



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:57 AM UTC

PDB ID : 8EUR / pdb_00008eur
Title : Co-crystal structure of Chaetomium glucosidase with compound 26
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2022-10-19
Resolution : 2.61 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

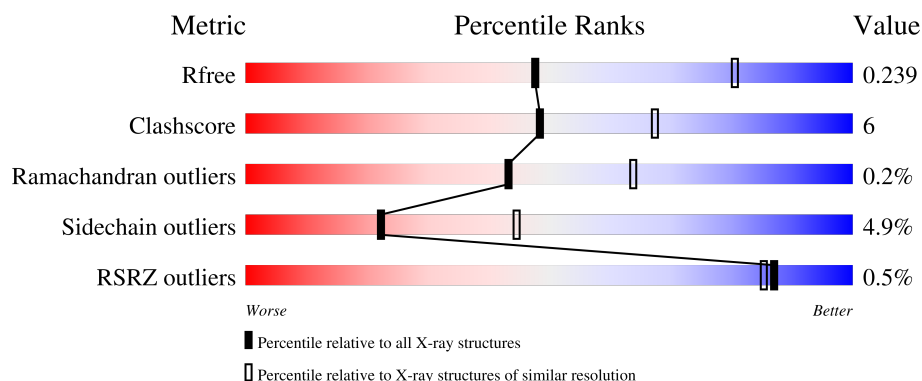
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	77% 15% • 7%
1	B	819	79% 12% • 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12395 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	1	0
			6067	3899	1023	1132	13			
1	B	764	Total	C	N	O	S	0	0	0
			6075	3899	1020	1143	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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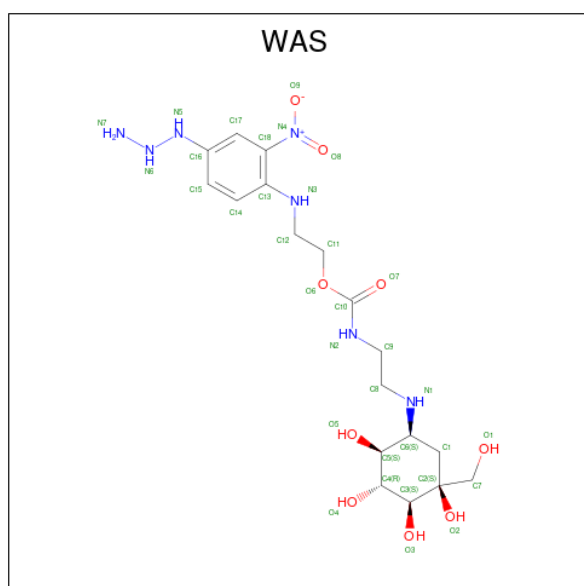
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	CYS	-	expression tag	UNP G0SFD1
A	25	VAL	-	expression tag	UNP G0SFD1
A	26	ALA	-	expression tag	UNP G0SFD1
A	27	GLU	-	expression tag	UNP G0SFD1
A	28	THR	-	expression tag	UNP G0SFD1
A	29	GLY	-	expression tag	UNP G0SFD1
A	810	SER	-	expression tag	UNP 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 2-{[2-nitro-4-(triazan-1-yl)phenyl]amino}ethyl (2-{[(1S,2S,3R,4S,5S)-2,3,4,5-tetrahydroxy-5-(hydroxymethyl)cyclohexyl]amino}ethyl)carbamate (CCD ID: WAS) (formula: $C_{18}H_{31}N_7O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	18	7	9		
2	B	1	Total	C	N	O	0	0
			34	18	7	9		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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).



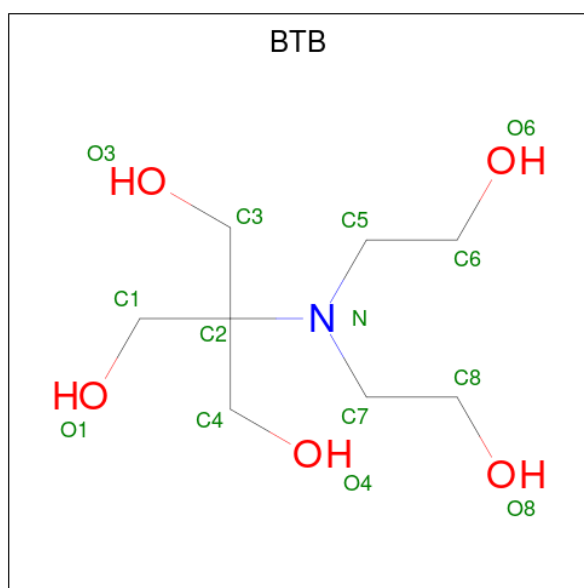
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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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	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-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



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

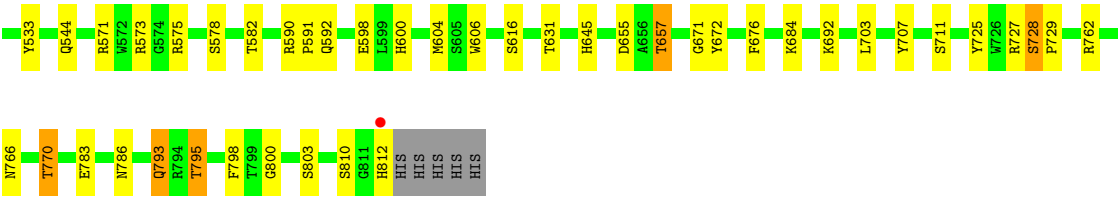
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	47	Total	O	0	0
			47	47		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	136.33Å 178.95Å 180.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.94 – 2.61 46.94 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.94-2.61) 99.9 (46.94-2.61)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.184 , 0.239 0.183 , 0.239	Depositor DCC
R_{free} test set	3441 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12395	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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: SO4, WAS, BTB, GOL

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	0.58	0/6246	1.13	15/8505 (0.2%)
1	B	0.60	2/6251 (0.0%)	1.12	11/8508 (0.1%)
All	All	0.59	2/12497 (0.0%)	1.13	26/17013 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	HIS	CE1-NE2	6.20	1.38	1.32
1	B	645	HIS	CE1-NE2	5.07	1.37	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	684	LYS	CB-CA-C	9.11	122.77	109.11
1	A	575	ARG	CB-CA-C	8.04	122.80	109.53
1	A	755	THR	CB-CA-C	-7.86	98.54	110.88
1	A	126	THR	CA-CB-OG1	-6.71	99.53	109.60
1	B	657	THR	CB-CA-C	-6.27	97.94	111.11
1	A	339	LYS	CB-CA-C	6.16	121.11	110.45
1	A	802	THR	CA-CB-OG1	-6.13	100.40	109.60
1	B	631	THR	CA-CB-OG1	-5.91	100.73	109.60
1	A	448	TYR	CB-CA-C	5.84	121.88	110.67
1	B	300	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	582	THR	CA-CB-OG1	-5.78	100.94	109.60
1	A	280	LYS	N-CA-CB	5.53	116.96	110.71
1	A	573	ARG	CG-CD-NE	-5.42	100.07	112.00
1	A	684	LYS	CB-CA-C	5.38	117.86	109.42
1	B	575	ARG	CB-CA-C	5.30	120.31	109.76
1	B	126	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	52	PRO	N-CA-C	-5.14	104.86	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LYS	CB-CA-C	-5.04	104.90	111.15
1	B	270	PRO	CB-CA-C	5.03	117.06	110.92
1	B	592	GLN	CB-CA-C	5.03	115.93	110.15
1	A	574	GLY	CA-C-N	-5.02	114.66	122.09
1	A	574	GLY	C-N-CA	-5.02	114.66	122.09
1	B	481	HIS	CB-CA-C	5.02	118.39	109.65
1	B	39	GLU	CB-CA-C	5.01	118.81	110.90
1	A	267	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	788	GLU	CB-CG-CD	5.00	121.11	112.60

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	6067	0	5734	73	0
1	B	6075	0	5734	57	0
2	A	34	0	0	1	0
2	B	34	0	0	1	0
3	A	6	0	8	1	0
3	B	6	0	8	2	0
4	A	20	0	0	0	0
4	B	25	0	0	2	0
5	B	14	0	19	1	0
6	A	67	0	0	0	0
6	B	47	0	0	0	0
All	All	12395	0	11503	131	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (131) 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:783:GLU:OE1	1:B:795:THR:HG23	1.51	1.08
1:A:550:LYS:HE2	1:A:550:LYS:HA	1.48	0.93
1:B:786:ASN:HB2	1:B:793:GLN:OE1	1.70	0.92
1:B:812:HIS:HD2	3:B:902:GOL:O2	1.61	0.82
1:B:766:ASN:O	1:B:770:THR:HG23	1.82	0.79
1:B:450:LEU:HB3	4:B:907:SO4:O4	1.83	0.78
1:A:110:ARG:NH2	1:A:323:GLN:HG3	2.07	0.69
1:A:550:LYS:HA	1:A:550:LYS:CE	2.22	0.69
1:A:451:MET:CE	1:A:540:LEU:HB3	2.22	0.68
1:A:489:PHE:CE1	1:A:610:MET:HE3	2.31	0.66
1:A:451:MET:HE1	1:A:540:LEU:HB3	1.78	0.65
1:B:766:ASN:O	1:B:770:THR:CG2	2.44	0.65
1:A:251:LEU:HD23	1:A:277:LEU:HD21	1.79	0.64
1:A:569:ALA:HB1	1:A:599:LEU:HD22	1.79	0.64
1:B:762:ARG:HD2	4:B:906:SO4:O3	1.97	0.64
1:B:194:ARG:CG	1:B:194:ARG:HH11	2.10	0.63
1:B:812:HIS:CD2	3:B:902:GOL:O2	2.50	0.63
1:A:659:ASP:HB3	1:A:661:PHE:H	1.63	0.62
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.36	0.61
1:B:590:ARG:HB3	1:B:591:PRO:CD	2.30	0.61
1:A:757:ARG:HH22	3:A:902:GOL:H2	1.65	0.60
1:A:416:PHE:CD2	1:A:795:THR:HG23	2.37	0.59
1:B:140:SER:HB3	1:B:303:PHE:O	2.03	0.59
1:B:451:MET:CE	1:B:544:GLN:HB2	2.33	0.59
1:B:728:SER:N	1:B:729:PRO:CD	2.67	0.58
1:B:128:SER:O	1:B:143:ALA:HA	2.05	0.57
1:B:451:MET:HE2	1:B:544:GLN:HB2	1.87	0.56
1:B:385:GLY:HA2	1:B:387:TRP:CZ3	2.41	0.56
1:A:727:ARG:O	1:A:728:SER:HB3	2.04	0.55
1:B:727:ARG:O	1:B:728:SER:HB3	2.07	0.55
1:A:234[B]:THR:HA	1:A:285:ASN:OD1	2.07	0.54
1:B:65:ILE:HD13	1:B:197:ALA:HB1	1.90	0.54
1:A:244:LYS:HB3	1:A:245:PRO:HD3	1.90	0.54
1:A:607:VAL:O	1:A:611:VAL:HG22	2.08	0.54
1:A:569:ALA:HA	1:A:604:MET:CE	2.38	0.53
1:A:550:LYS:HE2	1:A:550:LYS:CA	2.27	0.53
1:B:194:ARG:HH11	1:B:194:ARG:HG3	1.74	0.53
1:A:594:PRO:HA	1:A:598:GLU:OE1	2.10	0.52
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.44	0.52
1:A:451:MET:SD	1:A:455:GLY:HA2	2.50	0.51
1:A:234[A]:THR:HA	1:A:285:ASN:OD1	2.10	0.51
1:B:571:ARG:HB3	1:B:573:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:901:WAS:N1	2:A:901:WAS:O2	2.44	0.51
1:A:481:HIS:H	1:A:481:HIS:CD2	2.28	0.51
1:A:678:PHE:CE1	1:A:741:GLN:HB3	2.46	0.51
1:A:233:LEU:HD22	1:B:265:VAL:HG23	1.93	0.51
1:B:590:ARG:HB3	1:B:591:PRO:HD2	1.93	0.50
1:A:434:ASP:OD2	1:A:807:LYS:HD3	2.11	0.50
1:A:354:MET:HE1	1:A:781:ALA:HB2	1.94	0.50
1:A:553:ALA:O	1:A:573:ARG:NH2	2.40	0.50
1:B:600:HIS:HA	1:B:655:ASP:OD1	2.11	0.50
1:A:106:TYR:CD2	1:A:360:GLY:HA2	2.46	0.49
1:A:672:TYR:CZ	1:A:711:SER:HA	2.47	0.49
1:B:258:LEU:HD11	1:B:274:VAL:HG22	1.94	0.49
1:A:728:SER:N	1:A:729:PRO:CD	2.75	0.49
1:A:623:ALA:O	1:A:626:ASP:HB2	2.12	0.49
1:A:723:GLU:O	1:A:794:ARG:NH1	2.40	0.49
1:A:234[A]:THR:CG2	1:A:284:GLY:HA2	2.43	0.49
1:A:64:ARG:HD3	1:A:408:PHE:CE1	2.48	0.49
1:A:71:THR:HB	1:A:163:PHE:CZ	2.47	0.48
1:A:161:VAL:HG11	1:A:299:PHE:HE1	1.77	0.48
1:A:212:ILE:O	1:A:212:ILE:HG13	2.12	0.48
1:B:101:TYR:HA	1:B:115:SER:O	2.12	0.48
1:B:728:SER:H	1:B:729:PRO:CD	2.26	0.48
1:B:707:TYR:HA	1:B:770:THR:HG21	1.96	0.48
1:A:251:LEU:HD23	1:A:277:LEU:CD2	2.44	0.48
1:A:736:TYR:OH	1:A:807:LYS:HE3	2.14	0.48
1:B:441:LEU:HD22	1:B:533:TYR:CE1	2.49	0.48
1:A:44:ASN:ND2	1:A:519:LEU:HD22	2.28	0.47
1:B:427:PHE:CE2	1:B:487:THR:HG21	2.49	0.47
1:A:39:GLU:HA	1:A:39:GLU:OE2	2.13	0.47
1:A:569:ALA:HA	1:A:604:MET:HE2	1.95	0.47
1:B:194:ARG:HG3	1:B:194:ARG:NH1	2.29	0.47
1:B:106:TYR:CE2	1:B:360:GLY:HA2	2.50	0.47
1:A:313:THR:O	1:A:316:ASP:HB2	2.14	0.46
1:A:428:HIS:O	1:A:431:PRO:HD2	2.16	0.46
1:B:728:SER:N	1:B:729:PRO:HD3	2.29	0.46
1:A:659:ASP:HB2	1:A:663:GLU:H	1.80	0.46
1:B:485:PRO:HB3	1:B:606:TRP:CE2	2.51	0.46
1:A:570:TYR:HB3	1:A:603:LEU:HG	1.98	0.46
1:B:194:ARG:HA	1:B:199:GLY:O	2.15	0.46
1:A:519:LEU:HD23	1:A:519:LEU:HA	1.73	0.46
1:B:798:PHE:C	1:B:800:GLY:HA3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:SER:HB3	1:B:185:TYR:CD2	2.51	0.45
1:A:101:TYR:HA	1:A:115:SER:O	2.15	0.45
1:A:128:SER:O	1:A:143:ALA:HA	2.17	0.45
1:A:256:ASP:OD2	1:B:262:LYS:HE3	2.15	0.45
1:A:110:ARG:HD2	1:A:110:ARG:HA	1.67	0.45
1:B:134:GLY:O	1:B:139:GLY:HA2	2.17	0.45
1:B:331:ARG:NH1	1:B:435:TRP:O	2.49	0.45
1:A:451:MET:HE3	1:A:540:LEU:HD22	1.99	0.45
1:B:425:GLU:HG2	1:B:447:TRP:NE1	2.31	0.45
2:B:901:WAS:C10	2:B:901:WAS:N3	2.80	0.45
1:B:71:THR:HB	1:B:163:PHE:CZ	2.52	0.44
1:B:433:ALA:O	1:B:498:ARG:NH2	2.51	0.44
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.52	0.44
1:B:786:ASN:CB	1:B:793:GLN:OE1	2.55	0.44
1:A:49:LEU:HD22	1:A:138:GLY:HA3	1.99	0.44
1:A:110:ARG:HH21	1:A:323:GLN:HG3	1.81	0.44
1:A:106:TYR:CE2	1:A:360:GLY:HA2	2.53	0.44
1:A:241:TRP:CE2	1:A:242:GLN:HG2	2.52	0.44
1:A:672:TYR:CE2	1:A:711:SER:HA	2.52	0.44
1:A:110:ARG:HH22	1:A:323:GLN:HG3	1.82	0.44
1:A:675:LEU:O	1:A:676:PHE:C	2.61	0.44
1:A:720:GLY:HA2	1:A:724:ASN:OD1	2.18	0.44
5:B:903:BTB:H41	5:B:903:BTB:H72	1.72	0.44
1:A:373:ARG:O	1:A:375:TYR:HD1	2.01	0.43
1:B:105:GLU:HA	1:B:356:SER:OG	2.18	0.43
1:A:75:TRP:HA	1:A:160:ILE:O	2.19	0.43
1:B:145:ILE:HD13	1:B:301:ILE:CD1	2.49	0.43
1:A:545:PHE:CE1	1:A:611:VAL:HG13	2.53	0.42
1:A:719:TYR:CE1	1:A:728:SER:HB2	2.54	0.42
1:A:805:VAL:HA	1:A:808:ILE:HD12	2.00	0.42
1:B:142:ALA:HB3	1:B:317:LEU:HD13	2.01	0.42
1:B:145:ILE:O	1:B:298:GLU:HA	2.19	0.42
1:B:727:ARG:O	1:B:728:SER:CB	2.67	0.42
1:A:176:ALA:HA	1:A:191:LEU:HD23	2.01	0.42
1:A:375:TYR:O	1:A:376:ALA:C	2.63	0.41
1:B:451:MET:HE1	1:B:544:GLN:HB2	2.02	0.41
1:A:636:ALA:O	1:A:640:ASN:HB2	2.19	0.41
1:B:591:PRO:HD2	1:B:598:GLU:OE2	2.21	0.41
1:B:270:PRO:HA	1:B:271:PRO:HD3	2.01	0.41
1:A:110:ARG:HH22	1:A:323:GLN:HE21	1.69	0.41
1:B:41:GLY:O	1:B:45:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:GLY:HA2	1:B:703:LEU:HD21	2.03	0.41
1:B:672:TYR:CE2	1:B:711:SER:HB3	2.56	0.40
1:B:354:MET:HE3	1:B:803:SER:HA	2.02	0.40
1:A:240:LEU:HD22	1:A:286:VAL:CG2	2.52	0.40
1:A:130:VAL:HG21	1:A:320:GLU:HB3	2.03	0.40
1:A:451:MET:HE1	1:A:540:LEU:CB	2.50	0.40
1:B:376:ALA:HA	1:B:377:PRO:HD2	1.91	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%)	732 (96%)	28 (4%)	2 (0%)	36	56
1	B	760/819 (93%)	737 (97%)	22 (3%)	1 (0%)	48	69
All	All	1522/1638 (93%)	1469 (96%)	50 (3%)	3 (0%)	43	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	A	728	SER
1	B	728	SER

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	627/707 (89%)	596 (95%)	31 (5%)	22	44
1	B	631/707 (89%)	600 (95%)	31 (5%)	22	44
All	All	1258/1414 (89%)	1196 (95%)	62 (5%)	22	44

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	44	ASN
1	A	45	ASN
1	A	99	LYS
1	A	126	THR
1	A	155	LYS
1	A	158	LYS
1	A	212	ILE
1	A	218	ASP
1	A	343	GLN
1	A	348	LYS
1	A	349	LYS
1	A	438	ASP
1	A	445	LYS
1	A	470	LYS
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	676	PHE
1	A	692	LYS
1	A	748	GLN
1	A	753	LYS
1	A	758	ASP
1	A	765	LYS
1	A	773	ARG
1	A	805	VAL
1	A	807	LYS
1	B	33	GLU
1	B	42	ARG
1	B	44	ASN

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Mol	Chain	Res	Type
1	B	98	MET
1	B	105	GLU
1	B	126	THR
1	B	145	ILE
1	B	173	GLU
1	B	186	GLU
1	B	194	ARG
1	B	221	ARG
1	B	244	LYS
1	B	262	LYS
1	B	274	VAL
1	B	323	GLN
1	B	383	ASN
1	B	438	ASP
1	B	449	ASN
1	B	459	ARG
1	B	498	ARG
1	B	578	SER
1	B	604	MET
1	B	616	SER
1	B	657	THR
1	B	676	PHE
1	B	692	LYS
1	B	725	TYR
1	B	770	THR
1	B	793	GLN
1	B	795	THR
1	B	810	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	250	GLN
1	A	323	GLN
1	A	481	HIS
1	B	231	GLN
1	B	250	GLN
1	B	398	GLN
1	B	544	GLN
1	B	812	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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$
4	SO4	A	906	-	4,4,4	0.31	0	6,6,6	0.11	0
4	SO4	B	907	-	4,4,4	0.35	0	6,6,6	0.15	0
4	SO4	A	905	-	4,4,4	0.24	0	6,6,6	0.17	0
2	WAS	A	901	-	35,35,35	2.67	8 (22%)	39,48,48	2.38	10 (25%)
5	BTB	B	903	-	13,13,13	1.44	2 (15%)	7,16,16	1.05	0
4	SO4	B	906	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	A	904	-	4,4,4	0.25	0	6,6,6	0.09	0
3	GOL	B	902	-	5,5,5	0.16	0	5,5,5	0.59	0
4	SO4	B	904	-	4,4,4	0.48	0	6,6,6	0.33	0
4	SO4	B	908	-	4,4,4	0.29	0	6,6,6	0.14	0
4	SO4	B	905	-	4,4,4	0.26	0	6,6,6	0.18	0
3	GOL	A	902	-	5,5,5	0.10	0	5,5,5	0.50	0
2	WAS	B	901	-	35,35,35	2.56	7 (20%)	39,48,48	1.44	4 (10%)
4	SO4	A	903	-	4,4,4	0.36	0	6,6,6	0.29	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
2	WAS	A	901	-	-	9/21/47/47	0/2/2/2
5	BTB	B	903	-	-	7/21/21/21	-
3	GOL	B	902	-	-	0/4/4/4	-
3	GOL	A	902	-	-	3/4/4/4	-
2	WAS	B	901	-	-	10/21/47/47	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	WAS	O8-N4	11.69	1.42	1.22
2	B	901	WAS	O8-N4	11.00	1.41	1.22
2	A	901	WAS	C10-N2	6.87	1.48	1.34
2	B	901	WAS	C10-N2	6.72	1.48	1.34
2	B	901	WAS	C13-N3	3.69	1.47	1.37
2	A	901	WAS	O2-C2	-3.57	1.38	1.44
5	B	903	BTB	C2-N	3.55	1.55	1.48
2	B	901	WAS	O6-C10	3.46	1.42	1.35
2	A	901	WAS	C13-N3	2.99	1.45	1.37
2	B	901	WAS	O2-C2	-2.96	1.39	1.44
2	A	901	WAS	O7-C10	-2.84	1.16	1.21
2	B	901	WAS	N5-N6	2.82	1.44	1.41
2	A	901	WAS	O6-C10	2.78	1.40	1.35
2	A	901	WAS	C16-N5	2.70	1.48	1.39
2	B	901	WAS	C16-N5	2.65	1.47	1.39
2	A	901	WAS	N5-N6	2.41	1.44	1.41
5	B	903	BTB	C7-N	2.25	1.51	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	WAS	O6-C10-N2	9.49	126.27	110.62
2	A	901	WAS	O6-C10-O7	-5.26	114.17	124.26
2	B	901	WAS	O6-C10-N2	5.09	119.02	110.62
2	A	901	WAS	C16-C17-C18	3.76	122.08	119.57
2	A	901	WAS	O2-C2-C7	3.75	113.23	108.25
2	A	901	WAS	O7-C10-N2	-3.60	119.52	124.93
2	A	901	WAS	C17-C18-C13	-3.44	118.41	121.55
2	A	901	WAS	O2-C2-C3	-3.00	101.81	108.40
2	A	901	WAS	C1-C6-C5	-2.93	106.77	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	WAS	O6-C10-O7	-2.72	119.04	124.26
2	A	901	WAS	C18-C13-N3	-2.41	119.24	123.38
2	B	901	WAS	C16-N5-N6	2.36	122.84	116.79
2	A	901	WAS	C16-N5-N6	2.32	122.74	116.79
2	B	901	WAS	O5-C5-C6	2.21	114.00	109.40

There are no chirality outliers.

All (29) torsion outliers are listed below:

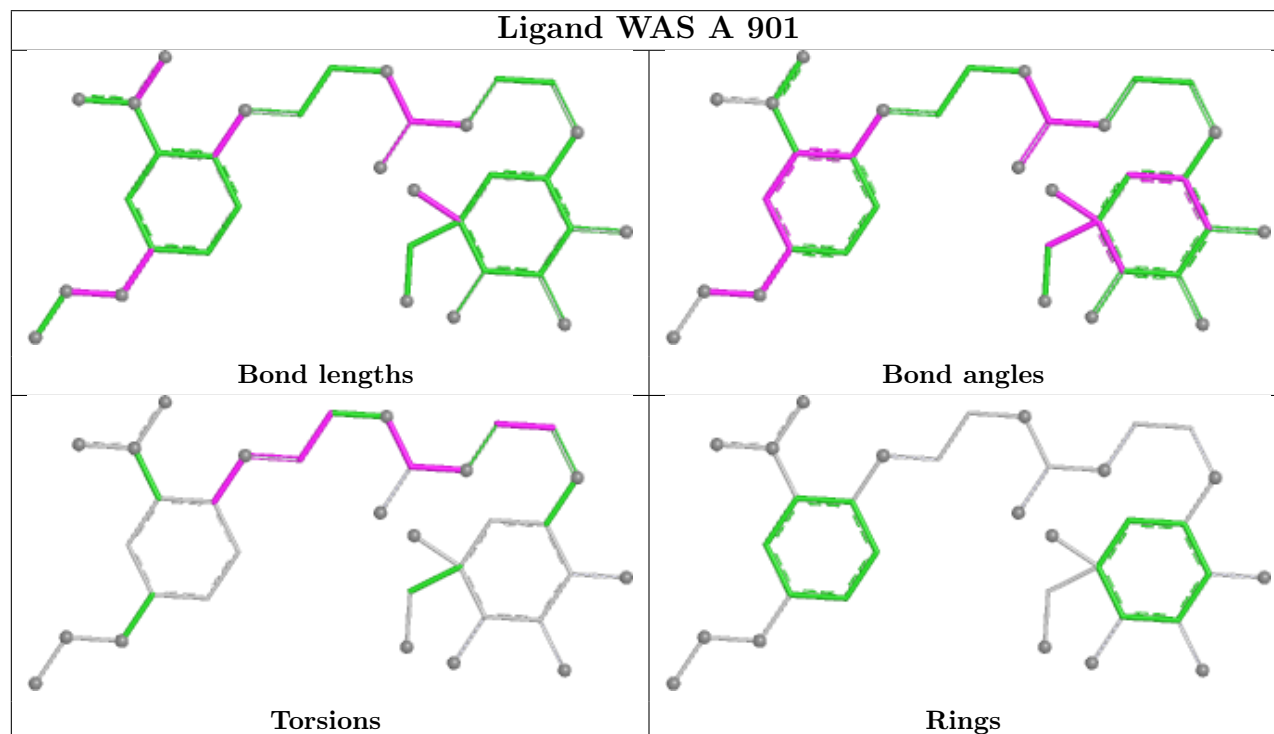
Mol	Chain	Res	Type	Atoms
2	A	901	WAS	O6-C10-N2-C9
2	A	901	WAS	O7-C10-N2-C9
2	B	901	WAS	O6-C10-N2-C9
5	B	903	BTB	O1-C1-C2-C3
5	B	903	BTB	O1-C1-C2-N
5	B	903	BTB	C1-C2-C4-O4
5	B	903	BTB	C3-C2-C4-O4
5	B	903	BTB	N-C2-C4-O4
2	A	901	WAS	O7-C10-O6-C11
2	A	901	WAS	N1-C8-C9-N2
2	A	901	WAS	N2-C10-O6-C11
2	B	901	WAS	O6-C11-C12-N3
2	B	901	WAS	O7-C10-N2-C9
5	B	903	BTB	N-C7-C8-O8
2	B	901	WAS	N1-C8-C9-N2
2	A	901	WAS	O6-C11-C12-N3
2	A	901	WAS	C18-C13-N3-C12
3	A	902	GOL	O1-C1-C2-C3
3	A	902	GOL	O1-C1-C2-O2
2	B	901	WAS	C11-C12-N3-C13
2	B	901	WAS	C17-C16-N5-N6
3	A	902	GOL	O2-C2-C3-O3
2	B	901	WAS	C15-C16-N5-N6
2	A	901	WAS	C14-C13-N3-C12
2	B	901	WAS	C1-C6-N1-C8
2	B	901	WAS	C5-C6-N1-C8
2	A	901	WAS	C11-C12-N3-C13
2	B	901	WAS	C8-C9-N2-C10
5	B	903	BTB	C4-C2-N-C7

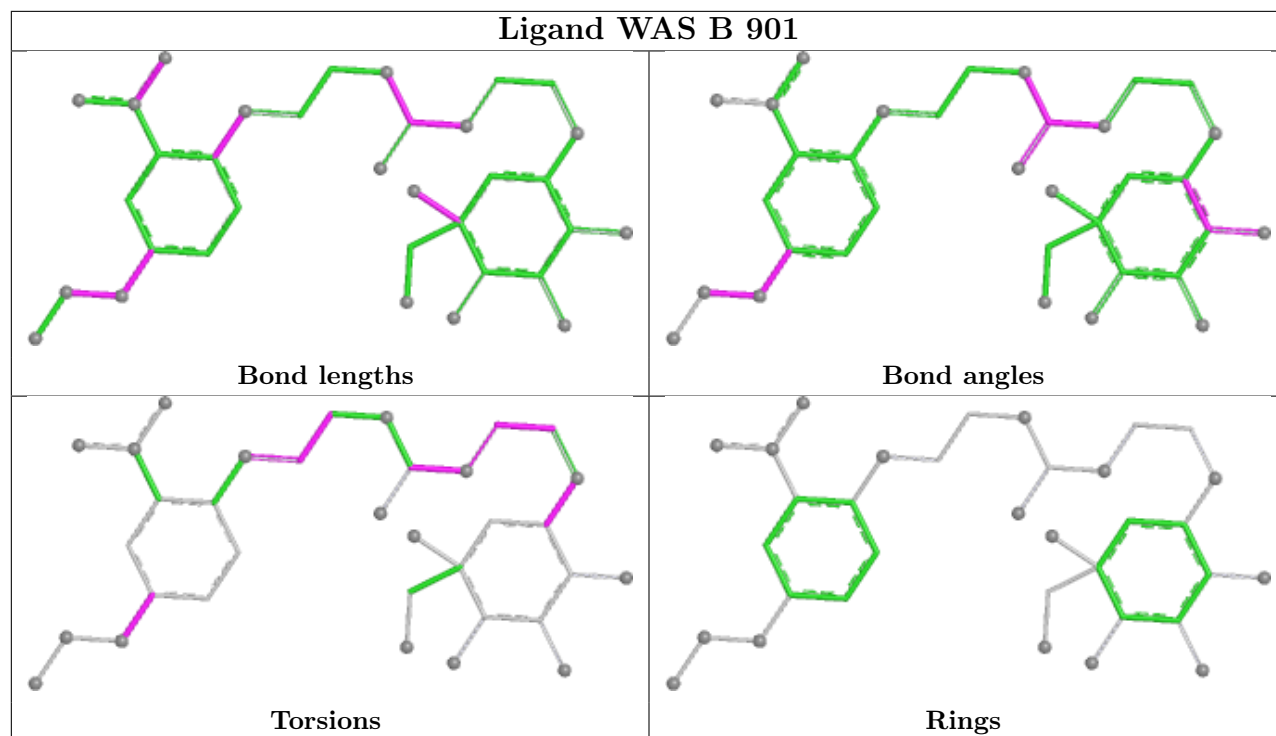
There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	907	SO4	1	0
2	A	901	WAS	1	0
5	B	903	BTB	1	0
4	B	906	SO4	1	0
3	B	902	GOL	2	0
3	A	902	GOL	1	0
2	B	901	WAS	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%)	-0.48	6 (0%)	82 80	22, 45, 73, 100	1 (0%)
1	B	764/819 (93%)	-0.49	2 (0%)	90 88	27, 46, 74, 97	0
All	All	1529/1638 (93%)	-0.48	8 (0%)	87 85	22, 46, 73, 100	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	3.8
1	B	518	THR	3.1
1	A	560	ASP	3.0
1	B	812	HIS	2.8
1	A	36	LEU	2.4
1	A	812	HIS	2.4
1	A	661	PHE	2.2
1	A	660	GLU	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 oligosaccharides in this entry.

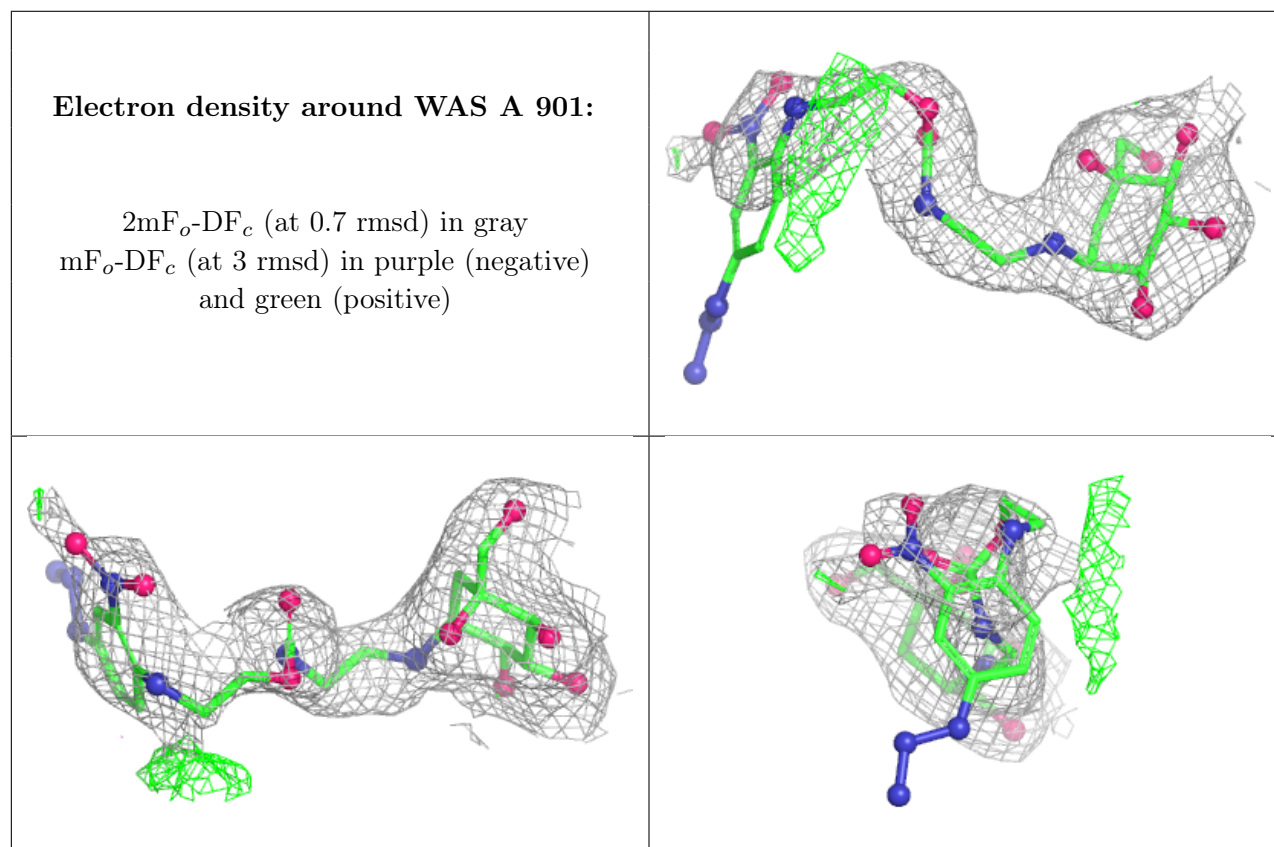
6.4 Ligands [i](#)

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.

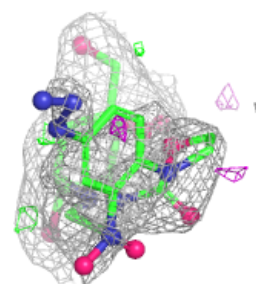
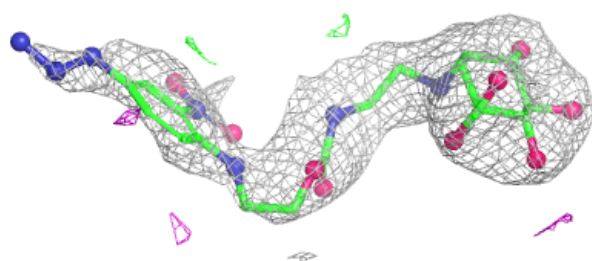
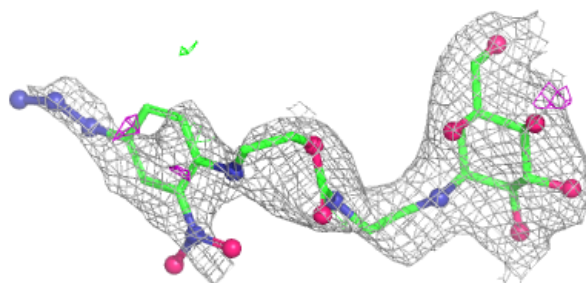
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	908	5/5	0.65	0.12	98,99,107,111	0
4	SO4	A	906	5/5	0.80	0.12	97,115,119,130	0
3	GOL	A	902	6/6	0.82	0.15	59,68,77,83	0
5	BTB	B	903	14/14	0.85	0.15	61,83,95,96	0
3	GOL	B	902	6/6	0.89	0.14	59,65,70,81	0
4	SO4	A	904	5/5	0.90	0.14	85,85,90,92	0
2	WAS	A	901	34/34	0.92	0.14	31,75,150,164	0
2	WAS	B	901	34/34	0.93	0.12	35,78,122,125	0
4	SO4	A	905	5/5	0.94	0.23	74,75,79,95	0
4	SO4	B	906	5/5	0.94	0.10	64,75,85,87	0
4	SO4	B	905	5/5	0.95	0.10	56,69,82,85	0
4	SO4	B	907	5/5	0.95	0.13	65,75,80,101	0
4	SO4	B	904	5/5	0.97	0.07	37,42,55,62	0
4	SO4	A	903	5/5	0.99	0.04	41,42,46,48	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 WAS 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 ⓘ

There are no such residues in this entry.