



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:37 PM UTC

PDB ID : 9UD7 / pdb\_00009ud7  
Title : Crystal structure of human glutaminy cyclase in complex with Inhibitor CL7  
Authors : Li, G.-B.; Ning, X.-L.; Meng, F.-B.; Chen, Y.-T.  
Deposited on : 2025-04-06  
Resolution : 2.49 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

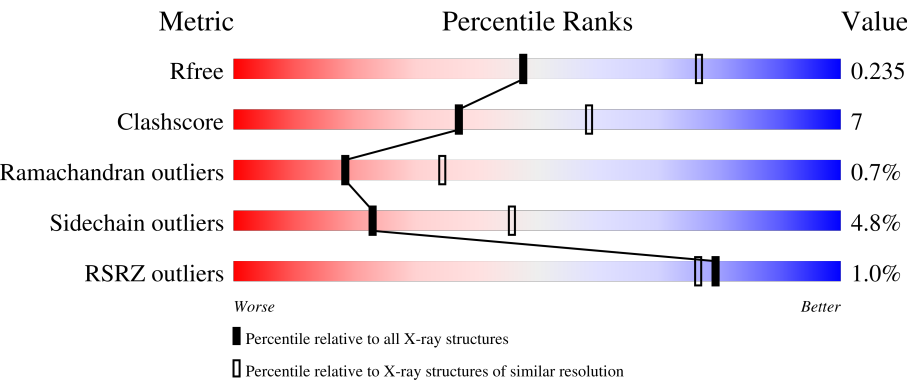
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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 <sub>free</sub>	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	<div><div>%</div><div><div></div><div>76%</div><div>12%</div><div>•</div><div>10%</div></div></div>
1	B	361	<div><div>%</div><div><div></div><div>77%</div><div>11%</div><div>•</div><div>11%</div></div></div>
1	C	361	<div><div>%</div><div><div></div><div>73%</div><div>15%</div><div>•</div><div>11%</div></div></div>
1	D	361	<div><div>%</div><div><div></div><div>72%</div><div>17%</div><div>•</div><div>11%</div></div></div>
1	E	361	<div><div>%</div><div><div></div><div>75%</div><div>13%</div><div>•</div><div>10%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	361	<div> <div>%</div> <div> </div> <div>77% 11% • 11%</div> </div>

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
4	MG	D	406	-	-	-	X
5	GOL	B	406	-	X	-	-
5	GOL	B	407	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17035 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.

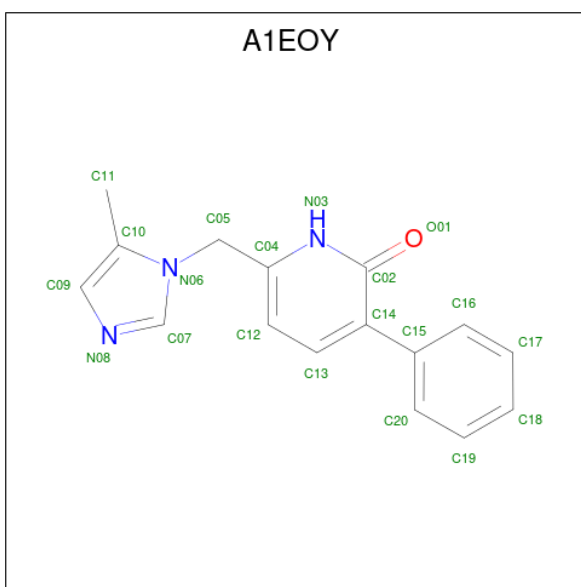
- Molecule 1 is a protein called Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2617	1677	451	480	9			
1	B	323	Total	C	N	O	S	0	1	0
			2618	1678	453	478	9			
1	C	323	Total	C	N	O	S	0	0	0
			2610	1673	450	478	9			
1	D	323	Total	C	N	O	S	8	1	0
			2618	1679	451	479	9			
1	E	324	Total	C	N	O	S	0	1	0
			2626	1682	452	483	9			
1	F	323	Total	C	N	O	S	0	0	0
			2610	1673	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		
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 6-[(5-methylimidazol-1-yl)methyl]-3-phenyl-1H-pyridin-2-one (CCD ID: A1EOY) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	16	3	1		
3	B	1	Total	C	N	O	0	0
			20	16	3	1		
3	C	1	Total	C	N	O	0	0
			20	16	3	1		
3	D	1	Total	C	N	O	0	0
			20	16	3	1		
3	E	1	Total	C	N	O	0	0
			20	16	3	1		
3	F	1	Total	C	N	O	0	0
			20	16	3	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	B	3	Total	Mg	0	0
			3	3		
4	C	1	Total	Mg	0	0
			1	1		
4	D	4	Total	Mg	0	0
			4	4		
4	E	3	Total	Mg	0	0
			3	3		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



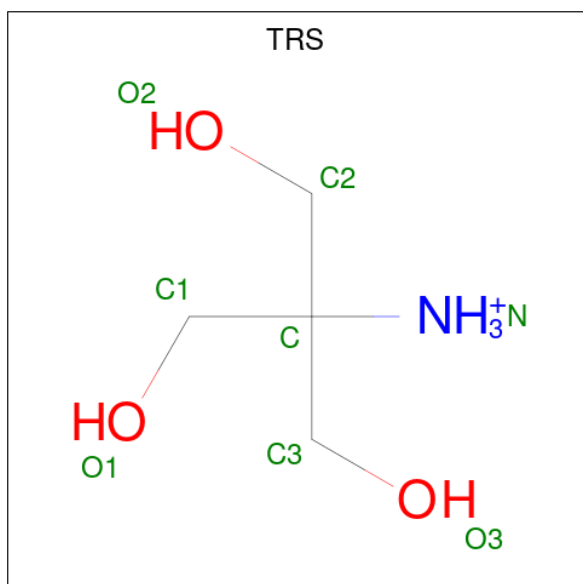
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	189	Total	O	0	0
			189	189		
7	B	194	Total	O	0	0
			194	194		
7	C	199	Total	O	0	0
			199	199		
7	D	155	Total	O	0	0
			155	155		

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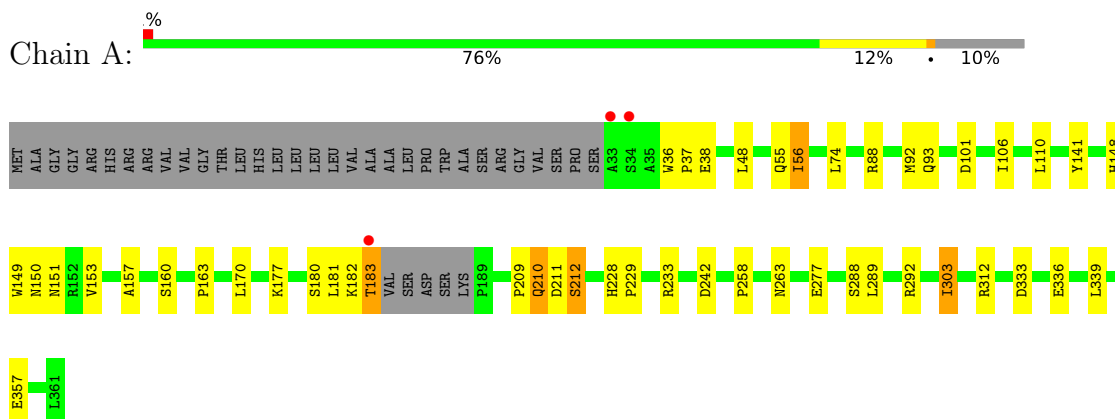
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	190	Total 190	O 190	0	0
7	F	158	Total 158	O 158	0	0



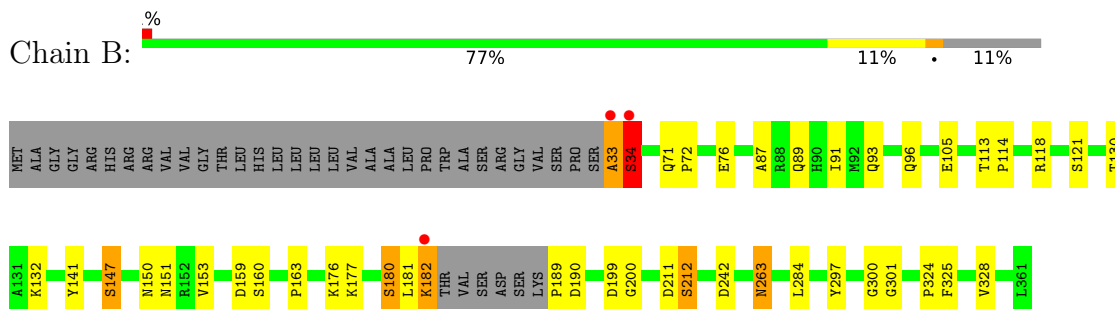
### 3 Residue-property plots [i](#)

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.

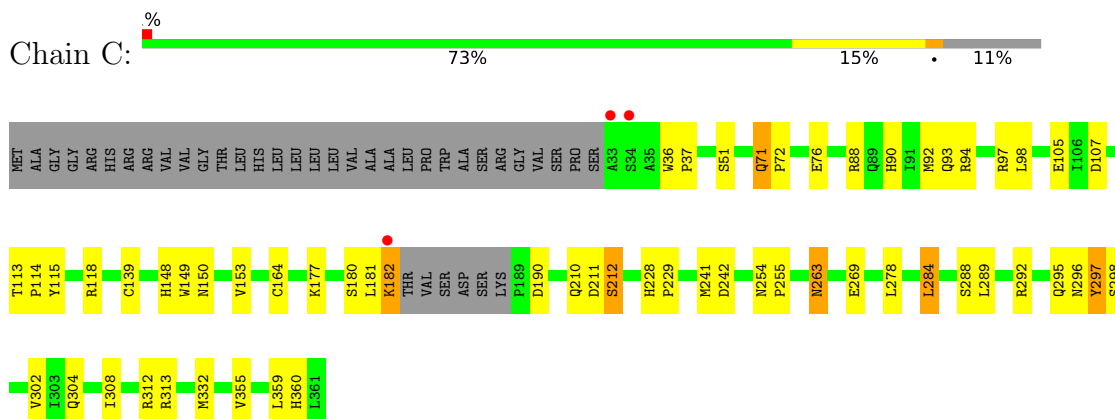
- Molecule 1: Glutaminyl-peptide cyclotransferase



- Molecule 1: Glutaminyl-peptide cyclotransferase

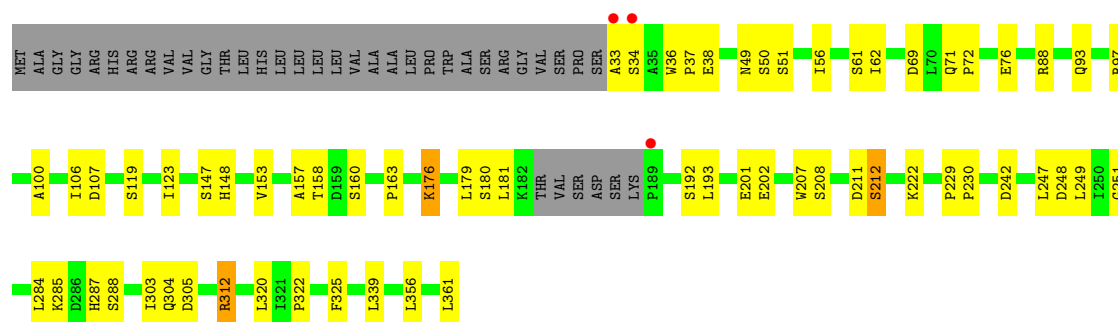


- Molecule 1: Glutaminyl-peptide cyclotransferase




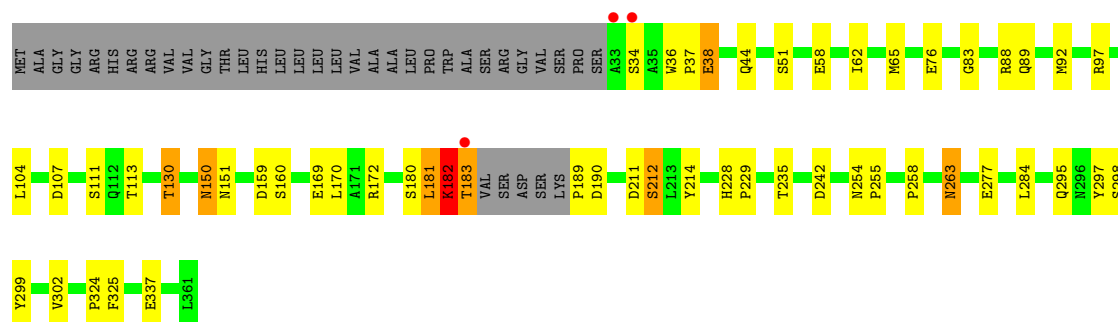
## ● Molecule 1: Glutaminyl-peptide cyclotransferase

Chain D: 




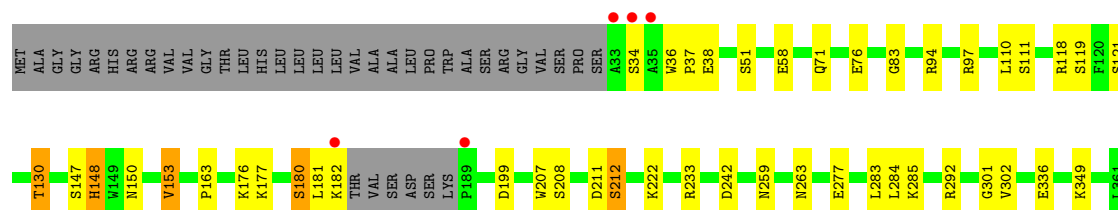
## ● Molecule 1: Glutaminyl-peptide cyclotransferase

Chain E: 



## ● Molecule 1: Glutaminyl-peptide cyclotransferase

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.43Å 181.57Å 89.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.82 – 2.49 71.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (71.82-2.49) 99.9 (71.82-2.49)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.160 , 0.230 0.172 , 0.235	Depositor DCC
$R_{free}$ test set	2000 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, GOL, ZN, TRS, A1EOY

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	1.14	0/2694	0.82	0/3666
1	B	1.12	0/2698	0.86	2/3670 (0.1%)
1	C	1.10	2/2687 (0.1%)	0.82	0/3656
1	D	1.01	0/2695	0.80	0/3667
1	E	1.13	0/2703	0.82	0/3678
1	F	1.06	0/2687	0.83	0/3656
All	All	1.09	2/16164 (0.0%)	0.83	2/21993 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	71	GLN	C-N	-6.62	1.26	1.33
1	C	313	ARG	CZ-NH2	-5.26	1.26	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ALA	CA-C-N	5.61	131.80	121.70
1	B	33	ALA	C-N-CA	5.61	131.80	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	181	LEU	Peptide
1	C	181	LEU	Peptide
1	E	181	LEU	Peptide

## 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	2617	0	2536	36	0
1	B	2618	0	2542	30	0
1	C	2610	0	2529	42	0
1	D	2618	0	2539	44	0
1	E	2626	0	2541	32	0
1	F	2610	0	2529	29	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	20	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	20	0	0	2	0
3	E	20	0	0	0	0
3	F	20	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
5	A	18	0	24	3	0
5	B	12	0	16	8	0
5	C	30	0	40	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	18	0	24	3	0
5	E	12	0	16	2	0
5	F	12	0	16	2	0
6	C	8	0	12	2	0
7	A	189	0	0	17	1
7	B	194	0	0	11	0
7	C	199	0	0	17	1
7	D	155	0	0	19	0
7	E	190	0	0	11	0
7	F	158	0	0	19	0
All	All	17035	0	15364	221	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 7.

All (221) 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)
5:B:407:GOL:H12	7:B:654:HOH:O	1.32	1.28
1:C:241:MET:SD	7:C:692:HOH:O	2.19	0.98
1:B:105:GLU:OE2	7:B:501:HOH:O	1.84	0.95
5:D:409:GOL:H12	7:D:625:HOH:O	1.68	0.92
1:B:118[A]:ARG:NH1	7:B:504:HOH:O	2.04	0.90
5:B:407:GOL:O1	7:B:502:HOH:O	1.86	0.90
1:D:69:ASP:OD2	7:D:501:HOH:O	1.95	0.84
3:D:402:A1EOY:N03	7:D:504:HOH:O	2.11	0.83
1:B:297:TYR:OH	7:B:503:HOH:O	1.92	0.82
1:C:296:ASN:OD1	7:C:501:HOH:O	1.98	0.80
1:C:139:CYS:SG	7:C:667:HOH:O	2.41	0.77
5:F:405:GOL:O1	7:F:501:HOH:O	2.02	0.77
1:B:263:ASN:HB3	5:B:407:GOL:O1	1.86	0.75
1:A:183:THR:OG1	7:A:501:HOH:O	2.07	0.73
1:D:33:ALA:N	7:D:506:HOH:O	2.22	0.72
1:F:150:ASN:OD1	7:F:502:HOH:O	2.07	0.72
1:F:130:THR:HB	7:F:620:HOH:O	1.92	0.70
1:C:107:ASP:OD2	7:C:503:HOH:O	2.08	0.70
1:D:208:SER:OG	7:D:503:HOH:O	2.10	0.69
1:C:304:GLN:HG2	7:C:502:HOH:O	1.92	0.69
1:E:277:GLU:OE2	7:E:501:HOH:O	2.10	0.69
1:C:269:GLU:OE2	7:C:504:HOH:O	2.09	0.69
1:A:56:ILE:CG1	7:A:626:HOH:O	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:ASP:OD2	7:E:502:HOH:O	2.10	0.69
1:D:37:PRO:O	7:D:502:HOH:O	2.10	0.68
1:B:324:PRO:HA	5:B:406:GOL:H12	1.74	0.68
1:C:164:CYS:HA	7:C:667:HOH:O	1.92	0.68
1:A:38:GLU:OE1	1:D:147:SER:OG	2.11	0.67
1:A:56:ILE:HG12	7:A:626:HOH:O	1.95	0.67
5:A:408:GOL:H12	7:A:652:HOH:O	1.94	0.67
1:A:277:GLU:OE2	7:A:502:HOH:O	2.12	0.67
1:B:33:ALA:N	1:B:34:SER:O	2.27	0.66
1:E:182:LYS:O	1:E:183:THR:O	2.13	0.66
1:D:304:GLN:NE2	7:D:507:HOH:O	2.23	0.65
1:B:189:PRO:CD	7:B:515:HOH:O	2.46	0.64
1:B:150:ASN:O	1:B:150:ASN:ND2	2.32	0.63
1:A:289:LEU:O	1:A:292:ARG:HG3	2.00	0.61
1:C:36:TRP:CG	1:C:37:PRO:HD3	2.37	0.60
1:C:105:GLU:OE1	7:C:505:HOH:O	2.16	0.60
1:E:299:TYR:O	7:E:504:HOH:O	2.16	0.60
1:F:51:SER:HB2	7:F:514:HOH:O	2.00	0.60
1:F:211:ASP:O	1:F:212:SER:HB3	2.00	0.60
1:C:177:LYS:NZ	7:C:516:HOH:O	2.34	0.60
1:C:332:MET:HB2	5:C:408:GOL:H12	1.84	0.59
1:D:312:ARG:NH1	7:D:509:HOH:O	2.33	0.59
1:E:190:ASP:OD1	7:E:503:HOH:O	2.16	0.59
1:E:92:MET:HE2	1:E:104:LEU:HD13	1.84	0.59
1:C:93:GLN:HB2	5:C:407:GOL:O1	2.03	0.58
1:E:324:PRO:HA	5:E:406:GOL:H11	1.85	0.58
1:A:101:ASP:OD1	7:A:503:HOH:O	2.17	0.58
1:B:325:PHE:H	5:B:406:GOL:H12	1.70	0.57
1:F:302:VAL:HG21	7:F:655:HOH:O	2.04	0.57
1:C:211:ASP:O	1:C:212:SER:HB3	2.04	0.57
1:A:48:LEU:CD1	7:A:626:HOH:O	2.53	0.57
1:B:76:GLU:HG3	1:B:153:VAL:CG1	2.36	0.56
1:B:189:PRO:N	7:B:515:HOH:O	2.39	0.56
1:F:283:LEU:O	1:F:349:LYS:NZ	2.37	0.56
1:F:94:ARG:NH1	7:F:503:HOH:O	2.19	0.55
1:D:211:ASP:O	1:D:212:SER:HB3	2.05	0.55
5:F:405:GOL:H11	7:F:587:HOH:O	2.06	0.55
1:C:308:ILE:O	1:C:312:ARG:HG2	2.07	0.54
1:F:207:TRP:N	7:F:510:HOH:O	2.40	0.54
1:B:132:LYS:NZ	1:B:190:ASP:OD2	2.41	0.53
1:D:93:GLN:HB3	7:D:633:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ARG:O	1:E:92:MET:HG3	2.08	0.53
1:B:147:SER:OG	1:D:38:GLU:OE1	2.25	0.53
1:C:355:VAL:HG11	7:C:697:HOH:O	2.08	0.53
1:A:148:HIS:CD2	1:A:153:VAL:HG22	2.44	0.53
1:A:211:ASP:O	1:A:212:SER:HB3	2.08	0.53
1:E:263:ASN:HB3	7:E:565:HOH:O	2.08	0.53
1:B:33:ALA:HB3	1:B:34:SER:O	2.09	0.52
1:E:150:ASN:O	1:E:151:ASN:HB2	2.07	0.52
1:A:101:ASP:OD1	1:A:101:ASP:O	2.27	0.52
1:B:121:SER:O	1:B:141:TYR:OH	2.26	0.52
5:B:407:GOL:C2	7:B:505:HOH:O	2.55	0.51
1:E:189:PRO:HD3	7:E:612:HOH:O	2.09	0.51
1:E:130:THR:HB	7:E:655:HOH:O	2.09	0.51
1:D:160:SER:C	1:D:163:PRO:HD2	2.36	0.50
1:E:97:ARG:HD3	7:E:606:HOH:O	2.10	0.50
1:B:211:ASP:O	1:B:212:SER:HB3	2.11	0.50
1:C:289:LEU:O	1:C:292:ARG:HD2	2.11	0.50
1:A:312:ARG:HD3	5:A:408:GOL:O1	2.11	0.50
1:C:93:GLN:HB2	5:C:407:GOL:O2	2.11	0.50
1:E:189:PRO:CD	7:E:612:HOH:O	2.59	0.50
1:A:228:HIS:HA	1:A:229:PRO:C	2.37	0.50
1:F:259:ASN:OD1	7:F:504:HOH:O	2.19	0.49
1:B:328:VAL:HG22	7:B:674:HOH:O	2.12	0.49
1:D:312:ARG:NH1	7:D:513:HOH:O	2.39	0.49
1:F:336:GLU:OE1	7:F:505:HOH:O	2.20	0.49
1:A:36:TRP:CG	1:A:37:PRO:HD3	2.48	0.49
1:F:110:LEU:HA	1:F:118:ARG:O	2.13	0.48
1:F:181:LEU:O	1:F:182:LYS:HB2	2.14	0.48
1:A:303:ILE:HD13	7:A:573:HOH:O	2.14	0.48
1:D:62:ILE:N	7:D:508:HOH:O	2.32	0.48
1:F:76:GLU:O	1:F:83:GLY:HA3	2.14	0.48
1:F:302:VAL:HG23	7:F:561:HOH:O	2.14	0.48
1:C:148:HIS:CD2	1:C:153:VAL:HG22	2.48	0.47
1:C:308:ILE:HG23	5:C:406:GOL:H2	1.95	0.47
1:D:49:ASN:OD1	1:D:49:ASN:C	2.57	0.47
1:C:278:LEU:HB3	1:C:284:LEU:HD13	1.96	0.47
1:E:211:ASP:O	1:E:212:SER:HB3	2.12	0.47
1:D:158:THR:HG22	1:D:251:GLY:HA3	1.95	0.47
1:E:36:TRP:CG	1:E:37:PRO:HD3	2.48	0.47
1:F:51:SER:N	7:F:514:HOH:O	2.38	0.47
1:F:148:HIS:CE1	1:F:153:VAL:CG2	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLN:NE2	7:C:526:HOH:O	2.48	0.47
1:C:263:ASN:HB3	7:C:593:HOH:O	2.15	0.47
1:E:254:ASN:N	1:E:255:PRO:CD	2.77	0.47
1:D:284:LEU:N	7:D:505:HOH:O	2.20	0.47
1:F:51:SER:CB	7:F:514:HOH:O	2.61	0.47
1:C:72:PRO:HG2	1:C:90:HIS:CE1	2.49	0.46
1:A:92:MET:SD	1:A:106:ILE:HD11	2.55	0.46
1:A:357:GLU:OE1	7:A:504:HOH:O	2.21	0.46
1:D:38:GLU:HG2	7:D:620:HOH:O	2.16	0.46
1:B:113:THR:HB	1:B:114:PRO:CD	2.45	0.46
1:C:359:LEU:O	1:C:360:HIS:HB2	2.16	0.46
1:F:180:SER:O	1:F:180:SER:OG	2.34	0.46
1:A:333:ASP:OD2	5:A:407:GOL:C1	2.64	0.46
1:B:89:GLN:O	1:B:93:GLN:HG2	2.16	0.46
1:B:33:ALA:N	1:B:34:SER:C	2.73	0.45
1:D:88:ARG:HG3	1:D:123:ILE:HD11	1.98	0.45
1:B:76:GLU:HG3	1:B:153:VAL:HG11	1.98	0.45
1:F:302:VAL:CG2	7:F:561:HOH:O	2.63	0.45
1:B:71:GLN:N	1:B:72:PRO:CD	2.80	0.45
1:A:177:LYS:O	1:A:180:SER:HB3	2.17	0.45
1:A:209:PRO:HD2	1:A:210:GLN:OE1	2.16	0.45
1:C:71:GLN:N	1:C:72:PRO:CD	2.79	0.45
1:D:33:ALA:O	1:D:34:SER:OG	2.28	0.45
1:B:325:PHE:H	5:B:406:GOL:C1	2.29	0.45
1:C:88:ARG:O	1:C:92:MET:HG3	2.16	0.45
1:E:228:HIS:HA	1:E:229:PRO:C	2.42	0.45
1:B:159:ASP:N	1:B:160:SER:HA	2.31	0.45
1:E:113:THR:HG22	1:E:214:TYR:CE1	2.52	0.45
1:D:285:LYS:NZ	7:D:529:HOH:O	2.49	0.44
1:D:356:LEU:HD22	1:D:361:LEU:HB2	1.99	0.44
1:A:150:ASN:O	1:A:151:ASN:HB2	2.17	0.44
1:F:285:LYS:HE3	7:F:578:HOH:O	2.16	0.44
1:A:312:ARG:NH2	7:A:516:HOH:O	2.44	0.44
1:D:181:LEU:HA	7:D:544:HOH:O	2.16	0.44
1:C:118:ARG:HH21	6:C:401:TRS:HN1	1.65	0.44
1:C:76:GLU:HG3	1:C:153:VAL:CG1	2.47	0.44
1:D:61:SER:HA	7:D:508:HOH:O	2.18	0.44
1:A:160:SER:C	1:A:163:PRO:HD2	2.43	0.44
1:A:303:ILE:HG12	7:A:573:HOH:O	2.17	0.44
1:B:87:ALA:O	1:B:91:ILE:HG13	2.17	0.44
1:C:94:ARG:O	1:C:97:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:TRP:CG	1:D:37:PRO:HD3	2.53	0.44
3:D:402:A1EOY:C11	7:D:504:HOH:O	2.65	0.44
1:E:325:PHE:CD1	5:E:406:GOL:H12	2.53	0.44
1:E:76:GLU:O	1:E:83:GLY:HA3	2.18	0.43
1:A:170:LEU:C	1:A:170:LEU:HD23	2.43	0.43
1:B:113:THR:HB	1:B:114:PRO:HD2	2.00	0.43
1:D:148:HIS:CD2	1:D:153:VAL:HG22	2.53	0.43
1:B:160:SER:C	1:B:163:PRO:HD2	2.43	0.43
1:A:303:ILE:CD1	7:A:573:HOH:O	2.65	0.43
1:C:113:THR:HB	1:C:114:PRO:HD2	2.00	0.43
1:D:287:HIS:O	5:D:408:GOL:H11	2.18	0.43
1:A:56:ILE:HB	7:A:626:HOH:O	2.19	0.43
1:A:177:LYS:NZ	7:A:525:HOH:O	2.50	0.43
1:D:229:PRO:O	1:D:230:PRO:C	2.62	0.43
1:C:36:TRP:N	1:C:37:PRO:CD	2.82	0.43
1:C:93:GLN:HB2	5:C:407:GOL:C1	2.49	0.43
1:C:228:HIS:HA	1:C:229:PRO:C	2.42	0.43
5:C:409:GOL:H2	7:C:590:HOH:O	2.18	0.43
1:D:207:TRP:CG	7:D:621:HOH:O	2.71	0.43
1:D:76:GLU:HG3	1:D:153:VAL:HG13	1.99	0.43
1:E:189:PRO:CG	7:E:668:HOH:O	2.66	0.42
1:C:304:GLN:NE2	7:C:502:HOH:O	1.98	0.42
1:D:176:LYS:H	1:D:176:LYS:HG3	1.65	0.42
1:D:325:PHE:H	5:D:407:GOL:H32	1.84	0.42
1:A:48:LEU:HD12	7:A:626:HOH:O	2.19	0.42
1:B:182:LYS:NZ	7:B:530:HOH:O	2.52	0.42
1:D:157:ALA:HB1	1:D:339:LEU:HD21	2.01	0.42
1:C:149:TRP:O	1:C:150:ASN:C	2.61	0.42
1:E:258:PRO:HB3	1:E:297:TYR:CZ	2.55	0.42
1:F:277:GLU:OE2	1:F:277:GLU:HA	2.20	0.42
1:A:88:ARG:HD3	1:A:141:TYR:OH	2.20	0.42
1:D:106:ILE:CD1	1:D:123:ILE:HG12	2.50	0.42
1:D:248:ASP:OD2	1:D:305:ASP:OD2	2.38	0.42
1:D:192:SER:OG	1:D:193:LEU:N	2.52	0.42
1:E:182:LYS:O	1:E:183:THR:C	2.62	0.42
1:F:36:TRP:CG	1:F:37:PRO:HD3	2.55	0.42
1:F:121:SER:O	1:F:199:ASP:HB2	2.19	0.42
1:A:177:LYS:HG3	7:A:675:HOH:O	2.19	0.42
1:C:71:GLN:N	1:C:72:PRO:HD2	2.35	0.42
1:D:249:LEU:HB2	1:D:322:PRO:HD2	2.02	0.42
1:E:36:TRP:N	1:E:37:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:GLU:OE1	1:F:147:SER:OG	2.36	0.42
1:D:71:GLN:N	1:D:72:PRO:CD	2.83	0.41
1:D:36:TRP:N	1:D:37:PRO:CD	2.82	0.41
1:E:62:ILE:HD12	1:E:65:MET:HE2	2.02	0.41
1:A:56:ILE:CB	7:A:626:HOH:O	2.67	0.41
1:A:148:HIS:NE2	1:A:153:VAL:HG22	2.35	0.41
1:B:199:ASP:OD1	1:B:200:GLY:N	2.53	0.41
1:C:190:ASP:OD1	7:C:507:HOH:O	2.21	0.41
1:D:247:LEU:CD2	1:D:320:LEU:HD12	2.50	0.41
1:E:181:LEU:O	1:E:182:LYS:CB	2.68	0.41
1:F:130:THR:HG22	7:F:642:HOH:O	2.20	0.41
1:C:98:LEU:O	7:C:506:HOH:O	2.21	0.41
1:C:355:VAL:HG21	7:C:697:HOH:O	2.20	0.41
1:D:107:ASP:OD2	1:D:222:LYS:NZ	2.50	0.41
1:E:169:GLU:CD	1:E:172:ARG:HH21	2.29	0.41
1:A:149:TRP:CD2	1:A:150:ASN:HB2	2.56	0.41
5:B:407:GOL:H31	7:B:664:HOH:O	2.20	0.41
1:E:170:LEU:C	1:E:170:LEU:HD23	2.46	0.41
1:A:157:ALA:HB1	1:A:339:LEU:HD21	2.02	0.41
1:E:302:VAL:HG11	7:E:570:HOH:O	2.20	0.41
1:F:119:SER:HB3	7:F:597:HOH:O	2.20	0.41
1:D:100:ALA:HA	1:D:179:LEU:HD12	2.03	0.40
1:F:177:LYS:O	1:F:180:SER:HB3	2.21	0.40
1:C:115:TYR:HE2	6:C:401:TRS:H32	1.85	0.40
1:D:56:ILE:HD11	1:D:356:LEU:CD1	2.50	0.40
1:D:312:ARG:NE	7:D:513:HOH:O	2.44	0.40
1:C:182:LYS:HD3	1:C:182:LYS:HA	1.81	0.40
1:C:254:ASN:N	1:C:255:PRO:CD	2.85	0.40
1:F:222:LYS:NZ	7:F:507:HOH:O	2.29	0.40
1:F:119:SER:CB	7:F:597:HOH:O	2.69	0.40
1:A:74:LEU:HD13	1:A:336:GLU:HB2	2.04	0.40
1:B:177:LYS:O	1:B:180:SER:HB3	2.20	0.40
1:D:201:GLU:OE1	1:D:202:GLU:HG2	2.22	0.40
1:E:159:ASP:N	1:E:160:SER:HA	2.36	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)
7:A:630:HOH:O	7:C:668:HOH:O[4_554]	2.02	0.18

## 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	320/361 (89%)	305 (95%)	12 (4%)	3 (1%)	14	27
1	B	320/361 (89%)	302 (94%)	14 (4%)	4 (1%)	9	18
1	C	319/361 (88%)	304 (95%)	13 (4%)	2 (1%)	21	38
1	D	320/361 (89%)	300 (94%)	19 (6%)	1 (0%)	36	55
1	E	321/361 (89%)	304 (95%)	15 (5%)	2 (1%)	21	38
1	F	319/361 (88%)	297 (93%)	20 (6%)	2 (1%)	21	38
All	All	1919/2166 (89%)	1812 (94%)	93 (5%)	14 (1%)	18	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	SER
1	B	212	SER
1	E	182	LYS
1	B	300	GLY
1	B	301	GLY
1	C	212	SER
1	C	297	TYR
1	D	212	SER
1	E	212	SER
1	F	212	SER
1	F	301	GLY
1	A	181	LEU
1	A	212	SER
1	A	258	PRO

### 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	285/314 (91%)	273 (96%)	12 (4%)	26	52
1	B	285/314 (91%)	274 (96%)	11 (4%)	28	55
1	C	284/314 (90%)	272 (96%)	12 (4%)	26	52
1	D	285/314 (91%)	274 (96%)	11 (4%)	28	55
1	E	286/314 (91%)	267 (93%)	19 (7%)	15	32
1	F	284/314 (90%)	266 (94%)	18 (6%)	16	34
All	All	1709/1884 (91%)	1626 (95%)	83 (5%)	23	45

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	56	ILE
1	A	93	GLN
1	A	110	LEU
1	A	182	LYS
1	A	183	THR
1	A	210	GLN
1	A	233	ARG
1	A	242	ASP
1	A	263	ASN
1	A	288	SER
1	A	303	ILE
1	B	34	SER
1	B	96	GLN
1	B	130	THR
1	B	147	SER
1	B	151	ASN
1	B	176	LYS
1	B	180	SER
1	B	182	LYS
1	B	242	ASP
1	B	263	ASN
1	B	284	LEU
1	C	51	SER
1	C	180	SER
1	C	182	LYS
1	C	210	GLN

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Mol	Chain	Res	Type
1	C	242	ASP
1	C	263	ASN
1	C	284	LEU
1	C	288	SER
1	C	295	GLN
1	C	297	TYR
1	C	298	SER
1	C	302	VAL
1	D	50	SER
1	D	51	SER
1	D	97	ARG
1	D	119	SER
1	D	176	LYS
1	D	180	SER
1	D	242	ASP
1	D	288	SER
1	D	303[A]	ILE
1	D	303[B]	ILE
1	D	312	ARG
1	E	34	SER
1	E	38	GLU
1	E	44	GLN
1	E	51	SER
1	E	58	GLU
1	E	89	GLN
1	E	111	SER
1	E	130	THR
1	E	150	ASN
1	E	180	SER
1	E	182	LYS
1	E	183	THR
1	E	235	THR
1	E	242	ASP
1	E	263	ASN
1	E	284	LEU
1	E	295	GLN
1	E	298	SER
1	E	337	GLU
1	F	34	SER
1	F	38	GLU
1	F	58	GLU
1	F	71	GLN

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Mol	Chain	Res	Type
1	F	97	ARG
1	F	111	SER
1	F	130	THR
1	F	148	HIS
1	F	153	VAL
1	F	163	PRO
1	F	176	LYS
1	F	180	SER
1	F	208	SER
1	F	233	ARG
1	F	242	ASP
1	F	263	ASN
1	F	284	LEU
1	F	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	96	GLN
1	A	112	GLN
1	A	194	GLN
1	B	90	HIS
1	B	96	GLN
1	B	304	GLN
1	E	41	ASN
1	E	194	GLN
1	E	218	HIS
1	E	254	ASN
1	F	44	GLN
1	F	218	HIS

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 21 are monoatomic - leaving 24 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$
6	TRS	C	401	-	7,7,7	0.75	0	9,9,9	1.43	2 (22%)
5	GOL	C	409	-	5,5,5	0.53	0	5,5,5	1.41	0
5	GOL	D	408	-	5,5,5	0.44	0	5,5,5	0.35	0
5	GOL	B	406	-	5,5,5	0.63	0	5,5,5	1.98	2 (40%)
3	A1EOY	A	402	2	21,22,22	2.96	9 (42%)	20,30,30	1.61	5 (25%)
5	GOL	A	407	-	5,5,5	0.35	0	5,5,5	0.58	0
5	GOL	F	405	-	5,5,5	0.30	0	5,5,5	0.98	0
5	GOL	C	406	-	5,5,5	0.19	0	5,5,5	0.92	0
5	GOL	D	409	-	5,5,5	0.38	0	5,5,5	1.01	0
3	A1EOY	F	402	2	21,22,22	2.17	8 (38%)	20,30,30	2.16	8 (40%)
3	A1EOY	D	402	2	21,22,22	3.13	11 (52%)	20,30,30	1.77	6 (30%)
5	GOL	C	405	-	5,5,5	0.70	0	5,5,5	1.16	0
3	A1EOY	C	403	2	21,22,22	2.61	8 (38%)	20,30,30	2.59	8 (40%)
5	GOL	C	407	-	5,5,5	0.44	0	5,5,5	1.01	0
5	GOL	F	404	-	5,5,5	0.73	0	5,5,5	1.35	0
5	GOL	A	406	-	5,5,5	0.63	0	5,5,5	1.37	1 (20%)
3	A1EOY	E	402	2	21,22,22	3.22	12 (57%)	20,30,30	2.20	8 (40%)
5	GOL	E	406	-	5,5,5	0.67	0	5,5,5	1.04	0
5	GOL	D	407	-	5,5,5	0.68	0	5,5,5	1.20	1 (20%)
5	GOL	E	407	-	5,5,5	0.47	0	5,5,5	1.12	1 (20%)
3	A1EOY	B	402	2	21,22,22	2.79	10 (47%)	20,30,30	2.07	8 (40%)
5	GOL	B	407	-	5,5,5	0.86	0	5,5,5	1.25	0
5	GOL	C	408	-	5,5,5	0.34	0	5,5,5	0.57	0
5	GOL	A	408	-	5,5,5	0.63	0	5,5,5	0.58	0



In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TRS	C	401	-	-	7/9/9/9	-
5	GOL	C	409	-	-	3/4/4/4	-
5	GOL	D	408	-	-	2/4/4/4	-
5	GOL	B	406	-	-	4/4/4/4	-
3	A1EOY	A	402	2	-	1/8/8/8	0/3/3/3
5	GOL	A	407	-	-	4/4/4/4	-
5	GOL	F	405	-	-	0/4/4/4	-
5	GOL	C	406	-	-	2/4/4/4	-
5	GOL	D	409	-	-	2/4/4/4	-
3	A1EOY	F	402	2	-	0/8/8/8	0/3/3/3
3	A1EOY	D	402	2	-	1/8/8/8	0/3/3/3
5	GOL	C	405	-	-	1/4/4/4	-
3	A1EOY	C	403	2	-	0/8/8/8	0/3/3/3
5	GOL	C	407	-	-	2/4/4/4	-
5	GOL	F	404	-	-	2/4/4/4	-
5	GOL	A	406	-	-	4/4/4/4	-
3	A1EOY	E	402	2	-	1/8/8/8	0/3/3/3
5	GOL	E	406	-	-	2/4/4/4	-
5	GOL	D	407	-	-	4/4/4/4	-
5	GOL	E	407	-	-	4/4/4/4	-
3	A1EOY	B	402	2	-	1/8/8/8	0/3/3/3
5	GOL	B	407	-	-	2/4/4/4	-
5	GOL	C	408	-	-	4/4/4/4	-
5	GOL	A	408	-	-	2/4/4/4	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	A1EOY	C04-N03	6.96	1.47	1.37
3	E	402	A1EOY	C10-N06	-6.85	1.27	1.38
3	A	402	A1EOY	C10-N06	-6.46	1.27	1.38
3	D	402	A1EOY	C10-N06	-6.37	1.28	1.38
3	B	402	A1EOY	C10-N06	-6.05	1.28	1.38
3	C	403	A1EOY	C10-N06	-5.93	1.28	1.38
3	B	402	A1EOY	C12-C04	5.25	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	A1EOY	C04-N03	5.06	1.44	1.37
3	F	402	A1EOY	C10-N06	-4.98	1.30	1.38
3	D	402	A1EOY	C04-N03	4.89	1.44	1.37
3	D	402	A1EOY	O01-C02	-4.84	1.14	1.23
3	E	402	A1EOY	C13-C14	4.76	1.46	1.37
3	E	402	A1EOY	C09-N08	-4.56	1.29	1.37
3	E	402	A1EOY	C12-C04	4.44	1.47	1.37
3	D	402	A1EOY	C13-C14	4.43	1.45	1.37
3	B	402	A1EOY	C04-N03	4.42	1.43	1.37
3	D	402	A1EOY	C12-C04	4.30	1.47	1.37
3	E	402	A1EOY	C02-N03	4.27	1.46	1.38
3	A	402	A1EOY	C13-C14	4.23	1.45	1.37
3	C	403	A1EOY	C04-N03	4.21	1.43	1.37
3	C	403	A1EOY	C12-C04	4.19	1.47	1.37
3	D	402	A1EOY	C20-C15	-4.15	1.33	1.39
3	E	402	A1EOY	O01-C02	-4.15	1.15	1.23
3	B	402	A1EOY	C02-N03	4.10	1.46	1.38
3	D	402	A1EOY	C02-N03	4.08	1.46	1.38
3	E	402	A1EOY	C07-N06	-3.96	1.30	1.36
3	F	402	A1EOY	C02-N03	3.90	1.46	1.38
3	F	402	A1EOY	C04-N03	3.89	1.43	1.37
3	A	402	A1EOY	C12-C04	3.78	1.46	1.37
3	A	402	A1EOY	O01-C02	-3.69	1.16	1.23
3	B	402	A1EOY	O01-C02	-3.60	1.16	1.23
3	C	403	A1EOY	C02-N03	3.60	1.45	1.38
3	A	402	A1EOY	C09-N08	-3.53	1.31	1.37
3	D	402	A1EOY	C09-N08	-3.52	1.31	1.37
3	C	403	A1EOY	O01-C02	-3.47	1.17	1.23
3	D	402	A1EOY	C16-C15	-3.24	1.34	1.39
3	B	402	A1EOY	C14-C02	3.10	1.50	1.46
3	F	402	A1EOY	C12-C04	3.07	1.44	1.37
3	A	402	A1EOY	C07-N06	-3.01	1.31	1.36
3	E	402	A1EOY	C16-C15	-2.96	1.34	1.39
3	B	402	A1EOY	C13-C14	2.93	1.43	1.37
3	F	402	A1EOY	C09-N08	-2.81	1.32	1.37
3	C	403	A1EOY	C13-C14	2.79	1.42	1.37
3	A	402	A1EOY	C02-N03	2.75	1.44	1.38
3	C	403	A1EOY	C19-C20	-2.71	1.34	1.38
3	B	402	A1EOY	C09-N08	-2.63	1.33	1.37
3	D	402	A1EOY	C17-C16	-2.50	1.34	1.38
3	B	402	A1EOY	C13-C12	2.47	1.48	1.41
3	E	402	A1EOY	C13-C12	2.44	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	A1EOY	C13-C12	2.43	1.47	1.41
3	A	402	A1EOY	C20-C15	-2.23	1.36	1.39
3	F	402	A1EOY	O01-C02	-2.16	1.19	1.23
3	B	402	A1EOY	C07-N06	-2.14	1.33	1.36
3	C	403	A1EOY	C16-C15	-2.12	1.36	1.39
3	F	402	A1EOY	C11-C10	2.10	1.53	1.49
3	F	402	A1EOY	C20-C15	-2.09	1.36	1.39
3	E	402	A1EOY	C05-N06	-2.08	1.43	1.46
3	E	402	A1EOY	C11-C10	2.05	1.53	1.49

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	A1EOY	O01-C02-C14	-5.62	118.04	125.19
3	C	403	A1EOY	C13-C12-C04	5.13	123.73	118.91
3	C	403	A1EOY	C12-C04-N03	-5.13	115.04	119.53
3	E	402	A1EOY	O01-C02-C14	-4.74	119.16	125.19
3	E	402	A1EOY	C13-C14-C02	-4.62	116.78	119.39
3	C	403	A1EOY	C15-C14-C02	4.56	125.58	120.05
3	B	402	A1EOY	O01-C02-C14	-4.52	119.44	125.19
3	F	402	A1EOY	C11-C10-N06	4.42	128.06	122.80
3	B	402	A1EOY	C12-C13-C14	-3.92	119.16	123.35
3	B	402	A1EOY	C13-C12-C04	3.80	122.48	118.91
3	E	402	A1EOY	C15-C14-C02	3.76	124.61	120.05
3	D	402	A1EOY	O01-C02-C14	-3.73	120.45	125.19
3	C	403	A1EOY	C13-C14-C02	-3.61	117.35	119.39
3	A	402	A1EOY	O01-C02-C14	-3.55	120.68	125.19
5	B	406	GOL	O3-C3-C2	-3.49	94.69	110.38
3	C	403	A1EOY	C15-C14-C13	-3.31	117.04	121.62
3	D	402	A1EOY	C11-C10-N06	3.25	126.66	122.80
3	D	402	A1EOY	C12-C13-C14	-3.21	119.93	123.35
3	A	402	A1EOY	C15-C14-C13	-3.08	117.37	121.62
3	F	402	A1EOY	C12-C04-N03	-3.07	116.84	119.53
6	C	401	TRS	C2-C-N	2.95	115.70	108.17
3	C	403	A1EOY	C12-C13-C14	-2.88	120.28	123.35
6	C	401	TRS	C3-C-C1	-2.75	103.33	110.66
3	B	402	A1EOY	C09-N08-C07	-2.74	101.66	105.24
3	E	402	A1EOY	C13-C12-C04	2.65	121.40	118.91
5	B	406	GOL	O2-C2-C3	-2.60	98.40	109.18
3	A	402	A1EOY	C15-C14-C02	2.59	123.19	120.05
5	D	407	GOL	O1-C1-C2	-2.47	99.24	110.38
3	E	402	A1EOY	C11-C10-N06	2.45	125.71	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	A1EOY	O01-C02-C14	-2.42	122.12	125.19
3	E	402	A1EOY	C12-C04-N03	-2.36	117.47	119.53
3	C	403	A1EOY	C17-C16-C15	-2.35	118.06	120.36
3	F	402	A1EOY	C20-C15-C14	-2.31	117.67	120.98
3	B	402	A1EOY	C12-C04-N03	-2.28	117.53	119.53
5	A	406	GOL	O2-C2-C1	-2.26	99.81	109.18
3	D	402	A1EOY	C13-C12-C04	2.25	121.03	118.91
3	E	402	A1EOY	C15-C14-C13	-2.23	118.54	121.62
3	A	402	A1EOY	C12-C13-C14	-2.21	120.99	123.35
3	A	402	A1EOY	C17-C16-C15	-2.17	118.23	120.36
3	F	402	A1EOY	C15-C14-C02	2.15	122.65	120.05
3	F	402	A1EOY	C13-C14-C02	-2.13	118.19	119.39
5	E	407	GOL	C3-C2-C1	-2.13	103.97	111.80
3	F	402	A1EOY	C20-C15-C16	2.12	121.26	118.57
3	B	402	A1EOY	C20-C15-C16	2.12	121.26	118.57
3	E	402	A1EOY	C12-C13-C14	-2.12	121.09	123.35
3	B	402	A1EOY	C20-C15-C14	-2.09	117.98	120.98
3	F	402	A1EOY	O01-C02-N03	2.07	124.01	120.11
3	D	402	A1EOY	C18-C17-C16	-2.02	117.75	120.24
3	B	402	A1EOY	C11-C10-N06	2.02	125.20	122.80
3	D	402	A1EOY	C16-C15-C14	-2.02	118.09	120.98

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1EOY	N03-C04-C05-N06
3	B	402	A1EOY	N03-C04-C05-N06
3	D	402	A1EOY	N03-C04-C05-N06
3	E	402	A1EOY	N03-C04-C05-N06
5	A	407	GOL	O1-C1-C2-O2
5	A	407	GOL	C1-C2-C3-O3
5	B	407	GOL	O1-C1-C2-C3
5	C	406	GOL	O1-C1-C2-O2
5	C	407	GOL	C1-C2-C3-O3
5	C	409	GOL	O1-C1-C2-C3
5	D	407	GOL	O1-C1-C2-C3
5	D	409	GOL	C1-C2-C3-O3
5	E	406	GOL	O1-C1-C2-O2
5	E	406	GOL	O1-C1-C2-C3
5	E	407	GOL	O1-C1-C2-C3
5	F	404	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	C	401	TRS	C1-C-C2-O2
6	C	401	TRS	C3-C-C2-O2
6	C	401	TRS	N-C-C2-O2
5	A	406	GOL	O1-C1-C2-O2
5	D	407	GOL	O1-C1-C2-O2
5	E	407	GOL	O2-C2-C3-O3
5	A	406	GOL	O1-C1-C2-C3
5	A	406	GOL	C1-C2-C3-O3
5	A	407	GOL	O1-C1-C2-C3
5	A	408	GOL	O1-C1-C2-C3
5	B	406	GOL	O1-C1-C2-C3
5	B	406	GOL	C1-C2-C3-O3
5	C	406	GOL	O1-C1-C2-C3
5	C	408	GOL	O1-C1-C2-C3
5	C	408	GOL	C1-C2-C3-O3
5	D	407	GOL	C1-C2-C3-O3
5	D	408	GOL	C1-C2-C3-O3
5	E	407	GOL	C1-C2-C3-O3
5	A	407	GOL	O2-C2-C3-O3
5	B	407	GOL	O1-C1-C2-O2
5	C	408	GOL	O2-C2-C3-O3
5	C	409	GOL	O1-C1-C2-O2
5	E	407	GOL	O1-C1-C2-O2
5	F	404	GOL	O1-C1-C2-O2
6	C	401	TRS	C1-C-C3-O3
5	A	406	GOL	O2-C2-C3-O3
5	B	406	GOL	O2-C2-C3-O3
5	C	405	GOL	O2-C2-C3-O3
5	C	407	GOL	O2-C2-C3-O3
5	D	407	GOL	O2-C2-C3-O3
5	D	409	GOL	O2-C2-C3-O3
6	C	401	TRS	N-C-C3-O3
5	C	409	GOL	O2-C2-C3-O3
6	C	401	TRS	C2-C-C3-O3
5	A	408	GOL	O1-C1-C2-O2
5	B	406	GOL	O1-C1-C2-O2
5	D	408	GOL	O2-C2-C3-O3
6	C	401	TRS	C3-C-C1-O1
5	C	408	GOL	O1-C1-C2-O2

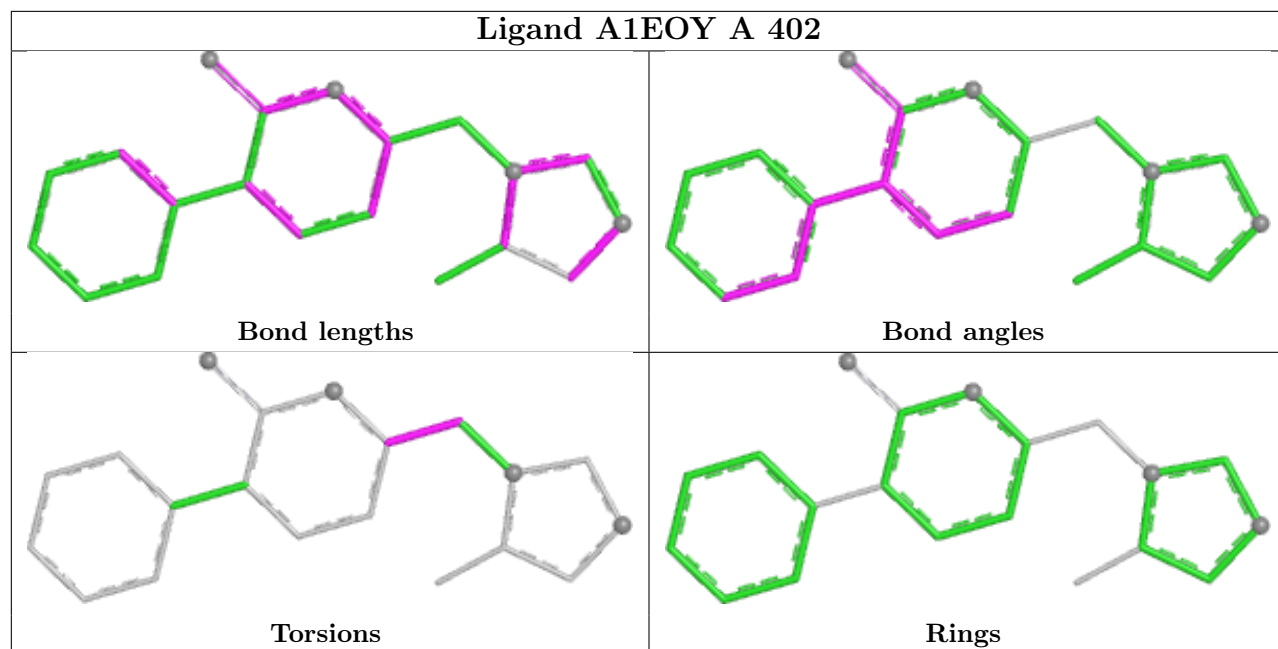
There are no ring outliers.

15 monomers are involved in 28 short contacts:

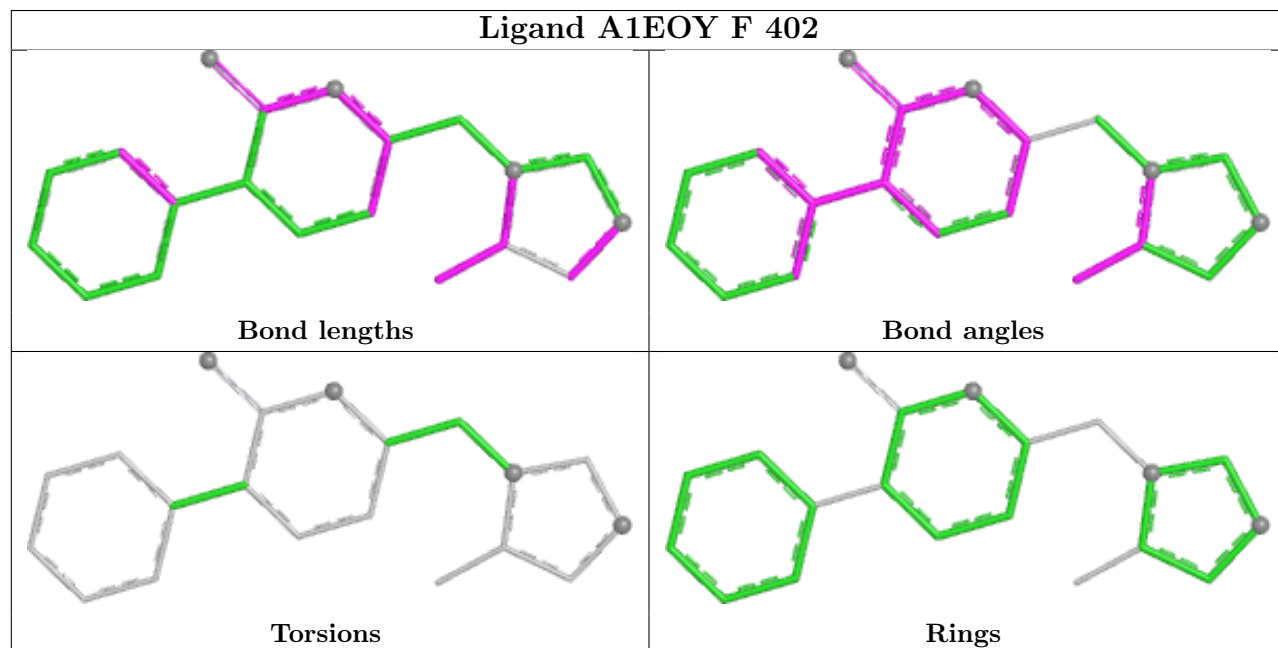
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	401	TRS	2	0
5	C	409	GOL	1	0
5	D	408	GOL	1	0
5	B	406	GOL	3	0
5	A	407	GOL	1	0
5	F	405	GOL	2	0
5	C	406	GOL	1	0
5	D	409	GOL	1	0
3	D	402	A1EOY	2	0
5	C	407	GOL	3	0
5	E	406	GOL	2	0
5	D	407	GOL	1	0
5	B	407	GOL	5	0
5	C	408	GOL	1	0
5	A	408	GOL	2	0

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

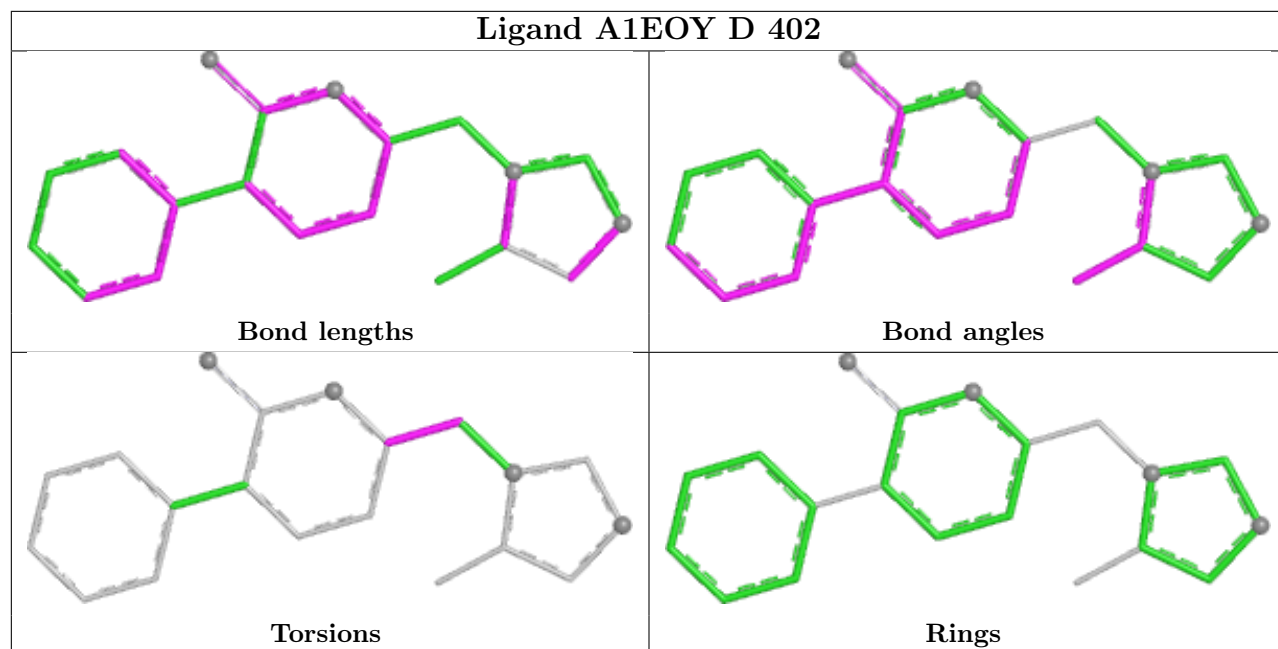
## Ligand A1EOY A 402



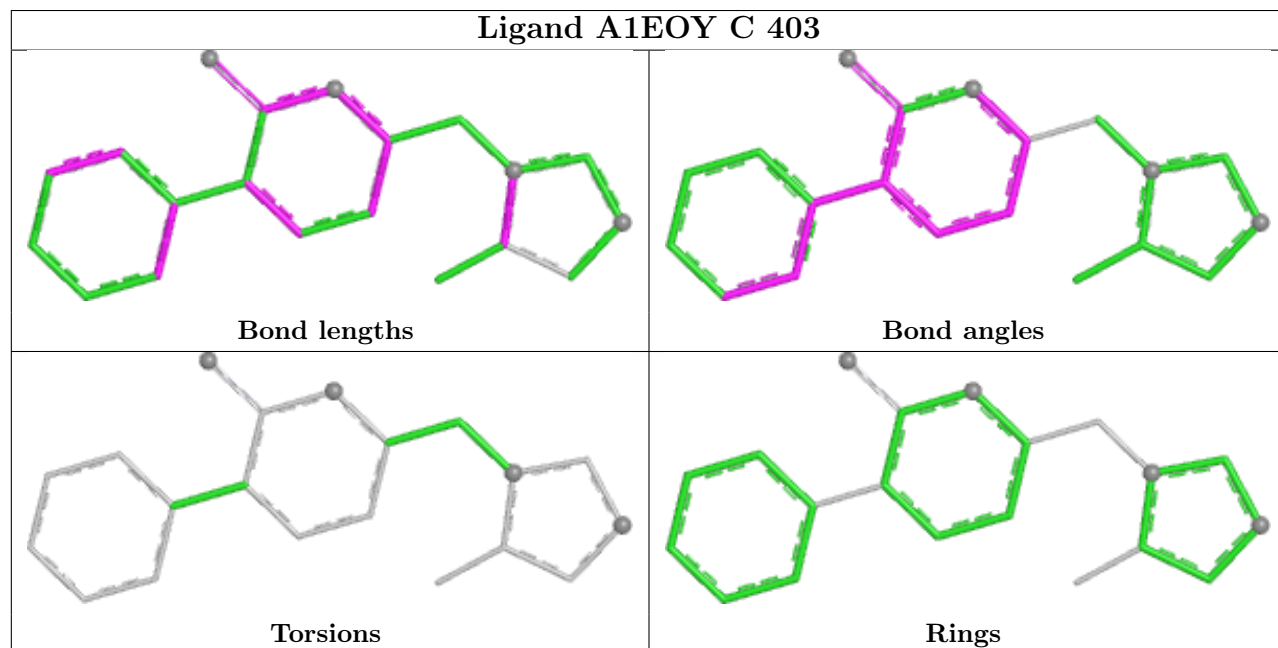
## Ligand A1EOY F 402



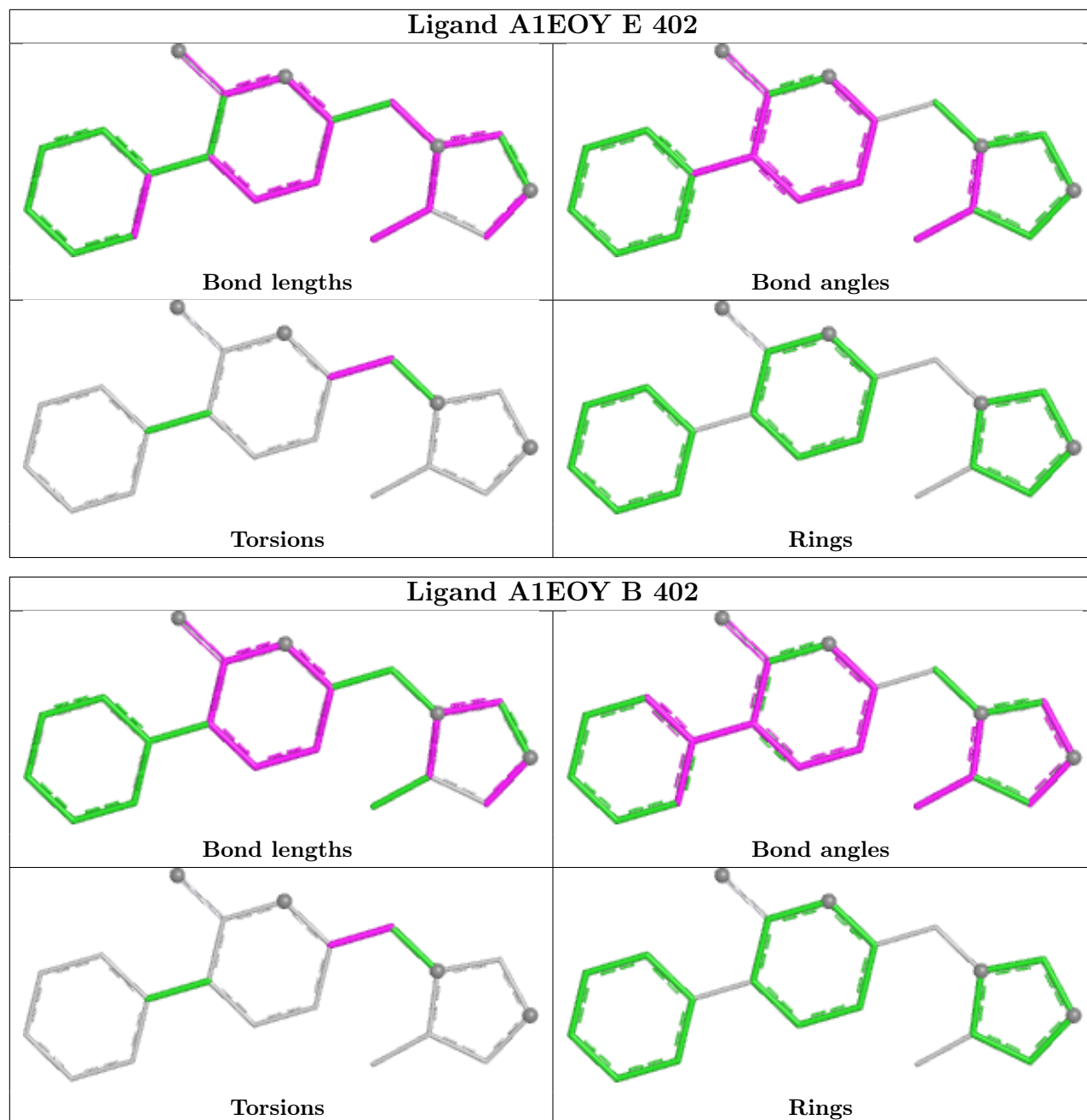
## Ligand A1EOY D 402



## Ligand A1EOY C 403







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	324/361 (89%)	-0.46	3 (0%)	81 78	25, 34, 54, 142	0
1	B	323/361 (89%)	-0.43	3 (0%)	81 78	22, 34, 53, 113	1 (0%)
1	C	323/361 (89%)	-0.45	3 (0%)	81 78	23, 35, 55, 122	0
1	D	322/361 (89%)	-0.23	3 (0%)	81 78	27, 41, 62, 129	0
1	E	324/361 (89%)	-0.43	3 (0%)	81 78	20, 35, 57, 143	1 (0%)
1	F	323/361 (89%)	-0.34	5 (1%)	72 68	28, 39, 58, 118	0
All	All	1939/2166 (89%)	-0.39	20 (1%)	79 76	20, 37, 58, 143	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ALA	7.0
1	E	33	ALA	6.0
1	D	33	ALA	4.9
1	C	33	ALA	4.8
1	B	33	ALA	4.2
1	E	34	SER	3.8
1	A	34	SER	3.7
1	E	183	THR	3.5
1	F	33	ALA	3.3
1	C	34	SER	3.2
1	A	183	THR	2.9
1	F	35	ALA	2.6
1	D	189	PRO	2.6
1	B	34	SER	2.3
1	C	182	LYS	2.2
1	F	182	LYS	2.2
1	F	189	PRO	2.2
1	B	182	LYS	2.1
1	D	34	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	34	SER	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MG	D	406	1/1	0.65	0.59	30,30,30,30	0
4	MG	B	405	1/1	0.73	0.19	71,71,71,71	0
5	GOL	E	407	6/6	0.78	0.17	55,62,71,74	0
5	GOL	C	406	6/6	0.80	0.23	58,66,69,87	0
5	GOL	B	407	6/6	0.82	0.23	48,51,57,57	0
5	GOL	A	408	6/6	0.83	0.17	52,54,66,67	0
5	GOL	F	405	6/6	0.83	0.17	58,65,73,75	0
5	GOL	C	409	6/6	0.84	0.19	52,61,73,77	0
6	TRS	C	401	8/8	0.84	0.14	47,64,74,76	0
5	GOL	C	407	6/6	0.86	0.21	60,78,80,82	0
4	MG	D	405	1/1	0.86	0.27	62,62,62,62	0
5	GOL	D	409	6/6	0.86	0.15	48,56,59,64	0
5	GOL	A	406	6/6	0.90	0.14	37,45,53,60	0
5	GOL	D	408	6/6	0.90	0.09	48,61,62,63	0
5	GOL	B	406	6/6	0.91	0.12	43,47,52,56	0
5	GOL	C	408	6/6	0.91	0.10	44,49,58,64	0
4	MG	E	404	1/1	0.92	0.10	64,64,64,64	0
5	GOL	A	407	6/6	0.92	0.09	47,58,63,64	0
4	MG	E	405	1/1	0.93	0.15	51,51,51,51	0
5	GOL	C	405	6/6	0.94	0.09	39,40,44,59	0
4	MG	F	403	1/1	0.94	0.07	18,18,18,18	0
5	GOL	E	406	6/6	0.95	0.09	39,46,52,53	0

*Continued on next page...*

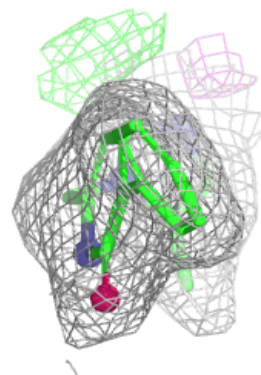
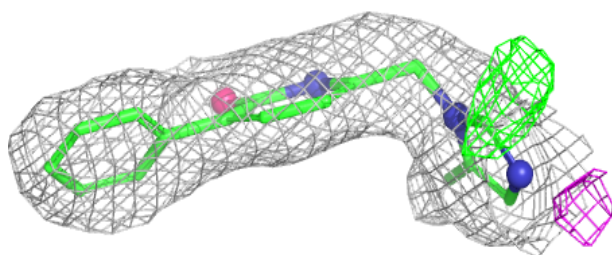
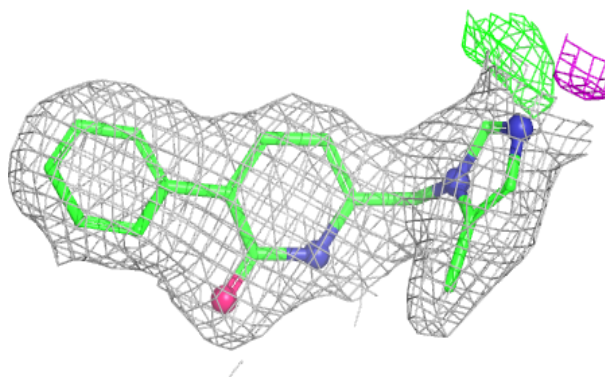
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	D	407	6/6	0.95	0.09	39,43,50,54	0
5	GOL	F	404	6/6	0.95	0.09	38,48,54,56	0
3	A1EOY	F	402	20/20	0.95	0.08	22,31,38,40	0
4	MG	A	404	1/1	0.95	0.09	52,52,52,52	0
3	A1EOY	C	403	20/20	0.96	0.07	26,29,36,41	0
3	A1EOY	E	402	20/20	0.96	0.07	25,30,41,41	0
3	A1EOY	A	402	20/20	0.96	0.07	21,30,38,41	0
3	A1EOY	B	402	20/20	0.96	0.08	27,32,38,38	0
4	MG	D	404	1/1	0.97	0.04	38,38,38,38	0
4	MG	B	404	1/1	0.97	0.11	52,52,52,52	0
4	MG	A	405	1/1	0.97	0.04	47,47,47,47	0
3	A1EOY	D	402	20/20	0.98	0.06	26,34,39,41	0
4	MG	A	403	1/1	0.98	0.03	19,19,19,19	0
4	MG	C	404	1/1	0.99	0.02	17,17,17,17	0
4	MG	D	403	1/1	0.99	0.04	14,14,14,14	0
4	MG	E	403	1/1	0.99	0.02	19,19,19,19	0
4	MG	B	403	1/1	0.99	0.03	21,21,21,21	0
2	ZN	D	401	1/1	1.00	0.06	27,27,27,27	0
2	ZN	E	401	1/1	1.00	0.03	27,27,27,27	0
2	ZN	F	401	1/1	1.00	0.04	26,26,26,26	0
2	ZN	A	401	1/1	1.00	0.03	25,25,25,25	0
2	ZN	B	401	1/1	1.00	0.03	26,26,26,26	0
2	ZN	C	402	1/1	1.00	0.03	28,28,28,28	0

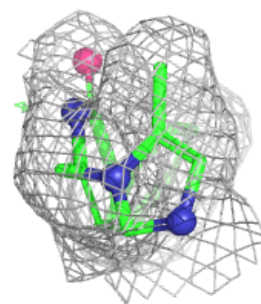
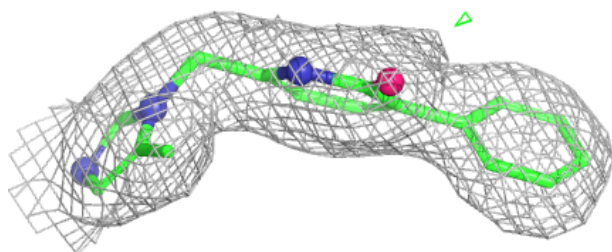
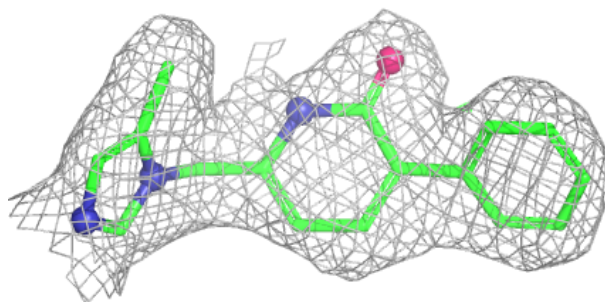
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1EOY 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)

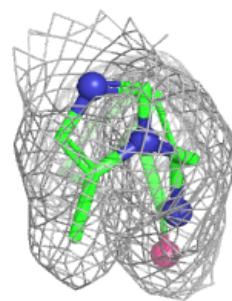
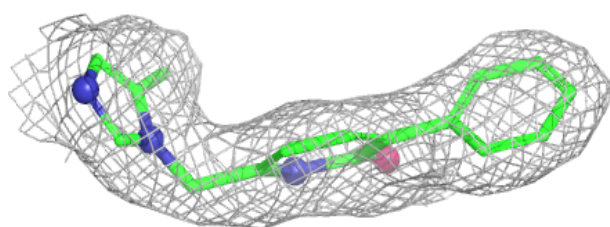
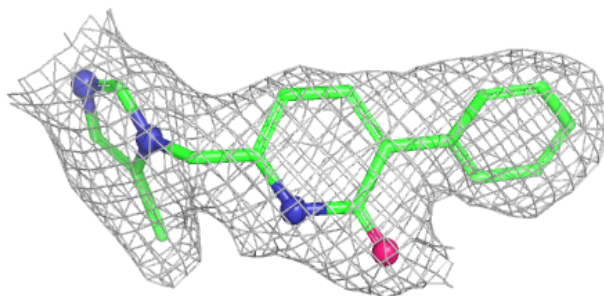
**Electron density around A1EOY C 403:**

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

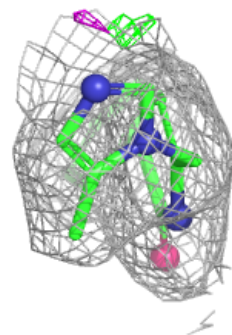
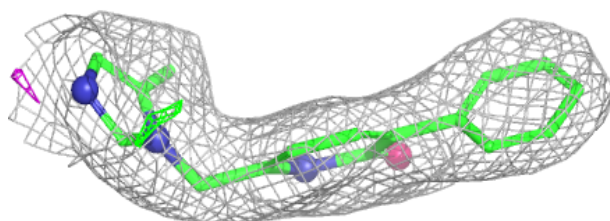
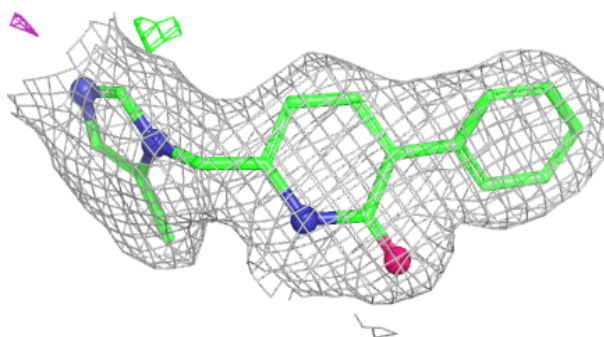


**Electron density around A1EOY E 402:**

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

**Electron density around A1EOY A 402:**

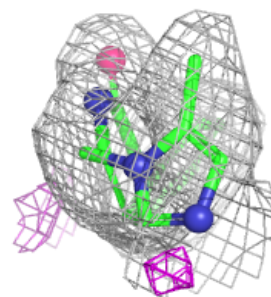
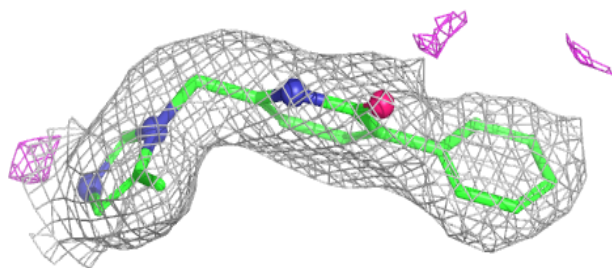
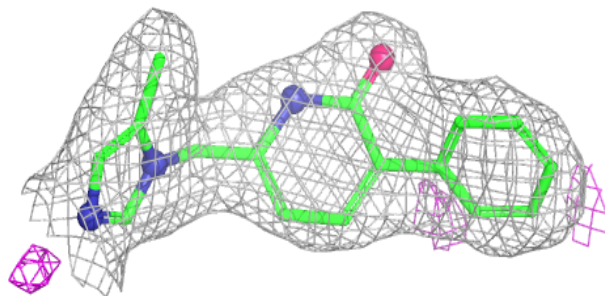
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



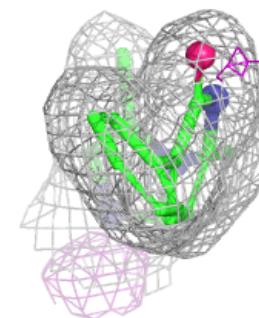
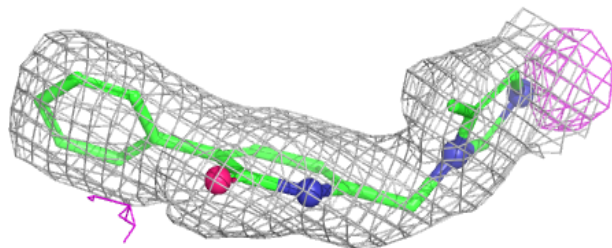
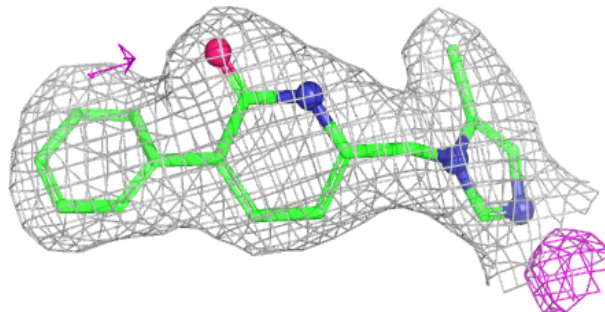


**Electron density around A1EOY B 402:**

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

**Electron density around A1EOY D 402:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.