



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2026 – 05:16 pm BST

PDB ID : 29SX / pdb_000029sx
Title : Crystal structure of carbonic anhydrase XII with 2-(benzylthio)phenyl sulfamate
Authors : Paketuryte-Latve, V.; Smirnov, A.; Manakova, E.N.; Grazulis, S.
Deposited on : 2026-04-07
Resolution : 1.85 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 Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

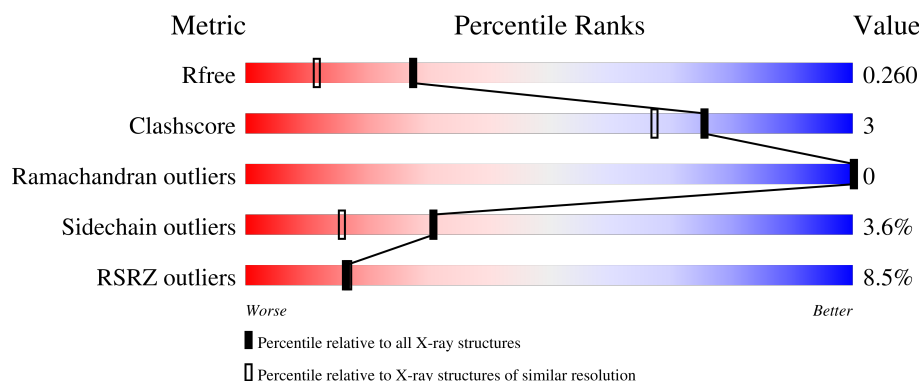
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	263	 7% 89% 9% ..
1	B	263	 11% 90% 8% ..
1	C	263	 11% 89% 9% ..
1	D	263	 4% 91% 8% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8904 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 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	2	0
			2091	1326	356	402	7			
1	B	261	Total	C	N	O	S	0	3	0
			2112	1342	359	402	9			
1	C	261	Total	C	N	O	S	0	2	0
			2114	1343	360	404	7			
1	D	261	Total	C	N	O	S	0	1	0
			2106	1339	359	401	7			

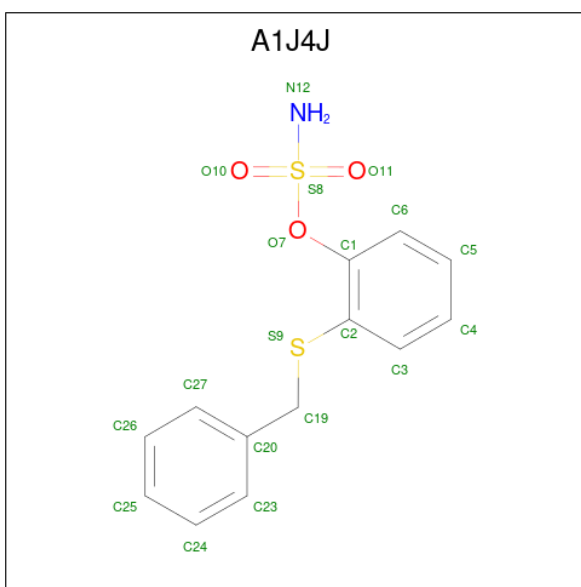
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O43570
B	1	MET	-	initiating methionine	UNP O43570
C	1	MET	-	initiating methionine	UNP O43570
D	1	MET	-	initiating methionine	UNP O43570

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

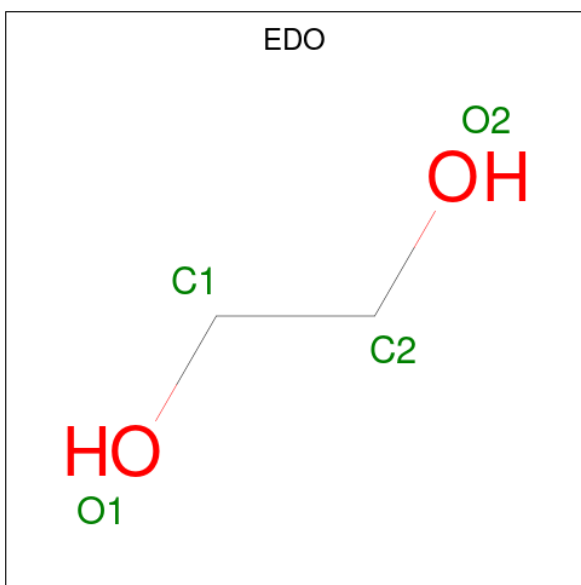
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is [2-(phenylmethylsulfanyl)phenyl] sulfamate (CCD ID: A1J4J) (formula: C₁₃H₁₃NO₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			19	13	1	3	2		
3	B	1	Total	C	N	O	S	0	0
			19	13	1	3	2		
3	C	1	Total	C	N	O	S	0	0
			19	13	1	3	2		
3	D	1	Total	C	N	O	S	0	0
			19	13	1	3	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

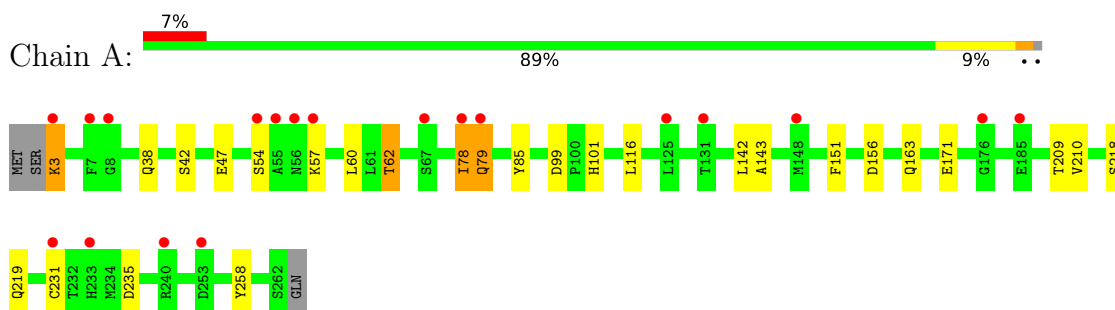
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		
5	B	99	Total	O	0	0
			99	99		
5	C	87	Total	O	0	0
			87	87		
5	D	121	Total	O	0	0
			121	121		

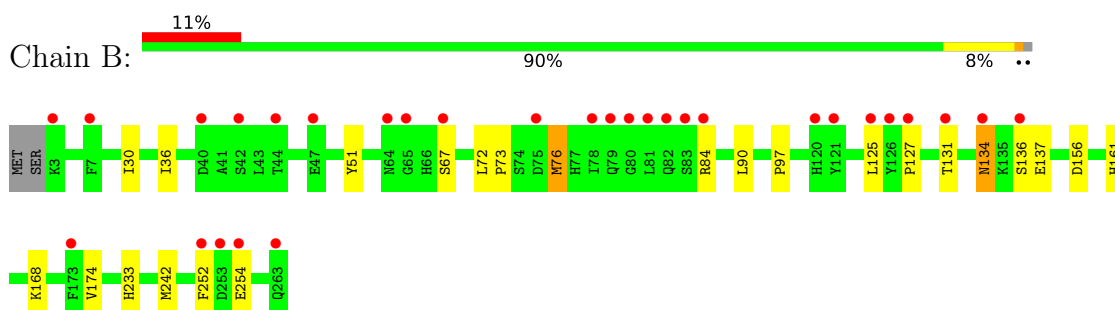
3 Residue-property plots

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.

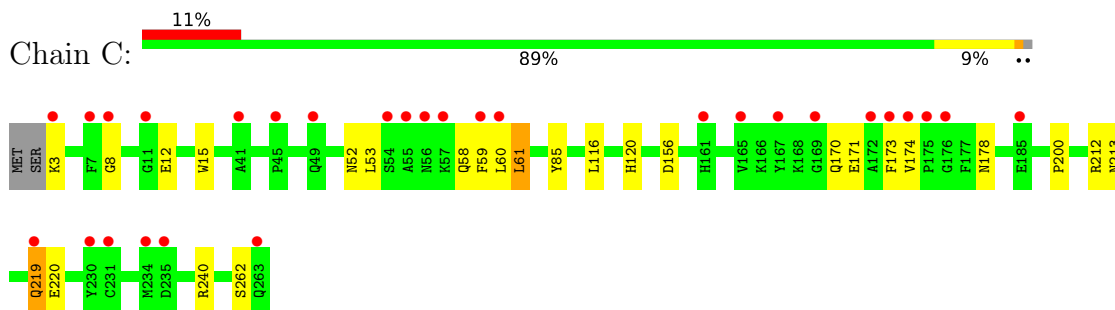
• Molecule 1: Carbonic anhydrase 12



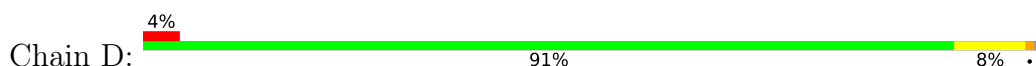
• Molecule 1: Carbonic anhydrase 12

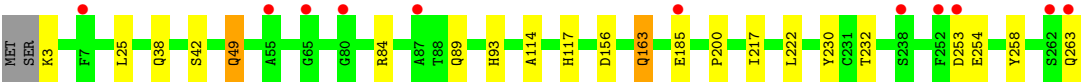


• Molecule 1: Carbonic anhydrase 12



• Molecule 1: Carbonic anhydrase 12





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.58Å 74.61Å 92.03Å 90.00° 108.80° 90.00°	Depositor
Resolution (Å)	73.45 – 1.85 73.45 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (73.45-1.85) 98.7 (73.45-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.214 , 0.261 0.215 , 0.260	Depositor DCC
R_{free} test set	8257 reflections (9.72%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7099e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1J4J, ZN, EDO

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	0/2153	1.09	0/2934
1	B	0.69	0/2175	1.14	0/2961
1	C	0.59	0/2177	1.05	0/2964
1	D	0.67	0/2169	1.15	0/2953
All	All	0.65	0/8674	1.11	0/11812

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	76[B]	MET	Mainchain
1	C	240	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	2091	0	1971	12	0
1	B	2112	0	1998	14	0
1	C	2114	0	2002	12	0
1	D	2106	0	1999	11	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	19	0	0	1	0
3	B	19	0	0	1	0
3	C	19	0	0	0	0
3	D	19	0	0	0	0
4	D	4	0	6	0	0
5	A	90	0	0	0	0
5	B	99	0	0	0	0
5	C	87	0	0	1	0
5	D	121	0	0	1	0
All	All	8904	0	7976	49	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 3.

All (49) 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)
3:B:302:A1J4J:N12	3:B:302:A1J4J:C6	2.26	0.97
3:A:302:A1J4J:C6	3:A:302:A1J4J:N12	2.32	0.91
1:A:47:GLU:HB2	1:A:79:GLN:HG3	1.65	0.78
1:A:60:LEU:HD11	1:A:171:GLU:HB3	1.73	0.71
1:D:163:GLN:HE21	1:D:163:GLN:H	1.44	0.66
1:C:212:ARG:HH11	1:C:213:ASN:HD21	1.52	0.57
1:B:72:LEU:HB3	1:B:76[B]:MET:CE	2.36	0.56
1:B:72:LEU:HB3	1:B:76[B]:MET:HE3	1.87	0.56
1:B:168:LYS:HE2	1:B:233:HIS:CE1	2.41	0.55
1:B:73:PRO:HD2	1:B:76[B]:MET:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:HB	1:A:171:GLU:HG2	1.91	0.53
1:C:58:GLN:HB3	1:C:173:PHE:HB3	1.90	0.53
1:D:217:ILE:HD11	1:D:222:LEU:HG	1.94	0.50
1:C:8:GLY:HA2	1:D:25:LEU:HD21	1.94	0.50
1:B:134:ASN:N	1:B:134:ASN:HD22	2.11	0.49
1:C:212:ARG:NH1	1:C:213:ASN:HD21	2.11	0.49
1:B:51:TYR:CD1	1:B:76[B]:MET:HG3	2.49	0.48
1:B:90:LEU:C	1:B:90:LEU:HD12	2.39	0.47
1:D:230:TYR:CD1	1:D:230:TYR:N	2.83	0.47
1:C:61:LEU:HG	1:C:174:VAL:HG21	1.96	0.47
1:C:85:TYR:HB3	1:C:120:HIS:HB3	1.98	0.46
1:D:38:GLN:O	1:D:258:TYR:HA	2.15	0.46
1:B:30:ILE:HD12	1:B:252:PHE:CE2	2.51	0.46
1:C:53:LEU:HD13	1:C:59:PHE:CE2	2.51	0.46
1:D:253:ASP:O	1:D:254:GLU:HB2	2.14	0.46
1:B:97:PRO:HG2	1:D:42:SER:HB3	1.97	0.45
1:A:54:SER:HB3	1:A:57:LYS:HB2	1.99	0.45
1:B:161:HIS:CD2	1:B:174:VAL:HG22	2.52	0.45
1:C:52:ASN:HA	1:C:178:ASN:HA	1.99	0.45
1:B:127:PRO:HD2	1:B:131:THR:HG21	1.98	0.45
1:A:78:ILE:HG13	1:A:85:TYR:HB2	2.00	0.44
1:B:76[B]:MET:HB2	1:B:76[B]:MET:HE2	1.75	0.44
1:C:12:GLU:HA	1:C:15:TRP:CE2	2.52	0.44
1:A:235:ASP:OD1	1:A:235:ASP:C	2.60	0.44
1:D:93:HIS:O	1:D:114:ALA:HB1	2.17	0.44
1:D:49:GLN:HE21	1:D:49:GLN:HA	1.82	0.43
1:A:151:PHE:HA	1:A:218:SER:HB3	2.00	0.43
1:C:60:LEU:HD11	1:C:171:GLU:HB3	2.00	0.43
1:B:67:SER:HA	1:B:242:MET:SD	2.59	0.43
1:A:3:LYS:HB2	1:A:3:LYS:HE3	1.60	0.42
1:C:219:GLN:HG3	1:C:220:GLU:OE1	2.19	0.42
1:A:99:ASP:OD1	1:A:101:HIS:HD2	2.03	0.42
1:D:185:GLU:HG3	5:D:445:HOH:O	2.19	0.42
1:A:38:GLN:O	1:A:258:TYR:HA	2.20	0.42
1:B:36:ILE:HD12	1:B:36:ILE:C	2.46	0.41
1:C:170:GLN:HA	5:C:481:HOH:O	2.18	0.41
1:D:93:HIS:CD2	1:D:117:HIS:CE1	3.07	0.41
1:A:143:ALA:HB3	1:A:210:VAL:HG22	2.02	0.41
1:A:142:LEU:HD23	1:A:209:THR:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
1	B	262/263 (100%)	255 (97%)	7 (3%)	0	100	100
1	C	261/263 (99%)	252 (97%)	9 (3%)	0	100	100
1	D	260/263 (99%)	251 (96%)	9 (4%)	0	100	100
All	All	1043/1052 (99%)	1012 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	232/235 (99%)	222 (96%)	10 (4%)	26	11
1	B	234/235 (100%)	227 (97%)	7 (3%)	36	21
1	C	235/235 (100%)	228 (97%)	7 (3%)	36	21
1	D	234/235 (100%)	225 (96%)	9 (4%)	29	14
All	All	935/940 (100%)	902 (96%)	33 (4%)	31	16

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	42	SER

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Mol	Chain	Res	Type
1	A	62	THR
1	A	78	ILE
1	A	79	GLN
1	A	116	LEU
1	A	156	ASP
1	A	163	GLN
1	A	219	GLN
1	A	231	CYS
1	B	84	ARG
1	B	125	LEU
1	B	134	ASN
1	B	136	SER
1	B	137	GLU
1	B	156	ASP
1	B	254	GLU
1	C	3	LYS
1	C	61	LEU
1	C	116	LEU
1	C	156	ASP
1	C	200	PRO
1	C	219	GLN
1	C	262	SER
1	D	3	LYS
1	D	49	GLN
1	D	84	ARG
1	D	89	GLN
1	D	156	ASP
1	D	163	GLN
1	D	200	PRO
1	D	232	THR
1	D	263	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	33	HIS
1	A	58	GLN
1	A	82	GLN
1	A	111	HIS
1	A	163	GLN
1	A	203	ASN

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Mol	Chain	Res	Type
1	B	66	HIS
1	B	101	HIS
1	B	134	ASN
1	B	178	ASN
1	B	203	ASN
1	B	213	ASN
1	B	219	GLN
1	B	250	GLN
1	C	82	GLN
1	C	111	HIS
1	C	161	HIS
1	C	213	ASN
1	C	219	GLN
1	C	263	GLN
1	D	49	GLN
1	D	66	HIS
1	D	79	GLN
1	D	101	HIS
1	D	110	GLN
1	D	163	GLN
1	D	203	ASN
1	D	213	ASN

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	A1J4J	A	302	2	20,20,20	7.57	4 (20%)	27,27,27	5.04	8 (29%)
3	A1J4J	B	302	2	20,20,20	5.43	4 (20%)	27,27,27	6.57	10 (37%)
3	A1J4J	C	302	-	20,20,20	5.64	6 (30%)	27,27,27	2.60	5 (18%)
3	A1J4J	D	303	2	20,20,20	6.06	5 (25%)	27,27,27	3.09	5 (18%)
4	EDO	D	302	-	3,3,3	0.78	0	2,2,2	1.33	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
3	A1J4J	A	302	2	-	3/10/10/10	0/2/2/2
3	A1J4J	B	302	2	-	1/10/10/10	0/2/2/2
3	A1J4J	C	302	-	-	0/10/10/10	0/2/2/2
3	A1J4J	D	303	2	-	0/10/10/10	0/2/2/2
4	EDO	D	302	-	-	0/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	A1J4J	S8-N12	24.87	1.85	1.58
3	B	302	A1J4J	S8-N12	19.71	1.80	1.58
3	D	303	A1J4J	S8-N12	16.91	1.77	1.58
3	A	302	A1J4J	O10-S8	16.29	1.55	1.42
3	A	302	A1J4J	O11-S8	15.29	1.54	1.42
3	D	303	A1J4J	O10-S8	14.98	1.54	1.42
3	C	302	A1J4J	O11-S8	14.21	1.53	1.42
3	C	302	A1J4J	S8-N12	13.71	1.73	1.58
3	C	302	A1J4J	O10-S8	13.52	1.53	1.42
3	D	303	A1J4J	O11-S8	11.17	1.51	1.42
3	B	302	A1J4J	O10-S8	8.70	1.49	1.42
3	D	303	A1J4J	O7-S8	8.52	1.71	1.61
3	B	302	A1J4J	O11-S8	7.98	1.48	1.42
3	B	302	A1J4J	O7-S8	6.66	1.69	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	A1J4J	O7-S8	6.29	1.68	1.61
3	A	302	A1J4J	O7-S8	4.05	1.66	1.61
3	D	303	A1J4J	O7-C1	-3.03	1.36	1.42
3	C	302	A1J4J	O7-C1	-2.47	1.37	1.42
3	C	302	A1J4J	C27-C20	2.01	1.43	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	A1J4J	O10-S8-N12	23.26	144.28	109.14
3	B	302	A1J4J	O11-S8-O10	-20.81	100.28	119.97
3	A	302	A1J4J	O10-S8-N12	20.23	139.71	109.14
3	D	303	A1J4J	O11-S8-O10	-13.97	106.75	119.97
3	A	302	A1J4J	O11-S8-O10	-12.22	108.40	119.97
3	C	302	A1J4J	O11-S8-O10	-11.83	108.78	119.97
3	B	302	A1J4J	O7-S8-N12	-6.62	90.21	106.61
3	A	302	A1J4J	O7-S8-N12	-5.86	92.10	106.61
3	B	302	A1J4J	C1-O7-S8	-5.79	107.41	118.50
3	A	302	A1J4J	C3-C2-C1	5.33	124.96	118.73
3	A	302	A1J4J	O11-S8-N12	-5.17	101.32	109.14
3	B	302	A1J4J	C6-C1-C2	-5.15	113.58	120.32
3	B	302	A1J4J	O7-C1-C6	4.88	128.13	119.32
3	B	302	A1J4J	C3-C2-C1	4.78	124.31	118.73
3	D	303	A1J4J	O7-S8-N12	4.09	116.74	106.61
3	B	302	A1J4J	O11-S8-N12	-4.04	103.04	109.14
3	A	302	A1J4J	C6-C1-C2	-3.16	116.19	120.32
3	C	302	A1J4J	C19-S9-C2	-3.06	97.19	102.73
3	A	302	A1J4J	C1-O7-S8	-2.94	112.87	118.50
3	D	303	A1J4J	O7-C1-C6	2.72	124.23	119.32
3	A	302	A1J4J	O7-C1-C6	2.72	124.23	119.32
3	C	302	A1J4J	O7-C1-C2	-2.65	117.02	119.31
3	D	303	A1J4J	O7-C1-C2	-2.54	117.11	119.31
3	C	302	A1J4J	O7-C1-C6	2.53	123.89	119.32
3	B	302	A1J4J	C5-C6-C1	2.51	124.33	119.71
3	C	302	A1J4J	O7-S8-O11	2.10	111.65	105.27
3	D	303	A1J4J	C19-S9-C2	-2.08	98.97	102.73
3	B	302	A1J4J	C19-S9-C2	-2.02	99.06	102.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	A1J4J	C1-O7-S8-N12
3	B	302	A1J4J	C1-O7-S8-N12
3	A	302	A1J4J	S9-C19-C20-C27
3	A	302	A1J4J	S9-C19-C20-C23

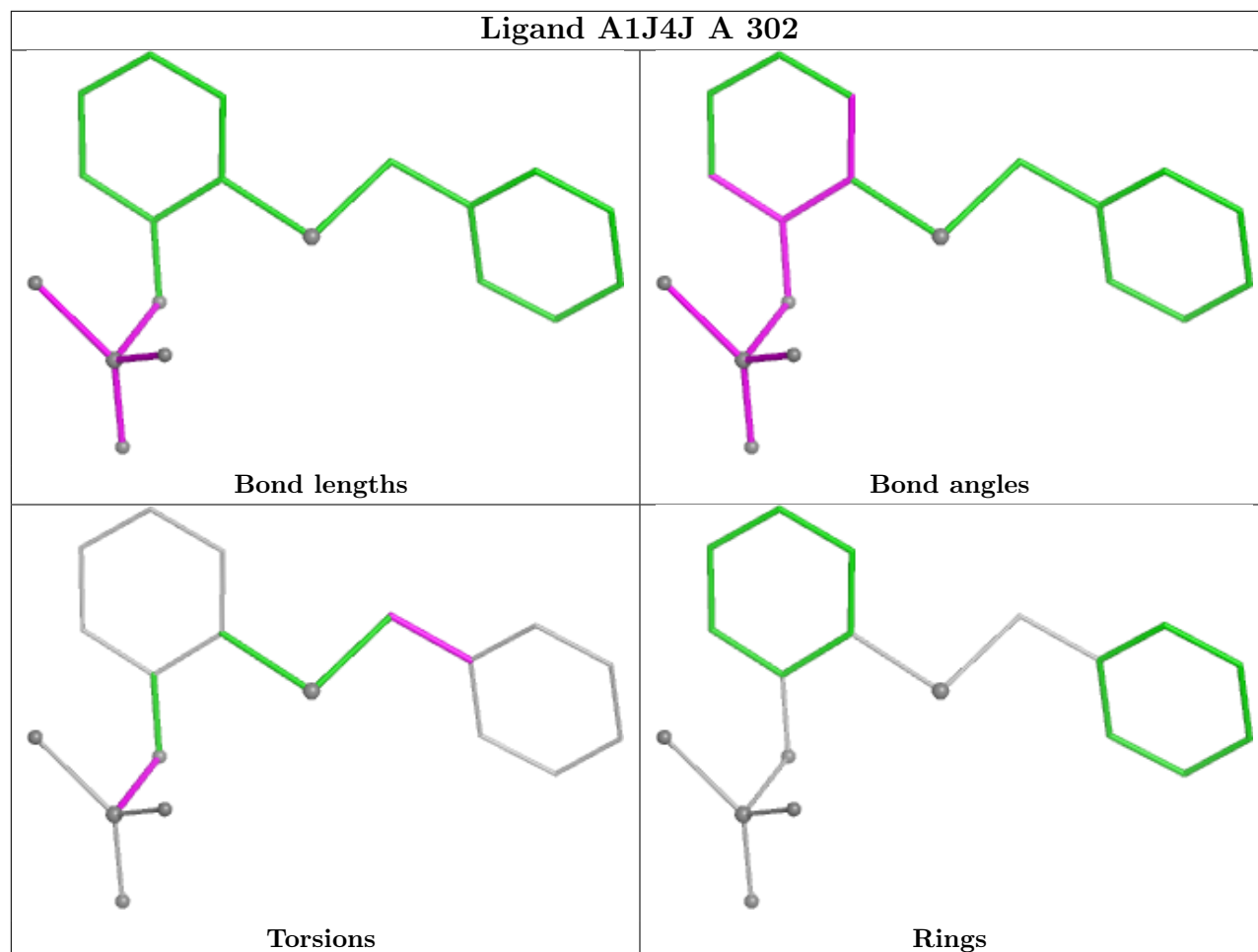
There are no ring outliers.

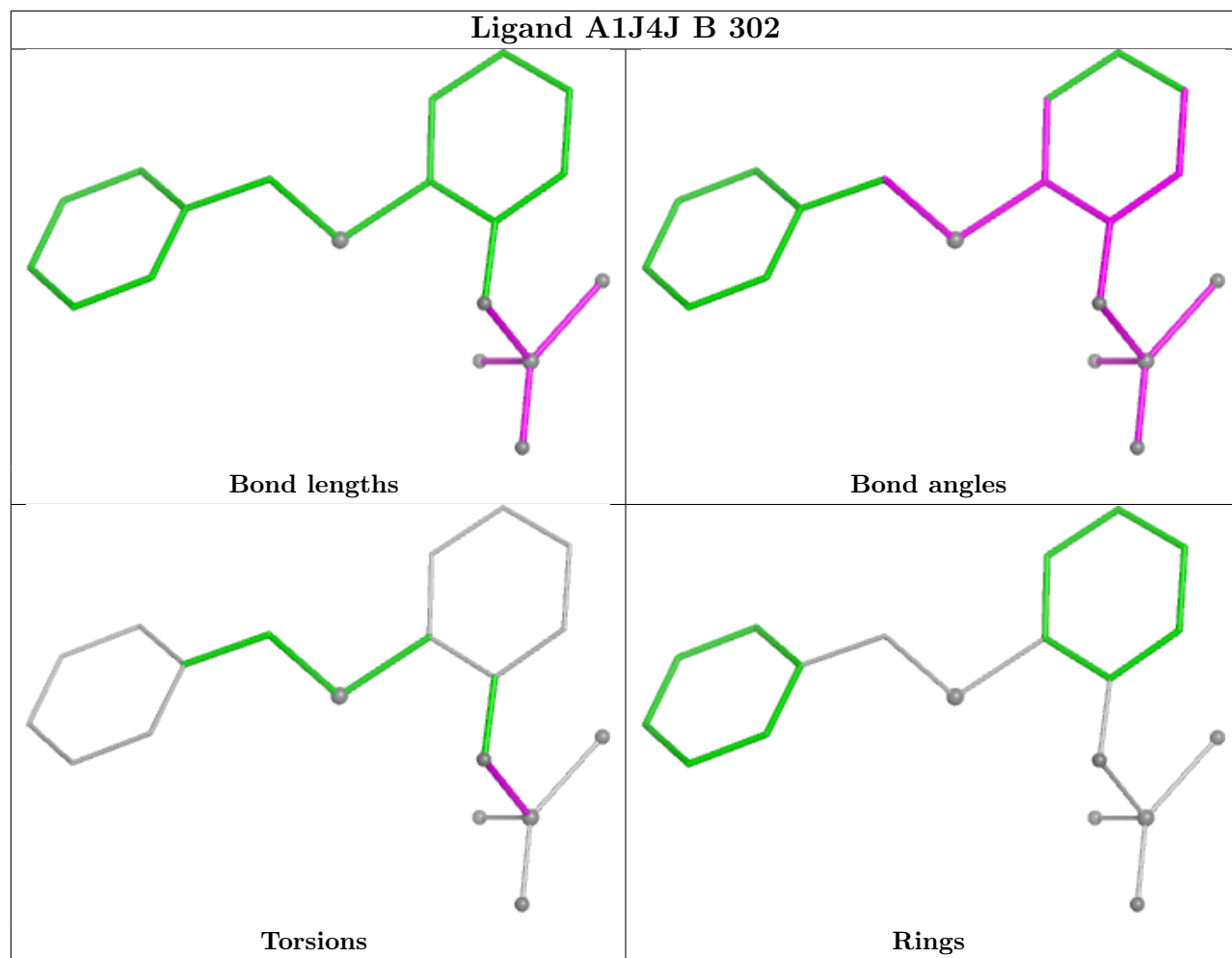
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	A1J4J	1	0
3	B	302	A1J4J	1	0

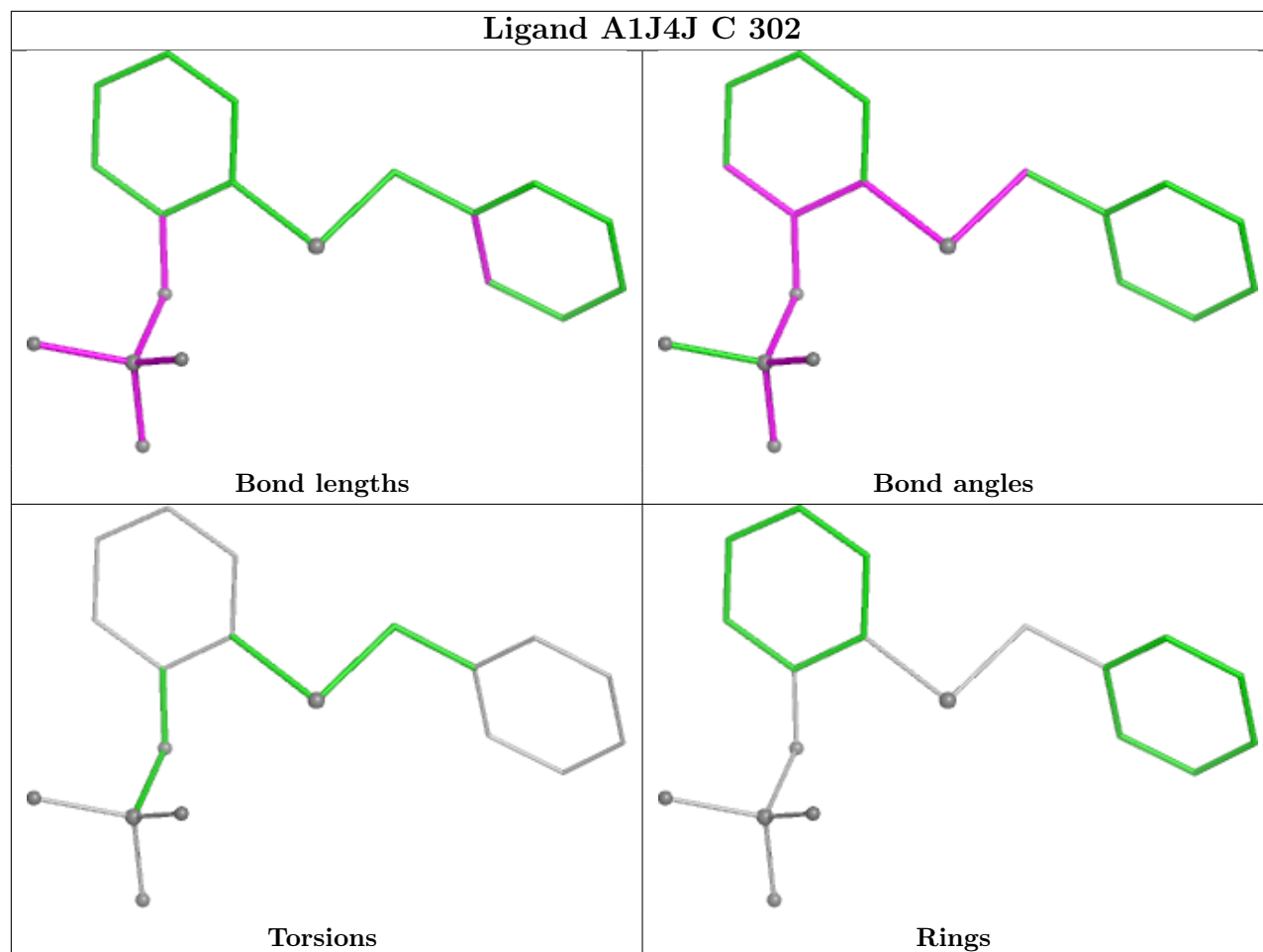
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

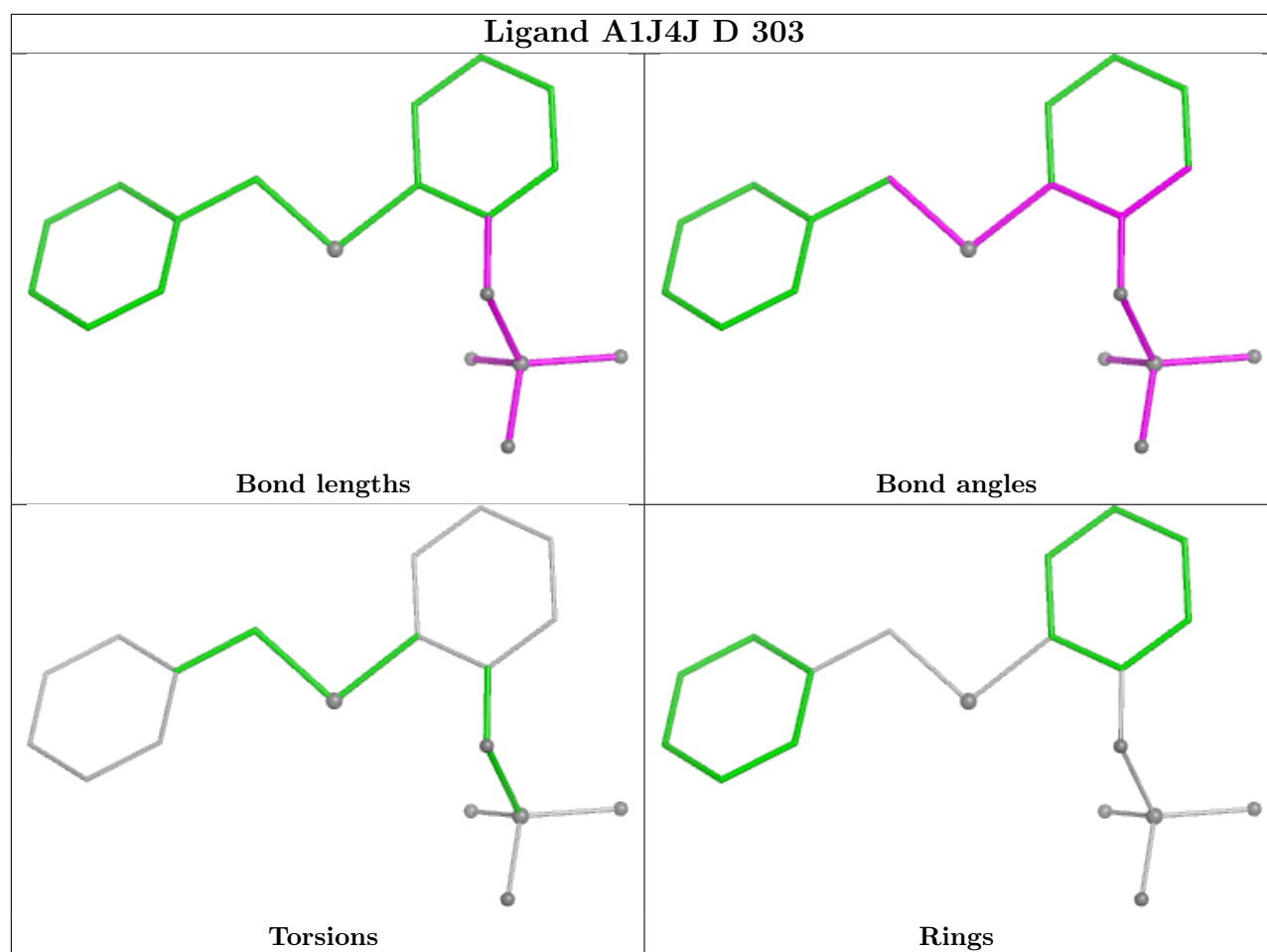
Ligand A1J4J A 302





Ligand A1J4J C 302





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	260/263 (98%)	0.66	19 (7%)	21 23	15, 30, 48, 68	2 (0%)
1	B	261/263 (99%)	0.80	30 (11%)	9 9	13, 25, 48, 67	3 (1%)
1	C	261/263 (99%)	0.78	29 (11%)	10 10	12, 31, 54, 76	2 (0%)
1	D	261/263 (99%)	0.54	11 (4%)	40 44	14, 25, 43, 70	1 (0%)
All	All	1043/1052 (99%)	0.69	89 (8%)	16 17	12, 27, 50, 76	8 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	GLN	5.6
1	B	81	LEU	5.5
1	C	7	PHE	4.7
1	B	65	GLY	4.6
1	A	78	ILE	4.4
1	A	253	ASP	4.3
1	B	84	ARG	4.2
1	C	169	GLY	4.1
1	B	83	SER	4.1
1	A	67[A]	SER	3.8
1	B	79	GLN	3.7
1	A	231	CYS	3.7
1	C	167	TYR	3.5
1	B	40	ASP	3.4
1	C	56	ASN	3.4
1	B	80	GLY	3.4
1	D	65	GLY	3.4
1	B	131	THR	3.3
1	C	57	LYS	3.3
1	A	55	ALA	3.3
1	C	174	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	8	GLY	3.2
1	B	126	TYR	3.1
1	D	238	SER	3.1
1	B	134	ASN	3.0
1	B	263	GLN	2.9
1	C	55	ALA	2.9
1	C	231	CYS	2.9
1	B	252	PHE	2.8
1	D	7	PHE	2.8
1	C	219	GLN	2.8
1	A	3	LYS	2.8
1	C	3	LYS	2.8
1	B	64	ASN	2.7
1	B	254	GLU	2.7
1	B	127	PRO	2.7
1	D	262	SER	2.7
1	A	240	ARG	2.7
1	C	41	ALA	2.7
1	D	80	GLY	2.7
1	B	125	LEU	2.6
1	A	8	GLY	2.6
1	A	185	GLU	2.6
1	B	3	LYS	2.6
1	D	55	ALA	2.5
1	A	54	SER	2.5
1	B	136	SER	2.5
1	C	185	GLU	2.5
1	B	253	ASP	2.5
1	C	161	HIS	2.5
1	A	56	ASN	2.4
1	B	7	PHE	2.4
1	C	45	PRO	2.4
1	C	165	VAL	2.4
1	C	230	TYR	2.4
1	A	7	PHE	2.4
1	C	175	PRO	2.4
1	A	125	LEU	2.3
1	C	176	GLY	2.3
1	C	49	GLN	2.3
1	C	59	PHE	2.3
1	A	233	HIS	2.3
1	B	121	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	173	PHE	2.2
1	C	172	ALA	2.2
1	D	252	PHE	2.2
1	C	263	GLN	2.2
1	C	234	MET	2.2
1	B	120	HIS	2.2
1	C	11	GLY	2.2
1	D	87	ALA	2.2
1	B	75	ASP	2.2
1	D	253	ASP	2.2
1	A	57	LYS	2.2
1	B	42	SER	2.1
1	C	54	SER	2.1
1	A	79	GLN	2.1
1	C	173	PHE	2.1
1	A	131	THR	2.1
1	A	176	GLY	2.1
1	D	185	GLU	2.1
1	C	60	LEU	2.1
1	C	235	ASP	2.0
1	B	47	GLU	2.0
1	B	67	SER	2.0
1	A	148	MET	2.0
1	B	78	ILE	2.0
1	B	44	THR	2.0
1	D	263	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

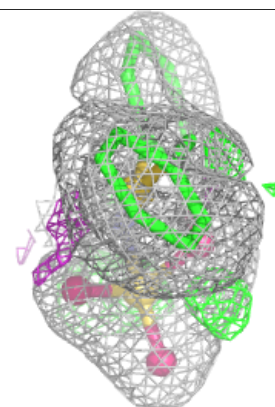
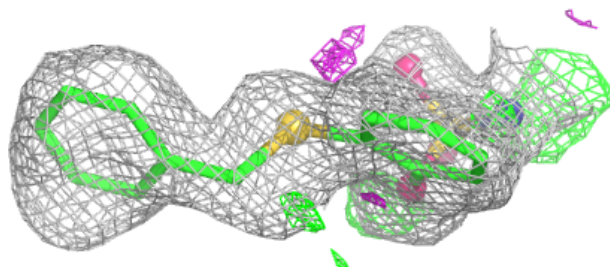
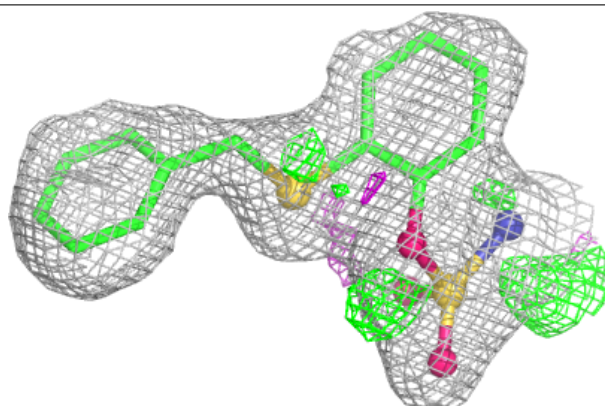
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	D	302	4/4	0.80	0.18	32,34,39,39	0
3	A1J4J	B	302	19/19	0.93	0.10	15,28,46,48	0
3	A1J4J	D	303	19/19	0.95	0.10	22,28,46,46	0
3	A1J4J	A	302	19/19	0.95	0.09	18,32,51,51	0
3	A1J4J	C	302	19/19	0.96	0.08	28,36,48,49	0
2	ZN	B	301	1/1	0.98	0.03	18,18,18,18	0
2	ZN	D	301	1/1	0.99	0.02	16,16,16,16	0
2	ZN	A	301	1/1	0.99	0.02	20,20,20,20	0
2	ZN	C	301	1/1	0.99	0.02	19,19,19,19	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.

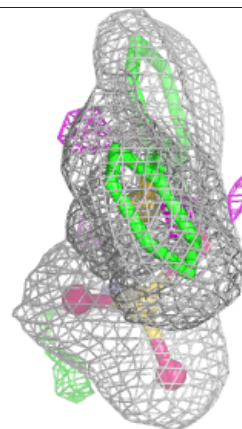
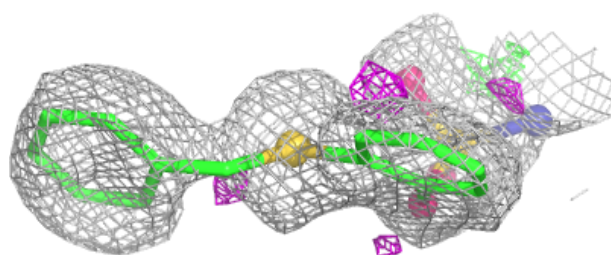
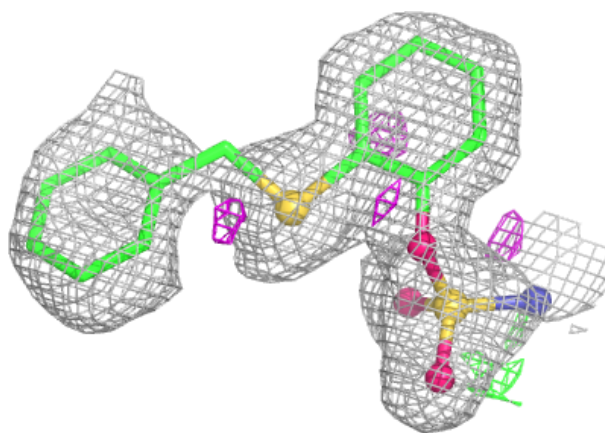
Electron density around A1J4J B 302:

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

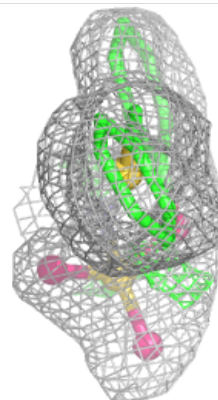
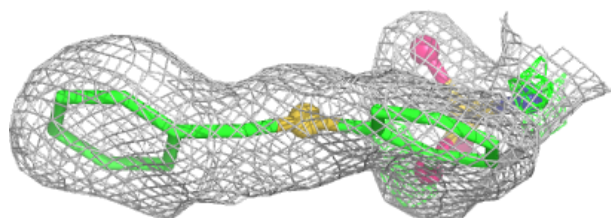
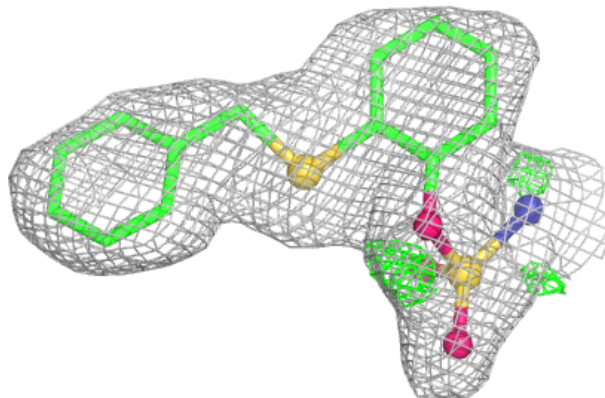


Electron density around A1J4J D 303:

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

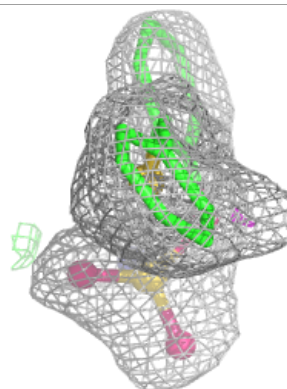
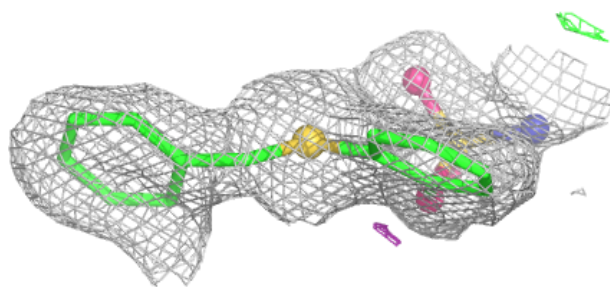
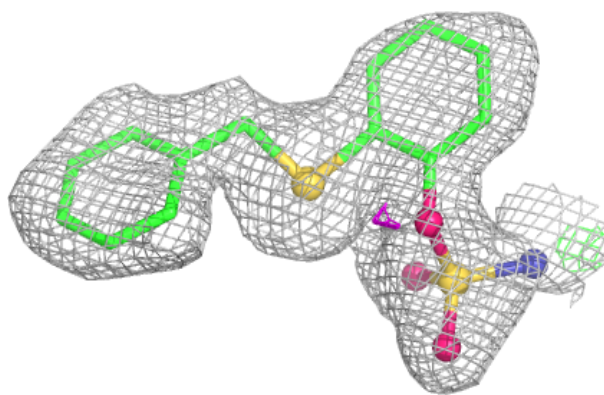
**Electron density around A1J4J A 302:**

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



Electron density around A1J4J 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.