



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 03:11 PM EDT

PDB ID : 5EOM  
Title : Structure of full-length human MAB21L1 with bound CTP  
Authors : de Oliveira Mann, C.C.; Witte, G.; Hopfner, K.-P.  
Deposited on : 2015-11-10  
Resolution : 2.55 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:

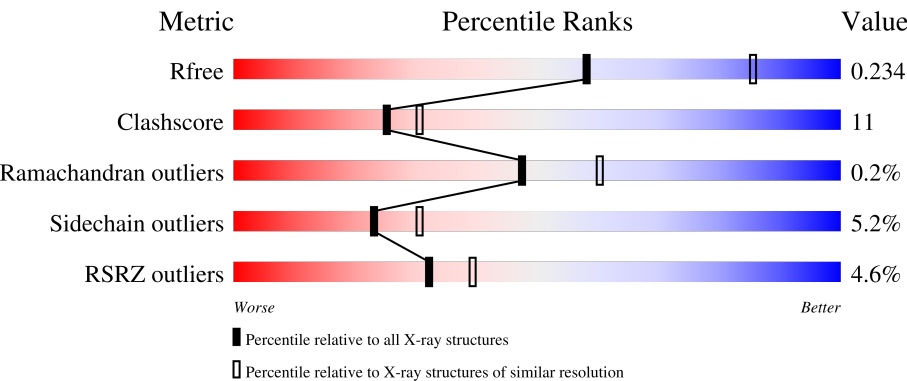
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 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 2.55 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>	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	362	<div><div></div><div>81%13% . .</div></div>
1	B	362	<div><div>3%</div><div>73%22% . .</div></div>
1	C	362	<div><div>%</div><div>79%17% . .</div></div>
1	D	362	<div><div>11%</div><div>71%22% . 6%</div></div>
1	E	362	<div><div>2%</div><div>73%20% . .</div></div>

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Mol	Chain	Length	Quality of chain
1	F	362	
1	G	362	
1	H	362	
1	I	362	
1	J	362	

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
2	CIT	C	401	-	-	X	-
2	CIT	F	401	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28115 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 Protein mab-21-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	2	0
			2821	1790	506	505	20			
1	B	349	Total	C	N	O	S	0	0	0
			2792	1771	494	507	20			
1	D	342	Total	C	N	O	S	0	0	0
			2749	1748	492	490	19			
1	E	348	Total	C	N	O	S	0	1	0
			2806	1779	503	507	17			
1	F	339	Total	C	N	O	S	0	0	0
			2721	1732	482	490	17			
1	G	352	Total	C	N	O	S	0	0	0
			2824	1790	506	508	20			
1	H	345	Total	C	N	O	S	0	0	0
			2767	1759	491	497	20			
1	I	346	Total	C	N	O	S	0	0	0
			2783	1767	499	499	18			
1	J	286	Total	C	N	O	S	0	0	0
			2304	1467	415	407	15			
1	C	353	Total	C	N	O	S	0	2	0
			2846	1804	510	511	21			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q13394
A	-1	ALA	-	expression tag	UNP Q13394
A	0	MET	-	expression tag	UNP Q13394
A	1	ASP	-	expression tag	UNP Q13394
B	-2	GLY	-	expression tag	UNP Q13394
B	-1	ALA	-	expression tag	UNP Q13394
B	0	MET	-	expression tag	UNP Q13394
B	1	ASP	-	expression tag	UNP Q13394
D	-2	GLY	-	expression tag	UNP Q13394

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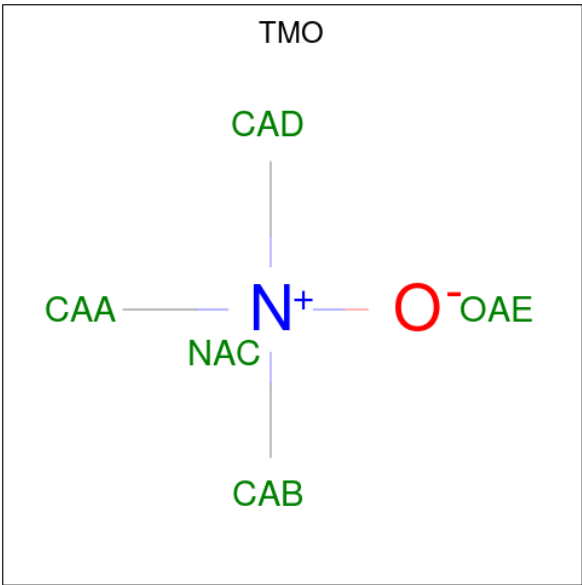
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	expression tag	UNP Q13394
D	0	MET	-	expression tag	UNP Q13394
D	1	ASP	-	expression tag	UNP Q13394
E	-2	GLY	-	expression tag	UNP Q13394
E	-1	ALA	-	expression tag	UNP Q13394
E	0	MET	-	expression tag	UNP Q13394
E	1	ASP	-	expression tag	UNP Q13394
F	-2	GLY	-	expression tag	UNP Q13394
F	-1	ALA	-	expression tag	UNP Q13394
F	0	MET	-	expression tag	UNP Q13394
F	1	ASP	-	expression tag	UNP Q13394
G	-2	GLY	-	expression tag	UNP Q13394
G	-1	ALA	-	expression tag	UNP Q13394
G	0	MET	-	expression tag	UNP Q13394
G	1	ASP	-	expression tag	UNP Q13394
H	-2	GLY	-	expression tag	UNP Q13394
H	-1	ALA	-	expression tag	UNP Q13394
H	0	MET	-	expression tag	UNP Q13394
H	1	ASP	-	expression tag	UNP Q13394
I	-2	GLY	-	expression tag	UNP Q13394
I	-1	ALA	-	expression tag	UNP Q13394
I	0	MET	-	expression tag	UNP Q13394
I	1	ASP	-	expression tag	UNP Q13394
J	-2	GLY	-	expression tag	UNP Q13394
J	-1	ALA	-	expression tag	UNP Q13394
J	0	MET	-	expression tag	UNP Q13394
J	1	ASP	-	expression tag	UNP Q13394
C	-2	GLY	-	expression tag	UNP Q13394
C	-1	ALA	-	expression tag	UNP Q13394
C	0	MET	-	expression tag	UNP Q13394
C	1	ASP	-	expression tag	UNP Q13394

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



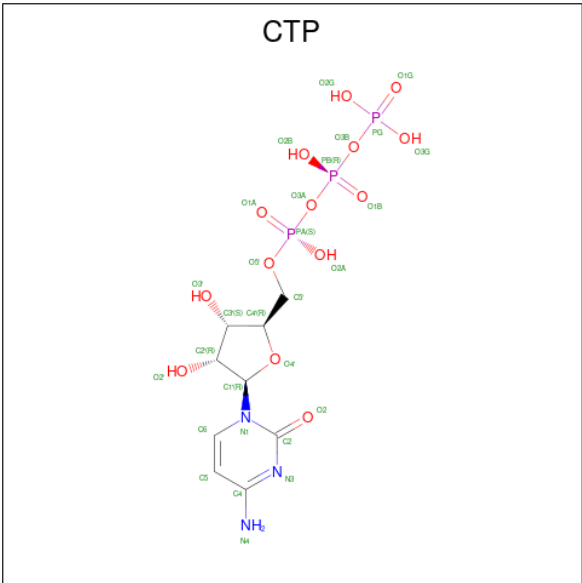
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is trimethylamine oxide (three-letter code: TMO) (formula:  $C_3H_9NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	F	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula:  $C_9H_{16}N_3O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	B	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	D	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	E	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	F	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	G	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	H	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	I	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	J	1	Total	C	N	O	P	0	0
			29	9	3	14	3		
4	C	1	Total	C	N	O	P	0	0
			29	9	3	14	3		

- Molecule 5 is water.

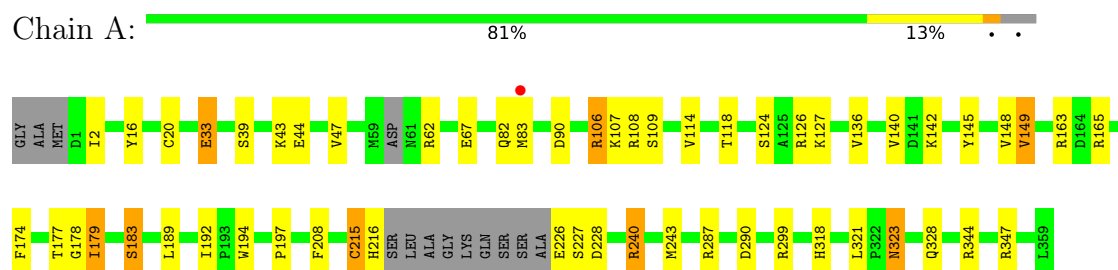
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	27	Total	O	0	0
			27	27		
5	D	21	Total	O	0	0
			21	21		
5	E	26	Total	O	0	0
			26	26		
5	F	38	Total	O	0	0
			38	38		
5	G	17	Total	O	0	0
			17	17		
5	H	18	Total	O	0	0
			18	18		
5	I	18	Total	O	0	0
			18	18		
5	J	16	Total	O	0	0
			16	16		
5	C	30	Total	O	0	0
			30	30		



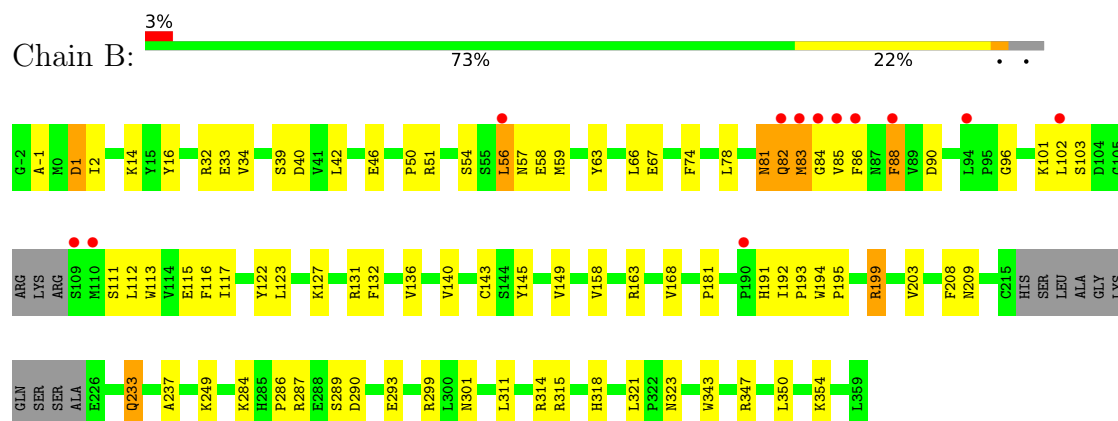
### 3 Residue-property plots [i](#)

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.

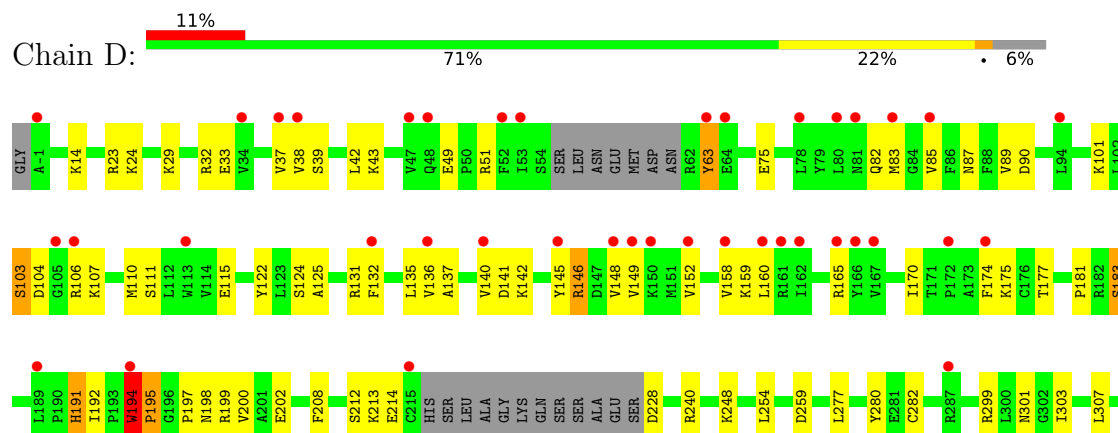
#### • Molecule 1: Protein mab-21-like 1



#### • Molecule 1: Protein mab-21-like 1

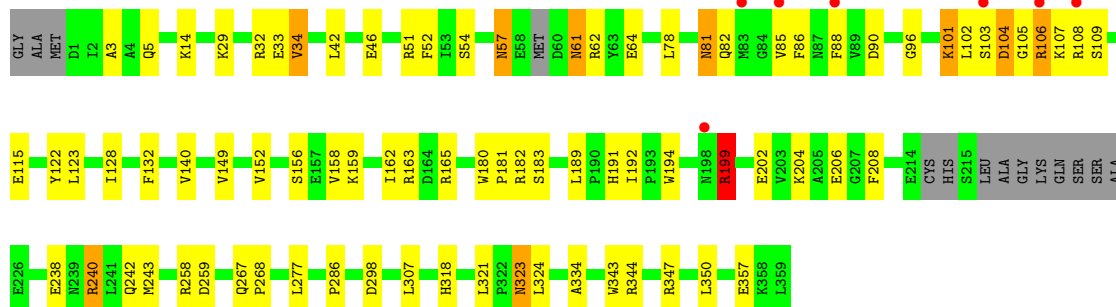
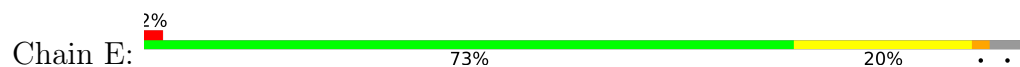


#### • Molecule 1: Protein mab-21-like 1

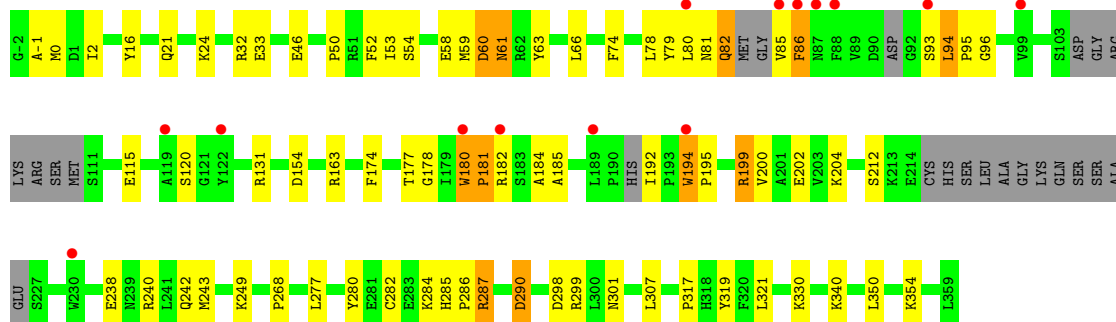




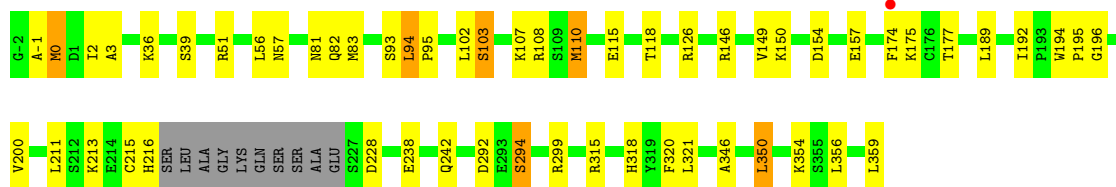
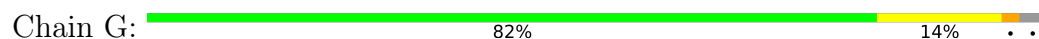
• Molecule 1: Protein mab-21-like 1



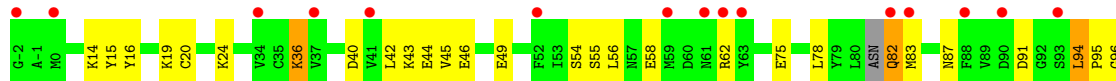
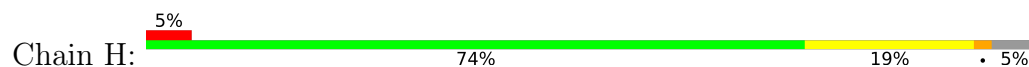
• Molecule 1: Protein mab-21-like 1

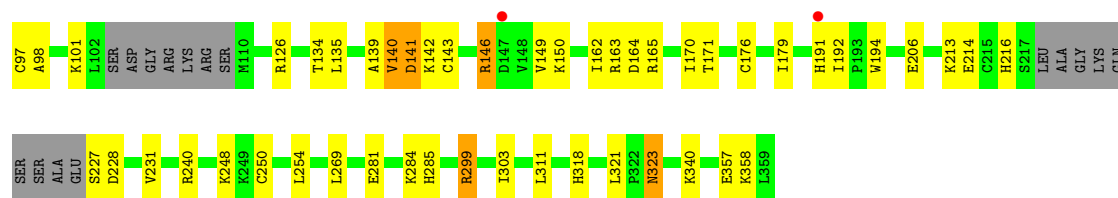


• Molecule 1: Protein mab-21-like 1

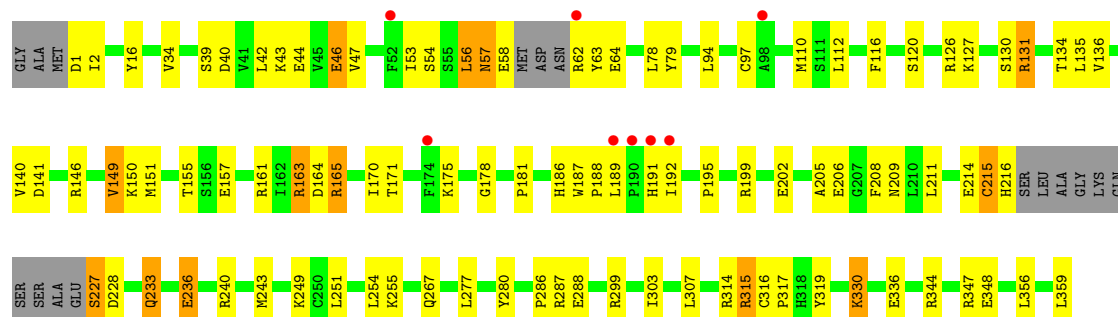


• Molecule 1: Protein mab-21-like 1

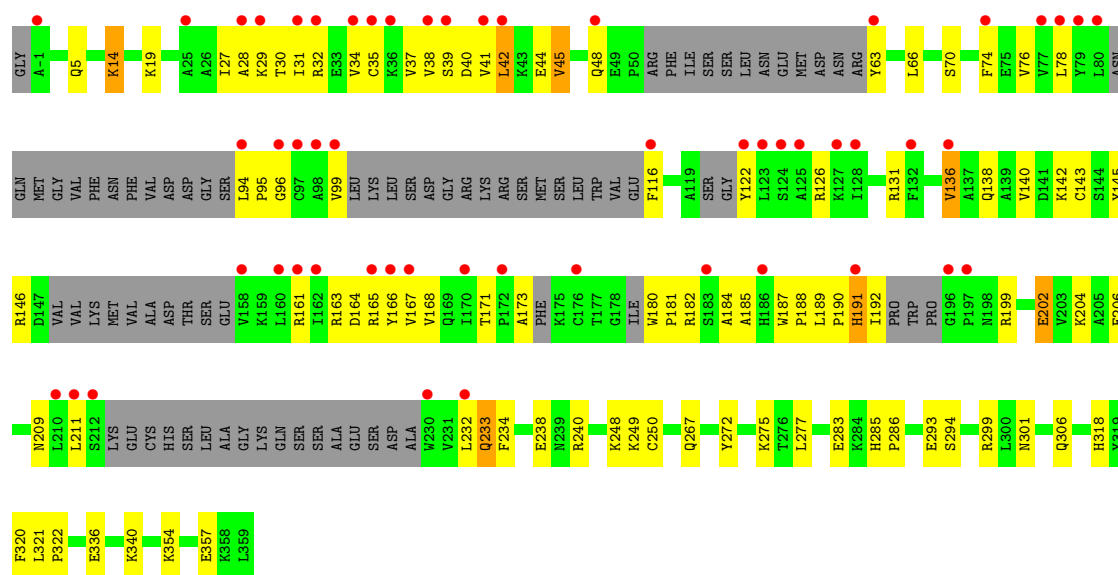




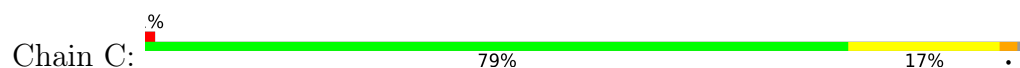
• Molecule 1: Protein mab-21-like 1

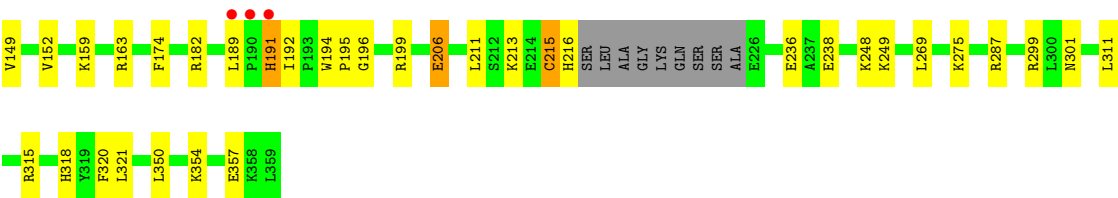


• Molecule 1: Protein mab-21-like 1



• Molecule 1: Protein mab-21-like 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.00Å 177.76Å 134.94Å 90.00° 97.58° 90.00°	Depositor
Resolution (Å)	49.98 – 2.55 49.98 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.98-2.55) 99.8 (49.98-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.199 , 0.227 0.205 , 0.234	Depositor DCC
$R_{free}$ test set	1670 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.2	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.4	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	28115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.80% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TMO, CTP, CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/2886	0.48	0/3897
1	B	0.25	0/2850	0.45	0/3852
1	C	0.25	0/2912	0.45	0/3933
1	D	0.28	0/2807	0.51	1/3792 (0.0%)
1	E	0.26	0/2867	0.47	1/3873 (0.0%)
1	F	0.32	1/2775 (0.0%)	0.50	0/3748
1	G	0.25	0/2884	0.44	0/3897
1	H	0.26	0/2825	0.46	0/3817
1	I	0.38	2/2842 (0.1%)	0.54	4/3840 (0.1%)
1	J	0.27	0/2345	0.46	1/3159 (0.0%)
All	All	0.28	3/27993 (0.0%)	0.48	7/37808 (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	E	0	2
1	J	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	319	TYR	CD2-CE2	-9.56	1.25	1.39
1	F	319	TYR	CD2-CE2	-6.11	1.30	1.39
1	I	46	GLU	CB-CG	-5.61	1.41	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	42	LEU	CA-CB-CG	6.65	130.59	115.30
1	D	194	TRP	CA-CB-CG	6.46	125.97	113.70
1	I	215	CYS	CB-CA-C	-5.80	98.79	110.40
1	I	319	TYR	OH-CZ-CE2	-5.66	104.82	120.10
1	E	199	ARG	CG-CD-NE	-5.23	100.81	111.80
1	I	319	TYR	CD1-CE1-CZ	-5.11	115.20	119.80
1	I	319	TYR	CE1-CZ-OH	5.06	133.76	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	61	ASN	Peptide
1	J	136	VAL	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	2821	0	2860	47	0
1	B	2792	0	2813	68	1
1	C	2846	0	2882	38	0
1	D	2749	0	2791	71	0
1	E	2806	0	2839	58	0
1	F	2721	0	2755	65	1
1	G	2824	0	2854	43	0
1	H	2767	0	2795	64	0
1	I	2783	0	2817	77	0
1	J	2304	0	2347	85	0
2	A	13	0	5	1	0
2	B	13	0	5	2	0
2	C	13	0	5	7	0
2	D	13	0	5	2	0
2	E	13	0	5	0	0
2	F	13	0	5	1	0
2	G	13	0	5	2	0
2	H	26	0	10	1	0
2	I	13	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	9	1	0
3	C	10	0	18	0	0
3	F	5	0	9	0	0
4	A	29	0	12	1	0
4	B	29	0	12	0	0
4	C	29	0	12	0	0
4	D	29	0	12	1	0
4	E	29	0	12	2	0
4	F	29	0	12	1	0
4	G	29	0	12	0	0
4	H	29	0	12	3	0
4	I	29	0	12	2	0
4	J	29	0	12	0	0
5	A	51	0	0	0	0
5	B	27	0	0	0	0
5	C	30	0	0	0	0
5	D	21	0	0	0	0
5	E	26	0	0	1	0
5	F	38	0	0	1	0
5	G	17	0	0	0	0
5	H	18	0	0	4	0
5	I	18	0	0	2	0
5	J	16	0	0	3	0
All	All	28115	0	27959	599	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 11.

All (599) 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:J:187:TRP:CE3	1:J:204:LYS:HE3	1.70	1.26
1:E:103:SER:O	1:E:106:ARG:HB2	1.34	1.23
1:J:187:TRP:CZ3	1:J:204:LYS:HE3	1.74	1.21
1:J:187:TRP:CE3	1:J:204:LYS:CE	2.34	1.09
1:E:104:ASP:OD1	1:E:105:GLY:N	1.93	1.02
1:J:187:TRP:HZ3	1:J:204:LYS:HG3	1.27	0.99
1:D:198:ASN:HD21	1:J:204:LYS:HD2	1.29	0.98
1:F:177:THR:O	1:I:205:ALA:HB1	1.64	0.97
4:E:402:CTP:O2A	5:E:501:HOH:O	1.80	0.97
1:F:60:ASP:O	1:F:61:ASN:HB2	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:314:ARG:NH1	1:I:336:GLU:OE2	1.99	0.95
1:J:180:TRP:CD1	1:J:185:ALA:HA	2.02	0.95
1:J:187:TRP:O	1:J:204:LYS:NZ	2.00	0.95
1:F:32:ARG:NH1	1:F:58:GLU:OE1	2.01	0.93
1:F:340:LYS:NZ	5:F:501:HOH:O	2.01	0.93
1:J:187:TRP:HE3	1:J:204:LYS:CE	1.80	0.92
1:H:248:LYS:NZ	4:H:403:CTP:O3G	2.04	0.91
1:E:103:SER:O	1:E:106:ARG:CB	2.20	0.89
1:J:31:ILE:HG23	1:J:32:ARG:HG2	1.55	0.87
1:I:206:GLU:OE1	1:I:240:ARG:NH2	2.08	0.86
1:J:187:TRP:HE3	1:J:204:LYS:HE2	1.39	0.85
1:D:197:PRO:HG2	1:D:199:ARG:HE	1.41	0.85
1:J:187:TRP:CZ3	1:J:204:LYS:CE	2.54	0.85
1:I:202:GLU:HB3	1:I:240:ARG:HD2	1.59	0.85
1:I:57:ASN:O	1:I:62:ARG:O	1.96	0.84
1:A:344:ARG:NH1	2:C:401:CIT:O3	2.10	0.83
1:E:61:ASN:O	1:E:62[A]:ARG:HG3	1.79	0.82
1:I:155:THR:OG1	1:I:157:GLU:OE1	1.98	0.80
1:J:187:TRP:HZ3	1:J:204:LYS:CG	1.94	0.79
1:J:187:TRP:CZ3	1:J:204:LYS:HG3	2.16	0.78
1:D:280:TYR:OH	1:D:317:PRO:O	2.00	0.78
1:J:180:TRP:HE1	1:J:184:ALA:C	1.87	0.78
1:D:194:TRP:HZ2	1:D:282:CYS:HB3	1.49	0.78
1:E:33:GLU:HG2	1:E:163:ARG:HH12	1.46	0.77
1:F:180:TRP:CE3	1:F:180:TRP:HA	2.19	0.77
1:I:215:CYS:O	1:I:216:HIS:CG	2.38	0.76
1:H:44:GLU:OE2	1:H:142:LYS:HG3	1.84	0.76
1:E:194:TRP:HB2	1:E:286:PRO:HB3	1.66	0.76
1:I:151:MET:SD	5:I:504:HOH:O	2.44	0.75
1:I:287:ARG:NH1	5:I:501:HOH:O	2.19	0.75
1:F:180:TRP:HA	1:F:180:TRP:HE3	1.52	0.75
1:F:52:PHE:HA	1:F:80:LEU:HD13	1.68	0.74
1:C:108:ARG:NH2	1:C:118:THR:O	2.21	0.73
1:A:344:ARG:HH11	2:C:401:CIT:C5	2.00	0.73
1:A:163:ARG:HH11	1:A:165:ARG:NH2	1.87	0.73
1:F:194:TRP:HB2	1:F:286:PRO:HB3	1.72	0.72
1:F:280:TYR:OH	1:F:317:PRO:O	2.07	0.72
1:C:14:LYS:NZ	1:C:357:GLU:OE1	2.23	0.72
1:J:180:TRP:NE1	1:J:185:ALA:HA	2.04	0.71
1:A:192:ILE:HG22	1:A:194:TRP:H	1.56	0.71
1:I:175:LYS:HG3	1:I:209:ASN:HD21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:LYS:HG3	1:I:209:ASN:ND2	2.06	0.70
1:J:180:TRP:CD1	1:J:185:ALA:CA	2.74	0.70
1:C:192:ILE:HG22	1:C:194:TRP:H	1.56	0.70
1:I:215:CYS:O	1:I:216:HIS:CD2	2.46	0.69
1:D:85:VAL:HB	1:D:107:LYS:HD3	1.74	0.69
1:F:199:ARG:HA	1:F:202:GLU:HB2	1.73	0.69
1:J:192:ILE:HG23	1:J:286:PRO:HG3	1.73	0.69
1:F:184:ALA:HB2	1:F:321:LEU:HD23	1.75	0.69
1:F:96:GLY:HA2	1:F:321:LEU:HD13	1.74	0.68
1:A:62[B]:ARG:HH21	1:A:62[B]:ARG:HG2	1.58	0.68
1:D:14:LYS:NZ	1:D:357:GLU:OE2	2.27	0.67
1:G:192:ILE:HG22	1:G:194:TRP:H	1.60	0.67
1:E:96:GLY:HA3	1:E:324:LEU:HD21	1.77	0.67
1:E:323:ASN:OD1	1:E:323:ASN:N	2.17	0.67
1:F:180:TRP:HB2	1:F:185:ALA:HA	1.76	0.66
1:I:63:TYR:H	4:I:402:CTP:HN41	1.44	0.66
1:I:280:TYR:OH	1:I:317:PRO:O	2.13	0.66
1:E:61:ASN:O	1:E:62[B]:ARG:HG3	1.95	0.66
1:D:198:ASN:ND2	1:J:204:LYS:HD2	2.06	0.66
1:I:206:GLU:HB2	1:I:240:ARG:HH21	1.61	0.66
1:B:112:LEU:HD12	1:G:83:MET:HB3	1.76	0.66
1:A:33:GLU:OE2	1:A:163:ARG:NH2	2.29	0.65
1:E:104:ASP:CG	1:E:105:GLY:H	1.97	0.65
1:G:215:CYS:SG	1:G:216:HIS:N	2.62	0.65
1:I:215:CYS:SG	1:I:216:HIS:N	2.66	0.65
1:I:277:LEU:HD11	1:I:307:LEU:HD13	1.78	0.65
1:F:54:SER:HA	1:F:78:LEU:HD11	1.78	0.65
1:I:344:ARG:NH2	1:I:348:GLU:OE1	2.30	0.65
1:H:299:ARG:HH11	1:H:299:ARG:HA	1.62	0.65
1:C:191:HIS:CD2	1:C:191:HIS:H	2.12	0.65
1:D:49:GLU:OE2	1:D:51:ARG:NH1	2.30	0.65
1:G:3:ALA:HB1	1:I:347:ARG:HH12	1.62	0.65
1:E:14:LYS:NZ	1:E:357:GLU:OE2	2.29	0.64
1:A:106:ARG:O	1:A:107:LYS:HG3	1.97	0.64
1:H:44:GLU:OE2	1:H:143:CYS:HA	1.97	0.64
1:H:192:ILE:HG22	1:H:194:TRP:H	1.62	0.64
1:F:32:ARG:NH1	1:F:63:TYR:OH	2.31	0.64
1:F:180:TRP:CB	1:F:185:ALA:HA	2.27	0.64
1:J:32:ARG:HD3	1:J:35:CYS:SG	2.37	0.64
1:F:81:ASN:OD1	1:F:82:GLN:N	2.31	0.63
1:D:37:VAL:HG22	1:D:145:TYR:HD2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:PHE:CE2	1:E:123:LEU:HD22	2.33	0.63
1:A:323:ASN:OD1	1:A:323:ASN:N	2.30	0.63
1:D:194:TRP:CZ2	1:D:282:CYS:HB3	2.32	0.63
2:I:401:CIT:O7	2:I:401:CIT:O4	2.17	0.63
1:B:192:ILE:HG22	1:B:194:TRP:H	1.62	0.63
1:J:238:GLU:HG3	1:J:275:LYS:NZ	2.13	0.63
1:C:49:GLU:HG3	1:C:135:LEU:HD11	1.80	0.63
1:I:136:VAL:O	1:I:140:VAL:HG13	1.99	0.63
1:E:51:ARG:NH2	1:E:115:GLU:OE1	2.25	0.62
1:F:301:ASN:ND2	1:F:350:LEU:HD21	2.13	0.62
1:J:5:GLN:NE2	5:J:502:HOH:O	2.31	0.62
1:J:48:GLN:HG2	1:J:138:GLN:HE22	1.64	0.62
1:D:37:VAL:HG22	1:D:145:TYR:CD2	2.34	0.62
1:J:143:CYS:O	1:J:146:ARG:NH2	2.30	0.62
1:A:2:ILE:HG12	1:D:301:ASN:HD21	1.64	0.62
1:G:195:PRO:HG2	1:G:200:VAL:HG22	1.82	0.62
1:B:301:ASN:HD21	1:B:350:LEU:HD22	1.63	0.62
1:J:187:TRP:CE3	1:J:204:LYS:HE2	2.18	0.62
1:A:108:ARG:NH1	1:A:108:ARG:HB2	2.14	0.62
1:I:199:ARG:NH2	1:I:288:GLU:OE2	2.33	0.62
1:F:81:ASN:HD21	1:F:85:VAL:HG13	1.64	0.61
1:C:354:LYS:HZ2	2:C:401:CIT:H42	1.65	0.61
1:A:126:ARG:HH22	1:A:226:GLU:HG3	1.65	0.61
1:E:206:GLU:OE2	1:E:240:ARG:HD2	2.00	0.61
1:J:63:TYR:N	5:J:503:HOH:O	2.34	0.61
1:G:107:LYS:NZ	1:G:110:MET:SD	2.60	0.61
2:G:401:CIT:O3	2:G:401:CIT:O7	2.18	0.60
1:C:82:GLN:HG2	1:C:84:GLY:H	1.64	0.60
1:D:104:ASP:OD2	1:D:107:LYS:HE3	2.01	0.60
1:H:149:VAL:HG23	1:H:162:ILE:HG12	1.84	0.60
1:G:-1:ALA:HB2	1:I:1:ASP:OD2	2.02	0.60
1:B:33:GLU:OE2	1:B:163:ARG:HD2	2.01	0.60
1:E:96:GLY:HA2	1:E:321:LEU:HD13	1.83	0.60
1:I:146:ARG:HH22	1:I:150:LYS:HA	1.67	0.59
1:A:126:ARG:NH1	1:A:227:SER:O	2.35	0.59
1:E:46:GLU:HG2	1:E:52:PHE:O	2.01	0.59
1:J:181:PRO:HG2	1:J:232:LEU:HD13	1.84	0.59
1:C:354:LYS:NZ	2:C:401:CIT:H42	2.17	0.59
1:B:2:ILE:HG23	1:C:350:LEU:HD21	1.84	0.59
1:F:86:PHE:CZ	1:F:178:GLY:HA2	2.37	0.59
1:I:140:VAL:O	1:I:146:ARG:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:LEU:HD12	1:J:95:PRO:HD2	1.84	0.59
1:F:115:GLU:OE2	1:F:131:ARG:NH2	2.33	0.59
1:I:53:ILE:O	1:I:78:LEU:HD11	2.03	0.59
1:G:0:MET:HG2	1:G:3:ALA:HB3	1.85	0.59
1:D:146:ARG:NH1	1:D:149:VAL:O	2.36	0.59
1:C:189:LEU:HB3	1:C:191:HIS:HD2	1.68	0.59
1:H:82:GLN:N	1:H:82:GLN:OE1	2.36	0.58
1:A:90:ASP:OD2	1:A:183:SER:OG	2.16	0.58
1:H:54:SER:HA	1:H:78:LEU:HD11	1.85	0.58
1:A:44:GLU:OE1	1:A:142:LYS:NZ	2.27	0.58
1:E:101:LYS:HG3	1:E:122:TYR:CE1	2.39	0.58
1:F:240:ARG:NH1	1:F:243:MET:SD	2.77	0.58
1:A:215:CYS:SG	1:A:216:HIS:N	2.78	0.57
1:J:14:LYS:NZ	1:J:357:GLU:OE1	2.37	0.57
1:B:343:TRP:CE2	1:B:347:ARG:HD2	2.39	0.57
1:B:39:SER:HA	1:B:56:LEU:HD22	1.85	0.57
1:B:96:GLY:HA2	1:B:321:LEU:HD13	1.86	0.57
1:D:85:VAL:HG21	1:D:111:SER:HB2	1.87	0.57
1:D:248:LYS:NZ	1:D:248:LYS:HB3	2.20	0.57
1:A:124:SER:OG	1:A:228:ASP:OD2	2.13	0.57
1:J:32:ARG:HG3	1:J:63:TYR:CZ	2.40	0.57
1:C:215:CYS:O	1:C:216:HIS:ND1	2.37	0.57
1:G:51:ARG:NH2	1:G:115:GLU:OE2	2.28	0.57
1:C:145:TYR:O	1:C:149:VAL:HG23	2.05	0.57
1:J:299:ARG:HH11	1:J:299:ARG:HA	1.70	0.57
1:B:84:GLY:HA2	1:G:177:THR:H	1.70	0.56
1:J:32:ARG:HG3	1:J:63:TYR:CE1	2.40	0.56
1:E:54:SER:HA	1:E:78:LEU:HD11	1.87	0.56
1:H:323:ASN:OD1	1:H:323:ASN:N	2.35	0.56
1:F:194:TRP:CD1	1:F:195:PRO:HA	2.40	0.56
1:I:150:LYS:HG3	1:I:161:ARG:HB3	1.87	0.56
1:J:35:CYS:HA	1:J:38:VAL:HG23	1.85	0.56
1:J:209:ASN:HB2	1:J:233:GLN:HG2	1.87	0.56
1:D:131:ARG:O	1:D:135:LEU:HD13	2.05	0.56
1:E:81:ASN:ND2	1:C:87:ASN:OD1	2.30	0.56
1:H:141:ASP:HA	1:H:146:ARG:CZ	2.36	0.56
1:B:203:VAL:HG13	1:B:237:ALA:HB1	1.85	0.56
1:E:189:LEU:HB3	1:E:191:HIS:HD2	1.69	0.56
1:H:269:LEU:HD21	1:H:311:LEU:HD21	1.87	0.56
1:I:209:ASN:HB2	1:I:233:GLN:HG2	1.86	0.56
1:I:146:ARG:NH2	1:I:149:VAL:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:LYS:NZ	1:H:54:SER:HB3	2.20	0.55
1:B:57:ASN:HB3	1:B:59:MET:HE2	1.87	0.55
1:E:33:GLU:HG2	1:E:163:ARG:NH1	2.19	0.55
1:F:52:PHE:HA	1:F:80:LEU:CD1	2.35	0.55
1:H:163:ARG:O	1:H:163:ARG:HG3	2.05	0.55
1:H:206:GLU:OE2	1:H:240:ARG:NH2	2.40	0.55
1:J:28:ALA:O	1:J:31:ILE:HG22	2.06	0.55
1:J:165:ARG:NH1	5:J:505:HOH:O	2.39	0.55
1:J:189:LEU:HB2	1:J:191:HIS:CE1	2.42	0.55
1:D:90:ASP:OD2	1:D:183:SER:OG	2.20	0.55
1:A:108:ARG:HB2	1:A:108:ARG:HH11	1.71	0.55
1:D:145:TYR:HB3	1:D:148:VAL:HG22	1.88	0.55
1:G:3:ALA:HB1	1:I:347:ARG:NH1	2.21	0.55
1:I:141:ASP:OD1	1:I:146:ARG:NE	2.40	0.55
1:C:206:GLU:HG2	1:C:236:GLU:HB3	1.88	0.55
1:B:299:ARG:HA	1:B:299:ARG:HH11	1.72	0.55
1:F:33:GLU:OE2	1:F:163:ARG:HD2	2.06	0.55
1:F:94:LEU:HG	1:F:95:PRO:HD2	1.88	0.55
1:J:74:PHE:HB2	1:J:168:VAL:HG22	1.87	0.55
1:H:163:ARG:HE	1:H:165:ARG:HH12	1.53	0.54
1:A:126:ARG:NH2	1:A:226:GLU:HG3	2.22	0.54
1:H:91:ASP:O	1:H:94:LEU:HD11	2.07	0.54
1:B:354:LYS:NZ	2:B:401:CIT:H41	2.21	0.54
1:B:249:LYS:NZ	1:B:293:GLU:OE2	2.35	0.54
1:D:63:TYR:N	1:D:63:TYR:CD2	2.74	0.54
1:B:51:ARG:NH2	1:B:115:GLU:OE2	2.40	0.54
1:D:132:PHE:CD2	1:D:158:VAL:HG21	2.43	0.54
1:I:189:LEU:H	1:I:192:ILE:HD12	1.73	0.54
2:D:401:CIT:O3	2:D:401:CIT:O7	2.18	0.54
1:J:187:TRP:CZ3	1:J:204:LYS:CG	2.83	0.54
1:E:42:LEU:O	1:E:46:GLU:HG3	2.08	0.53
1:J:181:PRO:HG2	1:J:232:LEU:CD1	2.37	0.53
1:D:49:GLU:CD	1:D:51:ARG:HE	2.12	0.53
1:D:192:ILE:HG22	1:D:194:TRP:HA	1.89	0.53
1:B:66:LEU:HD11	1:B:74:PHE:HB3	1.89	0.53
1:I:146:ARG:HD2	1:I:146:ARG:O	2.08	0.53
1:J:116:PHE:HZ	1:J:131:ARG:HD2	1.73	0.53
1:B:102:LEU:HG	1:B:103:SER:O	2.09	0.53
1:B:86:PHE:CE1	1:B:123:LEU:HB2	2.43	0.53
1:D:75:GLU:OE1	1:D:213:LYS:NZ	2.42	0.53
1:G:211:LEU:HD23	1:G:213:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:41:VAL:HA	1:J:143:CYS:SG	2.49	0.53
1:F:340:LYS:NZ	1:F:340:LYS:HB2	2.24	0.53
1:I:46:GLU:OE2	1:I:54:SER:N	2.42	0.53
1:I:79:TYR:CE1	1:I:175:LYS:HE2	2.44	0.53
1:B:111:SER:OG	1:B:112:LEU:N	2.41	0.52
1:J:32:ARG:NH1	1:J:66:LEU:HD13	2.24	0.52
1:B:42:LEU:O	1:B:46:GLU:HG3	2.08	0.52
1:F:180:TRP:CD1	1:F:204:LYS:HE2	2.43	0.52
1:H:42:LEU:HD11	1:H:170:ILE:HD13	1.92	0.52
1:I:42:LEU:HD11	1:I:170:ILE:HD13	1.92	0.52
2:C:401:CIT:H42	2:C:401:CIT:O1	2.08	0.52
1:D:152:VAL:HB	1:D:159:LYS:HB2	1.91	0.52
1:F:79:TYR:O	1:F:80:LEU:HG	2.08	0.52
1:H:75:GLU:HG3	5:H:506:HOH:O	2.10	0.52
1:H:140:VAL:HG13	1:H:146:ARG:HH21	1.74	0.52
1:F:287:ARG:H	1:F:287:ARG:HD2	1.75	0.52
1:G:-1:ALA:O	1:G:2:ILE:HG22	2.10	0.52
1:H:62:ARG:NH2	4:H:403:CTP:O1G	2.42	0.52
1:J:32:ARG:CZ	1:J:66:LEU:HD13	2.39	0.52
1:G:102:LEU:HD21	1:G:108:ARG:HB2	1.92	0.52
1:H:24:LYS:HE2	4:H:403:CTP:O1B	2.10	0.52
1:H:284:LYS:HB3	1:H:285:HIS:HD2	1.74	0.52
1:E:82:GLN:HE21	1:E:85:VAL:H	1.56	0.52
1:D:101:LYS:HE2	1:D:122:TYR:CE1	2.45	0.51
1:E:90:ASP:OD2	1:E:183:SER:N	2.38	0.51
1:C:301:ASN:HD21	1:C:350:LEU:HD13	1.75	0.51
1:D:198:ASN:OD1	1:J:204:LYS:HD3	2.10	0.51
1:D:131:ARG:NH1	1:D:135:LEU:HD11	2.25	0.51
1:B:-1:ALA:HA	1:B:2:ILE:HG22	1.92	0.51
1:D:195:PRO:CG	1:D:199:ARG:HB2	2.41	0.51
1:F:284:LYS:HG2	1:F:285:HIS:CD2	2.45	0.51
1:H:94:LEU:HD22	1:H:98:ALA:HA	1.91	0.51
1:J:44:GLU:OE1	1:J:142:LYS:NZ	2.34	0.51
1:B:181:PRO:HD3	1:B:208:PHE:CD1	2.45	0.51
1:E:192:ILE:HG22	1:E:194:TRP:H	1.76	0.51
1:C:196:GLY:O	1:C:199:ARG:N	2.39	0.51
1:C:82:GLN:HB2	1:C:174:PHE:CE1	2.46	0.51
1:F:194:TRP:HB2	1:F:286:PRO:CB	2.38	0.50
1:B:1:ASP:HB3	1:F:-1:ALA:HB2	1.91	0.50
1:D:38:VAL:HG22	1:D:160:LEU:HD12	1.92	0.50
1:D:136:VAL:HG21	1:D:158:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLY:HA3	1:G:175:LYS:O	2.11	0.50
1:B:86:PHE:CZ	1:B:123:LEU:HB2	2.45	0.50
1:I:39:SER:O	1:I:43:LYS:HG2	2.12	0.50
1:F:268:PRO:HA	1:F:330:LYS:HD2	1.92	0.50
1:I:356:LEU:HD23	1:I:359:LEU:HD12	1.94	0.50
1:D:191:HIS:HB2	1:D:192:ILE:HD12	1.93	0.50
1:H:149:VAL:O	1:H:150:LYS:NZ	2.38	0.50
1:A:189:LEU:HD12	1:A:192:ILE:HD12	1.94	0.50
1:G:82:GLN:HB3	1:G:174:PHE:CE1	2.47	0.50
1:H:44:GLU:HB2	1:H:139:ALA:HB1	1.94	0.50
1:J:171:THR:HG21	1:J:211:LEU:HB3	1.93	0.50
1:D:277:LEU:HD23	1:D:280:TYR:CD2	2.47	0.50
1:E:152:VAL:HB	1:E:159:LYS:HB2	1.93	0.50
1:F:180:TRP:O	1:F:185:ALA:HB2	2.11	0.50
1:F:301:ASN:HD21	1:F:350:LEU:HD21	1.76	0.50
1:G:94:LEU:HD22	1:G:95:PRO:HD2	1.93	0.50
1:G:238:GLU:O	1:G:242:GLN:HG3	2.12	0.50
1:J:320:PHE:O	1:J:322:PRO:HD3	2.12	0.50
1:H:284:LYS:HB3	1:H:285:HIS:CD2	2.47	0.50
1:B:50:PRO:HB2	1:G:107:LYS:HZ3	1.77	0.49
1:B:86:PHE:CE2	1:B:123:LEU:HD22	2.47	0.49
1:F:194:TRP:CZ3	1:F:282:CYS:HB3	2.47	0.49
1:I:131:ARG:NH1	1:I:135:LEU:HD11	2.26	0.49
1:C:354:LYS:NZ	2:C:401:CIT:C4	2.76	0.49
1:E:82:GLN:HE21	1:E:85:VAL:N	2.10	0.49
1:F:81:ASN:HD22	1:F:174:PHE:HD1	1.59	0.49
1:F:354:LYS:NZ	2:F:401:CIT:H42	2.27	0.49
1:B:88:PHE:CE1	1:B:90:ASP:HB2	2.47	0.49
1:D:145:TYR:O	1:D:149:VAL:HG12	2.13	0.49
1:F:277:LEU:HD23	1:F:280:TYR:CD2	2.48	0.49
1:J:187:TRP:HZ3	1:J:204:LYS:CE	2.19	0.49
1:A:126:ARG:H	1:A:228:ASP:CG	2.16	0.49
1:E:104:ASP:O	1:E:105:GLY:C	2.51	0.49
1:J:96:GLY:HA2	1:J:321:LEU:HD13	1.94	0.49
1:G:196:GLY:O	1:G:200:VAL:HG23	2.13	0.49
1:J:40:ASP:HB3	1:J:145:TYR:HE2	1.77	0.49
1:A:145:TYR:O	1:A:149:VAL:HG23	2.13	0.49
1:G:346:ALA:O	1:G:350:LEU:HG	2.13	0.49
1:B:101:LYS:HE2	1:B:122:TYR:CE1	2.48	0.48
1:H:40:ASP:OD2	1:H:143:CYS:HB2	2.13	0.48
1:I:46:GLU:OE2	1:I:53:ILE:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HG12	1:D:301:ASN:ND2	2.28	0.48
1:D:29:LYS:HA	1:D:32:ARG:CZ	2.43	0.48
1:E:132:PHE:CD2	1:E:158:VAL:HG21	2.48	0.48
1:H:281:GLU:HG3	1:H:303:ILE:HG12	1.95	0.48
1:A:178:GLY:HA2	1:H:179:ILE:HD13	1.94	0.48
1:B:354:LYS:HZ1	2:B:401:CIT:H41	1.78	0.48
1:F:287:ARG:HG2	1:F:290:ASP:H	1.79	0.48
1:G:238:GLU:HG3	1:G:320:PHE:HE2	1.78	0.48
1:B:136:VAL:O	1:B:140:VAL:HG13	2.13	0.48
1:E:238:GLU:O	1:E:242:GLN:HG3	2.14	0.48
1:G:82:GLN:HB3	1:G:174:PHE:HE1	1.78	0.48
1:H:176:CYS:HB3	1:H:179:ILE:HD11	1.95	0.48
1:I:57:ASN:OD1	1:I:57:ASN:N	2.46	0.48
1:D:141:ASP:HA	1:D:146:ARG:HG2	1.95	0.48
1:F:277:LEU:HD11	1:F:307:LEU:HD13	1.95	0.48
1:E:123:LEU:HD11	1:E:128:ILE:HD11	1.96	0.48
1:G:108:ARG:NH2	1:G:118:THR:O	2.47	0.48
1:H:15:TYR:CD1	1:H:19:LYS:HG3	2.49	0.48
1:I:195:PRO:HA	1:I:286:PRO:HB2	1.96	0.48
1:I:206:GLU:HG2	1:I:236:GLU:HB2	1.95	0.48
1:I:267:GLN:O	1:I:330:LYS:NZ	2.28	0.48
1:F:66:LEU:HD11	1:F:74:PHE:HB3	1.96	0.47
1:I:54:SER:OG	1:I:56:LEU:CD2	2.62	0.47
1:B:82:GLN:HG2	1:B:85:VAL:HG12	1.95	0.47
1:F:299:ARG:HA	1:F:299:ARG:HD3	1.69	0.47
1:H:58:GLU:H	1:H:58:GLU:CD	2.17	0.47
1:D:301:ASN:OD1	1:D:350:LEU:HD11	2.15	0.47
1:H:14:LYS:NZ	1:H:357:GLU:OE1	2.43	0.47
1:B:195:PRO:HB2	1:B:199:ARG:HG2	1.96	0.47
1:D:195:PRO:HD2	1:D:200:VAL:HG23	1.97	0.47
1:I:94:LEU:HB3	1:I:97:CYS:HB2	1.97	0.47
1:J:39:SER:HA	1:J:42:LEU:HB3	1.95	0.47
2:A:401:CIT:O3	2:A:401:CIT:O7	2.31	0.47
1:A:136:VAL:O	1:A:140:VAL:HG13	2.15	0.47
1:A:177:THR:HG21	1:H:87:ASN:HD22	1.80	0.47
1:B:58:GLU:HB2	1:B:63:TYR:CE2	2.49	0.47
1:D:299:ARG:HA	1:D:299:ARG:HH11	1.78	0.47
1:G:126:ARG:HD2	1:G:228:ASP:HB3	1.97	0.47
1:I:171:THR:HG21	1:I:211:LEU:HB3	1.97	0.47
1:I:206:GLU:CG	1:I:236:GLU:HB2	2.45	0.47
1:B:40:ASP:OD2	1:B:143:CYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ALA:HB2	1:G:350:LEU:HD13	1.96	0.47
1:E:85:VAL:O	1:E:102:LEU:HD12	2.14	0.47
1:E:103:SER:O	1:E:106:ARG:CG	2.62	0.47
1:F:194:TRP:CG	1:F:195:PRO:HA	2.49	0.47
1:H:281:GLU:HG3	1:H:303:ILE:CG1	2.45	0.47
1:C:16:TYR:CD1	1:C:249:LYS:HG3	2.49	0.47
1:A:62[B]:ARG:HG2	1:A:62[B]:ARG:NH2	2.27	0.47
1:A:299:ARG:HA	1:A:299:ARG:HD3	1.72	0.47
1:E:33:GLU:OE2	1:E:163:ARG:NH1	2.48	0.47
1:E:90:ASP:OD1	1:E:183:SER:OG	2.33	0.47
1:J:189:LEU:HB3	1:J:190:PRO:HD2	1.97	0.47
1:A:62[B]:ARG:NH1	4:A:403:CTP:H2'	2.29	0.46
1:B:193:PRO:HG2	1:B:286:PRO:HG3	1.96	0.46
1:H:140:VAL:O	1:H:146:ARG:NE	2.38	0.46
1:J:37:VAL:HA	1:J:145:TYR:CE2	2.50	0.46
1:J:233:GLN:HG3	1:J:234:PHE:N	2.30	0.46
1:I:163:ARG:HA	1:I:163:ARG:HE	1.81	0.46
1:E:199:ARG:NH1	1:E:202:GLU:OE1	2.46	0.46
1:J:27:ILE:O	1:J:31:ILE:HB	2.16	0.46
1:A:106:ARG:C	1:A:107:LYS:HG3	2.35	0.46
1:A:318:HIS:HB3	1:A:321:LEU:O	2.16	0.46
1:H:91:ASP:O	1:H:94:LEU:CD1	2.64	0.46
1:C:192:ILE:HG22	1:C:194:TRP:N	2.29	0.46
1:D:82:GLN:HB3	1:D:174:PHE:CE1	2.50	0.46
1:I:44:GLU:O	1:I:47:VAL:HG22	2.15	0.46
1:J:240:ARG:HH11	1:J:240:ARG:HG2	1.80	0.46
1:H:340:LYS:NZ	5:H:507:HOH:O	2.47	0.46
1:I:315:ARG:HD2	1:I:317:PRO:HD3	1.98	0.46
1:J:42:LEU:HA	1:J:45:VAL:HG13	1.98	0.46
1:H:15:TYR:CE1	1:H:19:LYS:HG3	2.51	0.46
1:G:3:ALA:CB	1:I:347:ARG:HH12	2.28	0.46
1:D:145:TYR:HB3	1:D:148:VAL:CG2	2.45	0.46
1:F:24:LYS:HE2	4:F:403:CTP:O2B	2.16	0.46
1:J:267:GLN:N	1:J:267:GLN:OE1	2.48	0.46
1:C:189:LEU:HB3	1:C:191:HIS:CD2	2.51	0.46
1:A:118:THR:HG22	1:A:127:LYS:NZ	2.30	0.45
1:B:101:LYS:HG2	1:B:102:LEU:N	2.31	0.45
1:F:298:ASP:HB3	1:F:299:ARG:HH12	1.81	0.45
1:D:107:LYS:HA	1:D:110:MET:HG3	1.98	0.45
1:C:301:ASN:ND2	1:C:350:LEU:HD13	2.31	0.45
1:C:33:GLU:OE2	1:C:163:ARG:HD2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:HIS:CD2	1:C:191:HIS:N	2.84	0.45
1:A:108:ARG:HG2	1:A:114:VAL:HG23	1.98	0.45
1:D:194:TRP:CB	1:D:195:PRO:HD3	2.47	0.45
1:C:269:LEU:HD21	1:C:311:LEU:HD21	1.97	0.45
1:D:42:LEU:HD11	1:D:170:ILE:HD13	1.99	0.45
1:F:194:TRP:HA	1:F:195:PRO:HA	1.58	0.45
1:G:149:VAL:O	1:G:150:LYS:HD2	2.16	0.45
1:C:91:ASP:OD2	1:C:93:SER:OG	2.33	0.45
1:C:299:ARG:HA	1:C:299:ARG:HD3	1.72	0.45
1:B:1:ASP:CB	1:F:-1:ALA:HB2	2.46	0.45
1:F:177:THR:OG1	1:I:178:GLY:CA	2.65	0.45
1:H:43:LYS:HA	1:H:46:GLU:HG2	1.98	0.45
1:I:251:LEU:HD11	1:I:255:LYS:HE3	1.98	0.45
1:J:136:VAL:O	1:J:140:VAL:HG13	2.17	0.45
1:B:83:MET:O	1:G:82:GLN:NE2	2.49	0.45
1:I:78:LEU:HD12	1:I:78:LEU:HA	1.74	0.45
1:F:195:PRO:HD2	1:F:200:VAL:HG22	1.99	0.45
1:B:84:GLY:HA2	1:G:177:THR:OG1	2.16	0.45
1:D:197:PRO:CG	1:D:199:ARG:HH11	2.30	0.45
1:E:163:ARG:O	1:E:165:ARG:HG2	2.17	0.45
1:H:163:ARG:HE	1:H:165:ARG:NH1	2.14	0.45
1:B:14:LYS:HB3	1:B:14:LYS:HE2	1.84	0.44
1:B:81:ASN:HD21	1:G:103:SER:CB	2.29	0.44
1:B:82:GLN:HE21	1:B:82:GLN:C	2.21	0.44
1:B:318:HIS:HB3	1:B:321:LEU:O	2.17	0.44
1:B:54:SER:HB3	1:B:78:LEU:HD11	2.00	0.44
1:B:116:PHE:HZ	1:B:131:ARG:HG2	1.82	0.44
1:D:137:ALA:O	1:D:140:VAL:HG12	2.17	0.44
1:D:194:TRP:HB3	1:D:195:PRO:HD3	1.99	0.44
1:D:194:TRP:HE3	1:D:194:TRP:C	2.21	0.44
2:D:401:CIT:O2	2:D:401:CIT:H42	2.18	0.44
1:H:213:LYS:HG3	1:H:231:VAL:HG21	1.98	0.44
1:H:269:LEU:HD11	1:H:311:LEU:HD11	1.98	0.44
1:J:187:TRP:HA	1:J:188:PRO:HA	1.64	0.44
1:A:43:LYS:HD2	1:A:43:LYS:HA	1.66	0.44
1:I:16:TYR:CD1	1:I:249:LYS:HG3	2.53	0.44
1:E:240:ARG:HA	1:E:243:MET:CE	2.47	0.44
1:J:19:LYS:NZ	1:J:357:GLU:O	2.37	0.44
1:F:50:PRO:O	1:F:53:ILE:HG12	2.17	0.44
1:H:171:THR:N	5:H:506:HOH:O	2.51	0.44
1:C:238:GLU:HG3	1:C:320:PHE:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:TRP:HE3	1:D:194:TRP:O	2.00	0.44
1:F:180:TRP:HB3	1:F:185:ALA:HA	2.00	0.44
1:F:238:GLU:O	1:F:242:GLN:HG3	2.18	0.44
1:D:124:SER:OG	1:D:228:ASP:OD2	2.15	0.44
1:D:140:VAL:O	1:D:146:ARG:HG2	2.17	0.44
1:H:96:GLY:HA2	1:H:321:LEU:HD13	1.99	0.44
1:H:254:LEU:HD11	1:H:303:ILE:HG21	1.98	0.44
1:J:78:LEU:O	1:J:173:ALA:N	2.42	0.44
1:B:284:LYS:HE2	1:B:284:LYS:HB3	1.83	0.44
1:H:43:LYS:HZ1	1:H:54:SER:HB3	1.82	0.44
1:I:141:ASP:HA	1:I:146:ARG:HG2	2.00	0.44
1:E:258:ARG:NH2	1:E:259:ASP:OD1	2.50	0.44
1:J:32:ARG:NH2	1:J:63:TYR:HB2	2.33	0.44
1:A:179:ILE:HG23	1:A:208:PHE:HE1	1.83	0.43
1:B:323:ASN:OD1	1:B:323:ASN:N	2.42	0.43
1:D:23:ARG:NH1	1:D:259:ASP:OD2	2.51	0.43
1:E:140:VAL:HB	1:E:149:VAL:HG13	2.00	0.43
1:H:45:VAL:HG13	1:H:135:LEU:HB3	1.99	0.43
1:J:66:LEU:HD12	1:J:76:VAL:HG22	2.00	0.43
1:A:148:VAL:HB	1:A:163:ARG:HG2	1.99	0.43
1:B:194:TRP:HB2	1:B:286:PRO:CB	2.48	0.43
1:B:209:ASN:HB2	1:B:233:GLN:HG2	1.99	0.43
1:D:87:ASN:N	1:D:101:LYS:O	2.39	0.43
1:J:32:ARG:NH2	1:J:66:LEU:HD22	2.33	0.43
1:J:202:GLU:O	1:J:206:GLU:HG2	2.18	0.43
1:C:318:HIS:HB3	1:C:321:LEU:O	2.18	0.43
1:E:82:GLN:HG3	1:E:85:VAL:HG22	1.99	0.43
1:E:106:ARG:HA	1:E:106:ARG:NE	2.34	0.43
1:G:189:LEU:HB2	1:G:192:ILE:CD1	2.48	0.43
1:I:299:ARG:HA	1:I:299:ARG:HD3	1.74	0.43
1:A:287:ARG:HG3	1:A:290:ASP:OD2	2.18	0.43
1:B:51:ARG:HD2	1:B:112:LEU:CD2	2.49	0.43
1:B:113:TRP:O	1:B:117:ILE:HG13	2.18	0.43
1:J:234:PHE:O	1:J:238:GLU:HG2	2.17	0.43
1:G:299:ARG:HA	1:G:299:ARG:HD3	1.77	0.43
1:I:116:PHE:CD1	1:I:127:LYS:HG3	2.53	0.43
1:J:32:ARG:CZ	1:J:63:TYR:HB2	2.48	0.43
1:I:126:ARG:HG3	1:I:228:ASP:OD1	2.19	0.43
1:D:181:PRO:HD3	1:D:208:PHE:CD1	2.54	0.43
1:E:268:PRO:HG3	1:E:334:ALA:HB1	2.00	0.43
1:G:56:LEU:HD23	1:G:56:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:LEU:HD13	1:H:97:CYS:O	2.18	0.43
1:I:40:ASP:HA	1:I:43:LYS:HG2	2.00	0.43
1:I:315:ARG:CD	1:I:317:PRO:HD3	2.48	0.43
1:J:336:GLU:OE2	1:J:340:LYS:HE2	2.18	0.43
1:A:226:GLU:HG2	1:A:227:SER:N	2.34	0.43
1:B:145:TYR:O	1:B:149:VAL:HG23	2.19	0.43
1:B:287:ARG:HD3	1:B:289:SER:OG	2.19	0.43
1:D:340:LYS:HE3	1:D:340:LYS:HB2	1.76	0.43
1:E:62[B]:ARG:NH1	4:E:402:CTP:H2'	2.33	0.43
1:H:318:HIS:HB3	1:H:321:LEU:O	2.19	0.43
1:C:152:VAL:HB	1:C:159:LYS:HB2	2.01	0.43
1:D:83:MET:HB2	1:D:85:VAL:HG13	2.01	0.43
1:H:162:ILE:C	1:H:164:ASP:H	2.22	0.43
1:C:211:LEU:HD23	1:C:213:LYS:HE3	2.01	0.42
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.44	0.42
1:E:181:PRO:HD3	1:E:208:PHE:CD1	2.54	0.42
1:H:358:LYS:HD3	1:H:358:LYS:HA	1.82	0.42
1:I:146:ARG:NH2	1:I:150:LYS:HA	2.33	0.42
1:I:315:ARG:HD3	1:I:316:CYS:N	2.34	0.42
1:B:16:TYR:CD1	1:B:249:LYS:HG3	2.54	0.42
1:B:132:PHE:CD2	1:B:158:VAL:HG21	2.55	0.42
1:B:343:TRP:CZ2	1:B:347:ARG:HD2	2.55	0.42
1:I:227:SER:HB3	1:I:228:ASP:H	1.46	0.42
1:J:192:ILE:HD13	1:J:283:GLU:HG2	2.00	0.42
1:J:299:ARG:HH11	1:J:299:ARG:CA	2.31	0.42
1:A:197:PRO:HG3	3:A:402:TMO:HABA	2.01	0.42
1:B:287:ARG:HB3	1:B:290:ASP:OD2	2.19	0.42
1:F:194:TRP:CD2	1:F:195:PRO:HB3	2.55	0.42
1:I:130:SER:O	1:I:134:THR:HG23	2.18	0.42
1:C:16:TYR:HA	1:C:20:CYS:HB2	2.02	0.42
1:A:44:GLU:O	1:A:47:VAL:HG22	2.18	0.42
1:D:195:PRO:HD2	1:D:200:VAL:CG2	2.49	0.42
1:G:356:LEU:HD23	1:G:359:LEU:HD12	2.02	0.42
1:H:36:LYS:HD2	1:H:36:LYS:HA	1.74	0.42
1:B:51:ARG:HG2	1:G:107:LYS:HZ1	1.85	0.42
1:B:301:ASN:ND2	1:B:350:LEU:HD22	2.34	0.42
1:D:254:LEU:HD11	1:D:303:ILE:HG21	2.02	0.42
1:E:343:TRP:CZ2	1:E:347:ARG:HD3	2.55	0.42
1:H:16:TYR:O	1:H:20:CYS:HB2	2.20	0.42
1:H:284:LYS:HB3	1:H:284:LYS:HE2	1.97	0.42
1:I:240:ARG:HA	1:I:243:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:272:TYR:OH	1:J:318:HIS:NE2	2.50	0.42
1:B:195:PRO:CB	1:B:199:ARG:HG2	2.50	0.42
1:G:350:LEU:HG	1:G:350:LEU:H	1.67	0.42
2:C:401:CIT:O3	2:C:401:CIT:O7	2.22	0.42
1:A:82:GLN:HB3	1:A:174:PHE:CE1	2.55	0.42
1:E:57:ASN:OD1	1:E:57:ASN:N	2.52	0.42
1:F:115:GLU:OE2	1:F:131:ARG:NH1	2.52	0.42
2:I:401:CIT:O1	2:I:401:CIT:H42	2.19	0.42
1:J:180:TRP:HE1	1:J:185:ALA:N	2.18	0.42
1:E:29:LYS:HA	1:E:32:ARG:NH1	2.35	0.42
1:E:277:LEU:HD11	1:E:307:LEU:HD13	2.02	0.42
1:H:45:VAL:HG13	1:H:135:LEU:HD23	2.01	0.42
1:I:254:LEU:HD11	1:I:303:ILE:HG21	2.02	0.42
1:J:238:GLU:HG3	1:J:275:LYS:HZ3	1.83	0.42
1:A:16:TYR:O	1:A:20:CYS:HB2	2.19	0.41
1:B:116:PHE:HD1	1:B:127:LYS:HB3	1.84	0.41
1:E:191:HIS:CD2	1:E:191:HIS:H	2.38	0.41
1:H:228:ASP:OD1	1:H:228:ASP:O	2.37	0.41
2:H:401:CIT:H21	1:J:354:LYS:NZ	2.35	0.41
1:I:62:ARG:HG3	1:I:63:TYR:H	1.84	0.41
1:D:175:LYS:HE3	1:D:177:THR:CG2	2.50	0.41
1:F:287:ARG:HD3	1:F:290:ASP:HB2	2.02	0.41
1:I:164:ASP:HB3	1:I:165:ARG:HH11	1.84	0.41
1:F:46:GLU:HG2	1:I:110:MET:SD	2.60	0.41
1:H:46:GLU:HA	1:H:49:GLU:O	2.20	0.41
1:I:189:LEU:HD13	1:I:191:HIS:HE1	1.86	0.41
4:I:402:CTP:O3G	4:I:402:CTP:H3'	2.20	0.41
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.83	0.41
1:F:79:TYR:C	1:F:80:LEU:HG	2.41	0.41
1:F:180:TRP:O	1:F:181:PRO:O	2.38	0.41
1:G:157:GLU:OE2	1:G:213:LYS:HB2	2.19	0.41
1:B:85:VAL:O	1:B:86:PHE:CD2	2.73	0.41
1:D:195:PRO:HG2	1:D:199:ARG:HB2	2.00	0.41
1:D:202:GLU:CD	1:D:240:ARG:HD2	2.41	0.41
1:E:5:GLN:NE2	1:E:298:ASP:OD2	2.53	0.41
1:F:16:TYR:CD1	1:F:249:LYS:HG3	2.55	0.41
1:I:187:TRP:HA	1:I:188:PRO:HA	1.78	0.41
1:J:191:HIS:CG	1:J:192:ILE:HD12	2.55	0.41
1:J:277:LEU:HD22	1:J:306:GLN:HG3	2.02	0.41
1:F:93:SER:OG	1:F:94:LEU:N	2.51	0.41
1:G:354:LYS:HZ3	2:G:401:CIT:HO7	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:PRO:HG2	1:H:216:HIS:NE2	2.36	0.41
1:J:161:ARG:HA	1:J:167:VAL:HG22	2.01	0.41
1:J:249:LYS:NZ	1:J:293:GLU:OE1	2.43	0.41
1:C:83[A]:MET:HG2	1:C:111:SER:HA	2.03	0.41
1:A:240:ARG:O	1:A:243:MET:HE2	2.21	0.41
1:D:32:ARG:NH2	1:D:33:GLU:OE2	2.54	0.41
1:D:197:PRO:HD2	1:D:199:ARG:HH11	1.86	0.41
1:C:89:VAL:HB	1:C:99:VAL:HG12	2.03	0.41
1:A:163:ARG:O	1:A:165:ARG:HG3	2.20	0.41
1:B:311:LEU:O	1:B:314:ARG:NH1	2.51	0.41
1:F:81:ASN:O	1:F:82:GLN:NE2	2.53	0.41
1:G:194:TRP:CG	1:G:195:PRO:HA	2.56	0.41
1:H:87:ASN:N	1:H:101:LYS:O	2.37	0.41
1:H:146:ARG:O	1:H:150:LYS:NZ	2.48	0.41
1:H:164:ASP:OD1	5:H:501:HOH:O	2.22	0.41
1:I:181:PRO:HD3	1:I:208:PHE:CD2	2.56	0.41
1:J:299:ARG:HA	1:J:299:ARG:HD3	1.84	0.41
1:A:347:ARG:HA	1:A:347:ARG:HD2	1.86	0.41
1:B:34:VAL:HG13	1:B:168:VAL:HG21	2.03	0.41
1:B:194:TRP:HB2	1:B:286:PRO:HB3	2.03	0.41
1:D:24:LYS:HE2	4:D:402:CTP:O2B	2.21	0.41
1:D:125:ALA:HB1	1:D:212:SER:HB2	2.02	0.41
1:D:202:GLU:OE2	1:D:240:ARG:HD2	2.21	0.41
1:E:106:ARG:HA	1:E:106:ARG:HE	1.86	0.41
1:E:318:HIS:HB3	1:E:321:LEU:O	2.20	0.41
1:G:93:SER:O	1:G:94:LEU:HD23	2.21	0.41
1:G:292:ASP:OD2	1:G:294:SER:OG	2.39	0.41
1:G:318:HIS:HB3	1:G:321:LEU:O	2.20	0.41
1:I:116:PHE:HD1	1:I:127:LYS:HG3	1.86	0.41
1:I:186:HIS:HB2	1:I:189:LEU:HD21	2.03	0.41
1:I:356:LEU:HA	1:I:359:LEU:HD12	2.02	0.41
1:C:215:CYS:O	1:C:216:HIS:CG	2.74	0.41
1:B:112:LEU:HD23	1:B:112:LEU:O	2.21	0.41
1:D:277:LEU:HD11	1:D:307:LEU:HD13	2.03	0.41
1:H:126:ARG:HH12	1:H:227:SER:N	2.19	0.41
1:C:58:GLU:HB2	1:C:63:TYR:CE1	2.56	0.41
1:C:238:GLU:HB3	1:C:275:LYS:HE2	2.03	0.41
1:H:299:ARG:HA	1:H:299:ARG:HD3	1.63	0.40
1:I:161:ARG:NH1	1:I:164:ASP:O	2.55	0.40
1:J:181:PRO:O	1:J:185:ALA:HB2	2.20	0.40
1:E:34:VAL:HG22	1:E:162:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:VAL:HG23	1:E:86:PHE:CG	2.55	0.40
1:J:31:ILE:O	1:J:34:VAL:HG12	2.21	0.40
1:J:180:TRP:NE1	1:J:185:ALA:CA	2.78	0.40
1:C:194:TRP:CD1	1:C:195:PRO:HA	2.56	0.40
1:D:103:SER:H	1:D:107:LYS:HD2	1.86	0.40
1:D:132:PHE:O	1:D:136:VAL:HG23	2.21	0.40
1:E:107:LYS:O	1:E:109:SER:N	2.53	0.40
1:F:180:TRP:O	1:F:181:PRO:C	2.58	0.40
1:F:285:HIS:HA	1:F:287:ARG:HH21	1.86	0.40
1:J:163:ARG:HH21	1:J:165:ARG:CZ	2.34	0.40
1:A:179:ILE:HG23	1:A:208:PHE:CE1	2.57	0.40
1:D:299:ARG:HA	1:D:299:ARG:HD3	1.71	0.40
1:E:180:TRP:CD2	1:E:204:LYS:HG2	2.56	0.40
1:J:48:GLN:HG2	1:J:138:GLN:NE2	2.33	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:NH1	1:F:154:ASP:OD2[2_846]	2.13	0.07

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/362 (95%)	337 (98%)	8 (2%)	0	100	100
1	B	343/362 (95%)	333 (97%)	10 (3%)	0	100	100
1	C	351/362 (97%)	344 (98%)	7 (2%)	0	100	100
1	D	336/362 (93%)	320 (95%)	15 (4%)	1 (0%)	41	51
1	E	343/362 (95%)	333 (97%)	8 (2%)	2 (1%)	25	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	327/362 (90%)	310 (95%)	15 (5%)	2 (1%)	25	34
1	G	348/362 (96%)	339 (97%)	9 (3%)	0	100	100
1	H	337/362 (93%)	326 (97%)	11 (3%)	0	100	100
1	I	340/362 (94%)	335 (98%)	5 (2%)	0	100	100
1	J	266/362 (74%)	255 (96%)	11 (4%)	0	100	100
All	All	3336/3620 (92%)	3232 (97%)	99 (3%)	5 (0%)	47	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	195	PRO
1	E	108	ARG
1	E	104	ASP
1	F	61	ASN
1	F	181	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	311/317 (98%)	299 (96%)	12 (4%)	32	44
1	B	307/317 (97%)	296 (96%)	11 (4%)	35	47
1	C	313/317 (99%)	290 (93%)	23 (7%)	14	18
1	D	301/317 (95%)	286 (95%)	15 (5%)	24	33
1	E	309/317 (98%)	294 (95%)	15 (5%)	25	34
1	F	299/317 (94%)	282 (94%)	17 (6%)	20	27
1	G	310/317 (98%)	297 (96%)	13 (4%)	30	40
1	H	304/317 (96%)	289 (95%)	15 (5%)	25	34
1	I	306/317 (96%)	288 (94%)	18 (6%)	19	25
1	J	251/317 (79%)	231 (92%)	20 (8%)	12	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3011/3170 (95%)	2852 (95%)	159 (5%)	23	30

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	39	SER
1	A	67	GLU
1	A	106	ARG
1	A	109	SER
1	A	149	VAL
1	A	179	ILE
1	A	183	SER
1	A	215	CYS
1	A	240	ARG
1	A	323	ASN
1	A	328	GLN
1	B	1	ASP
1	B	56	LEU
1	B	67	GLU
1	B	81	ASN
1	B	82	GLN
1	B	83	MET
1	B	88	PHE
1	B	191	HIS
1	B	199	ARG
1	B	233	GLN
1	B	315	ARG
1	D	39	SER
1	D	43	LYS
1	D	63	TYR
1	D	89	VAL
1	D	103	SER
1	D	106	ARG
1	D	115	GLU
1	D	142	LYS
1	D	146	ARG
1	D	165	ARG
1	D	183	SER
1	D	191	HIS
1	D	194	TRP
1	D	214	GLU

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Mol	Chain	Res	Type
1	D	315	ARG
1	E	34	VAL
1	E	57	ASN
1	E	64	GLU
1	E	81	ASN
1	E	88	PHE
1	E	101	LYS
1	E	106	ARG
1	E	156	SER
1	E	182	ARG
1	E	199	ARG
1	E	240	ARG
1	E	267	GLN
1	E	323	ASN
1	E	344	ARG
1	E	350	LEU
1	F	0	MET
1	F	2	ILE
1	F	21	GLN
1	F	59	MET
1	F	60	ASP
1	F	82	GLN
1	F	86	PHE
1	F	94	LEU
1	F	120	SER
1	F	180	TRP
1	F	182	ARG
1	F	192	ILE
1	F	194	TRP
1	F	199	ARG
1	F	212	SER
1	F	287	ARG
1	F	290	ASP
1	G	0	MET
1	G	36	LYS
1	G	39	SER
1	G	57	ASN
1	G	81	ASN
1	G	94	LEU
1	G	103	SER
1	G	110	MET
1	G	146	ARG

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Mol	Chain	Res	Type
1	G	154	ASP
1	G	294	SER
1	G	315	ARG
1	G	350	LEU
1	H	36	LYS
1	H	55	SER
1	H	56	LEU
1	H	82	GLN
1	H	83	MET
1	H	94	LEU
1	H	134	THR
1	H	140	VAL
1	H	141	ASP
1	H	146	ARG
1	H	191	HIS
1	H	214	GLU
1	H	250	CYS
1	H	299	ARG
1	H	323	ASN
1	I	2	ILE
1	I	34	VAL
1	I	56	LEU
1	I	57	ASN
1	I	58	GLU
1	I	64	GLU
1	I	112	LEU
1	I	120	SER
1	I	131	ARG
1	I	149	VAL
1	I	163	ARG
1	I	165	ARG
1	I	214	GLU
1	I	227	SER
1	I	233	GLN
1	I	236	GLU
1	I	315	ARG
1	I	330	LYS
1	J	14	LYS
1	J	29	LYS
1	J	30	THR
1	J	45	VAL
1	J	70	SER

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Mol	Chain	Res	Type
1	J	99	VAL
1	J	122	TYR
1	J	126	ARG
1	J	164	ASP
1	J	166	TYR
1	J	182	ARG
1	J	191	HIS
1	J	199	ARG
1	J	202	GLU
1	J	233	GLN
1	J	248	LYS
1	J	250	CYS
1	J	285	HIS
1	J	294	SER
1	J	301	ASN
1	C	2	ILE
1	C	5	GLN
1	C	47	VAL
1	C	62[A]	ARG
1	C	62[B]	ARG
1	C	67	GLU
1	C	77	VAL
1	C	83[A]	MET
1	C	83[B]	MET
1	C	99	VAL
1	C	103	SER
1	C	107	LYS
1	C	108	ARG
1	C	115	GLU
1	C	131	ARG
1	C	138	GLN
1	C	182	ARG
1	C	191	HIS
1	C	206	GLU
1	C	215	CYS
1	C	248	LYS
1	C	287	ARG
1	C	315	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	87	ASN
1	A	301	ASN
1	B	57	ASN
1	B	81	ASN
1	B	82	GLN
1	B	301	ASN
1	D	285	HIS
1	E	48	GLN
1	E	82	GLN
1	E	191	HIS
1	E	261	HIS
1	E	271	ASN
1	F	21	GLN
1	F	82	GLN
1	G	82	GLN
1	G	191	HIS
1	H	82	GLN
1	H	87	ASN
1	H	242	GLN
1	I	191	HIS
1	I	271	ASN
1	C	48	GLN
1	C	81	ASN
1	C	191	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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	TMO	A	402	-	4,4,4	1.89	3 (75%)	6,6,6	0.24	0
2	CIT	A	401	-	12,12,12	1.00	0	17,17,17	1.62	1 (5%)
4	CTP	C	404	-	26,30,30	0.86	0	39,47,47	1.12	2 (5%)
4	CTP	F	403	-	26,30,30	0.87	0	39,47,47	1.08	3 (7%)
2	CIT	I	401	-	12,12,12	1.00	0	17,17,17	1.68	4 (23%)
3	TMO	C	402	-	4,4,4	1.91	2 (50%)	6,6,6	0.22	0
2	CIT	D	401	-	12,12,12	1.00	0	17,17,17	1.63	3 (17%)
2	CIT	F	401	-	12,12,12	1.01	0	17,17,17	1.85	6 (35%)
3	TMO	F	402	-	4,4,4	1.86	1 (25%)	6,6,6	0.23	0
4	CTP	E	402	-	26,30,30	0.87	0	39,47,47	1.11	3 (7%)
4	CTP	I	402	-	26,30,30	0.88	0	39,47,47	1.18	3 (7%)
4	CTP	H	403	-	26,30,30	0.87	0	39,47,47	1.12	3 (7%)
2	CIT	B	401	-	12,12,12	0.99	0	17,17,17	1.66	2 (11%)
4	CTP	G	402	-	26,30,30	0.86	0	39,47,47	1.08	2 (5%)
2	CIT	E	401	-	12,12,12	1.03	0	17,17,17	1.57	3 (17%)
2	CIT	H	401	-	12,12,12	0.99	0	17,17,17	1.59	2 (11%)
4	CTP	B	402	-	26,30,30	0.86	0	39,47,47	1.09	3 (7%)
2	CIT	H	402	-	12,12,12	1.03	0	17,17,17	1.56	2 (11%)
4	CTP	J	401	-	26,30,30	0.87	0	39,47,47	1.14	4 (10%)
4	CTP	D	402	-	26,30,30	0.87	0	39,47,47	1.12	3 (7%)
3	TMO	C	403	-	4,4,4	1.87	2 (50%)	6,6,6	0.22	0
2	CIT	G	401	-	12,12,12	1.01	0	17,17,17	1.59	2 (11%)
2	CIT	C	401	-	12,12,12	1.16	1 (8%)	17,17,17	1.35	2 (11%)
4	CTP	A	403	-	26,30,30	0.86	0	39,47,47	1.11	3 (7%)

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
2	CIT	A	401	-	-	4/16/16/16	-
4	CTP	C	404	-	-	3/22/38/38	0/2/2/2
4	CTP	F	403	-	-	8/22/38/38	0/2/2/2
2	CIT	I	401	-	-	8/16/16/16	-
2	CIT	D	401	-	-	10/16/16/16	-
2	CIT	F	401	-	-	13/16/16/16	-
4	CTP	E	402	-	-	5/22/38/38	0/2/2/2
4	CTP	I	402	-	-	10/22/38/38	0/2/2/2
4	CTP	H	403	-	-	6/22/38/38	0/2/2/2
2	CIT	B	401	-	-	4/16/16/16	-
4	CTP	G	402	-	-	7/22/38/38	0/2/2/2
2	CIT	E	401	-	-	5/16/16/16	-
2	CIT	H	401	-	-	7/16/16/16	-
4	CTP	B	402	-	-	5/22/38/38	0/2/2/2
2	CIT	H	402	-	-	8/16/16/16	-
4	CTP	J	401	-	-	3/22/38/38	0/2/2/2
4	CTP	D	402	-	-	6/22/38/38	0/2/2/2
2	CIT	G	401	-	-	8/16/16/16	-
2	CIT	C	401	-	-	8/16/16/16	-
4	CTP	A	403	-	-	1/22/38/38	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	CIT	C3-C6	-2.24	1.51	1.53
3	C	402	TMO	CAA-NAC	-2.11	1.45	1.48
3	A	402	TMO	CAA-NAC	-2.07	1.45	1.48
3	C	402	TMO	CAB-NAC	-2.06	1.45	1.48
3	C	403	TMO	CAB-NAC	-2.02	1.45	1.48
3	C	403	TMO	CAA-NAC	-2.02	1.45	1.48
3	F	402	TMO	CAD-NAC	-2.01	1.45	1.48
3	A	402	TMO	CAB-NAC	-2.01	1.45	1.48
3	A	402	TMO	CAD-NAC	-2.00	1.45	1.48

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	CIT	O6-C6-C3	4.50	120.86	113.05
2	A	401	CIT	O6-C6-C3	4.40	120.69	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	CIT	O6-C6-C3	4.36	120.62	113.05
2	I	401	CIT	O6-C6-C3	4.25	120.42	113.05
2	F	401	CIT	O6-C6-C3	4.05	120.08	113.05
2	G	401	CIT	O6-C6-C3	4.01	120.02	113.05
2	H	402	CIT	O6-C6-C3	3.96	119.93	113.05
2	D	401	CIT	O6-C6-C3	3.92	119.86	113.05
2	H	401	CIT	O6-C6-C3	3.68	119.44	113.05
4	C	404	CTP	PB-O3B-PG	-3.56	120.59	132.83
4	E	402	CTP	PB-O3B-PG	-3.55	120.66	132.83
4	B	402	CTP	PB-O3B-PG	-3.50	120.81	132.83
4	H	403	CTP	PB-O3A-PA	-3.48	120.90	132.83
4	A	403	CTP	PB-O3B-PG	-3.43	121.05	132.83
4	G	402	CTP	PB-O3B-PG	-3.31	121.45	132.83
4	I	402	CTP	PB-O3A-PA	-3.31	121.48	132.83
2	C	401	CIT	O6-C6-C3	3.26	118.71	113.05
4	D	402	CTP	PB-O3B-PG	-3.24	121.72	132.83
4	C	404	CTP	PB-O3A-PA	-3.22	121.78	132.83
4	I	402	CTP	PB-O3B-PG	-3.20	121.86	132.83
4	D	402	CTP	PB-O3A-PA	-3.17	121.94	132.83
4	F	403	CTP	PB-O3B-PG	-3.07	122.29	132.83
2	F	401	CIT	O2-C1-C2	3.02	124.04	114.35
4	J	401	CTP	PB-O3A-PA	-2.99	122.56	132.83
4	F	403	CTP	PB-O3A-PA	-2.93	122.77	132.83
4	B	402	CTP	PB-O3A-PA	-2.92	122.80	132.83
4	A	403	CTP	PB-O3A-PA	-2.90	122.86	132.83
4	H	403	CTP	PB-O3B-PG	-2.86	123.00	132.83
4	G	402	CTP	PB-O3A-PA	-2.85	123.05	132.83
4	J	401	CTP	PB-O3B-PG	-2.84	123.08	132.83
4	E	402	CTP	PB-O3A-PA	-2.58	123.97	132.83
2	C	401	CIT	O5-C6-C3	-2.55	118.65	122.25
2	F	401	CIT	C3-C2-C1	2.45	119.75	113.81
4	F	403	CTP	C3'-C2'-C1'	2.43	106.04	101.43
2	D	401	CIT	O2-C1-C2	2.41	122.09	114.35
4	H	403	CTP	C3'-C2'-C1'	2.40	105.98	101.43
4	B	402	CTP	C3'-C2'-C1'	2.40	105.98	101.43
2	F	401	CIT	O2-C1-O1	-2.36	117.42	123.30
4	D	402	CTP	C3'-C2'-C1'	2.32	105.83	101.43
2	F	401	CIT	O4-C5-C4	2.29	121.71	114.35
2	I	401	CIT	C4-C3-C2	2.28	115.09	109.16
4	E	402	CTP	C3'-C2'-C1'	2.21	105.63	101.43
2	H	401	CIT	O2-C1-O1	-2.20	117.82	123.30
4	J	401	CTP	C3'-C2'-C1'	2.18	105.57	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	CIT	O2-C1-O1	-2.17	117.89	123.30
2	D	401	CIT	O2-C1-O1	-2.15	117.94	123.30
4	I	402	CTP	C3'-C2'-C1'	2.15	105.51	101.43
2	E	401	CIT	O2-C1-O1	-2.14	117.97	123.30
2	E	401	CIT	O4-C5-C4	2.12	121.16	114.35
4	A	403	CTP	C3'-C2'-C1'	2.09	105.40	101.43
2	G	401	CIT	C3-C4-C5	-2.07	108.79	113.81
2	I	401	CIT	O4-C5-C4	2.06	120.97	114.35
2	B	401	CIT	O2-C1-C2	2.05	120.93	114.35
2	H	402	CIT	O4-C5-C4	2.03	120.88	114.35
2	F	401	CIT	O4-C5-O3	-2.02	118.26	123.30
4	J	401	CTP	O3G-PG-O3B	2.00	111.36	104.64

There are no chirality outliers.

All (129) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CIT	C2-C3-C4-C5
2	B	401	CIT	O7-C3-C6-O5
2	B	401	CIT	O7-C3-C6-O6
2	B	401	CIT	C4-C3-C6-O5
2	B	401	CIT	C4-C3-C6-O6
2	D	401	CIT	C2-C3-C4-C5
2	D	401	CIT	O7-C3-C4-C5
2	D	401	CIT	C6-C3-C4-C5
2	D	401	CIT	C2-C3-C6-O5
2	D	401	CIT	C2-C3-C6-O6
2	D	401	CIT	O7-C3-C6-O5
2	D	401	CIT	O7-C3-C6-O6
2	E	401	CIT	O7-C3-C6-O5
2	E	401	CIT	O7-C3-C6-O6
2	E	401	CIT	C4-C3-C6-O5
2	E	401	CIT	C4-C3-C6-O6
2	G	401	CIT	C2-C3-C4-C5
2	G	401	CIT	O7-C3-C4-C5
2	G	401	CIT	C6-C3-C4-C5
2	G	401	CIT	O7-C3-C6-O5
2	G	401	CIT	O7-C3-C6-O6
2	G	401	CIT	C4-C3-C6-O5
2	G	401	CIT	C4-C3-C6-O6
2	H	401	CIT	C2-C3-C6-O5
2	H	401	CIT	C2-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
2	H	401	CIT	O7-C3-C6-O5
2	H	401	CIT	O7-C3-C6-O6
2	I	401	CIT	C1-C2-C3-C4
2	I	401	CIT	C1-C2-C3-C6
2	I	401	CIT	C2-C3-C4-C5
2	I	401	CIT	O7-C3-C4-C5
2	I	401	CIT	C6-C3-C4-C5
2	C	401	CIT	O7-C3-C6-O5
2	C	401	CIT	O7-C3-C6-O6
2	C	401	CIT	C4-C3-C6-O5
2	C	401	CIT	C4-C3-C6-O6
4	B	402	CTP	C5'-O5'-PA-O2A
4	B	402	CTP	C5'-O5'-PA-O3A
4	D	402	CTP	C3'-C4'-C5'-O5'
4	D	402	CTP	O4'-C4'-C5'-O5'
4	D	402	CTP	C5'-O5'-PA-O1A
4	D	402	CTP	C5'-O5'-PA-O2A
4	D	402	CTP	C5'-O5'-PA-O3A
4	E	402	CTP	C5'-O5'-PA-O1A
4	E	402	CTP	C5'-O5'-PA-O3A
4	F	403	CTP	C5'-O5'-PA-O2A
4	F	403	CTP	C5'-O5'-PA-O3A
4	G	402	CTP	O4'-C4'-C5'-O5'
4	G	402	CTP	C5'-O5'-PA-O3A
4	H	403	CTP	O4'-C4'-C5'-O5'
4	H	403	CTP	C5'-O5'-PA-O1A
4	H	403	CTP	C5'-O5'-PA-O2A
4	H	403	CTP	C5'-O5'-PA-O3A
4	I	402	CTP	C3'-C4'-C5'-O5'
4	I	402	CTP	O4'-C4'-C5'-O5'
4	I	402	CTP	C5'-O5'-PA-O1A
4	I	402	CTP	C5'-O5'-PA-O2A
4	I	402	CTP	C5'-O5'-PA-O3A
4	I	402	CTP	PB-O3B-PG-O2G
4	G	402	CTP	C3'-C4'-C5'-O5'
4	H	403	CTP	C3'-C4'-C5'-O5'
4	C	404	CTP	O4'-C4'-C5'-O5'
2	A	401	CIT	C6-C3-C4-C5
2	F	401	CIT	C1-C2-C3-O7
2	F	401	CIT	C1-C2-C3-C6
2	I	401	CIT	C1-C2-C3-O7
4	B	402	CTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	J	401	CTP	O4'-C4'-C5'-O5'
4	C	404	CTP	C3'-C4'-C5'-O5'
4	B	402	CTP	C3'-C4'-C5'-O5'
4	J	401	CTP	C3'-C4'-C5'-O5'
2	D	401	CIT	C1-C2-C3-C4
2	D	401	CIT	C1-C2-C3-C6
2	F	401	CIT	C6-C3-C4-C5
4	F	403	CTP	O4'-C4'-C5'-O5'
2	A	401	CIT	O7-C3-C4-C5
2	H	402	CIT	C2-C3-C4-C5
2	H	402	CIT	O7-C3-C4-C5
2	H	402	CIT	C2-C3-C6-O5
2	H	402	CIT	C2-C3-C6-O6
2	F	401	CIT	C1-C2-C3-C4
2	H	402	CIT	C6-C3-C4-C5
2	C	401	CIT	C6-C3-C4-C5
4	G	402	CTP	PB-O3A-PA-O5'
4	F	403	CTP	PB-O3B-PG-O1G
2	D	401	CIT	C1-C2-C3-O7
2	H	401	CIT	C1-C2-C3-O7
4	E	402	CTP	PB-O3B-PG-O2G
4	I	402	CTP	PA-O3A-PB-O2B
4	B	402	CTP	C5'-O5'-PA-O1A
4	F	403	CTP	C5'-O5'-PA-O1A
4	G	402	CTP	C5'-O5'-PA-O2A
4	F	403	CTP	C3'-C4'-C5'-O5'
2	F	401	CIT	C2-C3-C6-O6
2	F	401	CIT	C4-C3-C6-O6
2	H	402	CIT	C4-C3-C6-O5
2	H	402	CIT	C4-C3-C6-O6
2	F	401	CIT	C2-C3-C4-C5
2	G	401	CIT	C1-C2-C3-C4
2	H	402	CIT	C1-C2-C3-O7
2	C	401	CIT	O7-C3-C4-C5
2	A	401	CIT	C1-C2-C3-C4
2	E	401	CIT	C1-C2-C3-O7
2	C	401	CIT	C2-C3-C4-C5
2	F	401	CIT	O7-C3-C6-O6
2	F	401	CIT	C2-C3-C6-O5
4	D	402	CTP	PB-O3A-PA-O1A
4	E	402	CTP	O4'-C4'-C5'-O5'
2	F	401	CIT	C3-C4-C5-O3

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Mol	Chain	Res	Type	Atoms
2	F	401	CIT	C3-C4-C5-O4
2	I	401	CIT	C3-C4-C5-O3
2	C	401	CIT	C2-C3-C6-O6
4	F	403	CTP	PB-O3B-PG-O2G
4	F	403	CTP	PB-O3B-PG-O3G
4	I	402	CTP	PB-O3B-PG-O3G
4	J	401	CTP	PG-O3B-PB-O3A
2	F	401	CIT	O1-C1-C2-C3
2	H	401	CIT	C3-C4-C5-O3
4	C	404	CTP	C5'-O5'-PA-O3A
2	I	401	CIT	C3-C4-C5-O4
4	G	402	CTP	PG-O3B-PB-O1B
4	G	402	CTP	PG-O3B-PB-O2B
4	I	402	CTP	PA-O3A-PB-O1B
2	F	401	CIT	O2-C1-C2-C3
4	A	403	CTP	C5'-O5'-PA-O1A
4	E	402	CTP	C3'-C4'-C5'-O5'
4	H	403	CTP	PB-O3B-PG-O1G
4	I	402	CTP	PB-O3B-PG-O1G
2	H	401	CIT	C3-C4-C5-O4

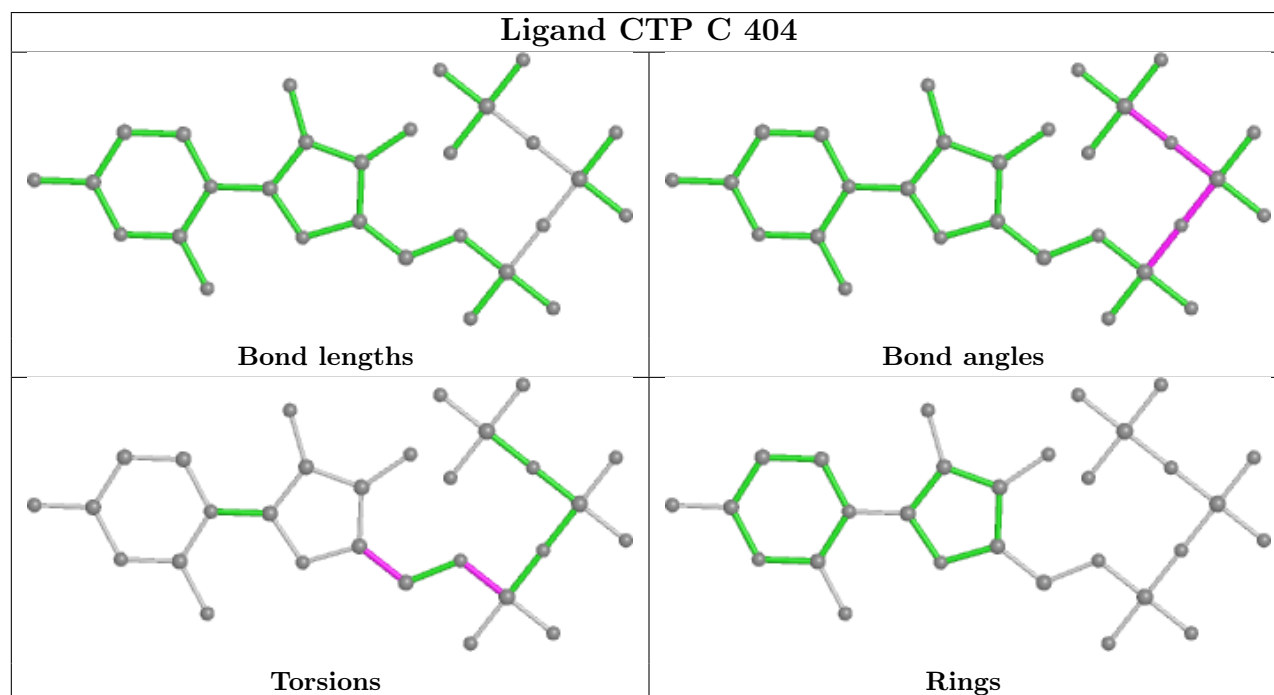
There are no ring outliers.

15 monomers are involved in 29 short contacts:

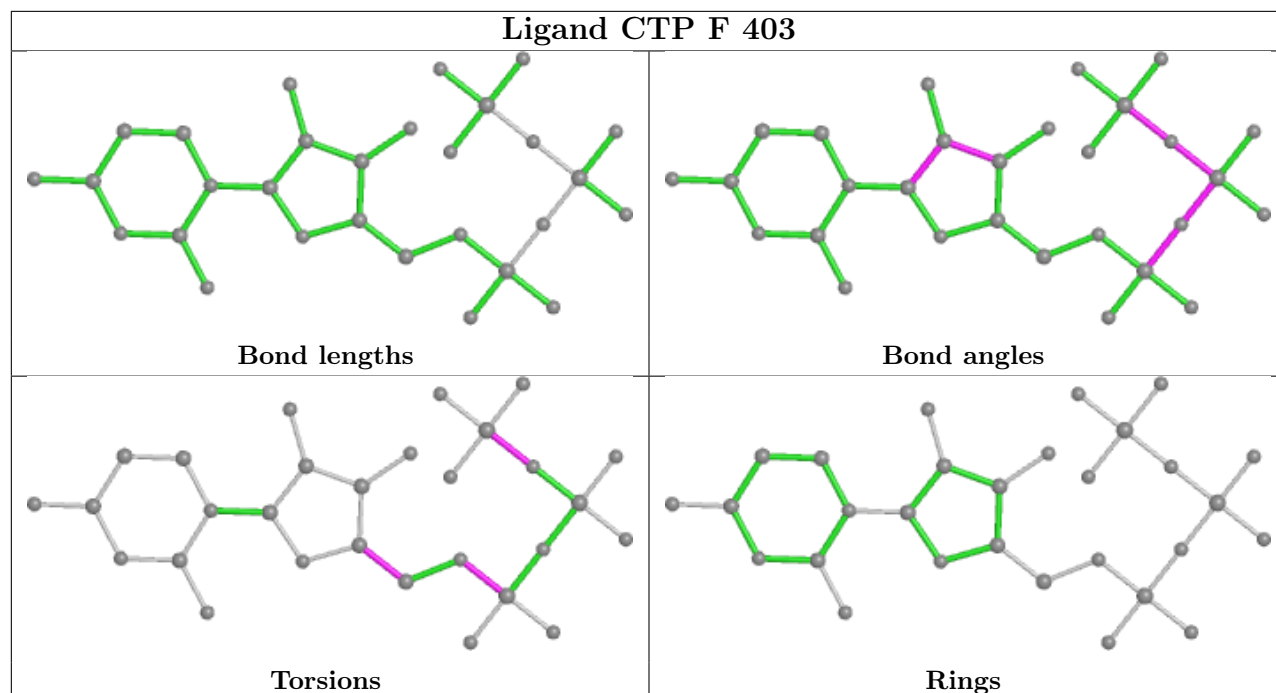
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	TMO	1	0
2	A	401	CIT	1	0
4	F	403	CTP	1	0
2	I	401	CIT	2	0
2	D	401	CIT	2	0
2	F	401	CIT	1	0
4	E	402	CTP	2	0
4	I	402	CTP	2	0
4	H	403	CTP	3	0
2	B	401	CIT	2	0
2	H	401	CIT	1	0
4	D	402	CTP	1	0
2	G	401	CIT	2	0
2	C	401	CIT	7	0
4	A	403	CTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

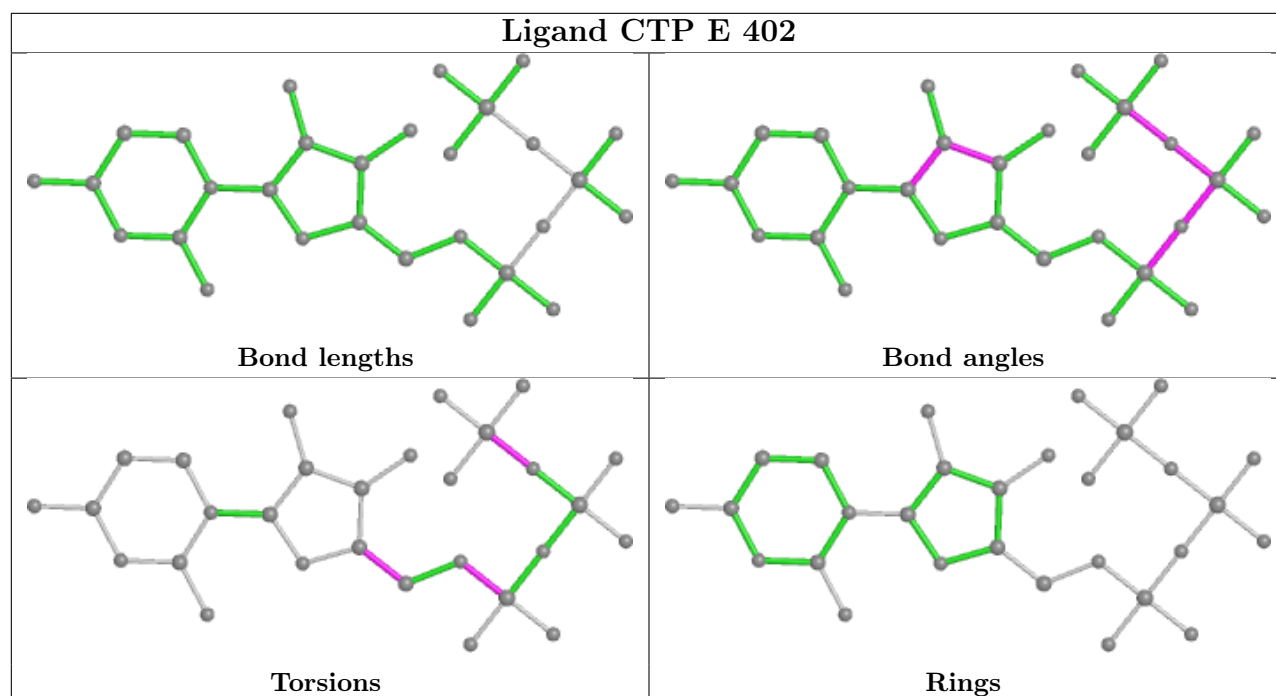
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



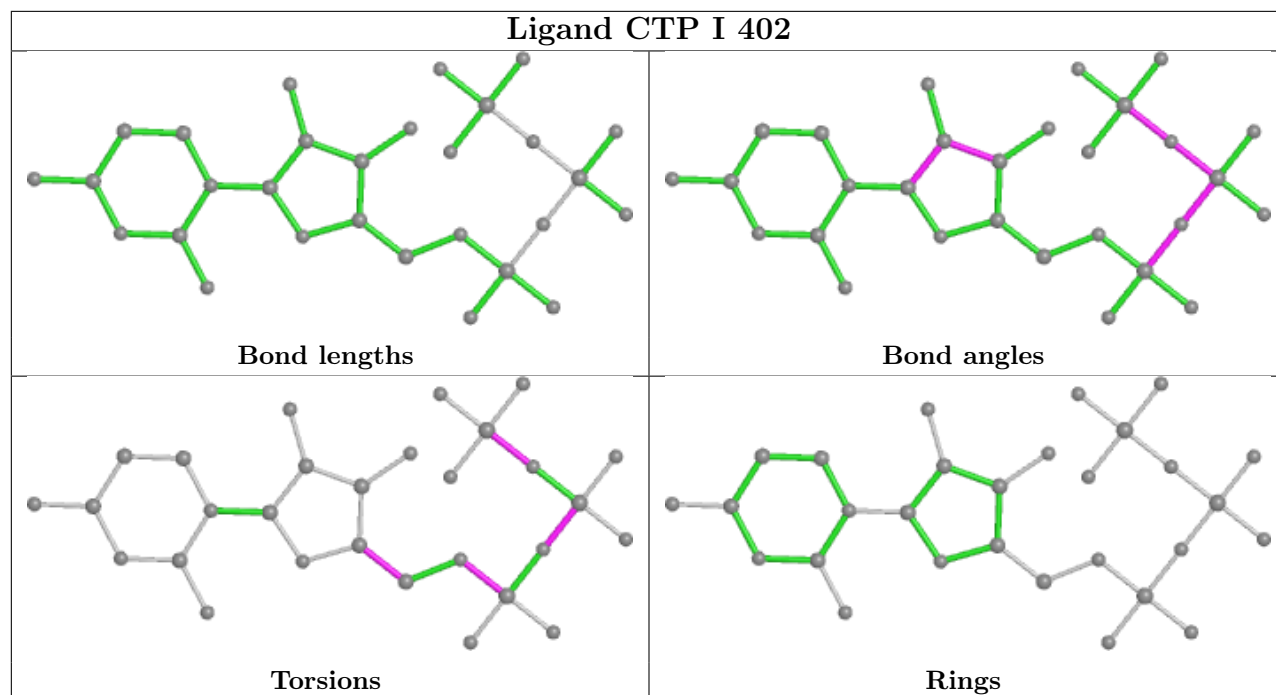
## Ligand CTP F 403



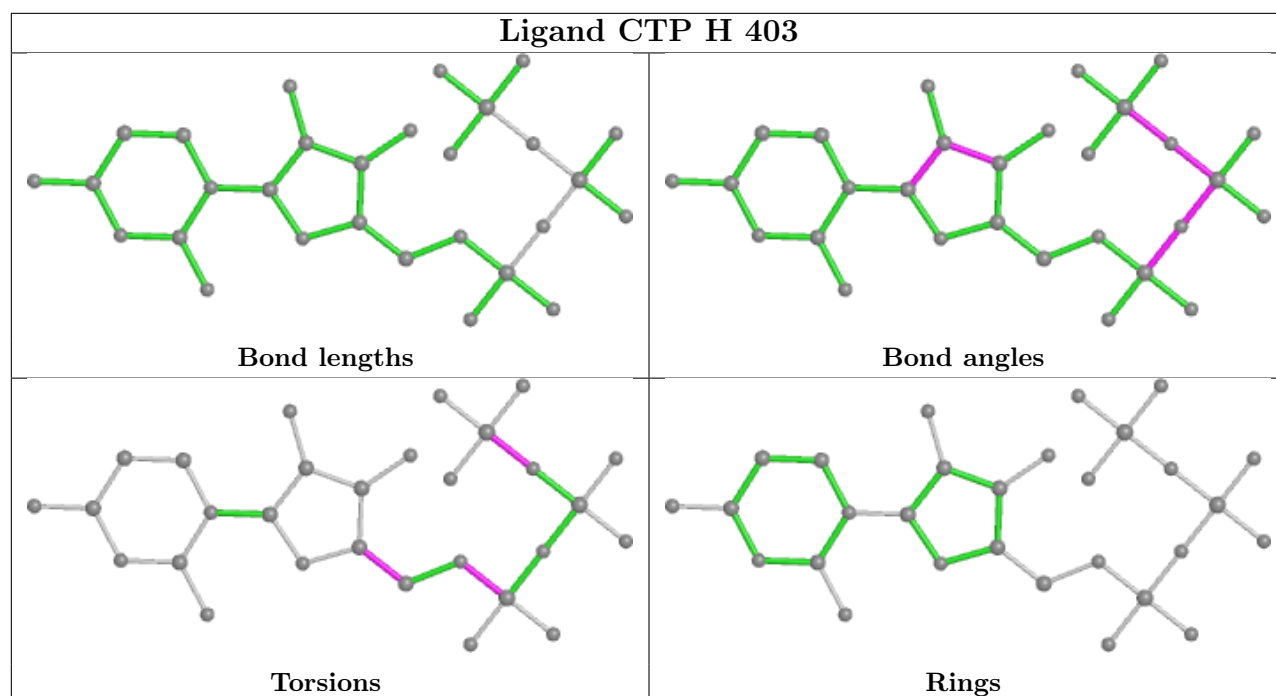
## Ligand CTP E 402

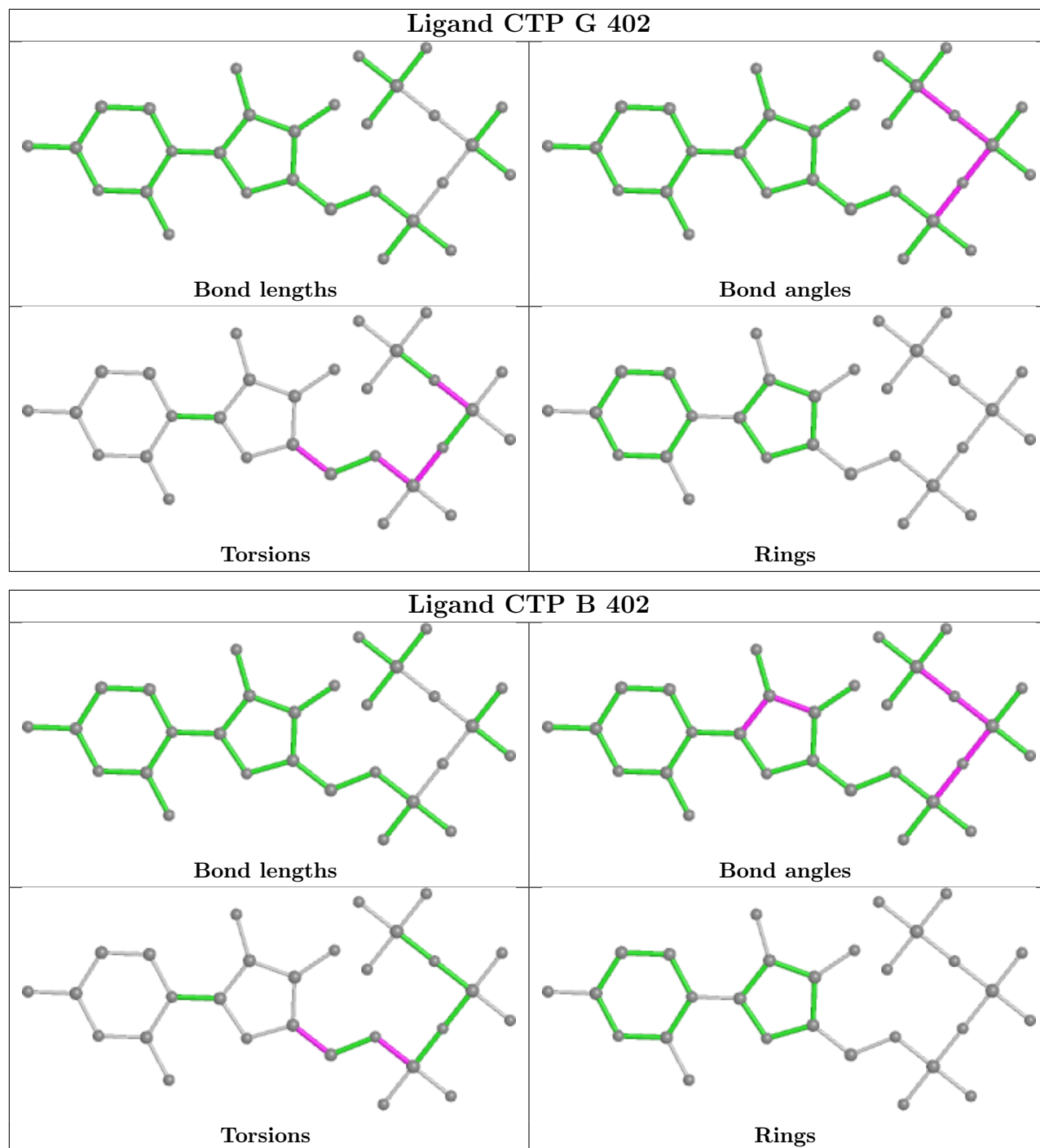


## Ligand CTP I 402



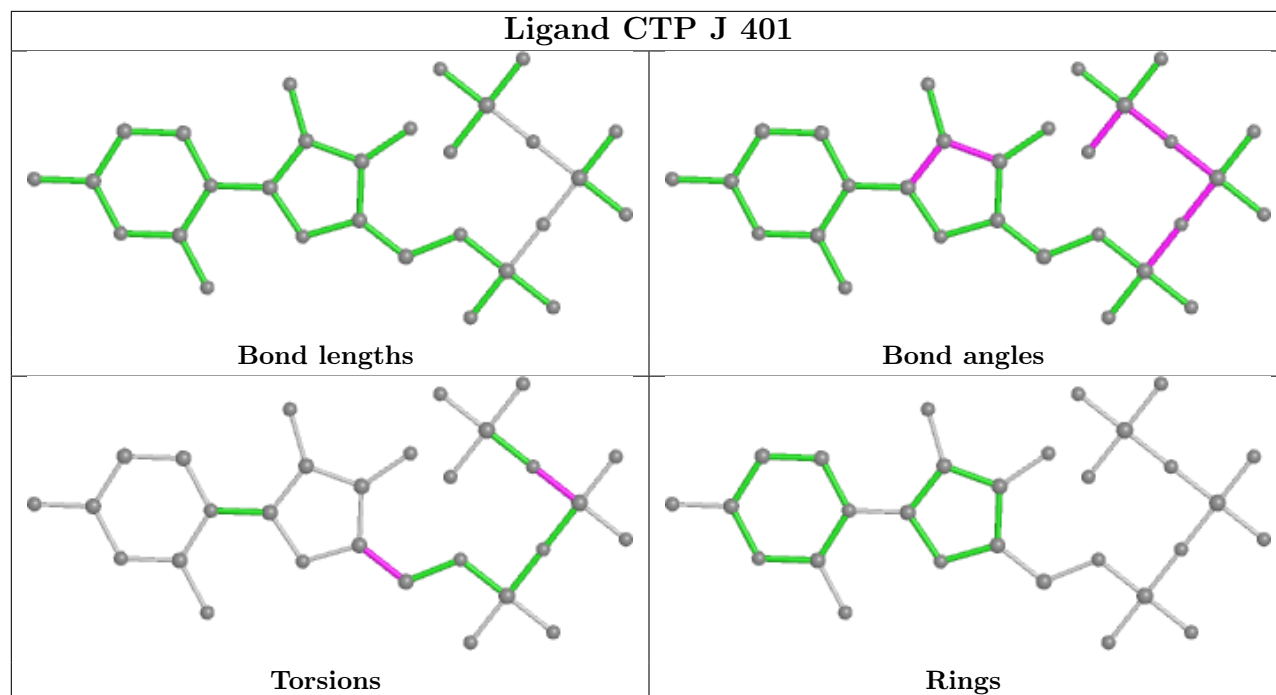
## Ligand CTP H 403



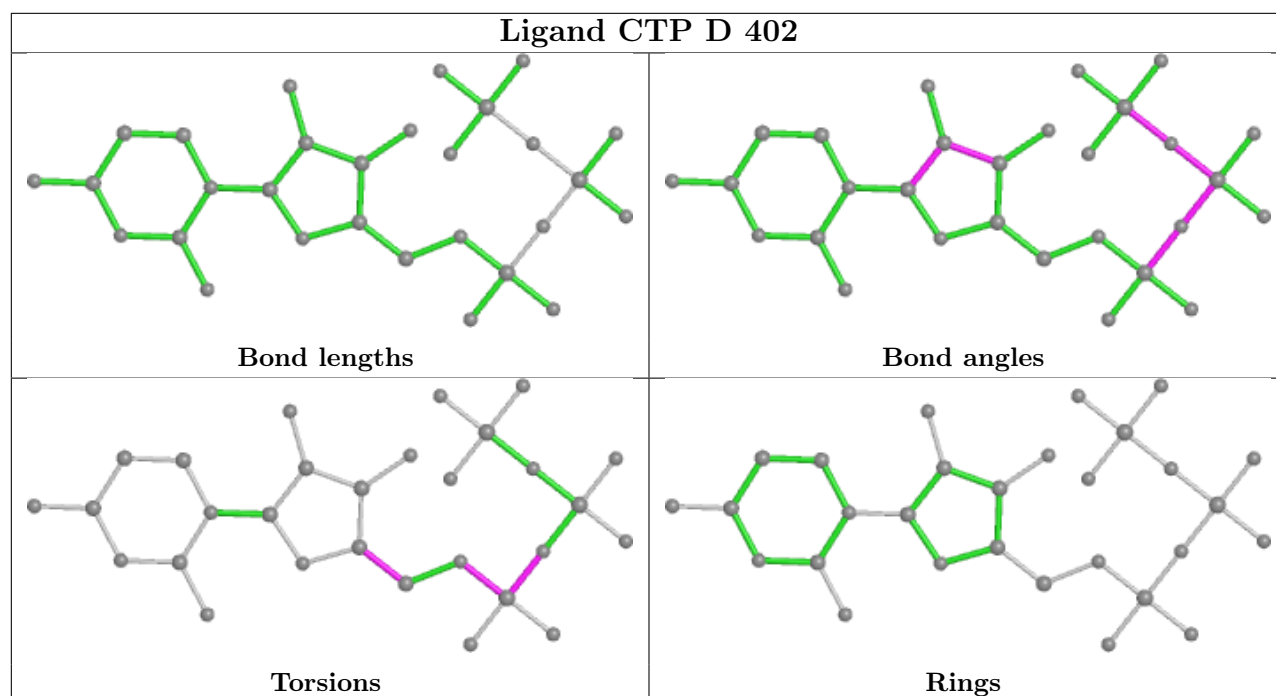


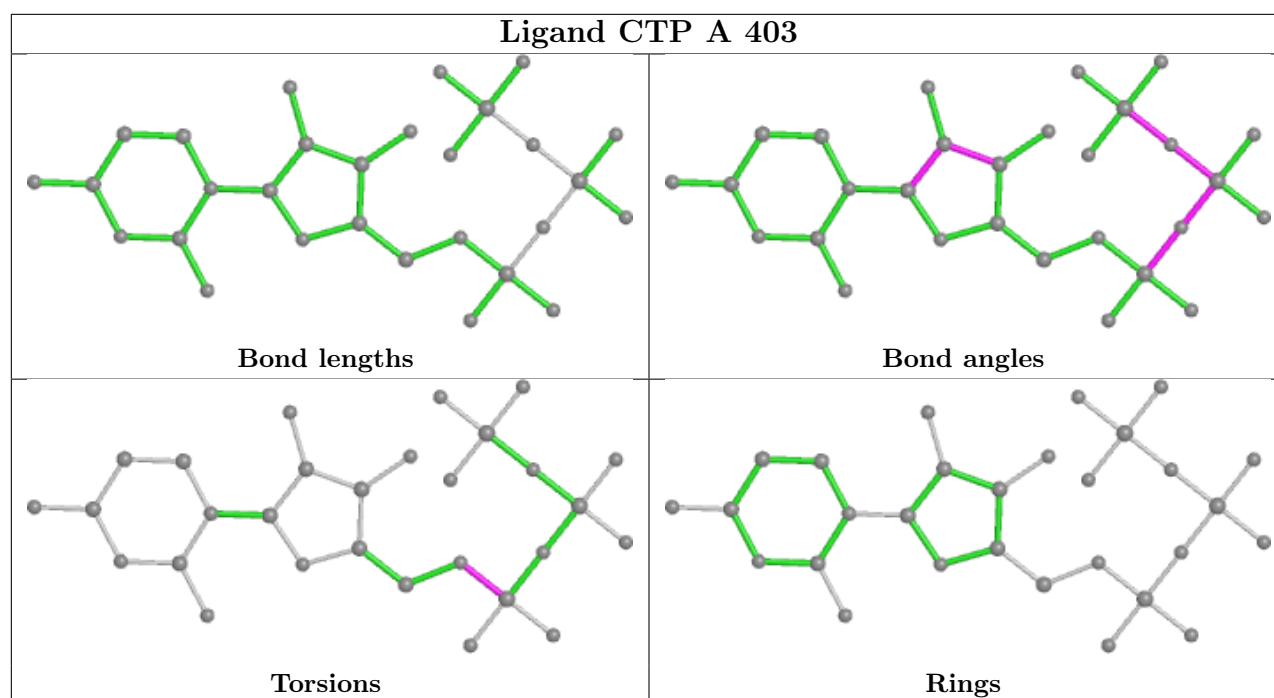


## Ligand CTP J 401



## Ligand CTP D 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, 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	349/362 (96%)	-0.03	1 (0%) <span>94</span> <span>96</span>	44, 73, 126, 176	0
1	B	349/362 (96%)	0.01	12 (3%) <span>45</span> <span>52</span>	49, 78, 134, 170	0
1	C	353/362 (97%)	-0.11	4 (1%) <span>80</span> <span>85</span>	47, 71, 125, 183	0
1	D	342/362 (94%)	0.54	40 (11%) <span>4</span> <span>6</span>	41, 102, 170, 202	0
1	E	348/362 (96%)	-0.03	7 (2%) <span>65</span> <span>72</span>	48, 80, 134, 195	0
1	F	339/362 (93%)	0.05	14 (4%) <span>37</span> <span>44</span>	42, 84, 143, 184	0
1	G	352/362 (97%)	-0.12	1 (0%) <span>94</span> <span>96</span>	47, 84, 132, 186	0
1	H	345/362 (95%)	0.17	17 (4%) <span>29</span> <span>35</span>	43, 95, 163, 194	0
1	I	346/362 (95%)	0.11	8 (2%) <span>60</span> <span>67</span>	55, 101, 148, 203	0
1	J	286/362 (79%)	0.89	54 (18%) <span>1</span> <span>1</span>	49, 114, 182, 215	0
All	All	3409/3620 (94%)	0.13	158 (4%) <span>32</span> <span>39</span>	41, 85, 157, 215	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	166	TYR	12.6
1	J	35	CYS	10.4
1	J	132	PHE	8.1
1	J	38	VAL	7.6
1	J	31	ILE	6.7
1	J	32	ARG	6.4
1	D	148	VAL	6.3
1	B	110	MET	5.9
1	J	158	VAL	5.9
1	H	63	TYR	5.6
1	H	61	ASN	5.2
1	J	210	LEU	5.1
1	D	53	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	J	232	LEU	5.0
1	J	123	LEU	5.0
1	J	98	ALA	4.9
1	F	87	ASN	4.8
1	D	83	MET	4.8
1	J	80	LEU	4.7
1	D	165	ARG	4.6
1	F	88	PHE	4.6
1	D	161	ARG	4.6
1	J	162	ILE	4.6
1	I	52	PHE	4.5
1	D	160	LEU	4.4
1	J	34	VAL	4.4
1	F	194	TRP	4.4
1	D	63	TYR	4.4
1	J	116	PHE	4.4
1	B	88	PHE	4.2
1	D	174	PHE	4.2
1	I	62	ARG	4.2
1	D	80	LEU	4.2
1	H	83	MET	4.1
1	J	186	HIS	4.1
1	J	191	HIS	4.0
1	J	160	LEU	4.0
1	E	83	MET	3.9
1	A	83[A]	MET	3.8
1	H	41	VAL	3.8
1	D	113	TRP	3.8
1	J	97	CYS	3.8
1	J	29	LYS	3.7
1	J	167	VAL	3.7
1	I	192	ILE	3.6
1	D	106	ARG	3.6
1	D	52	PHE	3.6
1	E	88	PHE	3.6
1	D	38	VAL	3.6
1	F	182	ARG	3.6
1	J	36	LYS	3.6
1	J	136	VAL	3.6
1	J	172	PRO	3.4
1	J	127	LYS	3.4
1	B	102	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	172	PRO	3.4
1	E	106	ARG	3.3
1	H	37	VAL	3.3
1	H	34	VAL	3.3
1	D	145	TYR	3.2
1	J	94	LEU	3.2
1	D	215	CYS	3.2
1	J	77	VAL	3.2
1	D	47	VAL	3.2
1	F	119	ALA	3.1
1	J	230	TRP	3.1
1	I	189	LEU	3.1
1	J	96	GLY	3.0
1	D	149	VAL	3.0
1	D	162	ILE	3.0
1	D	158	VAL	3.0
1	J	212	SER	3.0
1	J	128	ILE	2.9
1	F	122	TYR	2.9
1	J	28	ALA	2.9
1	B	86	PHE	2.9
1	D	166	TYR	2.9
1	D	132	PHE	2.9
1	G	174	PHE	2.9
1	J	42	LEU	2.9
1	J	41	VAL	2.8
1	I	190	PRO	2.8
1	J	211	LEU	2.8
1	H	191	HIS	2.8
1	F	189	LEU	2.8
1	C	190	PRO	2.8
1	B	85	VAL	2.8
1	D	194	TRP	2.8
1	H	88	PHE	2.8
1	J	197	PRO	2.8
1	D	167	VAL	2.7
1	D	-1	ALA	2.7
1	D	78	LEU	2.7
1	B	94	LEU	2.6
1	F	86	PHE	2.6
1	H	93	SER	2.6
1	J	176	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	189	LEU	2.6
1	D	105	GLY	2.6
1	J	122	TYR	2.6
1	J	196	GLY	2.6
1	I	191	HIS	2.6
1	J	79	TYR	2.6
1	J	-1	ALA	2.5
1	F	80	LEU	2.5
1	H	0	MET	2.5
1	E	85	VAL	2.5
1	J	165	ARG	2.5
1	D	136	VAL	2.5
1	J	78	LEU	2.5
1	F	180	TRP	2.5
1	F	230	TRP	2.5
1	H	52	PHE	2.5
1	J	39	SER	2.5
1	H	82	GLN	2.5
1	H	90	ASP	2.4
1	D	94	LEU	2.4
1	D	287	ARG	2.4
1	E	108	ARG	2.4
1	J	99	VAL	2.4
1	D	34	VAL	2.4
1	F	99	VAL	2.4
1	D	48	GLN	2.4
1	F	93	SER	2.3
1	J	161	ARG	2.3
1	D	64	GLU	2.3
1	D	37	VAL	2.3
1	B	109	SER	2.3
1	J	170	ILE	2.3
1	C	-2	GLY	2.3
1	H	147	ASP	2.3
1	J	25	ALA	2.3
1	E	198	ASN	2.2
1	B	84	GLY	2.2
1	E	103	SER	2.2
1	J	183	SER	2.2
1	J	124	SER	2.2
1	D	85	VAL	2.2
1	H	59	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	189	LEU	2.2
1	J	48	GLN	2.1
1	D	140	VAL	2.1
1	H	62	ARG	2.1
1	I	174	PHE	2.1
1	C	191	HIS	2.1
1	D	81	ASN	2.1
1	J	74	PHE	2.1
1	H	-2	GLY	2.1
1	F	85	VAL	2.1
1	J	63	TYR	2.1
1	B	56	LEU	2.1
1	J	125	ALA	2.1
1	D	152	VAL	2.1
1	B	82	GLN	2.1
1	B	83	MET	2.0
1	D	150	LYS	2.0
1	I	98	ALA	2.0
1	B	190	PRO	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 monosaccharides 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
3	TMO	C	403	5/5	0.83	0.40	130,130,132,137	0
2	CIT	C	401	13/13	0.84	0.14	86,104,126,130	0
4	CTP	I	402	29/29	0.84	0.22	117,146,189,197	0
2	CIT	I	401	13/13	0.85	0.24	104,112,141,144	0

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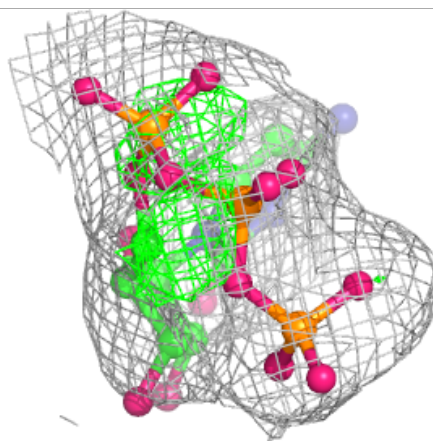
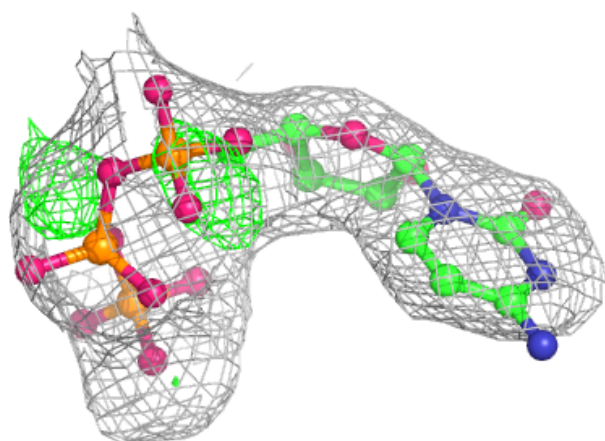
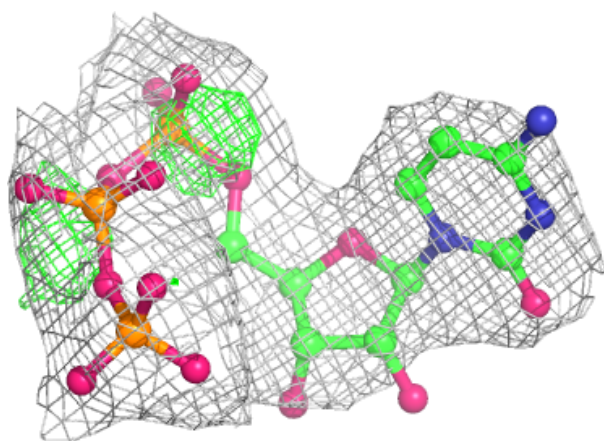
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	G	401	13/13	0.87	0.19	107,119,134,139	0
2	CIT	A	401	13/13	0.88	0.19	88,115,146,147	0
2	CIT	H	401	13/13	0.88	0.14	93,123,140,142	0
2	CIT	D	401	13/13	0.89	0.15	78,109,137,142	0
2	CIT	F	401	13/13	0.90	0.12	94,115,131,134	0
3	TMO	F	402	5/5	0.90	0.26	109,113,116,116	0
2	CIT	B	401	13/13	0.91	0.13	84,94,123,129	0
3	TMO	A	402	5/5	0.92	0.18	109,112,113,115	0
4	CTP	H	403	29/29	0.93	0.16	82,124,129,130	0
2	CIT	H	402	13/13	0.93	0.11	106,115,124,128	0
4	CTP	J	401	29/29	0.93	0.18	91,126,136,157	0
2	CIT	E	401	13/13	0.94	0.10	87,100,110,117	0
3	TMO	C	402	5/5	0.94	0.55	97,103,104,109	0
4	CTP	D	402	29/29	0.95	0.19	82,117,129,130	0
4	CTP	B	402	29/29	0.97	0.14	55,77,94,119	0
4	CTP	E	402	29/29	0.97	0.14	60,78,89,108	0
4	CTP	G	402	29/29	0.97	0.15	74,94,110,114	0
4	CTP	C	404	29/29	0.97	0.15	52,75,92,99	0
4	CTP	F	403	29/29	0.98	0.14	55,68,82,94	0
4	CTP	A	403	29/29	0.98	0.17	45,64,83,85	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.



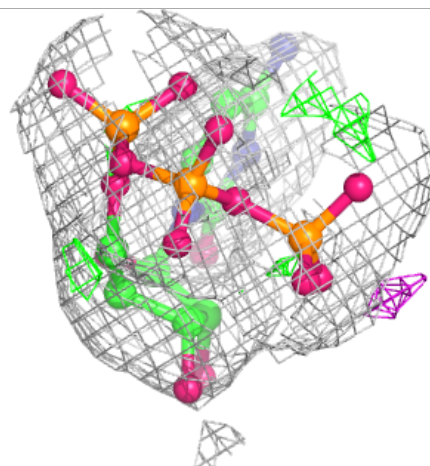
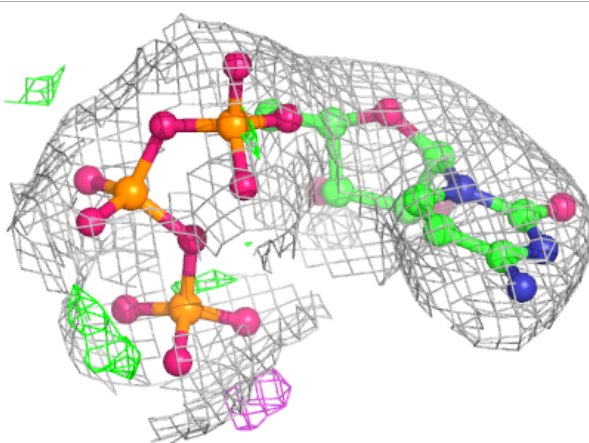
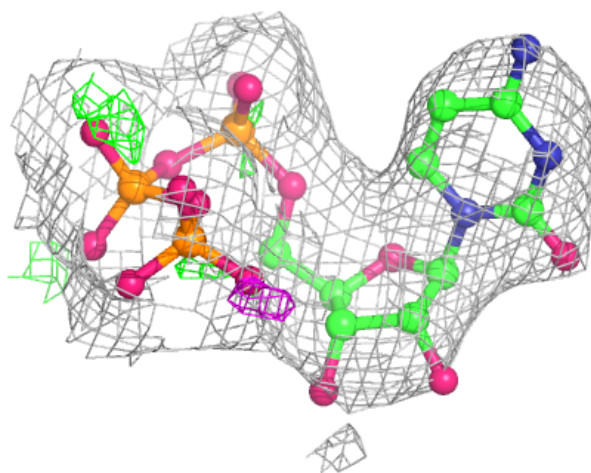
**Electron density around CTP I 402:**

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



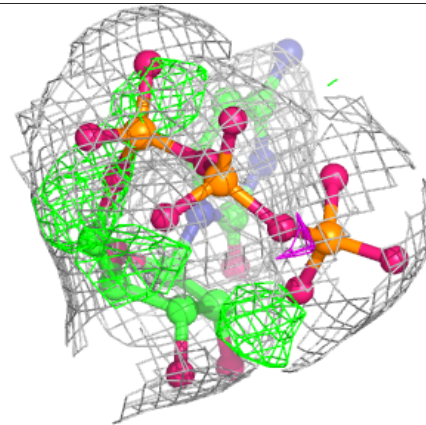
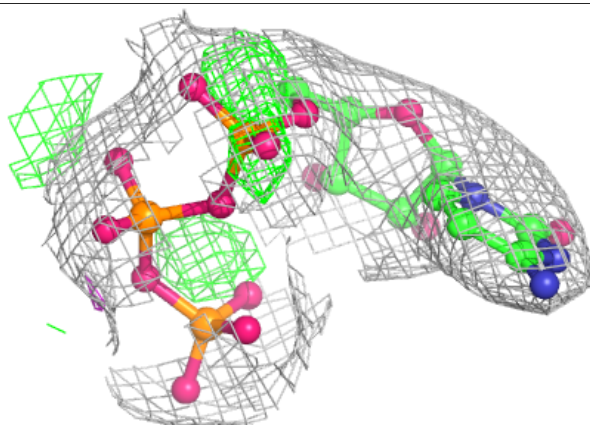
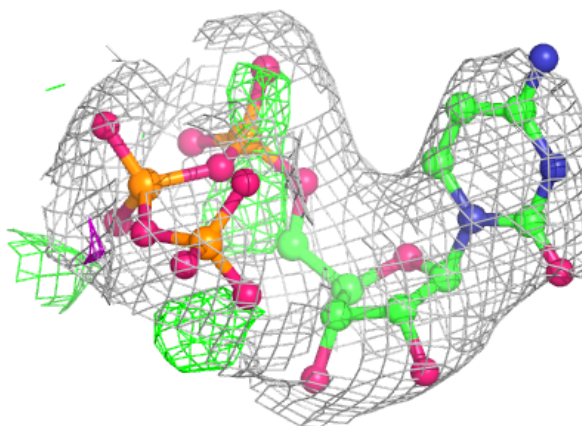
**Electron density around CTP H 403:**

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



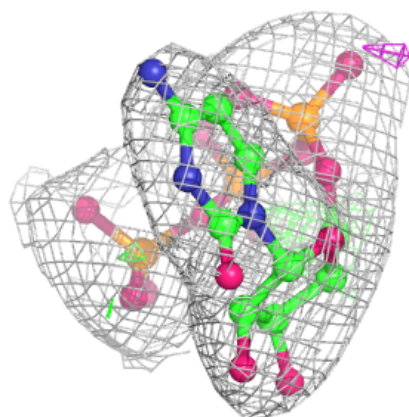
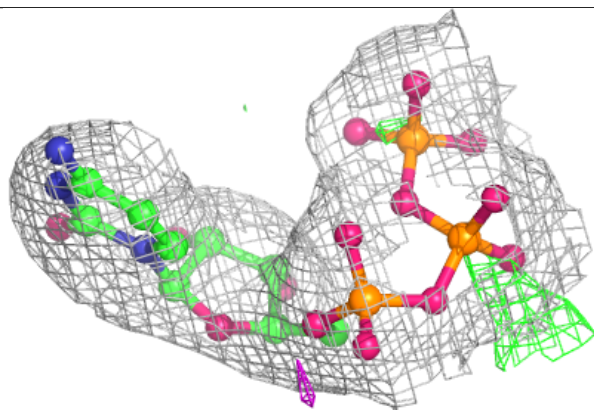
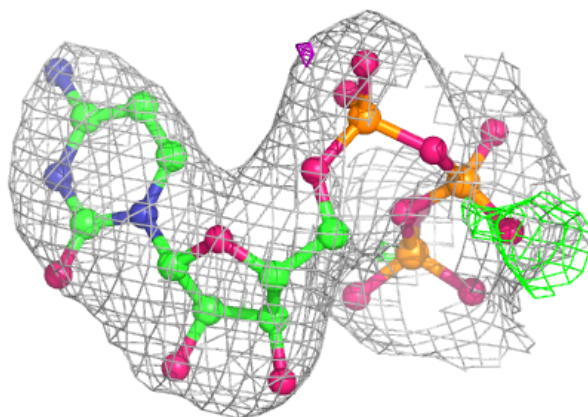
**Electron density around CTP J 401:**

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

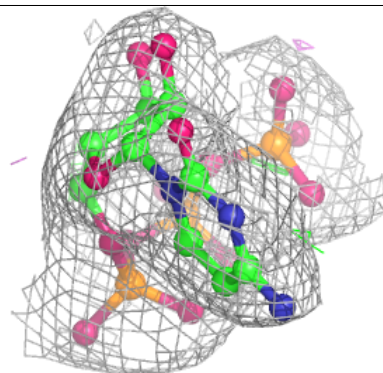
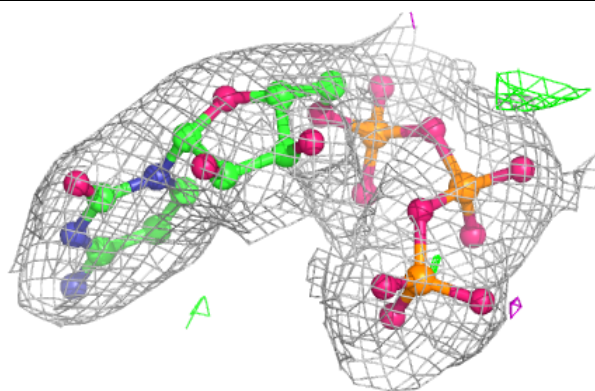
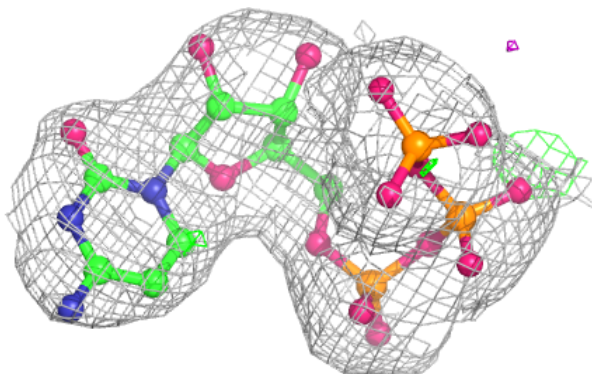


**Electron density around CTP D 402:**

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

**Electron density around CTP B 402:**

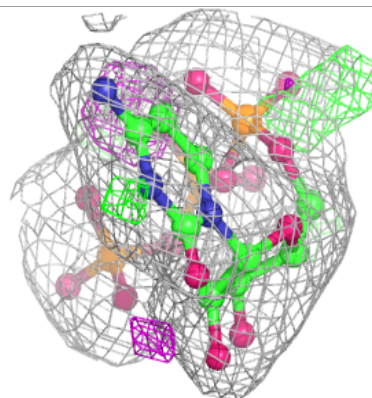
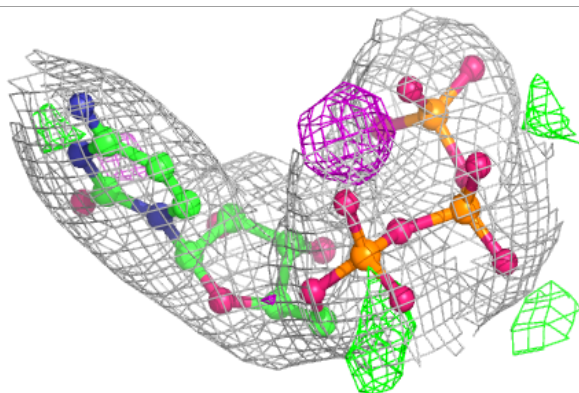
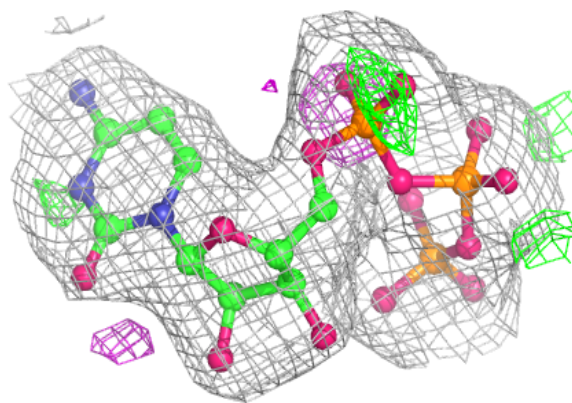
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



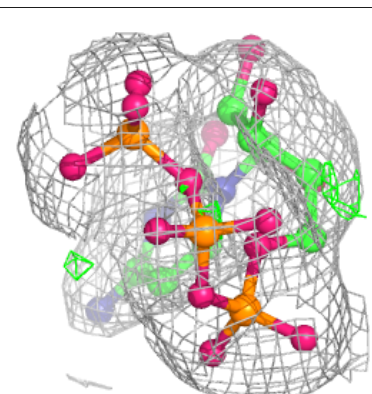
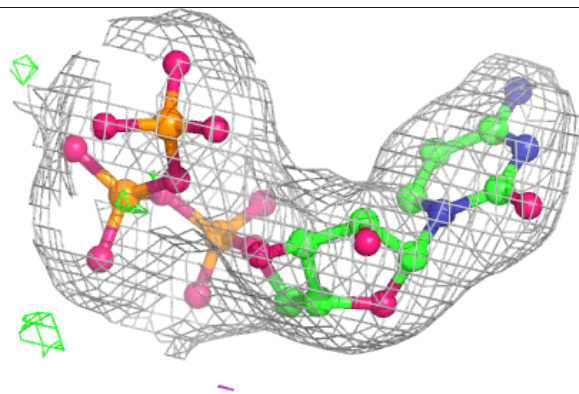
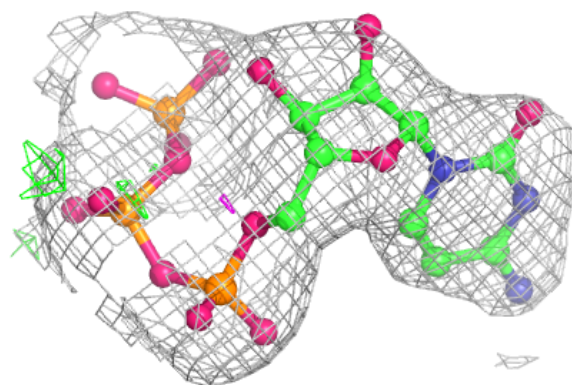


**Electron density around CTP E 402:**

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

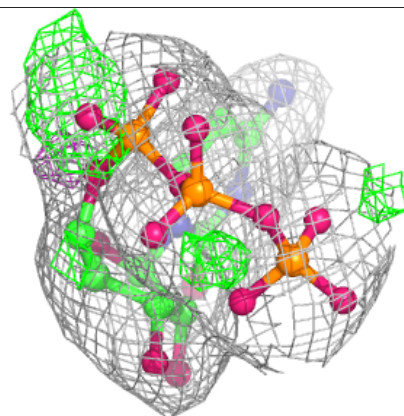
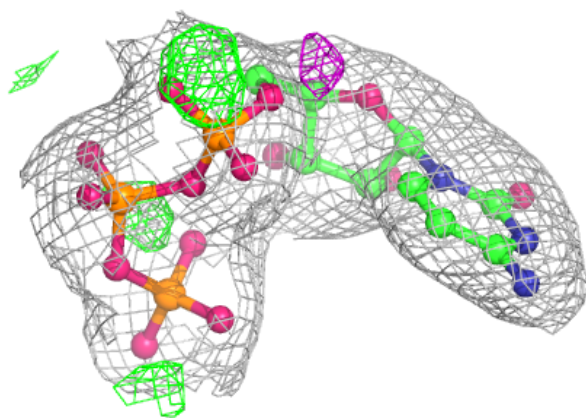
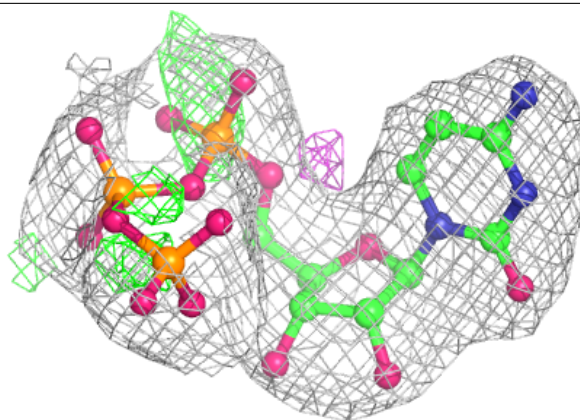
**Electron density around CTP G 402:**

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



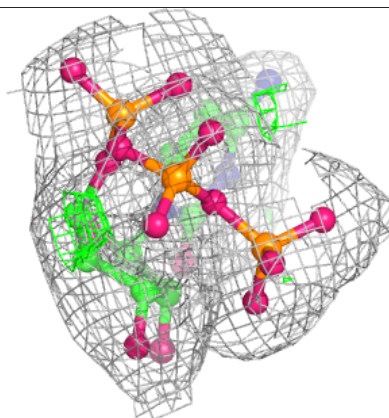
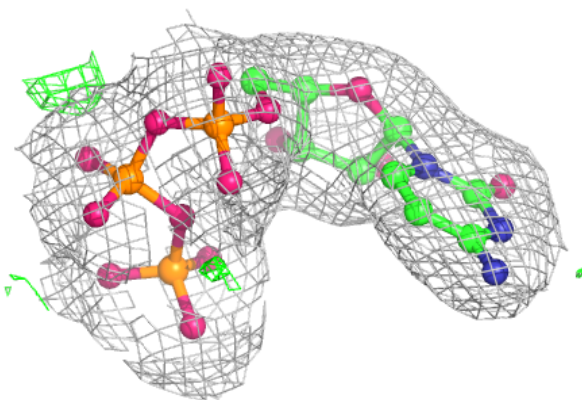
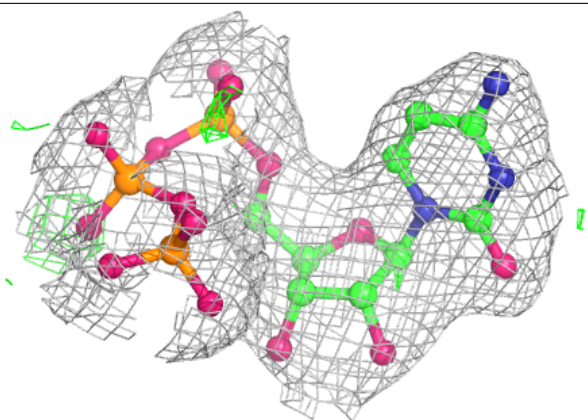
**Electron density around CTP C 404:**

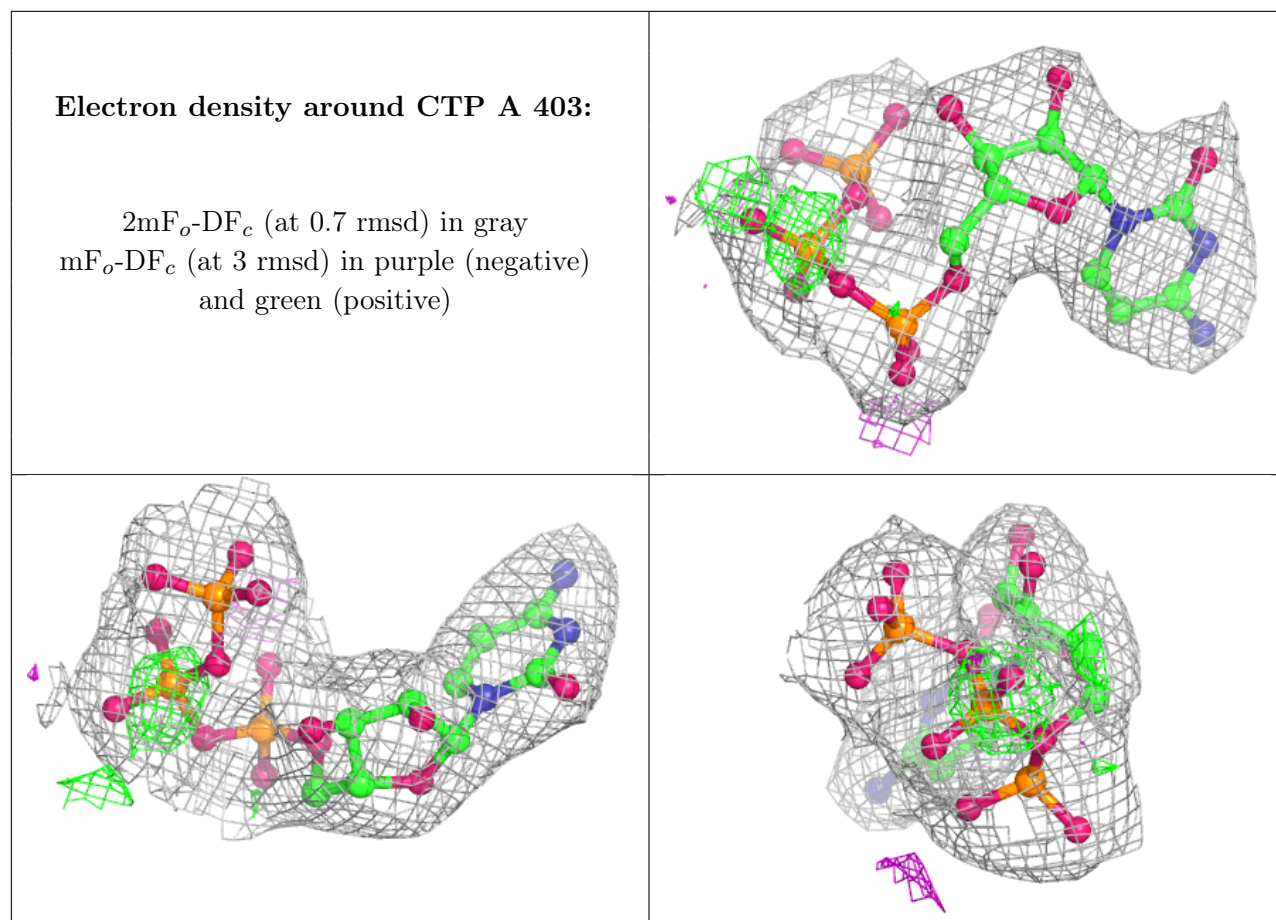
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CTP F 403:**

$2mF_o-DF_c$  (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.