



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 3, 2025 – 06:10 PM JST

PDB ID : 9ISD
Title : Crystal structure of human secretory glutaminyl cyclase in complex with the inhibitor N-(1H-benzo[d]imidazol-5-yl)-1-phenylmethanesulfonamide (compound 5)
Authors : Li, G.-B.; Yu, J.-L.; Zhou, C.; Ning, X.-L.; Mou, J.; Wu, J.-W.; Meng, F.-B.
Deposited on : 2024-07-17
Resolution : 2.37 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

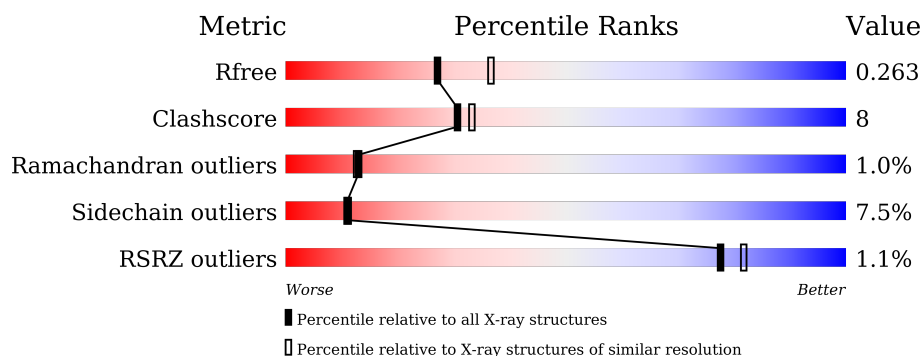
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	361	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	361	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	361	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	361	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	361	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	361	
1	G	361	
1	H	361	
1	I	361	
1	J	361	
1	K	361	
1	L	361	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DMF	C	403	-	-	X	-
7	PEG	E	403	-	-	X	-
7	PEG	J	403	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 63602 atoms, of which 30566 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total	C	H	N	O	S	0	0	0
			5138	1673	2528	450	478	9			
1	B	323	Total	C	H	N	O	S	0	0	0
			5141	1673	2531	450	478	9			
1	C	323	Total	C	H	N	O	S	0	0	0
			5138	1673	2528	450	478	9			
1	D	323	Total	C	H	N	O	S	0	0	0
			5139	1673	2529	450	478	9			
1	E	323	Total	C	H	N	O	S	0	0	0
			5140	1673	2530	450	478	9			
1	F	323	Total	C	H	N	O	S	0	0	0
			5140	1673	2530	450	478	9			
1	G	323	Total	C	H	N	O	S	0	0	0
			5140	1673	2530	450	478	9			
1	H	323	Total	C	H	N	O	S	0	0	0
			5139	1673	2529	450	478	9			
1	I	323	Total	C	H	N	O	S	0	0	0
			5139	1673	2529	450	478	9			
1	J	323	Total	C	H	N	O	S	0	0	0
			5139	1673	2529	450	478	9			
1	K	323	Total	C	H	N	O	S	0	0	0
			5139	1673	2529	450	478	9			
1	L	323	Total	C	H	N	O	S	0	0	0
			5139	1673	2529	450	478	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

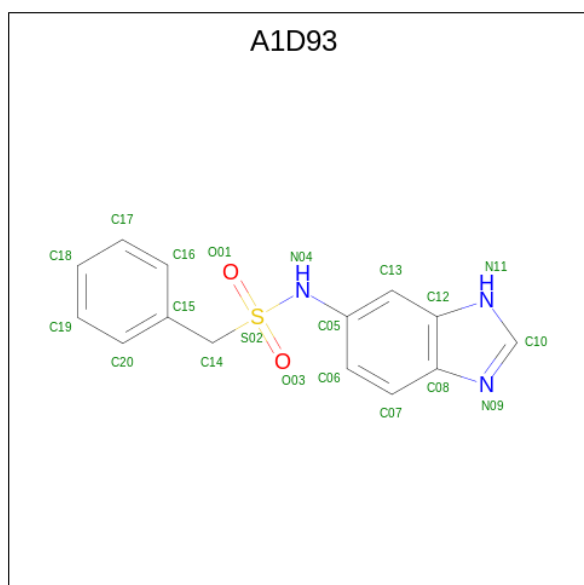
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		
2	G	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	I	1	Total	Zn	0	0
			1	1		
2	J	1	Total	Zn	0	0
			1	1		
2	K	1	Total	Zn	0	0
			1	1		
2	L	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-(1H-benzo[d]imidazol-5-yl)-1-phenylmethanesulfonamide (three-letter code: A1D93) (formula: C₁₄H₁₃N₃O₂S) (labeled as "Ligand of Interest" by depositor).



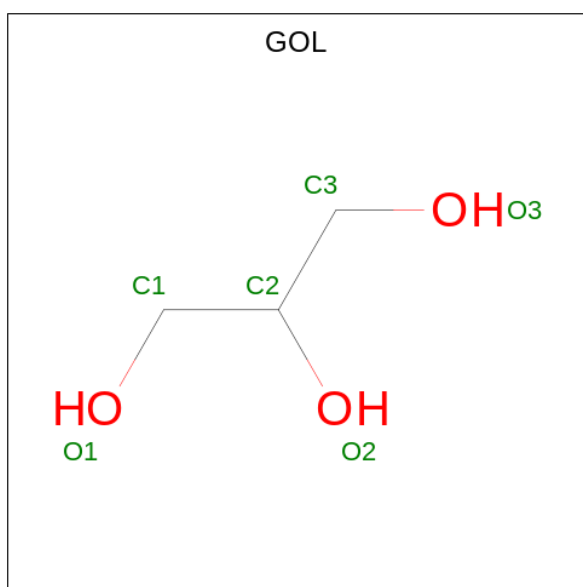
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			33	14	13	3	2	1		

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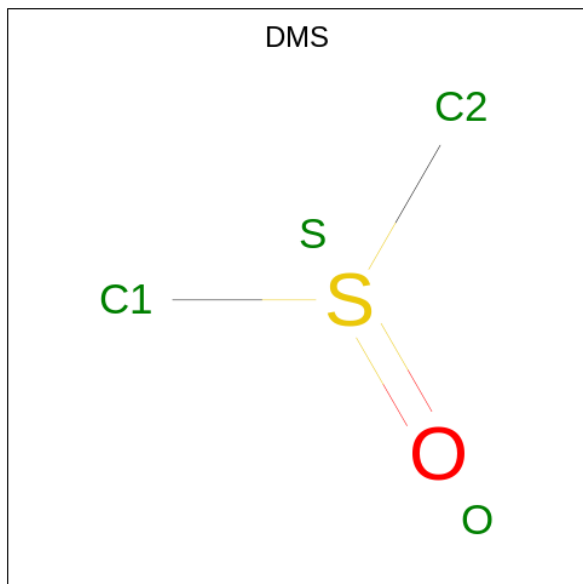
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	C	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	D	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	E	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	F	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	G	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	H	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	I	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	J	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	K	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	L	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



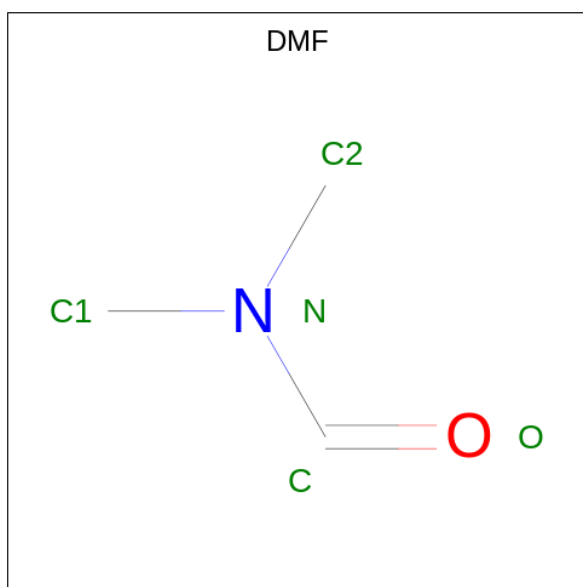
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			11	3	5	3		
4	F	1	Total	C	H	O	0	0
			11	3	5	3		
4	I	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



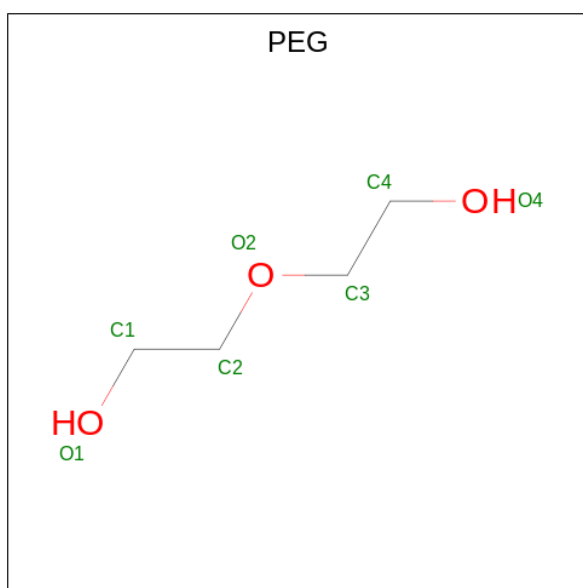
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula: C_3H_7NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			12	3	7	1	1		
6	E	1	Total	C	H	N	O	0	0
			12	3	7	1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	H	O	0	0
			17	4	10	3		
7	E	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	J	1	Total	C	H	O	0	0
			17	4	10	3		

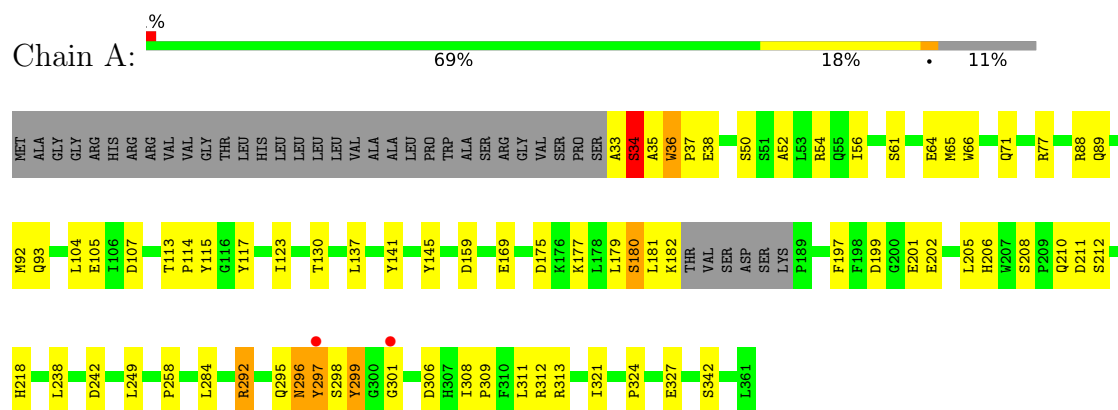
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	145	Total	O	0	0
			145	145		
8	B	148	Total	O	0	0
			148	148		
8	C	131	Total	O	0	0
			131	131		
8	D	115	Total	O	0	0
			115	115		
8	E	128	Total	O	0	0
			128	128		
8	F	120	Total	O	0	0
			120	120		
8	G	109	Total	O	0	0
			109	109		
8	H	123	Total	O	0	0
			123	123		
8	I	81	Total	O	0	0
			81	81		
8	J	85	Total	O	0	0
			85	85		
8	K	120	Total	O	0	0
			120	120		
8	L	102	Total	O	0	0
			102	102		

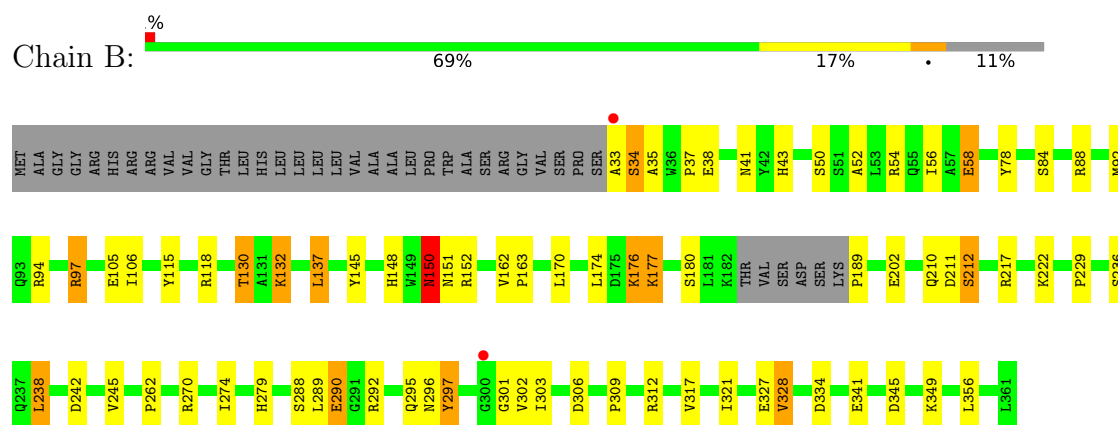
3 Residue-property plots

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.

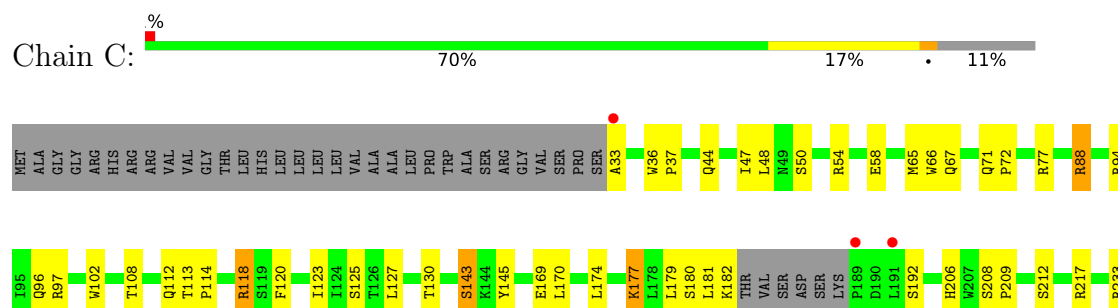
• Molecule 1: Glutaminyl-peptide cyclotransferase

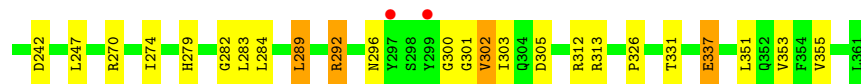


• Molecule 1: Glutaminyl-peptide cyclotransferase

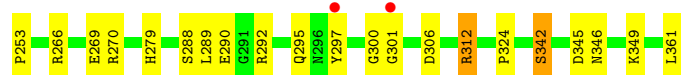
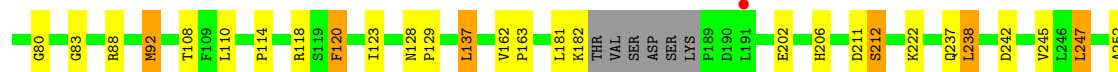
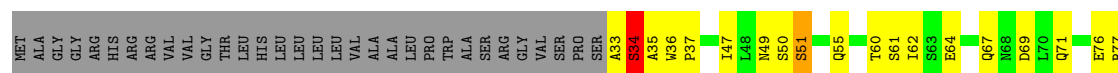


• Molecule 1: Glutaminyl-peptide cyclotransferase

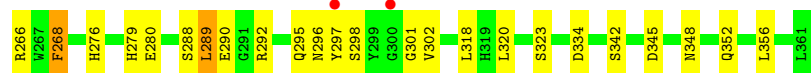
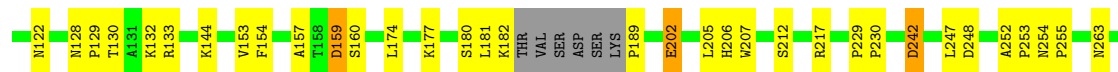
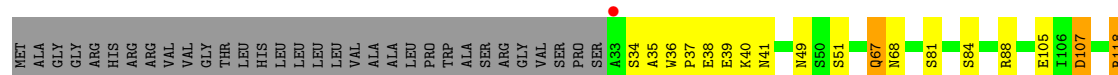




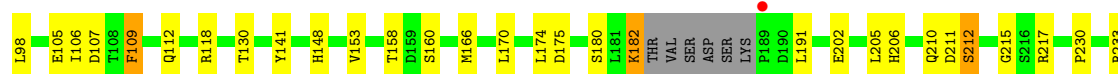
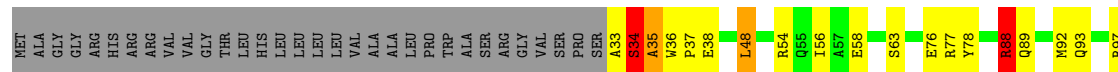
• Molecule 1: Glutaminyl-peptide cyclotransferase



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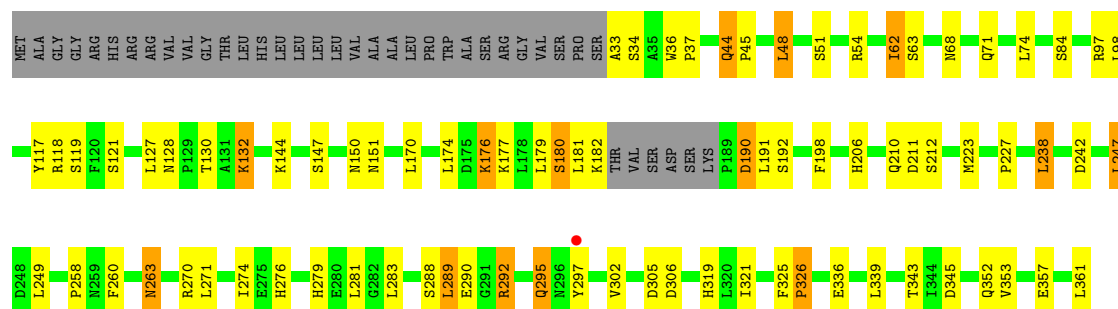


• Molecule 1: Glutaminyl-peptide cyclotransferase

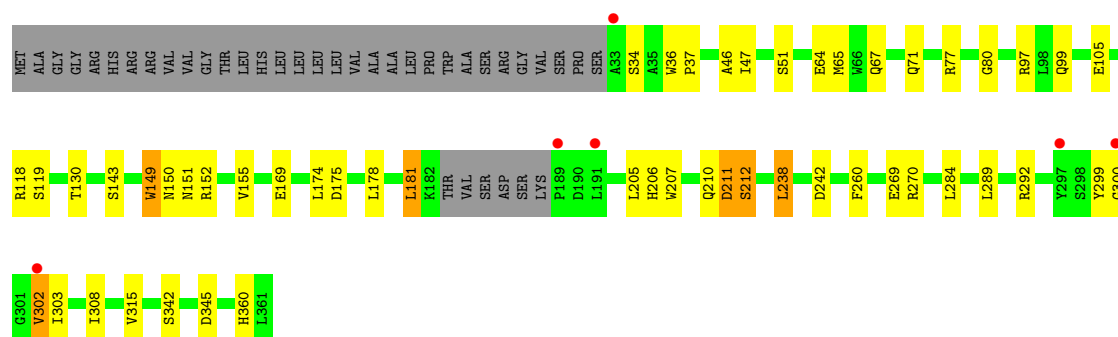
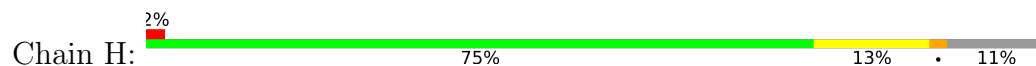


• Molecule 1: Glutaminyl-peptide cyclotransferase

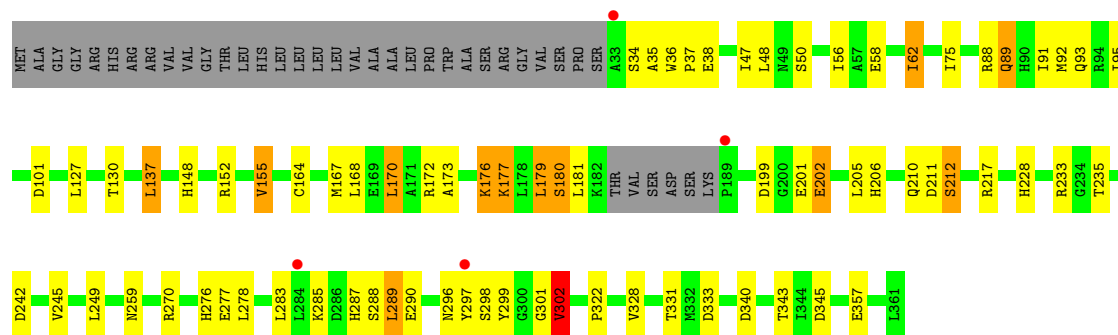




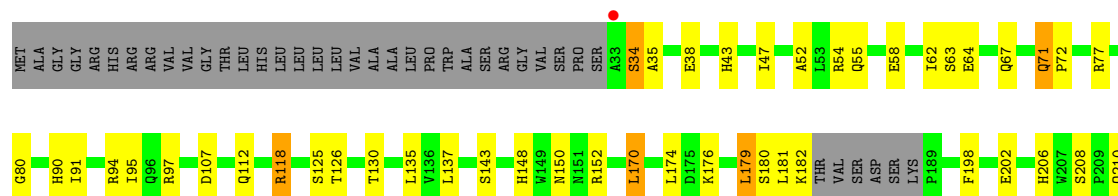
• Molecule 1: Glutaminyl-peptide cyclotransferase



• Molecule 1: Glutaminyl-peptide cyclotransferase



• Molecule 1: Glutaminyl-peptide cyclotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	114.54Å 116.48Å 122.75Å 96.21° 114.92° 109.69°	Depositor
Resolution (Å)	39.21 – 2.37 39.21 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.21-2.37) 98.5 (39.21-2.37)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.189 , 0.262 0.191 , 0.263	Depositor DCC
R_{free} test set	209564 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	63602	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.31% 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: A1D93, PEG, DMS, DMF, 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	1.07	9/2687 (0.3%)	1.05	15/3656 (0.4%)
1	B	1.04	9/2687 (0.3%)	1.04	7/3656 (0.2%)
1	C	1.02	2/2687 (0.1%)	1.02	7/3656 (0.2%)
1	D	0.96	1/2687 (0.0%)	0.96	8/3656 (0.2%)
1	E	1.05	5/2687 (0.2%)	1.03	8/3656 (0.2%)
1	F	1.09	8/2687 (0.3%)	1.04	15/3656 (0.4%)
1	G	0.91	1/2687 (0.0%)	0.92	7/3656 (0.2%)
1	H	1.01	8/2687 (0.3%)	0.94	3/3656 (0.1%)
1	I	0.91	3/2687 (0.1%)	0.91	4/3656 (0.1%)
1	J	0.91	2/2687 (0.1%)	0.93	6/3656 (0.2%)
1	K	1.01	5/2687 (0.2%)	1.03	11/3656 (0.3%)
1	L	0.93	4/2687 (0.1%)	0.96	9/3656 (0.2%)
All	All	0.99	57/32244 (0.2%)	0.99	100/43872 (0.2%)

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	GLU	CG-CD	8.76	1.65	1.51
1	A	201	GLU	CB-CG	7.35	1.66	1.52
1	B	115	TYR	CD2-CE2	7.17	1.50	1.39
1	E	207	TRP	CB-CG	7.17	1.63	1.50
1	C	66	TRP	CB-CG	-7.04	1.37	1.50

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	ARG	NE-CZ-NH2	12.15	126.38	120.30
1	L	312	ARG	NE-CZ-NH1	10.77	125.69	120.30
1	F	238	LEU	CA-CB-CG	9.62	137.44	115.30
1	A	312	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	K	217	ARG	NE-CZ-NH1	8.67	124.63	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2610	2528	2529	31	0
1	B	2610	2531	2529	46	1
1	C	2610	2528	2529	38	0
1	D	2610	2529	2529	35	0
1	E	2610	2530	2529	43	0
1	F	2610	2530	2529	42	0
1	G	2610	2530	2529	54	1
1	H	2610	2529	2529	17	0
1	I	2610	2529	2529	49	0
1	J	2610	2529	2529	48	0
1	K	2610	2529	2529	49	0
1	L	2610	2529	2529	57	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	20	13	0	0	0
3	B	20	13	0	0	0
3	C	20	13	0	0	0
3	D	20	13	0	0	0
3	E	20	13	0	0	0
3	F	20	13	0	0	0
3	G	20	13	0	1	0
3	H	20	13	0	0	0
3	I	20	13	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	20	13	0	0	0
3	K	20	13	0	0	0
3	L	20	13	0	0	0
4	A	6	5	8	2	0
4	F	6	5	8	0	0
4	I	6	5	8	2	0
5	B	4	0	6	3	0
5	D	4	0	6	0	0
6	C	5	7	7	4	0
6	E	5	7	7	2	0
7	D	7	10	10	2	0
7	E	7	10	10	4	0
7	J	7	10	10	4	0
8	A	145	0	0	6	0
8	B	148	0	0	13	0
8	C	131	0	0	6	0
8	D	115	0	0	7	0
8	E	128	0	0	10	0
8	F	120	0	0	2	0
8	G	109	0	0	13	0
8	H	123	0	0	2	0
8	I	81	0	0	6	0
8	J	85	0	0	8	0
8	K	120	0	0	10	0
8	L	102	0	0	7	0
All	All	33036	30566	30428	507	1

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 8.

The worst 5 of 507 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ARG:O	1:A:295:GLN:NE2	1.69	1.25
1:C:312:ARG:NH1	8:C:501:HOH:O	1.72	1.19
1:K:342:SER:O	1:K:346:ASN:ND2	2.02	0.93
1:E:34:SER:OG	8:E:501:HOH:O	1.89	0.90
1:L:60:THR:OG1	1:L:169:GLU:OE2	1.92	0.87

All (1) 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)
1:B:151:ASN:OD1	1:G:33:ALA:N[1_455]	2.13	0.07

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	319/361 (88%)	300 (94%)	17 (5%)	2 (1%)	22	24
1	B	319/361 (88%)	295 (92%)	20 (6%)	4 (1%)	10	8
1	C	319/361 (88%)	298 (93%)	17 (5%)	4 (1%)	10	8
1	D	319/361 (88%)	293 (92%)	25 (8%)	1 (0%)	37	43
1	E	319/361 (88%)	308 (97%)	10 (3%)	1 (0%)	37	43
1	F	319/361 (88%)	293 (92%)	21 (7%)	5 (2%)	8	6
1	G	319/361 (88%)	294 (92%)	21 (7%)	4 (1%)	10	8
1	H	319/361 (88%)	297 (93%)	18 (6%)	4 (1%)	10	8
1	I	319/361 (88%)	295 (92%)	22 (7%)	2 (1%)	22	24
1	J	319/361 (88%)	293 (92%)	24 (8%)	2 (1%)	22	24
1	K	319/361 (88%)	292 (92%)	23 (7%)	4 (1%)	10	8
1	L	319/361 (88%)	285 (89%)	27 (8%)	7 (2%)	5	4
All	All	3828/4332 (88%)	3543 (93%)	245 (6%)	40 (1%)	13	13

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	B	34	SER
1	B	212	SER
1	B	297	TYR
1	B	302	VAL

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	284/314 (90%)	263 (93%)	21 (7%)	11	11
1	B	284/314 (90%)	264 (93%)	20 (7%)	12	13
1	C	284/314 (90%)	263 (93%)	21 (7%)	11	11
1	D	284/314 (90%)	263 (93%)	21 (7%)	11	11
1	E	284/314 (90%)	266 (94%)	18 (6%)	15	16
1	F	284/314 (90%)	265 (93%)	19 (7%)	13	14
1	G	284/314 (90%)	258 (91%)	26 (9%)	7	6
1	H	284/314 (90%)	266 (94%)	18 (6%)	15	16
1	I	284/314 (90%)	262 (92%)	22 (8%)	10	10
1	J	284/314 (90%)	257 (90%)	27 (10%)	7	6
1	K	284/314 (90%)	265 (93%)	19 (7%)	13	14
1	L	284/314 (90%)	260 (92%)	24 (8%)	8	8
All	All	3408/3768 (90%)	3152 (92%)	256 (8%)	11	11

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	360	HIS
1	L	125	SER
1	E	296	ASN
1	E	288	SER
1	L	160	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	279	HIS
1	L	89	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 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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	A1D93	C	402	2	19,22,22	1.38	4 (21%)	23,31,31	2.71	5 (21%)
3	A1D93	J	402	2	19,22,22	1.67	5 (26%)	23,31,31	2.78	4 (17%)
6	DMF	C	403	-	4,4,4	1.00	0	4,4,4	1.32	1 (25%)
7	PEG	D	404	-	6,6,6	0.74	0	5,5,5	0.65	0
6	DMF	E	404	-	4,4,4	0.54	0	4,4,4	0.34	0
3	A1D93	A	402	2	19,22,22	1.72	4 (21%)	23,31,31	2.07	6 (26%)
3	A1D93	L	401	2	19,22,22	1.57	3 (15%)	23,31,31	1.54	5 (21%)
4	GOL	A	403	-	5,5,5	0.69	0	5,5,5	1.96	2 (40%)
5	DMS	B	403	-	3,3,3	0.71	0	3,3,3	1.76	2 (66%)
3	A1D93	D	402	2	19,22,22	1.72	4 (21%)	23,31,31	1.65	4 (17%)
3	A1D93	B	402	2	19,22,22	1.72	6 (31%)	23,31,31	1.75	6 (26%)
3	A1D93	I	402	2	19,22,22	1.59	4 (21%)	23,31,31	2.38	6 (26%)
7	PEG	J	403	-	6,6,6	0.88	0	5,5,5	0.91	0
3	A1D93	H	401	2	19,22,22	1.98	5 (26%)	23,31,31	4.30	7 (30%)
3	A1D93	E	402	2	19,22,22	1.27	2 (10%)	23,31,31	1.94	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1D93	G	401	2	19,22,22	1.92	4 (21%)	23,31,31	2.02	5 (21%)
4	GOL	F	403	-	5,5,5	0.71	0	5,5,5	1.24	0
5	DMS	D	403	-	3,3,3	0.86	0	3,3,3	1.79	1 (33%)
3	A1D93	F	402	2	19,22,22	2.07	7 (36%)	23,31,31	2.40	5 (21%)
3	A1D93	K	401	2	19,22,22	1.44	3 (15%)	23,31,31	2.69	6 (26%)
7	PEG	E	403	-	6,6,6	1.54	1 (16%)	5,5,5	1.63	2 (40%)
4	GOL	I	403	-	5,5,5	0.81	0	5,5,5	0.74	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	A1D93	C	402	2	-	0/10/10/10	0/3/3/3
3	A1D93	J	402	2	-	2/10/10/10	0/3/3/3
6	DMF	C	403	-	-	0/2/2/2	-
7	PEG	D	404	-	-	2/4/4/4	-
6	DMF	E	404	-	-	2/2/2/2	-
3	A1D93	A	402	2	-	0/10/10/10	0/3/3/3
3	A1D93	L	401	2	-	0/10/10/10	0/3/3/3
4	GOL	A	403	-	-	2/4/4/4	-
3	A1D93	D	402	2	-	0/10/10/10	0/3/3/3
3	A1D93	B	402	2	-	2/10/10/10	0/3/3/3
3	A1D93	I	402	2	-	2/10/10/10	0/3/3/3
7	PEG	J	403	-	-	1/4/4/4	-
3	A1D93	H	401	2	-	4/10/10/10	0/3/3/3
3	A1D93	E	402	2	-	0/10/10/10	0/3/3/3
3	A1D93	G	401	2	-	0/10/10/10	0/3/3/3
4	GOL	F	403	-	-	2/4/4/4	-
3	A1D93	F	402	2	-	1/10/10/10	0/3/3/3
3	A1D93	K	401	2	-	3/10/10/10	0/3/3/3
7	PEG	E	403	-	-	2/4/4/4	-
4	GOL	I	403	-	-	0/4/4/4	-

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	401	A1D93	S02-N04	4.94	1.72	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	401	A1D93	O01-S02	4.69	1.50	1.43
3	D	402	A1D93	S02-N04	4.68	1.72	1.62
3	H	401	A1D93	O03-S02	4.67	1.50	1.43
3	A	402	A1D93	O01-S02	3.86	1.49	1.43

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	A1D93	O01-S02-C14	-16.57	83.07	108.30
3	J	402	A1D93	O03-S02-O01	-11.47	102.73	119.35
3	K	401	A1D93	O03-S02-O01	-9.98	104.90	119.35
3	H	401	A1D93	O03-S02-O01	-8.54	106.98	119.35
3	C	402	A1D93	O03-S02-O01	-8.42	107.15	119.35

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	401	A1D93	S02-C14-C15-C20
3	H	401	A1D93	S02-C14-C15-C16
4	F	403	GOL	O1-C1-C2-C3
7	D	404	PEG	O1-C1-C2-O2
7	D	404	PEG	O2-C3-C4-O4

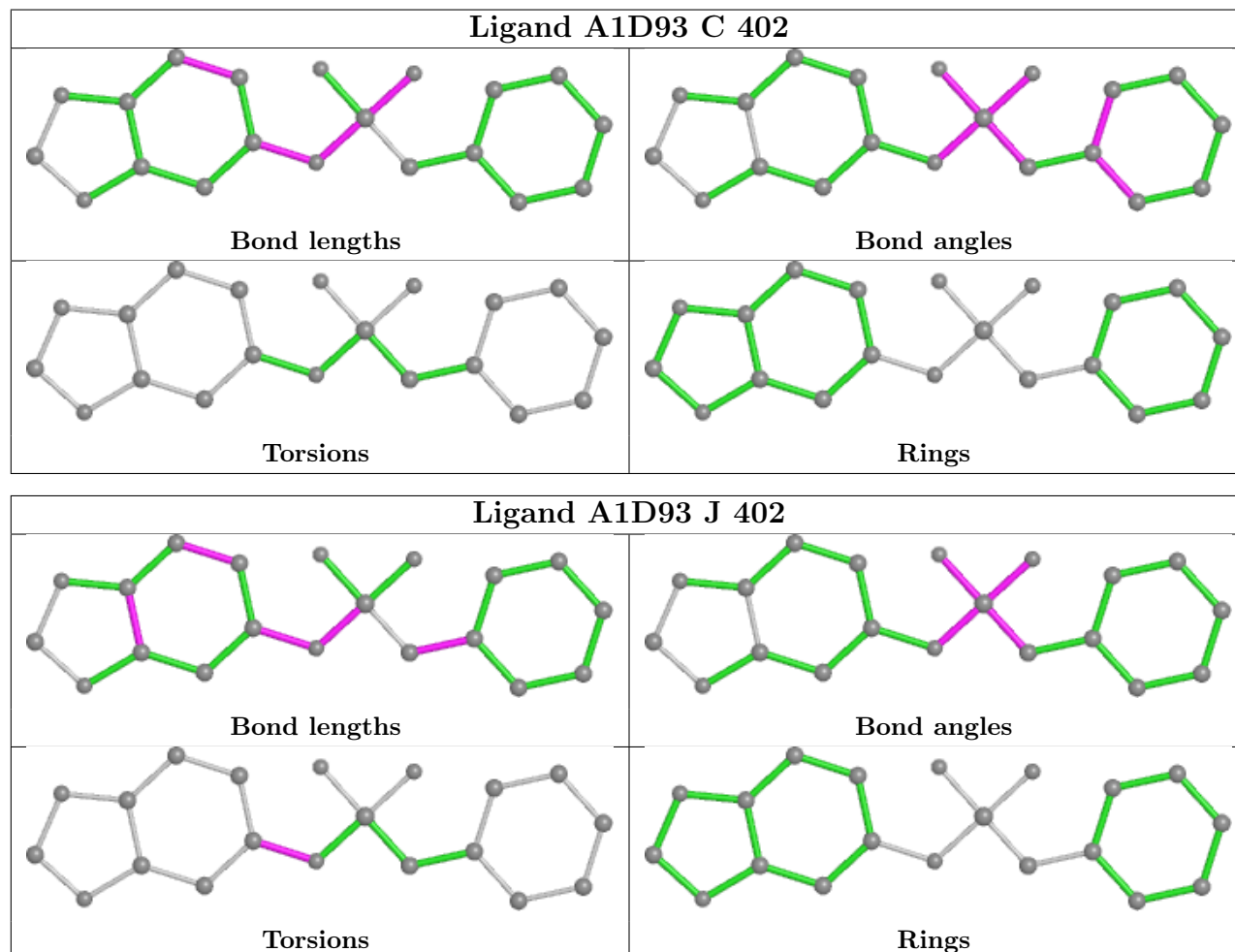
There are no ring outliers.

10 monomers are involved in 25 short contacts:

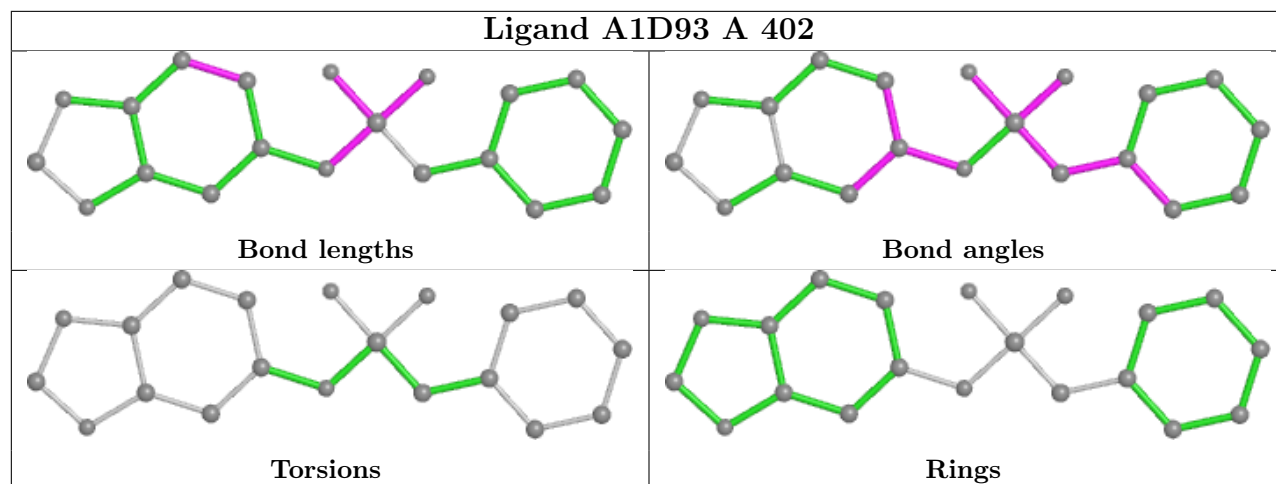
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	403	DMF	4	0
7	D	404	PEG	2	0
6	E	404	DMF	2	0
4	A	403	GOL	2	0
5	B	403	DMS	3	0
3	I	402	A1D93	1	0
7	J	403	PEG	4	0
3	G	401	A1D93	1	0
7	E	403	PEG	4	0
4	I	403	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

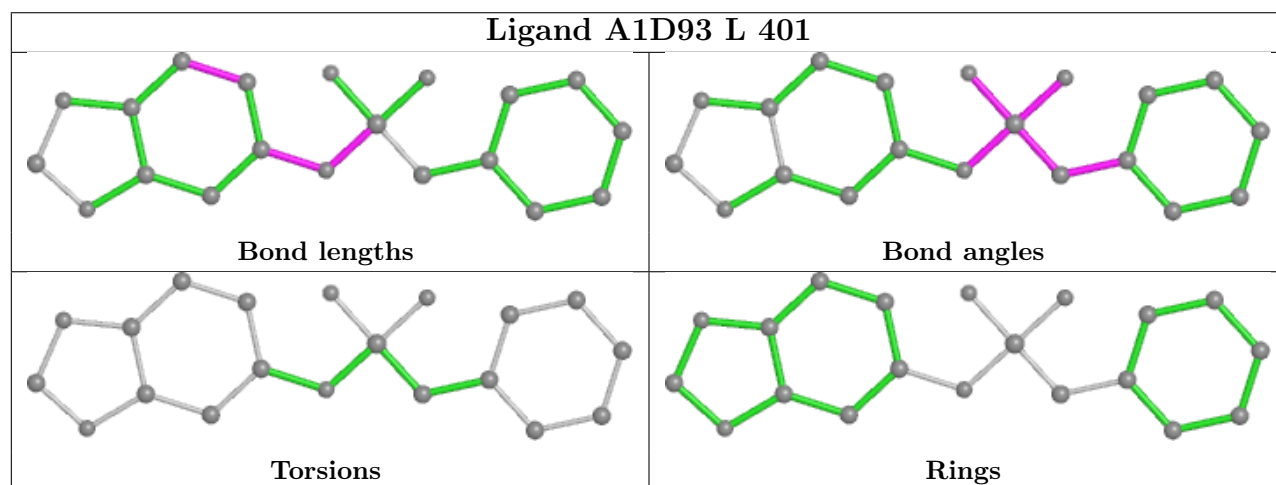
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



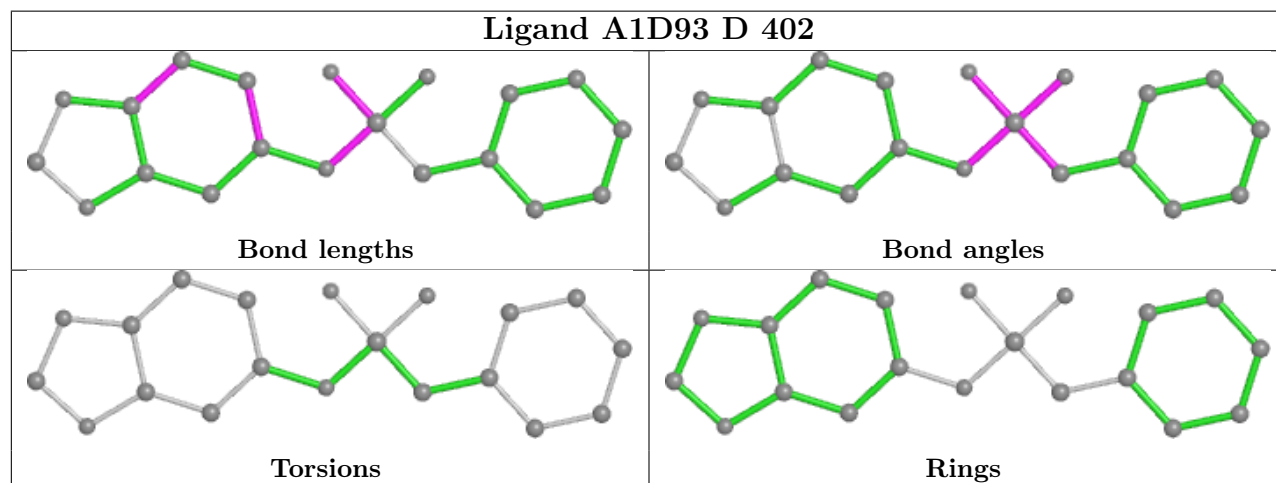
Ligand A1D93 A 402



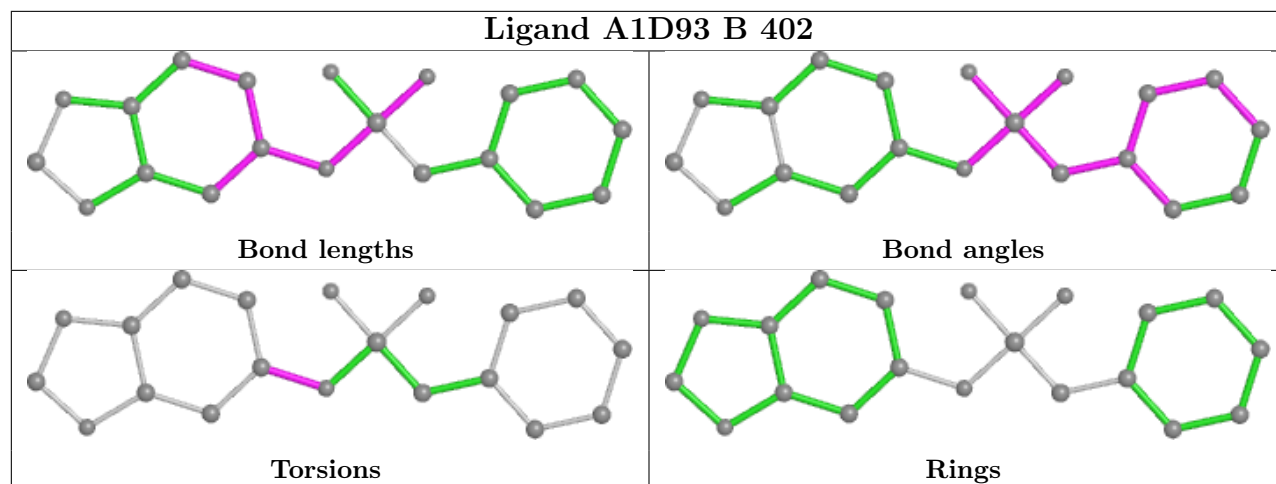
Ligand A1D93 L 401



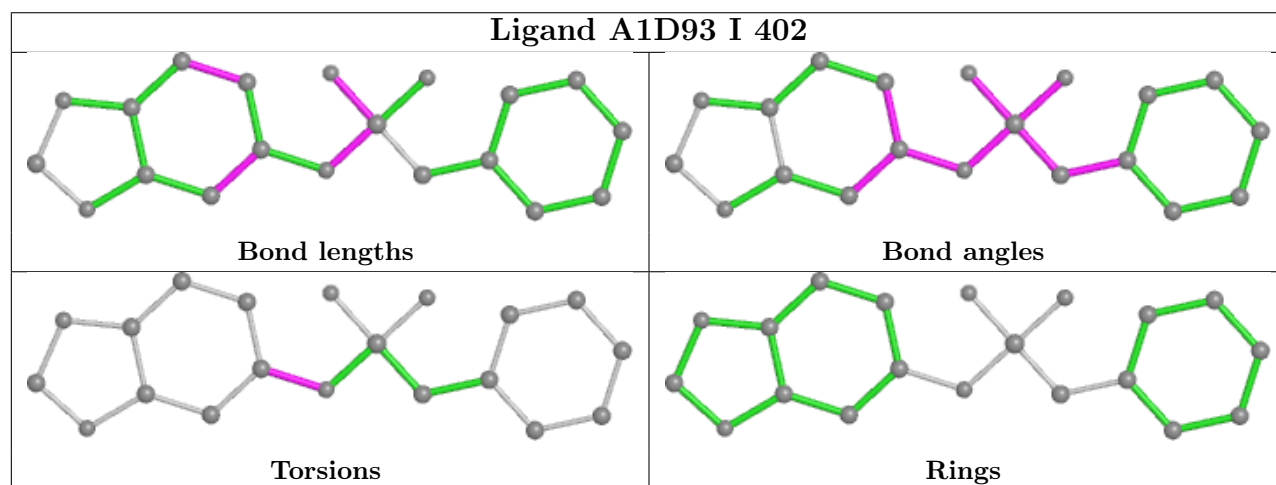
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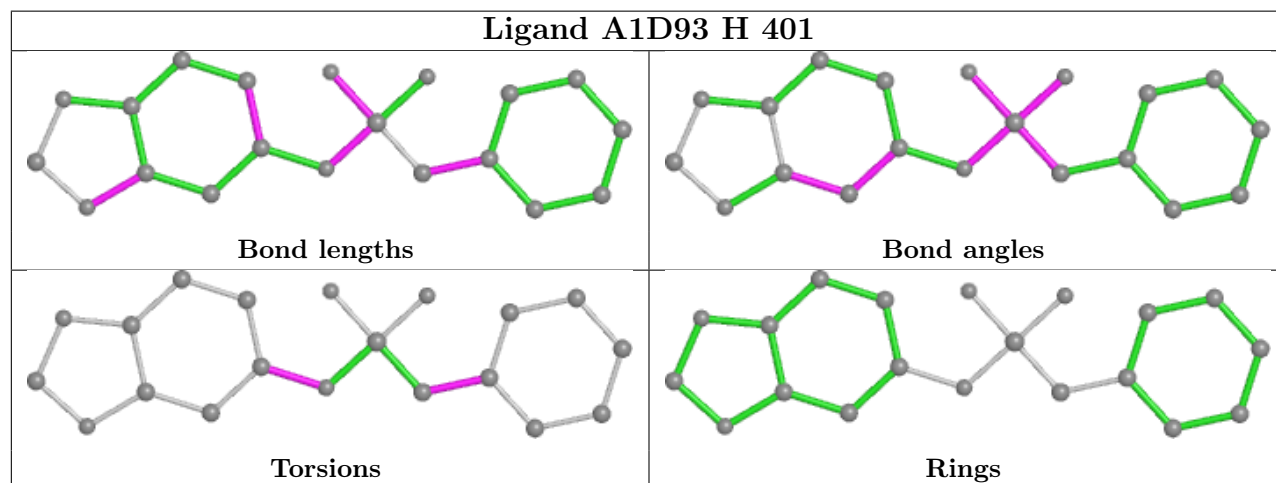
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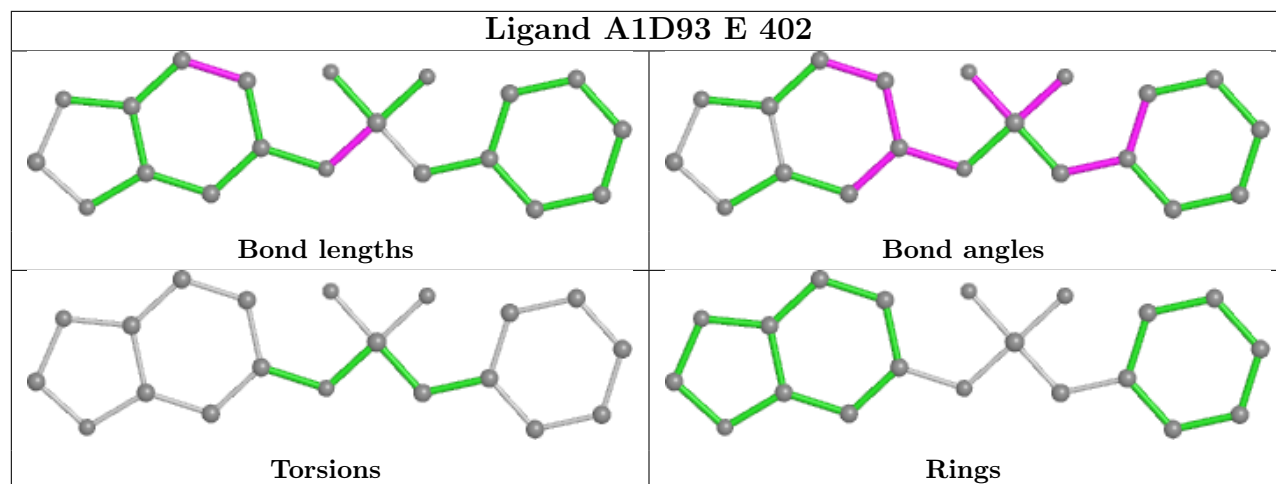
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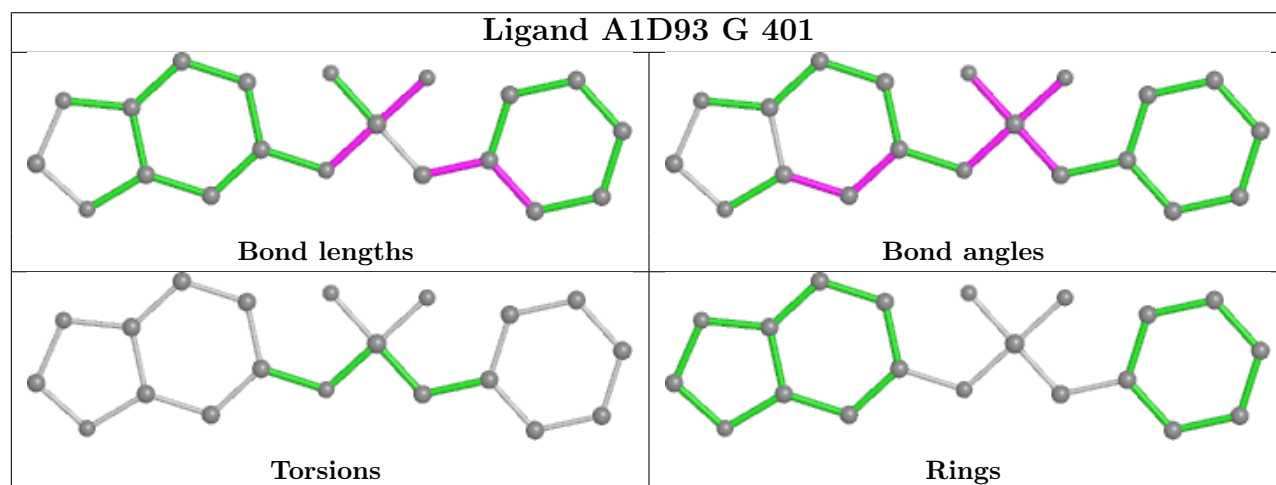
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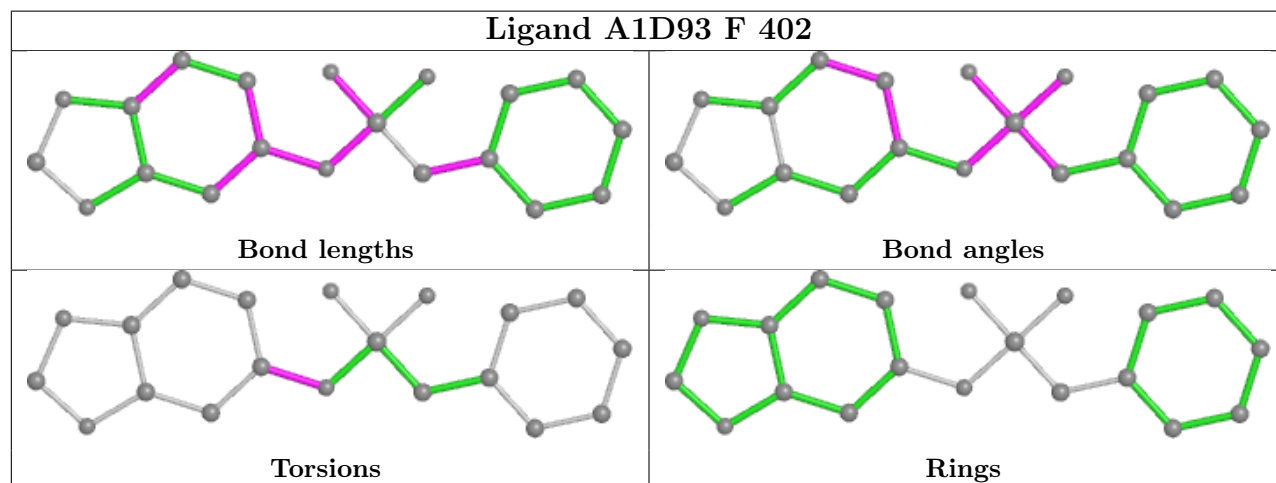
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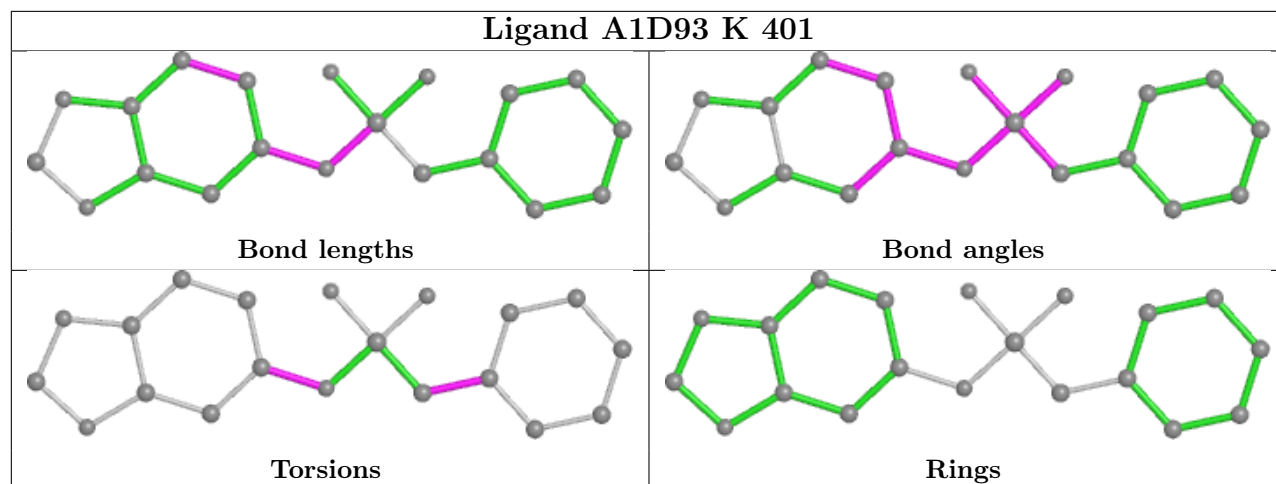


Ligand A1D93 G 401



Ligand A1D93 F 402





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/361 (89%)	-0.54	2 (0%) 85 88	34, 48, 73, 110	0
1	B	323/361 (89%)	-0.46	2 (0%) 85 88	32, 48, 71, 101	0
1	C	323/361 (89%)	-0.31	5 (1%) 71 76	37, 51, 77, 114	0
1	D	323/361 (89%)	-0.37	3 (0%) 81 84	32, 53, 81, 115	0
1	E	323/361 (89%)	-0.37	3 (0%) 81 84	29, 50, 75, 114	0
1	F	323/361 (89%)	-0.33	2 (0%) 85 88	36, 52, 79, 101	0
1	G	323/361 (89%)	-0.18	1 (0%) 90 91	35, 58, 88, 110	0
1	H	323/361 (89%)	-0.30	6 (1%) 66 71	35, 54, 81, 117	0
1	I	323/361 (89%)	-0.08	4 (1%) 76 80	41, 60, 90, 111	0
1	J	323/361 (89%)	-0.14	3 (0%) 81 84	38, 62, 93, 126	0
1	K	323/361 (89%)	-0.25	4 (1%) 76 80	38, 54, 81, 113	0
1	L	323/361 (89%)	-0.14	8 (2%) 58 64	37, 58, 85, 126	0
All	All	3876/4332 (89%)	-0.29	43 (1%) 77 82	29, 54, 84, 126	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	33	ALA	4.2
1	K	33	ALA	3.8
1	L	297	TYR	3.5
1	B	300	GLY	3.4
1	I	297	TYR	3.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	DMS	D	403	4/4	0.69	0.21	57,63,73,101	0
5	DMS	B	403	4/4	0.76	0.21	47,60,74,95	0
4	GOL	I	403	6/6	0.85	0.14	50,59,71,72	0
4	GOL	A	403	6/6	0.89	0.12	39,51,66,74	0
7	PEG	J	403	7/7	0.89	0.12	42,52,72,72	0
7	PEG	E	403	7/7	0.90	0.14	41,54,66,66	0
7	PEG	D	404	7/7	0.90	0.19	47,60,68,76	0
6	DMF	E	404	5/5	0.91	0.14	46,55,63,64	0
6	DMF	C	403	5/5	0.91	0.13	51,63,68,68	0
4	GOL	F	403	6/6	0.92	0.09	46,55,66,69	0
3	A1D93	K	401	20/20	0.95	0.07	37,48,58,63	0
3	A1D93	C	402	20/20	0.96	0.07	37,48,57,64	0
3	A1D93	G	401	20/20	0.97	0.07	34,50,69,70	0
3	A1D93	H	401	20/20	0.97	0.08	33,47,67,70	0
3	A1D93	I	402	20/20	0.97	0.09	41,54,77,85	0
3	A1D93	J	402	20/20	0.97	0.08	40,52,67,68	0
3	A1D93	D	402	20/20	0.97	0.07	37,49,61,66	0
3	A1D93	L	401	20/20	0.97	0.07	36,53,74,87	0
3	A1D93	E	402	20/20	0.97	0.07	36,49,66,73	0
3	A1D93	F	402	20/20	0.97	0.06	35,48,61,64	0
3	A1D93	A	402	20/20	0.98	0.06	29,45,57,65	0
3	A1D93	B	402	20/20	0.98	0.06	31,41,59,69	0
2	ZN	I	401	1/1	0.99	0.04	47,47,47,47	0
2	ZN	B	401	1/1	1.00	0.02	40,40,40,40	0
2	ZN	C	401	1/1	1.00	0.01	35,35,35,35	0
2	ZN	D	401	1/1	1.00	0.03	42,42,42,42	0
2	ZN	E	401	1/1	1.00	0.03	39,39,39,39	0
2	ZN	F	401	1/1	1.00	0.05	42,42,42,42	0
2	ZN	G	400	1/1	1.00	0.03	43,43,43,43	0
2	ZN	H	400	1/1	1.00	0.04	39,39,39,39	0
2	ZN	A	401	1/1	1.00	0.05	40,40,40,40	0
2	ZN	J	401	1/1	1.00	0.01	42,42,42,42	0

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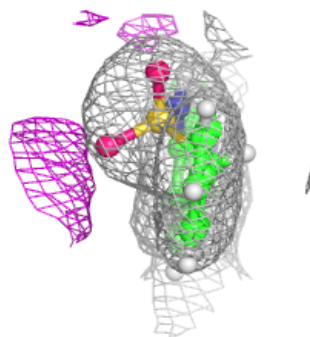
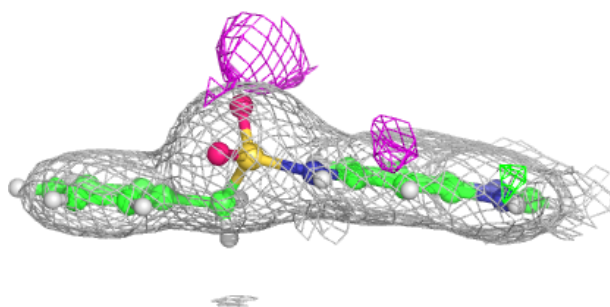
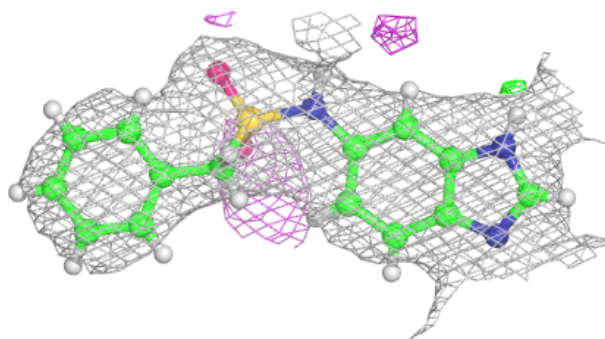
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	K	400	1/1	1.00	0.01	41,41,41,41	0
2	ZN	L	400	1/1	1.00	0.02	44,44,44,44	0

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.

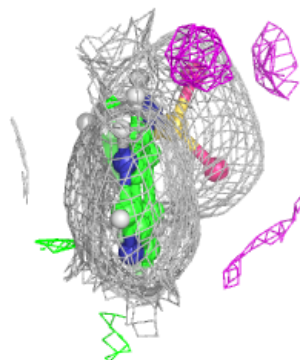
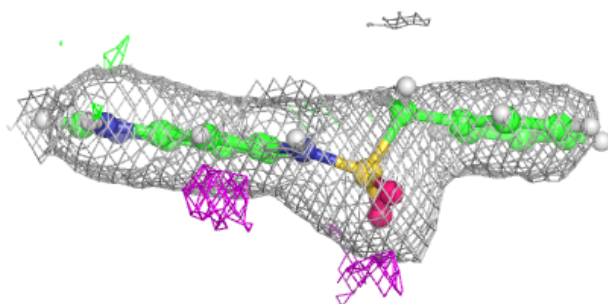
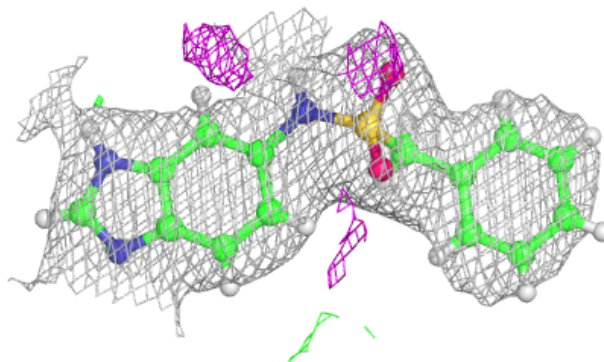
Electron density around A1D93 K 401:

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

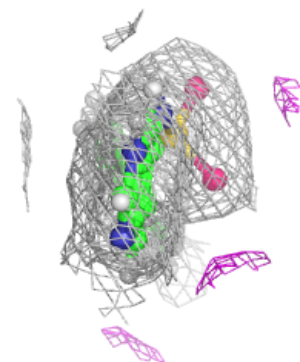
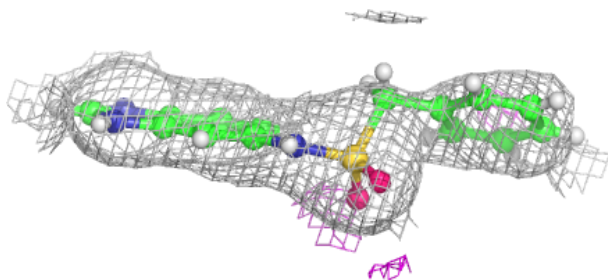
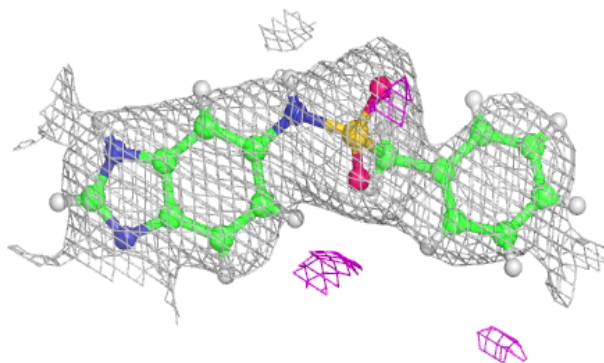


Electron density around A1D93 C 402:

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

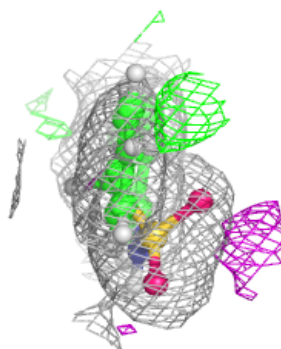
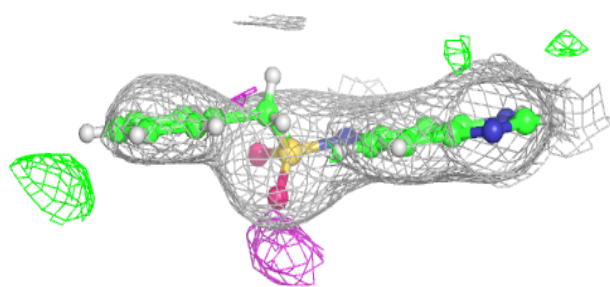
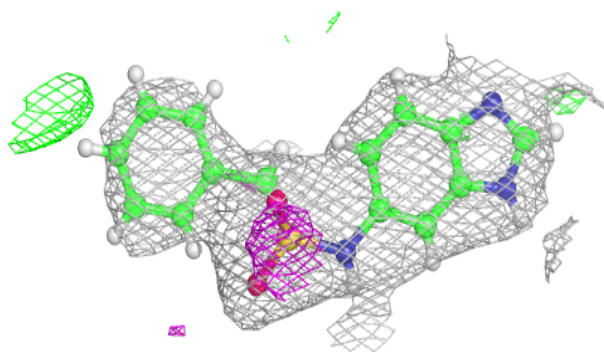
**Electron density around A1D93 G 401:**

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

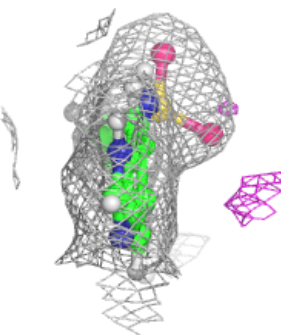
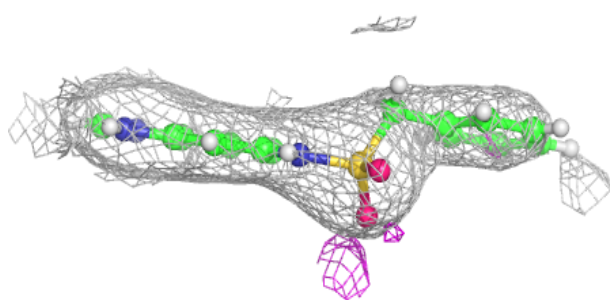
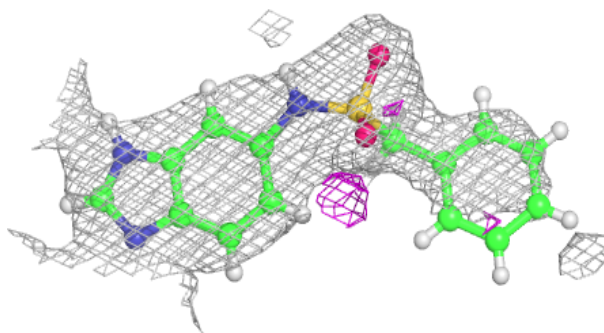


Electron density around A1D93 H 401:

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

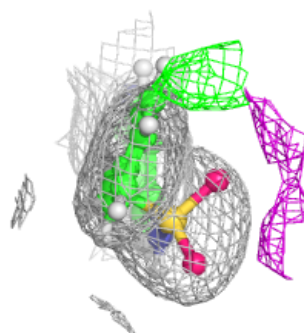
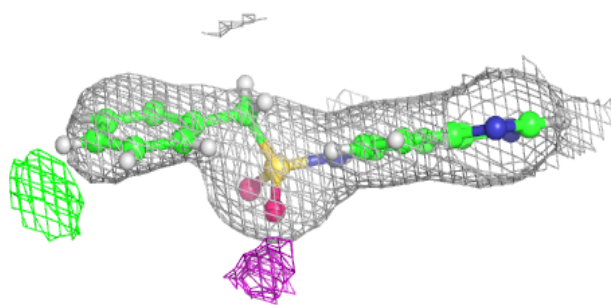
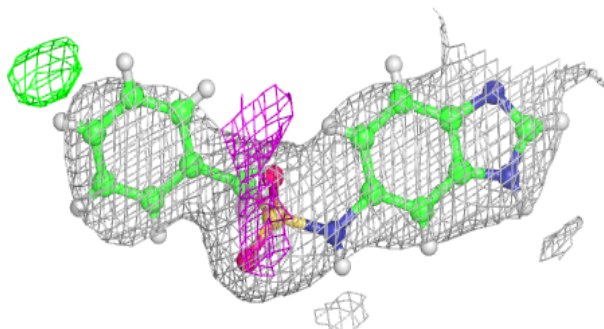
**Electron density around A1D93 I 402:**

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

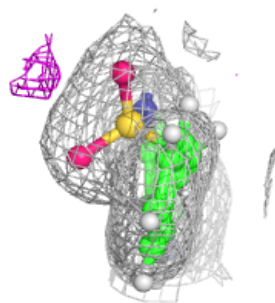
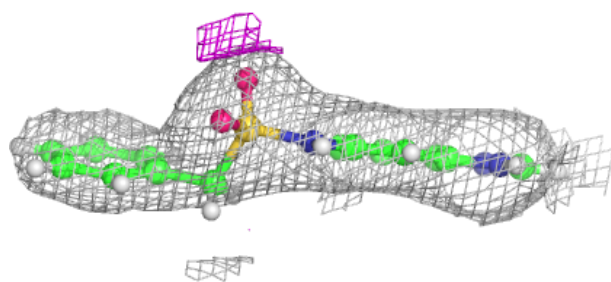
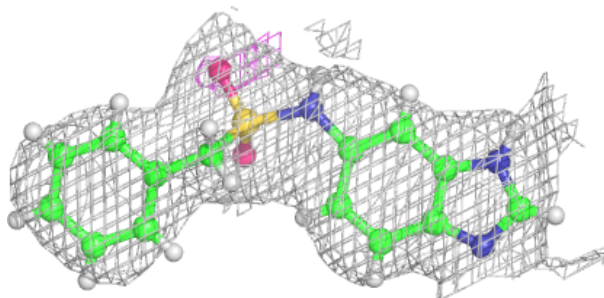


Electron density around A1D93 J 402:

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

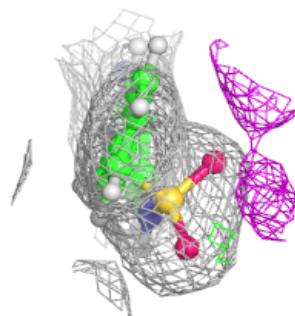
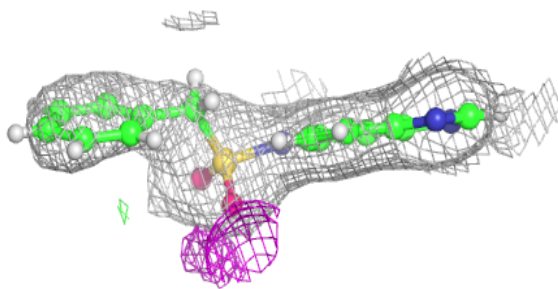
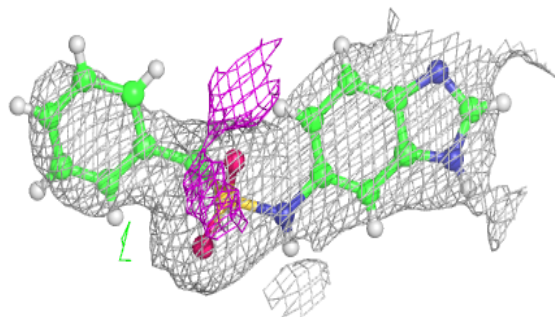
**Electron density around A1D93 D 402:**

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

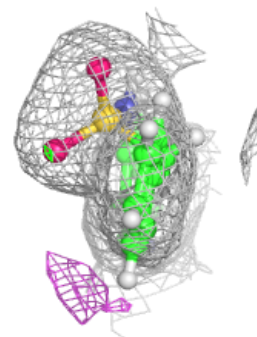
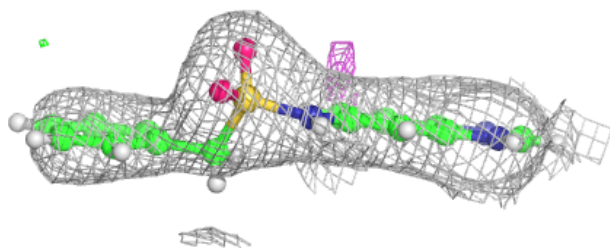
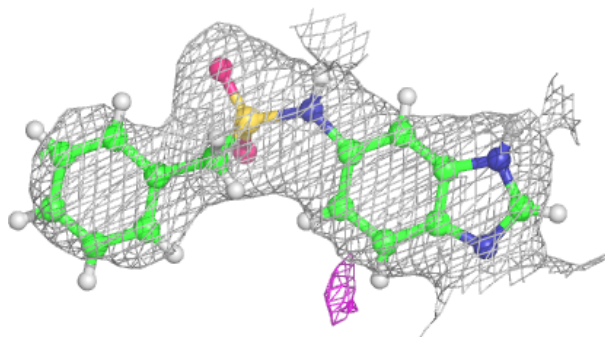


Electron density around A1D93 L 401:

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

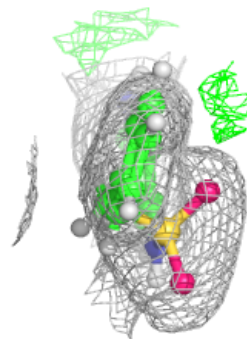
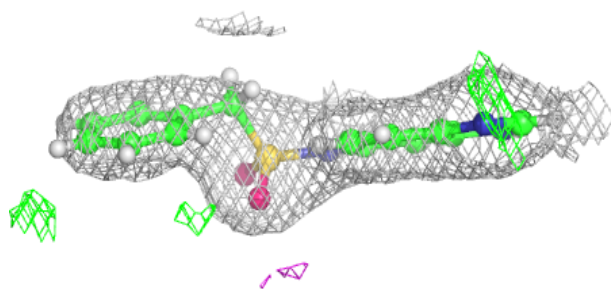
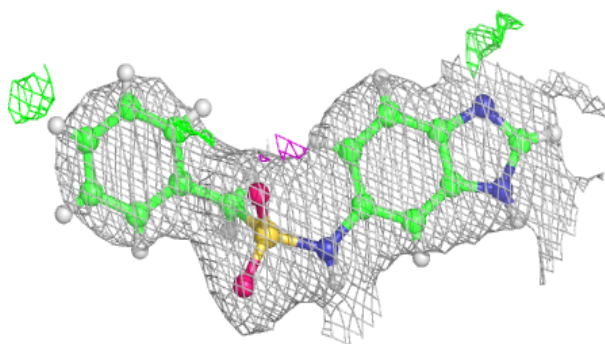
**Electron density around A1D93 E 402:**

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

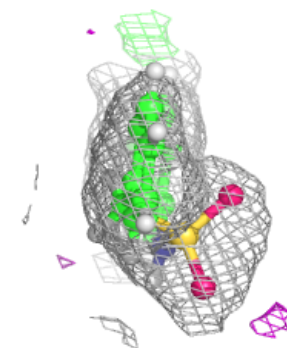
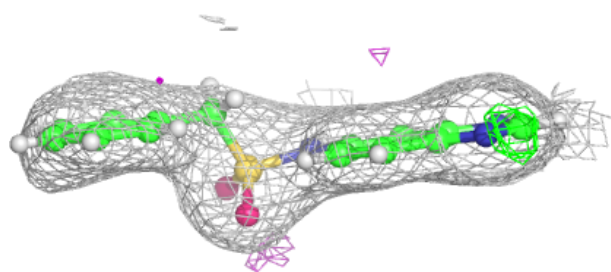
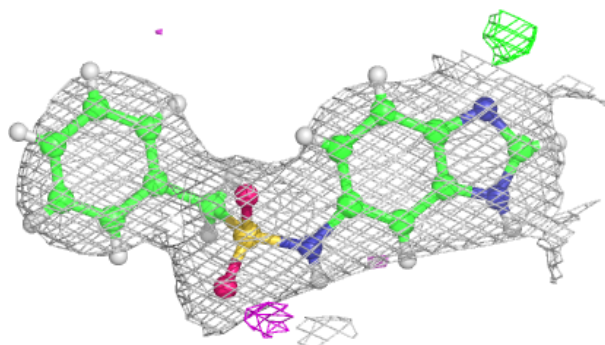


Electron density around A1D93 F 402:

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

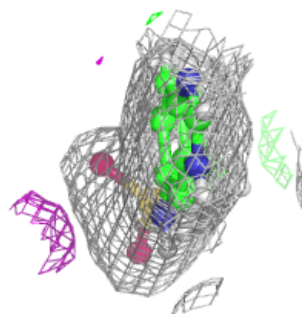
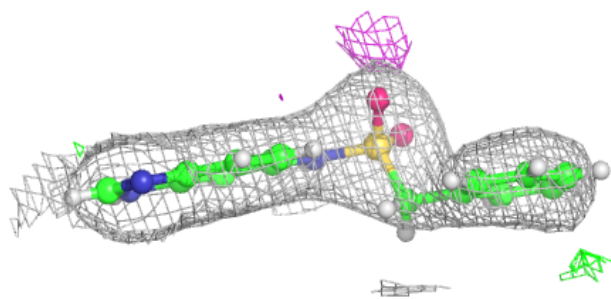
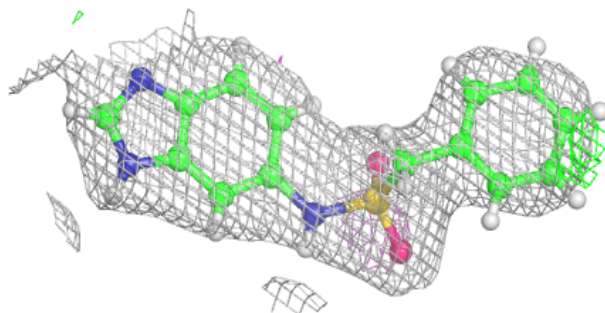
**Electron density around A1D93 A 402:**

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



Electron density around A1D93 B 402:

$2mF_o - DF_c$ (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.