



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:52 PM UTC

PDB ID : 4ZY0 / pdb_00004zy0
Title : X-ray crystal structure of PfA-M17 in complex with hydroxamic acid-based inhibitor 10q
Authors : Drinkwater, N.; McGowan, S.
Deposited on : 2015-05-21
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

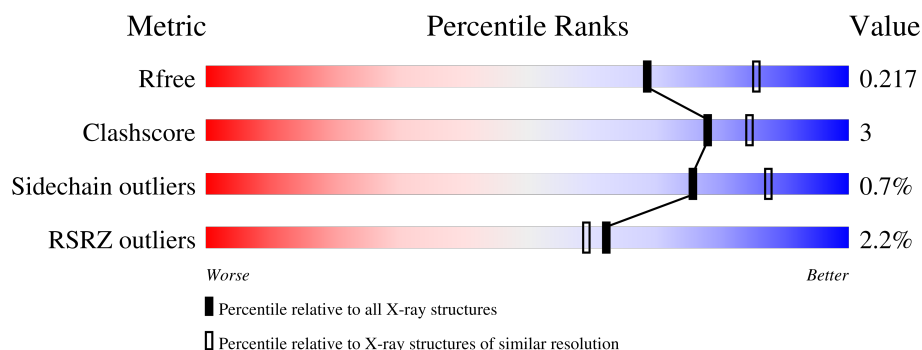
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	522	2% 90% 9%
1	B	522	5% 91% 8%
1	C	522	2% 92% 7%
1	D	522	% 92% 7%
1	E	522	% 91% 7%
1	F	522	4% 91% 7%

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Mol	Chain	Length	Quality of chain
1	G	522	%93%7% .
1	H	522	3%91%8% .
1	I	522	2%93%6% .
1	J	522	2%91%8% .
1	K	522	%91%6% .
1	L	522	3%89%8% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 51006 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 Probable M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			3970	2548	638	765	19			
1	B	518	Total	C	N	O	S	0	0	0
			3910	2512	632	747	19			
1	C	517	Total	C	N	O	S	0	0	0
			3934	2531	636	748	19			
1	D	513	Total	C	N	O	S	0	1	0
			3931	2532	634	745	20			
1	E	509	Total	C	N	O	S	0	0	0
			3891	2505	624	743	19			
1	F	510	Total	C	N	O	S	0	0	0
			3841	2470	619	733	19			
1	G	519	Total	C	N	O	S	0	0	0
			3964	2547	639	759	19			
1	H	517	Total	C	N	O	S	0	1	0
			3934	2528	637	749	20			
1	I	518	Total	C	N	O	S	0	0	0
			3948	2537	638	753	20			
1	J	514	Total	C	N	O	S	0	0	0
			3926	2530	635	741	20			
1	K	508	Total	C	N	O	S	0	0	0
			3901	2512	627	743	19			
1	L	511	Total	C	N	O	S	0	0	0
			3846	2474	621	732	19			

There are 36 discrepancies between the modelled and reference sequences:

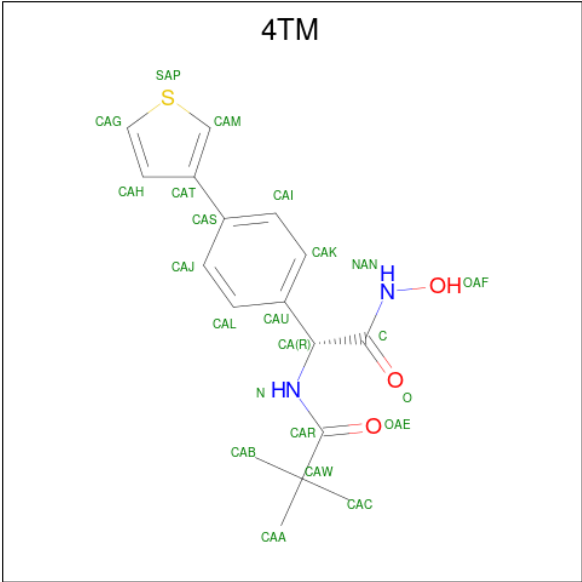
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
E	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
F	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
G	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
H	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
I	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
J	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
K	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
L	546	GLN	ASN	engineered mutation	UNP A0A024V0B1

- Molecule 2 is N-{(1R)-2-(hydroxyamino)-2-oxo-1-[4-(thiophen-3-yl)phenyl]ethyl}-2,2-dimethylpropanamide (CCD ID: 4TM) (formula: C₁₇H₂₀N₂O₃S).

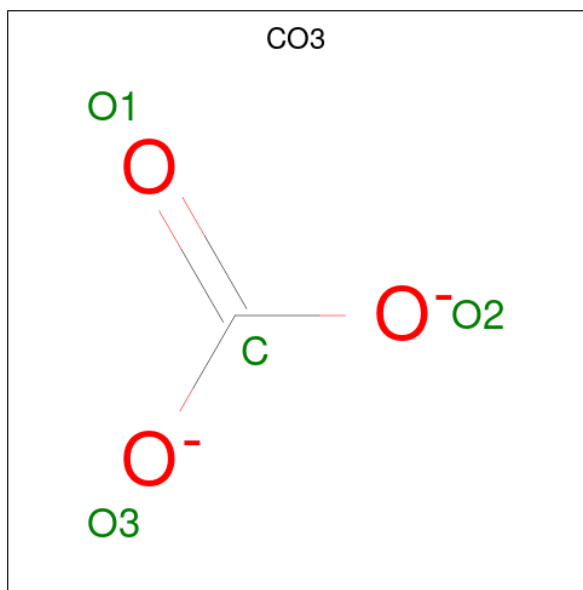


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	C	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	D	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	E	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	F	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	G	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	H	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	I	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	J	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	K	1	Total	C	N	O	S	0	0
			23	17	2	3	1		
2	L	1	Total	C	N	O	S	0	0
			23	17	2	3	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

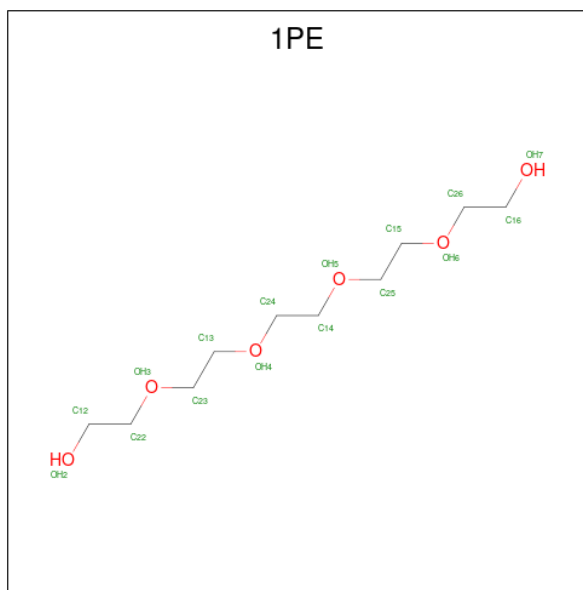
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	F	2	Total 2	Zn 2	0	0
3	G	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	J	2	Total 2	Zn 2	0	0
3	K	2	Total 2	Zn 2	0	0
3	L	2	Total 2	Zn 2	0	0

- Molecule 4 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 1 3	0	0
4	B	1	Total C O 4 1 3	0	0
4	C	1	Total C O 4 1 3	0	0
4	D	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0
4	G	1	Total C O 4 1 3	0	0
4	H	1	Total C O 4 1 3	0	0
4	I	1	Total C O 4 1 3	0	0
4	J	1	Total C O 4 1 3	0	0
4	K	1	Total C O 4 1 3	0	0
4	L	1	Total C O 4 1 3	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



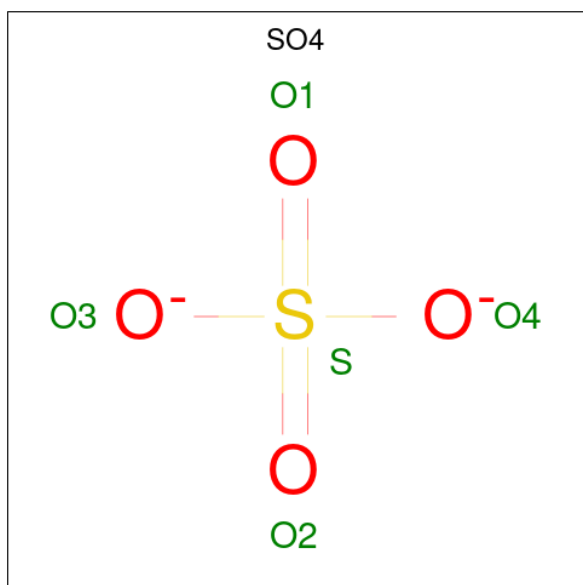
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 9 6 3	0	0
5	A	1	Total C O 6 4 2	0	0
5	A	1	Total C O 6 4 2	0	0
5	B	1	Total C O 10 7 3	0	0
5	C	1	Total C O 12 8 4	0	0
5	C	1	Total C O 11 8 3	0	0
5	D	1	Total C O 11 7 4	0	0
5	D	1	Total C O 10 6 4	0	0
5	E	1	Total C O 12 8 4	0	0
5	E	1	Total C O 12 8 4	0	0
5	F	1	Total C O 11 7 4	0	0
5	F	1	Total C O 7 4 3	0	0
5	F	1	Total C O 10 6 4	0	0
5	G	1	Total C O 9 6 3	0	0
5	G	1	Total C O 12 8 4	0	0
5	H	1	Total C O 10 7 3	0	0
5	H	1	Total C O 10 7 3	0	0
5	I	1	Total C O 13 9 4	0	0
5	I	1	Total C O 9 6 3	0	0
5	J	1	Total C O 10 7 3	0	0
5	J	1	Total C O 10 7 3	0	0
5	K	1	Total C O 12 8 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			12	8	4		
5	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	295	Total	O	0	0
			295	295		
8	B	237	Total	O	0	0
			237	237		
8	C	283	Total	O	0	0
			283	283		
8	D	304	Total	O	0	0
			304	304		
8	E	348	Total	O	0	0
			348	348		
8	F	214	Total	O	0	0
			214	214		
8	G	297	Total	O	0	0
			297	297		
8	H	222	Total	O	0	0
			222	222		
8	I	269	Total	O	0	0
			269	269		
8	J	292	Total	O	0	0
			292	292		

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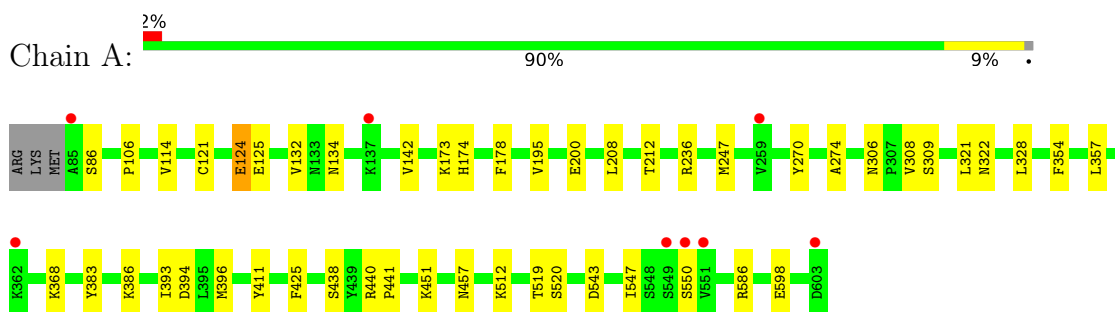
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	287	Total 287	O 287	0	0
8	L	243	Total 243	O 243	0	0

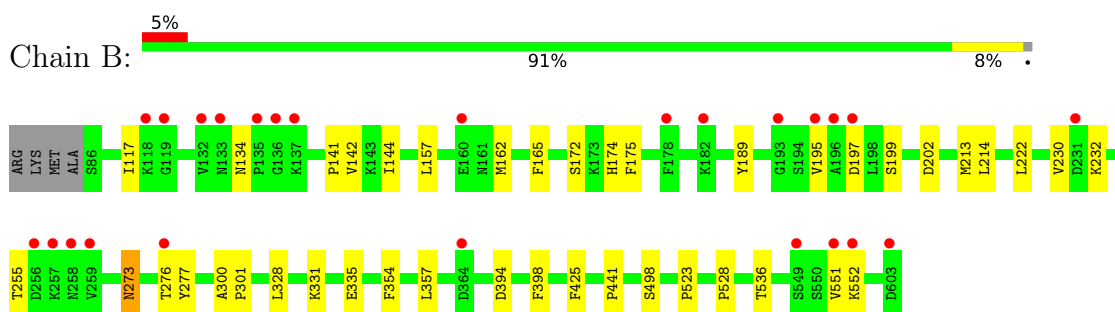
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

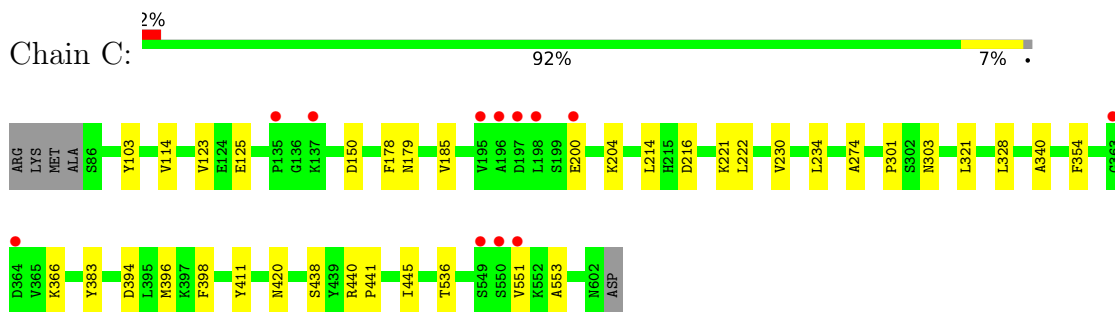
- Molecule 1: Probable M17 family aminopeptidase



- Molecule 1: Probable M17 family aminopeptidase

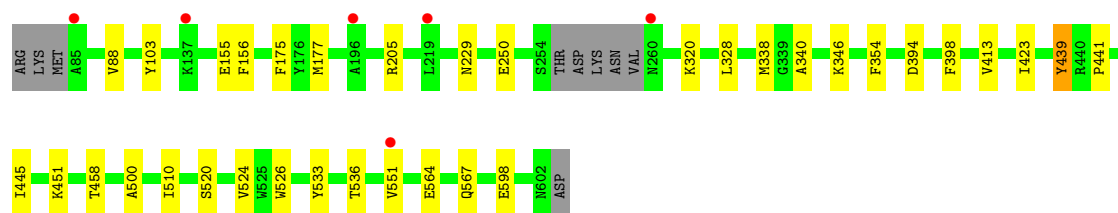


- Molecule 1: Probable M17 family aminopeptidase

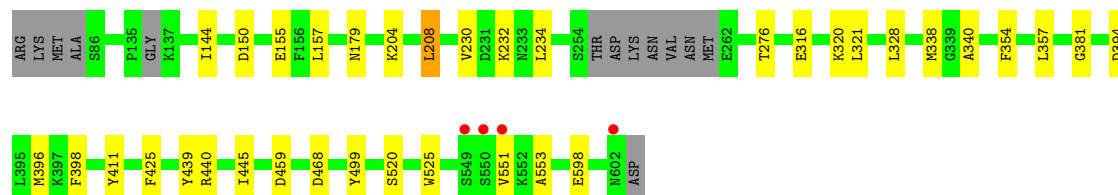
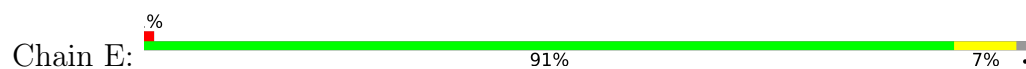


- Molecule 1: Probable M17 family aminopeptidase

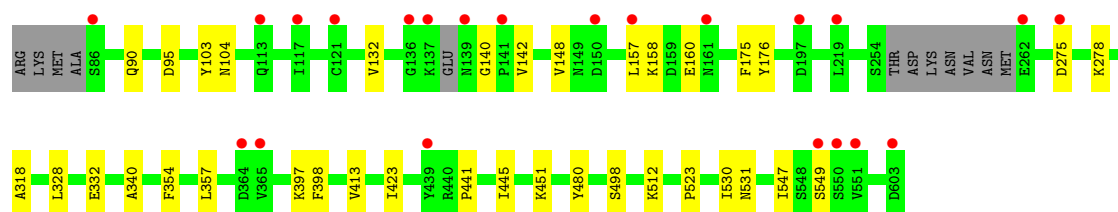
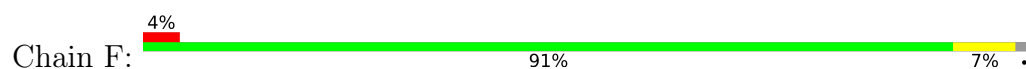




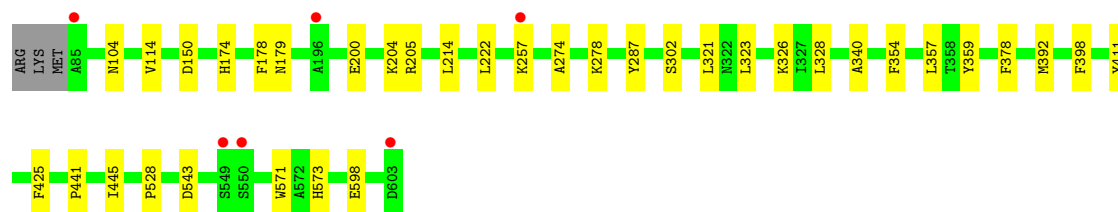
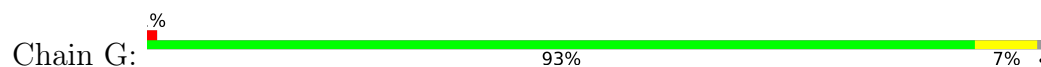
- Molecule 1: Probable M17 family aminopeptidase



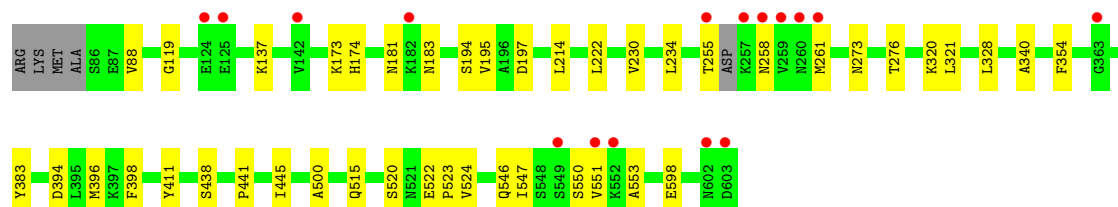
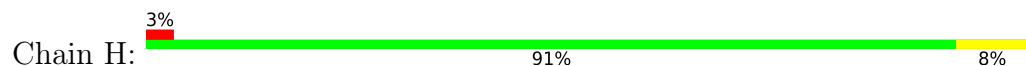
- Molecule 1: Probable M17 family aminopeptidase

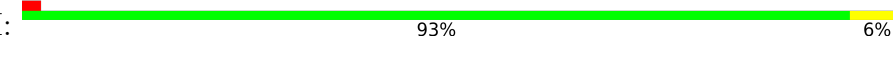


- Molecule 1: Probable M17 family aminopeptidase



- Molecule 1: Probable M17 family aminopeptidase



- Chain I: 

- Chain J: 
- 
- ARG LYS MET A85 P96 V123 V132 K137 V142 K143 I144 E155 F156 L157 M162 F175 E200 L214 L219 L222 N229 V230 L234 S254 THR ASP LYS ASN VAL N260 N303 E316 K320 L321 L328 Y341 F354 C361
- M392 I393 C394 Y411 G412 V413 I423 A428 R440 P441 D459 S498 P523 V524 W525 P528 Y533 T536 S549 S550 V551 K563 Q567 L601 N602 D603

- [illegible]

- Chain L: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.72Å 176.07Å 230.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 2.20 48.63 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.63-2.20) 88.4 (48.63-2.20)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.198 , 0.244 (Not available) , 0.217	Depositor DCC
R_{free} test set	17813 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51006	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8453e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 4TM, GOL, SO4, 1PE, CO3, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/4051	0.71	2/5500 (0.0%)
1	B	0.33	0/3988	0.71	0/5424
1	C	0.32	0/4012	0.70	0/5448
1	D	0.33	0/4011	0.70	1/5438 (0.0%)
1	E	0.32	0/3967	0.69	0/5382
1	F	0.31	0/3917	0.72	4/5326 (0.1%)
1	G	0.32	0/4042	0.69	0/5486
1	H	0.32	0/4014	0.71	1/5450 (0.0%)
1	I	0.32	0/4026	0.68	0/5466
1	J	0.32	0/4003	0.69	0/5427
1	K	0.32	0/3976	0.70	0/5389
1	L	0.34	0/3923	0.73	2/5336 (0.0%)
All	All	0.32	0/47930	0.70	10/65072 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	551	VAL	N-CA-C	-8.09	105.60	113.53
1	F	549	SER	CA-C-N	7.46	135.13	121.70
1	F	549	SER	C-N-CA	7.46	135.13	121.70
1	L	138	GLU	N-CA-C	6.28	121.01	113.23
1	A	134	ASN	CA-C-N	5.69	126.02	119.93
1	A	134	ASN	C-N-CA	5.69	126.02	119.93
1	F	140	GLY	CA-C-N	5.30	125.28	120.03
1	F	140	GLY	C-N-CA	5.30	125.28	120.03
1	H	119	GLY	N-CA-C	-5.13	107.92	114.85
1	D	551	VAL	N-CA-C	5.06	119.86	109.34

There are no chirality outliers.

There are no planarity outliers.

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	3970	0	3866	30	0
1	B	3910	0	3778	25	0
1	C	3934	0	3848	22	0
1	D	3931	0	3869	19	0
1	E	3891	0	3809	22	0
1	F	3841	0	3705	22	0
1	G	3964	0	3871	23	0
1	H	3934	0	3831	25	0
1	I	3948	0	3864	23	0
1	J	3926	0	3866	27	0
1	K	3901	0	3837	20	0
1	L	3846	0	3709	26	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
2	E	23	0	0	0	0
2	F	23	0	0	0	0
2	G	23	0	0	1	0
2	H	23	0	0	0	0
2	I	23	0	0	0	0
2	J	23	0	0	1	0
2	K	23	0	0	0	0
2	L	23	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	21	0	20	1	0
5	B	10	0	10	0	0
5	C	23	0	26	0	0
5	D	21	0	26	2	0
5	E	24	0	28	3	0
5	F	28	0	34	6	0
5	G	21	0	22	1	0
5	H	20	0	20	2	0
5	I	22	0	24	4	0
5	J	20	0	20	3	0
5	K	24	0	28	0	0
5	L	10	0	13	2	0
6	A	10	0	0	0	0
6	B	15	0	0	1	0
6	C	15	0	0	1	0
6	D	5	0	0	0	0
6	E	10	0	0	0	0
6	F	5	0	0	1	0
6	G	10	0	0	1	0
6	H	20	0	0	0	0
6	I	5	0	0	0	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	10	0	0	2	0
7	C	6	0	8	0	0
7	G	6	0	8	0	0
8	A	295	0	0	7	0
8	B	237	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	283	0	0	2	0
8	D	304	0	0	3	0
8	E	348	0	0	3	0
8	F	214	0	0	1	0
8	G	297	0	0	3	0
8	H	222	0	0	1	0
8	I	269	0	0	1	0
8	J	292	0	0	3	0
8	K	287	0	0	2	0
8	L	243	0	0	0	0
All	All	51006	0	46140	260	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 3.

All (260) 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:L:104:ASN:HD21	5:L:1005:1PE:H161	1.29	0.95
1:L:104:ASN:ND2	5:L:1005:1PE:H161	1.96	0.80
1:I:320:LYS:HZ1	5:I:1005:1PE:H142	1.48	0.77
1:A:512:LYS:NZ	8:A:1101:HOH:O	2.19	0.76
1:F:451:LYS:HG2	5:F:1005:1PE:H262	1.70	0.73
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.70	0.72
1:A:386:LYS:HE3	1:A:396:MET:HE2	1.73	0.70
1:I:360:LYS:NZ	1:I:422:GLU:OE1	2.25	0.69
1:K:338:MET:HE2	1:K:468:ASP:HB3	1.75	0.69
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.74	0.69
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.75	0.69
1:A:451:LYS:HG2	1:B:255:THR:HG21	1.72	0.69
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.76	0.67
1:I:567:GLN:NE2	8:I:1102:HOH:O	2.25	0.67
5:E:1006:1PE:OH6	8:E:1101:HOH:O	2.12	0.67
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.60	0.67
1:J:316:GLU:HG3	5:J:1005:1PE:H221	1.76	0.67
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.77	0.66
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.76	0.66
1:I:396:MET:SD	1:I:398:PHE:HE2	2.19	0.66
1:G:205:ARG:NE	8:G:1104:HOH:O	2.29	0.65
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.63	0.64
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.81	0.63
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.79	0.63
1:C:366:LYS:HG3	1:C:420:ASN:HB3	1.81	0.61
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.82	0.61
1:I:326:LYS:HE3	1:I:328:LEU:HD11	1.83	0.60
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.84	0.60
1:F:531:ASN:HB2	5:F:1006:1PE:H141	1.83	0.60
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.83	0.59
6:B:1008:SO4:O3	1:E:499:TYR:OH	2.18	0.59
1:H:320:LYS:HZ1	5:H:1006:1PE:H142	1.67	0.59
1:A:368:LYS:NZ	8:A:1110:HOH:O	2.34	0.58
1:H:137:LYS:O	1:H:194:SER:OG	2.21	0.58
1:J:320:LYS:HZ1	5:J:1005:1PE:H142	1.67	0.58
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.86	0.57
1:G:104:ASN:ND2	6:G:1008:SO4:O4	2.37	0.57
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.69	0.57
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.86	0.57
1:H:546:GLN:HG3	1:H:547:ILE:HG23	1.86	0.57
1:D:500:ALA:HB3	1:D:524:VAL:HG22	1.87	0.57
1:L:531:ASN:ND2	6:L:1006:SO4:O3	2.32	0.57
1:E:232:LYS:NZ	1:E:276:THR:O	2.36	0.56
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.87	0.56
1:A:322:ASN:ND2	8:A:1105:HOH:O	2.30	0.56
1:A:173:LYS:NZ	8:A:1114:HOH:O	2.38	0.55
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.88	0.55
1:D:320:LYS:HE2	5:D:1005:1PE:H152	1.87	0.55
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.88	0.55
1:A:440:ARG:NH1	8:A:1115:HOH:O	2.39	0.55
1:I:551:VAL:HG12	1:I:553:ALA:H	1.72	0.55
1:L:138:GLU:N	1:L:139:ASN:HA	2.22	0.55
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.89	0.55
1:C:536:THR:HG21	1:C:551:VAL:HG23	1.88	0.54
1:F:158:LYS:HG2	1:F:160:GLU:H	1.72	0.54
1:A:106:PRO:HD2	1:A:247:MET:HE1	1.89	0.54
1:G:278:LYS:NZ	8:G:1111:HOH:O	2.39	0.54
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.89	0.54
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.89	0.54
1:F:530:ILE:HG23	5:F:1006:1PE:H242	1.90	0.54
1:F:480:TYR:OH	1:F:512:LYS:NZ	2.34	0.53
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.90	0.53
1:C:103:TYR:N	6:C:1008:SO4:O3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.91	0.53
1:L:413:VAL:HG11	1:L:423:ILE:HD12	1.91	0.53
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.91	0.52
1:B:144:ILE:HD12	1:B:157:LEU:HB3	1.91	0.52
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.90	0.52
1:J:320:LYS:NZ	5:J:1005:1PE:H142	2.25	0.52
1:H:550:SER:OG	1:H:551:VAL:N	2.42	0.52
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.91	0.51
1:J:214:LEU:HD11	1:J:222:LEU:HD22	1.91	0.51
1:A:520:SER:HB3	1:A:598:GLU:HG3	1.93	0.51
1:F:90:GLN:NE2	1:F:95:ASP:O	2.39	0.51
1:C:204:LYS:NZ	8:C:1113:HOH:O	2.44	0.51
1:G:114:VAL:HG12	1:G:274:ALA:HB1	1.92	0.50
1:G:287:TYR:OH	1:G:598:GLU:OE2	2.28	0.50
1:H:258:ASN:HB3	1:H:261:MET:HB2	1.93	0.50
1:C:396:MET:SD	1:C:398:PHE:HE2	2.35	0.50
1:F:451:LYS:HG2	5:F:1005:1PE:H152	1.93	0.50
1:B:195:VAL:HG12	1:B:197:ASP:H	1.77	0.50
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.94	0.50
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.94	0.49
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.94	0.49
1:K:331:LYS:O	1:K:335:GLU:HG3	2.12	0.49
1:L:504:GLY:HA3	1:L:510:ILE:HD11	1.95	0.49
1:A:208:LEU:O	1:A:212:THR:HG23	2.13	0.49
1:E:396:MET:SD	1:E:398:PHE:HE2	2.35	0.49
1:B:199:SER:OG	1:B:202:ASP:OD2	2.27	0.49
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.95	0.49
1:E:316:GLU:HG3	5:E:1005:1PE:H251	1.95	0.49
1:G:392:MET:HE3	2:G:1001:4TM:SAP	2.53	0.49
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.95	0.49
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.94	0.49
1:K:230:VAL:HG13	1:K:234:LEU:HB3	1.94	0.49
1:L:103:TYR:OH	1:L:316:GLU:OE2	2.24	0.48
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.48	0.48
1:K:364:ASP:O	1:K:420:ASN:HA	2.13	0.48
1:K:480:TYR:OH	1:K:512:LYS:NZ	2.34	0.48
1:F:397:LYS:NZ	8:F:1113:HOH:O	2.47	0.48
1:J:563:LYS:NZ	8:J:2515:HOH:O	2.46	0.48
1:B:165:PHE:HB3	1:B:189:TYR:OH	2.14	0.47
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.96	0.47
1:E:320:LYS:HB3	5:E:1006:1PE:H252	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.95	0.47
1:G:543:ASP:CG	1:H:255:THR:H	2.21	0.47
1:F:451:LYS:HE3	5:F:1005:1PE:H242	1.96	0.47
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.95	0.47
1:F:275:ASP:HA	1:F:278:LYS:HE3	1.96	0.47
1:J:392:MET:HE3	2:J:1001:4TM:SAP	2.55	0.47
1:D:451:LYS:NZ	1:D:564:GLU:O	2.47	0.47
1:F:413:VAL:HG11	1:F:423:ILE:HD12	1.95	0.47
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.96	0.47
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.96	0.47
1:D:413:VAL:HG11	1:D:423:ILE:HD12	1.96	0.47
1:G:326:LYS:HE3	1:G:328:LEU:HD11	1.97	0.47
1:I:108:HIS:CD2	5:I:1006:1PE:H142	2.50	0.47
1:B:331:LYS:O	1:B:335:GLU:HG3	2.15	0.47
1:E:520:SER:HB3	1:E:598:GLU:HG3	1.96	0.47
1:E:338:MET:HE3	1:E:468:ASP:HB3	1.96	0.46
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.98	0.46
1:K:338:MET:HE1	1:K:354:PHE:CE2	2.50	0.46
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.96	0.46
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.50	0.46
1:L:214:LEU:HD21	1:L:222:LEU:HD22	1.97	0.46
1:I:498:SER:O	1:I:523:PRO:HG2	2.16	0.46
1:K:164:LYS:NZ	8:K:1116:HOH:O	2.49	0.46
1:C:125:GLU:HG3	1:C:221:LYS:HD2	1.96	0.46
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.98	0.46
1:K:396:MET:SD	1:K:398:PHE:HE2	2.39	0.46
5:G:1007:1PE:H142	5:G:1007:1PE:H152	1.70	0.46
1:H:195:VAL:HG12	1:H:197:ASP:H	1.81	0.46
1:L:275:ASP:HA	1:L:278:LYS:HD2	1.98	0.46
1:D:103:TYR:HB3	5:D:1006:1PE:H261	1.97	0.45
1:J:132:VAL:HG11	1:J:144:ILE:HD13	1.97	0.45
1:H:553:ALA:N	8:H:1120:HOH:O	2.50	0.45
1:J:440:ARG:NH1	8:J:2517:HOH:O	2.48	0.45
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.99	0.45
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.98	0.45
1:A:393:ILE:HA	1:A:396:MET:HG2	1.99	0.45
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.99	0.45
1:K:440:ARG:NH2	8:K:1117:HOH:O	2.49	0.45
1:D:533:TYR:O	1:D:536:THR:HG22	2.16	0.45
1:E:150:ASP:OD1	1:E:179:ASN:HB2	2.16	0.45
1:L:498:SER:O	1:L:523:PRO:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:137:LYS:CB	1:L:140:GLY:H	2.30	0.45
1:B:214:LEU:HD21	1:B:222:LEU:HD22	1.98	0.45
1:C:114:VAL:HG12	1:C:274:ALA:HB1	1.99	0.45
1:F:103:TYR:HB3	5:F:1007:1PE:H252	1.99	0.45
1:I:195:VAL:HG12	1:I:197:ASP:H	1.81	0.45
1:D:156:PHE:CG	1:D:177:MET:HE1	2.52	0.45
1:I:525:TRP:CE2	1:J:528:PRO:HD3	2.52	0.45
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.52	0.44
1:B:157:LEU:HA	1:B:162:MET:HE3	1.97	0.44
1:B:551:VAL:HG12	1:B:552:LYS:O	2.17	0.44
1:A:394:ASP:HA	1:C:441:PRO:HB2	2.00	0.44
1:I:411:TYR:HE1	5:I:1006:1PE:H232	1.82	0.44
1:A:200:GLU:OE1	1:A:200:GLU:N	2.49	0.44
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.99	0.44
1:F:318:ALA:HB2	1:F:357:LEU:HD22	2.00	0.44
1:K:144:ILE:HG13	1:K:157:LEU:HD22	2.00	0.44
1:G:257:LYS:NZ	8:G:1121:HOH:O	2.45	0.44
1:H:181:ASN:HD22	1:H:183:ASN:HD21	1.64	0.44
1:C:214:LEU:HD21	1:C:222:LEU:HD22	2.00	0.44
1:F:104:ASN:N	6:F:1008:SO4:O4	2.44	0.44
1:G:528:PRO:HB3	1:L:525:TRP:CZ3	2.53	0.44
1:I:114:VAL:HG12	1:I:274:ALA:HB1	2.00	0.44
1:J:341:TYR:CE1	1:J:428:ALA:HB1	2.53	0.44
1:L:114:VAL:HG12	1:L:274:ALA:HB1	1.99	0.44
1:C:216:ASP:HB3	8:E:1179:HOH:O	2.18	0.43
1:G:302:SER:OG	1:G:378:PHE:HB2	2.18	0.43
1:C:383:TYR:HE2	1:C:438:SER:HB2	1.82	0.43
1:D:205:ARG:NH2	8:D:1128:HOH:O	2.51	0.43
1:L:307:PRO:HD3	1:L:377:THR:OG1	2.17	0.43
1:B:134:ASN:ND2	1:B:141:PRO:O	2.51	0.43
1:D:520:SER:HB3	1:D:598:GLU:HG3	2.01	0.43
1:F:498:SER:O	1:F:523:PRO:HG2	2.19	0.43
1:H:500:ALA:HB3	1:H:524:VAL:HG22	1.99	0.43
5:A:1005:1PE:H131	8:A:1251:HOH:O	2.17	0.43
1:C:123:VAL:HG12	1:C:185:VAL:HG21	2.01	0.43
1:E:551:VAL:C	1:E:553:ALA:H	2.25	0.43
1:G:441:PRO:HB2	1:H:394:ASP:HA	2.00	0.43
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.99	0.43
1:D:338:MET:HE2	8:D:1178:HOH:O	2.19	0.43
1:J:230:VAL:HG12	1:J:234:LEU:HD23	2.00	0.43
1:J:321:LEU:HD11	1:J:411:TYR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:439:TYR:H	1:K:439:TYR:HD2	1.65	0.43
1:A:121:CYS:HA	1:A:270:TYR:CE2	2.54	0.43
1:A:124:GLU:HB3	1:A:125:GLU:H	1.66	0.43
1:A:543:ASP:CG	1:B:255:THR:HG22	2.44	0.43
1:B:300:ALA:HA	1:B:301:PRO:HD3	1.89	0.43
1:D:346:LYS:O	8:D:1101:HOH:O	2.20	0.43
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.54	0.43
1:H:520:SER:HB3	1:H:598:GLU:HG3	1.99	0.43
1:E:357:LEU:HB2	1:E:425:PHE:HB2	2.01	0.42
1:E:381:GLY:HA2	1:E:459:ASP:OD1	2.18	0.42
1:I:321:LEU:HD11	1:I:411:TYR:HA	2.01	0.42
1:L:300:ALA:HA	1:L:301:PRO:HD3	1.84	0.42
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.90	0.42
1:E:321:LEU:HD11	1:E:411:TYR:HA	2.01	0.42
1:J:533:TYR:O	1:J:536:THR:HG22	2.19	0.42
1:B:273:ASN:O	1:B:276:THR:HG22	2.20	0.42
1:D:340:ALA:HA	1:D:445:ILE:HD12	2.01	0.42
1:K:198:LEU:HD22	1:K:202:ASP:HB3	2.00	0.42
1:C:551:VAL:HG12	1:C:553:ALA:H	1.85	0.42
1:D:439:TYR:OH	1:D:458:THR:O	2.31	0.42
1:J:229:ASN:ND2	8:J:2511:HOH:O	2.39	0.42
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.01	0.42
1:G:571:TRP:CZ2	1:G:573:HIS:HB2	2.54	0.42
1:H:273:ASN:O	1:H:276:THR:OG1	2.35	0.42
1:C:301:PRO:HB2	1:C:303:ASN:OD1	2.20	0.42
1:E:440:ARG:NH2	8:E:1122:HOH:O	2.49	0.42
1:A:457:ASN:HB2	1:A:547:ILE:HD13	2.02	0.42
1:B:357:LEU:HB2	1:B:425:PHE:HB2	2.01	0.42
1:B:528:PRO:HB3	1:E:525:TRP:CZ3	2.55	0.42
1:E:230:VAL:HG13	1:E:234:LEU:HB3	2.00	0.42
1:I:396:MET:SD	1:I:398:PHE:CE2	3.06	0.42
1:I:536:THR:HG21	1:I:551:VAL:HG23	2.01	0.42
1:A:586:ARG:NH2	8:A:1122:HOH:O	2.46	0.42
1:B:230:VAL:O	1:B:277:TYR:OH	2.30	0.42
1:C:230:VAL:HG12	1:C:234:LEU:HD23	2.01	0.42
1:L:546:GLN:HG2	1:L:547:ILE:HG23	2.02	0.42
1:A:236:ARG:NH2	1:A:519:THR:O	2.52	0.41
1:G:150:ASP:OD1	1:G:179:ASN:HB2	2.19	0.41
1:I:316:GLU:HG3	5:I:1005:1PE:H231	2.02	0.41
1:B:172:SER:HB2	1:B:213:MET:HE3	2.01	0.41
1:D:510:ILE:HD13	1:D:526:TRP:NE1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:168:LYS:O	1:I:171:THR:HB	2.21	0.41
1:K:300:ALA:HA	1:K:301:PRO:HD3	1.80	0.41
1:A:306:ASN:H	1:A:309:SER:HG	1.68	0.41
1:B:498:SER:O	1:B:523:PRO:HG2	2.20	0.41
1:H:173:LYS:HA	1:H:173:LYS:HD3	1.94	0.41
1:L:451:LYS:NZ	1:L:564:GLU:O	2.53	0.41
1:H:522:GLU:HA	1:H:523:PRO:HD2	1.91	0.41
1:L:104:ASN:HB2	6:L:1007:SO4:O4	2.21	0.41
1:A:86:SER:HB2	1:A:308:VAL:HG13	2.03	0.41
1:B:174:HIS:HB3	1:F:175:PHE:CE1	2.56	0.41
1:C:440:ARG:NH2	8:C:1130:HOH:O	2.54	0.41
1:G:323:LEU:HD22	1:G:359:TYR:HB2	2.02	0.41
1:L:488:THR:HG21	1:L:555:SER:HA	2.02	0.41
1:A:383:TYR:HE2	1:A:438:SER:HB2	1.86	0.41
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.56	0.41
1:J:498:SER:O	1:J:523:PRO:HG2	2.20	0.41
1:K:160:GLU:CD	1:K:160:GLU:H	2.28	0.41
1:C:150:ASP:OD1	1:C:179:ASN:HB2	2.21	0.40
1:J:156:PHE:O	1:J:162:MET:HE3	2.21	0.40
1:H:396:MET:SD	1:H:398:PHE:HE2	2.45	0.40
1:J:413:VAL:HG11	1:J:423:ILE:HD12	2.02	0.40
1:E:204:LYS:HE3	1:E:204:LYS:HB2	1.86	0.40
1:L:340:ALA:HA	1:L:445:ILE:HD12	2.03	0.40
1:G:204:LYS:HE3	1:G:204:LYS:HB2	1.89	0.40
1:H:214:LEU:HD21	1:H:222:LEU:HD22	2.03	0.40
1:H:320:LYS:HZ1	5:H:1006:1PE:H132	1.86	0.40
1:I:520:SER:HB3	1:I:598:GLU:HG3	2.03	0.40
1:J:96:PRO:HG2	1:J:303:ASN:O	2.21	0.40
1:J:381:GLY:HA2	1:J:459:ASP:OD1	2.22	0.40
1:B:175:PHE:HD1	1:F:176:TYR:HB2	1.87	0.40
1:F:148:VAL:HG21	1:F:157:LEU:HD12	2.04	0.40
1:H:383:TYR:HE2	1:H:438:SER:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	420/450 (93%)	417 (99%)	3 (1%)	76	87
1	B	408/450 (91%)	404 (99%)	4 (1%)	68	81
1	C	415/450 (92%)	414 (100%)	1 (0%)	87	94
1	D	416/450 (92%)	409 (98%)	7 (2%)	53	69
1	E	413/450 (92%)	411 (100%)	2 (0%)	81	90
1	F	400/450 (89%)	397 (99%)	3 (1%)	73	85
1	G	418/450 (93%)	416 (100%)	2 (0%)	81	90
1	H	414/450 (92%)	412 (100%)	2 (0%)	81	90
1	I	419/450 (93%)	416 (99%)	3 (1%)	76	87
1	J	414/450 (92%)	412 (100%)	2 (0%)	81	90
1	K	416/450 (92%)	413 (99%)	3 (1%)	76	87
1	L	399/450 (89%)	394 (99%)	5 (1%)	61	76
All	All	4952/5400 (92%)	4915 (99%)	37 (1%)	76	87

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	GLU
1	A	195	VAL
1	A	550	SER
1	B	117	ILE
1	B	232	LYS
1	B	273	ASN
1	B	398	PHE
1	C	200	GLU
1	D	88	VAL
1	D	229[A]	ASN
1	D	229[B]	ASN
1	D	250	GLU
1	D	398	PHE
1	D	439	TYR

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Mol	Chain	Res	Type
1	D	567	GLN
1	E	208	LEU
1	E	439	TYR
1	F	332	GLU
1	F	398	PHE
1	F	547	ILE
1	G	200	GLU
1	G	398	PHE
1	H	88	VAL
1	H	515	GLN
1	I	171	THR
1	I	185	VAL
1	I	567	GLN
1	J	567	GLN
1	J	601	LEU
1	K	117	ILE
1	K	160	GLU
1	K	439	TYR
1	L	104	ASN
1	L	398	PHE
1	L	439	TYR
1	L	551	VAL
1	L	568	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	437	ASN
1	B	139	ASN
1	B	215	HIS
1	B	272	ASN
1	B	515	GLN
1	B	567	GLN
1	C	152	GLN
1	C	420	ASN
1	C	602	ASN
1	D	152	GLN
1	D	174	HIS
1	D	437	ASN
1	D	568	ASN
1	E	113	GLN

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Mol	Chain	Res	Type
1	F	174	HIS
1	F	521	ASN
1	F	567	GLN
1	G	139	ASN
1	G	437	ASN
1	H	183	ASN
1	I	515	GLN
1	I	521	ASN
1	J	139	ASN
1	J	183	ASN
1	J	567	GLN
1	J	568	ASN
1	K	420	ASN
1	L	104	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 97 ligands modelled in this entry, 24 are monoatomic - leaving 73 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
5	1PE	I	1005	-	12,12,15	0.65	0	11,11,14	0.36	0
5	1PE	K	1006	-	11,11,15	0.59	0	10,10,14	0.39	0
6	SO4	C	1009	-	4,4,4	0.24	0	6,6,6	0.06	0
5	1PE	A	1007	-	5,5,15	0.70	0	4,4,14	0.37	0
4	CO3	F	1004	-	3,3,3	0.89	0	2,3,3	0.27	0
4	CO3	I	1004	-	3,3,3	0.87	0	2,3,3	0.23	0
6	SO4	E	1007	-	4,4,4	0.22	0	6,6,6	0.11	0
5	1PE	E	1006	-	11,11,15	0.57	0	10,10,14	0.45	0
6	SO4	G	1009	-	4,4,4	0.25	0	6,6,6	0.08	0
6	SO4	K	1007	-	4,4,4	0.22	0	6,6,6	0.09	0
5	1PE	J	1006	-	9,9,15	0.55	0	8,8,14	0.33	0
5	1PE	L	1005	-	9,9,15	0.90	0	8,8,14	0.39	0
2	4TM	C	1001	3	23,24,24	2.31	2 (8%)	32,34,34	1.20	4 (12%)
6	SO4	J	1007	-	4,4,4	0.24	0	6,6,6	0.19	0
5	1PE	F	1007	-	9,9,15	0.89	0	8,8,14	0.43	0
2	4TM	G	1001	3	23,24,24	2.32	2 (8%)	32,34,34	1.36	5 (15%)
2	4TM	A	1001	3	23,24,24	2.29	2 (8%)	32,34,34	1.11	3 (9%)
2	4TM	E	1001	3	23,24,24	2.29	2 (8%)	32,34,34	1.29	4 (12%)
6	SO4	C	1010	-	4,4,4	0.22	0	6,6,6	0.08	0
5	1PE	C	1007	-	10,10,15	0.58	0	9,9,14	0.36	0
4	CO3	H	1004	-	3,3,3	0.75	0	2,3,3	0.05	0
5	1PE	E	1005	-	11,11,15	0.58	0	10,10,14	0.48	0
5	1PE	A	1006	-	5,5,15	0.68	0	4,4,14	0.55	0
5	1PE	K	1005	-	11,11,15	0.60	0	10,10,14	0.39	0
7	GOL	C	1005	-	5,5,5	0.33	0	5,5,5	0.31	0
6	SO4	L	1007	-	4,4,4	0.24	0	6,6,6	0.22	0
6	SO4	H	1009	-	4,4,4	0.23	0	6,6,6	0.10	0
4	CO3	B	1004	-	3,3,3	0.77	0	2,3,3	0.15	0
5	1PE	A	1005	-	8,8,15	0.57	0	7,7,14	0.29	0
2	4TM	B	1001	3	23,24,24	2.21	2 (8%)	32,34,34	1.14	3 (9%)
6	SO4	H	1008	-	4,4,4	0.25	0	6,6,6	0.07	0
2	4TM	J	1001	3	23,24,24	2.39	2 (8%)	32,34,34	1.24	3 (9%)
2	4TM	K	1001	3	23,24,24	2.41	3 (13%)	32,34,34	1.26	4 (12%)
6	SO4	D	1007	-	4,4,4	0.24	0	6,6,6	0.11	0
6	SO4	G	1008	-	4,4,4	0.23	0	6,6,6	0.09	0
4	CO3	E	1004	-	3,3,3	0.90	0	2,3,3	0.26	0
5	1PE	D	1006	-	9,9,15	0.89	0	8,8,14	0.43	0
5	1PE	F	1006	-	6,6,15	0.63	0	5,5,14	0.50	0
2	4TM	H	1001	3	23,24,24	2.19	2 (8%)	32,34,34	1.24	3 (9%)
5	1PE	I	1006	-	8,8,15	0.54	0	7,7,14	0.37	0
6	SO4	B	1006	-	4,4,4	0.26	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CO3	K	1004	-	3,3,3	0.85	0	2,3,3	0.14	0
6	SO4	L	1006	-	4,4,4	0.25	0	6,6,6	0.08	0
6	SO4	C	1008	-	4,4,4	0.24	0	6,6,6	0.08	0
7	GOL	G	1005	-	5,5,5	0.34	0	5,5,5	0.36	0
2	4TM	F	1001	3	23,24,24	2.50	3 (13%)	32,34,34	1.23	4 (12%)
5	1PE	B	1005	-	9,9,15	0.55	0	8,8,14	0.39	0
6	SO4	H	1007	-	4,4,4	0.25	0	6,6,6	0.06	0
5	1PE	J	1005	-	9,9,15	0.56	0	8,8,14	0.32	0
4	CO3	D	1004	-	3,3,3	0.85	0	2,3,3	0.19	0
5	1PE	H	1006	-	9,9,15	0.57	0	8,8,14	0.31	0
6	SO4	I	1007	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	F	1008	-	4,4,4	0.24	0	6,6,6	0.07	0
2	4TM	L	1001	3	23,24,24	2.31	2 (8%)	32,34,34	1.23	4 (12%)
6	SO4	E	1008	-	4,4,4	0.24	0	6,6,6	0.07	0
5	1PE	H	1005	-	9,9,15	0.55	0	8,8,14	0.35	0
4	CO3	L	1004	-	3,3,3	0.86	0	2,3,3	0.17	0
5	1PE	C	1006	-	11,11,15	0.62	0	10,10,14	0.37	0
5	1PE	F	1005	-	10,10,15	0.85	0	9,9,14	0.35	0
6	SO4	A	1009	-	4,4,4	0.24	0	6,6,6	0.10	0
4	CO3	G	1004	-	3,3,3	0.90	0	2,3,3	0.18	0
6	SO4	H	1010	-	4,4,4	0.23	0	6,6,6	0.12	0
5	1PE	G	1007	-	11,11,15	0.66	0	10,10,14	0.40	0
5	1PE	G	1006	-	8,8,15	0.54	0	7,7,14	0.40	0
6	SO4	A	1008	-	4,4,4	0.22	0	6,6,6	0.08	0
4	CO3	J	1004	-	3,3,3	0.77	0	2,3,3	0.06	0
4	CO3	C	1004	-	3,3,3	0.88	0	2,3,3	0.33	0
5	1PE	D	1005	-	10,10,15	0.89	0	9,9,14	0.31	0
2	4TM	D	1001	3	23,24,24	2.22	2 (8%)	32,34,34	1.16	3 (9%)
6	SO4	B	1007	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	B	1008	-	4,4,4	0.23	0	6,6,6	0.09	0
2	4TM	I	1001	3	23,24,24	2.17	2 (8%)	32,34,34	0.99	2 (6%)
4	CO3	A	1004	-	3,3,3	0.86	0	2,3,3	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	I	1005	-	-	6/10/10/13	-
5	1PE	K	1006	-	-	3/9/9/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	A	1007	-	-	1/3/3/13	-
5	1PE	E	1006	-	-	8/9/9/13	-
5	1PE	J	1006	-	-	7/7/7/13	-
5	1PE	L	1005	-	-	6/7/7/13	-
2	4TM	C	1001	3	-	0/24/24/24	0/2/2/2
5	1PE	F	1007	-	-	3/7/7/13	-
2	4TM	G	1001	3	-	0/24/24/24	0/2/2/2
2	4TM	A	1001	3	-	1/24/24/24	0/2/2/2
2	4TM	E	1001	3	-	2/24/24/24	0/2/2/2
5	1PE	E	1005	-	-	7/9/9/13	-
5	1PE	A	1006	-	-	2/3/3/13	-
5	1PE	K	1005	-	-	6/9/9/13	-
7	GOL	C	1005	-	-	2/4/4/4	-
5	1PE	A	1005	-	-	3/6/6/13	-
2	4TM	D	1001	3	-	1/24/24/24	0/2/2/2
2	4TM	B	1001	3	-	0/24/24/24	0/2/2/2
2	4TM	J	1001	3	-	3/24/24/24	0/2/2/2
2	4TM	K	1001	3	-	0/24/24/24	0/2/2/2
5	1PE	D	1006	-	-	3/7/7/13	-
5	1PE	F	1006	-	-	2/4/4/13	-
2	4TM	H	1001	3	-	0/24/24/24	0/2/2/2
5	1PE	I	1006	-	-	3/6/6/13	-
7	GOL	G	1005	-	-	2/4/4/4	-
2	4TM	F	1001	3	-	0/24/24/24	0/2/2/2
5	1PE	B	1005	-	-	4/7/7/13	-
5	1PE	J	1005	-	-	3/7/7/13	-
5	1PE	H	1006	-	-	5/7/7/13	-
2	4TM	L	1001	3	-	2/24/24/24	0/2/2/2
5	1PE	H	1005	-	-	4/7/7/13	-
5	1PE	C	1006	-	-	6/9/9/13	-
5	1PE	F	1005	-	-	7/8/8/13	-
5	1PE	G	1007	-	-	6/9/9/13	-
5	1PE	G	1006	-	-	6/6/6/13	-
5	1PE	D	1005	-	-	4/8/8/13	-
5	1PE	C	1007	-	-	6/8/8/13	-
2	4TM	I	1001	3	-	0/24/24/24	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1001	4TM	CAU-CA	-8.14	1.40	1.52
2	F	1001	4TM	CAU-CA	-8.09	1.40	1.52
2	L	1001	4TM	CAU-CA	-8.00	1.40	1.52
2	K	1001	4TM	CAU-CA	-8.00	1.40	1.52
2	C	1001	4TM	CAU-CA	-7.86	1.40	1.52
2	A	1001	4TM	CAU-CA	-7.75	1.40	1.52
2	E	1001	4TM	CAU-CA	-7.74	1.40	1.52
2	G	1001	4TM	CAU-CA	-7.57	1.41	1.52
2	G	1001	4TM	CAS-CAT	-7.56	1.33	1.48
2	J	1001	4TM	CAS-CAT	-7.50	1.33	1.48
2	K	1001	4TM	CAS-CAT	-7.41	1.34	1.48
2	B	1001	4TM	CAU-CA	-7.30	1.41	1.52
2	H	1001	4TM	CAU-CA	-7.27	1.41	1.52
2	B	1001	4TM	CAS-CAT	-7.24	1.34	1.48
2	C	1001	4TM	CAS-CAT	-7.20	1.34	1.48
2	D	1001	4TM	CAS-CAT	-7.19	1.34	1.48
2	A	1001	4TM	CAS-CAT	-7.13	1.34	1.48
2	E	1001	4TM	CAS-CAT	-7.08	1.34	1.48
2	I	1001	4TM	CAU-CA	-7.07	1.41	1.52
2	F	1001	4TM	CAS-CAT	-7.06	1.34	1.48
2	D	1001	4TM	CAU-CA	-7.06	1.41	1.52
2	H	1001	4TM	CAS-CAT	-7.03	1.34	1.48
2	L	1001	4TM	CAS-CAT	-6.91	1.35	1.48
2	I	1001	4TM	CAS-CAT	-6.85	1.35	1.48
2	F	1001	4TM	OAF-NAN	4.59	1.51	1.40
2	K	1001	4TM	OAF-NAN	2.42	1.45	1.40

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1001	4TM	CAT-CAM-SAP	-3.72	104.88	112.33
2	J	1001	4TM	CAT-CAM-SAP	-3.66	105.01	112.33
2	K	1001	4TM	CAT-CAM-SAP	-3.57	105.18	112.33
2	B	1001	4TM	CAT-CAM-SAP	-3.47	105.40	112.33
2	C	1001	4TM	CAT-CAM-SAP	-3.44	105.45	112.33
2	D	1001	4TM	CAT-CAM-SAP	-3.39	105.54	112.33
2	H	1001	4TM	CAT-CAM-SAP	-3.38	105.56	112.33
2	L	1001	4TM	CAT-CAM-SAP	-3.28	105.78	112.33
2	E	1001	4TM	CAT-CAM-SAP	-3.25	105.82	112.33
2	F	1001	4TM	CAT-CAM-SAP	-3.14	106.05	112.33
2	A	1001	4TM	CAT-CAM-SAP	-3.11	106.10	112.33
2	L	1001	4TM	CAW-CAR-N	-3.05	113.33	117.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1001	4TM	CAH-CAT-CAM	3.03	115.48	111.17
2	I	1001	4TM	CAT-CAM-SAP	-3.00	106.33	112.33
2	G	1001	4TM	CAS-CAT-CAH	-2.97	120.00	124.69
2	F	1001	4TM	CAW-CAR-N	-2.97	113.45	117.49
2	J	1001	4TM	CAH-CAT-CAM	2.88	115.26	111.17
2	K	1001	4TM	CAH-CAT-CAM	2.82	115.18	111.17
2	H	1001	4TM	CAW-CAR-N	-2.81	113.66	117.49
2	D	1001	4TM	CAW-CAR-N	-2.80	113.68	117.49
2	F	1001	4TM	CAH-CAT-CAM	2.78	115.12	111.17
2	E	1001	4TM	CAH-CAT-CAM	2.76	115.10	111.17
2	E	1001	4TM	CAK-CAU-CA	-2.76	116.35	120.78
2	A	1001	4TM	CAH-CAT-CAM	2.71	115.03	111.17
2	B	1001	4TM	CAH-CAT-CAM	2.67	114.97	111.17
2	C	1001	4TM	CAH-CAT-CAM	2.62	114.89	111.17
2	C	1001	4TM	CAW-CAR-N	-2.60	113.94	117.49
2	D	1001	4TM	CAH-CAT-CAM	2.56	114.81	111.17
2	H	1001	4TM	CAH-CAT-CAM	2.50	114.72	111.17
2	L	1001	4TM	CAH-CAT-CAM	2.47	114.69	111.17
2	I	1001	4TM	CAH-CAT-CAM	2.45	114.66	111.17
2	J	1001	4TM	CAW-CAR-N	-2.42	114.19	117.49
2	C	1001	4TM	CAS-CAT-CAH	-2.38	120.93	124.69
2	E	1001	4TM	CAL-CAU-CA	2.32	124.50	120.78
2	B	1001	4TM	CAW-CAR-N	-2.29	114.37	117.49
2	K	1001	4TM	CAK-CAU-CA	-2.24	117.19	120.78
2	G	1001	4TM	CAK-CAU-CA	-2.21	117.24	120.78
2	L	1001	4TM	CAS-CAT-CAH	-2.18	121.25	124.69
2	G	1001	4TM	CAI-CAS-CAT	-2.17	118.13	121.16
2	K	1001	4TM	CAS-CAT-CAH	-2.14	121.31	124.69
2	A	1001	4TM	CAW-CAR-N	-2.12	114.61	117.49
2	F	1001	4TM	CAS-CAT-CAH	-2.06	121.43	124.69

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	1005	1PE	OH5-C14-C24-OH4
5	K	1006	1PE	OH5-C14-C24-OH4
5	C	1006	1PE	OH5-C14-C24-OH4
5	D	1005	1PE	OH5-C14-C24-OH4
5	K	1005	1PE	OH5-C14-C24-OH4
5	J	1006	1PE	OH4-C13-C23-OH3
5	K	1006	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
5	A	1005	1PE	OH4-C13-C23-OH3
5	H	1005	1PE	OH5-C14-C24-OH4
5	I	1005	1PE	OH5-C14-C24-OH4
5	G	1006	1PE	OH4-C13-C23-OH3
5	G	1007	1PE	OH5-C14-C24-OH4
5	L	1005	1PE	OH6-C15-C25-OH5
5	G	1007	1PE	OH4-C13-C23-OH3
5	I	1005	1PE	OH4-C13-C23-OH3
5	K	1005	1PE	OH4-C13-C23-OH3
5	B	1005	1PE	OH5-C14-C24-OH4
5	I	1005	1PE	OH6-C15-C25-OH5
5	B	1005	1PE	OH4-C13-C23-OH3
5	H	1005	1PE	OH4-C13-C23-OH3
5	C	1007	1PE	OH4-C13-C23-OH3
5	J	1005	1PE	OH4-C13-C23-OH3
5	A	1005	1PE	OH5-C14-C24-OH4
5	F	1005	1PE	OH6-C15-C25-OH5
5	C	1007	1PE	C23-C13-OH4-C24
5	C	1006	1PE	OH6-C15-C25-OH5
5	E	1006	1PE	OH6-C15-C25-OH5
5	G	1007	1PE	OH6-C15-C25-OH5
7	C	1005	GOL	C1-C2-C3-O3
5	A	1007	1PE	OH6-C15-C25-OH5
5	E	1005	1PE	OH6-C15-C25-OH5
5	L	1005	1PE	OH5-C14-C24-OH4
5	I	1005	1PE	C14-C24-OH4-C13
5	F	1007	1PE	OH6-C15-C25-OH5
5	K	1005	1PE	OH6-C15-C25-OH5
5	E	1005	1PE	OH5-C14-C24-OH4
5	C	1007	1PE	OH5-C14-C24-OH4
5	F	1007	1PE	OH7-C16-C26-OH6
5	G	1006	1PE	OH5-C14-C24-OH4
5	C	1006	1PE	OH4-C13-C23-OH3
5	F	1006	1PE	OH5-C14-C24-OH4
5	G	1007	1PE	C15-C25-OH5-C14
5	E	1006	1PE	OH5-C14-C24-OH4
5	F	1005	1PE	OH7-C16-C26-OH6
5	B	1005	1PE	C12-C22-OH3-C23
5	K	1005	1PE	C12-C22-OH3-C23
5	A	1006	1PE	OH6-C15-C25-OH5
7	C	1005	GOL	O2-C2-C3-O3
5	J	1005	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
5	F	1005	1PE	C14-C24-OH4-C13
5	C	1007	1PE	C24-C14-OH5-C25
5	H	1006	1PE	C24-C14-OH5-C25
5	C	1007	1PE	C15-C25-OH5-C14
5	J	1006	1PE	C24-C14-OH5-C25
5	G	1007	1PE	C25-C15-OH6-C26
5	F	1007	1PE	C16-C26-OH6-C15
5	J	1006	1PE	C23-C13-OH4-C24
5	C	1006	1PE	C24-C14-OH5-C25
5	F	1005	1PE	C15-C25-OH5-C14
5	E	1005	1PE	C24-C14-OH5-C25
5	D	1005	1PE	C25-C15-OH6-C26
5	E	1006	1PE	C14-C24-OH4-C13
5	H	1005	1PE	C12-C22-OH3-C23
5	J	1006	1PE	C13-C23-OH3-C22
5	I	1006	1PE	C12-C22-OH3-C23
5	F	1005	1PE	C16-C26-OH6-C15
5	E	1006	1PE	C23-C13-OH4-C24
5	I	1006	1PE	C14-C24-OH4-C13
5	G	1006	1PE	C12-C22-OH3-C23
5	A	1005	1PE	C13-C23-OH3-C22
5	C	1007	1PE	C12-C22-OH3-C23
5	L	1005	1PE	C16-C26-OH6-C15
5	C	1006	1PE	C23-C13-OH4-C24
5	G	1006	1PE	C14-C24-OH4-C13
5	I	1005	1PE	C15-C25-OH5-C14
5	E	1006	1PE	C15-C25-OH5-C14
5	F	1005	1PE	OH5-C14-C24-OH4
5	A	1006	1PE	C24-C14-OH5-C25
5	C	1006	1PE	C12-C22-OH3-C23
5	H	1005	1PE	C23-C13-OH4-C24
5	E	1005	1PE	C14-C24-OH4-C13
5	E	1005	1PE	OH4-C13-C23-OH3
5	G	1007	1PE	C13-C23-OH3-C22
5	E	1005	1PE	C12-C22-OH3-C23
5	G	1006	1PE	C13-C23-OH3-C22
5	L	1005	1PE	C15-C25-OH5-C14
5	I	1005	1PE	C25-C15-OH6-C26
5	E	1006	1PE	C12-C22-OH3-C23
5	J	1006	1PE	C14-C24-OH4-C13
2	E	1001	4TM	NAN-C-CA-N
2	J	1001	4TM	NAN-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	L	1001	4TM	NAN-C-CA-N
5	D	1006	1PE	C16-C26-OH6-C15
5	D	1006	1PE	C25-C15-OH6-C26
5	F	1005	1PE	C25-C15-OH6-C26
5	J	1006	1PE	OH5-C14-C24-OH4
5	K	1006	1PE	C23-C13-OH4-C24
5	E	1005	1PE	C23-C13-OH4-C24
5	J	1006	1PE	C12-C22-OH3-C23
7	G	1005	GOL	C1-C2-C3-O3
5	I	1006	1PE	OH5-C14-C24-OH4
5	K	1005	1PE	C23-C13-OH4-C24
5	H	1006	1PE	C12-C22-OH3-C23
2	E	1001	4TM	O-C-CA-N
2	J	1001	4TM	O-C-CA-N
5	H	1006	1PE	OH4-C13-C23-OH3
5	F	1006	1PE	C15-C25-OH5-C14
5	D	1005	1PE	C24-C14-OH5-C25
5	E	1006	1PE	C24-C14-OH5-C25
5	B	1005	1PE	C14-C24-OH4-C13
5	K	1005	1PE	C24-C14-OH5-C25
5	L	1005	1PE	C24-C14-OH5-C25
5	D	1006	1PE	OH6-C15-C25-OH5
5	E	1006	1PE	OH4-C13-C23-OH3
2	J	1001	4TM	NAN-C-CA-CAU
5	G	1006	1PE	C23-C13-OH4-C24
5	H	1006	1PE	C14-C24-OH4-C13
5	D	1005	1PE	C15-C25-OH5-C14
5	L	1005	1PE	OH7-C16-C26-OH6
5	H	1006	1PE	OH5-C14-C24-OH4
7	G	1005	GOL	O2-C2-C3-O3
2	L	1001	4TM	NAN-C-CA-CAU
2	A	1001	4TM	NAN-C-CA-N
2	D	1001	4TM	NAN-C-CA-N

There are no ring outliers.

22 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1005	1PE	2	0
5	E	1006	1PE	2	0
5	L	1005	1PE	2	0
5	F	1007	1PE	1	0

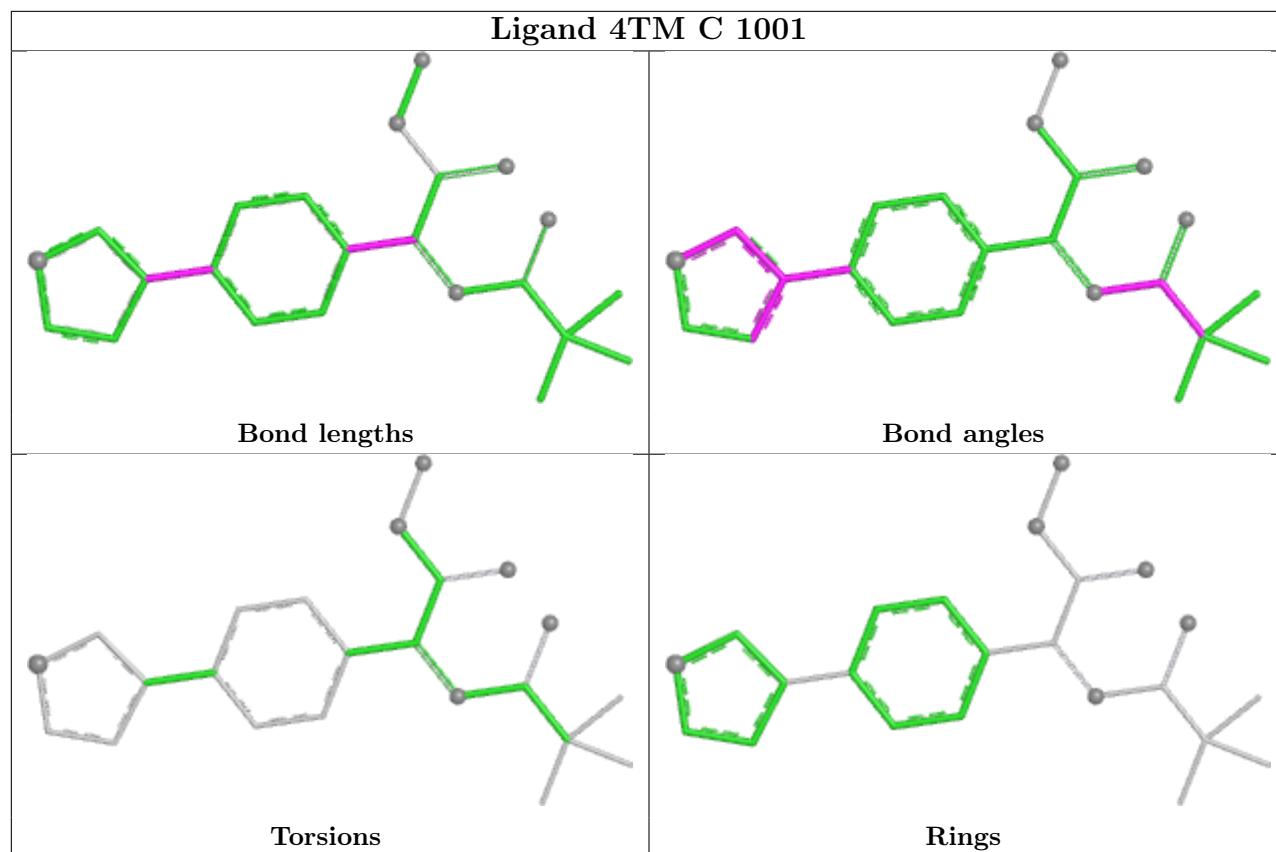
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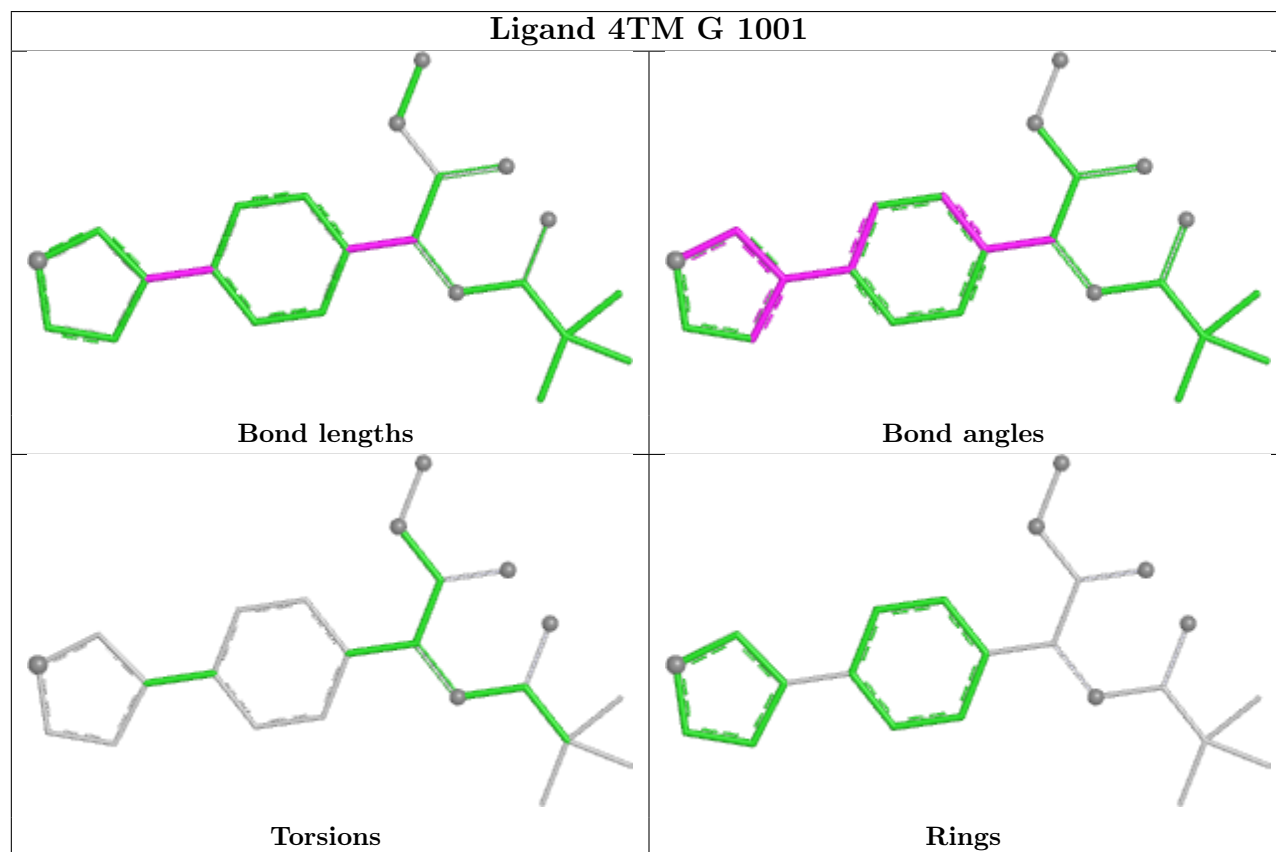
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1001	4TM	1	0
5	E	1005	1PE	1	0
6	L	1007	SO4	1	0
5	A	1005	1PE	1	0
2	J	1001	4TM	1	0
6	G	1008	SO4	1	0
5	D	1006	1PE	1	0
5	F	1006	1PE	2	0
5	I	1006	1PE	2	0
6	L	1006	SO4	1	0
6	C	1008	SO4	1	0
5	J	1005	1PE	3	0
5	H	1006	1PE	2	0
6	F	1008	SO4	1	0
5	F	1005	1PE	3	0
5	G	1007	1PE	1	0
5	D	1005	1PE	1	0
6	B	1008	SO4	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.

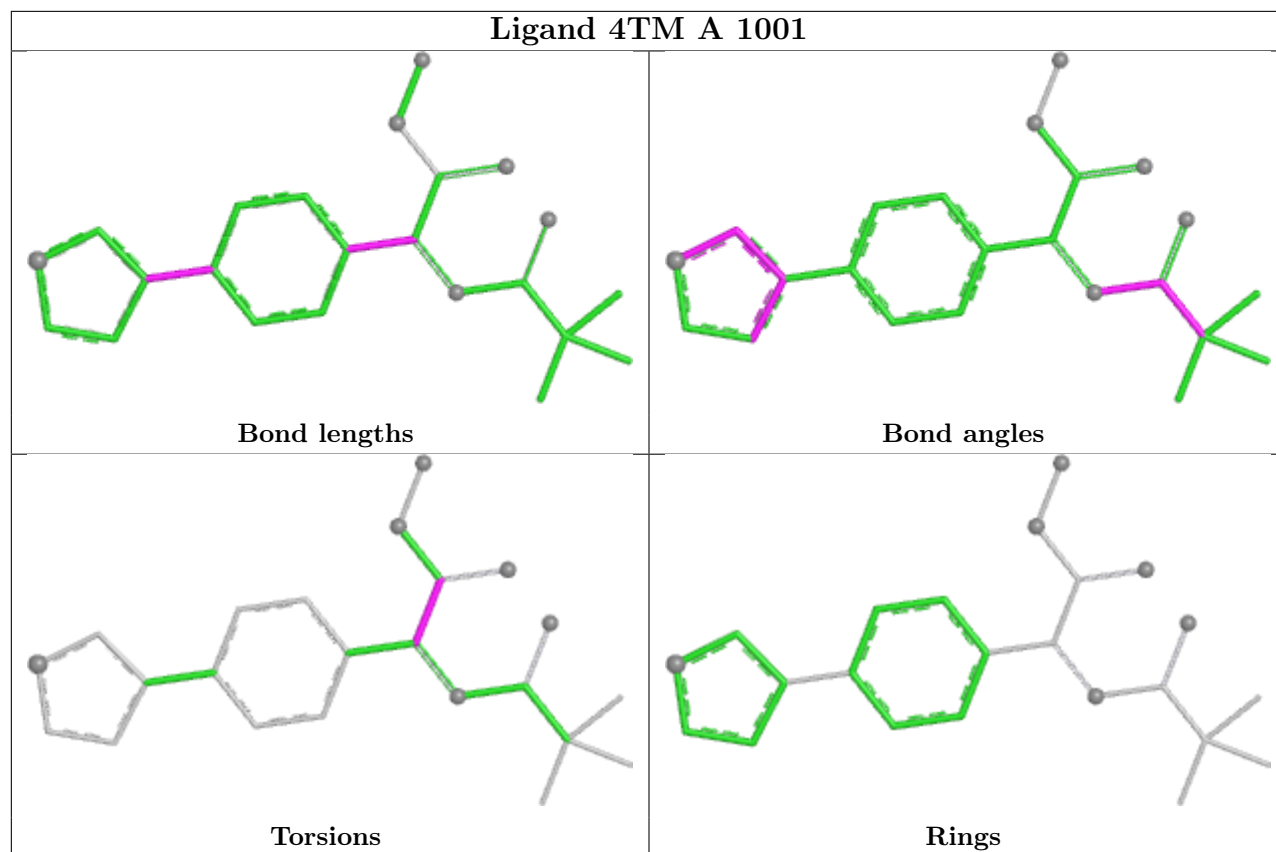
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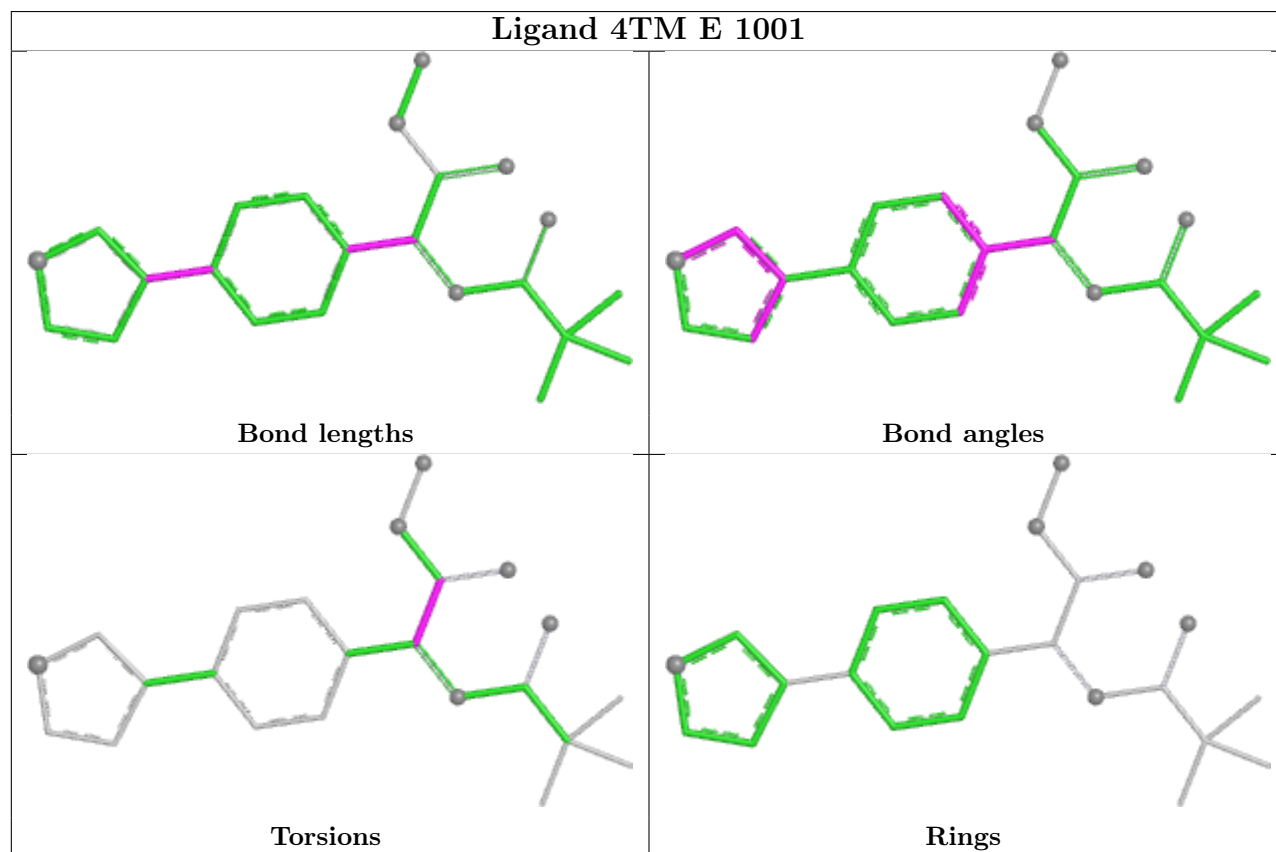
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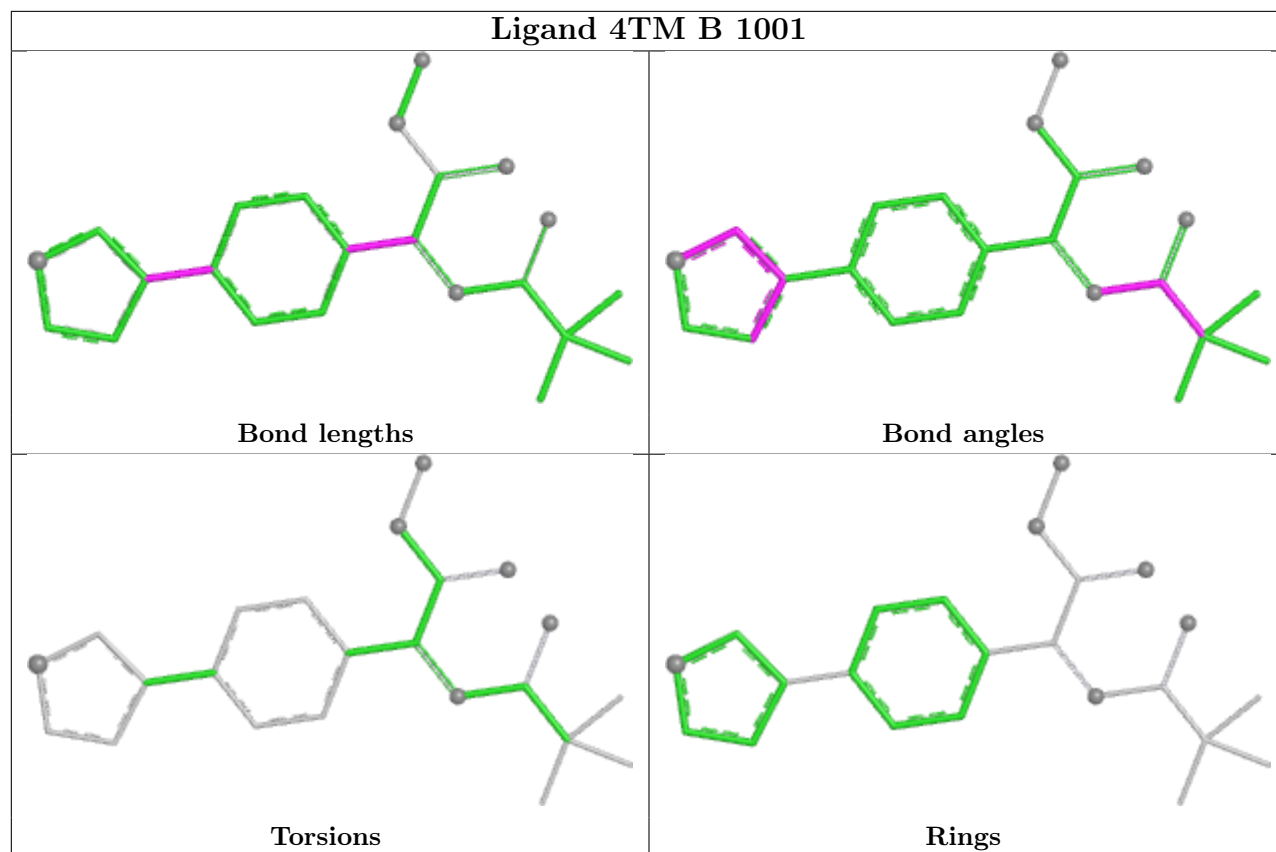
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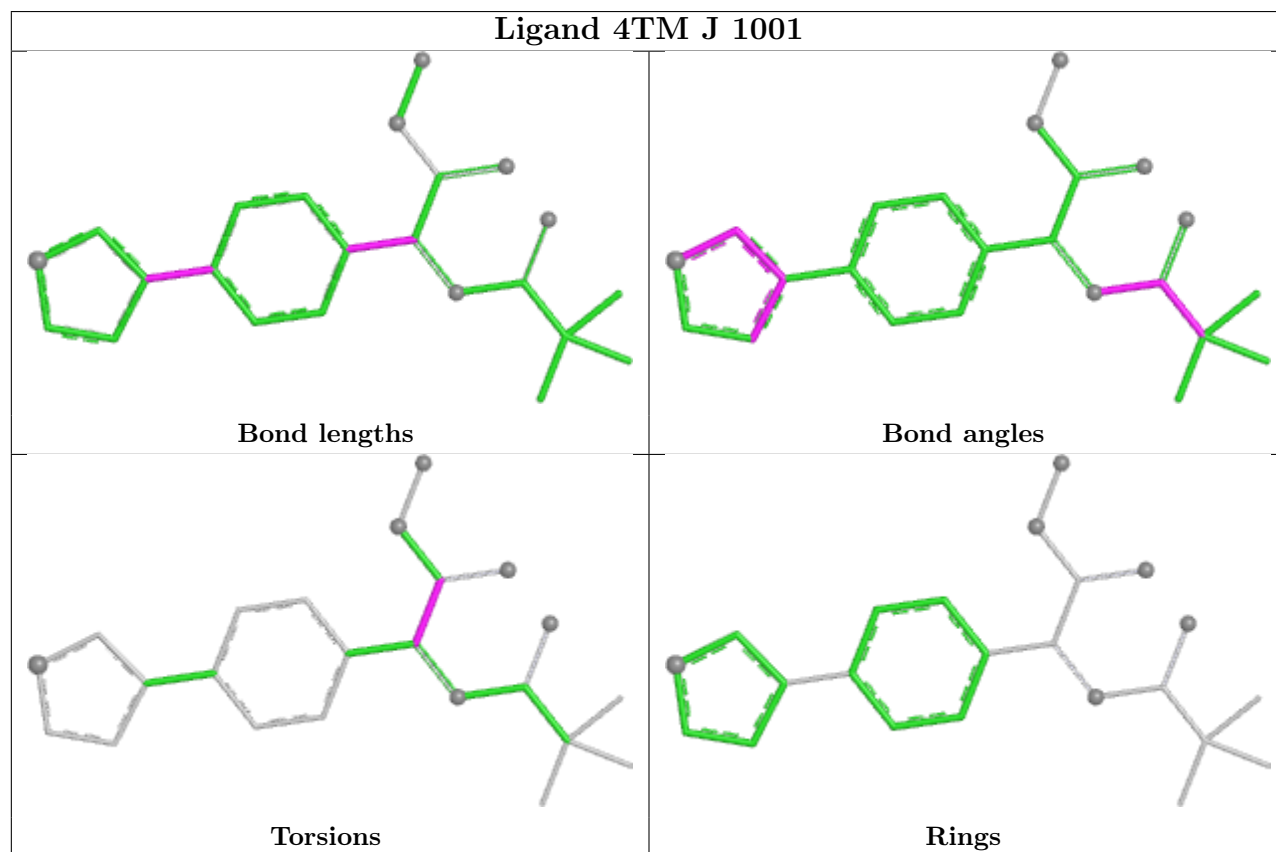
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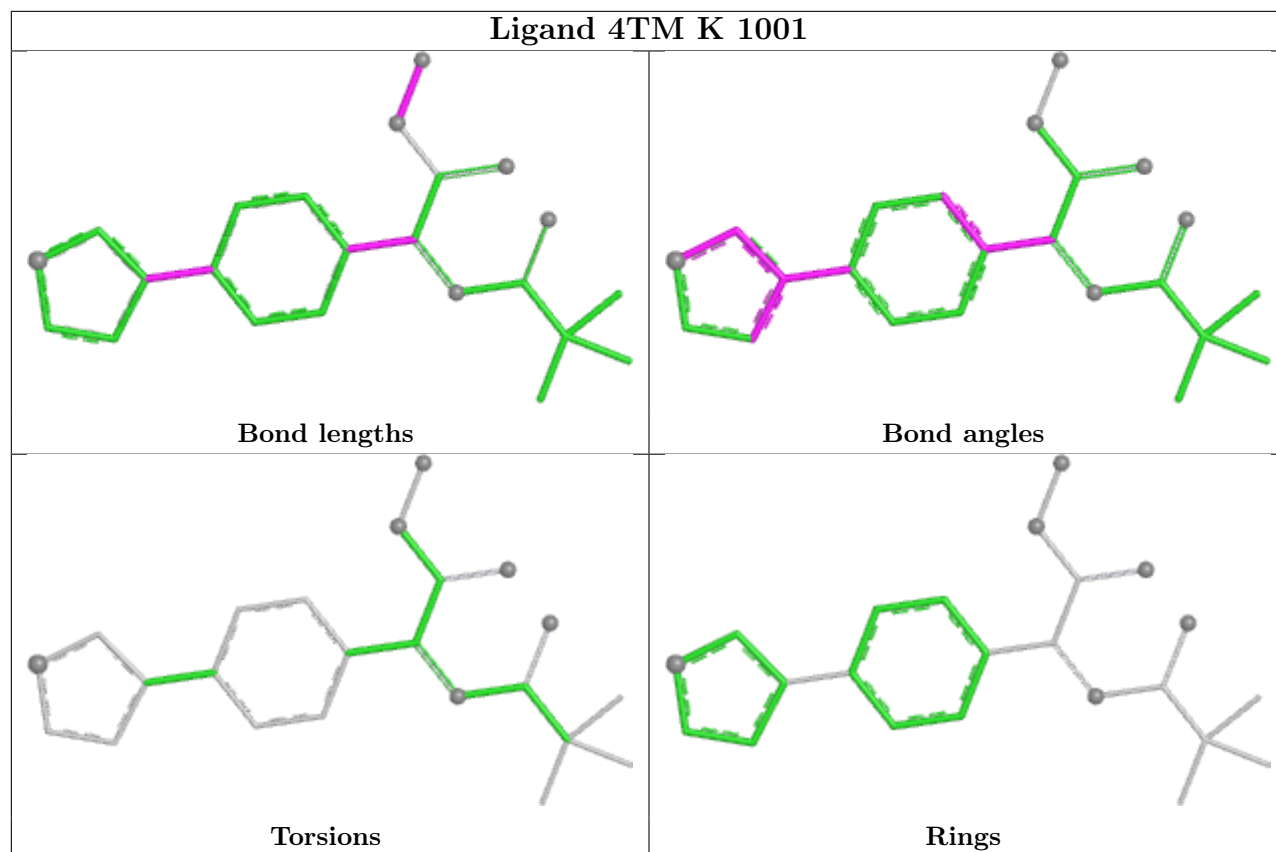
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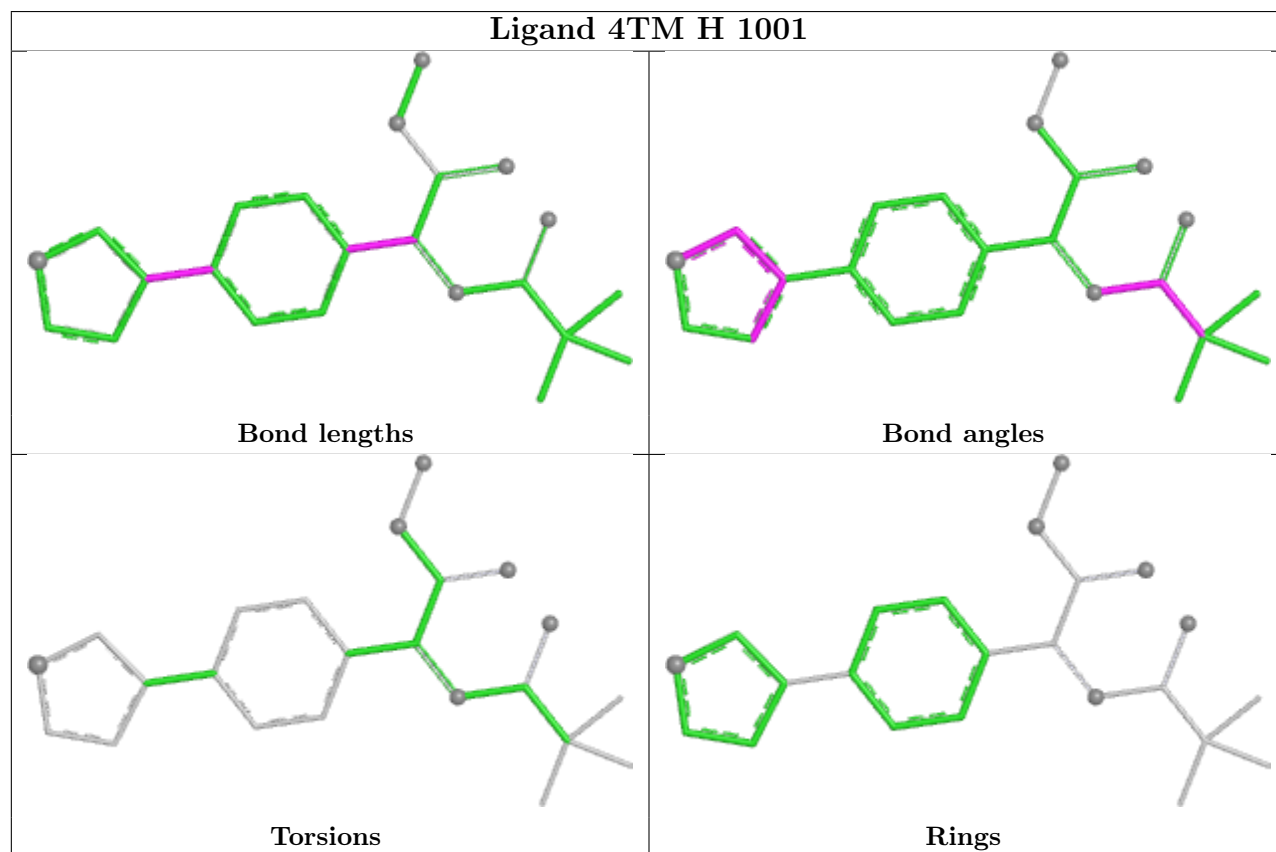
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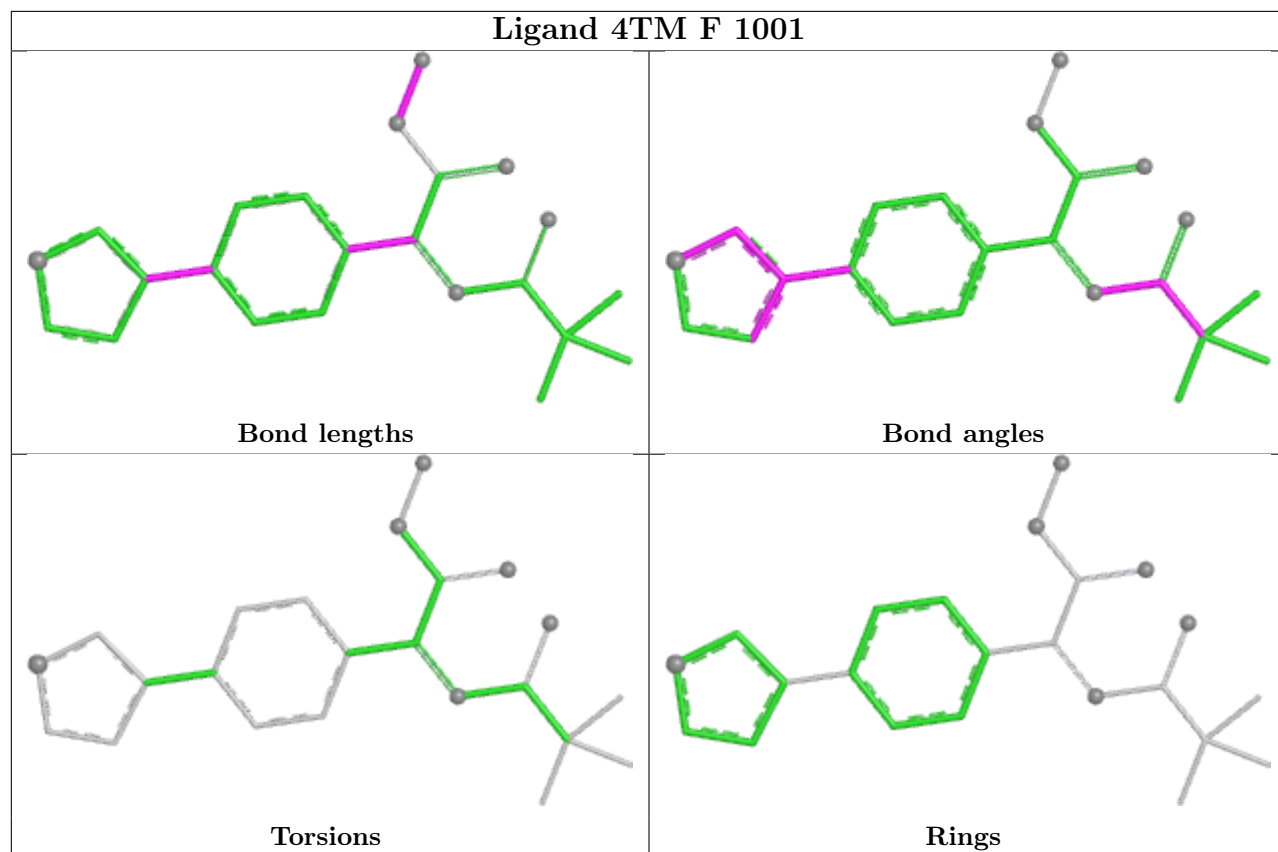
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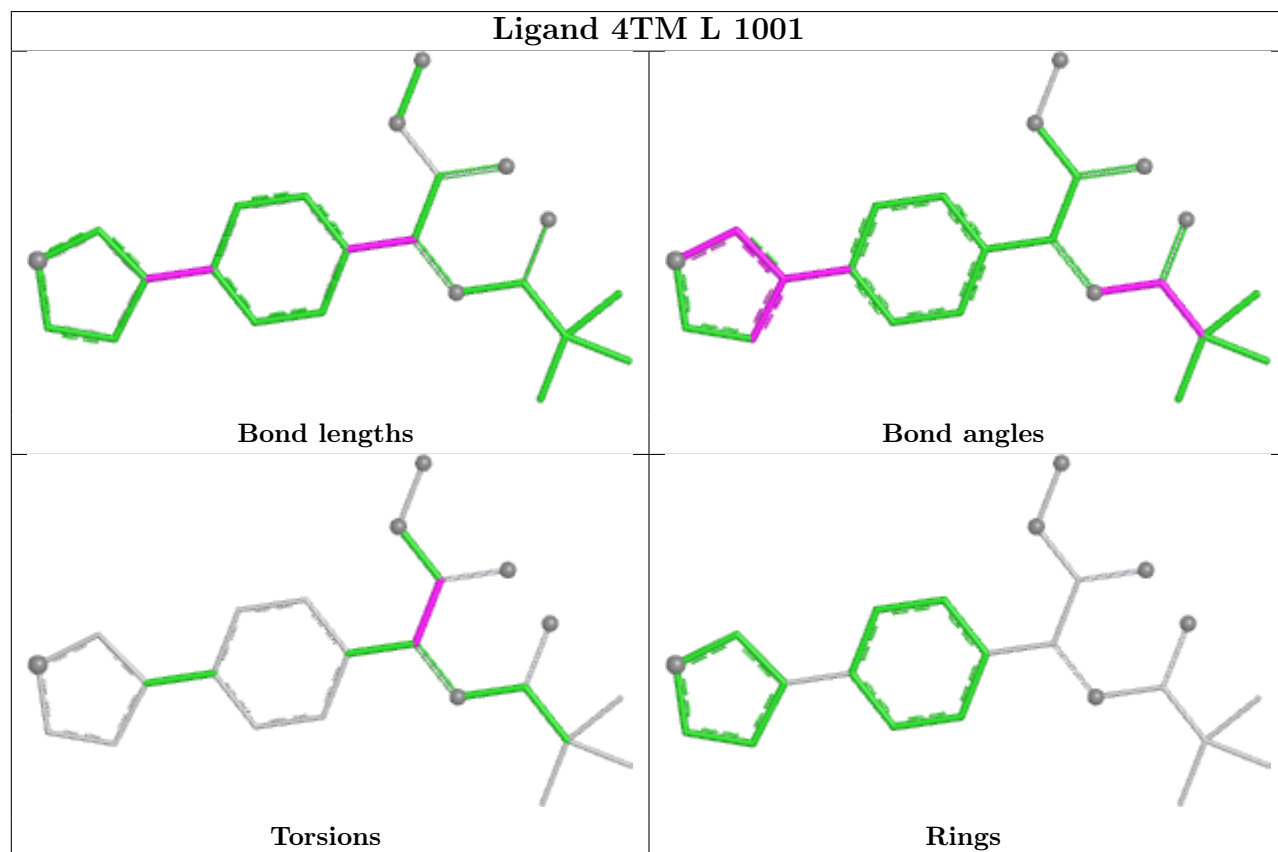
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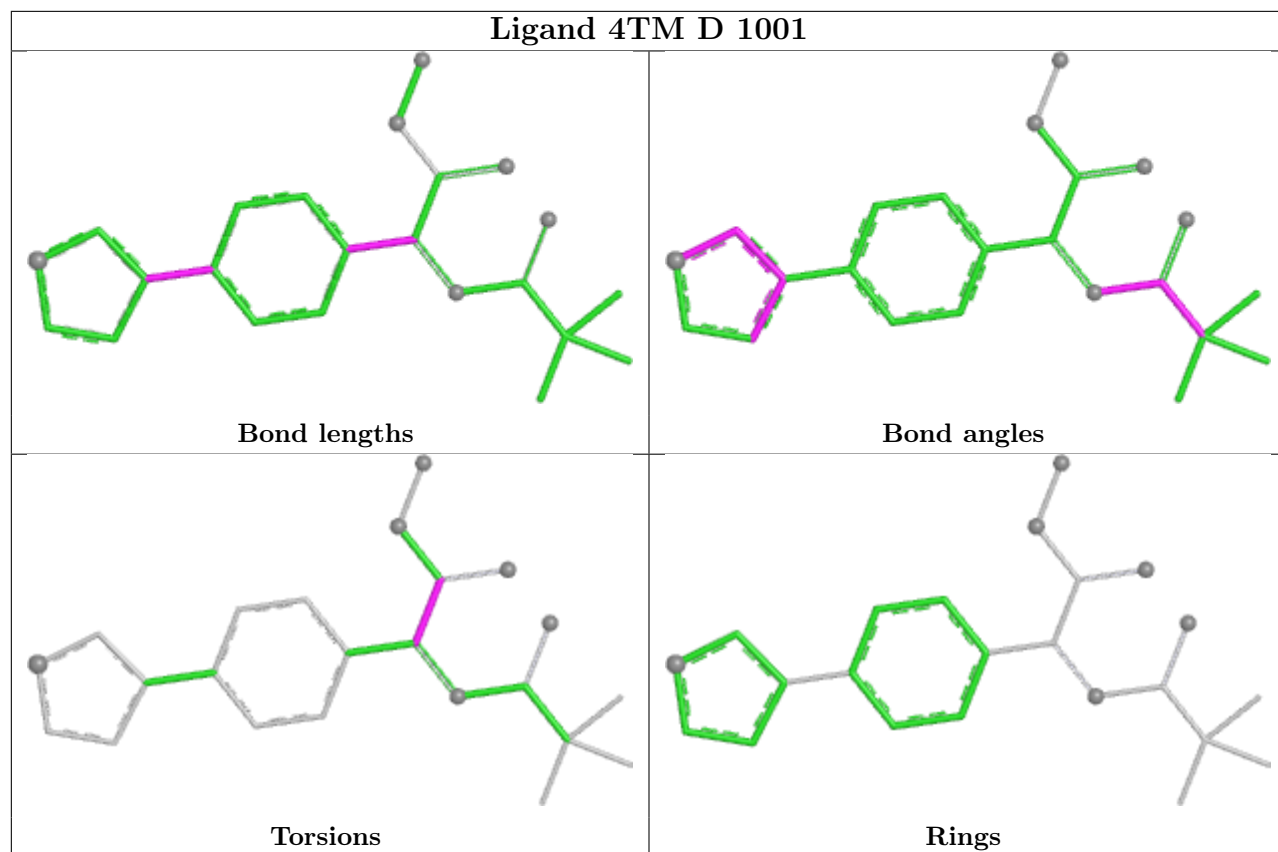
Ligand 4TM F 1001



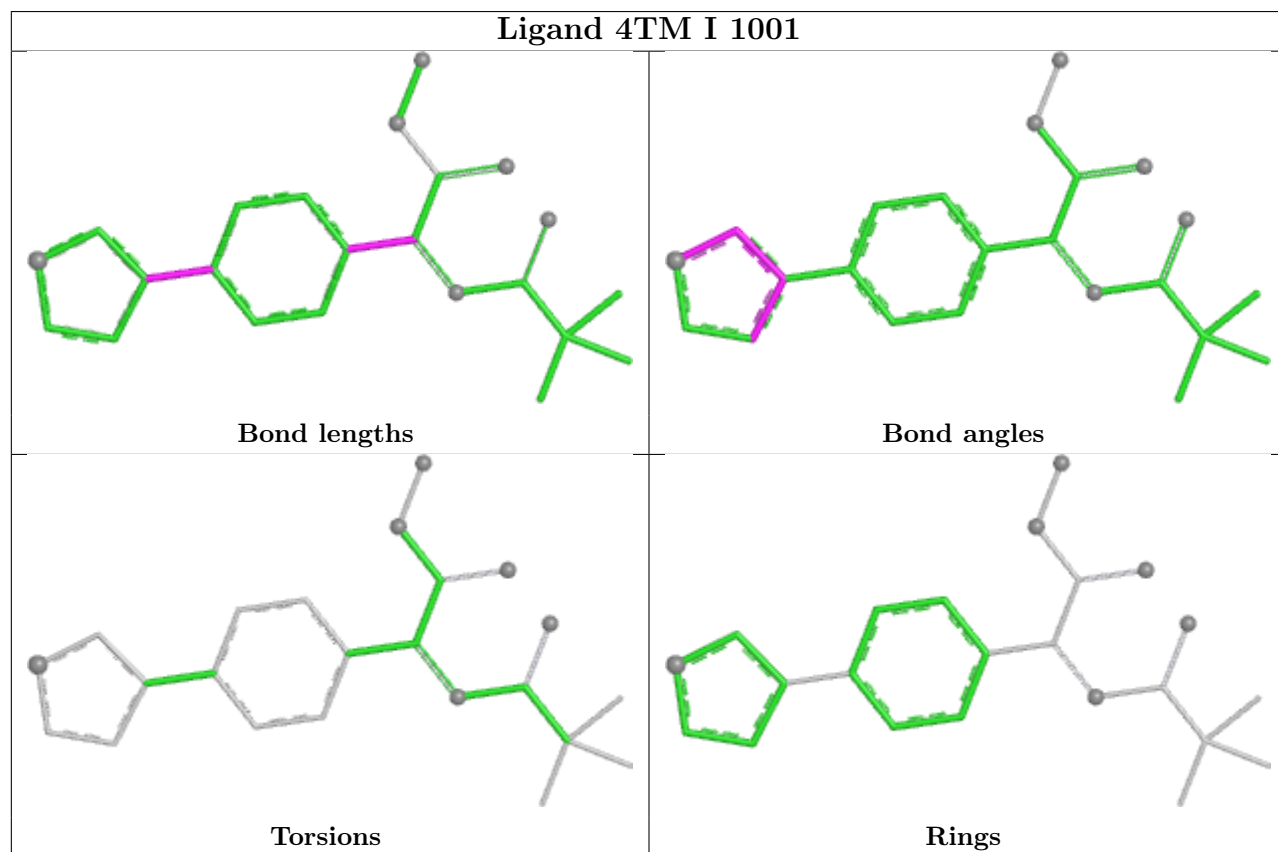
Ligand 4TM L 1001



Ligand 4TM D 1001



Ligand 4TM I 1001



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	519/522 (99%)	-0.12	8 (1%) 72 69	15, 25, 49, 95	6 (1%)
1	B	518/522 (99%)	0.17	25 (4%) 35 32	14, 27, 66, 92	4 (0%)
1	C	517/522 (99%)	-0.06	12 (2%) 61 58	13, 25, 55, 84	5 (0%)
1	D	513/522 (98%)	-0.21	6 (1%) 76 74	16, 24, 44, 73	7 (1%)
1	E	509/522 (97%)	-0.27	4 (0%) 82 80	16, 24, 39, 77	1 (0%)
1	F	510/522 (97%)	0.20	22 (4%) 40 36	18, 32, 62, 94	1 (0%)
1	G	519/522 (99%)	-0.14	6 (1%) 76 74	16, 24, 46, 81	3 (0%)
1	H	517/522 (99%)	0.13	16 (3%) 51 48	16, 28, 64, 83	8 (1%)
1	I	518/522 (99%)	-0.02	8 (1%) 72 69	15, 27, 53, 102	7 (1%)
1	J	514/522 (98%)	-0.14	9 (1%) 67 64	16, 25, 45, 71	8 (1%)
1	K	508/522 (97%)	-0.20	3 (0%) 85 83	16, 25, 42, 67	3 (0%)
1	L	511/522 (97%)	0.08	14 (2%) 56 53	15, 28, 54, 106	7 (1%)
All	All	6173/6264 (98%)	-0.05	133 (2%) 62 59	13, 26, 55, 106	60 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	138	GLU	5.8
1	F	549	SER	5.3
1	E	551	VAL	5.2
1	I	603	ASP	4.9
1	J	603	ASP	4.8
1	H	603	ASP	4.7
1	B	603	ASP	4.7
1	H	259	VAL	4.5
1	A	549	SER	4.5
1	F	603	ASP	4.4
1	H	257	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	549	SER	4.2
1	D	551	VAL	4.2
1	A	603	ASP	4.1
1	L	551	VAL	3.9
1	D	260	ASN	3.9
1	C	550	SER	3.9
1	I	549	SER	3.9
1	L	136	GLY	3.8
1	H	549	SER	3.8
1	B	257	LYS	3.7
1	B	259	VAL	3.7
1	A	85	ALA	3.7
1	H	255	THR	3.7
1	G	603	ASP	3.6
1	L	603	ASP	3.6
1	L	139	ASN	3.6
1	J	260	ASN	3.5
1	F	364	ASP	3.4
1	G	550	SER	3.3
1	I	550	SER	3.3
1	B	135	PRO	3.3
1	A	551	VAL	3.3
1	I	121	CYS	3.3
1	L	550	SER	3.3
1	F	550	SER	3.3
1	B	256	ASP	3.2
1	B	364	ASP	3.2
1	F	139	ASN	3.2
1	F	551	VAL	3.1
1	B	119	GLY	3.1
1	E	550	SER	3.1
1	J	219	LEU	3.1
1	H	261	MET	3.1
1	K	439	TYR	3.0
1	G	549	SER	3.0
1	A	550	SER	3.0
1	C	196	ALA	3.0
1	J	137	LYS	2.9
1	L	137	LYS	2.9
1	B	118	LYS	2.8
1	B	231	ASP	2.8
1	J	200	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	197	ASP	2.7
1	C	549	SER	2.7
1	G	85	ALA	2.7
1	H	363	GLY	2.7
1	B	552	LYS	2.6
1	J	85	ALA	2.6
1	I	364	ASP	2.6
1	K	549	SER	2.6
1	B	196	ALA	2.5
1	C	137	LYS	2.5
1	F	137	LYS	2.5
1	A	137	LYS	2.5
1	H	552	LYS	2.5
1	B	276	THR	2.4
1	K	551	VAL	2.4
1	L	161	ASN	2.4
1	F	136	GLY	2.4
1	C	197	ASP	2.4
1	L	140	GLY	2.4
1	B	195	VAL	2.4
1	J	123	VAL	2.4
1	I	602	ASN	2.3
1	A	362	LYS	2.3
1	G	196	ALA	2.3
1	C	198	LEU	2.3
1	D	85	ALA	2.3
1	L	549	SER	2.3
1	H	551	VAL	2.3
1	F	262	GLU	2.3
1	B	132	VAL	2.3
1	B	178	PHE	2.3
1	C	551	VAL	2.3
1	F	121	CYS	2.3
1	L	196	ALA	2.3
1	F	365	VAL	2.3
1	H	602	ASN	2.2
1	L	146	SER	2.2
1	G	257	LYS	2.2
1	F	117	ILE	2.2
1	A	259	VAL	2.2
1	B	258	ASN	2.2
1	H	124	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	182	LYS	2.2
1	C	195	VAL	2.2
1	C	364	ASP	2.2
1	B	136	GLY	2.2
1	B	160	GLU	2.2
1	D	137	LYS	2.2
1	F	86	SER	2.2
1	F	219	LEU	2.2
1	F	141	PRO	2.2
1	C	200	GLU	2.2
1	D	219	LEU	2.1
1	F	157	LEU	2.1
1	J	549	SER	2.1
1	F	439	TYR	2.1
1	F	150	ASP	2.1
1	F	161	ASN	2.1
1	F	275	ASP	2.1
1	H	260	ASN	2.1
1	L	364	ASP	2.1
1	C	135	PRO	2.1
1	H	142	VAL	2.1
1	D	196	ALA	2.1
1	E	549	SER	2.1
1	L	262	GLU	2.1
1	I	551	VAL	2.1
1	J	551	VAL	2.1
1	C	363	GLY	2.1
1	B	137	LYS	2.1
1	I	196	ALA	2.1
1	B	133	ASN	2.1
1	E	602	ASN	2.1
1	B	193	GLY	2.1
1	F	113	GLN	2.0
1	B	551	VAL	2.0
1	H	125	GLU	2.0
1	F	197	ASP	2.0
1	H	258	ASN	2.0
1	B	182	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	1PE	H	1006	10/16	0.69	0.23	60,65,67,67	0
5	1PE	F	1005	11/16	0.71	0.20	44,59,68,68	0
6	SO4	C	1009	5/5	0.71	0.15	103,103,103,104	0
6	SO4	H	1009	5/5	0.71	0.18	94,96,96,97	0
5	1PE	H	1005	10/16	0.72	0.22	43,50,59,60	0
5	1PE	K	1005	12/16	0.72	0.18	46,52,59,59	0
7	GOL	C	1005	6/6	0.74	0.19	70,70,71,71	0
6	SO4	C	1010	5/5	0.75	0.15	81,81,81,83	0
6	SO4	B	1008	5/5	0.77	0.15	81,82,83,85	0
7	GOL	G	1005	6/6	0.77	0.16	57,57,57,59	0
5	1PE	J	1005	10/16	0.78	0.17	43,47,54,55	0
5	1PE	G	1007	12/16	0.78	0.17	48,51,54,55	0
6	SO4	K	1007	5/5	0.78	0.14	81,82,82,83	0
5	1PE	C	1006	12/16	0.78	0.18	50,59,61,61	0
5	1PE	B	1005	10/16	0.78	0.19	47,54,59,59	0
5	1PE	E	1005	12/16	0.79	0.17	46,49,51,51	0
6	SO4	H	1008	5/5	0.79	0.14	78,79,81,82	0
6	SO4	L	1006	5/5	0.80	0.14	79,80,80,82	0
6	SO4	I	1007	5/5	0.81	0.14	84,85,86,86	0
5	1PE	A	1006	6/16	0.81	0.20	48,50,53,56	0
6	SO4	F	1008	5/5	0.81	0.11	91,92,92,93	0
5	1PE	I	1005	13/16	0.81	0.15	43,45,55,55	0
5	1PE	F	1007	10/16	0.81	0.16	44,49,56,58	0
6	SO4	G	1009	5/5	0.82	0.12	80,81,81,81	0
5	1PE	J	1006	10/16	0.82	0.17	37,48,55,56	0
6	SO4	H	1010	5/5	0.83	0.16	74,75,77,77	0
5	1PE	D	1005	11/16	0.83	0.16	45,53,66,67	0
5	1PE	A	1007	6/16	0.84	0.15	43,43,44,45	0
5	1PE	I	1006	9/16	0.84	0.14	39,39,41,43	0
5	1PE	A	1005	9/16	0.84	0.14	34,36,37,38	0
5	1PE	D	1006	10/16	0.85	0.14	39,45,58,59	0
6	SO4	C	1008	5/5	0.85	0.13	76,77,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	1PE	G	1006	9/16	0.85	0.14	33,37,45,48	0
6	SO4	A	1009	5/5	0.85	0.12	76,76,78,78	0
6	SO4	E	1007	5/5	0.85	0.19	78,79,80,82	0
5	1PE	C	1007	11/16	0.86	0.15	30,42,50,51	0
6	SO4	L	1007	5/5	0.86	0.11	72,72,73,73	0
6	SO4	E	1008	5/5	0.86	0.15	81,81,82,82	0
6	SO4	B	1007	5/5	0.86	0.13	86,87,87,88	0
6	SO4	G	1008	5/5	0.87	0.14	72,72,73,74	0
5	1PE	K	1006	12/16	0.89	0.12	38,40,55,55	0
5	1PE	E	1006	12/16	0.90	0.11	33,38,49,50	0
5	1PE	L	1005	10/16	0.91	0.10	30,35,53,53	0
5	1PE	F	1006	7/16	0.92	0.12	44,44,50,51	0
2	4TM	I	1001	23/23	0.92	0.10	14,22,33,89	0
2	4TM	D	1001	23/23	0.92	0.09	14,25,34,56	0
2	4TM	E	1001	23/23	0.93	0.08	16,20,32,46	0
2	4TM	C	1001	23/23	0.93	0.09	16,24,34,39	0
2	4TM	K	1001	23/23	0.93	0.10	20,25,41,44	0
6	SO4	A	1008	5/5	0.93	0.14	60,60,61,61	0
2	4TM	L	1001	23/23	0.93	0.09	15,22,35,40	0
2	4TM	B	1001	23/23	0.93	0.09	13,26,34,60	0
2	4TM	J	1001	23/23	0.94	0.08	13,21,30,55	0
2	4TM	G	1001	23/23	0.94	0.08	15,19,32,34	0
2	4TM	F	1001	23/23	0.94	0.08	19,24,34,46	0
2	4TM	H	1001	23/23	0.95	0.08	13,25,32,48	0
4	CO3	E	1004	4/4	0.95	0.07	23,26,27,31	0
4	CO3	H	1004	4/4	0.95	0.07	21,23,23,25	0
2	4TM	A	1001	23/23	0.96	0.07	14,22,32,43	0
4	CO3	G	1004	4/4	0.96	0.07	20,24,25,25	0
4	CO3	C	1004	4/4	0.96	0.08	19,23,23,27	0
4	CO3	I	1004	4/4	0.96	0.08	24,24,25,27	0
4	CO3	K	1004	4/4	0.96	0.10	21,22,22,25	0
4	CO3	F	1004	4/4	0.97	0.06	22,24,24,26	0
4	CO3	D	1004	4/4	0.97	0.05	23,23,24,24	0
4	CO3	L	1004	4/4	0.97	0.05	22,23,23,24	0
4	CO3	A	1004	4/4	0.97	0.05	23,24,24,25	0
4	CO3	B	1004	4/4	0.98	0.04	16,18,18,22	0
4	CO3	J	1004	4/4	0.98	0.05	23,23,23,24	0
6	SO4	J	1007	5/5	0.98	0.05	22,23,25,26	0
6	SO4	B	1006	5/5	0.98	0.05	23,23,25,25	0
3	ZN	F	1003	1/1	0.99	0.02	21,21,21,21	0
3	ZN	H	1003	1/1	0.99	0.01	20,20,20,20	0
6	SO4	H	1007	5/5	0.99	0.04	20,21,23,24	0

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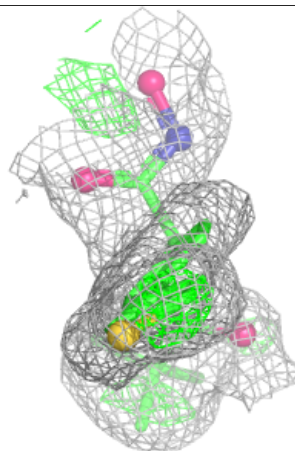
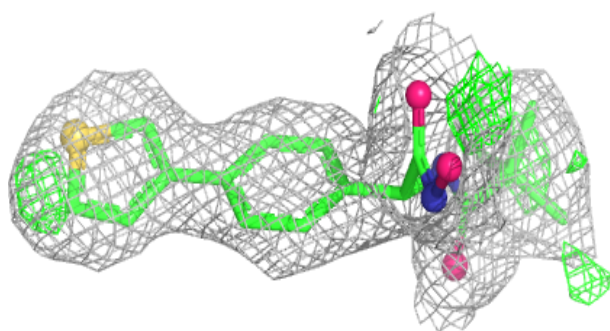
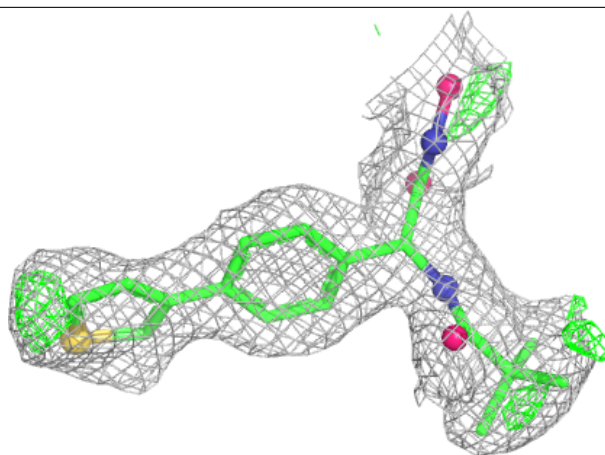
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	I	1002	1/1	0.99	0.03	17,17,17,17	0
3	ZN	I	1003	1/1	0.99	0.04	22,22,22,22	0
3	ZN	J	1002	1/1	0.99	0.03	21,21,21,21	0
3	ZN	J	1003	1/1	0.99	0.01	25,25,25,25	0
3	ZN	L	1002	1/1	0.99	0.02	22,22,22,22	0
3	ZN	L	1003	1/1	0.99	0.03	22,22,22,22	0
6	SO4	D	1007	5/5	0.99	0.04	25,25,25,28	0
3	ZN	C	1003	1/1	0.99	0.03	23,23,23,23	0
3	ZN	D	1003	1/1	0.99	0.02	24,24,24,24	0
3	ZN	F	1002	1/1	0.99	0.03	27,27,27,27	0
3	ZN	K	1002	1/1	1.00	0.01	21,21,21,21	0
3	ZN	K	1003	1/1	1.00	0.01	24,24,24,24	0
3	ZN	E	1003	1/1	1.00	0.01	21,21,21,21	0
3	ZN	B	1002	1/1	1.00	0.03	21,21,21,21	0
3	ZN	B	1003	1/1	1.00	0.02	16,16,16,16	0
3	ZN	G	1002	1/1	1.00	0.02	23,23,23,23	0
3	ZN	G	1003	1/1	1.00	0.01	18,18,18,18	0
3	ZN	H	1002	1/1	1.00	0.01	24,24,24,24	0
3	ZN	C	1002	1/1	1.00	0.02	18,18,18,18	0
3	ZN	A	1002	1/1	1.00	0.01	19,19,19,19	0
3	ZN	D	1002	1/1	1.00	0.02	21,21,21,21	0
3	ZN	A	1003	1/1	1.00	0.01	18,18,18,18	0
3	ZN	E	1002	1/1	1.00	0.01	24,24,24,24	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.

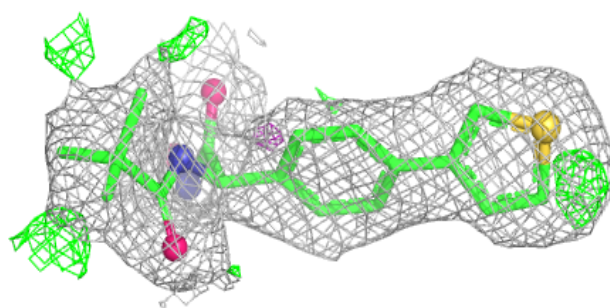
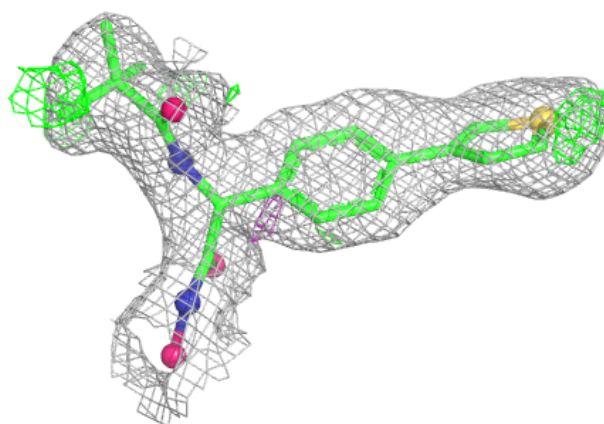
Electron density around 4TM I 1001:

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



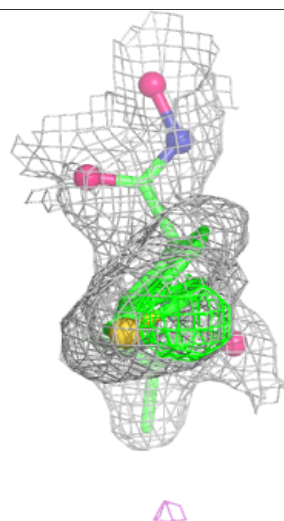
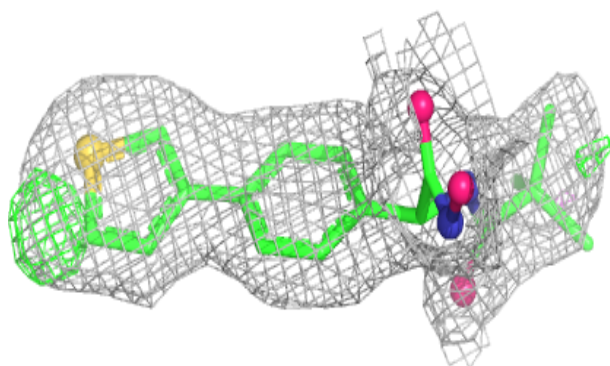
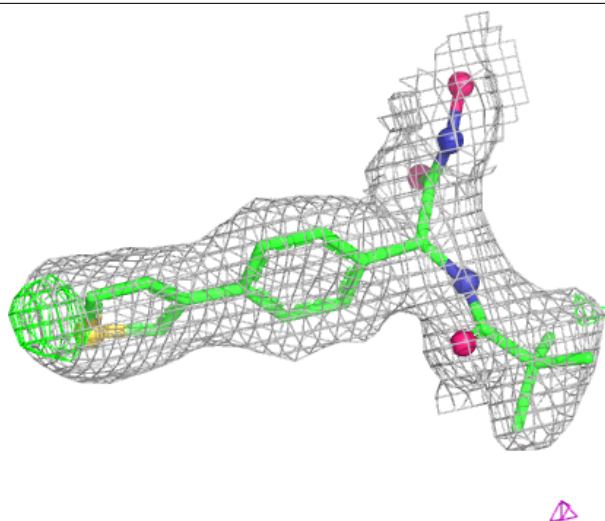
Electron density around 4TM D 1001:

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



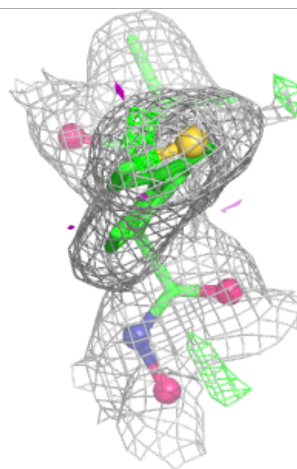
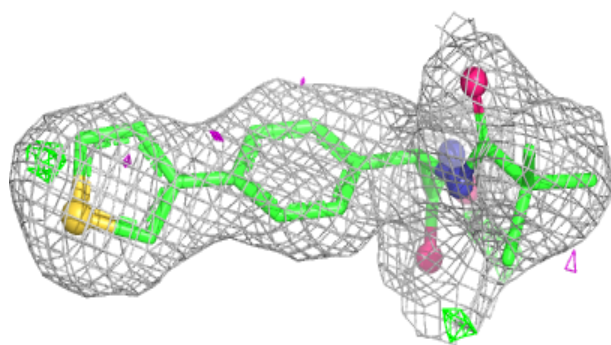
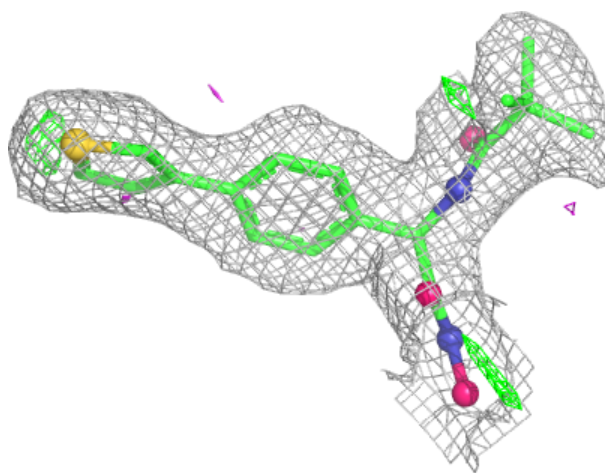
Electron density around 4TM E 1001:

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



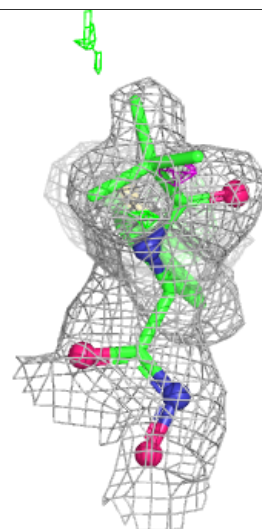
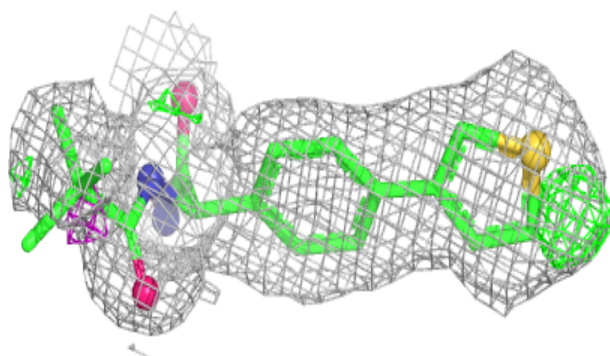
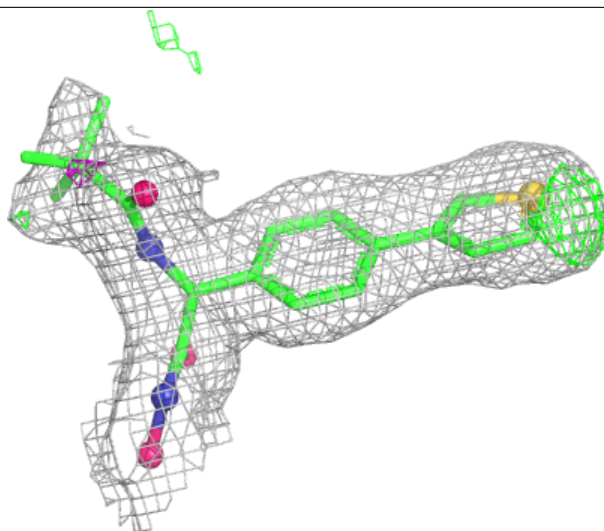
Electron density around 4TM C 1001:

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



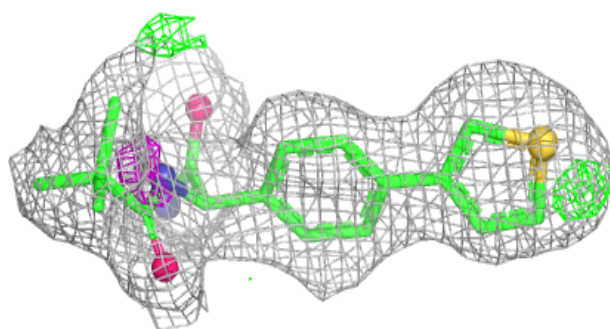
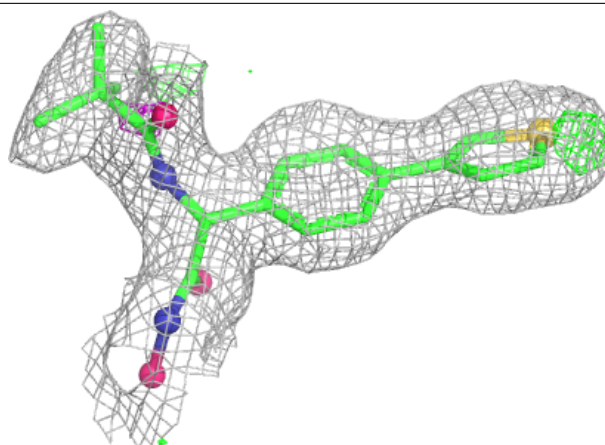
Electron density around 4TM K 1001:

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



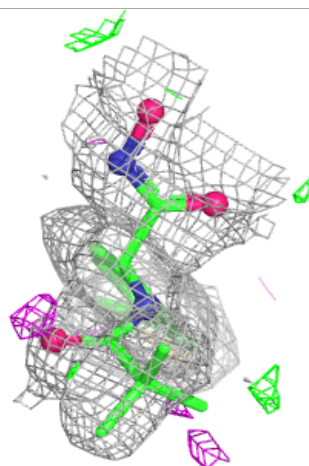
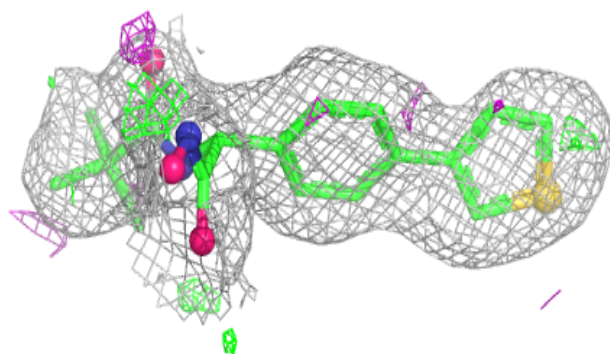
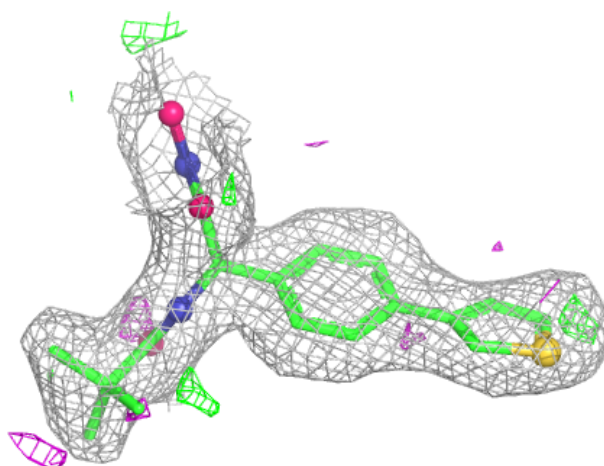
Electron density around 4TM L 1001:

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



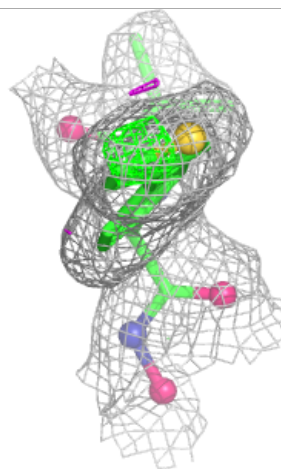
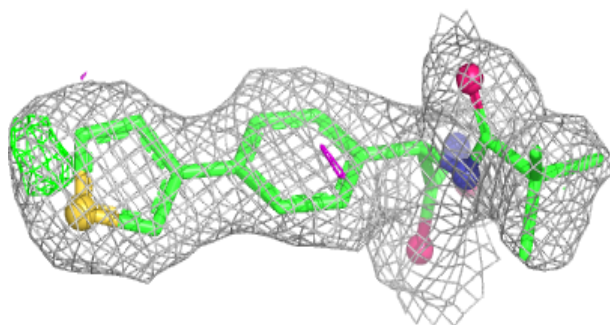
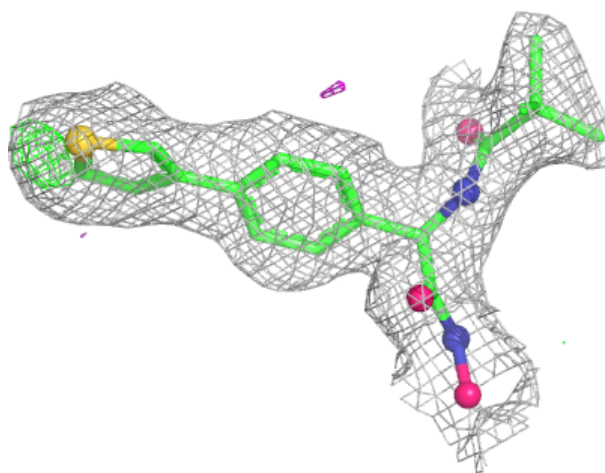
Electron density around 4TM B 1001:

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



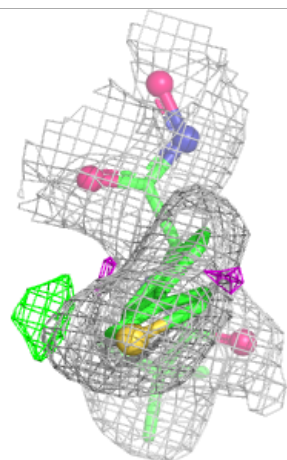
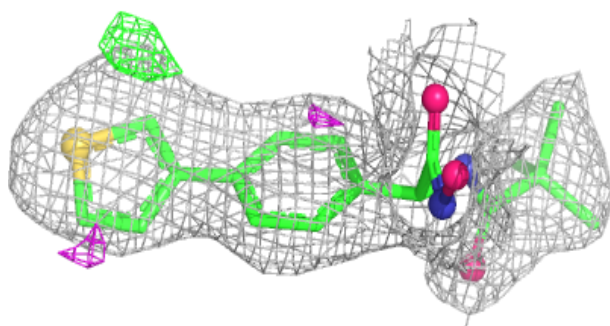
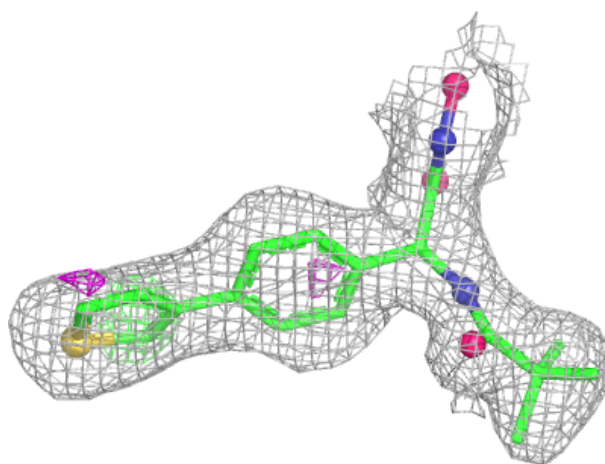
Electron density around 4TM J 1001:

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



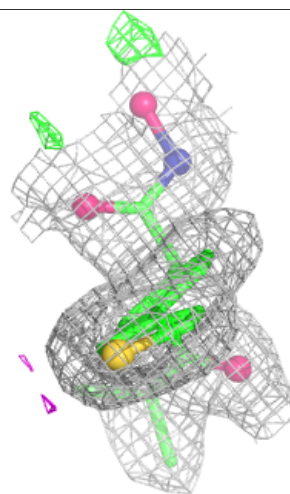
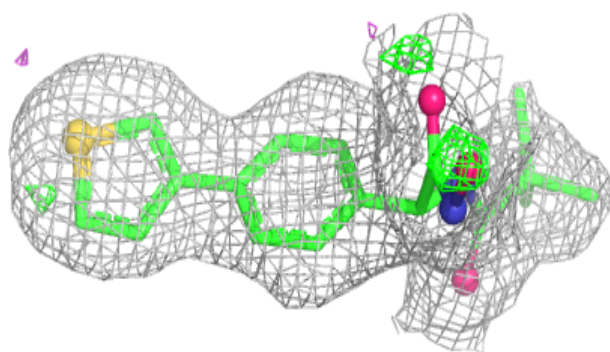
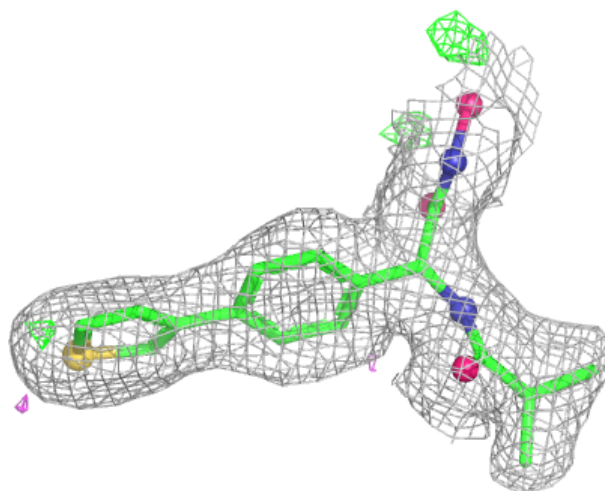
Electron density around 4TM G 1001:

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



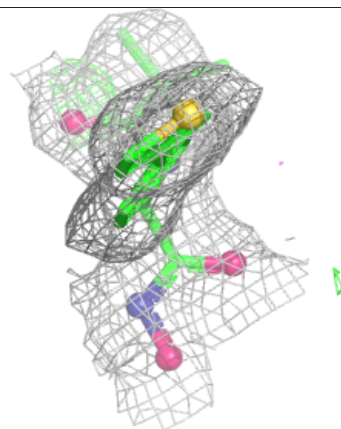
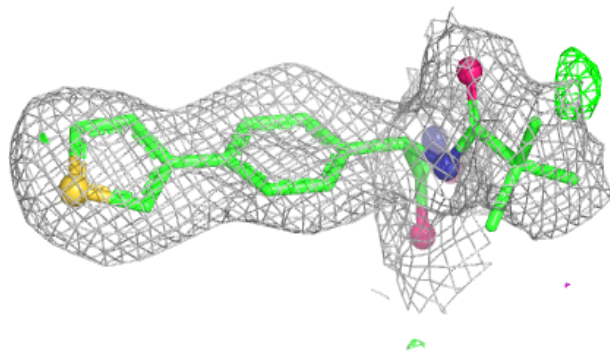
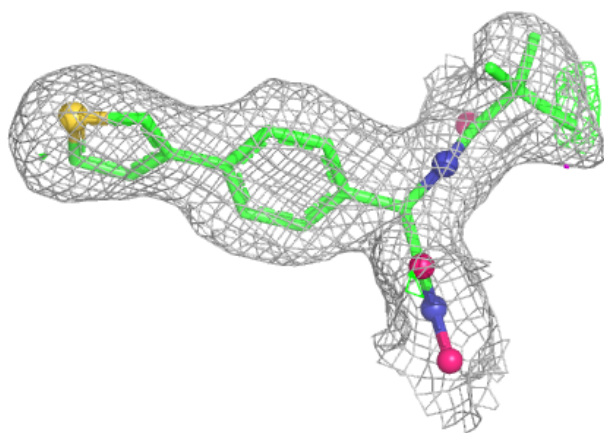
Electron density around 4TM F 1001:

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



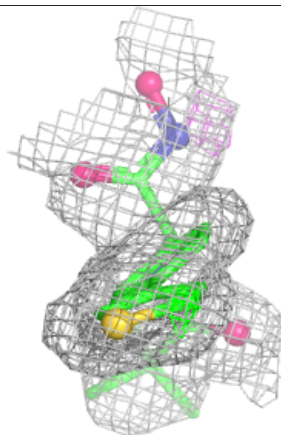
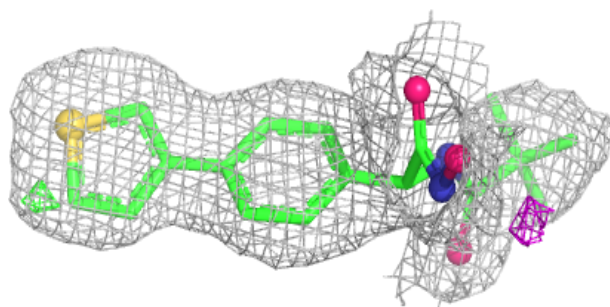
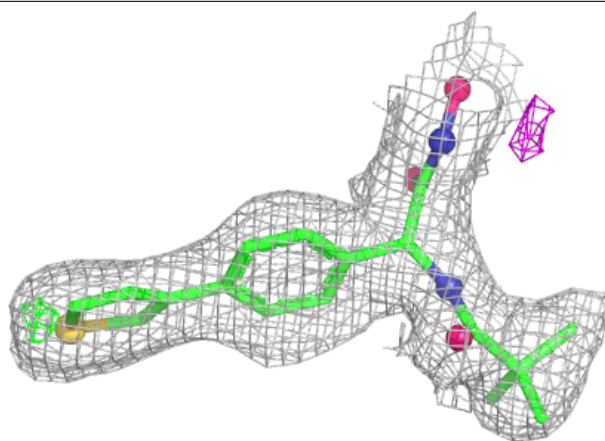
Electron density around 4TM H 1001:

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



Electron density around 4TM A 1001:

$2mF_o - DF_c$ (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.