



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:42 AM UTC

PDB ID : 8Q18 / pdb_00008q18
Title : The Crystal Structure of Human Carbonic Anhydrase IX in Complex with Sulfonamide
Authors : Leitans, J.; Tars, K.
Deposited on : 2023-07-31
Resolution : 2.13 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

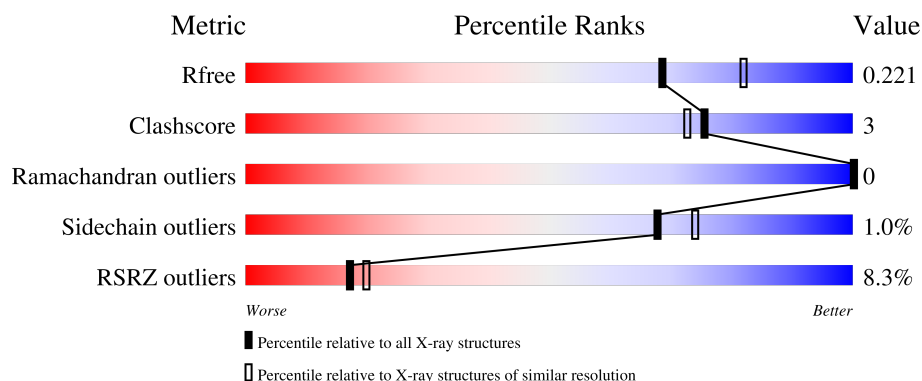
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	257	9% 89% 9% .
1	B	257	8% 89% 7% ..
1	C	257	7% 84% 13% .
1	D	257	8% 88% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8533 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
			1926	1230	340	352	4			
1	B	251	Total	C	N	O	S	0	1	0
			1927	1230	340	353	4			
1	C	251	Total	C	N	O	S	0	0	0
			1920	1226	336	354	4			
1	D	251	Total	C	N	O	S	0	1	0
			1937	1236	340	357	4			

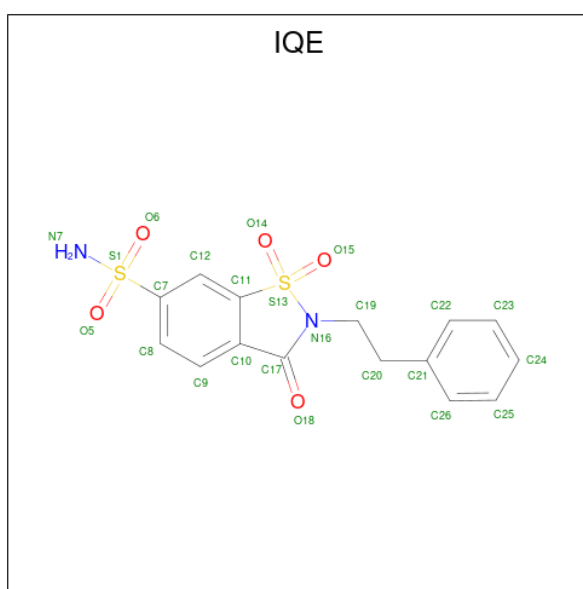
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP Q16790
A	4	PRO	-	expression tag	UNP Q16790
A	42	SER	CYS	engineered mutation	UNP Q16790
A	214	GLN	ASN	engineered mutation	UNP Q16790
B	3	GLY	-	expression tag	UNP Q16790
B	4	PRO	-	expression tag	UNP Q16790
B	42	SER	CYS	engineered mutation	UNP Q16790
B	214	GLN	ASN	engineered mutation	UNP Q16790
C	3	GLY	-	expression tag	UNP Q16790
C	4	PRO	-	expression tag	UNP Q16790
C	42	SER	CYS	engineered mutation	UNP Q16790
C	214	GLN	ASN	engineered mutation	UNP Q16790
D	3	GLY	-	expression tag	UNP Q16790
D	4	PRO	-	expression tag	UNP Q16790
D	42	SER	CYS	engineered mutation	UNP Q16790
D	214	GLN	ASN	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 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is 1,1,3-tris(oxidanylidene)-2-(2-phenylethyl)-1,2-benzothiazole-6-sulfonamide (CCD ID: IQE) (formula: C₁₅H₁₄N₂O₅S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 24 15 2 5 2	0	0
3	B	1	Total C N O S 24 15 2 5 2	0	0
3	C	1	Total C N O S 24 15 2 5 2	0	0
3	D	1	Total C N O S 24 15 2 5 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

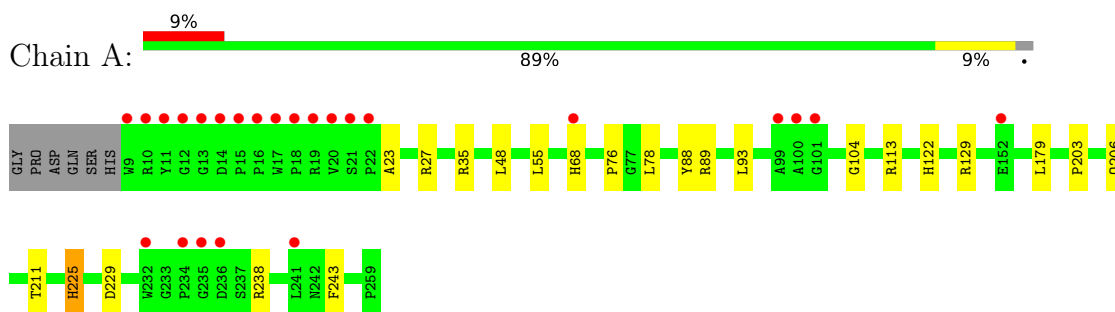
- Molecule 5 is water.

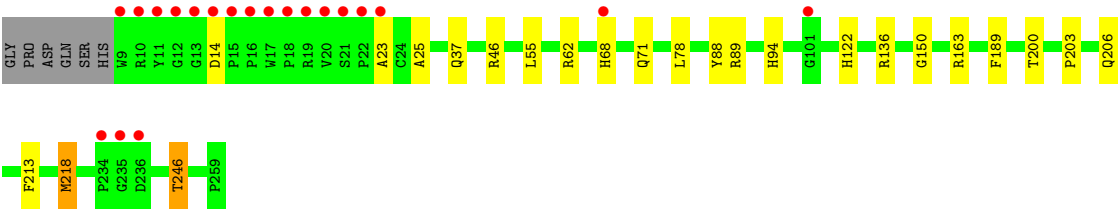
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	140	Total	O	0	0
			140	140		
5	B	165	Total	O	0	0
			165	165		
5	C	164	Total	O	0	0
			164	164		
5	D	230	Total	O	0	0
			230	230		

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





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	152.10Å 152.10Å 171.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.01 – 2.13 61.01 – 2.13	Depositor EDS
% Data completeness (in resolution range)	98.0 (61.01-2.13) 98.0 (61.01-2.13)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.175 , 0.217 0.182 , 0.221	Depositor DCC
R_{free} test set	4080 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8533	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IQE, GOL, 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	0.65	2/1984 (0.1%)	0.93	0/2712
1	B	0.69	2/1985 (0.1%)	0.97	3/2715 (0.1%)
1	C	0.65	1/1978 (0.1%)	0.94	1/2706 (0.0%)
1	D	0.70	2/1998 (0.1%)	0.97	1/2731 (0.0%)
All	All	0.67	7/7945 (0.1%)	0.95	5/10864 (0.0%)

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	5
1	B	0	4
1	C	0	5
1	D	0	4
All	All	0	18

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	HIS	CE1-NE2	5.48	1.38	1.32
1	C	94	HIS	CE1-NE2	5.34	1.37	1.32
1	A	225	HIS	CE1-NE2	5.32	1.37	1.32
1	D	68	HIS	CE1-NE2	5.30	1.37	1.32
1	B	68	HIS	CE1-NE2	5.30	1.37	1.32
1	A	68	HIS	CE1-NE2	5.22	1.37	1.32
1	B	107	HIS	CE1-NE2	5.05	1.37	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	ASP	CA-CB-CG	6.40	119.00	112.60
1	C	131	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	245	ALA	CA-C-N	5.69	128.84	120.82
1	B	245	ALA	C-N-CA	5.69	128.84	120.82
1	D	246	THR	CB-CA-C	5.13	118.24	109.72

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ARG	Sidechain
1	A	129	ARG	Sidechain
1	A	27	ARG	Sidechain
1	A	35	ARG	Sidechain
1	A	89	ARG	Sidechain
1	B	129	ARG	Sidechain
1	B	14	ASP	Peptide
1	B	64	ARG	Sidechain
1	B	89[A]	ARG	Sidechain
1	C	113	ARG	Sidechain
1	C	129	ARG	Sidechain
1	C	136	ARG	Sidechain
1	C	35	ARG	Sidechain
1	C	89	ARG	Sidechain
1	D	136	ARG	Sidechain
1	D	163	ARG	Sidechain
1	D	46	ARG	Sidechain
1	D	62	ARG	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	1926	0	1869	12	0
1	B	1927	0	1859	8	0
1	C	1920	0	1851	17	0
1	D	1937	0	1882	12	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	0	0	0
3	B	24	0	0	1	0
3	C	24	0	0	1	0
3	D	24	0	0	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	1	0
5	A	140	0	0	1	0
5	B	165	0	0	1	1
5	C	164	0	0	2	1
5	D	230	0	0	1	1
All	All	8533	0	7493	46	2

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 3.

All (46) 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:191:ARG:HE	1:B:214:GLN:NE2	1.93	0.66
1:D:150:GLY:HA3	1:D:218:MET:HE3	1.78	0.65
1:C:55:LEU:HD21	1:C:78:LEU:HD11	1.81	0.63
1:D:23:ALA:HB3	1:D:203:PRO:O	2.00	0.60
1:C:94:HIS:C	1:C:95:LEU:HD12	2.27	0.60
1:D:71:GLN:HE22	4:D:303:GOL:H31	1.68	0.58
1:D:189:PHE:HD1	1:D:213:PHE:HE1	1.52	0.58
1:A:225:HIS:NE2	1:A:229:ASP:OD2	2.39	0.56
1:B:147:LEU:HD22	1:B:217:VAL:CG2	2.36	0.56
1:C:153:GLU:HG3	5:C:439:HOH:O	2.06	0.56
1:B:98:GLY:HA2	1:B:241:LEU:HD23	1.89	0.54
1:B:191:ARG:HE	1:B:214:GLN:HE21	1.57	0.53
1:A:23:ALA:HB3	1:A:203:PRO:O	2.08	0.52
1:C:61:LEU:HD13	1:C:178:GLY:HA2	1.90	0.52
1:C:200:THR:OG1	3:C:302:IQE:N7	2.42	0.52
1:D:88:TYR:HB3	1:D:122:HIS:HB3	1.91	0.51
1:D:55:LEU:HD21	1:D:78:LEU:HD11	1.93	0.50
1:A:55:LEU:HD21	1:A:78:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:THR:O	1:C:230:THR:OG1	2.28	0.48
1:A:238:ARG:HH11	1:A:238:ARG:HG2	1.78	0.48
1:B:89[B]:ARG:HG2	5:B:504:HOH:O	2.13	0.47
1:C:63:LEU:HD11	1:C:70:VAL:HG22	1.95	0.47
1:C:14:ASP:HB3	1:C:15:PRO:HA	1.97	0.46
1:A:76:PRO:HG2	1:D:89:ARG:CZ	2.46	0.46
1:A:48:LEU:HD11	1:A:211:THR:HG21	1.99	0.45
1:C:54:GLN:HE22	1:D:206:GLN:HE22	1.63	0.45
1:C:88:TYR:HB3	1:C:122:HIS:HB3	1.97	0.45
1:C:163:ARG:NH1	1:C:166:GLU:OE1	2.50	0.45
1:B:55:LEU:HD21	1:B:78:LEU:HD11	1.98	0.44
1:D:37:GLN:NE2	5:D:413:HOH:O	2.50	0.43
1:C:232:TRP:CD1	5:C:527:HOH:O	2.71	0.43
1:A:88:TYR:HB3	1:A:122:HIS:HB3	2.00	0.43
1:A:104:GLY:HA2	1:A:243:PHE:CD2	2.54	0.43
1:A:179:LEU:HD23	1:A:179:LEU:N	2.33	0.43
1:B:200:THR:OG1	3:B:302:IQE:N7	2.52	0.42
1:A:206:GLN:NE2	5:A:401:HOH:O	2.34	0.42
1:C:60:GLU:C	1:C:61:LEU:HD12	2.44	0.42
1:A:93:LEU:C	1:A:93:LEU:HD12	2.45	0.42
1:C:18:PRO:HA	1:C:21:SER:O	2.20	0.42
1:D:200:THR:OG1	3:D:302:IQE:N7	2.52	0.42
1:C:156:ALA:HA	1:D:25:ALA:HB1	2.02	0.41
1:B:88:TYR:HB3	1:B:122:HIS:HB3	2.00	0.41
1:C:163:ARG:HH11	1:C:166:GLU:CD	2.28	0.41
1:D:78:LEU:HD12	1:D:78:LEU:N	2.36	0.40
1:C:29:GLN:OE1	1:C:204:CYS:HB3	2.22	0.40
1:A:238:ARG:HG2	1:A:238:ARG:NH1	2.35	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:512:HOH:O	5:B:512:HOH:O[2_555]	1.97	0.23
5:C:509:HOH:O	5:D:558:HOH:O[8_444]	2.16	0.04

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	249/257 (97%)	240 (96%)	9 (4%)	0	100	100
1	B	250/257 (97%)	242 (97%)	8 (3%)	0	100	100
1	C	249/257 (97%)	240 (96%)	9 (4%)	0	100	100
1	D	250/257 (97%)	246 (98%)	4 (2%)	0	100	100
All	All	998/1028 (97%)	968 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	200/210 (95%)	200 (100%)	0	100	100
1	B	199/210 (95%)	196 (98%)	3 (2%)	57	63
1	C	199/210 (95%)	197 (99%)	2 (1%)	68	74
1	D	203/210 (97%)	200 (98%)	3 (2%)	57	63
All	All	801/840 (95%)	793 (99%)	8 (1%)	68	74

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	ASP
1	B	152	GLU

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Mol	Chain	Res	Type
1	B	229	ASP
1	C	37	GLN
1	C	147	LEU
1	D	14	ASP
1	D	218	MET
1	D	246	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	71	GLN
1	A	154	ASN
1	B	37	GLN
1	B	194	GLN
1	B	214	GLN
1	C	54	GLN
1	C	71	GLN
1	C	159	GLN
1	C	175	GLN
1	C	194	GLN
1	C	225	HIS
1	D	37	GLN
1	D	71	GLN
1	D	240	GLN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	GOL	C	303	-	5,5,5	0.10	0	5,5,5	0.39	0
4	GOL	B	303	-	5,5,5	0.19	0	5,5,5	0.51	0
3	IQE	C	302	2	26,26,26	2.97	8 (30%)	36,40,40	6.20	18 (50%)
3	IQE	D	302	2	26,26,26	3.15	9 (34%)	36,40,40	6.02	22 (61%)
3	IQE	B	302	2	26,26,26	2.98	10 (38%)	36,40,40	6.35	21 (58%)
3	IQE	A	302	2	26,26,26	2.99	9 (34%)	36,40,40	6.16	21 (58%)
4	GOL	D	303	-	5,5,5	0.13	0	5,5,5	0.31	0
4	GOL	A	303	-	5,5,5	0.18	0	5,5,5	0.33	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
4	GOL	C	303	-	-	0/4/4/4	-
4	GOL	B	303	-	-	3/4/4/4	-
3	IQE	C	302	2	-	6/11/31/31	0/3/3/3
3	IQE	D	302	2	-	8/11/31/31	0/3/3/3
3	IQE	B	302	2	-	8/11/31/31	0/3/3/3
3	IQE	A	302	2	-	7/11/31/31	0/3/3/3
4	GOL	D	303	-	-	4/4/4/4	-
4	GOL	A	303	-	-	4/4/4/4	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	IQE	C10-C11	9.82	1.51	1.38
3	C	302	IQE	C10-C11	9.56	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	IQE	C10-C11	9.48	1.50	1.38
3	D	302	IQE	C10-C11	9.32	1.50	1.38
3	D	302	IQE	C7-S1	-6.01	1.67	1.77
3	D	302	IQE	C11-S13	-5.82	1.67	1.75
3	B	302	IQE	C11-S13	-5.56	1.68	1.75
3	C	302	IQE	C7-S1	-5.04	1.69	1.77
3	C	302	IQE	C11-S13	-4.91	1.69	1.75
3	A	302	IQE	C12-C7	4.85	1.47	1.39
3	A	302	IQE	C11-S13	-4.84	1.69	1.75
3	B	302	IQE	C12-C7	4.63	1.47	1.39
3	B	302	IQE	C7-S1	-4.26	1.70	1.77
3	A	302	IQE	C12-C11	4.12	1.46	1.39
3	C	302	IQE	O15-S13	4.08	1.47	1.43
3	A	302	IQE	C7-S1	-3.92	1.71	1.77
3	D	302	IQE	S1-N7	3.89	1.68	1.60
3	D	302	IQE	O15-S13	3.83	1.47	1.43
3	C	302	IQE	C12-C11	3.78	1.45	1.39
3	C	302	IQE	C12-C7	3.67	1.45	1.39
3	D	302	IQE	C12-C11	3.64	1.45	1.39
3	D	302	IQE	O18-C17	3.53	1.29	1.22
3	B	302	IQE	C12-C11	3.50	1.45	1.39
3	A	302	IQE	C8-C7	3.49	1.44	1.38
3	D	302	IQE	C8-C7	3.41	1.44	1.38
3	D	302	IQE	C12-C7	3.39	1.45	1.39
3	A	302	IQE	S1-N7	3.34	1.67	1.60
3	B	302	IQE	O18-C17	3.31	1.29	1.22
3	A	302	IQE	O18-C17	3.28	1.29	1.22
3	C	302	IQE	O18-C17	3.27	1.29	1.22
3	C	302	IQE	C8-C7	3.01	1.43	1.38
3	B	302	IQE	C10-C17	2.52	1.52	1.48
3	B	302	IQE	C8-C7	2.50	1.42	1.38
3	B	302	IQE	S1-N7	2.46	1.65	1.60
3	A	302	IQE	O15-S13	2.27	1.45	1.43
3	B	302	IQE	O15-S13	2.14	1.45	1.43

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	IQE	C12-C11-C10	-16.58	114.31	123.55
3	B	302	IQE	O6-S1-C7	-16.56	88.64	107.35
3	C	302	IQE	O6-S1-O5	-16.33	93.68	118.80
3	D	302	IQE	C12-C11-C10	-16.30	114.46	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	IQE	C12-C11-C10	-15.47	114.92	123.55
3	A	302	IQE	O6-S1-C7	-14.57	90.89	107.35
3	D	302	IQE	O6-S1-C7	-14.53	90.93	107.35
3	B	302	IQE	O6-S1-O5	-14.32	96.77	118.80
3	B	302	IQE	O5-S1-N7	13.74	127.16	107.35
3	C	302	IQE	O5-S1-N7	13.74	127.16	107.35
3	B	302	IQE	C12-C11-C10	-13.41	116.07	123.55
3	A	302	IQE	O6-S1-O5	-12.29	99.90	118.80
3	D	302	IQE	O6-S1-O5	-12.01	100.32	118.80
3	C	302	IQE	O15-S13-C11	10.84	126.06	111.23
3	B	302	IQE	C17-N16-S13	-10.58	108.75	115.13
3	A	302	IQE	O5-S1-N7	10.55	122.57	107.35
3	D	302	IQE	O5-S1-C7	10.43	119.14	107.35
3	A	302	IQE	O5-S1-C7	10.31	119.00	107.35
3	D	302	IQE	O5-S1-N7	10.20	122.06	107.35
3	A	302	IQE	O15-S13-C11	9.93	124.82	111.23
3	B	302	IQE	C11-S13-N16	9.90	99.55	92.54
3	C	302	IQE	O15-S13-N16	-9.82	101.62	109.98
3	D	302	IQE	O15-S13-C11	9.12	123.72	111.23
3	A	302	IQE	C17-N16-S13	-8.37	110.08	115.13
3	B	302	IQE	O14-S13-N16	-8.14	103.05	109.98
3	C	302	IQE	O6-S1-C7	-8.13	98.16	107.35
3	D	302	IQE	C17-N16-S13	-8.00	110.30	115.13
3	B	302	IQE	O15-S13-C11	7.99	122.17	111.23
3	C	302	IQE	C7-S1-N7	7.90	119.40	108.40
3	C	302	IQE	C11-S13-N16	7.63	97.94	92.54
3	C	302	IQE	C17-N16-S13	-7.47	110.62	115.13
3	A	302	IQE	C11-S13-N16	7.46	97.82	92.54
3	A	302	IQE	C11-C10-C17	-7.41	104.31	112.30
3	D	302	IQE	O14-S13-N16	-7.19	103.86	109.98
3	D	302	IQE	C11-C10-C17	-7.15	104.59	112.30
3	C	302	IQE	C11-C10-C17	-7.01	104.75	112.30
3	B	302	IQE	C7-S1-N7	6.91	118.02	108.40
3	A	302	IQE	O15-S13-O14	-6.80	105.24	116.29
3	D	302	IQE	O15-S13-O14	-6.79	105.25	116.29
3	D	302	IQE	C11-S13-N16	6.67	97.26	92.54
3	B	302	IQE	C11-C10-C17	-6.48	105.31	112.30
3	C	302	IQE	O6-S1-N7	-6.47	98.02	107.35
3	C	302	IQE	O15-S13-O14	-6.32	106.02	116.29
3	A	302	IQE	O14-S13-N16	-6.23	104.68	109.98
3	A	302	IQE	C10-C17-N16	5.81	116.71	108.56
3	D	302	IQE	C10-C17-N16	5.74	116.61	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	IQE	C10-C17-N16	5.70	116.55	108.56
3	C	302	IQE	C10-C17-N16	5.47	116.23	108.56
3	B	302	IQE	O18-C17-C10	-4.64	119.67	128.66
3	B	302	IQE	O6-S1-N7	-4.48	100.90	107.35
3	B	302	IQE	C9-C8-C7	4.47	123.79	119.44
3	B	302	IQE	O15-S13-O14	-4.30	109.30	116.29
3	D	302	IQE	O18-C17-C10	-4.22	120.49	128.66
3	A	302	IQE	C7-C12-C11	4.13	125.10	120.22
3	A	302	IQE	C8-C7-C12	-4.12	115.58	120.68
3	C	302	IQE	O18-C17-C10	-4.11	120.69	128.66
3	A	302	IQE	O18-C17-C10	-4.05	120.81	128.66
3	C	302	IQE	C9-C8-C7	3.90	123.23	119.44
3	B	302	IQE	O5-S1-C7	3.89	111.75	107.35
3	A	302	IQE	C12-C7-S1	3.86	126.31	119.34
3	B	302	IQE	C8-C7-C12	-3.85	115.92	120.68
3	D	302	IQE	C12-C7-S1	3.78	126.17	119.34
3	D	302	IQE	O6-S1-N7	3.55	112.47	107.35
3	A	302	IQE	O6-S1-N7	3.46	112.35	107.35
3	C	302	IQE	C8-C7-C12	-3.16	116.77	120.68
3	D	302	IQE	C9-C8-C7	3.10	122.45	119.44
3	A	302	IQE	C9-C10-C17	3.00	134.62	129.59
3	B	302	IQE	C12-C7-S1	2.98	124.72	119.34
3	A	302	IQE	C9-C8-C7	2.90	122.26	119.44
3	B	302	IQE	C9-C10-C17	2.84	134.35	129.59
3	D	302	IQE	O14-S13-C11	2.69	114.92	111.23
3	C	302	IQE	C7-C12-C11	2.65	123.35	120.22
3	B	302	IQE	C7-C12-C11	2.64	123.34	120.22
3	D	302	IQE	C8-C7-S1	-2.57	116.23	119.72
3	D	302	IQE	C8-C7-C12	-2.54	117.53	120.68
3	D	302	IQE	C7-C12-C11	2.54	123.23	120.22
3	C	302	IQE	C9-C10-C17	2.42	133.66	129.59
3	A	302	IQE	O15-S13-N16	-2.42	107.92	109.98
3	D	302	IQE	C9-C10-C11	2.35	122.39	119.87
3	A	302	IQE	O14-S13-C11	2.23	114.28	111.23
3	B	302	IQE	O15-S13-N16	-2.09	108.20	109.98
3	D	302	IQE	C9-C10-C17	2.04	133.01	129.59

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	IQE	C20-C19-N16-S13

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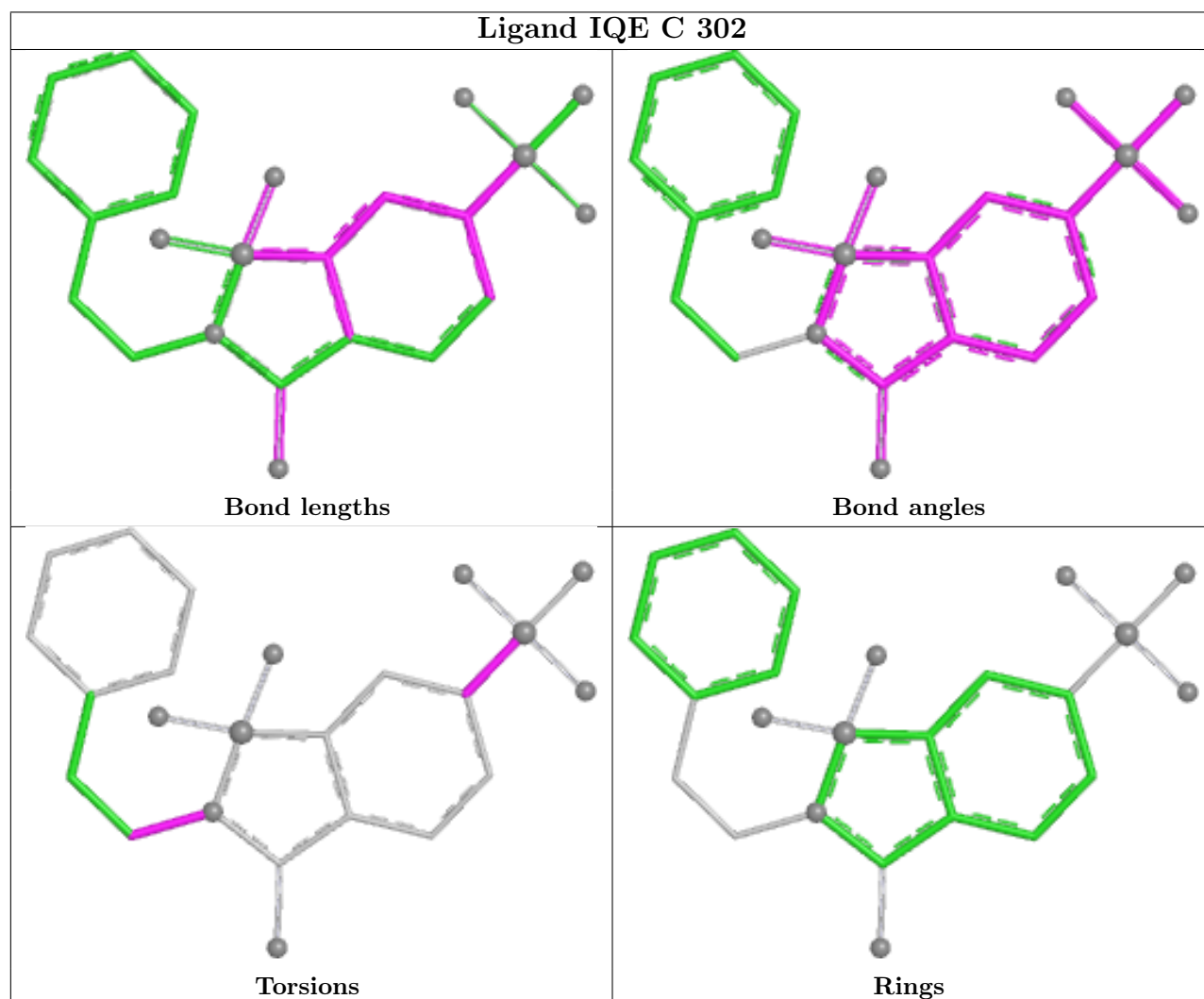
Mol	Chain	Res	Type	Atoms
3	A	302	IQE	C20-C19-N16-C17
3	A	302	IQE	N16-C19-C20-C21
3	B	302	IQE	C20-C19-N16-C17
3	C	302	IQE	C20-C19-N16-C17
3	D	302	IQE	C20-C19-N16-C17
4	A	303	GOL	O1-C1-C2-O2
4	A	303	GOL	O1-C1-C2-C3
4	A	303	GOL	C1-C2-C3-O3
4	B	303	GOL	O1-C1-C2-C3
4	D	303	GOL	O1-C1-C2-C3
4	D	303	GOL	C1-C2-C3-O3
4	D	303	GOL	O2-C2-C3-O3
4	A	303	GOL	O2-C2-C3-O3
4	B	303	GOL	O1-C1-C2-O2
4	D	303	GOL	O1-C1-C2-O2
3	C	302	IQE	C12-C7-S1-O6
3	C	302	IQE	C8-C7-S1-N7
3	C	302	IQE	C8-C7-S1-O6
3	B	302	IQE	C12-C7-S1-N7
3	B	302	IQE	C8-C7-S1-N7
3	C	302	IQE	C12-C7-S1-N7
4	B	303	GOL	C1-C2-C3-O3
3	B	302	IQE	C12-C7-S1-O6
3	B	302	IQE	C8-C7-S1-O6
3	D	302	IQE	C19-C20-C21-C22
3	D	302	IQE	C19-C20-C21-C26
3	D	302	IQE	C8-C7-S1-O6
3	D	302	IQE	C12-C7-S1-O6
3	D	302	IQE	C8-C7-S1-N7
3	D	302	IQE	C12-C7-S1-N7
3	A	302	IQE	C8-C7-S1-O6
3	A	302	IQE	C12-C7-S1-O6
3	A	302	IQE	C8-C7-S1-N7
3	A	302	IQE	C12-C7-S1-N7
3	B	302	IQE	C19-C20-C21-C22
3	B	302	IQE	C20-C19-N16-S13
3	C	302	IQE	C20-C19-N16-S13
3	D	302	IQE	C20-C19-N16-S13
3	B	302	IQE	C19-C20-C21-C26

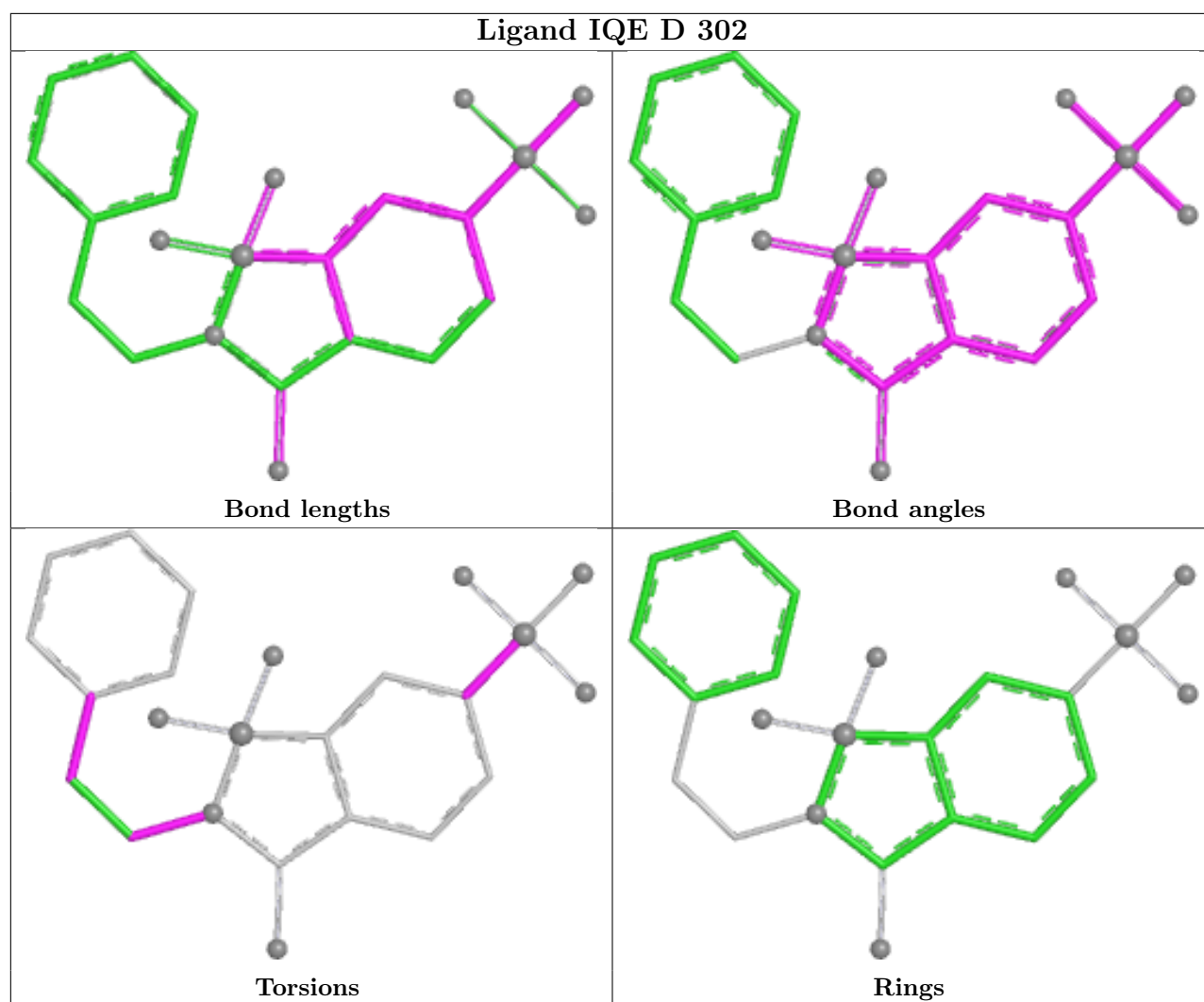
There are no ring outliers.

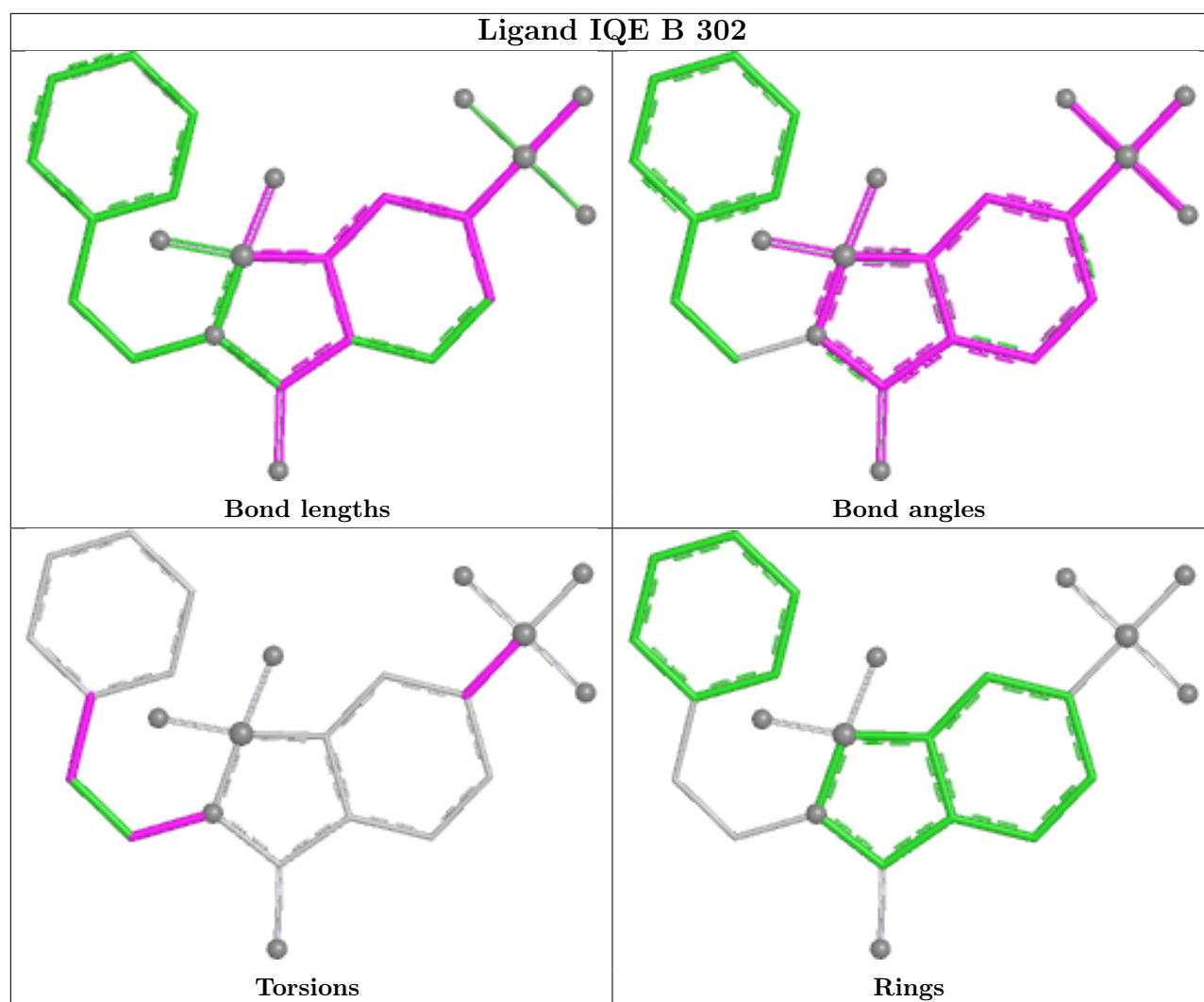
4 monomers are involved in 4 short contacts:

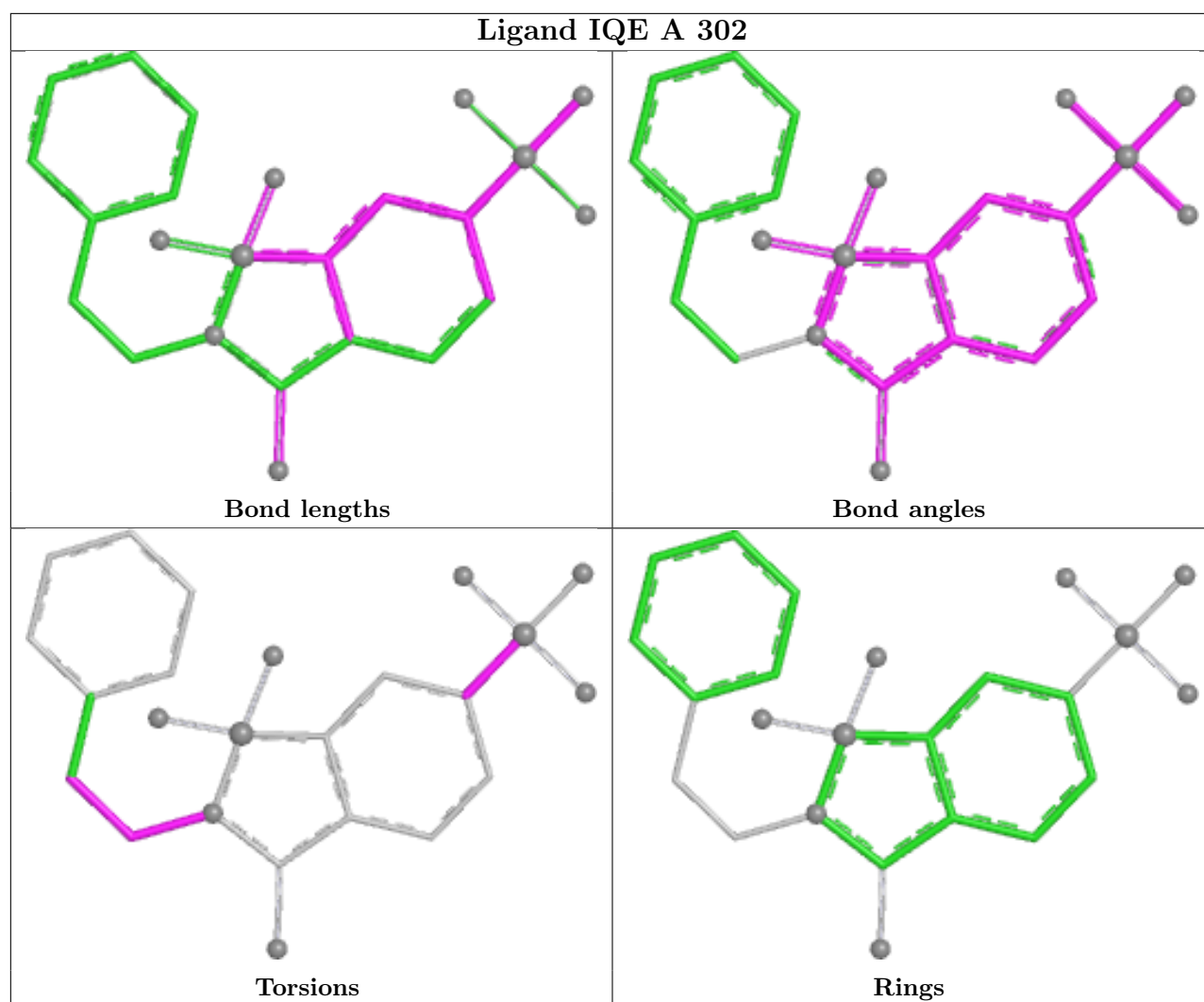
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	IQE	1	0
3	D	302	IQE	1	0
3	B	302	IQE	1	0
4	D	303	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	251/257 (97%)	0.41	24 (9%) 13 15	21, 37, 81, 154	0
1	B	251/257 (97%)	0.17	20 (7%) 18 21	14, 30, 82, 158	1 (0%)
1	C	251/257 (97%)	0.35	19 (7%) 20 23	21, 37, 76, 106	0
1	D	251/257 (97%)	0.02	20 (7%) 18 21	15, 25, 77, 147	1 (0%)
All	All	1004/1028 (97%)	0.24	83 (8%) 17 20	14, 32, 82, 158	2 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	PRO	8.2
1	D	10	ARG	6.4
1	D	12	GLY	6.4
1	D	15	PRO	6.2
1	A	9	TRP	6.1
1	B	16	PRO	5.8
1	D	9	TRP	5.8
1	A	15	PRO	5.7
1	B	11	TYR	5.5
1	D	20	VAL	5.2
1	C	15	PRO	5.2
1	D	16	PRO	5.2
1	D	236	ASP	5.1
1	A	16	PRO	5.1
1	D	19	ARG	4.9
1	D	17	TRP	4.6
1	A	236	ASP	4.6
1	D	18	PRO	4.6
1	A	20	VAL	4.5
1	B	232	TRP	4.5
1	B	20	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	11	TYR	4.3
1	D	14	ASP	4.2
1	C	13	GLY	4.1
1	B	12	GLY	4.1
1	B	13	GLY	4.0
1	A	18	PRO	4.0
1	C	12	GLY	3.9
1	C	11	TYR	3.9
1	C	232	TRP	3.7
1	A	13	GLY	3.7
1	C	234	PRO	3.5
1	C	236	ASP	3.5
1	B	9	TRP	3.4
1	B	236	ASP	3.4
1	A	11	TYR	3.4
1	A	10	ARG	3.4
1	A	12	GLY	3.4
1	C	16	PRO	3.3
1	A	17	TRP	3.3
1	D	13	GLY	3.2
1	D	235	GLY	3.2
1	C	9	TRP	3.2
1	A	14	ASP	3.1
1	B	19	ARG	3.0
1	A	232	TRP	3.0
1	C	17	TRP	3.0
1	C	20	VAL	3.0
1	C	235	GLY	3.0
1	D	68	HIS	2.9
1	A	68	HIS	2.9
1	A	22	PRO	2.8
1	B	101	GLY	2.8
1	B	17	TRP	2.8
1	B	14	ASP	2.8
1	C	225	HIS	2.7
1	A	100	ALA	2.6
1	D	22	PRO	2.6
1	C	102	ARG	2.6
1	C	14	ASP	2.5
1	D	234	PRO	2.4
1	C	19	ARG	2.4
1	A	241	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	101	GLY	2.3
1	C	101	GLY	2.3
1	B	100	ALA	2.3
1	A	152	GLU	2.2
1	B	21	SER	2.2
1	B	225	HIS	2.2
1	B	18	PRO	2.2
1	A	235	GLY	2.2
1	A	21	SER	2.2
1	A	19	ARG	2.2
1	C	10	ARG	2.2
1	B	10	ARG	2.1
1	D	23	ALA	2.1
1	D	21	SER	2.1
1	A	234	PRO	2.0
1	A	99	ALA	2.0
1	C	100	ALA	2.0
1	B	68	HIS	2.0
1	B	226	THR	2.0
1	A	101	GLY	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
4	GOL	A	303	6/6	0.79	0.24	60,70,79,80	0
3	IQE	D	302	24/24	0.82	0.24	40,73,101,105	0
4	GOL	B	303	6/6	0.83	0.23	68,77,81,83	0

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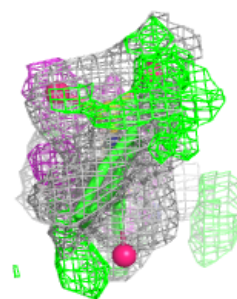
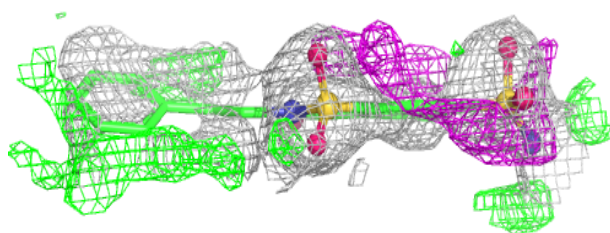
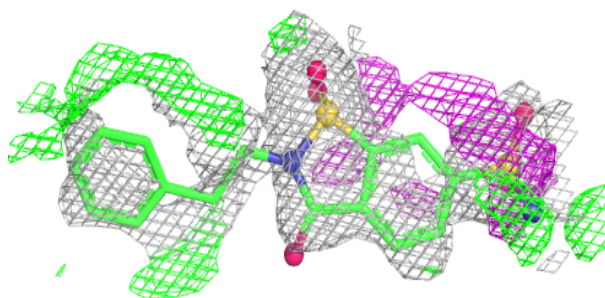
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	D	303	6/6	0.85	0.20	57,64,66,69	0
3	IQE	A	302	24/24	0.89	0.18	36,69,84,88	0
4	GOL	C	303	6/6	0.92	0.14	55,59,60,63	0
3	IQE	C	302	24/24	0.93	0.15	39,60,96,97	0
3	IQE	B	302	24/24	0.95	0.12	30,49,69,74	0
2	ZN	A	301	1/1	0.99	0.02	29,29,29,29	0
2	ZN	C	301	1/1	0.99	0.03	32,32,32,32	0
2	ZN	B	301	1/1	1.00	0.02	27,27,27,27	0
2	ZN	D	301	1/1	1.00	0.02	24,24,24,24	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.

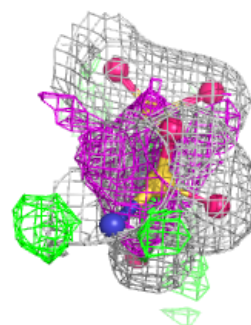
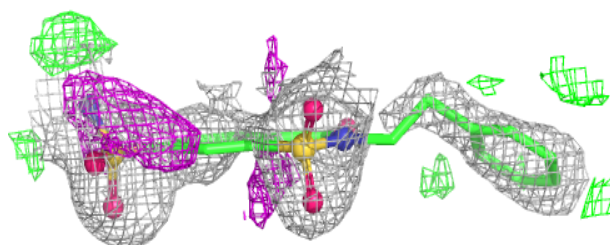
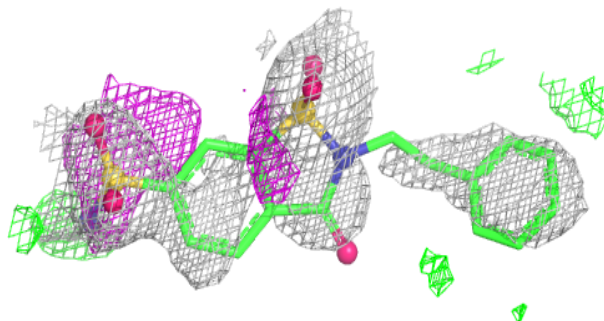
Electron density around IQE D 302:

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

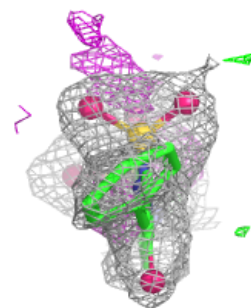
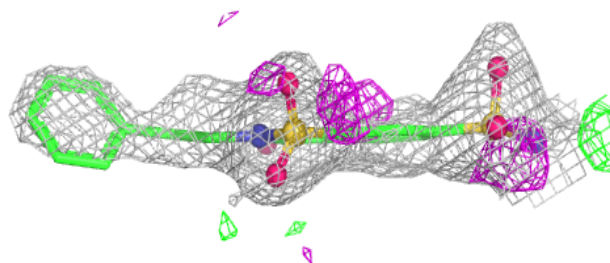
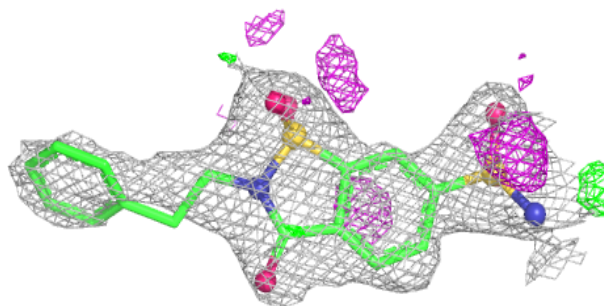


Electron density around IQE A 302:

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

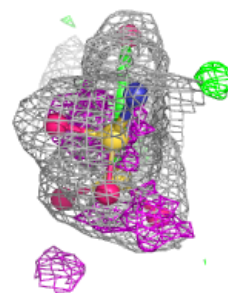
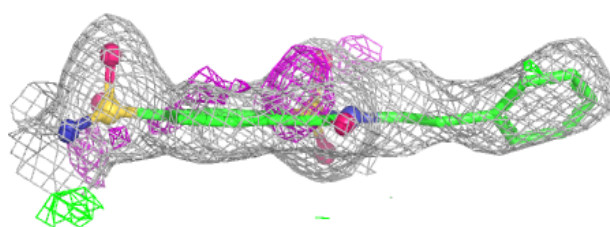
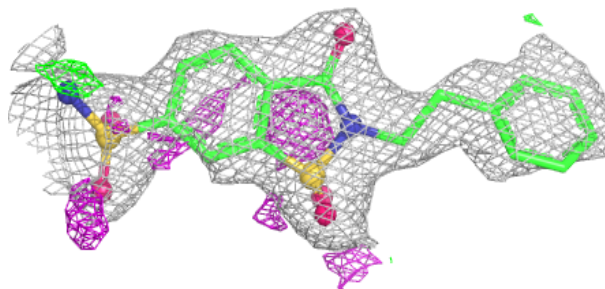
**Electron density around IQE C 302:**

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



Electron density around IQE 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.