Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 05:46 AM EDT

PDB ID	:	4ZY0
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 (i) 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 (i)) were used in the production of this report:

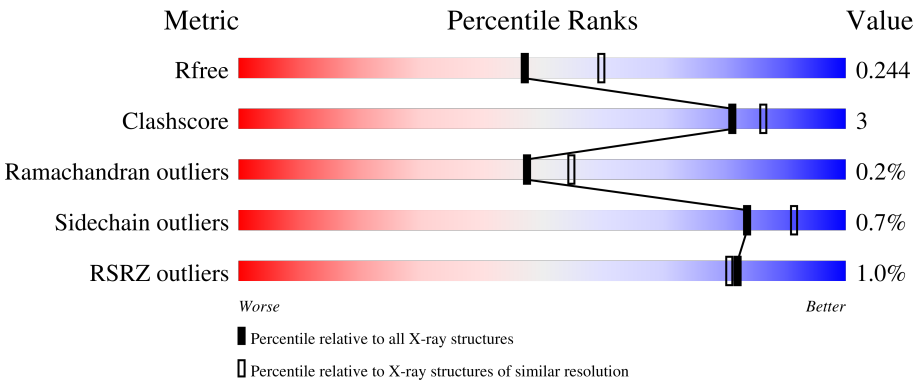
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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 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 <=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	.% 91% 9% •
1	B	522	2% 92% 7% •
1	C	522	.% 92% 7% •
1	D	522	93% 5% •
1	E	522	91% 6% •

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Mol	Chain	Length	Quality of chain
1	F	522	2% 91% 7%
1	G	522	93% 6%
1	H	522	2% 90% 8%
1	I	522	% 93% 6%
1	J	522	% 91% 8%
1	K	522	92% 5%
1	L	522	% 90% 8%

2 Entry composition (i)

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

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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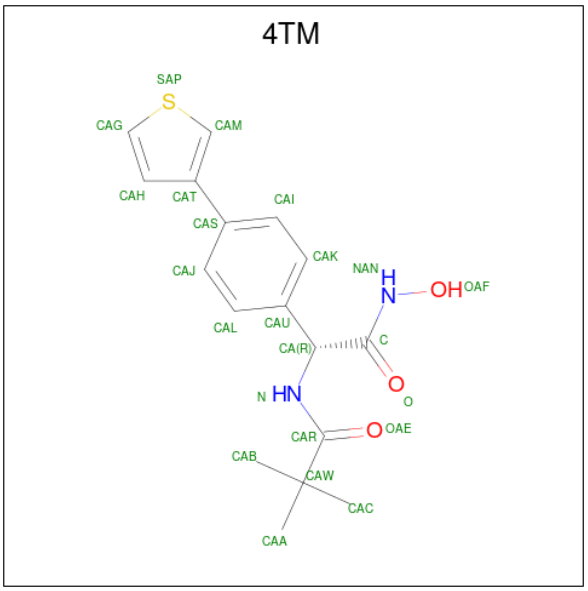
Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
C	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
D	515	GLN	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 (three-letter code: 4TM) (formula: $C_{17}H_{20}N_2O_3S$).

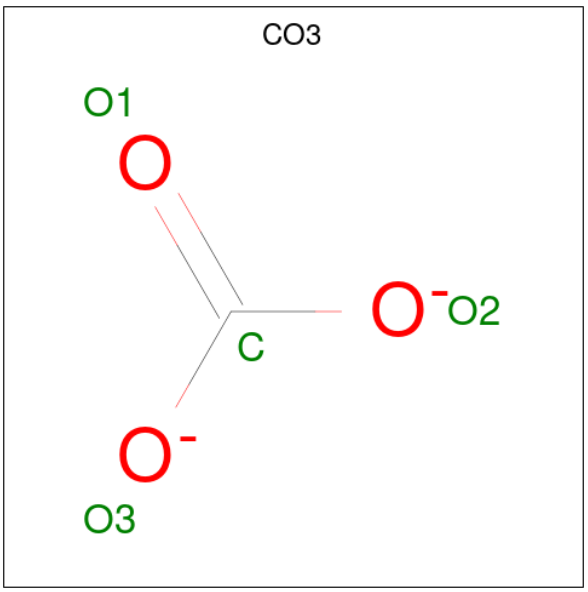


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	23	17	2	3	1	0	0
2	B	1	23	17	2	3	1	0	0
2	C	1	23	17	2	3	1	0	0
2	D	1	23	17	2	3	1	0	0
2	E	1	23	17	2	3	1	0	0
2	F	1	23	17	2	3	1	0	0
2	G	1	23	17	2	3	1	0	0
2	H	1	23	17	2	3	1	0	0
2	I	1	23	17	2	3	1	0	0
2	J	1	23	17	2	3	1	0	0
2	K	1	23	17	2	3	1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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

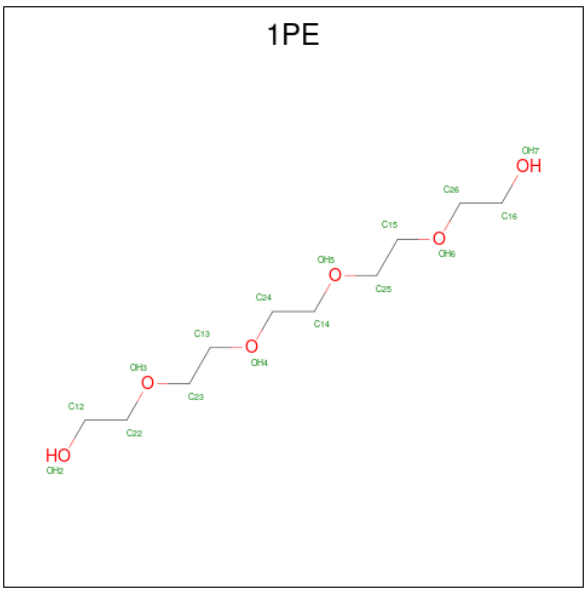
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0
3	E	2	2	2	0	0
3	F	2	2	2	0	0
3	G	2	2	2	0	0
3	H	2	2	2	0	0
3	I	2	2	2	0	0
3	J	2	2	2	0	0
3	K	2	2	2	0	0
3	L	2	2	2	0	0

- Molecule 4 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

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



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

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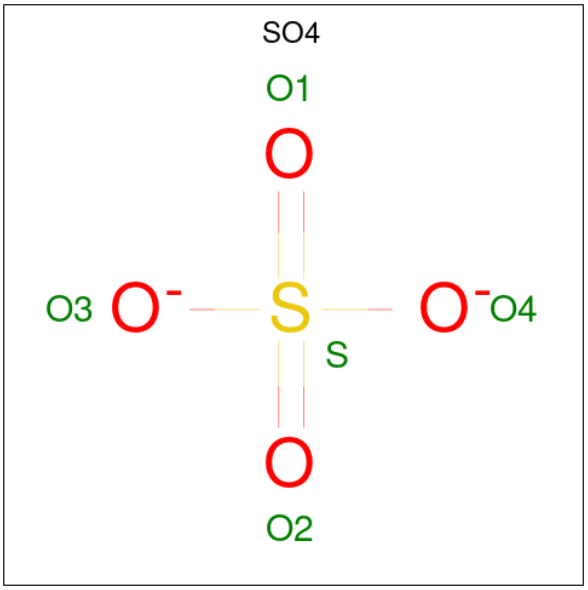
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	K	1	12	8	4	0	0
			Total	C	O		
5	L	1	10	6	4	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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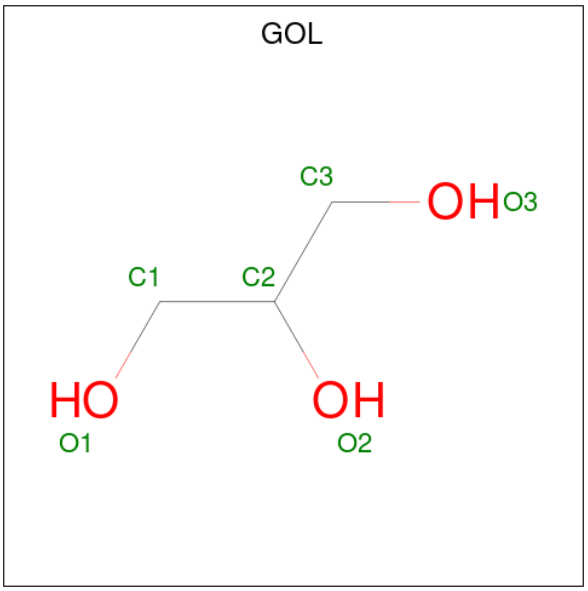
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	E	1	5	4	1	0	0
			Total	O	S		
6	E	1	5	4	1	0	0
			Total	O	S		
6	F	1	5	4	1	0	0
			Total	O	S		
6	G	1	5	4	1	0	0
			Total	O	S		
6	G	1	5	4	1	0	0
			Total	O	S		
6	H	1	5	4	1	0	0
			Total	O	S		
6	H	1	5	4	1	0	0
			Total	O	S		
6	H	1	5	4	1	0	0
			Total	O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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

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

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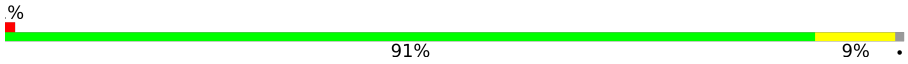
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	K	287	287	287	0	0
			Total	O		
8	L	243	243	243	0	0

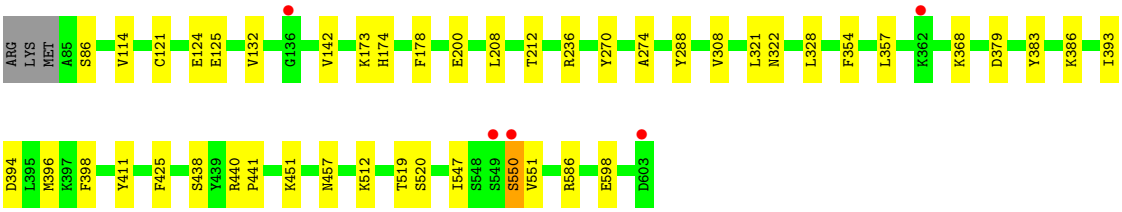
3 Residue-property plots (i)

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

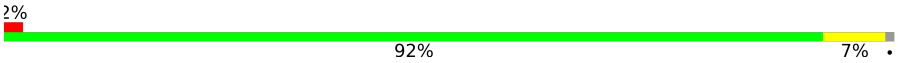
Chain A:

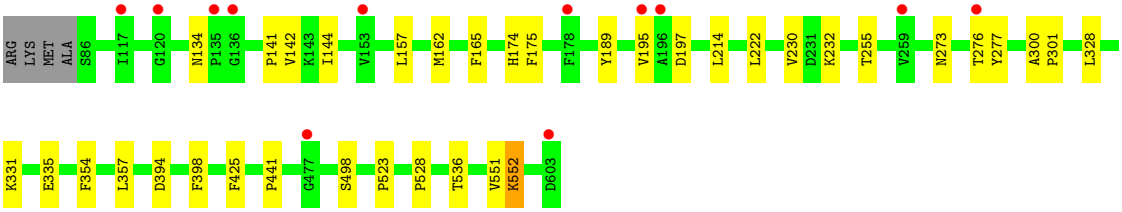




• Molecule 1: Probable M17 family aminopeptidase

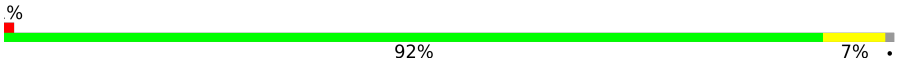
Chain B:

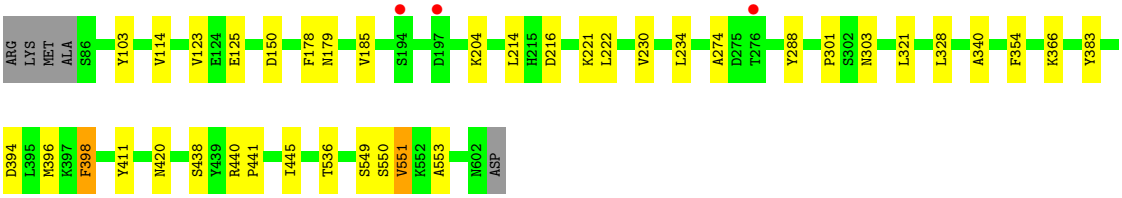




• Molecule 1: Probable M17 family aminopeptidase

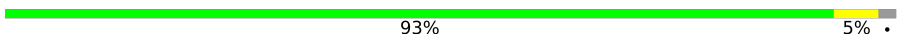
Chain C:

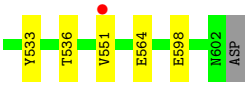




• Molecule 1: Probable M17 family aminopeptidase

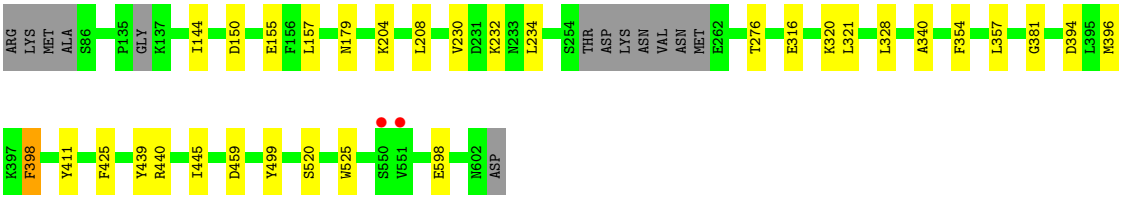
Chain D:





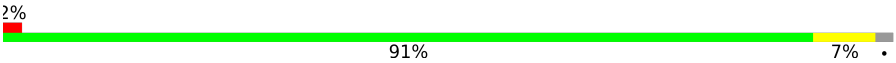
• Molecule 1: Probable M17 family aminopeptidase

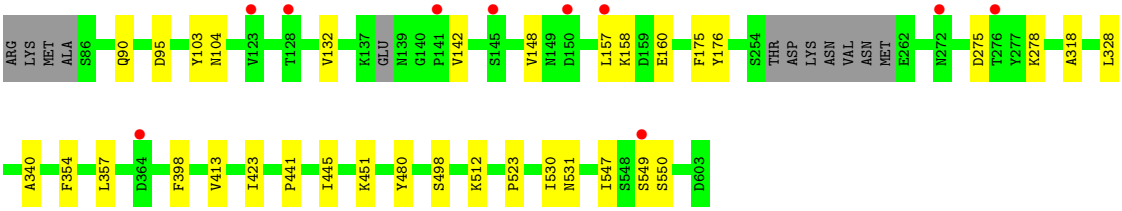
Chain E:



• Molecule 1: Probable M17 family aminopeptidase

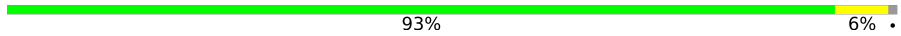
Chain F:

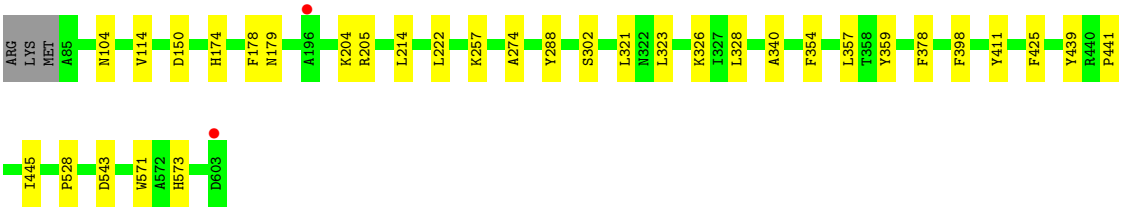




• Molecule 1: Probable M17 family aminopeptidase

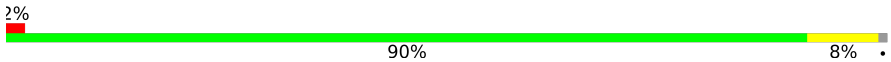
Chain G:

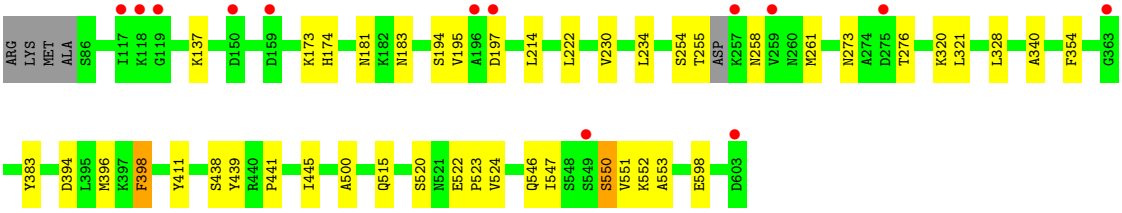




• Molecule 1: Probable M17 family aminopeptidase

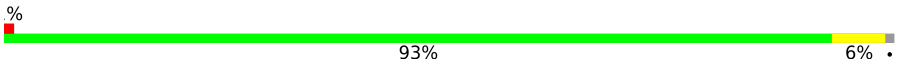
Chain H:

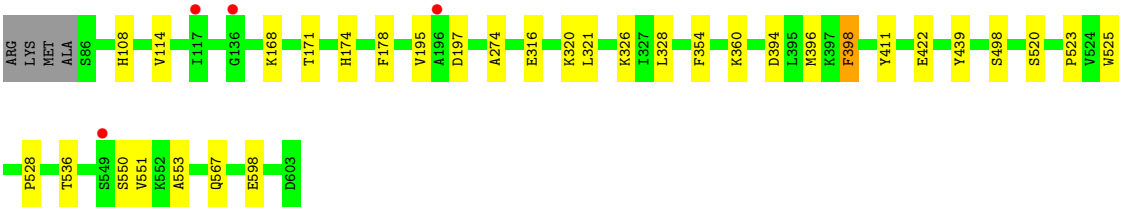




• Molecule 1: Probable M17 family aminopeptidase

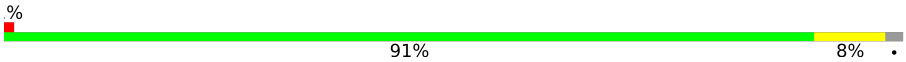
Chain I:

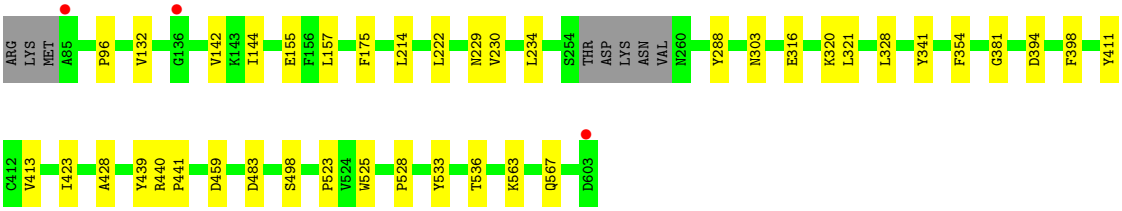




• Molecule 1: Probable M17 family aminopeptidase

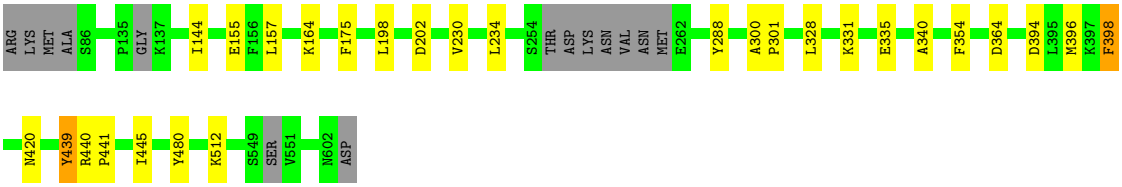
Chain J:





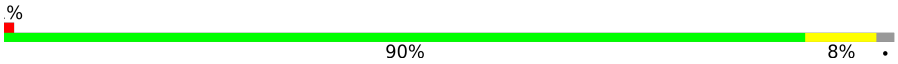
• Molecule 1: Probable M17 family aminopeptidase

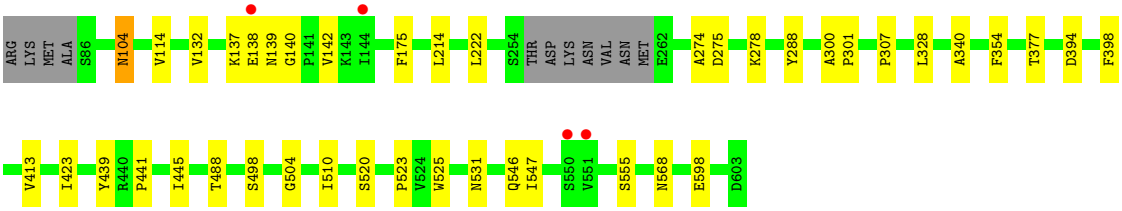
Chain K:



• Molecule 1: Probable M17 family aminopeptidase

Chain L:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.44 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.198 , 0.244 0.200 , 0.244	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 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4TM, GOL, SO4, ZN, 1PE, CO3

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	0.27	0/4051	0.43	0/5500
1	B	0.27	0/3988	0.42	0/5424
1	C	0.26	0/4012	0.42	0/5448
1	D	0.26	0/4011	0.42	0/5438
1	E	0.26	0/3967	0.42	0/5382
1	F	0.25	0/3917	0.42	1/5326 (0.0%)
1	G	0.26	0/4042	0.42	0/5486
1	H	0.26	0/4014	0.41	0/5450
1	I	0.26	0/4026	0.41	0/5466
1	J	0.26	0/4003	0.42	0/5427
1	K	0.26	0/3976	0.43	0/5389
1	L	0.27	0/3923	0.43	0/5336
All	All	0.26	0/47930	0.42	1/65072 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	549	SER	C-N-CA	5.37	135.13	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	28	0
1	B	3910	0	3778	21	0
1	C	3934	0	3848	22	0
1	D	3931	0	3869	17	0
1	E	3891	0	3809	20	0
1	F	3841	0	3705	21	0
1	G	3964	0	3871	20	0
1	H	3934	0	3831	25	0
1	I	3948	0	3864	25	0
1	J	3926	0	3866	25	0
1	K	3901	0	3837	17	0
1	L	3846	0	3709	24	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	0	0
2	H	23	0	0	0	0
2	I	23	0	0	0	0
2	J	23	0	0	0	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	6	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
8	C	283	0	0	2	0
8	D	304	0	0	2	0
8	E	348	0	0	3	0
8	F	214	0	0	0	0
8	G	297	0	0	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	243	0	0	0	0
All	All	51006	0	46140	242	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 (242) 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: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: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:I:360:LYS:NZ	1:I:422:GLU:OE1	2.25	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
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:H:137:LYS:O	1:H:194:SER:OG	2.21	0.58
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:320:LYS:HZ1	5:J:1005:1PE:H142	1.68	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: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: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
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:F:480:TYR:OH	1:F:512:LYS:NZ	2.34	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:386:LYS:HE3	1:A:396:MET:HE2	1.93	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:H:258:ASN:HB3	1:H:261:MET:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:257:LYS:NZ	8:G:1121:HOH:O	2.45	0.48
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.48	0.48
1:I:320:LYS:HZ1	5:I:1005:1PE:H142	1.79	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: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
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.95	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: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:H:441:PRO:HB2	1:I:394:ASP:HA	1.98	0.46
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.96	0.46
1:A:379:ASP:HB3	1:A:396:MET:HE2	1.97	0.46
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:368:LYS:NZ	8:A:1110:HOH:O	2.34	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:G:441:PRO:HB2	1:H:394:ASP:HA	2.00	0.43
1:G:543:ASP:CG	1:H:255:THR:H	2.21	0.43
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.99	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:320:LYS:NZ	5:I:1005:1PE:H142	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:D:510:ILE:HD13	1:D:526:TRP:NE1	2.35	0.41
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: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: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:I:320:LYS:HZ1	5:I:1005:1PE:H132	1.86	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:C:150:ASP:OD1	1:C:179:ASN:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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)

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	518/522 (99%)	501 (97%)	15 (3%)	2 (0%)	34	37
1	B	516/522 (99%)	496 (96%)	19 (4%)	1 (0%)	47	55
1	C	515/522 (99%)	500 (97%)	12 (2%)	3 (1%)	25	26
1	D	510/522 (98%)	498 (98%)	11 (2%)	1 (0%)	47	55
1	E	503/522 (96%)	490 (97%)	13 (3%)	0	100	100
1	F	504/522 (97%)	487 (97%)	16 (3%)	1 (0%)	47	55
1	G	517/522 (99%)	502 (97%)	15 (3%)	0	100	100
1	H	514/522 (98%)	498 (97%)	13 (2%)	3 (1%)	25	26
1	I	516/522 (99%)	504 (98%)	11 (2%)	1 (0%)	47	55
1	J	510/522 (98%)	498 (98%)	12 (2%)	0	100	100
1	K	500/522 (96%)	488 (98%)	12 (2%)	0	100	100
1	L	507/522 (97%)	494 (97%)	13 (3%)	0	100	100
All	All	6130/6264 (98%)	5956 (97%)	162 (3%)	12 (0%)	47	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	550	SER
1	H	552	LYS
1	A	551	VAL
1	B	552	LYS
1	C	549	SER
1	C	551	VAL
1	D	551	VAL
1	I	550	SER
1	A	550	SER
1	C	550	SER
1	H	254	SER
1	H	550	SER

5.3.2 Protein sidechains (i)

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%)	84	91
1	B	408/450 (91%)	406 (100%)	2 (0%)	88	94
1	C	415/450 (92%)	413 (100%)	2 (0%)	88	94
1	D	416/450 (92%)	412 (99%)	4 (1%)	76	86
1	E	413/450 (92%)	411 (100%)	2 (0%)	88	94
1	F	400/450 (89%)	398 (100%)	2 (0%)	88	94
1	G	418/450 (93%)	415 (99%)	3 (1%)	84	91
1	H	414/450 (92%)	411 (99%)	3 (1%)	84	91
1	I	419/450 (93%)	417 (100%)	2 (0%)	88	94
1	J	414/450 (92%)	409 (99%)	5 (1%)	71	83
1	K	416/450 (92%)	413 (99%)	3 (1%)	84	91
1	L	399/450 (89%)	394 (99%)	5 (1%)	69	81
All	All	4952/5400 (92%)	4916 (99%)	36 (1%)	84	91

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	TYR
1	A	398	PHE
1	A	550	SER
1	B	232	LYS
1	B	398	PHE
1	C	288	TYR
1	C	398	PHE
1	D	229[A]	ASN
1	D	229[B]	ASN
1	D	398	PHE
1	D	439	TYR
1	E	398	PHE
1	E	439	TYR
1	F	398	PHE
1	F	547	ILE
1	G	288	TYR
1	G	398	PHE
1	G	439	TYR
1	H	398	PHE
1	H	439	TYR
1	H	515	GLN
1	I	398	PHE
1	I	439	TYR
1	J	288	TYR
1	J	398	PHE
1	J	439	TYR
1	J	483	ASP
1	J	567	GLN
1	K	288	TYR
1	K	398	PHE
1	K	439	TYR
1	L	104	ASN
1	L	288	TYR
1	L	398	PHE
1	L	439	TYR
1	L	568	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	272	ASN
1	E	273	ASN
1	F	567	GLN

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Mol	Chain	Res	Type
1	H	181	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 monosaccharides 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	$\#\|Z\| > 2$
2	4TM	J	1001	3	24,24,24	2.49	5 (20%)	30,34,34	2.54	5 (16%)
2	4TM	B	1001	3	24,24,24	2.35	4 (16%)	30,34,34	2.39	6 (20%)
2	4TM	E	1001	3	24,24,24	2.40	4 (16%)	30,34,34	2.39	6 (20%)
5	1PE	D	1006	-	9,9,15	0.89	0	8,8,14	0.43	0
4	CO3	I	1004	-	2,3,3	0.39	0	2,3,3	0.27	0
5	1PE	I	1006	-	8,8,15	0.54	0	7,7,14	0.38	0
5	1PE	K	1005	-	11,11,15	0.59	0	10,10,14	0.40	0
4	CO3	D	1004	-	2,3,3	0.41	0	2,3,3	0.23	0
4	CO3	K	1004	-	2,3,3	0.39	0	2,3,3	0.19	0
2	4TM	C	1001	3	24,24,24	2.39	4 (16%)	30,34,34	2.46	5 (16%)
6	SO4	H	1008	-	4,4,4	0.15	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	4TM	D	1001	3	24,24,24	2.36	4 (16%)	30,34,34	2.37	5 (16%)
4	CO3	G	1004	-	2,3,3	0.37	0	2,3,3	0.22	0
5	1PE	K	1006	-	11,11,15	0.59	0	10,10,14	0.40	0
6	SO4	A	1008	-	4,4,4	0.13	0	6,6,6	0.07	0
6	SO4	B	1006	-	4,4,4	0.17	0	6,6,6	0.11	0
5	1PE	J	1005	-	9,9,15	0.56	0	8,8,14	0.33	0
6	SO4	B	1008	-	4,4,4	0.15	0	6,6,6	0.07	0
6	SO4	C	1008	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	B	1007	-	4,4,4	0.14	0	6,6,6	0.04	0
2	4TM	K	1001	3	24,24,24	2.54	6 (25%)	30,34,34	2.53	5 (16%)
5	1PE	L	1005	-	9,9,15	0.89	0	8,8,14	0.40	0
2	4TM	H	1001	3	24,24,24	2.32	4 (16%)	30,34,34	2.43	6 (20%)
5	1PE	C	1006	-	11,11,15	0.62	0	10,10,14	0.38	0
2	4TM	I	1001	3	24,24,24	2.29	5 (20%)	30,34,34	2.10	4 (13%)
6	SO4	D	1007	-	4,4,4	0.15	0	6,6,6	0.09	0
2	4TM	G	1001	3	24,24,24	2.44	4 (16%)	30,34,34	2.68	5 (16%)
5	1PE	G	1006	-	8,8,15	0.53	0	7,7,14	0.41	0
6	SO4	J	1007	-	4,4,4	0.15	0	6,6,6	0.17	0
4	CO3	F	1004	-	2,3,3	0.41	0	2,3,3	0.30	0
5	1PE	F	1006	-	6,6,15	0.62	0	5,5,14	0.50	0
5	1PE	G	1007	-	11,11,15	0.65	0	10,10,14	0.40	0
6	SO4	E	1008	-	4,4,4	0.15	0	6,6,6	0.04	0
4	CO3	E	1004	-	2,3,3	0.41	0	2,3,3	0.31	0
6	SO4	H	1007	-	4,4,4	0.15	0	6,6,6	0.07	0
5	1PE	F	1007	-	9,9,15	0.89	0	8,8,14	0.43	0
5	1PE	I	1005	-	12,12,15	0.64	0	11,11,14	0.37	0
7	GOL	G	1005	-	5,5,5	0.33	0	5,5,5	0.32	0
6	SO4	C	1010	-	4,4,4	0.13	0	6,6,6	0.07	0
6	SO4	H	1009	-	4,4,4	0.13	0	6,6,6	0.08	0
2	4TM	F	1001	3	24,24,24	2.53	5 (20%)	30,34,34	2.32	5 (16%)
6	SO4	H	1010	-	4,4,4	0.14	0	6,6,6	0.09	0
6	SO4	K	1007	-	4,4,4	0.12	0	6,6,6	0.08	0
6	SO4	A	1009	-	4,4,4	0.15	0	6,6,6	0.07	0
4	CO3	H	1004	-	2,3,3	0.42	0	2,3,3	0.09	0
5	1PE	D	1005	-	10,10,15	0.89	0	9,9,14	0.31	0
6	SO4	E	1007	-	4,4,4	0.14	0	6,6,6	0.11	0
7	GOL	C	1005	-	5,5,5	0.33	0	5,5,5	0.27	0
5	1PE	B	1005	-	9,9,15	0.55	0	8,8,14	0.40	0
4	CO3	B	1004	-	2,3,3	0.40	0	2,3,3	0.19	0
4	CO3	A	1004	-	2,3,3	0.39	0	2,3,3	0.17	0
4	CO3	J	1004	-	2,3,3	0.41	0	2,3,3	0.10	0
4	CO3	L	1004	-	2,3,3	0.42	0	2,3,3	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	1PE	A	1005	-	8,8,15	0.56	0	7,7,14	0.29	0
5	1PE	H	1006	-	9,9,15	0.57	0	8,8,14	0.31	0
6	SO4	C	1009	-	4,4,4	0.15	0	6,6,6	0.04	0
6	SO4	G	1009	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	L	1006	-	4,4,4	0.15	0	6,6,6	0.06	0
6	SO4	G	1008	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	L	1007	-	4,4,4	0.14	0	6,6,6	0.20	0
4	CO3	C	1004	-	2,3,3	0.40	0	2,3,3	0.37	0
5	1PE	A	1007	-	5,5,15	0.69	0	4,4,14	0.37	0
5	1PE	H	1005	-	9,9,15	0.55	0	8,8,14	0.35	0
6	SO4	I	1007	-	4,4,4	0.13	0	6,6,6	0.06	0
5	1PE	F	1005	-	10,10,15	0.85	0	9,9,14	0.35	0
6	SO4	F	1008	-	4,4,4	0.15	0	6,6,6	0.05	0
5	1PE	A	1006	-	5,5,15	0.67	0	4,4,14	0.55	0
5	1PE	C	1007	-	10,10,15	0.58	0	9,9,14	0.38	0
5	1PE	E	1006	-	11,11,15	0.57	0	10,10,14	0.46	0
2	4TM	L	1001	3	24,24,24	2.37	4 (16%)	30,34,34	2.38	5 (16%)
5	1PE	J	1006	-	9,9,15	0.54	0	8,8,14	0.34	0
5	1PE	E	1005	-	11,11,15	0.58	0	10,10,14	0.50	0
2	4TM	A	1001	3	24,24,24	2.43	5 (20%)	30,34,34	2.23	5 (16%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	C	1006	-	-	6/9/9/13	-
2	4TM	I	1001	3	-	0/24/24/24	0/2/2/2
2	4TM	G	1001	3	-	0/24/24/24	0/2/2/2
5	1PE	G	1006	-	-	6/6/6/13	-
5	1PE	F	1006	-	-	2/4/4/13	-
5	1PE	G	1007	-	-	6/9/9/13	-
5	1PE	F	1007	-	-	3/7/7/13	-
5	1PE	I	1005	-	-	6/10/10/13	-
7	GOL	G	1005	-	-	1/4/4/4	-
2	4TM	F	1001	3	-	0/24/24/24	0/2/2/2
5	1PE	D	1005	-	-	4/8/8/13	-
7	GOL	C	1005	-	-	2/4/4/4	-
5	1PE	B	1005	-	-	4/7/7/13	-
5	1PE	H	1006	-	-	5/7/7/13	-
5	1PE	A	1005	-	-	3/6/6/13	-
5	1PE	A	1007	-	-	1/3/3/13	-
5	1PE	H	1005	-	-	4/7/7/13	-
5	1PE	F	1005	-	-	7/8/8/13	-
5	1PE	A	1006	-	-	2/3/3/13	-
5	1PE	C	1007	-	-	6/8/8/13	-
5	1PE	E	1006	-	-	8/9/9/13	-
2	4TM	L	1001	3	-	1/24/24/24	0/2/2/2
5	1PE	J	1006	-	-	7/7/7/13	-
5	1PE	E	1005	-	-	7/9/9/13	-
2	4TM	A	1001	3	-	0/24/24/24	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1001	4TM	CAU-CA	-7.67	1.40	1.52
2	F	1001	4TM	CAU-CA	-7.62	1.40	1.52
2	L	1001	4TM	CAU-CA	-7.54	1.40	1.52
2	K	1001	4TM	CAU-CA	-7.53	1.40	1.52
2	C	1001	4TM	CAU-CA	-7.41	1.40	1.52
2	A	1001	4TM	CAU-CA	-7.30	1.40	1.52
2	E	1001	4TM	CAU-CA	-7.29	1.40	1.52
2	G	1001	4TM	CAU-CA	-7.13	1.41	1.52
2	B	1001	4TM	CAU-CA	-6.87	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1001	4TM	CAU-CA	-6.84	1.41	1.52
2	I	1001	4TM	CAU-CA	-6.66	1.41	1.52
2	D	1001	4TM	CAU-CA	-6.64	1.41	1.52
2	G	1001	4TM	CAT-CAS	-6.15	1.33	1.49
2	J	1001	4TM	CAT-CAS	-6.11	1.33	1.49
2	K	1001	4TM	CAT-CAS	-6.04	1.34	1.49
2	B	1001	4TM	CAT-CAS	-5.91	1.34	1.49
2	C	1001	4TM	CAT-CAS	-5.87	1.34	1.49
2	D	1001	4TM	CAT-CAS	-5.87	1.34	1.49
2	A	1001	4TM	CAT-CAS	-5.82	1.34	1.49
2	E	1001	4TM	CAT-CAS	-5.78	1.34	1.49
2	F	1001	4TM	CAT-CAS	-5.76	1.34	1.49
2	H	1001	4TM	CAT-CAS	-5.74	1.34	1.49
2	L	1001	4TM	CAT-CAS	-5.64	1.35	1.49
2	I	1001	4TM	CAT-CAS	-5.60	1.35	1.49
2	K	1001	4TM	CAM-CAT	-5.08	1.34	1.37
2	B	1001	4TM	CAM-CAT	-5.07	1.34	1.37
2	G	1001	4TM	CAM-CAT	-4.98	1.34	1.37
2	D	1001	4TM	CAM-CAT	-4.92	1.34	1.37
2	E	1001	4TM	CAM-CAT	-4.90	1.34	1.37
2	A	1001	4TM	CAM-CAT	-4.88	1.34	1.37
2	H	1001	4TM	CAM-CAT	-4.84	1.34	1.37
2	J	1001	4TM	CAM-CAT	-4.70	1.34	1.37
2	G	1001	4TM	CAH-CAT	-4.59	1.35	1.42
2	F	1001	4TM	CAH-CAT	-4.48	1.35	1.42
2	K	1001	4TM	CAH-CAT	-4.47	1.35	1.42
2	L	1001	4TM	CAH-CAT	-4.44	1.35	1.42
2	C	1001	4TM	CAM-CAT	-4.43	1.34	1.37
2	A	1001	4TM	CAH-CAT	-4.41	1.35	1.42
2	J	1001	4TM	CAH-CAT	-4.39	1.35	1.42
2	C	1001	4TM	CAH-CAT	-4.38	1.35	1.42
2	L	1001	4TM	CAM-CAT	-4.35	1.34	1.37
2	F	1001	4TM	OAF-NAN	4.34	1.51	1.40
2	D	1001	4TM	CAH-CAT	-4.33	1.35	1.42
2	H	1001	4TM	CAH-CAT	-4.28	1.35	1.42
2	E	1001	4TM	CAH-CAT	-4.22	1.35	1.42
2	F	1001	4TM	CAM-CAT	-4.21	1.34	1.37
2	B	1001	4TM	CAH-CAT	-4.17	1.36	1.42
2	I	1001	4TM	CAH-CAT	-4.16	1.36	1.42
2	I	1001	4TM	CAM-CAT	-4.04	1.34	1.37
2	I	1001	4TM	CAM-SAP	-2.98	1.67	1.70
2	K	1001	4TM	CAM-SAP	-2.31	1.68	1.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1001	4TM	CAM-SAP	-2.29	1.68	1.70
2	K	1001	4TM	OAF-NAN	2.27	1.45	1.40
2	A	1001	4TM	CAM-SAP	-2.27	1.68	1.70

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1001	4TM	CAT-CAM-SAP	-11.49	104.88	112.29
2	J	1001	4TM	CAT-CAM-SAP	-11.29	105.01	112.29
2	K	1001	4TM	CAT-CAM-SAP	-11.02	105.18	112.29
2	B	1001	4TM	CAT-CAM-SAP	-10.69	105.40	112.29
2	C	1001	4TM	CAT-CAM-SAP	-10.61	105.45	112.29
2	D	1001	4TM	CAT-CAM-SAP	-10.47	105.54	112.29
2	H	1001	4TM	CAT-CAM-SAP	-10.43	105.56	112.29
2	L	1001	4TM	CAT-CAM-SAP	-10.11	105.78	112.29
2	E	1001	4TM	CAT-CAM-SAP	-10.03	105.82	112.29
2	F	1001	4TM	CAT-CAM-SAP	-9.67	106.05	112.29
2	A	1001	4TM	CAT-CAM-SAP	-9.60	106.10	112.29
2	I	1001	4TM	CAT-CAM-SAP	-9.24	106.33	112.29
2	G	1001	4TM	CAH-CAT-CAS	-6.86	120.00	126.32
2	C	1001	4TM	CAH-CAT-CAS	-5.84	120.93	126.32
2	L	1001	4TM	CAH-CAT-CAS	-5.50	121.25	126.32
2	K	1001	4TM	CAH-CAT-CAS	-5.44	121.31	126.32
2	F	1001	4TM	CAH-CAT-CAS	-5.30	121.43	126.32
2	H	1001	4TM	CAH-CAT-CAS	-5.17	121.56	126.32
2	E	1001	4TM	CAH-CAT-CAS	-5.04	121.67	126.32
2	A	1001	4TM	CAH-CAT-CAS	-4.54	122.13	126.32
2	D	1001	4TM	CAH-CAT-CAS	-4.46	122.21	126.32
2	J	1001	4TM	CAH-CAT-CAS	-4.46	122.21	126.32
2	B	1001	4TM	CAH-CAT-CAS	-4.06	122.58	126.32
2	I	1001	4TM	CAM-CAT-CAS	-4.04	122.07	127.58
2	B	1001	4TM	CAM-CAT-CAS	-3.76	122.45	127.58
2	J	1001	4TM	CAM-CAT-CAS	-3.70	122.53	127.58
2	A	1001	4TM	CAM-CAT-CAS	-3.48	122.84	127.58
2	D	1001	4TM	CAM-CAT-CAS	-3.38	122.97	127.58
2	I	1001	4TM	CAH-CAT-CAS	-3.31	123.27	126.32
2	E	1001	4TM	CAM-CAT-CAS	-3.19	123.23	127.58
2	L	1001	4TM	CAW-CAR-N	-3.15	113.33	117.66
2	F	1001	4TM	CAW-CAR-N	-3.06	113.45	117.66
2	F	1001	4TM	CAM-CAT-CAS	-3.03	123.44	127.58
2	K	1001	4TM	CAM-CAT-CAS	-2.98	123.51	127.58
2	H	1001	4TM	CAW-CAR-N	-2.91	113.66	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	4TM	CAW-CAR-N	-2.89	113.68	117.66
2	H	1001	4TM	CAM-CAT-CAS	-2.83	123.72	127.58
2	J	1001	4TM	CAG-SAP-CAM	2.81	98.10	92.37
2	K	1001	4TM	CAG-SAP-CAM	2.76	98.00	92.37
2	E	1001	4TM	CAK-CAU-CA	-2.71	116.35	120.80
2	C	1001	4TM	CAW-CAR-N	-2.70	113.94	117.66
2	B	1001	4TM	CAG-SAP-CAM	2.65	97.78	92.37
2	G	1001	4TM	CAG-SAP-CAM	2.65	97.77	92.37
2	L	1001	4TM	CAM-CAT-CAS	-2.58	124.06	127.58
2	D	1001	4TM	CAG-SAP-CAM	2.56	97.60	92.37
2	H	1001	4TM	CAG-SAP-CAM	2.54	97.55	92.37
2	J	1001	4TM	CAW-CAR-N	-2.52	114.19	117.66
2	C	1001	4TM	CAG-SAP-CAM	2.51	97.48	92.37
2	C	1001	4TM	CAM-CAT-CAS	-2.50	124.17	127.58
2	I	1001	4TM	CAG-SAP-CAM	2.47	97.40	92.37
2	E	1001	4TM	CAG-SAP-CAM	2.39	97.25	92.37
2	B	1001	4TM	CAW-CAR-N	-2.39	114.37	117.66
2	A	1001	4TM	CAG-SAP-CAM	2.31	97.07	92.37
2	E	1001	4TM	CAL-CAU-CA	2.25	124.50	120.80
2	G	1001	4TM	CAM-CAT-CAS	-2.25	124.52	127.58
2	L	1001	4TM	CAG-SAP-CAM	2.25	96.95	92.37
2	A	1001	4TM	CAW-CAR-N	-2.22	114.61	117.66
2	K	1001	4TM	CAK-CAU-CA	-2.20	117.19	120.80
2	G	1001	4TM	CAK-CAU-CA	-2.17	117.24	120.80
2	B	1001	4TM	CAU-CA-C	2.12	112.93	108.16
2	H	1001	4TM	CAU-CA-C	2.12	112.92	108.16
2	F	1001	4TM	CAG-SAP-CAM	2.10	96.64	92.37

There are no chirality outliers.

All (121) torsion outliers are listed below:

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

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

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

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

There are no ring outliers.

20 monomers are involved in 32 short contacts:

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

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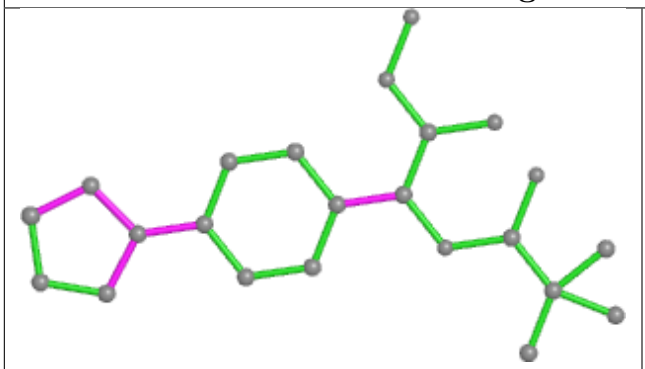
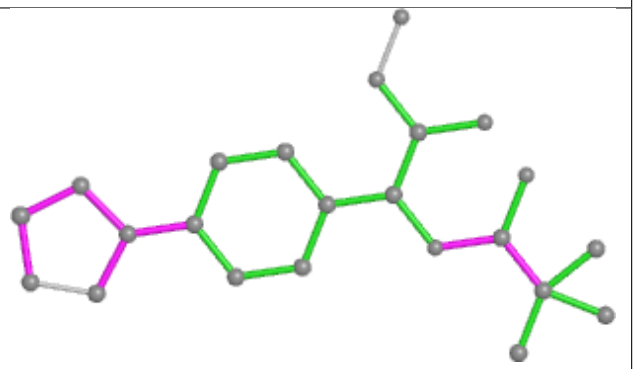
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1005	1PE	1	0
5	A	1005	1PE	1	0
5	H	1006	1PE	2	0
6	L	1006	SO4	1	0
6	G	1008	SO4	1	0
6	L	1007	SO4	1	0
5	F	1005	1PE	3	0
6	F	1008	SO4	1	0
5	E	1006	1PE	2	0
5	E	1005	1PE	1	0

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 then 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.

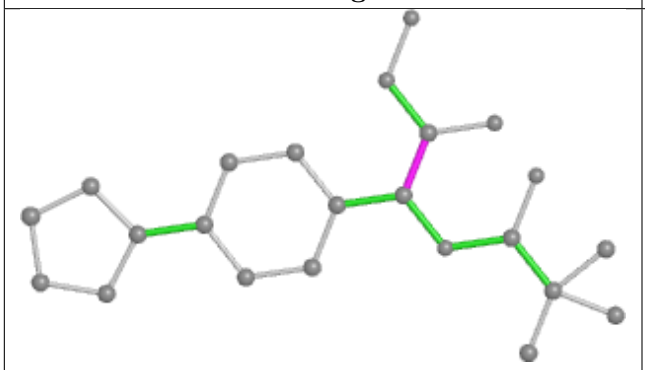
Ligand 4TM J 1001



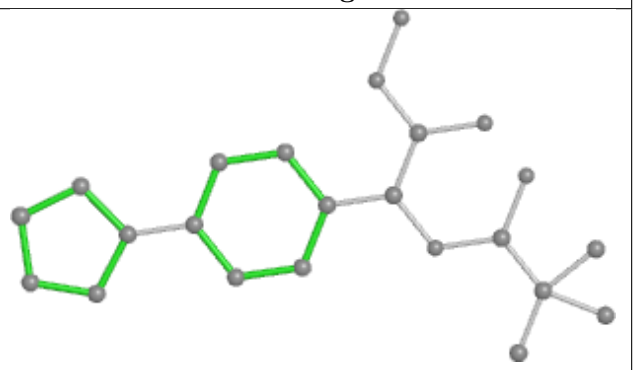
Bond lengths



Bond angles

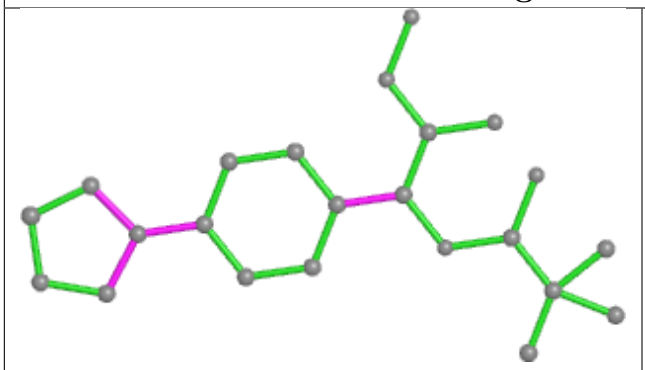


Torsions

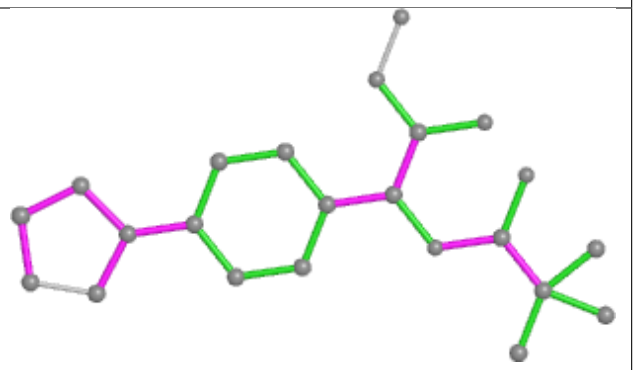


Rings

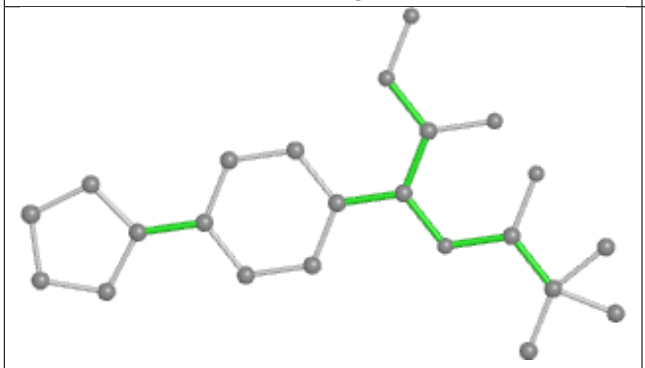
Ligand 4TM B 1001



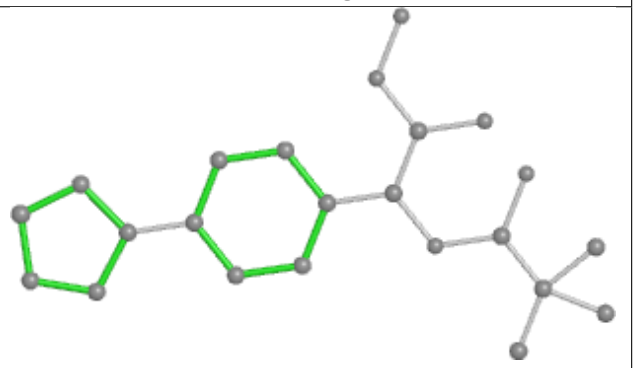
Bond lengths



Bond angles

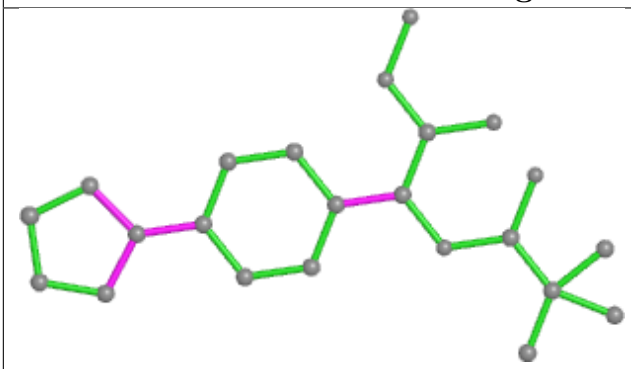


Torsions

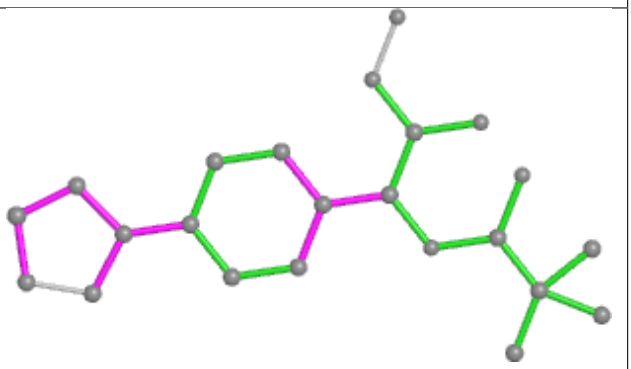


Rings

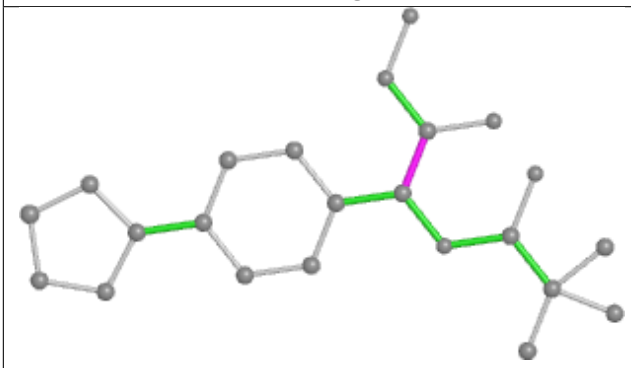
Ligand 4TM E 1001



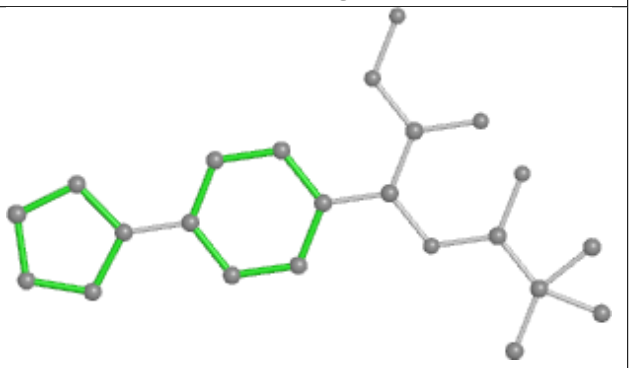
Bond lengths



Bond angles

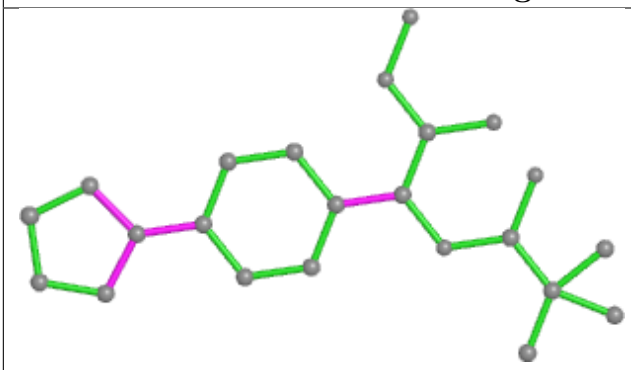


Torsions



Rings

Ligand 4TM C 1001



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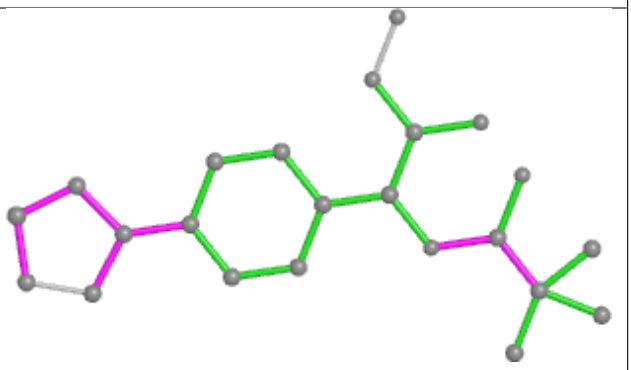
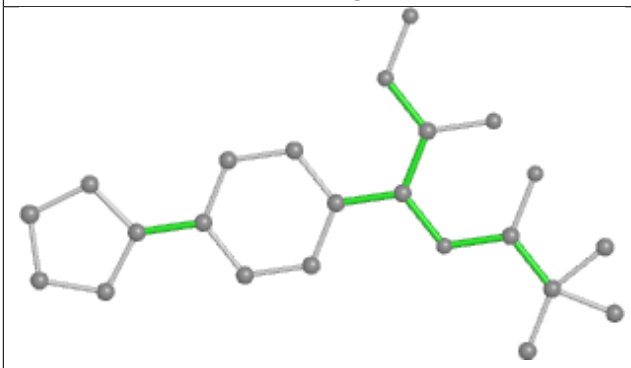


Bond angles



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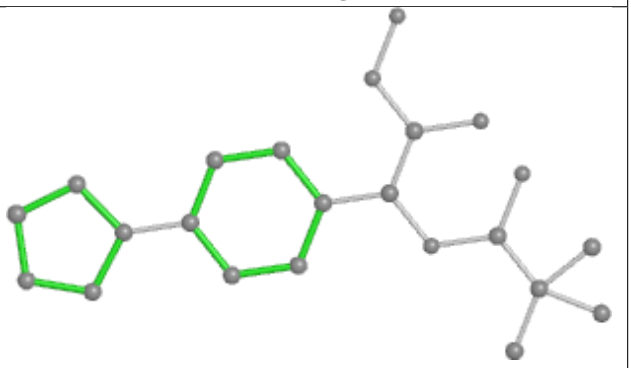
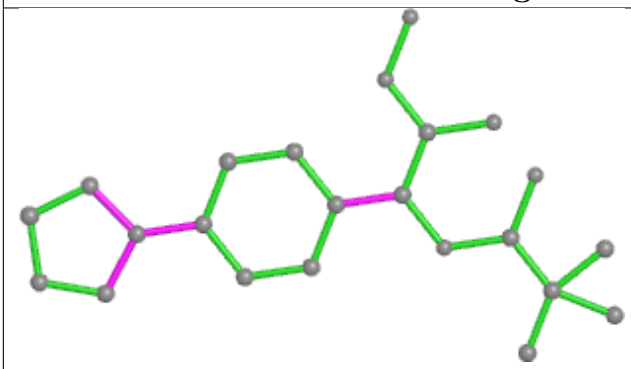


Rings

Ligand 4TM D 1001



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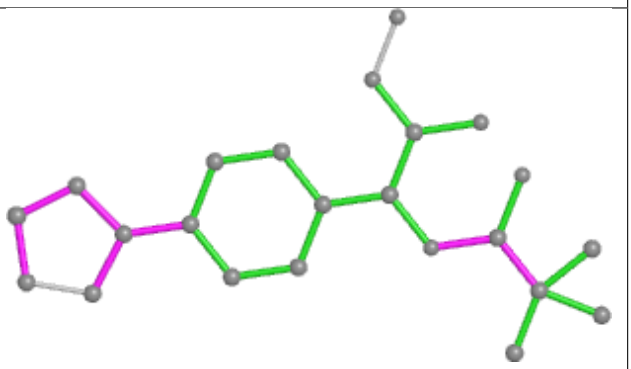

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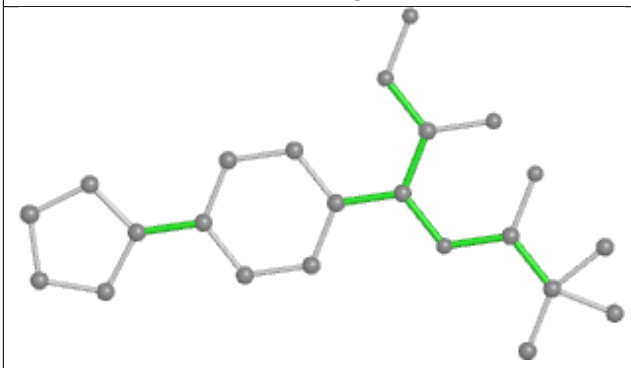

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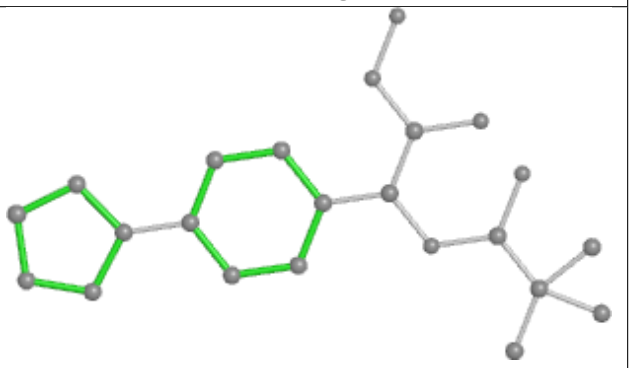

Rings

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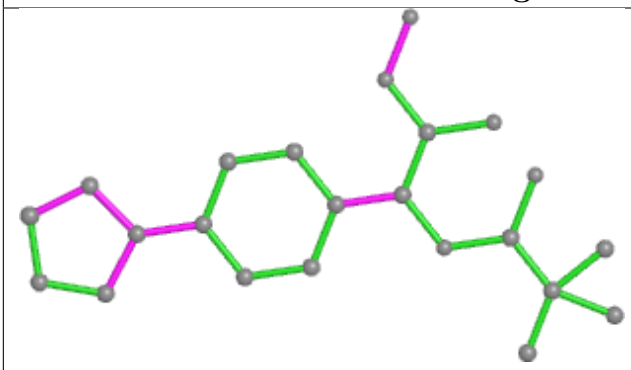

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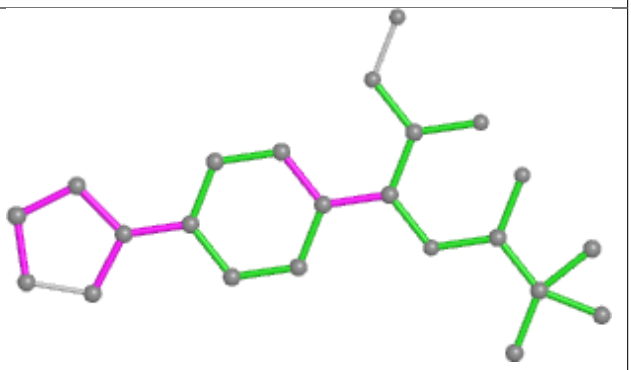

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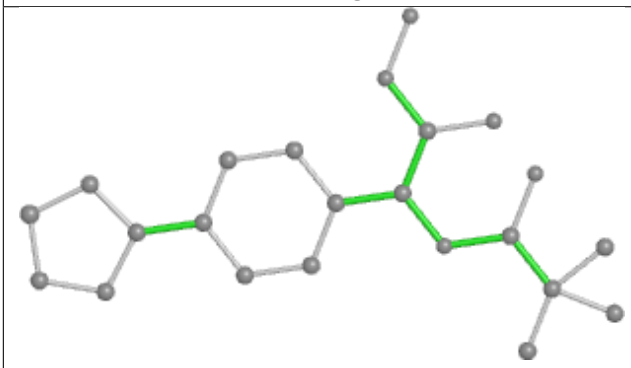

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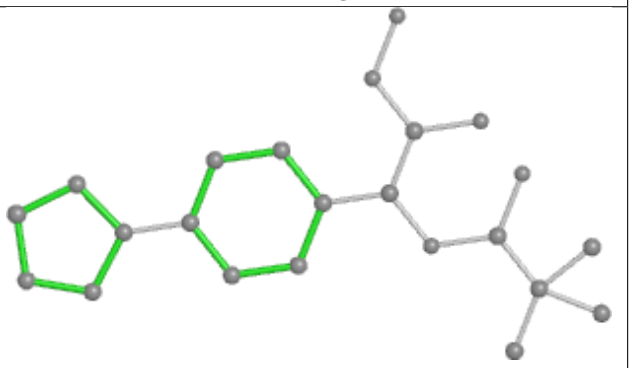

Rings

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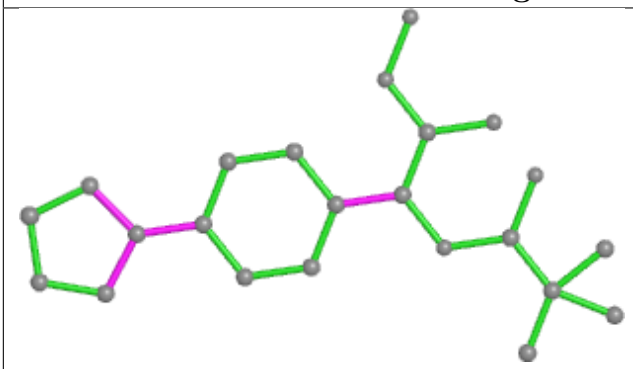

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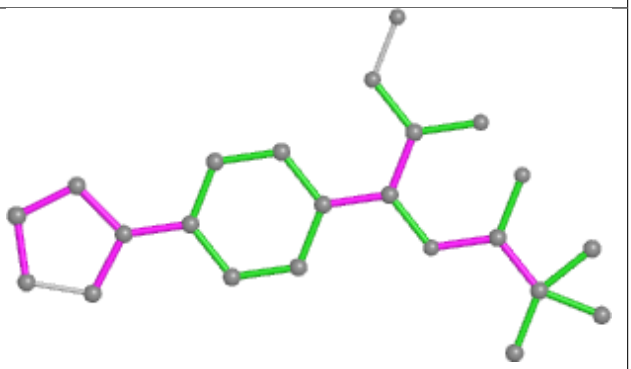

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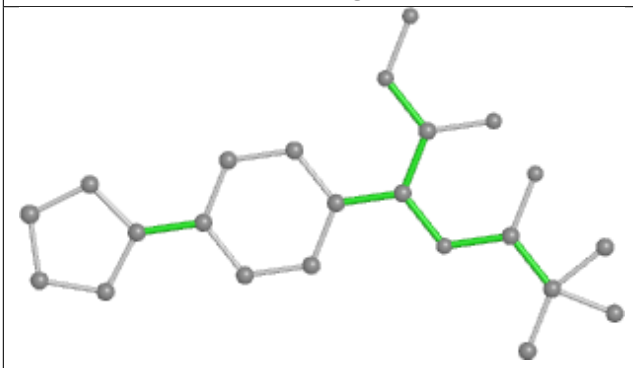

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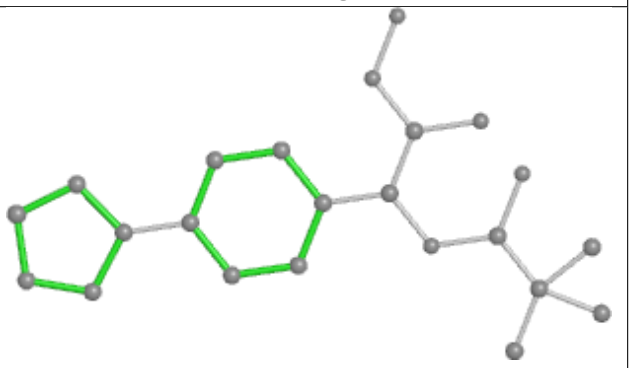

Rings

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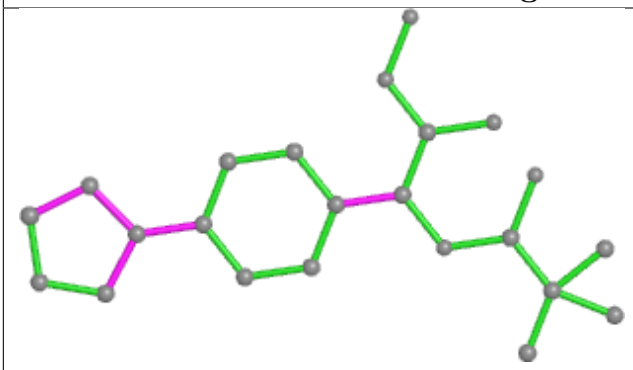

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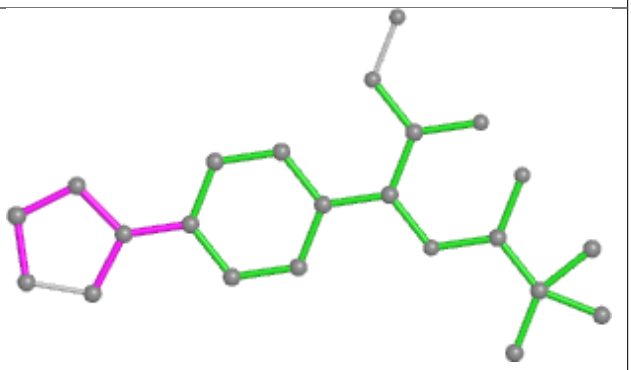

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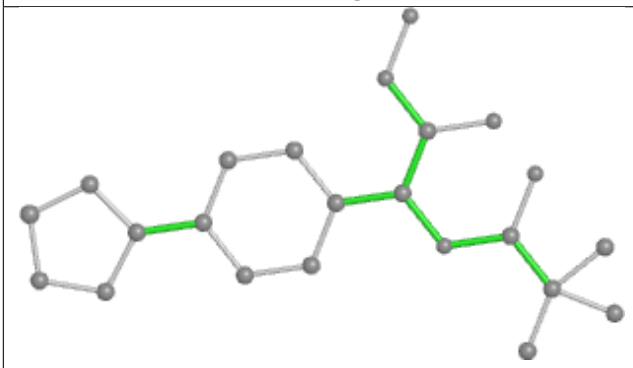

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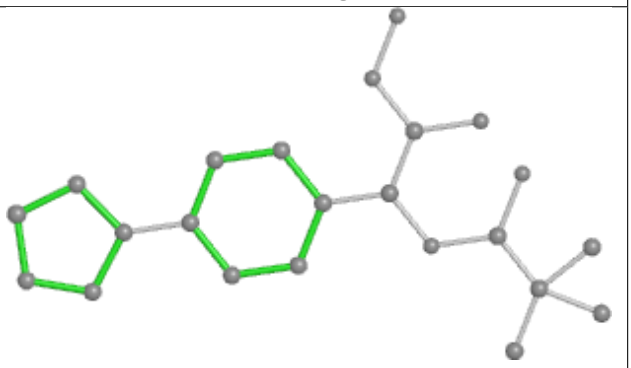
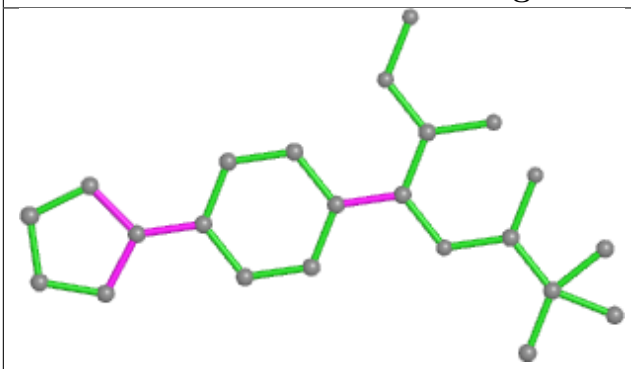


Rings

Ligand 4TM G 1001



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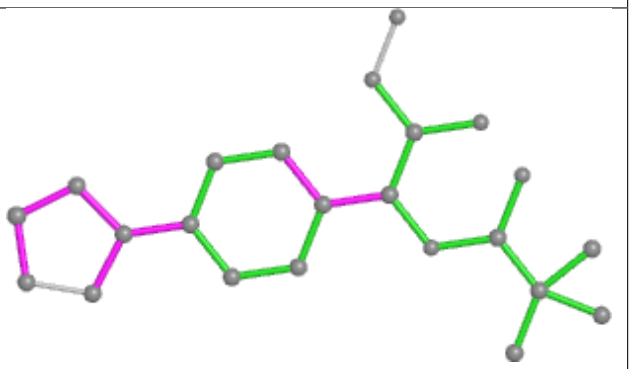
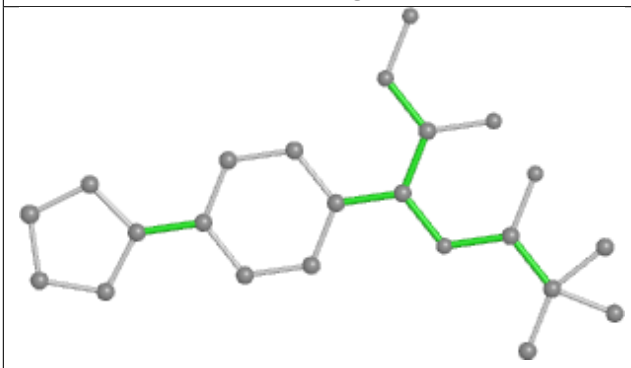


Bond angles



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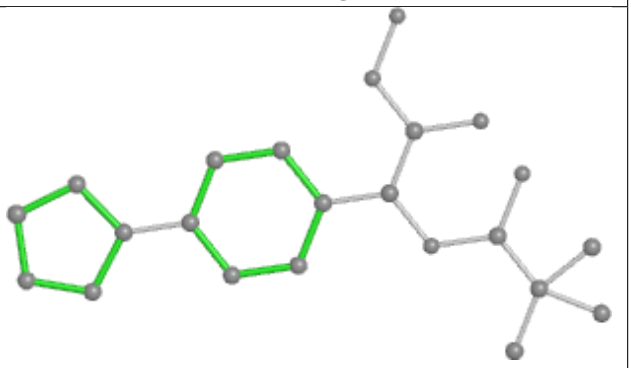
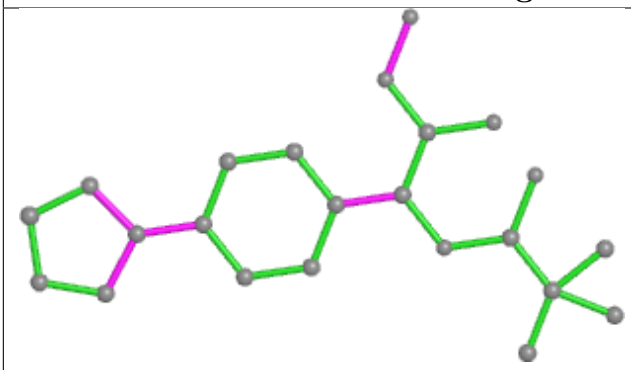


Rings

Ligand 4TM F 1001



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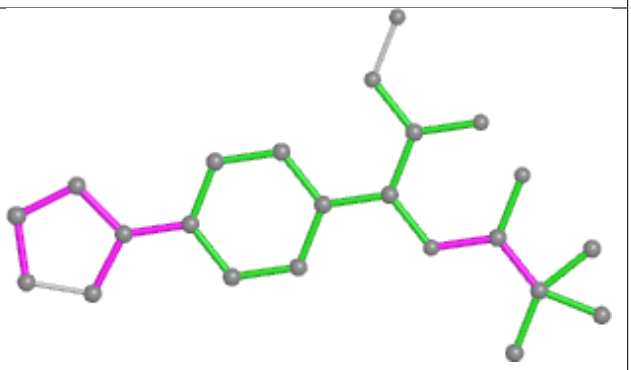

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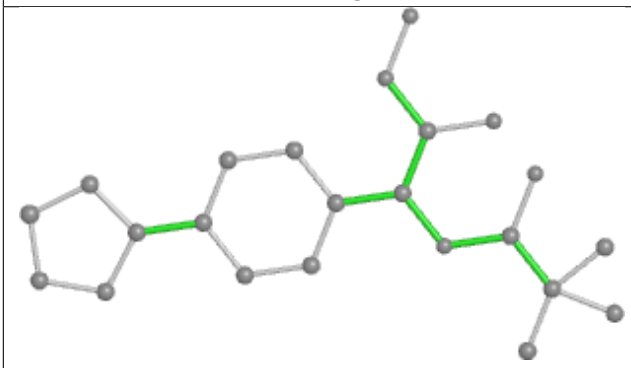

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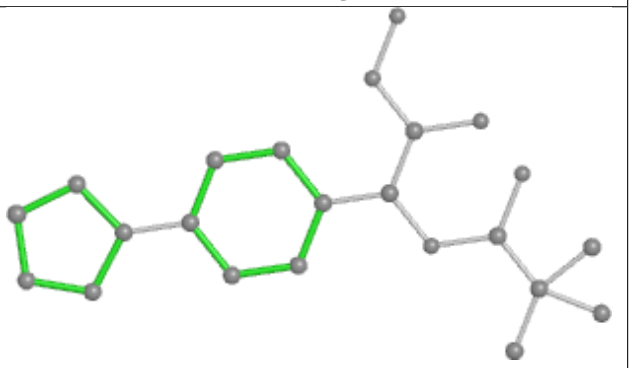
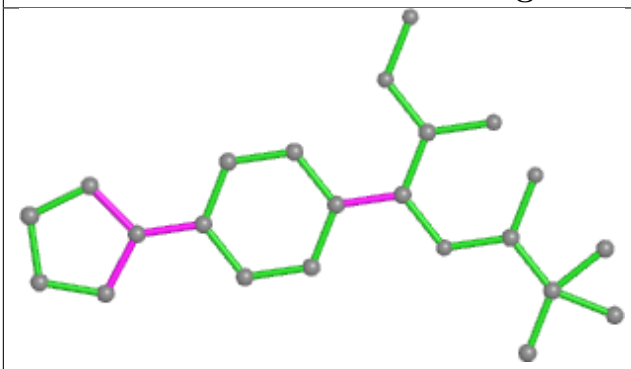


Rings

Ligand 4TM L 1001



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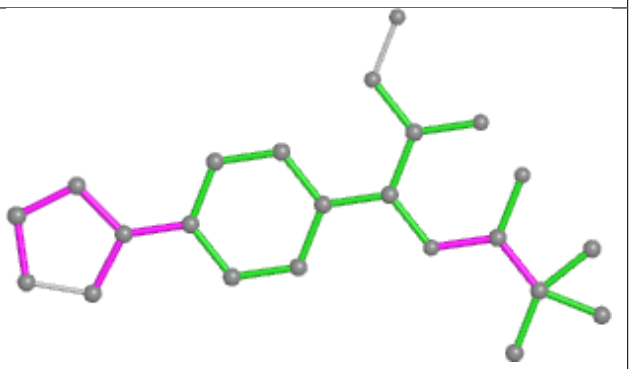
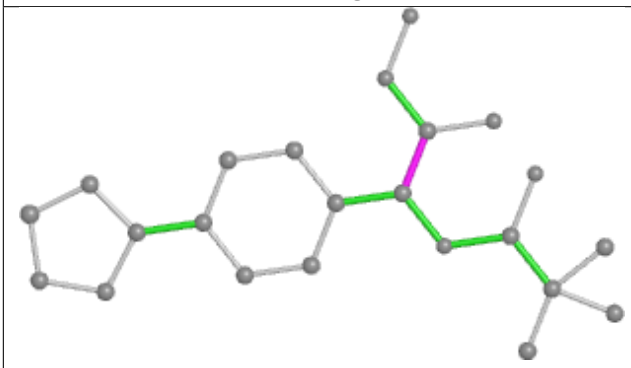


Bond angles



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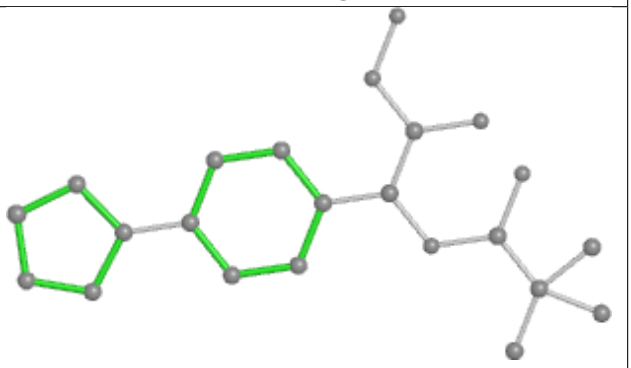
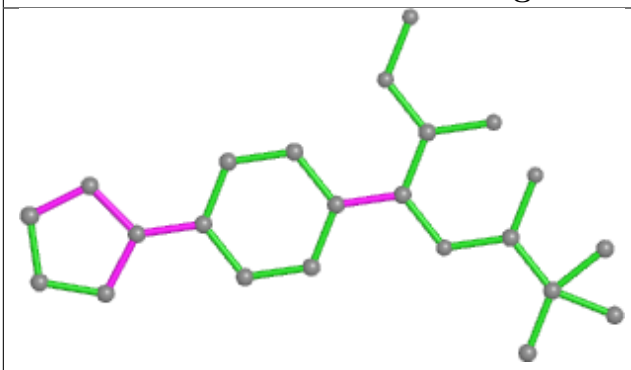
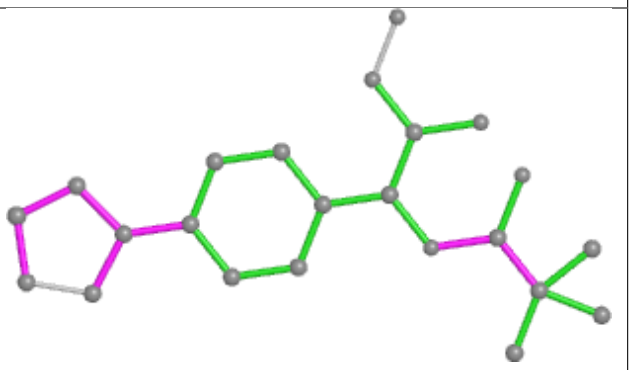


Rings

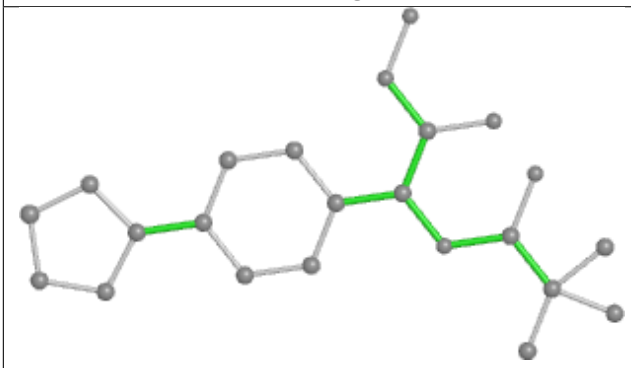
Ligand 4TM A 1001



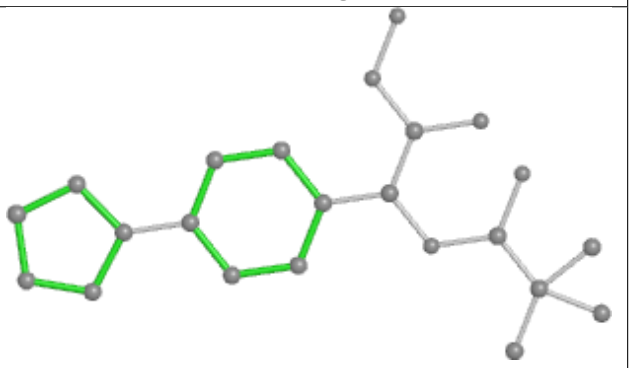
Bond lengths



Bond angles



Torsions



Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.42	5 (0%)	82	81	15, 25, 49, 95	5 (0%)
1	B	518/522 (99%)	-0.24	12 (2%)	60	58	14, 27, 66, 92	4 (0%)
1	C	517/522 (99%)	-0.39	3 (0%)	89	88	13, 25, 55, 84	5 (0%)
1	D	513/522 (98%)	-0.57	1 (0%)	95	94	16, 24, 44, 73	6 (1%)
1	E	509/522 (97%)	-0.56	2 (0%)	92	91	16, 24, 39, 77	1 (0%)
1	F	510/522 (97%)	-0.23	10 (1%)	65	63	18, 32, 62, 94	1 (0%)
1	G	519/522 (99%)	-0.44	2 (0%)	92	91	16, 24, 46, 81	3 (0%)
1	H	517/522 (99%)	-0.23	13 (2%)	57	55	16, 28, 64, 83	7 (1%)
1	I	518/522 (99%)	-0.36	4 (0%)	86	85	15, 27, 53, 102	7 (1%)
1	J	514/522 (98%)	-0.55	3 (0%)	89	88	16, 25, 46, 71	8 (1%)
1	K	508/522 (97%)	-0.54	0	100	100	16, 25, 42, 67	3 (0%)
1	L	511/522 (97%)	-0.37	4 (0%)	86	85	15, 28, 54, 106	7 (1%)
All	All	6173/6264 (98%)	-0.41	59 (0%)	82	81	13, 26, 55, 106	57 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	138	GLU	4.6
1	I	196	ALA	3.8
1	H	259	VAL	3.5
1	A	603	ASP	3.3
1	G	603	ASP	3.2
1	H	257	LYS	3.1
1	L	551	VAL	3.0
1	H	159	ASP	3.0
1	B	136	GLY	2.9
1	H	603	ASP	2.9
1	F	141	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	117	ILE	2.8
1	I	136	GLY	2.8
1	B	120	GLY	2.8
1	A	549	SER	2.7
1	B	196	ALA	2.7
1	F	128	THR	2.7
1	F	150	ASP	2.7
1	I	549	SER	2.7
1	H	118	LYS	2.6
1	F	364	ASP	2.6
1	F	549	SER	2.6
1	H	197	ASP	2.5
1	L	144	ILE	2.5
1	H	196	ALA	2.4
1	F	157	LEU	2.4
1	G	196	ALA	2.4
1	B	135	PRO	2.4
1	A	362	LYS	2.4
1	L	550	SER	2.4
1	J	136	GLY	2.4
1	F	145	SER	2.4
1	B	259	VAL	2.4
1	B	117	ILE	2.4
1	B	195	VAL	2.4
1	E	551	VAL	2.3
1	J	603	ASP	2.3
1	F	123	VAL	2.3
1	H	549	SER	2.3
1	E	550	SER	2.2
1	D	551	VAL	2.2
1	H	363	GLY	2.2
1	F	276	THR	2.2
1	B	477	GLY	2.2
1	B	603	ASP	2.1
1	F	272	ASN	2.1
1	B	153	VAL	2.1
1	C	197	ASP	2.1
1	C	194	SER	2.1
1	H	119	GLY	2.1
1	H	117	ILE	2.1
1	H	150	ASP	2.1
1	B	276	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	276	THR	2.1
1	B	178	PHE	2.1
1	J	85	ALA	2.1
1	A	550	SER	2.0
1	A	136	GLY	2.0
1	H	275	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1PE	H	1006	10/16	0.68	0.27	60,65,67,67	0
5	1PE	H	1005	10/16	0.72	0.27	43,50,59,60	0
5	1PE	D	1005	11/16	0.74	0.22	45,53,66,67	0
5	1PE	F	1005	11/16	0.76	0.22	44,59,68,68	0
5	1PE	K	1005	12/16	0.77	0.19	46,52,59,59	0
5	1PE	C	1006	12/16	0.78	0.16	50,59,61,61	0
5	1PE	E	1005	12/16	0.78	0.17	46,49,51,51	0
5	1PE	D	1006	10/16	0.81	0.20	39,45,58,59	0
7	GOL	C	1005	6/6	0.81	0.20	70,70,71,71	0
7	GOL	G	1005	6/6	0.81	0.18	57,57,57,59	0
5	1PE	J	1005	10/16	0.82	0.16	43,47,54,55	0
5	1PE	B	1005	10/16	0.83	0.24	47,54,59,59	0
5	1PE	G	1007	12/16	0.83	0.17	48,51,54,55	0
5	1PE	J	1006	10/16	0.84	0.18	37,48,55,56	0
5	1PE	F	1007	10/16	0.85	0.18	44,49,56,58	0
5	1PE	I	1006	9/16	0.86	0.13	39,39,41,43	0
5	1PE	G	1006	9/16	0.86	0.16	33,37,45,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1PE	C	1007	11/16	0.86	0.17	30,42,50,51	0
6	SO4	B	1008	5/5	0.87	0.27	81,82,83,85	0
5	1PE	A	1005	9/16	0.87	0.17	34,36,37,38	0
5	1PE	I	1005	13/16	0.87	0.17	43,45,55,55	0
5	1PE	L	1005	10/16	0.88	0.13	30,35,53,53	0
5	1PE	A	1006	6/16	0.88	0.24	48,50,53,56	0
6	SO4	H	1010	5/5	0.90	0.27	74,75,77,77	0
6	SO4	H	1008	5/5	0.90	0.23	78,79,81,82	0
6	SO4	H	1009	5/5	0.90	0.19	94,96,96,97	0
5	1PE	K	1006	12/16	0.91	0.15	38,40,55,55	0
6	SO4	K	1007	5/5	0.91	0.16	81,82,82,83	0
6	SO4	C	1009	5/5	0.92	0.20	103,103,103,104	0
6	SO4	E	1007	5/5	0.92	0.28	78,79,80,82	0
2	4TM	K	1001	23/23	0.92	0.14	20,25,41,44	0
5	1PE	A	1007	6/16	0.92	0.11	43,43,44,45	0
6	SO4	C	1010	5/5	0.93	0.17	81,81,81,83	0
5	1PE	F	1006	7/16	0.93	0.17	44,44,50,51	0
6	SO4	L	1006	5/5	0.93	0.27	79,80,80,82	0
2	4TM	I	1001	23/23	0.93	0.13	14,22,33,89	0
2	4TM	L	1001	23/23	0.93	0.11	15,22,35,40	0
6	SO4	G	1008	5/5	0.94	0.17	72,72,73,74	0
2	4TM	E	1001	23/23	0.94	0.10	16,20,32,46	0
6	SO4	A	1009	5/5	0.94	0.12	76,76,78,78	0
6	SO4	B	1007	5/5	0.94	0.14	86,87,87,88	0
6	SO4	I	1007	5/5	0.94	0.20	84,85,86,86	0
5	1PE	E	1006	12/16	0.94	0.14	33,38,49,50	0
2	4TM	B	1001	23/23	0.94	0.12	13,26,34,60	0
2	4TM	C	1001	23/23	0.94	0.13	16,24,34,39	0
2	4TM	D	1001	23/23	0.94	0.12	14,25,34,56	0
2	4TM	H	1001	23/23	0.95	0.10	13,25,32,48	0
2	4TM	F	1001	23/23	0.95	0.10	19,24,34,46	0
2	4TM	J	1001	23/23	0.95	0.12	13,21,30,55	0
6	SO4	F	1008	5/5	0.95	0.18	91,92,92,93	0
2	4TM	G	1001	23/23	0.95	0.12	15,19,32,34	0
6	SO4	L	1007	5/5	0.95	0.20	72,72,73,73	0
6	SO4	G	1009	5/5	0.95	0.09	80,81,81,81	0
6	SO4	C	1008	5/5	0.95	0.18	76,77,78,78	0
2	4TM	A	1001	23/23	0.96	0.11	14,22,32,43	0
6	SO4	E	1008	5/5	0.96	0.21	81,81,82,82	0
6	SO4	A	1008	5/5	0.97	0.12	60,60,61,61	0
4	CO3	C	1004	4/4	0.97	0.08	19,23,23,27	0
4	CO3	D	1004	4/4	0.97	0.10	23,23,24,24	0

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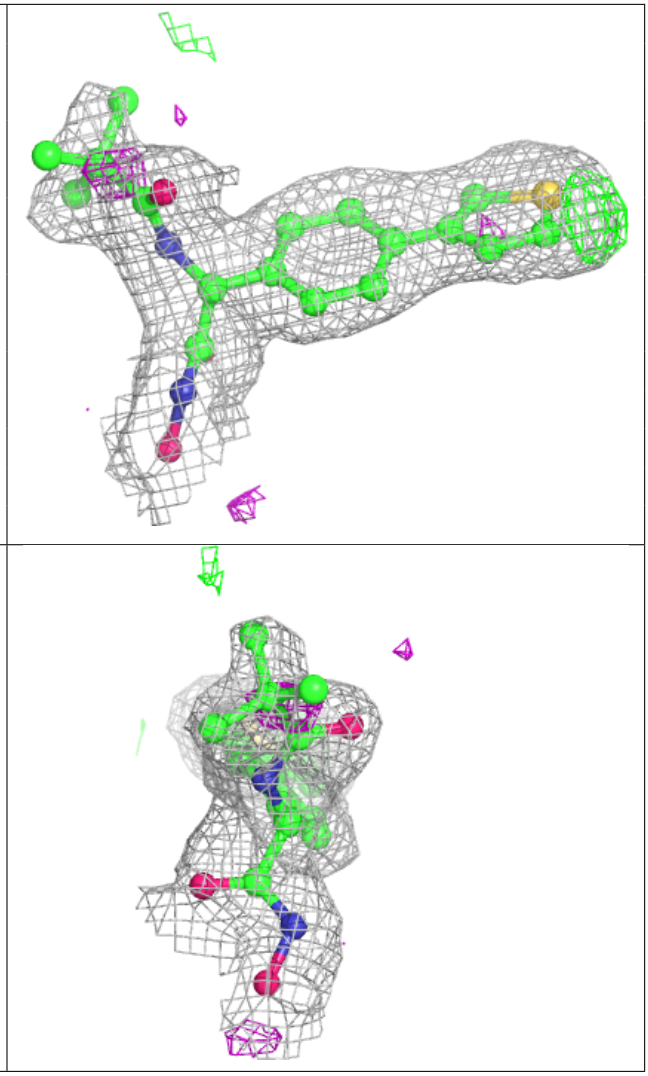
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CO3	E	1004	4/4	0.97	0.11	23,26,27,31	0
4	CO3	F	1004	4/4	0.97	0.10	22,24,24,26	0
4	CO3	G	1004	4/4	0.97	0.09	20,24,25,25	0
4	CO3	H	1004	4/4	0.97	0.10	21,23,23,25	0
6	SO4	B	1006	5/5	0.98	0.09	23,23,25,25	0
4	CO3	J	1004	4/4	0.98	0.10	23,23,23,24	0
4	CO3	K	1004	4/4	0.98	0.08	21,22,22,25	0
4	CO3	A	1004	4/4	0.98	0.10	23,24,24,25	0
4	CO3	I	1004	4/4	0.98	0.06	24,24,25,27	0
3	ZN	D	1003	1/1	0.99	0.06	24,24,24,24	0
3	ZN	E	1003	1/1	0.99	0.08	21,21,21,21	0
3	ZN	F	1002	1/1	0.99	0.10	27,27,27,27	0
3	ZN	F	1003	1/1	0.99	0.09	21,21,21,21	0
6	SO4	D	1007	5/5	0.99	0.07	25,25,25,28	0
3	ZN	H	1002	1/1	0.99	0.05	24,24,24,24	0
3	ZN	H	1003	1/1	0.99	0.07	20,20,20,20	0
3	ZN	I	1002	1/1	0.99	0.11	17,17,17,17	0
4	CO3	L	1004	4/4	0.99	0.12	22,23,23,24	0
3	ZN	I	1003	1/1	0.99	0.10	22,22,22,22	0
6	SO4	H	1007	5/5	0.99	0.07	20,21,23,24	0
3	ZN	J	1002	1/1	0.99	0.09	21,21,21,21	0
3	ZN	K	1002	1/1	0.99	0.10	21,21,21,21	0
3	ZN	K	1003	1/1	0.99	0.09	24,24,24,24	0
3	ZN	L	1002	1/1	0.99	0.08	22,22,22,22	0
6	SO4	J	1007	5/5	0.99	0.10	22,23,25,26	0
3	ZN	L	1003	1/1	0.99	0.10	22,22,22,22	0
3	ZN	A	1003	1/1	0.99	0.09	18,18,18,18	0
4	CO3	B	1004	4/4	0.99	0.07	16,18,18,22	0
3	ZN	C	1002	1/1	0.99	0.10	18,18,18,18	0
3	ZN	C	1003	1/1	0.99	0.10	23,23,23,23	0
3	ZN	G	1003	1/1	1.00	0.09	18,18,18,18	0
3	ZN	B	1003	1/1	1.00	0.06	16,16,16,16	0
3	ZN	E	1002	1/1	1.00	0.08	24,24,24,24	0
3	ZN	A	1002	1/1	1.00	0.07	19,19,19,19	0
3	ZN	B	1002	1/1	1.00	0.04	21,21,21,21	0
3	ZN	D	1002	1/1	1.00	0.09	21,21,21,21	0
3	ZN	J	1003	1/1	1.00	0.07	25,25,25,25	0
3	ZN	G	1002	1/1	1.00	0.08	23,23,23,23	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.

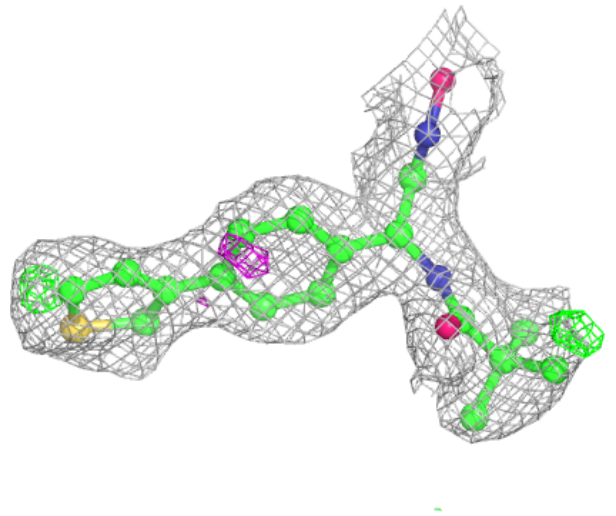
Electron density around 4TM K 1001:

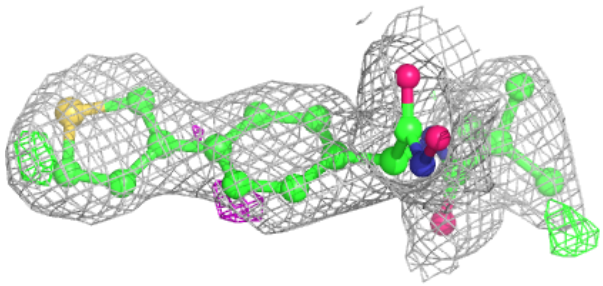
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

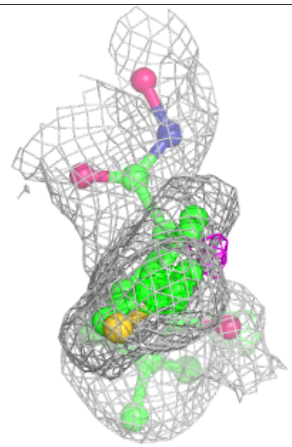


Electron density around 4TM I 1001:

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

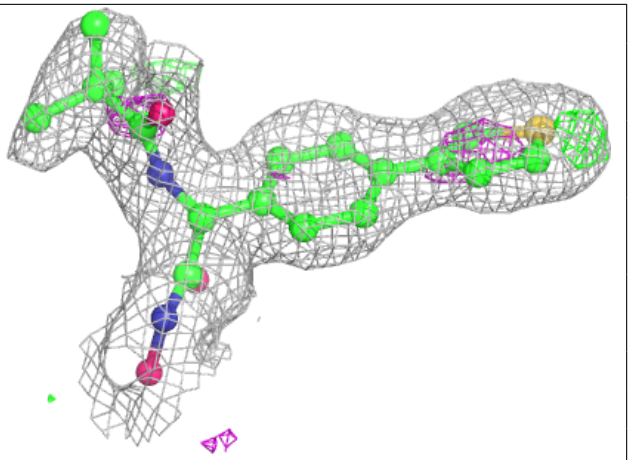


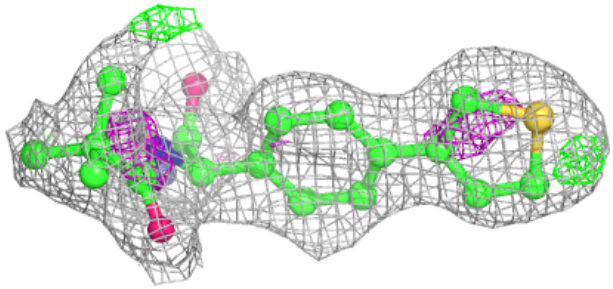


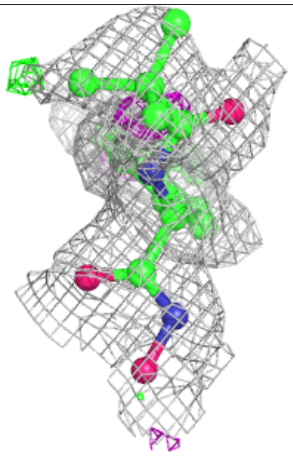


Electron density around 4TM L 1001:

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

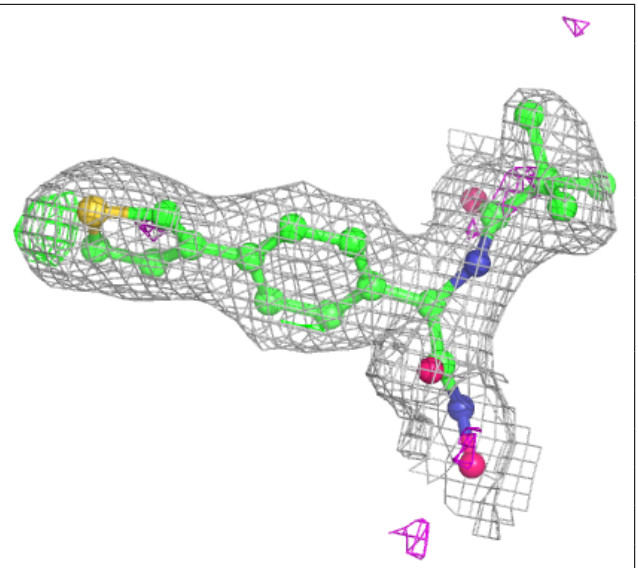


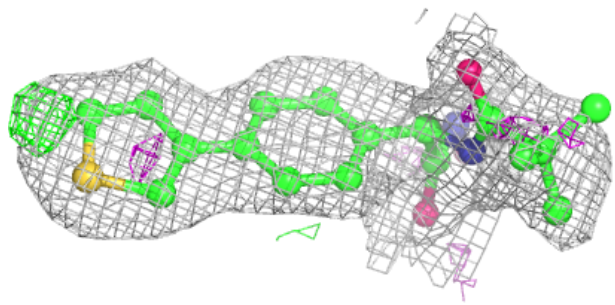




Electron density around 4TM E 1001:

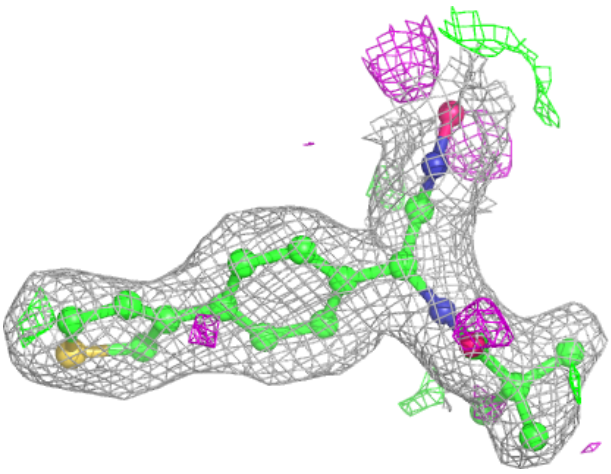
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

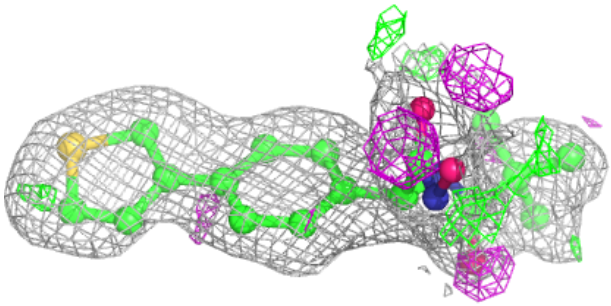


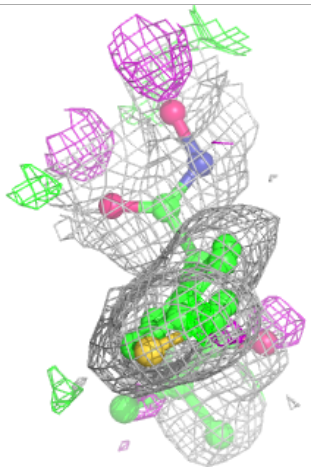


Electron density around 4TM B 1001:

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

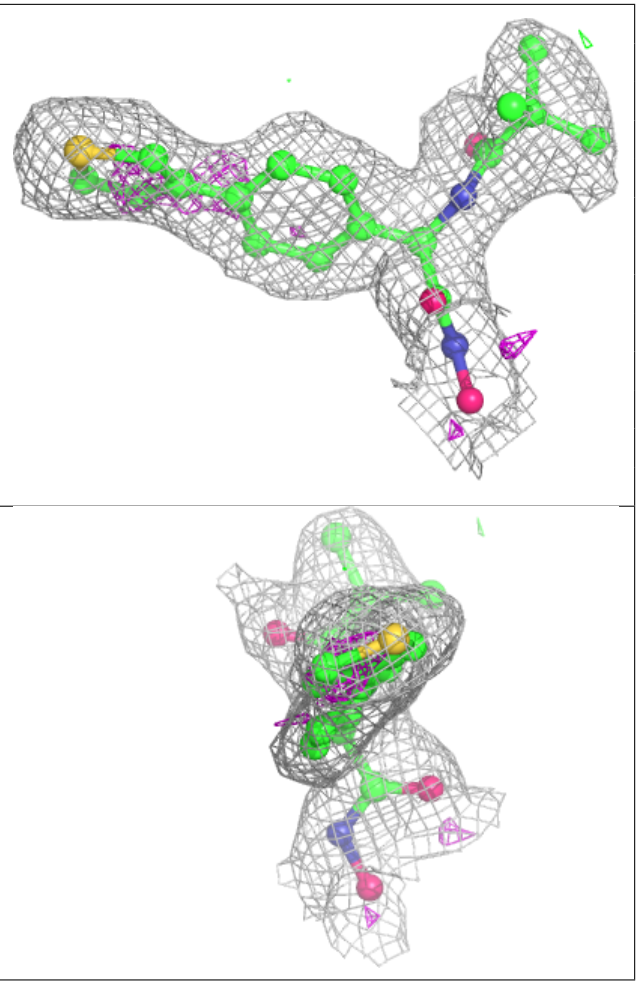






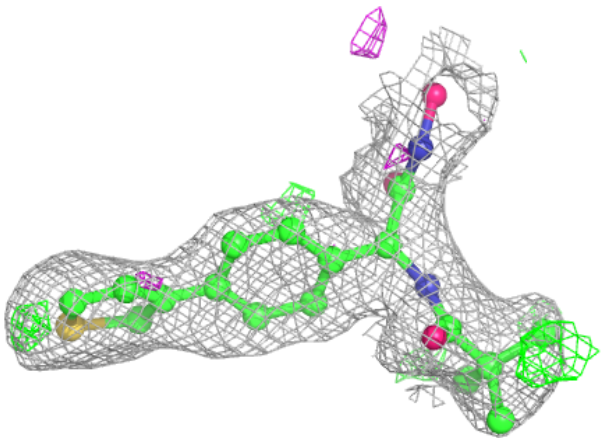
Electron density around 4TM C 1001:

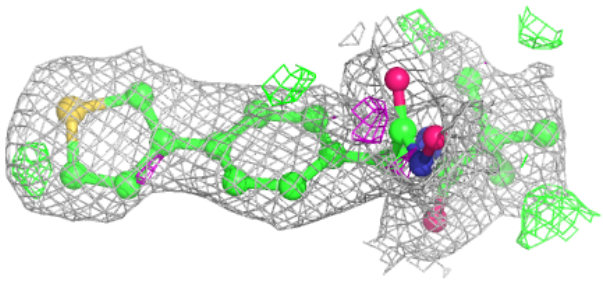
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

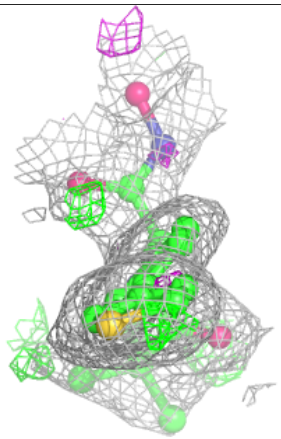


Electron density around 4TM D 1001:

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

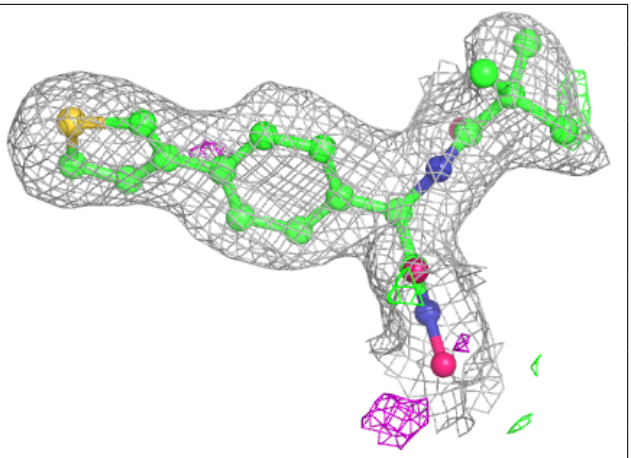


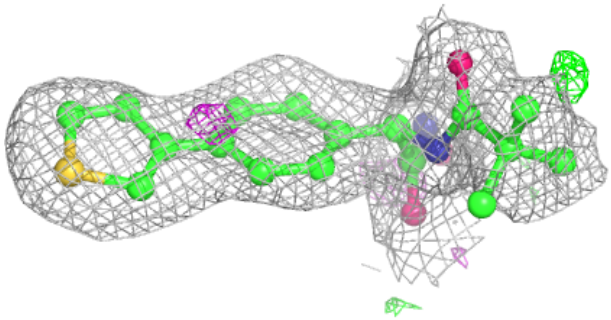


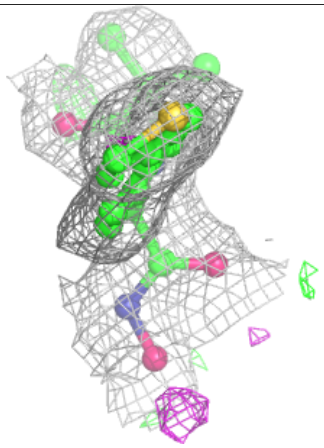


Electron density around 4TM H 1001:

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

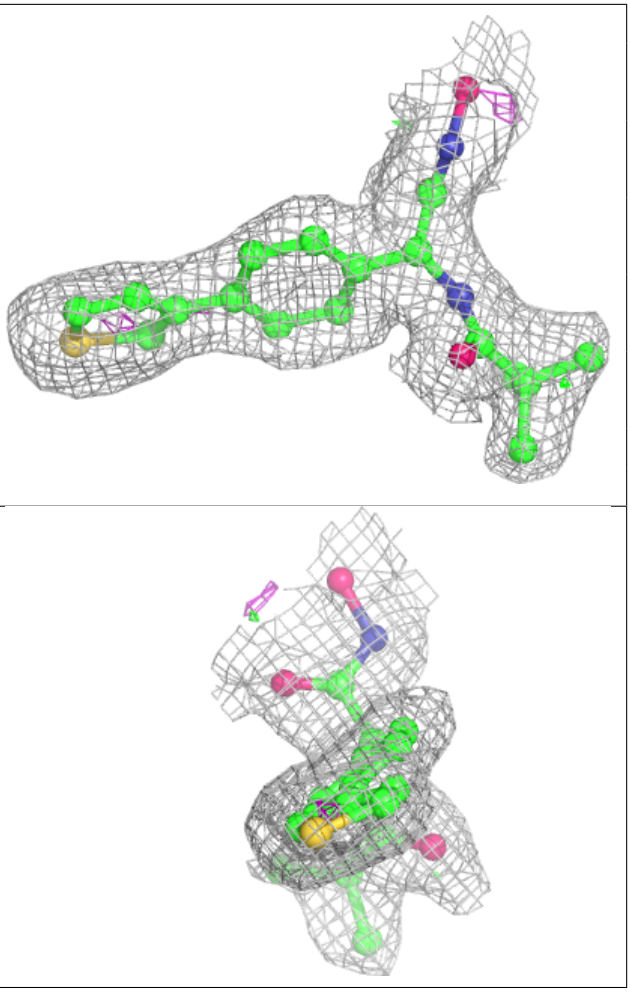






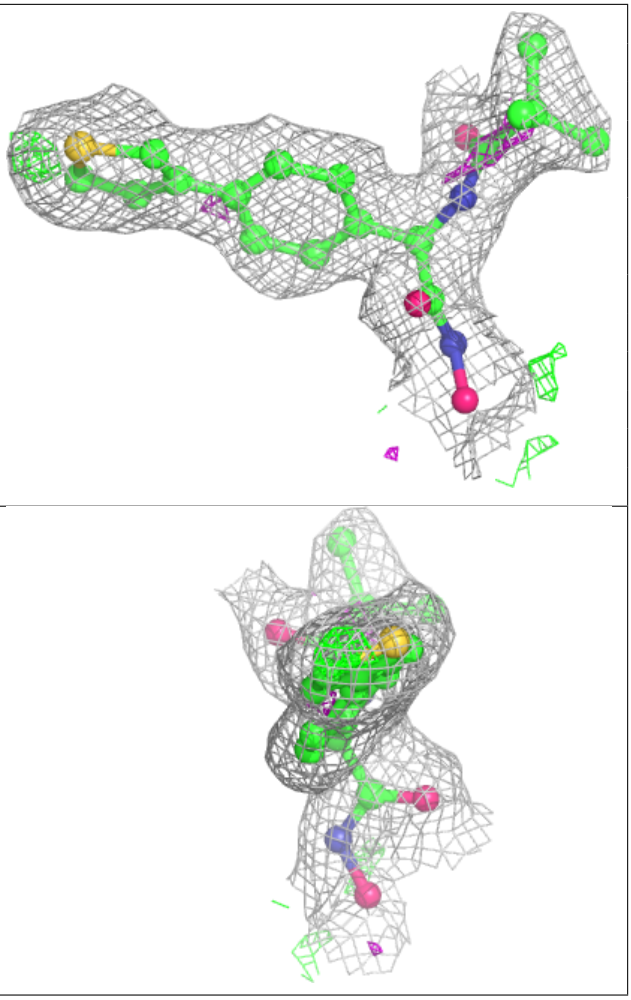
Electron density around 4TM F 1001:

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



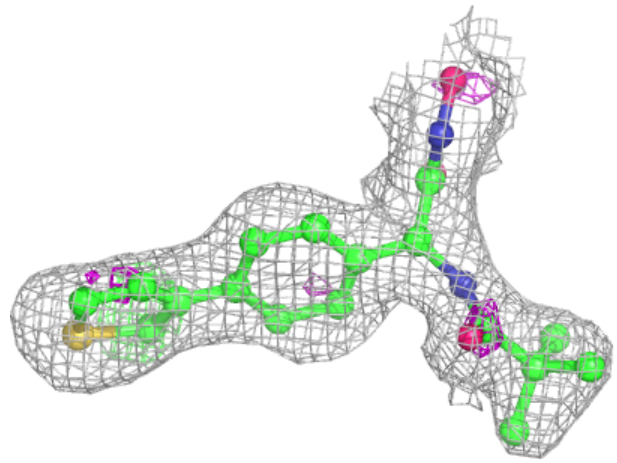
Electron density around 4TM J 1001:

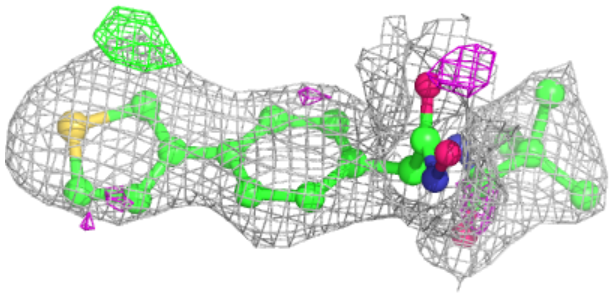
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

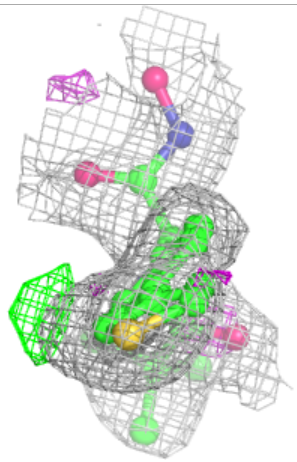


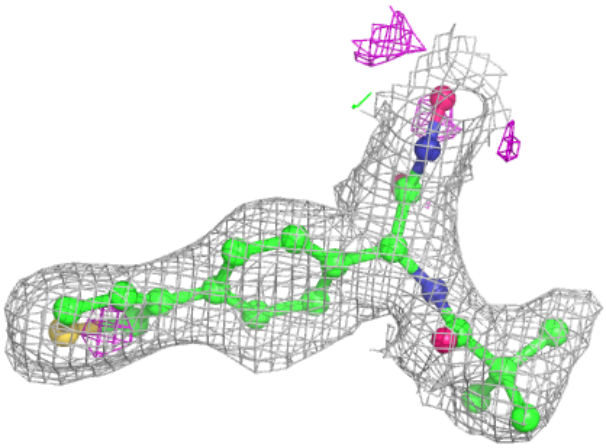
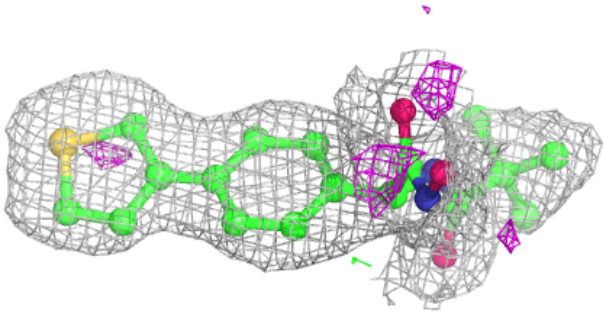
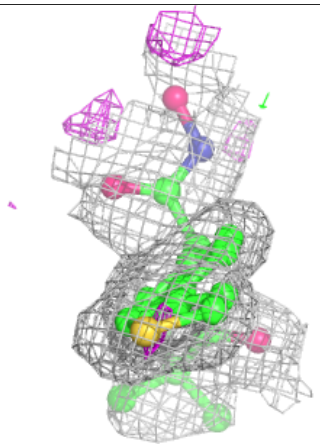
Electron density around 4TM G 1001:

$2mF_o$-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.