Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 01:28 PM EDT

PDB ID	:	8EPR
Title	:	Co-crystal structure of Chaetomium glucosidase with compound 19
Authors	:	Karade, S.S.; Mariuzza, R.A.
Deposited on	:	2022-10-06
Resolution	:	1.99 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 (i) 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 (i)) were used in the production of this report:

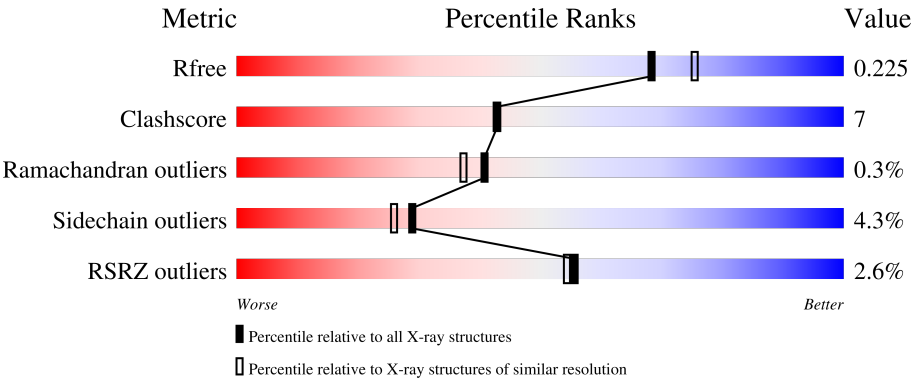
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	4% 81% 11% • 7%
1	B	819	% 81% 11% • 7%

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
3	GOL	A	903	-	-	X	-
3	GOL	B	905	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13580 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	763	Total	C	N	O	S	0	3	0
			6072	3903	1024	1132	13			
1	B	764	Total	C	N	O	S	0	1	0
			6070	3893	1018	1146	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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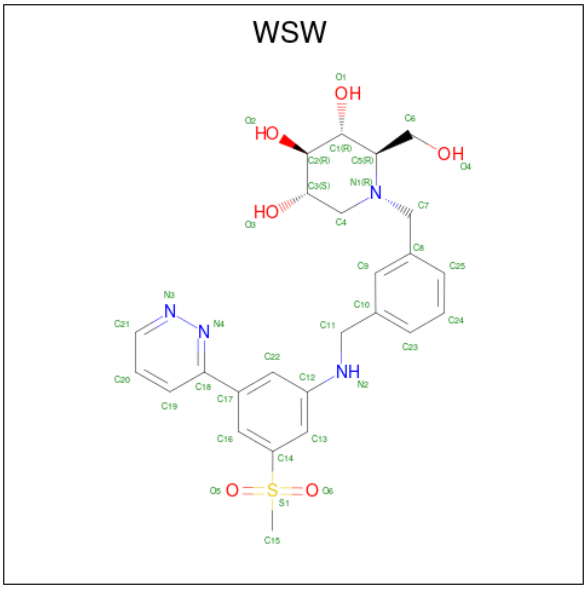
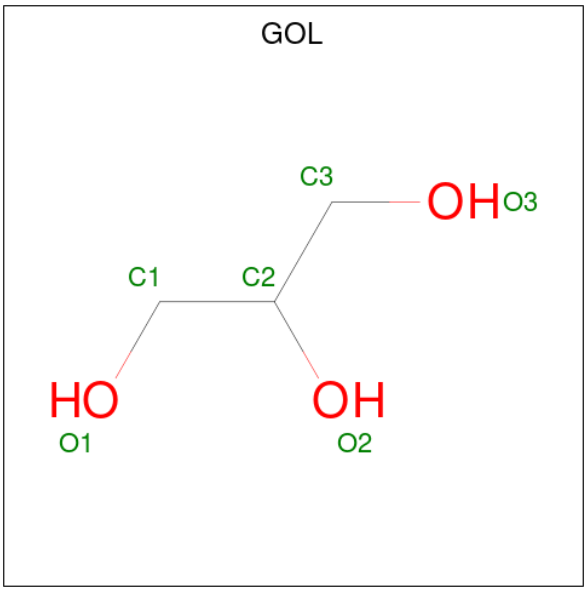
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLU	-	expression tag	UNP G0SFD1
B	28	THR	-	expression tag	UNP G0SFD1
B	29	GLY	-	expression tag	UNP G0SFD1
B	810	SER	-	expression tag	UNP G0SFD1
B	811	GLY	-	expression tag	UNP G0SFD1
B	812	HIS	-	expression tag	UNP G0SFD1
B	813	HIS	-	expression tag	UNP 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-{[3-({[(5M)-3-(methanesulfonyl)-5-(pyridazin-3-yl)phenyl]amino}methyl)phenyl]methyl}piperidine-3,4,5-triol (three-letter code: WSW) (formula: $C_{25}H_{30}N_4O_6S$) (labeled as "Ligand of Interest" by depositor).



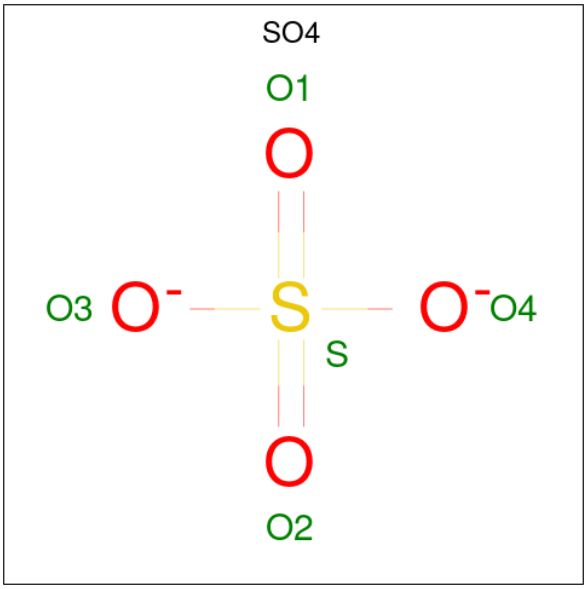
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			36	25	4	6	1		
2	B	1	Total	C	N	O	S	0	0
			36	25	4	6	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



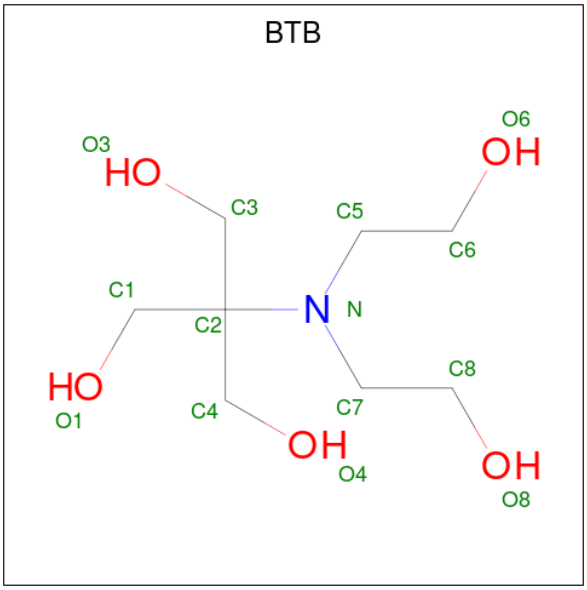
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



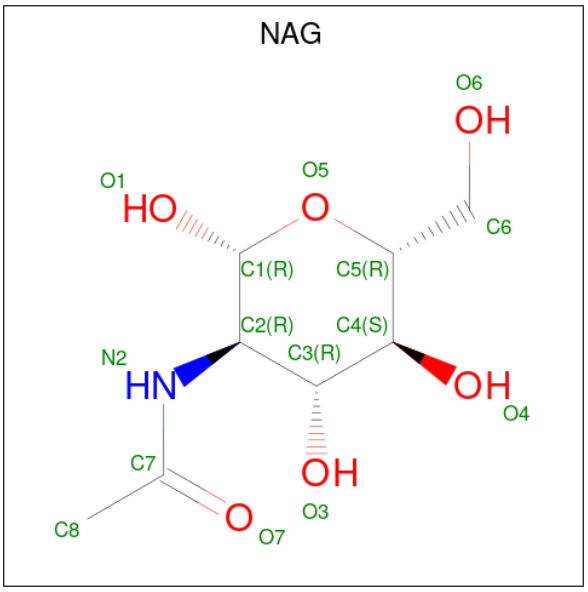
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

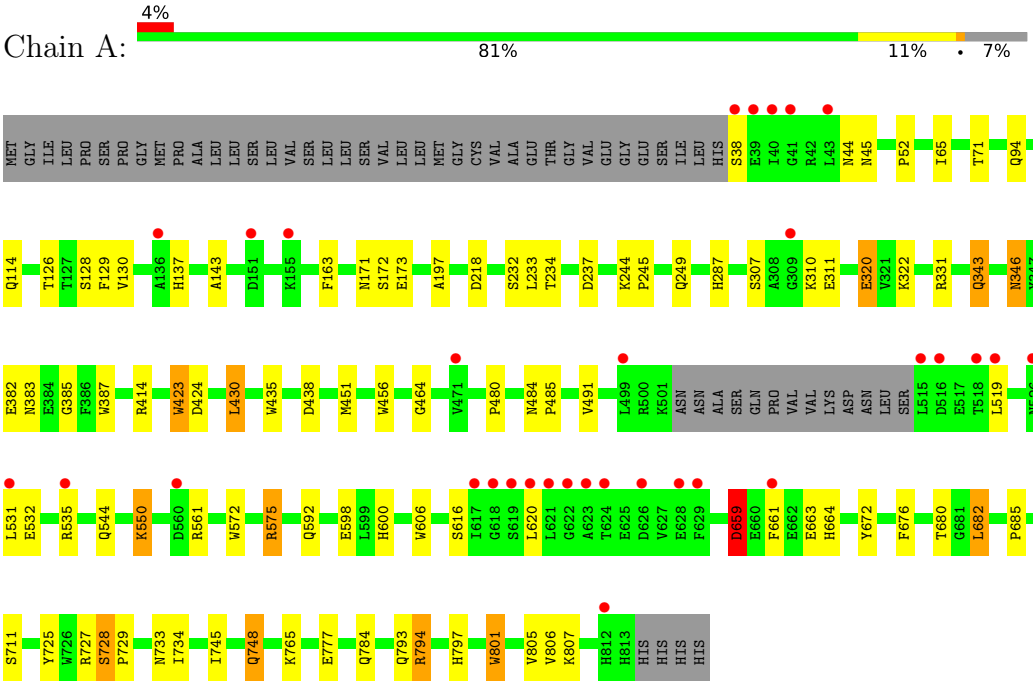
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	595	Total O 595 595	0	0
7	B	678	Total O 678 678	0	0

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.

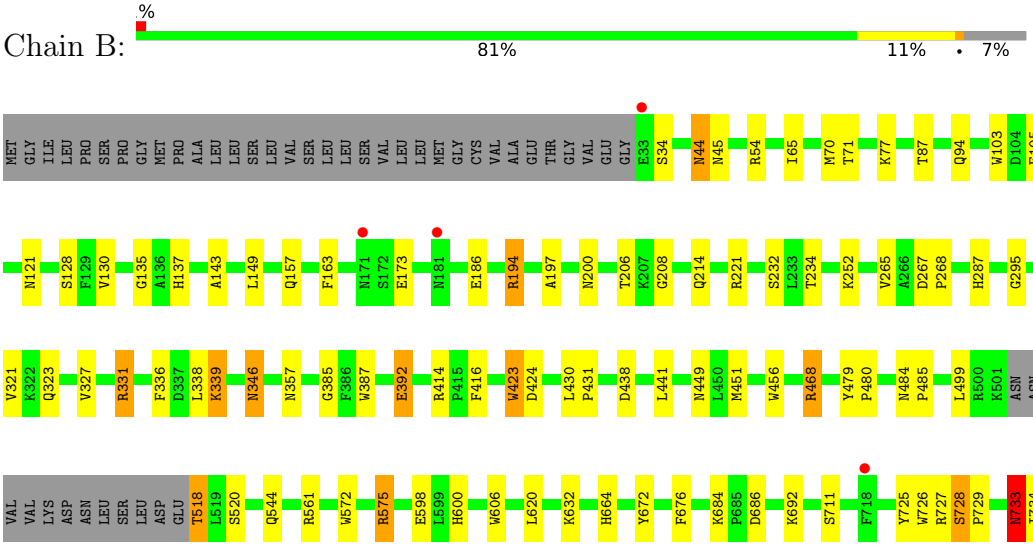
• Molecule 1: Chaetomium alpha glucosidase

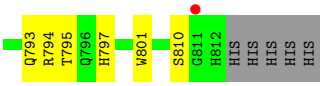
Chain A:



• Molecule 1: Chaetomium alpha glucosidase

Chain B:




Q793
R794
T795
Q796
H797
W801
S810
G811
H812
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	135.62Å 178.74Å 179.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.78 – 1.99 46.74 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.78-1.99) 99.6 (46.74-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.187 , 0.225 0.187 , 0.225	Depositor DCC
R_{free} test set	7398 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13580	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, SO4, WSW, 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	0.48	0/6256	0.71	8/8515 (0.1%)
1	B	0.49	0/6246	0.70	7/8506 (0.1%)
All	All	0.49	0/12502	0.70	15/17021 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	659	ASP	CB-CA-C	-8.42	93.57	110.40
1	B	733	ASN	N-CA-CB	-7.35	97.37	110.60
1	A	575	ARG	CB-CA-C	6.79	123.98	110.40
1	A	805[A]	VAL	CA-C-O	5.91	132.52	120.10
1	A	805[B]	VAL	CA-C-O	5.91	132.52	120.10
1	B	575	ARG	CB-CA-C	5.87	122.14	110.40
1	A	748	GLN	CB-CA-C	-5.71	98.97	110.40
1	B	392	GLU	CB-CA-C	5.67	121.74	110.40
1	A	777	GLU	CB-CA-C	5.61	121.62	110.40
1	A	806[A]	VAL	CA-C-O	5.60	131.86	120.10
1	A	806[B]	VAL	CA-C-O	5.60	131.86	120.10
1	B	331	ARG	CG-CD-NE	-5.50	100.24	111.80
1	B	45	ASN	CB-CA-C	5.13	120.67	110.40
1	B	468	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	468	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	6072	0	5762	78	0
1	B	6070	0	5701	82	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
3	A	18	0	24	6	0
3	B	12	0	16	5	0
4	A	15	0	0	1	0
4	B	20	0	0	0	0
5	B	14	0	19	1	0
6	B	14	0	13	0	0
7	A	595	0	0	10	0
7	B	678	0	0	16	0
All	All	13580	0	11535	161	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 7.

All (161) 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:208:GLY:HA2	3:B:905:GOL:O1	1.54	1.08
1:B:632:LYS:HE3	7:B:1520:HOH:O	1.57	1.02
1:A:659:ASP:HB3	1:A:661:PHE:H	1.25	1.00
1:B:561:ARG:HE	1:B:664:HIS:HD2	1.10	0.98
1:B:572:TRP:H	1:B:600:HIS:HD2	1.15	0.94
1:A:561:ARG:HE	1:A:664:HIS:HD2	1.07	0.93
1:A:171:ASN:H	3:A:903:GOL:H31	1.34	0.92
1:A:572:TRP:H	1:A:600:HIS:HD2	1.18	0.90
1:A:310:LYS:HA	7:A:1457:HOH:O	1.73	0.88
1:B:684:LYS:CB	7:B:1537:HOH:O	2.25	0.83
1:A:234[B]:THR:HG22	7:B:1021:HOH:O	1.80	0.81
1:A:561:ARG:HE	1:A:664:HIS:CD2	1.97	0.80
1:A:685:PRO:HG3	1:A:748:GLN:HE22	1.48	0.78
1:A:114:GLN:HE22	1:A:414:ARG:HH22	1.31	0.76
1:B:797:HIS:HD2	7:B:1564:HOH:O	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLY:HA2	3:B:905:GOL:HO1	1.48	0.76
1:A:346:ASN:H	1:A:346:ASN:HD22	1.36	0.73
1:B:561:ARG:HE	1:B:664:HIS:CD2	1.99	0.73
3:B:905:GOL:H11	7:B:1134:HOH:O	1.87	0.73
1:B:114:GLN:HE22	1:B:414:ARG:HH22	1.35	0.72
1:A:44:ASN:HD21	1:A:109:ARG:HH22	1.37	0.71
1:A:343:GLN:HE21	1:A:343:GLN:H	1.37	0.71
1:B:572:TRP:H	1:B:600:HIS:CD2	2.05	0.70
1:B:346:ASN:HD22	1:B:346:ASN:H	1.39	0.70
1:A:233:LEU:HD22	1:B:265:VAL:HG23	1.72	0.70
1:A:234[B]:THR:HG21	1:B:268:PRO:HG3	1.73	0.69
1:A:659:ASP:HB3	1:A:661:PHE:N	2.06	0.68
1:B:784:GLN:HE21	1:B:793:GLN:HE21	1.42	0.66
1:A:126:THR:HG22	7:A:1402:HOH:O	1.95	0.66
1:A:171:ASN:H	3:A:903:GOL:C3	2.08	0.66
1:B:114:GLN:NE2	1:B:414:ARG:HH12	1.94	0.65
1:A:561:ARG:NE	1:A:664:HIS:HD2	1.89	0.65
1:B:797:HIS:CD2	7:B:1564:HOH:O	2.43	0.65
1:B:518:THR:HG23	1:B:520:SER:HB2	1.78	0.64
1:A:114:GLN:NE2	1:A:414:ARG:HH12	1.96	0.64
1:A:234[A]:THR:HG23	7:B:1021:HOH:O	1.97	0.64
1:B:561:ARG:NE	1:B:664:HIS:HD2	1.91	0.64
1:B:54:ARG:CZ	1:B:70:MET:HE2	2.28	0.63
1:B:87:THR:HB	1:B:121:ASN:HD21	1.64	0.62
3:A:903:GOL:H11	7:A:1348:HOH:O	1.98	0.62
1:B:726:TRP:HH2	1:B:733:ASN:HD22	1.47	0.62
1:B:252:LYS:HE3	7:B:1553:HOH:O	1.99	0.61
1:A:784:GLN:HE22	1:A:794:ARG:HH21	1.47	0.61
1:A:130:VAL:HG21	1:A:320:GLU:HB3	1.83	0.61
1:B:430:LEU:HB2	1:B:431:PRO:HD3	1.84	0.59
1:B:103:TRP:H	1:B:357:ASN:ND2	1.99	0.59
1:A:659:ASP:HB2	1:A:663:GLU:H	1.66	0.59
1:B:451:MET:CE	1:B:544:GLN:HB2	2.33	0.59
1:B:128[A]:SER:O	1:B:143:ALA:HA	2.02	0.59
1:A:128:SER:O	1:A:143:ALA:HA	2.03	0.58
1:B:769:GLU:HG3	7:B:1109:HOH:O	2.04	0.57
1:A:103:TRP:H	1:A:357:ASN:ND2	2.02	0.57
1:A:784:GLN:HE21	1:A:793:GLN:HE21	1.52	0.57
1:A:451:MET:CE	1:A:544:GLN:HB2	2.34	0.57
1:A:575:ARG:HH22	1:A:592:GLN:HE22	1.52	0.57
1:B:44:ASN:ND2	1:B:109:ARG:HH12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:HD22	1:A:346:ASN:N	2.02	0.56
1:B:572:TRP:N	1:B:600:HIS:HD2	1.96	0.56
1:B:214:GLN:NE2	7:B:1002:HOH:O	2.38	0.56
1:A:550:LYS:HE3	7:A:1484:HOH:O	2.06	0.55
1:A:598:GLU:OE2	1:A:600:HIS:HE1	1.89	0.55
1:B:77:LYS:H	1:B:121:ASN:ND2	2.04	0.55
1:B:103:TRP:H	1:B:357:ASN:HD21	1.55	0.55
1:A:572:TRP:H	1:A:600:HIS:CD2	2.10	0.55
1:A:572:TRP:N	1:A:600:HIS:HD2	1.98	0.54
1:B:346:ASN:HD22	1:B:346:ASN:N	2.05	0.54
1:B:65:ILE:HD13	1:B:197:ALA:HB1	1.90	0.54
1:A:114:GLN:HE21	1:A:414:ARG:HH12	1.55	0.54
1:A:784:GLN:NE2	1:A:794:ARG:HH21	2.04	0.54
1:B:518:THR:N	7:B:1003:HOH:O	2.39	0.54
1:A:171:ASN:N	3:A:903:GOL:H31	2.13	0.54
1:B:130:VAL:CG1	1:B:321:VAL:HG22	2.37	0.54
1:B:727:ARG:O	1:B:728:SER:HB3	2.07	0.54
1:B:784:GLN:NE2	1:B:793:GLN:HE21	2.06	0.54
1:B:194:ARG:HB2	1:B:200:ASN:HD22	1.72	0.54
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.43	0.54
1:A:94:GLN:OE1	1:A:797:HIS:HE1	1.91	0.53
1:B:94:GLN:OE1	1:B:797:HIS:HE1	1.92	0.53
1:B:130:VAL:HG11	1:B:321:VAL:CG2	2.39	0.53
1:A:550:LYS:CE	7:A:1484:HOH:O	2.57	0.53
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.43	0.53
1:B:451:MET:HE1	1:B:544:GLN:HB2	1.91	0.52
1:B:114:GLN:HE21	1:B:414:ARG:HH12	1.57	0.52
1:B:728:SER:N	1:B:729:PRO:CD	2.73	0.51
1:B:339:LYS:HD2	1:B:810:SER:O	2.10	0.51
1:B:130:VAL:HG11	1:B:321:VAL:HG23	1.92	0.50
1:A:331:ARG:NH1	1:A:435:TRP:O	2.45	0.50
1:A:727:ARG:O	1:A:728:SER:HB3	2.11	0.50
1:B:206:THR:OG1	3:B:905:GOL:H12	2.11	0.50
1:B:130:VAL:CG1	1:B:321:VAL:CG2	2.90	0.50
1:B:208:GLY:CA	3:B:905:GOL:O1	2.43	0.50
1:A:343:GLN:H	1:A:343:GLN:NE2	2.08	0.50
1:B:44:ASN:HD21	1:B:109:ARG:HH22	1.58	0.50
1:B:54:ARG:NE	1:B:70:MET:CE	2.75	0.50
1:A:382:GLU:HB2	7:A:1071:HOH:O	2.10	0.49
1:B:339:LYS:HE2	1:B:810:SER:O	2.13	0.49
1:A:728:SER:N	1:A:729:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TRP:H	1:A:357:ASN:HD21	1.61	0.48
1:B:221:ARG:HD2	7:B:1504:HOH:O	2.13	0.48
1:A:137:HIS:HD2	1:A:307:SER:OG	1.96	0.48
1:B:327:VAL:HG13	7:B:1546:HOH:O	2.14	0.48
1:A:451:MET:HE1	1:A:544:GLN:HB2	1.94	0.48
1:B:423:TRP:H	1:B:484:ASN:ND2	2.11	0.48
1:B:234:THR:O	5:B:902:BTB:H52	2.13	0.47
1:A:423:TRP:H	1:A:484:ASN:ND2	2.12	0.47
1:A:451:MET:HE2	1:A:544:GLN:HB2	1.96	0.47
1:B:451:MET:HE2	1:B:544:GLN:HB2	1.96	0.47
1:A:784:GLN:NE2	1:A:793:GLN:HE21	2.11	0.47
1:B:672:TYR:CG	1:B:734:ILE:HG21	2.50	0.47
1:A:65:ILE:HD13	1:A:197:ALA:HB1	1.96	0.46
1:B:728:SER:N	1:B:729:PRO:HD3	2.29	0.46
1:B:733:ASN:HB3	1:B:734:ILE:H	1.30	0.46
1:A:532:GLU:OE1	1:A:535:ARG:HD2	2.15	0.46
1:B:137:HIS:HD2	1:B:307:SER:HB2	1.81	0.46
1:A:44:ASN:ND2	1:A:109:ARG:HH12	2.14	0.46
1:B:336:PHE:O	1:B:338:LEU:HD13	2.17	0.45
1:A:172:SER:HB3	3:A:903:GOL:O3	2.16	0.45
1:A:690:LEU:HD11	1:A:745:ILE:HD11	1.99	0.45
1:A:232:SER:OG	1:A:287:HIS:HD2	2.00	0.44
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.52	0.44
1:B:485:PRO:HB3	1:B:606:TRP:CE2	2.52	0.44
1:A:232:SER:OG	1:A:287:HIS:CD2	2.70	0.44
1:B:137:HIS:HD2	1:B:307:SER:CB	2.30	0.44
1:A:672:TYR:CG	1:A:734:ILE:HG21	2.52	0.44
1:B:479:TYR:HA	1:B:480:PRO:HD3	1.86	0.44
1:A:385:GLY:HA2	1:A:387:TRP:CH2	2.53	0.44
1:A:52:PRO:HD3	1:A:129:PHE:CE2	2.53	0.44
1:A:485:PRO:HB3	1:A:606:TRP:CE2	2.53	0.44
1:B:598:GLU:OE2	1:B:600:HIS:HE1	2.01	0.44
1:B:149:LEU:CD1	1:B:295:GLY:HA2	2.48	0.43
1:A:383:ASN:HB2	7:A:1082:HOH:O	2.18	0.43
1:A:765:LYS:CE	7:A:1120:HOH:O	2.66	0.43
1:A:550:LYS:HB3	1:A:550:LYS:HE2	1.72	0.43
1:A:234[B]:THR:CG2	7:B:1021:HOH:O	2.54	0.43
1:A:244:LYS:HB3	1:A:245:PRO:HD3	2.00	0.43
1:A:784:GLN:HE22	1:A:794:ARG:NH2	2.16	0.43
1:A:71:THR:HB	1:A:163:PHE:CZ	2.54	0.43
1:B:726:TRP:HH2	1:B:733:ASN:ND2	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ASP:HB3	7:B:1217:HOH:O	2.19	0.42
1:B:672:TYR:CZ	1:B:711:SER:HA	2.54	0.42
1:B:157:GLN:NE2	7:B:1016:HOH:O	2.47	0.42
1:B:135:GLY:HA3	1:B:307:SER:HB3	2.02	0.42
1:B:728:SER:H	1:B:729:PRO:CD	2.32	0.42
1:A:430:LEU:HD13	1:A:491:VAL:HG22	2.00	0.42
1:B:575:ARG:HE	1:B:575:ARG:HB2	1.65	0.42
1:A:464:GLY:HA2	4:A:905:SO4:O1	2.19	0.42
1:A:672:TYR:CZ	1:A:711:SER:HA	2.55	0.42
1:A:728:SER:N	1:A:729:PRO:HD3	2.34	0.41
3:A:903:GOL:H12	7:A:1064:HOH:O	2.21	0.41
1:A:348:LYS:HE2	7:A:1098:HOH:O	2.20	0.41
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.91	0.41
1:A:680:THR:OG1	1:A:682:LEU:HD22	2.20	0.41
1:B:194:ARG:HD2	1:B:200:ASN:HD21	1.85	0.41
1:A:456:TRP:CD2	1:A:480:PRO:HA	2.56	0.41
1:B:71:THR:HB	1:B:163:PHE:CZ	2.55	0.41
1:B:385:GLY:HA2	1:B:387:TRP:CH2	2.56	0.41
1:B:416:PHE:CD2	1:B:795:THR:HB	2.56	0.41
1:B:232:SER:OG	1:B:287:HIS:CD2	2.74	0.40
1:A:575:ARG:HE	1:A:575:ARG:HB2	1.70	0.40
1:B:620:LEU:HD12	1:B:620:LEU:HA	1.91	0.40
1:B:456:TRP:CD2	1:B:480:PRO:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	762/819 (93%)	744 (98%)	16 (2%)	2 (0%)	41	37
1	B	761/819 (93%)	746 (98%)	13 (2%)	2 (0%)	41	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1523/1638 (93%)	1490 (98%)	29 (2%)	4 (0%)	41 37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	728	SER
1	B	728	SER
1	A	659	ASP
1	B	733	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	630/707 (89%)	603 (96%)	27 (4%)	29 26
1	B	629/707 (89%)	602 (96%)	27 (4%)	29 26
All	All	1259/1414 (89%)	1205 (96%)	54 (4%)	29 26

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	45	ASN
1	A	173	GLU
1	A	218	ASP
1	A	237	ASP
1	A	249	GLN
1	A	311	GLU
1	A	320	GLU
1	A	322	LYS
1	A	343	GLN
1	A	346	ASN
1	A	423	TRP
1	A	424	ASP
1	A	430	LEU

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Mol	Chain	Res	Type
1	A	438	ASP
1	A	519	LEU
1	A	531	LEU
1	A	550	LYS
1	A	616	SER
1	A	620	LEU
1	A	676	PHE
1	A	682	LEU
1	A	693	LEU
1	A	725	TYR
1	A	794	ARG
1	A	801	TRP
1	A	807	LYS
1	B	34	SER
1	B	44	ASN
1	B	105	GLU
1	B	173	GLU
1	B	186	GLU
1	B	194	ARG
1	B	307	SER
1	B	311	GLU
1	B	323	GLN
1	B	331	ARG
1	B	339	LYS
1	B	346	ASN
1	B	392	GLU
1	B	423	TRP
1	B	424	ASP
1	B	438	ASP
1	B	441	LEU
1	B	449	ASN
1	B	468	ARG
1	B	499	LEU
1	B	518	THR
1	B	676	PHE
1	B	686	ASP
1	B	692	LYS
1	B	725	TYR
1	B	794	ARG
1	B	801	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	45	ASN
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	398	GLN
1	A	484	ASN
1	A	494	ASN
1	A	544	GLN
1	A	592	GLN
1	A	600	HIS
1	A	664	HIS
1	A	741	GLN
1	A	748	GLN
1	A	784	GLN
1	A	797	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	200	ASN
1	B	214	GLN
1	B	287	HIS
1	B	346	ASN
1	B	357	ASN
1	B	476	GLN
1	B	484	ASN
1	B	600	HIS
1	B	664	HIS
1	B	733	ASN
1	B	748	GLN
1	B	784	GLN
1	B	797	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
3	GOL	A	902	-	5,5,5	0.22	0	5,5,5	0.39	0
2	WSW	B	901	-	39,39,39	2.93	15 (38%)	55,56,56	1.94	11 (20%)
5	BTB	B	902	-	13,13,13	1.25	2 (15%)	7,16,16	0.54	0
4	SO4	A	905	-	4,4,4	0.47	0	6,6,6	0.24	0
4	SO4	B	908	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	A	907	-	4,4,4	0.34	0	6,6,6	0.16	0
3	GOL	B	903	-	5,5,5	0.47	0	5,5,5	0.56	0
4	SO4	B	907	-	4,4,4	0.30	0	6,6,6	0.11	0
3	GOL	B	905	-	5,5,5	0.08	0	5,5,5	0.34	0
4	SO4	B	909	-	4,4,4	0.22	0	6,6,6	0.14	0
3	GOL	A	904	-	5,5,5	0.19	0	5,5,5	0.38	0
3	GOL	A	903	-	5,5,5	0.17	0	5,5,5	0.37	0
2	WSW	A	901	-	39,39,39	3.38	16 (41%)	55,56,56	2.99	20 (36%)
6	NAG	B	904	1	14,14,15	0.73	0	17,19,21	2.70	4 (23%)
4	SO4	B	906	-	4,4,4	0.65	0	6,6,6	0.08	0
4	SO4	A	906	-	4,4,4	0.34	0	6,6,6	0.11	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
3	GOL	A	902	-	-	4/4/4/4	-
2	WSW	B	901	-	-	2/21/41/41	0/4/4/4
5	BTB	B	902	-	-	1/21/21/21	-
3	GOL	B	903	-	-	2/4/4/4	-
3	GOL	B	905	-	-	4/4/4/4	-
3	GOL	A	904	-	-	4/4/4/4	-
3	GOL	A	903	-	-	0/4/4/4	-
2	WSW	A	901	-	-	4/21/41/41	0/4/4/4
6	NAG	B	904	1	-	2/6/23/26	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	WSW	C14-S1	9.25	1.87	1.77
2	A	901	WSW	C7-N1	-9.24	1.31	1.47
2	A	901	WSW	O5-S1	8.49	1.67	1.44
2	B	901	WSW	O5-S1	8.40	1.67	1.44
2	A	901	WSW	O6-S1	8.25	1.67	1.44
2	B	901	WSW	O6-S1	7.38	1.64	1.44
2	B	901	WSW	C7-N1	-7.29	1.35	1.47
2	A	901	WSW	C3-C2	-4.98	1.45	1.52
2	B	901	WSW	C14-S1	4.70	1.82	1.77
2	B	901	WSW	C4-C3	4.66	1.58	1.52
2	B	901	WSW	C7-C8	3.85	1.58	1.51
2	B	901	WSW	C6-C5	3.78	1.58	1.52
2	A	901	WSW	C4-C3	3.67	1.57	1.52
2	B	901	WSW	C1-C5	3.42	1.60	1.53
2	A	901	WSW	C7-C8	3.33	1.57	1.51
2	B	901	WSW	O2-C2	3.23	1.50	1.43
2	B	901	WSW	C3-C2	-3.21	1.47	1.52
2	A	901	WSW	C9-C10	3.18	1.44	1.39
2	A	901	WSW	C16-C14	2.90	1.44	1.39
2	A	901	WSW	C17-C18	2.79	1.53	1.48
5	B	902	BTB	C3-C2	2.77	1.57	1.53
2	B	901	WSW	C20-C19	2.61	1.44	1.38
2	A	901	WSW	C16-C17	2.56	1.44	1.39
2	A	901	WSW	O2-C2	2.53	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	WSW	C9-C8	2.39	1.43	1.39
2	B	901	WSW	C17-C18	2.37	1.52	1.48
5	B	902	BTB	C4-C2	2.24	1.56	1.53
2	A	901	WSW	C19-C18	2.17	1.43	1.38
2	A	901	WSW	C18-N4	-2.16	1.30	1.34
2	B	901	WSW	C11-C10	2.05	1.55	1.51
2	A	901	WSW	C2-C1	-2.02	1.47	1.52
2	A	901	WSW	C9-C8	2.01	1.42	1.39
2	B	901	WSW	C15-S1	2.01	1.83	1.75

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	904	NAG	C1-O5-C5	9.90	125.60	112.19
2	A	901	WSW	C16-C14-S1	8.49	125.81	119.06
2	A	901	WSW	C22-C17-C18	-7.45	109.80	120.59
2	A	901	WSW	O5-S1-C14	7.07	114.02	108.25
2	B	901	WSW	O6-S1-C14	6.67	113.69	108.25
2	A	901	WSW	C16-C17-C18	6.38	129.83	120.59
2	A	901	WSW	C21-N3-N4	6.23	124.02	118.99
2	B	901	WSW	C15-S1-C14	5.52	111.11	104.58
2	A	901	WSW	C17-C18-N4	5.40	124.35	115.97
2	A	901	WSW	O6-S1-O5	-4.92	109.45	117.92
2	A	901	WSW	C6-C5-C1	-4.79	105.56	112.90
2	B	901	WSW	O6-S1-O5	-4.58	110.03	117.92
2	A	901	WSW	C19-C20-C21	-4.55	112.18	118.91
2	B	901	WSW	C6-C5-C1	-4.33	106.27	112.90
2	A	901	WSW	C19-C18-C17	-3.79	114.54	121.93
2	A	901	WSW	C7-N1-C5	3.78	120.61	112.97
2	B	901	WSW	C18-N4-N3	3.75	124.34	119.11
2	A	901	WSW	C13-C14-S1	-3.73	116.11	119.06
2	A	901	WSW	C11-N2-C12	-3.42	113.34	122.15
2	A	901	WSW	C15-S1-C14	3.42	108.62	104.58
6	B	904	NAG	O5-C1-C2	2.98	115.99	111.29
2	B	901	WSW	C7-N1-C5	2.92	118.87	112.97
2	A	901	WSW	O4-C6-C5	-2.84	105.32	111.42
2	B	901	WSW	C7-N1-C4	2.71	115.51	110.31
2	B	901	WSW	C17-C18-N4	2.54	119.90	115.97
2	A	901	WSW	C20-C19-C18	2.52	122.33	118.90
2	B	901	WSW	C20-C21-N3	-2.49	118.07	123.46
6	B	904	NAG	O5-C5-C4	2.39	116.65	110.83
2	A	901	WSW	C11-C10-C23	-2.39	115.96	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	WSW	C7-C8-C9	2.16	124.41	120.25
2	B	901	WSW	C21-N3-N4	2.10	120.69	118.99
6	B	904	NAG	C4-C3-C2	2.08	114.06	111.02
2	B	901	WSW	C10-C11-N2	-2.04	108.45	113.77
2	A	901	WSW	C24-C23-C10	-2.04	117.50	120.63
2	A	901	WSW	C22-C12-N2	-2.03	115.60	120.77

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	GOL	O1-C1-C2-C3
3	A	904	GOL	O1-C1-C2-O2
3	A	904	GOL	O1-C1-C2-C3
3	A	904	GOL	C1-C2-C3-O3
3	A	904	GOL	O2-C2-C3-O3
3	B	903	GOL	C1-C2-C3-O3
3	B	905	GOL	O1-C1-C2-C3
6	B	904	NAG	C4-C5-C6-O6
6	B	904	NAG	O5-C5-C6-O6
3	A	902	GOL	O1-C1-C2-O2
2	A	901	WSW	C16-C14-S1-C15
2	A	901	WSW	C13-C14-S1-C15
2	A	901	WSW	C13-C14-S1-O5
3	A	902	GOL	C1-C2-C3-O3
3	B	905	GOL	C1-C2-C3-O3
3	A	902	GOL	O2-C2-C3-O3
3	B	903	GOL	O2-C2-C3-O3
3	B	905	GOL	O1-C1-C2-O2
2	A	901	WSW	C16-C14-S1-O5
5	B	902	BTB	N-C7-C8-O8
3	B	905	GOL	O2-C2-C3-O3
2	B	901	WSW	C13-C14-S1-O5
2	B	901	WSW	C16-C14-S1-O5

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	BTB	1	0
4	A	905	SO4	1	0

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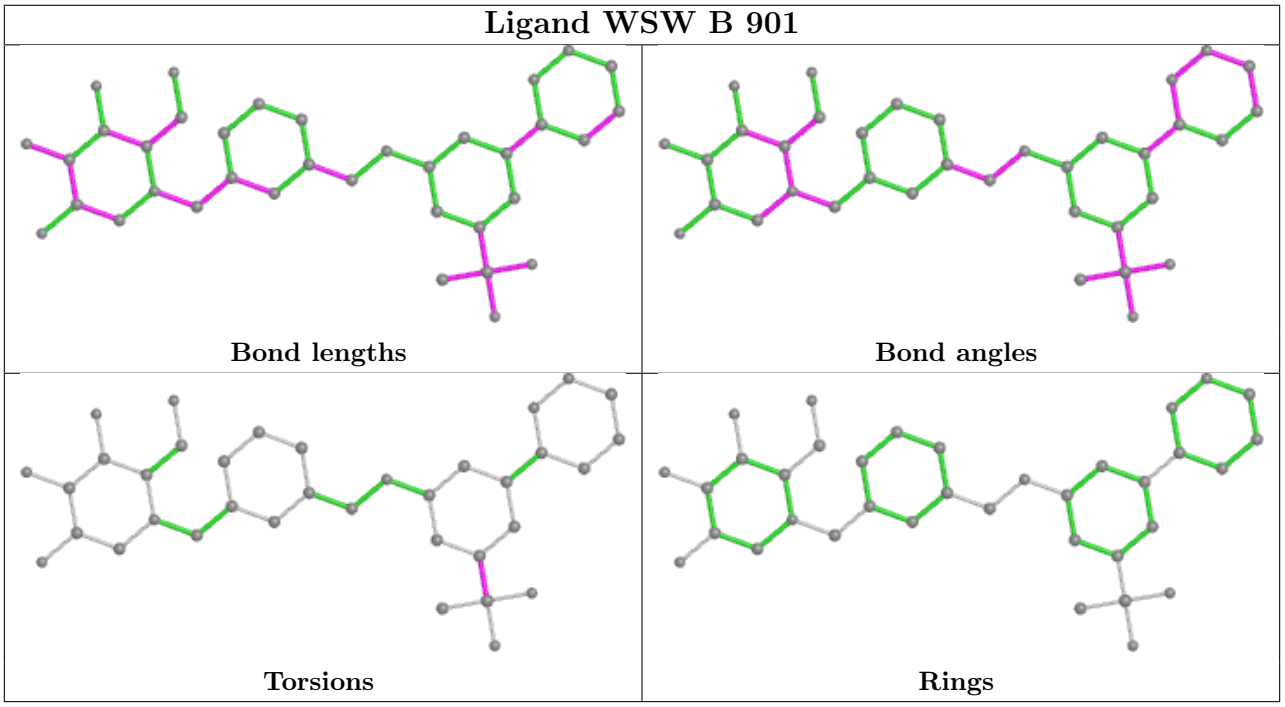
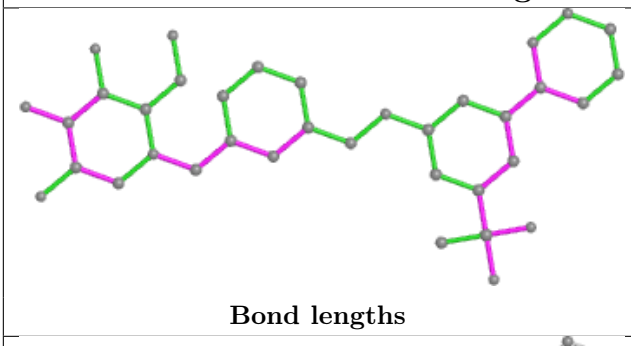
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	905	GOL	5	0
3	A	903	GOL	6	0

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 then 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.

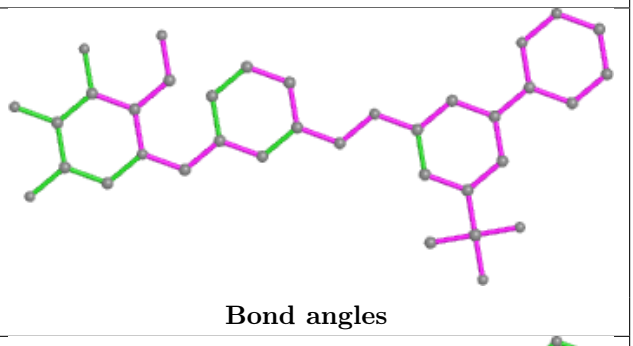
Ligand WSW B 901



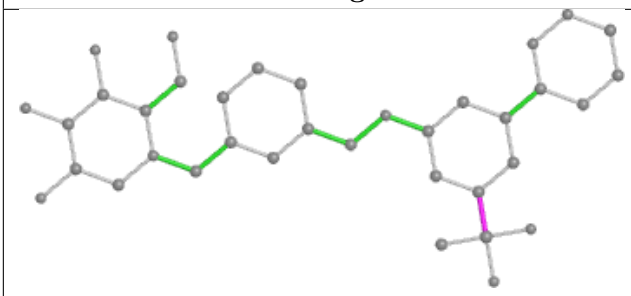
Ligand WSW A 901



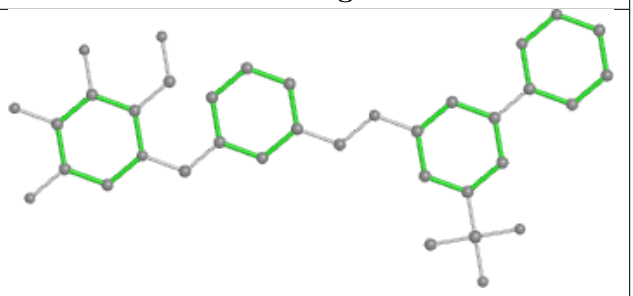
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	763/819 (93%)	0.11	35 (4%) 32 31	19, 30, 52, 81	0
1	B	764/819 (93%)	-0.10	5 (0%) 87 87	18, 28, 44, 77	0
All	All	1527/1638 (93%)	0.00	40 (2%) 56 54	18, 29, 49, 81	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	THR	5.4
1	A	40	ILE	4.6
1	A	515	LEU	4.3
1	A	43	LEU	3.8
1	A	629	PHE	3.8
1	A	531	LEU	3.8
1	A	516	ASP	3.5
1	A	38	SER	3.4
1	B	33	GLU	3.3
1	A	151	ASP	3.3
1	A	39	GLU	3.3
1	A	309	GLY	3.2
1	A	519	LEU	3.1
1	A	661	PHE	3.0
1	A	529	VAL	3.0
1	A	560	ASP	2.9
1	B	181	ASN	2.9
1	A	499	LEU	2.8
1	A	527	PRO	2.8
1	A	619	SER	2.8
1	A	41	GLY	2.7
1	A	136	ALA	2.6
1	A	623	ALA	2.6
1	A	622	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	621	LEU	2.5
1	A	624	THR	2.5
1	B	171	ASN	2.5
1	A	620	LEU	2.4
1	A	530	GLY	2.4
1	B	718	PHE	2.3
1	A	626	ASP	2.3
1	A	471	VAL	2.2
1	A	526	ASN	2.2
1	A	535	ARG	2.2
1	A	617	ILE	2.1
1	A	812	HIS	2.1
1	B	811	GLY	2.1
1	A	618	GLY	2.1
1	A	628	GLU	2.1
1	A	155	LYS	2.1

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 monosaccharides 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, 95^{th} 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
3	GOL	A	903	6/6	0.85	0.23	46,49,55,61	0
5	BTB	B	902	14/14	0.85	0.15	36,48,55,55	0
6	NAG	B	904	14/15	0.86	0.24	46,54,61,76	0
3	GOL	B	905	6/6	0.89	0.22	45,50,59,63	0
3	GOL	A	902	6/6	0.90	0.18	45,51,56,59	0
3	GOL	B	903	6/6	0.91	0.20	21,34,41,45	0
3	GOL	A	904	6/6	0.92	0.17	53,61,64,68	0

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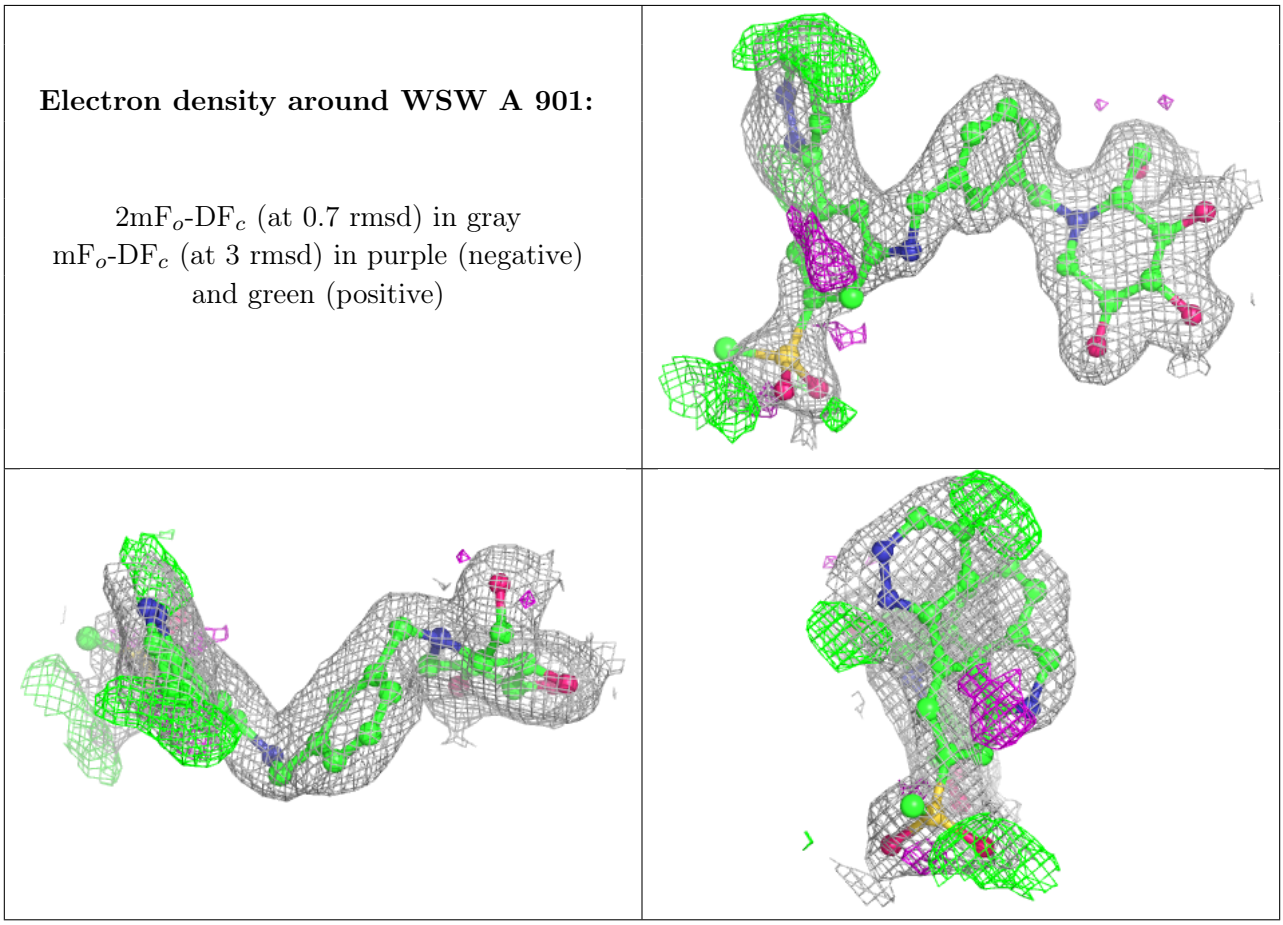
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	WSW	A	901	36/36	0.93	0.17	18,27,73,77	0
4	SO4	B	909	5/5	0.95	0.25	47,48,59,64	0
2	WSW	B	901	36/36	0.95	0.12	16,24,48,50	0
4	SO4	B	908	5/5	0.95	0.17	53,57,63,65	0
4	SO4	A	906	5/5	0.96	0.14	68,70,71,75	0
4	SO4	A	907	5/5	0.97	0.14	38,49,57,58	0
4	SO4	B	907	5/5	0.97	0.13	38,46,54,59	0
4	SO4	A	905	5/5	0.98	0.14	34,36,41,42	0
4	SO4	B	906	5/5	0.99	0.11	31,32,42,46	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.

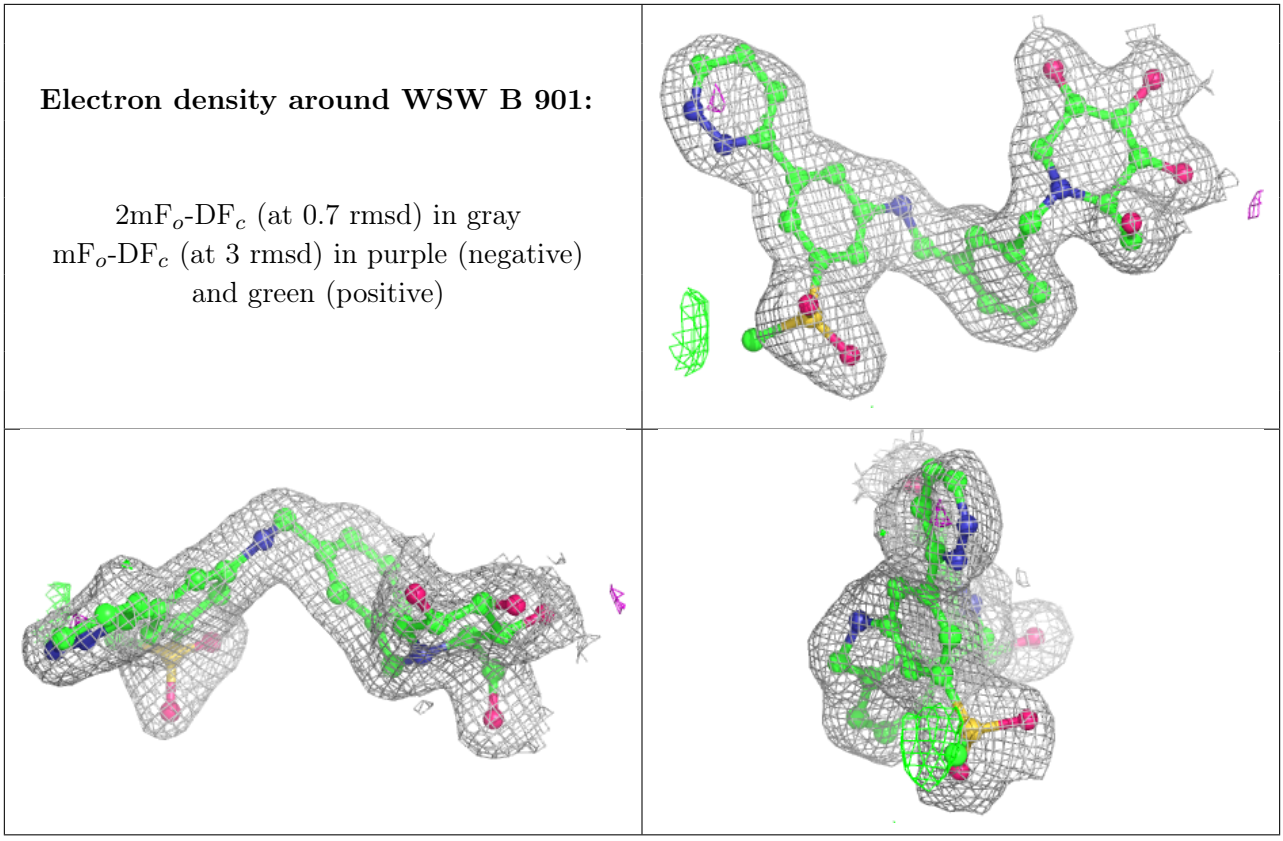
Electron density around WSW A 901:

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



Electron density around WSW B 901:

$2mF_o$-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.