



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 02:31 AM UTC

PDB ID : 6QUT / pdb_00006qut
Title : Three dimensional structure of human carbonic anhydrase IX in complex with benzenesulfonamide
Authors : Leitans, J.; Tars, K.
Deposited on : 2019-02-28
Resolution : 1.96 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

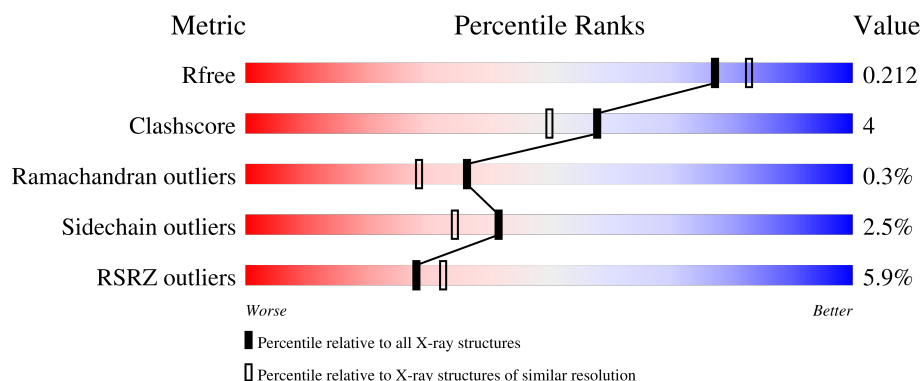
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	251	7% 88% 10% .
1	B	251	8% 86% 11% .
1	C	251	2% 86% 13% .
1	D	251	6% 92% 8% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8639 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 Carbonic anhydrase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1939	1236	343	356	4			
1	B	251	Total	C	N	O	S	0	0	0
			1939	1236	343	356	4			
1	C	251	Total	C	N	O	S	0	0	0
			1942	1237	343	358	4			
1	D	251	Total	C	N	O	S	0	0	0
			1930	1231	337	358	4			

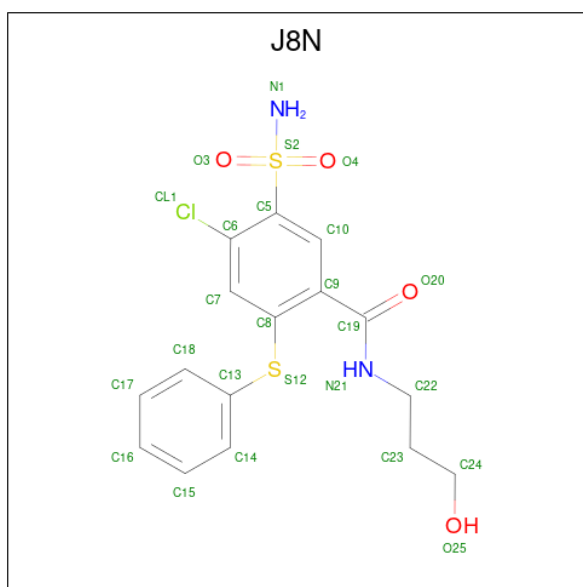
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	CYS	engineered mutation	UNP Q16790
B	41	SER	CYS	engineered mutation	UNP Q16790
C	41	SER	CYS	engineered mutation	UNP Q16790
D	41	SER	CYS	engineered mutation	UNP Q16790

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-chloranyl- {N}-(3-oxidanylpropyl)-2-phenylsulfanyl-5-sulfamoyl-benzamide (CCD ID: J8N) (formula: C₁₆H₁₇ClN₂O₄S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 25	C 16	Cl 1	N 2	O 4	S 2	0	0
3	B	1	Total 25	C 16	Cl 1	N 2	O 4	S 2	0	0
3	C	1	Total 25	C 16	Cl 1	N 2	O 4	S 2	0	0
3	C	1	Total 25	C 16	Cl 1	N 2	O 4	S 2	0	0
3	D	1	Total 25	C 16	Cl 1	N 2	O 4	S 2	0	0
3	D	1	Total 25	C 16	Cl 1	N 2	O 4	S 2	0	0

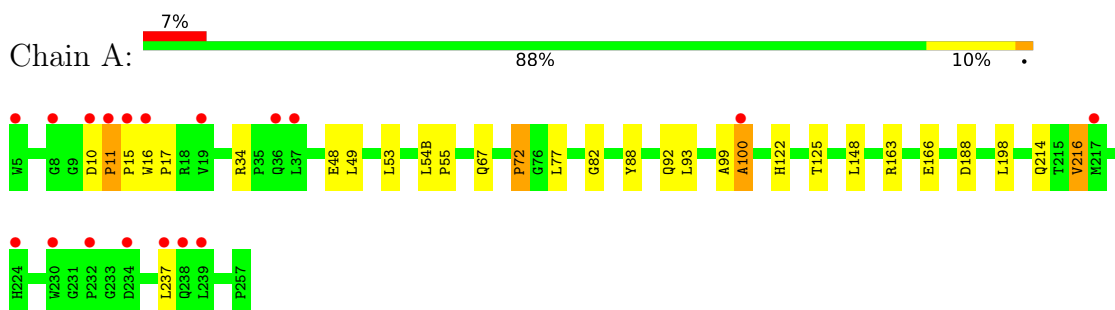
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total	O	0	0
			156	156		
4	B	171	Total	O	0	0
			171	171		
4	C	235	Total	O	0	0
			235	235		
4	D	173	Total	O	0	0
			173	173		

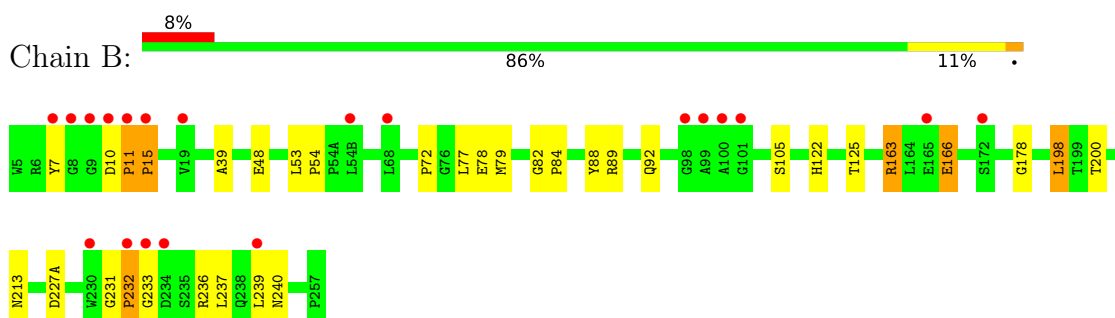
3 Residue-property plots [i](#)

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.

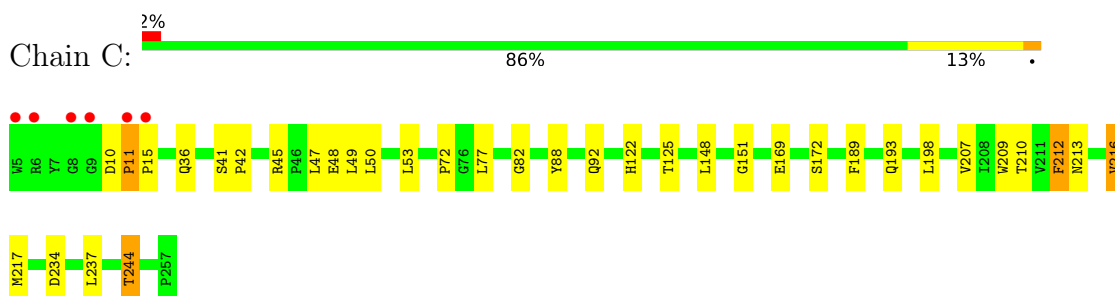
- Molecule 1: Carbonic anhydrase 9



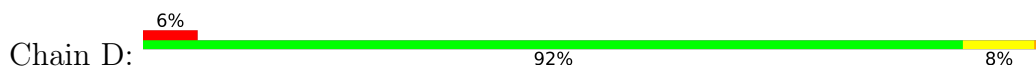
- Molecule 1: Carbonic anhydrase 9

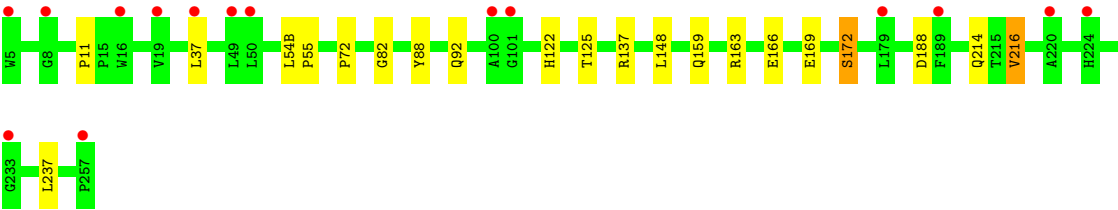


- Molecule 1: Carbonic anhydrase 9



- Molecule 1: Carbonic anhydrase 9





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	151.73Å 151.73Å 174.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.86 – 1.96 75.86 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.2 (75.86-1.96) 99.2 (75.86-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.173 , 0.205 0.181 , 0.212	Depositor DCC
R_{free} test set	5616 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8639	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: J8N, ZN

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	1.28	4/1997 (0.2%)	1.29	3/2728 (0.1%)
1	B	1.30	6/1997 (0.3%)	1.42	6/2728 (0.2%)
1	C	1.32	4/2000 (0.2%)	1.24	4/2732 (0.1%)
1	D	1.17	4/1988 (0.2%)	1.25	3/2718 (0.1%)
All	All	1.27	18/7982 (0.2%)	1.30	16/10906 (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	A	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	11	PRO	C-N	27.34	1.69	1.33
1	A	125	THR	C-N	21.34	1.63	1.33
1	A	11	PRO	C-N	19.20	1.78	1.33
1	B	72	PRO	C-N	18.59	1.59	1.33
1	B	125	THR	C-N	18.10	1.61	1.33
1	A	72	PRO	C-N	17.88	1.63	1.33
1	C	125	THR	C-N	17.82	1.58	1.33
1	B	82	GLY	C-N	17.20	1.53	1.33
1	D	11	PRO	C-N	13.84	1.66	1.33
1	B	11	PRO	C-N	13.64	1.65	1.33
1	D	82	GLY	C-N	11.37	1.47	1.33
1	C	72	PRO	C-N	11.24	1.49	1.33
1	D	125	THR	C-N	11.10	1.50	1.33
1	D	72	PRO	C-N	11.03	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	GLY	C-N	7.42	1.51	1.33
1	A	82	GLY	C-N	5.83	1.47	1.33
1	B	105	SER	C-O	5.29	1.30	1.23
1	B	198	LEU	C-O	5.14	1.29	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	PRO	CA-C-N	19.68	144.44	119.84
1	B	11	PRO	C-N-CA	19.68	144.44	119.84
1	B	11	PRO	C-N-CD	-7.84	92.86	125.00
1	A	34	ARG	CB-CA-C	7.62	118.10	110.33
1	A	11	PRO	CA-C-N	7.53	129.25	119.84
1	A	11	PRO	C-N-CA	7.53	129.25	119.84
1	C	213	ASN	CA-CB-CG	7.05	119.66	112.60
1	C	244	THR	CB-CA-C	6.66	120.43	109.70
1	B	84	PRO	CA-N-CD	6.27	120.78	112.00
1	D	82	GLY	O-C-N	5.95	127.72	121.77
1	D	137	ARG	CG-CD-NE	-5.73	99.39	112.00
1	C	212	PHE	CA-C-N	5.58	127.70	120.44
1	C	212	PHE	C-N-CA	5.58	127.70	120.44
1	B	72	PRO	O-C-N	5.41	129.46	122.91
1	D	125	THR	O-C-N	-5.39	115.26	122.43
1	B	213	ASN	CA-CB-CG	5.10	117.70	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	PRO	Mainchain

5.2 Too-close contacts [i](#)

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	1939	0	1886	17	0
1	B	1939	0	1886	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1942	0	1888	21	0
1	D	1930	0	1866	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	25	0	0	2	0
3	B	25	0	0	4	0
3	C	50	0	0	2	0
3	D	50	0	0	1	0
4	A	156	0	0	0	0
4	B	171	0	0	0	0
4	C	235	0	0	2	0
4	D	173	0	0	2	0
All	All	8639	0	7526	69	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 4.

All (69) 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:C:11:PRO:C	1:C:15:PRO:N	1.69	1.49
1:A:11:PRO:C	1:A:15:PRO:N	1.78	1.38
1:C:198:LEU:HD22	3:C:302:J8N:CL1	2.29	0.69
1:C:189:PHE:HD1	1:C:212:PHE:HE2	1.41	0.68
1:B:53:LEU:HD21	1:B:77:LEU:HD11	1.76	0.67
1:D:188:ASP:H	1:D:214:GLN:NE2	1.93	0.66
3:B:302:J8N:O20	3:B:302:J8N:C24	2.43	0.66
1:A:11:PRO:C	1:A:15:PRO:CD	2.71	0.62
1:D:188:ASP:H	1:D:214:GLN:HE22	1.48	0.59
1:B:78:GLU:HG2	1:B:89:ARG:NE	2.17	0.58
1:A:198:LEU:HD22	3:A:302:J8N:CL1	2.42	0.57
1:A:163:ARG:HD2	1:A:166:GLU:OE1	2.04	0.57
1:A:53:LEU:HD21	1:A:77:LEU:HD11	1.87	0.56
1:C:11:PRO:C	1:C:15:PRO:CA	2.72	0.56
1:C:189:PHE:HD1	1:C:212:PHE:CE2	2.23	0.56
1:D:88:TYR:HB3	1:D:122:HIS:HB3	1.89	0.55
1:B:227(A):ASP:O	1:B:236:ARG:NH1	2.39	0.54
1:B:198:LEU:HD22	3:B:302:J8N:CL1	2.44	0.54
1:C:217:MET:HE1	4:C:454:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:GLU:O	1:C:172:SER:HB2	2.07	0.53
1:A:10:ASP:HA	1:A:11:PRO:C	2.33	0.53
3:B:302:J8N:C24	3:B:302:J8N:C19	2.86	0.52
1:C:151:GLY:HA3	1:C:217:MET:HE3	1.91	0.52
1:D:148:LEU:HD22	1:D:216:VAL:HG22	1.91	0.51
1:C:88:TYR:HB3	1:C:122:HIS:HB3	1.91	0.51
1:D:169:GLU:O	1:D:172:SER:HB2	2.11	0.51
1:C:53:LEU:HD21	1:C:77:LEU:HD11	1.93	0.51
1:D:148:LEU:HD22	1:D:216:VAL:CG2	2.41	0.51
1:B:231:GLY:O	1:B:232:PRO:C	2.53	0.50
1:A:54(B):LEU:HA	1:A:55:PRO:C	2.39	0.48
1:C:148:LEU:HD22	1:C:216:VAL:HG22	1.96	0.48
1:B:163:ARG:NH1	1:B:166:GLU:OE1	2.45	0.47
1:C:45:ARG:HG2	4:C:403:HOH:O	2.14	0.47
1:D:163:ARG:HD2	1:D:166:GLU:OE1	2.14	0.47
1:B:7:TYR:CE2	1:B:240:ASN:HB2	2.50	0.47
1:C:47:LEU:HD11	1:C:210:THR:HG21	1.97	0.47
3:D:303:J8N:O20	3:D:303:J8N:S12	2.72	0.47
1:C:151:GLY:CA	1:C:217:MET:HE3	2.44	0.47
1:A:88:TYR:HB3	1:A:122:HIS:HB3	1.98	0.46
1:A:188:ASP:H	1:A:214:GLN:NE2	2.15	0.45
1:D:148:LEU:CD2	1:D:216:VAL:HG22	2.47	0.45
1:B:54:PRO:O	1:B:178:GLY:HA3	2.17	0.45
3:C:303:J8N:O20	3:C:303:J8N:S12	2.75	0.45
1:A:11:PRO:HA	1:A:15:PRO:CD	2.47	0.45
1:B:10:ASP:HA	1:B:11:PRO:C	2.42	0.44
1:B:11:PRO:CB	1:B:15:PRO:HD2	2.36	0.43
1:B:88:TYR:HB3	1:B:122:HIS:HB3	2.01	0.43
1:D:159:GLN:NE2	4:D:402:HOH:O	2.36	0.43
1:A:99:ALA:O	1:A:100:ALA:C	2.61	0.43
1:C:198:LEU:HD23	1:C:207:VAL:HG21	2.00	0.43
1:D:188:ASP:N	1:D:214:GLN:HE22	2.15	0.42
1:B:78:GLU:HG2	1:B:89:ARG:HE	1.82	0.42
1:A:11:PRO:CA	1:A:15:PRO:CD	2.98	0.42
1:A:67:GLN:NE2	3:A:302:J8N:O25	2.52	0.42
1:A:148:LEU:HD22	1:A:216:VAL:HG22	2.02	0.42
1:B:231:GLY:O	1:B:233:GLY:N	2.52	0.42
1:C:36:GLN:HE21	1:C:36:GLN:HB3	1.74	0.41
1:A:16:TRP:N	1:A:17:PRO:CD	2.84	0.41
1:A:48:GLU:C	1:A:49:LEU:HD12	2.46	0.41
1:B:39:ALA:HB1	1:C:42:PRO:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:O	1:B:79:MET:HA	2.19	0.41
1:C:189:PHE:CD1	1:C:212:PHE:HE2	2.30	0.41
1:D:54(B):LEU:HA	1:D:55:PRO:C	2.46	0.41
1:C:10:ASP:HA	1:C:11:PRO:C	2.45	0.40
1:B:200:THR:HG21	3:B:302:J8N:C22	2.52	0.40
1:C:48:GLU:C	1:C:49:LEU:HD12	2.46	0.40
1:C:193:GLN:HA	1:C:209:TRP:O	2.21	0.40
1:D:163:ARG:NH2	4:D:408:HOH:O	2.46	0.40
1:A:93:LEU:C	1:A:93:LEU:HD12	2.45	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	249/251 (99%)	242 (97%)	6 (2%)	1 (0%)	30	21
1	B	249/251 (99%)	240 (96%)	7 (3%)	2 (1%)	16	8
1	C	249/251 (99%)	246 (99%)	3 (1%)	0	100	100
1	D	249/251 (99%)	242 (97%)	7 (3%)	0	100	100
All	All	996/1004 (99%)	970 (97%)	23 (2%)	3 (0%)	36	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	232	PRO
1	B	15	PRO
1	A	100	ALA

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	203/205 (99%)	200 (98%)	3 (2%)	57	54
1	B	203/205 (99%)	198 (98%)	5 (2%)	42	34
1	C	204/205 (100%)	197 (97%)	7 (3%)	32	23
1	D	202/205 (98%)	197 (98%)	5 (2%)	42	34
All	All	812/820 (99%)	792 (98%)	20 (2%)	42	34

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	216	VAL
1	A	237	LEU
1	B	92	GLN
1	B	163	ARG
1	B	166	GLU
1	B	237	LEU
1	B	239	LEU
1	C	41	SER
1	C	50	LEU
1	C	92	GLN
1	C	216	VAL
1	C	234	ASP
1	C	237	LEU
1	C	244	THR
1	D	37	LEU
1	D	92	GLN
1	D	172	SER
1	D	216	VAL
1	D	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	67	GLN
1	A	175	GLN
1	A	193	GLN
1	A	214	GLN
1	A	224	HIS
1	B	36	GLN
1	B	52	GLN
1	B	67	GLN
1	B	193	GLN
1	B	224	HIS
1	C	36	GLN
1	C	67	GLN
1	C	205	GLN
1	C	245	GLN
1	D	67	GLN
1	D	213	ASN
1	D	214	GLN
1	D	224	HIS

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
3	J8N	B	302	2	26,26,26	3.22	5 (19%)	36,36,36	2.27	15 (41%)
3	J8N	D	302	2	26,26,26	2.97	7 (26%)	36,36,36	2.26	11 (30%)
3	J8N	C	303	-	26,26,26	2.28	8 (30%)	36,36,36	3.77	20 (55%)
3	J8N	A	302	2	26,26,26	3.22	6 (23%)	36,36,36	2.82	12 (33%)
3	J8N	D	303	-	26,26,26	2.78	7 (26%)	36,36,36	3.99	17 (47%)
3	J8N	C	302	2	26,26,26	3.13	9 (34%)	36,36,36	2.20	11 (30%)

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
3	J8N	B	302	2	-	3/19/19/19	0/2/2/2
3	J8N	D	302	2	-	3/19/19/19	0/2/2/2
3	J8N	C	303	-	-	3/19/19/19	0/2/2/2
3	J8N	A	302	2	-	1/19/19/19	0/2/2/2
3	J8N	D	303	-	-	4/19/19/19	0/2/2/2
3	J8N	C	302	2	-	1/19/19/19	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	J8N	C5-S2	-11.73	1.63	1.77
3	A	302	J8N	C5-S2	-11.54	1.63	1.77
3	D	303	J8N	C5-S2	-11.25	1.63	1.77
3	C	302	J8N	C5-S2	-10.88	1.64	1.77
3	D	302	J8N	C5-S2	-10.76	1.64	1.77
3	B	302	J8N	C6-C5	7.39	1.49	1.40
3	A	302	J8N	C6-C5	6.35	1.48	1.40
3	C	303	J8N	C5-S2	-6.31	1.69	1.77
3	B	302	J8N	C13-S12	-6.31	1.66	1.77
3	A	302	J8N	C8-S12	-6.29	1.68	1.78
3	D	302	J8N	C6-C5	6.09	1.48	1.40
3	C	302	J8N	C9-C8	5.76	1.50	1.40
3	D	302	J8N	C9-C8	5.31	1.49	1.40
3	C	302	J8N	C6-C5	5.22	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	J8N	C9-C8	4.99	1.48	1.40
3	A	302	J8N	C13-S12	-4.83	1.68	1.77
3	C	303	J8N	C13-S12	-4.43	1.69	1.77
3	C	302	J8N	C8-S12	-4.38	1.71	1.78
3	C	302	J8N	C13-S12	-4.38	1.69	1.77
3	A	302	J8N	C9-C8	4.16	1.47	1.40
3	D	303	J8N	C9-C8	4.03	1.47	1.40
3	B	302	J8N	C9-C8	4.01	1.47	1.40
3	C	303	J8N	C22-N21	-3.40	1.38	1.46
3	D	302	J8N	C8-S12	-3.36	1.73	1.78
3	D	302	J8N	C13-S12	-3.18	1.71	1.77
3	D	303	J8N	C22-N21	-3.02	1.39	1.46
3	A	302	J8N	O3-S2	2.88	1.48	1.43
3	D	303	J8N	O3-S2	2.77	1.48	1.43
3	D	302	J8N	C17-C18	2.73	1.43	1.38
3	C	303	J8N	C15-C14	2.58	1.43	1.38
3	C	302	J8N	C10-C5	-2.52	1.35	1.39
3	D	303	J8N	C6-CL1	2.47	1.79	1.73
3	B	302	J8N	C6-CL1	2.41	1.79	1.73
3	C	302	J8N	C15-C14	2.36	1.42	1.38
3	C	303	J8N	O20-C19	2.30	1.28	1.23
3	D	302	J8N	O3-S2	2.23	1.47	1.43
3	C	303	J8N	C14-C13	-2.12	1.35	1.39
3	C	303	J8N	C8-S12	-2.07	1.75	1.78
3	D	303	J8N	C19-N21	2.07	1.38	1.33
3	D	303	J8N	C6-C5	2.06	1.43	1.40
3	C	302	J8N	C17-C18	2.05	1.42	1.38
3	C	302	J8N	O4-S2	2.04	1.47	1.43

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	303	J8N	C9-C19-N21	13.36	143.30	117.32
3	C	303	J8N	C9-C19-N21	12.86	142.32	117.32
3	A	302	J8N	O4-S2-O3	-9.43	104.30	118.80
3	D	303	J8N	O4-S2-O3	-7.41	107.40	118.80
3	D	303	J8N	O20-C19-N21	-7.25	108.46	122.59
3	A	302	J8N	O4-S2-C5	7.17	117.67	107.26
3	D	303	J8N	C5-C6-CL1	7.13	126.67	121.52
3	D	303	J8N	O20-C19-C9	-7.00	108.20	121.03
3	C	303	J8N	O20-C19-N21	-6.95	109.06	122.59
3	C	303	J8N	O20-C19-C9	-6.89	108.40	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	J8N	C5-C6-CL1	-6.58	116.76	121.52
3	D	303	J8N	C13-S12-C8	6.42	111.41	102.97
3	C	303	J8N	C22-N21-C19	6.40	136.58	122.11
3	C	302	J8N	O4-S2-O3	-6.35	109.03	118.80
3	D	302	J8N	O4-S2-O3	-5.45	110.42	118.80
3	C	303	J8N	C7-C6-C5	5.40	126.58	121.36
3	C	303	J8N	C10-C5-S2	5.31	124.61	118.26
3	D	303	J8N	C22-N21-C19	5.13	133.71	122.11
3	B	302	J8N	O20-C19-C9	-4.99	111.89	121.03
3	D	302	J8N	O3-S2-N1	4.93	114.46	107.35
3	A	302	J8N	C5-S2-N1	4.79	116.88	108.28
3	D	303	J8N	C7-C6-CL1	-4.71	110.73	118.45
3	D	302	J8N	C10-C5-S2	4.53	123.68	118.26
3	C	302	J8N	O3-S2-N1	4.37	113.66	107.35
3	B	302	J8N	C9-C19-N21	4.30	125.69	117.32
3	B	302	J8N	C22-C23-C24	-4.14	106.66	112.95
3	D	302	J8N	C10-C5-C6	-4.12	114.02	118.33
3	D	302	J8N	O3-S2-C5	4.09	113.20	107.26
3	D	303	J8N	C10-C5-S2	4.06	123.11	118.26
3	D	303	J8N	C6-C5-S2	-4.04	118.63	123.47
3	C	303	J8N	C6-C7-C8	-3.76	116.37	120.27
3	C	303	J8N	C10-C9-C19	3.75	127.85	117.21
3	D	303	J8N	C10-C9-C19	3.74	127.82	117.21
3	C	302	J8N	C7-C6-C5	3.72	124.96	121.36
3	C	302	J8N	C13-S12-C8	3.61	107.71	102.97
3	D	302	J8N	C7-C6-C5	3.53	124.78	121.36
3	C	303	J8N	C13-S12-C8	3.51	107.59	102.97
3	D	303	J8N	O3-S2-C5	3.49	112.33	107.26
3	C	302	J8N	C10-C5-S2	3.46	122.40	118.26
3	C	303	J8N	C7-C6-CL1	-3.46	112.78	118.45
3	B	302	J8N	O4-S2-O3	-3.46	113.48	118.80
3	C	303	J8N	O4-S2-C5	-3.44	102.25	107.26
3	A	302	J8N	C7-C6-C5	3.38	124.64	121.36
3	D	302	J8N	C5-C6-CL1	-3.38	119.07	121.52
3	B	302	J8N	C8-C9-C19	-3.28	112.76	122.09
3	B	302	J8N	C18-C13-C14	3.21	124.06	118.85
3	B	302	J8N	O3-S2-C5	-3.19	102.62	107.26
3	C	303	J8N	C10-C5-C6	-3.15	115.04	118.33
3	A	302	J8N	C10-C5-S2	3.10	121.97	118.26
3	B	302	J8N	C5-C6-CL1	-3.09	119.28	121.52
3	A	302	J8N	O4-S2-N1	-3.07	102.92	107.35
3	A	302	J8N	O20-C19-C9	-3.07	115.40	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	J8N	O3-S2-C5	3.06	111.70	107.26
3	C	302	J8N	O4-S2-C5	3.06	111.70	107.26
3	B	302	J8N	C10-C9-C8	3.02	123.09	118.68
3	C	303	J8N	C5-S2-N1	3.02	113.70	108.28
3	A	302	J8N	C10-C5-C6	-2.99	115.20	118.33
3	C	302	J8N	C22-C23-C24	2.97	117.46	112.95
3	C	302	J8N	O3-S2-C5	-2.92	103.02	107.26
3	D	302	J8N	O20-C19-C9	-2.90	115.72	121.03
3	C	303	J8N	O4-S2-O3	-2.84	114.42	118.80
3	D	303	J8N	C7-C8-S12	-2.72	112.21	118.49
3	C	302	J8N	C5-C6-CL1	-2.65	119.60	121.52
3	C	303	J8N	C6-C5-S2	-2.61	120.34	123.47
3	B	302	J8N	C5-S2-N1	2.60	112.95	108.28
3	C	303	J8N	C23-C22-N21	2.59	119.47	112.20
3	C	302	J8N	C10-C5-C6	-2.58	115.63	118.33
3	C	303	J8N	C22-C23-C24	-2.53	109.10	112.95
3	D	302	J8N	C16-C15-C14	2.53	123.36	120.24
3	B	302	J8N	C23-C22-N21	2.53	119.28	112.20
3	B	302	J8N	O3-S2-N1	2.49	110.94	107.35
3	D	302	J8N	C13-S12-C8	2.47	106.21	102.97
3	B	302	J8N	C10-C9-C19	2.44	124.14	117.21
3	B	302	J8N	C7-C8-S12	2.41	124.06	118.49
3	C	303	J8N	C18-C13-C14	2.37	122.71	118.85
3	D	303	J8N	C8-C9-C19	-2.34	115.44	122.09
3	A	302	J8N	C10-C9-C8	2.29	122.03	118.68
3	D	303	J8N	C9-C8-S12	2.23	126.76	121.05
3	D	302	J8N	C9-C19-N21	2.22	121.63	117.32
3	A	302	J8N	C7-C8-S12	2.20	123.56	118.49
3	D	303	J8N	C5-S2-N1	2.13	112.11	108.28
3	C	302	J8N	C9-C8-S12	2.08	126.37	121.05
3	C	303	J8N	C10-C9-C8	-2.08	115.65	118.68
3	B	302	J8N	C22-N21-C19	-2.03	117.50	122.11
3	A	302	J8N	C9-C19-N21	2.02	121.25	117.32
3	D	303	J8N	O4-S2-C5	2.02	110.20	107.26

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	J8N	C9-C19-N21-C22
3	B	302	J8N	O20-C19-N21-C22
3	B	302	J8N	N21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	D	303	J8N	N21-C22-C23-C24
3	D	303	J8N	O20-C19-N21-C22
3	D	303	J8N	C9-C19-N21-C22
3	C	303	J8N	C9-C19-N21-C22
3	C	303	J8N	O20-C19-N21-C22
3	D	302	J8N	C9-C8-S12-C13
3	C	302	J8N	C9-C8-S12-C13
3	C	303	J8N	N21-C22-C23-C24
3	D	303	J8N	C22-C23-C24-O25
3	D	302	J8N	C10-C5-S2-N1
3	D	302	J8N	C6-C5-S2-N1
3	A	302	J8N	C7-C8-S12-C13

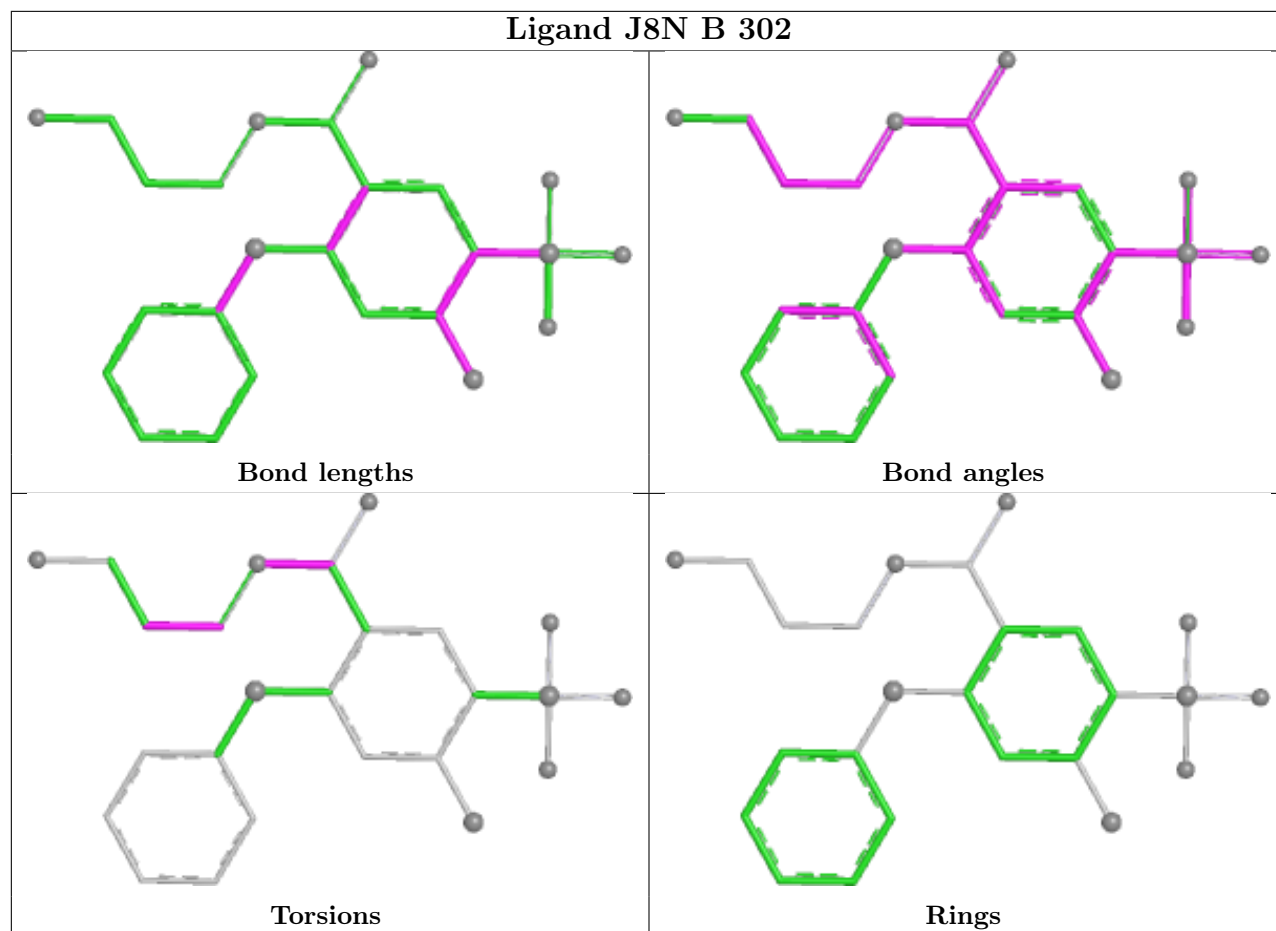
There are no ring outliers.

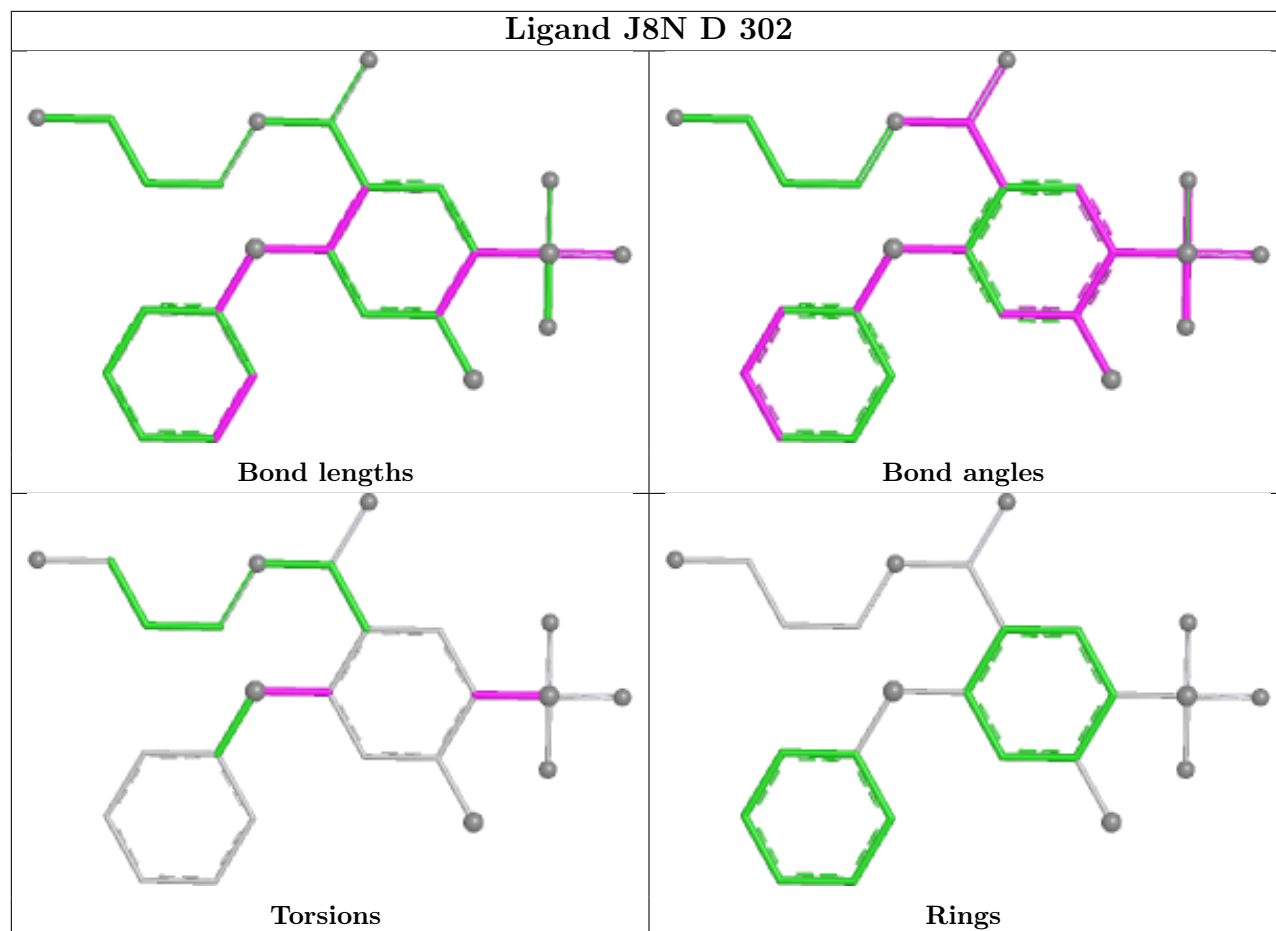
5 monomers are involved in 9 short contacts:

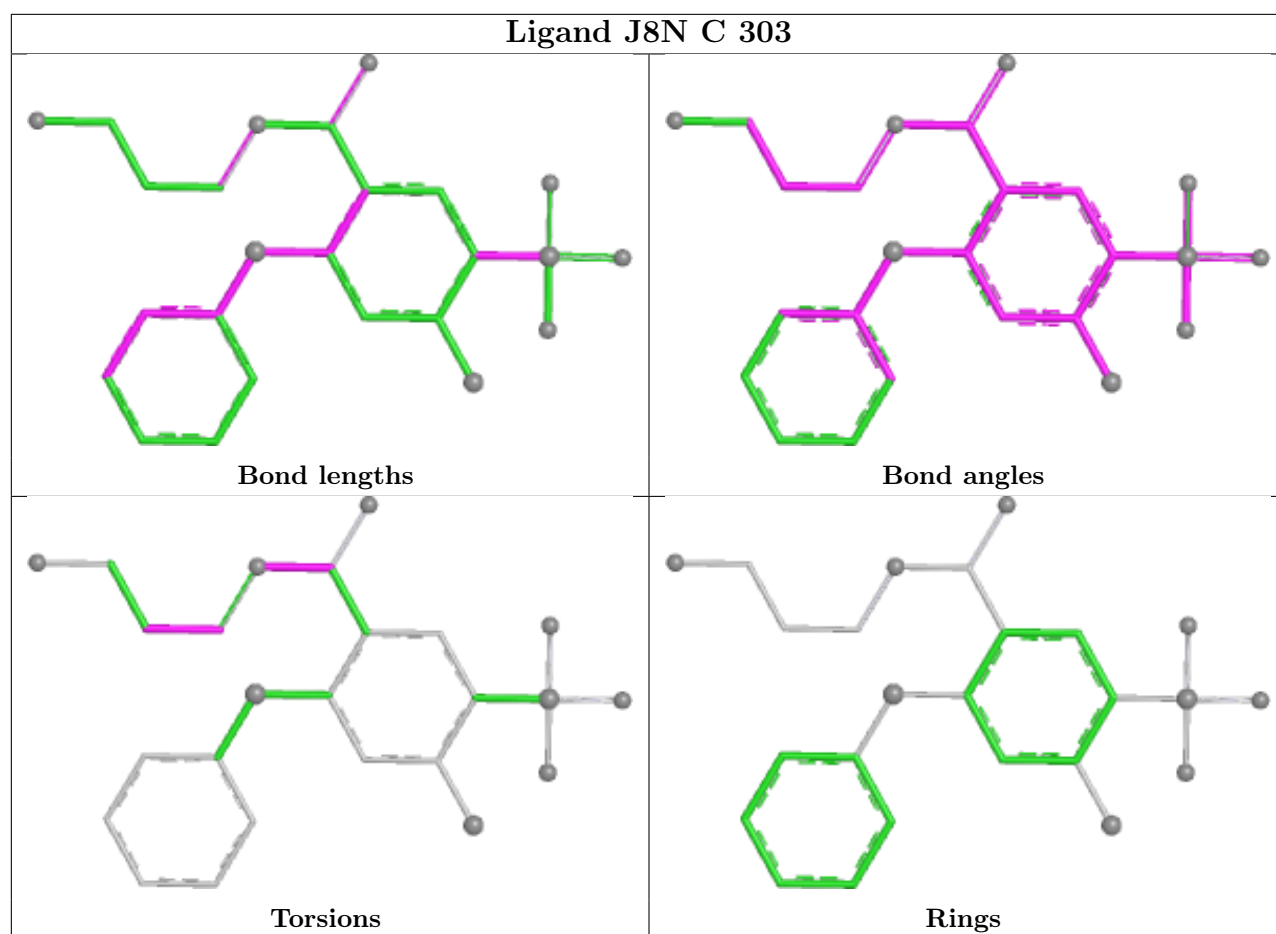
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	J8N	4	0
3	C	303	J8N	1	0
3	A	302	J8N	2	0
3	D	303	J8N	1	0
3	C	302	J8N	1	0

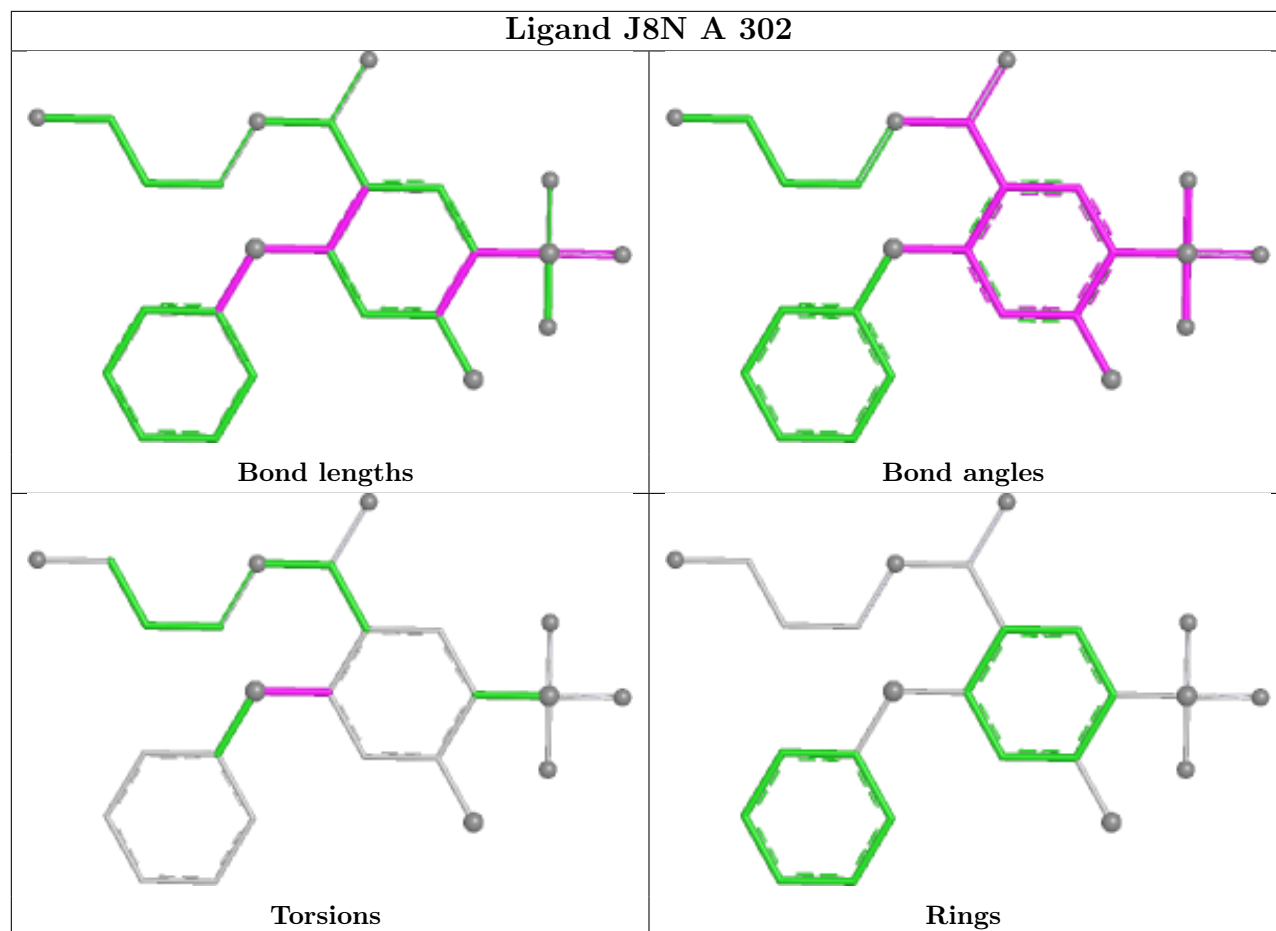
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

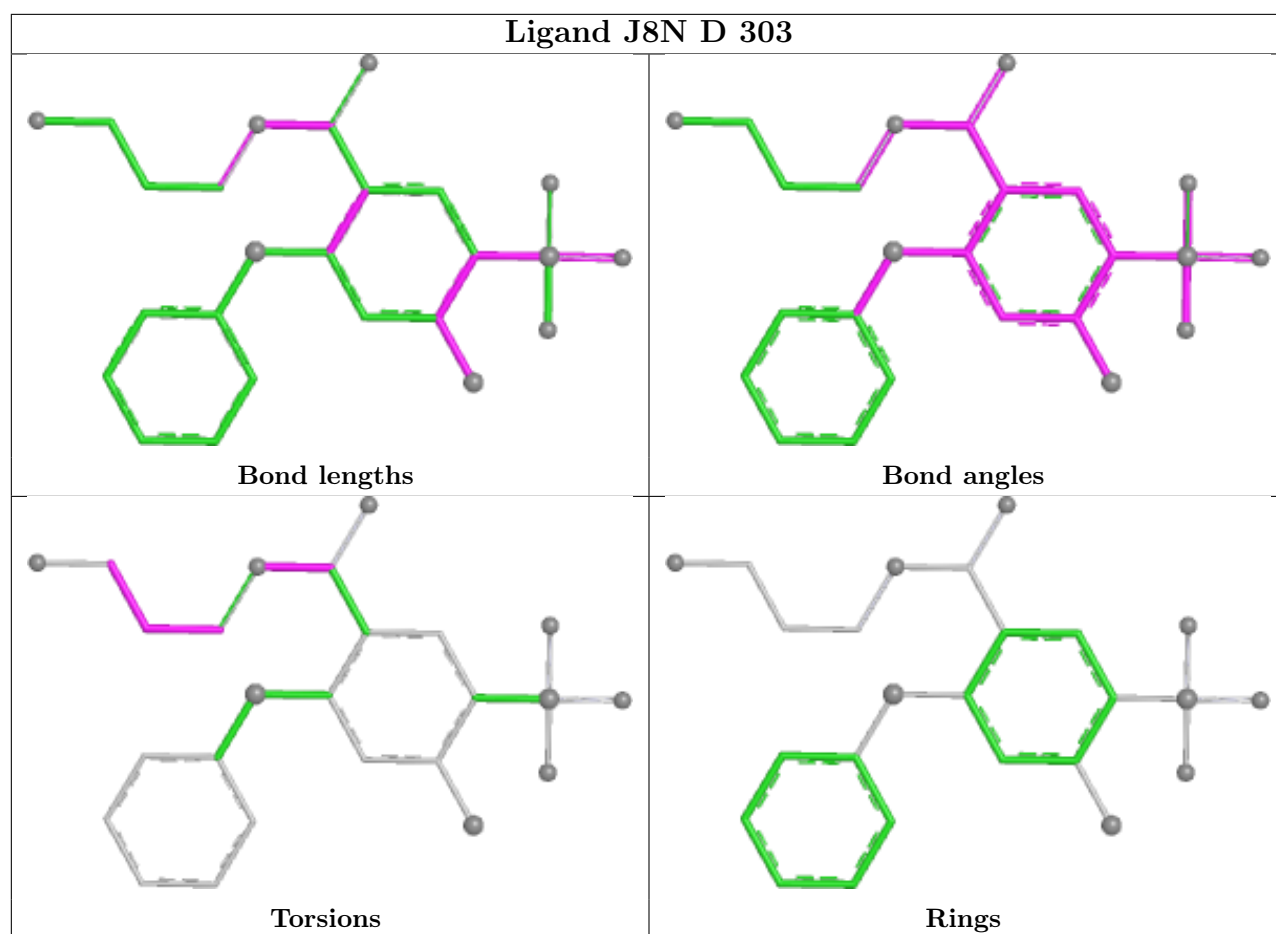
Ligand J8N B 302

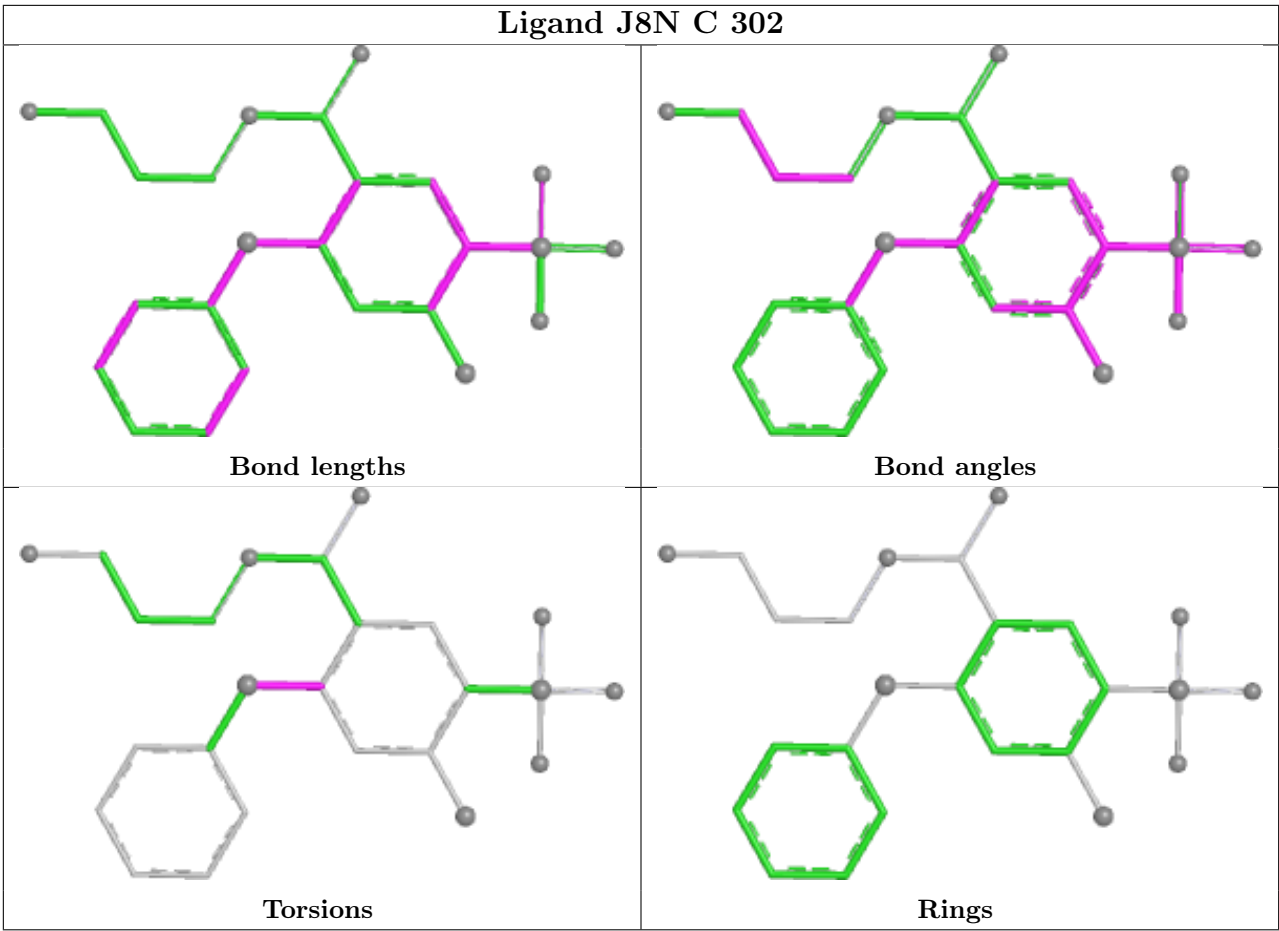












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	11:PRO	C	15:PRO	N	1.78
1	C	11:PRO	C	15:PRO	N	1.69

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	11:PRO	C	15:PRO	N	1.66
1	B	11:PRO	C	15:PRO	N	1.65
1	A	72:PRO	C	76:GLY	N	1.63
1	A	125:THR	C	127:ALA	N	1.63
1	B	125:THR	C	127:ALA	N	1.61

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	251/251 (100%)	0.65	18 (7%) 21 25	26, 42, 69, 87	1 (0%)
1	B	251/251 (100%)	0.55	20 (7%) 18 21	22, 35, 67, 100	0
1	C	251/251 (100%)	0.07	6 (2%) 59 66	19, 30, 50, 78	0
1	D	251/251 (100%)	0.47	15 (5%) 27 32	25, 38, 60, 79	0
All	All	1004/1004 (100%)	0.44	59 (5%) 28 32	19, 36, 65, 100	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ASP	6.7
1	A	230	TRP	4.3
1	B	8	GLY	4.2
1	B	232	PRO	3.8
1	B	11	PRO	3.7
1	B	100	ALA	3.6
1	D	189	PHE	3.4
1	B	9	GLY	3.3
1	C	5	TRP	3.2
1	D	257	PRO	3.1
1	A	11	PRO	3.0
1	B	234	ASP	2.9
1	B	101	GLY	2.9
1	A	237	LEU	2.9
1	A	100	ALA	2.9
1	A	8	GLY	2.9
1	B	7	TYR	2.8
1	C	8	GLY	2.8
1	B	19	VAL	2.8
1	A	232	PRO	2.8
1	A	239	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	172	SER	2.7
1	D	5	TRP	2.7
1	A	36	GLN	2.7
1	C	11	PRO	2.7
1	B	10	ASP	2.6
1	B	230	TRP	2.6
1	A	224	HIS	2.5
1	A	37	LEU	2.5
1	B	98	GLY	2.5
1	D	100	ALA	2.5
1	A	19	VAL	2.5
1	C	9	GLY	2.4
1	B	15	PRO	2.4
1	A	15	PRO	2.4
1	B	233	GLY	2.4
1	D	16	TRP	2.4
1	B	54(B)	LEU	2.3
1	D	8	GLY	2.3
1	D	50	LEU	2.3
1	C	6	ARG	2.3
1	B	165	GLU	2.3
1	B	68	LEU	2.2
1	A	234	ASP	2.2
1	B	99	ALA	2.2
1	A	16	TRP	2.2
1	B	239	LEU	2.2
1	D	179	LEU	2.2
1	D	233	GLY	2.2
1	D	19	VAL	2.1
1	D	224	HIS	2.1
1	D	220	ALA	2.1
1	C	15	PRO	2.1
1	D	49	LEU	2.1
1	A	5	TRP	2.1
1	D	37	LEU	2.1
1	D	101	GLY	2.0
1	A	238	GLN	2.0
1	A	217	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

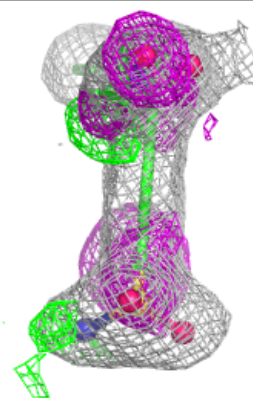
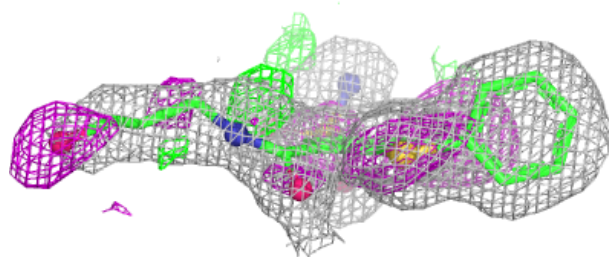
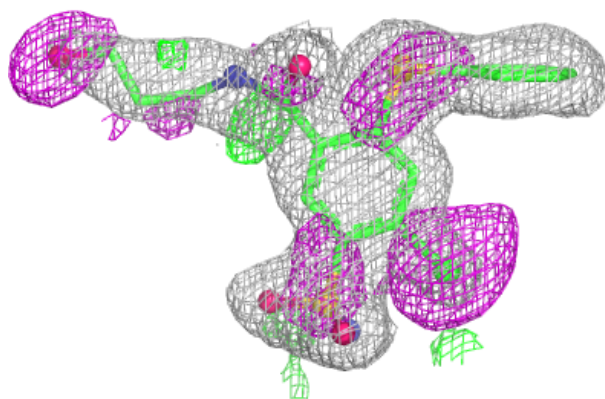
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	J8N	C	303	25/25	0.91	0.11	24,27,34,37	0
3	J8N	D	303	25/25	0.93	0.11	25,28,34,38	0
3	J8N	B	302	25/25	0.97	0.08	28,39,56,57	0
3	J8N	D	302	25/25	0.97	0.09	27,35,53,58	0
3	J8N	C	302	25/25	0.97	0.09	25,32,50,52	0
3	J8N	A	302	25/25	0.98	0.07	31,42,48,50	0
2	ZN	A	301	1/1	0.99	0.02	33,33,33,33	0
2	ZN	B	301	1/1	1.00	0.01	29,29,29,29	0
2	ZN	C	301	1/1	1.00	0.01	22,22,22,22	0
2	ZN	D	301	1/1	1.00	0.02	27,27,27,27	0

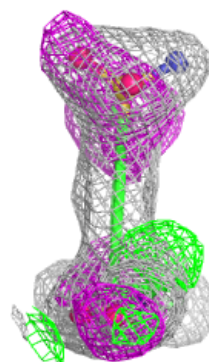
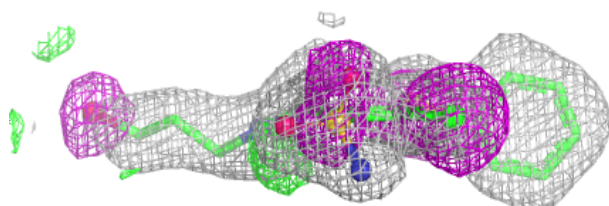
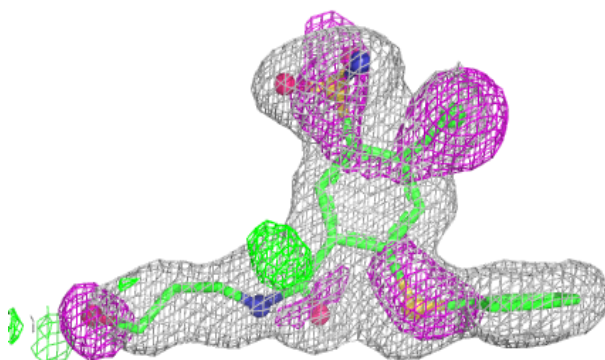
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around J8N C 303:

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

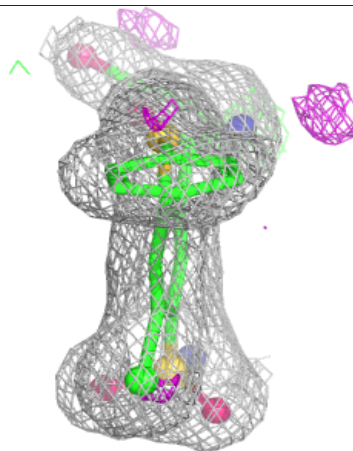
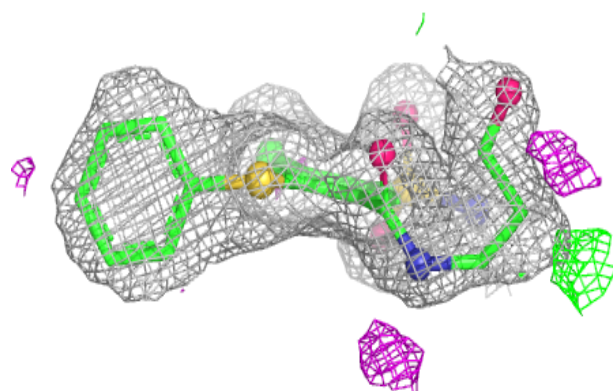
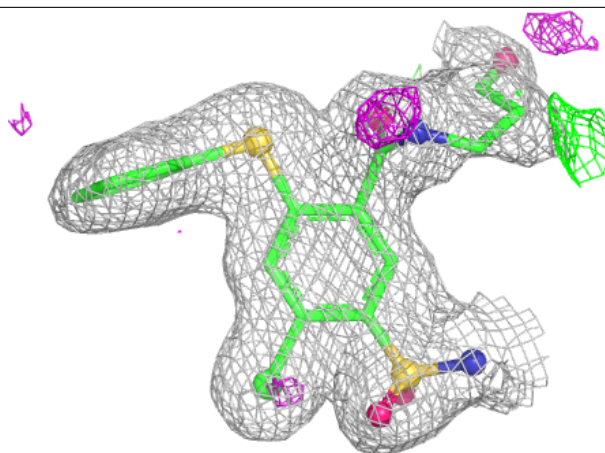
**Electron density around J8N D 303:**

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



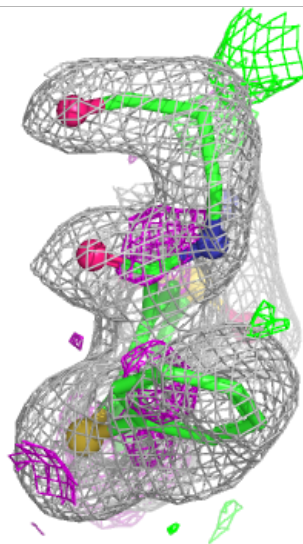
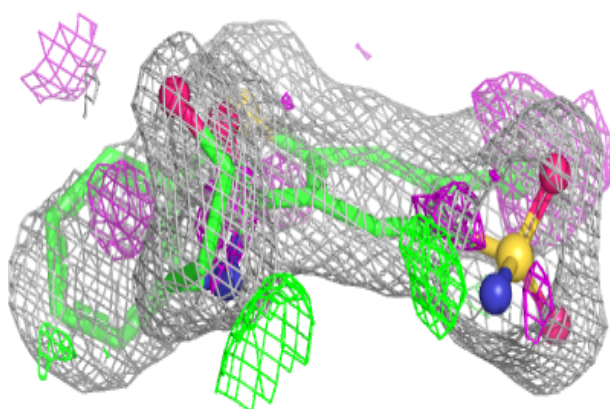
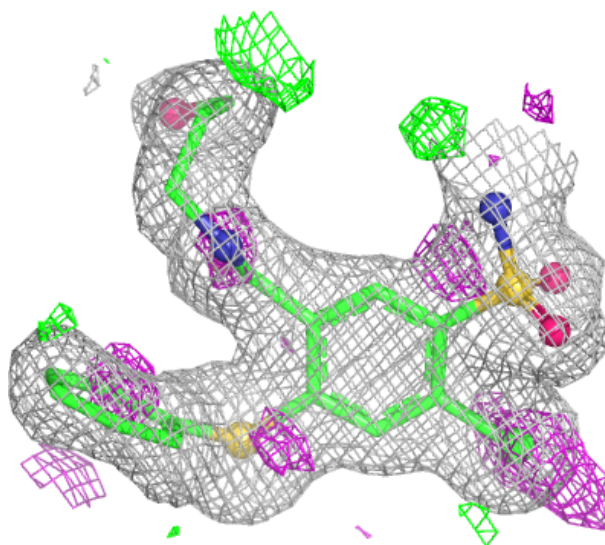
Electron density around J8N B 302:

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



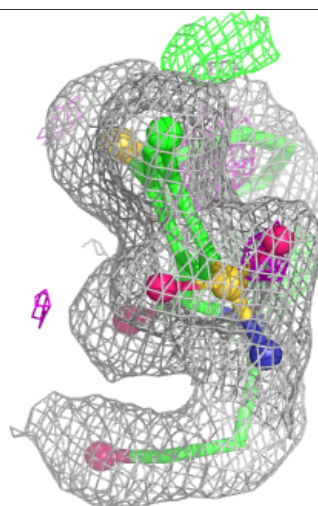
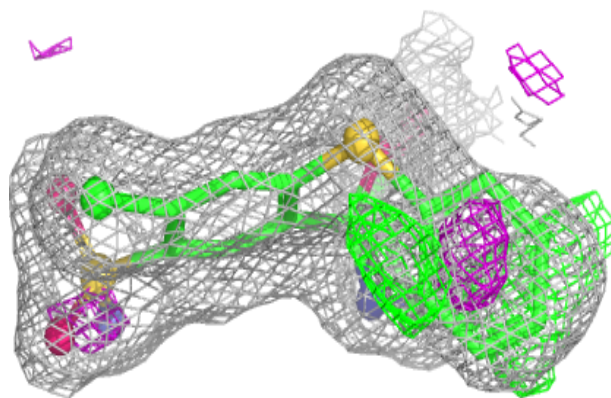
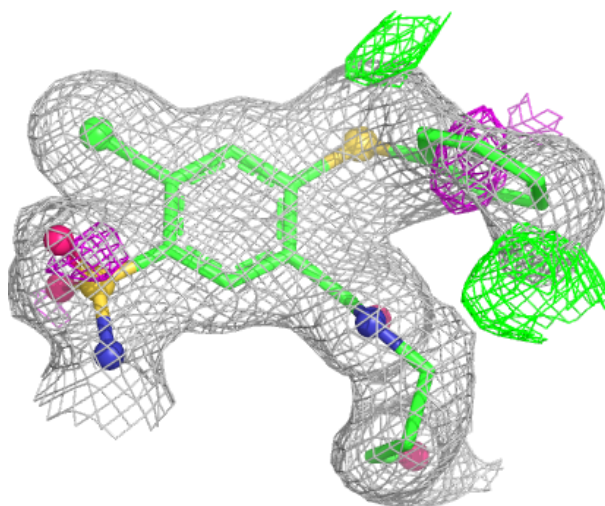
Electron density around J8N D 302:

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



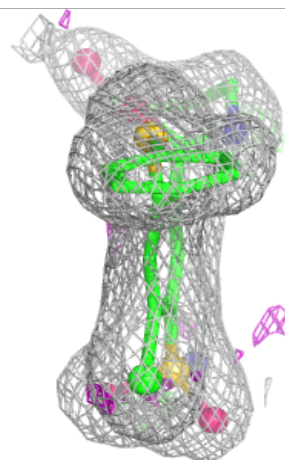
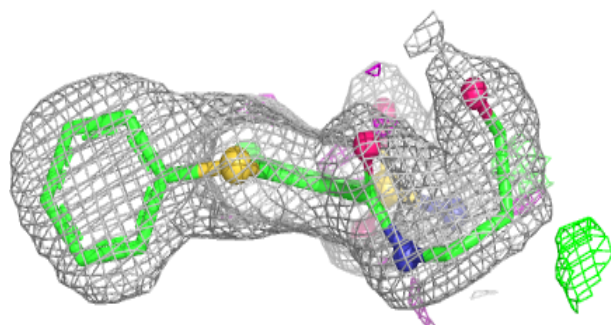
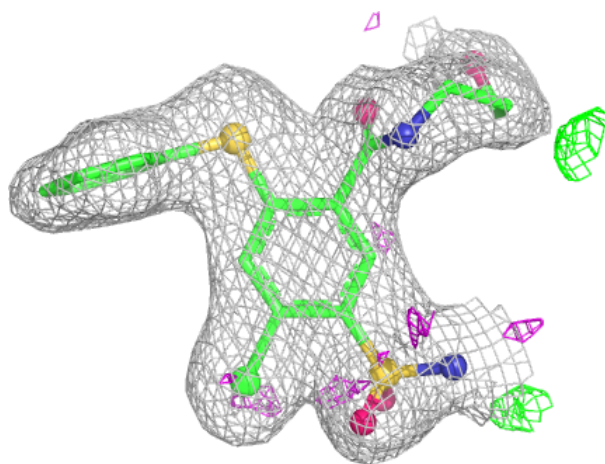
Electron density around J8N C 302:

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



Electron density around J8N A 302:

$2mF_o-DF_c$ (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.