



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:03 AM EDT

PDB ID : 7QEA / pdb_00007qea
Title : Crystal structure of fluorescein-di-Beta-D-glucuronide bound to a mutant of SN243 (D415A)
Authors : Neun, S.; Brear, P.; Campbell, E.; Omari, K.; Wagner, O.; Hyvonen, M.; Hollfelder, F.
Deposited on : 2021-12-01
Resolution : 2.28 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

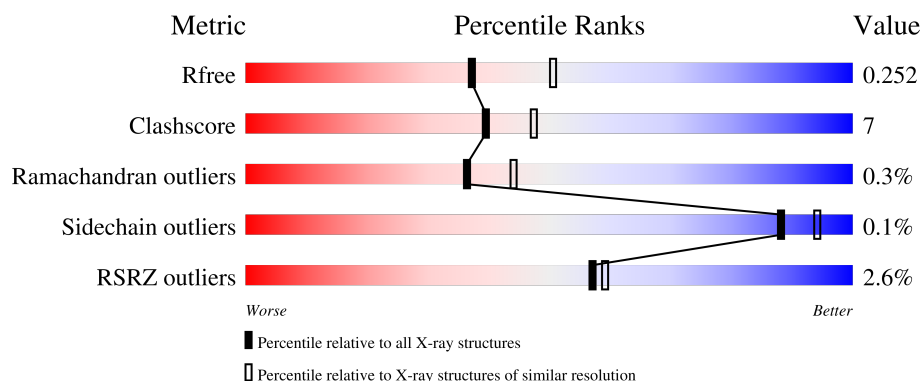
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

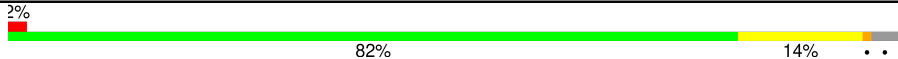
The reported resolution of this entry is 2.28 Å.

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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	759	
1	B	759	

2 Entry composition [i](#)

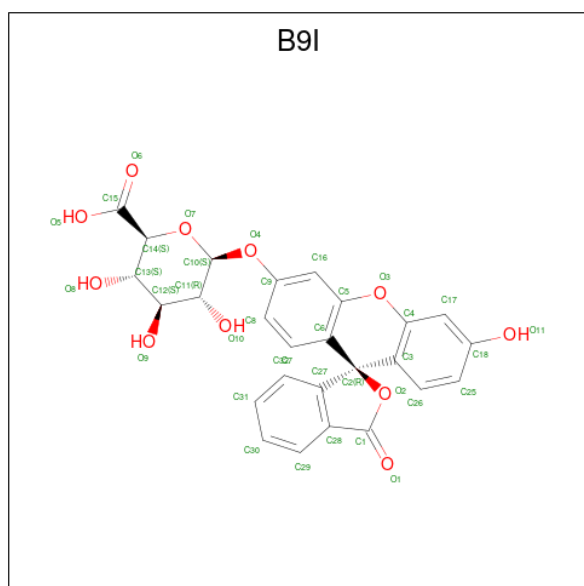
There are 6 unique types of molecules in this entry. The entry contains 11694 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SN243.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	2	0
			5623	3525	923	1155	20			
1	B	739	Total	C	N	O	S	0	1	0
			5627	3527	923	1157	20			

- Molecule 2 is (2 {S},3 {S},4 {S},5 {R},6 {S})-3,4,5-tris(oxidanyl)-6-[(1 {R})-6'-oxidanyl-3-oxidanylidene-spiro[2-benzofuran-1,9'-xanthene]-3'-yl]oxy-oxane-2-carboxylic acid (CCD ID: B9I) (formula: C₂₆H₂₀O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	Zn	0	0
			22	22		
3	B	16	Total	Zn	0	0
			16	16		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

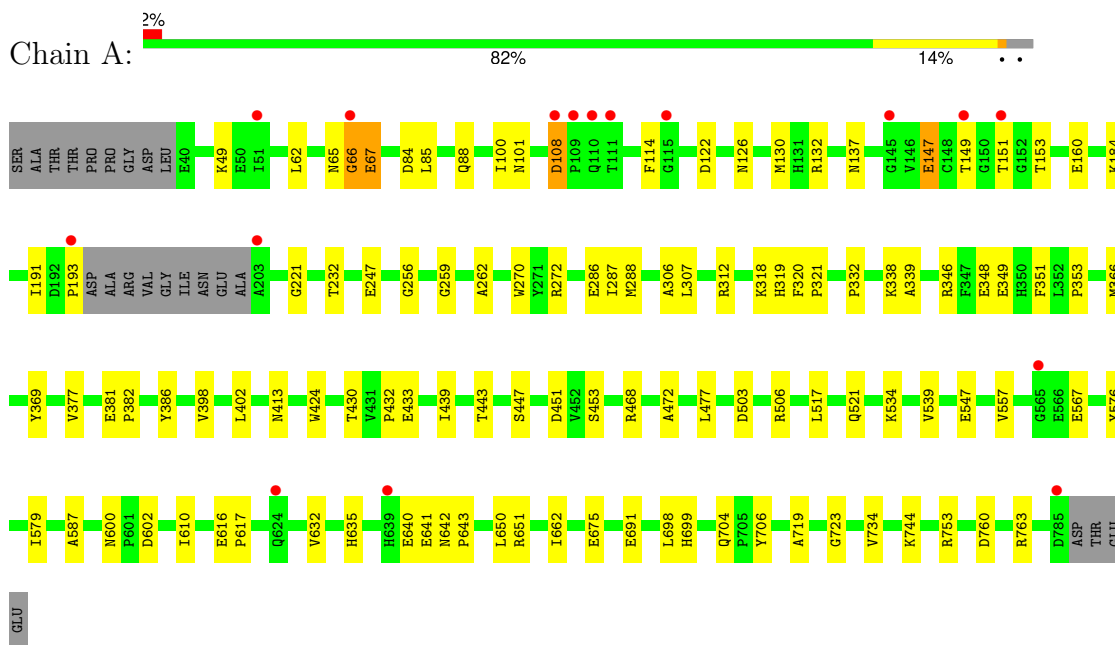
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	174	Total O 174 174	0	0
6	B	134	Total O 134 134	0	0

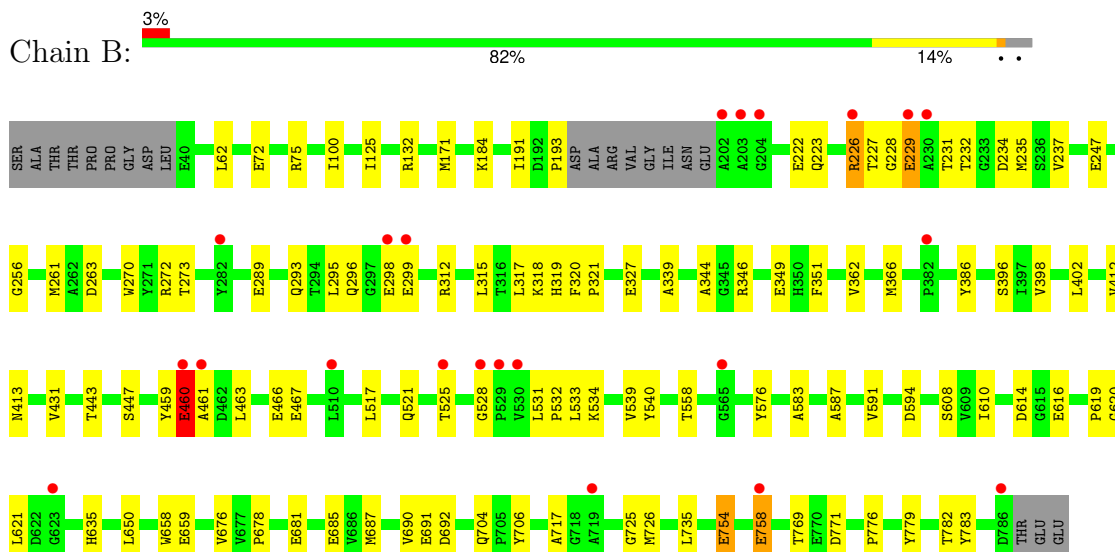
3 Residue-property plots

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: SN243



• Molecule 1: SN243



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.27Å 81.56Å 93.39Å 66.64° 89.38° 89.57°	Depositor
Resolution (Å)	51.11 – 2.28 51.11 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.3 (51.11-2.28) 96.3 (51.11-2.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.198 , 0.252 0.202 , 0.252	Depositor DCC
R_{free} test set	3981 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l 0.016 for -h,k,k-l 0.007 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11694	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: ACT, B9I, ZN, 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	0.45	0/5748	0.71	16/7837 (0.2%)
1	B	0.51	6/5752 (0.1%)	0.71	15/7843 (0.2%)
All	All	0.48	6/11500 (0.1%)	0.71	31/15680 (0.2%)

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	A	0	2
1	B	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	431	VAL	CA-CB	15.33	1.62	1.54
1	B	754	GLU	CB-CG	6.29	1.71	1.52
1	B	299	GLU	CD-OE1	6.05	1.36	1.25
1	B	229	GLU	CB-CG	5.77	1.69	1.52
1	B	229	GLU	CG-CD	5.35	1.65	1.52
1	B	460	GLU	CB-CG	5.12	1.67	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	754	GLU	CA-CB-CG	10.39	134.89	114.10
1	A	651	ARG	CG-CD-NE	-9.16	91.84	112.00
1	A	66	GLY	CA-C-N	-8.74	107.44	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GLY	C-N-CA	-8.74	107.44	123.01
1	B	228	GLY	CA-C-N	8.09	135.24	122.62
1	B	228	GLY	C-N-CA	8.09	135.24	122.62
1	B	229	GLU	CB-CG-CD	7.56	125.46	112.60
1	B	229	GLU	N-CA-C	7.50	121.35	109.50
1	B	299	GLU	CA-CB-CG	7.49	129.08	114.10
1	B	298	GLU	N-CA-C	7.24	122.22	112.88
1	B	460	GLU	CA-C-N	-6.97	111.49	122.65
1	B	460	GLU	C-N-CA	-6.97	111.49	122.65
1	B	754	GLU	CG-CD-OE2	-6.79	102.78	118.40
1	A	108	ASP	CB-CG-OD2	-6.61	103.21	118.40
1	A	567	GLU	N-CA-C	6.43	119.30	110.24
1	A	108	ASP	N-CA-C	-6.24	99.91	109.64
1	B	226	ARG	CG-CD-NE	6.19	125.62	112.00
1	A	67	GLU	CG-CD-OE2	-6.18	104.19	118.40
1	A	147	GLU	CB-CA-C	-6.14	99.32	111.60
1	A	147	GLU	CA-CB-CG	6.01	126.11	114.10
1	A	651	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	B	229	GLU	CA-CB-CG	5.82	125.73	114.10
1	B	758	GLU	CB-CG-CD	-5.75	102.82	112.60
1	A	108	ASP	CB-CG-OD1	5.63	131.35	118.40
1	A	108	ASP	CB-CA-C	-5.53	102.95	109.47
1	A	651	ARG	CB-CG-CD	5.29	123.47	111.30
1	A	651	ARG	CD-NE-CZ	5.24	131.73	124.40
1	A	67	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	754	GLU	CB-CA-C	5.13	120.52	110.67
1	A	67	GLU	CA-CB-CG	-5.06	103.99	114.10
1	B	754	GLU	CG-CD-OE1	5.04	130.00	118.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ASP	Sidechain
1	A	675	GLU	Sidechain
1	B	460	GLU	Sidechain

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	5623	0	5292	64	0
1	B	5627	0	5294	83	0
2	A	37	0	0	0	0
2	B	37	0	0	0	0
3	A	22	0	0	0	0
3	B	16	0	0	0	0
4	A	4	0	3	0	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	174	0	0	1	0
6	B	134	0	0	0	0
All	All	11694	0	10589	147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (147) 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:229:GLU:OE1	1:B:231:THR:CG2	1.75	1.32
1:B:758:GLU:OE2	1:B:769:THR:HA	1.32	1.29
1:B:229:GLU:OE1	1:B:231:THR:HG23	0.99	1.15
1:B:226:ARG:NH1	1:B:234:ASP:OD2	2.00	0.94
1:A:641:GLU:HG2	1:A:642:ASN:H	1.29	0.92
1:B:317:LEU:HD13	1:B:362:VAL:HG21	1.52	0.91
1:B:758:GLU:OE2	1:B:769:THR:CA	2.23	0.81
1:A:147:GLU:OE2	6:A:901:HOH:O	2.00	0.79
1:B:226:ARG:HH12	1:B:234:ASP:CG	1.91	0.78
1:B:229:GLU:CD	1:B:231:THR:HG23	2.08	0.77
1:B:346:ARG:HG3	1:B:346:ARG:HH11	1.54	0.72
1:B:327:GLU:OE1	1:B:608:SER:HB2	1.90	0.70
1:B:346:ARG:HG2	1:B:349:GLU:OE1	1.93	0.67
1:A:232:THR:HB	1:A:286:GLU:HG3	1.76	0.67
1:B:459:TYR:HE1	1:B:466:GLU:HB2	1.62	0.63
1:A:247:GLU:HG2	1:A:312:ARG:HH11	1.64	0.62
1:B:412:VAL:HG12	1:B:443:THR:HG23	1.82	0.62
1:B:125:ILE:HD12	1:B:171:MET:HE3	1.84	0.60
1:B:525:THR:OG1	1:B:528:GLY:O	2.20	0.60
1:A:49:LYS:NZ	1:A:62:LEU:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:GLU:HG3	1:B:226:ARG:CZ	2.33	0.59
1:B:247:GLU:HG2	1:B:312:ARG:HH11	1.67	0.59
1:A:101:ASN:HB2	1:A:130:MET:HE1	1.85	0.58
1:A:451:ASP:OD1	1:A:453:SER:HB3	2.04	0.58
1:A:339:ALA:HB2	1:A:610:ILE:HD11	1.87	0.57
1:A:287:ILE:HG22	1:A:288:MET:HE2	1.87	0.57
1:B:782:THR:HG22	1:B:783:TYR:O	2.05	0.57
1:A:65:ASN:OD1	1:A:67:GLU:N	2.33	0.57
1:B:539:VAL:HG22	1:B:576:TYR:HB2	1.89	0.54
1:B:318:LYS:HB2	1:B:319:HIS:CD2	2.42	0.54
1:B:386:TYR:HD1	1:B:396:SER:HG	1.55	0.53
1:A:318:LYS:HB2	1:A:319:HIS:CD2	2.43	0.53
1:B:531:LEU:HD23	1:B:533:LEU:CD1	2.39	0.53
1:A:114:PHE:HB2	1:A:160:GLU:OE2	2.07	0.52
1:B:289:GLU:OE2	1:B:293:GLN:NE2	2.42	0.52
1:B:681:GLU:O	1:B:685:GLU:HG3	2.09	0.52
1:B:517:LEU:HD22	1:B:726:MET:HE1	1.90	0.52
1:A:122:ASP:OD1	1:A:126:ASN:ND2	2.37	0.52
1:A:398:VAL:O	1:A:402:LEU:HB3	2.09	0.52
1:A:587:ALA:HB1	1:A:650:LEU:HD12	1.91	0.52
1:A:506:ARG:HH11	1:A:506:ARG:HG3	1.75	0.51
1:A:100:ILE:HG23	1:A:447:SER:HA	1.92	0.51
1:B:459:TYR:CE1	1:B:466:GLU:HB2	2.43	0.51
1:B:531:LEU:HB3	1:B:783:TYR:CE1	2.46	0.51
1:B:261:MET:HE3	1:B:263:ASP:OD2	2.12	0.50
1:B:658:TRP:CD1	1:B:659:GLU:HG3	2.46	0.50
1:A:65:ASN:OD1	1:A:66:GLY:N	2.43	0.50
1:A:247:GLU:HG2	1:A:312:ARG:NH1	2.26	0.50
1:B:318:LYS:HB2	1:B:319:HIS:CG	2.47	0.50
1:A:641:GLU:CG	1:A:642:ASN:H	2.13	0.50
1:A:468:ARG:HH12	1:A:472:ALA:HB2	1.77	0.49
1:A:547:GLU:HG3	1:A:557:VAL:HG11	1.93	0.49
1:A:640:GLU:HG2	1:A:641:GLU:H	1.77	0.49
1:B:521:GLN:NE2	1:B:717:ALA:O	2.46	0.49
1:B:346:ARG:CG	1:B:349:GLU:OE1	2.60	0.49
1:A:366:MET:HA	1:A:413:ASN:O	2.12	0.49
1:A:85:LEU:HD23	1:A:477:LEU:HD13	1.95	0.49
1:B:620:GLY:O	1:B:621:LEU:HD23	2.14	0.48
1:A:662:ILE:HG12	1:A:753:ARG:NH1	2.28	0.48
1:A:262:ALA:HB1	1:A:353:PRO:HB2	1.96	0.48
1:B:226:ARG:CZ	1:B:234:ASP:OD2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LEU:HD13	1:B:315:LEU:HD21	1.96	0.47
1:B:690:VAL:O	1:B:692:ASP:N	2.47	0.47
1:A:332:PRO:HB2	1:A:369:TYR:HB2	1.95	0.47
1:A:699:HIS:NE2	1:A:723:GLY:HA3	2.29	0.47
1:A:521:GLN:O	1:A:719:ALA:HA	2.13	0.47
1:A:430:THR:OG1	1:A:432:PRO:HD2	2.14	0.47
1:A:306:ALA:O	1:A:307:LEU:HD23	2.14	0.47
1:B:344:ALA:HB1	1:B:346:ARG:NH1	2.29	0.47
1:B:534:LYS:HD3	1:B:576:TYR:OH	2.15	0.47
1:A:503:ASP:HA	1:A:506:ARG:NH1	2.30	0.47
1:B:100:ILE:HD12	1:B:132:ARG:HB3	1.97	0.47
1:B:229:GLU:OE1	1:B:231:THR:HG21	1.96	0.47
1:A:641:GLU:HG2	1:A:642:ASN:N	2.07	0.46
1:B:320:PHE:CD1	1:B:321:PRO:HA	2.50	0.46
1:B:461:ALA:HB3	1:B:463:LEU:HD13	1.97	0.46
1:B:704:GLN:O	1:B:706:TYR:N	2.49	0.46
1:B:223:GLN:HE22	1:B:229:GLU:HG3	1.81	0.46
1:A:616:GLU:HG2	1:A:617:PRO:HD2	1.98	0.45
1:B:193:PRO:HG3	1:B:725:GLY:HA2	1.97	0.45
1:B:467:GLU:H	1:B:467:GLU:CD	2.24	0.45
1:A:346:ARG:HD2	1:A:349:GLU:OE1	2.16	0.45
1:B:339:ALA:HB2	1:B:610:ILE:HD11	1.98	0.45
1:B:229:GLU:HG3	1:B:231:THR:N	2.32	0.45
1:A:579:ILE:HB	1:A:698:LEU:HD23	1.99	0.45
1:B:533:LEU:HD22	1:B:735:LEU:HB3	1.99	0.45
1:B:398:VAL:O	1:B:402:LEU:HB3	2.17	0.44
1:A:184:LYS:HA	1:A:256:GLY:O	2.18	0.44
1:A:270:TRP:CE2	1:A:272:ARG:HB2	2.53	0.44
1:A:662:ILE:HG12	1:A:753:ARG:HH11	1.82	0.44
1:B:270:TRP:O	1:B:273:THR:HG23	2.17	0.44
1:A:377:VAL:HA	1:A:386:TYR:CE2	2.52	0.44
1:B:676:VAL:HG12	1:B:678:PRO:O	2.17	0.44
1:B:227:THR:HG22	1:B:229:GLU:CB	2.47	0.44
1:A:100:ILE:HD12	1:A:132:ARG:HB3	1.98	0.44
1:B:234:ASP:O	1:B:237:VAL:HG22	2.18	0.43
1:B:346:ARG:HG3	1:B:346:ARG:NH1	2.28	0.43
1:A:191:ILE:O	1:A:193:PRO:HD3	2.18	0.43
1:A:640:GLU:HG2	1:A:641:GLU:N	2.33	0.43
1:A:338:LYS:HE2	1:A:424:TRP:CE3	2.54	0.43
1:B:232:THR:O	1:B:235:MET:HE3	2.18	0.43
1:B:591:VAL:HB	1:B:594:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HG23	1:B:447:SER:HA	2.01	0.43
1:A:381:GLU:HA	1:A:382:PRO:HD3	1.82	0.43
1:B:223:GLN:NE2	1:B:229:GLU:HG3	2.34	0.43
1:B:583:ALA:HB3	1:B:706:TYR:CZ	2.54	0.43
1:B:587:ALA:HB1	1:B:650:LEU:HD12	2.00	0.43
1:B:227:THR:HG22	1:B:229:GLU:HB3	2.01	0.43
1:A:320:PHE:CD1	1:A:321:PRO:HA	2.54	0.42
1:B:191:ILE:O	1:B:193:PRO:HD3	2.19	0.42
1:B:318:LYS:HA	1:B:319:HIS:HA	1.74	0.42
1:A:640:GLU:OE2	1:A:643:PRO:HA	2.19	0.42
1:B:776:PRO:HD2	1:B:779:TYR:HB2	2.01	0.42
1:A:259:GLY:HA2	1:A:318:LYS:HG2	2.01	0.42
1:B:531:LEU:HA	1:B:532:PRO:C	2.44	0.42
1:A:439:ILE:HA	1:A:443:THR:O	2.19	0.42
1:B:223:GLN:NE2	1:B:229:GLU:CG	2.82	0.42
1:A:430:THR:HG22	1:A:433:GLU:OE1	2.20	0.42
1:A:468:ARG:NH1	1:A:472:ALA:HB2	2.35	0.42
1:A:600:ASN:OD1	1:A:602:ASP:HB2	2.19	0.42
1:A:632:VAL:HA	1:A:635:HIS:CE1	2.55	0.42
1:B:619:PRO:HB2	1:B:635:HIS:CD2	2.55	0.42
1:A:137:ASN:ND2	1:A:153:THR:HG22	2.35	0.42
1:B:296:GLN:HE21	1:B:296:GLN:HB3	1.64	0.42
1:B:366:MET:HA	1:B:413:ASN:O	2.20	0.41
1:B:351:PHE:C	1:B:351:PHE:CD1	2.98	0.41
1:A:760:ASP:OD2	1:A:763:ARG:NH2	2.48	0.41
1:A:351:PHE:C	1:A:351:PHE:CD1	2.99	0.41
1:B:614:ASP:OD2	1:B:616:GLU:HG2	2.21	0.41
1:B:270:TRP:CE2	1:B:272:ARG:HB2	2.55	0.41
1:A:221:GLY:HA2	1:A:744:LYS:HG2	2.03	0.41
1:A:704:GLN:O	1:A:706:TYR:N	2.54	0.41
1:A:534:LYS:HA	1:A:534:LYS:HD2	1.76	0.41
1:A:539:VAL:HG22	1:A:576:TYR:HB2	2.03	0.41
1:B:226:ARG:NH2	1:B:234:ASP:OD2	2.53	0.41
1:B:754:GLU:HG3	1:B:771:ASP:OD1	2.21	0.41
1:A:84:ASP:O	1:A:88:GLN:HG3	2.21	0.41
1:B:62:LEU:N	1:B:72:GLU:OE2	2.54	0.41
1:A:517:LEU:HD23	1:A:734:VAL:HG11	2.03	0.40
1:B:184:LYS:HA	1:B:256:GLY:O	2.22	0.40
1:B:531:LEU:HD23	1:B:533:LEU:HD13	2.01	0.40
1:A:348:GLU:HA	1:A:351:PHE:CE2	2.56	0.40
1:B:346:ARG:CD	1:B:349:GLU:OE1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:TYR:CD1	1:B:558:THR:HG23	2.56	0.40
1:B:687:MET:O	1:B:690:VAL:HG12	2.22	0.40
1:B:75:ARG:HE	1:B:75:ARG:HB2	1.60	0.40
1:B:620:GLY:C	1:B:621:LEU:HD23	2.46	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	735/759 (97%)	710 (97%)	22 (3%)	3 (0%)	30	36
1	B	736/759 (97%)	715 (97%)	20 (3%)	1 (0%)	48	59
All	All	1471/1518 (97%)	1425 (97%)	42 (3%)	4 (0%)	36	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	THR
1	B	691	GLU
1	A	151	THR
1	A	691	GLU

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	591/606 (98%)	591 (100%)	0	100	100
1	B	591/606 (98%)	590 (100%)	1 (0%)	87	93
All	All	1182/1212 (98%)	1181 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	460	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	123	ASN
1	A	128	GLN
1	A	759	GLN
1	B	123	ASN
1	B	128	GLN
1	B	131	HIS
1	B	186	ASN
1	B	350	HIS
1	B	704	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](#)

Of 45 ligands modelled in this entry, 38 are monoatomic - leaving 7 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	$\# Z > 2$
5	SO4	A	825	-	4,4,4	0.34	0	6,6,6	0.52	0
5	SO4	A	826	-	4,4,4	0.25	0	6,6,6	0.09	0
2	B9I	B	801	-	42,42,42	0.72	1 (2%)	64,65,65	0.96	3 (4%)
2	B9I	A	801	-	42,42,42	0.63	1 (2%)	64,65,65	1.12	4 (6%)
4	ACT	A	824	-	3,3,3	1.78	1 (33%)	3,3,3	1.54	0
5	SO4	A	827	-	4,4,4	0.22	0	6,6,6	0.49	0
5	SO4	B	818	-	4,4,4	0.30	0	6,6,6	0.16	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	B9I	B	801	-	-	4/8/59/59	0/6/6/6
2	B9I	A	801	-	-	4/8/59/59	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	B9I	O5-C15	-3.33	1.20	1.30
4	A	824	ACT	CH3-C	2.69	1.59	1.49
2	A	801	B9I	O5-C15	-2.57	1.22	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	B9I	C10-O7-C14	4.02	118.82	112.23
2	B	801	B9I	C10-O7-C14	2.77	116.78	112.23
2	A	801	B9I	O7-C14-C15	2.31	113.38	106.14
2	A	801	B9I	O2-C2-C27	-2.22	99.85	101.65
2	B	801	B9I	C9-O4-C10	2.09	120.76	117.82
2	A	801	B9I	O7-C10-C11	2.04	114.56	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	B9I	C2-O2-C1	-2.03	109.06	110.97

There are no chirality outliers.

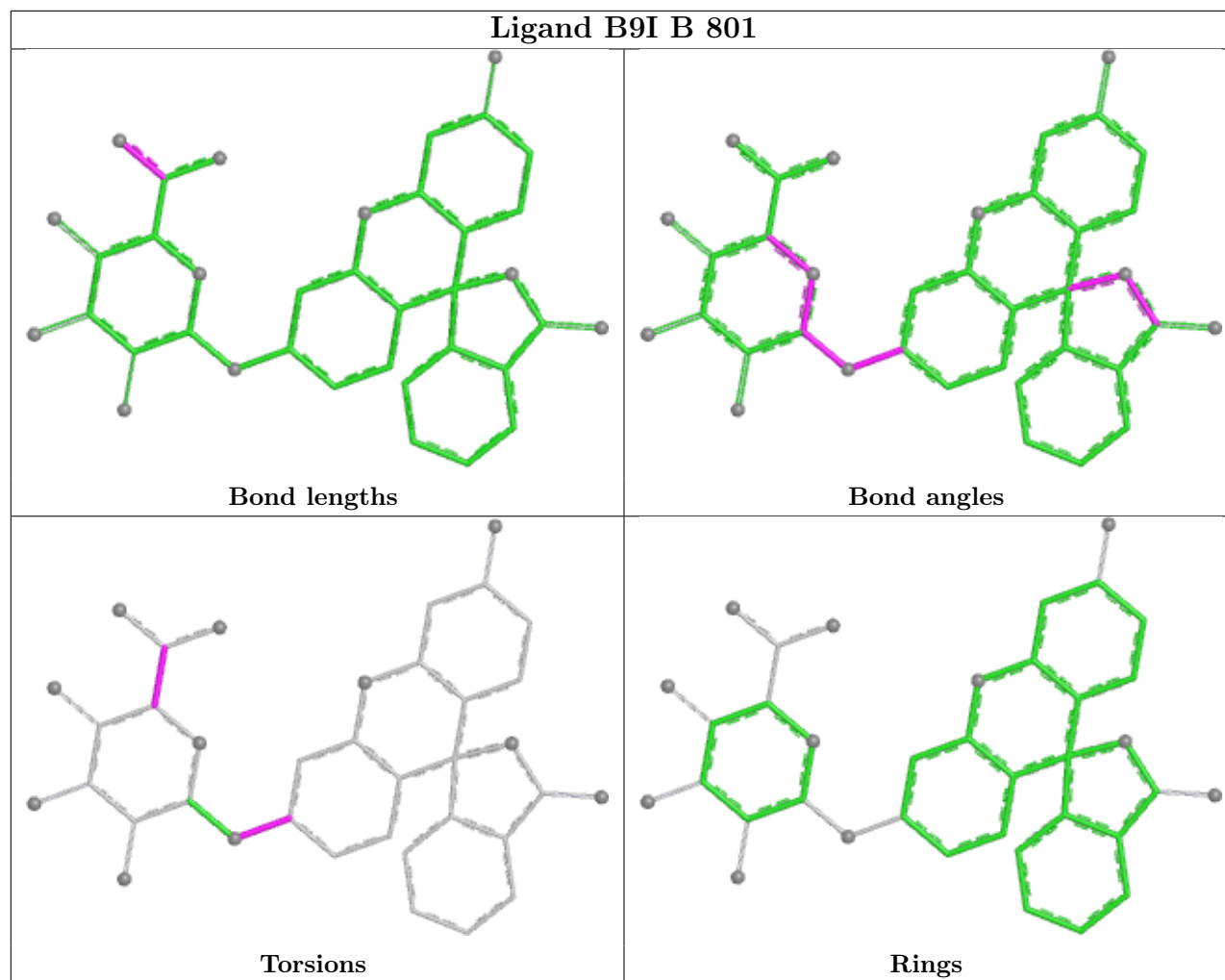
All (8) torsion outliers are listed below:

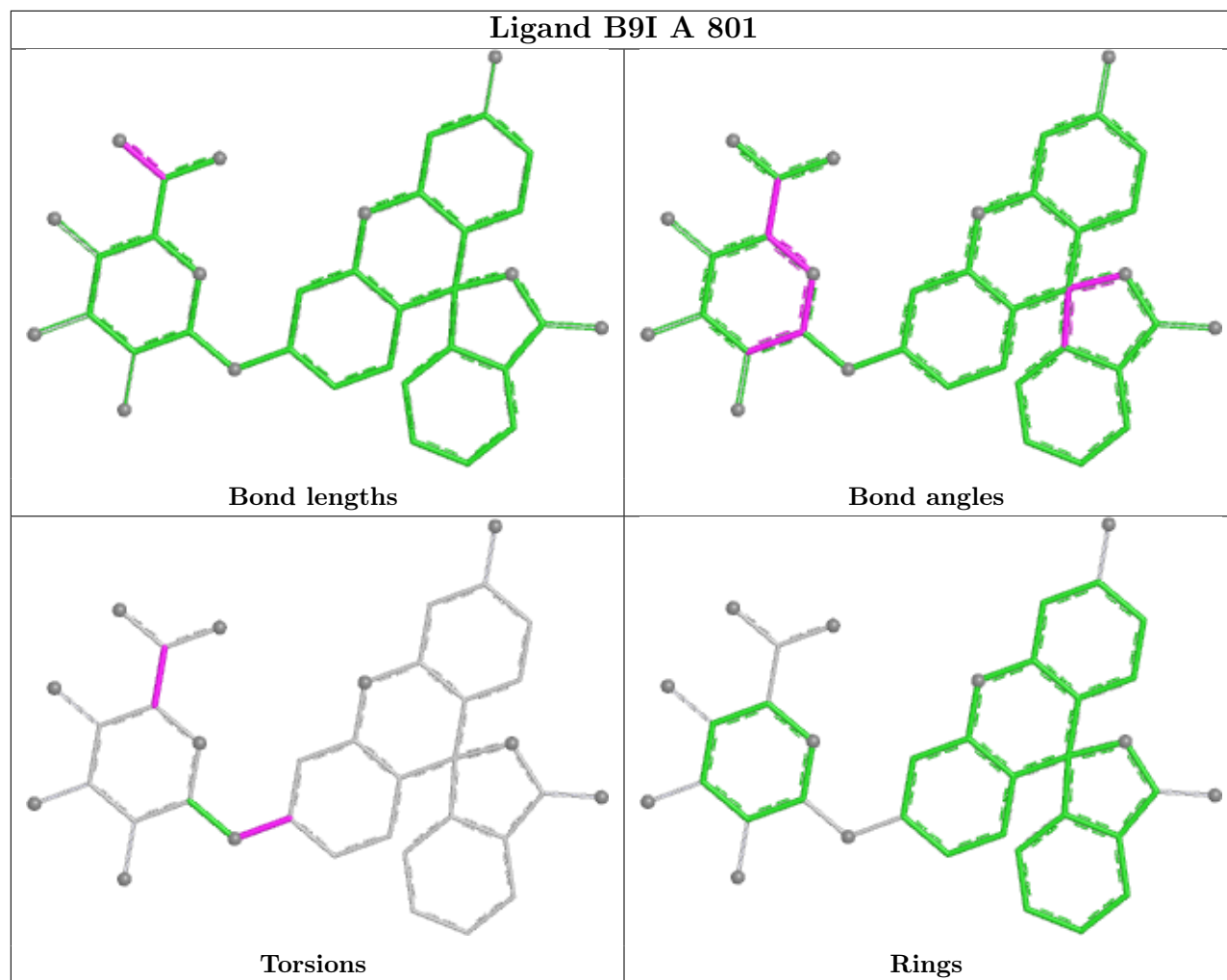
Mol	Chain	Res	Type	Atoms
2	A	801	B9I	C13-C14-C15-O6
2	A	801	B9I	C13-C14-C15-O5
2	B	801	B9I	C13-C14-C15-O6
2	B	801	B9I	C13-C14-C15-O5
2	A	801	B9I	C16-C9-O4-C10
2	A	801	B9I	C8-C9-O4-C10
2	B	801	B9I	C8-C9-O4-C10
2	B	801	B9I	C16-C9-O4-C10

There are no ring outliers.

No monomer is involved in short contacts.

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

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(Å ²)	Q<0.9
1	A	737/759 (97%)	0.03	16 (2%) 62 64	20, 46, 80, 111	2 (0%)
1	B	739/759 (97%)	0.30	22 (2%) 52 54	29, 53, 82, 121	1 (0%)
All	All	1476/1518 (97%)	0.17	38 (2%) 57 59	20, 50, 81, 121	3 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	GLY	6.5
1	B	202	ALA	3.7
1	B	298	GLU	3.6
1	A	565	GLY	3.4
1	A	110	GLN	3.4
1	B	203	ALA	3.2
1	A	66	GLY	3.2
1	B	528	GLY	3.2
1	A	151	THR	3.0
1	A	639	HIS	3.0
1	A	115	GLY	3.0
1	A	109	PRO	3.0
1	B	382	PRO	3.0
1	A	785	ASP	2.7
1	B	529	PRO	2.7
1	B	226	ARG	2.6
1	B	282	TYR	2.6
1	B	758	GLU	2.6
1	A	149	THR	2.6
1	B	299	GLU	2.5
1	A	193	PRO	2.5
1	B	229	GLU	2.5
1	A	108	ASP	2.5
1	B	230	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	623	GLY	2.4
1	B	461	ALA	2.4
1	B	525	THR	2.4
1	A	624[A]	GLN	2.3
1	A	111	THR	2.3
1	B	786	ASP	2.3
1	A	51	ILE	2.2
1	B	719	ALA	2.2
1	A	145	GLY	2.2
1	B	530	VAL	2.1
1	B	460	GLU	2.1
1	B	510	LEU	2.1
1	B	565	GLY	2.1
1	A	203	ALA	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(Å ²)	Q<0.9
3	ZN	A	809	1/1	0.65	0.14	139,139,139,139	0
3	ZN	A	807	1/1	0.77	0.09	133,133,133,133	0
3	ZN	A	803	1/1	0.79	0.09	143,143,143,143	0
5	SO4	A	825	5/5	0.79	0.11	54,71,77,93	0
5	SO4	A	827	5/5	0.80	0.09	74,84,101,112	0
3	ZN	B	816	1/1	0.82	0.09	127,127,127,127	0
3	ZN	A	806	1/1	0.82	0.12	119,119,119,119	0
3	ZN	A	816	1/1	0.82	0.12	112,112,112,112	0
5	SO4	A	826	5/5	0.83	0.10	96,100,106,120	0

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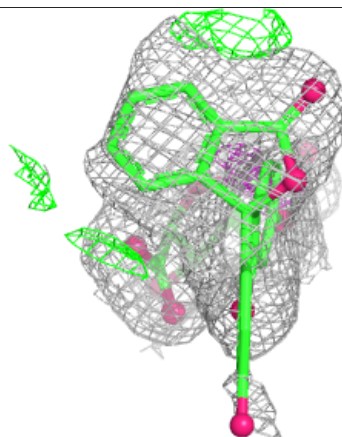
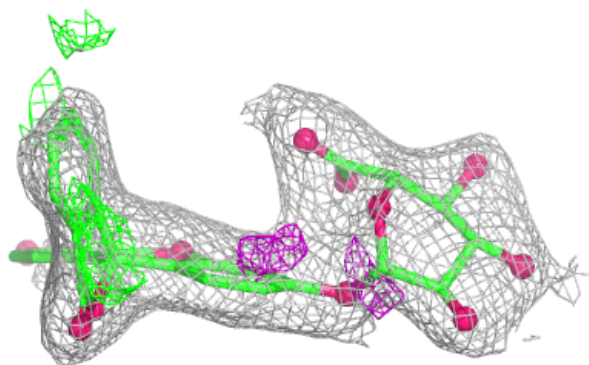
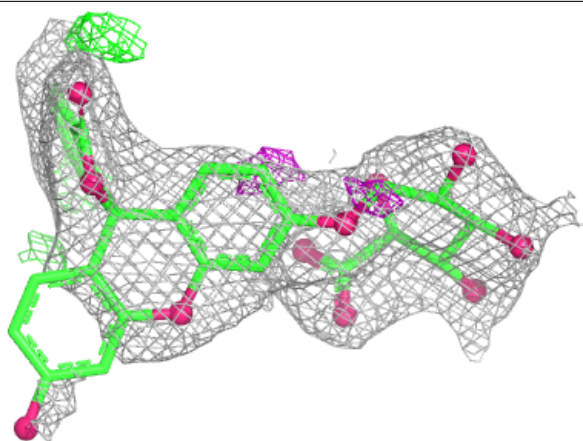
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	B	813	1/1	0.86	0.20	139,139,139,139	0
2	B9I	B	801	37/37	0.86	0.14	47,66,104,113	0
4	ACT	A	824	4/4	0.86	0.23	45,59,67,70	0
2	B9I	A	801	37/37	0.87	0.14	39,63,89,102	0
3	ZN	A	804	1/1	0.87	0.15	121,121,121,121	0
5	SO4	B	818	5/5	0.87	0.10	84,86,105,107	0
3	ZN	B	805	1/1	0.89	0.10	108,108,108,108	0
3	ZN	B	804	1/1	0.89	0.12	110,110,110,110	0
3	ZN	B	806	1/1	0.90	0.07	135,135,135,135	0
3	ZN	A	821	1/1	0.90	0.10	111,111,111,111	0
3	ZN	A	810	1/1	0.91	0.12	101,101,101,101	0
3	ZN	A	817	1/1	0.91	0.08	124,124,124,124	0
3	ZN	B	817	1/1	0.91	0.21	93,93,93,93	0
3	ZN	A	815	1/1	0.91	0.13	119,119,119,119	0
3	ZN	B	811	1/1	0.92	0.16	104,104,104,104	0
3	ZN	B	802	1/1	0.92	0.12	124,124,124,124	0
3	ZN	A	811	1/1	0.92	0.07	107,107,107,107	0
3	ZN	A	823	1/1	0.93	0.08	106,106,106,106	0
3	ZN	A	819	1/1	0.93	0.07	106,106,106,106	0
3	ZN	B	812	1/1	0.94	0.26	78,78,78,78	0
3	ZN	B	810	1/1	0.94	0.06	93,93,93,93	0
3	ZN	A	822	1/1	0.94	0.09	88,88,88,88	0
3	ZN	B	803	1/1	0.95	0.06	92,92,92,92	0
3	ZN	A	820	1/1	0.96	0.07	100,100,100,100	0
3	ZN	B	809	1/1	0.97	0.07	73,73,73,73	0
3	ZN	A	805	1/1	0.97	0.11	76,76,76,76	0
3	ZN	B	815	1/1	0.98	0.04	79,79,79,79	0
3	ZN	B	807	1/1	0.98	0.11	57,57,57,57	0
3	ZN	A	812	1/1	0.99	0.09	57,57,57,57	0
3	ZN	B	808	1/1	0.99	0.12	62,62,62,62	0
3	ZN	A	818	1/1	0.99	0.03	50,50,50,50	0
3	ZN	A	813	1/1	0.99	0.07	78,78,78,78	0
3	ZN	A	814	1/1	0.99	0.07	70,70,70,70	0
3	ZN	A	808	1/1	0.99	0.03	55,55,55,55	0
3	ZN	A	802	1/1	0.99	0.02	58,58,58,58	0
3	ZN	B	814	1/1	0.99	0.06	77,77,77,77	0

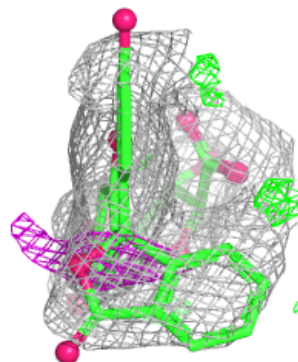
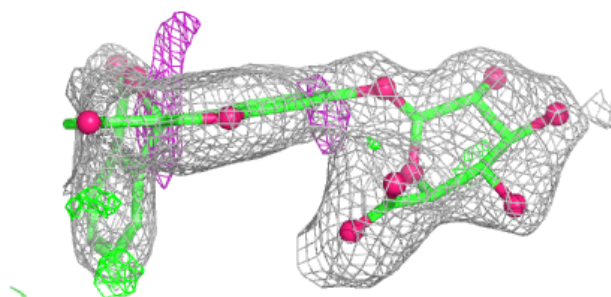
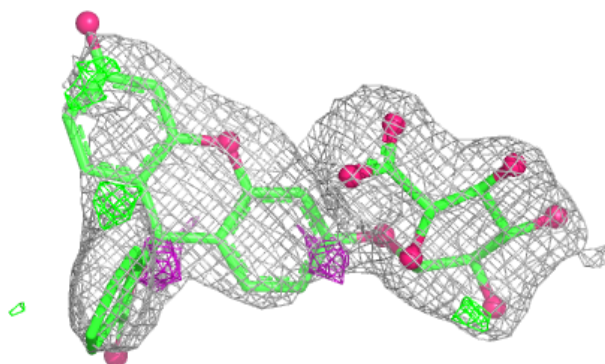
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B9I B 801:

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

**Electron density around B9I A 801:**

$2mF_o-DF_c$ (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.