



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:01 AM UTC

PDB ID : 8EPO / pdb_00008epo
Title : Co-crystal structure of Chaetomium glucosidase with compound 18
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2022-10-06
Resolution : 2.20 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

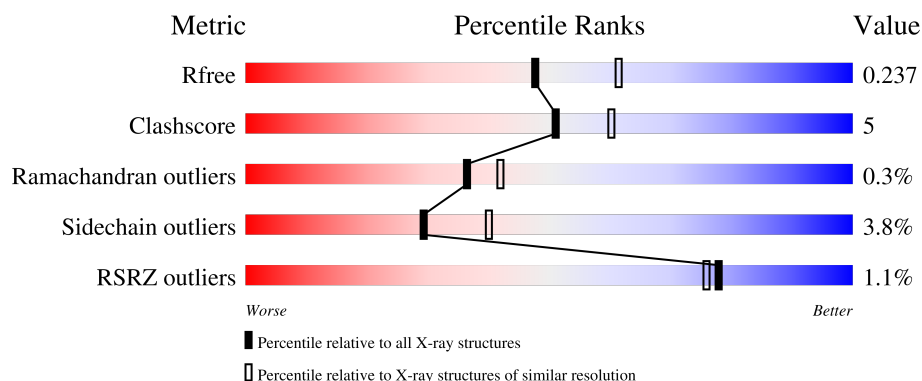
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12629 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chaetomium alpha glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	2	0
			6071	3904	1023	1131	13			
1	B	764	Total	C	N	O	S	0	0	0
			6060	3890	1019	1138	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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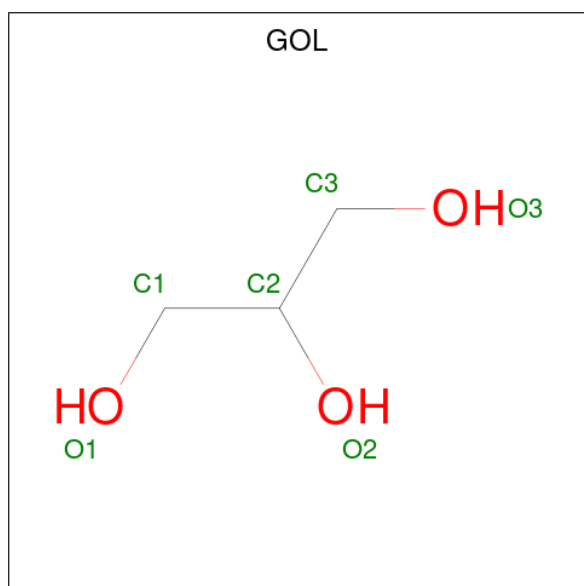
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	CYS	-	expression tag	UNP G0SFD1
A	25	VAL	-	expression tag	UNP G0SFD1
A	26	ALA	-	expression tag	UNP G0SFD1
A	27	GLU	-	expression tag	UNP G0SFD1
A	28	THR	-	expression tag	UNP G0SFD1
A	29	GLY	-	expression tag	UNP G0SFD1
A	810	SER	-	expression tag	UNP 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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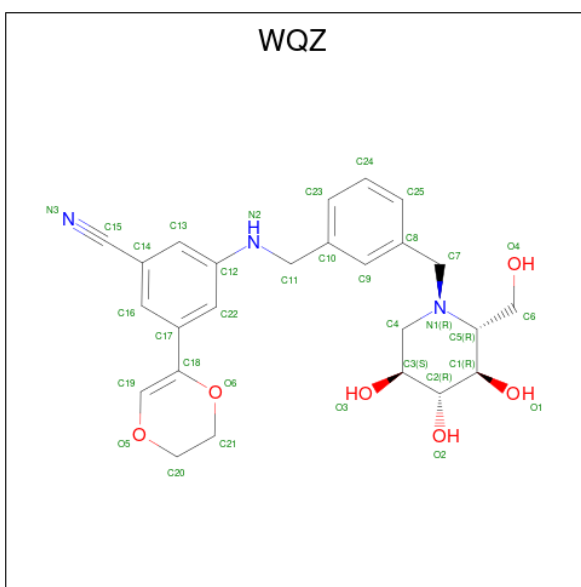
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLU	-	expression tag	UNP G0SFD1
B	28	THR	-	expression tag	UNP G0SFD1
B	29	GLY	-	expression tag	UNP G0SFD1
B	810	SER	-	expression tag	UNP G0SFD1
B	811	GLY	-	expression tag	UNP G0SFD1
B	812	HIS	-	expression tag	UNP G0SFD1
B	813	HIS	-	expression tag	UNP 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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is (3P)-3-(5,6-dihydro-1,4-dioxin-2-yl)-5-{[(3-{[(2R,3R,4R,5S)-3,4,5-trihydroxy-2-(hydroxymethyl)piperidin-1-yl]methyl}phenyl)methyl]amino}benzonitrile (CCD ID: WQZ) (formula: $C_{25}H_{29}N_3O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	25	3	6		
3	B	1	Total	C	N	O	0	0
			34	25	3	6		

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



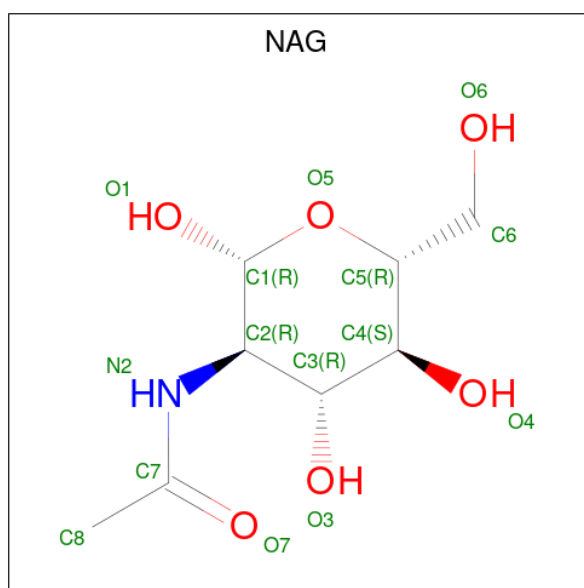
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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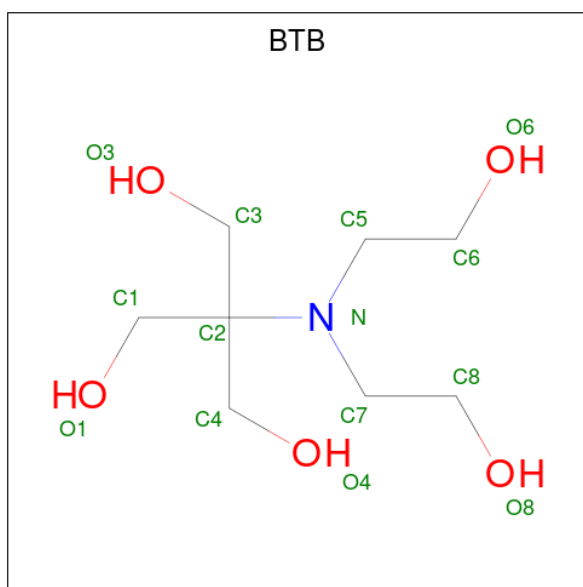
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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



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

- Molecule 6 is 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
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

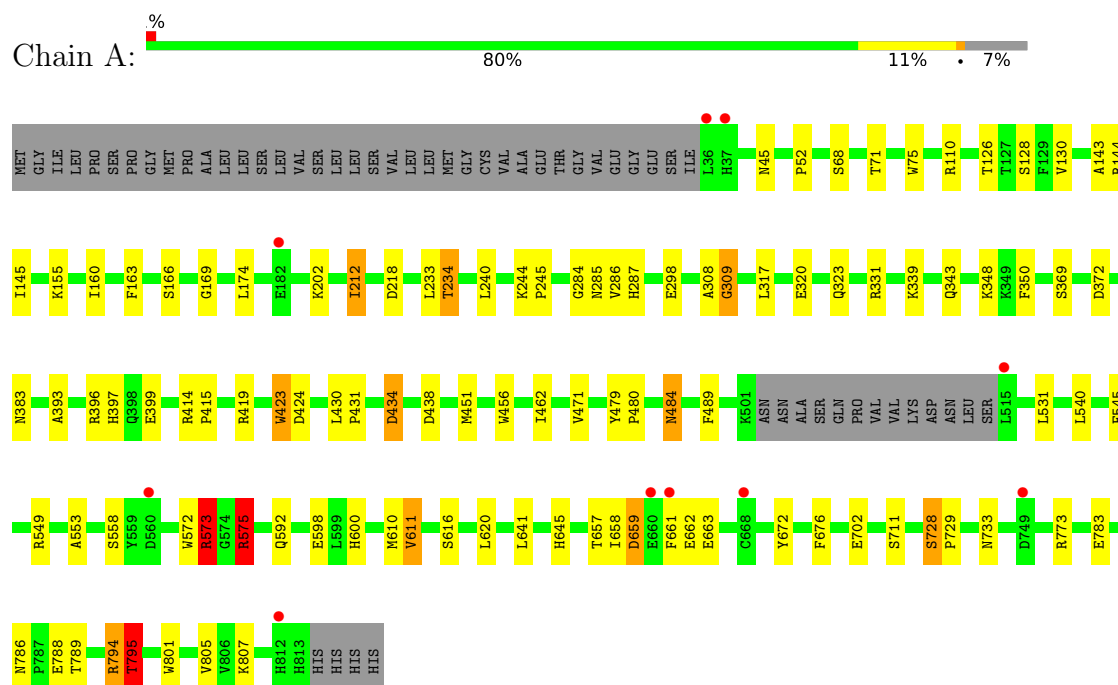
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	161	Total O 161 161	0	0
7	B	184	Total O 184 184	0	0

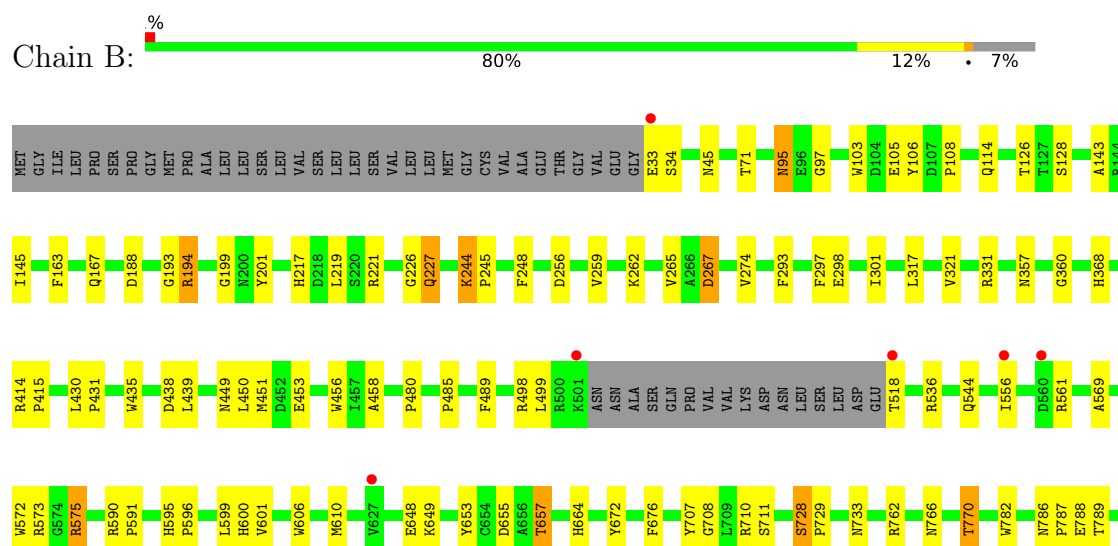
3 Residue-property plots

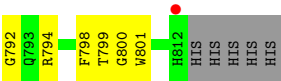
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Chaetomium alpha glucosidase



• Molecule 1: Chaetomium alpha glucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	136.94Å 178.61Å 180.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.20 46.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.86-2.20) 98.7 (46.86-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.190 , 0.237 0.194 , 0.237	Depositor DCC
R_{free} test set	5405 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12629	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: BTB, SO4, WQZ, NAG, 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	1.07	3/6253 (0.0%)	1.40	11/8515 (0.1%)
1	B	1.06	0/6236	1.40	9/8491 (0.1%)
All	All	1.06	3/12489 (0.0%)	1.40	20/17006 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	702	GLU	CA-C	5.95	1.55	1.52
1	A	471	VAL	N-CA	5.42	1.50	1.45
1	A	68	SER	C-O	5.03	1.27	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	575	ARG	CB-CA-C	9.52	125.59	109.50
1	A	575	ARG	CB-CA-C	9.49	125.74	109.51
1	A	795	THR	CA-CB-OG1	-7.08	98.98	109.60
1	B	45	ASN	CB-CA-C	6.95	121.88	110.90
1	A	212	ILE	CB-CA-C	6.28	118.00	110.78
1	B	45	ASN	N-CA-C	-6.08	104.58	111.14
1	B	188	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	248	PHE	CA-CB-CG	-5.68	108.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	708	GLY	CA-C-O	-5.66	117.10	122.13
1	A	479	TYR	CB-CA-C	5.56	117.58	110.13
1	A	794	ARG	CB-CG-CD	5.54	124.05	111.30
1	B	267	ASP	CB-CA-C	5.46	116.27	108.68
1	B	556	ILE	CA-C-N	5.36	128.24	120.79
1	B	556	ILE	C-N-CA	5.36	128.24	120.79
1	A	795	THR	CB-CA-C	5.31	118.50	109.84
1	A	484	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	573	ARG	CG-CD-NE	-5.20	100.56	112.00
1	A	52	PRO	N-CA-C	-5.17	105.50	112.48
1	A	434	ASP	N-CA-C	-5.04	105.67	111.07
1	A	611	VAL	N-CA-CB	5.02	116.42	110.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	657	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6071	0	5745	53	0
1	B	6060	0	5707	71	0
2	A	6	0	8	0	0
2	B	6	0	8	3	0
3	A	34	0	0	1	0
3	B	34	0	0	1	0
4	A	25	0	0	1	0
4	B	20	0	0	2	0
5	B	14	0	13	0	0
6	B	14	0	19	0	0
7	A	161	0	0	2	0
7	B	184	0	0	0	0
All	All	12629	0	11500	123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:TRP:H	1:B:600:HIS:HD2	1.25	0.84
1:B:458:ALA:H	2:B:1002:GOL:HO1	1.23	0.83
1:B:561:ARG:HE	1:B:664:HIS:HD2	1.27	0.83
1:A:383:ASN:HB2	7:A:1178:HOH:O	1.81	0.79
1:B:561:ARG:HE	1:B:664:HIS:CD2	2.09	0.69
1:B:458:ALA:N	2:B:1002:GOL:O1	2.21	0.69
1:B:217:HIS:HD2	1:B:219:LEU:H	1.39	0.68
1:B:786:ASN:HD22	1:B:789:THR:H	1.43	0.66
1:B:766:ASN:O	1:B:770:THR:HG23	1.95	0.66
1:B:794:ARG:NH1	3:B:1004:WQZ:C15	2.60	0.65
1:A:451:MET:HE1	1:A:540:LEU:HB3	1.79	0.65
1:B:572:TRP:H	1:B:600:HIS:CD2	2.13	0.63
1:A:434:ASP:OD2	1:A:807:LYS:HD3	1.98	0.62
1:B:217:HIS:HE1	1:B:267:ASP:O	1.82	0.62
1:A:350:PHE:CZ	1:A:805[B]:VAL:HG11	2.36	0.61
1:A:451:MET:CE	1:A:540:LEU:HB3	2.31	0.60
1:A:783:GLU:OE1	1:A:795:THR:HB	2.02	0.59
1:A:110:ARG:NH2	1:A:323:GLN:HG3	2.17	0.59
1:B:331:ARG:NH1	1:B:435:TRP:O	2.34	0.59
1:B:114:GLN:HE22	1:B:414:ARG:HH22	1.52	0.58
1:B:561:ARG:NE	1:B:664:HIS:HD2	2.00	0.57
1:B:450:LEU:O	2:B:1002:GOL:H12	2.05	0.57
1:A:572:TRP:H	1:A:600:HIS:HD2	1.51	0.57
1:A:598:GLU:OE2	1:A:600:HIS:HE1	1.88	0.56
1:A:451:MET:HE1	1:A:540:LEU:CA	2.35	0.56
1:B:114:GLN:NE2	1:B:414:ARG:HH12	2.05	0.55
1:A:423:TRP:H	1:A:484:ASN:HD22	1.55	0.54
1:B:485:PRO:HB3	1:B:606:TRP:CE2	2.42	0.54
1:B:728:SER:N	1:B:729:PRO:CD	2.72	0.53
1:B:786:ASN:ND2	1:B:788:GLU:H	2.06	0.53
1:B:569:ALA:HB1	1:B:599:LEU:HD22	1.90	0.53
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.44	0.52
1:B:128:SER:O	1:B:143:ALA:HA	2.09	0.52
1:B:95:ASN:HD22	1:B:95:ASN:C	2.18	0.52
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.45	0.52
1:A:553:ALA:O	1:A:573:ARG:NH2	2.38	0.51
1:A:451:MET:HE1	1:A:540:LEU:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LEU:HB2	1:B:431:PRO:HD3	1.93	0.51
1:A:786:ASN:HD22	1:A:789:THR:H	1.60	0.50
1:A:128:SER:O	1:A:143:ALA:HA	2.12	0.50
1:A:545:PHE:CZ	1:A:549:ARG:HD2	2.47	0.50
1:B:451:MET:HE1	1:B:544:GLN:HB2	1.94	0.50
1:A:240:LEU:HD22	1:A:286:VAL:CG2	2.42	0.50
1:A:598:GLU:OE2	1:A:600:HIS:CE1	2.65	0.50
1:B:226:GLY:H	1:B:227:GLN:HE22	1.60	0.49
1:B:728:SER:N	1:B:729:PRO:HD3	2.27	0.49
1:B:766:ASN:O	1:B:770:THR:CG2	2.60	0.49
1:A:233:LEU:HD22	1:B:265:VAL:HG23	1.93	0.49
1:A:423:TRP:H	1:A:484:ASN:ND2	2.11	0.49
1:A:126:THR:HG22	7:A:1198:HOH:O	2.12	0.49
1:A:659:ASP:HB3	1:A:661:PHE:H	1.78	0.48
1:B:103:TRP:H	1:B:357:ASN:ND2	2.10	0.48
1:B:226:GLY:H	1:B:227:GLN:NE2	2.12	0.48
1:B:782:TRP:CG	1:B:792:GLY:HA3	2.48	0.47
1:A:71:THR:HB	1:A:163:PHE:CZ	2.50	0.47
1:B:762:ARG:NH1	4:B:1007:SO4:O1	2.48	0.47
1:A:372:ASP:OD1	1:A:372:ASP:C	2.58	0.47
1:A:575:ARG:HH22	1:A:592:GLN:HE22	1.63	0.47
1:B:707:TYR:HA	1:B:770:THR:HG21	1.97	0.47
1:B:451:MET:CE	1:B:544:GLN:HB2	2.44	0.47
1:B:145:ILE:CD1	1:B:301:ILE:CD1	2.93	0.46
1:B:601:VAL:HG21	1:B:653:TYR:HB3	1.98	0.46
1:B:108:PRO:HG2	1:B:439:LEU:HD22	1.96	0.46
1:B:600:HIS:HA	1:B:655:ASP:OD1	2.16	0.46
1:B:728:SER:H	1:B:729:PRO:CD	2.28	0.46
1:A:659:ASP:HB2	1:A:663:GLU:H	1.80	0.46
1:B:572:TRP:N	1:B:600:HIS:HD2	2.04	0.46
1:A:308:ALA:O	1:A:309:GLY:O	2.34	0.46
1:A:419:ARG:HD2	1:A:462:ILE:HG12	1.98	0.46
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.50	0.46
1:A:130:VAL:HG21	1:A:320:GLU:HB3	1.98	0.45
1:B:244:LYS:HB3	1:B:245:PRO:HD3	1.98	0.45
1:B:145:ILE:O	1:B:298:GLU:HA	2.16	0.44
1:B:167:GLN:NE2	1:B:201:TYR:OH	2.50	0.44
1:B:733:ASN:HB3	1:B:801:TRP:CG	2.51	0.44
1:A:451:MET:HE1	1:A:540:LEU:HA	2.00	0.44
1:A:234:THR:HG22	1:A:284:GLY:HA2	2.00	0.44
1:A:144:ARG:HB2	1:A:317:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:THR:HB	1:B:163:PHE:CZ	2.53	0.44
1:B:145:ILE:CD1	1:B:301:ILE:HD11	2.47	0.44
1:B:798:PHE:C	1:B:800:GLY:HA3	2.42	0.44
1:B:672:TYR:CE2	1:B:711:SER:HB3	2.53	0.44
1:A:489:PHE:CE1	1:A:610:MET:HE3	2.53	0.44
1:B:194:ARG:HA	1:B:199:GLY:O	2.18	0.43
1:B:499:LEU:HD23	1:B:499:LEU:HA	1.90	0.43
1:B:595:HIS:ND1	1:B:596:PRO:HD2	2.32	0.43
1:B:193:GLY:HA3	1:B:201:TYR:CZ	2.53	0.43
1:A:393:ALA:O	1:A:396:ARG:HB2	2.18	0.43
1:A:672:TYR:CE2	1:A:711:SER:HA	2.53	0.43
1:A:728:SER:N	1:A:729:PRO:CD	2.81	0.43
1:B:590:ARG:HB3	1:B:591:PRO:CD	2.48	0.43
1:A:244:LYS:HB3	1:A:245:PRO:HD3	2.00	0.43
1:B:244:LYS:CB	1:B:245:PRO:HD3	2.49	0.43
1:A:430:LEU:HB2	1:A:431:PRO:HD3	2.00	0.43
1:A:672:TYR:CZ	1:A:711:SER:HA	2.54	0.43
1:B:145:ILE:HD11	1:B:301:ILE:CD1	2.49	0.43
1:B:33:GLU:HB3	1:B:536:ARG:HH12	1.83	0.43
1:B:456:TRP:CD2	1:B:480:PRO:HA	2.54	0.42
1:A:174:LEU:HD23	1:A:287:HIS:CD2	2.54	0.42
1:A:166:SER:HA	1:A:285:ASN:O	2.19	0.42
1:B:368:HIS:HD2	4:B:1005:SO4:O3	2.02	0.42
1:B:489:PHE:CE1	1:B:610:MET:HE3	2.55	0.42
1:A:575:ARG:HH22	1:A:592:GLN:NE2	2.17	0.42
1:B:317:LEU:O	1:B:321:VAL:HG23	2.19	0.42
1:B:799:THR:N	1:B:800:GLY:HA3	2.34	0.42
1:A:641:LEU:O	1:A:645:HIS:HB2	2.19	0.42
1:A:424:ASP:OD1	3:A:1002:WQZ:O1	2.38	0.41
1:B:786:ASN:ND2	1:B:789:THR:H	2.14	0.41
1:B:256:ASP:O	1:B:259:VAL:HG22	2.20	0.41
1:B:293:PHE:CG	1:B:297:PHE:HB3	2.56	0.41
1:A:169:GLY:HA3	4:A:1007:SO4:O3	2.21	0.41
1:A:397:HIS:HD2	1:A:399:GLU:OE2	2.04	0.41
1:A:145:ILE:O	1:A:298:GLU:HA	2.21	0.41
1:A:75:TRP:HA	1:A:160:ILE:O	2.21	0.41
1:B:672:TYR:CE1	1:B:711:SER:HA	2.56	0.41
1:B:710:ARG:HG2	1:B:787:PRO:HB3	2.02	0.41
1:A:658:ILE:CG2	1:A:662:GLU:HA	2.51	0.41
1:B:414:ARG:N	1:B:415:PRO:HD2	2.36	0.41
1:A:414:ARG:N	1:A:415:PRO:HD2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ASN:ND2	1:A:788:GLU:H	2.19	0.40
1:B:95:ASN:HD22	1:B:97:GLY:H	1.70	0.40
1:B:106:TYR:CD2	1:B:360:GLY:HA2	2.57	0.40
1:B:106:TYR:CE2	1:B:360:GLY:HA2	2.56	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	763/819 (93%)	734 (96%)	26 (3%)	3 (0%)	30	34
1	B	760/819 (93%)	740 (97%)	19 (2%)	1 (0%)	48	57
All	All	1523/1638 (93%)	1474 (97%)	45 (3%)	4 (0%)	36	42

All (4) Ramachandran outliers are listed below:

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

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	628/707 (89%)	603 (96%)	25 (4%)	28	38
1	B	627/707 (89%)	605 (96%)	22 (4%)	32	43
All	All	1255/1414 (89%)	1208 (96%)	47 (4%)	29	41

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	155	LYS
1	A	202	LYS
1	A	212	ILE
1	A	218	ASP
1	A	234	THR
1	A	331	ARG
1	A	339	LYS
1	A	343	GLN
1	A	348	LYS
1	A	369	SER
1	A	423	TRP
1	A	438	ASP
1	A	531	LEU
1	A	558	SER
1	A	573	ARG
1	A	575	ARG
1	A	611	VAL
1	A	616	SER
1	A	620	LEU
1	A	657	THR
1	A	676	PHE
1	A	773	ARG
1	A	794	ARG
1	A	795	THR
1	B	34	SER
1	B	95	ASN
1	B	105	GLU
1	B	126	THR
1	B	194	ARG
1	B	221	ARG
1	B	227	GLN
1	B	244	LYS
1	B	262	LYS
1	B	274	VAL

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Mol	Chain	Res	Type
1	B	438	ASP
1	B	449	ASN
1	B	453	GLU
1	B	498	ARG
1	B	518	THR
1	B	573	ARG
1	B	575	ARG
1	B	648	GLU
1	B	649	LYS
1	B	657	THR
1	B	676	PHE
1	B	770	THR

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

Mol	Chain	Res	Type
1	A	85	GLN
1	A	120	GLN
1	A	157	GLN
1	A	167	GLN
1	A	200	ASN
1	A	231	GLN
1	A	249	GLN
1	A	323	GLN
1	A	397	HIS
1	A	461	GLN
1	A	478	GLN
1	A	481	HIS
1	A	484	ASN
1	A	494	ASN
1	A	592	GLN
1	A	600	HIS
1	A	639	HIS
1	A	786	ASN
1	A	793	GLN
1	A	813	HIS
1	B	95	ASN
1	B	114	GLN
1	B	120	GLN
1	B	137	HIS
1	B	167	GLN
1	B	217	HIS

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Mol	Chain	Res	Type
1	B	227	GLN
1	B	242	GLN
1	B	249	GLN
1	B	323	GLN
1	B	357	ASN
1	B	368	HIS
1	B	398	GLN
1	B	481	HIS
1	B	484	ASN
1	B	600	HIS
1	B	664	HIS
1	B	748	GLN
1	B	786	ASN
1	B	793	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	1002	-	5,5,5	0.35	0	5,5,5	0.72	0
4	SO4	B	1006	-	4,4,4	0.24	0	6,6,6	0.18	0
4	SO4	B	1007	-	4,4,4	0.34	0	6,6,6	0.15	0
4	SO4	B	1005	-	4,4,4	0.43	0	6,6,6	0.35	0
2	GOL	A	1001	-	5,5,5	0.13	0	5,5,5	0.47	0
3	WQZ	A	1002	-	37,37,37	3.99	16 (43%)	48,51,51	4.57	18 (37%)
4	SO4	A	1003	-	4,4,4	0.38	0	6,6,6	0.41	0
4	SO4	A	1007	-	4,4,4	0.33	0	6,6,6	0.10	0
5	NAG	B	1001	1	14,14,15	0.88	0	17,19,21	1.88	6 (35%)
4	SO4	A	1005	-	4,4,4	0.33	0	6,6,6	0.17	0
3	WQZ	B	1004	-	37,37,37	3.72	14 (37%)	48,51,51	4.08	7 (14%)
4	SO4	A	1006	-	4,4,4	0.29	0	6,6,6	0.13	0
6	BTB	B	1003	-	13,13,13	1.75	3 (23%)	7,16,16	0.95	0
4	SO4	A	1004	-	4,4,4	0.26	0	6,6,6	0.22	0
4	SO4	B	1008	-	4,4,4	0.24	0	6,6,6	0.20	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	GOL	B	1002	-	-	2/4/4/4	-
2	GOL	A	1001	-	-	4/4/4/4	-
3	WQZ	A	1002	-	-	0/17/45/45	0/4/4/4
5	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
3	WQZ	B	1004	-	-	2/17/45/45	0/4/4/4
6	BTB	B	1003	-	-	6/21/21/21	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	WQZ	C15-N3	14.07	1.45	1.14
3	A	1002	WQZ	C15-N3	13.89	1.45	1.14
3	A	1002	WQZ	C7-N1	-12.15	1.26	1.47
3	B	1004	WQZ	C7-N1	-10.66	1.29	1.47
3	A	1002	WQZ	C19-C18	9.50	1.55	1.35
3	B	1004	WQZ	C19-C18	8.40	1.53	1.35
6	B	1003	BTB	C2-N	4.74	1.57	1.48
3	A	1002	WQZ	C3-C2	-4.65	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	WQZ	C14-C15	4.50	1.54	1.44
3	A	1002	WQZ	C7-C8	4.27	1.59	1.51
3	A	1002	WQZ	O6-C18	4.21	1.43	1.37
3	B	1004	WQZ	C14-C15	4.04	1.53	1.44
3	B	1004	WQZ	O6-C18	3.99	1.42	1.37
3	B	1004	WQZ	C7-C8	3.83	1.58	1.51
3	A	1002	WQZ	C17-C18	3.58	1.56	1.48
3	B	1004	WQZ	C17-C18	3.41	1.55	1.48
3	A	1002	WQZ	C12-N2	3.25	1.47	1.38
3	B	1004	WQZ	C12-N2	2.86	1.46	1.38
3	B	1004	WQZ	C3-C2	-2.86	1.48	1.52
3	B	1004	WQZ	O2-C2	2.82	1.49	1.43
3	A	1002	WQZ	C2-C1	-2.69	1.45	1.52
3	A	1002	WQZ	O5-C19	2.67	1.43	1.36
3	B	1004	WQZ	C4-C3	2.56	1.55	1.52
3	B	1004	WQZ	O5-C19	2.44	1.42	1.36
3	B	1004	WQZ	C2-C1	-2.42	1.46	1.52
3	B	1004	WQZ	C24-C23	2.40	1.43	1.38
6	B	1003	BTB	C5-N	2.38	1.51	1.48
3	A	1002	WQZ	C16-C14	2.38	1.43	1.39
3	A	1002	WQZ	O2-C2	2.32	1.48	1.43
3	A	1002	WQZ	C16-C17	2.22	1.42	1.39
3	A	1002	WQZ	C9-C8	2.12	1.42	1.39
6	B	1003	BTB	C7-N	2.06	1.50	1.48
3	A	1002	WQZ	C9-C10	2.02	1.42	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	WQZ	C14-C15-N3	-26.36	112.81	177.87
3	B	1004	WQZ	C14-C15-N3	-25.14	115.83	177.87
3	A	1002	WQZ	C17-C18-C19	-10.35	114.65	126.30
3	B	1004	WQZ	C17-C18-C19	-9.35	115.77	126.30
3	A	1002	WQZ	O6-C18-C17	6.63	119.26	112.28
3	A	1002	WQZ	C24-C23-C10	-3.87	115.17	120.61
3	B	1004	WQZ	O6-C18-C17	3.77	116.24	112.28
3	A	1002	WQZ	C6-C5-C1	-3.76	107.28	112.93
3	A	1002	WQZ	C16-C14-C15	3.55	124.33	119.55
3	A	1002	WQZ	C7-C8-C9	3.27	126.44	120.27
5	B	1001	NAG	C4-C3-C2	3.25	115.77	111.02
3	A	1002	WQZ	O1-C1-C5	3.13	115.60	109.87
5	B	1001	NAG	C3-C4-C5	-3.05	104.70	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	WQZ	O2-C2-C3	-3.02	103.90	110.05
3	A	1002	WQZ	C11-C10-C23	-3.00	114.82	120.94
3	A	1002	WQZ	C23-C10-C9	2.96	122.63	118.55
5	B	1001	NAG	O4-C4-C5	2.87	116.40	109.32
3	A	1002	WQZ	C25-C8-C9	-2.83	114.65	118.55
3	A	1002	WQZ	C7-N1-C5	2.73	118.41	112.94
3	B	1004	WQZ	C7-N1-C5	2.71	118.35	112.94
5	B	1001	NAG	C2-N2-C7	2.69	126.50	122.90
3	A	1002	WQZ	C3-C2-C1	-2.69	106.14	110.86
3	B	1004	WQZ	O4-C6-C5	-2.66	105.67	111.55
3	A	1002	WQZ	C13-C14-C15	-2.64	116.00	119.55
3	A	1002	WQZ	C25-C24-C23	2.53	123.50	120.24
5	B	1001	NAG	O3-C3-C2	-2.36	104.49	109.40
3	B	1004	WQZ	O2-C2-C1	-2.36	104.82	110.38
5	B	1001	NAG	C6-C5-C4	2.10	118.16	113.02
3	A	1002	WQZ	C20-O5-C19	2.08	119.97	114.18
3	B	1004	WQZ	C6-C5-C1	-2.03	109.88	112.93
3	A	1002	WQZ	C16-C17-C18	2.02	123.52	120.25

There are no chirality outliers.

All (14) torsion outliers are listed below:

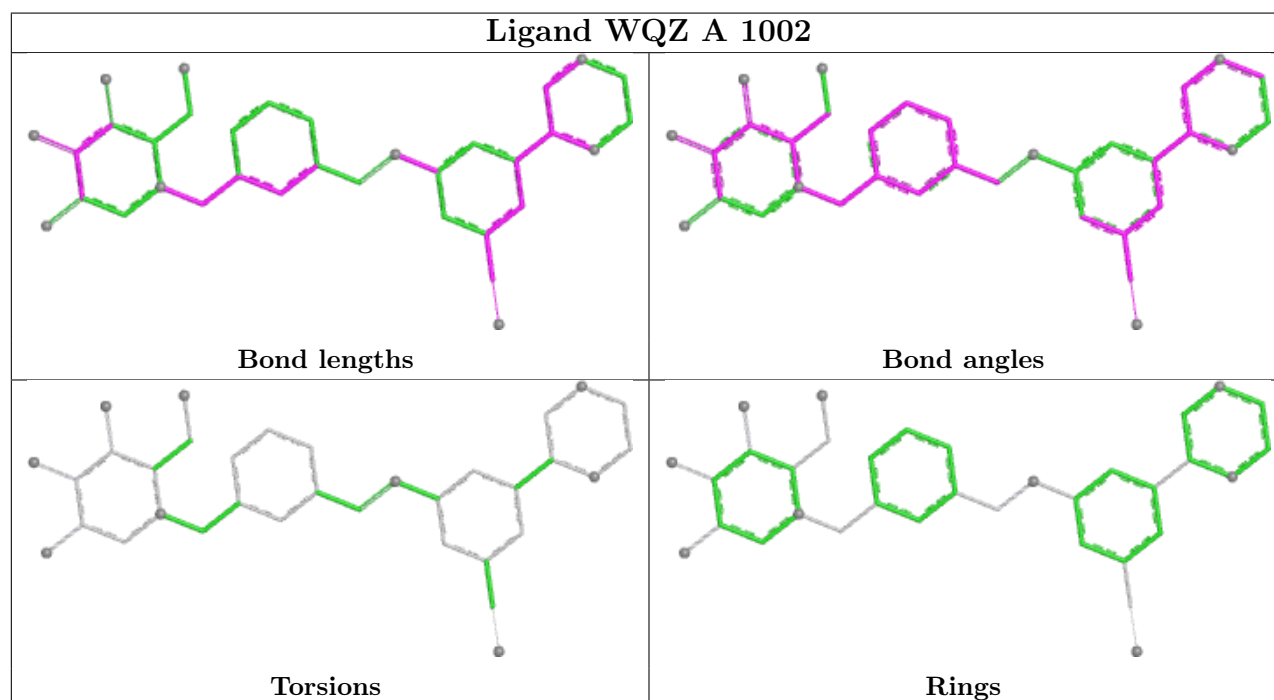
Mol	Chain	Res	Type	Atoms
2	A	1001	GOL	C1-C2-C3-O3
2	B	1002	GOL	O1-C1-C2-C3
6	B	1003	BTB	C4-C2-C3-O3
6	B	1003	BTB	C1-C2-C4-O4
6	B	1003	BTB	C3-C2-C4-O4
6	B	1003	BTB	N-C2-C4-O4
2	B	1002	GOL	O1-C1-C2-O2
6	B	1003	BTB	N-C7-C8-O8
2	A	1001	GOL	O1-C1-C2-C3
2	A	1001	GOL	O2-C2-C3-O3
2	A	1001	GOL	O1-C1-C2-O2
3	B	1004	WQZ	C16-C17-C18-C19
3	B	1004	WQZ	C22-C17-C18-C19
6	B	1003	BTB	N-C2-C3-O3

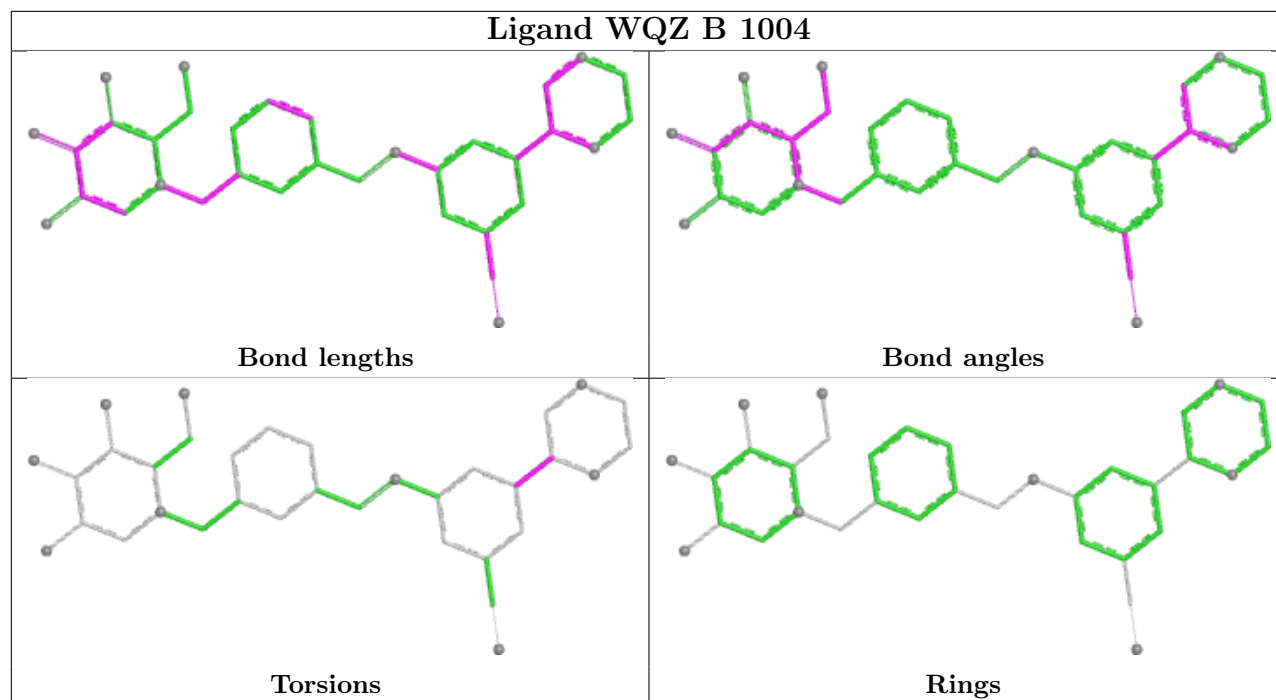
There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	GOL	3	0
4	B	1007	SO4	1	0
4	B	1005	SO4	1	0
3	A	1002	WQZ	1	0
4	A	1007	SO4	1	0
3	B	1004	WQZ	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%)	-0.12	10 (1%) 75 73	21, 42, 69, 93	2 (0%)
1	B	764/819 (93%)	-0.15	7 (0%) 81 79	27, 43, 66, 86	0
All	All	1529/1638 (93%)	-0.13	17 (1%) 78 76	21, 42, 67, 93	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	812	HIS	4.4
1	B	518	THR	4.2
1	A	515	LEU	4.1
1	A	560	ASP	3.7
1	A	36	LEU	3.3
1	A	660	GLU	3.1
1	A	661	PHE	2.9
1	A	182	GLU	2.8
1	A	812	HIS	2.7
1	A	749	ASP	2.4
1	B	560	ASP	2.4
1	B	501	LYS	2.3
1	B	627	VAL	2.3
1	B	556	ILE	2.1
1	A	668	CYS	2.1
1	B	33	GLU	2.1
1	A	37	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

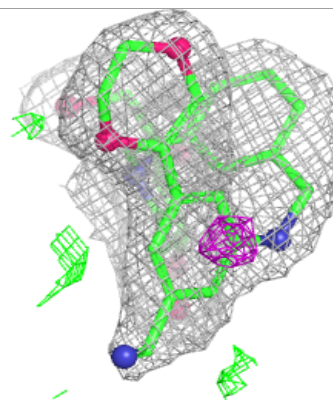
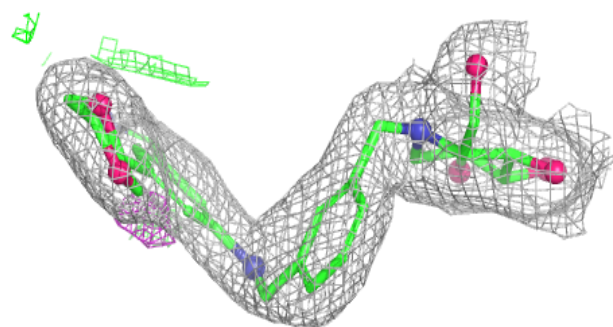
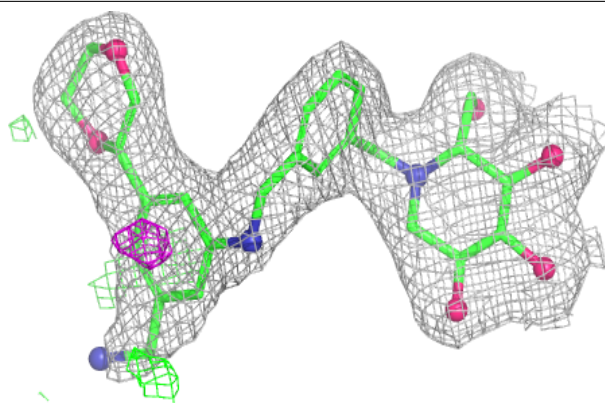
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	1008	5/5	0.79	0.11	72,88,91,93	0
5	NAG	B	1001	14/15	0.81	0.13	55,70,77,77	0
4	SO4	A	1007	5/5	0.82	0.11	91,97,104,108	0
4	SO4	A	1006	5/5	0.85	0.10	83,83,99,108	0
6	BTB	B	1003	14/14	0.86	0.13	52,76,83,83	0
4	SO4	A	1004	5/5	0.88	0.10	56,59,71,78	0
2	GOL	B	1002	6/6	0.89	0.12	39,51,51,52	0
4	SO4	A	1005	5/5	0.91	0.14	61,82,92,98	0
2	GOL	A	1001	6/6	0.92	0.12	62,69,72,78	0
3	WQZ	A	1002	34/34	0.95	0.10	28,38,66,70	0
4	SO4	B	1006	5/5	0.95	0.08	45,62,69,72	0
4	SO4	B	1007	5/5	0.95	0.06	53,74,80,88	0
3	WQZ	B	1004	34/34	0.97	0.08	26,39,84,88	0
4	SO4	B	1005	5/5	0.98	0.06	39,40,49,60	0
4	SO4	A	1003	5/5	0.98	0.05	43,44,45,47	0

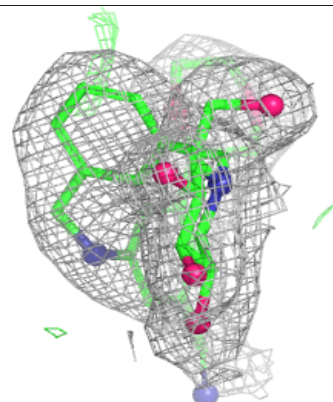
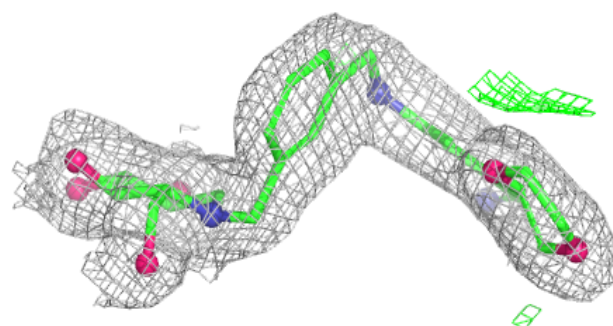
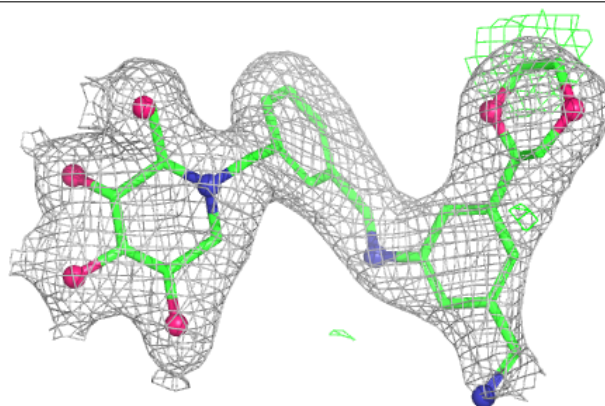
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around WQZ A 1002:

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

**Electron density around WQZ B 1004:**

$2mF_o-DF_c$ (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.