11526	122	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 (122) 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:B:572:TRP:H	1:B:600:HIS:HD2	1.26	0.81
1:B:561:ARG:HE	1:B:664:HIS:HD2	1.31	0.79
1:A:559:TYR:CE1	1:A:658:ILE:HD13	2.21	0.75
1:B:217:HIS:HD2	1:B:219:LEU:H	1.40	0.68
1:B:786:ASN:HD22	1:B:789:THR:H	1.41	0.68
1:A:468:ARG:NE	5:A:909:SO4:O1	2.24	0.67
1:B:766:ASN:O	1:B:770:THR:HG23	1.96	0.66
1:B:561:ARG:HE	1:B:664:HIS:CD2	2.16	0.64
1:B:65:ILE:HD13	1:B:197:ALA:HB1	1.79	0.64
1:A:559:TYR:CD1	1:A:658:ILE:HD13	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:MET:HE1	1:A:540:LEU:HB3	1.80	0.61
1:B:217:HIS:HE1	1:B:267:ASP:O	1.82	0.61
1:B:591:PRO:HD2	1:B:598:GLU:OE2	2.00	0.61
1:B:786:ASN:HB2	1:B:793:GLN:NE2	2.16	0.60
1:B:786:ASN:HD21	1:B:788:GLU:HB2	1.68	0.58
1:A:451:MET:HE1	1:A:540:LEU:CB	2.35	0.56
1:B:145:ILE:CD1	1:B:301:ILE:CD1	2.84	0.56
1:B:786:ASN:ND2	1:B:788:GLU:H	2.04	0.56
1:B:707:TYR:HA	1:B:770:THR:HG21	1.88	0.56
1:A:434:ASP:OD2	1:A:807:LYS:HD3	2.06	0.55
1:A:451:MET:HE1	1:A:540:LEU:CA	2.36	0.55
1:B:256:ASP:O	1:B:259:VAL:HG22	2.07	0.55
1:A:572:TRP:H	1:A:600:HIS:HD2	1.53	0.55
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.42	0.55
1:B:95:ASN:HD22	1:B:95:ASN:C	2.15	0.54
1:B:71:THR:HB	1:B:163:PHE:CZ	2.43	0.54
1:A:244:LYS:HB3	1:A:245:PRO:HD3	1.89	0.54
1:A:794:ARG:NH2	2:A:901[A]:WT0:O5	2.41	0.53
1:A:553:ALA:O	1:A:573:ARG:NH2	2.36	0.52
1:B:728:SER:N	1:B:729:PRO:CD	2.73	0.52
1:B:794:ARG:NH1	2:B:901:WT0:O6	2.41	0.52
1:B:44:ASN:HD22	1:B:109:ARG:HH12	1.57	0.51
1:A:545:PHE:CZ	1:A:549:ARG:HD2	2.46	0.51
1:B:44:ASN:ND2	1:B:109:ARG:HH12	2.08	0.50
1:A:110:ARG:HH21	1:A:323:GLN:HG3	1.76	0.50
1:B:134:GLY:O	1:B:139:GLY:HA2	2.12	0.50
1:A:451:MET:CE	1:A:540:LEU:HB3	2.42	0.49
1:B:128:SER:O	1:B:143:ALA:HA	2.11	0.49
1:A:564:TYR:OH	1:A:635:ASP:OD2	2.20	0.49
1:B:149:LEU:HD11	1:B:295:GLY:HA2	1.93	0.49
1:B:114:GLN:HE22	1:B:414:ARG:HH22	1.59	0.49
1:A:128:SER:O	1:A:143:ALA:HA	2.12	0.49
1:B:600:HIS:HA	1:B:655:ASP:OD1	2.13	0.48
1:B:203:LEU:HD11	1:B:301:ILE:CG2	2.43	0.48
1:B:145:ILE:HD13	1:B:301:ILE:HD11	1.96	0.48
1:B:728:SER:N	1:B:729:PRO:HD3	2.28	0.48
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.47	0.48
1:A:451:MET:CE	1:A:540:LEU:HD22	2.44	0.48
1:A:786:ASN:ND2	1:A:788:GLU:H	2.12	0.47
1:A:71:THR:HB	1:A:163:PHE:CZ	2.50	0.47
1:B:451:MET:HE1	1:B:544:GLN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.49	0.47
1:A:65:ILE:HD13	1:A:197:ALA:HB1	1.96	0.47
1:A:451:MET:HE1	1:A:540:LEU:HA	1.95	0.47
1:B:414:ARG:N	1:B:415:PRO:HD2	2.31	0.47
1:B:103:TRP:H	1:B:357:ASN:ND2	2.11	0.46
1:A:685:PRO:HG3	1:A:748:GLN:HE22	1.80	0.46
1:A:167:GLN:NE2	1:A:201:TYR:OH	2.48	0.46
1:B:430:LEU:HB2	1:B:431:PRO:HD3	1.97	0.46
1:B:766:ASN:O	1:B:770:THR:CG2	2.62	0.46
1:A:598:GLU:OE2	1:A:600:HIS:HE1	1.98	0.46
1:B:485:PRO:HB3	1:B:606:TRP:CE2	2.50	0.46
1:B:733:ASN:HB3	1:B:801:TRP:CG	2.50	0.46
1:A:641:LEU:O	1:A:645:HIS:HB2	2.15	0.46
1:A:569:ALA:HA	1:A:604:MET:CE	2.46	0.45
1:B:672:TYR:CE1	1:B:711:SER:HA	2.52	0.45
1:A:249:GLN:HE21	1:B:262:LYS:HZ3	1.63	0.45
1:B:368:HIS:HD2	5:B:905:SO4:O3	2.00	0.45
1:B:728:SER:H	1:B:729:PRO:CD	2.30	0.45
1:A:223[B]:ARG:NH2	1:A:257:TRP:CE2	2.85	0.45
1:B:203:LEU:HD11	1:B:301:ILE:HG23	1.97	0.45
1:B:179:SER:HB3	1:B:185:TYR:CD2	2.52	0.44
1:B:782:TRP:CG	1:B:792:GLY:HA3	2.52	0.44
1:B:102:GLY:HA3	1:B:357:ASN:HD21	1.82	0.44
1:A:233:LEU:HD22	1:B:265:VAL:HG23	1.99	0.44
1:B:97:GLY:HA3	7:B:1028:HOH:O	2.16	0.44
1:B:114:GLN:NE2	1:B:414:ARG:HH12	2.16	0.44
1:A:350:PHE:CZ	1:A:805:VAL:HG11	2.52	0.44
1:A:485:PRO:HB3	1:A:606:TRP:CE2	2.53	0.44
1:A:451:MET:HE3	1:A:540:LEU:HD22	1.98	0.44
1:A:569:ALA:HB1	1:A:599:LEU:HD22	2.00	0.44
1:B:167:GLN:NE2	1:B:201:TYR:OH	2.51	0.44
1:A:672:TYR:CG	1:A:734:ILE:HG21	2.53	0.44
1:A:158:LYS:HD3	1:A:272:TRP:CD1	2.53	0.44
1:A:728:SER:N	1:A:729:PRO:CD	2.81	0.44
1:A:110:ARG:NH2	1:A:323:GLN:HG3	2.32	0.43
1:A:489:PHE:CE1	1:A:610:MET:HE3	2.53	0.43
1:B:145:ILE:O	1:B:298:GLU:HA	2.18	0.43
1:B:106:TYR:CE2	1:B:360:GLY:HA2	2.53	0.43
1:A:397:HIS:HD2	1:A:399:GLU:OE2	2.02	0.43
1:A:105:GLU:OE2	1:A:325:THR:HG23	2.18	0.43
1:B:707:TYR:CA	1:B:770:THR:HG21	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LYS:HD2	1:A:810:SER:O	2.18	0.43
1:A:550:LYS:HE2	1:A:550:LYS:HA	2.01	0.42
1:B:451:MET:CE	1:B:544:GLN:HB2	2.49	0.42
1:B:456:TRP:CD2	1:B:480:PRO:HA	2.54	0.42
1:B:425:GLU:HG2	1:B:447:TRP:NE1	2.35	0.42
1:A:234[A]:THR:CG2	1:A:284:GLY:HA2	2.50	0.42
1:B:799:THR:N	1:B:800:GLY:HA3	2.34	0.42
1:B:608:GLY:O	1:B:611:VAL:HG12	2.19	0.42
1:A:552:GLN:HB3	1:A:603:LEU:HD21	2.02	0.42
1:B:672:TYR:CG	1:B:734:ILE:HG21	2.55	0.42
1:A:166:SER:HA	1:A:285:ASN:O	2.20	0.42
1:A:430:LEU:HB2	1:A:431:PRO:HD3	2.01	0.42
1:A:783:GLU:OE1	1:A:795:THR:HB	2.20	0.42
1:A:234[B]:THR:HA	1:A:285:ASN:OD1	2.20	0.41
1:A:240:LEU:HD22	1:A:286:VAL:CG2	2.50	0.41
1:B:489:PHE:CE1	1:B:610:MET:HE3	2.55	0.41
1:A:212:ILE:HD11	7:A:1053:HOH:O	2.20	0.41
1:B:81:TYR:OH	1:B:269:PRO:HD2	2.21	0.41
1:B:572:TRP:N	1:B:600:HIS:HD2	2.04	0.41
1:B:149:LEU:CD1	1:B:295:GLY:HA2	2.51	0.41
1:A:234[B]:THR:HG21	1:B:268:PRO:HG3	2.02	0.41
1:B:234:THR:O	6:B:903:BTB:H51	2.20	0.41
1:B:494:ASN:O	1:B:497:GLU:HB3	2.21	0.41
1:A:249:GLN:HE21	1:B:262:LYS:NZ	2.19	0.41
1:A:685:PRO:HG3	1:A:748:GLN:NE2	2.36	0.40
1:B:571:ARG:HB3	1:B:573:ARG:HH21	1.86	0.40
1:B:411:ILE:HA	1:B:412:PRO:HD3	1.91	0.40
1:B:729:PRO:HA	1:B:787:PRO:HD3	2.03	0.40
1:A:614:LEU:HB3	1:A:630:TYR:CE2	2.57	0.40
1:B:763:LEU:O	1:B:764:ARG:C	2.63	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	763/819 (93%)	743 (97%)	18 (2%)	2 (0%)	36	41
1	B	762/819 (93%)	741 (97%)	20 (3%)	1 (0%)	48	56
All	All	1525/1638 (93%)	1484 (97%)	38 (2%)	3 (0%)	43	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	728	SER
1	B	728	SER
1	A	659	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	625/707 (88%)	601 (96%)	24 (4%)	29	38
1	B	631/707 (89%)	609 (96%)	22 (4%)	32	41
All	All	1256/1414 (89%)	1210 (96%)	46 (4%)	30	39

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	45	ASN
1	A	105	GLU
1	A	202	LYS
1	A	218	ASP
1	A	339	LYS
1	A	343	GLN
1	A	348	LYS
1	A	438	ASP
1	A	445	LYS

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Mol	Chain	Res	Type
1	A	531	LEU
1	A	550	LYS
1	A	558	SER
1	A	573	ARG
1	A	575	ARG
1	A	611	VAL
1	A	657	THR
1	A	658	ILE
1	A	676	PHE
1	A	773	ARG
1	A	786	ASN
1	A	795	THR
1	A	805	VAL
1	A	807	LYS
1	B	42	ARG
1	B	95	ASN
1	B	105	GLU
1	B	126	THR
1	B	194	ARG
1	B	227	GLN
1	B	244	LYS
1	B	262	LYS
1	B	274	VAL
1	B	413	SER
1	B	423	TRP
1	B	449	ASN
1	B	453	GLU
1	B	518	THR
1	B	573	ARG
1	B	604	MET
1	B	632	LYS
1	B	657	THR
1	B	676	PHE
1	B	692	LYS
1	B	705	SER
1	B	770	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	157	GLN

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Mol	Chain	Res	Type
1	A	167	GLN
1	A	231	GLN
1	A	249	GLN
1	A	323	GLN
1	A	368	HIS
1	A	397	HIS
1	A	398	GLN
1	A	461	GLN
1	A	478	GLN
1	A	481	HIS
1	A	484	ASN
1	A	544	GLN
1	A	592	GLN
1	A	600	HIS
1	A	639	HIS
1	A	748	GLN
1	A	786	ASN
1	A	793	GLN
1	B	44	ASN
1	B	46	GLN
1	B	95	ASN
1	B	114	GLN
1	B	120	GLN
1	B	137	HIS
1	B	167	GLN
1	B	217	HIS
1	B	227	GLN
1	B	249	GLN
1	B	357	ASN
1	B	368	HIS
1	B	398	GLN
1	B	461	GLN
1	B	481	HIS
1	B	484	ASN
1	B	600	HIS
1	B	664	HIS
1	B	786	ASN
1	B	793	GLN

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 ⓘ

24 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	$\# Z > 2$
6	BTB	B	903	-	13,13,13	1.51	3 (23%)	7,16,16	0.52	0
4	GOL	B	904	-	5,5,5	0.19	0	5,5,5	0.47	0
5	SO4	A	911	-	4,4,4	0.28	0	6,6,6	0.14	0
5	SO4	A	908	-	4,4,4	0.38	0	6,6,6	0.37	0
5	SO4	A	906	-	4,4,4	0.25	0	6,6,6	0.12	0
3	NAG	B	902	1	14,14,15	0.83	0	17,19,21	1.45	4 (23%)
2	WT0	A	901[B]	-	33,33,33	3.68	12 (36%)	46,48,48	2.65	11 (23%)
5	SO4	A	910	-	4,4,4	0.27	0	6,6,6	0.28	0
4	GOL	A	903	-	5,5,5	0.09	0	5,5,5	0.26	0
5	SO4	A	912	-	4,4,4	0.30	0	6,6,6	0.06	0
5	SO4	B	909	-	4,4,4	0.25	0	6,6,6	0.12	0
5	SO4	A	907	-	4,4,4	0.28	0	6,6,6	0.09	0
2	WT0	A	901[A]	-	33,33,33	3.63	11 (33%)	46,48,48	2.19	9 (19%)
3	NAG	A	902	1	14,14,15	0.85	1 (7%)	17,19,21	1.56	4 (23%)
5	SO4	A	909	-	4,4,4	0.26	0	6,6,6	0.17	0
5	SO4	A	913	-	4,4,4	0.30	0	6,6,6	0.15	0
2	WT0	B	901	-	33,33,33	3.34	10 (30%)	46,48,48	2.44	15 (32%)
5	SO4	B	907	-	4,4,4	0.39	0	6,6,6	0.15	0
5	SO4	B	905	-	4,4,4	0.41	0	6,6,6	0.23	0
4	GOL	A	904	-	5,5,5	0.09	0	5,5,5	0.26	0
5	SO4	A	914	-	4,4,4	0.26	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	906	-	4,4,4	0.30	0	6,6,6	0.15	0
5	SO4	B	908	-	4,4,4	0.21	0	6,6,6	0.17	0
5	SO4	A	905	-	4,4,4	0.26	0	6,6,6	0.13	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	GOL	A	903	-	-	4/4/4/4	-
3	NAG	B	902	1	-	0/6/23/26	0/1/1/1
6	BTB	B	903	-	-	4/21/21/21	-
4	GOL	A	904	-	-	0/4/4/4	-
2	WT0	A	901[A]	-	-	5/17/37/37	0/3/3/3
4	GOL	B	904	-	-	2/4/4/4	-
3	NAG	A	902	1	-	4/6/23/26	0/1/1/1
2	WT0	B	901	-	-	2/17/37/37	0/3/3/3
2	WT0	A	901[B]	-	-	6/17/37/37	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901[B]	WT0	C7-N1	-13.80	1.24	1.47
2	A	901[A]	WT0	C7-N1	-13.79	1.24	1.47
2	B	901	WT0	C7-N1	-11.62	1.27	1.47
2	A	901[A]	WT0	O6-S1	9.14	1.66	1.44
2	A	901[B]	WT0	O6-S1	8.96	1.66	1.44
2	B	901	WT0	O5-S1	8.63	1.65	1.44
2	B	901	WT0	O6-S1	8.59	1.65	1.44
2	A	901[A]	WT0	O5-S1	8.49	1.65	1.44
2	A	901[B]	WT0	O5-S1	8.46	1.65	1.44
2	A	901[B]	WT0	C14-S1	4.64	1.81	1.77
2	A	901[B]	WT0	C3-C2	-4.48	1.45	1.52
2	A	901[A]	WT0	C3-C2	-4.41	1.45	1.52
2	A	901[A]	WT0	C14-S1	3.66	1.80	1.77
2	B	901	WT0	C7-C8	3.60	1.57	1.51
2	B	901	WT0	C14-S1	3.47	1.80	1.77
2	B	901	WT0	C3-C2	-3.42	1.47	1.52
6	B	903	BTB	C3-C2	3.41	1.57	1.53
2	B	901	WT0	BR1-C17	3.11	1.96	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	903	BTB	C4-C2	3.09	1.56	1.53
2	A	901[A]	WT0	C12-N2	2.94	1.47	1.38
2	A	901[B]	WT0	C4-C3	2.94	1.56	1.52
2	A	901[A]	WT0	C4-C3	2.90	1.56	1.52
2	A	901[B]	WT0	BR1-C17	2.87	1.96	1.90
2	A	901[B]	WT0	O2-C2	2.84	1.50	1.43
2	A	901[A]	WT0	O2-C2	2.78	1.49	1.43
2	B	901	WT0	O2-C2	2.63	1.49	1.43
2	A	901[B]	WT0	C12-N2	2.62	1.46	1.38
2	A	901[B]	WT0	C15-S1	2.40	1.83	1.75
2	A	901[B]	WT0	C7-C8	2.37	1.55	1.51
2	A	901[A]	WT0	C7-C8	2.33	1.55	1.51
2	A	901[A]	WT0	C15-S1	2.33	1.83	1.75
6	B	903	BTB	C1-C2	2.32	1.56	1.53
3	A	902	NAG	C1-C2	2.26	1.55	1.52
2	B	901	WT0	C15-S1	2.22	1.83	1.75
2	A	901[B]	WT0	C2-C1	-2.16	1.46	1.52
2	B	901	WT0	C4-C3	2.13	1.55	1.52
2	A	901[A]	WT0	C2-C1	-2.12	1.46	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901[B]	WT0	O6-S1-C14	10.15	116.12	108.23
2	B	901	WT0	C13-C14-S1	-8.33	112.33	119.02
2	B	901	WT0	C16-C14-S1	8.24	125.64	119.02
2	A	901[B]	WT0	O6-S1-O5	-7.36	105.52	117.99
2	A	901[A]	WT0	C13-C14-S1	6.86	124.53	119.02
2	A	901[B]	WT0	O5-S1-C14	-6.81	102.94	108.23
2	A	901[A]	WT0	O6-S1-O5	-6.77	106.50	117.99
2	A	901[B]	WT0	C15-S1-C14	6.01	111.17	104.55
2	A	901[A]	WT0	O6-S1-C15	5.84	117.04	108.47
2	A	901[A]	WT0	C16-C14-S1	-4.85	115.12	119.02
2	B	901	WT0	O6-S1-O5	-4.18	110.91	117.99
2	A	901[B]	WT0	C16-C14-S1	3.39	121.75	119.02
3	A	902	NAG	C8-C7-N2	3.31	121.60	116.12
2	B	901	WT0	C11-C10-C19	-3.21	114.38	120.94
2	A	901[B]	WT0	C6-C5-C1	-3.14	108.20	112.93
2	B	901	WT0	C19-C10-C9	3.14	122.88	118.55
3	B	902	NAG	O4-C4-C5	3.08	116.91	109.32
2	A	901[A]	WT0	C6-C5-C1	-3.07	108.31	112.93
2	A	901[A]	WT0	BR1-C17-C16	-3.04	114.93	119.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	WT0	O5-S1-C15	2.88	112.69	108.47
3	B	902	NAG	C1-O5-C5	2.85	116.01	112.19
2	A	901[A]	WT0	BR1-C17-C18	2.76	123.15	119.23
3	B	902	NAG	C3-C4-C5	-2.74	105.26	110.23
2	A	901[B]	WT0	BR1-C17-C16	2.68	123.03	119.23
2	B	901	WT0	C10-C11-N2	-2.64	106.29	113.60
2	B	901	WT0	C7-N1-C5	2.63	118.19	112.94
2	B	901	WT0	C6-C5-C1	-2.63	108.98	112.93
2	B	901	WT0	O6-S1-C14	2.56	110.22	108.23
2	A	901[B]	WT0	O6-S1-C15	2.54	112.20	108.47
2	A	901[B]	WT0	C7-N1-C4	2.47	115.25	110.33
2	B	901	WT0	BR1-C17-C16	2.43	122.67	119.23
2	B	901	WT0	C20-C19-C10	-2.38	117.27	120.61
2	A	901[B]	WT0	C7-N1-C5	2.35	117.65	112.94
3	A	902	NAG	O7-C7-N2	-2.28	117.95	121.98
2	B	901	WT0	O2-C2-C1	-2.28	105.01	110.38
2	A	901[B]	WT0	C13-C14-S1	-2.26	117.20	119.02
2	B	901	WT0	C8-C7-N1	2.15	116.22	112.73
3	A	902	NAG	C3-C4-C5	-2.14	106.35	110.23
3	B	902	NAG	C4-C3-C2	2.10	114.09	111.02
3	A	902	NAG	O5-C5-C6	2.07	111.70	107.66
2	B	901	WT0	C7-C8-C9	2.06	124.16	120.27
2	A	901[A]	WT0	C7-N1-C5	2.03	116.99	112.94
2	A	901[A]	WT0	C7-N1-C4	2.01	114.34	110.33

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901[B]	WT0	C13-C14-S1-C15
2	A	901[B]	WT0	C16-C14-S1-C15
3	A	902	NAG	C8-C7-N2-C2
3	A	902	NAG	O7-C7-N2-C2
4	A	903	GOL	C1-C2-C3-O3
4	A	903	GOL	O2-C2-C3-O3
6	B	903	BTB	C1-C2-C3-O3
6	B	903	BTB	C4-C2-C3-O3
6	B	903	BTB	N-C2-C3-O3
2	A	901[B]	WT0	C10-C11-N2-C12
3	A	902	NAG	O5-C5-C6-O6
2	A	901[A]	WT0	C10-C11-N2-C12
4	A	903	GOL	O1-C1-C2-C3

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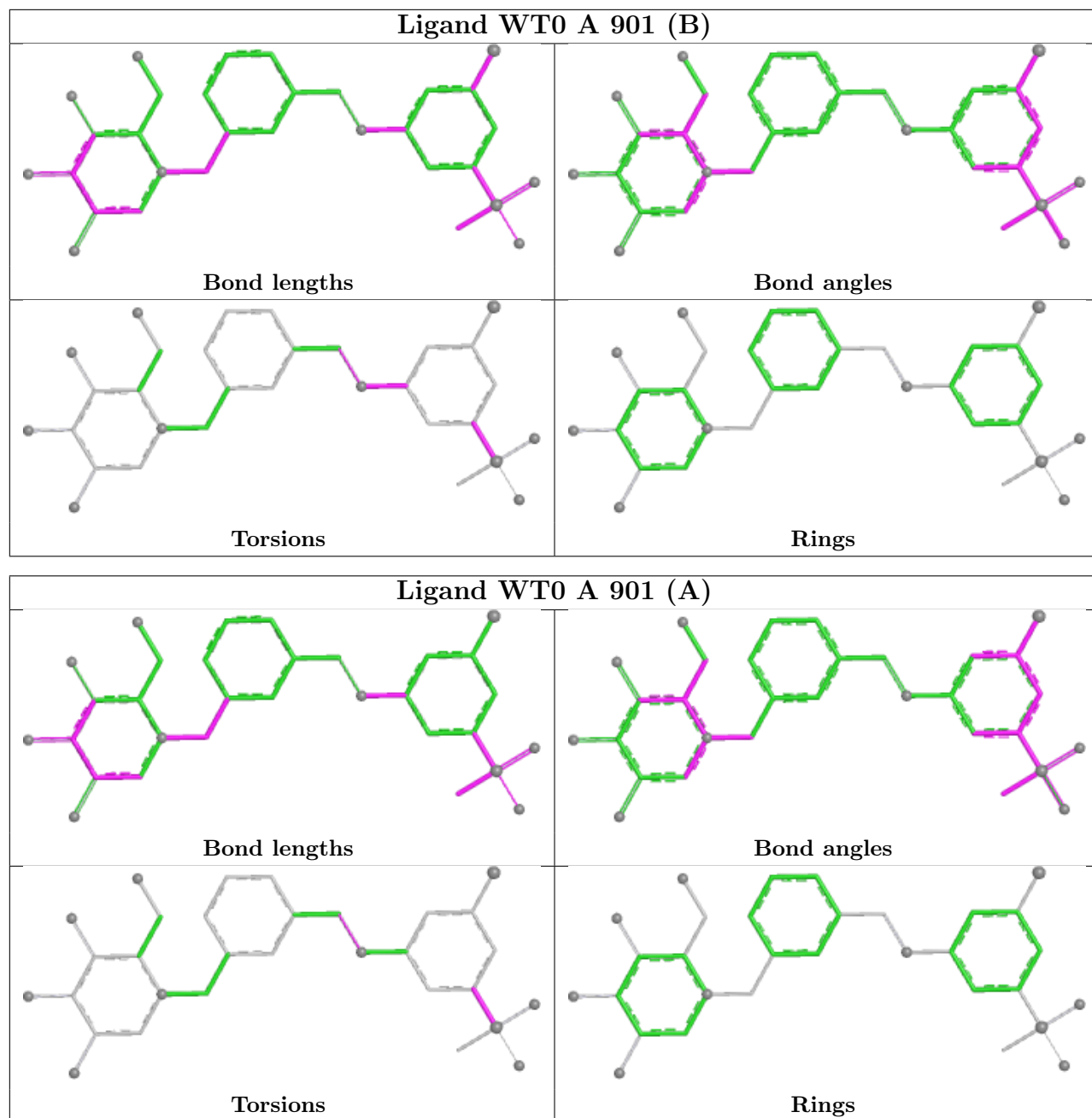
Mol	Chain	Res	Type	Atoms
6	B	903	BTB	N-C7-C8-O8
2	A	901[A]	WT0	C16-C14-S1-O5
2	A	901[A]	WT0	C13-C14-S1-O5
2	A	901[B]	WT0	C13-C14-S1-O5
2	A	901[B]	WT0	C16-C14-S1-O5
4	A	903	GOL	O1-C1-C2-O2
4	B	904	GOL	O1-C1-C2-O2
2	A	901[A]	WT0	C16-C14-S1-C15
2	A	901[A]	WT0	C13-C14-S1-C15
3	A	902	NAG	C4-C5-C6-O6
2	B	901	WT0	C13-C14-S1-O5
2	A	901[B]	WT0	C13-C12-N2-C11
4	B	904	GOL	O1-C1-C2-C3
2	B	901	WT0	C16-C14-S1-O5

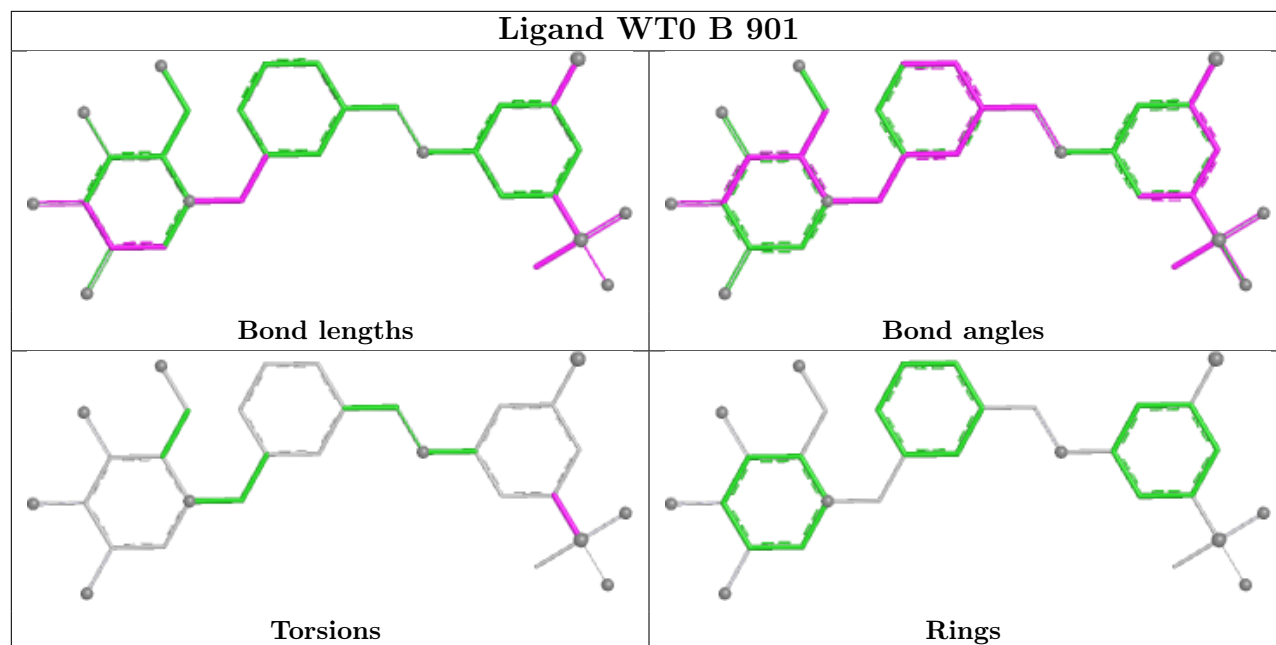
There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	903	BTB	1	0
2	A	901[A]	WT0	1	0
5	A	909	SO4	1	0
2	B	901	WT0	1	0
5	B	905	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

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	765/819 (93%)	-0.03	14 (1%) 67 65	23, 44, 71, 95	2 (0%)
1	B	766/819 (93%)	-0.09	7 (0%) 81 79	29, 44, 67, 100	0
All	All	1531/1638 (93%)	-0.06	21 (1%) 73 72	23, 44, 69, 100	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	ASP	6.5
1	A	36	LEU	5.6
1	B	812	HIS	5.0
1	B	517	GLU	4.3
1	A	560	ASP	3.3
1	A	661	PHE	3.1
1	A	182	GLU	2.9
1	A	170	GLU	2.9
1	A	812	HIS	2.8
1	A	660	GLU	2.8
1	A	658	ILE	2.7
1	A	515	LEU	2.7
1	B	33	GLU	2.4
1	A	310	LYS	2.3
1	A	37	HIS	2.3
1	B	170	GLU	2.2
1	A	180	GLU	2.2
1	B	252	LYS	2.1
1	A	181	ASN	2.1
1	A	272	TRP	2.1
1	B	556	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

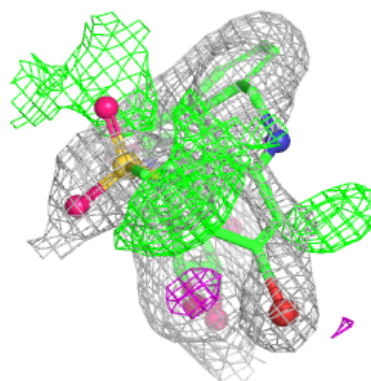
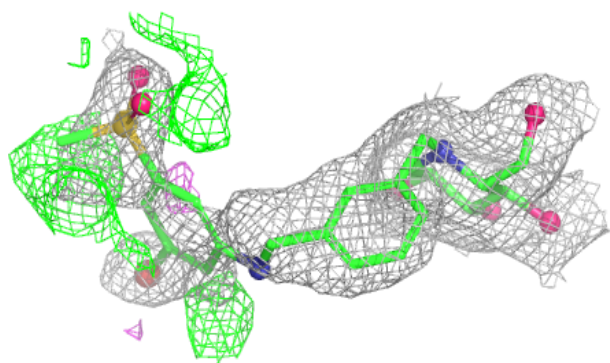
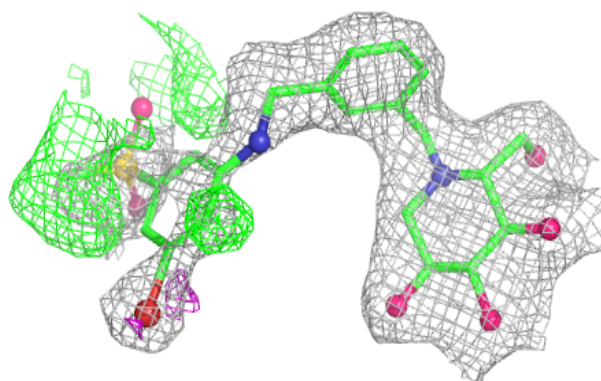
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	907	5/5	0.54	0.12	99,112,126,130	0
3	NAG	A	902	14/15	0.73	0.17	93,117,123,124	0
3	NAG	B	902	14/15	0.76	0.14	57,68,74,77	0
5	SO4	A	913	5/5	0.78	0.10	79,86,93,94	0
5	SO4	B	909	5/5	0.78	0.09	81,81,88,96	0
5	SO4	A	905	5/5	0.79	0.09	81,89,98,102	0
2	WT0	A	901[A]	31/31	0.82	0.21	31,41,67,74	31
2	WT0	A	901[B]	31/31	0.82	0.21	32,45,77,102	31
5	SO4	B	906	5/5	0.83	0.10	73,79,84,87	0
5	SO4	A	911	5/5	0.84	0.10	78,79,87,103	0
5	SO4	A	914	5/5	0.84	0.08	76,79,89,92	0
5	SO4	A	909	5/5	0.87	0.09	72,77,88,99	0
5	SO4	A	912	5/5	0.87	0.12	106,110,124,126	0
4	GOL	A	904	6/6	0.88	0.14	71,77,84,86	0
5	SO4	A	910	5/5	0.88	0.14	65,68,79,82	0
6	BTB	B	903	14/14	0.88	0.12	58,74,77,79	0
4	GOL	A	903	6/6	0.91	0.12	55,64,69,74	0
2	WT0	B	901	31/31	0.92	0.13	31,45,132,145	0
5	SO4	B	907	5/5	0.93	0.08	57,70,75,84	0
5	SO4	A	906	5/5	0.94	0.11	58,60,65,74	0
4	GOL	B	904	6/6	0.95	0.10	33,46,49,52	0
5	SO4	B	908	5/5	0.95	0.08	44,61,63,69	0
5	SO4	B	905	5/5	0.97	0.07	40,40,49,57	0
5	SO4	A	908	5/5	0.98	0.04	43,43,47,49	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.

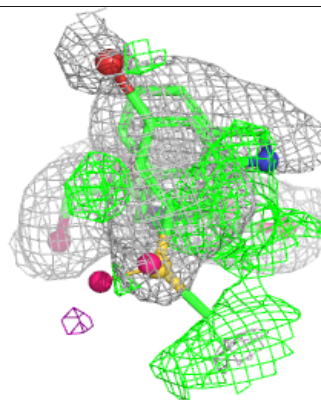
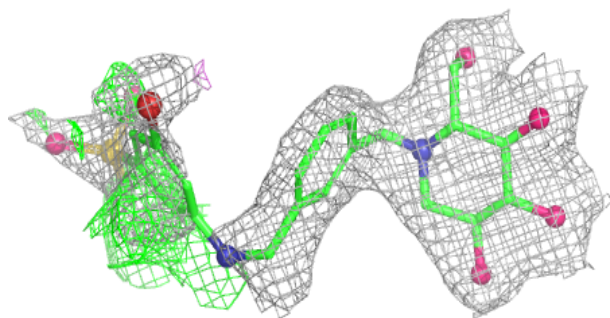
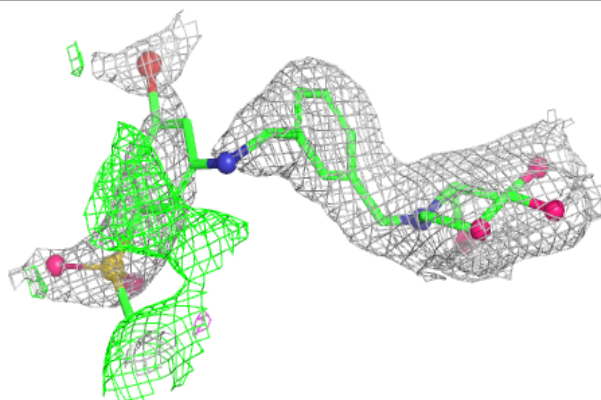
Electron density around WT0 A 901 (A):

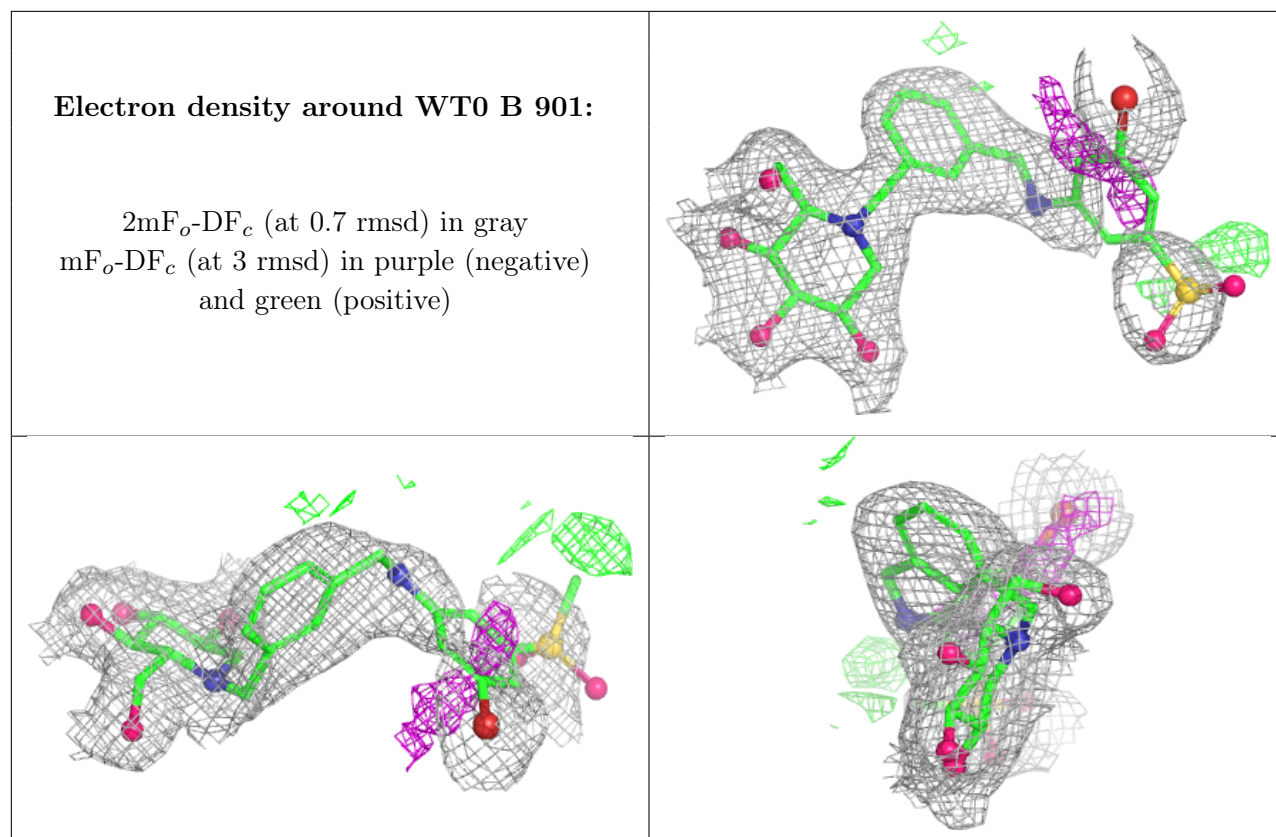
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around WT0 A 901 (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.