



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:03 PM UTC

PDB ID : 9LZV / pdb_00009lzv
Title : Crystal structure of human glutaminy cyclase in complex with Inhibitor M-42
Authors : Li, G.-B.; Meng, F.-B.; Mou, J.
Deposited on : 2025-02-22
Resolution : 2.33 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

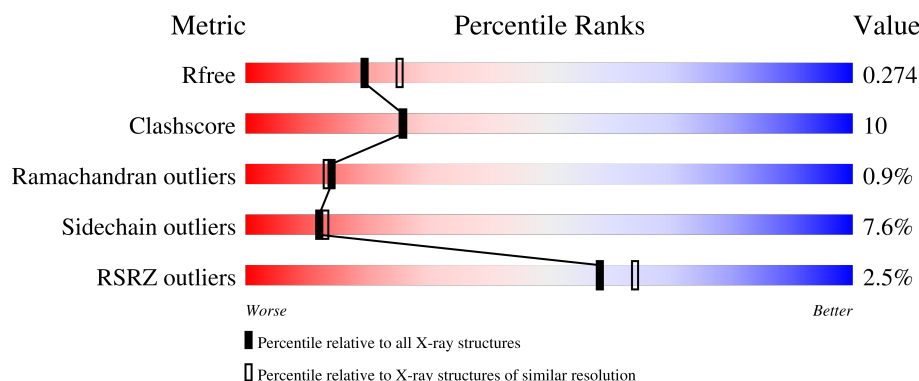
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	329	<div> <div>2%</div> <div>74%</div> <div>19%</div> <div>5%</div> <div>.</div> </div>
1	B	329	<div> <div>3%</div> <div>73%</div> <div>22%</div> <div>.</div> <div>.</div> </div>
1	C	329	<div> <div>3%</div> <div>73%</div> <div>22%</div> <div>.</div> <div>.</div> </div>
1	D	329	<div> <div>3%</div> <div>73%</div> <div>22%</div> <div>.</div> <div>.</div> </div>
1	E	329	<div> <div>2%</div> <div>74%</div> <div>22%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	329	<div><div></div><div>2%</div><div>75%</div><div>20%</div><div>..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16890 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

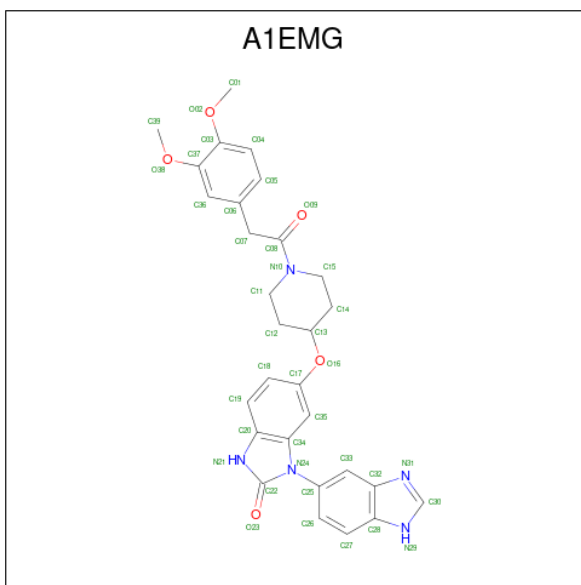
- Molecule 1 is a protein called Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2609	1673	450	477	9			
1	B	323	Total	C	N	O	S	0	1	0
			2620	1679	454	478	9			
1	C	323	Total	C	N	O	S	0	1	0
			2617	1677	452	479	9			
1	D	323	Total	C	N	O	S	0	1	0
			2620	1679	454	478	9			
1	E	323	Total	C	N	O	S	0	0	0
			2609	1673	450	477	9			
1	F	323	Total	C	N	O	S	0	0	0
			2609	1673	450	477	9			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 3-(1H-benzimidazol-5-yl)-5-[1-[2-(3,4-dimethoxyphenyl)ethanoyl]piperidin-4-yl]oxy-1H-benzimidazol-2-one (CCD ID: A1EMG) (formula: C₂₉H₂₉N₅O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			39	29	5	5		
3	B	1	Total	C	N	O	0	0
			39	29	5	5		
3	C	1	Total	C	N	O	0	0
			39	29	5	5		
3	D	1	Total	C	N	O	0	0
			39	29	5	5		
3	E	1	Total	C	N	O	0	0
			39	29	5	5		
3	F	1	Total	C	N	O	0	0
			39	29	5	5		

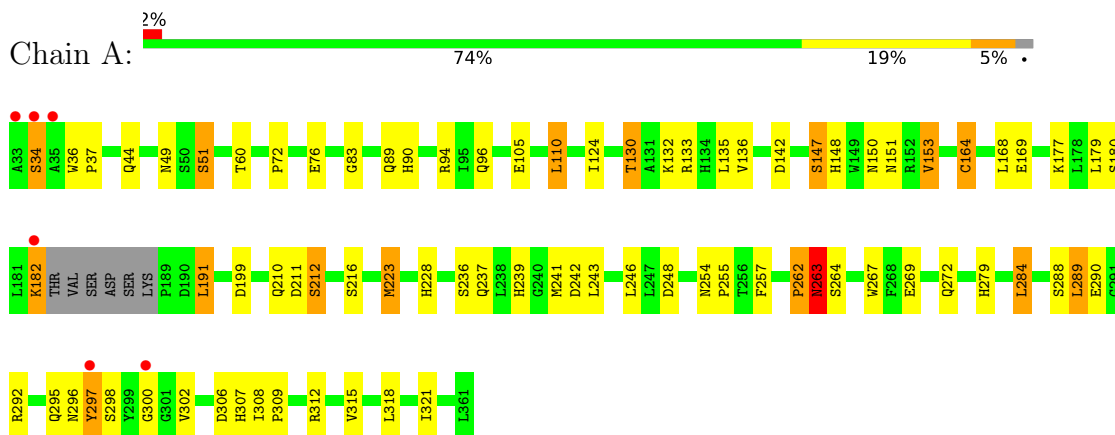
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	172	Total	O	0	0
			172	172		
4	B	175	Total	O	0	0
			175	175		
4	C	151	Total	O	0	0
			151	151		
4	D	155	Total	O	0	0
			155	155		
4	E	145	Total	O	0	0
			145	145		
4	F	168	Total	O	0	0
			168	168		

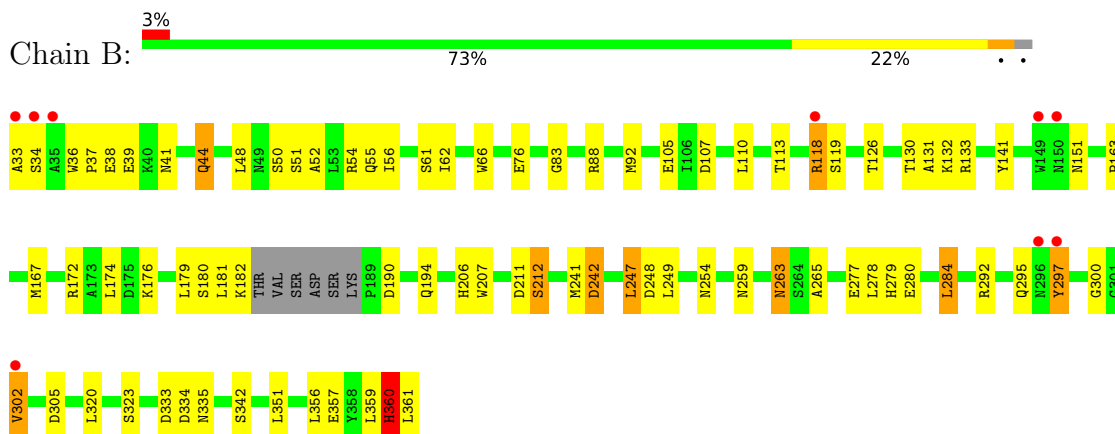
3 Residue-property plots [i](#)

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.

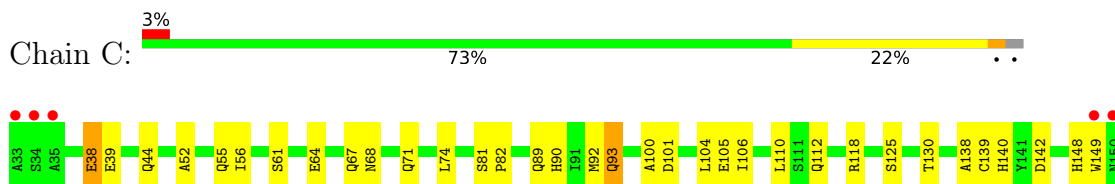
- Molecule 1: Glutaminyl-peptide cyclotransferase

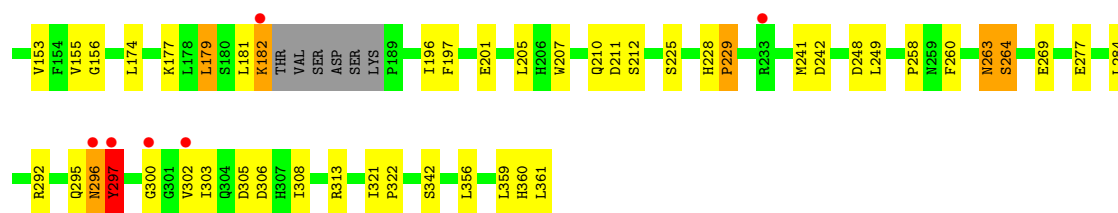


- Molecule 1: Glutaminyl-peptide cyclotransferase

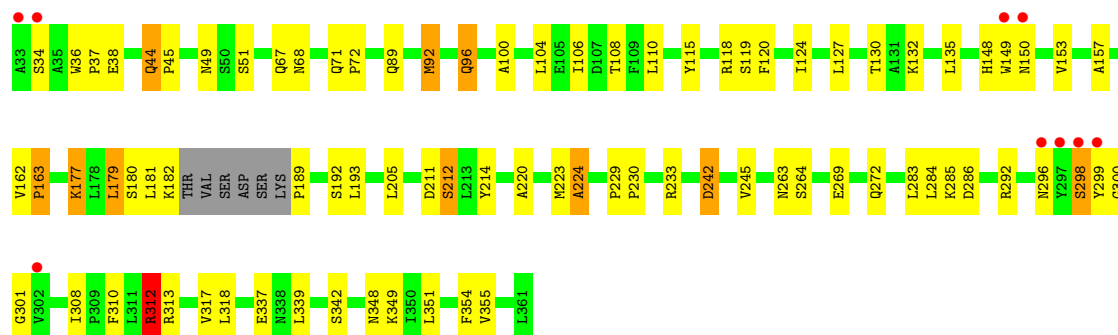
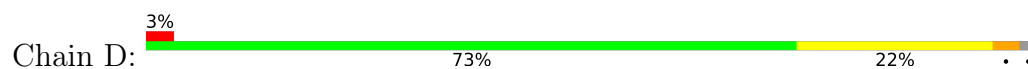


- Molecule 1: Glutaminyl-peptide cyclotransferase

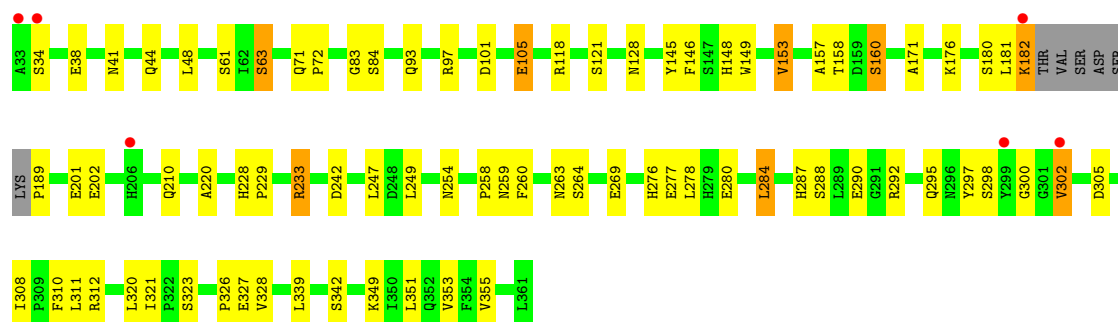
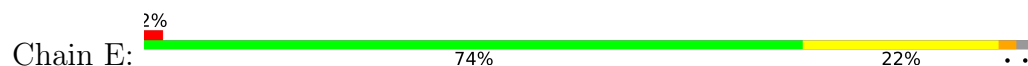




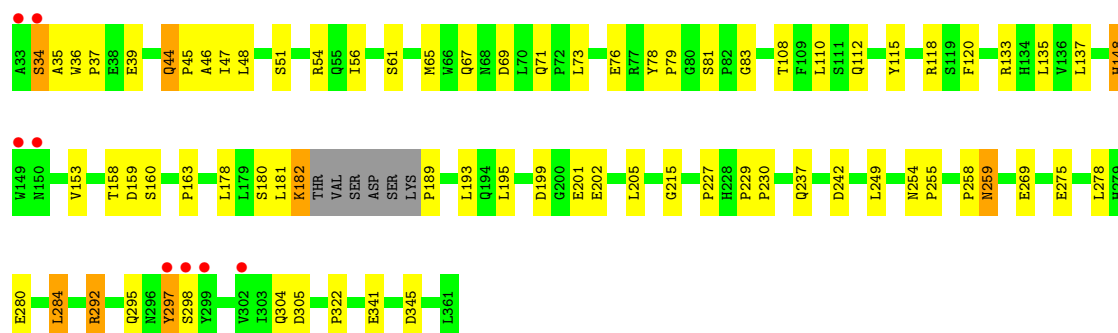
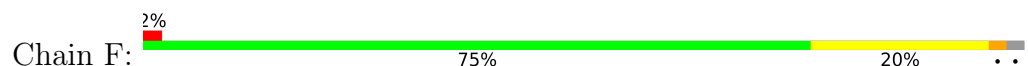
● Molecule 1: Glutaminyl-peptide cyclotransferase



● Molecule 1: Glutaminyl-peptide cyclotransferase



● Molecule 1: Glutaminyl-peptide cyclotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	186.61Å 88.77Å 156.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.06 – 2.33 45.06 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.06-2.33) 98.4 (45.06-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.200 , 0.274 0.208 , 0.274	Depositor DCC
R_{free} test set	2000 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16890	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: ZN, A1EMG

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	1.05	2/2686 (0.1%)	0.99	4/3656 (0.1%)
1	B	1.04	1/2697 (0.0%)	0.97	1/3670 (0.0%)
1	C	1.00	2/2694 (0.1%)	0.95	1/3667 (0.0%)
1	D	0.96	0/2697	0.93	3/3670 (0.1%)
1	E	1.01	2/2686 (0.1%)	0.99	2/3656 (0.1%)
1	F	1.00	1/2686 (0.0%)	0.96	0/3656
All	All	1.01	8/16146 (0.0%)	0.97	11/21975 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	SER	C-O	-7.46	1.18	1.25
1	E	323	SER	CA-C	-6.49	1.44	1.52
1	C	229	PRO	CB-CG	-5.99	1.27	1.51
1	A	110	LEU	CG-CD1	-5.80	1.33	1.52
1	E	308	ILE	CB-CG2	-5.73	1.33	1.52
1	C	139	CYS	CB-SG	-5.56	1.62	1.81
1	F	47	ILE	CG1-CD1	-5.55	1.30	1.51
1	A	136	VAL	CB-CG2	-5.15	1.35	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	SER	N-CA-C	-9.59	90.37	110.80
1	E	233	ARG	NE-CZ-NH2	-7.40	112.54	119.20
1	E	233	ARG	CG-CD-NE	-7.18	96.21	112.00
1	C	297	TYR	N-CA-C	-7.17	95.53	110.80
1	A	164	CYS	CA-CB-SG	6.28	128.83	114.40
1	D	312	ARG	CG-CD-NE	5.95	125.10	112.00
1	A	297	TYR	N-CA-C	-5.62	99.10	108.32
1	A	263	ASN	N-CA-C	5.35	122.20	110.80
1	B	297	TYR	CA-CB-CG	5.33	123.49	113.90
1	D	312	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	D	312	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	263	ASN	Peptide
1	C	296[A]	ASN	Mainchain
1	C	296[B]	ASN	Mainchain

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	2609	0	2529	45	0
1	B	2620	0	2541	44	0
1	C	2617	0	2534	52	0
1	D	2620	0	2541	52	0
1	E	2609	0	2529	48	0
1	F	2609	0	2529	53	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
3	A	39	0	0	1	0
3	B	39	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	39	0	0	1	0
3	D	39	0	0	0	0
3	E	39	0	0	0	0
3	F	39	0	0	1	0
4	A	172	0	0	14	0
4	B	175	0	0	16	1
4	C	151	0	0	18	0
4	D	155	0	0	11	0
4	E	145	0	0	20	0
4	F	168	0	0	22	1
All	All	16890	0	15203	296	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 10.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ASN:ND2	4:C:502:HOH:O	1.99	0.95
1:E:105:GLU:OE2	4:E:501:HOH:O	1.84	0.93
1:E:259:ASN:ND2	4:E:504:HOH:O	2.04	0.91
1:A:267:TRP:NE1	4:A:502:HOH:O	2.07	0.85
1:F:275:GLU:OE1	4:F:501:HOH:O	1.94	0.84
1:E:41:ASN:OD1	4:E:502:HOH:O	1.94	0.84
1:E:101:ASP:OD2	4:E:503:HOH:O	1.94	0.83
1:C:101:ASP:O	4:C:501:HOH:O	1.95	0.83
1:F:237:GLN:OE1	4:F:502:HOH:O	2.01	0.79
1:B:277:GLU:OE2	4:B:501:HOH:O	2.01	0.78
1:D:242:ASP:O	4:D:502:HOH:O	2.02	0.78
1:D:269:GLU:OE2	4:D:501:HOH:O	2.01	0.78
1:F:112:GLN:O	4:F:503:HOH:O	2.04	0.75
1:C:56:ILE:O	4:C:503:HOH:O	2.05	0.75
1:F:280:GLU:OE2	4:F:504:HOH:O	2.04	0.75
1:C:361:LEU:C	4:C:609:HOH:O	2.30	0.75
1:B:126:THR:HG22	1:B:194:GLN:HG3	1.70	0.72
1:E:181:LEU:O	1:E:182:LYS:HB2	1.89	0.72
1:A:289:LEU:O	4:A:503:HOH:O	2.08	0.71
1:F:292:ARG:HD2	4:F:595:HOH:O	1.89	0.71
1:E:171:ALA:O	4:E:505:HOH:O	2.08	0.71
1:C:39:GLU:OE1	4:C:504:HOH:O	2.09	0.71
1:B:39:GLU:OE1	4:B:502:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ILE:O	4:F:505:HOH:O	2.09	0.69
1:B:241:MET:O	4:B:503:HOH:O	2.10	0.69
1:C:105:GLU:OE2	4:C:505:HOH:O	2.11	0.69
1:A:306:ASP:OD2	4:A:505:HOH:O	2.11	0.68
1:F:304:GLN:NE2	4:F:507:HOH:O	2.18	0.68
1:F:108:THR:HA	1:F:120:PHE:O	1.93	0.68
1:D:313:ARG:NH1	4:D:504:HOH:O	2.09	0.68
1:A:296:ASN:N	4:A:501:HOH:O	2.05	0.68
1:D:214:TYR:O	4:D:506:HOH:O	2.10	0.67
1:D:337:GLU:O	4:D:505:HOH:O	2.10	0.67
1:D:189:PRO:N	4:D:512:HOH:O	2.28	0.66
1:B:357:GLU:OE1	4:B:504:HOH:O	2.13	0.66
1:D:127:LEU:HA	4:D:511:HOH:O	1.96	0.66
1:D:192:SER:OG	1:D:193:LEU:N	2.25	0.65
1:E:146:PHE:O	4:E:507:HOH:O	2.14	0.65
1:A:105:GLU:OE1	4:A:506:HOH:O	2.14	0.65
1:E:202:GLU:OE1	4:E:506:HOH:O	2.13	0.65
1:E:263:ASN:ND2	4:E:515:HOH:O	2.30	0.64
1:B:280:GLU:OE2	4:B:505:HOH:O	2.15	0.64
1:E:339:LEU:O	4:E:508:HOH:O	2.16	0.63
1:C:302:VAL:HG11	4:C:539:HOH:O	1.99	0.62
1:B:211:ASP:O	1:B:212:SER:HB3	1.99	0.61
1:A:60:THR:OG1	1:A:169:GLU:OE2	2.16	0.61
1:B:44:GLN:NE2	4:B:514:HOH:O	2.34	0.60
1:E:300:GLY:HA3	4:E:614:HOH:O	2.01	0.60
1:F:76:GLU:OE2	4:F:506:HOH:O	2.16	0.59
1:F:229:PRO:O	1:F:230:PRO:C	2.45	0.59
1:D:44:GLN:HG3	1:D:45:PRO:HD2	1.84	0.59
1:B:33:ALA:N	4:B:517:HOH:O	2.35	0.59
1:C:302:VAL:CG1	4:C:539:HOH:O	2.51	0.59
1:F:181:LEU:HD21	4:F:649:HOH:O	2.02	0.58
1:F:189:PRO:N	4:F:522:HOH:O	2.37	0.58
1:B:52:ALA:O	1:B:56:ILE:HG12	2.04	0.58
1:C:302:VAL:HG12	1:C:303:ILE:H	1.68	0.57
1:B:133:ARG:HB3	1:B:242:ASP:OD1	2.04	0.57
1:D:92:MET:HE3	1:D:106:ILE:HG12	1.85	0.57
1:E:233:ARG:HG2	4:E:609:HOH:O	2.05	0.57
1:C:277:GLU:OE1	4:C:507:HOH:O	2.18	0.56
1:D:211:ASP:O	1:D:212:SER:HB3	2.05	0.56
1:A:211:ASP:O	1:A:212:SER:HB3	2.04	0.56
1:D:130:THR:HG22	1:D:130:THR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:TYR:HA	4:E:549:HOH:O	2.05	0.56
1:A:296:ASN:CA	4:A:501:HOH:O	2.51	0.56
1:E:305:ASP:HA	4:E:532:HOH:O	2.05	0.55
1:A:241:MET:HE2	1:A:315:VAL:HG11	1.88	0.55
1:A:308:ILE:HB	1:A:309:PRO:HD3	1.87	0.55
1:B:292:ARG:NH1	4:B:520:HOH:O	2.39	0.55
1:D:348:ASN:OD1	4:D:508:HOH:O	2.18	0.54
1:C:52:ALA:N	4:C:513:HOH:O	2.40	0.54
1:C:207:TRP:CD1	4:C:519:HOH:O	2.61	0.54
1:D:100:ALA:HA	1:D:179:LEU:HD13	1.90	0.54
1:A:147:SER:OG	1:C:38:GLU:OE1	2.26	0.53
1:D:157:ALA:HB1	1:D:339:LEU:HD11	1.90	0.53
1:B:207:TRP:NE1	4:B:522:HOH:O	2.41	0.53
1:F:67:GLN:NE2	4:F:523:HOH:O	2.39	0.53
1:E:228:HIS:HA	1:E:229:PRO:C	2.34	0.53
1:A:150:ASN:O	1:A:150:ASN:CG	2.52	0.53
4:C:513:HOH:O	1:E:63:SER:HB3	2.07	0.53
1:F:181:LEU:CG	4:F:649:HOH:O	2.56	0.52
1:C:359:LEU:O	1:C:360:HIS:HB2	2.08	0.52
1:C:248:ASP:OD2	1:C:305:ASP:OD2	2.27	0.52
1:C:177:LYS:HD3	4:C:609:HOH:O	2.09	0.52
1:D:92:MET:HG2	1:D:104:LEU:HD13	1.91	0.52
1:F:269:GLU:CD	4:F:510:HOH:O	2.52	0.52
1:C:248:ASP:O	1:C:322:PRO:HD3	2.10	0.52
1:E:258:PRO:HB3	1:E:297:TYR:CE1	2.45	0.52
1:E:258:PRO:HB3	1:E:297:TYR:HE1	1.75	0.52
1:C:207:TRP:NE1	4:C:519:HOH:O	2.43	0.52
1:E:297:TYR:HD1	1:E:298:SER:O	1.93	0.52
1:F:36:TRP:CG	1:F:37:PRO:HD3	2.45	0.51
1:E:349:LYS:O	1:E:353:VAL:HG23	2.09	0.51
1:E:351:LEU:O	1:E:355:VAL:HG23	2.09	0.51
1:D:298:SER:OG	4:D:507:HOH:O	2.16	0.51
1:F:345:ASP:OD1	4:F:508:HOH:O	2.19	0.51
1:C:258:PRO:HG2	1:C:260:PHE:CZ	2.46	0.51
1:D:96:GLN:NE2	4:D:519:HOH:O	2.39	0.50
1:F:181:LEU:O	1:F:182:LYS:HB2	2.11	0.50
1:B:48:LEU:HB3	1:B:52:ALA:HB3	1.93	0.50
1:E:278:LEU:HB3	1:E:284:LEU:HD13	1.92	0.50
1:B:207:TRP:CD1	4:B:522:HOH:O	2.63	0.50
1:D:245:VAL:HG22	1:D:318:LEU:HD23	1.92	0.50
1:D:162:VAL:HB	1:D:163:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:PRO:O	4:F:509:HOH:O	2.20	0.50
1:A:76:GLU:HG3	1:A:153:VAL:HG13	1.94	0.50
1:B:263:ASN:OD1	4:B:506:HOH:O	2.19	0.50
1:F:78:TYR:CE1	1:F:81:SER:HB3	2.46	0.50
1:A:49:ASN:ND2	4:A:525:HOH:O	2.45	0.50
1:F:148:HIS:ND1	1:F:148:HIS:N	2.59	0.50
1:C:181:LEU:O	1:C:182:LYS:HB2	2.12	0.49
1:C:292:ARG:NH2	1:C:296[A]:ASN:H	2.09	0.49
1:B:172:ARG:NH2	4:B:513:HOH:O	2.34	0.49
1:C:56:ILE:HA	4:C:503:HOH:O	2.10	0.49
1:E:277:GLU:O	1:E:278:LEU:C	2.55	0.49
1:C:71:GLN:HA	1:C:74:LEU:HD12	1.94	0.49
1:C:138:ALA:HA	1:C:196:ILE:O	2.12	0.49
1:D:285:LYS:O	1:D:286:ASP:C	2.55	0.49
1:D:115:TYR:OH	1:D:205:LEU:HD21	2.12	0.49
1:A:72:PRO:HG2	1:A:90:HIS:CE1	2.48	0.48
1:E:201:GLU:OE1	1:E:202:GLU:HG2	2.12	0.48
1:A:279:HIS:N	1:A:284:LEU:HD22	2.27	0.48
3:C:402:A1EMG:C18	3:C:402:A1EMG:C12	2.91	0.48
1:E:158:THR:O	1:E:160:SER:HA	2.13	0.48
1:A:133:ARG:O	1:A:191:LEU:HA	2.12	0.48
1:E:189:PRO:N	4:E:526:HOH:O	2.45	0.48
1:B:302:VAL:HG23	4:B:523:HOH:O	2.14	0.48
1:C:308:ILE:HD11	4:C:539:HOH:O	2.14	0.48
1:B:174:LEU:HD13	1:B:356:LEU:HG	1.96	0.48
1:C:292:ARG:NH2	1:C:296[B]:ASN:H	2.11	0.48
1:F:258:PRO:HB3	1:F:297:TYR:CE2	2.49	0.48
1:A:302:VAL:HG12	4:A:540:HOH:O	2.12	0.48
1:D:110:LEU:HA	1:D:118[B]:ARG:O	2.14	0.48
1:D:148:HIS:CD2	1:D:153:VAL:HG22	2.49	0.48
1:D:110:LEU:HA	1:D:118[A]:ARG:O	2.14	0.48
1:E:258:PRO:HG2	1:E:260:PHE:CZ	2.48	0.47
1:A:248:ASP:HB3	1:A:321:ILE:HD12	1.97	0.47
3:A:402:A1EMG:C18	3:A:402:A1EMG:C12	2.92	0.47
1:C:100:ALA:HA	1:C:179:LEU:HD13	1.95	0.47
1:C:302:VAL:HG12	1:C:303:ILE:N	2.29	0.47
1:D:36:TRP:N	1:D:37:PRO:CD	2.77	0.47
1:D:263:ASN:ND2	4:D:526:HOH:O	2.42	0.47
1:D:36:TRP:CD1	1:D:132:LYS:HD2	2.50	0.47
1:F:269:GLU:OE1	4:F:510:HOH:O	2.20	0.47
1:C:81:SER:HB2	1:C:82:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:LEU:HB3	1:E:284:LEU:CD1	2.45	0.47
1:A:76:GLU:HG3	1:A:153:VAL:CG1	2.44	0.47
1:A:142:ASP:HB3	1:A:199:ASP:OD1	2.15	0.47
1:C:292:ARG:HH22	1:C:296[B]:ASN:CG	2.22	0.47
1:F:259:ASN:ND2	4:F:534:HOH:O	2.48	0.47
1:F:292:ARG:CD	4:F:595:HOH:O	2.54	0.47
1:A:223:MET:HG2	1:A:237:GLN:HB3	1.97	0.47
1:B:88:ARG:HD3	1:B:141:TYR:OH	2.13	0.47
1:B:181:LEU:O	1:B:182:LYS:HG2	2.14	0.47
1:F:115:TYR:OH	1:F:205:LEU:HD21	2.15	0.47
1:F:71:GLN:O	1:F:73:LEU:N	2.47	0.47
1:B:259:ASN:HD21	1:B:265:ALA:HA	1.80	0.47
1:D:229:PRO:O	1:D:230:PRO:C	2.55	0.47
1:B:248:ASP:OD2	1:B:305:ASP:OD2	2.34	0.46
1:A:83:GLY:N	4:A:504:HOH:O	2.11	0.46
1:E:71:GLN:HB2	1:E:72:PRO:HD3	1.96	0.46
1:F:135:LEU:O	1:F:193:LEU:HD12	2.16	0.46
1:A:49:ASN:OD1	1:A:51:SER:N	2.47	0.46
1:E:290:GLU:HB2	4:E:564:HOH:O	2.15	0.46
1:C:302:VAL:CG1	1:C:303:ILE:H	2.29	0.46
1:B:118[A]:ARG:NH1	4:B:532:HOH:O	2.49	0.46
1:C:142:ASP:N	1:C:142:ASP:OD1	2.47	0.46
1:D:110:LEU:HD12	1:D:119:SER:HA	1.98	0.46
1:E:61:SER:HA	4:E:555:HOH:O	2.15	0.45
1:E:284:LEU:HD23	1:E:287:HIS:CG	2.51	0.45
1:E:328:VAL:HG22	4:E:620:HOH:O	2.16	0.45
1:F:78:TYR:O	1:F:79:PRO:C	2.59	0.45
1:A:36:TRP:N	1:A:37:PRO:CD	2.80	0.45
1:C:140:HIS:CE1	1:C:201:GLU:OE1	2.69	0.45
1:B:359:LEU:O	1:B:360:HIS:HB2	2.16	0.45
1:A:302:VAL:CG1	4:A:540:HOH:O	2.65	0.45
1:C:67:GLN:OE1	1:C:68:ASN:ND2	2.50	0.45
1:D:181:LEU:O	1:D:182:LYS:HG2	2.17	0.45
1:E:97:ARG:HD3	4:E:524:HOH:O	2.16	0.45
1:F:278:LEU:HB3	1:F:284:LEU:HD13	1.98	0.45
3:B:402:A1EMG:C18	3:B:402:A1EMG:C12	2.95	0.45
1:E:249:LEU:HD12	1:E:321:ILE:HD11	1.99	0.45
1:F:48:LEU:N	1:F:48:LEU:HD23	2.31	0.44
1:B:130:THR:O	1:B:131:ALA:C	2.58	0.44
1:D:264:SER:OG	1:D:317:VAL:O	2.30	0.44
1:E:128:ASN:OD1	1:E:181:LEU:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HA	1:A:228:HIS:NE2	2.32	0.44
1:F:159:ASP:N	1:F:160:SER:HA	2.33	0.44
1:F:189:PRO:CD	4:F:630:HOH:O	2.65	0.44
1:A:269:GLU:HB2	4:A:635:HOH:O	2.18	0.44
1:C:228:HIS:HA	1:C:229:PRO:C	2.43	0.44
1:E:326:PRO:O	1:E:327:GLU:C	2.60	0.44
1:D:181:LEU:O	1:D:182:LYS:CB	2.65	0.44
1:F:178:LEU:O	1:F:181:LEU:HB2	2.18	0.44
1:F:304:GLN:O	1:F:305:ASP:HB2	2.18	0.44
1:A:255:PRO:HB2	1:A:257:PHE:CE1	2.53	0.44
1:D:149:TRP:CE3	1:D:150:ASN:HB2	2.53	0.44
1:E:83:GLY:O	1:E:84:SER:C	2.61	0.44
1:C:305:ASP:OD1	1:C:306:ASP:N	2.46	0.44
1:E:157:ALA:HB1	1:E:339:LEU:HD11	2.00	0.44
1:B:36:TRP:CG	1:B:37:PRO:HD3	2.53	0.44
1:D:124:ILE:N	1:D:124:ILE:HD12	2.33	0.44
1:E:182:LYS:HA	1:E:182:LYS:HD3	1.84	0.44
1:E:254:ASN:HB3	4:E:510:HOH:O	2.18	0.44
1:B:132:LYS:HG3	1:B:190:ASP:OD2	2.18	0.43
1:C:181:LEU:O	1:C:182:LYS:CB	2.65	0.43
1:C:211:ASP:O	1:C:212:SER:HB3	2.18	0.43
1:F:51:SER:HA	1:F:54:ARG:NH2	2.33	0.43
1:F:158:THR:C	1:F:160:SER:HA	2.42	0.43
1:C:249:LEU:HD12	1:C:321:ILE:HD11	2.00	0.43
1:D:71:GLN:N	1:D:72:PRO:CD	2.82	0.43
1:A:246:LEU:HD22	1:A:307:HIS:HB3	2.00	0.43
1:C:92:MET:SD	1:C:106:ILE:HD11	2.59	0.43
1:C:241:MET:HE2	1:C:241:MET:HB3	1.84	0.43
1:D:354:PHE:CD1	1:D:354:PHE:C	2.97	0.43
1:B:356:LEU:HD23	1:B:361:LEU:HB2	2.01	0.43
1:D:67:GLN:HG2	1:D:68:ASN:OD1	2.18	0.43
1:D:135:LEU:O	1:D:193:LEU:HD12	2.18	0.43
1:E:220:ALA:HB2	1:E:310:PHE:CZ	2.53	0.43
1:A:269:GLU:HA	1:A:272:GLN:HE21	1.83	0.43
1:B:61:SER:HB3	4:B:513:HOH:O	2.18	0.43
1:B:62:ILE:O	1:B:66:TRP:HB2	2.19	0.43
1:B:279:HIS:O	1:B:280:GLU:C	2.60	0.43
1:C:302:VAL:HG13	4:C:591:HOH:O	2.19	0.43
1:C:313:ARG:NH1	4:C:506:HOH:O	2.14	0.43
1:C:174:LEU:HD22	1:C:356:LEU:HD11	2.01	0.42
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:TYR:CG	1:D:300:GLY:N	2.87	0.42
1:E:311:LEU:O	1:E:312:ARG:C	2.62	0.42
1:C:81:SER:CB	1:C:82:PRO:CD	2.96	0.42
1:C:197:PHE:CD1	1:C:197:PHE:N	2.87	0.42
1:A:228:HIS:HB2	1:A:237:GLN:HG3	2.00	0.42
1:B:105:GLU:OE1	1:B:107:ASP:HB2	2.20	0.42
1:B:247:LEU:HD23	1:B:320:LEU:HD12	2.01	0.42
1:A:262:PRO:O	1:A:264:SER:N	2.52	0.42
1:A:243:LEU:HD11	1:A:318:LEU:HB2	2.02	0.42
1:A:290:GLU:HA	4:A:503:HOH:O	2.19	0.42
1:B:38:GLU:O	1:B:41:ASN:HB2	2.19	0.42
1:B:333:ASP:O	1:B:335:ASN:N	2.52	0.42
1:F:44:GLN:HG3	1:F:45:PRO:HD2	2.01	0.42
1:F:65:MET:O	1:F:69:ASP:HB2	2.19	0.42
1:F:181:LEU:HG	4:F:649:HOH:O	2.19	0.42
1:B:206:HIS:HB3	4:B:540:HOH:O	2.19	0.42
1:D:272:GLN:HE22	1:D:296:ASN:HB3	1.85	0.42
1:B:163:PRO:O	1:B:167:MET:HG3	2.20	0.42
1:D:177:LYS:O	1:D:180:SER:HB3	2.19	0.42
1:E:48:LEU:HD12	1:E:353:VAL:HG13	2.02	0.42
1:A:236:SER:O	1:A:239:HIS:HB2	2.19	0.42
1:E:302:VAL:HB	4:E:519:HOH:O	2.20	0.42
1:A:130:THR:O	1:A:130:THR:OG1	2.33	0.41
1:B:181:LEU:O	1:B:182:LYS:CB	2.67	0.41
1:D:36:TRP:CG	1:D:37:PRO:HD3	2.55	0.41
1:D:108:THR:HA	1:D:120:PHE:O	2.19	0.41
1:F:201:GLU:OE1	1:F:202:GLU:HG2	2.19	0.41
1:B:126:THR:HG22	1:B:194:GLN:CG	2.45	0.41
1:F:35:ALA:O	1:F:36:TRP:C	2.63	0.41
1:D:299:TYR:CD2	1:D:301:GLY:O	2.74	0.41
1:F:159:ASP:OD1	3:F:402:A1EMG:C30	2.69	0.41
1:F:254:ASN:N	1:F:255:PRO:CD	2.82	0.41
1:B:76:GLU:O	1:B:83:GLY:HA3	2.20	0.41
1:E:276:HIS:O	1:E:280:GLU:HG2	2.21	0.41
1:F:46:ALA:HB3	4:F:552:HOH:O	2.21	0.41
1:F:189:PRO:HD3	4:F:630:HOH:O	2.21	0.41
1:F:199:ASP:O	1:F:215:GLY:HA3	2.21	0.41
1:A:312:ARG:NH1	4:A:534:HOH:O	2.53	0.41
1:C:61:SER:OG	1:C:64:GLU:HG2	2.21	0.41
1:E:247:LEU:CD2	1:E:320:LEU:HD12	2.50	0.41
1:F:137:LEU:O	1:F:195:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASN:ND2	4:A:524:HOH:O	2.44	0.41
1:E:148:HIS:NE2	1:E:153:VAL:HG22	2.36	0.41
1:F:71:GLN:C	1:F:73:LEU:H	2.27	0.41
1:F:76:GLU:O	1:F:83:GLY:HA3	2.20	0.41
1:B:50:SER:O	1:B:54:ARG:HG3	2.20	0.41
1:C:89:GLN:O	1:C:90:HIS:C	2.64	0.41
1:D:220:ALA:HB2	1:D:310:PHE:CE1	2.55	0.41
1:D:308:ILE:O	1:D:312:ARG:HB2	2.20	0.41
1:A:94:ARG:HD2	1:A:94:ARG:HA	1.88	0.41
1:B:248:ASP:O	1:B:249:LEU:HB2	2.20	0.41
1:C:104:LEU:CD2	1:C:125:SER:HB2	2.51	0.41
1:D:49:ASN:OD1	1:D:49:ASN:C	2.63	0.40
1:F:36:TRP:CD1	1:F:37:PRO:HD3	2.55	0.40
1:A:148:HIS:CE1	1:A:153:VAL:CG2	3.04	0.40
1:A:182:LYS:HD3	1:A:182:LYS:HA	1.92	0.40
1:C:155:VAL:O	1:C:156:GLY:C	2.62	0.40
1:D:283:LEU:O	1:D:349:LYS:NZ	2.48	0.40
1:F:249:LEU:HB2	1:F:322:PRO:HD2	2.03	0.40
1:B:278:LEU:HB3	1:B:284:LEU:HD13	2.02	0.40
1:C:92:MET:O	1:C:93:GLN:C	2.60	0.40
1:F:39:GLU:HB3	1:F:133:ARG:NH1	2.37	0.40
1:A:124:ILE:N	1:A:124:ILE:HD12	2.36	0.40
1:A:164:CYS:O	1:A:168:LEU:HG	2.22	0.40
1:D:223:MET:O	1:D:224:ALA:C	2.61	0.40
1:D:299:TYR:HD2	1:D:301:GLY:O	2.05	0.40
1:D:351:LEU:O	1:D:355:VAL:HG23	2.21	0.40
1:A:148:HIS:CE1	1:A:153:VAL:HG22	2.57	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)
4:B:644:HOH:O	4:F:640:HOH:O[1_545]	1.84	0.36

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	319/329 (97%)	288 (90%)	25 (8%)	6 (2%)	6	4
1	B	320/329 (97%)	294 (92%)	22 (7%)	4 (1%)	9	7
1	C	320/329 (97%)	296 (92%)	21 (7%)	3 (1%)	14	13
1	D	320/329 (97%)	296 (92%)	22 (7%)	2 (1%)	21	22
1	E	319/329 (97%)	300 (94%)	18 (6%)	1 (0%)	36	41
1	F	319/329 (97%)	287 (90%)	31 (10%)	1 (0%)	36	41
All	All	1917/1974 (97%)	1761 (92%)	139 (7%)	17 (1%)	14	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	300	GLY
1	B	212	SER
1	C	264	SER
1	E	264	SER
1	B	300	GLY
1	B	334	ASP
1	C	300	GLY
1	D	212	SER
1	A	34	SER
1	A	262	PRO
1	B	360	HIS
1	A	212	SER
1	D	224	ALA
1	F	34	SER
1	A	179	LEU
1	C	297	TYR

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	284/290 (98%)	258 (91%)	26 (9%)	8	8
1	B	285/290 (98%)	260 (91%)	25 (9%)	9	9
1	C	285/290 (98%)	263 (92%)	22 (8%)	12	12
1	D	285/290 (98%)	268 (94%)	17 (6%)	17	20
1	E	284/290 (98%)	261 (92%)	23 (8%)	11	11
1	F	284/290 (98%)	266 (94%)	18 (6%)	16	19
All	All	1707/1740 (98%)	1576 (92%)	131 (8%)	12	12

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	51	SER
1	A	89	GLN
1	A	96	GLN
1	A	110	LEU
1	A	130	THR
1	A	135	LEU
1	A	147	SER
1	A	151	ASN
1	A	153	VAL
1	A	177	LYS
1	A	180	SER
1	A	182	LYS
1	A	191	LEU
1	A	210	GLN
1	A	216	SER
1	A	223	MET
1	A	242	ASP
1	A	254	ASN
1	A	284	LEU
1	A	288	SER
1	A	289	LEU
1	A	292	ARG
1	A	295	GLN
1	A	297	TYR
1	A	298	SER
1	B	34	SER
1	B	44	GLN
1	B	51	SER
1	B	55	GLN

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Mol	Chain	Res	Type
1	B	92	MET
1	B	110	LEU
1	B	113	THR
1	B	118[A]	ARG
1	B	118[B]	ARG
1	B	119	SER
1	B	151	ASN
1	B	176	LYS
1	B	179	LEU
1	B	180	SER
1	B	242	ASP
1	B	247	LEU
1	B	254	ASN
1	B	263	ASN
1	B	284	LEU
1	B	295	GLN
1	B	297	TYR
1	B	302	VAL
1	B	342	SER
1	B	351	LEU
1	B	360	HIS
1	C	38	GLU
1	C	44	GLN
1	C	55	GLN
1	C	93	GLN
1	C	110	LEU
1	C	112	GLN
1	C	118	ARG
1	C	130	THR
1	C	148	HIS
1	C	149	TRP
1	C	153	VAL
1	C	179	LEU
1	C	182	LYS
1	C	210	GLN
1	C	225	SER
1	C	242	ASP
1	C	264	SER
1	C	269	GLU
1	C	284	LEU
1	C	295	GLN
1	C	297	TYR

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Mol	Chain	Res	Type
1	C	342	SER
1	D	34	SER
1	D	38	GLU
1	D	44	GLN
1	D	51	SER
1	D	89	GLN
1	D	92	MET
1	D	96	GLN
1	D	163	PRO
1	D	177	LYS
1	D	179	LEU
1	D	233	ARG
1	D	242	ASP
1	D	284	LEU
1	D	292	ARG
1	D	298	SER
1	D	312	ARG
1	D	342	SER
1	E	34	SER
1	E	38	GLU
1	E	44	GLN
1	E	63	SER
1	E	93	GLN
1	E	105	GLU
1	E	118	ARG
1	E	121	SER
1	E	149	TRP
1	E	153	VAL
1	E	160	SER
1	E	176	LYS
1	E	180	SER
1	E	182	LYS
1	E	210	GLN
1	E	242	ASP
1	E	269	GLU
1	E	284	LEU
1	E	288	SER
1	E	292	ARG
1	E	295	GLN
1	E	302	VAL
1	E	342	SER
1	F	34	SER

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Mol	Chain	Res	Type
1	F	44	GLN
1	F	61	SER
1	F	110	LEU
1	F	118	ARG
1	F	148	HIS
1	F	153	VAL
1	F	163	PRO
1	F	180	SER
1	F	182	LYS
1	F	242	ASP
1	F	259	ASN
1	F	284	LEU
1	F	292	ARG
1	F	295	GLN
1	F	297	TYR
1	F	298	SER
1	F	341	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	67	GLN
1	A	148	HIS
1	A	276	HIS
1	A	279	HIS
1	A	360	HIS
1	B	151	ASN
1	C	41	ASN
1	C	68	ASN
1	C	71	GLN
1	C	90	HIS
1	C	206	HIS
1	C	304	GLN
1	D	41	ASN
1	D	67	GLN
1	D	68	ASN
1	D	128	ASN
1	D	218	HIS
1	E	41	ASN
1	E	99	GLN
1	E	206	HIS

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Mol	Chain	Res	Type
1	E	210	GLN
1	E	304	GLN
1	E	348	ASN
1	F	41	ASN
1	F	112	GLN
1	F	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A1EMG	B	402	2	44,44,44	2.23	11 (25%)	62,63,63	2.00	13 (20%)
3	A1EMG	A	402	2	44,44,44	2.36	14 (31%)	62,63,63	2.37	21 (33%)
3	A1EMG	E	402	2	44,44,44	2.70	13 (29%)	62,63,63	2.61	23 (37%)
3	A1EMG	C	402	2	44,44,44	2.37	13 (29%)	62,63,63	2.35	24 (38%)
3	A1EMG	D	402	2	44,44,44	2.56	19 (43%)	62,63,63	2.76	18 (29%)
3	A1EMG	F	402	2	44,44,44	2.14	14 (31%)	62,63,63	2.80	20 (32%)

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	A1EMG	B	402	2	-	6/20/30/30	0/6/6/6
3	A1EMG	A	402	2	-	7/20/30/30	0/6/6/6
3	A1EMG	E	402	2	-	8/20/30/30	0/6/6/6
3	A1EMG	C	402	2	-	7/20/30/30	0/6/6/6
3	A1EMG	D	402	2	-	6/20/30/30	0/6/6/6
3	A1EMG	F	402	2	-	9/20/30/30	0/6/6/6

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	A1EMG	C22-N21	7.56	1.45	1.37
3	D	402	A1EMG	C22-N21	6.58	1.44	1.37
3	E	402	A1EMG	C15-N10	6.56	1.58	1.47
3	C	402	A1EMG	C12-C13	-6.35	1.34	1.51
3	D	402	A1EMG	C14-C13	-6.05	1.35	1.51
3	E	402	A1EMG	C11-N10	5.72	1.57	1.47
3	A	402	A1EMG	C12-C13	-5.65	1.36	1.51
3	B	402	A1EMG	C12-C13	-5.64	1.36	1.51
3	E	402	A1EMG	C12-C13	-5.64	1.36	1.51
3	A	402	A1EMG	C14-C13	-5.62	1.36	1.51
3	B	402	A1EMG	C14-C13	-5.56	1.36	1.51
3	D	402	A1EMG	C15-N10	5.31	1.56	1.47
3	F	402	A1EMG	C11-N10	5.14	1.56	1.47
3	A	402	A1EMG	C15-N10	5.06	1.56	1.47
3	D	402	A1EMG	O23-C22	-5.00	1.14	1.23
3	B	402	A1EMG	C11-N10	4.82	1.55	1.47
3	B	402	A1EMG	C15-N10	4.75	1.55	1.47
3	C	402	A1EMG	C11-N10	4.74	1.55	1.47
3	A	402	A1EMG	C22-N21	4.71	1.42	1.37
3	F	402	A1EMG	C15-N10	4.71	1.55	1.47
3	C	402	A1EMG	C15-N10	4.69	1.55	1.47
3	D	402	A1EMG	C12-C13	-4.66	1.38	1.51
3	E	402	A1EMG	C14-C13	-4.60	1.39	1.51
3	A	402	A1EMG	C11-N10	4.49	1.55	1.47
3	C	402	A1EMG	C14-C13	-4.43	1.39	1.51
3	C	402	A1EMG	O23-C22	-4.39	1.15	1.23
3	E	402	A1EMG	C20-N21	4.30	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	A1EMG	C08-N10	4.26	1.43	1.35
3	E	402	A1EMG	C08-N10	4.18	1.43	1.35
3	F	402	A1EMG	C12-C13	-4.16	1.40	1.51
3	A	402	A1EMG	C20-N21	4.06	1.46	1.38
3	F	402	A1EMG	C20-N21	4.02	1.46	1.38
3	B	402	A1EMG	C08-N10	3.92	1.42	1.35
3	C	402	A1EMG	C20-N21	3.85	1.45	1.38
3	D	402	A1EMG	C11-N10	3.84	1.53	1.47
3	C	402	A1EMG	O38-C37	3.79	1.43	1.37
3	C	402	A1EMG	C28-C32	-3.75	1.34	1.40
3	F	402	A1EMG	C14-C13	-3.74	1.41	1.51
3	B	402	A1EMG	C22-N21	3.73	1.41	1.37
3	E	402	A1EMG	C28-C32	-3.71	1.34	1.40
3	C	402	A1EMG	C08-N10	3.65	1.42	1.35
3	A	402	A1EMG	O23-C22	-3.55	1.16	1.23
3	D	402	A1EMG	C20-N21	3.44	1.45	1.38
3	C	402	A1EMG	O09-C08	-3.39	1.15	1.23
3	E	402	A1EMG	C34-N24	3.38	1.46	1.40
3	D	402	A1EMG	C28-C32	-3.35	1.35	1.40
3	F	402	A1EMG	C25-N24	-3.26	1.39	1.44
3	A	402	A1EMG	C34-N24	3.16	1.45	1.40
3	D	402	A1EMG	O09-C08	-3.15	1.16	1.23
3	F	402	A1EMG	O02-C03	3.12	1.42	1.37
3	F	402	A1EMG	C28-C32	-3.11	1.35	1.40
3	D	402	A1EMG	C37-C03	-3.10	1.34	1.40
3	E	402	A1EMG	O38-C37	3.08	1.42	1.37
3	E	402	A1EMG	O09-C08	-2.98	1.16	1.23
3	B	402	A1EMG	C20-N21	2.98	1.44	1.38
3	A	402	A1EMG	C28-C32	-2.92	1.36	1.40
3	D	402	A1EMG	C28-N29	-2.92	1.33	1.37
3	A	402	A1EMG	C30-N29	-2.88	1.28	1.35
3	E	402	A1EMG	C32-N31	-2.88	1.34	1.39
3	A	402	A1EMG	C32-N31	-2.86	1.34	1.39
3	A	402	A1EMG	C28-N29	-2.84	1.33	1.37
3	B	402	A1EMG	O23-C22	-2.82	1.18	1.23
3	A	402	A1EMG	O09-C08	-2.78	1.17	1.23
3	D	402	A1EMG	C33-C32	2.57	1.43	1.40
3	D	402	A1EMG	C08-N10	2.56	1.40	1.35
3	F	402	A1EMG	O09-C08	-2.52	1.17	1.23
3	D	402	A1EMG	C30-N29	-2.51	1.29	1.35
3	B	402	A1EMG	C32-N31	-2.45	1.35	1.39
3	A	402	A1EMG	C08-N10	2.41	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	A1EMG	C32-N31	-2.37	1.35	1.39
3	B	402	A1EMG	O09-C08	-2.37	1.17	1.23
3	F	402	A1EMG	C22-N21	2.31	1.39	1.37
3	D	402	A1EMG	C34-N24	2.27	1.44	1.40
3	F	402	A1EMG	C37-C03	-2.26	1.36	1.40
3	C	402	A1EMG	C22-N21	2.26	1.39	1.37
3	F	402	A1EMG	C34-N24	2.21	1.44	1.40
3	D	402	A1EMG	C07-C08	-2.21	1.49	1.52
3	E	402	A1EMG	C28-N29	-2.20	1.34	1.37
3	C	402	A1EMG	C28-N29	-2.13	1.34	1.37
3	D	402	A1EMG	O16-C17	2.13	1.42	1.38
3	D	402	A1EMG	C35-C34	-2.10	1.36	1.39
3	D	402	A1EMG	O02-C03	2.06	1.40	1.37
3	C	402	A1EMG	C26-C27	-2.02	1.35	1.38
3	B	402	A1EMG	C07-C08	2.00	1.54	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	A1EMG	C11-N10-C15	-9.60	93.11	112.68
3	D	402	A1EMG	C11-N10-C15	-9.01	94.31	112.68
3	C	402	A1EMG	C11-N10-C15	-8.79	94.76	112.68
3	D	402	A1EMG	N21-C22-N24	8.42	110.44	106.35
3	D	402	A1EMG	C20-N21-C22	-8.24	105.21	110.27
3	E	402	A1EMG	C11-N10-C15	-7.86	96.65	112.68
3	D	402	A1EMG	C34-N24-C22	-7.30	105.44	109.22
3	B	402	A1EMG	C11-N10-C15	-7.26	97.88	112.68
3	E	402	A1EMG	C17-O16-C13	7.08	131.98	119.18
3	F	402	A1EMG	C15-C14-C13	7.05	117.95	110.32
3	F	402	A1EMG	C33-C25-N24	-6.97	112.21	119.42
3	E	402	A1EMG	C01-O02-C03	-6.75	107.62	117.51
3	F	402	A1EMG	C34-N24-C22	6.47	112.57	109.22
3	A	402	A1EMG	C11-N10-C15	-6.46	99.51	112.68
3	F	402	A1EMG	C39-O38-C37	-6.22	108.39	117.51
3	F	402	A1EMG	N21-C22-N24	-5.96	103.45	106.35
3	D	402	A1EMG	C17-O16-C13	5.70	129.49	119.18
3	C	402	A1EMG	C12-C11-N10	5.60	121.64	110.66
3	E	402	A1EMG	C07-C06-C05	-5.50	112.81	120.89
3	A	402	A1EMG	C26-C25-N24	5.48	126.01	119.72
3	A	402	A1EMG	C11-C12-C13	5.10	115.84	110.32
3	F	402	A1EMG	C17-O16-C13	5.01	128.25	119.18
3	A	402	A1EMG	C33-C25-N24	-5.00	114.24	119.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	A1EMG	C15-C14-C13	4.90	115.63	110.32
3	F	402	A1EMG	O16-C13-C12	4.54	118.90	108.31
3	B	402	A1EMG	C17-O16-C13	4.44	127.20	119.18
3	A	402	A1EMG	O09-C08-C07	4.31	128.47	121.61
3	D	402	A1EMG	O16-C13-C12	4.27	118.28	108.31
3	C	402	A1EMG	C20-N21-C22	-4.20	107.69	110.27
3	A	402	A1EMG	C17-O16-C13	4.20	126.77	119.18
3	D	402	A1EMG	C20-C34-N24	4.14	110.17	106.19
3	B	402	A1EMG	C11-C12-C13	4.13	114.79	110.32
3	B	402	A1EMG	C14-C15-N10	4.12	118.73	110.66
3	E	402	A1EMG	O02-C03-C04	-3.95	117.64	124.30
3	B	402	A1EMG	C20-N21-C22	-3.90	107.88	110.27
3	B	402	A1EMG	C12-C11-N10	3.89	118.28	110.66
3	F	402	A1EMG	C15-N10-C08	3.87	135.59	122.83
3	E	402	A1EMG	C12-C11-N10	3.81	118.13	110.66
3	E	402	A1EMG	C15-C14-C13	3.80	114.44	110.32
3	B	402	A1EMG	O16-C13-C12	3.78	117.13	108.31
3	E	402	A1EMG	C15-N10-C08	3.73	135.12	122.83
3	A	402	A1EMG	N21-C22-N24	3.70	108.14	106.35
3	C	402	A1EMG	O23-C22-N21	-3.68	124.31	127.49
3	C	402	A1EMG	O02-C03-C37	3.68	120.39	115.40
3	D	402	A1EMG	C01-O02-C03	-3.63	112.18	117.51
3	C	402	A1EMG	C17-O16-C13	3.60	125.68	119.18
3	A	402	A1EMG	C25-N24-C34	3.59	130.16	124.24
3	E	402	A1EMG	C20-C34-N24	3.58	109.62	106.19
3	A	402	A1EMG	C20-N21-C22	-3.56	108.09	110.27
3	E	402	A1EMG	C14-C13-C12	3.54	118.89	111.67
3	F	402	A1EMG	C26-C25-N24	3.53	123.78	119.72
3	C	402	A1EMG	O09-C08-N10	-3.52	115.86	122.12
3	A	402	A1EMG	C34-N24-C22	-3.46	107.43	109.22
3	E	402	A1EMG	C35-C34-C20	-3.44	118.74	121.55
3	A	402	A1EMG	O09-C08-N10	-3.43	116.02	122.12
3	E	402	A1EMG	C07-C06-C36	3.43	125.58	120.38
3	A	402	A1EMG	C35-C34-C20	-3.42	118.76	121.55
3	E	402	A1EMG	C11-C12-C13	3.37	113.97	110.32
3	B	402	A1EMG	C01-O02-C03	-3.29	112.69	117.51
3	D	402	A1EMG	C11-N10-C08	3.28	133.63	122.83
3	E	402	A1EMG	O02-C03-C37	3.27	119.83	115.40
3	C	402	A1EMG	N21-C22-N24	3.26	107.93	106.35
3	A	402	A1EMG	C14-C15-N10	3.25	117.04	110.66
3	F	402	A1EMG	C14-C13-C12	3.25	118.30	111.67
3	E	402	A1EMG	C04-C05-C06	-3.11	116.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	A1EMG	O16-C13-C12	3.06	115.46	108.31
3	C	402	A1EMG	C15-N10-C08	3.04	132.84	122.83
3	C	402	A1EMG	C11-C12-C13	3.03	113.60	110.32
3	D	402	A1EMG	C35-C34-C20	-3.02	119.08	121.55
3	F	402	A1EMG	O16-C13-C14	-3.01	101.31	108.31
3	E	402	A1EMG	C27-C28-C32	-2.93	118.89	122.10
3	F	402	A1EMG	O23-C22-N24	2.91	130.66	125.50
3	B	402	A1EMG	O09-C08-N10	-2.91	116.95	122.12
3	B	402	A1EMG	O09-C08-C07	2.91	126.23	121.61
3	A	402	A1EMG	C20-C34-N24	2.89	108.97	106.19
3	E	402	A1EMG	C36-C37-C03	-2.89	116.12	119.83
3	A	402	A1EMG	C15-N10-C08	2.89	132.35	122.83
3	C	402	A1EMG	C11-N10-C08	2.88	132.31	122.83
3	C	402	A1EMG	C07-C06-C05	-2.85	116.69	120.89
3	D	402	A1EMG	C25-N24-C22	2.80	128.94	124.33
3	D	402	A1EMG	C15-N10-C08	2.80	132.05	122.83
3	D	402	A1EMG	C19-C20-C34	-2.79	118.70	121.33
3	A	402	A1EMG	C28-N29-C30	2.71	109.83	106.73
3	B	402	A1EMG	C15-N10-C08	2.70	131.74	122.83
3	C	402	A1EMG	O16-C13-C12	2.69	114.58	108.31
3	F	402	A1EMG	C11-C12-C13	2.62	113.16	110.32
3	D	402	A1EMG	O16-C13-C14	-2.59	102.27	108.31
3	A	402	A1EMG	O16-C13-C14	-2.59	102.27	108.31
3	F	402	A1EMG	C11-N10-C08	2.57	131.29	122.83
3	D	402	A1EMG	C14-C15-N10	2.54	115.65	110.66
3	C	402	A1EMG	C18-C17-C35	-2.53	117.10	120.50
3	E	402	A1EMG	C14-C15-N10	2.50	115.56	110.66
3	C	402	A1EMG	O02-C03-C04	-2.47	120.13	124.30
3	A	402	A1EMG	O16-C13-C12	2.37	113.83	108.31
3	C	402	A1EMG	O38-C37-C03	2.36	118.60	115.40
3	B	402	A1EMG	C11-N10-C08	2.29	130.37	122.83
3	C	402	A1EMG	C34-N24-C22	-2.29	108.03	109.22
3	B	402	A1EMG	C27-C28-C32	-2.26	119.62	122.10
3	F	402	A1EMG	C26-C25-C33	2.25	123.59	119.12
3	F	402	A1EMG	C01-O02-C03	-2.24	114.23	117.51
3	F	402	A1EMG	C19-C18-C17	2.22	122.27	119.73
3	E	402	A1EMG	C05-C06-C36	2.22	121.60	118.55
3	D	402	A1EMG	C18-C17-C35	-2.19	117.56	120.50
3	C	402	A1EMG	C25-N24-C22	2.16	127.89	124.33
3	C	402	A1EMG	C19-C20-C34	-2.15	119.30	121.33
3	F	402	A1EMG	C27-C26-C25	-2.13	117.61	120.30
3	C	402	A1EMG	C19-C18-C17	2.13	122.16	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1EMG	C27-C28-N29	2.11	134.12	130.74
3	E	402	A1EMG	C04-C03-C37	2.11	122.51	119.71
3	E	402	A1EMG	C34-C35-C17	2.10	122.31	118.02
3	F	402	A1EMG	C36-C37-C03	2.09	122.51	119.83
3	A	402	A1EMG	O16-C17-C35	-2.09	108.94	119.60
3	D	402	A1EMG	C34-C35-C17	2.08	122.28	118.02
3	C	402	A1EMG	C07-C06-C36	2.08	123.54	120.38
3	A	402	A1EMG	O23-C22-N21	-2.04	125.73	127.49
3	C	402	A1EMG	C20-C34-N24	2.03	108.14	106.19
3	D	402	A1EMG	O09-C08-N10	-2.02	118.52	122.12
3	E	402	A1EMG	C20-N21-C22	-2.01	109.04	110.27
3	C	402	A1EMG	N29-C30-N31	-2.01	110.81	113.87

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1EMG	C12-C13-O16-C17
3	B	402	A1EMG	C12-C13-O16-C17
3	C	402	A1EMG	C12-C13-O16-C17
3	D	402	A1EMG	C12-C13-O16-C17
3	E	402	A1EMG	C12-C13-O16-C17
3	F	402	A1EMG	C12-C13-O16-C17
3	E	402	A1EMG	C37-C03-O02-C01
3	E	402	A1EMG	C04-C03-O02-C01
3	C	402	A1EMG	C26-C25-N24-C34
3	F	402	A1EMG	C03-C37-O38-C39
3	C	402	A1EMG	C03-C37-O38-C39
3	B	402	A1EMG	C26-C25-N24-C34
3	F	402	A1EMG	C26-C25-N24-C34
3	F	402	A1EMG	C36-C37-O38-C39
3	C	402	A1EMG	C36-C37-O38-C39
3	A	402	A1EMG	C33-C25-N24-C34
3	B	402	A1EMG	C33-C25-N24-C34
3	C	402	A1EMG	C33-C25-N24-C34
3	D	402	A1EMG	C37-C03-O02-C01
3	E	402	A1EMG	C26-C25-N24-C34
3	E	402	A1EMG	C36-C06-C07-C08
3	F	402	A1EMG	C36-C06-C07-C08
3	E	402	A1EMG	C05-C06-C07-C08
3	F	402	A1EMG	C05-C06-C07-C08
3	A	402	A1EMG	C36-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
3	D	402	A1EMG	C04-C03-O02-C01
3	A	402	A1EMG	C05-C06-C07-C08
3	D	402	A1EMG	C36-C06-C07-C08
3	D	402	A1EMG	C05-C06-C07-C08
3	A	402	A1EMG	C26-C25-N24-C34
3	E	402	A1EMG	C33-C25-N24-C34
3	B	402	A1EMG	C36-C06-C07-C08
3	F	402	A1EMG	C18-C17-O16-C13
3	B	402	A1EMG	C05-C06-C07-C08
3	B	402	A1EMG	C14-C13-O16-C17
3	D	402	A1EMG	C14-C13-O16-C17
3	E	402	A1EMG	C14-C13-O16-C17
3	A	402	A1EMG	C18-C17-O16-C13
3	F	402	A1EMG	C35-C17-O16-C13
3	A	402	A1EMG	C35-C17-O16-C13
3	F	402	A1EMG	C33-C25-N24-C34
3	C	402	A1EMG	C37-C03-O02-C01
3	C	402	A1EMG	C18-C17-O16-C13

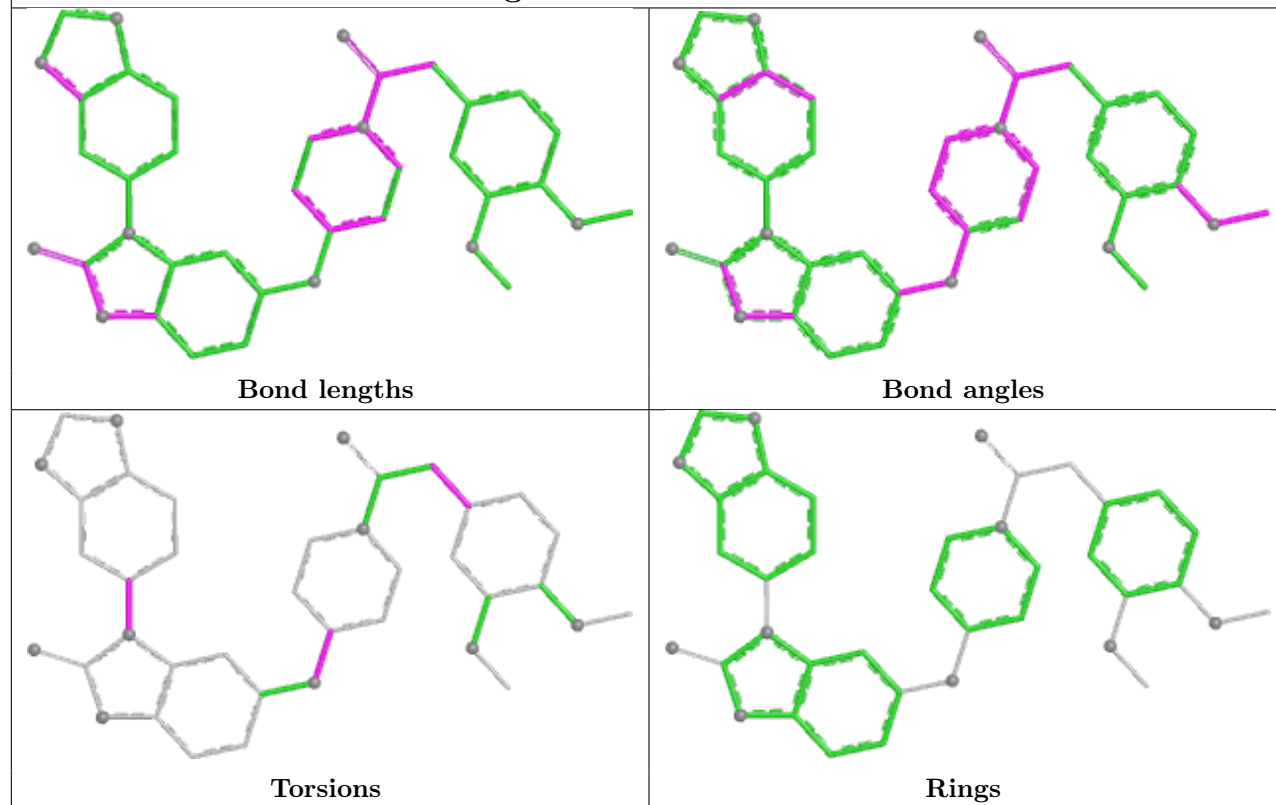
There are no ring outliers.

4 monomers are involved in 4 short contacts:

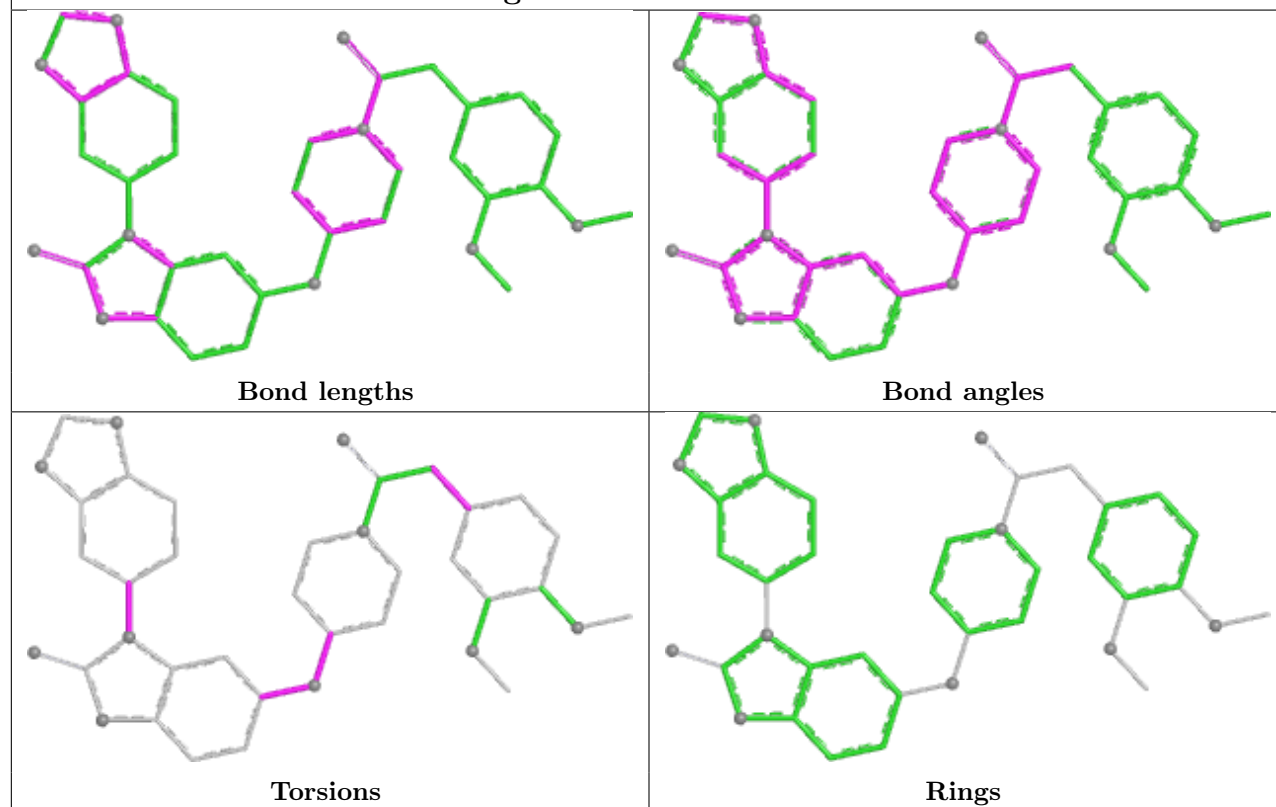
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	A1EMG	1	0
3	A	402	A1EMG	1	0
3	C	402	A1EMG	1	0
3	F	402	A1EMG	1	0

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

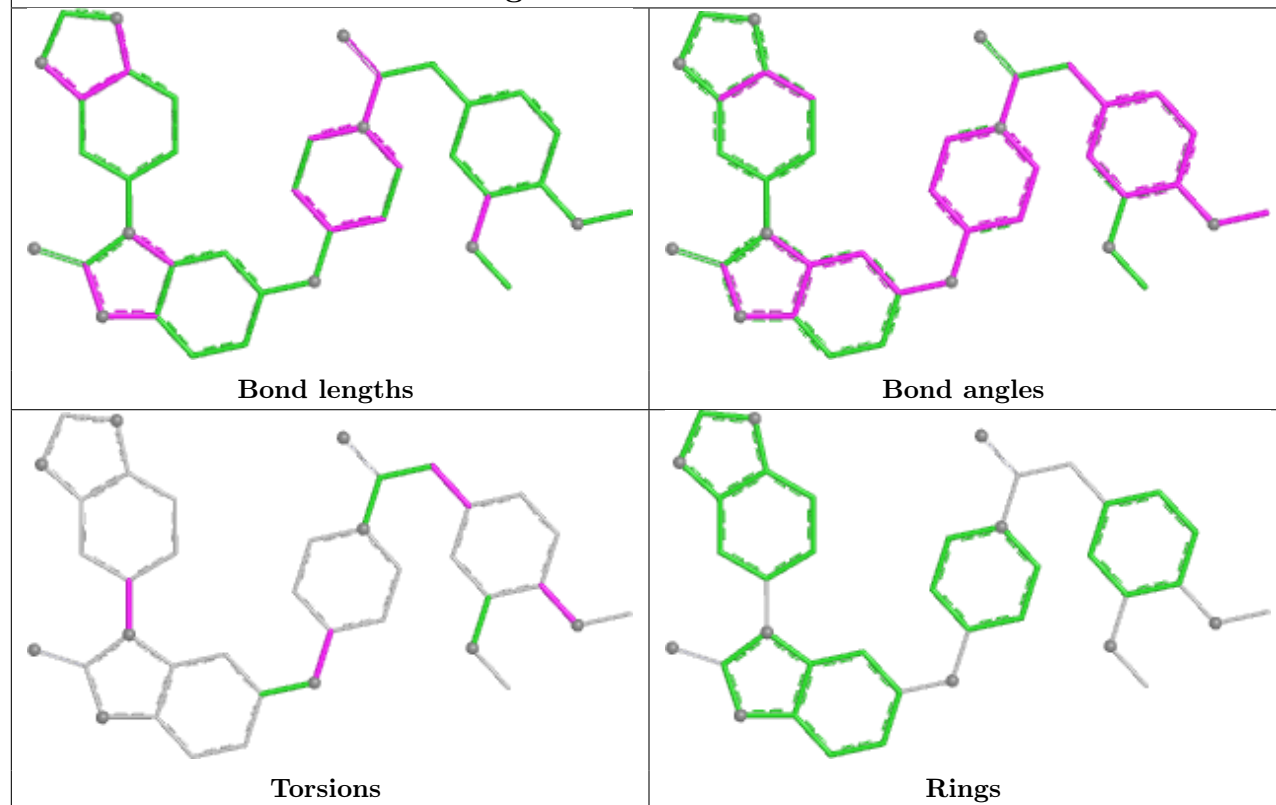
Ligand A1EMG B 402



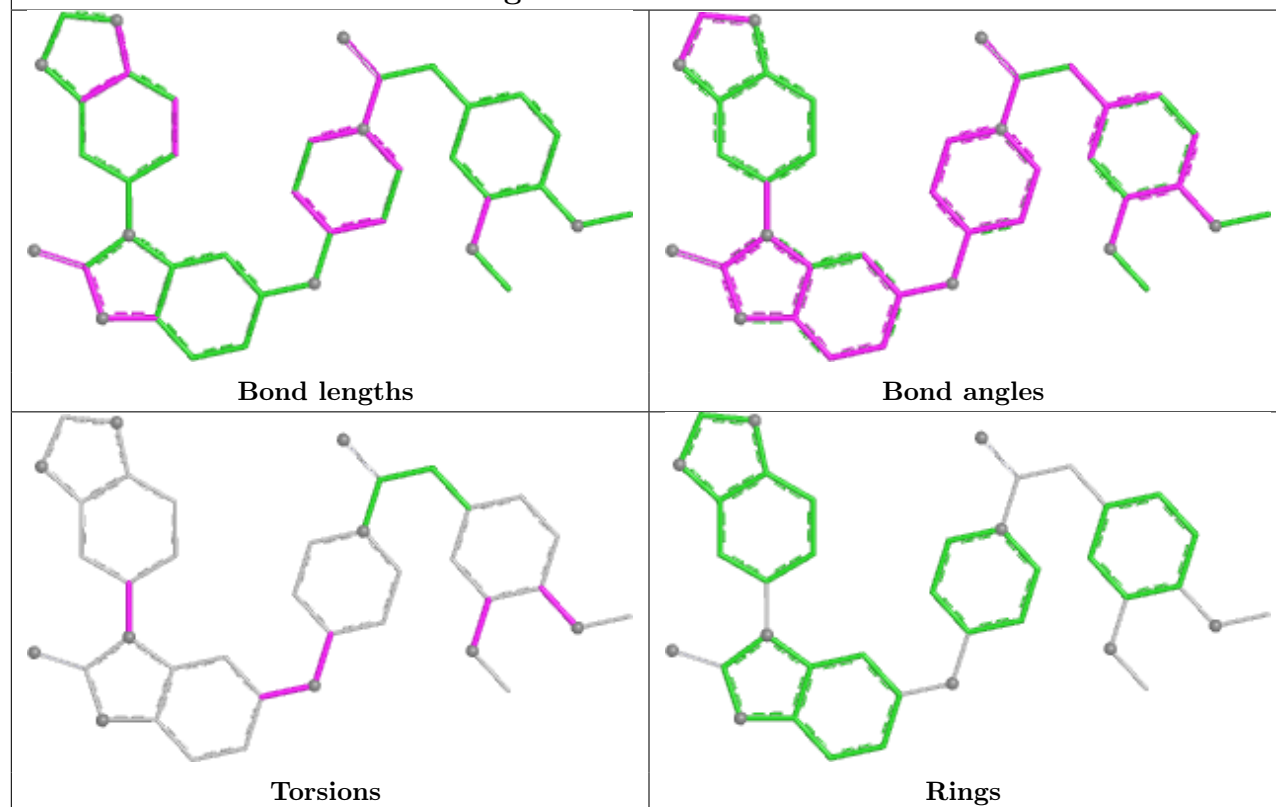
Ligand A1EMG A 402



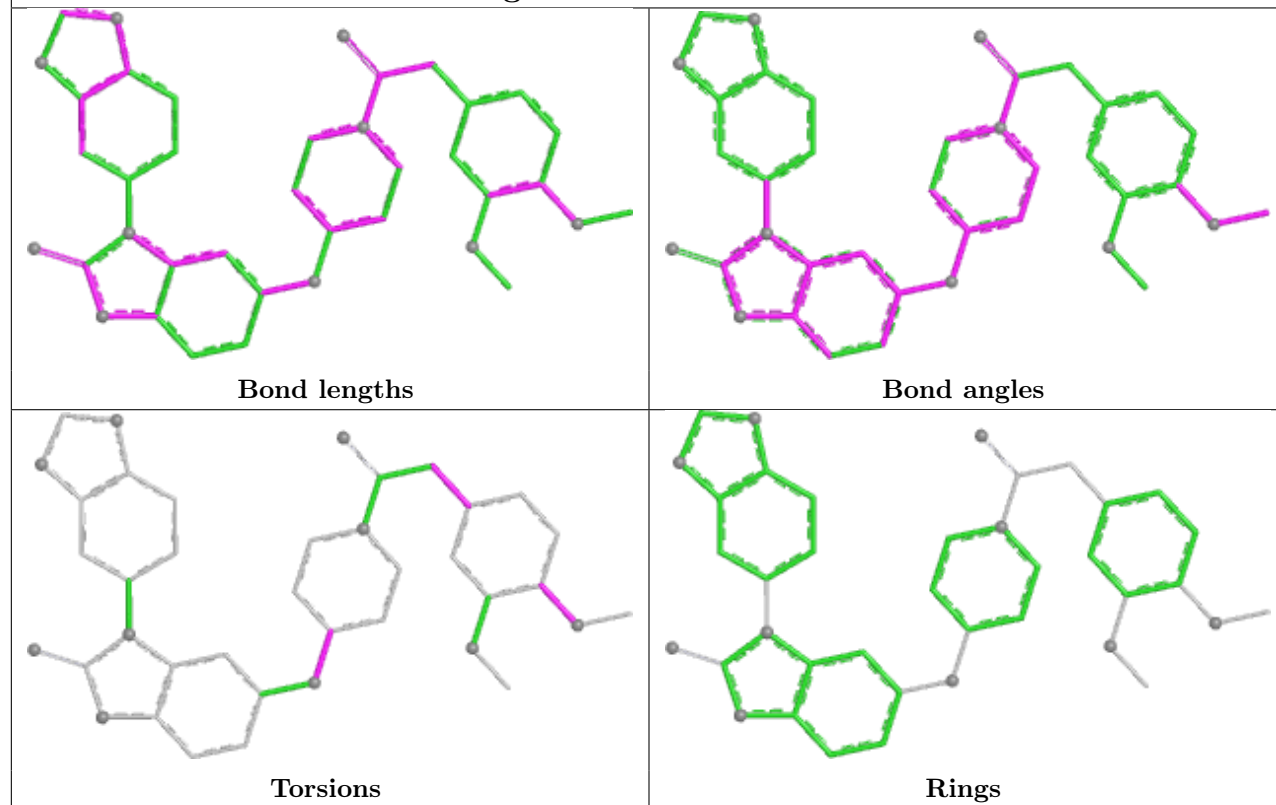
Ligand A1EMG E 402



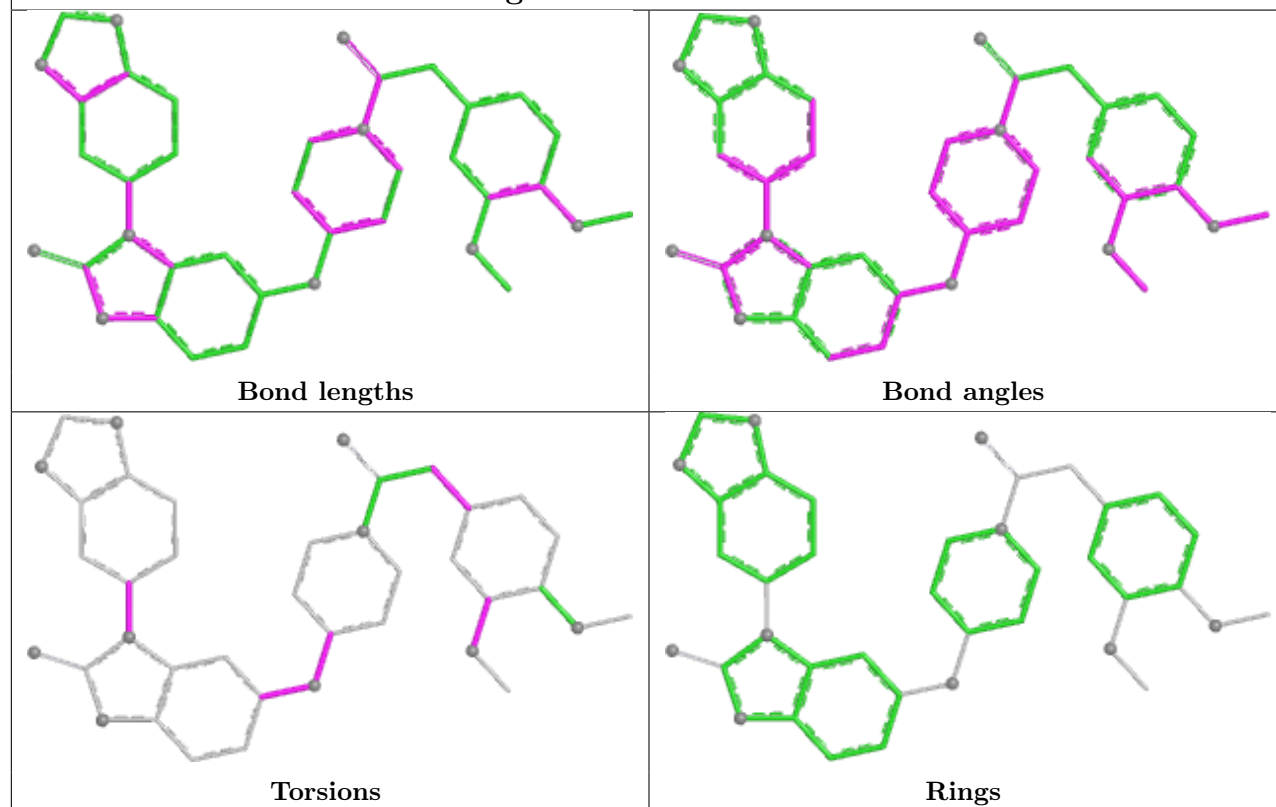
Ligand A1EMG C 402



Ligand A1EMG D 402



Ligand A1EMG 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	323/329 (98%)	-0.19	6 (1%) 66 71	5, 15, 34, 78	0
1	B	323/329 (98%)	-0.15	9 (2%) 55 61	5, 15, 36, 65	1 (0%)
1	C	323/329 (98%)	-0.08	11 (3%) 48 54	6, 17, 37, 81	1 (0%)
1	D	323/329 (98%)	-0.05	9 (2%) 55 61	6, 18, 38, 60	1 (0%)
1	E	323/329 (98%)	-0.12	6 (1%) 66 71	6, 17, 36, 70	0
1	F	323/329 (98%)	-0.14	8 (2%) 58 64	5, 16, 38, 65	0
All	All	1938/1974 (98%)	-0.12	49 (2%) 58 64	5, 16, 37, 81	3 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ALA	11.5
1	C	33	ALA	9.8
1	E	33	ALA	8.8
1	A	34	SER	7.8
1	B	34	SER	6.6
1	F	33	ALA	6.5
1	B	33	ALA	6.4
1	B	150	ASN	5.3
1	D	33	ALA	5.3
1	C	34	SER	5.3
1	B	149	TRP	4.6
1	D	149	TRP	4.5
1	C	302	VAL	4.4
1	D	34	SER	4.4
1	C	296[A]	ASN	4.4
1	F	34	SER	4.2
1	E	34	SER	4.1
1	F	150	ASN	4.0
1	E	302	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	298	SER	3.8
1	F	302	VAL	3.7
1	F	149	TRP	3.7
1	D	297	TYR	3.6
1	D	302	VAL	3.5
1	C	149	TRP	3.4
1	B	297	TYR	3.4
1	D	299	TYR	3.3
1	B	302	VAL	2.9
1	C	297	TYR	2.9
1	C	150	ASN	2.9
1	D	150	ASN	2.9
1	C	300	GLY	2.8
1	B	296	ASN	2.8
1	B	118[A]	ARG	2.8
1	E	182	LYS	2.7
1	E	206	HIS	2.6
1	C	233	ARG	2.4
1	D	296	ASN	2.3
1	F	299	TYR	2.3
1	B	35	ALA	2.3
1	F	297	TYR	2.3
1	C	182	LYS	2.1
1	A	300	GLY	2.1
1	A	297	TYR	2.1
1	A	35	ALA	2.1
1	A	182	LYS	2.0
1	E	299	TYR	2.0
1	F	298	SER	2.0
1	C	35	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

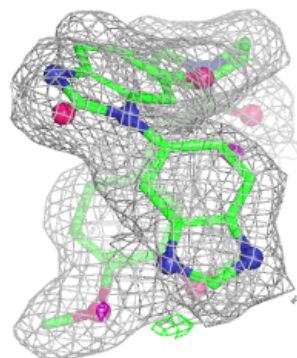
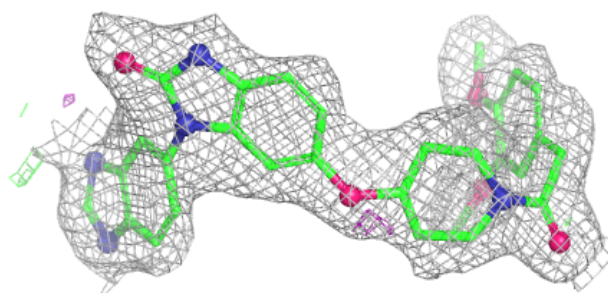
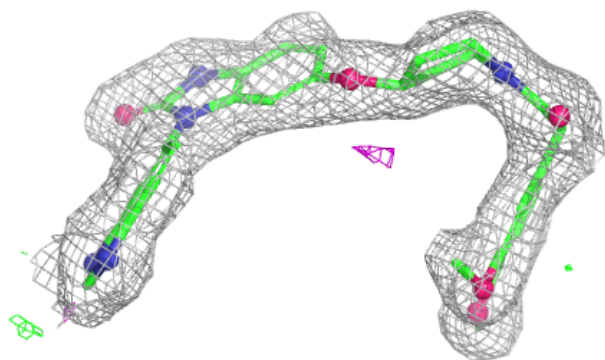
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1EMG	F	402	39/39	0.95	0.08	10,17,27,32	0
3	A1EMG	B	402	39/39	0.96	0.07	4,14,23,27	0
3	A1EMG	C	402	39/39	0.96	0.07	4,13,25,30	0
3	A1EMG	D	402	39/39	0.96	0.07	3,11,20,22	0
3	A1EMG	E	402	39/39	0.96	0.07	7,14,24,27	0
3	A1EMG	A	402	39/39	0.96	0.07	4,15,24,25	0
2	ZN	A	401	1/1	1.00	0.02	12,12,12,12	0
2	ZN	B	401	1/1	1.00	0.04	10,10,10,10	0
2	ZN	C	401	1/1	1.00	0.01	11,11,11,11	0
2	ZN	D	401	1/1	1.00	0.02	10,10,10,10	0
2	ZN	E	401	1/1	1.00	0.02	12,12,12,12	0
2	ZN	F	401	1/1	1.00	0.03	8,8,8,8	0

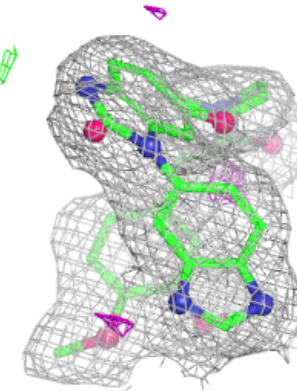
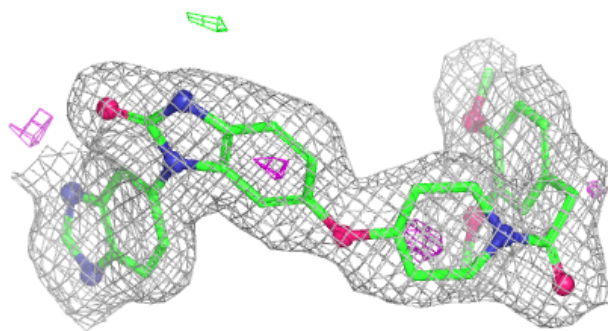
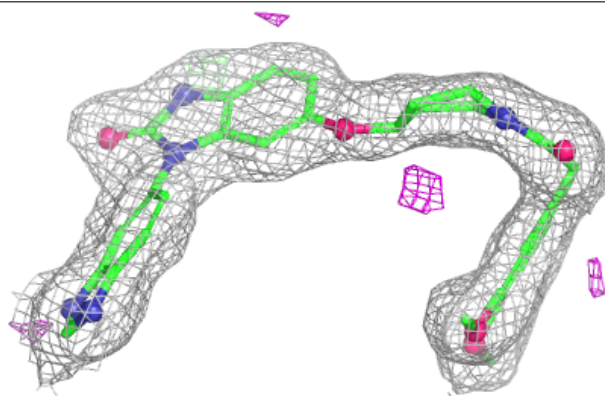
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1EMG 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)

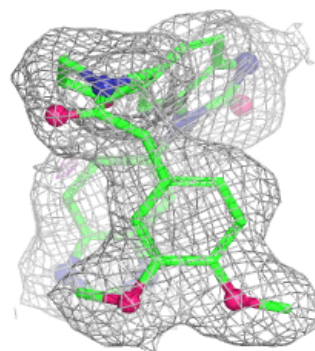
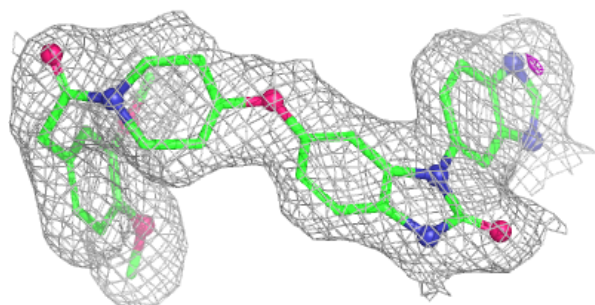
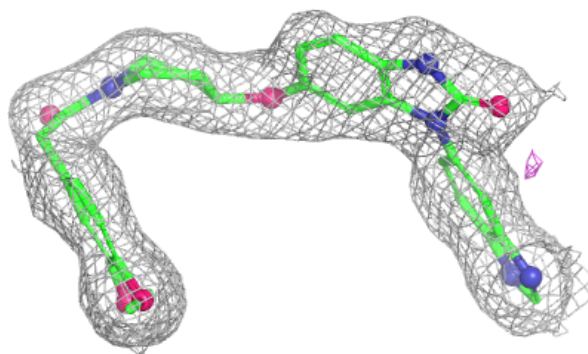
**Electron density around A1EMG B 402:**

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

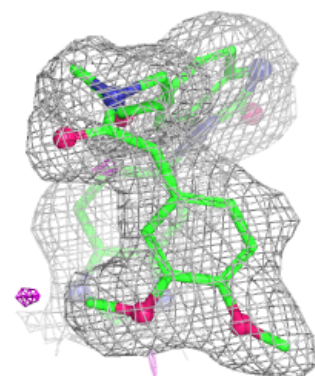
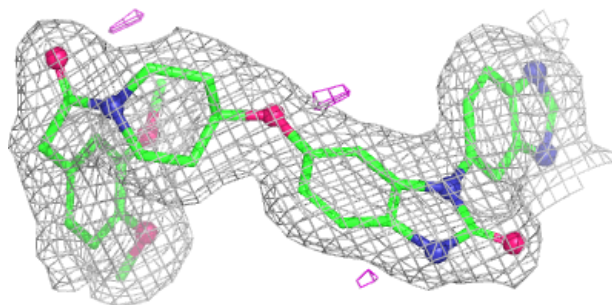
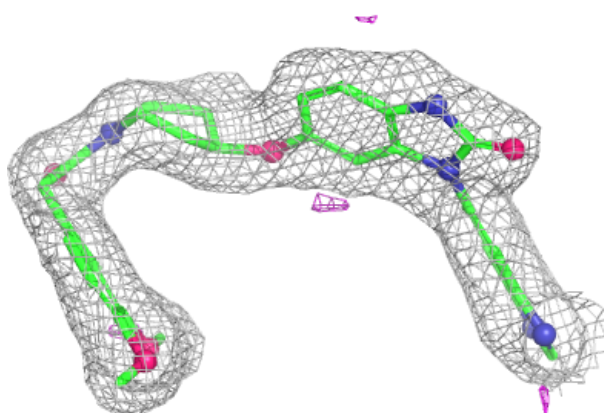


Electron density around A1EMG C 402:

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

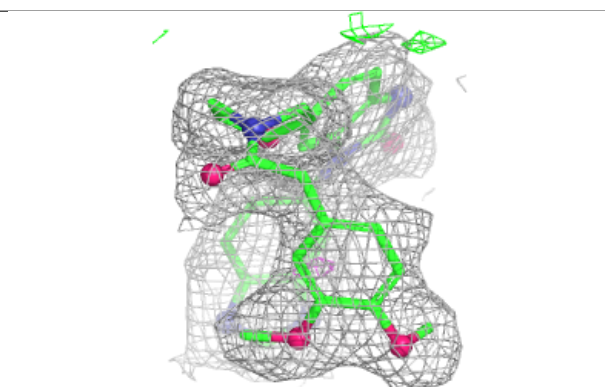
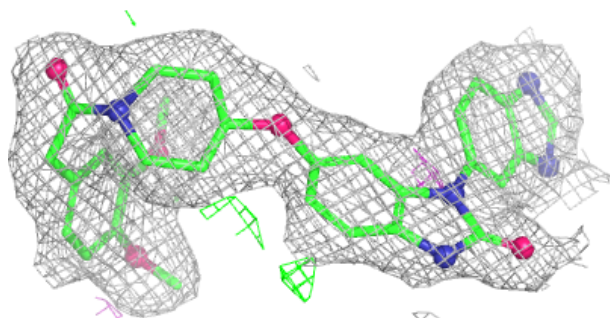
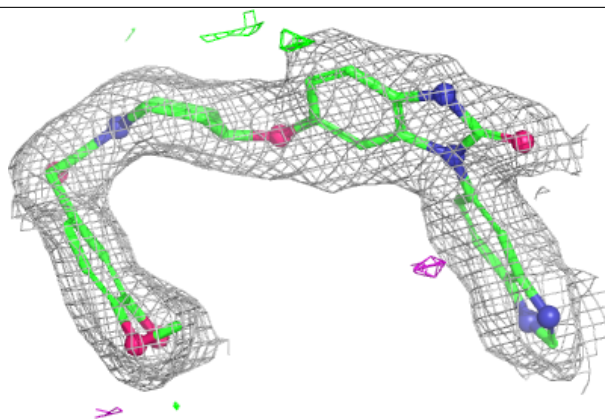
**Electron density around A1EMG D 402:**

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

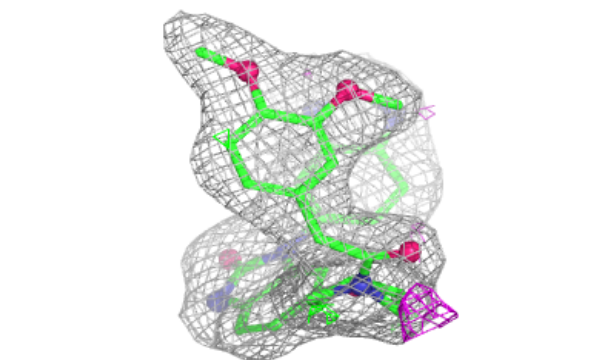
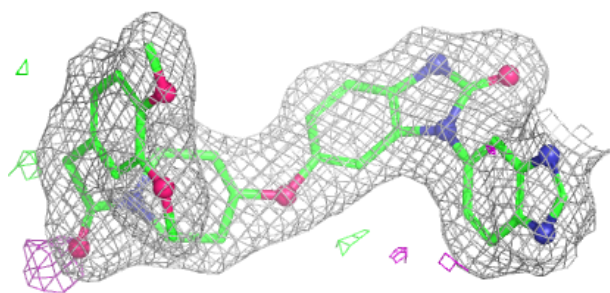
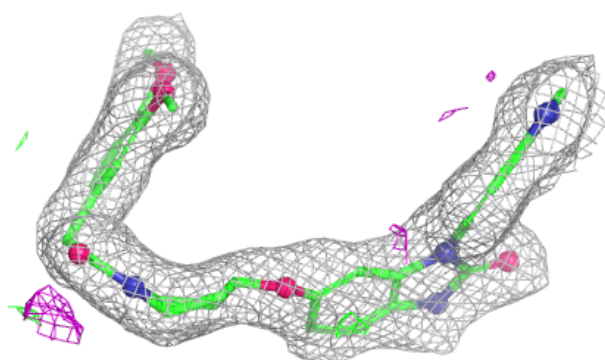


Electron density around A1EMG E 402:

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

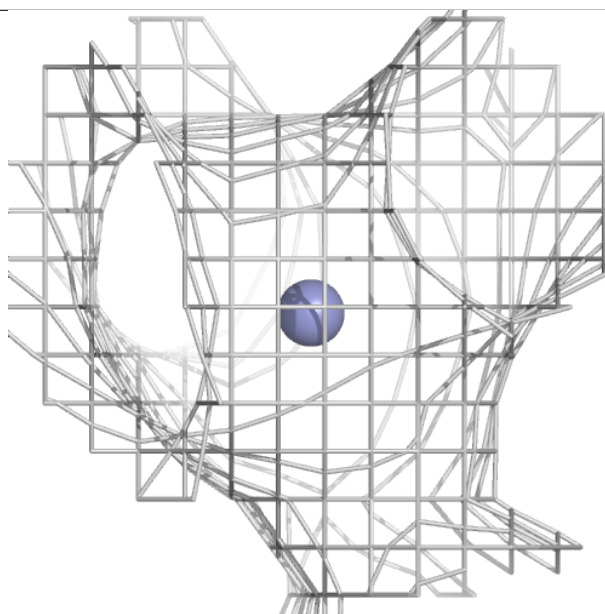
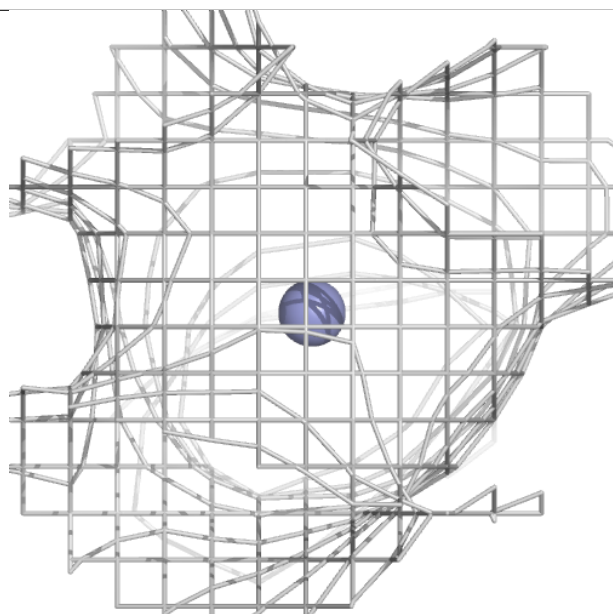
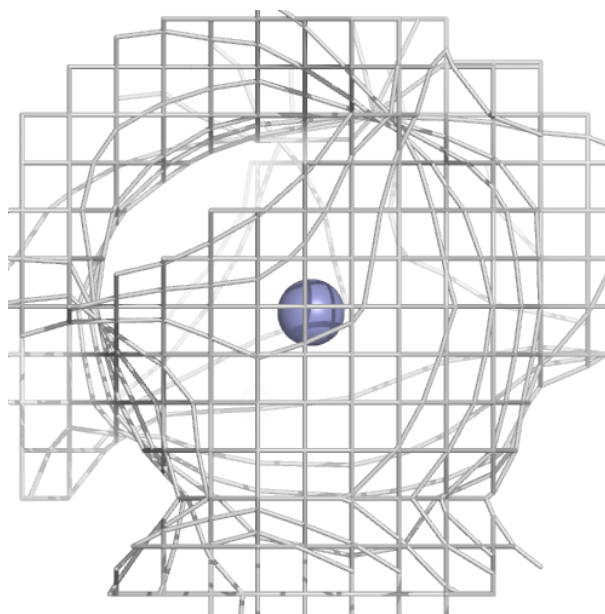
**Electron density around A1EMG A 402:**

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



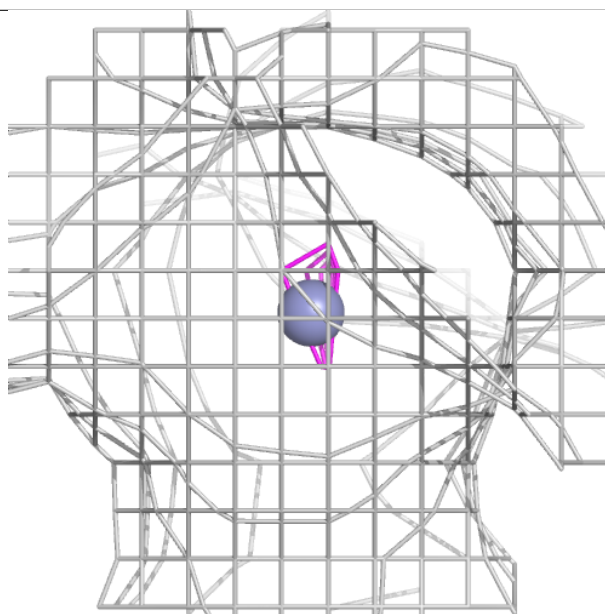
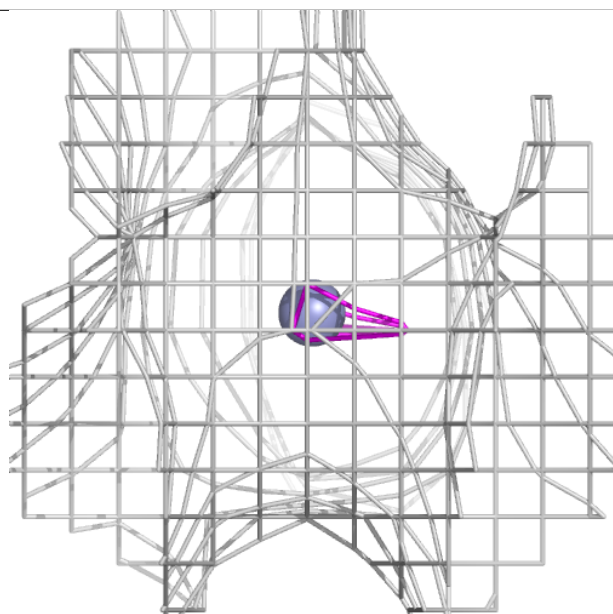
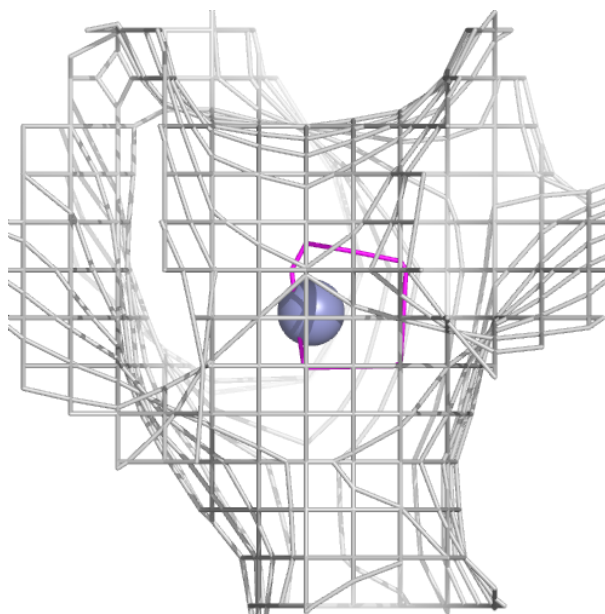
Electron density around ZN A 401:

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and green (positive)



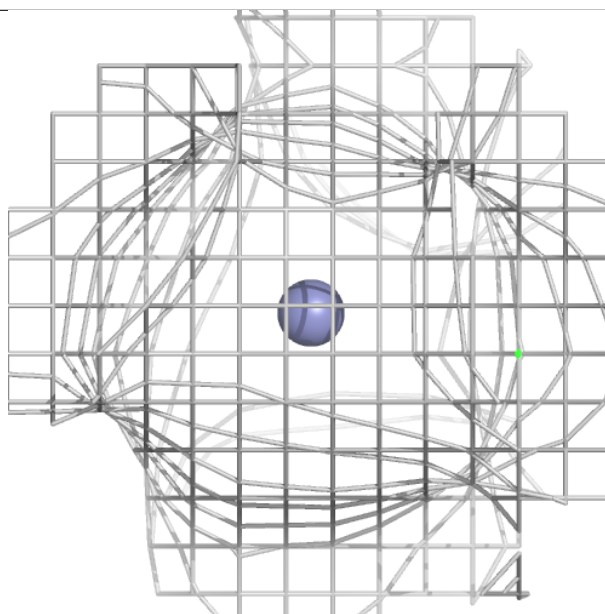
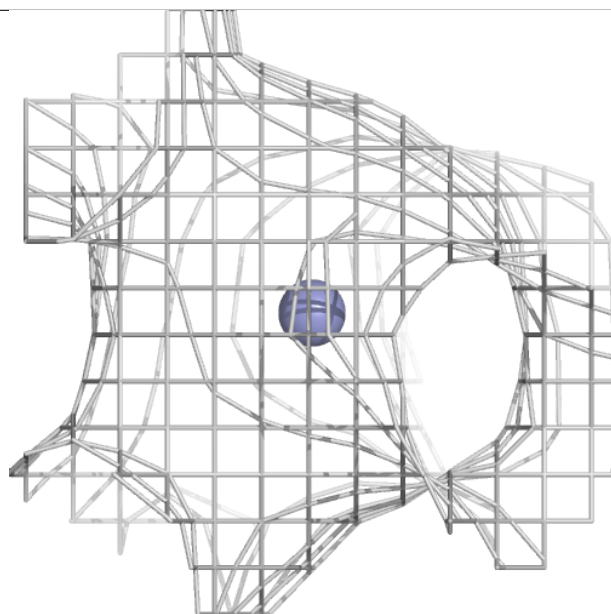
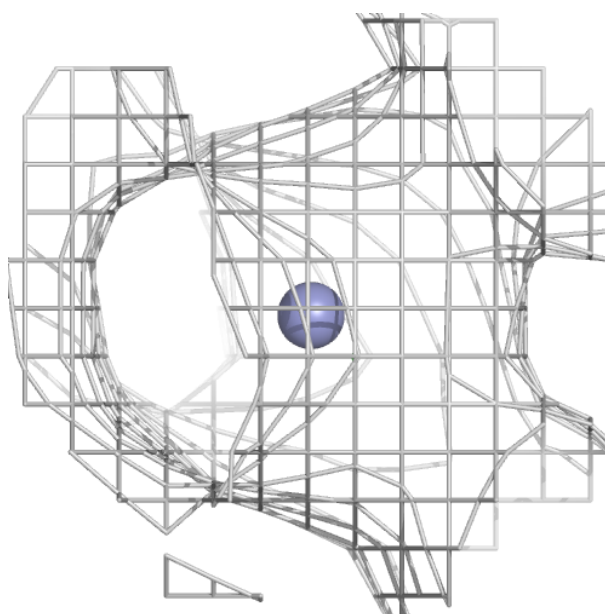
Electron density around ZN B 401:

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and green (positive)



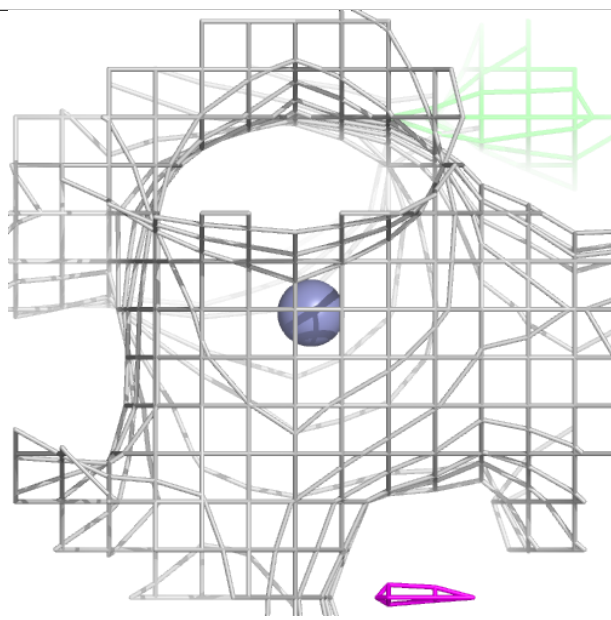
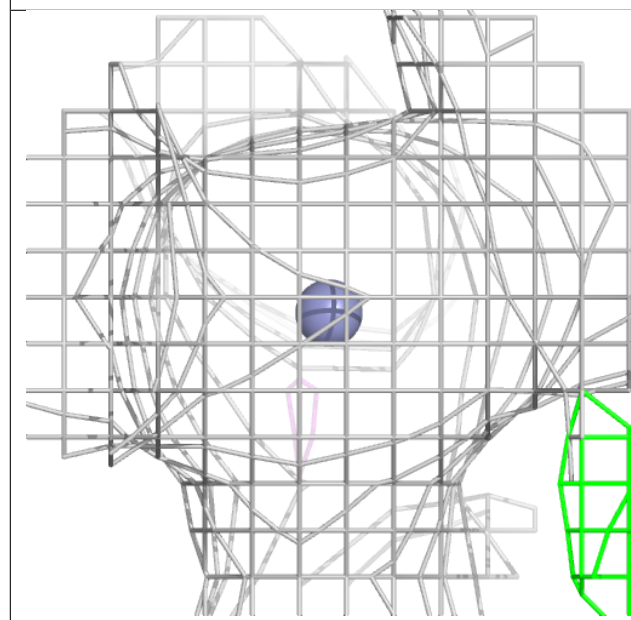
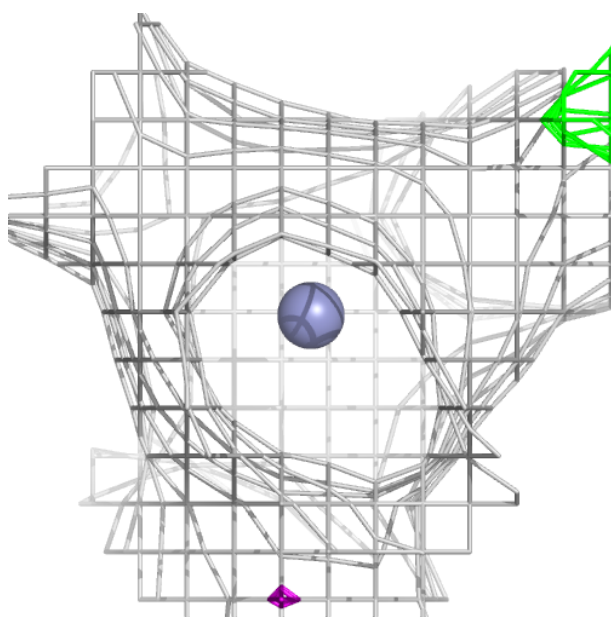
Electron density around ZN C 401:

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



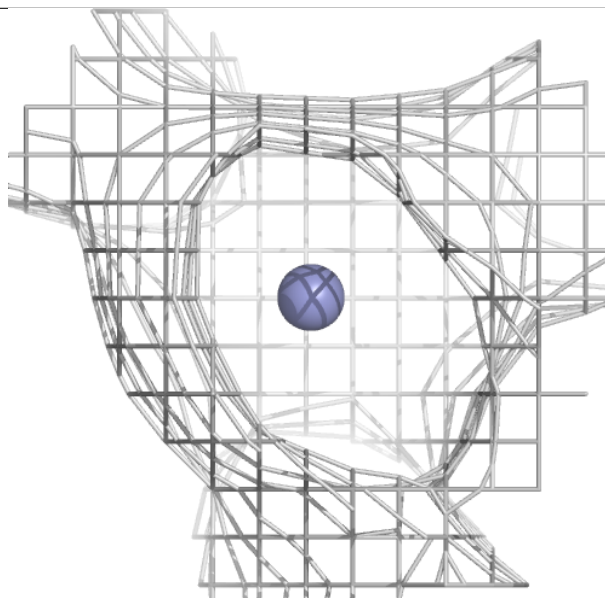
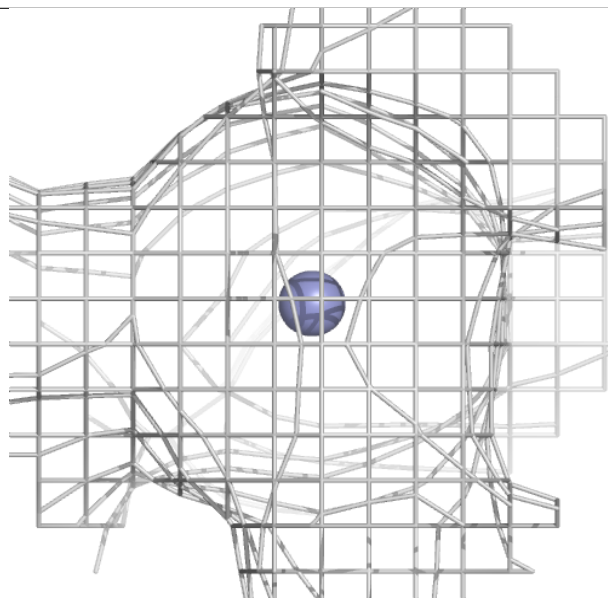
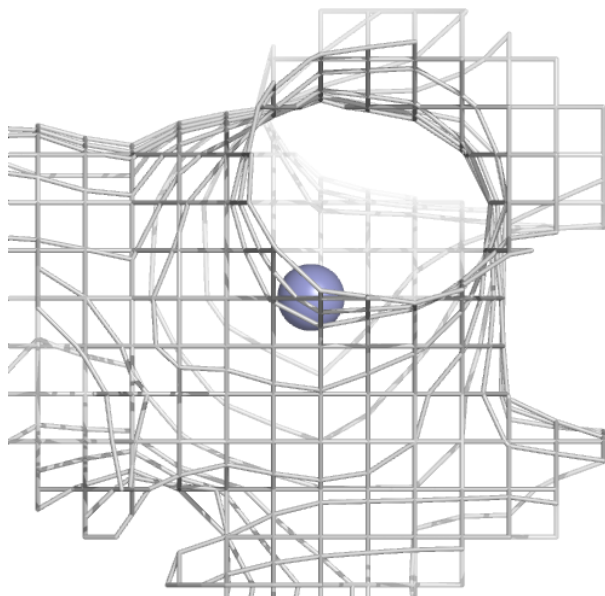
Electron density around ZN D 401:

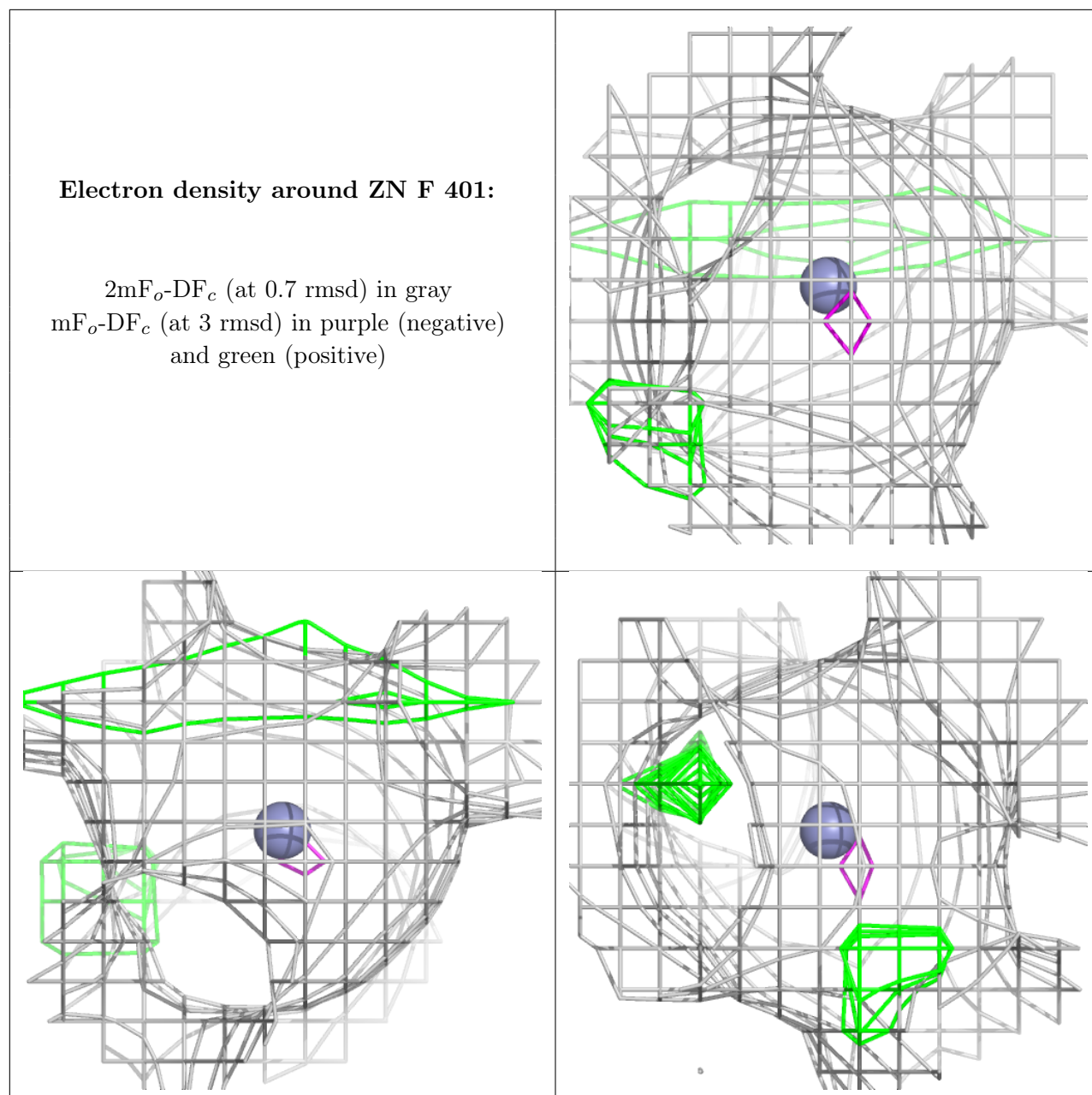
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN E 401:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.