



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:25 am BST

PDB ID : 1XDY
Title : Structural and Biochemical Identification of a Novel Bacterial Oxidoreductase, W-containing cofactor
Authors : Loschi, L.; Brokx, S.J.; Hills, T.L.; Zhang, G.; Bertero, M.G.; Lovering, A.L.; Weiner, J.H.; Strynadka, N.C.
Deposited on : 2004-09-08
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

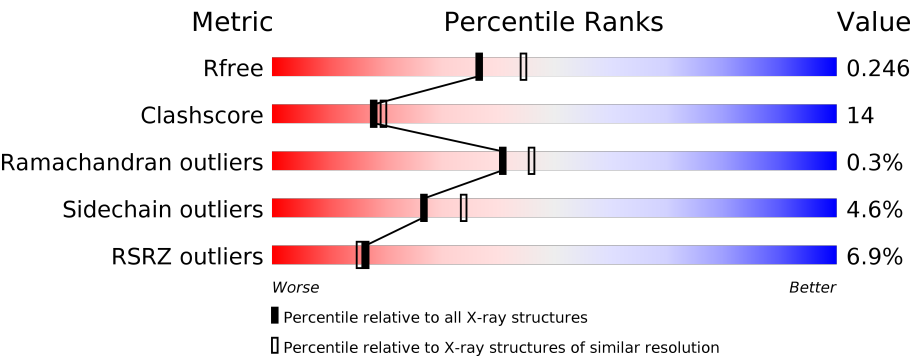
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






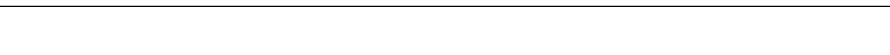
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	298	<div><div>3%</div><div><div></div><div>67%</div><div>18%</div><div>•</div><div>12%</div></div></div>
1	B	298	<div><div>9%</div><div><div></div><div>60%</div><div>27%</div><div>•</div><div>12%</div></div></div>
1	C	298	<div><div>3%</div><div><div></div><div>67%</div><div>19%</div><div>•</div><div>11%</div></div></div>
1	D	298	<div><div>%</div><div><div></div><div>65%</div><div>22%</div><div>•</div><div>12%</div></div></div>
1	E	298	<div><div>3%</div><div><div></div><div>69%</div><div>18%</div><div>•</div><div>12%</div></div></div>
1	F	298	<div><div>16%</div><div><div></div><div>60%</div><div>26%</div><div>•</div><div>12%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	298	
1	H	298	
1	I	298	
1	J	298	

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
3	MTE	A	301	X	-	-	-
3	MTE	B	302	X	-	-	-
3	MTE	C	303	X	-	-	-
3	MTE	D	304	X	-	-	-
3	MTE	E	305	X	-	-	-
3	MTE	F	306	X	-	-	-
3	MTE	G	307	X	-	-	-
3	MTE	H	308	X	-	-	-
3	MTE	I	309	X	-	-	-
3	MTE	J	310	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21369 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 Bacterial Sulfite Oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2093	1358	354	375	6			
1	B	262	Total	C	N	O	S	0	0	0
			2088	1354	353	375	6			
1	C	264	Total	C	N	O	S	0	0	0
			2102	1363	356	377	6			
1	D	263	Total	C	N	O	S	0	0	0
			2094	1357	355	376	6			
1	E	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			
1	F	262	Total	C	N	O	S	1	0	0
			2084	1352	352	374	6			
1	G	261	Total	C	N	O	S	0	0	0
			2079	1349	351	373	6			
1	H	264	Total	C	N	O	S	11	0	0
			2102	1363	356	377	6			
1	I	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			
1	J	262	Total	C	N	O	S	0	0	0
			2085	1351	353	375	6			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	ASP	ALA	SEE REMARK 999	UNP P76342
A	291	LEU	-	EXPRESSION TAG	UNP P76342
A	292	GLU	-	EXPRESSION TAG	UNP P76342
A	293	HIS	-	EXPRESSION TAG	UNP P76342
A	294	HIS	-	EXPRESSION TAG	UNP P76342
A	295	HIS	-	EXPRESSION TAG	UNP P76342
A	296	HIS	-	EXPRESSION TAG	UNP P76342
A	297	HIS	-	EXPRESSION TAG	UNP P76342
A	298	HIS	-	EXPRESSION TAG	UNP P76342

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Chain	Residue	Modelled	Actual	Comment	Reference
B	275	ASP	ALA	SEE REMARK 999	UNP P76342
B	291	LEU	-	EXPRESSION TAG	UNP P76342
B	292	GLU	-	EXPRESSION TAG	UNP P76342
B	293	HIS	-	EXPRESSION TAG	UNP P76342
B	294	HIS	-	EXPRESSION TAG	UNP P76342
B	295	HIS	-	EXPRESSION TAG	UNP P76342
B	296	HIS	-	EXPRESSION TAG	UNP P76342
B	297	HIS	-	EXPRESSION TAG	UNP P76342
B	298	HIS	-	EXPRESSION TAG	UNP P76342
C	275	ASP	ALA	SEE REMARK 999	UNP P76342
C	291	LEU	-	EXPRESSION TAG	UNP P76342
C	292	GLU	-	EXPRESSION TAG	UNP P76342
C	293	HIS	-	EXPRESSION TAG	UNP P76342
C	294	HIS	-	EXPRESSION TAG	UNP P76342
C	295	HIS	-	EXPRESSION TAG	UNP P76342
C	296	HIS	-	EXPRESSION TAG	UNP P76342
C	297	HIS	-	EXPRESSION TAG	UNP P76342
C	298	HIS	-	EXPRESSION TAG	UNP P76342
D	275	ASP	ALA	SEE REMARK 999	UNP P76342
D	291	LEU	-	EXPRESSION TAG	UNP P76342
D	292	GLU	-	EXPRESSION TAG	UNP P76342
D	293	HIS	-	EXPRESSION TAG	UNP P76342
D	294	HIS	-	EXPRESSION TAG	UNP P76342
D	295	HIS	-	EXPRESSION TAG	UNP P76342
D	296	HIS	-	EXPRESSION TAG	UNP P76342
D	297	HIS	-	EXPRESSION TAG	UNP P76342
D	298	HIS	-	EXPRESSION TAG	UNP P76342
E	275	ASP	ALA	SEE REMARK 999	UNP P76342
E	291	LEU	-	EXPRESSION TAG	UNP P76342
E	292	GLU	-	EXPRESSION TAG	UNP P76342
E	293	HIS	-	EXPRESSION TAG	UNP P76342
E	294	HIS	-	EXPRESSION TAG	UNP P76342
E	295	HIS	-	EXPRESSION TAG	UNP P76342
E	296	HIS	-	EXPRESSION TAG	UNP P76342
E	297	HIS	-	EXPRESSION TAG	UNP P76342
E	298	HIS	-	EXPRESSION TAG	UNP P76342
F	275	ASP	ALA	SEE REMARK 999	UNP P76342
F	291	LEU	-	EXPRESSION TAG	UNP P76342
F	292	GLU	-	EXPRESSION TAG	UNP P76342
F	293	HIS	-	EXPRESSION TAG	UNP P76342
F	294	HIS	-	EXPRESSION TAG	UNP P76342
F	295	HIS	-	EXPRESSION TAG	UNP P76342

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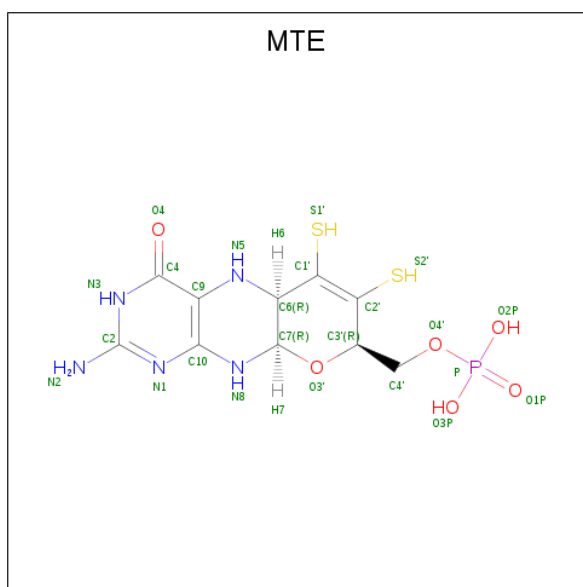
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Chain	Residue	Modelled	Actual	Comment	Reference
F	296	HIS	-	EXPRESSION TAG	UNP P76342
F	297	HIS	-	EXPRESSION TAG	UNP P76342
F	298	HIS	-	EXPRESSION TAG	UNP P76342
G	275	ASP	ALA	SEE REMARK 999	UNP P76342
G	291	LEU	-	EXPRESSION TAG	UNP P76342
G	292	GLU	-	EXPRESSION TAG	UNP P76342
G	293	HIS	-	EXPRESSION TAG	UNP P76342
G	294	HIS	-	EXPRESSION TAG	UNP P76342
G	295	HIS	-	EXPRESSION TAG	UNP P76342
G	296	HIS	-	EXPRESSION TAG	UNP P76342
G	297	HIS	-	EXPRESSION TAG	UNP P76342
G	298	HIS	-	EXPRESSION TAG	UNP P76342
H	275	ASP	ALA	SEE REMARK 999	UNP P76342
H	291	LEU	-	EXPRESSION TAG	UNP P76342
H	292	GLU	-	EXPRESSION TAG	UNP P76342
H	293	HIS	-	EXPRESSION TAG	UNP P76342
H	294	HIS	-	EXPRESSION TAG	UNP P76342
H	295	HIS	-	EXPRESSION TAG	UNP P76342
H	296	HIS	-	EXPRESSION TAG	UNP P76342
H	297	HIS	-	EXPRESSION TAG	UNP P76342
H	298	HIS	-	EXPRESSION TAG	UNP P76342
I	275	ASP	ALA	SEE REMARK 999	UNP P76342
I	291	LEU	-	EXPRESSION TAG	UNP P76342
I	292	GLU	-	EXPRESSION TAG	UNP P76342
I	293	HIS	-	EXPRESSION TAG	UNP P76342
I	294	HIS	-	EXPRESSION TAG	UNP P76342
I	295	HIS	-	EXPRESSION TAG	UNP P76342
I	296	HIS	-	EXPRESSION TAG	UNP P76342
I	297	HIS	-	EXPRESSION TAG	UNP P76342
I	298	HIS	-	EXPRESSION TAG	UNP P76342
J	275	ASP	ALA	SEE REMARK 999	UNP P76342
J	291	LEU	-	EXPRESSION TAG	UNP P76342
J	292	GLU	-	EXPRESSION TAG	UNP P76342
J	293	HIS	-	EXPRESSION TAG	UNP P76342
J	294	HIS	-	EXPRESSION TAG	UNP P76342
J	295	HIS	-	EXPRESSION TAG	UNP P76342
J	296	HIS	-	EXPRESSION TAG	UNP P76342
J	297	HIS	-	EXPRESSION TAG	UNP P76342
J	298	HIS	-	EXPRESSION TAG	UNP P76342

- Molecule 2 is TUNGSTEN ION (three-letter code: W) (formula: W).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total W 1 1	0	0
2	J	1	Total W 1 1	0	0
2	D	1	Total W 1 1	0	0
2	E	1	Total W 1 1	0	0
2	H	1	Total W 1 1	0	0
2	B	1	Total W 1 1	0	0
2	I	1	Total W 1 1	0	0
2	C	1	Total W 1 1	0	0
2	A	1	Total W 1 1	0	0
2	F	1	Total W 1 1	0	0

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆P₂).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	E	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	F	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	G	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	H	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	I	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	J	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

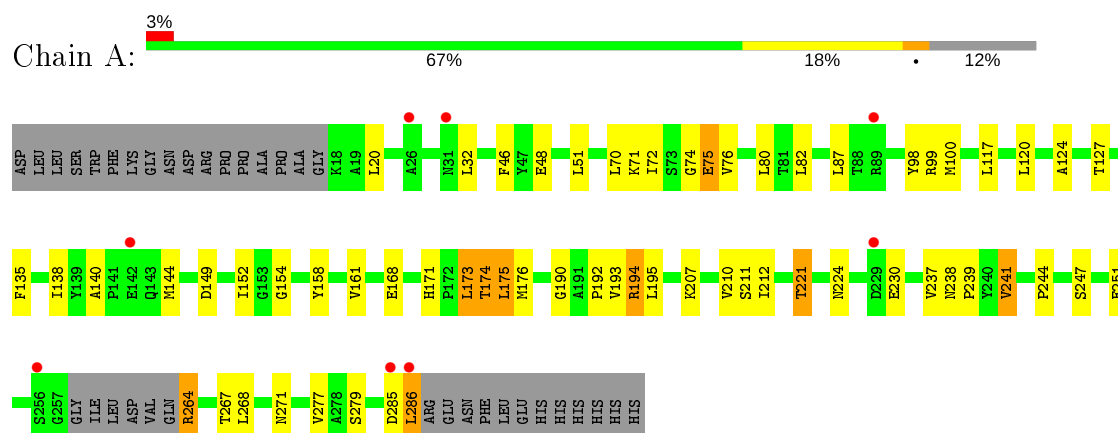
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	13	Total	O	0	0
			13	13		
4	C	32	Total	O	0	0
			32	32		
4	D	30	Total	O	0	0
			30	30		
4	E	29	Total	O	0	0
			29	29		
4	F	10	Total	O	0	0
			10	10		
4	G	22	Total	O	0	0
			22	22		
4	H	4	Total	O	0	0
			4	4		
4	I	12	Total	O	0	0
			12	12		
4	J	35	Total	O	0	0
			35	35		

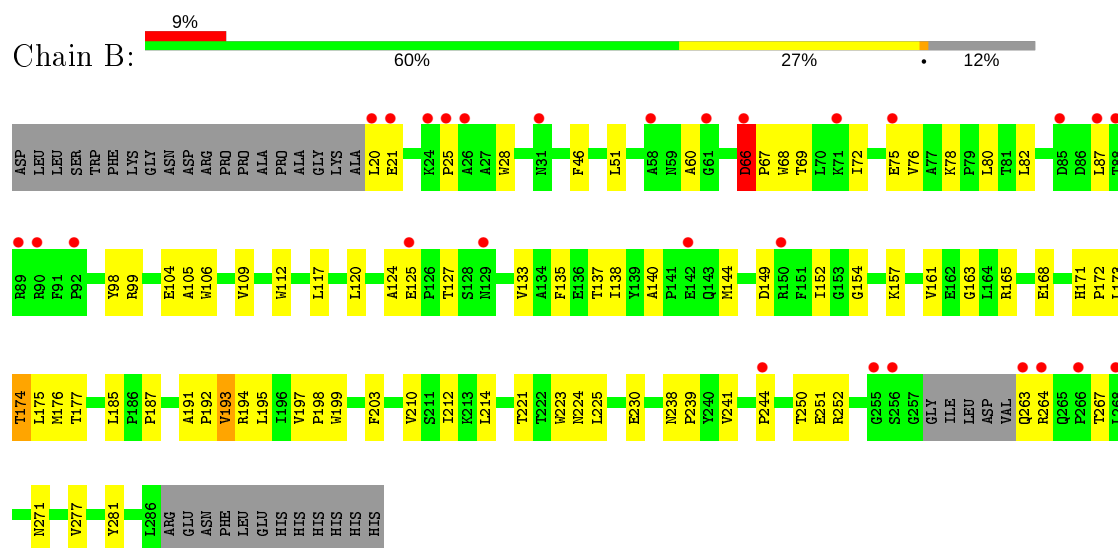
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

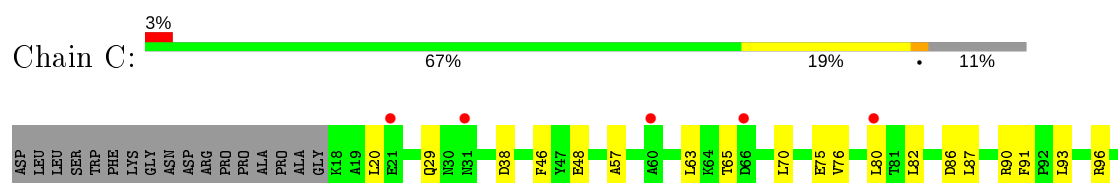
• Molecule 1: Bacterial Sulfite Oxidase

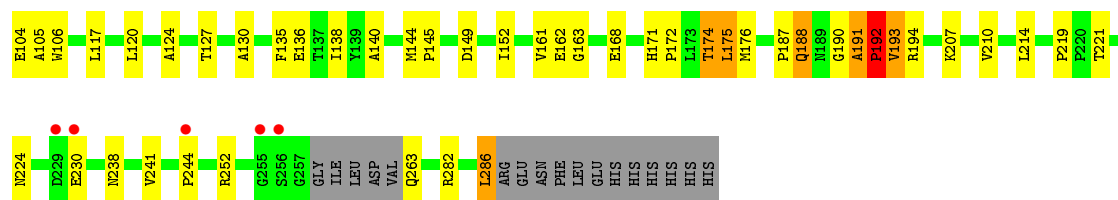


• Molecule 1: Bacterial Sulfite Oxidase

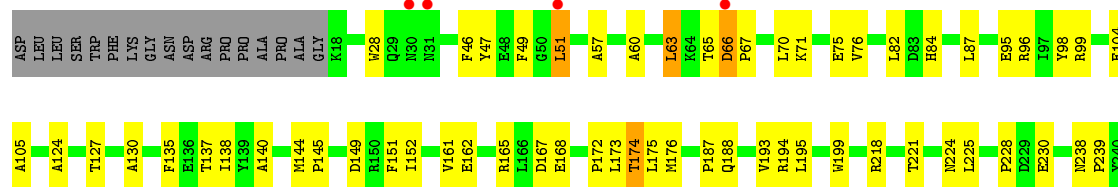


• Molecule 1: Bacterial Sulfite Oxidase

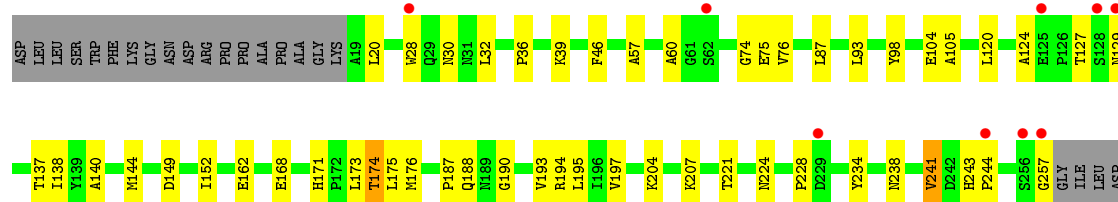




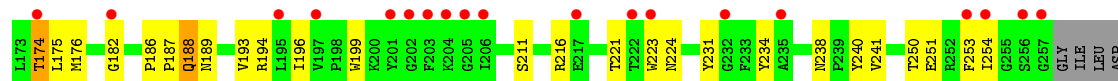
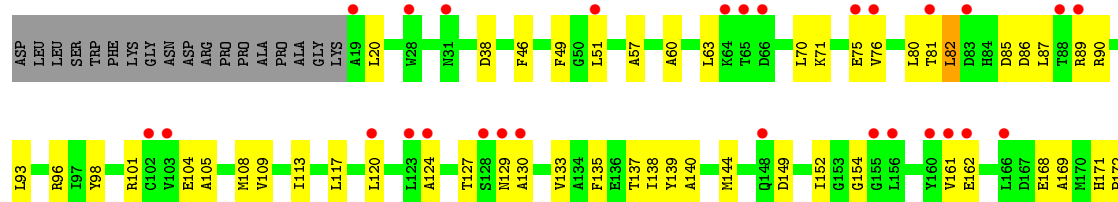
• Molecule 1: Bacterial Sulfite Oxidase



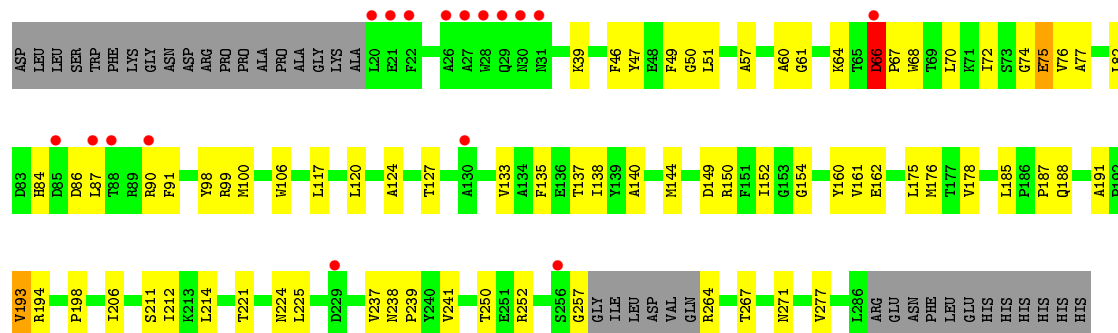
• Molecule 1: Bacterial Sulfite Oxidase



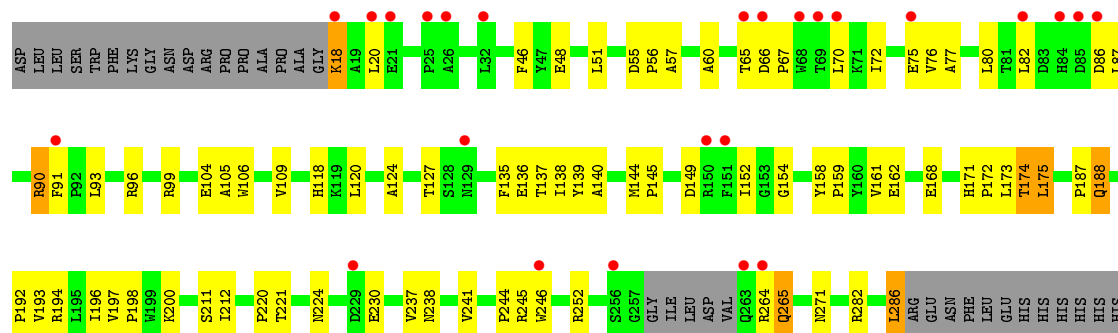
• Molecule 1: Bacterial Sulfite Oxidase



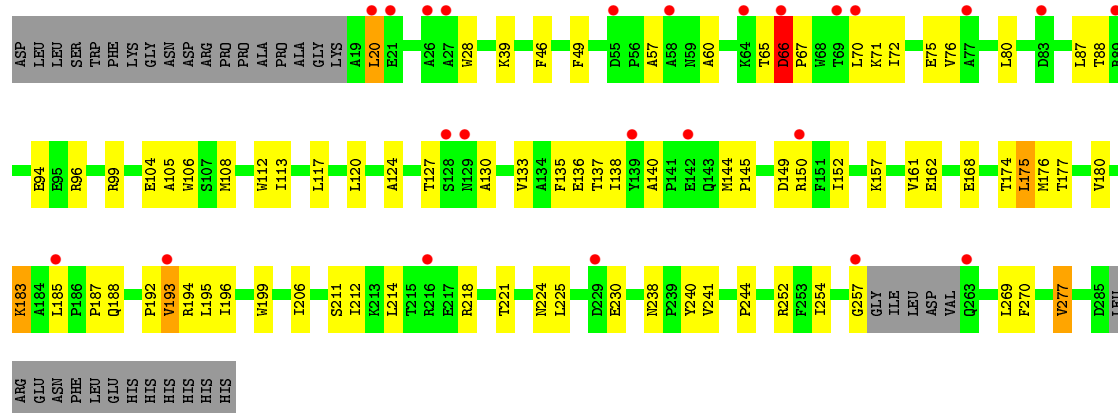
- Molecule 1: Bacterial Sulfite Oxidase



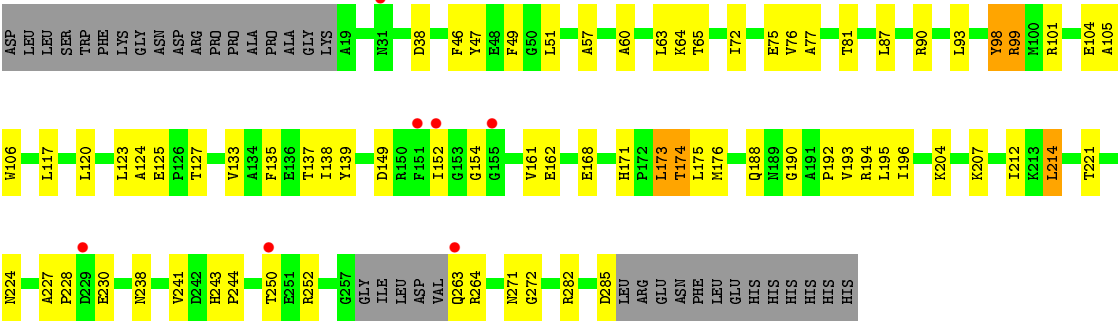
- Molecule 1: Bacterial Sulfite Oxidase



- Molecule 1: Bacterial Sulfite Oxidase



- Molecule 1: Bacterial Sulfite Oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.84Å 177.51Å 104.21Å 90.00° 109.73° 90.00°	Depositor
Resolution (Å)	38.96 – 2.20 38.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.96-2.20) 98.6 (38.96-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.258 0.213 , 0.246	Depositor DCC
R_{free} test set	4389 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21369	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: W, MTE

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	0.57	1/2158 (0.0%)	0.76	2/2942 (0.1%)
1	B	0.43	0/2153	0.69	2/2936 (0.1%)
1	C	0.51	0/2167	0.85	3/2954 (0.1%)
1	D	0.53	0/2159	0.77	1/2943 (0.0%)
1	E	0.55	0/2150	0.75	1/2932 (0.0%)
1	F	0.42	0/2149	0.69	0/2931
1	G	0.53	0/2144	0.75	1/2924 (0.0%)
1	H	0.40	0/2167	0.67	1/2954 (0.0%)
1	I	0.45	0/2150	0.70	1/2932 (0.0%)
1	J	0.58	0/2150	0.77	0/2932
All	All	0.50	1/21547 (0.0%)	0.74	12/29380 (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	A	0	1
1	E	0	1
1	J	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	ARG	CB-CG	-5.40	1.38	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	ALA	C-N-CD	-20.12	76.34	120.60
1	C	191	ALA	C-N-CA	13.52	178.78	122.00
1	A	175	LEU	CA-CB-CG	7.14	131.72	115.30
1	G	66	ASP	C-N-CD	7.09	143.29	128.40
1	B	66	ASP	C-N-CD	6.70	142.46	128.40
1	A	194	ARG	CG-CD-NE	-6.23	98.72	111.80
1	C	192	PRO	CA-N-CD	-5.92	103.21	111.50
1	I	66	ASP	C-N-CD	5.89	140.77	128.40
1	D	66	ASP	C-N-CD	5.83	140.65	128.40
1	E	197	VAL	N-CA-C	-5.82	95.29	111.00
1	B	109	VAL	N-CA-C	-5.30	96.69	111.00
1	H	109	VAL	N-CA-C	-5.23	96.88	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	TYR	Sidechain
1	E	234	TYR	Sidechain
1	J	98	TYR	Sidechain

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	2093	0	2067	49	0
1	B	2088	0	2057	62	0
1	C	2102	0	2075	53	0
1	D	2094	0	2064	63	0
1	E	2085	0	2051	46	0
1	F	2084	0	2054	63	0
1	G	2079	0	2049	54	0
1	H	2102	0	2075	58	0
1	I	2085	0	2051	67	0
1	J	2085	0	2051	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	24	0	9	0	0
3	B	24	0	9	0	0
3	C	24	0	9	0	0
3	D	24	0	9	0	0
3	E	24	0	9	0	0
3	F	24	0	9	0	0
3	G	24	0	9	0	0
3	H	24	0	9	0	0
3	I	24	0	9	0	0
3	J	24	0	9	0	0
4	A	35	0	0	1	0
4	B	13	0	0	1	0
4	C	32	0	0	2	0
4	D	30	0	0	0	0
4	E	29	0	0	1	0
4	F	10	0	0	0	0
4	G	22	0	0	1	0
4	H	4	0	0	0	0
4	I	12	0	0	0	0
4	J	35	0	0	2	0
All	All	21369	0	20684	565	0

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 14.

All (565) 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:D:250:THR:HG23	1:D:264:ARG:HH21	1.33	0.92
1:H:57:ALA:HA	1:H:188:GLN:HG2	1.51	0.92
1:B:20:LEU:HG	1:B:21:GLU:H	1.35	0.90
1:A:140:ALA:HB3	1:A:144:MET:HE3	1.52	0.88
1:E:140:ALA:HB3	1:E:144:MET:HE3	1.56	0.86
1:I:57:ALA:HA	1:I:188:GLN:HG2	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:ALA:HA	1:E:188:GLN:HG2	1.60	0.84
1:J:221:THR:HG21	4:J:440:HOH:O	1.76	0.84
1:E:87:LEU:HD13	1:E:193:VAL:HG22	1.59	0.83
1:J:250:THR:HG23	1:J:264:ARG:HE	1.44	0.82
1:G:250:THR:HG23	1:G:264:ARG:HH21	1.44	0.81
1:H:66:ASP:HB3	1:H:67:PRO:HD3	1.63	0.81
1:E:30:ASN:HD22	1:E:32:LEU:H	1.29	0.81
1:C:57:ALA:HA	1:C:188:GLN:HG2	1.60	0.81
1:D:230:GLU:HG2	1:D:244:PRO:HG2	1.61	0.80
1:G:76:VAL:HG13	1:G:124:ALA:O	1.82	0.79
1:E:57:ALA:HA	1:E:188:GLN:CG	2.12	0.79
1:J:57:ALA:HA	1:J:188:GLN:CG	2.13	0.79
1:A:87:LEU:HD13	1:A:193:VAL:HG22	1.62	0.79
1:F:211:SER:OG	1:H:282:ARG:HD3	1.84	0.78
1:A:76:VAL:HG13	1:A:124:ALA:O	1.83	0.78
1:D:75:GLU:HG3	1:D:127:THR:OG1	1.84	0.78
1:H:286:LEU:HD22	1:H:286:LEU:H	1.47	0.78
1:H:76:VAL:HG13	1:H:124:ALA:O	1.84	0.78
1:I:75:GLU:HG3	1:I:127:THR:OG1	1.84	0.78
1:I:230:GLU:HG2	1:I:244:PRO:HG2	1.66	0.78
1:I:28:TRP:CG	1:I:96:ARG:HG2	2.19	0.77
1:G:140:ALA:HB3	1:G:144:MET:HE3	1.65	0.77
1:H:168:GLU:O	1:H:174:THR:HG21	1.83	0.77
1:B:176:MET:HE1	1:B:195:LEU:HD13	1.65	0.77
1:C:57:ALA:HA	1:C:188:GLN:CG	2.15	0.77
1:J:230:GLU:HG2	1:J:244:PRO:HG2	1.64	0.77
1:G:87:LEU:HD13	1:G:193:VAL:HG22	1.66	0.77
1:I:72:ILE:HD13	1:I:212:ILE:HB	1.67	0.76
1:J:149:ASP:HB3	1:J:152:ILE:HB	1.68	0.76
1:C:65:THR:HB	1:C:192:PRO:CD	2.16	0.76
1:D:57:ALA:HA	1:D:188:GLN:CG	2.16	0.76
1:D:87:LEU:HD13	1:D:193:VAL:HG22	1.67	0.75
1:H:57:ALA:HA	1:H:188:GLN:CG	2.16	0.74
1:J:87:LEU:HD13	1:J:193:VAL:CG2	2.17	0.74
1:B:99:ARG:HG3	1:B:271:ASN:ND2	2.03	0.74
1:C:221:THR:HG21	4:C:426:HOH:O	1.85	0.74
1:I:57:ALA:HA	1:I:188:GLN:CG	2.18	0.73
1:J:221:THR:HG22	1:J:224:ASN:H	1.53	0.73
1:H:230:GLU:HG2	1:H:244:PRO:HG2	1.68	0.73
1:H:87:LEU:HD13	1:H:193:VAL:HG22	1.69	0.72
1:C:238:ASN:HB3	1:C:241:VAL:HG12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:ASN:HB3	1:J:241:VAL:HG12	1.72	0.72
1:A:221:THR:HG22	1:A:224:ASN:H	1.55	0.71
1:A:168:GLU:O	1:A:174:THR:HG21	1.91	0.71
1:I:87:LEU:HD13	1:I:193:VAL:HG22	1.73	0.71
1:C:140:ALA:HB3	1:C:144:MET:HE3	1.71	0.71
1:H:238:ASN:HB3	1:H:241:VAL:HG12	1.72	0.71
1:F:57:ALA:HA	1:F:188:GLN:CG	2.21	0.70
1:I:137:THR:HG22	1:I:138:ILE:N	2.06	0.70
1:I:39:LYS:NZ	1:I:257:GLY:H	1.89	0.70
1:G:57:ALA:HA	1:G:188:GLN:HG3	1.73	0.70
1:C:168:GLU:O	1:C:174:THR:HG21	1.92	0.70
1:D:162:GLU:OE2	1:D:221:THR:HG23	1.91	0.70
1:E:238:ASN:HB3	1:E:241:VAL:CG1	2.22	0.70
1:A:99:ARG:HD2	1:A:271:ASN:O	1.91	0.69
1:H:60:ALA:HB1	1:H:187:PRO:HB2	1.75	0.69
1:F:60:ALA:HB1	1:F:187:PRO:HB2	1.72	0.69
1:C:187:PRO:HA	1:C:191:ALA:HB2	1.75	0.69
1:A:176:MET:HE1	1:A:195:LEU:HD13	1.76	0.68
1:B:87:LEU:HD13	1:B:193:VAL:HG22	1.75	0.68
1:C:65:THR:HB	1:C:192:PRO:HD3	1.74	0.68
1:H:96:ARG:HD2	1:H:175:LEU:HD13	1.75	0.68
1:I:133:VAL:HG22	1:I:214:LEU:HD13	1.75	0.68
1:I:162:GLU:OE2	1:I:221:THR:HG23	1.94	0.68
1:J:75:GLU:HG3	1:J:127:THR:OG1	1.93	0.68
1:H:162:GLU:OE2	1:H:221:THR:HG23	1.94	0.68
1:J:168:GLU:O	1:J:174:THR:HG21	1.93	0.68
1:B:230:GLU:HG2	1:B:244:PRO:HG2	1.74	0.68
1:E:87:LEU:HD13	1:E:193:VAL:CG2	2.24	0.68
1:G:51:LEU:HD21	1:G:154:GLY:CA	2.23	0.68
1:F:120:LEU:O	1:F:120:LEU:HD23	1.93	0.68
1:H:149:ASP:HB3	1:H:152:ILE:HB	1.75	0.67
1:I:66:ASP:HB3	1:I:67:PRO:HD3	1.75	0.67
1:A:32:LEU:HD11	1:A:99:ARG:HH11	1.59	0.67
1:D:238:ASN:HB3	1:D:241:VAL:HG12	1.77	0.67
1:G:51:LEU:HD21	1:G:154:GLY:N	2.09	0.67
1:A:51:LEU:HD21	1:A:154:GLY:CA	2.25	0.66
1:J:87:LEU:HD22	1:J:193:VAL:HG21	1.77	0.66
1:E:221:THR:HG22	1:E:224:ASN:H	1.60	0.66
1:B:241:VAL:HG13	4:B:413:HOH:O	1.96	0.66
1:D:250:THR:HG23	1:D:264:ARG:NH2	2.07	0.66
1:F:87:LEU:HD13	1:F:193:VAL:CG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:THR:CG2	1:J:264:ARG:HE	2.08	0.66
1:B:238:ASN:HB3	1:B:241:VAL:CG1	2.26	0.66
1:F:238:ASN:HB3	1:F:241:VAL:HG12	1.78	0.66
1:J:57:ALA:HA	1:J:188:GLN:HG3	1.77	0.66
1:A:99:ARG:HG3	1:A:271:ASN:ND2	2.11	0.65
1:G:221:THR:HG22	1:G:224:ASN:H	1.61	0.65
1:E:241:VAL:HG13	4:E:427:HOH:O	1.95	0.65
1:D:57:ALA:HA	1:D:188:GLN:HG2	1.80	0.64
1:I:76:VAL:HG13	1:I:124:ALA:O	1.97	0.64
1:C:238:ASN:HB3	1:C:241:VAL:CG1	2.27	0.64
1:F:51:LEU:HD21	1:F:154:GLY:CA	2.27	0.64
1:D:149:ASP:OD2	1:D:152:ILE:HG12	1.97	0.64
1:J:63:LEU:HD12	1:J:65:THR:HG23	1.80	0.64
1:I:180:VAL:HG12	1:I:185:LEU:HD23	1.78	0.64
1:D:135:PHE:O	1:D:161:VAL:HG23	1.98	0.64
1:H:57:ALA:CA	1:H:188:GLN:HG2	2.25	0.63
1:B:117:LEU:HD13	1:B:176:MET:HE3	1.79	0.63
1:F:51:LEU:HD21	1:F:154:GLY:HA3	1.81	0.63
1:F:162:GLU:OE2	1:F:221:THR:HG23	1.97	0.63
1:B:168:GLU:O	1:B:174:THR:HG21	1.99	0.63
1:E:57:ALA:CA	1:E:188:GLN:HG2	2.26	0.63
1:H:286:LEU:N	1:H:286:LEU:HD22	2.14	0.62
1:I:57:ALA:CA	1:I:188:GLN:HG2	2.29	0.62
1:B:76:VAL:HG11	1:B:124:ALA:HB1	1.82	0.62
1:F:75:GLU:HG3	1:F:127:THR:OG1	1.98	0.62
1:I:140:ALA:H	1:I:144:MET:HE3	1.64	0.62
1:E:162:GLU:OE2	1:E:221:THR:HG23	1.99	0.62
1:B:238:ASN:HB3	1:B:241:VAL:HG12	1.80	0.62
1:D:28:TRP:CG	1:D:96:ARG:HG2	2.34	0.62
1:J:176:MET:HE1	1:J:195:LEU:HD13	1.81	0.62
1:B:75:GLU:HG3	1:B:127:THR:OG1	2.00	0.62
1:D:76:VAL:HG13	1:D:124:ALA:O	2.00	0.61
1:C:57:ALA:CA	1:C:188:GLN:HG2	2.30	0.61
1:H:221:THR:HG22	1:H:224:ASN:H	1.65	0.61
1:A:149:ASP:HB3	1:A:152:ILE:HB	1.82	0.61
1:H:197:VAL:HG11	1:H:200:LYS:HD2	1.82	0.61
1:J:57:ALA:HA	1:J:188:GLN:HG2	1.82	0.61
1:C:187:PRO:HA	1:C:191:ALA:CB	2.30	0.61
1:G:72:ILE:HD13	1:G:212:ILE:HB	1.81	0.60
1:I:221:THR:HG22	1:I:224:ASN:H	1.67	0.60
1:J:99:ARG:HD3	1:J:271:ASN:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ALA:HB1	1:E:187:PRO:HB2	1.84	0.60
1:J:149:ASP:OD2	1:J:152:ILE:HG12	2.01	0.60
1:B:99:ARG:HD2	1:B:271:ASN:O	2.02	0.60
1:A:75:GLU:HG3	1:A:127:THR:OG1	2.02	0.60
1:G:135:PHE:O	1:G:161:VAL:HG23	2.01	0.60
1:G:72:ILE:HG13	1:G:120:LEU:HD21	1.84	0.60
1:I:20:LEU:HD23	1:I:88:THR:HG21	1.84	0.59
1:J:117:LEU:HD13	1:J:176:MET:HE3	1.83	0.59
1:B:250:THR:HG23	1:B:264:ARG:NH2	2.16	0.59
1:H:82:LEU:HD12	1:H:82:LEU:N	2.17	0.59
1:C:241:VAL:HG13	4:C:435:HOH:O	2.01	0.59
1:D:51:LEU:HD23	1:D:152:ILE:O	2.03	0.59
1:D:250:THR:CG2	1:D:264:ARG:HH21	2.12	0.59
1:F:221:THR:HG22	1:F:224:ASN:H	1.67	0.59
1:F:76:VAL:HG11	1:F:124:ALA:HB1	1.84	0.58
1:C:87:LEU:HD13	1:C:193:VAL:HG22	1.85	0.58
1:F:82:LEU:HD12	1:F:82:LEU:N	2.18	0.58
1:I:199:TRP:CD2	1:I:277:VAL:HG21	2.37	0.58
1:H:18:LYS:HA	1:H:18:LYS:NZ	2.18	0.58
1:A:176:MET:CE	1:A:195:LEU:HD13	2.32	0.58
1:D:176:MET:HE1	1:D:195:LEU:HD13	1.85	0.58
1:D:168:GLU:O	1:D:174:THR:HG21	2.04	0.58
1:H:75:GLU:HG3	1:H:127:THR:OG1	2.04	0.58
1:I:39:LYS:HZ1	1:I:257:GLY:H	1.52	0.58
1:B:98:TYR:HE1	1:B:175:LEU:HD22	1.68	0.57
1:D:57:ALA:HA	1:D:188:GLN:HG3	1.85	0.57
1:I:137:THR:CG2	1:I:138:ILE:N	2.67	0.57
1:D:66:ASP:HB3	1:D:67:PRO:HD3	1.86	0.57
1:G:250:THR:CG2	1:G:264:ARG:HH21	2.16	0.57
1:G:99:ARG:HG3	1:G:271:ASN:ND2	2.18	0.57
1:G:66:ASP:O	1:G:84:HIS:HB2	2.04	0.57
1:A:99:ARG:NH2	1:A:268:LEU:HD12	2.20	0.57
1:E:140:ALA:HB3	1:E:144:MET:CE	2.32	0.57
1:F:129:ASN:HB3	1:F:216:ARG:NH1	2.20	0.57
1:A:285:ASP:O	1:A:286:LEU:HB3	2.05	0.57
1:F:135:PHE:O	1:F:161:VAL:HG23	2.05	0.57
1:H:238:ASN:HB3	1:H:241:VAL:CG1	2.33	0.57
1:E:120:LEU:HD23	1:E:120:LEU:O	2.05	0.57
1:F:250:THR:HG23	1:F:264:ARG:HH21	1.70	0.57
1:I:168:GLU:O	1:I:174:THR:HG21	2.05	0.57
1:A:238:ASN:HB3	1:A:241:VAL:CG1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:ASP:HB3	1:E:152:ILE:HB	1.85	0.56
1:I:238:ASN:HB3	1:I:241:VAL:HG12	1.86	0.56
1:I:28:TRP:CB	1:I:96:ARG:HG2	2.35	0.56
1:A:80:LEU:HD23	1:A:80:LEU:H	1.71	0.56
1:F:57:ALA:HA	1:F:188:GLN:HG3	1.86	0.56
1:G:133:VAL:HG22	1:G:214:LEU:HD13	1.88	0.56
1:B:120:LEU:HD23	1:B:120:LEU:O	2.06	0.56
1:B:60:ALA:HB1	1:B:187:PRO:HB2	1.87	0.56
1:C:65:THR:HB	1:C:192:PRO:CG	2.36	0.56
1:A:239:PRO:HB3	1:A:267:THR:HB	1.88	0.56
1:H:120:LEU:O	1:H:120:LEU:HD23	2.05	0.56
1:B:69:THR:O	1:B:210:VAL:HG23	2.06	0.55
1:E:285:ASP:N	1:E:285:ASP:OD2	2.39	0.55
1:G:57:ALA:HA	1:G:188:GLN:CG	2.36	0.55
1:A:285:ASP:OD1	1:A:286:LEU:N	2.38	0.55
1:B:20:LEU:HG	1:B:21:GLU:N	2.14	0.55
1:F:211:SER:HB2	1:H:282:ARG:NH2	2.21	0.55
1:I:49:PHE:CZ	1:I:144:MET:HG2	2.41	0.55
1:E:39:LYS:NZ	1:E:257:GLY:H	2.05	0.55
1:F:234:TYR:CD2	1:F:286:LEU:HB3	2.41	0.55
1:C:149:ASP:OD2	1:C:152:ILE:HG12	2.06	0.55
1:C:93:LEU:HD12	1:C:93:LEU:N	2.21	0.55
1:G:117:LEU:HD13	1:G:176:MET:HE3	1.88	0.55
1:C:65:THR:HB	1:C:192:PRO:HG3	1.88	0.54
1:J:133:VAL:HG22	1:J:214:LEU:HD13	1.89	0.54
1:D:225:LEU:O	1:D:228:PRO:HD3	2.07	0.54
1:D:96:ARG:NH1	1:D:172:PRO:O	2.40	0.54
1:F:171:HIS:ND1	1:F:172:PRO:HD2	2.22	0.54
1:J:138:ILE:HG12	1:J:139:TYR:N	2.22	0.54
1:D:75:GLU:HG3	1:D:127:THR:HG1	1.70	0.54
1:F:82:LEU:CD1	1:F:82:LEU:N	2.71	0.54
1:G:60:ALA:HB1	1:G:187:PRO:HB2	1.90	0.54
1:H:87:LEU:HD13	1:H:193:VAL:CG2	2.36	0.54
1:D:263:GLN:HE21	1:D:264:ARG:H	1.54	0.54
1:G:238:ASN:HB3	1:G:241:VAL:HG12	1.90	0.54
1:J:117:LEU:HD13	1:J:176:MET:CE	2.38	0.54
1:D:238:ASN:HB3	1:D:241:VAL:CG1	2.37	0.54
1:E:30:ASN:ND2	1:E:32:LEU:H	2.03	0.54
1:D:28:TRP:CB	1:D:96:ARG:HG2	2.38	0.54
1:J:51:LEU:HD21	1:J:154:GLY:CA	2.38	0.53
1:A:87:LEU:HD13	1:A:193:VAL:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:VAL:HG13	1:C:124:ALA:O	2.08	0.53
1:F:87:LEU:HD22	1:F:193:VAL:HG21	1.89	0.53
1:H:66:ASP:HB3	1:H:67:PRO:CD	2.37	0.53
1:J:238:ASN:HB3	1:J:241:VAL:CG1	2.37	0.53
1:F:57:ALA:HA	1:F:188:GLN:HG2	1.90	0.53
1:F:20:LEU:HD11	1:F:113:ILE:HG21	1.91	0.53
1:I:140:ALA:H	1:I:144:MET:CE	2.21	0.53
1:C:75:GLU:HG3	1:C:127:THR:OG1	2.09	0.53
1:E:76:VAL:HG13	1:E:124:ALA:O	2.08	0.53
1:I:20:LEU:H	1:I:20:LEU:HD12	1.73	0.53
1:B:192:PRO:HG2	1:B:193:VAL:HG23	1.90	0.53
1:B:117:LEU:HD13	1:B:176:MET:CE	2.38	0.53
1:C:190:GLY:HA3	1:C:207:LYS:HB3	1.91	0.53
1:E:238:ASN:HB3	1:E:241:VAL:HG13	1.92	0.52
1:J:90:ARG:NH1	1:J:123:LEU:HD11	2.24	0.52
1:H:220:PRO:HB3	1:J:285:ASP:OD1	2.10	0.52
1:C:230:GLU:HG2	1:C:244:PRO:HG2	1.91	0.52
1:A:138:ILE:HG23	1:A:144:MET:CE	2.40	0.52
1:C:120:LEU:C	1:C:120:LEU:HD23	2.30	0.52
1:F:98:TYR:HE1	1:F:175:LEU:HD22	1.74	0.52
1:I:20:LEU:HD23	1:I:88:THR:CG2	2.39	0.52
1:D:104:GLU:O	1:D:105:ALA:HB3	2.10	0.52
1:D:221:THR:HG22	1:D:224:ASN:H	1.74	0.52
1:G:162:GLU:OE2	1:G:221:THR:HG23	2.10	0.52
1:B:149:ASP:HB3	1:B:152:ILE:HB	1.92	0.52
1:H:120:LEU:HD23	1:H:120:LEU:C	2.30	0.52
1:E:98:TYR:HE1	1:E:175:LEU:HD22	1.75	0.51
1:B:99:ARG:HG3	1:B:271:ASN:HD21	1.75	0.51
1:I:149:ASP:HB3	1:I:152:ILE:HB	1.92	0.51
1:D:241:VAL:HG13	1:D:241:VAL:O	2.11	0.51
1:F:238:ASN:HB3	1:F:241:VAL:CG1	2.40	0.51
1:G:106:TRP:HA	1:G:252:ARG:O	2.10	0.51
1:J:57:ALA:CA	1:J:188:GLN:HG2	2.40	0.51
1:G:82:LEU:HD12	1:G:82:LEU:N	2.25	0.51
1:I:106:TRP:HA	1:I:252:ARG:O	2.11	0.51
1:J:76:VAL:HG13	1:J:124:ALA:O	2.10	0.51
1:A:117:LEU:HD13	1:A:176:MET:HE3	1.93	0.51
1:B:104:GLU:O	1:B:105:ALA:HB3	2.10	0.51
1:B:51:LEU:HD21	1:B:154:GLY:CA	2.40	0.51
1:C:138:ILE:HG23	1:C:144:MET:CE	2.41	0.51
1:A:99:ARG:HH21	1:A:268:LEU:HD12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:CG1	1:B:281:TYR:HE2	2.24	0.51
1:G:150:ARG:NH1	1:I:240:TYR:HA	2.26	0.51
1:B:137:THR:HG22	1:B:138:ILE:N	2.25	0.51
1:H:136:GLU:HB3	1:H:211:SER:HB3	1.92	0.51
1:B:171:HIS:CE1	1:B:172:PRO:HG2	2.46	0.51
1:C:190:GLY:CA	1:C:207:LYS:HB3	2.40	0.51
1:C:75:GLU:HB3	1:C:130:ALA:HB2	1.92	0.50
1:F:76:VAL:CG1	1:F:124:ALA:HB1	2.40	0.50
1:F:137:THR:HG22	1:F:138:ILE:N	2.26	0.50
1:F:138:ILE:HG12	1:F:139:TYR:N	2.26	0.50
1:J:241:VAL:O	1:J:241:VAL:HG13	2.10	0.50
1:A:48:GLU:HG3	1:A:158:TYR:CE2	2.46	0.50
1:G:239:PRO:HG3	1:G:267:THR:O	2.12	0.50
1:D:149:ASP:HB3	1:D:152:ILE:HB	1.93	0.50
1:J:63:LEU:C	1:J:63:LEU:HD13	2.32	0.50
1:A:192:PRO:HG2	1:A:193:VAL:HG23	1.93	0.50
1:J:65:THR:HB	1:J:192:PRO:HD3	1.93	0.50
1:A:190:GLY:HA3	1:A:207:LYS:HG2	1.92	0.50
1:F:96:ARG:HD2	1:F:175:LEU:HD13	1.92	0.50
1:H:241:VAL:HG13	1:H:241:VAL:O	2.12	0.50
1:D:49:PHE:CE2	1:D:60:ALA:HA	2.47	0.50
1:F:104:GLU:O	1:F:105:ALA:HB3	2.12	0.50
1:J:98:TYR:HE1	1:J:175:LEU:HD22	1.77	0.50
1:A:72:ILE:HD13	1:A:212:ILE:HB	1.94	0.50
1:F:140:ALA:H	1:F:144:MET:CE	2.24	0.50
1:D:221:THR:HB	1:D:224:ASN:HB3	1.93	0.50
1:F:86:ASP:O	1:F:90:ARG:HB2	2.11	0.50
1:D:98:TYR:HE1	1:D:175:LEU:HD22	1.76	0.49
1:B:251:GLU:O	1:B:264:ARG:HA	2.12	0.49
1:F:223:TRP:HE3	1:F:231:TYR:CE2	2.31	0.49
1:C:93:LEU:CD1	1:C:93:LEU:N	2.74	0.49
1:D:173:LEU:HD11	1:D:276:GLN:NE2	2.28	0.49
1:F:117:LEU:HD13	1:F:176:MET:CE	2.41	0.49
1:G:39:LYS:NZ	1:G:257:GLY:O	2.34	0.49
1:G:239:PRO:HB3	1:G:267:THR:HB	1.93	0.49
1:E:137:THR:HG22	1:E:138:ILE:N	2.26	0.49
1:J:63:LEU:HD12	1:J:65:THR:CG2	2.41	0.49
1:D:28:TRP:HB3	1:D:96:ARG:HG2	1.93	0.49
1:F:171:HIS:CG	1:F:172:PRO:HD2	2.47	0.49
1:D:75:GLU:HB3	1:D:130:ALA:HB2	1.94	0.49
1:D:82:LEU:N	1:D:82:LEU:HD12	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:GLU:OE1	1:E:204:LYS:NZ	2.45	0.49
1:H:139:TYR:HB2	1:H:159:PRO:HB3	1.95	0.49
1:J:224:ASN:O	1:J:228:PRO:HG3	2.13	0.49
1:E:104:GLU:O	1:E:105:ALA:HB3	2.13	0.48
1:H:245:ARG:O	1:H:246:TRP:HB3	2.13	0.48
1:I:96:ARG:HD3	1:I:175:LEU:HD13	1.95	0.48
1:J:77:ALA:HB3	1:J:125:GLU:HB2	1.95	0.48
1:E:168:GLU:O	1:E:174:THR:HG21	2.13	0.48
1:F:140:ALA:H	1:F:144:MET:HE3	1.78	0.48
1:F:250:THR:HG23	1:F:264:ARG:NH2	2.28	0.48
1:G:185:LEU:O	1:G:191:ALA:HB2	2.12	0.48
1:H:90:ARG:HB3	1:H:91:PHE:CD1	2.48	0.48
1:A:251:GLU:HA	1:A:264:ARG:HH22	1.78	0.48
1:G:117:LEU:HD13	1:G:176:MET:CE	2.43	0.48
1:B:210:VAL:O	1:B:210:VAL:HG22	2.12	0.48
1:C:286:LEU:HD13	1:C:286:LEU:N	2.28	0.48
1:C:80:LEU:N	1:C:80:LEU:HD23	2.28	0.48
1:D:176:MET:CE	1:D:195:LEU:HD13	2.43	0.48
1:A:211:SER:OG	1:C:282:ARG:HD3	2.12	0.48
1:A:80:LEU:HD23	1:A:80:LEU:N	2.29	0.48
1:B:106:TRP:HA	1:B:252:ARG:O	2.13	0.48
1:H:48:GLU:HG3	1:H:158:TYR:CE2	2.48	0.48
1:D:263:GLN:HA	1:D:263:GLN:NE2	2.27	0.48
1:H:135:PHE:O	1:H:161:VAL:HG23	2.14	0.48
1:G:120:LEU:HD23	1:G:120:LEU:O	2.14	0.47
1:C:136:GLU:OE1	1:E:282:ARG:HD3	2.14	0.47
1:H:171:HIS:O	1:H:174:THR:HG23	2.14	0.47
1:J:87:LEU:HD13	1:J:193:VAL:HG22	1.93	0.47
1:G:99:ARG:HD2	1:G:271:ASN:O	2.14	0.47
1:G:74:GLY:O	1:G:76:VAL:N	2.43	0.47
1:H:80:LEU:H	1:H:80:LEU:HD23	1.78	0.47
1:J:171:HIS:ND1	1:J:173:LEU:HB2	2.28	0.47
1:J:175:LEU:HD23	1:J:175:LEU:H	1.79	0.47
1:J:272:GLY:HA2	4:J:434:HOH:O	2.14	0.47
1:B:87:LEU:CD1	1:B:193:VAL:HG22	2.43	0.47
1:C:29:GLN:HG2	1:G:61:GLY:HA3	1.95	0.47
1:A:140:ALA:HB3	1:A:144:MET:CE	2.35	0.47
1:D:245:ARG:O	1:D:246:TRP:HB3	2.14	0.47
1:B:199:TRP:CD1	1:B:277:VAL:HG11	2.49	0.47
1:B:51:LEU:HD21	1:B:154:GLY:HA3	1.97	0.47
1:G:75:GLU:HG3	1:G:127:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:PHE:CE2	1:J:60:ALA:HA	2.49	0.47
1:B:176:MET:CE	1:B:195:LEU:HD13	2.41	0.47
1:B:66:ASP:O	1:B:67:PRO:C	2.51	0.47
1:F:168:GLU:O	1:F:174:THR:HG21	2.15	0.47
1:B:149:ASP:OD2	1:B:152:ILE:HG12	2.14	0.47
1:D:51:LEU:HD21	1:D:151:PHE:O	2.14	0.47
1:F:240:TYR:HA	1:I:150:ARG:NH1	2.30	0.47
1:G:66:ASP:O	1:G:68:TRP:N	2.47	0.47
1:H:140:ALA:HB3	1:H:144:MET:HE3	1.97	0.47
1:I:60:ALA:HB1	1:I:187:PRO:HB2	1.95	0.47
1:F:140:ALA:HB3	1:F:144:MET:HE3	1.97	0.47
1:I:112:TRP:CE3	1:I:177:THR:HG21	2.50	0.47
1:I:138:ILE:O	1:I:144:MET:HE1	2.15	0.47
1:C:96:ARG:HD2	1:C:175:LEU:HD13	1.97	0.47
1:A:135:PHE:O	1:A:161:VAL:HG23	2.14	0.46
1:D:57:ALA:CA	1:D:188:GLN:HG2	2.42	0.46
1:E:75:GLU:HG3	1:E:127:THR:OG1	2.15	0.46
1:G:237:VAL:HG21	1:G:271:ASN:HB2	1.97	0.46
1:A:171:HIS:ND1	1:A:173:LEU:HB2	2.31	0.46
1:B:185:LEU:O	1:B:191:ALA:HB2	2.16	0.46
1:D:60:ALA:HB1	1:D:187:PRO:HB2	1.97	0.46
1:F:223:TRP:CE3	1:F:231:TYR:CE2	3.03	0.46
1:E:39:LYS:HZ1	1:E:257:GLY:H	1.64	0.46
1:I:175:LEU:HD23	1:I:196:ILE:HB	1.98	0.46
1:I:136:GLU:HB3	1:I:211:SER:HB3	1.96	0.46
1:C:162:GLU:OE2	1:C:221:THR:HG23	2.16	0.46
1:F:120:LEU:C	1:F:120:LEU:HD23	2.36	0.46
1:J:104:GLU:O	1:J:105:ALA:HB3	2.16	0.46
1:D:63:LEU:HD13	1:D:65:THR:CG2	2.45	0.46
1:B:133:VAL:HG22	1:B:214:LEU:HD13	1.97	0.46
1:B:221:THR:HG22	1:B:224:ASN:H	1.81	0.46
1:F:109:VAL:HG23	1:F:253:PHE:HE1	1.80	0.46
1:H:211:SER:OG	1:J:282:ARG:HD3	2.16	0.46
1:H:264:ARG:O	1:H:265:GLN:HB3	2.15	0.46
1:I:133:VAL:HG22	1:I:214:LEU:CD1	2.44	0.46
1:I:221:THR:HB	1:I:224:ASN:HB3	1.98	0.46
1:D:95:GLU:O	1:D:96:ARG:HG3	2.16	0.45
1:A:286:LEU:C	1:A:286:LEU:HD22	2.36	0.45
1:A:82:LEU:N	1:A:82:LEU:HD12	2.31	0.45
1:B:76:VAL:CG1	1:B:124:ALA:HB1	2.45	0.45
1:I:66:ASP:HB3	1:I:67:PRO:CD	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:VAL:HG11	1:A:124:ALA:HB1	1.97	0.45
1:A:277:VAL:HG12	1:A:277:VAL:O	2.15	0.45
1:B:25:PRO:HB2	1:B:28:TRP:CD1	2.51	0.45
1:B:171:HIS:CG	1:B:172:PRO:HD2	2.51	0.45
1:F:80:LEU:N	1:F:80:LEU:HD23	2.32	0.45
1:I:238:ASN:HB3	1:I:241:VAL:CG1	2.47	0.45
1:C:144:MET:HA	1:C:145:PRO:HD2	1.85	0.45
1:C:135:PHE:O	1:C:161:VAL:HG23	2.17	0.45
1:F:108:MET:HG2	1:F:254:ILE:HB	1.99	0.45
1:F:76:VAL:HG13	1:F:124:ALA:O	2.16	0.45
1:F:171:HIS:ND1	1:F:172:PRO:CD	2.80	0.45
1:I:221:THR:O	1:I:225:LEU:HB2	2.17	0.45
1:E:39:LYS:NZ	1:E:257:GLY:N	2.65	0.45
1:F:113:ILE:HD11	1:F:182:GLY:HA2	1.99	0.45
1:I:72:ILE:CD1	1:I:212:ILE:HB	2.41	0.45
1:J:72:ILE:HD13	1:J:212:ILE:HB	1.99	0.45
1:F:285:ASP:OD1	1:F:286:LEU:N	2.50	0.45
1:G:50:GLY:HA2	1:G:152:ILE:O	2.17	0.45
1:J:106:TRP:HA	1:J:252:ARG:O	2.18	0.45
1:B:112:TRP:CE3	1:B:177:THR:HG21	2.53	0.44
1:C:221:THR:HG22	1:C:224:ASN:H	1.82	0.44
1:G:238:ASN:HB3	1:G:241:VAL:CG1	2.46	0.44
1:I:135:PHE:O	1:I:161:VAL:HG23	2.16	0.44
1:D:140:ALA:H	1:D:144:MET:HE3	1.82	0.44
1:E:39:LYS:HZ1	1:E:257:GLY:N	2.16	0.44
1:D:82:LEU:CD1	1:D:82:LEU:N	2.81	0.44
1:F:57:ALA:CA	1:F:188:GLN:HG2	2.47	0.44
1:G:90:ARG:HB3	1:G:91:PHE:CD1	2.52	0.44
1:B:76:VAL:HG12	1:B:78:LYS:N	2.33	0.44
1:C:82:LEU:HD12	1:C:82:LEU:N	2.32	0.44
1:B:82:LEU:N	1:B:82:LEU:HD12	2.32	0.44
1:C:171:HIS:CG	1:C:172:PRO:HD2	2.53	0.44
1:C:117:LEU:HD13	1:C:176:MET:CE	2.48	0.44
1:C:63:LEU:CD1	1:C:65:THR:HG22	2.48	0.44
1:D:199:TRP:CD1	1:D:277:VAL:HG11	2.53	0.44
1:F:101:ARG:NE	1:F:251:GLU:OE2	2.51	0.44
1:I:120:LEU:HD23	1:I:120:LEU:O	2.18	0.44
1:I:183:LYS:HG2	1:I:183:LYS:H	1.65	0.44
1:I:80:LEU:HD23	1:I:80:LEU:N	2.33	0.44
1:J:190:GLY:CA	1:J:207:LYS:HB3	2.48	0.44
1:B:133:VAL:O	1:B:163:GLY:HA2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:VAL:HG11	1:D:124:ALA:HB1	1.99	0.44
1:H:138:ILE:HG23	1:H:144:MET:CE	2.48	0.44
1:J:135:PHE:O	1:J:161:VAL:HG23	2.17	0.44
1:J:243:HIS:O	1:J:244:PRO:C	2.57	0.44
1:C:106:TRP:HA	1:C:252:ARG:O	2.18	0.44
1:G:76:VAL:HG11	1:G:124:ALA:HB1	1.99	0.44
1:H:82:LEU:CD1	1:H:82:LEU:N	2.81	0.44
1:C:57:ALA:HA	1:C:188:GLN:HG3	1.96	0.43
1:D:137:THR:HG22	1:D:138:ILE:N	2.32	0.43
1:D:165:ARG:NH2	1:D:167:ASP:OD2	2.47	0.43
1:D:87:LEU:CD1	1:D:193:VAL:HG22	2.41	0.43
1:E:57:ALA:HA	1:E:188:GLN:HG3	1.96	0.43
1:I:75:GLU:HB3	1:I:130:ALA:HB2	1.98	0.43
1:I:87:LEU:CD1	1:I:193:VAL:HG22	2.46	0.43
1:J:51:LEU:HD21	1:J:154:GLY:HA3	1.98	0.43
1:H:137:THR:HG22	1:H:138:ILE:N	2.33	0.43
1:H:196:ILE:HG22	1:H:198:PRO:HD3	2.00	0.43
1:E:190:GLY:HA2	1:E:207:LYS:HB3	2.00	0.43
1:B:72:ILE:HD13	1:B:212:ILE:HB	2.00	0.43
1:D:76:VAL:CG1	1:D:124:ALA:HB1	2.49	0.43
1:A:230:GLU:HG2	1:A:244:PRO:HG2	1.99	0.43
1:E:75:GLU:CG	1:E:129:ASN:HB2	2.49	0.43
1:G:149:ASP:HB3	1:G:152:ILE:HB	2.01	0.43
1:G:98:TYR:CE1	1:G:198:PRO:HG3	2.53	0.43
1:B:66:ASP:O	1:B:68:TRP:N	2.52	0.43
1:C:86:ASP:O	1:C:90:ARG:HB2	2.18	0.43
1:D:140:ALA:HB3	1:D:144:MET:HE3	2.00	0.43
1:E:224:ASN:O	1:E:228:PRO:HG3	2.19	0.43
1:H:104:GLU:O	1:H:105:ALA:HB3	2.19	0.43
1:A:51:LEU:HD21	1:A:154:GLY:N	2.34	0.43
1:C:138:ILE:HG23	1:C:144:MET:HE1	2.01	0.43
1:F:186:PRO:HG2	1:F:189:ASN:OD1	2.19	0.43
1:H:80:LEU:N	1:H:80:LEU:HD23	2.34	0.43
1:B:80:LEU:HD23	1:B:80:LEU:N	2.34	0.43
1:C:163:GLY:HA3	1:C:219:PRO:HG2	2.00	0.43
1:D:140:ALA:HB3	1:D:144:MET:CE	2.49	0.43
1:I:104:GLU:O	1:I:105:ALA:HB3	2.18	0.43
1:A:138:ILE:HG23	1:A:144:MET:HE1	2.00	0.42
1:B:238:ASN:CB	1:B:241:VAL:HG12	2.47	0.42
1:D:63:LEU:HD13	1:D:65:THR:HG22	2.00	0.42
1:G:82:LEU:HB3	1:G:86:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ARG:HB3	1:G:91:PHE:CE1	2.53	0.42
1:I:117:LEU:HD13	1:I:176:MET:CE	2.49	0.42
1:J:214:LEU:CD2	1:J:214:LEU:N	2.82	0.42
1:J:63:LEU:HD13	1:J:64:LYS:N	2.34	0.42
1:C:149:ASP:HB3	1:C:152:ILE:HB	2.00	0.42
1:E:138:ILE:HG23	1:E:144:MET:CE	2.49	0.42
1:E:204:LYS:HE3	1:E:204:LYS:HB3	1.89	0.42
1:F:49:PHE:CE2	1:F:60:ALA:HA	2.53	0.42
1:G:160:TYR:CD1	1:G:206:ILE:HG13	2.53	0.42
1:G:66:ASP:O	1:G:67:PRO:C	2.52	0.42
1:H:144:MET:HA	1:H:145:PRO:HD2	1.83	0.42
1:H:55:ASP:HB2	1:H:56:PRO:HD3	2.01	0.42
1:I:20:LEU:N	1:I:20:LEU:HD12	2.33	0.42
1:J:263:GLN:HG3	1:J:264:ARG:H	1.83	0.42
1:A:71:LYS:HB2	1:A:71:LYS:HE3	1.84	0.42
1:F:133:VAL:HG21	1:F:169:ALA:CB	2.49	0.42
1:B:140:ALA:H	1:B:144:MET:HE3	1.84	0.42
1:F:199:TRP:CD1	1:F:277:VAL:HG11	2.54	0.42
1:H:86:ASP:O	1:H:90:ARG:HB2	2.19	0.42
1:J:227:ALA:N	1:J:228:PRO:HD3	2.34	0.42
1:C:171:HIS:O	1:C:174:THR:HG23	2.19	0.42
1:D:140:ALA:H	1:D:144:MET:CE	2.33	0.42
1:F:238:ASN:ND2	1:I:157:LYS:HE3	2.34	0.42
1:I:28:TRP:CD1	1:I:96:ARG:HG2	2.52	0.42
1:J:175:LEU:CD2	1:J:196:ILE:HB	2.50	0.42
1:C:286:LEU:CD1	1:C:286:LEU:N	2.82	0.42
1:E:138:ILE:HG23	1:E:144:MET:HE1	2.02	0.42
1:B:171:HIS:HE1	1:B:173:LEU:HD13	1.84	0.42
1:C:104:GLU:O	1:C:105:ALA:HB3	2.19	0.42
1:C:90:ARG:HB3	1:C:91:PHE:CD1	2.54	0.42
1:D:239:PRO:HB3	1:D:267:THR:HB	2.01	0.42
1:G:49:PHE:CE2	1:G:60:ALA:HA	2.54	0.42
1:H:286:LEU:CD2	1:H:286:LEU:H	2.26	0.42
1:H:72:ILE:HD13	1:H:212:ILE:HB	2.00	0.42
1:E:243:HIS:O	1:E:244:PRO:C	2.58	0.42
1:E:277:VAL:O	1:E:278:ALA:C	2.58	0.42
1:F:101:ARG:HD3	1:F:251:GLU:OE2	2.20	0.42
1:G:138:ILE:HG23	1:G:144:MET:CE	2.50	0.42
1:G:178:VAL:C	1:G:185:LEU:HG	2.40	0.42
1:G:47:TYR:CE2	1:G:51:LEU:HD22	2.55	0.42
1:I:94:GLU:O	1:I:113:ILE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:135:PHE:CB	1:I:206:ILE:HG21	2.49	0.42
1:D:71:LYS:HE3	1:D:71:LYS:HB2	1.76	0.42
1:A:237:VAL:HG21	1:A:271:ASN:HB2	2.01	0.42
1:A:99:ARG:NH2	1:A:268:LEU:CD1	2.83	0.42
1:B:221:THR:O	1:B:225:LEU:HD13	2.19	0.42
1:B:157:LYS:HE3	1:D:238:ASN:ND2	2.35	0.42
1:E:98:TYR:CE1	1:E:175:LEU:HD22	2.55	0.42
1:I:65:THR:HB	1:I:192:PRO:HG3	2.01	0.42
1:A:100:MET:HG2	4:A:428:HOH:O	2.20	0.41
1:B:263:GLN:OE1	1:B:263:GLN:HA	2.20	0.41
1:G:137:THR:HG22	1:G:138:ILE:N	2.35	0.41
1:H:51:LEU:HD21	1:H:154:GLY:CA	2.49	0.41
1:I:108:MET:HG2	1:I:254:ILE:HB	2.02	0.41
1:C:48:GLU:OE2	1:C:48:GLU:N	2.46	0.41
1:D:66:ASP:O	1:D:84:HIS:HB2	2.20	0.41
1:G:277:VAL:CG1	1:G:277:VAL:O	2.68	0.41
1:G:76:VAL:CG1	1:G:77:ALA:N	2.83	0.41
1:I:176:MET:HE1	1:I:195:LEU:HD13	2.02	0.41
1:B:135:PHE:O	1:B:161:VAL:HG23	2.20	0.41
1:B:197:VAL:HA	1:B:198:PRO:HD2	1.86	0.41
1:E:171:HIS:ND1	1:E:173:LEU:HB2	2.36	0.41
1:F:149:ASP:HB3	1:F:152:ILE:HB	2.03	0.41
1:F:175:LEU:HD23	1:F:196:ILE:HB	2.03	0.41
1:B:20:LEU:CG	1:B:21:GLU:H	2.12	0.41
1:F:71:LYS:HB2	1:F:71:LYS:HE3	1.81	0.41
1:H:106:TRP:HA	1:H:252:ARG:O	2.20	0.41
1:I:71:LYS:HB2	1:I:71:LYS:HE3	1.84	0.41
1:A:277:VAL:O	1:A:277:VAL:CG1	2.68	0.41
1:A:74:GLY:O	1:A:76:VAL:N	2.47	0.41
1:I:137:THR:CG2	1:I:138:ILE:H	2.32	0.41
1:J:101:ARG:NH1	1:J:105:ALA:HA	2.35	0.41
1:D:47:TYR:N	1:D:47:TYR:CD1	2.89	0.41
1:J:137:THR:HG22	1:J:138:ILE:N	2.35	0.41
1:E:176:MET:CE	1:E:195:LEU:HD13	2.51	0.41
1:D:224:ASN:O	1:D:228:PRO:HG3	2.20	0.41
1:G:161:VAL:HG22	1:G:162:GLU:N	2.36	0.41
1:H:65:THR:HB	1:H:192:PRO:HD3	2.03	0.41
1:H:93:LEU:N	1:H:93:LEU:HD12	2.36	0.41
1:J:214:LEU:HD22	1:J:214:LEU:N	2.35	0.41
1:A:285:ASP:OD1	1:A:286:LEU:HD13	2.20	0.41
1:B:239:PRO:HB3	1:B:267:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:VAL:CG1	1:H:77:ALA:N	2.83	0.41
1:A:138:ILE:HG23	1:A:144:MET:HE2	2.03	0.41
1:F:85:ASP:O	1:F:89:ARG:HB2	2.21	0.41
1:I:144:MET:HA	1:I:145:PRO:HD2	1.87	0.41
1:I:70:LEU:HD12	1:I:193:VAL:HG21	2.03	0.41
1:I:269:LEU:O	1:I:270:PHE:HB2	2.20	0.41
1:I:66:ASP:O	1:I:67:PRO:C	2.56	0.41
1:J:162:GLU:OE1	1:J:204:LYS:HD2	2.21	0.41
1:B:203:PHE:HB2	1:B:223:TRP:CD1	2.55	0.40
1:B:66:ASP:HB3	1:B:67:PRO:CD	2.51	0.40
1:E:36:PRO:HG2	1:E:39:LYS:HD2	2.04	0.40
1:E:28:TRP:CH2	1:E:173:LEU:CD1	3.04	0.40
1:H:237:VAL:HG21	1:H:271:ASN:HB2	2.04	0.40
1:J:99:ARG:HG3	1:J:271:ASN:ND2	2.36	0.40
1:E:173:LEU:HD12	1:E:173:LEU:HA	1.78	0.40
1:E:74:GLY:O	1:E:76:VAL:N	2.52	0.40
1:G:100:MET:HG2	4:G:421:HOH:O	2.21	0.40
1:H:171:HIS:CG	1:H:172:PRO:HD2	2.57	0.40
1:J:190:GLY:HA2	1:J:207:LYS:HB3	2.03	0.40
1:J:47:TYR:C	1:J:49:PHE:N	2.73	0.40
1:A:51:LEU:HD21	1:A:154:GLY:HA3	2.00	0.40
1:C:138:ILE:HG23	1:C:144:MET:HE2	2.02	0.40
1:F:75:GLU:HB3	1:F:130:ALA:HB2	2.02	0.40
1:D:144:MET:HA	1:D:145:PRO:HD2	1.88	0.40
1:I:161:VAL:HG22	1:I:162:GLU:N	2.36	0.40
1:J:87:LEU:HD13	1:J:193:VAL:HG23	2.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/298 (87%)	249 (96%)	9 (4%)	1 (0%)	34	37
1	B	258/298 (87%)	242 (94%)	15 (6%)	1 (0%)	34	37
1	C	260/298 (87%)	246 (95%)	13 (5%)	1 (0%)	34	37
1	D	259/298 (87%)	248 (96%)	11 (4%)	0	100	100
1	E	258/298 (87%)	241 (93%)	17 (7%)	0	100	100
1	F	258/298 (87%)	243 (94%)	15 (6%)	0	100	100
1	G	257/298 (86%)	242 (94%)	13 (5%)	2 (1%)	19	19
1	H	260/298 (87%)	236 (91%)	23 (9%)	1 (0%)	34	37
1	I	258/298 (87%)	239 (93%)	18 (7%)	1 (0%)	34	37
1	J	258/298 (87%)	244 (95%)	14 (5%)	0	100	100
All	All	2585/2980 (87%)	2430 (94%)	148 (6%)	7 (0%)	41	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	192	PRO
1	G	75	GLU
1	A	75	GLU
1	B	66	ASP
1	G	66	ASP
1	H	265	GLN
1	I	66	ASP

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	219/249 (88%)	204 (93%)	15 (7%)	16	17
1	B	219/249 (88%)	213 (97%)	6 (3%)	44	57
1	C	220/249 (88%)	207 (94%)	13 (6%)	19	23
1	D	219/249 (88%)	211 (96%)	8 (4%)	34	43
1	E	218/249 (88%)	211 (97%)	7 (3%)	39	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	218/249 (88%)	206 (94%)	12 (6%)	21	26
1	G	218/249 (88%)	210 (96%)	8 (4%)	34	43
1	H	220/249 (88%)	207 (94%)	13 (6%)	19	23
1	I	218/249 (88%)	209 (96%)	9 (4%)	30	39
1	J	218/249 (88%)	208 (95%)	10 (5%)	27	34
All	All	2187/2490 (88%)	2086 (95%)	101 (5%)	27	34

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	46	PHE
1	A	70	LEU
1	A	120	LEU
1	A	173	LEU
1	A	174	THR
1	A	175	LEU
1	A	194	ARG
1	A	210	VAL
1	A	221	THR
1	A	241	VAL
1	A	247	SER
1	A	264	ARG
1	A	279	SER
1	A	286	LEU
1	B	46	PHE
1	B	125	GLU
1	B	165	ARG
1	B	174	THR
1	B	193	VAL
1	B	194	ARG
1	C	20	LEU
1	C	38	ASP
1	C	46	PHE
1	C	70	LEU
1	C	174	THR
1	C	175	LEU
1	C	188	GLN
1	C	193	VAL
1	C	194	ARG

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Mol	Chain	Res	Type
1	C	210	VAL
1	C	214	LEU
1	C	263	GLN
1	C	286	LEU
1	D	46	PHE
1	D	51	LEU
1	D	63	LEU
1	D	70	LEU
1	D	99	ARG
1	D	174	THR
1	D	194	ARG
1	D	218	ARG
1	E	20	LEU
1	E	46	PHE
1	E	93	LEU
1	E	174	THR
1	E	194	ARG
1	E	241	VAL
1	E	285	ASP
1	F	38	ASP
1	F	46	PHE
1	F	63	LEU
1	F	70	LEU
1	F	81	THR
1	F	82	LEU
1	F	93	LEU
1	F	174	THR
1	F	188	GLN
1	F	194	ARG
1	F	279	SER
1	F	286	LEU
1	G	46	PHE
1	G	64	LYS
1	G	70	LEU
1	G	175	LEU
1	G	193	VAL
1	G	194	ARG
1	G	211	SER
1	G	225	LEU
1	H	18	LYS
1	H	20	LEU
1	H	46	PHE

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Mol	Chain	Res	Type
1	H	70	LEU
1	H	90	ARG
1	H	99	ARG
1	H	118	HIS
1	H	173	LEU
1	H	174	THR
1	H	175	LEU
1	H	188	GLN
1	H	194	ARG
1	H	286	LEU
1	I	20	LEU
1	I	46	PHE
1	I	99	ARG
1	I	175	LEU
1	I	183	LYS
1	I	193	VAL
1	I	194	ARG
1	I	218	ARG
1	I	277	VAL
1	J	38	ASP
1	J	46	PHE
1	J	81	THR
1	J	93	LEU
1	J	99	ARG
1	J	120	LEU
1	J	173	LEU
1	J	174	THR
1	J	194	ARG
1	J	214	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	GLN
1	D	263	GLN
1	D	276	GLN
1	E	30	ASN
1	G	59	ASN
1	J	31	ASN
1	J	263	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MTE	C	303	2	21,26,26	3.16	12 (57%)	21,40,40	6.51	13 (61%)
3	MTE	H	308	2	21,26,26	3.53	11 (52%)	21,40,40	5.96	15 (71%)
3	MTE	B	302	2	21,26,26	3.22	12 (57%)	21,40,40	5.99	15 (71%)
3	MTE	G	307	2	21,26,26	3.23	11 (52%)	21,40,40	6.40	12 (57%)
3	MTE	I	309	2	21,26,26	3.62	11 (52%)	21,40,40	6.14	13 (61%)
3	MTE	A	301	2	21,26,26	3.43	12 (57%)	21,40,40	6.27	12 (57%)
3	MTE	J	310	2	21,26,26	3.50	10 (47%)	21,40,40	6.55	13 (61%)
3	MTE	D	304	2	21,26,26	3.17	11 (52%)	21,40,40	6.04	13 (61%)
3	MTE	E	305	2	21,26,26	2.89	9 (42%)	21,40,40	6.53	13 (61%)
3	MTE	F	306	2	21,26,26	3.44	10 (47%)	21,40,40	6.29	16 (76%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MTE	C	303	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	H	308	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	B	302	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	G	307	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	I	309	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	A	301	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	J	310	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	D	304	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	E	305	2	1/1/6/8	0/6/34/34	0/3/3/3
3	MTE	F	306	2	1/1/6/8	0/6/34/34	0/3/3/3

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	309	MTE	C4'-C3'	-10.16	1.38	1.52
3	H	308	MTE	C4'-C3'	-9.50	1.39	1.52
3	J	310	MTE	C4'-C3'	-9.27	1.39	1.52
3	F	306	MTE	C4'-C3'	-9.02	1.39	1.52
3	G	307	MTE	C4'-C3'	-8.93	1.39	1.52
3	A	301	MTE	C4'-C3'	-8.44	1.40	1.52
3	B	302	MTE	C4'-C3'	-7.91	1.41	1.52
3	C	303	MTE	C4'-C3'	-7.89	1.41	1.52
3	D	304	MTE	C4'-C3'	-7.82	1.41	1.52
3	E	305	MTE	C4'-C3'	-7.64	1.41	1.52
3	H	308	MTE	C9-C10	7.33	1.55	1.41
3	F	306	MTE	C9-C10	6.91	1.54	1.41
3	G	307	MTE	C9-C10	6.68	1.54	1.41
3	J	310	MTE	C9-C10	6.66	1.54	1.41
3	C	303	MTE	C9-C10	6.39	1.53	1.41
3	I	309	MTE	C9-C10	6.35	1.53	1.41
3	E	305	MTE	C9-C10	6.29	1.53	1.41
3	B	302	MTE	C9-C10	6.25	1.53	1.41
3	D	304	MTE	C9-C10	6.16	1.53	1.41
3	I	309	MTE	C6-N5	5.88	1.53	1.45
3	I	309	MTE	P-O4'	-5.67	1.42	1.60
3	H	308	MTE	P-O4'	-5.39	1.42	1.60
3	A	301	MTE	C9-C10	5.32	1.51	1.41
3	J	310	MTE	P-O4'	-5.19	1.43	1.60
3	J	310	MTE	C6-N5	5.18	1.52	1.45
3	C	303	MTE	P-O4'	-5.07	1.43	1.60
3	F	306	MTE	P-O4'	-4.92	1.44	1.60
3	F	306	MTE	C6-N5	4.92	1.52	1.45
3	A	301	MTE	P-O1P	-4.88	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	310	MTE	O3'-C7	4.80	1.50	1.43
3	B	302	MTE	P-O4'	-4.64	1.45	1.60
3	B	302	MTE	C6-N5	4.58	1.51	1.45
3	D	304	MTE	O3'-C3'	4.55	1.49	1.43
3	A	301	MTE	C6-N5	4.52	1.51	1.45
3	D	304	MTE	P-O4'	-4.46	1.45	1.60
3	A	301	MTE	P-O4'	-4.45	1.45	1.60
3	E	305	MTE	P-O4'	-4.29	1.46	1.60
3	D	304	MTE	O3'-C7	4.17	1.49	1.43
3	G	307	MTE	C6-N5	4.10	1.51	1.45
3	A	301	MTE	C2-N3	-4.02	1.28	1.35
3	G	307	MTE	C9-N5	3.89	1.46	1.38
3	H	308	MTE	C6-N5	3.87	1.50	1.45
3	A	301	MTE	O3'-C3'	3.84	1.48	1.43
3	G	307	MTE	P-O4'	-3.72	1.48	1.60
3	F	306	MTE	C9-N5	3.64	1.45	1.38
3	E	305	MTE	C6-N5	3.59	1.50	1.45
3	J	310	MTE	C9-N5	3.59	1.45	1.38
3	H	308	MTE	O3'-C7	3.58	1.48	1.43
3	I	309	MTE	C9-N5	3.57	1.45	1.38
3	H	308	MTE	P-O1P	-3.56	1.39	1.50
3	A	301	MTE	C4-N3	3.56	1.39	1.33
3	B	302	MTE	C9-N5	3.54	1.45	1.38
3	F	306	MTE	C4-N3	3.51	1.39	1.33
3	D	304	MTE	C6-N5	3.51	1.50	1.45
3	E	305	MTE	C7-C6	3.49	1.56	1.53
3	C	303	MTE	C9-N5	3.48	1.45	1.38
3	B	302	MTE	P-O1P	-3.48	1.39	1.50
3	F	306	MTE	O3'-C3'	3.48	1.48	1.43
3	C	303	MTE	C4-N3	3.45	1.39	1.33
3	A	301	MTE	C9-N5	3.42	1.45	1.38
3	C	303	MTE	C6-N5	3.33	1.50	1.45
3	G	307	MTE	C2-N3	-3.28	1.29	1.35
3	H	308	MTE	C4-N3	3.23	1.38	1.33
3	H	308	MTE	C9-N5	3.09	1.44	1.38
3	F	306	MTE	P-O1P	-3.04	1.40	1.50
3	C	303	MTE	O3'-C3'	2.91	1.47	1.43
3	J	310	MTE	C2-N3	-2.87	1.30	1.35
3	I	309	MTE	C2-N3	-2.87	1.30	1.35
3	G	307	MTE	O3'-C3'	2.87	1.47	1.43
3	J	310	MTE	C4-N3	2.85	1.38	1.33
3	C	303	MTE	O3'-C7	2.82	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	MTE	O3'-C7	2.77	1.47	1.43
3	D	304	MTE	C2-N3	-2.75	1.30	1.35
3	H	308	MTE	O3'-C3'	2.75	1.47	1.43
3	A	301	MTE	C2'-C1'	2.67	1.52	1.35
3	F	306	MTE	O3'-C7	2.67	1.47	1.43
3	D	304	MTE	P-O1P	-2.65	1.42	1.50
3	E	305	MTE	P-O1P	-2.64	1.42	1.50
3	I	309	MTE	P-O1P	-2.64	1.42	1.50
3	I	309	MTE	O3'-C7	2.53	1.47	1.43
3	B	302	MTE	C4-N3	2.52	1.37	1.33
3	A	301	MTE	O3'-C7	2.51	1.47	1.43
3	J	310	MTE	P-O1P	-2.51	1.42	1.50
3	B	302	MTE	C2-N3	-2.49	1.31	1.35
3	J	310	MTE	C2-N2	-2.47	1.29	1.33
3	I	309	MTE	C4-N3	2.44	1.37	1.33
3	E	305	MTE	C2-N2	-2.44	1.29	1.33
3	G	307	MTE	C4-C9	2.43	1.44	1.41
3	C	303	MTE	P-O1P	-2.40	1.42	1.50
3	A	301	MTE	C2-N2	-2.40	1.29	1.33
3	C	303	MTE	C2-N3	-2.37	1.31	1.35
3	G	307	MTE	C4-N3	2.29	1.37	1.33
3	B	302	MTE	O4'-C4'	2.24	1.53	1.44
3	I	309	MTE	O3'-C3'	2.20	1.46	1.43
3	G	307	MTE	P-O1P	-2.20	1.43	1.50
3	D	304	MTE	C9-N5	2.14	1.42	1.38
3	G	307	MTE	C2'-C1'	2.11	1.49	1.35
3	E	305	MTE	O4'-C4'	2.11	1.52	1.44
3	H	308	MTE	C2'-C1'	2.09	1.49	1.35
3	I	309	MTE	C2'-C1'	2.09	1.49	1.35
3	F	306	MTE	C2'-C1'	2.09	1.49	1.35
3	B	302	MTE	C4-C9	2.08	1.44	1.41
3	E	305	MTE	C2-N3	-2.07	1.31	1.35
3	D	304	MTE	C4-N3	2.06	1.36	1.33
3	H	308	MTE	C2-N3	-2.04	1.31	1.35
3	D	304	MTE	C2'-C1'	2.03	1.48	1.35
3	C	303	MTE	O4'-C4'	2.01	1.52	1.44
3	C	303	MTE	C2'-C1'	2.00	1.48	1.35
3	B	302	MTE	C2-N1	2.00	1.39	1.35

All (135) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	305	MTE	O3'-C7-C6	-24.51	92.61	108.96
3	J	310	MTE	O3'-C7-C6	-24.48	92.63	108.96
3	C	303	MTE	O3'-C7-C6	-24.35	92.72	108.96
3	G	307	MTE	O3'-C7-C6	-23.05	93.59	108.96
3	A	301	MTE	O3'-C7-C6	-22.85	93.73	108.96
3	F	306	MTE	O3'-C7-C6	-22.67	93.84	108.96
3	D	304	MTE	O3'-C7-C6	-21.85	94.39	108.96
3	I	309	MTE	O3'-C7-C6	-21.57	94.58	108.96
3	B	302	MTE	O3'-C7-C6	-21.24	94.80	108.96
3	H	308	MTE	O3'-C7-C6	-20.93	95.00	108.96
3	I	309	MTE	C4-C9-N5	11.49	128.76	119.12
3	F	306	MTE	C4-C9-N5	11.32	128.62	119.12
3	G	307	MTE	C4-C9-N5	11.31	128.61	119.12
3	J	310	MTE	C4-C9-N5	11.28	128.58	119.12
3	A	301	MTE	C4-C9-N5	11.06	128.40	119.12
3	B	302	MTE	C4-C9-N5	10.88	128.25	119.12
3	D	304	MTE	C4-C9-N5	10.86	128.24	119.12
3	H	308	MTE	C4-C9-N5	10.86	128.23	119.12
3	E	305	MTE	C4-C9-N5	10.74	128.14	119.12
3	C	303	MTE	C4-C9-N5	10.51	127.94	119.12
3	C	303	MTE	C2-N1-C10	7.63	131.64	114.54
3	D	304	MTE	C2-N1-C10	7.59	131.56	114.54
3	A	301	MTE	C2-N1-C10	7.58	131.54	114.54
3	I	309	MTE	C2-N1-C10	7.45	131.25	114.54
3	G	307	MTE	C2-N1-C10	7.45	131.23	114.54
3	F	306	MTE	C2-N1-C10	7.35	131.01	114.54
3	H	308	MTE	C2-N1-C10	7.32	130.96	114.54
3	E	305	MTE	C2-N1-C10	7.29	130.89	114.54
3	J	310	MTE	C2-N1-C10	7.28	130.87	114.54
3	B	302	MTE	C2-N1-C10	7.16	130.59	114.54
3	E	305	MTE	C7-C6-C1'	5.34	122.50	110.53
3	H	308	MTE	C7-C6-C1'	5.25	122.31	110.53
3	D	304	MTE	C7-C6-C1'	5.13	122.03	110.53
3	I	309	MTE	N3-C2-N1	-5.12	117.39	125.42
3	G	307	MTE	C7-C6-C1'	5.03	121.80	110.53
3	G	307	MTE	N3-C2-N1	-5.02	117.54	125.42
3	B	302	MTE	C7-C6-C1'	5.02	121.79	110.53
3	A	301	MTE	C7-C6-C1'	5.00	121.74	110.53
3	C	303	MTE	C7-C6-C1'	4.88	121.47	110.53
3	F	306	MTE	N3-C2-N1	-4.82	117.86	125.42
3	I	309	MTE	C7-C6-C1'	4.80	121.29	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	304	MTE	N3-C2-N1	-4.72	118.02	125.42
3	G	307	MTE	O3'-C7-N8	4.71	113.41	108.57
3	H	308	MTE	N3-C2-N1	-4.70	118.05	125.42
3	J	310	MTE	N3-C2-N1	-4.69	118.06	125.42
3	A	301	MTE	N3-C2-N1	-4.65	118.13	125.42
3	C	303	MTE	O3'-C7-N8	4.63	113.32	108.57
3	C	303	MTE	N3-C2-N1	-4.62	118.17	125.42
3	B	302	MTE	N3-C2-N1	-4.58	118.23	125.42
3	F	306	MTE	C7-C6-C1'	4.54	120.72	110.53
3	J	310	MTE	C7-C6-C1'	4.48	120.58	110.53
3	E	305	MTE	N3-C2-N1	-4.46	118.43	125.42
3	A	301	MTE	O3'-C7-N8	4.37	113.06	108.57
3	I	309	MTE	C10-N8-C7	4.16	131.83	123.67
3	J	310	MTE	C10-N8-C7	4.15	131.80	123.67
3	B	302	MTE	C10-N8-C7	4.10	131.70	123.67
3	J	310	MTE	O3'-C7-N8	4.09	112.78	108.57
3	F	306	MTE	C10-N8-C7	4.03	131.57	123.67
3	I	309	MTE	O3'-C7-N8	4.00	112.68	108.57
3	G	307	MTE	C10-N8-C7	3.93	131.37	123.67
3	A	301	MTE	C10-N8-C7	3.92	131.35	123.67
3	E	305	MTE	C10-N8-C7	3.87	131.26	123.67
3	H	308	MTE	C10-N8-C7	3.71	130.94	123.67
3	F	306	MTE	O3'-C7-N8	3.68	112.35	108.57
3	B	302	MTE	O4'-P-O1P	3.62	116.63	106.47
3	D	304	MTE	C10-N8-C7	3.61	130.75	123.67
3	C	303	MTE	C10-N8-C7	3.46	130.46	123.67
3	G	307	MTE	C4-N3-C2	3.40	121.34	115.93
3	H	308	MTE	O4'-P-O1P	3.38	115.94	106.47
3	C	303	MTE	O4'-P-O1P	3.28	115.68	106.47
3	B	302	MTE	O3P-P-O2P	3.28	120.16	107.64
3	H	308	MTE	O3'-C7-N8	3.22	111.88	108.57
3	G	307	MTE	N2-C2-N1	3.18	122.20	117.25
3	E	305	MTE	O4'-P-O1P	3.15	115.30	106.47
3	F	306	MTE	O4'-P-O1P	3.13	115.26	106.47
3	I	309	MTE	O4'-P-O1P	3.12	115.22	106.47
3	I	309	MTE	O3P-P-O2P	3.11	119.52	107.64
3	G	307	MTE	C9-C10-N8	-3.07	115.32	118.13
3	F	306	MTE	C9-C10-N8	-3.05	115.34	118.13
3	G	307	MTE	O3P-P-O2P	3.05	119.29	107.64
3	E	305	MTE	O3P-P-O2P	3.00	119.09	107.64
3	I	309	MTE	C4-N3-C2	2.90	120.54	115.93
3	B	302	MTE	O3'-C7-N8	2.86	111.51	108.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	306	MTE	O3P-P-O2P	2.85	118.53	107.64
3	H	308	MTE	C4-N3-C2	2.83	120.43	115.93
3	I	309	MTE	N2-C2-N1	2.83	121.66	117.25
3	B	302	MTE	C9-C10-N8	-2.82	115.55	118.13
3	H	308	MTE	O3P-P-O2P	2.82	118.42	107.64
3	J	310	MTE	C9-C10-N8	-2.80	115.56	118.13
3	D	304	MTE	C4-N3-C2	2.80	120.37	115.93
3	J	310	MTE	O4'-P-O1P	2.78	114.27	106.47
3	D	304	MTE	N2-C2-N3	2.73	121.50	117.25
3	D	304	MTE	O3P-P-O2P	2.73	118.07	107.64
3	J	310	MTE	C4-N3-C2	2.67	120.17	115.93
3	F	306	MTE	N2-C2-N3	2.67	121.40	117.25
3	D	304	MTE	O4'-P-O1P	2.66	113.95	106.47
3	E	305	MTE	N2-C2-N3	2.63	121.35	117.25
3	E	305	MTE	C4-N3-C2	2.62	120.09	115.93
3	J	310	MTE	N2-C2-N1	2.55	121.21	117.25
3	E	305	MTE	O3'-C7-N8	2.53	111.17	108.57
3	C	303	MTE	N2-C2-N3	2.53	121.19	117.25
3	H	308	MTE	O3P-P-O4'	-2.51	100.04	106.73
3	B	302	MTE	N2-C2-N3	2.51	121.16	117.25
3	H	308	MTE	C9-C10-N8	-2.50	115.84	118.13
3	A	301	MTE	O4'-P-O1P	2.49	113.47	106.47
3	H	308	MTE	N2-C2-N3	2.48	121.11	117.25
3	B	302	MTE	C4-N3-C2	2.48	119.87	115.93
3	E	305	MTE	C9-N5-C6	2.47	128.95	120.00
3	I	309	MTE	C9-C10-N8	-2.46	115.88	118.13
3	F	306	MTE	O3P-P-O4'	-2.46	100.19	106.73
3	C	303	MTE	C9-C10-N8	-2.42	115.91	118.13
3	A	301	MTE	N2-C2-N1	2.42	121.02	117.25
3	F	306	MTE	C4-N3-C2	2.42	119.77	115.93
3	I	309	MTE	N2-C2-N3	2.38	120.95	117.25
3	A	301	MTE	C4-N3-C2	2.36	119.68	115.93
3	C	303	MTE	O3P-P-O2P	2.34	116.58	107.64
3	C	303	MTE	C4-N3-C2	2.32	119.61	115.93
3	A	301	MTE	N2-C2-N3	2.32	120.86	117.25
3	H	308	MTE	N2-C2-N1	2.30	120.84	117.25
3	F	306	MTE	N2-C2-N1	2.24	120.74	117.25
3	A	301	MTE	O3P-P-O2P	2.24	116.19	107.64
3	J	310	MTE	N2-C2-N3	2.23	120.72	117.25
3	J	310	MTE	O3P-P-O2P	2.23	116.15	107.64
3	G	307	MTE	C9-N5-C6	2.23	128.07	120.00
3	H	308	MTE	O2P-P-O1P	-2.20	102.07	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	MTE	N2-C2-N1	2.18	120.64	117.25
3	B	302	MTE	N2-C2-N1	2.16	120.61	117.25
3	F	306	MTE	O2P-P-O1P	-2.10	102.46	110.68
3	B	302	MTE	O3P-P-O4'	-2.10	101.16	106.73
3	F	306	MTE	C9-N5-C6	2.07	127.52	120.00
3	D	304	MTE	N2-C2-N1	2.07	120.47	117.25
3	D	304	MTE	C9-N5-C6	2.06	127.47	120.00
3	D	304	MTE	C9-C10-N8	-2.04	116.27	118.13
3	B	302	MTE	C9-N5-C6	2.03	127.37	120.00
3	E	305	MTE	C9-C10-N8	-2.03	116.27	118.13

All (10) chirality outliers are listed below:

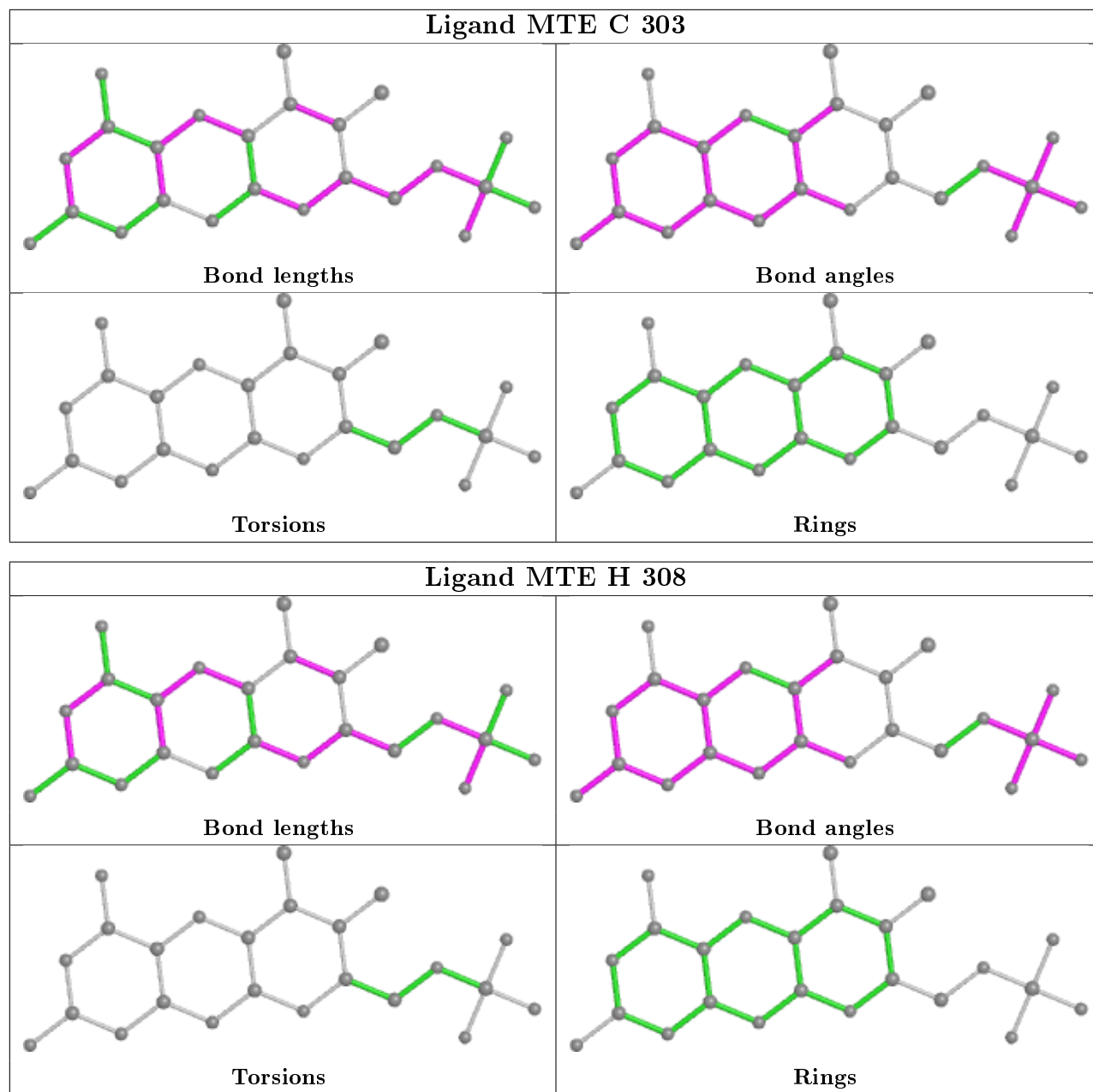
Mol	Chain	Res	Type	Atom
3	I	309	MTE	C6
3	C	303	MTE	C6
3	G	307	MTE	C6
3	B	302	MTE	C6
3	E	305	MTE	C6
3	A	301	MTE	C6
3	J	310	MTE	C6
3	D	304	MTE	C6
3	H	308	MTE	C6
3	F	306	MTE	C6

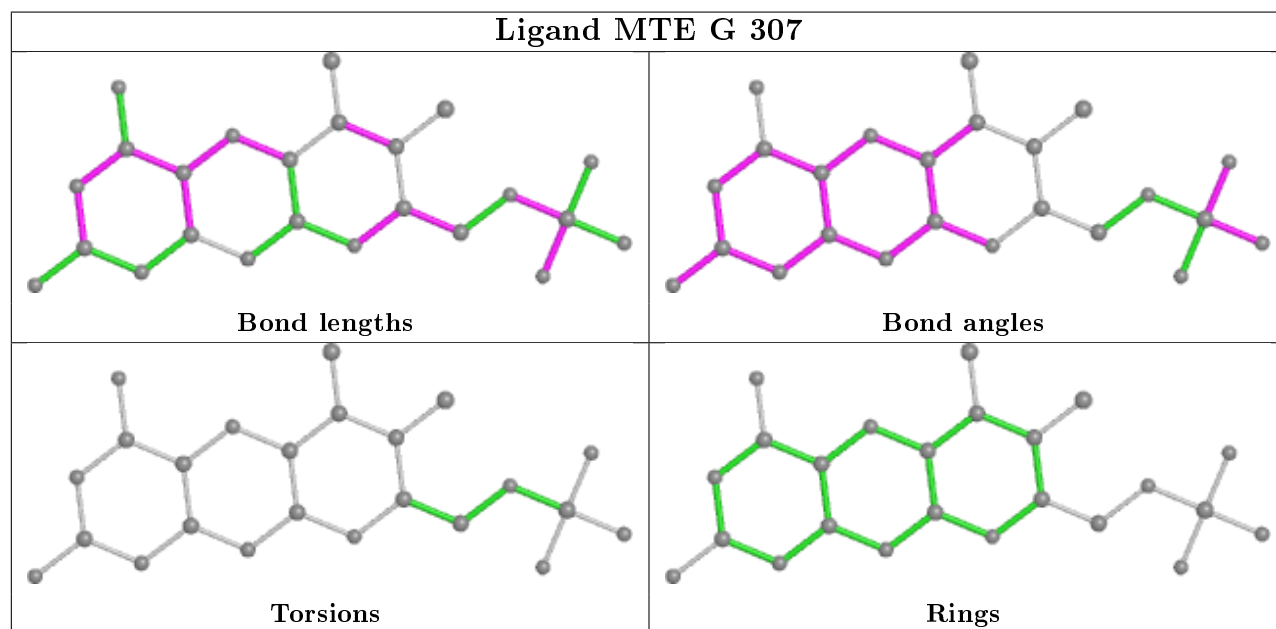
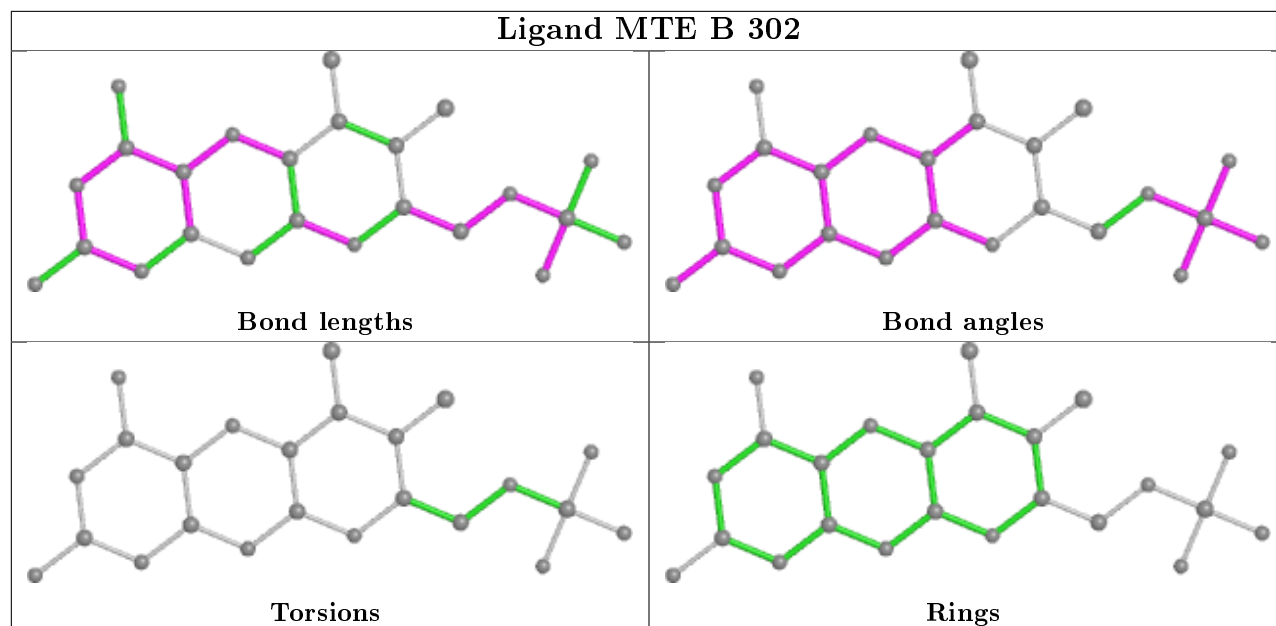
There are no torsion outliers.

There are no ring outliers.

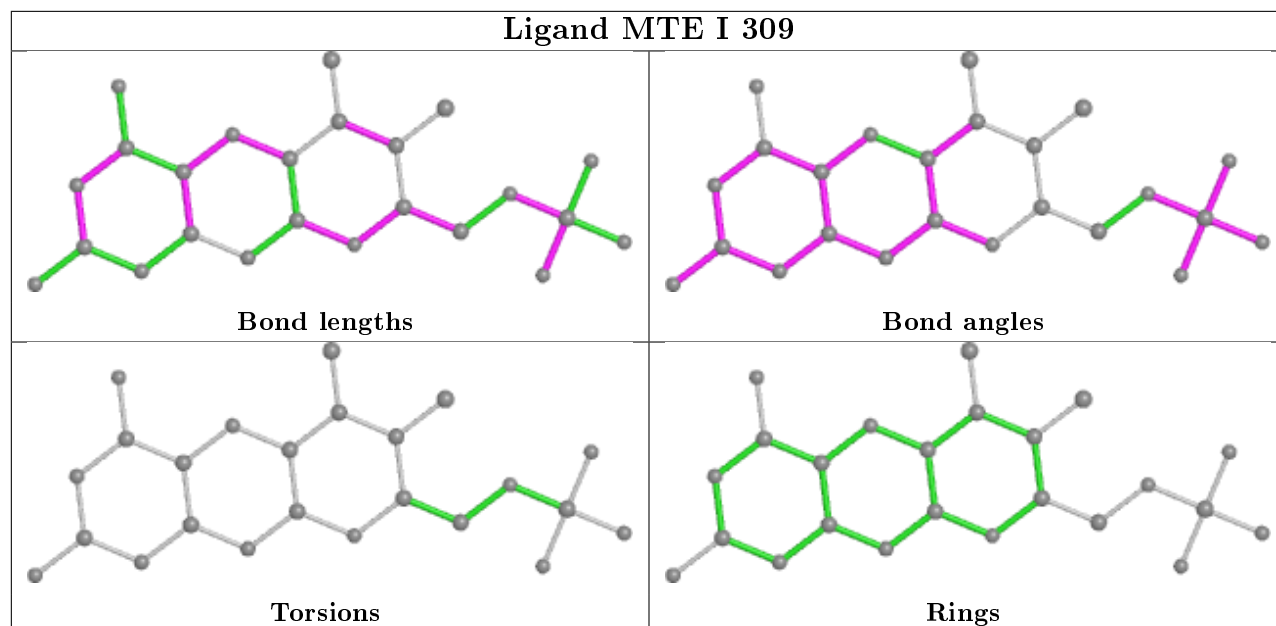
No monomer is involved in short contacts.

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.

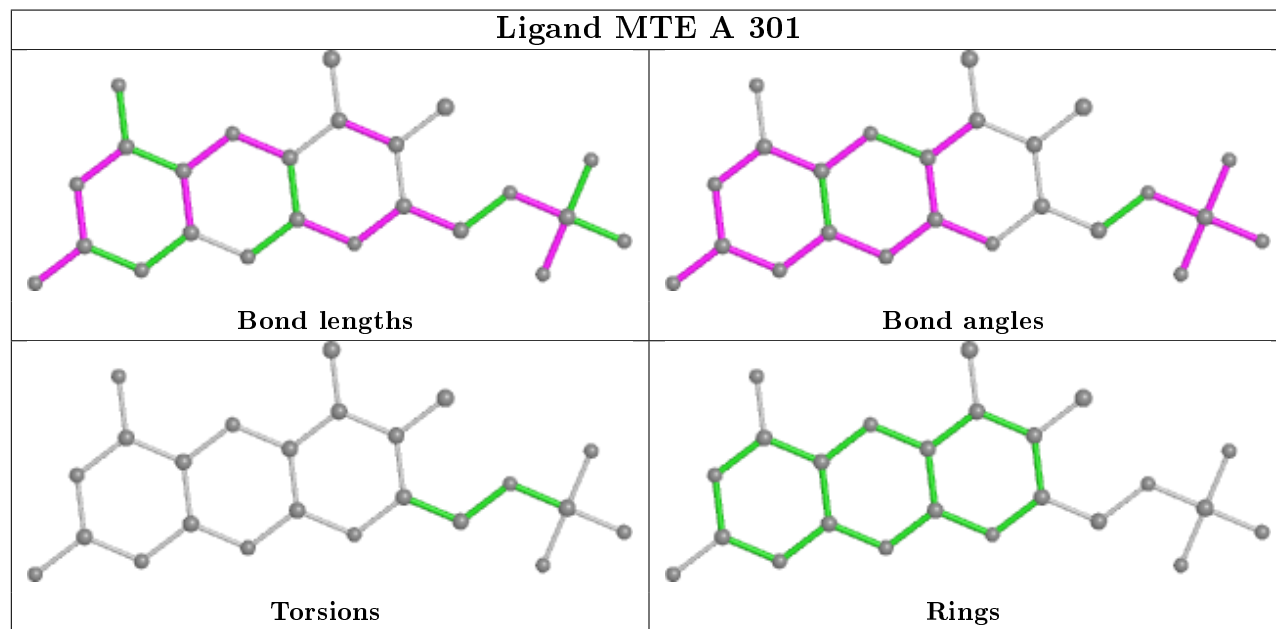




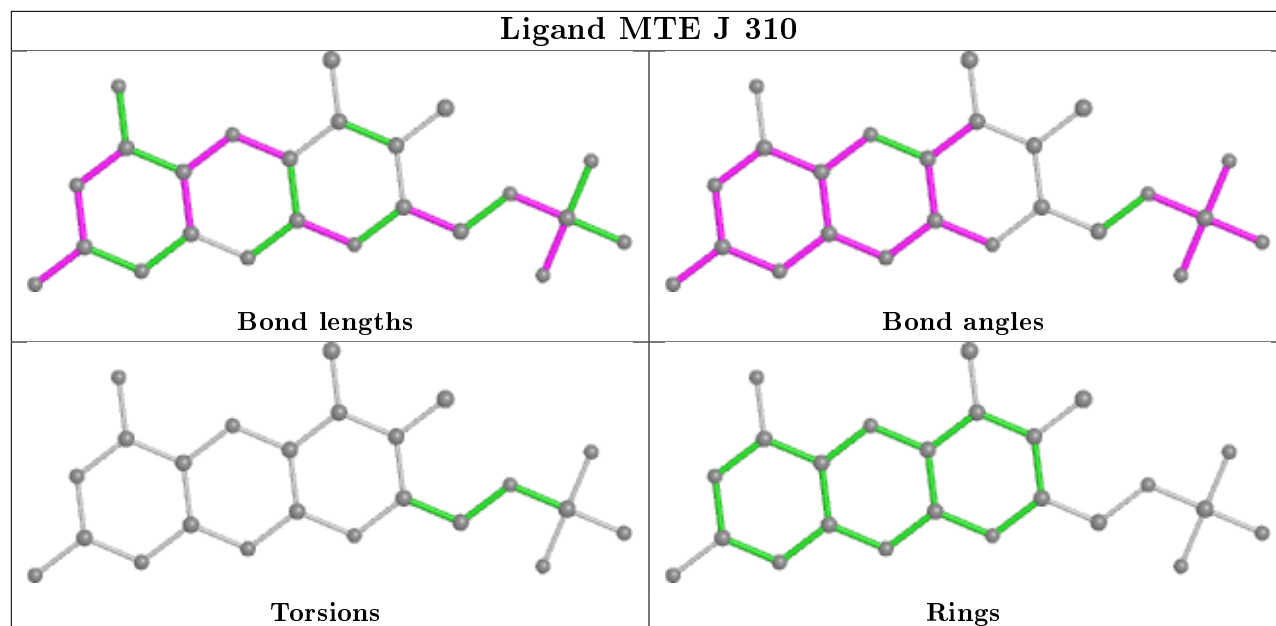
Ligand MTE I 309



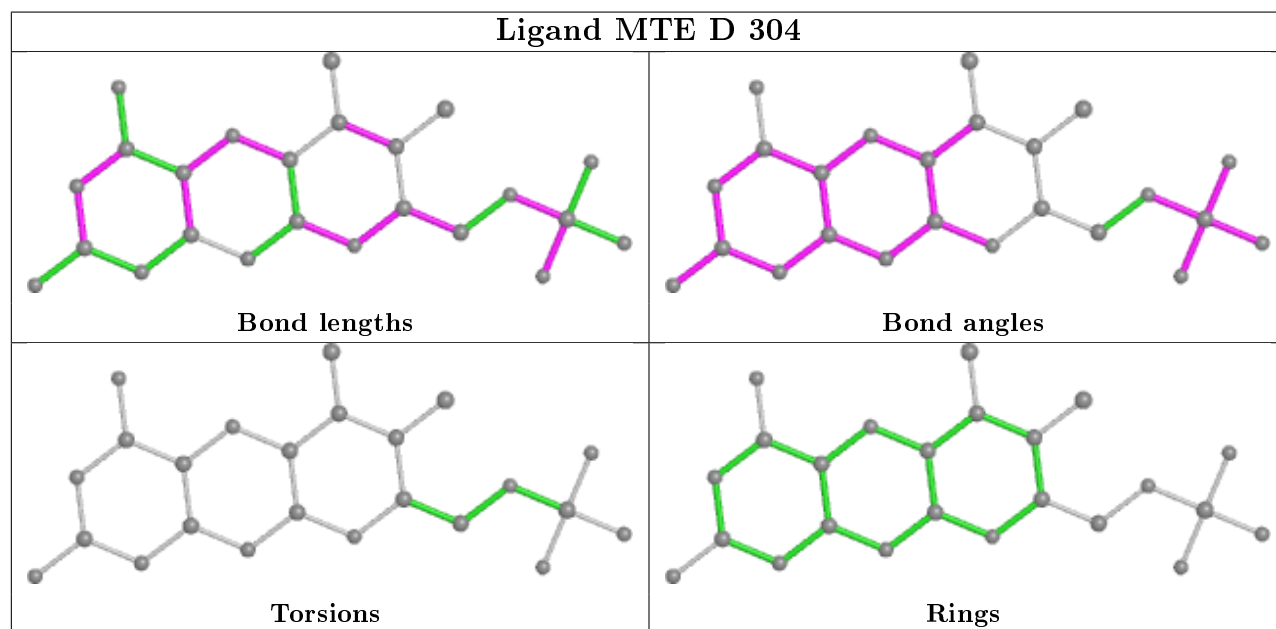
Ligand MTE A 301

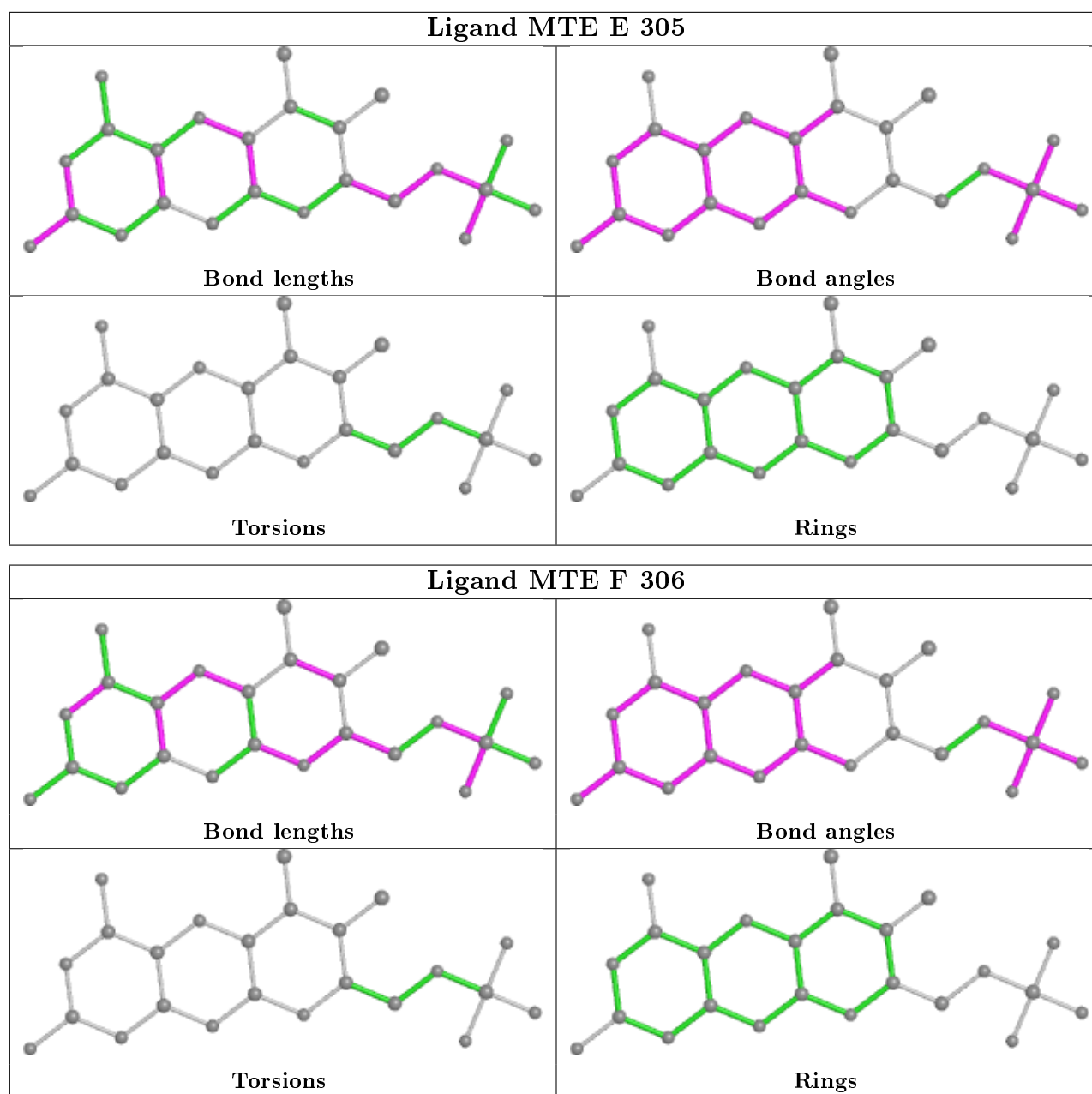


Ligand MTE J 310



Ligand MTE D 304





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	263/298 (88%)	0.17	8 (3%) 50 48	22, 46, 78, 95	0
1	B	262/298 (87%)	0.66	28 (10%) 6 5	33, 68, 94, 106	0
1	C	264/298 (88%)	0.19	10 (3%) 40 38	22, 49, 78, 90	0
1	D	263/298 (88%)	0.20	4 (1%) 73 72	24, 46, 76, 92	0
1	E	262/298 (87%)	0.19	10 (3%) 40 38	25, 46, 80, 97	0
1	F	262/298 (87%)	1.01	48 (18%) 1 1	36, 64, 88, 94	1 (0%)
1	G	261/298 (87%)	0.41	17 (6%) 18 17	21, 49, 84, 100	0
1	H	263/298 (88%)	0.66	25 (9%) 8 7	36, 68, 95, 102	0
1	I	262/298 (87%)	0.72	24 (9%) 9 7	34, 61, 90, 106	0
1	J	262/298 (87%)	0.16	7 (2%) 54 52	20, 44, 73, 91	0
All	All	2624/2980 (88%)	0.44	181 (6%) 16 15	20, 54, 88, 106	1 (0%)

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	31	ASN	7.6
1	F	130	ALA	7.1
1	G	66	ASP	5.5
1	F	120	LEU	5.3
1	B	256	SER	4.6
1	J	263	GLN	4.5
1	H	26	ALA	4.5
1	E	256	SER	4.4
1	B	89	ARG	4.4
1	F	65	THR	4.3
1	B	125	GLU	4.3
1	F	88	THR	4.3
1	A	31	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	28	TRP	4.0
1	I	26	ALA	4.0
1	H	20	LEU	3.9
1	F	129	ASN	3.9
1	C	229	ASP	3.9
1	F	223	TRP	3.8
1	B	66	ASP	3.8
1	F	256	SER	3.8
1	I	229	ASP	3.8
1	H	91	PHE	3.7
1	I	263	GLN	3.7
1	B	255	GLY	3.7
1	E	263	GLN	3.7
1	F	31	ASN	3.7
1	F	206	ILE	3.7
1	I	150	ARG	3.6
1	A	26	ALA	3.6
1	B	61	GLY	3.6
1	I	89	ARG	3.6
1	H	256	SER	3.6
1	I	257	GLY	3.5
1	E	257	GLY	3.5
1	C	256	SER	3.5
1	J	151	PHE	3.5
1	G	22	PHE	3.4
1	H	86	ASP	3.4
1	I	64	LYS	3.4
1	F	156	LEU	3.4
1	I	66	ASP	3.4
1	F	166	LEU	3.4
1	B	264	ARG	3.3
1	F	203	PHE	3.3
1	F	253	PHE	3.3
1	F	28	TRP	3.3
1	I	55	ASP	3.3
1	B	85	ASP	3.3
1	F	205	GLY	3.2
1	B	58	ALA	3.2
1	I	20	LEU	3.2
1	H	70	LEU	3.2
1	G	30	ASN	3.2
1	G	90	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	160	TYR	3.2
1	H	85	ASP	3.2
1	F	66	ASP	3.1
1	I	58	ALA	3.1
1	F	64	LYS	3.1
1	B	87	LEU	3.1
1	A	285	ASP	3.1
1	B	263	GLN	3.1
1	A	256	SER	3.0
1	F	124	ALA	3.0
1	J	229	ASP	3.0
1	C	31	ASN	3.0
1	C	21	GLU	2.9
1	B	26	ALA	2.9
1	H	25	PRO	2.9
1	H	151	PHE	2.9
1	I	69	THR	2.8
1	B	21	GLU	2.8
1	F	19	ALA	2.8
1	H	75	GLU	2.8
1	F	89	ARG	2.8
1	F	103	VAL	2.8
1	H	263	GLN	2.8
1	F	51	LEU	2.8
1	F	204	LYS	2.8
1	F	257	GLY	2.7
1	C	230	GLU	2.7
1	F	148	GLN	2.7
1	H	69	THR	2.7
1	B	129	ASN	2.7
1	I	129	ASN	2.7
1	F	123	LEU	2.7
1	H	82	LEU	2.7
1	G	229	ASP	2.7
1	A	142	GLU	2.7
1	B	31	ASN	2.7
1	G	85	ASP	2.7
1	E	125	GLU	2.6
1	G	27	ALA	2.6
1	G	88	THR	2.6
1	I	185	LEU	2.6
1	F	217	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	195	LEU	2.6
1	I	21	GLU	2.6
1	I	70	LEU	2.5
1	F	202	GLY	2.5
1	D	66	ASP	2.5
1	G	256	SER	2.5
1	I	77	ALA	2.5
1	H	32	LEU	2.5
1	I	193	VAL	2.5
1	B	88	THR	2.5
1	F	232	GLY	2.5
1	G	20	LEU	2.5
1	H	18	LYS	2.5
1	C	255	GLY	2.5
1	F	201	TYR	2.4
1	I	139	TYR	2.4
1	E	244	PRO	2.4
1	F	197	VAL	2.4
1	F	254	ILE	2.4
1	D	31	ASN	2.4
1	F	128	SER	2.4
1	E	129	ASN	2.4
1	H	65	THR	2.4
1	H	246	TRP	2.4
1	B	20	LEU	2.4
1	G	26	ALA	2.4
1	G	29	GLN	2.4
1	E	62	SER	2.4
1	F	182	GLY	2.3
1	F	235	ALA	2.3
1	D	30	ASN	2.3
1	A	89	ARG	2.3
1	B	92	PRO	2.3
1	I	128	SER	2.3
1	A	286	LEU	2.2
1	F	222	THR	2.2
1	J	250	THR	2.2
1	F	162	GLU	2.2
1	C	244	PRO	2.2
1	I	83	ASP	2.2
1	E	28	TRP	2.2
1	A	229	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	71	LYS	2.2
1	F	161	VAL	2.2
1	C	66	ASP	2.2
1	E	229	ASP	2.2
1	J	152	ILE	2.2
1	H	150	ARG	2.2
1	B	24	LYS	2.2
1	G	87	LEU	2.2
1	H	264	ARG	2.2
1	I	142	GLU	2.2
1	B	25	PRO	2.2
1	G	21	GLU	2.1
1	F	81	THR	2.1
1	C	80	LEU	2.1
1	B	90	ARG	2.1
1	F	75	GLU	2.1
1	H	84	HIS	2.1
1	F	76	VAL	2.1
1	H	229	ASP	2.1
1	B	150	ARG	2.1
1	B	75	GLU	2.1
1	E	128	SER	2.1
1	F	102	CYS	2.1
1	H	68	TRP	2.1
1	H	66	ASP	2.1
1	C	60	ALA	2.1
1	I	27	ALA	2.1
1	F	264	ARG	2.1
1	H	129	ASN	2.1
1	J	31	ASN	2.1
1	H	21	GLU	2.1
1	D	51	LEU	2.1
1	G	130	ALA	2.1
1	F	174	THR	2.0
1	J	155	GLY	2.0
1	B	142	GLU	2.0
1	F	155	GLY	2.0
1	B	244	PRO	2.0
1	B	266	PRO	2.0
1	F	83	ASP	2.0
1	B	268	LEU	2.0
1	I	216	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

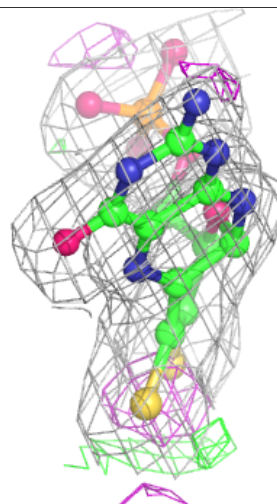
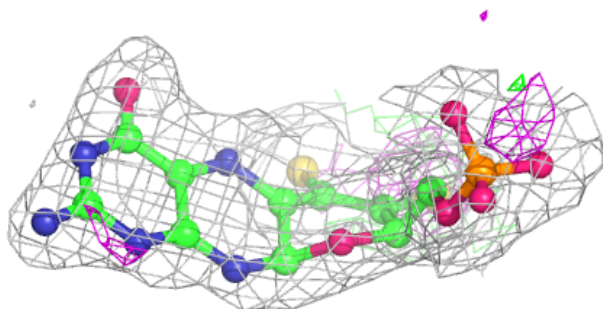
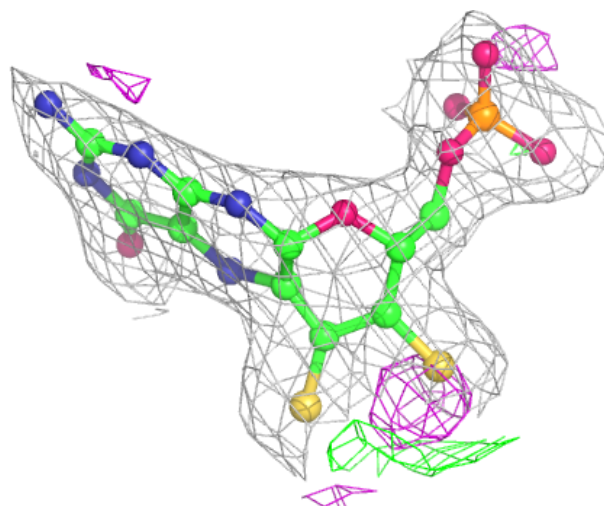
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MTE	I	309	24/24	0.94	0.14	26,42,49,50	0
3	MTE	C	303	24/24	0.95	0.13	15,32,39,42	0
3	MTE	H	308	24/24	0.95	0.15	30,43,48,50	0
2	W	I	409	1/1	0.96	0.15	42,42,42,42	0
3	MTE	F	306	24/24	0.96	0.19	26,38,46,47	0
3	MTE	J	310	24/24	0.97	0.15	8,22,28,29	0
3	MTE	D	304	24/24	0.97	0.14	18,28,35,38	0
3	MTE	G	307	24/24	0.97	0.16	17,26,32,36	0
3	MTE	B	302	24/24	0.97	0.14	22,39,50,56	0
3	MTE	E	305	24/24	0.98	0.13	8,22,33,36	0
3	MTE	A	301	24/24	0.98	0.15	16,23,30,32	0
2	W	F	406	1/1	0.98	0.14	41,41,41,41	0
2	W	B	402	1/1	0.99	0.12	43,43,43,43	0
2	W	H	408	1/1	0.99	0.13	41,41,41,41	0
2	W	J	410	1/1	0.99	0.16	30,30,30,30	0
2	W	E	405	1/1	1.00	0.14	32,32,32,32	0
2	W	A	401	1/1	1.00	0.15	28,28,28,28	0
2	W	D	404	1/1	1.00	0.14	32,32,32,32	0
2	W	G	407	1/1	1.00	0.14	29,29,29,29	0
2	W	C	403	1/1	1.00	0.15	32,32,32,32	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.

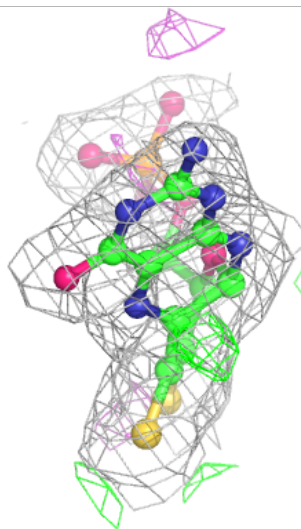
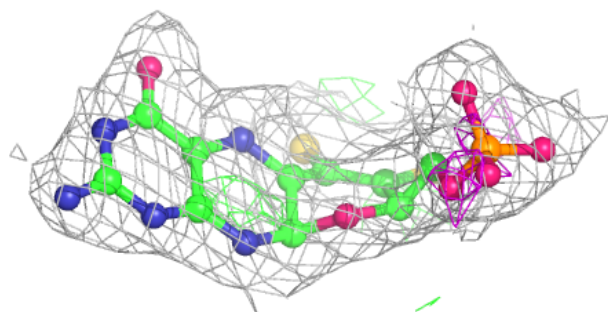
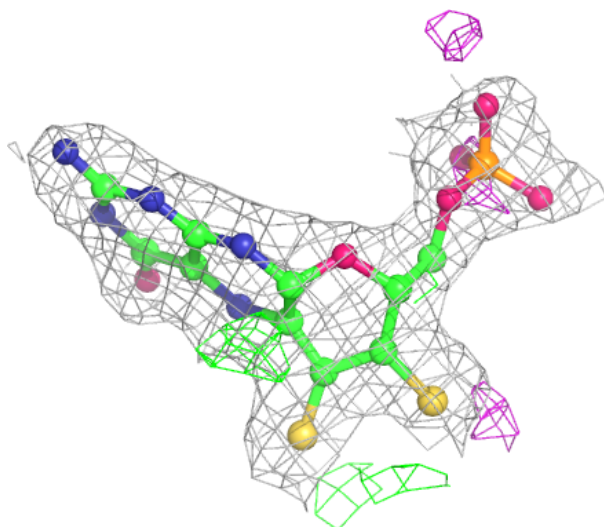
Electron density around MTE I 309:

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



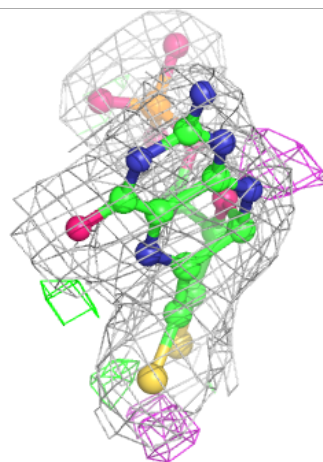
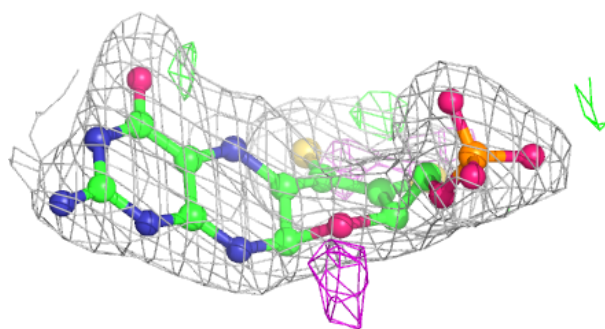
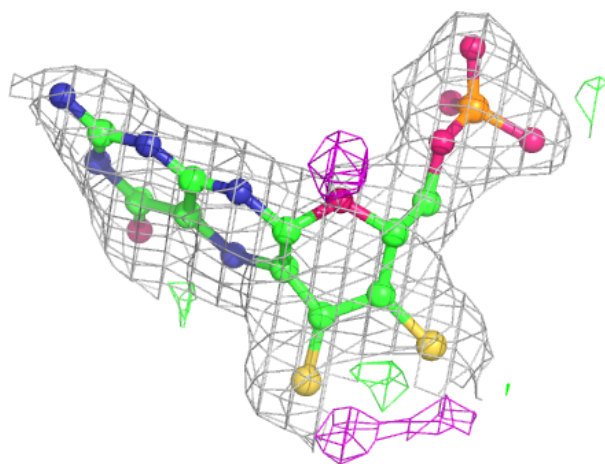
Electron density around MTE C 303:

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



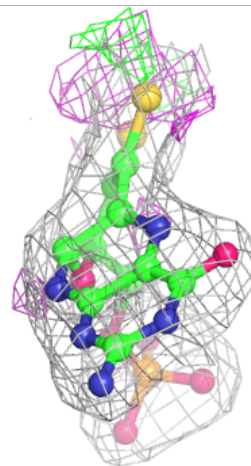
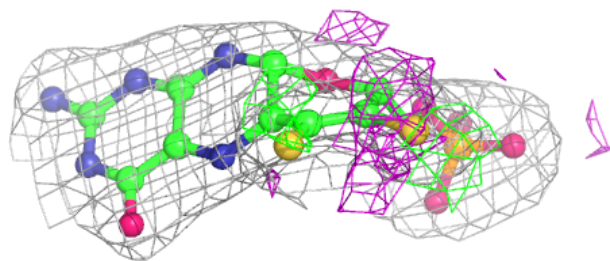
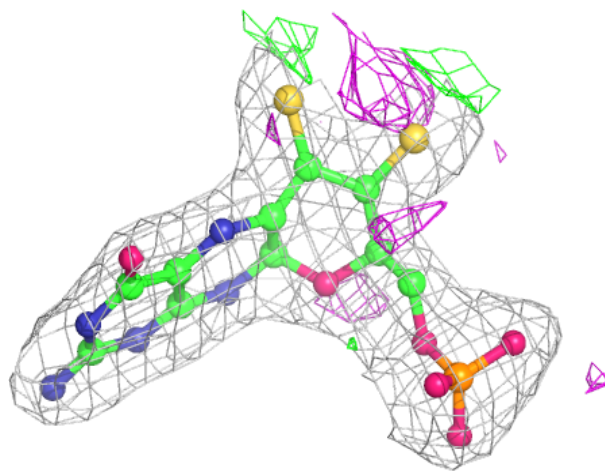
Electron density around MTE H 308:

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



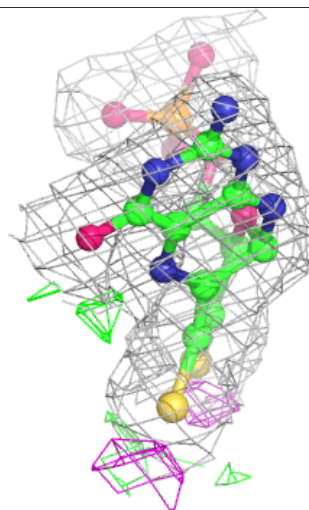
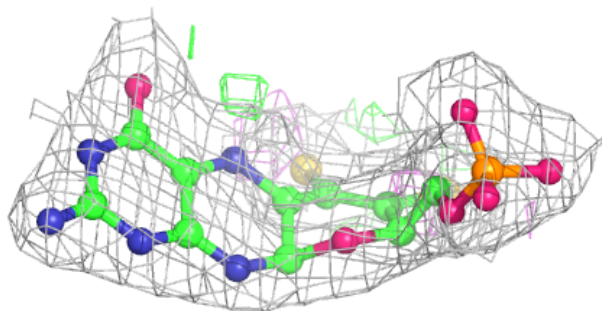
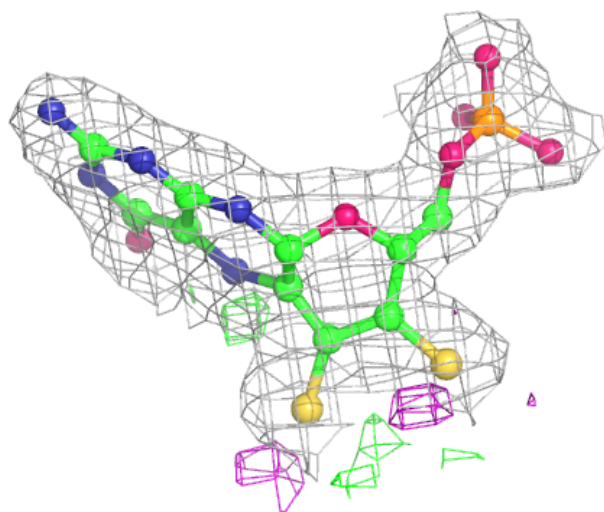
Electron density around MTE F 306:

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



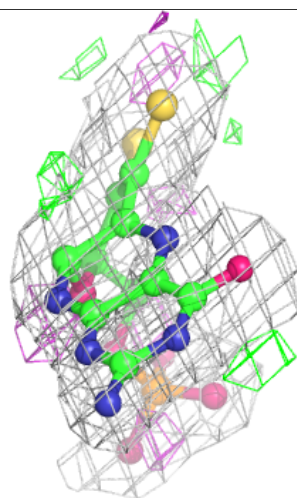
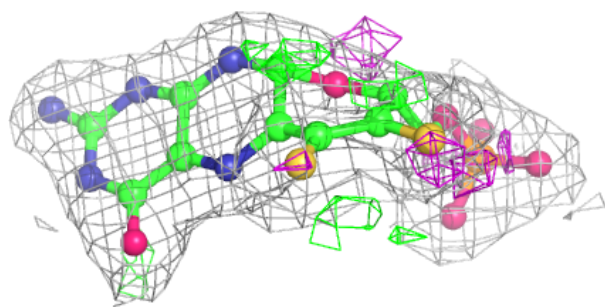
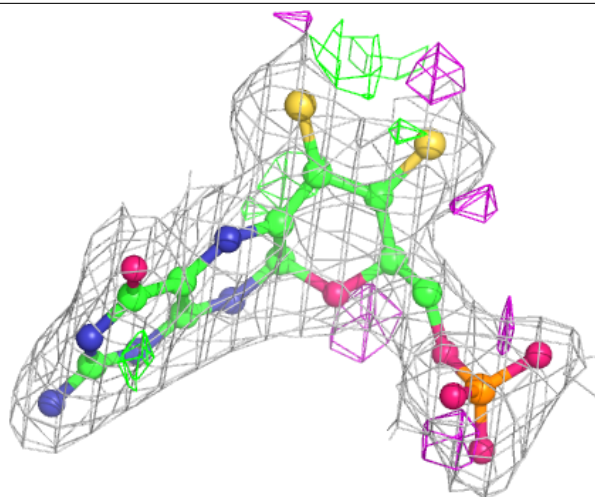
Electron density around MTE J 310:

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



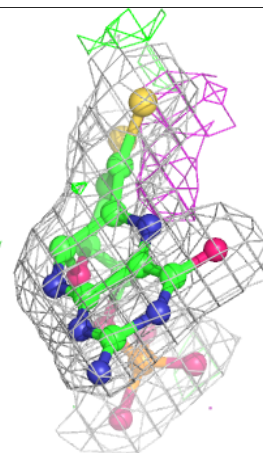
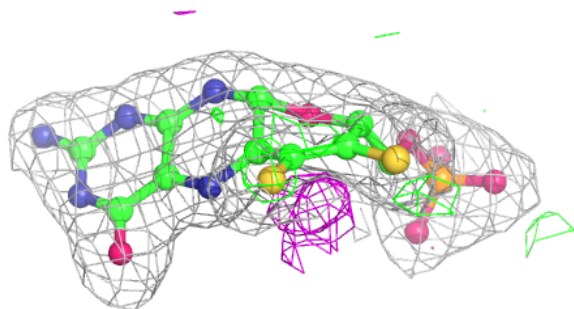
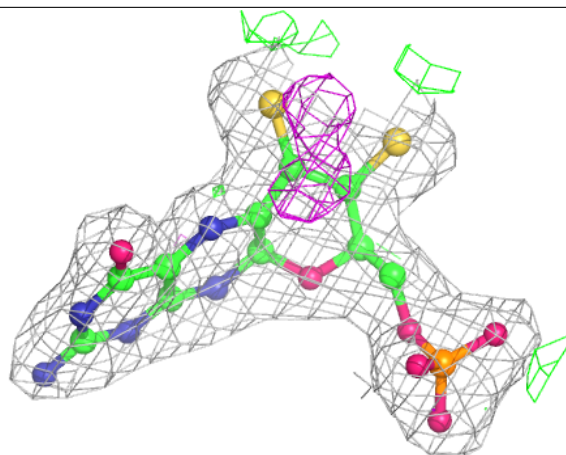
Electron density around MTE D 304:

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



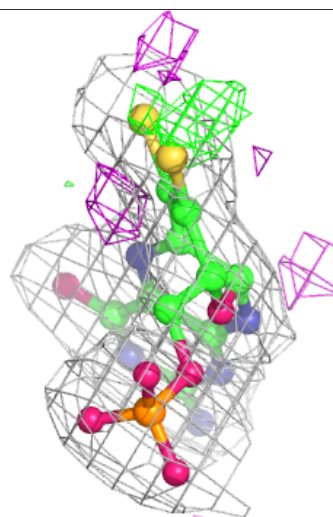
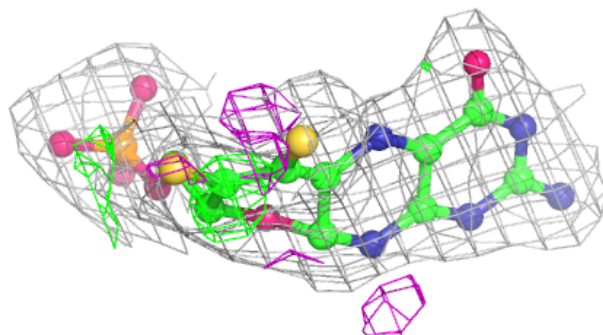
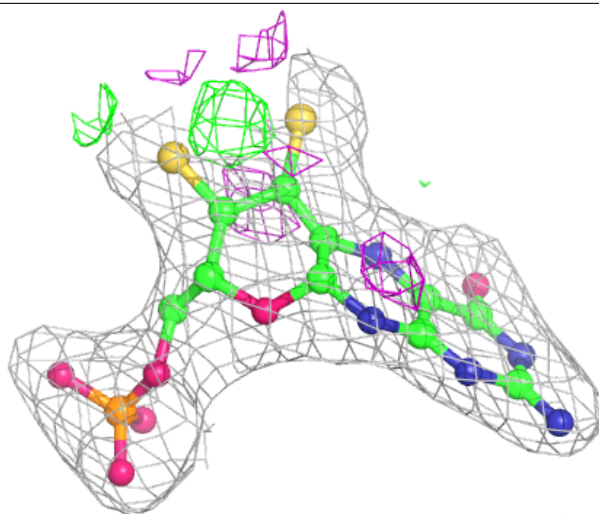
Electron density around MTE G 307:

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



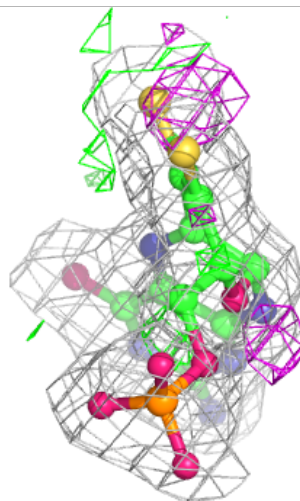
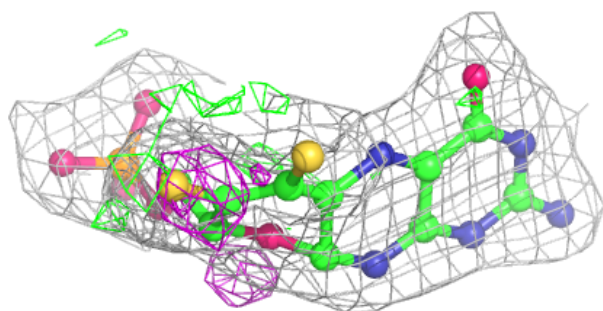
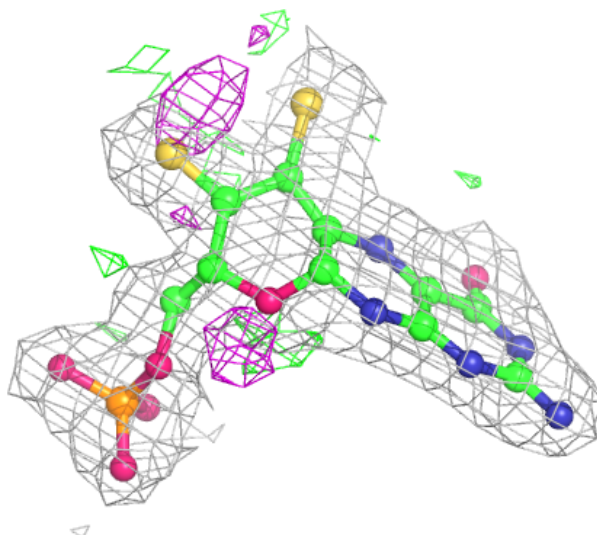
Electron density around MTE B 302:

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



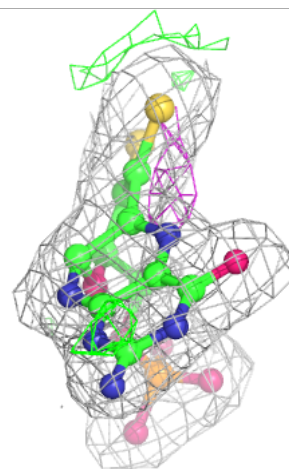
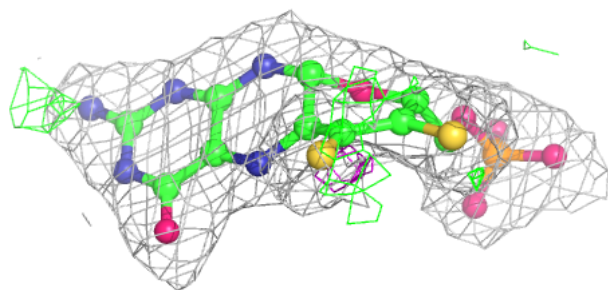
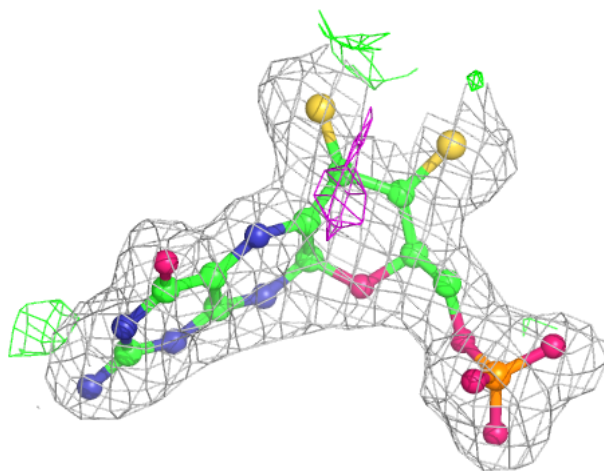
Electron density around MTE E 305:

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



Electron density around MTE A 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.