



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 07:34 PM EDT

PDB ID : 4ZX9
Title : X-ray crystal structure of PfA-M17 in complex with hydroxamic acid-based inhibitor 10b
Authors : Drinkwater, N.; McGowan, S.
Deposited on : 2015-05-20
Resolution : 2.60 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 : 4.02b-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

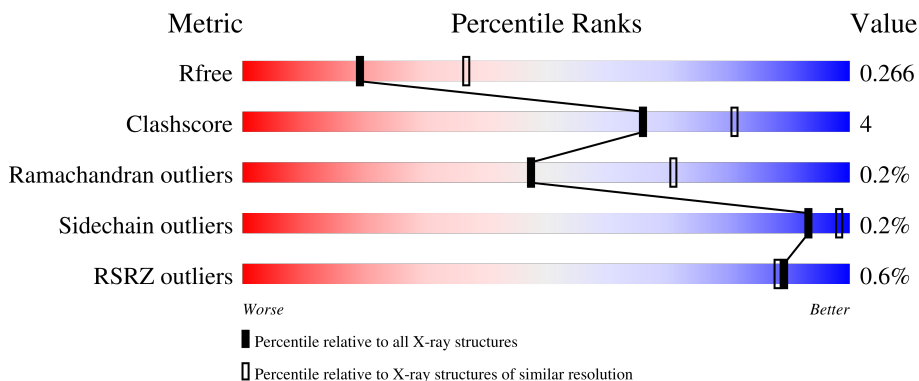
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	
1	B	522	
1	C	522	
1	D	522	
1	E	522	

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Mol	Chain	Length	Quality of chain
1	F	522	 <p>87% 11%</p>
1	G	522	 <p>92% 7%</p>
1	H	522	 <p>87% 12%</p>
1	I	522	 <p>90% 9%</p>
1	J	522	 <p>85% 12%</p>
1	K	522	 <p>87% 10%</p>
1	L	522	 <p>86% 12%</p>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 48710 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	3966	2543	637	767	19	0	0	0
1	B	516	3869	2483	630	737	19	0	0	0
1	C	517	3926	2521	633	753	19	0	0	0
1	D	513	3881	2500	628	733	20	0	0	0
1	E	509	3873	2492	622	740	19	0	0	0
1	F	511	3837	2467	618	733	19	0	0	0
1	G	519	3961	2542	638	762	19	0	0	0
1	H	517	3896	2504	633	740	19	0	0	0
1	I	518	3953	2540	636	757	20	0	0	0
1	J	512	3921	2524	632	745	20	0	0	0
1	K	508	3882	2499	626	738	19	0	0	0
1	L	511	3835	2468	619	729	19	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

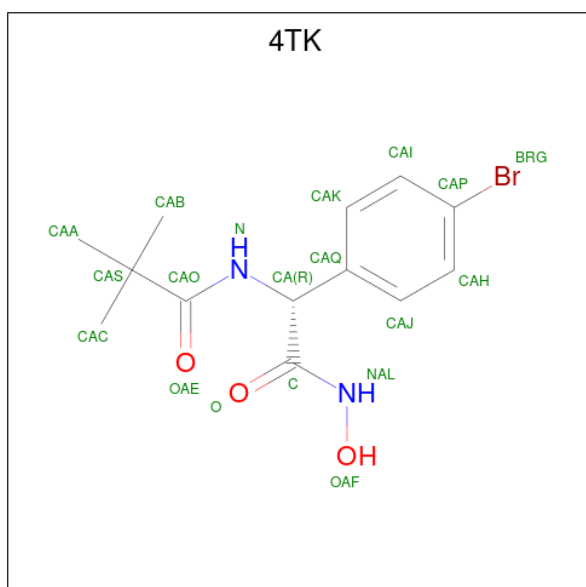
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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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)-1-(4-bromophenyl)-2-(hydroxyamino)-2-oxoethyl]-2,2-dimethylpropanamide (three-letter code: 4TK) (formula: C₁₃H₁₇BrN₂O₃).

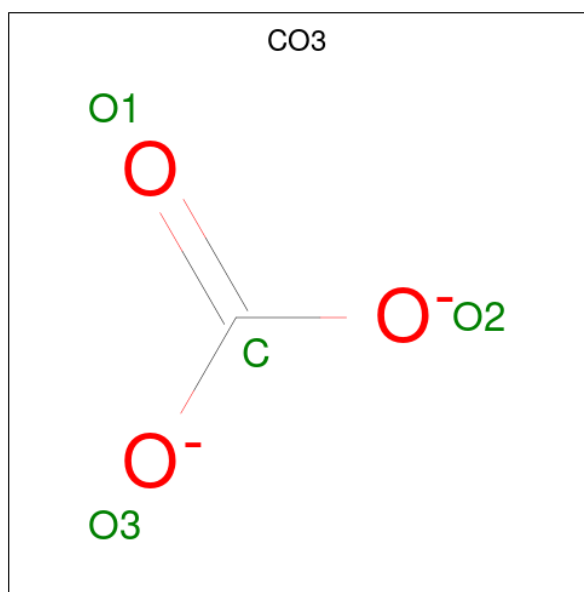


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
2	A	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	B	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	C	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	D	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	E	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	F	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	G	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	H	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	I	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	J	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	K	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		
2	L	1	Total	Br	C	N	O	0	0
			19	1	13	2	3		

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

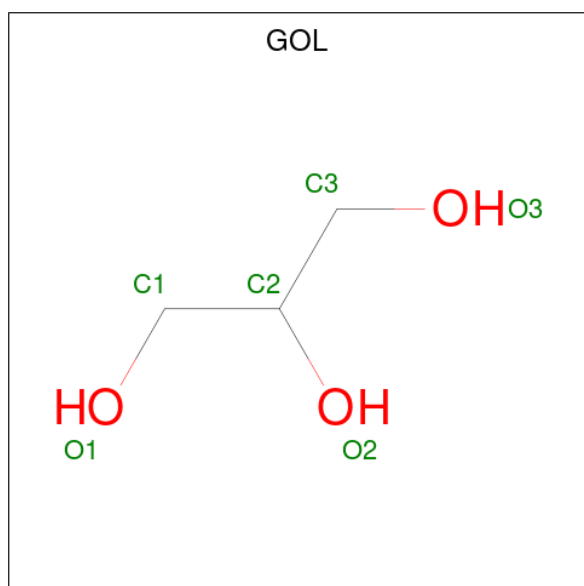
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0
3	J	2	Total Zn 2 2	0	0
3	K	2	Total Zn 2 2	0	0
3	L	2	Total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

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



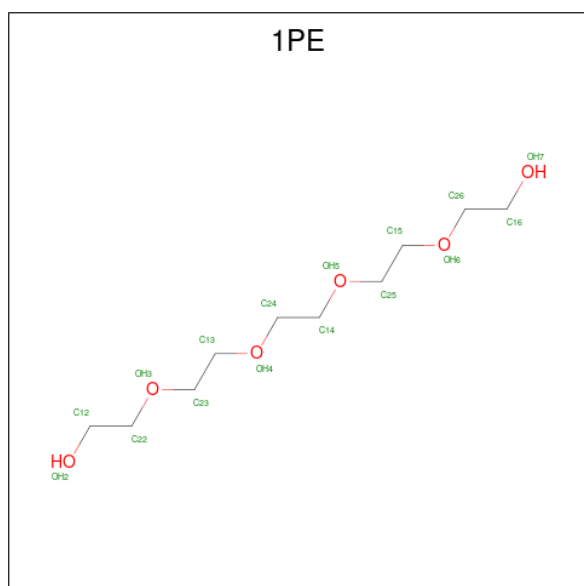
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 1 3	0	0
4	B	1	Total C O 4 1 3	0	0
4	C	1	Total C O 4 1 3	0	0
4	D	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0
4	G	1	Total C O 4 1 3	0	0
4	H	1	Total C O 4 1 3	0	0
4	I	1	Total C O 4 1 3	0	0
4	J	1	Total C O 4 1 3	0	0
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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



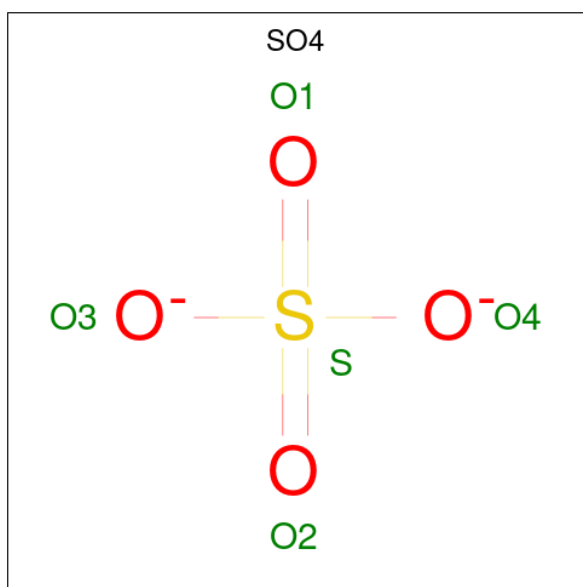
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 6 3	0	0
6	A	1	Total C O 12 8 4	0	0
6	B	1	Total C O 10 7 3	0	0
6	C	1	Total C O 13 9 4	0	0
6	C	1	Total C O 9 6 3	0	0
6	D	1	Total C O 10 7 3	0	0
6	D	1	Total C O 10 7 3	0	0

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	I	1	Total	O	S	0	0
			5	4	1		
7	I	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	O	S	0	0
			4	2	1	1		
8	D	1	Total	C	O	S	0	0
			4	2	1	1		
8	G	1	Total	C	O	S	0	0
			4	2	1	1		
8	I	1	Total	C	O	S	0	0
			4	2	1	1		
8	J	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	119	Total	O	0	0
			119	119		
9	B	109	Total	O	0	0
			109	109		
9	C	90	Total	O	0	0
			90	90		
9	D	86	Total	O	0	0
			86	86		
9	E	131	Total	O	0	0
			131	131		
9	F	79	Total	O	0	0
			79	79		
9	G	120	Total	O	0	0
			120	120		

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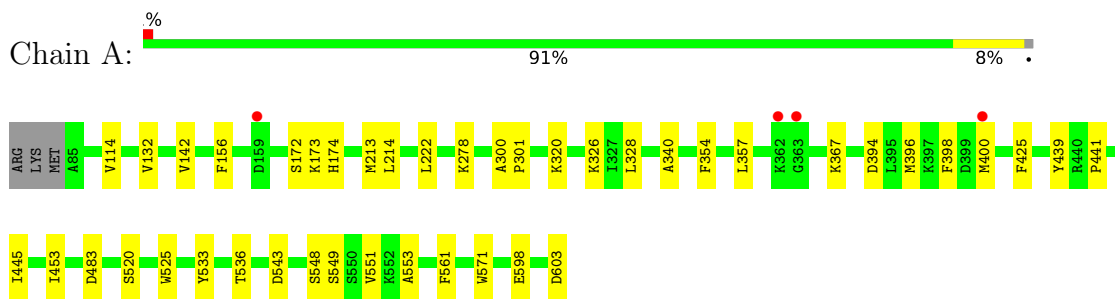
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	102	Total 102	O 102	0	0
9	I	116	Total 116	O 116	0	0
9	J	104	Total 104	O 104	0	0
9	K	150	Total 150	O 150	0	0
9	L	99	Total 99	O 99	0	0

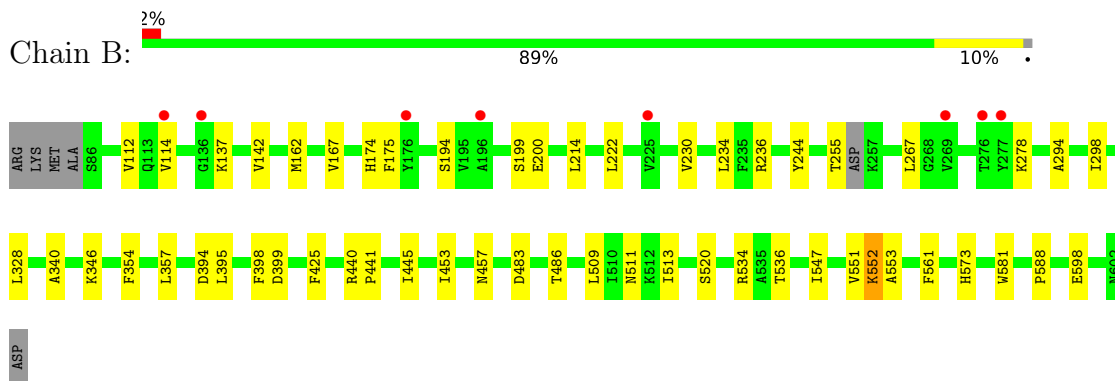
3 Residue-property plots [i](#)

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.

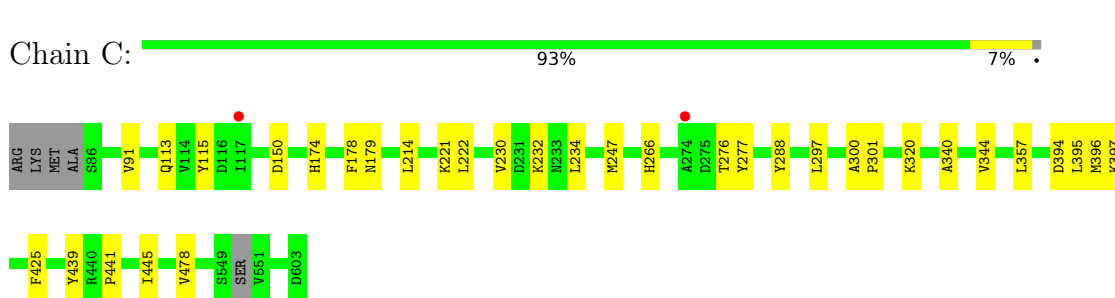
- Molecule 1: Probable M17 family aminopeptidase



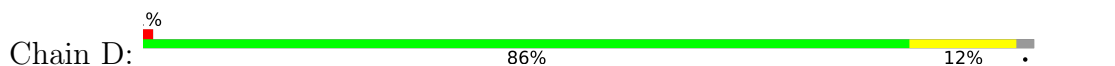
- Molecule 1: Probable M17 family aminopeptidase

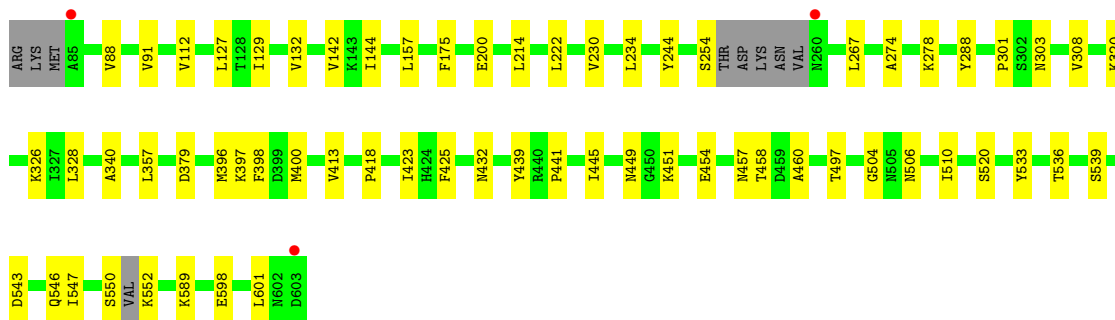


- Molecule 1: Probable M17 family aminopeptidase



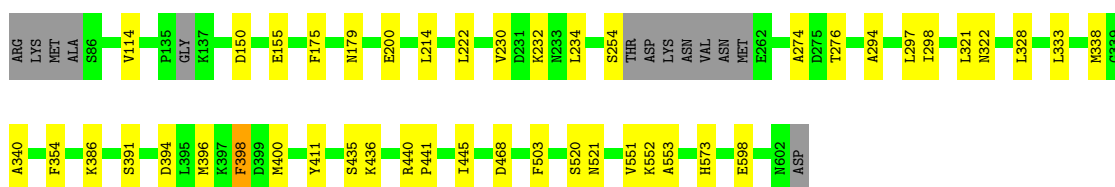
- Molecule 1: Probable M17 family aminopeptidase





- Molecule 1: Probable M17 family aminopeptidase

Chain E: 89% 8%



- Molecule 1: Probable M17 family aminopeptidase

Chain F: 87% 11%



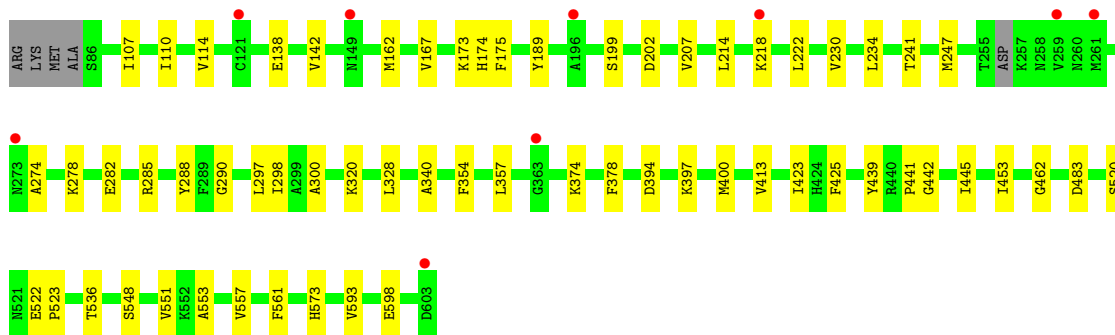
- Molecule 1: Probable M17 family aminopeptidase

Chain G: 92% 7%

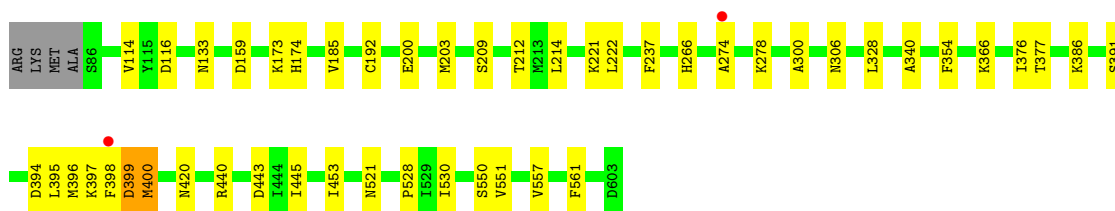
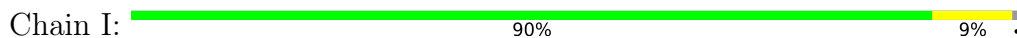


- Molecule 1: Probable M17 family aminopeptidase

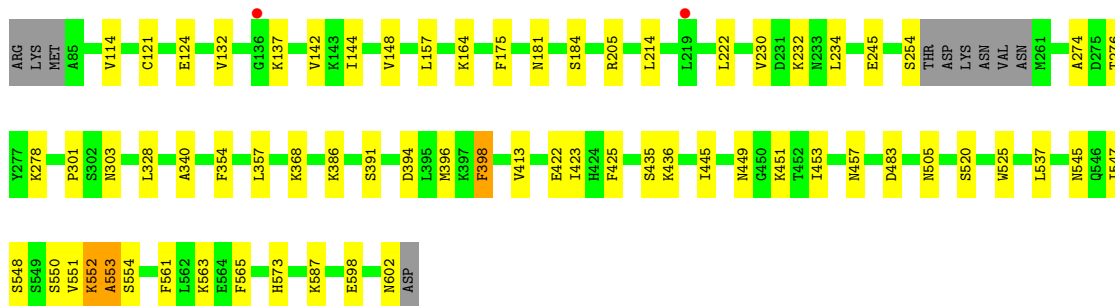
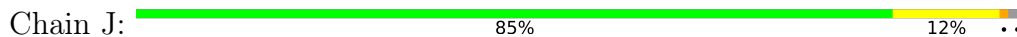
Chain H: 87% 12%



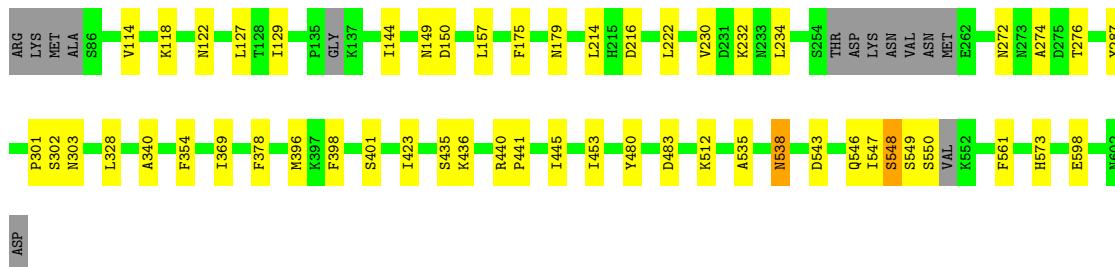
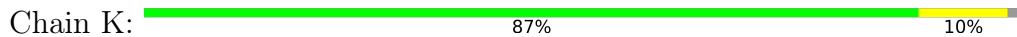
• Molecule 1: Probable M17 family aminopeptidase



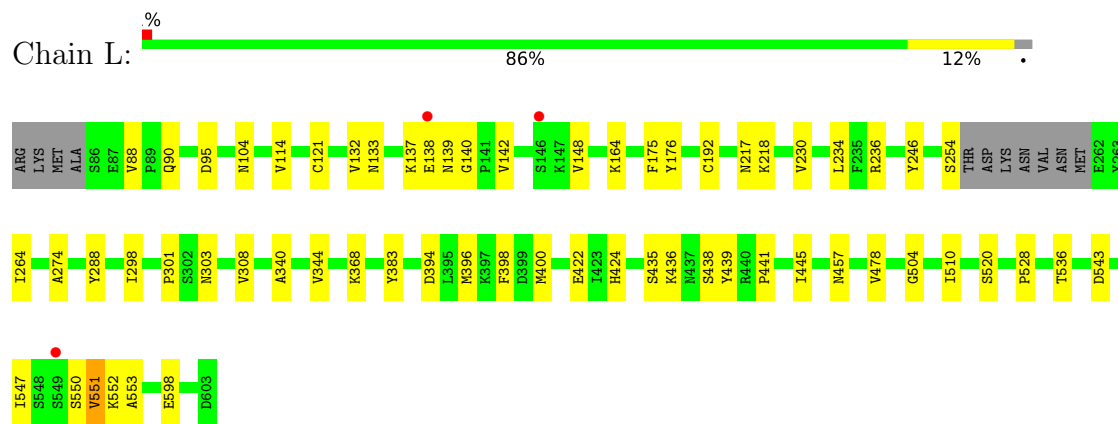
• Molecule 1: Probable M17 family aminopeptidase



• Molecule 1: Probable M17 family aminopeptidase



• Molecule 1: Probable M17 family aminopeptidase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.85Å 176.97Å 229.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.74 – 2.60 48.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (46.74-2.60) 77.1 (48.48-2.60)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.221 , 0.267 0.223 , 0.266	Depositor DCC
R_{free} test set	9762 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtrriage
Anisotropy	0.802	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	48710	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.32 % 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 1.0098e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4TK, SO4, ZN, 1PE, DMS, GOL, 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	0.21	0/4044	0.38	0/5492
1	B	0.21	0/3946	0.37	0/5369
1	C	0.22	0/4003	0.37	0/5437
1	D	0.22	0/3957	0.38	0/5372
1	E	0.21	0/3949	0.37	0/5361
1	F	0.22	0/3913	0.39	0/5322
1	G	0.22	0/4039	0.38	0/5485
1	H	0.22	0/3973	0.38	0/5400
1	I	0.23	0/4031	0.39	0/5472
1	J	0.21	0/3998	0.37	0/5422
1	K	0.22	0/3957	0.39	0/5366
1	L	0.23	0/3912	0.39	0/5322
All	All	0.22	0/47722	0.38	0/64820

There are no bond length outliers.

There are no bond angle outliers.

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	3966	0	3862	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3869	0	3717	37	0
1	C	3926	0	3809	24	0
1	D	3881	0	3788	41	0
1	E	3873	0	3773	28	0
1	F	3837	0	3685	36	0
1	G	3961	0	3862	28	0
1	H	3896	0	3768	41	0
1	I	3953	0	3857	30	0
1	J	3921	0	3860	40	0
1	K	3882	0	3802	35	0
1	L	3835	0	3696	39	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	1	0
2	D	19	0	0	1	0
2	E	19	0	0	0	0
2	F	19	0	0	1	0
2	G	19	0	0	0	0
2	H	19	0	0	0	0
2	I	19	0	0	0	0
2	J	19	0	0	0	0
2	K	19	0	0	0	0
2	L	19	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	1	0
4	D	4	0	0	1	0
4	E	4	0	0	0	0
4	F	4	0	0	1	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	6	0	8	0	0
5	B	6	0	8	0	0
5	G	6	0	8	0	0
5	I	6	0	8	1	0
5	J	6	0	8	0	0
6	A	21	0	22	2	0
6	B	10	0	10	0	0
6	C	22	0	24	2	0
6	D	20	0	20	1	0
6	E	24	0	28	0	0
6	F	10	0	13	0	0
6	G	21	0	20	2	0
6	H	16	0	16	2	0
6	I	23	0	26	0	0
6	J	11	0	13	0	0
6	K	12	0	14	0	0
6	L	10	0	13	1	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	D	5	0	0	0	0
7	G	10	0	0	1	0
7	H	5	0	0	0	0
7	I	10	0	0	0	0
7	J	10	0	0	1	0
7	L	5	0	0	1	0
8	C	4	0	6	0	0
8	D	4	0	6	1	0
8	G	4	0	6	1	0
8	I	4	0	6	0	0
8	J	4	0	6	0	0
9	A	119	0	0	1	0
9	B	109	0	0	6	0
9	C	90	0	0	3	0
9	D	86	0	0	0	0
9	E	131	0	0	1	0
9	F	79	0	0	3	0
9	G	120	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	102	0	0	2	0
9	I	116	0	0	3	0
9	J	104	0	0	1	0
9	K	150	0	0	1	0
9	L	99	0	0	1	0
All	All	48710	0	45768	376	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 4.

All (376) 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:K:538:ASN:H	1:K:538:ASN:HD22	1.11	0.95
1:G:398:PHE:HE1	1:G:580:SER:HB3	1.31	0.92
1:L:176:TYR:OH	1:L:217:ASN:ND2	2.09	0.84
1:D:432:ASN:OD1	1:D:439:TYR:OH	1.96	0.82
1:K:538:ASN:HD22	1:K:538:ASN:N	1.77	0.82
1:G:551:VAL:HG21	1:G:557:VAL:HG21	1.63	0.80
1:B:553:ALA:O	9:B:1101:HOH:O	2.02	0.77
1:H:218:LYS:HE3	1:L:164:LYS:HA	1.69	0.75
1:L:550:SER:OG	1:L:551:VAL:N	2.20	0.73
1:C:320:LYS:HZ1	6:C:1006:1PE:H142	1.53	0.71
1:G:398:PHE:CE1	1:G:580:SER:HB3	2.21	0.70
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.56	0.70
1:I:366:LYS:HG3	1:I:420:ASN:HB3	1.74	0.69
1:C:232:LYS:NZ	1:C:276:THR:O	2.27	0.68
1:G:132:VAL:HG21	1:G:142:VAL:HG13	1.76	0.67
1:F:551:VAL:HA	1:F:552:LYS:HB2	1.77	0.67
1:B:114:VAL:O	1:B:278:LYS:NZ	2.28	0.66
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.76	0.66
1:J:551:VAL:O	1:J:553:ALA:N	2.29	0.66
1:L:536:THR:HG21	1:L:551:VAL:HG21	1.78	0.65
1:G:512:LYS:NZ	8:G:1006:DMS:O	2.29	0.65
1:H:300:ALA:O	9:H:1101:HOH:O	2.14	0.65
1:H:214:LEU:HD21	1:H:222:LEU:HD22	1.79	0.65
1:E:230:VAL:HG13	1:E:234:LEU:HB3	1.79	0.64
1:J:254:SER:OG	1:L:543:ASP:OD2	2.14	0.64
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.79	0.64
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.80	0.64
1:K:535:ALA:HA	1:K:538:ASN:HD21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:PRO:O	1:F:311:SER:OG	2.14	0.64
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.78	0.64
1:L:422:GLU:OE1	1:L:424:HIS:NE2	2.31	0.64
1:I:300:ALA:O	9:I:1101:HOH:O	2.15	0.64
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.80	0.64
1:H:110:ILE:O	1:H:285:ARG:NH2	2.30	0.64
1:K:232:LYS:NZ	1:K:276:THR:O	2.32	0.63
1:I:530:ILE:HA	5:I:1005:GOL:H31	1.79	0.63
1:A:551:VAL:HG12	1:A:553:ALA:H	1.64	0.62
1:E:232:LYS:NZ	1:E:276:THR:O	2.31	0.62
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.82	0.62
1:K:535:ALA:O	1:K:538:ASN:ND2	2.32	0.62
1:A:173:LYS:NZ	9:A:1105:HOH:O	2.33	0.62
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.81	0.62
1:D:379:ASP:OD1	1:D:432:ASN:ND2	2.22	0.62
1:E:551:VAL:O	1:E:553:ALA:N	2.33	0.62
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.82	0.62
1:I:395:LEU:O	1:I:397:LYS:N	2.31	0.61
1:D:379:ASP:HA	1:D:432:ASN:HB3	1.81	0.61
1:A:533:TYR:O	1:A:536:THR:HG22	2.01	0.61
1:G:164:LYS:NZ	7:J:1008:SO4:O2	2.33	0.61
1:E:440:ARG:NH2	9:E:1104:HOH:O	2.34	0.60
1:H:297:LEU:HB3	1:H:400:MET:HE1	1.82	0.60
1:K:538:ASN:N	1:K:538:ASN:ND2	2.45	0.60
1:I:551:VAL:HG21	1:I:557:VAL:HG21	1.83	0.60
1:G:483:ASP:OD1	1:G:573:HIS:ND1	2.31	0.60
1:D:88:VAL:HG12	1:D:308:VAL:HB	1.84	0.60
1:J:232:LYS:NZ	1:J:276:THR:O	2.34	0.60
1:H:114:VAL:O	1:H:278:LYS:NZ	2.34	0.60
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.83	0.60
1:I:306:ASN:ND2	9:I:1104:HOH:O	2.33	0.59
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.83	0.59
1:E:338:MET:HE3	1:E:468:ASP:HB3	1.84	0.59
1:G:411:TYR:HE1	6:G:1007:1PE:H132	1.67	0.59
1:B:440:ARG:NH1	9:B:1104:HOH:O	2.34	0.59
1:K:483:ASP:OD1	1:K:573:HIS:ND1	2.32	0.59
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.85	0.59
1:A:548:SER:OG	1:A:549:SER:N	2.36	0.59
1:L:368:LYS:HG2	1:L:478:VAL:HA	1.85	0.59
1:G:550:SER:O	1:G:552:LYS:N	2.31	0.59
1:L:114:VAL:HG12	1:L:274:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.85	0.58
1:F:357:LEU:HB2	1:F:425:PHE:HB2	1.84	0.58
1:J:124:GLU:OE2	1:J:181:ASN:ND2	2.36	0.58
1:G:395:LEU:O	1:G:398:PHE:HB3	2.03	0.58
1:B:114:VAL:HB	1:B:278:LYS:HZ3	1.69	0.58
1:F:396:MET:SD	1:F:398:PHE:HE2	2.27	0.58
1:F:480:TYR:OH	1:F:512:LYS:NZ	2.34	0.57
1:H:282:GLU:OE1	1:H:285:ARG:NH1	2.37	0.57
1:H:199:SER:OG	1:H:202:ASP:OD2	2.19	0.57
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.87	0.57
1:C:395:LEU:O	1:C:397:LYS:N	2.37	0.57
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.87	0.56
1:G:440:ARG:NH1	9:G:1110:HOH:O	2.37	0.56
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.86	0.56
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.87	0.56
1:D:504:GLY:HA3	1:D:510:ILE:HD11	1.86	0.56
1:E:520:SER:HB3	1:E:598:GLU:HG3	1.87	0.56
1:I:377:THR:O	9:I:1102:HOH:O	2.18	0.56
1:H:551:VAL:HG12	1:H:553:ALA:H	1.69	0.56
1:F:114:VAL:O	1:F:278:LYS:NZ	2.39	0.55
7:G:1011:SO4:O4	1:J:164:LYS:NZ	2.34	0.55
1:F:440:ARG:NH2	9:F:1108:HOH:O	2.39	0.55
1:H:320:LYS:HZ3	6:H:1006:1PE:H142	1.72	0.55
1:J:205:ARG:NH1	9:J:1107:HOH:O	2.39	0.55
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.70	0.55
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.89	0.55
1:B:175:PHE:HD1	1:F:176:TYR:HB2	1.72	0.54
1:D:320:LYS:HZ1	6:D:1006:1PE:H142	1.70	0.54
1:D:439:TYR:CE1	1:D:458:THR:HB	2.42	0.54
1:B:520:SER:HB3	1:B:598:GLU:HG3	1.88	0.54
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.90	0.54
1:C:221:LYS:HG3	1:C:266:HIS:HB2	1.89	0.54
1:J:245:GLU:OE1	1:J:587:LYS:NZ	2.30	0.54
1:F:361:SER:OG	1:F:418:PRO:O	2.20	0.54
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.89	0.54
1:F:150:ASP:OD2	1:F:179:ASN:HB2	2.06	0.54
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.88	0.54
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.88	0.53
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.89	0.53
1:G:244:TYR:HA	1:G:288:TYR:HE1	1.71	0.53
1:L:104:ASN:ND2	7:L:1006:SO4:O2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:ASP:OD1	1:I:159:ASP:N	2.41	0.53
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.91	0.53
1:J:368:LYS:HG2	1:J:422:GLU:HB3	1.91	0.53
1:I:221:LYS:HG3	1:I:266:HIS:HB2	1.90	0.53
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.89	0.53
1:C:344:VAL:HA	1:C:439:TYR:CE2	2.43	0.53
1:J:230:VAL:HG12	1:J:234:LEU:HD23	1.91	0.53
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.90	0.53
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.91	0.53
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.91	0.53
1:D:550:SER:O	1:D:552:LYS:N	2.42	0.52
1:I:398:PHE:C	1:I:400:MET:H	2.12	0.52
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.91	0.52
1:L:133:ASN:HB3	1:L:192:CYS:HB2	1.91	0.52
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.91	0.52
1:H:142:VAL:HG23	1:H:162:MET:HB3	1.90	0.52
1:E:333:LEU:HD21	1:E:354:PHE:HB2	1.90	0.52
1:F:364:ASP:OD1	1:F:420:ASN:ND2	2.43	0.52
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.91	0.52
1:C:113:GLN:OE1	1:C:115:TYR:OH	2.23	0.52
1:C:230:VAL:O	1:C:277:TYR:OH	2.20	0.52
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.92	0.52
1:F:254:SER:OG	1:F:255:THR:N	2.41	0.52
1:A:398:PHE:C	1:A:400:MET:H	2.13	0.52
1:C:357:LEU:HB2	1:C:425:PHE:HB2	1.90	0.51
1:J:449:ASN:HD21	1:J:451:LYS:HD2	1.75	0.51
1:I:200:GLU:OE1	1:I:200:GLU:N	2.31	0.51
1:F:344:VAL:HA	1:F:439:TYR:CE2	2.45	0.51
1:B:511:ASN:ND2	9:B:1110:HOH:O	2.38	0.51
1:H:114:VAL:HG12	1:H:274:ALA:HB1	1.92	0.51
1:C:297:LEU:O	9:C:1101:HOH:O	2.19	0.51
1:E:214:LEU:HD21	1:E:222:LEU:HD22	1.93	0.51
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.92	0.51
1:K:214:LEU:HD11	1:K:222:LEU:HD22	1.93	0.51
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.91	0.50
2:C:1001:4TK:NAL	4:C:1004:CO3:O3	2.44	0.50
1:L:88:VAL:HG22	1:L:308:VAL:HB	1.92	0.50
1:A:326:LYS:HE3	1:A:328:LEU:HD11	1.94	0.50
1:D:357:LEU:HB2	1:D:425:PHE:HB2	1.92	0.50
1:C:247:MET:HG3	1:C:288:TYR:OH	2.10	0.50
1:J:483:ASP:OD1	1:J:573:HIS:ND1	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.93	0.50
1:L:344:VAL:HA	1:L:439:TYR:CE2	2.47	0.50
1:A:320:LYS:HZ1	6:A:1007:1PE:H152	1.76	0.49
1:F:150:ASP:OD1	1:F:152:GLN:N	2.46	0.49
1:B:214:LEU:HD21	1:B:222:LEU:HD22	1.94	0.49
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.95	0.49
1:H:483:ASP:OD1	1:H:573:HIS:ND1	2.35	0.49
1:B:236:ARG:NH1	9:B:1118:HOH:O	2.43	0.48
1:D:326:LYS:HE3	1:D:328:LEU:HD21	1.94	0.48
1:I:209:SER:O	1:I:212:THR:OG1	2.28	0.48
1:A:214:LEU:HD21	1:A:222:LEU:HD22	1.94	0.48
1:H:397:LYS:O	1:H:400:MET:HG2	2.12	0.48
1:D:91:VAL:HB	1:F:346:LYS:HE3	1.94	0.48
1:L:236:ARG:NH1	9:L:1101:HOH:O	2.39	0.48
1:B:453:ILE:HD13	1:B:561:PHE:HZ	1.79	0.48
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.35	0.48
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.96	0.48
1:D:200:GLU:N	1:D:200:GLU:OE1	2.46	0.48
1:J:396:MET:SD	1:J:398:PHE:HE2	2.37	0.48
1:G:480:TYR:OH	1:G:512:LYS:NZ	2.39	0.48
1:H:413:VAL:HG11	1:H:423:ILE:HD12	1.95	0.48
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.96	0.47
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.96	0.47
1:H:442:GLY:O	9:H:1102:HOH:O	2.20	0.47
1:J:121:CYS:HB2	1:J:148:VAL:HG12	1.96	0.47
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.95	0.47
1:D:397:LYS:O	1:D:400:MET:HG2	2.15	0.47
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.96	0.47
1:D:506:ASN:O	1:D:510:ILE:HG12	2.14	0.47
1:K:122:ASN:OD1	1:K:149:ASN:HB2	2.15	0.47
1:J:598:GLU:OE1	1:J:602:ASN:ND2	2.43	0.47
1:H:320:LYS:NZ	6:H:1006:1PE:H142	2.30	0.47
1:J:301:PRO:HB2	1:J:303:ASN:OD1	2.15	0.47
1:K:230:VAL:HG12	1:K:234:LEU:HD23	1.96	0.47
1:K:548:SER:HA	1:K:549:SER:CB	2.44	0.47
1:A:520:SER:HB3	1:A:598:GLU:HG3	1.97	0.47
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.96	0.47
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.97	0.47
1:B:175:PHE:CD1	1:F:176:TYR:HB2	2.50	0.47
1:B:244:TYR:OH	1:B:588:PRO:O	2.31	0.47
1:D:439:TYR:N	1:D:439:TYR:CD2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1001:4TK:NAL	4:D:1004:CO3:O1	2.48	0.47
1:J:520:SER:HB3	1:J:598:GLU:HG3	1.97	0.47
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.97	0.46
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.97	0.46
1:E:396:MET:SD	1:E:398:PHE:HE2	2.38	0.46
1:K:543:ASP:OD2	1:L:254:SER:OG	2.26	0.46
1:A:453:ILE:HD13	1:A:561:PHE:HZ	1.80	0.46
1:G:164:LYS:NZ	1:J:184:SER:OG	2.48	0.46
1:D:449:ASN:HD21	1:D:451:LYS:HD2	1.79	0.46
1:I:173:LYS:NZ	1:K:216:ASP:O	2.35	0.46
1:J:548:SER:OG	1:J:551:VAL:HG23	2.15	0.46
1:B:553:ALA:N	9:B:1120:HOH:O	2.47	0.46
1:E:230:VAL:HG22	1:E:234:LEU:HD23	1.96	0.46
1:F:225:VAL:HG22	1:F:270:TYR:HB2	1.98	0.46
1:H:520:SER:HB3	1:H:598:GLU:HG3	1.97	0.46
1:I:440:ARG:NH1	1:I:443:ASP:OD2	2.49	0.46
1:L:504:GLY:HA3	1:L:510:ILE:HD11	1.98	0.46
1:B:395:LEU:O	1:B:398:PHE:HD2	1.98	0.46
1:E:150:ASP:OD2	1:E:179:ASN:HB2	2.15	0.46
1:H:374:LYS:HE3	1:H:462:GLY:HA3	1.96	0.46
1:L:550:SER:HG	1:L:551:VAL:H	1.62	0.46
1:D:396:MET:SD	1:D:398:PHE:HE2	2.37	0.46
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.98	0.46
1:H:453:ILE:HD13	1:H:561:PHE:HZ	1.81	0.46
1:J:457:ASN:HB2	1:J:547:ILE:HD13	1.97	0.46
1:D:457:ASN:HB2	1:D:547:ILE:HD13	1.97	0.46
1:F:230:VAL:O	1:F:277:TYR:OH	2.23	0.46
1:I:200:GLU:HA	1:I:203:MET:HB3	1.97	0.45
1:J:552:LYS:O	1:J:554:SER:N	2.48	0.45
1:F:413:VAL:HG11	1:F:423:ILE:HD13	1.99	0.45
1:C:300:ALA:O	9:C:1101:HOH:O	2.21	0.45
1:G:483:ASP:OD2	1:G:571:TRP:NE1	2.46	0.45
1:K:396:MET:SD	1:K:398:PHE:HE2	2.39	0.45
1:A:543:ASP:CG	1:B:255:THR:H	2.19	0.45
1:B:174:HIS:HB3	1:F:175:PHE:CD2	2.51	0.45
1:J:214:LEU:HD21	1:J:222:LEU:HD22	1.99	0.45
1:A:320:LYS:NZ	6:A:1007:1PE:H152	2.31	0.45
1:L:383:TYR:HE2	1:L:438:SER:HB2	1.80	0.45
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.99	0.45
6:C:1006:1PE:H142	6:C:1006:1PE:H132	1.69	0.45
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:GLU:HB2	1:I:237:PHE:CE2	2.52	0.45
1:K:114:VAL:HG12	1:K:274:ALA:HB1	1.99	0.45
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.98	0.45
1:I:114:VAL:HB	1:I:278:LYS:HG2	1.98	0.45
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.52	0.45
1:B:534:ARG:NE	9:B:1122:HOH:O	2.50	0.44
1:E:200:GLU:HG3	1:E:521:ASN:O	2.16	0.44
1:B:395:LEU:HD21	1:B:581:TRP:CD1	2.52	0.44
1:D:244:TYR:HA	1:D:288:TYR:HE1	1.82	0.44
1:H:218:LYS:HB2	1:L:164:LYS:HA	1.99	0.44
1:K:440:ARG:NH2	9:K:1119:HOH:O	2.49	0.44
1:L:217:ASN:OD1	1:L:218:LYS:N	2.49	0.44
1:E:503:PHE:HD1	1:E:573:HIS:HD1	1.65	0.44
1:H:175:PHE:CD1	1:L:176:TYR:HB2	2.51	0.44
1:H:247:MET:HG3	1:H:288:TYR:OH	2.18	0.44
1:J:274:ALA:O	1:J:278:LYS:HG3	2.18	0.44
1:D:413:VAL:HG11	1:D:423:ILE:HD12	2.00	0.44
1:I:133:ASN:HB3	1:I:192:CYS:HB2	1.99	0.44
1:I:386:LYS:HB3	1:I:391:SER:HB2	1.99	0.44
1:J:453:ILE:HD13	1:J:561:PHE:HZ	1.82	0.44
1:K:548:SER:CB	1:K:550:SER:H	2.30	0.44
1:E:321:LEU:HD11	1:E:411:TYR:HA	1.99	0.44
1:H:207:VAL:HG11	1:H:241:THR:HG22	1.99	0.44
1:H:298:ILE:HA	1:H:400:MET:SD	2.58	0.44
1:B:399:ASP:OD1	1:B:486:THR:OG1	2.33	0.44
1:I:200:GLU:HG3	1:I:521:ASN:HB3	1.99	0.44
1:K:398:PHE:O	1:K:401:SER:OG	2.27	0.44
1:A:172:SER:HB2	1:A:213:MET:HE1	2.00	0.44
1:B:457:ASN:HB2	1:B:547:ILE:HD13	2.00	0.44
1:J:435:SER:OG	1:J:436:LYS:N	2.51	0.44
6:L:1005:1PE:H262	6:L:1005:1PE:H251	1.71	0.44
1:D:254:SER:OG	1:F:543:ASP:OD2	2.24	0.43
1:D:533:TYR:O	1:D:536:THR:HG22	2.18	0.43
1:F:133:ASN:HA	1:F:167:VAL:HG21	1.99	0.43
1:J:505:ASN:HB3	1:J:563:LYS:HE2	2.00	0.43
1:G:301:PRO:HB2	1:G:303:ASN:OD1	2.18	0.43
1:E:294:ALA:O	1:E:298:ILE:HG13	2.18	0.43
1:G:441:PRO:HD2	1:H:378:PHE:CZ	2.52	0.43
1:E:386:LYS:HE3	1:E:396:MET:SD	2.58	0.43
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.01	0.43
1:H:548:SER:HB2	1:H:557:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:TYR:H	1:A:439:TYR:HD2	1.65	0.43
1:D:439:TYR:H	1:D:439:TYR:HD2	1.67	0.43
1:A:132:VAL:HG21	1:A:142:VAL:HG13	2.00	0.43
1:B:199:SER:OG	1:B:200:GLU:N	2.51	0.43
1:J:453:ILE:HD11	1:J:565:PHE:HZ	1.83	0.43
1:K:546:GLN:HG2	1:K:547:ILE:HG23	2.01	0.43
1:C:301:PRO:HA	1:C:397:LYS:HD2	2.01	0.43
1:D:127:LEU:HD11	1:D:129:ILE:HD11	2.00	0.43
1:G:441:PRO:HB2	1:H:394:ASP:HA	2.01	0.43
1:K:302:SER:OG	1:K:378:PHE:HB2	2.19	0.43
1:K:435:SER:OG	1:K:436:LYS:N	2.51	0.43
1:L:246:TYR:HE2	1:L:264:ILE:HG12	1.84	0.43
1:H:142:VAL:HG12	1:H:167:VAL:HG12	2.00	0.43
1:H:357:LEU:HB2	1:H:425:PHE:HB2	2.01	0.43
1:J:413:VAL:HG11	1:J:423:ILE:HD12	2.00	0.43
1:L:298:ILE:HG23	1:L:398:PHE:HA	2.00	0.43
1:L:137:LYS:CB	1:L:140:GLY:H	2.32	0.43
1:D:301:PRO:HB2	1:D:303:ASN:OD1	2.18	0.42
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.54	0.42
1:I:453:ILE:HD13	1:I:561:PHE:HZ	1.83	0.42
1:K:150:ASP:OD2	1:K:179:ASN:HB2	2.19	0.42
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.54	0.42
1:J:551:VAL:O	1:J:551:VAL:HG12	2.19	0.42
1:D:543:ASP:OD2	1:E:254:SER:OG	2.26	0.42
1:G:270:TYR:OH	6:G:1008:1PE:OH6	2.36	0.42
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.54	0.42
1:D:497:THR:O	1:D:589:LYS:NZ	2.52	0.42
1:K:214:LEU:HD21	1:K:222:LEU:HD22	2.01	0.42
1:H:174:HIS:HB3	1:L:175:PHE:CD2	2.54	0.42
1:A:156:PHE:CZ	8:D:1005:DMS:H11	2.55	0.42
1:B:551:VAL:HG12	1:B:552:LYS:O	2.19	0.42
1:C:230:VAL:HG23	1:C:234:LEU:HD23	2.02	0.42
1:C:478:VAL:N	9:C:1112:HOH:O	2.50	0.42
1:F:587:LYS:NZ	9:F:1109:HOH:O	2.39	0.42
1:K:127:LEU:HD11	1:K:129:ILE:HD11	2.01	0.42
1:D:418:PRO:HB3	1:D:601:LEU:HD23	2.02	0.42
1:E:338:MET:CE	1:E:468:ASP:HB3	2.50	0.42
1:E:435:SER:OG	1:E:436:LYS:N	2.53	0.42
1:F:207:VAL:HG11	1:F:241:THR:HG22	2.02	0.42
1:G:168:LYS:HB3	1:G:171:THR:OG1	2.20	0.42
1:J:386:LYS:HB3	1:J:391:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:453:ILE:HD13	1:K:561:PHE:HZ	1.85	0.42
1:A:367:LYS:HG2	1:A:603:ASP:OD2	2.20	0.42
1:H:522:GLU:HA	1:H:523:PRO:HD2	1.94	0.42
1:J:537:LEU:HA	1:J:545:ASN:HB2	2.01	0.42
1:K:144:ILE:HG13	1:K:157:LEU:HD22	2.01	0.42
1:L:457:ASN:HB2	1:L:547:ILE:HD13	2.01	0.42
1:L:552:LYS:HB3	1:L:553:ALA:H	1.72	0.42
1:C:395:LEU:C	1:C:397:LYS:H	2.23	0.42
2:F:1001:4TK:OAF	4:F:1004:CO3:O3	2.38	0.42
1:I:116:ASP:HA	1:I:274:ALA:HB2	2.01	0.42
1:J:114:VAL:HG12	1:J:274:ALA:HB1	2.00	0.42
1:D:144:ILE:HG13	1:D:157:LEU:HD22	2.01	0.41
1:L:90:GLN:NE2	1:L:95:ASP:O	2.51	0.41
1:B:357:LEU:HB2	1:B:425:PHE:HB2	2.02	0.41
1:D:112:VAL:HG22	1:D:267:LEU:HB3	2.01	0.41
1:D:230:VAL:HG12	1:D:234:LEU:HD23	2.01	0.41
1:D:460:ALA:O	1:D:546:GLN:NE2	2.52	0.41
1:G:520:SER:HB3	1:G:598:GLU:HG3	2.03	0.41
1:F:396:MET:HA	1:F:398:PHE:CD2	2.56	0.41
1:K:118:LYS:NZ	1:K:272:ASN:OD1	2.54	0.41
1:K:480:TYR:OH	1:K:512:LYS:NZ	2.35	0.41
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.83	0.41
1:D:214:LEU:HD11	1:D:222:LEU:HD22	2.03	0.41
1:K:287:TYR:OH	1:K:598:GLU:OE2	2.30	0.41
1:A:483:ASP:OD2	1:A:571:TRP:NE1	2.53	0.41
1:B:509:LEU:O	1:B:513:ILE:HG12	2.20	0.41
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.55	0.41
1:L:121:CYS:HB2	1:L:148:VAL:HG12	2.02	0.41
1:L:138:GLU:N	1:L:139:ASN:HA	2.35	0.41
1:B:112:VAL:HG22	1:B:267:LEU:HB3	2.03	0.41
1:B:142:VAL:HG12	1:B:167:VAL:HG12	2.02	0.41
1:B:346:LYS:HE3	1:C:91:VAL:HB	2.02	0.41
1:D:441:PRO:HB2	1:E:394:ASP:HA	2.02	0.41
1:E:297:LEU:HB3	1:E:400:MET:HE1	2.03	0.41
1:E:386:LYS:HB3	1:E:391:SER:HB2	2.02	0.41
1:L:301:PRO:HB2	1:L:303:ASN:OD1	2.21	0.41
1:B:137:LYS:O	1:B:194:SER:OG	2.29	0.41
1:B:294:ALA:O	1:B:298:ILE:HG13	2.21	0.41
1:C:150:ASP:OD2	1:C:179:ASN:HB2	2.21	0.41
1:C:174:HIS:HB3	1:E:175:PHE:CD2	2.56	0.41
1:D:274:ALA:O	1:D:278:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:364:ASP:O	1:F:420:ASN:HA	2.20	0.41
1:F:512:LYS:NZ	9:F:1112:HOH:O	2.43	0.41
1:I:376:ILE:HB	1:I:399:ASP:HB3	2.01	0.41
1:I:395:LEU:C	1:I:397:LYS:H	2.23	0.41
1:K:301:PRO:HB2	1:K:303:ASN:OD1	2.20	0.41
1:D:454:GLU:OE1	1:D:539:SER:OG	2.35	0.41
1:H:290:GLY:C	1:H:593:VAL:HG11	2.41	0.41
1:L:230:VAL:HG12	1:L:234:LEU:HD23	2.02	0.41
1:A:114:VAL:HB	1:A:278:LYS:HG2	2.02	0.40
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.56	0.40
1:F:504:GLY:HA3	1:F:510:ILE:HD11	2.03	0.40
1:F:549:SER:HA	1:F:550:SER:HA	1.67	0.40
1:K:369:ILE:HB	1:K:423:ILE:HD13	2.02	0.40
1:C:394:ASP:OD1	1:C:394:ASP:N	2.50	0.40
1:G:350:TYR:HA	1:G:351:PRO:HD3	1.91	0.40
1:H:107:ILE:HG12	1:H:247:MET:HG2	2.03	0.40
1:L:435:SER:OG	1:L:436:LYS:N	2.55	0.40
1:A:525:TRP:CZ3	1:F:528:PRO:HB3	2.55	0.40
1:F:323:LEU:HD22	1:F:359:TYR:HB2	2.04	0.40
1:J:214:LEU:HD11	1:J:222:LEU:HD22	2.03	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	517/522 (99%)	502 (97%)	14 (3%)	1 (0%)	47 71
1	B	512/522 (98%)	496 (97%)	15 (3%)	1 (0%)	47 71
1	C	513/522 (98%)	501 (98%)	11 (2%)	1 (0%)	47 71
1	D	507/522 (97%)	494 (97%)	13 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	503/522 (96%)	488 (97%)	14 (3%)	1 (0%)	47	71
1	F	505/522 (97%)	492 (97%)	13 (3%)	0	100	100
1	G	517/522 (99%)	501 (97%)	14 (3%)	2 (0%)	34	57
1	H	513/522 (98%)	493 (96%)	19 (4%)	1 (0%)	47	71
1	I	516/522 (99%)	502 (97%)	12 (2%)	2 (0%)	34	57
1	J	508/522 (97%)	491 (97%)	13 (3%)	4 (1%)	19	39
1	K	500/522 (96%)	485 (97%)	15 (3%)	0	100	100
1	L	507/522 (97%)	489 (96%)	16 (3%)	2 (0%)	34	57
All	All	6118/6264 (98%)	5934 (97%)	169 (3%)	15 (0%)	47	71

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	396	MET
1	E	552	LYS
1	G	551	VAL
1	I	396	MET
1	L	551	VAL
1	I	550	SER
1	J	552	LYS
1	J	553	ALA
1	A	396	MET
1	G	550	SER
1	J	137	LYS
1	J	550	SER
1	L	396	MET
1	B	552	LYS
1	H	138	GLU

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	422/450 (94%)	422 (100%)	0	100	100
1	B	401/450 (89%)	401 (100%)	0	100	100
1	C	413/450 (92%)	413 (100%)	0	100	100
1	D	406/450 (90%)	406 (100%)	0	100	100
1	E	409/450 (91%)	407 (100%)	2 (0%)	88	96
1	F	397/450 (88%)	397 (100%)	0	100	100
1	G	420/450 (93%)	419 (100%)	1 (0%)	93	98
1	H	405/450 (90%)	404 (100%)	1 (0%)	93	98
1	I	418/450 (93%)	415 (99%)	3 (1%)	84	94
1	J	417/450 (93%)	416 (100%)	1 (0%)	93	98
1	K	411/450 (91%)	409 (100%)	2 (0%)	88	96
1	L	397/450 (88%)	395 (100%)	2 (0%)	88	96
All	All	4916/5400 (91%)	4904 (100%)	12 (0%)	93	98

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	322	ASN
1	E	398	PHE
1	G	398	PHE
1	H	439	TYR
1	I	185	VAL
1	I	399	ASP
1	I	400	MET
1	J	398	PHE
1	K	538	ASN
1	K	548	SER
1	L	288	TYR
1	L	400	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	538	ASN
1	L	217	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 89 ligands modelled in this entry, 24 are monoatomic - leaving 65 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
4	CO3	D	1004	-	2,3,3	0.39	0	2,3,3	0.22	0
2	4TK	D	1001	3	19,19,19	1.95	2 (10%)	26,27,27	0.79	1 (3%)
4	CO3	F	1004	-	2,3,3	0.40	0	2,3,3	0.18	0
4	CO3	A	1004	-	2,3,3	0.40	0	2,3,3	0.18	0
2	4TK	I	1001	3	19,19,19	1.94	1 (5%)	26,27,27	0.82	0
5	GOL	J	1005	-	5,5,5	0.35	0	5,5,5	0.28	0
4	CO3	I	1004	-	2,3,3	0.41	0	2,3,3	0.26	0
5	GOL	A	1005	-	5,5,5	0.37	0	5,5,5	0.25	0
6	1PE	K	1005	-	11,11,15	0.60	0	10,10,14	0.36	0
6	1PE	D	1007	-	9,9,15	0.54	0	8,8,14	0.34	0
6	1PE	G	1009	-	5,5,15	0.68	0	4,4,14	0.42	0
7	SO4	G	1010	-	4,4,4	0.14	0	6,6,6	0.06	0
4	CO3	K	1004	-	2,3,3	0.39	0	2,3,3	0.14	0
6	1PE	G	1008	-	5,5,15	0.66	0	4,4,14	0.61	0
7	SO4	D	1008	-	4,4,4	0.15	0	6,6,6	0.05	0
5	GOL	I	1005	-	5,5,5	0.37	0	5,5,5	0.25	0
6	1PE	C	1006	-	12,12,15	0.64	0	11,11,14	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	B	1007	-	4,4,4	0.14	0	6,6,6	0.09	0
4	CO3	H	1004	-	2,3,3	0.39	0	2,3,3	0.20	0
6	1PE	A	1007	-	11,11,15	0.65	0	10,10,14	0.37	0
6	1PE	A	1006	-	8,8,15	0.53	0	7,7,14	0.39	0
2	4TK	C	1001	3	19,19,19	1.94	1 (5%)	26,27,27	0.85	0
2	4TK	K	1001	3	19,19,19	1.91	1 (5%)	26,27,27	0.87	0
2	4TK	A	1001	3	19,19,19	1.89	1 (5%)	26,27,27	0.75	0
4	CO3	E	1004	-	2,3,3	0.40	0	2,3,3	0.16	0
8	DMS	I	1006	-	3,3,3	0.66	0	3,3,3	0.52	0
2	4TK	G	1001	3	19,19,19	1.88	2 (10%)	26,27,27	0.81	0
2	4TK	H	1001	3	19,19,19	1.82	1 (5%)	26,27,27	0.86	0
8	DMS	D	1005	-	3,3,3	0.64	0	3,3,3	0.51	0
2	4TK	E	1001	3	19,19,19	1.99	1 (5%)	26,27,27	0.78	0
7	SO4	I	1010	-	4,4,4	0.14	0	6,6,6	0.06	0
2	4TK	J	1001	3	19,19,19	1.94	2 (10%)	26,27,27	0.77	1 (3%)
4	CO3	G	1004	-	2,3,3	0.40	0	2,3,3	0.21	0
6	1PE	F	1005	-	9,9,15	0.90	0	8,8,14	0.45	0
6	1PE	H	1006	-	9,9,15	0.54	0	8,8,14	0.40	0
5	GOL	G	1005	-	5,5,5	0.35	0	5,5,5	0.30	0
6	1PE	I	1007	-	11,11,15	0.57	0	10,10,14	0.46	0
8	DMS	G	1006	-	3,3,3	0.66	0	3,3,3	0.53	0
8	DMS	J	1006	-	3,3,3	0.67	0	3,3,3	0.52	0
5	GOL	B	1005	-	5,5,5	0.38	0	5,5,5	0.21	0
6	1PE	B	1006	-	9,9,15	0.54	0	8,8,14	0.32	0
4	CO3	C	1004	-	2,3,3	0.39	0	2,3,3	0.19	0
4	CO3	J	1004	-	2,3,3	0.40	0	2,3,3	0.22	0
6	1PE	D	1006	-	9,9,15	0.55	0	8,8,14	0.39	0
2	4TK	B	1001	3	19,19,19	1.91	1 (5%)	26,27,27	0.74	0
6	1PE	C	1007	-	8,8,15	0.52	0	7,7,14	0.42	0
7	SO4	A	1008	-	4,4,4	0.14	0	6,6,6	0.05	0
2	4TK	F	1001	3	19,19,19	1.99	2 (10%)	26,27,27	0.75	0
7	SO4	I	1009	-	4,4,4	0.14	0	6,6,6	0.04	0
6	1PE	G	1007	-	8,8,15	0.54	0	7,7,14	0.29	0
7	SO4	L	1006	-	4,4,4	0.14	0	6,6,6	0.05	0
8	DMS	C	1005	-	3,3,3	0.66	0	3,3,3	0.52	0
6	1PE	E	1006	-	11,11,15	0.58	0	10,10,14	0.39	0
7	SO4	G	1011	-	4,4,4	0.14	0	6,6,6	0.06	0
7	SO4	J	1008	-	4,4,4	0.15	0	6,6,6	0.05	0
7	SO4	J	1009	-	4,4,4	0.15	0	6,6,6	0.05	0
4	CO3	L	1004	-	2,3,3	0.41	0	2,3,3	0.15	0
7	SO4	H	1007	-	4,4,4	0.13	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	B	1004	-	2,3,3	0.39	0	2,3,3	0.20	0
6	1PE	E	1005	-	11,11,15	0.59	0	10,10,14	0.42	0
6	1PE	J	1007	-	10,10,15	0.85	0	9,9,14	0.38	0
6	1PE	L	1005	-	9,9,15	0.89	0	8,8,14	0.41	0
6	1PE	I	1008	-	10,10,15	0.56	0	9,9,14	0.38	0
6	1PE	H	1005	-	5,5,15	0.69	0	4,4,14	0.46	0
2	4TK	L	1001	3	19,19,19	1.96	2 (10%)	26,27,27	0.81	1 (3%)

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	4TK	D	1001	3	-	0/20/20/20	0/1/1/1
2	4TK	I	1001	3	-	1/20/20/20	0/1/1/1
5	GOL	J	1005	-	-	4/4/4/4	-
2	4TK	L	1001	3	-	0/20/20/20	0/1/1/1
6	1PE	K	1005	-	-	7/9/9/13	-
5	GOL	A	1005	-	-	2/4/4/4	-
6	1PE	D	1007	-	-	5/7/7/13	-
6	1PE	G	1009	-	-	3/3/3/13	-
6	1PE	G	1008	-	-	1/3/3/13	-
6	1PE	C	1006	-	-	6/10/10/13	-
6	1PE	A	1007	-	-	5/9/9/13	-
6	1PE	A	1006	-	-	4/6/6/13	-
2	4TK	C	1001	3	-	4/20/20/20	0/1/1/1
2	4TK	K	1001	3	-	3/20/20/20	0/1/1/1
2	4TK	A	1001	3	-	0/20/20/20	0/1/1/1
2	4TK	G	1001	3	-	0/20/20/20	0/1/1/1
2	4TK	H	1001	3	-	0/20/20/20	0/1/1/1
2	4TK	E	1001	3	-	0/20/20/20	0/1/1/1
2	4TK	J	1001	3	-	0/20/20/20	0/1/1/1
6	1PE	F	1005	-	-	3/7/7/13	-
6	1PE	H	1006	-	-	5/7/7/13	-
5	GOL	G	1005	-	-	4/4/4/4	-
6	1PE	I	1007	-	-	7/9/9/13	-
5	GOL	B	1005	-	-	2/4/4/4	-
6	1PE	B	1006	-	-	3/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	D	1006	-	-	2/7/7/13	-
2	4TK	B	1001	3	-	0/20/20/20	0/1/1/1
6	1PE	C	1007	-	-	3/6/6/13	-
2	4TK	F	1001	3	-	3/20/20/20	0/1/1/1
6	1PE	G	1007	-	-	4/6/6/13	-
6	1PE	E	1006	-	-	6/9/9/13	-
6	1PE	E	1005	-	-	7/9/9/13	-
6	1PE	J	1007	-	-	4/8/8/13	-
6	1PE	L	1005	-	-	2/7/7/13	-
6	1PE	I	1008	-	-	6/8/8/13	-
6	1PE	H	1005	-	-	2/3/3/13	-
5	GOL	I	1005	-	-	2/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1001	4TK	CAQ-CA	-8.31	1.39	1.52
2	F	1001	4TK	CAQ-CA	-8.09	1.39	1.52
2	C	1001	4TK	CAQ-CA	-8.04	1.39	1.52
2	I	1001	4TK	CAQ-CA	-8.02	1.39	1.52
2	L	1001	4TK	CAQ-CA	-8.00	1.39	1.52
2	J	1001	4TK	CAQ-CA	-8.00	1.39	1.52
2	K	1001	4TK	CAQ-CA	-7.98	1.39	1.52
2	B	1001	4TK	CAQ-CA	-7.93	1.39	1.52
2	A	1001	4TK	CAQ-CA	-7.92	1.39	1.52
2	D	1001	4TK	CAQ-CA	-7.90	1.39	1.52
2	H	1001	4TK	CAQ-CA	-7.64	1.40	1.52
2	G	1001	4TK	CAQ-CA	-7.60	1.40	1.52
2	D	1001	4TK	OAF-NAL	2.31	1.45	1.40
2	F	1001	4TK	OAF-NAL	2.16	1.45	1.40
2	G	1001	4TK	OAF-NAL	2.10	1.45	1.40
2	J	1001	4TK	OAF-NAL	2.06	1.45	1.40
2	L	1001	4TK	OAF-NAL	2.01	1.45	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	4TK	CAS-CAO-N	-2.33	114.46	117.66
2	L	1001	4TK	CAS-CAO-N	-2.07	114.82	117.66
2	J	1001	4TK	CAS-CAO-N	-2.04	114.86	117.66

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1005	GOL	O1-C1-C2-C3
5	G	1005	GOL	C1-C2-C3-O3
5	G	1005	GOL	O2-C2-C3-O3
5	J	1005	GOL	O1-C1-C2-C3
5	J	1005	GOL	C1-C2-C3-O3
6	B	1006	1PE	OH5-C14-C24-OH4
6	A	1007	1PE	OH4-C13-C23-OH3
6	A	1007	1PE	OH5-C14-C24-OH4
6	E	1006	1PE	OH5-C14-C24-OH4
6	G	1007	1PE	OH5-C14-C24-OH4
6	A	1007	1PE	OH6-C15-C25-OH5
6	D	1007	1PE	OH5-C14-C24-OH4
6	C	1006	1PE	OH4-C13-C23-OH3
6	C	1006	1PE	OH5-C14-C24-OH4
6	A	1006	1PE	OH4-C13-C23-OH3
6	I	1008	1PE	OH4-C13-C23-OH3
6	J	1007	1PE	OH5-C14-C24-OH4
6	C	1006	1PE	OH6-C15-C25-OH5
6	D	1006	1PE	OH4-C13-C23-OH3
6	C	1007	1PE	OH5-C14-C24-OH4
6	B	1006	1PE	OH4-C13-C23-OH3
6	E	1005	1PE	OH4-C13-C23-OH3
6	E	1005	1PE	OH5-C14-C24-OH4
6	D	1006	1PE	OH5-C14-C24-OH4
6	C	1006	1PE	C14-C24-OH4-C13
6	I	1007	1PE	OH6-C15-C25-OH5
6	J	1007	1PE	C16-C26-OH6-C15
5	B	1005	GOL	O1-C1-C2-C3
5	G	1005	GOL	O1-C1-C2-C3
5	I	1005	GOL	O1-C1-C2-C3
5	B	1005	GOL	O1-C1-C2-O2
5	J	1005	GOL	O2-C2-C3-O3
6	F	1005	1PE	OH5-C14-C24-OH4
6	G	1009	1PE	OH6-C15-C25-OH5
6	A	1006	1PE	OH5-C14-C24-OH4
5	A	1005	GOL	O1-C1-C2-O2
5	G	1005	GOL	O1-C1-C2-O2
5	J	1005	GOL	O1-C1-C2-O2
6	H	1006	1PE	OH4-C13-C23-OH3
6	L	1005	1PE	C25-C15-OH6-C26

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Mol	Chain	Res	Type	Atoms
6	C	1007	1PE	C12-C22-OH3-C23
6	J	1007	1PE	C15-C25-OH5-C14
6	I	1008	1PE	C12-C22-OH3-C23
5	I	1005	GOL	O1-C1-C2-O2
6	I	1008	1PE	C15-C25-OH5-C14
6	H	1006	1PE	C24-C14-OH5-C25
6	I	1007	1PE	C12-C22-OH3-C23
6	G	1009	1PE	C24-C14-OH5-C25
6	E	1005	1PE	OH6-C15-C25-OH5
6	E	1006	1PE	C24-C14-OH5-C25
6	H	1005	1PE	C24-C14-OH5-C25
6	H	1005	1PE	C15-C25-OH5-C14
6	D	1007	1PE	C14-C24-OH4-C13
6	I	1008	1PE	C23-C13-OH4-C24
6	K	1005	1PE	C23-C13-OH4-C24
6	G	1007	1PE	C14-C24-OH4-C13
6	A	1006	1PE	C23-C13-OH4-C24
6	D	1007	1PE	C12-C22-OH3-C23
6	F	1005	1PE	C16-C26-OH6-C15
6	E	1005	1PE	C15-C25-OH5-C14
6	K	1005	1PE	C14-C24-OH4-C13
6	I	1007	1PE	C23-C13-OH4-C24
6	C	1006	1PE	C15-C25-OH5-C14
6	I	1007	1PE	C24-C14-OH5-C25
6	E	1005	1PE	C12-C22-OH3-C23
6	G	1007	1PE	C24-C14-OH5-C25
6	I	1008	1PE	C13-C23-OH3-C22
6	E	1006	1PE	OH6-C15-C25-OH5
2	C	1001	4TK	O-C-CA-N
6	H	1006	1PE	C14-C24-OH4-C13
6	H	1006	1PE	C23-C13-OH4-C24
6	B	1006	1PE	C12-C22-OH3-C23
6	D	1007	1PE	C24-C14-OH5-C25
6	E	1005	1PE	C14-C24-OH4-C13
6	K	1005	1PE	C12-C22-OH3-C23
6	K	1005	1PE	C15-C25-OH5-C14
6	K	1005	1PE	OH4-C13-C23-OH3
2	C	1001	4TK	O-C-CA-CAQ
2	C	1001	4TK	NAL-C-CA-N
6	A	1006	1PE	C14-C24-OH4-C13
6	E	1006	1PE	OH4-C13-C23-OH3
6	A	1007	1PE	C15-C25-OH5-C14

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Mol	Chain	Res	Type	Atoms
6	A	1007	1PE	C25-C15-OH6-C26
6	C	1006	1PE	C25-C15-OH6-C26
6	I	1007	1PE	C15-C25-OH5-C14
6	G	1007	1PE	OH4-C13-C23-OH3
2	C	1001	4TK	NAL-C-CA-CAQ
2	F	1001	4TK	O-C-CA-N
6	H	1006	1PE	OH5-C14-C24-OH4
6	G	1009	1PE	C15-C25-OH5-C14
6	E	1006	1PE	C14-C24-OH4-C13
6	K	1005	1PE	OH5-C14-C24-OH4
6	I	1007	1PE	OH5-C14-C24-OH4
6	F	1005	1PE	OH6-C15-C25-OH5
6	C	1007	1PE	OH4-C13-C23-OH3
6	E	1005	1PE	C23-C13-OH4-C24
6	G	1008	1PE	OH6-C15-C25-OH5
6	K	1005	1PE	C13-C23-OH3-C22
6	J	1007	1PE	OH6-C15-C25-OH5
6	D	1007	1PE	OH4-C13-C23-OH3
6	L	1005	1PE	OH6-C15-C25-OH5
2	F	1001	4TK	O-C-CA-CAQ
2	K	1001	4TK	O-C-CA-CAQ
2	F	1001	4TK	NAL-C-CA-N
2	I	1001	4TK	NAL-C-CA-N
2	K	1001	4TK	O-C-CA-N
2	K	1001	4TK	NAL-C-CA-N
6	I	1007	1PE	OH4-C13-C23-OH3
6	I	1008	1PE	OH5-C14-C24-OH4
6	E	1006	1PE	C15-C25-OH5-C14

There are no ring outliers.

19 monomers are involved in 19 short contacts:

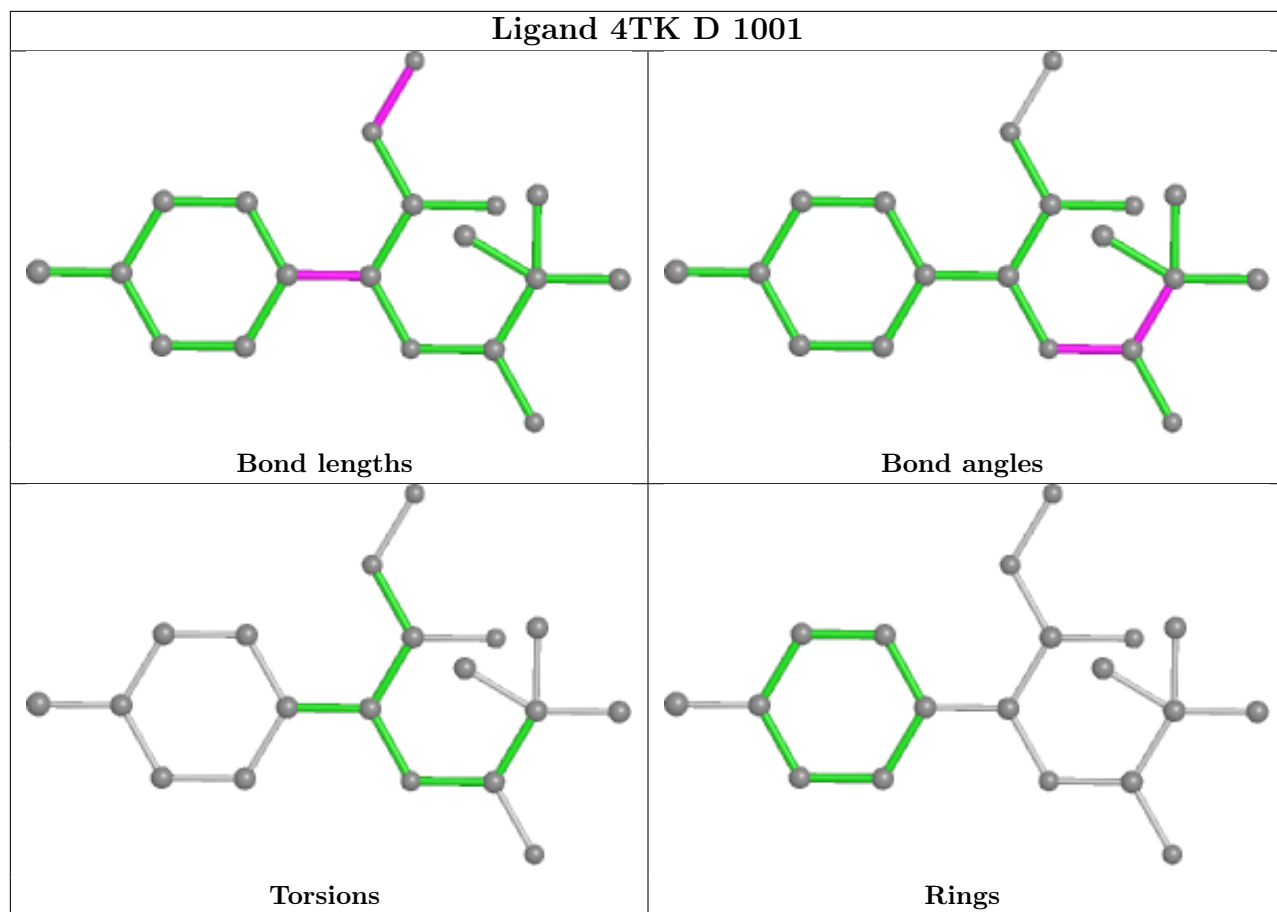
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1004	CO3	1	0
2	D	1001	4TK	1	0
4	F	1004	CO3	1	0
6	G	1008	1PE	1	0
5	I	1005	GOL	1	0
6	C	1006	1PE	2	0
6	A	1007	1PE	2	0
2	C	1001	4TK	1	0
8	D	1005	DMS	1	0

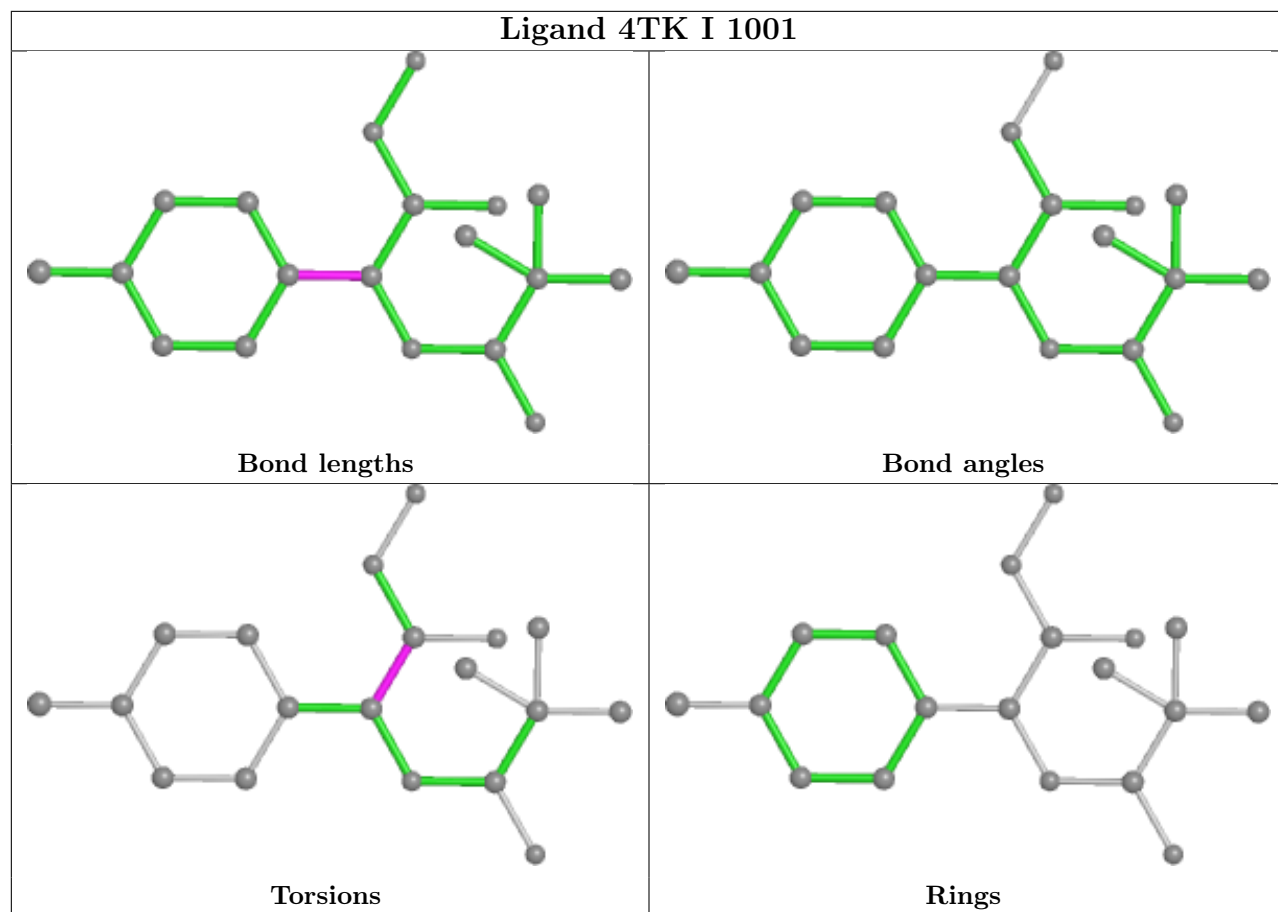
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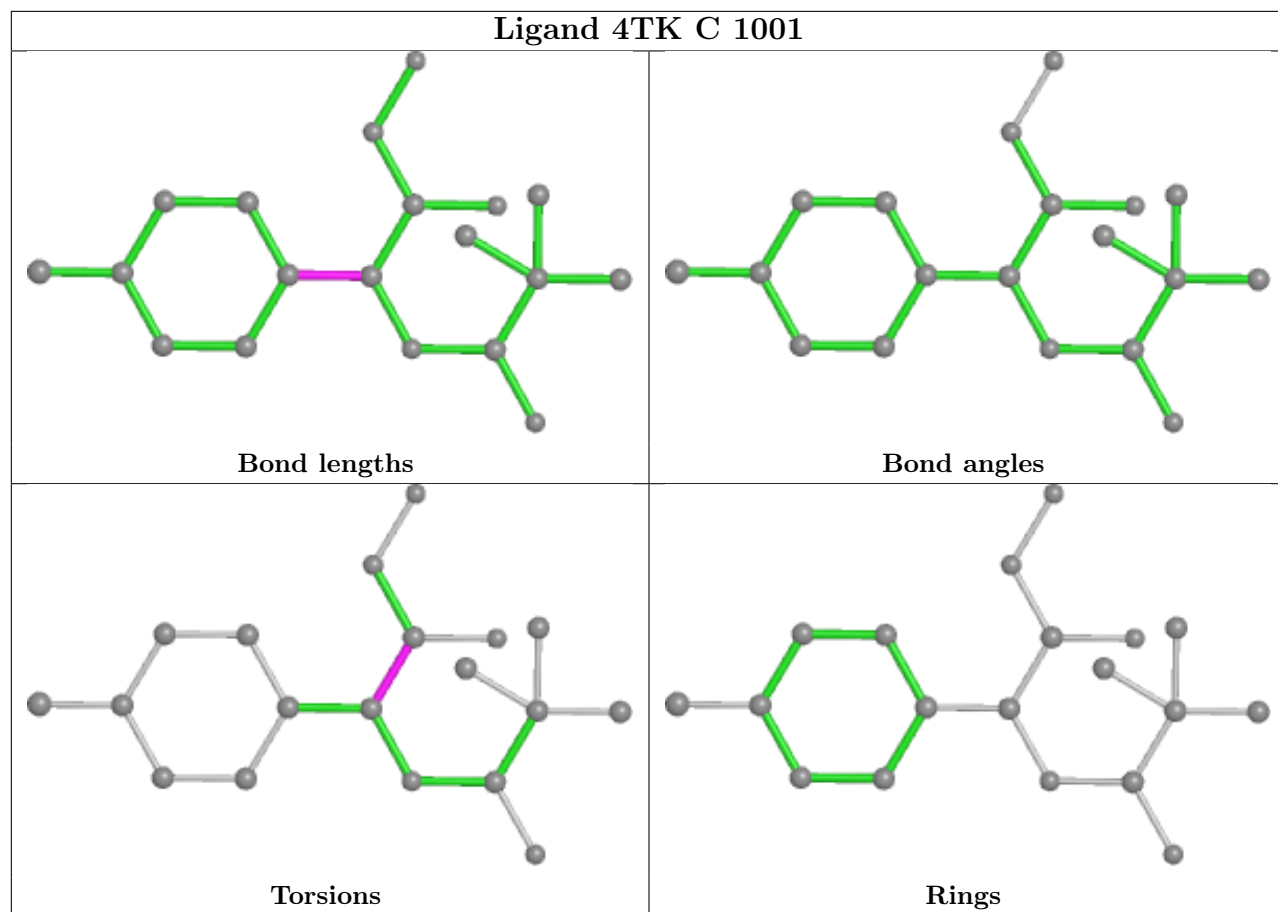
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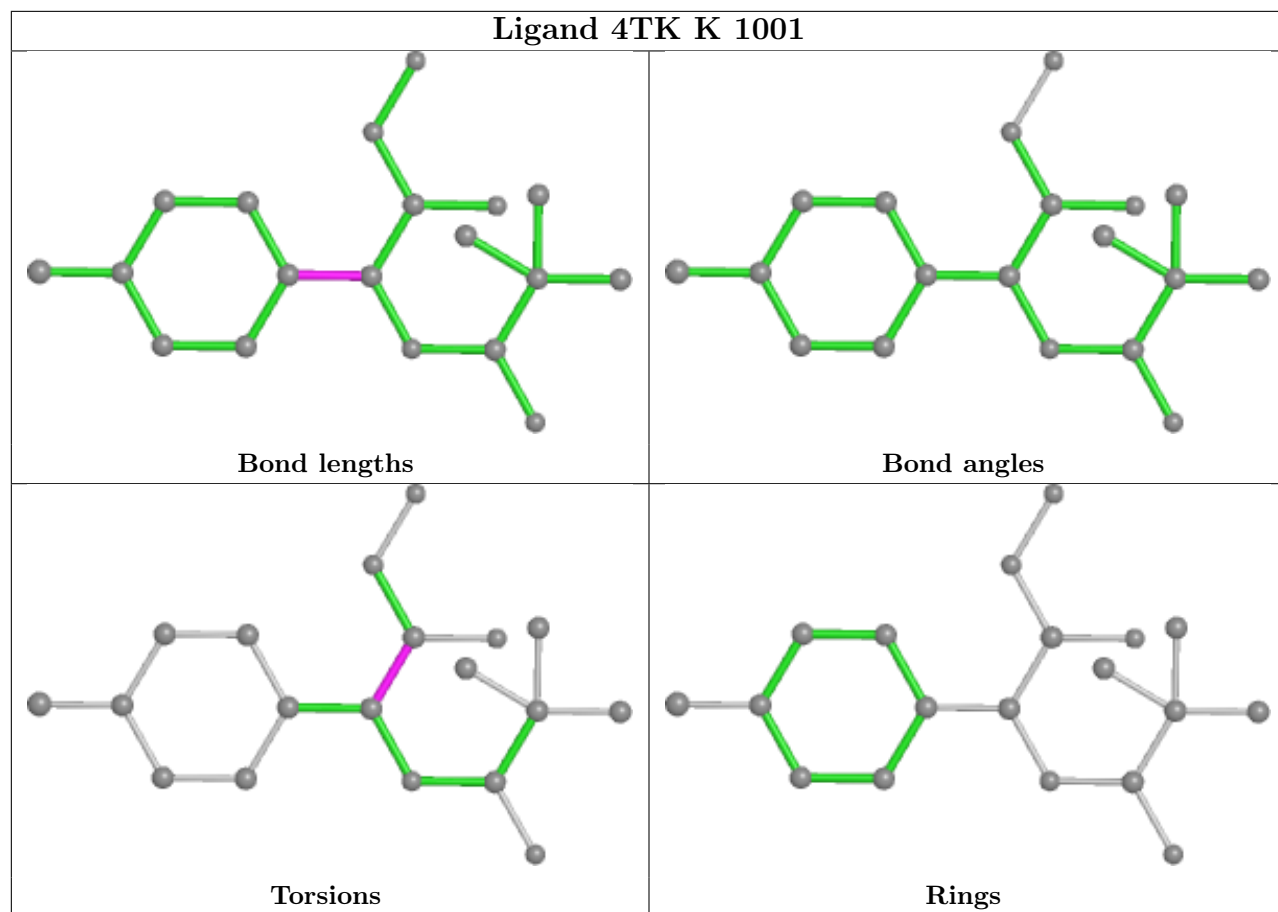
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1006	1PE	2	0
8	G	1006	DMS	1	0
4	C	1004	CO3	1	0
6	D	1006	1PE	1	0
2	F	1001	4TK	1	0
6	G	1007	1PE	1	0
7	L	1006	SO4	1	0
7	G	1011	SO4	1	0
7	J	1008	SO4	1	0
6	L	1005	1PE	1	0

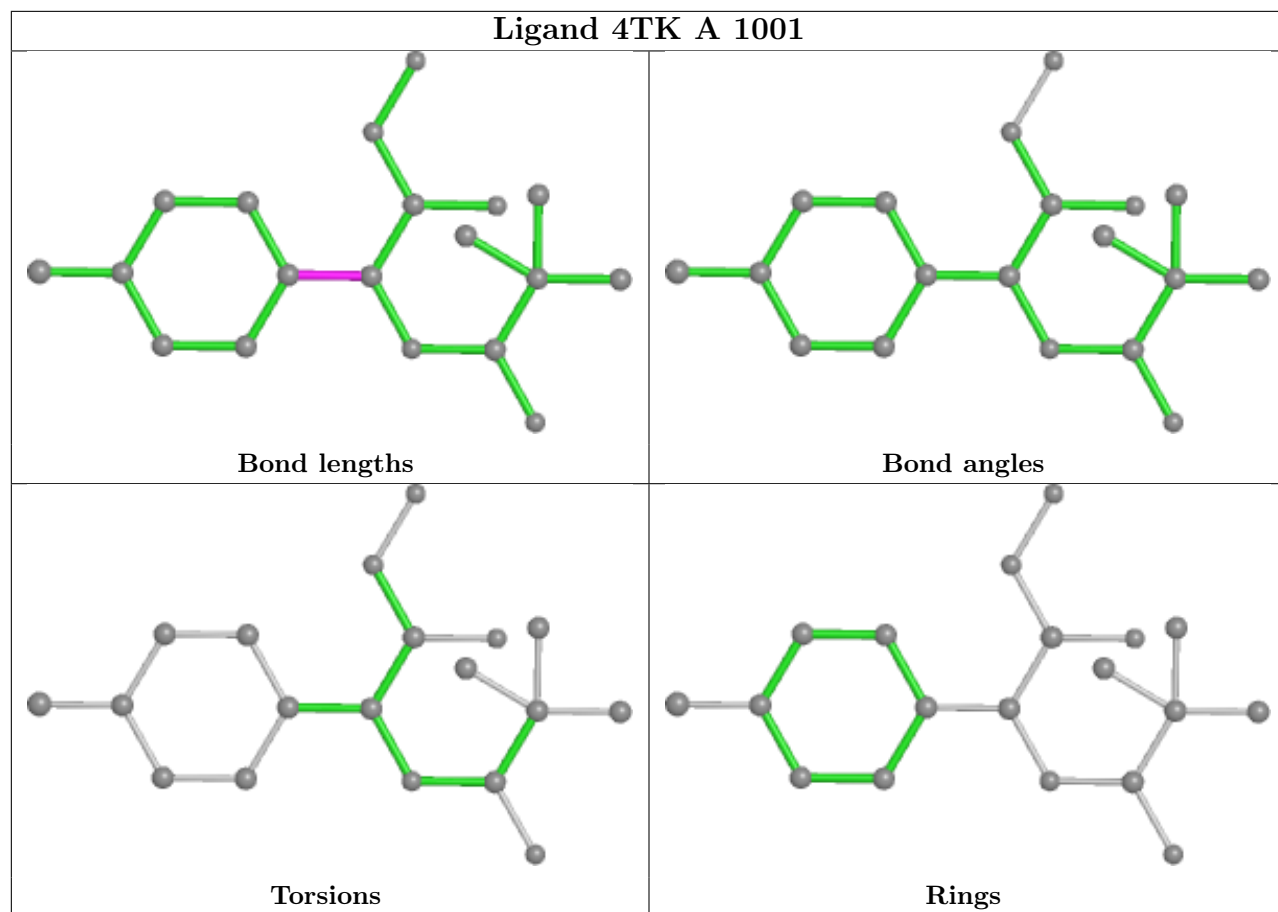
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

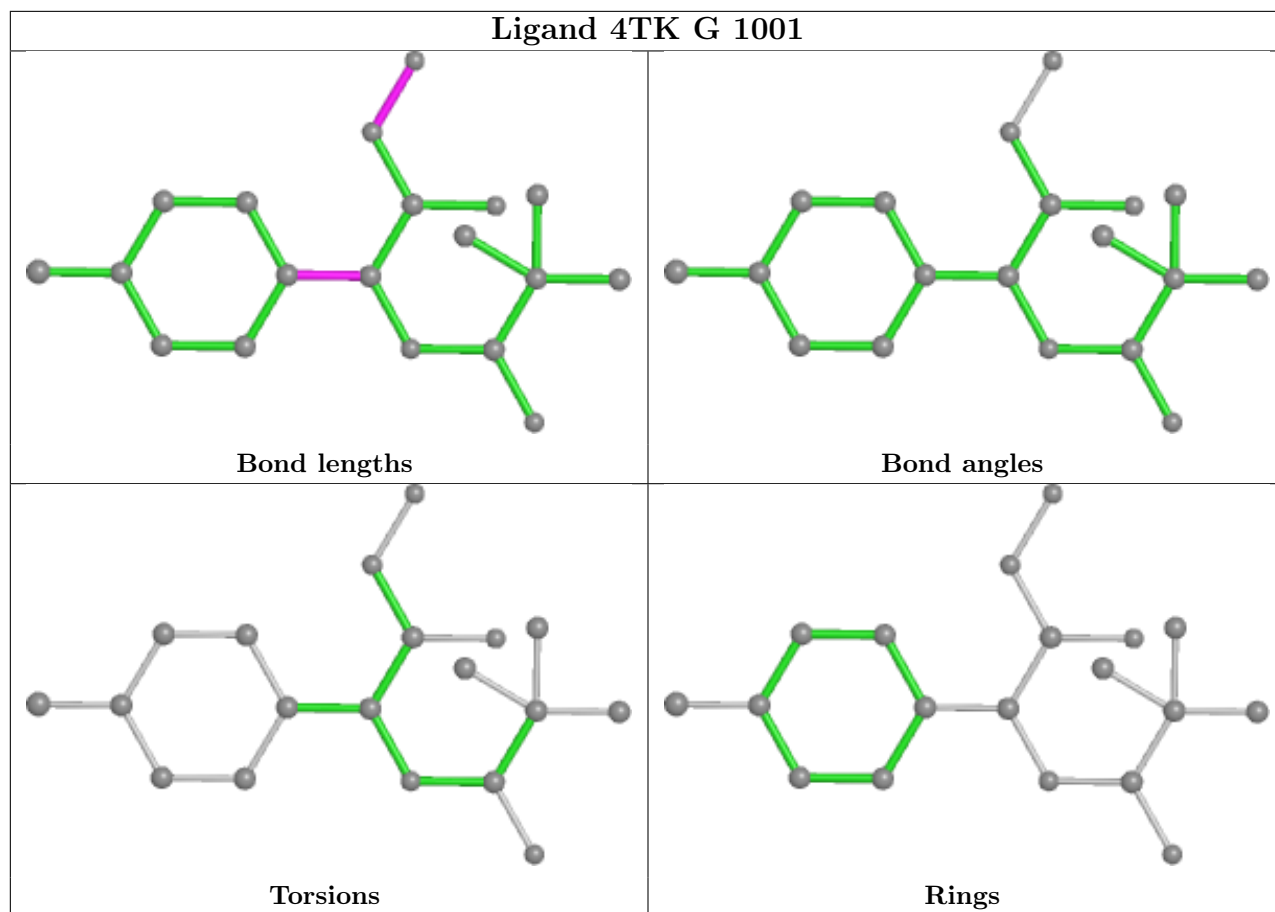


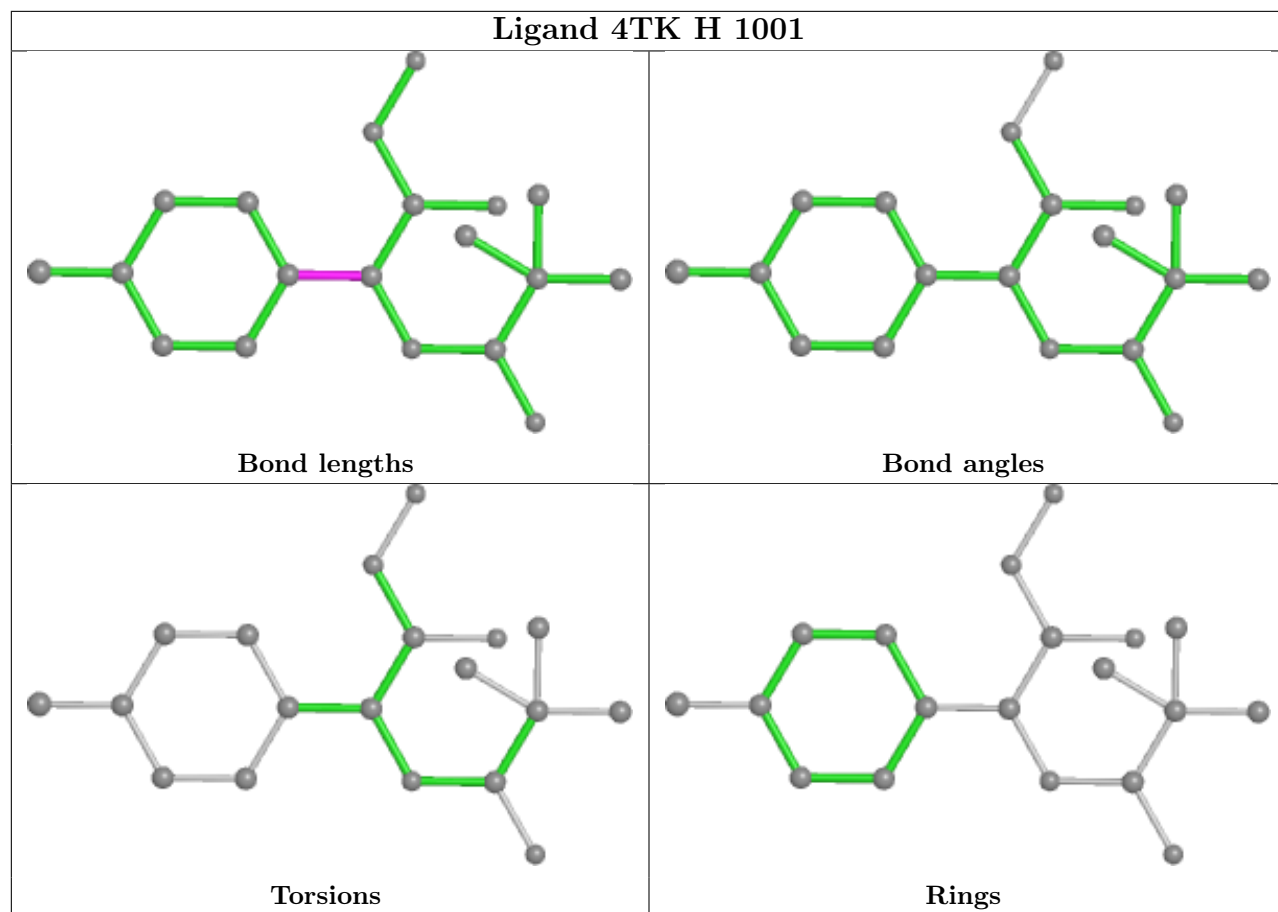


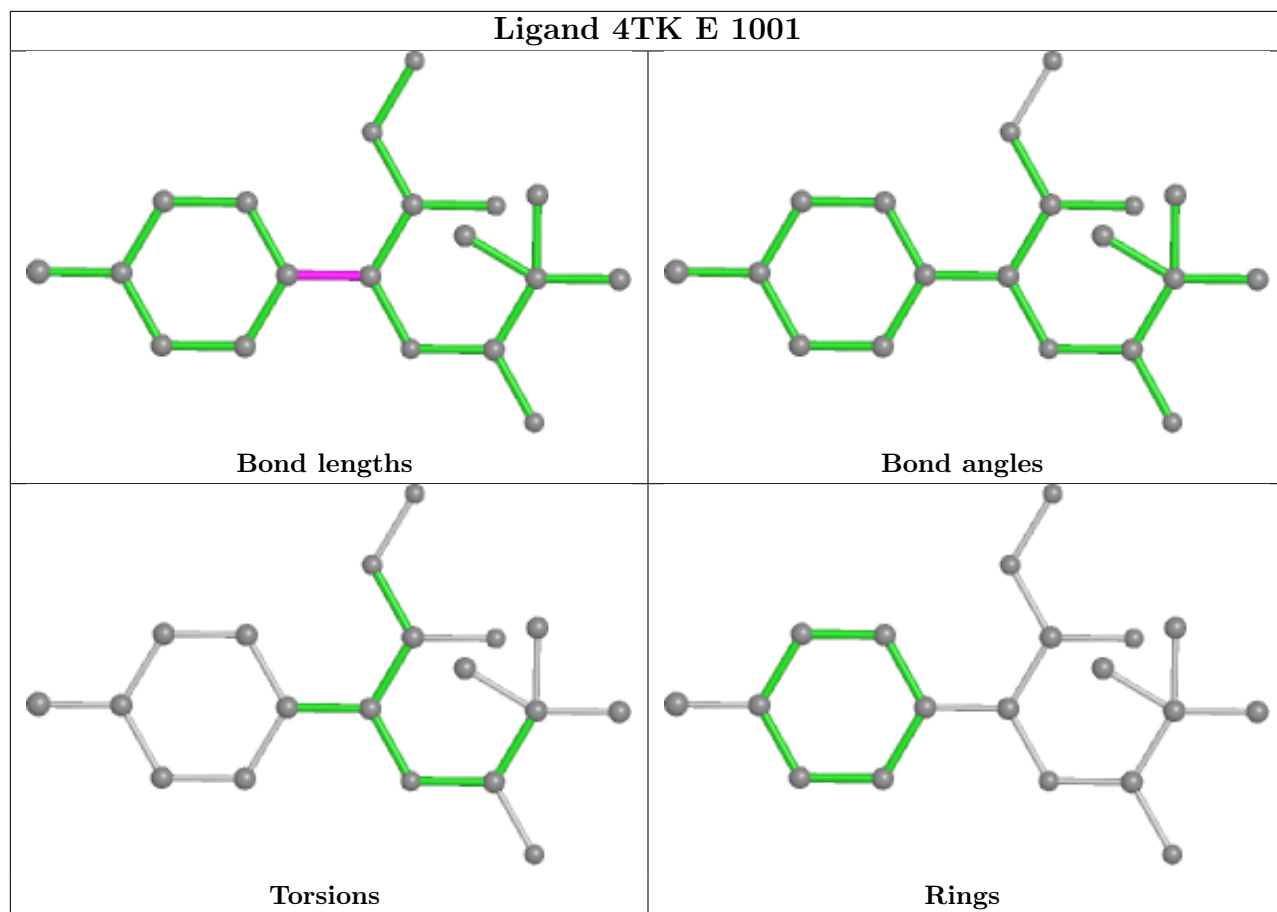


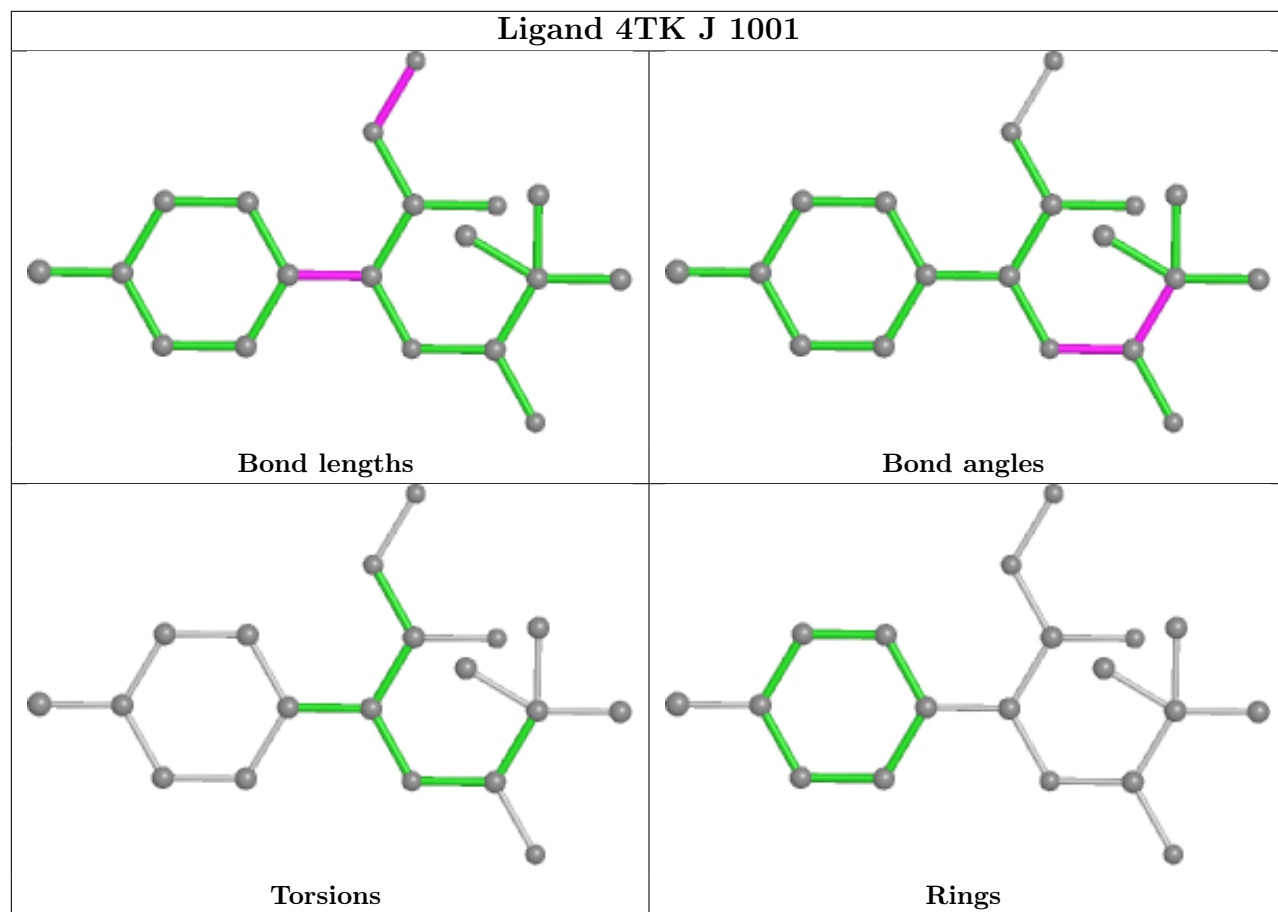


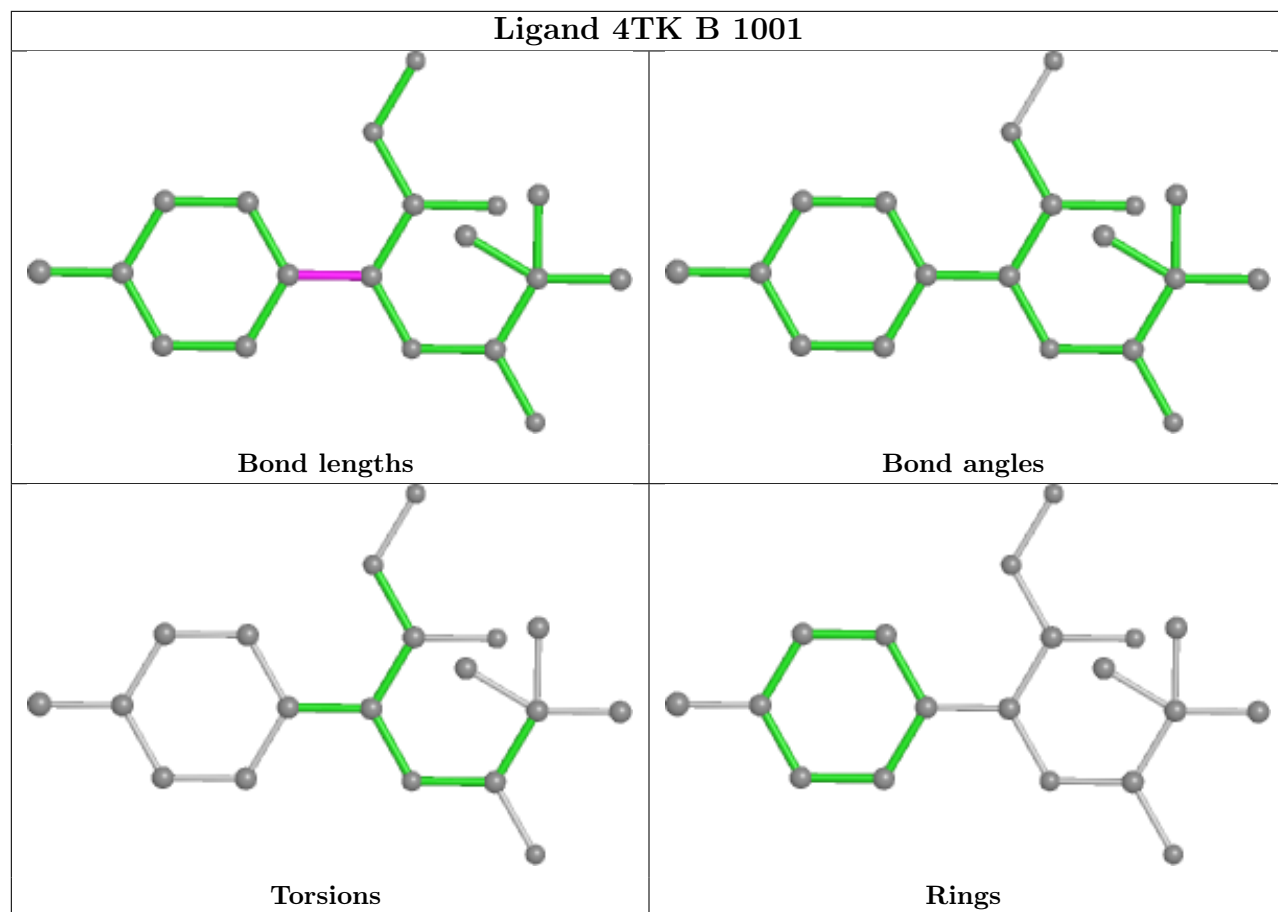


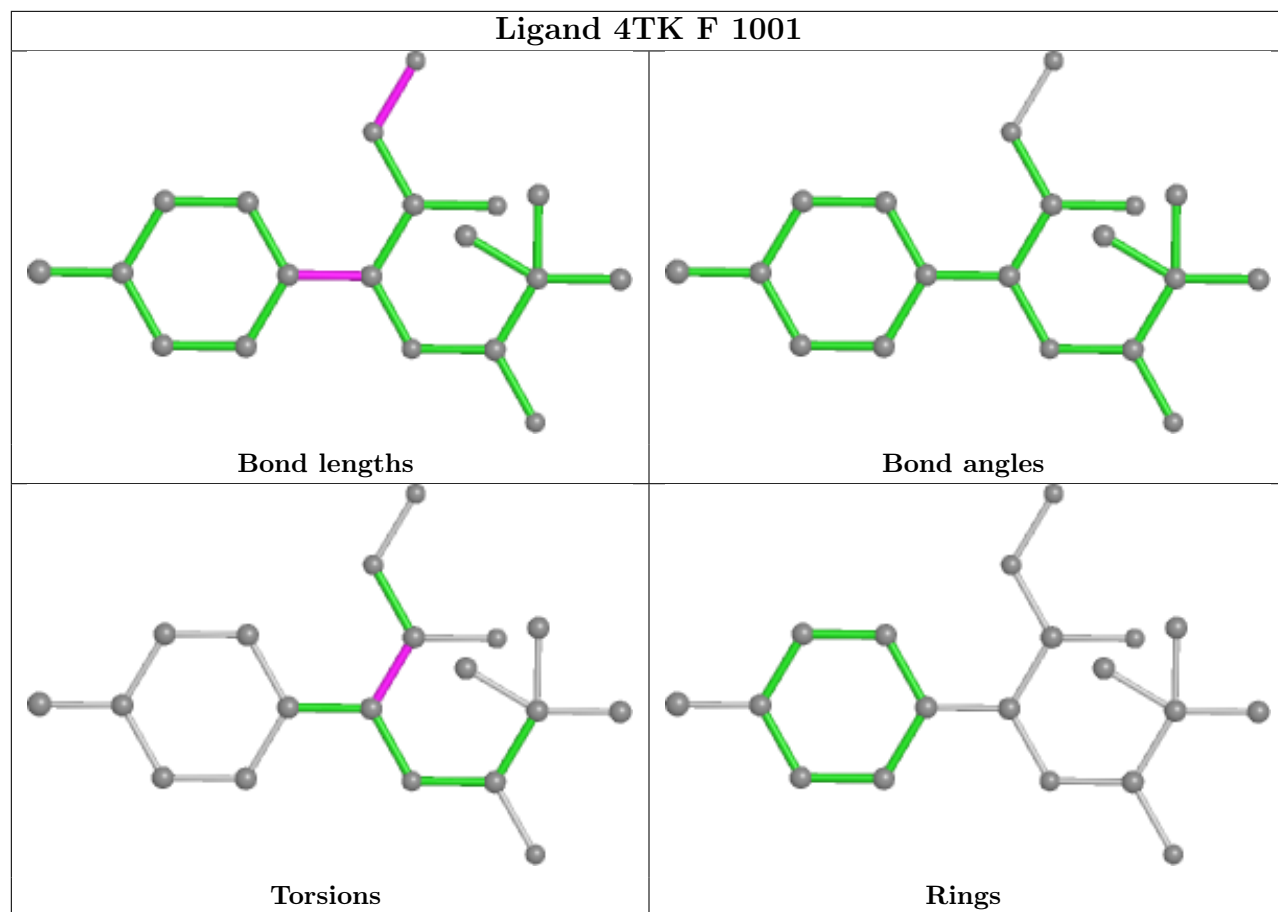


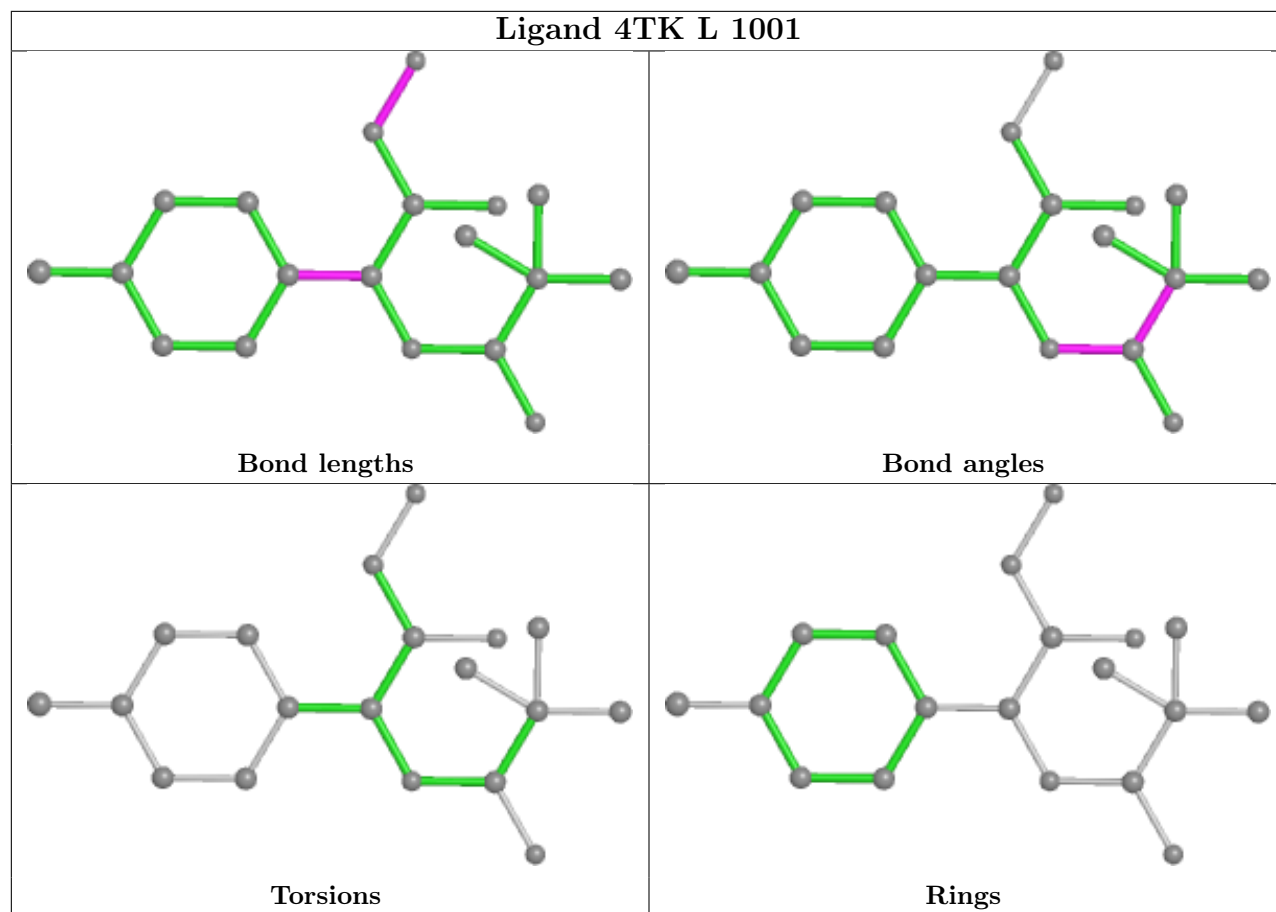












5.7 Other polymers [i](#)

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%)	-0.29	4 (0%) 86 84	18, 30, 48, 62	1 (0%)
1	B	516/522 (98%)	-0.11	8 (1%) 72 68	19, 30, 61, 74	4 (0%)
1	C	517/522 (99%)	-0.28	2 (0%) 92 91	20, 28, 48, 60	3 (0%)
1	D	513/522 (98%)	-0.40	3 (0%) 89 88	20, 28, 44, 61	2 (0%)
1	E	509/522 (97%)	-0.38	0 100 100	17, 28, 41, 57	5 (0%)
1	F	511/522 (97%)	-0.08	5 (0%) 82 80	23, 37, 59, 71	4 (0%)
1	G	519/522 (99%)	-0.32	1 (0%) 95 95	18, 29, 48, 65	5 (0%)
1	H	517/522 (99%)	-0.13	9 (1%) 70 66	20, 31, 60, 70	1 (0%)
1	I	518/522 (99%)	-0.23	2 (0%) 92 91	20, 31, 53, 65	2 (0%)
1	J	512/522 (98%)	-0.38	2 (0%) 92 91	20, 29, 47, 62	3 (0%)
1	K	508/522 (97%)	-0.38	0 100 100	19, 29, 42, 60	3 (0%)
1	L	511/522 (97%)	-0.26	3 (0%) 89 88	22, 33, 56, 71	3 (0%)
All	All	6170/6264 (98%)	-0.27	39 (0%) 89 88	17, 30, 54, 74	36 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	260	ASN	3.9
1	H	603	ASP	3.3
1	I	274	ALA	3.1
1	F	549	SER	3.1
1	B	196	ALA	3.0
1	C	274	ALA	3.0
1	B	136	GLY	2.9
1	H	259	VAL	2.9
1	J	219	LEU	2.8
1	G	362	LYS	2.7
1	F	146	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	85	ALA	2.7
1	H	363	GLY	2.6
1	B	276	THR	2.5
1	F	276	THR	2.5
1	C	117	ILE	2.5
1	D	603	ASP	2.5
1	L	146	SER	2.4
1	I	398	PHE	2.4
1	L	138	GLU	2.3
1	H	218	LYS	2.3
1	A	400	MET	2.3
1	B	176	TYR	2.3
1	F	272	ASN	2.3
1	H	273	ASN	2.2
1	A	362	LYS	2.2
1	L	549	SER	2.2
1	B	269	VAL	2.2
1	H	261	MET	2.2
1	A	363	GLY	2.1
1	F	121	CYS	2.1
1	B	225	VAL	2.1
1	B	277	TYR	2.1
1	J	136	GLY	2.1
1	H	121	CYS	2.0
1	H	196	ALA	2.0
1	H	149	ASN	2.0
1	A	159	ASP	2.0
1	B	114	VAL	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
8	DMS	G	1006	4/4	0.71	0.30	53,61,64,98	0
6	1PE	A	1007	12/16	0.79	0.23	36,43,52,52	0
6	1PE	B	1006	10/16	0.80	0.29	36,43,47,55	0
6	1PE	H	1006	10/16	0.80	0.28	35,50,64,68	0
5	GOL	G	1005	6/6	0.80	0.29	43,53,60,61	0
5	GOL	J	1005	6/6	0.81	0.20	37,38,40,48	0
6	1PE	D	1006	10/16	0.83	0.20	27,40,46,57	0
6	1PE	H	1005	6/16	0.83	0.21	30,35,38,46	0
6	1PE	F	1005	10/16	0.85	0.30	40,48,57,59	0
7	SO4	I	1010	5/5	0.86	0.17	64,68,72,87	0
6	1PE	L	1005	10/16	0.86	0.17	33,39,51,51	0
8	DMS	I	1006	4/4	0.86	0.35	41,46,62,81	0
6	1PE	E	1005	12/16	0.87	0.17	26,36,39,44	0
5	GOL	I	1005	6/6	0.88	0.21	28,32,34,39	0
6	1PE	G	1007	9/16	0.88	0.19	30,35,40,40	0
6	1PE	G	1008	6/16	0.88	0.20	34,39,40,42	0
6	1PE	G	1009	6/16	0.88	0.13	30,32,37,39	0
6	1PE	C	1006	13/16	0.88	0.33	32,48,56,62	0
8	DMS	J	1006	4/4	0.88	0.16	53,57,70,82	0
6	1PE	C	1007	9/16	0.89	0.16	24,28,34,40	0
7	SO4	G	1011	5/5	0.90	0.18	45,54,59,69	0
5	GOL	A	1005	6/6	0.90	0.24	32,36,45,46	0
6	1PE	I	1007	12/16	0.90	0.22	32,46,50,50	0
6	1PE	I	1008	11/16	0.90	0.21	36,42,49,49	0
5	GOL	B	1005	6/6	0.90	0.28	36,39,43,43	0
2	4TK	G	1001	19/19	0.91	0.23	18,23,31,38	19
2	4TK	D	1001	19/19	0.91	0.20	12,25,31,55	19
2	4TK	C	1001	19/19	0.92	0.18	21,24,31,58	19
2	4TK	A	1001	19/19	0.92	0.23	18,23,28,50	19
2	4TK	E	1001	19/19	0.92	0.22	18,22,28,39	19
2	4TK	B	1001	19/19	0.92	0.17	13,21,27,47	19
2	4TK	L	1001	19/19	0.92	0.22	17,22,28,38	19
6	1PE	J	1007	11/16	0.93	0.16	28,34,39,43	0
6	1PE	K	1005	12/16	0.93	0.18	18,32,58,64	0
2	4TK	I	1001	19/19	0.93	0.22	24,27,33,56	19
6	1PE	D	1007	10/16	0.93	0.16	33,36,44,45	0
2	4TK	J	1001	19/19	0.93	0.18	15,20,25,55	19
6	1PE	E	1006	12/16	0.93	0.17	25,32,59,63	0
2	4TK	F	1001	19/19	0.93	0.21	22,26,33,47	19
2	4TK	H	1001	19/19	0.93	0.18	17,23,27,51	19
4	CO3	K	1004	4/4	0.94	0.17	27,28,31,33	0

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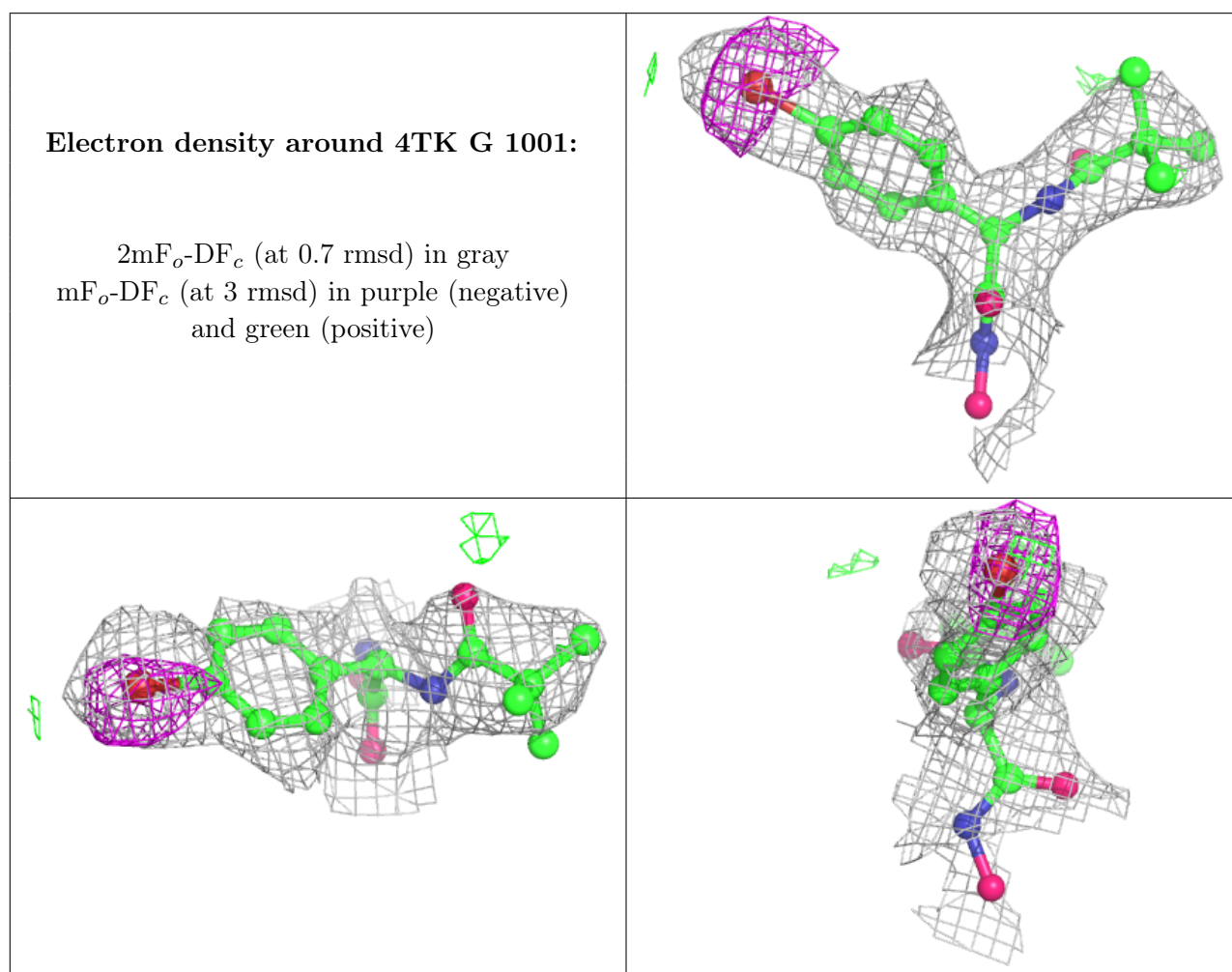
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	DMS	D	1005	4/4	0.94	0.25	31,34,52,52	0
2	4TK	K	1001	19/19	0.94	0.21	19,22,27,42	19
4	CO3	I	1004	4/4	0.94	0.17	27,28,28,31	0
6	1PE	A	1006	9/16	0.94	0.19	26,31,35,41	0
7	SO4	G	1010	5/5	0.95	0.14	47,56,60,62	0
8	DMS	C	1005	4/4	0.95	0.12	36,37,43,59	0
7	SO4	A	1008	5/5	0.95	0.11	52,53,56,66	0
4	CO3	D	1004	4/4	0.96	0.13	24,26,28,29	0
4	CO3	F	1004	4/4	0.96	0.11	28,28,30,32	0
4	CO3	G	1004	4/4	0.96	0.12	29,29,30,31	0
4	CO3	C	1004	4/4	0.96	0.15	24,29,31,31	0
4	CO3	J	1004	4/4	0.96	0.13	23,23,24,26	0
7	SO4	H	1007	5/5	0.97	0.08	19,23,27,28	0
3	ZN	K	1003	1/1	0.97	0.11	30,30,30,30	0
7	SO4	J	1008	5/5	0.97	0.33	41,44,47,54	0
7	SO4	L	1006	5/5	0.97	0.16	38,51,55,60	0
4	CO3	L	1004	4/4	0.97	0.16	24,24,27,28	0
4	CO3	A	1004	4/4	0.97	0.12	27,28,29,30	0
4	CO3	H	1004	4/4	0.97	0.14	23,24,27,30	0
3	ZN	H	1002	1/1	0.97	0.10	27,27,27,27	0
3	ZN	K	1002	1/1	0.97	0.12	29,29,29,29	0
3	ZN	C	1003	1/1	0.98	0.09	24,24,24,24	0
3	ZN	D	1003	1/1	0.98	0.08	27,27,27,27	0
7	SO4	I	1009	5/5	0.98	0.23	44,52,64,66	0
4	CO3	B	1004	4/4	0.98	0.10	20,21,23,27	0
3	ZN	F	1002	1/1	0.98	0.10	30,30,30,30	0
3	ZN	F	1003	1/1	0.98	0.13	31,31,31,31	0
4	CO3	E	1004	4/4	0.98	0.07	26,27,28,30	0
3	ZN	G	1002	1/1	0.98	0.09	32,32,32,32	0
3	ZN	A	1003	1/1	0.98	0.13	24,24,24,24	0
3	ZN	I	1003	1/1	0.98	0.09	29,29,29,29	0
3	ZN	C	1002	1/1	0.98	0.11	27,27,27,27	0
7	SO4	B	1007	5/5	0.99	0.07	22,23,25,25	0
7	SO4	D	1008	5/5	0.99	0.08	23,25,34,36	0
3	ZN	B	1003	1/1	0.99	0.10	26,26,26,26	0
3	ZN	H	1003	1/1	0.99	0.10	24,24,24,24	0
3	ZN	I	1002	1/1	0.99	0.13	26,26,26,26	0
3	ZN	E	1002	1/1	0.99	0.12	30,30,30,30	0
3	ZN	J	1002	1/1	0.99	0.08	29,29,29,29	0
3	ZN	J	1003	1/1	0.99	0.07	27,27,27,27	0
7	SO4	J	1009	5/5	0.99	0.08	24,29,32,40	0
3	ZN	E	1003	1/1	0.99	0.09	32,32,32,32	0

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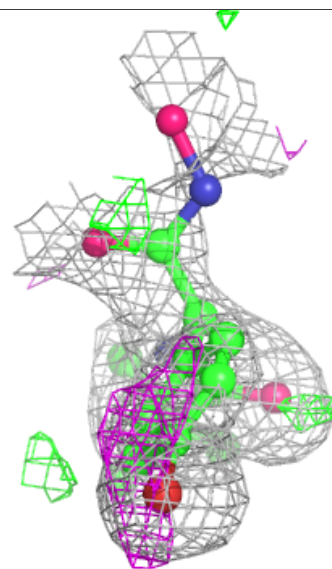
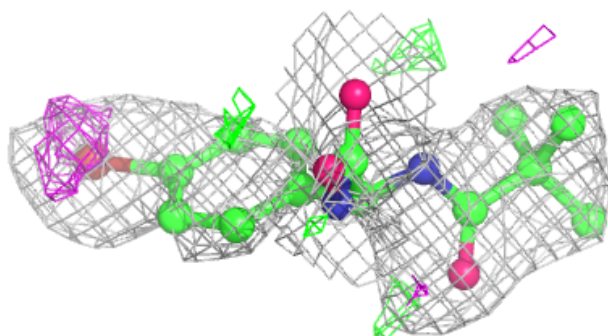
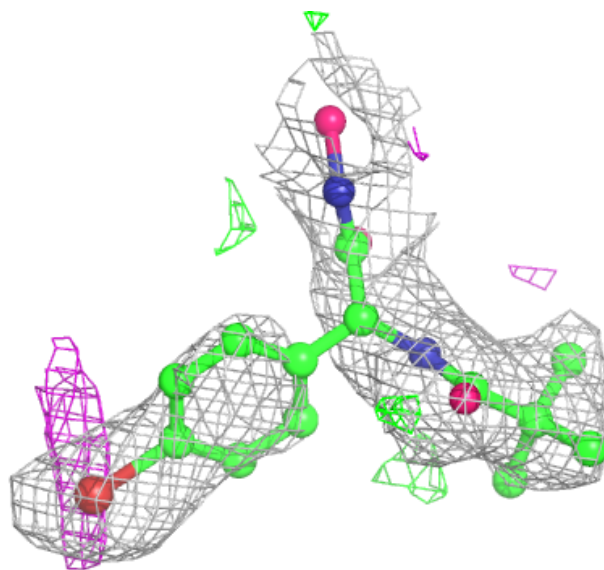
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	A	1002	1/1	0.99	0.10	31,31,31,31	0
3	ZN	L	1002	1/1	0.99	0.11	27,27,27,27	0
3	ZN	L	1003	1/1	0.99	0.13	27,27,27,27	0
3	ZN	B	1002	1/1	0.99	0.07	23,23,23,23	0
3	ZN	D	1002	1/1	0.99	0.08	26,26,26,26	0
3	ZN	G	1003	1/1	1.00	0.13	25,25,25,25	0

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.



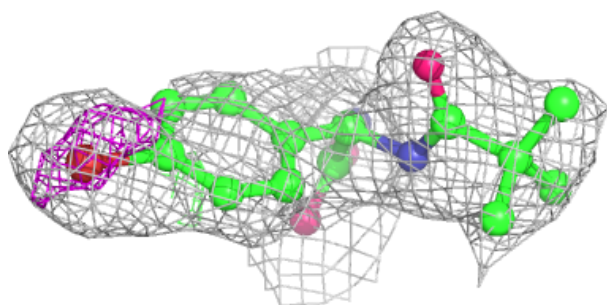
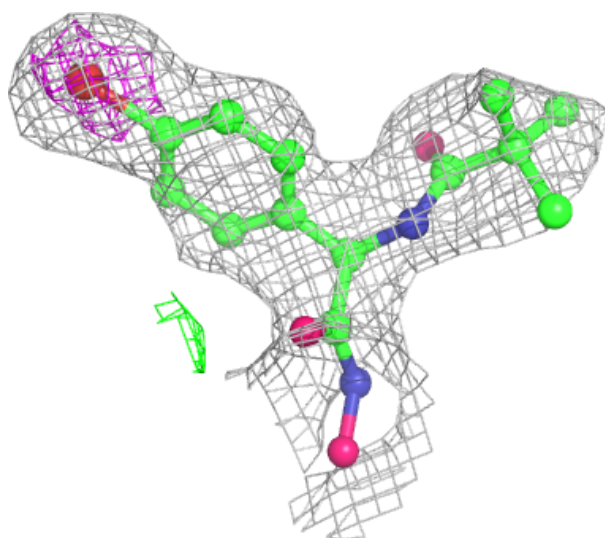
Electron density around 4TK D 1001:

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



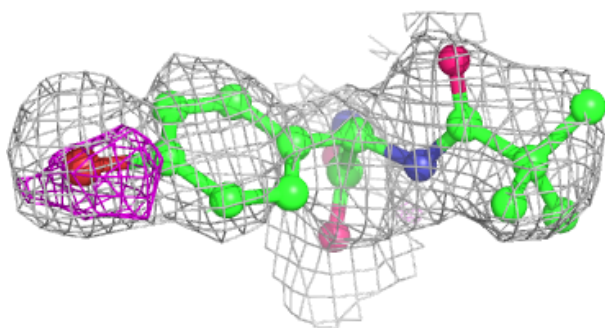
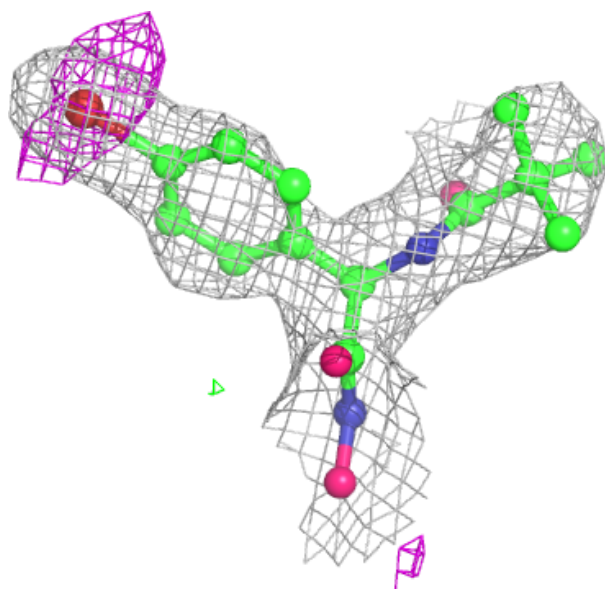
Electron density around 4TK C 1001:

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



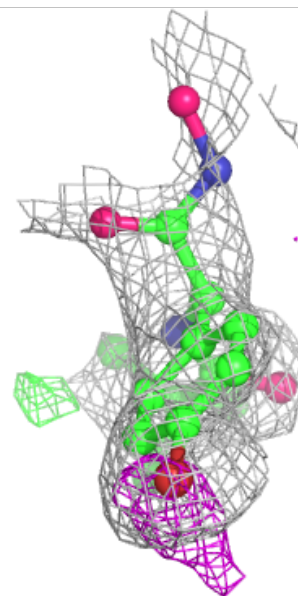
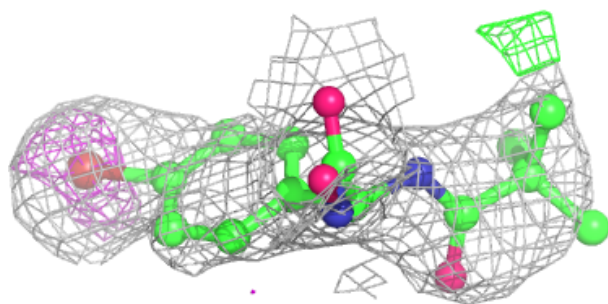
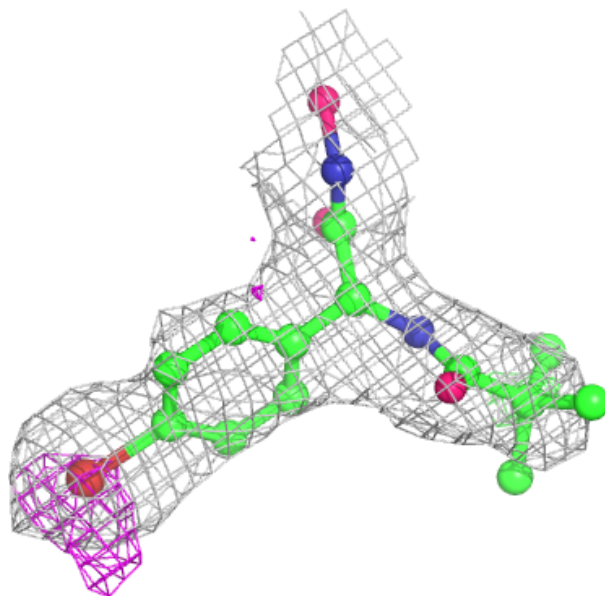
Electron density around 4TK A 1001:

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



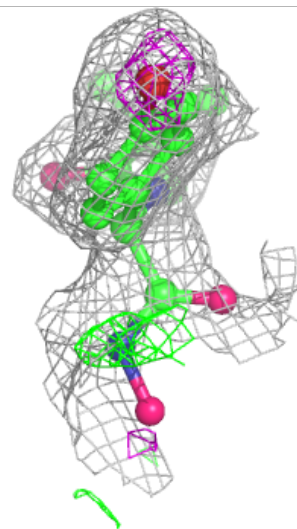
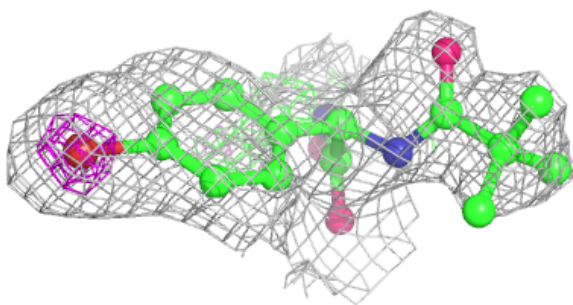
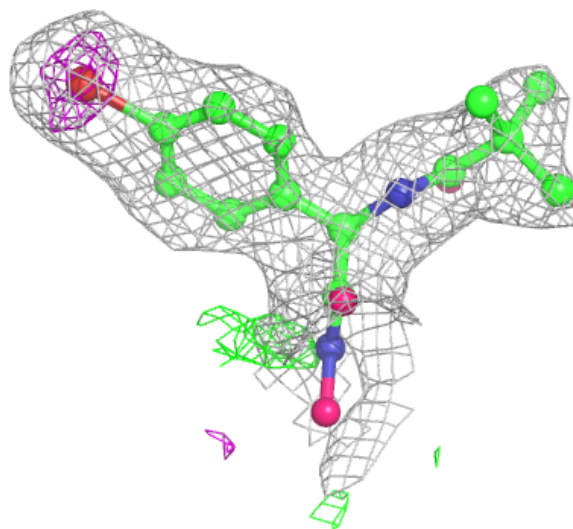
Electron density around 4TK E 1001:

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



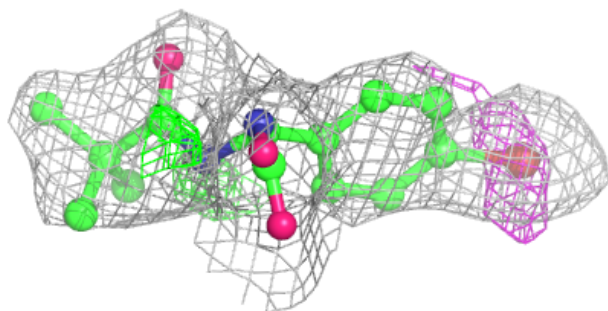
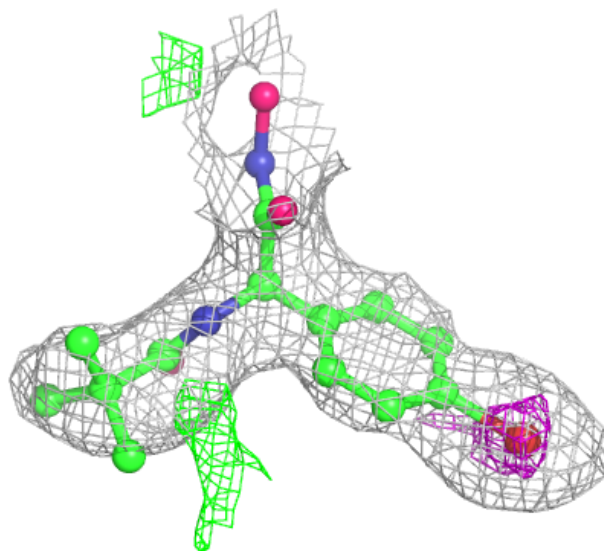
Electron density around 4TK B 1001:

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



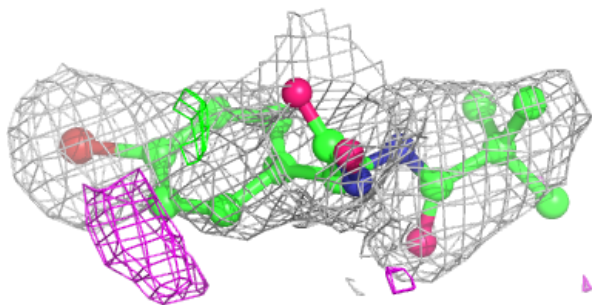
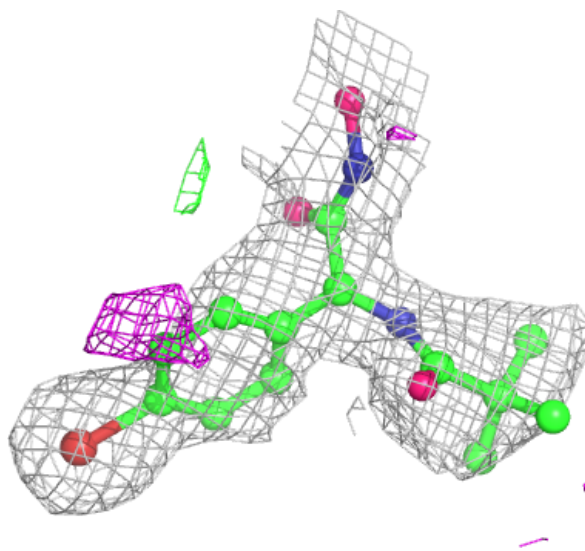
Electron density around 4TK L 1001:

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



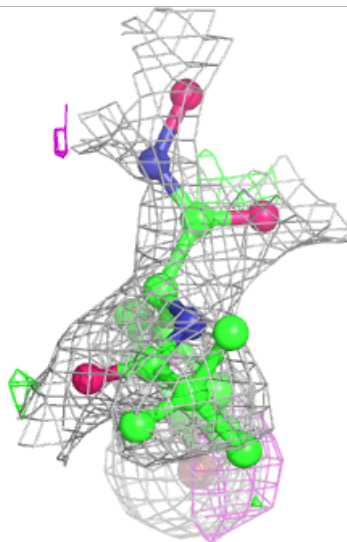
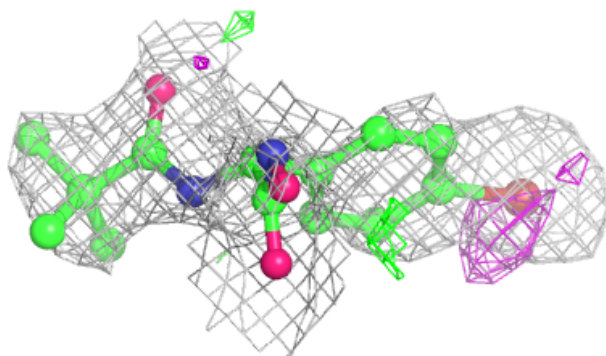
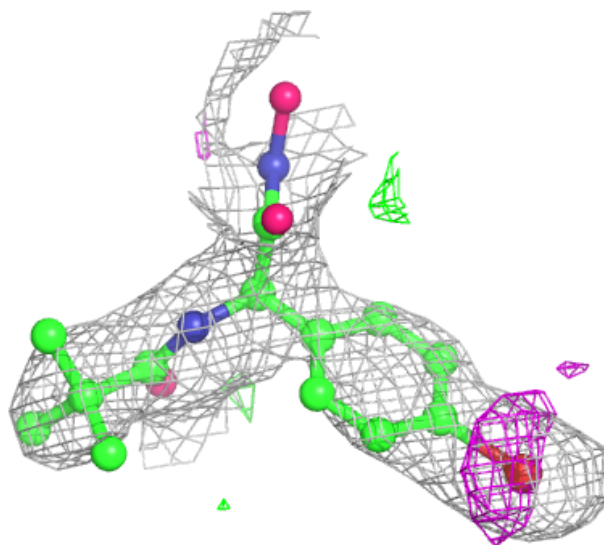
Electron density around 4TK I 1001:

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



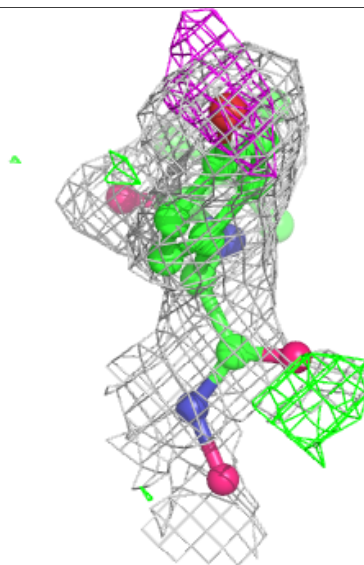
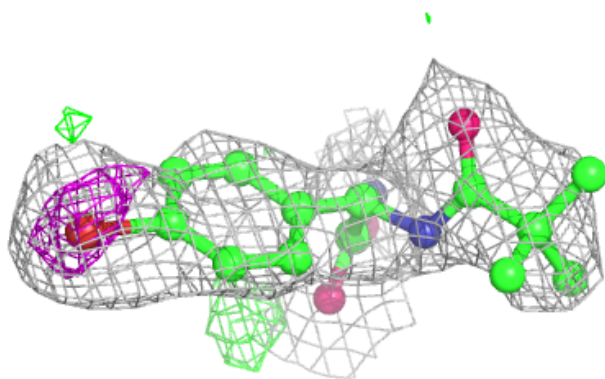
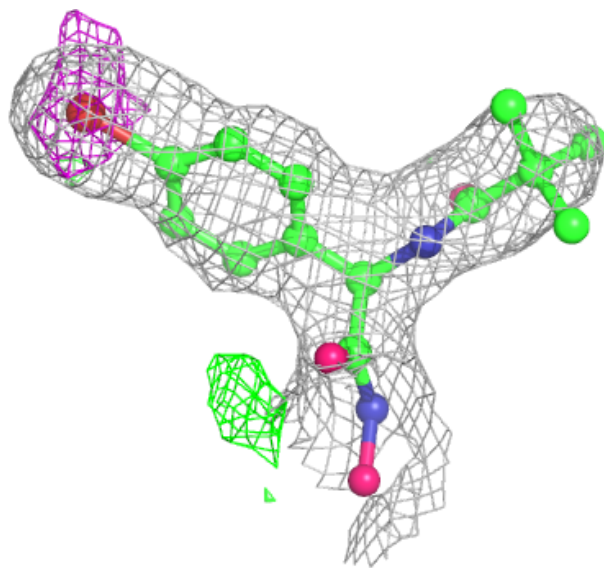
Electron density around 4TK J 1001:

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



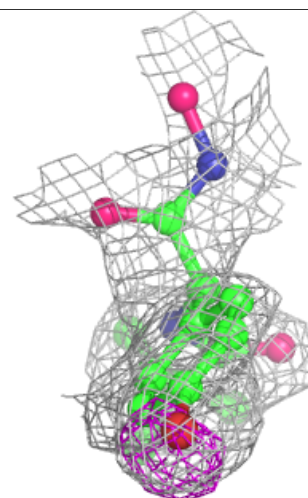
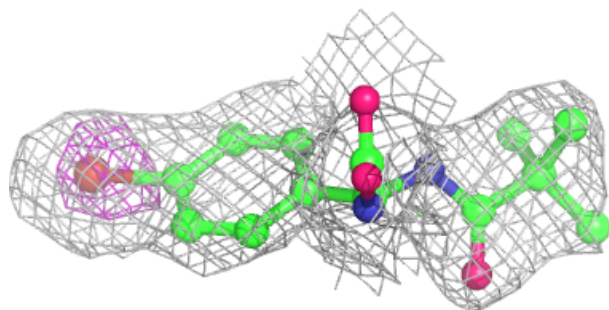
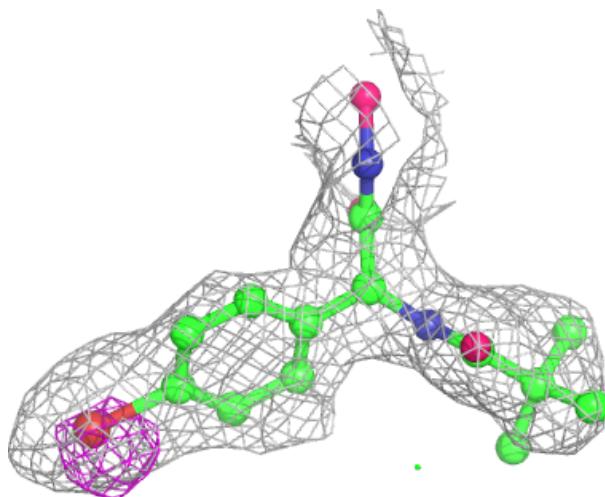
Electron density around 4TK F 1001:

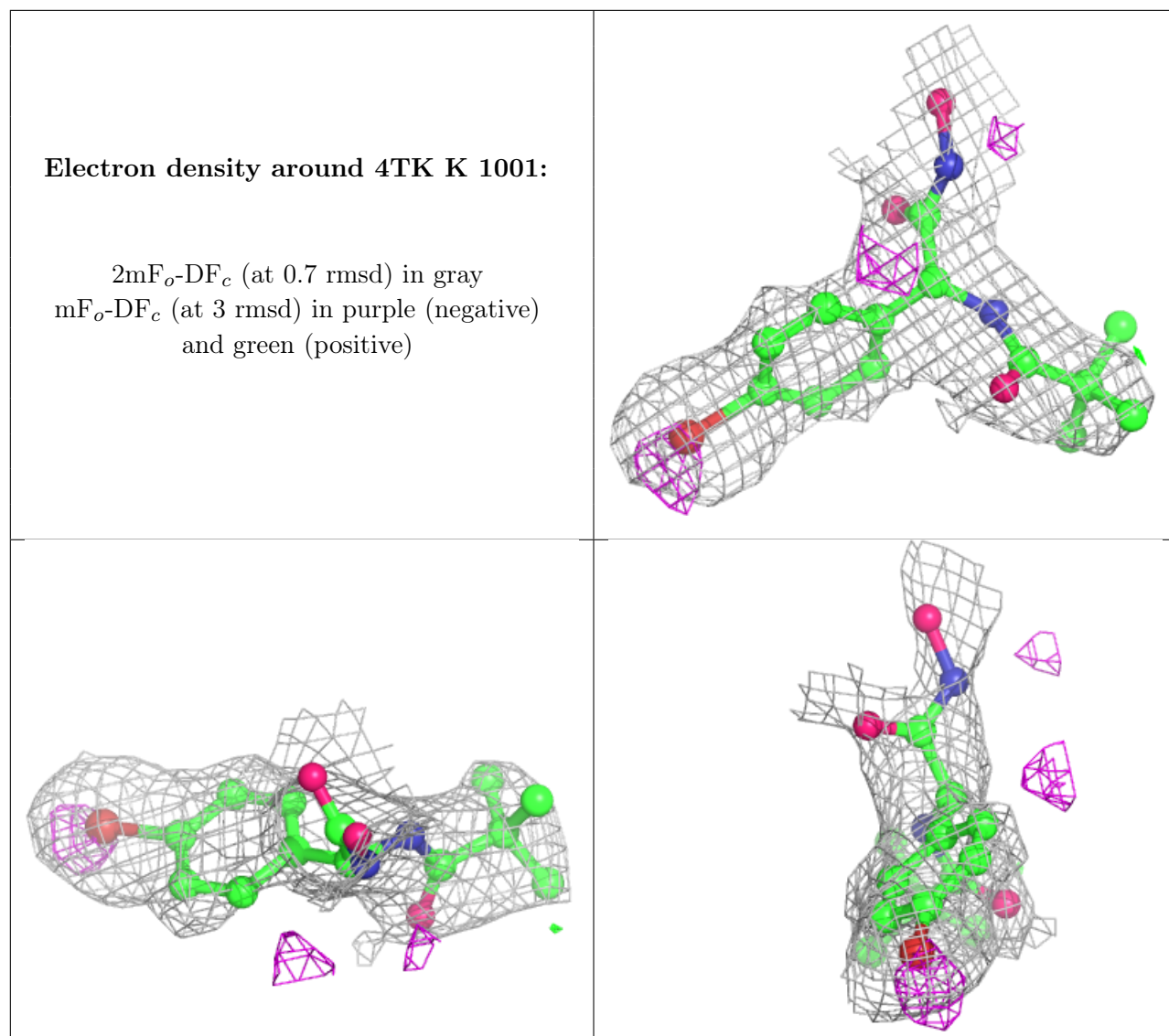
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4TK 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.