



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:37 AM UTC

PDB ID : 3U57 / pdb_00003u57
Title : Structures of Alkaloid Biosynthetic Glucosidases Decode Substrate Specificity
Authors : Xia, L.; Ruppert, M.; Wang, M.; Panjikar, S.; Lin, H.; Rajendran, C.; Barleben, L.; Stoeckigt, J.
Deposited on : 2011-10-11
Resolution : 2.43 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

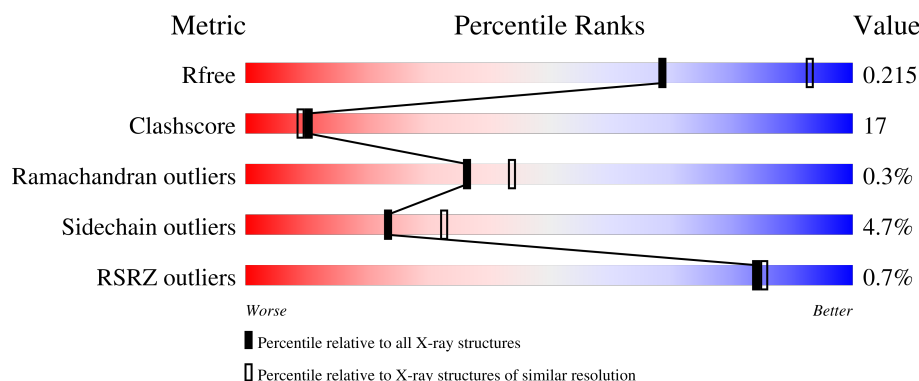
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

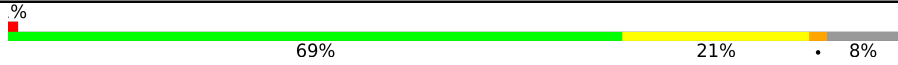
The reported resolution of this entry is 2.43 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	513	
1	B	513	

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.

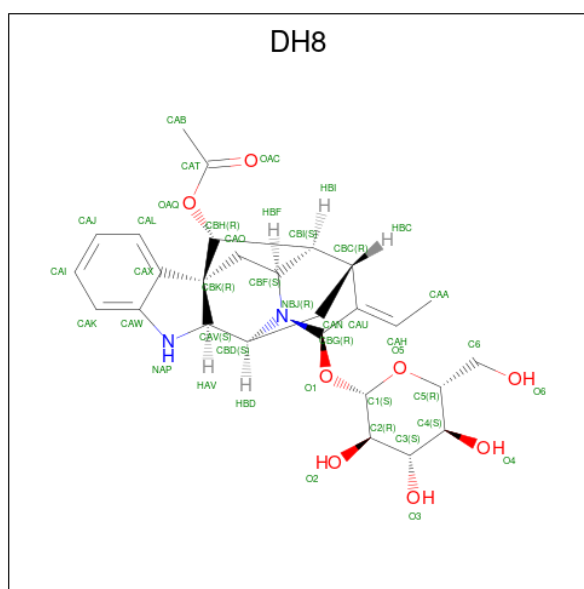
- Molecule 1 is a protein called Raucaffricine-O-beta-D-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total 3780	C 2417	N 645	O 705	S 13	0	0	0
1	B	471	Total 3780	C 2417	N 645	O 705	S 13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLN	GLU	engineered mutation	UNP Q9SPP9
B	186	GLN	GLU	engineered mutation	UNP Q9SPP9

- Molecule 2 is (2beta,7beta,16S,17R,19E,21beta)-21-(beta-D-glucopyranosyloxy)-2,7-dihydro-7,17-cyclosarpagan-17-yl acetate (CCD ID: DH8) (formula: C₂₇H₃₄N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	27	2	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			37	27	2	8		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	41	Total	O	0	0
			41	41		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	104.89Å 129.55Å 216.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.16 – 2.43 65.16 – 2.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.16-2.43) 98.6 (65.16-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.206 , 0.238 0.179 , 0.215	Depositor DCC
R_{free} test set	2762 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7729	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: CL, DH8

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	0.79	0/3891	0.94	6/5281 (0.1%)
1	B	0.79	0/3891	0.96	3/5281 (0.1%)
All	All	0.79	0/7782	0.95	9/10562 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	VAL	N-CA-C	6.12	116.28	110.53
1	A	38	GLU	N-CA-C	5.99	117.48	111.07
1	B	411	TYR	CA-C-N	-5.92	114.82	123.93
1	B	411	TYR	C-N-CA	-5.92	114.82	123.93
1	A	382	VAL	CA-C-N	5.33	125.34	119.90
1	A	382	VAL	C-N-CA	5.33	125.34	119.90
1	A	192	VAL	N-CA-C	5.06	115.28	110.53
1	A	396	TYR	CA-C-N	5.01	125.28	119.47
1	A	396	TYR	C-N-CA	5.01	125.28	119.47

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	3780	0	3583	117	0
1	B	3780	0	3583	134	0
2	A	37	0	34	2	0
2	B	37	0	34	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	52	0	0	1	0
4	B	41	0	0	10	0
All	All	7729	0	7234	253	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 17.

All (253) 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:313:PRO:HD2	1:A:316:MET:CE	1.58	1.33
1:B:281:TRP:CG	4:B:538:HOH:O	1.95	1.18
1:A:185:ASN:HD22	1:A:272:SER:HB3	1.08	1.15
1:A:313:PRO:CD	1:A:316:MET:CE	2.24	1.14
1:B:313:PRO:HD2	1:B:316:MET:HE3	1.16	1.14
1:A:316:MET:SD	4:A:545:HOH:O	2.03	1.13
1:B:281:TRP:CD1	4:B:538:HOH:O	2.05	1.09
1:A:313:PRO:CD	1:A:316:MET:HE3	1.81	1.09
1:B:16:ARG:HG2	1:B:16:ARG:HH11	1.03	1.09
1:A:16:ARG:HH11	1:A:16:ARG:HG2	1.17	1.04
1:A:185:ASN:HD22	1:A:272:SER:CB	1.71	1.02
1:B:313:PRO:CD	1:B:316:MET:HE3	1.91	0.98
1:B:53:THR:HG22	1:B:57:ARG:HD2	1.45	0.97
1:A:281:TRP:CD1	1:A:376:GLU:HG3	1.99	0.97
1:A:16:ARG:HH11	1:A:16:ARG:CG	1.77	0.96
1:A:276:GLN:N	1:A:299:MET:HE1	1.81	0.94
1:A:185:ASN:ND2	1:A:272:SER:HB3	1.82	0.94
1:B:16:ARG:HG2	1:B:16:ARG:NH1	1.82	0.92
1:A:313:PRO:HD2	1:A:316:MET:HE3	0.91	0.89
1:B:319:PHE:CD1	1:B:372:HIS:HD2	1.90	0.89
1:B:281:TRP:CD2	4:B:538:HOH:O	2.18	0.88
1:A:313:PRO:HG2	1:A:316:MET:HE2	1.54	0.88
1:A:16:ARG:HG2	1:A:16:ARG:NH1	1.89	0.86
1:A:73:ASP:OD1	1:A:76:HIS:HD2	1.58	0.85
1:B:73:ASP:OD1	1:B:76:HIS:HD2	1.60	0.85
1:B:319:PHE:CD1	1:B:372:HIS:CD2	2.64	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLN:H	1:A:299:MET:HE1	1.37	0.84
1:B:319:PHE:HD1	1:B:372:HIS:CD2	1.96	0.83
1:B:16:ARG:HH11	1:B:16:ARG:CG	1.92	0.82
1:A:276:GLN:NE2	1:A:350:SER:HB2	1.95	0.82
1:A:275:THR:HA	1:A:299:MET:HE3	1.60	0.82
1:B:155:LEU:O	1:B:245:HIS:CE1	2.34	0.80
1:A:302:TRP:HA	1:A:316:MET:HE1	1.63	0.80
1:B:313:PRO:HD2	1:B:316:MET:CE	2.08	0.79
1:A:333:LYS:HD2	1:A:333:LYS:O	1.83	0.78
1:B:276:GLN:N	1:B:299:MET:HE1	1.99	0.78
1:A:379:ARG:O	1:A:380:ASN:HB2	1.83	0.77
1:B:183:THR:OG1	1:B:250:HIS:HD2	1.68	0.77
1:A:244:HIS:HD2	1:A:312:TYR:OH	1.69	0.76
1:B:185:ASN:HD22	1:B:272:SER:CB	1.98	0.76
1:A:445:TYR:O	1:A:449:HIS:HD2	1.69	0.76
1:A:313:PRO:CG	1:A:316:MET:HE2	2.16	0.74
1:B:186:GLN:HE21	1:B:345:ASN:HD22	1.35	0.74
1:B:454:ARG:HD2	1:B:454:ARG:O	1.86	0.74
1:B:313:PRO:CD	1:B:316:MET:CE	2.66	0.73
1:A:276:GLN:HE21	1:A:350:SER:HB2	1.52	0.73
1:A:281:TRP:HD1	1:A:376:GLU:HG3	1.54	0.73
1:B:275:THR:HA	1:B:299:MET:HE3	1.69	0.73
1:B:281:TRP:CD1	1:B:376:GLU:HG3	2.23	0.73
1:B:185:ASN:ND2	1:B:272:SER:HB3	2.03	0.73
1:A:185:ASN:ND2	1:A:272:SER:CB	2.47	0.72
1:A:13:ASP:HB3	1:A:16:ARG:HG3	1.71	0.72
1:B:313:PRO:HG2	1:B:316:MET:CE	2.21	0.71
1:B:185:ASN:HD22	1:B:272:SER:HB2	1.57	0.70
1:A:381:GLY:O	1:A:383:PRO:HD3	1.91	0.70
1:A:415:LEU:HD11	1:A:464:LYS:CG	2.22	0.69
1:B:155:LEU:O	1:B:245:HIS:HE1	1.74	0.69
1:A:512:HIS:O	1:A:513:LYS:HD3	1.93	0.69
1:B:411:TYR:O	1:B:412:ASN:HB3	1.92	0.69
1:B:281:TRP:CE2	4:B:518:HOH:O	2.47	0.68
1:B:294:ARG:HD2	1:B:371:ILE:O	1.93	0.68
1:A:313:PRO:CG	1:A:316:MET:CE	2.72	0.68
1:B:73:ASP:OD1	1:B:76:HIS:CD2	2.46	0.68
1:B:258:LYS:HG3	1:B:262:GLN:OE1	1.94	0.68
1:B:392:TRP:CH2	2:B:1000:DH8:HB ^F	2.29	0.68
1:A:333:LYS:HD2	1:A:333:LYS:C	2.19	0.67
1:A:204:ARG:NH1	1:A:238:GLU:OE1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TRP:CD1	1:A:376:GLU:CG	2.76	0.66
1:A:178:VAL:C	1:A:179:LYS:HD2	2.20	0.66
1:A:276:GLN:H	1:A:299:MET:CE	2.08	0.66
1:A:183:THR:OG1	1:A:250:HIS:HD2	1.79	0.66
1:B:281:TRP:CE2	4:B:538:HOH:O	2.41	0.66
1:A:279:GLU:O	1:A:351:TYR:HA	1.95	0.66
1:A:415:LEU:CD1	1:A:464:LYS:HG2	2.26	0.65
1:A:415:LEU:HD11	1:A:464:LYS:HG3	1.79	0.65
1:B:411:TYR:O	1:B:412:ASN:CB	2.43	0.65
1:A:499:TYR:CD2	1:A:500:PRO:HD2	2.32	0.64
1:B:428:ASN:OD1	1:B:430:ASN:HB2	1.97	0.64
1:B:53:THR:HG22	1:B:57:ARG:CD	2.24	0.64
1:B:297:ASP:OD2	1:B:315:SER:OG	2.13	0.64
1:B:275:THR:HA	1:B:299:MET:CE	2.28	0.63
1:A:281:TRP:HD1	1:A:376:GLU:CG	2.09	0.63
1:B:278:MET:HE3	1:B:295:ALA:HB1	1.80	0.63
1:B:512:HIS:ND1	1:B:513:LYS:HD2	2.14	0.63
1:A:197:THR:O	1:A:206:ARG:HB2	1.98	0.63
1:B:276:GLN:H	1:B:299:MET:HE1	1.64	0.62
1:A:16:ARG:CG	1:A:16:ARG:NH1	2.49	0.62
1:A:313:PRO:CD	1:A:316:MET:HE2	2.25	0.62
1:B:204:ARG:NH1	1:B:238:GLU:OE2	2.32	0.62
1:A:379:ARG:O	1:A:380:ASN:CB	2.47	0.62
2:B:1000:DH8:CAL	2:B:1000:DH8:HABB	2.31	0.61
1:B:185:ASN:ND2	1:B:272:SER:CB	2.61	0.61
1:B:305:GLU:HB3	1:B:306:PRO:HD3	1.81	0.61
1:B:512:HIS:O	1:B:513:LYS:CD	2.49	0.61
1:A:271:ILE:HG12	1:A:272:SER:H	1.66	0.60
1:A:16:ARG:HH11	1:A:16:ARG:CB	2.15	0.59
1:A:294:ARG:HD2	1:A:371:ILE:O	2.03	0.59
1:B:445:TYR:O	1:B:449:HIS:HD2	1.86	0.59
1:B:281:TRP:NE1	4:B:518:HOH:O	2.36	0.58
1:B:508:MET:O	1:B:512:HIS:HB2	2.04	0.58
1:B:339:TYR:CD1	1:B:339:TYR:C	2.81	0.58
1:A:415:LEU:HD11	1:A:464:LYS:HG2	1.85	0.58
1:A:445:TYR:O	1:A:449:HIS:CD2	2.54	0.58
1:A:512:HIS:ND1	1:A:513:LYS:HD3	2.19	0.58
1:B:345:ASN:HB3	1:B:420:GLU:HB2	1.85	0.58
1:A:73:ASP:OD1	1:A:76:HIS:CD2	2.49	0.57
1:B:256:LEU:C	1:B:256:LEU:HD23	2.29	0.57
1:B:378:ASP:HB3	1:B:382:VAL:C	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:HIS:HD2	1:B:312:TYR:OH	1.88	0.57
1:B:14:ALA:O	1:B:17:ILE:HG22	2.05	0.57
1:B:302:TRP:HA	1:B:316:MET:HE1	1.87	0.57
1:B:313:PRO:CG	1:B:316:MET:CE	2.82	0.56
1:B:393:LEU:C	1:B:393:LEU:HD23	2.32	0.55
1:A:142:ASP:OD1	1:A:142:ASP:N	2.35	0.55
1:A:512:HIS:ND1	1:A:513:LYS:CD	2.69	0.55
1:B:271:ILE:HG12	1:B:272:SER:N	2.22	0.55
1:B:284:ASN:O	1:B:285:SER:C	2.50	0.55
1:B:476:GLU:O	1:B:479:GLU:HB2	2.07	0.55
1:A:313:PRO:CD	1:A:316:MET:HE1	2.32	0.54
1:B:243:THR:HG23	1:B:303:PHE:CE1	2.42	0.54
1:B:512:HIS:O	1:B:513:LYS:HB2	2.06	0.54
1:B:343:GLY:HA2	1:B:417:TYR:O	2.08	0.54
1:B:355:ALA:O	1:B:356:SER:C	2.51	0.54
1:B:512:HIS:O	1:B:513:LYS:CB	2.56	0.54
1:A:271:ILE:HG12	1:A:272:SER:N	2.23	0.53
1:A:281:TRP:NE1	1:A:376:GLU:HG3	2.22	0.53
1:A:397:PRO:HA	1:A:449:HIS:CE1	2.44	0.53
1:A:244:HIS:CD2	1:A:312:TYR:OH	2.56	0.53
1:B:415:LEU:HD12	1:B:462:ASN:ND2	2.24	0.53
1:A:411:TYR:O	1:A:412:ASN:CB	2.54	0.53
1:B:305:GLU:HG3	1:B:311:ASP:O	2.09	0.52
1:B:300:LEU:CD1	1:B:304:MET:HG2	2.38	0.52
1:A:392:TRP:CH2	2:A:1000:DH8:HB F	2.44	0.52
1:A:353:THR:HG22	1:A:374:THR:HB	1.92	0.52
1:A:421:ASN:ND2	1:A:466:TYR:OH	2.41	0.52
2:B:1000:DH8:CAL	2:B:1000:DH8:CAB	2.89	0.51
1:A:376:GLU:OE1	1:A:376:GLU:HA	2.11	0.50
1:B:313:PRO:HG2	1:B:316:MET:HE2	1.94	0.50
1:A:355:ALA:O	1:A:356:SER:C	2.55	0.50
1:A:176:ASP:CG	1:A:177:ARG:HD3	2.36	0.50
1:B:16:ARG:NH1	1:B:16:ARG:CG	2.61	0.50
1:B:338:SER:O	1:B:339:TYR:HB3	2.11	0.50
1:A:276:GLN:N	1:A:299:MET:CE	2.64	0.49
1:B:279:GLU:O	1:B:351:TYR:HA	2.11	0.49
1:B:300:LEU:HD11	1:B:304:MET:CG	2.42	0.49
1:A:14:ALA:O	1:A:17:ILE:HG22	2.11	0.49
1:B:512:HIS:C	1:B:513:LYS:HD2	2.37	0.49
1:A:434:SER:O	1:A:438:LYS:HE3	2.13	0.49
1:B:282:ASP:OD1	1:B:282:ASP:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:SER:O	1:B:319:PHE:HD2	1.94	0.49
1:B:445:TYR:O	1:B:449:HIS:CD2	2.66	0.48
1:B:449:HIS:HE1	4:B:542:HOH:O	1.96	0.48
1:A:42:ARG:NH2	1:B:494:ASP:OD2	2.47	0.48
1:A:179:LYS:HD2	1:A:179:LYS:N	2.29	0.48
1:A:427:LYS:O	1:A:428:ASN:HB2	2.13	0.47
1:A:281:TRP:CD1	1:A:376:GLU:CB	2.97	0.47
1:A:186:GLN:HG2	1:A:345:ASN:HD22	1.80	0.47
1:B:205:GLY:O	1:B:206:ARG:HB2	2.13	0.47
1:B:454:ARG:HD2	1:B:454:ARG:C	2.39	0.47
1:A:66:THR:HG22	1:B:493:ASN:OD1	2.15	0.47
1:A:273:HIS:CE1	1:A:303:PHE:HB3	2.49	0.47
1:A:281:TRP:HD1	1:A:376:GLU:CB	2.27	0.47
1:B:454:ARG:HA	1:B:454:ARG:HD3	1.68	0.47
1:B:406:TYR:CD2	1:B:406:TYR:C	2.93	0.47
1:B:512:HIS:ND1	1:B:512:HIS:C	2.72	0.46
1:A:512:HIS:O	1:A:513:LYS:CB	2.63	0.46
1:B:250:HIS:HE1	1:B:338:SER:O	1.98	0.46
1:B:327:PHE:C	1:B:328:SER:O	2.57	0.46
1:A:512:HIS:ND1	1:A:512:HIS:C	2.74	0.46
1:B:454:ARG:C	1:B:454:ARG:CD	2.88	0.46
1:B:313:PRO:CG	1:B:316:MET:HE3	2.44	0.46
1:A:185:ASN:ND2	1:A:272:SER:OG	2.48	0.46
1:A:186:GLN:N	1:A:187:PRO:CD	2.79	0.46
1:A:306:PRO:O	1:A:310:GLY:HA2	2.15	0.46
1:B:449:HIS:CE1	4:B:542:HOH:O	2.68	0.46
1:A:244:HIS:NE2	1:A:327:PHE:CE1	2.85	0.45
1:A:353:THR:HG23	1:A:354:ASN:O	2.16	0.45
1:B:204:ARG:NH1	1:B:238:GLU:CD	2.75	0.45
1:B:250:HIS:CE1	1:B:338:SER:O	2.69	0.45
1:B:323:ARG:CZ	1:B:365:PHE:CD1	2.99	0.45
1:B:176:ASP:CG	1:B:177:ARG:HD3	2.41	0.45
1:B:469:TRP:HA	1:B:470:SER:HA	1.57	0.45
1:A:454:ARG:NH1	1:A:457:MET:HB2	2.32	0.44
1:A:496:PHE:O	1:A:498:ARG:HD2	2.17	0.44
1:B:300:LEU:HD11	1:B:304:MET:HG3	2.00	0.44
1:B:449:HIS:O	1:B:453:VAL:HG23	2.16	0.44
1:A:409:LYS:NZ	1:A:409:LYS:HB3	2.32	0.44
1:A:36:GLN:O	1:A:474:ASN:HB2	2.16	0.44
1:B:445:TYR:CD2	1:B:445:TYR:C	2.94	0.44
1:B:339:TYR:CD1	1:B:339:TYR:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ILE:CG1	1:B:272:SER:N	2.80	0.43
1:A:275:THR:HG22	1:A:300:LEU:HD13	2.00	0.43
1:A:204:ARG:NH1	1:A:238:GLU:CD	2.76	0.43
1:A:393:LEU:C	1:A:393:LEU:HD23	2.43	0.43
2:B:1000:DH8:CAB	2:B:1000:DH8:HAL	2.48	0.43
1:B:195:TYR:CE2	1:B:242:VAL:HG21	2.52	0.43
1:A:315:SER:O	1:A:319:PHE:HD2	2.01	0.43
1:A:406:TYR:O	1:A:410:THR:OG1	2.35	0.43
1:B:17:ILE:HD12	1:B:21:ASP:OD2	2.18	0.43
1:B:281:TRP:HD1	1:B:376:GLU:HG3	1.77	0.43
1:B:294:ARG:NH1	1:B:372:HIS:O	2.52	0.43
1:A:185:ASN:HD21	1:A:345:ASN:HD21	1.67	0.43
1:B:327:PHE:O	1:B:328:SER:C	2.62	0.43
1:A:305:GLU:HG3	1:A:311:ASP:O	2.19	0.42
1:B:281:TRP:CD1	1:B:376:GLU:CG	2.99	0.42
1:A:469:TRP:HA	1:A:470:SER:HA	1.60	0.42
1:B:300:LEU:HD12	1:B:304:MET:HG2	2.02	0.42
1:B:314:LYS:H	1:B:314:LYS:HG2	1.63	0.42
1:A:58:ARG:N	1:A:59:PRO:CD	2.82	0.42
1:B:281:TRP:HD1	1:B:376:GLU:CG	2.33	0.42
1:A:128:LEU:HD11	1:A:177:ARG:HB3	2.01	0.42
1:B:439:ASP:OD2	1:B:503:SER:OG	2.26	0.42
1:B:366:SER:O	1:B:367:TYR:C	2.62	0.42
1:B:176:ASP:HB3	4:B:524:HOH:O	2.19	0.42
1:B:458:ASN:C	1:B:460:GLY:H	2.27	0.42
1:B:37:ILE:HG13	1:B:38:GLU:N	2.35	0.42
1:A:485:PHE:CE2	2:A:1000:DH8:H6A	2.54	0.42
1:B:403:ILE:HD12	1:B:403:ILE:HA	1.91	0.42
1:A:33:SER:HB3	1:A:140:HIS:CD2	2.54	0.42
1:B:195:TYR:CD2	1:B:242:VAL:HG21	2.55	0.42
1:B:79:LYS:HB2	4:B:539:HOH:O	2.19	0.41
1:B:393:LEU:C	1:B:393:LEU:CD2	2.93	0.41
1:A:19:ARG:HB2	1:A:511:PHE:HA	2.01	0.41
1:A:316:MET:O	1:A:320:VAL:HG23	2.21	0.41
1:A:512:HIS:O	1:A:513:LYS:HB2	2.19	0.41
1:B:273:HIS:CE1	1:B:303:PHE:HB3	2.56	0.41
1:B:454:ARG:O	1:B:454:ARG:CD	2.62	0.41
1:A:114:LYS:HA	1:A:114:LYS:HD3	1.80	0.41
1:A:305:GLU:HB3	1:A:306:PRO:HD3	2.02	0.41
1:B:128:LEU:C	1:B:130:ASN:N	2.76	0.41
1:A:512:HIS:C	1:A:513:LYS:HD3	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASN:O	1:B:286:ALA:N	2.54	0.41
1:A:351:TYR:HB2	1:A:376:GLU:O	2.20	0.41
1:B:192:VAL:O	1:B:196:ALA:HB3	2.20	0.41
1:B:238:GLU:N	1:B:239:PRO:CD	2.84	0.41
1:A:490:ILE:HG23	1:A:496:PHE:HA	2.03	0.41
1:B:186:GLN:N	1:B:187:PRO:CD	2.84	0.41
1:A:19:ARG:O	1:A:19:ARG:HG2	2.20	0.41
1:B:512:HIS:O	1:B:513:LYS:HD2	2.20	0.41
1:A:313:PRO:HG2	1:A:316:MET:CE	2.32	0.41
1:B:323:ARG:CZ	1:B:365:PHE:HD1	2.34	0.41
1:A:19:ARG:O	1:A:19:ARG:CG	2.69	0.41
1:B:36:GLN:O	1:B:474:ASN:HB2	2.21	0.41
1:A:413:VAL:HA	1:A:414:PRO:HD3	1.92	0.40
1:A:508:MET:O	1:A:512:HIS:HB2	2.21	0.40
1:B:344:LEU:HD12	1:B:404:LEU:HD23	2.03	0.40
1:B:423:VAL:HG22	1:B:424:ASP:H	1.86	0.40
1:A:182:MET:HE3	1:A:182:MET:HB2	1.82	0.40
1:A:397:PRO:O	1:A:400:ILE:HG22	2.22	0.40
1:B:58:ARG:N	1:B:59:PRO:CD	2.85	0.40
1:B:243:THR:HG23	1:B:303:PHE:CZ	2.57	0.40
1:B:281:TRP:HD1	1:B:376:GLU:HB2	1.87	0.40
2:B:1000:DH8:HAN	2:B:1000:DH8:HBH	1.82	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	465/513 (91%)	436 (94%)	28 (6%)	1 (0%)	43	53
1	B	465/513 (91%)	434 (93%)	29 (6%)	2 (0%)	30	36
All	All	930/1026 (91%)	870 (94%)	57 (6%)	3 (0%)	36	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	B	285	SER
1	B	459	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/435 (91%)	382 (96%)	15 (4%)	29	41
1	B	397/435 (91%)	375 (94%)	22 (6%)	19	26
All	All	794/870 (91%)	757 (95%)	37 (5%)	23	33

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	63	ARG
1	A	94	ARG
1	A	179	LYS
1	A	182	MET
1	A	255	GLU
1	A	263	ARG
1	A	272	SER
1	A	276	GLN
1	A	318	LYS
1	A	326	LYS
1	A	330	GLU
1	A	410	THR
1	A	434	SER
1	A	513	LYS
1	B	16	ARG
1	B	18	SER
1	B	53	THR
1	B	63	ARG
1	B	94	ARG

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Mol	Chain	Res	Type
1	B	179	LYS
1	B	206	ARG
1	B	232	THR
1	B	258	LYS
1	B	315	SER
1	B	316	MET
1	B	326	LYS
1	B	333	LYS
1	B	352	VAL
1	B	354	ASN
1	B	374	THR
1	B	378	ASP
1	B	409	LYS
1	B	415	LEU
1	B	447	GLN
1	B	454	ARG
1	B	513	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	76	HIS
1	A	140	HIS
1	A	185	ASN
1	A	244	HIS
1	A	250	HIS
1	A	276	GLN
1	A	372	HIS
1	A	380	ASN
1	A	421	ASN
1	A	449	HIS
1	A	452	ASN
1	B	12	ASN
1	B	76	HIS
1	B	185	ASN
1	B	186	GLN
1	B	244	HIS
1	B	250	HIS
1	B	273	HIS
1	B	372	HIS
1	B	449	HIS

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Mol	Chain	Res	Type
1	B	452	ASN
1	B	462	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	DH8	B	1000	-	39,43,43	1.39	4 (10%)	43,69,69	1.80	10 (23%)
2	DH8	A	1000	-	39,43,43	1.37	3 (7%)	43,69,69	1.57	8 (18%)

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	DH8	B	1000	-	-	6/12/99/99	0/1/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DH8	A	1000	-	-	4/12/99/99	0/1/7/7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	DH8	CAH-CAU	5.40	1.40	1.32
2	A	1000	DH8	CAH-CAU	5.25	1.40	1.32
2	A	1000	DH8	CAW-NAP	-2.82	1.35	1.39
2	B	1000	DH8	CAW-NAP	-2.78	1.35	1.39
2	A	1000	DH8	CAW-CAX	2.70	1.42	1.39
2	B	1000	DH8	O1-C1	2.05	1.47	1.41
2	B	1000	DH8	CAO-CBK	-2.04	1.50	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	DH8	OAQ-CAT-CAB	4.71	119.49	111.09
2	A	1000	DH8	OAQ-CAT-CAB	4.51	119.13	111.09
2	B	1000	DH8	OAQ-CBH-CBI	-4.32	100.28	111.24
2	A	1000	DH8	CAA-CAH-CAU	-3.72	121.22	126.25
2	B	1000	DH8	C1-O5-C5	-3.54	106.80	113.72
2	B	1000	DH8	CAA-CAH-CAU	-3.44	121.61	126.25
2	B	1000	DH8	CBH-OAQ-CAT	-3.34	113.05	117.79
2	A	1000	DH8	CBH-OAQ-CAT	-3.29	113.12	117.79
2	B	1000	DH8	CAK-CAW-CAX	-3.18	118.94	121.92
2	A	1000	DH8	C1-O5-C5	-3.06	107.75	113.72
2	A	1000	DH8	CBK-CAX-CAW	-2.68	105.50	108.89
2	A	1000	DH8	CAK-CAW-CAX	-2.51	119.57	121.92
2	B	1000	DH8	CBK-CAX-CAW	-2.42	105.83	108.89
2	B	1000	DH8	C1-C2-C3	2.41	115.07	110.01
2	B	1000	DH8	OAQ-CAT-OAC	-2.16	118.82	122.99
2	A	1000	DH8	CAL-CAX-CBK	2.15	134.04	130.21
2	A	1000	DH8	CAK-CAW-NAP	2.13	130.87	127.98
2	B	1000	DH8	CAK-CAW-NAP	2.06	130.78	127.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	DH8	NBJ-CBG-O1-C1
2	B	1000	DH8	NBJ-CBG-O1-C1

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Mol	Chain	Res	Type	Atoms
2	B	1000	DH8	CAB-CAT-OAQ-CBH
2	A	1000	DH8	CAB-CAT-OAQ-CBH
2	B	1000	DH8	OAC-CAT-OAQ-CBH
2	B	1000	DH8	O5-C1-O1-CBG
2	A	1000	DH8	OAC-CAT-OAQ-CBH
2	A	1000	DH8	O5-C1-O1-CBG
2	B	1000	DH8	CBI-CBH-OAQ-CAT
2	B	1000	DH8	CBK-CBH-OAQ-CAT

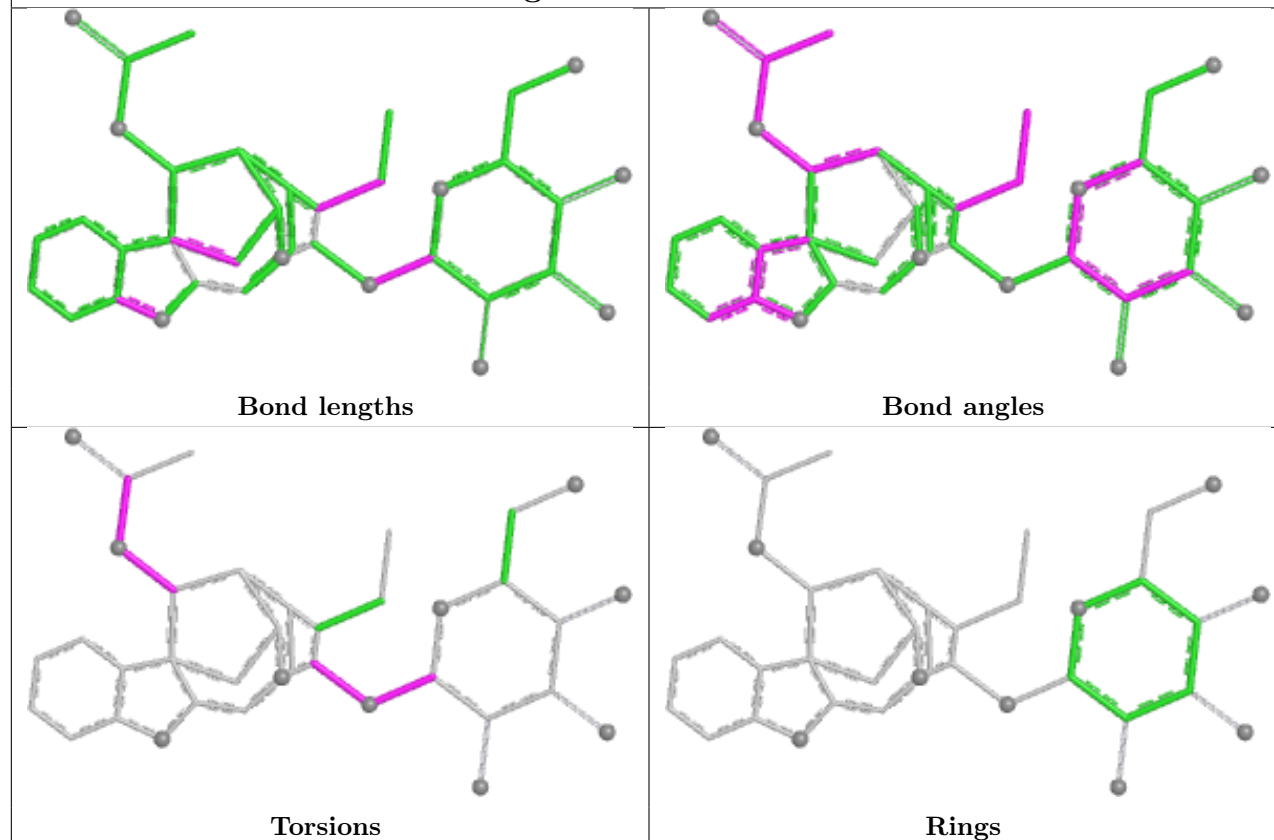
There are no ring outliers.

2 monomers are involved in 7 short contacts:

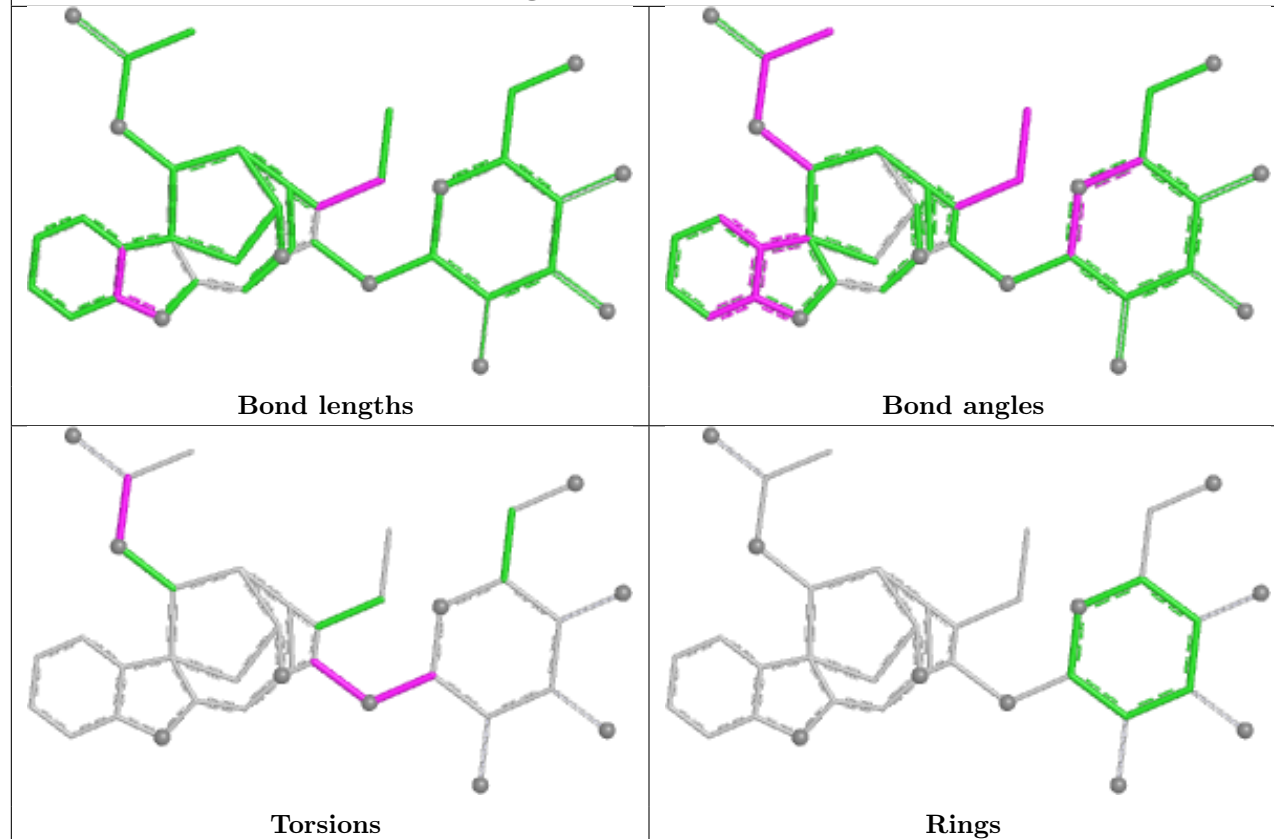
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	DH8	5	0
2	A	1000	DH8	2	0

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.

Ligand DH8 B 1000



Ligand DH8 A 1000



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 [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	471/513 (91%)	-0.48	4 (0%) 82 83	13, 31, 57, 76	0
1	B	471/513 (91%)	-0.41	3 (0%) 85 87	16, 33, 55, 72	0
All	All	942/1026 (91%)	-0.44	7 (0%) 84 85	13, 32, 56, 76	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	ARG	6.0
1	B	206	ARG	5.1
1	A	281	TRP	3.2
1	B	281	TRP	2.9
1	A	356	SER	2.9
1	A	231	SER	2.6
1	B	356	SER	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](#)

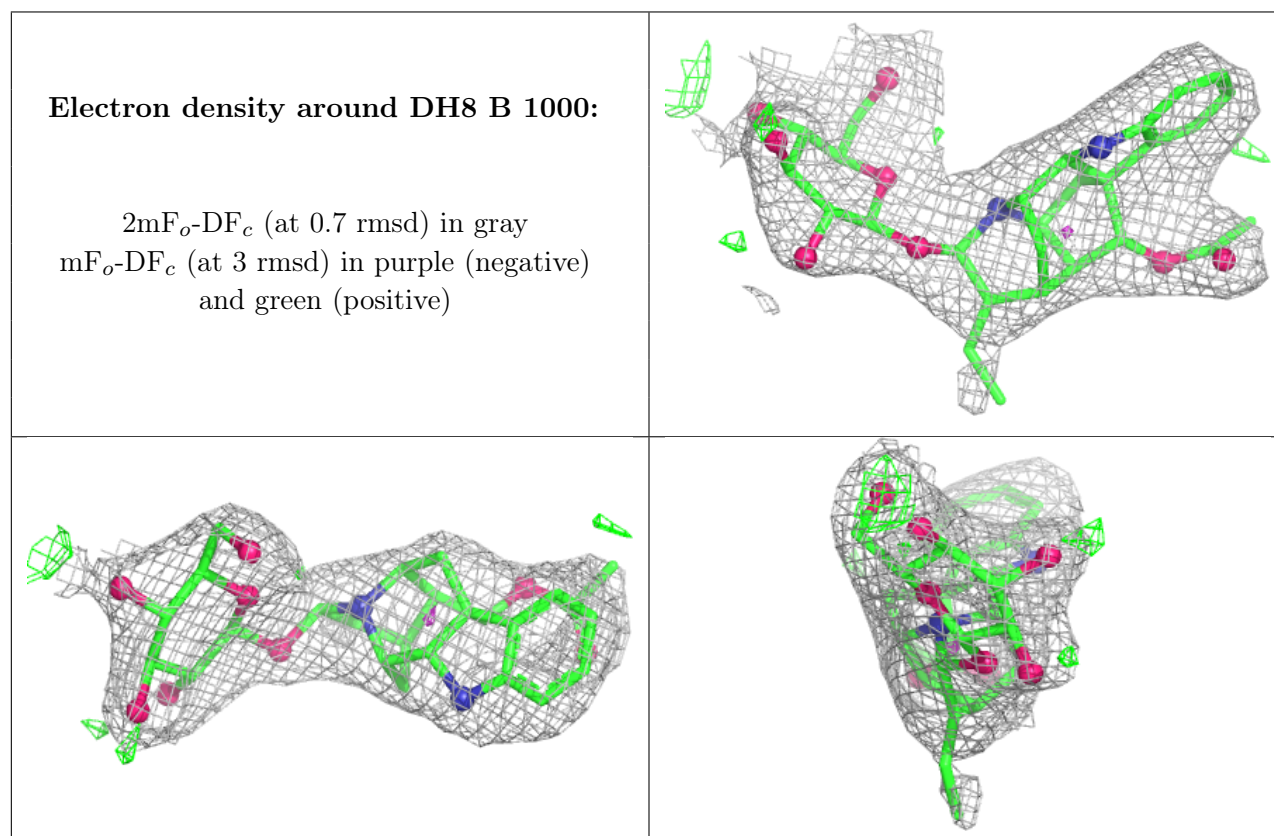
There are no oligosaccharides in this entry.

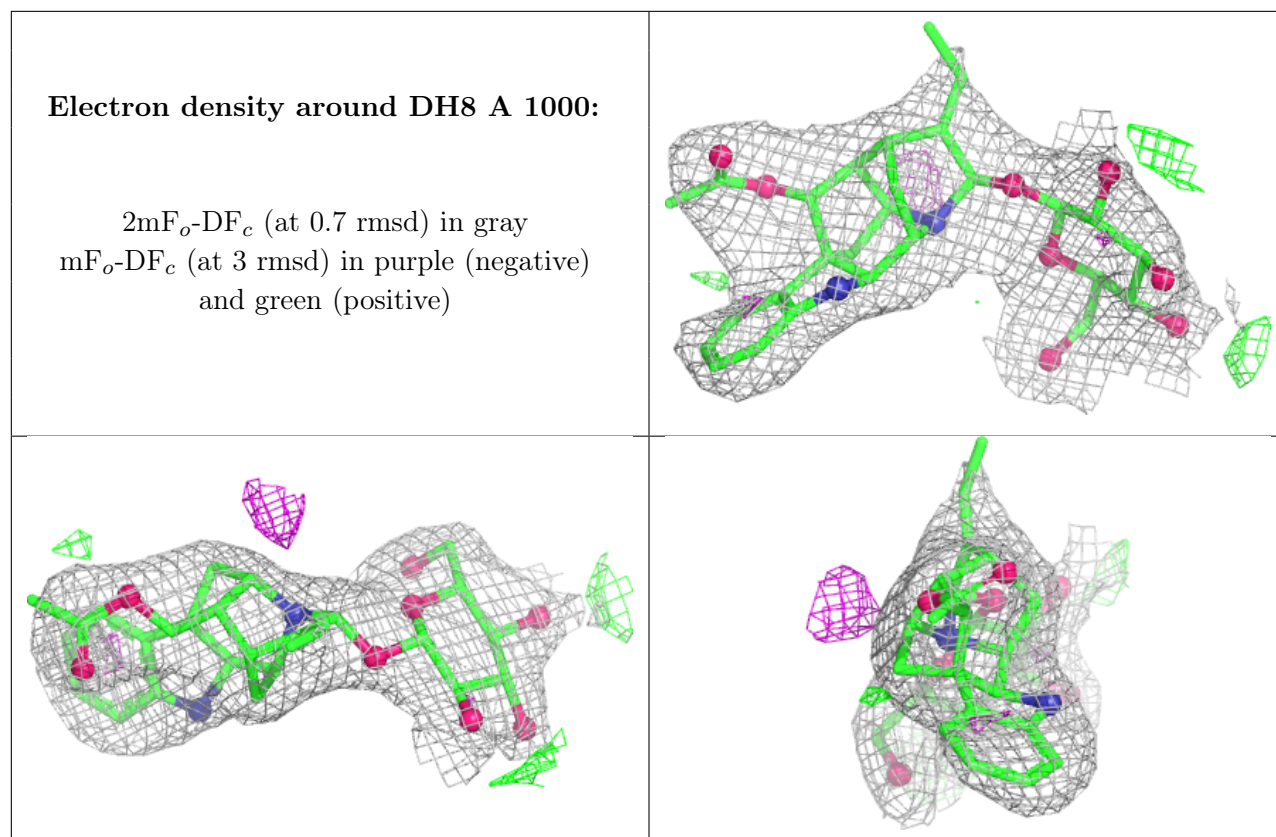
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	DH8	B	1000	37/37	0.90	0.12	57,61,63,64	0
2	DH8	A	1000	37/37	0.91	0.11	49,59,61,62	0
3	CL	B	514	1/1	0.96	0.20	34,34,34,34	0
3	CL	A	514	1/1	0.99	0.22	30,30,30,30	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.