



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:21 PM UTC

PDB ID : 9ISD / pdb_00009isd
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 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

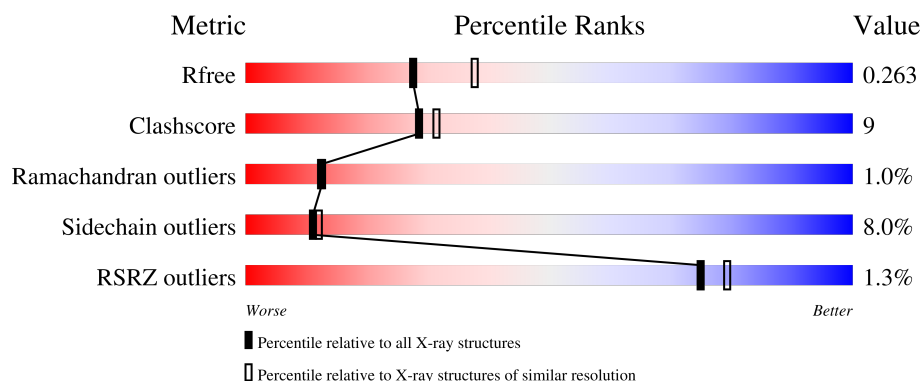
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

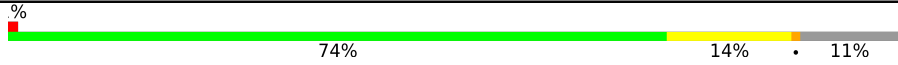
The reported resolution of this entry is 2.37 Å.

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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	
1	B	361	
1	C	361	
1	D	361	

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Mol	Chain	Length	Quality of chain
1	E	361	
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 (CCD ID: ZN) (formula: Zn).

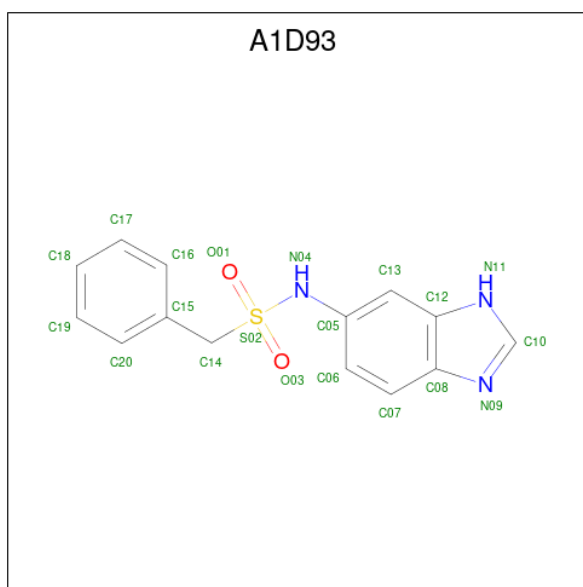
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

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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 (CCD ID: A1D93) (formula: C₁₄H₁₃N₃O₂S) (labeled as "Ligand of Interest" by depositor).



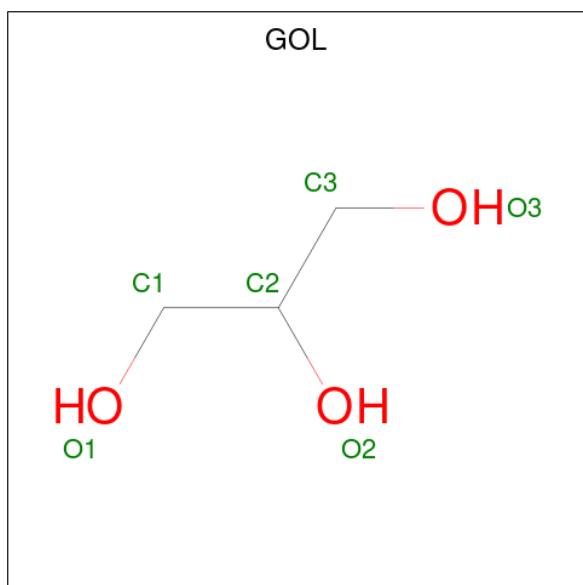
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			33	14	13	3	2	1		

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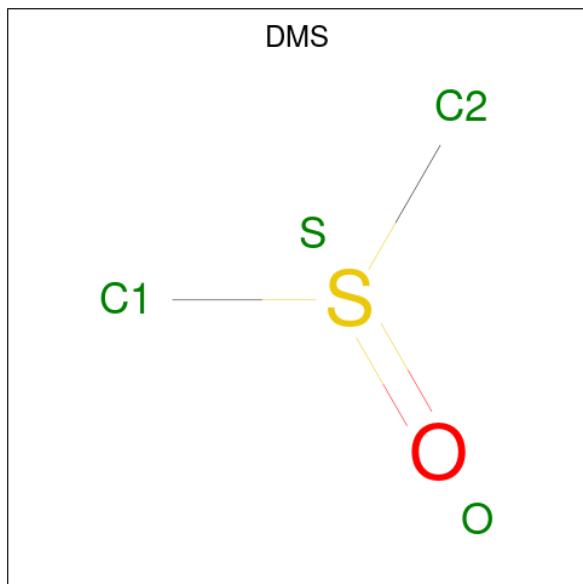
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	C	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	D	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	E	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	F	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	G	1	Total 33	C 14	H 13	N 3	O 2	S 1	0	0
3	H	1	Total 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



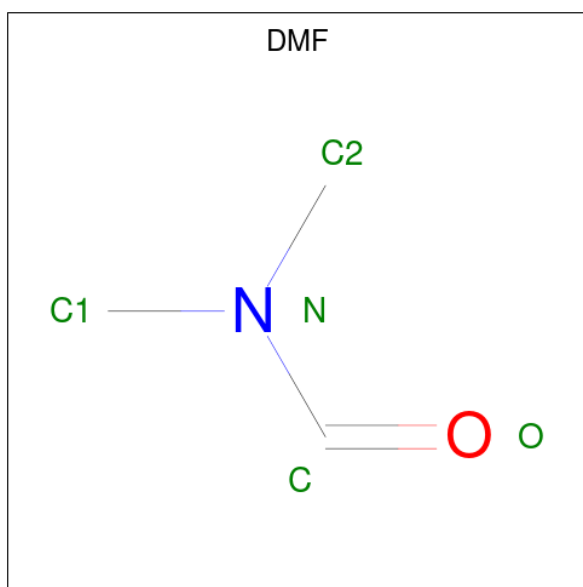
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			11	3	5	3		
4	F	1	Total	C	H	O	0	0
			11	3	5	3		
4	I	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



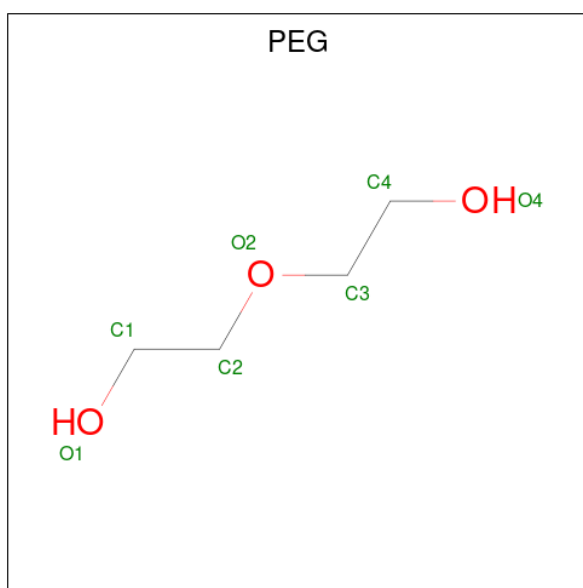
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is DIMETHYLFORMAMIDE (CCD ID: 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 (CCD ID: 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		

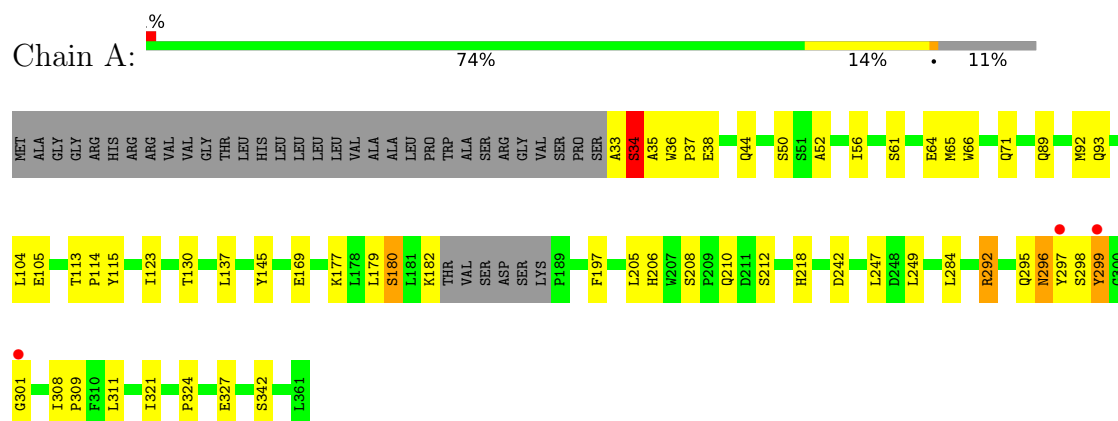
- Molecule 8 is water.

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		

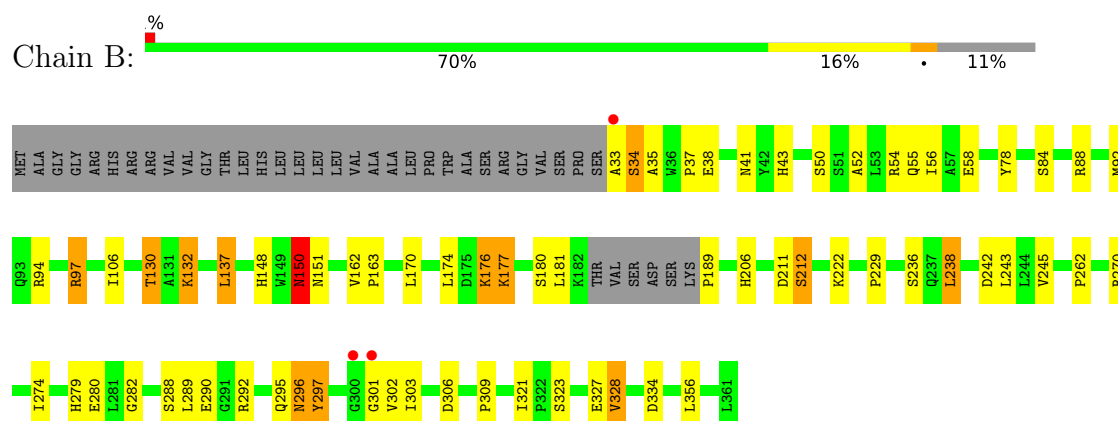
3 Residue-property plots [i](#)

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.

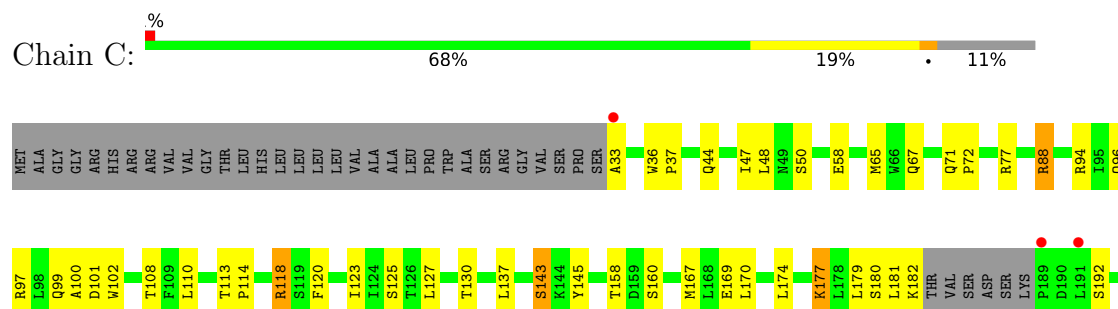
• Molecule 1: Glutaminyl-peptide cyclotransferase



• Molecule 1: Glutaminyl-peptide cyclotransferase

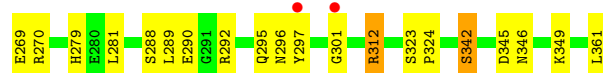
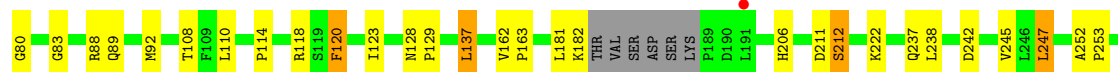
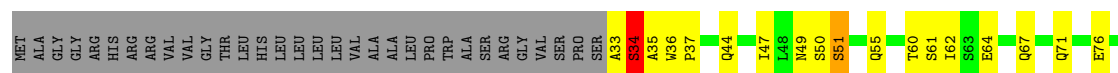


• Molecule 1: Glutaminyl-peptide cyclotransferase

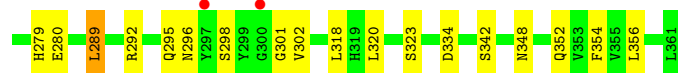
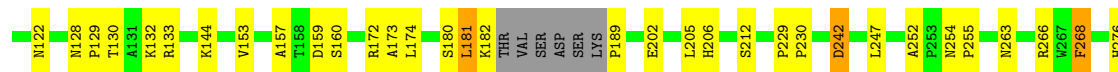
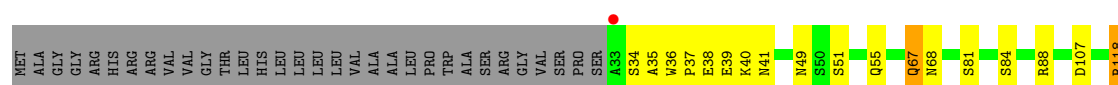




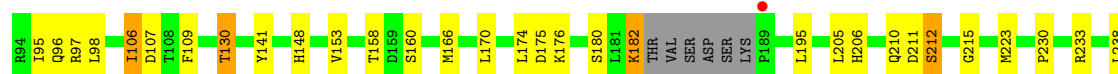
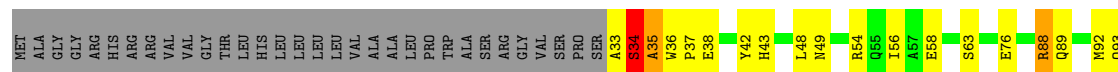
- Molecule 1: Glutaminyl-peptide cyclotransferase



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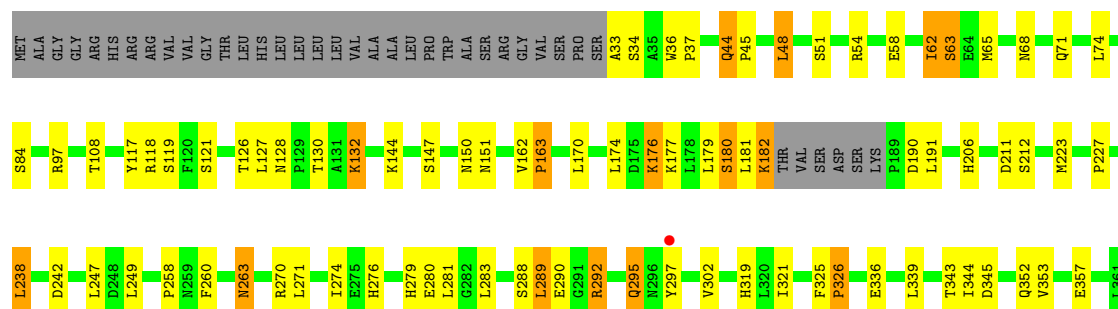


- Molecule 1: Glutaminyl-peptide cyclotransferase

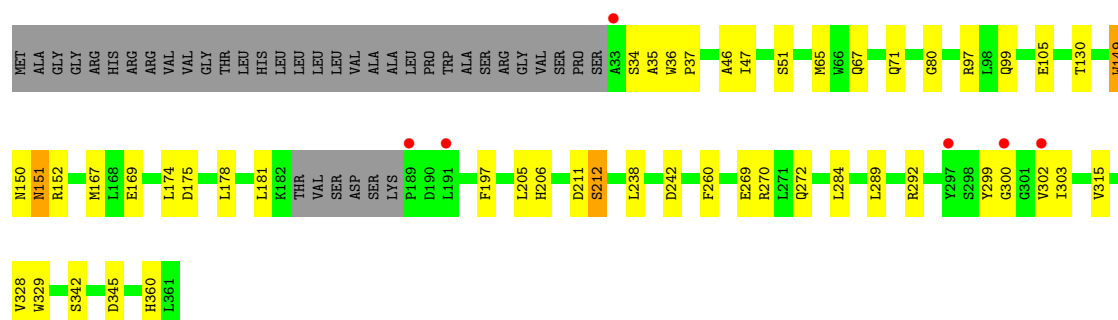
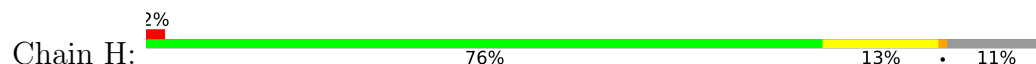


- Molecule 1: Glutaminyl-peptide cyclotransferase

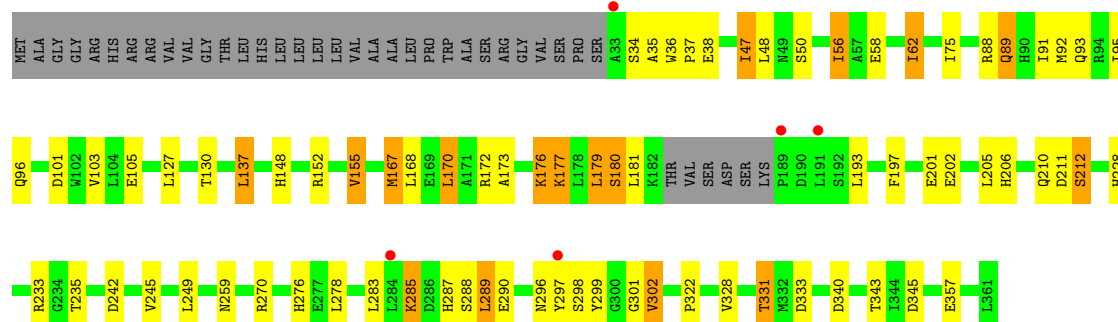




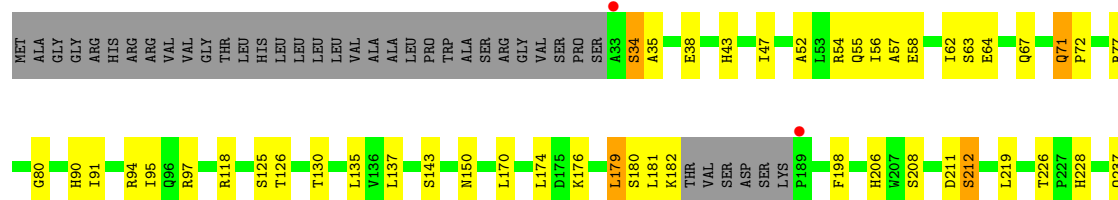
• Molecule 1: Glutaminyl-peptide cyclotransferase

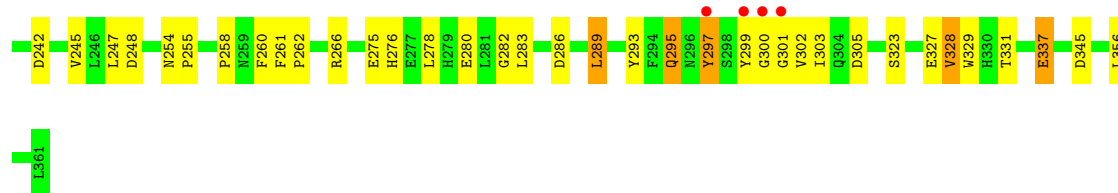


• Molecule 1: Glutaminyl-peptide cyclotransferase

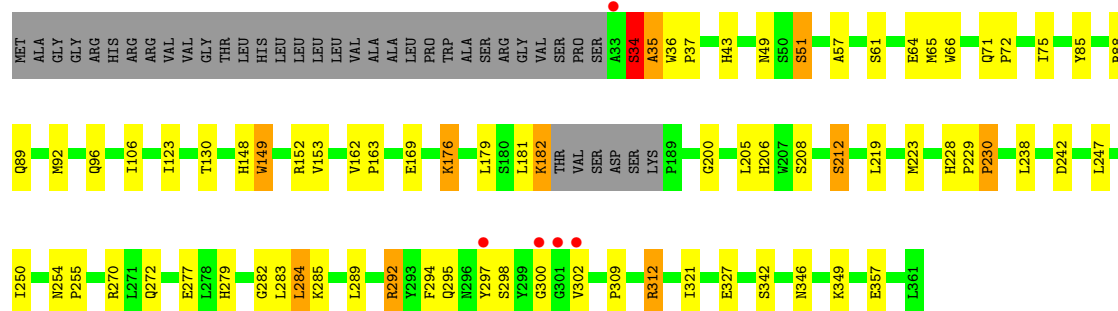


• Molecule 1: Glutaminyl-peptide cyclotransferase

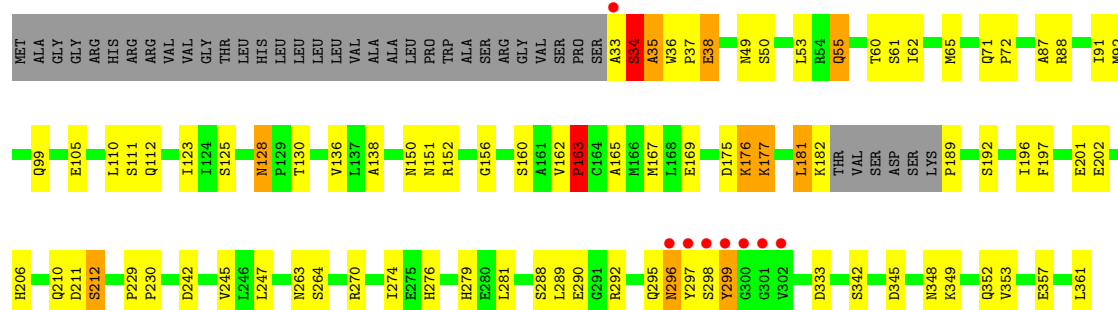




- Molecule 1: Glutaminyl-peptide cyclotransferase



- 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	2007 reflections (0.75%)	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: GOL, PEG, A1D93, DMF, DMS, 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	1.06	1/2687 (0.0%)	1.07	0/3656
1	B	1.06	2/2687 (0.1%)	1.08	1/3656 (0.0%)
1	C	1.05	2/2687 (0.1%)	1.08	4/3656 (0.1%)
1	D	0.97	1/2687 (0.0%)	1.04	2/3656 (0.1%)
1	E	1.04	0/2687	1.07	1/3656 (0.0%)
1	F	1.06	2/2687 (0.1%)	1.06	1/3656 (0.0%)
1	G	0.92	0/2687	0.96	0/3656
1	H	0.99	0/2687	0.99	0/3656
1	I	0.90	0/2687	0.97	0/3656
1	J	0.89	0/2687	0.96	2/3656 (0.1%)
1	K	1.00	1/2687 (0.0%)	1.06	3/3656 (0.1%)
1	L	0.94	1/2687 (0.0%)	0.99	3/3656 (0.1%)
All	All	0.99	10/32244 (0.0%)	1.03	17/43872 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	228	HIS	CA-C	9.31	1.62	1.53
1	K	228	HIS	CA-C	6.82	1.59	1.52
1	C	101	ASP	CA-CB	6.64	1.63	1.53
1	L	34	SER	CA-C	6.20	1.61	1.52
1	D	323	SER	CA-C	5.58	1.57	1.52
1	B	323	SER	CA-C	5.44	1.58	1.52
1	F	195	LEU	CG-CD2	-5.37	1.34	1.52
1	F	271	LEU	CG-CD2	-5.30	1.35	1.52
1	A	105	GLU	CG-CD	5.21	1.65	1.52
1	B	150	ASN	CB-CG	-5.18	1.39	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	ARG	NE-CZ-NH2	7.97	126.38	119.20
1	C	100	ALA	CA-C-N	-7.84	111.53	123.14
1	C	100	ALA	C-N-CA	-7.84	111.53	123.14
1	D	34	SER	CA-C-N	7.63	135.43	121.70
1	D	34	SER	C-N-CA	7.63	135.43	121.70
1	J	329	TRP	CA-C-N	6.65	131.58	122.07
1	J	329	TRP	C-N-CA	6.65	131.58	122.07
1	L	34	SER	CA-C-N	6.34	133.11	121.70
1	L	34	SER	C-N-CA	6.34	133.11	121.70
1	F	238	LEU	CA-CB-CG	6.04	137.44	116.30
1	K	34	SER	N-CA-C	5.51	118.23	109.96
1	K	200	GLY	N-CA-C	5.40	122.25	114.10
1	C	118	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	E	118	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	B	238	LEU	CA-CB-CG	5.23	134.61	116.30
1	L	138	ALA	N-CA-C	5.16	116.69	108.79
1	K	238	LEU	CA-CB-CG	5.15	134.33	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2610	2528	2529	31	0
1	B	2610	2531	2529	48	1
1	C	2610	2528	2529	42	0
1	D	2610	2529	2529	36	0
1	E	2610	2530	2529	45	0
1	F	2610	2530	2529	46	0
1	G	2610	2530	2529	58	1
1	H	2610	2529	2529	22	0
1	I	2610	2529	2529	55	0
1	J	2610	2529	2529	50	0
1	K	2610	2529	2529	52	0
1	L	2610	2529	2529	65	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
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
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	9	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	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	547	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 9.

All (547) 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
1:L:270:ARG:O	1:L:274:ILE:HD12	1.80	0.82
7:D:404:PEG:H12	8:D:501:HOH:O	1.81	0.81
1:G:177:LYS:NZ	8:G:502:HOH:O	2.14	0.80
1:C:47:ILE:O	8:C:502:HOH:O	2.00	0.80
1:C:233:ARG:NH2	1:D:80:GLY:O	2.15	0.79
1:I:228:HIS:O	1:I:235:THR:OG1	1.99	0.79
1:H:80:GLY:O	1:I:233:ARG:NH2	2.14	0.79
1:L:361:LEU:OXT	8:L:501:HOH:O	2.00	0.78
1:I:345:ASP:OD2	8:I:501:HOH:O	2.00	0.78
1:F:233:ARG:NH2	1:J:80:GLY:O	2.16	0.78
1:B:279:HIS:CD2	1:B:289:LEU:HD11	2.21	0.76
1:B:327:GLU:O	8:B:501:HOH:O	2.04	0.75
1:J:337:GLU:N	1:J:337:GLU:OE2	2.19	0.75
1:B:54:ARG:NH1	8:B:505:HOH:O	2.19	0.75
1:A:115:TYR:OH	8:A:501:HOH:O	2.03	0.75
1:L:279:HIS:ND1	1:L:289:LEU:HD11	2.02	0.74
1:B:33:ALA:HA	1:B:35:ALA:N	2.02	0.74
1:I:340:ASP:OD2	1:I:343:THR:HG23	1.88	0.73
1:K:342:SER:OG	8:K:501:HOH:O	2.07	0.72
1:J:43:HIS:O	1:J:266:ARG:NH2	2.23	0.72
1:L:270:ARG:NH2	1:L:357:GLU:OE1	2.19	0.72
1:G:118:ARG:NH2	8:G:504:HOH:O	2.23	0.71
1:G:190:ASP:OD2	8:G:501:HOH:O	2.08	0.71
1:L:279:HIS:CE1	1:L:289:LEU:HD11	2.26	0.71
1:K:85:TYR:CZ	1:K:89:GLN:NE2	2.58	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ALA:HB2	8:C:507:HOH:O	1.91	0.70
1:D:237:GLN:OE1	8:D:501:HOH:O	2.10	0.70
1:G:62:ILE:CG2	1:G:345:ASP:OD1	2.40	0.70
1:E:118:ARG:HE	6:E:404:DMF:H13	1.57	0.69
5:B:403:DMS:H22	8:B:522:HOH:O	1.91	0.69
1:J:328:VAL:O	1:J:331:THR:HG22	1.92	0.69
1:C:118:ARG:HH11	6:C:403:DMF:C	2.06	0.68
1:L:263:ASN:OD1	8:L:502:HOH:O	2.12	0.68
1:I:88:ARG:O	1:I:92:MET:HG3	1.94	0.68
1:I:328:VAL:O	1:I:331:THR:HB	1.94	0.67
1:L:34:SER:N	1:L:35:ALA:HB3	2.09	0.67
1:B:52:ALA:O	1:B:56:ILE:HD13	1.95	0.66
1:L:289:LEU:N	1:L:289:LEU:HD12	2.11	0.66
1:J:261:PHE:HE1	1:J:302:VAL:HG21	1.62	0.66
1:F:34:SER:O	1:F:35:ALA:CB	2.45	0.65
1:B:148:HIS:O	8:B:502:HOH:O	2.13	0.65
1:D:279:HIS:ND1	1:D:289:LEU:HG	2.11	0.65
1:F:33:ALA:N	1:F:34:SER:O	2.30	0.65
1:J:295:GLN:OE1	1:J:295:GLN:N	2.30	0.64
1:K:176:LYS:O	1:K:179:LEU:CD2	2.45	0.64
1:K:149:TRP:HA	8:K:507:HOH:O	1.96	0.64
1:G:68:ASN:ND2	8:G:506:HOH:O	2.30	0.64
1:B:301:GLY:O	1:B:303:ILE:N	2.31	0.64
1:A:296:ASN:O	1:A:296:ASN:ND2	2.26	0.64
1:L:88:ARG:O	1:L:92:MET:HG3	1.97	0.64
1:G:97:ARG:NH1	8:G:508:HOH:O	2.31	0.64
1:G:292:ARG:O	1:G:295:GLN:NE2	2.31	0.64
1:L:279:HIS:CE1	1:L:289:LEU:CD1	2.80	0.64
1:A:299:TYR:CE1	1:A:301:GLY:O	2.51	0.63
1:C:118:ARG:NH1	6:C:403:DMF:O	2.22	0.63
1:D:88:ARG:HG3	1:D:123:ILE:HD11	1.80	0.63
1:E:88:ARG:HH12	7:E:403:PEG:H21	1.62	0.63
1:L:276:HIS:O	1:L:276:HIS:ND1	2.31	0.63
1:D:34:SER:N	1:D:35:ALA:HB3	2.14	0.63
1:I:95:ILE:O	8:I:502:HOH:O	2.15	0.63
1:K:34:SER:HA	1:K:35:ALA:HB2	1.80	0.63
1:G:180:SER:O	1:G:181:LEU:HD23	1.98	0.63
1:D:88:ARG:O	1:D:92:MET:HG3	1.99	0.63
1:C:118:ARG:NH1	6:C:403:DMF:C	2.62	0.62
1:H:302:VAL:HG12	1:H:303:ILE:H	1.63	0.62
1:I:137:LEU:HD12	1:I:245:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ALA:O	1:B:38:GLU:HG2	2.01	0.61
1:L:167:MET:HE2	1:L:197:PHE:CZ	2.35	0.61
1:I:176:LYS:HD2	1:I:177:LYS:HG2	1.81	0.61
1:L:34:SER:N	1:L:35:ALA:CB	2.63	0.61
1:A:218:HIS:ND1	8:A:504:HOH:O	2.31	0.61
1:C:292:ARG:NH2	8:C:508:HOH:O	2.33	0.61
1:J:261:PHE:CE1	1:J:302:VAL:HG21	2.35	0.61
1:B:177:LYS:NZ	8:B:509:HOH:O	2.24	0.61
1:B:33:ALA:HA	1:B:35:ALA:H	1.64	0.60
1:L:49:ASN:O	1:L:53:LEU:HD12	2.02	0.60
1:G:270:ARG:NH2	1:G:357:GLU:OE1	2.33	0.60
1:G:65:MET:HE1	1:G:344:ILE:HG21	1.84	0.60
1:J:170:LEU:HD23	1:J:170:LEU:O	2.00	0.60
1:E:67:GLN:OE1	1:E:68:ASN:OD1	2.20	0.60
1:G:270:ARG:O	1:G:274:ILE:HD12	2.02	0.60
1:B:279:HIS:CG	1:B:289:LEU:HD11	2.37	0.59
1:K:148:HIS:C	8:K:507:HOH:O	2.46	0.59
1:G:336:GLU:HA	1:G:339:LEU:HD12	1.85	0.59
1:D:312:ARG:O	1:D:312:ARG:HG2	2.02	0.59
1:I:180:SER:O	1:I:180:SER:OG	2.19	0.58
1:A:145:TYR:CZ	4:A:403:GOL:H11	2.38	0.58
1:K:148:HIS:CD2	1:K:153:VAL:HG12	2.38	0.58
1:D:182:LYS:NZ	8:D:503:HOH:O	2.35	0.58
1:B:84:SER:OG	8:B:504:HOH:O	2.17	0.58
1:G:62:ILE:HG21	1:G:345:ASP:HB2	1.85	0.58
1:J:137:LEU:HD12	1:J:245:VAL:HB	1.86	0.58
1:J:211:ASP:O	1:J:212:SER:HB3	2.04	0.58
1:B:78:TYR:OH	8:B:503:HOH:O	2.15	0.58
1:G:279:HIS:CD2	1:G:289:LEU:HD13	2.38	0.58
1:E:348:ASN:O	1:E:352:GLN:HG3	2.04	0.57
1:F:107:ASP:OD1	8:F:501:HOH:O	2.17	0.57
1:L:189:PRO:HD3	8:L:590:HOH:O	2.02	0.57
1:J:179:LEU:HD23	1:J:179:LEU:O	2.05	0.57
1:A:65:MET:HG3	1:A:169:GLU:HB2	1.86	0.57
1:B:270:ARG:O	1:B:274:ILE:HD12	2.05	0.57
1:F:35:ALA:O	1:F:38:GLU:HG2	2.05	0.57
1:J:67:GLN:O	8:J:501:HOH:O	2.17	0.57
1:B:289:LEU:N	1:B:289:LEU:HD12	2.19	0.57
1:I:176:LYS:HD2	1:I:177:LYS:N	2.19	0.57
1:L:298:SER:O	1:L:299:TYR:C	2.47	0.57
1:B:211:ASP:O	1:B:212:SER:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:148:HIS:HA	1:I:152:ARG:O	2.04	0.56
1:E:36:TRP:CD2	1:E:37:PRO:HD3	2.40	0.56
1:C:47:ILE:HG22	1:C:48:LEU:N	2.20	0.56
1:F:33:ALA:CA	1:F:34:SER:O	2.54	0.56
1:E:229:PRO:O	1:E:230:PRO:C	2.47	0.56
1:G:179:LEU:C	1:G:181:LEU:H	2.12	0.56
1:G:326:PRO:HG2	8:G:594:HOH:O	2.06	0.56
1:L:292:ARG:NH1	8:L:503:HOH:O	2.31	0.56
1:J:299:TYR:CE2	1:J:301:GLY:O	2.58	0.56
1:K:149:TRP:N	8:K:507:HOH:O	2.37	0.56
1:E:174:LEU:HD22	1:E:356:LEU:HD11	1.89	0.55
1:K:34:SER:OG	1:K:35:ALA:HB2	2.06	0.55
1:G:270:ARG:O	1:G:274:ILE:CD1	2.55	0.55
1:F:270:ARG:NH2	1:F:357:GLU:OE1	2.35	0.55
1:A:301:GLY:HA3	1:C:300:GLY:O	2.06	0.55
1:D:61:SER:OG	1:D:64:GLU:CG	2.55	0.55
1:E:159:ASP:N	1:E:160:SER:HA	2.21	0.54
1:I:75:ILE:C	1:I:155:VAL:HG12	2.32	0.54
1:J:276:HIS:CE1	1:J:289:LEU:HD11	2.43	0.54
1:J:170:LEU:HD21	1:J:174:LEU:HD12	1.88	0.54
1:L:162:VAL:HB	1:L:163:PRO:HD3	1.89	0.54
1:A:61:SER:OG	1:A:64:GLU:HG2	2.07	0.54
1:L:99:GLN:HG3	1:L:175:ASP:OD2	2.08	0.54
1:K:34:SER:CA	1:K:35:ALA:HB2	2.37	0.54
1:F:33:ALA:HA	1:F:34:SER:C	2.33	0.54
1:I:276:HIS:CE1	1:I:289:LEU:HD11	2.43	0.54
1:L:33:ALA:HB3	1:L:35:ALA:HB3	1.89	0.54
1:C:270:ARG:O	1:C:274:ILE:HG13	2.08	0.53
1:D:47:ILE:HG12	1:D:270:ARG:NH2	2.23	0.53
1:E:268:PHE:CD1	1:E:268:PHE:C	2.85	0.53
1:E:49:ASN:OD1	1:E:51:SER:N	2.40	0.53
1:F:277:GLU:HG3	1:F:281:LEU:HD12	1.89	0.53
1:B:137:LEU:HD12	1:B:245:VAL:HB	1.90	0.53
1:L:176:LYS:NZ	1:L:177:LYS:HG3	2.24	0.53
1:A:33:ALA:HA	1:A:35:ALA:N	2.24	0.53
1:G:276:HIS:HB2	1:G:292:ARG:NH2	2.24	0.53
1:J:118:ARG:NE	7:J:403:PEG:O1	2.42	0.53
1:J:282:GLY:HA2	8:J:504:HOH:O	2.08	0.53
1:G:179:LEU:O	1:G:181:LEU:N	2.38	0.53
1:I:35:ALA:O	1:I:38:GLU:HG2	2.09	0.53
1:I:36:TRP:CG	1:I:37:PRO:HD3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:343:THR:OG1	8:G:503:HOH:O	2.19	0.53
1:H:178:LEU:O	1:H:181:LEU:HD12	2.09	0.53
1:I:287:HIS:CE1	1:I:288:SER:O	2.61	0.53
1:G:62:ILE:HD13	1:G:63:SER:H	1.74	0.52
1:F:36:TRP:CG	1:F:37:PRO:HD3	2.44	0.52
1:L:33:ALA:HB3	1:L:35:ALA:CB	2.39	0.52
1:K:312:ARG:O	8:K:502:HOH:O	2.19	0.52
1:F:170:LEU:C	1:F:170:LEU:HD23	2.35	0.52
1:F:89:GLN:O	1:F:93:GLN:HG3	2.09	0.52
1:G:325:PHE:O	1:G:326:PRO:C	2.53	0.52
1:F:285:LYS:NZ	1:F:346:ASN:OD1	2.42	0.52
1:I:101:ASP:O	1:I:127:LEU:HD23	2.10	0.52
1:K:35:ALA:HB2	8:K:517:HOH:O	2.09	0.52
1:F:34:SER:O	1:F:35:ALA:HB3	2.10	0.52
1:H:46:ALA:HB2	1:H:360:HIS:ND1	2.25	0.52
1:K:270:ARG:HH21	1:K:357:GLU:CD	2.18	0.52
1:L:87:ALA:O	1:L:91:ILE:HG13	2.10	0.52
1:F:276:HIS:HB2	1:F:292:ARG:NH2	2.25	0.51
1:K:284:LEU:O	1:K:285:LYS:HG3	2.10	0.51
1:A:180:SER:O	1:A:182:LYS:HE2	2.10	0.51
1:C:289:LEU:N	1:C:289:LEU:HD22	2.24	0.51
1:F:106:ILE:O	1:F:106:ILE:HG22	2.10	0.51
1:H:47:ILE:HD12	1:H:270:ARG:NH2	2.25	0.51
1:D:211:ASP:O	1:D:212:SER:HB3	2.09	0.51
1:I:249:LEU:HB2	1:I:322:PRO:HD2	1.93	0.51
1:L:292:ARG:O	1:L:295:GLN:NE2	2.43	0.51
1:B:170:LEU:C	1:B:170:LEU:HD23	2.35	0.51
1:C:301:GLY:O	1:C:302:VAL:HG22	2.11	0.51
1:E:189:PRO:HG3	8:E:610:HOH:O	2.10	0.51
1:L:279:HIS:CG	1:L:289:LEU:HD11	2.45	0.51
1:A:113:THR:HB	1:A:114:PRO:HD2	1.93	0.51
1:I:170:LEU:C	1:I:170:LEU:HD23	2.36	0.51
1:L:162:VAL:O	1:L:165:ALA:N	2.43	0.51
1:F:299:TYR:CE1	1:F:301:GLY:O	2.64	0.51
1:H:238:LEU:HD22	1:H:315:VAL:CG2	2.40	0.51
1:K:297:TYR:OH	1:L:298:SER:CB	2.59	0.51
1:E:118:ARG:HE	6:E:404:DMF:C1	2.24	0.51
1:E:189:PRO:CG	8:E:610:HOH:O	2.59	0.51
1:H:36:TRP:N	1:H:37:PRO:CD	2.74	0.51
1:E:39:GLU:OE2	8:E:502:HOH:O	2.18	0.50
1:K:149:TRP:CA	8:K:507:HOH:O	2.56	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:162:VAL:HB	1:L:163:PRO:CD	2.41	0.50
1:C:301:GLY:O	1:C:302:VAL:O	2.30	0.50
5:B:403:DMS:C2	8:B:522:HOH:O	2.52	0.50
1:L:65:MET:HG3	1:L:169:GLU:HB2	1.93	0.50
1:C:179:LEU:C	1:C:179:LEU:HD23	2.37	0.50
1:I:177:LYS:O	1:I:180:SER:HB3	2.12	0.50
1:B:295:GLN:HG3	1:B:297:TYR:HE1	1.77	0.50
1:B:88:ARG:NH2	8:B:511:HOH:O	2.31	0.50
1:C:77:ARG:HG2	1:C:143:SER:HB3	1.94	0.50
1:D:292:ARG:HD3	1:D:295:GLN:OE1	2.11	0.50
1:G:279:HIS:CD2	1:G:289:LEU:CD1	2.95	0.50
1:H:302:VAL:CG1	1:H:303:ILE:H	2.23	0.50
1:K:36:TRP:CD2	1:K:37:PRO:HD3	2.47	0.50
1:K:65:MET:HG3	1:K:169:GLU:HB2	1.94	0.50
1:B:296:ASN:O	1:B:297:TYR:HB3	2.11	0.50
1:F:166:MET:HG2	1:F:348:ASN:OD1	2.11	0.50
1:J:226:THR:HG21	1:J:237:GLN:NE2	2.27	0.50
1:L:33:ALA:C	1:L:35:ALA:CB	2.84	0.50
1:B:130:THR:HB	8:B:611:HOH:O	2.11	0.49
1:I:299:TYR:HE1	1:I:301:GLY:C	2.19	0.49
1:I:301:GLY:O	1:I:302:VAL:O	2.30	0.49
1:F:54:ARG:NH2	1:F:283:LEU:HD21	2.27	0.49
1:I:331:THR:HG22	1:I:333:ASP:H	1.77	0.49
1:K:247:LEU:HD23	1:K:250:ILE:CD1	2.42	0.49
1:I:179:LEU:O	1:I:179:LEU:HD23	2.13	0.49
1:I:201:GLU:OE1	1:I:202:GLU:HG2	2.13	0.49
1:D:36:TRP:CG	1:D:37:PRO:HD3	2.47	0.49
1:L:111:SER:OG	1:L:112:GLN:N	2.46	0.49
1:I:211:ASP:O	1:I:212:SER:HB3	2.11	0.49
1:I:302:VAL:HG12	8:I:510:HOH:O	2.12	0.49
1:B:279:HIS:CE1	1:B:289:LEU:CD1	2.96	0.49
1:G:319:HIS:ND1	8:G:511:HOH:O	2.35	0.49
1:F:285:LYS:HD3	1:F:285:LYS:N	2.28	0.49
1:L:348:ASN:O	1:L:352:GLN:HG3	2.13	0.49
1:G:263:ASN:ND2	8:G:515:HOH:O	2.40	0.48
1:J:174:LEU:HD22	1:J:356:LEU:HD11	1.94	0.48
1:K:321:ILE:O	1:K:321:ILE:HG23	2.12	0.48
1:E:39:GLU:O	1:E:40:LYS:C	2.56	0.48
1:D:114:PRO:HD3	8:D:592:HOH:O	2.14	0.48
1:G:127:LEU:O	1:G:128:ASN:HB2	2.13	0.48
1:G:223:MET:CB	1:G:238:LEU:HD23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:MET:HE2	1:H:197:PHE:CZ	2.48	0.48
1:L:128:ASN:OD1	1:L:192:SER:OG	2.16	0.48
1:C:145:TYR:OH	6:C:403:DMF:H13	2.14	0.48
1:F:276:HIS:HB2	1:F:292:ARG:HH22	1.78	0.48
1:I:47:ILE:CG2	1:I:48:LEU:N	2.77	0.48
1:A:66:TRP:O	1:A:71:GLN:HG3	2.13	0.48
1:F:285:LYS:HE3	1:F:349:LYS:HZ1	1.79	0.48
1:I:170:LEU:HD23	1:I:170:LEU:O	2.14	0.48
1:J:170:LEU:HD23	1:J:170:LEU:C	2.38	0.48
1:L:49:ASN:OD1	1:L:49:ASN:C	2.57	0.48
1:F:270:ARG:O	1:F:274:ILE:HG13	2.14	0.48
1:B:34:SER:O	1:B:34:SER:OG	2.32	0.47
1:C:170:LEU:O	1:C:174:LEU:HG	2.13	0.47
1:J:118:ARG:HD2	7:J:403:PEG:O1	2.14	0.47
1:J:258:PRO:HG2	1:J:260:PHE:CZ	2.49	0.47
1:J:276:HIS:ND1	1:J:289:LEU:HD11	2.29	0.47
1:K:61:SER:OG	1:K:64:GLU:HG2	2.14	0.47
1:L:33:ALA:CB	1:L:35:ALA:CB	2.92	0.47
1:L:270:ARG:C	1:L:274:ILE:HD12	2.39	0.47
1:F:48:LEU:CD1	1:F:56:ILE:HD11	2.44	0.47
1:D:181:LEU:O	1:D:182:LYS:HB2	2.15	0.47
1:E:301:GLY:C	1:E:302:VAL:HG13	2.39	0.47
1:F:33:ALA:CA	1:F:34:SER:C	2.86	0.47
1:G:54:ARG:HG2	1:G:283:LEU:HD21	1.96	0.47
1:I:299:TYR:HE1	1:I:301:GLY:O	1.95	0.47
1:J:52:ALA:O	1:J:55:GLN:HB2	2.14	0.47
1:K:208:SER:O	1:K:212:SER:OG	2.32	0.47
1:L:349:LYS:O	1:L:353:VAL:HG23	2.15	0.47
1:L:189:PRO:CD	8:L:590:HOH:O	2.59	0.47
1:D:182:LYS:NZ	8:D:506:HOH:O	2.40	0.47
1:D:33:ALA:C	1:D:35:ALA:HB3	2.39	0.47
1:E:247:LEU:HD23	1:E:320:LEU:HD12	1.96	0.47
1:J:94:ARG:NH1	8:J:502:HOH:O	2.18	0.47
1:G:270:ARG:O	1:G:274:ILE:HG13	2.15	0.47
1:I:331:THR:HG22	1:I:333:ASP:N	2.30	0.47
1:L:35:ALA:O	1:L:38:GLU:HB2	2.14	0.47
1:L:295:GLN:O	1:L:297:TYR:N	2.48	0.47
1:G:211:ASP:O	1:G:212:SER:HB3	2.14	0.47
1:K:289:LEU:O	1:K:292:ARG:HD2	2.15	0.47
1:L:88:ARG:HG3	1:L:123:ILE:HD11	1.97	0.47
1:B:35:ALA:C	1:B:37:PRO:CD	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:THR:O	1:F:160:SER:HA	2.15	0.46
1:H:260:PHE:HE1	1:H:299:TYR:CD2	2.32	0.46
1:J:54:ARG:O	1:J:58:GLU:HG3	2.14	0.46
1:F:282:GLY:HA2	8:F:572:HOH:O	2.14	0.46
1:G:48:LEU:N	1:G:48:LEU:HD23	2.31	0.46
1:B:279:HIS:NE2	1:B:289:LEU:CD1	2.78	0.46
1:C:282:GLY:C	1:C:283:LEU:HD23	2.41	0.46
1:E:36:TRP:CD2	1:E:132:LYS:HD2	2.50	0.46
1:E:84:SER:HB3	7:E:403:PEG:H22	1.97	0.46
1:F:130:THR:O	1:F:130:THR:CG2	2.61	0.46
1:I:62:ILE:HD13	1:I:345:ASP:HB2	1.97	0.46
1:A:177:LYS:NZ	8:A:509:HOH:O	2.47	0.46
1:G:276:HIS:HB2	1:G:292:ARG:HH22	1.79	0.46
1:L:264:SER:HA	8:L:514:HOH:O	2.15	0.46
1:A:182:LYS:HE2	1:A:182:LYS:HA	1.96	0.46
1:E:144:LYS:HB2	1:E:202:GLU:HG3	1.97	0.46
1:C:47:ILE:CG2	1:C:48:LEU:N	2.79	0.46
1:I:172:ARG:O	1:I:173:ALA:C	2.59	0.46
1:I:176:LYS:C	1:I:176:LYS:CD	2.89	0.46
1:A:180:SER:O	1:A:182:LYS:CE	2.64	0.46
1:B:321:ILE:O	1:B:321:ILE:CG2	2.64	0.46
1:B:321:ILE:O	1:B:321:ILE:HG23	2.15	0.46
1:B:43:HIS:ND1	8:B:512:HOH:O	2.36	0.45
1:B:296:ASN:OD1	8:B:507:HOH:O	2.21	0.45
1:A:249:LEU:HD12	1:A:321:ILE:HD11	1.98	0.45
1:D:163:PRO:HB3	1:D:247:LEU:HB2	1.98	0.45
1:F:174:LEU:O	1:F:175:ASP:C	2.58	0.45
1:H:149:TRP:O	1:H:152:ARG:N	2.33	0.45
1:H:167:MET:HE2	1:H:197:PHE:CE2	2.51	0.45
1:J:198:PHE:HE1	1:J:219:LEU:HD23	1.81	0.45
1:A:36:TRP:CD2	1:A:37:PRO:HD3	2.51	0.45
1:B:162:VAL:HB	1:B:163:PRO:CD	2.46	0.45
1:B:176:LYS:HD3	1:B:177:LYS:HG2	1.97	0.45
1:I:56:ILE:HD13	1:I:56:ILE:HA	1.90	0.45
1:K:36:TRP:N	1:K:37:PRO:HD2	2.31	0.45
1:L:33:ALA:O	1:L:34:SER:CB	2.64	0.45
1:L:176:LYS:HE3	1:L:177:LYS:CG	2.47	0.45
1:B:41:ASN:OD1	1:B:41:ASN:O	2.34	0.45
1:B:306:ASP:O	1:B:309:PRO:HD2	2.16	0.45
1:I:259:ASN:O	1:I:298:SER:HA	2.16	0.45
1:A:145:TYR:CZ	4:A:403:GOL:C1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASN:OD1	1:D:51:SER:N	2.50	0.45
1:J:77:ARG:HG2	1:J:143:SER:HB3	1.97	0.45
1:D:345:ASP:O	1:D:349:LYS:HG3	2.17	0.45
1:A:64:GLU:HB3	8:A:574:HOH:O	2.17	0.45
1:E:279:HIS:NE2	1:E:289:LEU:HD12	2.32	0.45
1:K:181:LEU:O	1:K:182:LYS:HB2	2.17	0.45
1:A:33:ALA:N	1:A:34:SER:CB	2.80	0.45
1:G:117:TYR:O	1:G:118:ARG:HG2	2.17	0.45
1:L:152:ARG:NH1	1:L:333:ASP:OD1	2.36	0.45
1:D:222:LYS:NZ	7:D:404:PEG:H12	2.32	0.44
1:D:252:ALA:HB1	1:D:253:PRO:HD2	1.99	0.44
1:G:44:GLN:NE2	8:G:520:HOH:O	2.50	0.44
1:I:301:GLY:C	8:I:510:HOH:O	2.59	0.44
1:I:301:GLY:O	1:I:302:VAL:C	2.60	0.44
1:E:266:ARG:HG3	1:E:266:ARG:HH11	1.82	0.44
1:E:279:HIS:C	1:E:279:HIS:CD2	2.96	0.44
1:F:301:GLY:O	1:F:302:VAL:C	2.60	0.44
1:I:176:LYS:CD	1:I:177:LYS:N	2.80	0.44
1:K:88:ARG:HG3	1:K:123:ILE:HD11	1.99	0.44
1:K:219:LEU:O	1:K:223:MET:HG3	2.17	0.44
1:C:65:MET:HG3	1:C:169:GLU:HB2	1.99	0.44
1:K:49:ASN:OD1	1:K:51:SER:N	2.51	0.44
1:A:36:TRP:CG	1:A:37:PRO:HD3	2.52	0.44
1:E:182:LYS:CE	8:E:515:HOH:O	2.65	0.44
1:E:252:ALA:HB3	8:E:583:HOH:O	2.16	0.44
8:A:573:HOH:O	3:G:401:A1D93:C18	2.66	0.44
1:F:182:LYS:HA	1:F:182:LYS:HZ3	1.82	0.44
1:I:176:LYS:CG	1:I:177:LYS:N	2.80	0.44
4:I:403:GOL:H32	8:I:527:HOH:O	2.18	0.44
1:J:295:GLN:HE21	1:J:297:TYR:HD2	1.66	0.44
1:L:167:MET:HE2	1:L:197:PHE:CE2	2.53	0.44
1:A:52:ALA:O	1:A:56:ILE:HG12	2.16	0.44
1:C:88:ARG:HA	1:C:123:ILE:HD11	1.99	0.44
1:E:35:ALA:O	1:E:38:GLU:HG2	2.17	0.44
1:F:274:ILE:HD13	1:F:353:VAL:HG12	2.00	0.44
1:G:279:HIS:CG	1:G:289:LEU:CD1	3.01	0.44
1:H:178:LEU:HD12	8:H:516:HOH:O	2.16	0.44
1:C:351:LEU:O	1:C:355:VAL:HG23	2.17	0.44
1:G:162:VAL:O	1:G:163:PRO:C	2.59	0.44
1:G:181:LEU:C	1:G:182:LYS:HG2	2.43	0.44
1:G:302:VAL:HG23	8:G:511:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:TRP:CD2	1:I:37:PRO:HD3	2.53	0.44
1:J:254:ASN:N	1:J:255:PRO:CD	2.80	0.44
1:L:162:VAL:O	1:L:163:PRO:C	2.60	0.44
1:C:274:ILE:HD13	1:C:353:VAL:HG12	2.00	0.44
1:C:276:HIS:C	1:C:276:HIS:HD1	2.25	0.44
1:E:133:ARG:NH2	1:E:242:ASP:OD2	2.47	0.44
1:L:62:ILE:HB	1:L:345:ASP:OD1	2.18	0.44
1:K:283:LEU:N	1:K:283:LEU:HD23	2.33	0.44
1:C:36:TRP:CG	1:C:37:PRO:HD3	2.53	0.43
1:F:88:ARG:HD3	1:F:141:TYR:OH	2.18	0.43
1:G:249:LEU:HD12	1:G:321:ILE:HD11	2.00	0.43
1:J:118:ARG:HE	7:J:403:PEG:C1	2.30	0.43
1:K:279:HIS:CD2	1:K:289:LEU:HG	2.53	0.43
1:L:71:GLN:N	1:L:72:PRO:CD	2.80	0.43
1:D:342:SER:O	1:D:346:ASN:ND2	2.51	0.43
1:F:356:LEU:HD22	1:F:361:LEU:HB3	2.01	0.43
1:G:144:LYS:HE2	8:G:587:HOH:O	2.18	0.43
1:J:299:TYR:CD2	1:J:301:GLY:O	2.71	0.43
1:K:272:GLN:HG2	1:K:294:PHE:O	2.17	0.43
1:L:201:GLU:OE2	1:L:202:GLU:HG2	2.17	0.43
1:C:181:LEU:O	1:C:182:LYS:CB	2.66	0.43
1:F:249:LEU:HD12	1:F:321:ILE:HD11	2.00	0.43
1:H:238:LEU:HD22	1:H:315:VAL:HG21	1.99	0.43
1:I:278:LEU:O	1:I:283:LEU:HB2	2.19	0.43
1:K:321:ILE:O	1:K:321:ILE:CG2	2.66	0.43
1:F:293:TYR:CD2	1:F:347:LEU:HD21	2.54	0.43
1:G:176:LYS:CE	1:G:177:LYS:HG3	2.49	0.43
1:H:345:ASP:OD1	8:H:501:HOH:O	2.21	0.43
1:J:35:ALA:HB1	1:J:38:GLU:OE2	2.18	0.43
1:K:71:GLN:N	1:K:72:PRO:CD	2.80	0.43
1:K:176:LYS:O	1:K:179:LEU:HD23	2.18	0.43
1:B:279:HIS:CE1	1:B:289:LEU:HD12	2.52	0.43
1:F:109:PHE:CZ	1:F:215:GLY:HA2	2.53	0.43
1:H:65:MET:HG3	1:H:169:GLU:HB2	2.00	0.43
1:J:248:ASP:OD2	1:J:305:ASP:OD2	2.37	0.43
1:D:76:GLU:O	1:D:83:GLY:HA3	2.19	0.43
1:D:295:GLN:NE2	8:D:508:HOH:O	2.45	0.43
1:I:176:LYS:CD	1:I:177:LYS:HG2	2.48	0.43
1:J:97:ARG:NH2	8:J:507:HOH:O	2.30	0.43
1:J:295:GLN:NE2	1:J:297:TYR:CD2	2.87	0.43
1:C:33:ALA:CB	8:C:507:HOH:O	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:LYS:H	1:G:176:LYS:HG3	1.68	0.43
1:G:270:ARG:O	1:G:274:ILE:CG1	2.67	0.43
1:E:263:ASN:OD1	1:E:263:ASN:C	2.62	0.43
1:G:223:MET:HB3	1:G:238:LEU:HD23	2.00	0.43
1:G:288:SER:HB2	1:G:290:GLU:OE1	2.19	0.43
1:J:91:ILE:O	1:J:95:ILE:HG12	2.19	0.43
1:K:92:MET:SD	1:K:106:ILE:HD11	2.59	0.43
1:B:189:PRO:O	8:B:506:HOH:O	2.20	0.43
1:H:35:ALA:C	1:H:37:PRO:HD2	2.44	0.43
1:H:211:ASP:O	1:H:212:SER:HB3	2.19	0.43
1:H:328:VAL:O	1:H:329:TRP:C	2.62	0.43
1:K:85:TYR:CE2	1:K:89:GLN:NE2	2.87	0.43
1:C:71:GLN:N	1:C:72:PRO:CD	2.81	0.43
1:E:268:PHE:HB2	1:E:318:LEU:HD11	2.00	0.43
1:J:90:HIS:ND1	8:J:503:HOH:O	2.19	0.43
1:K:270:ARG:HD2	1:K:270:ARG:HA	1.88	0.43
1:B:279:HIS:NE2	1:B:289:LEU:HD11	2.34	0.42
1:D:128:ASN:N	1:D:129:PRO:HD3	2.34	0.42
1:E:301:GLY:O	1:E:302:VAL:CG1	2.66	0.42
1:F:42:TYR:O	1:F:43:HIS:C	2.62	0.42
1:L:229:PRO:O	1:L:230:PRO:C	2.60	0.42
1:B:132:LYS:HG3	1:B:229:PRO:HD3	2.01	0.42
1:G:271:LEU:HA	1:G:274:ILE:HD12	2.01	0.42
1:H:99:GLN:HB2	1:H:175:ASP:OD2	2.19	0.42
1:L:181:LEU:O	1:L:182:LYS:HB2	2.19	0.42
1:A:308:ILE:N	1:A:309:PRO:CD	2.82	0.42
1:F:36:TRP:CD2	1:F:37:PRO:HD3	2.55	0.42
1:F:211:ASP:O	1:F:212:SER:HB3	2.18	0.42
1:G:179:LEU:C	1:G:181:LEU:N	2.77	0.42
1:L:36:TRP:C	1:L:38:GLU:H	2.26	0.42
1:L:211:ASP:O	1:L:212:SER:HB3	2.19	0.42
1:C:77:ARG:CG	1:C:143:SER:HB3	2.49	0.42
1:C:177:LYS:O	1:C:180:SER:OG	2.25	0.42
1:E:81:SER:O	7:E:403:PEG:H31	2.19	0.42
1:B:150:ASN:O	1:B:151:ASN:HB2	2.18	0.42
1:B:295:GLN:HG3	1:B:297:TYR:CE1	2.54	0.42
1:E:182:LYS:HE2	8:E:515:HOH:O	2.20	0.42
1:F:49:ASN:OD1	1:F:49:ASN:C	2.62	0.42
1:I:301:GLY:H	1:J:300:GLY:HA3	1.84	0.42
1:J:62:ILE:HB	1:J:345:ASP:OD1	2.19	0.42
1:C:158:THR:C	1:C:160:SER:HA	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:HIS:CD2	1:F:153:VAL:HG22	2.54	0.42
1:K:162:VAL:HB	1:K:163:PRO:HD3	2.02	0.42
1:K:277:GLU:O	1:K:277:GLU:HG3	2.20	0.42
1:C:108:THR:HA	1:C:120:PHE:O	2.20	0.42
1:K:182:LYS:HE2	8:K:544:HOH:O	2.18	0.42
1:A:295:GLN:O	1:A:297:TYR:N	2.44	0.42
1:C:102:TRP:CE3	1:C:127:LEU:HG	2.54	0.42
1:E:181:LEU:O	1:E:182:LYS:CB	2.68	0.42
1:G:227:PRO:HG3	1:L:110:LEU:HB2	2.01	0.42
1:L:36:TRP:CD2	1:L:37:PRO:HD3	2.54	0.42
1:L:136:VAL:HG11	1:L:196:ILE:HD12	2.02	0.42
1:C:94:ARG:O	1:C:97:ARG:HG2	2.19	0.42
1:E:88:ARG:NH1	7:E:403:PEG:H21	2.33	0.42
1:E:107:ASP:HB3	1:E:122:ASN:HB2	2.02	0.42
1:F:92:MET:SD	1:F:106:ILE:HD11	2.60	0.42
1:F:277:GLU:HG3	1:F:281:LEU:CD1	2.50	0.42
1:I:296:ASN:OD1	1:I:296:ASN:O	2.37	0.42
1:K:66:TRP:O	1:K:71:GLN:HG3	2.19	0.42
1:B:92:MET:SD	1:B:106:ILE:HD11	2.60	0.42
1:C:179:LEU:HD23	1:C:179:LEU:O	2.20	0.42
1:G:353:VAL:O	1:G:357:GLU:HG3	2.19	0.42
1:K:309:PRO:HA	1:K:312:ARG:HH11	1.84	0.42
1:E:354:PHE:CD1	1:E:354:PHE:C	2.98	0.41
1:F:223:MET:HE1	1:F:241:MET:SD	2.59	0.41
1:J:56:ILE:O	1:J:57:ALA:C	2.62	0.41
1:J:64:GLU:HG3	8:J:545:HOH:O	2.20	0.41
1:A:38:GLU:OE2	1:G:147:SER:OG	2.35	0.41
1:B:328:VAL:HG21	1:B:334:ASP:HA	2.02	0.41
1:C:208:SER:HB2	1:C:209:PRO:CD	2.50	0.41
1:L:33:ALA:C	1:L:35:ALA:HB2	2.45	0.41
1:L:295:GLN:O	1:L:296:ASN:C	2.61	0.41
1:B:33:ALA:HA	1:B:35:ALA:CB	2.49	0.41
1:G:132:LYS:HG2	8:G:501:HOH:O	2.20	0.41
3:I:402:A1D93:C18	8:J:547:HOH:O	2.68	0.41
1:K:282:GLY:C	1:K:283:LEU:HD23	2.45	0.41
1:B:35:ALA:C	1:B:37:PRO:HD2	2.45	0.41
1:B:280:GLU:C	1:B:282:GLY:H	2.27	0.41
1:D:110:LEU:HD12	1:D:118:ARG:O	2.20	0.41
1:G:62:ILE:HG12	1:G:63:SER:N	2.35	0.41
1:I:270:ARG:NH2	1:I:357:GLU:OE1	2.44	0.41
1:K:43:HIS:ND1	8:K:506:HOH:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:ALA:HB1	1:K:349:LYS:HE2	2.02	0.41
1:C:270:ARG:HH21	1:C:357:GLU:CD	2.25	0.41
1:E:254:ASN:N	1:E:255:PRO:CD	2.84	0.41
1:F:98:LEU:HB3	1:F:175:ASP:OD2	2.20	0.41
1:H:149:TRP:C	1:H:151:ASN:N	2.76	0.41
1:I:285:LYS:C	1:I:287:HIS:N	2.79	0.41
1:J:278:LEU:HD23	1:J:283:LEU:HD12	2.01	0.41
1:A:311:LEU:HD12	8:A:573:HOH:O	2.20	0.41
1:E:172:ARG:O	1:E:173:ALA:C	2.61	0.41
1:E:263:ASN:ND2	8:E:524:HOH:O	2.54	0.41
1:I:296:ASN:O	1:I:296:ASN:CG	2.64	0.41
1:K:254:ASN:N	1:K:255:PRO:HD3	2.35	0.41
1:I:91:ILE:HG23	1:I:168:LEU:HD21	2.03	0.41
1:I:301:GLY:HA3	1:J:300:GLY:C	2.45	0.41
1:J:181:LEU:O	1:J:182:LYS:HB2	2.20	0.41
1:K:229:PRO:O	1:K:230:PRO:C	2.62	0.41
1:C:97:ARG:NH1	8:C:509:HOH:O	2.37	0.41
1:D:36:TRP:CD2	1:D:37:PRO:HD3	2.55	0.41
1:G:36:TRP:N	1:G:37:PRO:CD	2.84	0.41
1:G:258:PRO:HG2	1:G:260:PHE:CZ	2.55	0.41
1:G:281:LEU:HD13	1:G:283:LEU:HD12	2.03	0.41
1:I:89:GLN:O	1:I:93:GLN:HG3	2.20	0.41
1:J:71:GLN:N	1:J:72:PRO:CD	2.83	0.41
1:L:33:ALA:O	1:L:34:SER:HB3	2.21	0.41
1:A:92:MET:HG2	1:A:104:LEU:HD13	2.03	0.41
1:B:174:LEU:HD22	1:B:356:LEU:HD11	2.03	0.41
1:B:270:ARG:HH22	5:B:403:DMS:H23	1.86	0.41
1:D:162:VAL:HB	1:D:163:PRO:HD3	2.03	0.41
1:I:343:THR:HG21	8:I:557:HOH:O	2.21	0.41
4:I:403:GOL:H31	1:J:262:PRO:HG3	2.03	0.41
1:K:152:ARG:HG2	8:K:545:HOH:O	2.21	0.41
1:L:33:ALA:C	1:L:35:ALA:HB3	2.46	0.41
1:L:36:TRP:CG	1:L:37:PRO:HD3	2.56	0.41
1:A:33:ALA:HA	1:A:35:ALA:H	1.84	0.41
1:C:279:HIS:ND1	1:C:289:LEU:HD13	2.36	0.41
1:D:61:SER:OG	1:D:64:GLU:HG3	2.20	0.41
1:D:62:ILE:O	1:D:62:ILE:HG13	2.21	0.41
1:E:181:LEU:O	1:E:182:LYS:HG2	2.21	0.41
1:G:170:LEU:HD12	1:G:352:GLN:HG3	2.02	0.41
1:C:167:MET:HE2	1:C:197:PHE:CE2	2.56	0.40
1:E:157:ALA:HB3	1:E:334:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:208:SER:HB3	1:J:211:ASP:H	1.86	0.40
1:J:275:GLU:OE2	1:J:293:TYR:N	2.40	0.40
1:C:113:THR:HB	1:C:114:PRO:HD2	2.03	0.40
1:D:88:ARG:NH1	8:D:515:HOH:O	2.54	0.40
1:D:296:ASN:O	1:D:297:TYR:C	2.63	0.40
1:D:301:GLY:HA3	1:K:300:GLY:O	2.21	0.40
1:E:128:ASN:N	1:E:129:PRO:CD	2.84	0.40
1:G:174:LEU:HA	1:G:176:LYS:CE	2.51	0.40
1:A:89:GLN:O	1:A:93:GLN:HG3	2.20	0.40
1:B:94:ARG:O	1:B:97:ARG:HG2	2.22	0.40
1:E:276:HIS:ND1	1:E:292:ARG:NH2	2.70	0.40
1:I:170:LEU:HB2	8:I:508:HOH:O	2.21	0.40
1:K:284:LEU:C	1:K:285:LYS:HG3	2.46	0.40
1:L:50:SER:HA	1:L:53:LEU:HD12	2.04	0.40
1:L:55:GLN:HG3	8:L:507:HOH:O	2.21	0.40
1:D:108:THR:HA	1:D:120:PHE:O	2.21	0.40
1:D:137:LEU:HD12	1:D:245:VAL:HB	2.04	0.40
1:G:44:GLN:HG3	1:G:45:PRO:HD2	2.04	0.40
1:I:167:MET:HE2	1:I:197:PHE:CZ	2.56	0.40
1:J:228:HIS:HB2	1:J:237:GLN:HG3	2.03	0.40
1:K:279:HIS:N	1:K:284:LEU:HD22	2.37	0.40
1:A:123:ILE:HB	1:A:197:PHE:HB2	2.02	0.40
1:E:342:SER:HB2	8:E:609:HOH:O	2.21	0.40
1:H:289:LEU:HD23	1:H:292:ARG:HG2	2.03	0.40
7:J:403:PEG:C2	8:J:508:HOH:O	2.69	0.40

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

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	319/361 (88%)	300 (94%)	17 (5%)	2 (1%)	21	24
1	B	319/361 (88%)	295 (92%)	20 (6%)	4 (1%)	9	8
1	C	319/361 (88%)	298 (93%)	17 (5%)	4 (1%)	9	8
1	D	319/361 (88%)	293 (92%)	25 (8%)	1 (0%)	36	43
1	E	319/361 (88%)	308 (97%)	10 (3%)	1 (0%)	36	43
1	F	319/361 (88%)	293 (92%)	21 (7%)	5 (2%)	7	6
1	G	319/361 (88%)	294 (92%)	21 (7%)	4 (1%)	9	8
1	H	319/361 (88%)	297 (93%)	18 (6%)	4 (1%)	9	8
1	I	319/361 (88%)	295 (92%)	22 (7%)	2 (1%)	21	24
1	J	319/361 (88%)	293 (92%)	24 (8%)	2 (1%)	21	24
1	K	319/361 (88%)	292 (92%)	23 (7%)	4 (1%)	9	8
1	L	319/361 (88%)	285 (89%)	27 (8%)	7 (2%)	5	3
All	All	3828/4332 (88%)	3543 (93%)	245 (6%)	40 (1%)	12	12

All (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
1	E	212	SER
1	F	34	SER
1	H	212	SER
1	I	302	VAL
1	K	35	ALA
1	L	35	ALA
1	A	212	SER
1	C	302	VAL
1	D	212	SER
1	F	35	ALA
1	F	212	SER
1	G	74	LEU
1	H	34	SER
1	H	150	ASN

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Mol	Chain	Res	Type
1	I	212	SER
1	K	312	ARG
1	L	34	SER
1	L	212	SER
1	L	299	TYR
1	C	212	SER
1	G	34	SER
1	G	180	SER
1	H	300	GLY
1	K	212	SER
1	L	156	GLY
1	J	34	SER
1	J	212	SER
1	G	326	PRO
1	L	296	ASN
1	C	50	SER
1	C	303	ILE
1	K	230	PRO
1	L	163	PRO
1	F	230	PRO
1	F	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%)	13	14
1	B	284/314 (90%)	260 (92%)	24 (8%)	10	11
1	C	284/314 (90%)	261 (92%)	23 (8%)	11	12
1	D	284/314 (90%)	261 (92%)	23 (8%)	11	12
1	E	284/314 (90%)	267 (94%)	17 (6%)	17	21
1	F	284/314 (90%)	260 (92%)	24 (8%)	10	11
1	G	284/314 (90%)	254 (89%)	30 (11%)	6	6
1	H	284/314 (90%)	268 (94%)	16 (6%)	19	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	284/314 (90%)	254 (89%)	30 (11%)	6	6
1	J	284/314 (90%)	259 (91%)	25 (9%)	9	10
1	K	284/314 (90%)	267 (94%)	17 (6%)	17	21
1	L	284/314 (90%)	261 (92%)	23 (8%)	11	12
All	All	3408/3768 (90%)	3135 (92%)	273 (8%)	11	12

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	44	GLN
1	A	50	SER
1	A	130	THR
1	A	137	LEU
1	A	179	LEU
1	A	180	SER
1	A	205	LEU
1	A	206	HIS
1	A	208	SER
1	A	210	GLN
1	A	242	ASP
1	A	247	LEU
1	A	284	LEU
1	A	292	ARG
1	A	296	ASN
1	A	298	SER
1	A	299	TYR
1	A	324	PRO
1	A	327	GLU
1	A	342	SER
1	B	50	SER
1	B	55	GLN
1	B	58	GLU
1	B	97	ARG
1	B	130	THR
1	B	132	LYS
1	B	137	LEU
1	B	150	ASN
1	B	176	LYS
1	B	177	LYS
1	B	180	SER

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Mol	Chain	Res	Type
1	B	181	LEU
1	B	206	HIS
1	B	222	LYS
1	B	236	SER
1	B	238	LEU
1	B	242	ASP
1	B	243	LEU
1	B	262	PRO
1	B	288	SER
1	B	290	GLU
1	B	292	ARG
1	B	296	ASN
1	B	328	VAL
1	C	44	GLN
1	C	58	GLU
1	C	67	GLN
1	C	88	ARG
1	C	96	GLN
1	C	99	GLN
1	C	110	LEU
1	C	125	SER
1	C	130	THR
1	C	137	LEU
1	C	143	SER
1	C	177	LYS
1	C	192	SER
1	C	206	HIS
1	C	242	ASP
1	C	284	LEU
1	C	289	LEU
1	C	290	GLU
1	C	292	ARG
1	C	296	ASN
1	C	312	ARG
1	C	331	THR
1	C	337	GLU
1	D	34	SER
1	D	44	GLN
1	D	50	SER
1	D	51	SER
1	D	55	GLN
1	D	60	THR

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Mol	Chain	Res	Type
1	D	67	GLN
1	D	71	GLN
1	D	89	GLN
1	D	120	PHE
1	D	137	LEU
1	D	206	HIS
1	D	238	LEU
1	D	242	ASP
1	D	247	LEU
1	D	269	GLU
1	D	281	LEU
1	D	288	SER
1	D	290	GLU
1	D	312	ARG
1	D	324	PRO
1	D	342	SER
1	D	361	LEU
1	E	41	ASN
1	E	55	GLN
1	E	67	GLN
1	E	130	THR
1	E	153	VAL
1	E	180	SER
1	E	181	LEU
1	E	205	LEU
1	E	206	HIS
1	E	242	ASP
1	E	268	PHE
1	E	280	GLU
1	E	289	LEU
1	E	295	GLN
1	E	296	ASN
1	E	298	SER
1	E	323	SER
1	F	34	SER
1	F	58	GLU
1	F	63	SER
1	F	76	GLU
1	F	88	ARG
1	F	95	ILE
1	F	96	GLN
1	F	97	ARG

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Mol	Chain	Res	Type
1	F	106	ILE
1	F	130	THR
1	F	176	LYS
1	F	180	SER
1	F	182	LYS
1	F	205	LEU
1	F	206	HIS
1	F	210	GLN
1	F	242	ASP
1	F	285	LYS
1	F	288	SER
1	F	297	TYR
1	F	299	TYR
1	F	302	VAL
1	F	304	GLN
1	F	321	ILE
1	G	44	GLN
1	G	48	LEU
1	G	51	SER
1	G	58	GLU
1	G	62	ILE
1	G	63	SER
1	G	71	GLN
1	G	84	SER
1	G	108	THR
1	G	119	SER
1	G	121	SER
1	G	126	THR
1	G	130	THR
1	G	132	LYS
1	G	150	ASN
1	G	151	ASN
1	G	163	PRO
1	G	176	LYS
1	G	182	LYS
1	G	191	LEU
1	G	206	HIS
1	G	238	LEU
1	G	242	ASP
1	G	247	LEU
1	G	263	ASN
1	G	280	GLU

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Mol	Chain	Res	Type
1	G	289	LEU
1	G	292	ARG
1	G	295	GLN
1	G	297	TYR
1	H	51	SER
1	H	67	GLN
1	H	71	GLN
1	H	97	ARG
1	H	105	GLU
1	H	130	THR
1	H	149	TRP
1	H	151	ASN
1	H	174	LEU
1	H	205	LEU
1	H	206	HIS
1	H	242	ASP
1	H	269	GLU
1	H	272	GLN
1	H	284	LEU
1	H	342	SER
1	I	34	SER
1	I	47	ILE
1	I	50	SER
1	I	56	ILE
1	I	58	GLU
1	I	62	ILE
1	I	89	GLN
1	I	96	GLN
1	I	103	VAL
1	I	105	GLU
1	I	130	THR
1	I	137	LEU
1	I	155	VAL
1	I	167	MET
1	I	170	LEU
1	I	176	LYS
1	I	177	LYS
1	I	179	LEU
1	I	180	SER
1	I	181	LEU
1	I	193	LEU
1	I	205	LEU

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Mol	Chain	Res	Type
1	I	206	HIS
1	I	210	GLN
1	I	242	ASP
1	I	285	LYS
1	I	289	LEU
1	I	290	GLU
1	I	297	TYR
1	I	331	THR
1	J	34	SER
1	J	47	ILE
1	J	63	SER
1	J	71	GLN
1	J	125	SER
1	J	126	THR
1	J	130	THR
1	J	135	LEU
1	J	150	ASN
1	J	176	LYS
1	J	179	LEU
1	J	180	SER
1	J	206	HIS
1	J	242	ASP
1	J	247	LEU
1	J	280	GLU
1	J	286	ASP
1	J	289	LEU
1	J	295	GLN
1	J	297	TYR
1	J	303	ILE
1	J	323	SER
1	J	327	GLU
1	J	328	VAL
1	J	337	GLU
1	K	34	SER
1	K	51	SER
1	K	75	ILE
1	K	96	GLN
1	K	130	THR
1	K	149	TRP
1	K	176	LYS
1	K	182	LYS
1	K	205	LEU

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Mol	Chain	Res	Type
1	K	206	HIS
1	K	242	ASP
1	K	284	LEU
1	K	292	ARG
1	K	295	GLN
1	K	298	SER
1	K	302	VAL
1	K	327	GLU
1	L	38	GLU
1	L	55	GLN
1	L	61	SER
1	L	105	GLU
1	L	125	SER
1	L	128	ASN
1	L	130	THR
1	L	150	ASN
1	L	151	ASN
1	L	160	SER
1	L	163	PRO
1	L	176	LYS
1	L	177	LYS
1	L	181	LEU
1	L	206	HIS
1	L	210	GLN
1	L	242	ASP
1	L	245	VAL
1	L	247	LEU
1	L	281	LEU
1	L	288	SER
1	L	290	GLU
1	L	342	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	194	GLN
1	A	237	GLN
1	A	259	ASN
1	A	276	HIS
1	B	44	GLN
1	B	67	GLN

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Mol	Chain	Res	Type
1	B	68	ASN
1	B	210	GLN
1	B	295	GLN
1	C	68	ASN
1	C	194	GLN
1	C	319	HIS
1	D	68	ASN
1	D	89	GLN
1	D	90	HIS
1	D	128	ASN
1	D	237	GLN
1	D	335	ASN
1	E	41	ASN
1	E	112	GLN
1	E	295	GLN
1	E	296	ASN
1	F	112	GLN
1	F	194	GLN
1	F	272	GLN
1	F	352	GLN
1	G	128	ASN
1	G	194	GLN
1	G	254	ASN
1	G	272	GLN
1	G	296	ASN
1	H	194	GLN
1	H	206	HIS
1	H	218	HIS
1	H	259	ASN
1	I	112	GLN
1	I	194	GLN
1	I	218	HIS
1	K	89	GLN
1	K	259	ASN
1	K	263	ASN
1	K	296	ASN
1	L	89	GLN
1	L	134	HIS
1	L	194	GLN
1	L	218	HIS
1	L	259	ASN
1	L	295	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	H	401	2	21,22,22	2.08	8 (38%)	29,31,31	3.83	6 (20%)
7	PEG	J	403	-	6,6,6	0.89	0	5,5,5	0.91	0
3	A1D93	I	402	2	21,22,22	1.69	5 (23%)	29,31,31	2.29	8 (27%)
5	DMS	D	403	-	3,3,3	0.88	0	3,3,3	1.83	1 (33%)
6	DMF	E	404	-	4,4,4	0.56	0	4,4,4	0.36	0
3	A1D93	A	402	2	21,22,22	1.82	7 (33%)	29,31,31	2.12	9 (31%)
4	GOL	F	403	-	5,5,5	0.73	0	5,5,5	1.32	0
6	DMF	C	403	-	4,4,4	1.04	0	4,4,4	1.37	1 (25%)
4	GOL	A	403	-	5,5,5	0.71	0	5,5,5	2.10	2 (40%)
3	A1D93	L	401	2	21,22,22	1.60	3 (14%)	29,31,31	1.43	4 (13%)
3	A1D93	K	401	2	21,22,22	1.52	4 (19%)	29,31,31	2.64	10 (34%)
7	PEG	E	403	-	6,6,6	1.55	1 (16%)	5,5,5	1.61	2 (40%)
3	A1D93	J	402	2	21,22,22	1.89	7 (33%)	29,31,31	2.56	7 (24%)
3	A1D93	G	401	2	21,22,22	2.02	7 (33%)	29,31,31	1.83	4 (13%)
3	A1D93	B	402	2	21,22,22	1.72	6 (28%)	29,31,31	1.64	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1D93	D	402	2	21,22,22	1.96	7 (33%)	29,31,31	1.61	5 (17%)
7	PEG	D	404	-	6,6,6	0.75	0	5,5,5	0.64	0
4	GOL	I	403	-	5,5,5	0.84	0	5,5,5	0.77	0
3	A1D93	C	402	2	21,22,22	1.42	4 (19%)	29,31,31	2.63	7 (24%)
3	A1D93	F	402	2	21,22,22	2.14	7 (33%)	29,31,31	2.35	10 (34%)
5	DMS	B	403	-	3,3,3	0.72	0	3,3,3	1.79	2 (66%)
3	A1D93	E	402	2	21,22,22	1.36	3 (14%)	29,31,31	1.99	7 (24%)

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	H	401	2	-	4/10/10/10	0/3/3/3
7	PEG	J	403	-	-	1/4/4/4	-
3	A1D93	I	402	2	-	2/10/10/10	0/3/3/3
6	DMF	E	404	-	-	2/2/2/2	-
3	A1D93	A	402	2	-	0/10/10/10	0/3/3/3
4	GOL	F	403	-	-	2/4/4/4	-
6	DMF	C	403	-	-	0/2/2/2	-
4	GOL	A	403	-	-	2/4/4/4	-
3	A1D93	L	401	2	-	0/10/10/10	0/3/3/3
3	A1D93	K	401	2	-	4/10/10/10	0/3/3/3
7	PEG	E	403	-	-	2/4/4/4	-
3	A1D93	J	402	2	-	2/10/10/10	0/3/3/3
3	A1D93	G	401	2	-	0/10/10/10	0/3/3/3
3	A1D93	B	402	2	-	2/10/10/10	0/3/3/3
3	A1D93	D	402	2	-	0/10/10/10	0/3/3/3
7	PEG	D	404	-	-	3/4/4/4	-
4	GOL	I	403	-	-	0/4/4/4	-
3	A1D93	C	402	2	-	0/10/10/10	0/3/3/3
3	A1D93	F	402	2	-	2/10/10/10	0/3/3/3
3	A1D93	E	402	2	-	0/10/10/10	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	401	A1D93	S02-N04	5.02	1.72	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	401	A1D93	O01-S02	4.86	1.50	1.43
3	H	401	A1D93	O03-S02	4.85	1.50	1.43
3	D	402	A1D93	S02-N04	4.75	1.72	1.62
3	F	402	A1D93	C07-C08	4.33	1.46	1.40
3	A	402	A1D93	O01-S02	4.00	1.49	1.43
3	F	402	A1D93	O03-S02	3.99	1.49	1.43
3	F	402	A1D93	S02-N04	3.79	1.70	1.62
3	G	401	A1D93	S02-N04	3.78	1.70	1.62
3	H	401	A1D93	S02-N04	3.78	1.70	1.62
3	J	402	A1D93	S02-N04	3.67	1.70	1.62
3	B	402	A1D93	O01-S02	3.65	1.48	1.43
3	K	401	A1D93	S02-N04	3.59	1.69	1.62
3	E	402	A1D93	S02-N04	3.53	1.69	1.62
3	D	402	A1D93	C07-C08	3.47	1.45	1.40
3	H	401	A1D93	C12-N11	-3.44	1.32	1.37
3	I	402	A1D93	S02-N04	3.30	1.69	1.62
3	K	401	A1D93	C07-C06	3.25	1.44	1.38
3	J	402	A1D93	C12-C08	-3.16	1.35	1.40
3	A	402	A1D93	O03-S02	3.15	1.47	1.43
3	I	402	A1D93	O03-S02	3.11	1.47	1.43
3	G	401	A1D93	C12-N11	-3.06	1.32	1.37
3	A	402	A1D93	C07-C08	3.05	1.44	1.40
3	H	401	A1D93	C14-C15	2.98	1.57	1.51
3	L	401	A1D93	C13-C12	2.97	1.44	1.39
3	D	402	A1D93	C13-C12	2.94	1.44	1.39
3	F	402	A1D93	C05-N04	2.84	1.47	1.43
3	B	402	A1D93	S02-N04	2.80	1.68	1.62
3	B	402	A1D93	C05-N04	2.79	1.47	1.43
3	B	402	A1D93	C07-C06	2.78	1.43	1.38
3	J	402	A1D93	C05-N04	2.72	1.47	1.43
3	H	401	A1D93	C06-C05	2.70	1.43	1.39
3	J	402	A1D93	C13-C12	2.64	1.43	1.39
7	E	403	PEG	C2-C1	2.64	1.63	1.49
3	I	402	A1D93	C07-C08	2.62	1.44	1.40
3	I	402	A1D93	C07-C06	2.62	1.43	1.38
3	C	402	A1D93	O01-S02	2.61	1.47	1.43
3	C	402	A1D93	S02-N04	2.60	1.68	1.62
3	F	402	A1D93	C06-C05	2.59	1.43	1.39
3	F	402	A1D93	C14-C15	2.59	1.56	1.51
3	G	401	A1D93	C16-C15	2.52	1.43	1.38
3	F	402	A1D93	C13-C05	2.51	1.43	1.39
3	A	402	A1D93	C08-N09	-2.50	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	A1D93	C06-C05	2.46	1.43	1.39
3	G	401	A1D93	C14-C15	2.45	1.56	1.51
3	B	402	A1D93	C08-N09	-2.45	1.35	1.39
3	D	402	A1D93	C12-C08	-2.43	1.36	1.40
3	K	401	A1D93	C07-C08	2.41	1.43	1.40
3	D	402	A1D93	C10-N11	-2.39	1.29	1.35
3	C	402	A1D93	C08-N09	-2.39	1.35	1.39
3	C	402	A1D93	C05-N04	2.37	1.46	1.43
3	J	402	A1D93	C07-C08	2.36	1.43	1.40
3	E	402	A1D93	C08-N09	-2.31	1.35	1.39
3	G	401	A1D93	C07-C08	2.31	1.43	1.40
3	G	401	A1D93	C13-C12	2.23	1.43	1.39
3	K	401	A1D93	C05-N04	2.21	1.46	1.43
3	D	402	A1D93	O03-S02	2.18	1.46	1.43
3	J	402	A1D93	C12-N11	-2.17	1.34	1.37
3	A	402	A1D93	S02-N04	2.17	1.67	1.62
3	H	401	A1D93	C12-C08	-2.14	1.37	1.40
3	I	402	A1D93	C13-C12	2.14	1.42	1.39
3	L	401	A1D93	C05-N04	2.10	1.46	1.43
3	B	402	A1D93	C06-C05	2.09	1.42	1.39
3	E	402	A1D93	C07-C06	2.09	1.42	1.38
3	H	401	A1D93	C13-C12	2.06	1.42	1.39
3	J	402	A1D93	C14-C15	2.04	1.55	1.51
3	A	402	A1D93	C07-C06	2.03	1.42	1.38
3	A	402	A1D93	C12-N11	-2.02	1.34	1.37
3	H	401	A1D93	C08-N09	-2.01	1.36	1.39

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	A1D93	O01-S02-C14	-16.46	83.07	108.33
3	J	402	A1D93	O03-S02-O01	-11.87	102.73	119.34
3	K	401	A1D93	O03-S02-O01	-10.33	104.90	119.34
3	H	401	A1D93	O03-S02-O01	-8.83	106.98	119.34
3	C	402	A1D93	O03-S02-O01	-8.72	107.15	119.34
3	I	402	A1D93	O03-S02-O01	-8.44	107.54	119.34
3	G	401	A1D93	O03-S02-O01	-7.72	108.54	119.34
3	C	402	A1D93	O01-S02-N04	6.94	124.03	107.23
3	A	402	A1D93	O03-S02-O01	-6.94	109.64	119.34
3	F	402	A1D93	O03-S02-O01	-6.36	110.45	119.34
3	E	402	A1D93	O03-S02-O01	-6.29	110.54	119.34
3	F	402	A1D93	O01-S02-C14	-5.90	99.27	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	A1D93	O01-S02-N04	5.20	119.82	107.23
3	B	402	A1D93	O03-S02-O01	-4.89	112.50	119.34
3	D	402	A1D93	O03-S02-O01	-4.74	112.71	119.34
3	L	401	A1D93	O03-S02-O01	-4.17	113.51	119.34
3	I	402	A1D93	O01-S02-C14	3.96	114.41	108.33
3	A	402	A1D93	O03-S02-C14	3.90	114.31	108.33
3	F	402	A1D93	N11-C10-N09	-3.77	108.13	113.87
3	K	401	A1D93	O01-S02-N04	3.74	116.29	107.23
3	C	402	A1D93	O01-S02-C14	-3.68	102.68	108.33
3	K	401	A1D93	O01-S02-C14	-3.57	102.85	108.33
3	B	402	A1D93	O03-S02-C14	3.53	113.75	108.33
3	H	401	A1D93	O03-S02-C14	3.49	113.69	108.33
3	L	401	A1D93	O03-S02-C14	3.46	113.64	108.33
3	L	401	A1D93	C15-C14-S02	3.32	119.21	112.44
3	K	401	A1D93	C07-C08-N09	3.15	135.43	129.62
3	F	402	A1D93	C07-C08-N09	3.14	135.42	129.62
3	F	402	A1D93	C07-C06-C05	-3.11	116.72	120.30
3	E	402	A1D93	C06-C05-N04	3.09	126.53	120.02
3	F	402	A1D93	C08-N09-C10	3.03	111.05	105.18
3	F	402	A1D93	C13-C12-C08	-2.97	117.77	122.17
4	A	403	GOL	O3-C3-C2	-2.97	97.03	110.38
4	A	403	GOL	C3-C2-C1	-2.96	100.93	111.80
3	H	401	A1D93	O03-S02-N04	2.95	114.38	107.23
3	J	402	A1D93	O01-S02-C14	-2.88	103.91	108.33
3	I	402	A1D93	C13-C05-N04	-2.87	112.94	119.92
3	C	402	A1D93	C16-C15-C20	2.83	122.44	118.23
3	G	401	A1D93	O01-S02-N04	2.81	114.02	107.23
3	K	401	A1D93	C07-C06-C05	-2.80	117.07	120.30
3	E	402	A1D93	C13-C05-N04	-2.76	113.21	119.92
3	K	401	A1D93	C06-C05-N04	2.75	125.81	120.02
3	I	402	A1D93	N11-C10-N09	-2.74	109.69	113.87
3	I	402	A1D93	C15-C14-S02	2.72	117.97	112.44
3	I	402	A1D93	C06-C05-N04	2.70	125.69	120.02
3	B	402	A1D93	C14-C15-C16	-2.69	117.31	120.56
3	E	402	A1D93	C07-C06-C05	-2.65	117.25	120.30
3	A	402	A1D93	C07-C08-N09	2.63	134.47	129.62
3	E	402	A1D93	C14-C15-C20	-2.59	117.43	120.56
3	A	402	A1D93	C13-C05-N04	-2.59	113.63	119.92
3	H	401	A1D93	N11-C10-N09	-2.59	109.93	113.87
3	E	402	A1D93	C13-C12-C08	-2.58	118.33	122.17
3	A	402	A1D93	C15-C14-S02	2.57	117.67	112.44
3	J	402	A1D93	O03-S02-C14	2.54	112.24	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	402	A1D93	C07-C06-C05	-2.54	117.38	120.30
3	A	402	A1D93	C06-C05-N04	2.53	125.34	120.02
3	A	402	A1D93	C08-C12-N11	2.52	110.33	106.15
3	D	402	A1D93	O01-S02-C14	2.51	112.18	108.33
3	B	402	A1D93	C18-C19-C20	2.49	123.31	120.24
7	E	403	PEG	O2-C2-C1	2.48	121.06	110.11
3	C	402	A1D93	C07-C08-N09	2.44	134.12	129.62
3	K	401	A1D93	C13-C05-N04	-2.44	114.00	119.92
3	D	402	A1D93	C07-C08-N09	2.43	134.10	129.62
5	D	403	DMS	O-S-C1	2.42	118.63	106.49
3	E	402	A1D93	C07-C08-N09	2.41	134.07	129.62
3	D	402	A1D93	O03-S02-C14	-2.39	104.66	108.33
3	J	402	A1D93	N11-C10-N09	-2.33	110.33	113.87
3	C	402	A1D93	O03-S02-C14	2.33	111.90	108.33
5	B	403	DMS	O-S-C1	2.30	118.00	106.49
3	B	402	A1D93	C19-C20-C15	-2.29	117.39	120.61
7	E	403	PEG	C3-O2-C2	2.22	122.98	113.26
3	G	401	A1D93	O03-S02-C14	2.22	111.74	108.33
3	D	402	A1D93	N11-C10-N09	-2.21	110.50	113.87
3	F	402	A1D93	C12-C08-N09	-2.20	103.64	108.39
3	F	402	A1D93	O01-S02-N04	2.17	112.49	107.23
3	I	402	A1D93	C07-C08-N09	2.15	133.59	129.62
3	A	402	A1D93	C14-C15-C16	-2.14	117.97	120.56
3	J	402	A1D93	C07-C08-N09	2.14	133.57	129.62
6	C	403	DMF	C2-N-C1	2.14	127.92	117.35
3	A	402	A1D93	C07-C06-C05	-2.14	117.84	120.30
3	L	401	A1D93	O01-S02-N04	-2.11	102.14	107.23
3	K	401	A1D93	C08-C12-N11	2.09	109.60	106.15
3	F	402	A1D93	C08-C12-N11	2.05	109.55	106.15
5	B	403	DMS	C2-S-C1	2.05	108.91	98.42
3	J	402	A1D93	C15-C14-S02	2.04	116.59	112.44
3	G	401	A1D93	C07-C08-N09	2.03	133.37	129.62
3	K	401	A1D93	O03-S02-N04	2.02	112.13	107.23
3	B	402	A1D93	N11-C10-N09	-2.02	110.80	113.87
3	J	402	A1D93	O03-S02-N04	2.02	112.11	107.23
3	C	402	A1D93	C06-C05-N04	2.01	124.26	120.02
3	K	401	A1D93	C07-C08-C12	-2.00	118.05	120.26

There are no chirality outliers.

All (28) torsion outliers are listed below:

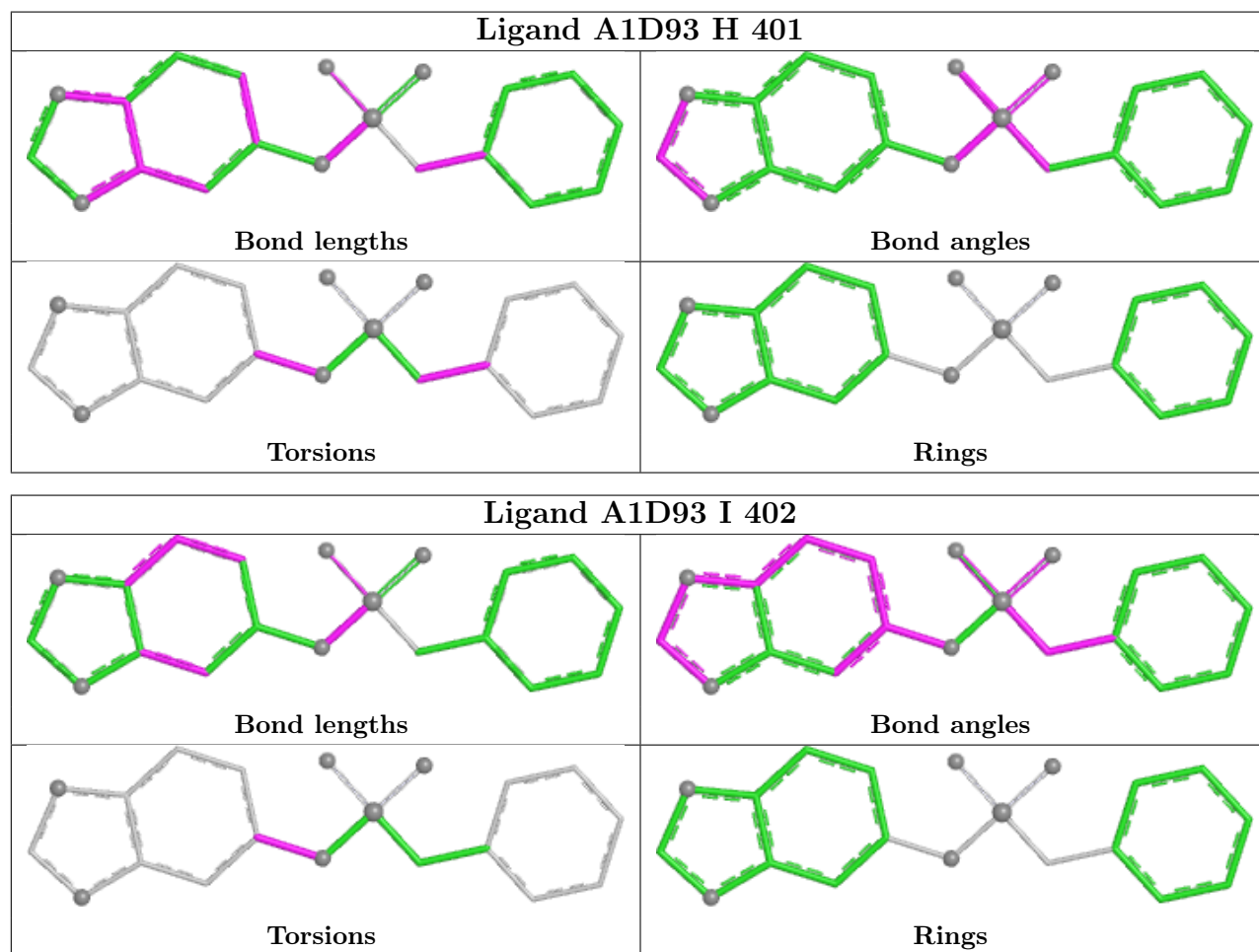
Mol	Chain	Res	Type	Atoms
3	H	401	A1D93	S02-C14-C15-C20
3	H	401	A1D93	S02-C14-C15-C16
4	F	403	GOL	O1-C1-C2-C3
7	D	404	PEG	O1-C1-C2-O2
7	D	404	PEG	O2-C3-C4-O4
4	A	403	GOL	O1-C1-C2-C3
4	F	403	GOL	O1-C1-C2-O2
7	E	403	PEG	O1-C1-C2-O2
3	K	401	A1D93	S02-C14-C15-C20
3	K	401	A1D93	S02-C14-C15-C16
7	J	403	PEG	O2-C3-C4-O4
6	E	404	DMF	O-C-N-C1
6	E	404	DMF	O-C-N-C2
7	E	403	PEG	C1-C2-O2-C3
3	B	402	A1D93	C06-C05-N04-S02
3	I	402	A1D93	C06-C05-N04-S02
3	I	402	A1D93	C13-C05-N04-S02
3	J	402	A1D93	C06-C05-N04-S02
3	H	401	A1D93	C13-C05-N04-S02
3	B	402	A1D93	C13-C05-N04-S02
3	H	401	A1D93	C06-C05-N04-S02
3	F	402	A1D93	C13-C05-N04-S02
4	A	403	GOL	O1-C1-C2-O2
3	K	401	A1D93	C06-C05-N04-S02
3	F	402	A1D93	C06-C05-N04-S02
3	J	402	A1D93	C13-C05-N04-S02
7	D	404	PEG	C1-C2-O2-C3
3	K	401	A1D93	C13-C05-N04-S02

There are no ring outliers.

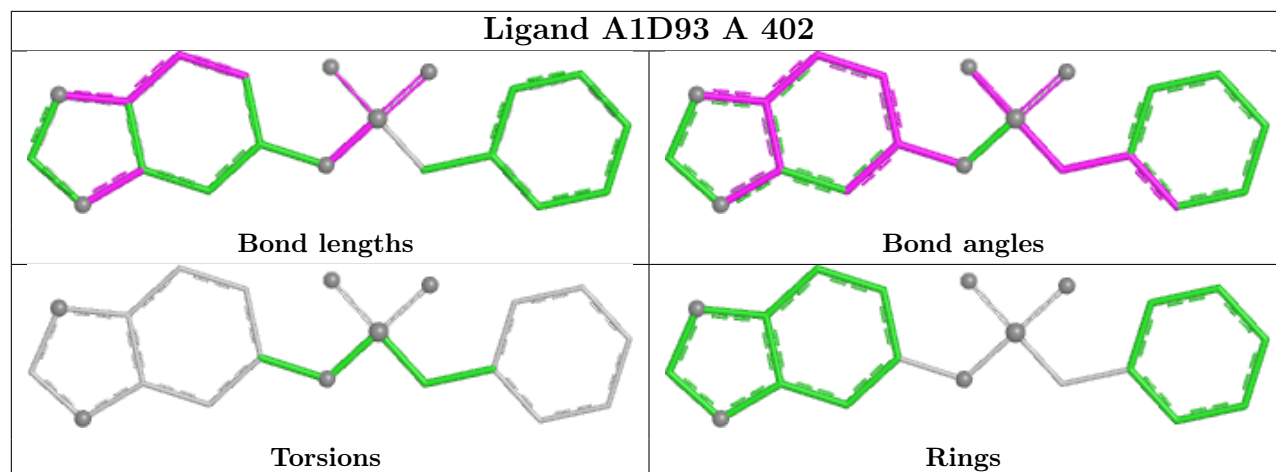
10 monomers are involved in 25 short contacts:

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

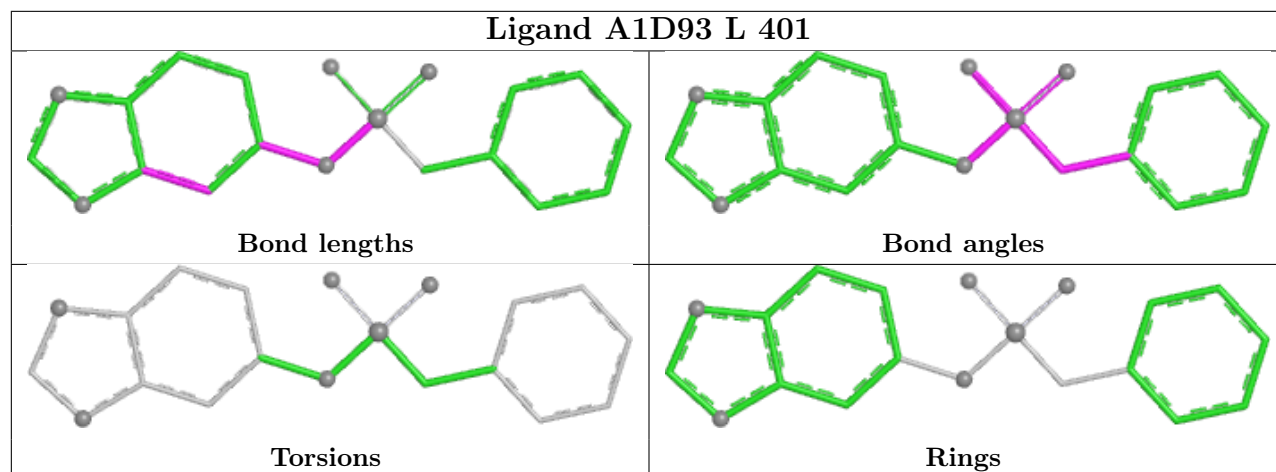
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



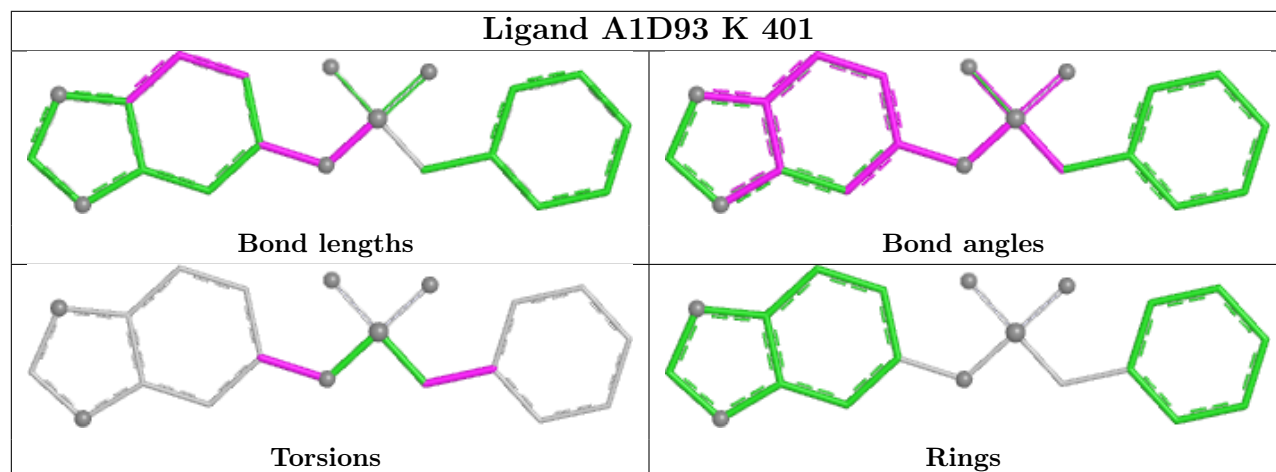
Ligand A1D93 A 402



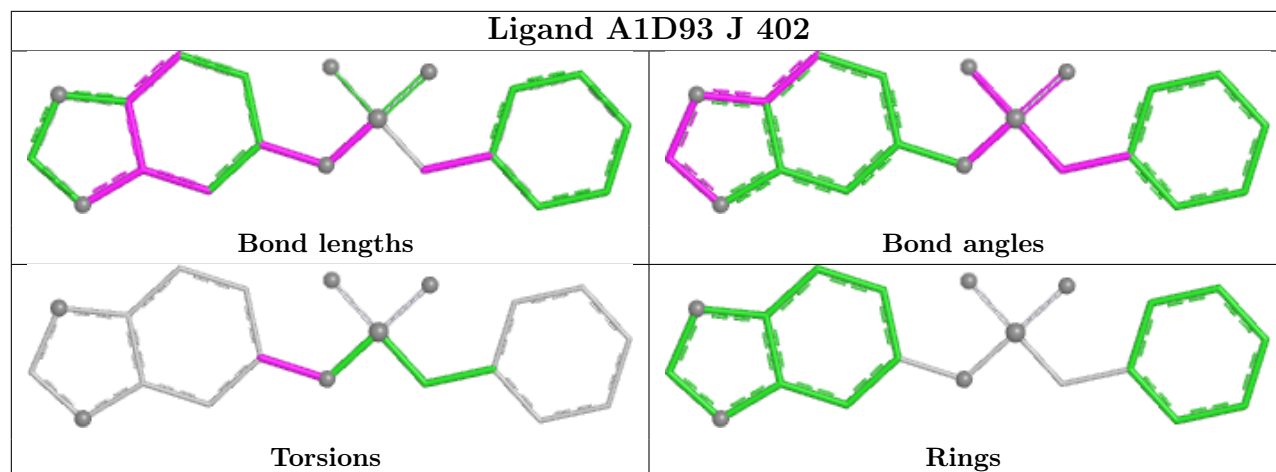
Ligand A1D93 L 401



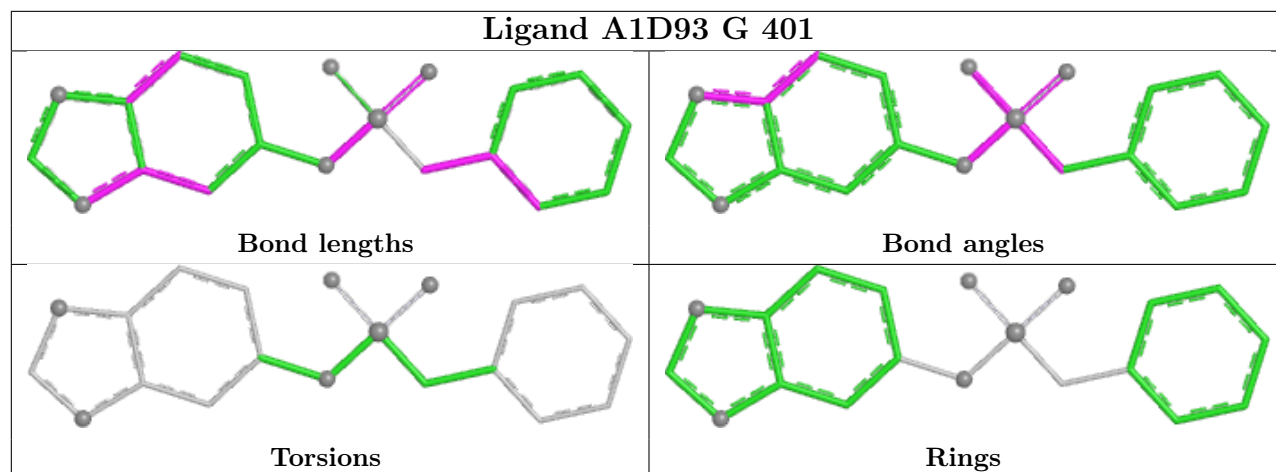
Ligand A1D93 K 401



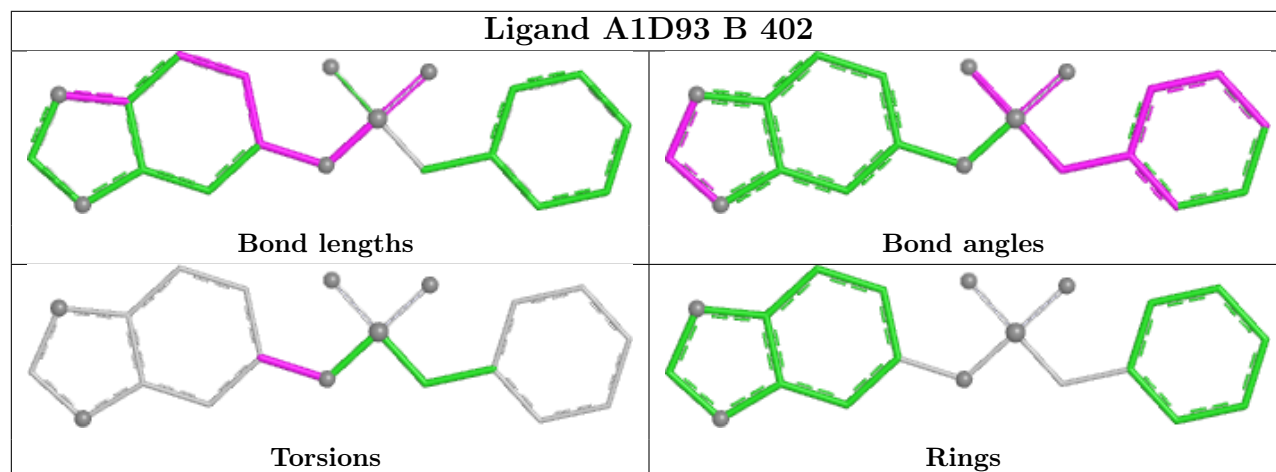
Ligand A1D93 J 402



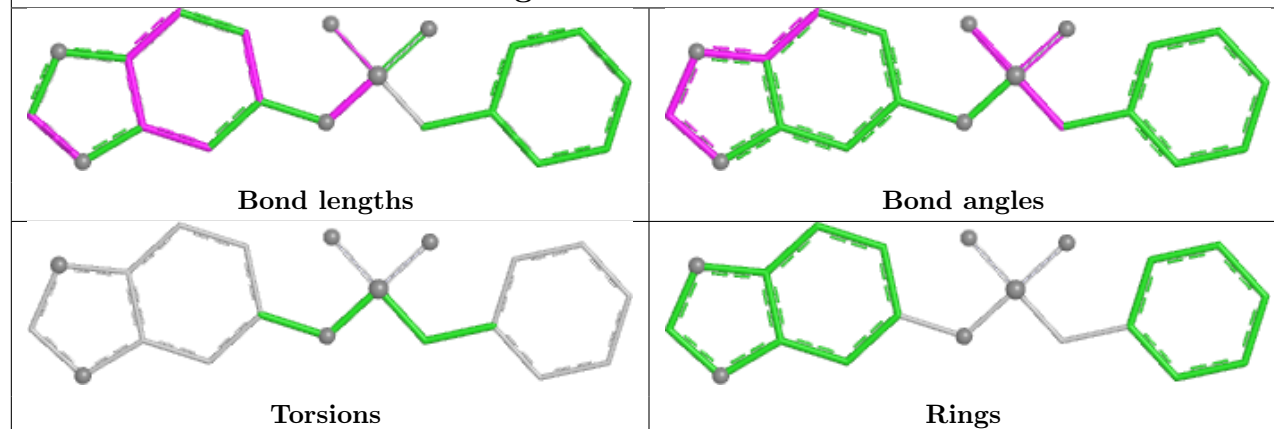
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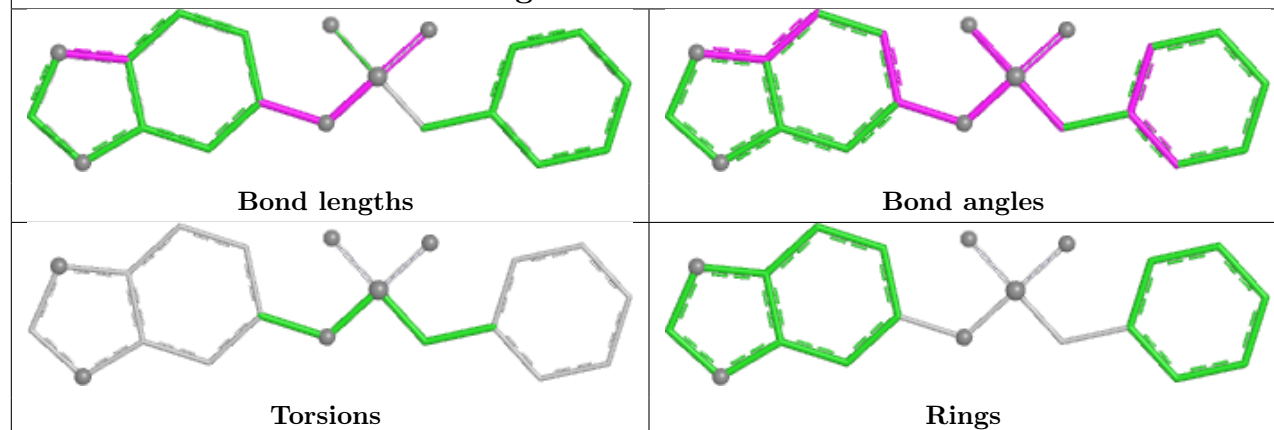
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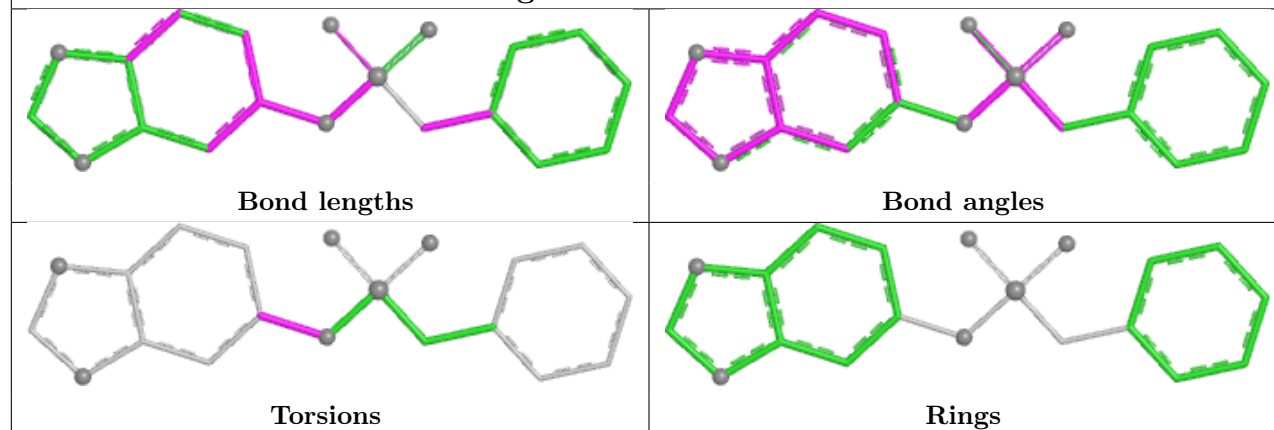
Ligand A1D93 D 402

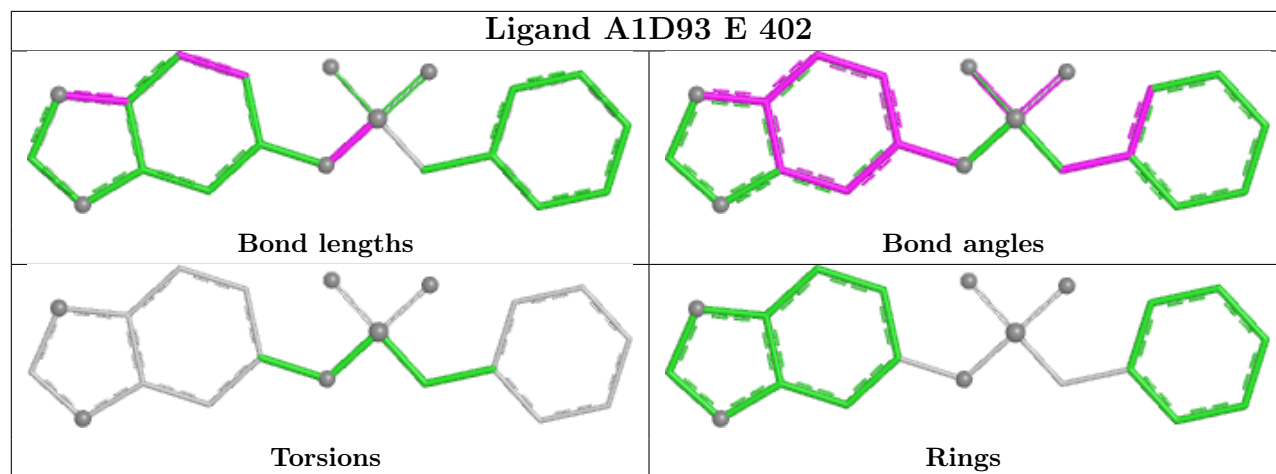


Ligand A1D93 C 402



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

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	323/361 (89%)	-0.43	3 (0%) 81 84	34, 48, 73, 110	0
1	B	323/361 (89%)	-0.35	3 (0%) 81 84	32, 48, 71, 101	0
1	C	323/361 (89%)	-0.20	5 (1%) 72 77	37, 51, 77, 114	0
1	D	323/361 (89%)	-0.26	3 (0%) 81 84	32, 53, 81, 115	0
1	E	323/361 (89%)	-0.27	3 (0%) 81 84	29, 50, 75, 114	0
1	F	323/361 (89%)	-0.22	3 (0%) 81 84	36, 52, 79, 101	0
1	G	323/361 (89%)	-0.08	1 (0%) 90 92	35, 58, 88, 110	0
1	H	323/361 (89%)	-0.19	6 (1%) 66 71	35, 54, 81, 117	0
1	I	323/361 (89%)	0.02	5 (1%) 72 77	41, 60, 90, 111	0
1	J	323/361 (89%)	-0.04	6 (1%) 66 71	38, 62, 93, 126	0
1	K	323/361 (89%)	-0.15	5 (1%) 72 77	38, 54, 81, 113	0
1	L	323/361 (89%)	-0.04	8 (2%) 58 64	37, 58, 85, 126	0
All	All	3876/4332 (89%)	-0.18	51 (1%) 75 79	29, 54, 84, 126	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	33	ALA	4.3
1	K	33	ALA	3.9
1	L	297	TYR	3.6
1	B	300	GLY	3.5
1	I	297	TYR	3.4
1	G	297	TYR	3.4
1	C	33	ALA	3.3
1	D	297	TYR	3.2
1	I	33	ALA	3.2
1	L	299	TYR	3.0
1	H	300	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	189	PRO	2.9
1	B	33	ALA	2.9
1	E	297	TYR	2.8
1	L	33	ALA	2.8
1	K	300	GLY	2.6
1	E	33	ALA	2.6
1	L	302	VAL	2.6
1	F	189	PRO	2.6
1	H	189	PRO	2.6
1	E	300	GLY	2.5
1	L	300	GLY	2.5
1	A	297	TYR	2.5
1	A	301	GLY	2.5
1	C	297	TYR	2.5
1	I	284	LEU	2.5
1	K	297	TYR	2.4
1	D	301	GLY	2.3
1	J	33	ALA	2.3
1	L	301	GLY	2.3
1	I	189	PRO	2.3
1	J	297	TYR	2.3
1	J	299	TYR	2.3
1	K	301	GLY	2.3
1	L	298	SER	2.2
1	C	299	TYR	2.2
1	F	297	TYR	2.2
1	H	297	TYR	2.2
1	H	302	VAL	2.2
1	C	191	LEU	2.1
1	D	191	LEU	2.1
1	H	191	LEU	2.1
1	L	296	ASN	2.1
1	A	299	TYR	2.1
1	J	300	GLY	2.1
1	B	301	GLY	2.1
1	J	301	GLY	2.1
1	I	191	LEU	2.0
1	J	189	PRO	2.0
1	K	302	VAL	2.0
1	F	284	LEU	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
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

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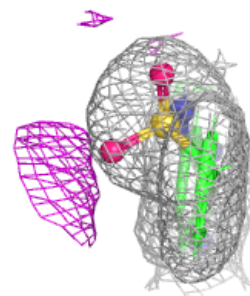
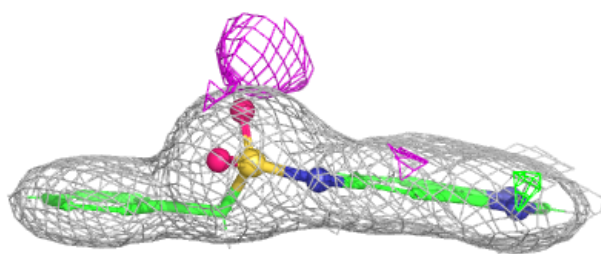
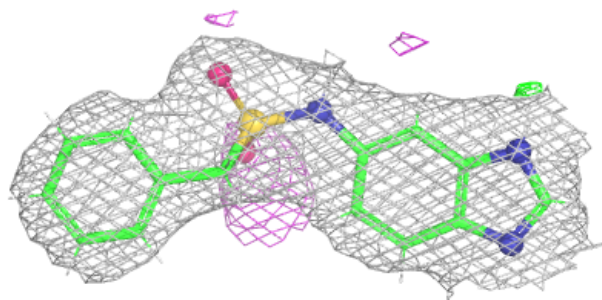
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	F	401	1/1	1.00	0.05	42,42,42,42	0
2	ZN	G	400	1/1	1.00	0.03	43,43,43,43	0
2	ZN	H	400	1/1	1.00	0.04	39,39,39,39	0
2	ZN	A	401	1/1	1.00	0.05	40,40,40,40	0
2	ZN	J	401	1/1	1.00	0.01	42,42,42,42	0
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.

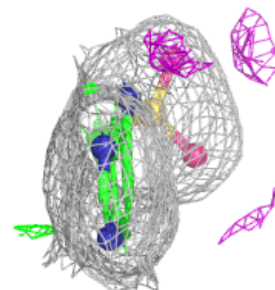
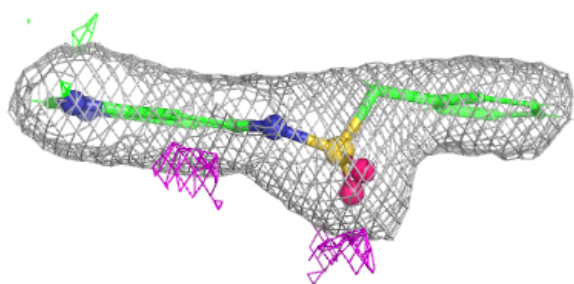
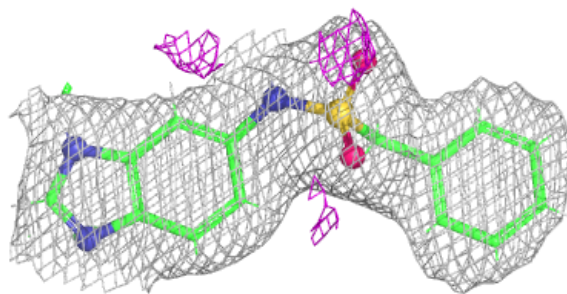
Electron density around A1D93 K 401:

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

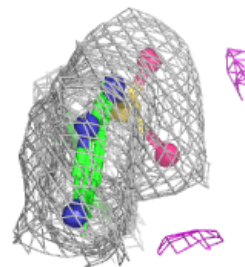
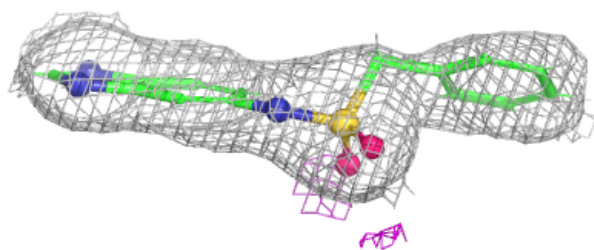
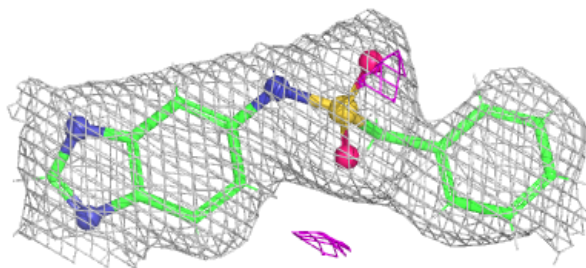


Electron density around A1D93 C 402:

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

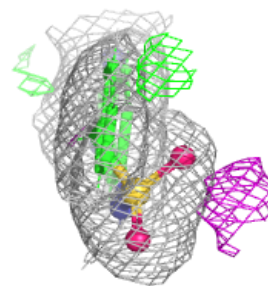
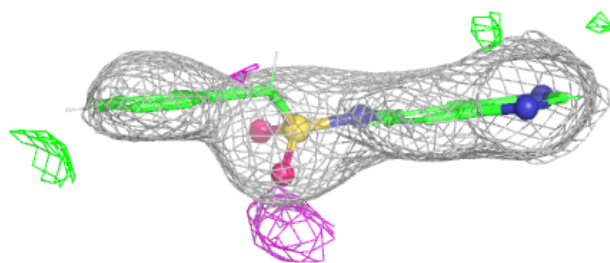
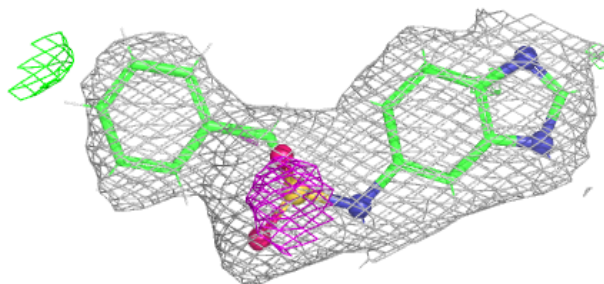
**Electron density around A1D93 G 401:**

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

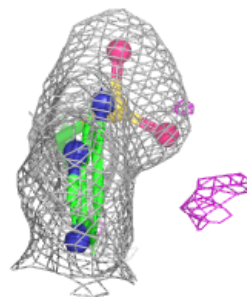
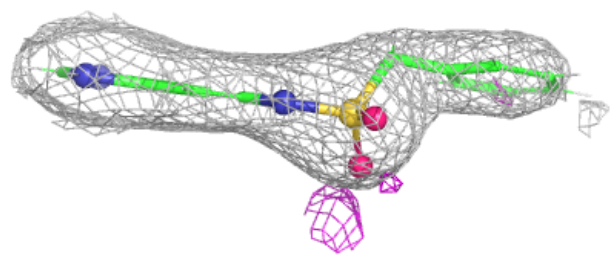
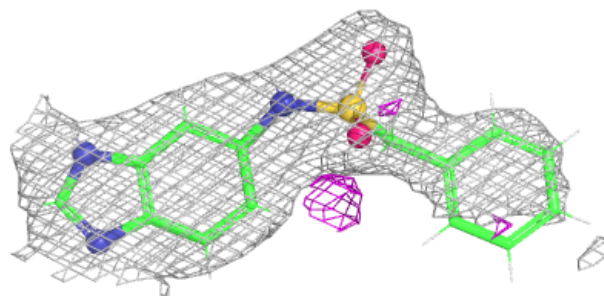


Electron density around A1D93 H 401:

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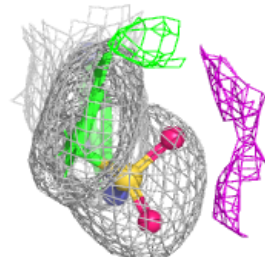
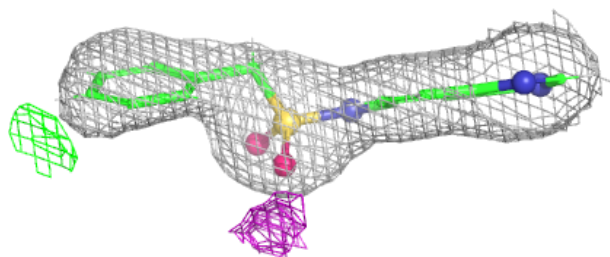
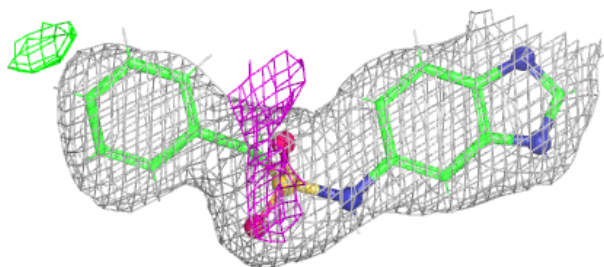
**Electron density around A1D93 I 402:**

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

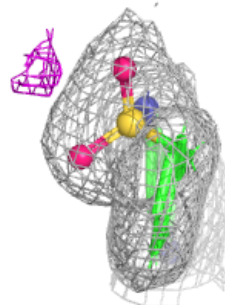
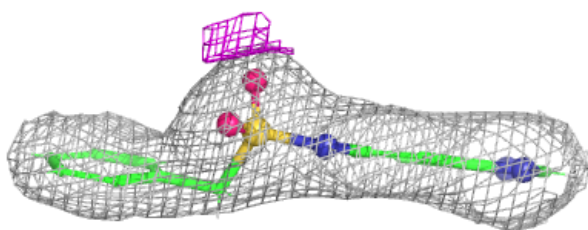
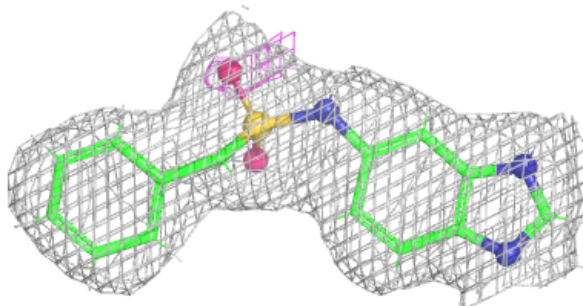


Electron density around A1D93 J 402:

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

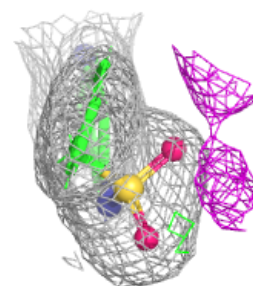
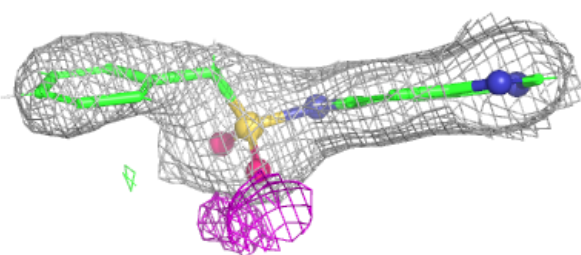
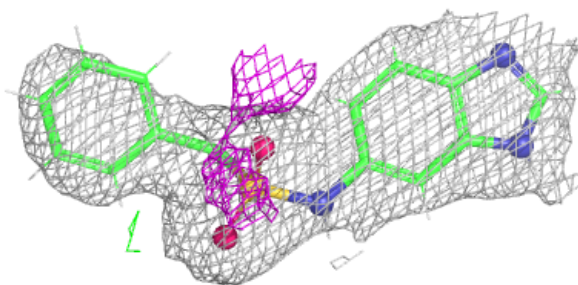
**Electron density around A1D93 D 402:**

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and green (positive)

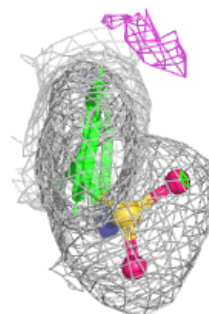
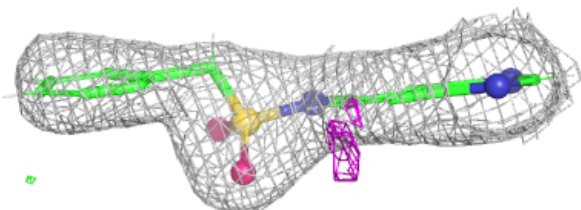
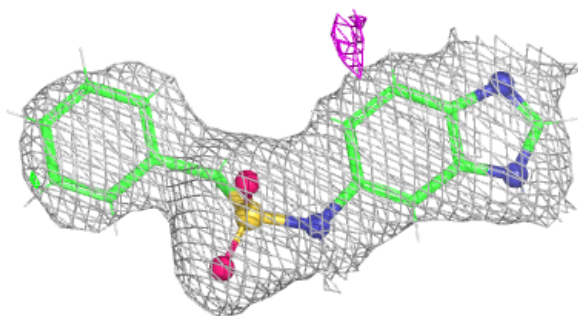


Electron density around A1D93 L 401:

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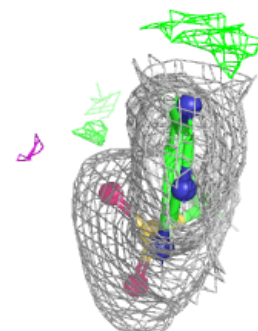
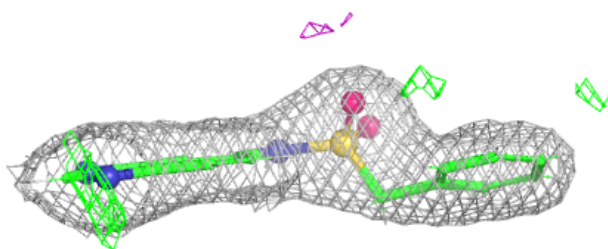
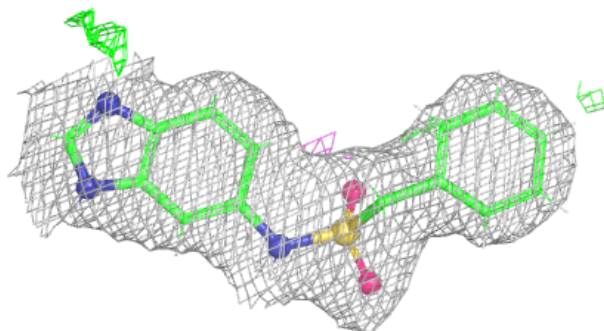
**Electron density around A1D93 E 402:**

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and green (positive)

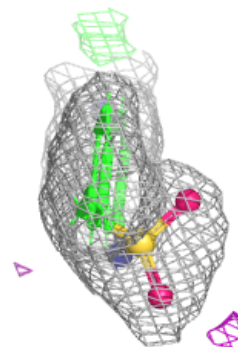
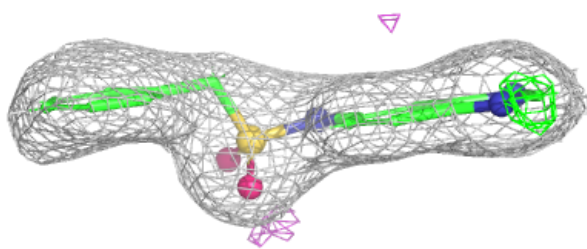
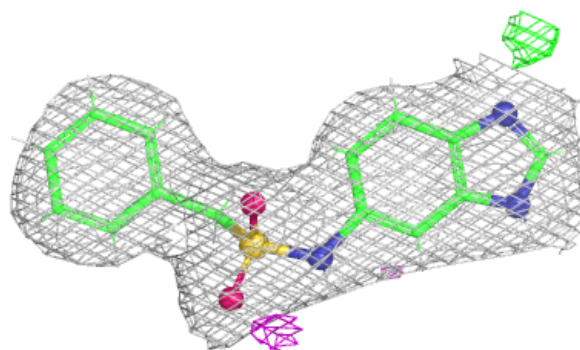


Electron density around A1D93 F 402:

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and green (positive)

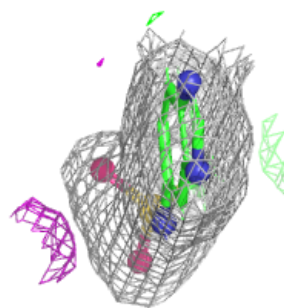
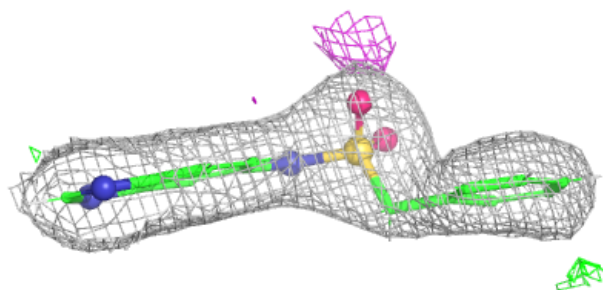
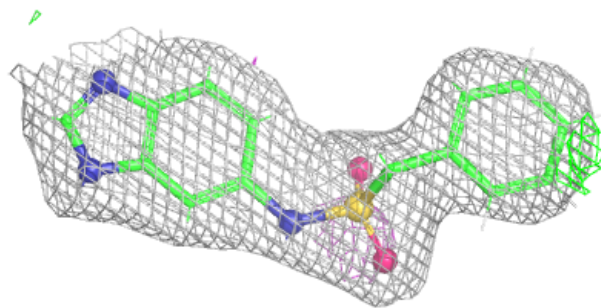
**Electron density around A1D93 A 402:**

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 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.