W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 15, 2023 – 10:22 AM EDT

PDB ID	:	8EUD
Title	:	Co-crystal structure of Chaetomium glucosidase with compound 22
Authors	:	Karade, S.S.; Mariuzza, R.A.
Deposited on	:	2022-10-18
Resolution	:	2.37 Å(reported)

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 ⓘ

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

The reported resolution of this entry is 2.37 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.
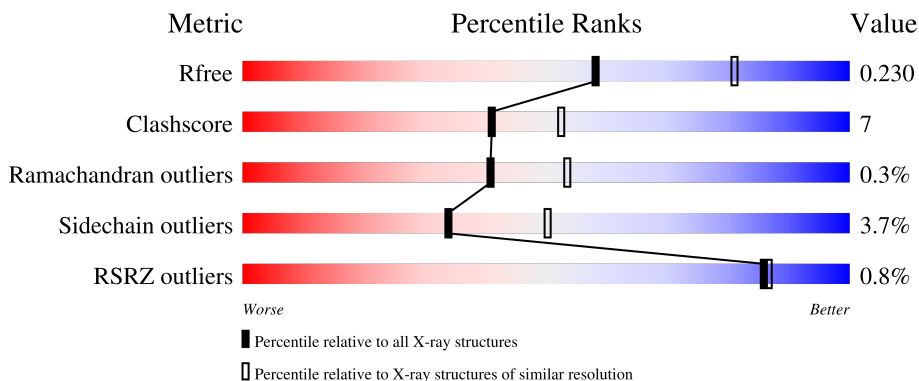
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	80% 11% · 7%
1	B	819	79% 13% · 6%

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
4	SO4	B	1009	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12749 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 6029	C 3870	N 1018	O 1128	S 13	0	1	0
1	B	767	Total 6041	C 3876	N 1019	O 1133	S 13	0	0	0

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-{6-[2-methyl-5-(pyrimidin-2-yl)-1H-benzimidazol-1-yl]hexyl}piperidine-3,4,5-triol (three-letter code: WUR) (formula: $C_{24}H_{33}N_5O_4$) (labeled as "Ligand of Interest" by depositor).
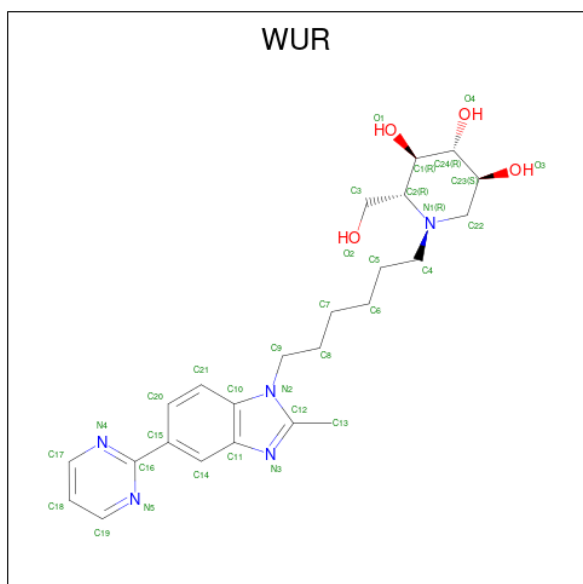
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 33	C 24	N 5	O 4	0	0
2	B	1	Total 33	C 24	N 5	O 4	0	0

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

GOL

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

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

SO4

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

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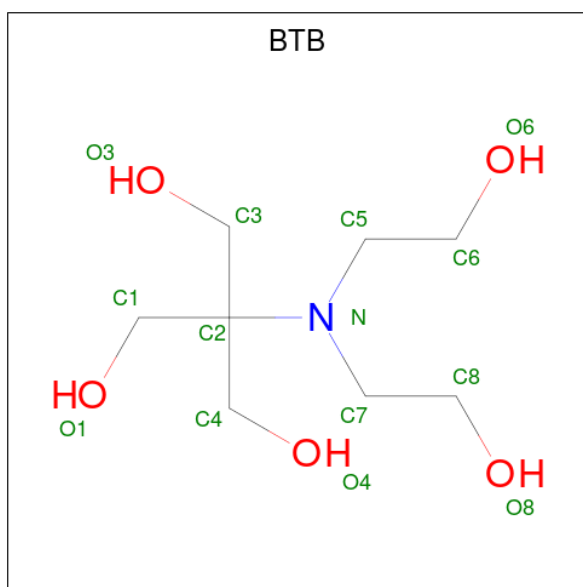| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
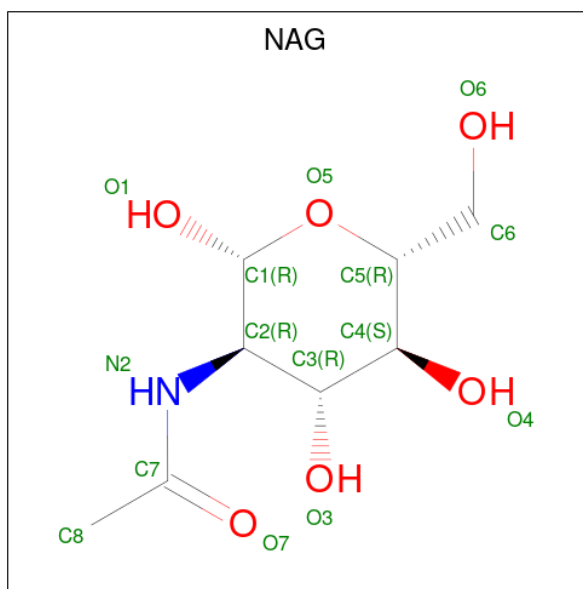
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).

BTB

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

- Molecule 7 is water.

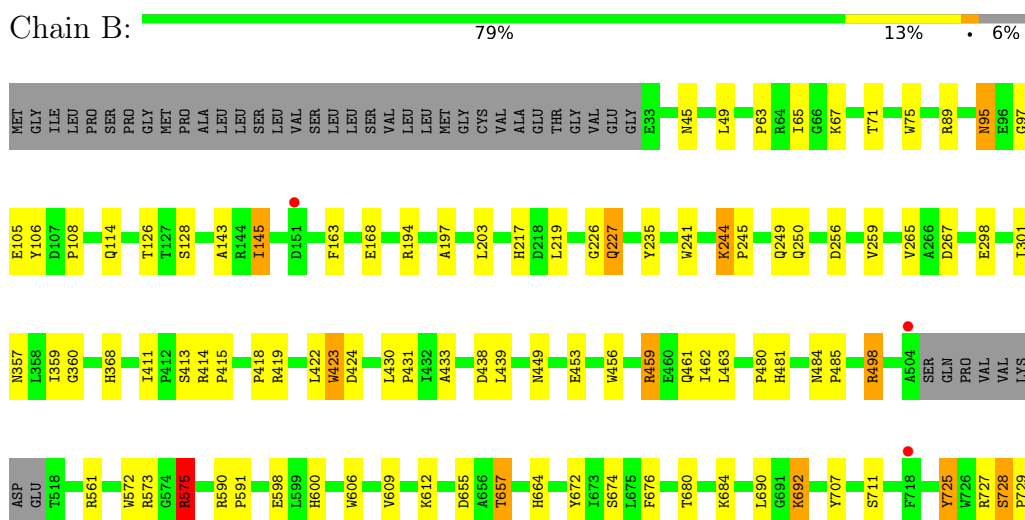| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	252	Total 252	O 252	0	0
7	B	270	Total 270	O 270	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Chaetomium alpha glucosidase

Chain A:

• Molecule 1: Chaetomium alpha glucosidase

Chain B:

R762 N766 T770 W782 E783 N786 P787 E788 T789 G792 Q793 Q796 H797 W801 T802 S803 V806 H812 HIS HIS HIS HIS HIS
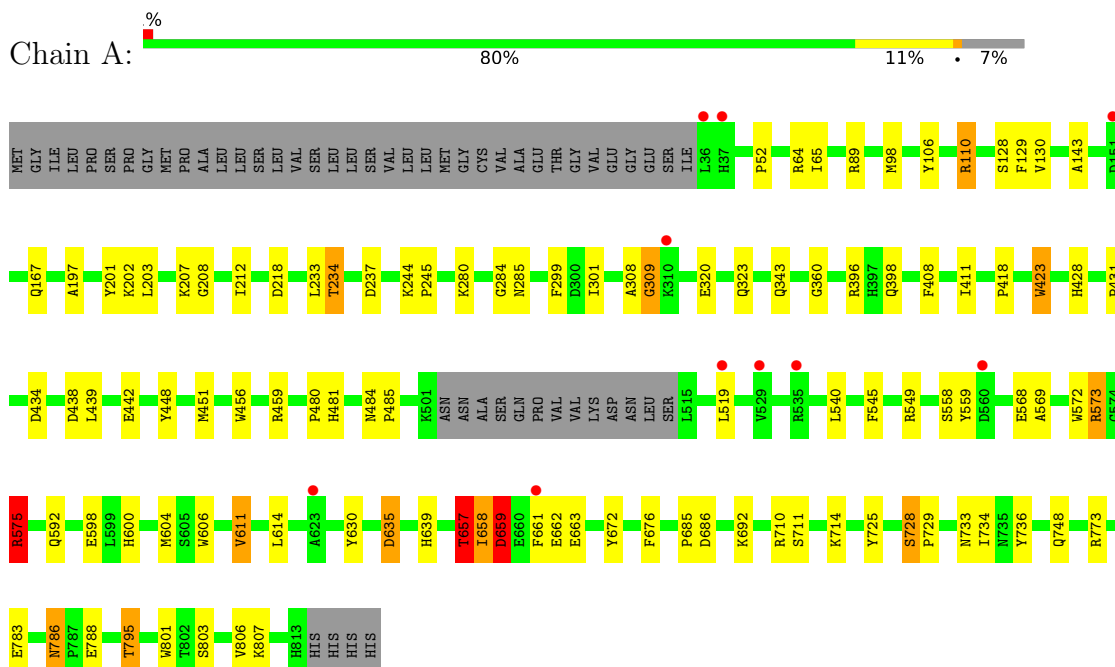
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	135.03Å 178.12Å 179.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.66 – 2.37 46.61 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.66-2.37) 99.4 (46.61-2.37)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , 0.230 0.178 , 0.230	Depositor DCC
R_{free} test set	4280 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 31.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12749	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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, WUR, BTB, SO4

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	0.47	0/6208	0.85	12/8460 (0.1%)
1	B	0.50	0/6217	0.90	14/8475 (0.2%)
All	All	0.48	0/12425	0.88	26/16935 (0.2%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	B	459	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	B	575	ARG	CG-CD-NE	-8.89	93.12	111.80
1	B	459	ARG	CG-CD-NE	-8.62	93.69	111.80
1	A	459	ARG	CG-CD-NE	-8.30	94.36	111.80

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	6029	0	5639	78	0
1	B	6041	0	5649	88	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	8	3	0
3	B	12	0	16	2	0
4	A	25	0	0	0	0
4	B	20	0	0	3	0
5	B	14	0	13	0	0
6	B	14	0	19	3	0
7	A	252	0	0	5	0
7	B	270	0	0	6	0
All	All	12749	0	11344	168	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.

The worst 5 of 168 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:MET:CE	1:A:540:LEU:HB3	1.83	1.07
1:A:795:THR:HG23	7:A:1002:HOH:O	1.60	0.99
1:A:657:THR:HG21	7:A:1056:HOH:O	1.63	0.96
1:A:451:MET:HE1	1:A:540:LEU:HB3	1.45	0.96
1:B:572:TRP:H	1:B:600:HIS:HD2	1.10	0.91

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	762/819 (93%)	733 (96%)	26 (3%)	3 (0%)	34	46
1	B	763/819 (93%)	742 (97%)	20 (3%)	1 (0%)	51	67
All	All	1525/1638 (93%)	1475 (97%)	46 (3%)	4 (0%)	41	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	A	659	ASP
1	A	728	SER
1	B	728	SER

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	616/707 (87%)	592 (96%)	24 (4%)	32	48
1	B	619/707 (88%)	597 (96%)	22 (4%)	35	51
All	All	1235/1414 (87%)	1189 (96%)	46 (4%)	34	50

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	227	GLN
1	B	449	ASN
1	B	244	LYS
1	B	423	TRP
1	B	575	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	ASN
1	B	664	HIS
1	B	368	HIS
1	B	484	ASN
1	B	786	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
4	SO4	A	905	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	A	906	-	4,4,4	0.32	0	6,6,6	0.22	0
4	SO4	B	1009	-	4,4,4	0.25	0	6,6,6	0.25	0
6	BTB	B	1002	-	13,13,13	0.98	1 (7%)	7,16,16	0.46	0
2	WUR	B	1005	-	33,36,36	2.46	6 (18%)	38,50,50	2.11	10 (26%)
3	GOL	B	1003	-	5,5,5	0.17	0	5,5,5	0.32	0
3	GOL	A	902	-	5,5,5	0.21	0	5,5,5	0.68	0
4	SO4	A	903	-	4,4,4	0.47	0	6,6,6	0.44	0
4	SO4	A	907	-	4,4,4	0.21	0	6,6,6	0.17	0
4	SO4	B	1008	-	4,4,4	0.28	0	6,6,6	0.14	0
5	NAG	B	1001	1	14,14,15	1.40	3 (21%)	17,19,21	2.59	7 (41%)
4	SO4	B	1007	-	4,4,4	0.56	0	6,6,6	0.20	0
4	SO4	B	1006	-	4,4,4	0.20	0	6,6,6	0.21	0
3	GOL	B	1004	-	5,5,5	0.20	0	5,5,5	0.73	0
4	SO4	A	904	-	4,4,4	0.30	0	6,6,6	0.07	0
2	WUR	A	901	-	33,36,36	2.61	7 (21%)	38,50,50	2.10	10 (26%)

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
6	BTB	B	1002	-	-	6/21/21/21	-
2	WUR	B	1005	-	-	6/15/35/35	0/4/4/4
3	GOL	B	1003	-	-	4/4/4/4	-
3	GOL	A	902	-	-	4/4/4/4	-
5	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	B	1004	-	-	2/4/4/4	-
2	WUR	A	901	-	-	2/15/35/35	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	WUR	C4-N1	-12.92	1.24	1.47
2	B	1005	WUR	C4-N1	-12.05	1.25	1.47
2	A	901	WUR	C23-C24	-2.87	1.48	1.52
2	B	1005	WUR	C13-C12	2.62	1.55	1.49
2	B	1005	WUR	C1-C24	-2.59	1.45	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	WUR	C17-N4-C16	7.64	124.06	116.08
2	B	1005	WUR	C19-N5-C16	6.21	122.57	116.08
5	B	1001	NAG	C2-N2-C7	5.77	131.13	122.90
2	B	1005	WUR	C17-N4-C16	5.52	121.85	116.08
5	B	1001	NAG	O4-C4-C5	4.66	120.87	109.30

There are no chirality outliers.
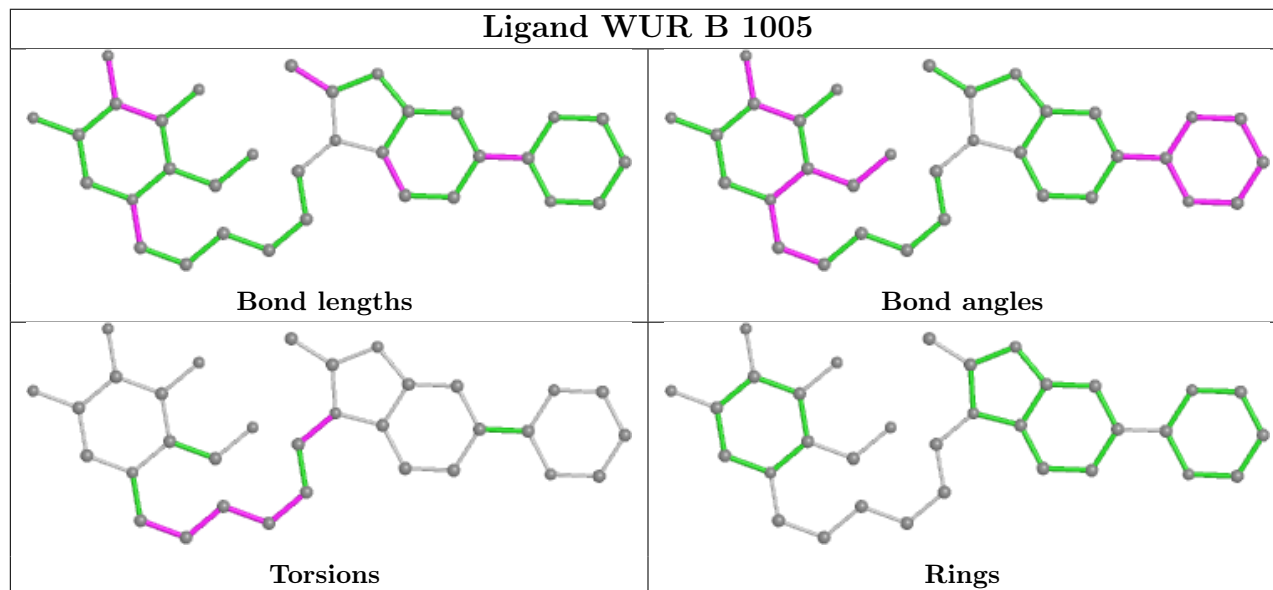
5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	GOL	C1-C2-C3-O3
3	B	1003	GOL	C1-C2-C3-O3
3	B	1003	GOL	O2-C2-C3-O3
3	B	1004	GOL	O1-C1-C2-C3
6	B	1002	BTB	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1009	SO4	2	0
6	B	1002	BTB	3	0
3	B	1003	GOL	2	0
3	A	902	GOL	3	0
4	B	1007	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 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 WUR B 1005

Bond lengths

Bond angles

Torsions

Rings

Ligand WUR A 901

Bond lengths

Bond angles

Torsions

Rings
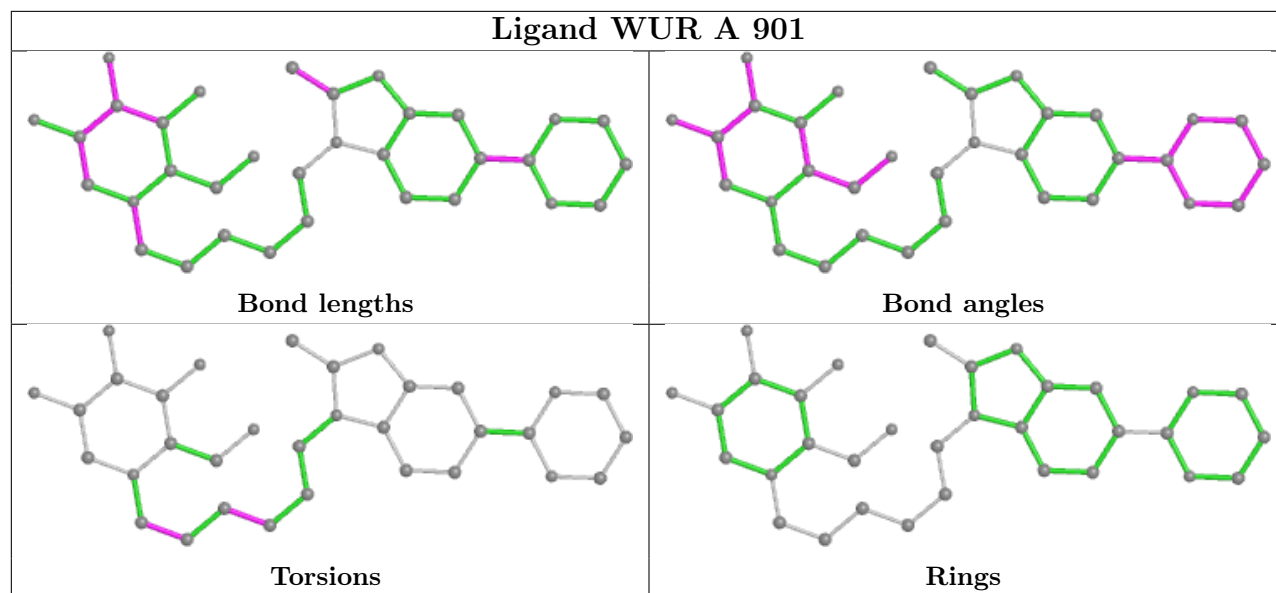
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	765/819 (93%)	-0.28	10 (1%) 77	78	15, 28, 50, 78	0
1	B	767/819 (93%)	-0.40	3 (0%) 92	93	15, 27, 46, 102	0
All	All	1532/1638 (93%)	-0.34	13 (0%) 86	86	15, 27, 49, 102	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	ALA	4.8
1	A	560	ASP	3.4
1	A	661	PHE	3.3
1	A	37	HIS	2.7
1	A	151	ASP	2.5

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

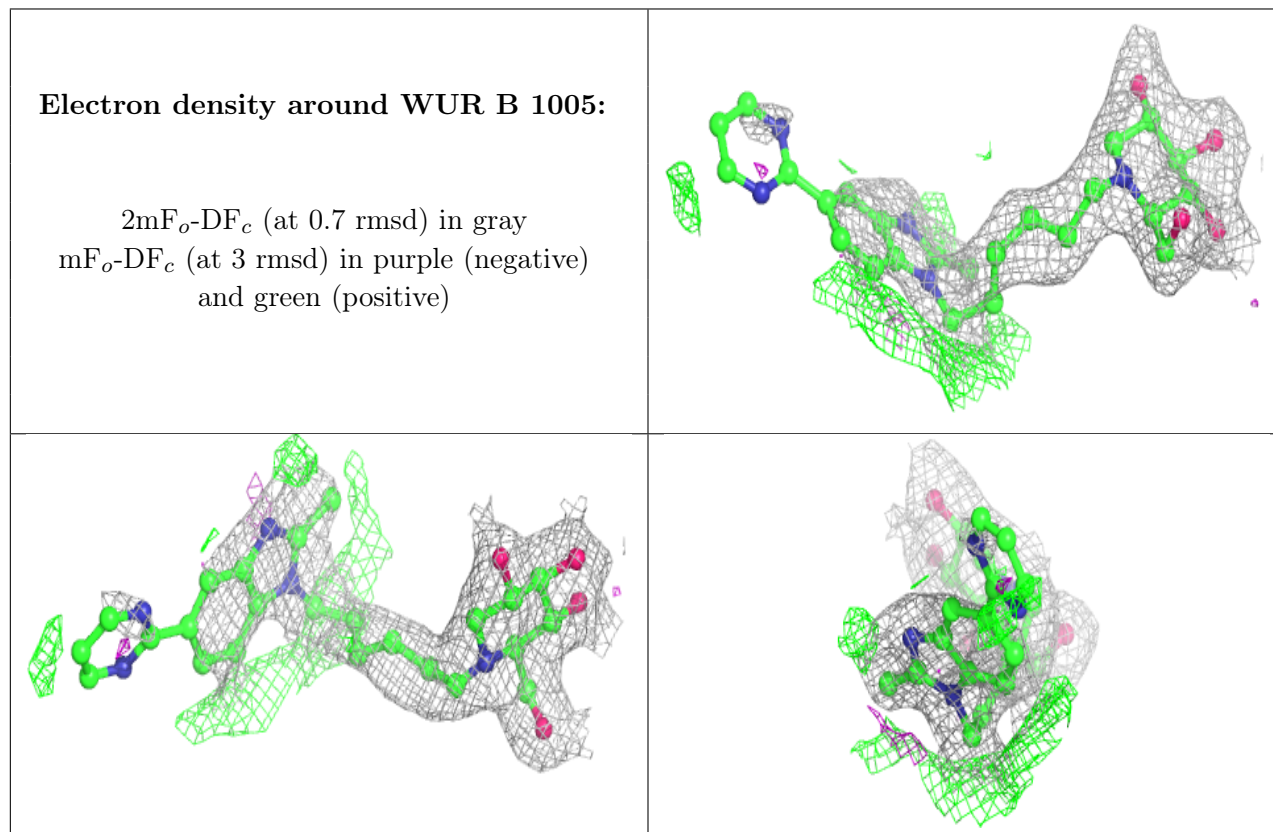There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.
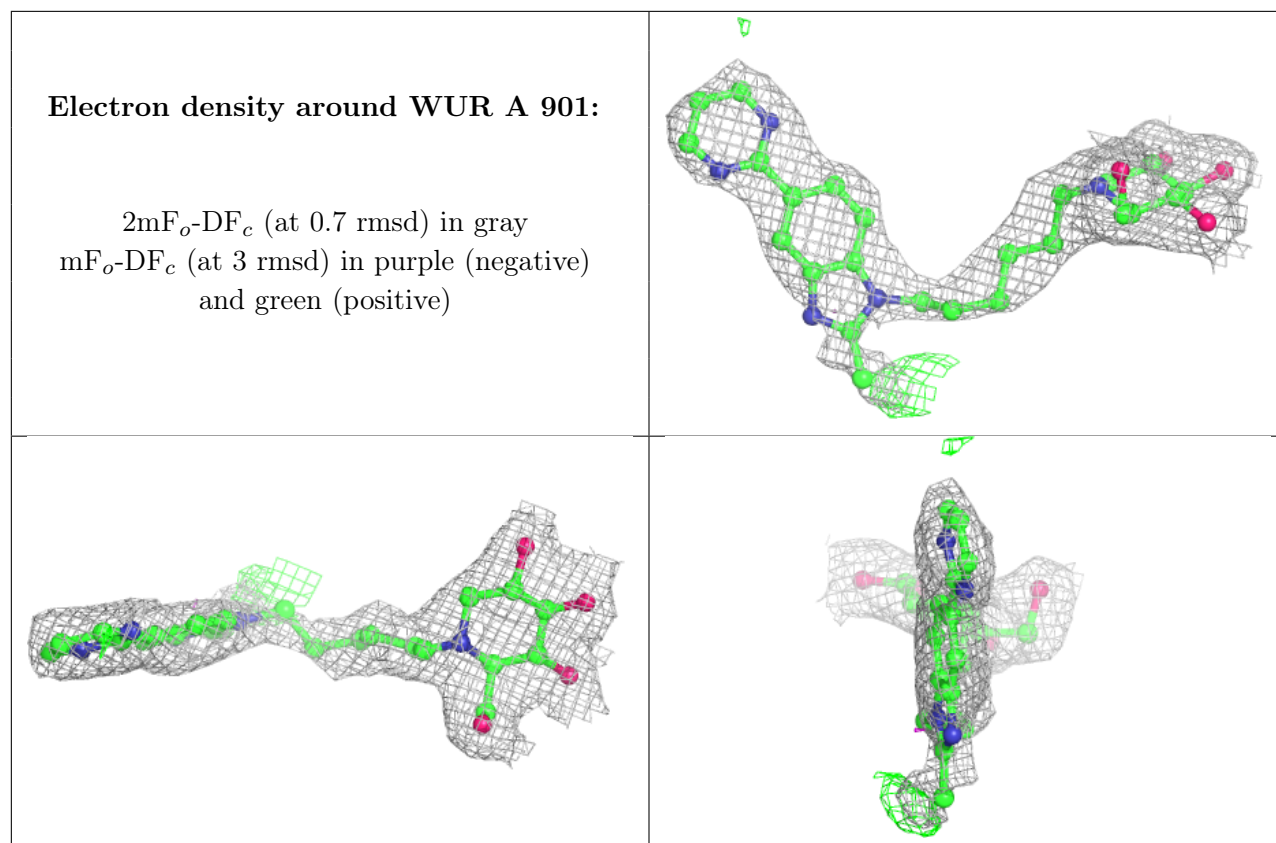
6.4 Ligands ⓘ

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
6	BTB	B	1002	14/14	0.90	0.14	40,46,48,50	0
3	GOL	A	902	6/6	0.91	0.24	39,52,59,63	0
5	NAG	B	1001	14/15	0.92	0.20	30,43,50,52	0
4	SO4	A	907	5/5	0.92	0.22	65,66,78,79	0
3	GOL	B	1003	6/6	0.94	0.13	38,42,46,52	0
2	WUR	B	1005	33/33	0.94	0.20	17,76,131,147	0
3	GOL	B	1004	6/6	0.95	0.13	21,28,33,37	0
2	WUR	A	901	33/33	0.96	0.17	17,48,88,93	0
4	SO4	B	1006	5/5	0.97	0.10	41,46,50,58	0
4	SO4	A	906	5/5	0.97	0.13	50,53,64,69	0
4	SO4	A	905	5/5	0.97	0.11	54,55,64,68	0
4	SO4	B	1009	5/5	0.98	0.15	41,42,52,59	0
4	SO4	A	904	5/5	0.98	0.16	54,55,63,67	0
4	SO4	B	1008	5/5	0.98	0.17	39,45,51,53	0
4	SO4	A	903	5/5	0.99	0.12	23,26,31,33	0
4	SO4	B	1007	5/5	0.99	0.10	27,27,33,34	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 WUR B 1005:

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

Electron density around WUR A 901:

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

6.5 Other polymers (i)

There are no such residues in this entry.