



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:09 PM BST

PDB ID : 4ZYQ
Title : X-ray crystal structure of PfA-M17 in complex with hydroxamic acid-based inhibitor 10s
Authors : Drinkwater, N.; McGowan, S.
Deposited on : 2015-05-22
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 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 : 2.13.1
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) : 2.13.1

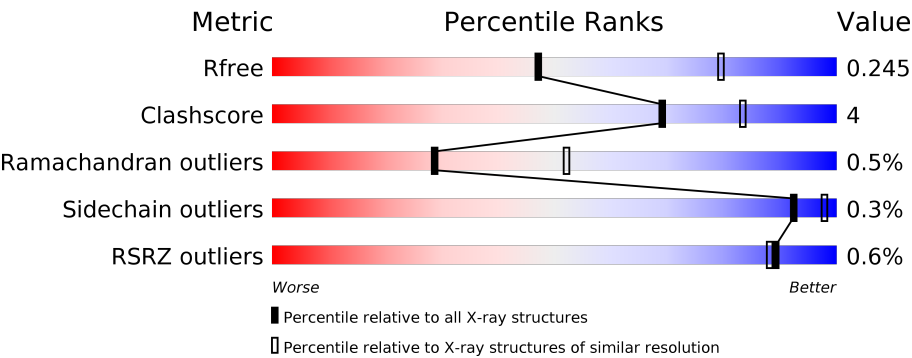
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	522	<div><div>%</div><div><div></div><div>89%</div><div>10%</div><div>.</div></div></div>
1	B	522	<div><div>2%</div><div><div></div><div>88%</div><div>10%</div><div>.</div></div></div>
1	C	522	<div><div></div><div><div></div><div>89%</div><div>10%</div><div>.</div></div></div>
1	D	522	<div><div></div><div><div></div><div>87%</div><div>11%</div><div>..</div></div></div>
1	E	522	<div><div></div><div><div></div><div>89%</div><div>8%</div><div>.</div></div></div>
1	F	522	<div><div>%</div><div><div></div><div>90%</div><div>8%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	522	 90% 9% .
1	H	522	 87% 11% .
1	I	522	 90% 9% .
1	J	522	 88% 10% ..
1	K	522	 89% 8% .
1	L	522	 90% 8% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CO3	J	1004	-	-	X	-
6	SO4	B	1006	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 49414 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable M17 family aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3942	2531	634	758	19			
1	B	516	Total	C	N	O	S	0	0	0
			3893	2504	633	737	19			
1	C	516	Total	C	N	O	S	0	0	0
			3935	2530	635	751	19			
1	D	514	Total	C	N	O	S	0	0	0
			3911	2519	632	740	20			
1	E	509	Total	C	N	O	S	0	0	0
			3884	2502	623	740	19			
1	F	511	Total	C	N	O	S	0	0	0
			3843	2472	620	732	19			
1	G	519	Total	C	N	O	S	0	0	0
			3970	2550	639	762	19			
1	H	516	Total	C	N	O	S	0	0	0
			3890	2501	633	737	19			
1	I	518	Total	C	N	O	S	0	0	0
			3939	2532	637	751	19			
1	J	513	Total	C	N	O	S	0	0	0
			3922	2523	633	746	20			
1	K	508	Total	C	N	O	S	0	0	0
			3891	2507	624	741	19			
1	L	511	Total	C	N	O	S	0	0	0
			3827	2462	617	729	19			

There are 36 discrepancies between the modelled and reference sequences:

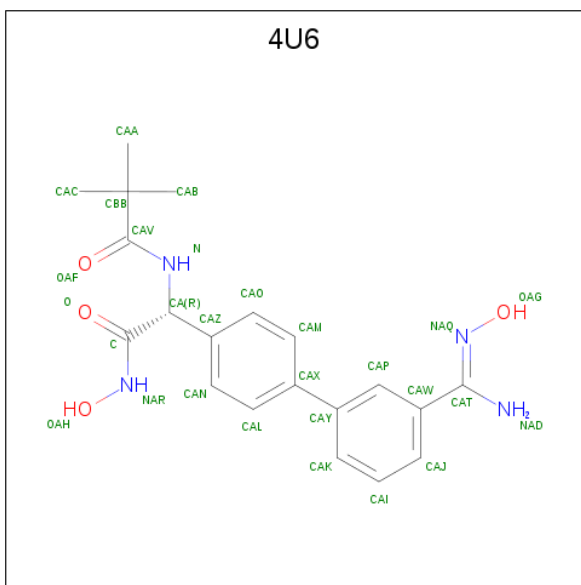
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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

- Molecule 2 is N-[(1R)-2-(hydroxyamino)-1-[3'-(N'-hydroxycarbamimidoyl)biphenyl-4-yl]-2-oxoethyl]-2,2-dimethylpropanamide (three-letter code: 4U6) (formula: C₂₀H₂₄N₄O₄).

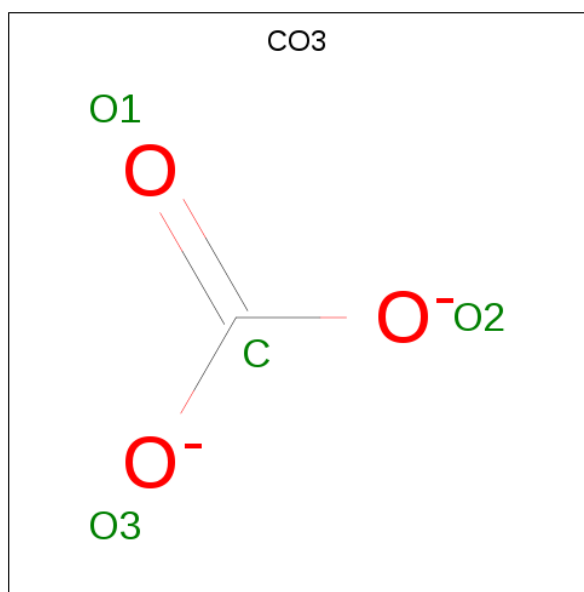


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 28	C 20	N 4	O 4	0	0
2	B	1	Total 28	C 20	N 4	O 4	0	0
2	C	1	Total 28	C 20	N 4	O 4	0	0
2	D	1	Total 28	C 20	N 4	O 4	0	0
2	E	1	Total 28	C 20	N 4	O 4	0	0
2	F	1	Total 28	C 20	N 4	O 4	0	0
2	G	1	Total 28	C 20	N 4	O 4	0	0
2	H	1	Total 28	C 20	N 4	O 4	0	0
2	I	1	Total 28	C 20	N 4	O 4	0	0
2	J	1	Total 28	C 20	N 4	O 4	0	0
2	K	1	Total 28	C 20	N 4	O 4	0	0
2	L	1	Total 28	C 20	N 4	O 4	0	0

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

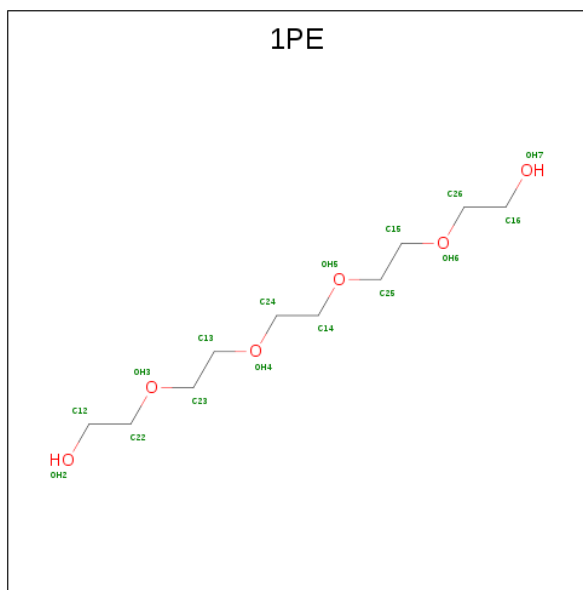
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total 2	Zn 2	0	0
3	J	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	K	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0
3	L	2	Total 2	Zn 2	0	0
3	F	2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

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



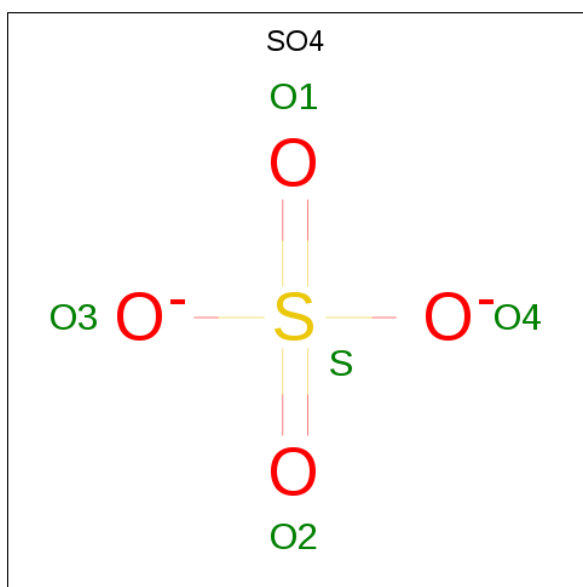
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 1 3	0	0
4	B	1	Total C O 4 1 3	0	0
4	C	1	Total C O 4 1 3	0	0
4	D	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0
4	G	1	Total C O 4 1 3	0	0
4	H	1	Total C O 4 1 3	0	0
4	I	1	Total C O 4 1 3	0	0
4	J	1	Total C O 4 1 3	0	0
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 PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	162	Total	O	0	0
			162	162		
7	B	148	Total	O	0	0
			148	148		
7	C	168	Total	O	0	0
			168	168		
7	D	196	Total	O	0	0
			196	196		

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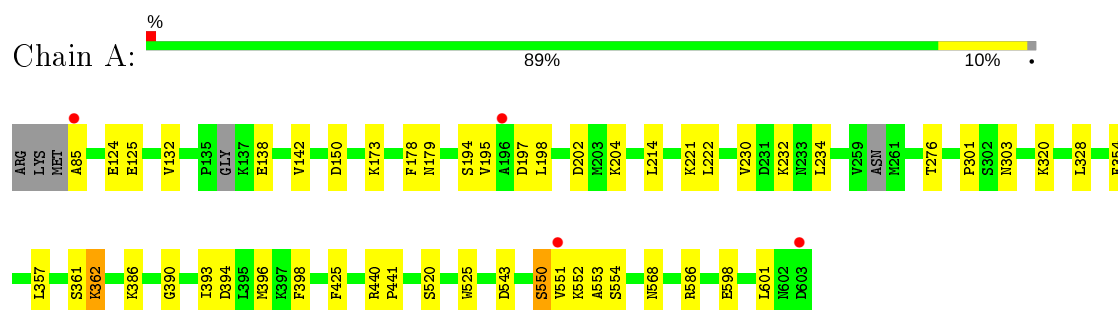
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	204	Total 204	O 204	0	0
7	F	126	Total 126	O 126	0	0
7	G	167	Total 167	O 167	0	0
7	H	127	Total 127	O 127	0	0
7	I	144	Total 144	O 144	0	0
7	J	148	Total 148	O 148	0	0
7	K	189	Total 189	O 189	0	0
7	L	134	Total 134	O 134	0	0

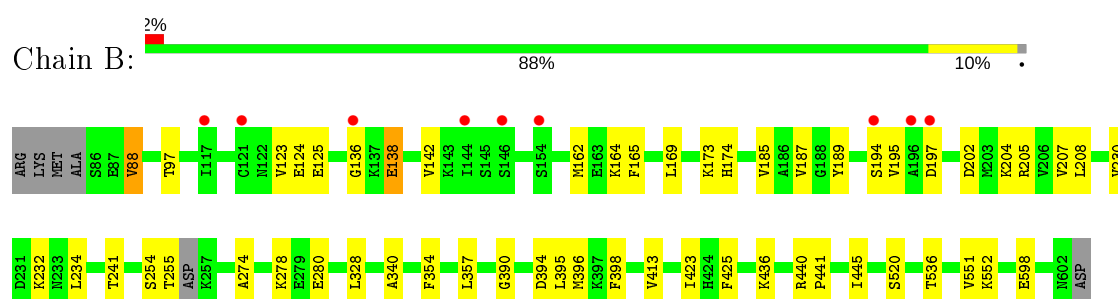
3 Residue-property plots

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.

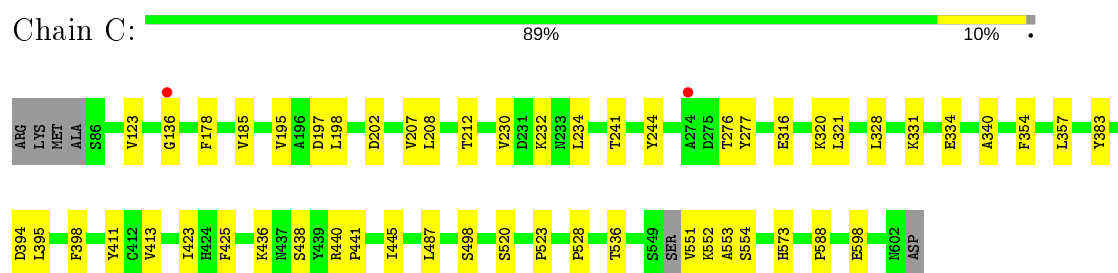
- Molecule 1: Probable M17 family aminopeptidase



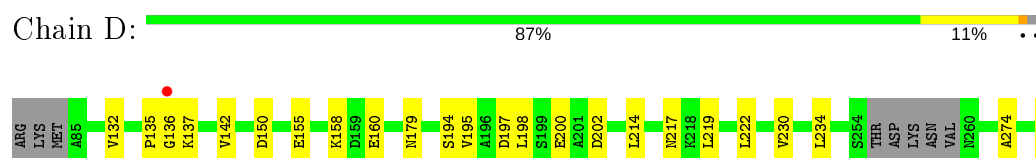
- Molecule 1: Probable M17 family aminopeptidase

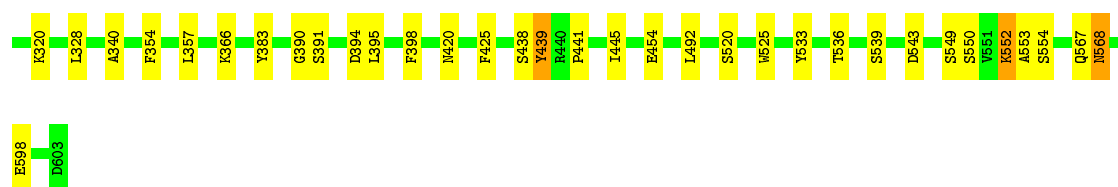


- Molecule 1: Probable M17 family aminopeptidase



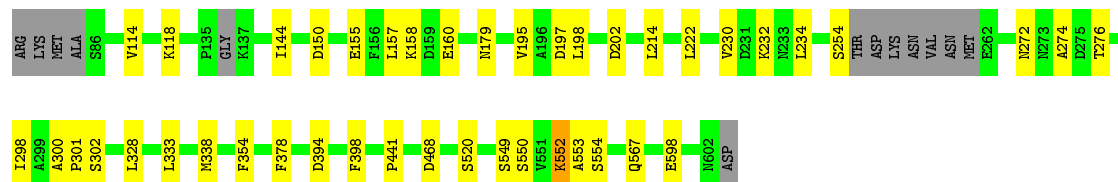
- Molecule 1: Probable M17 family aminopeptidase





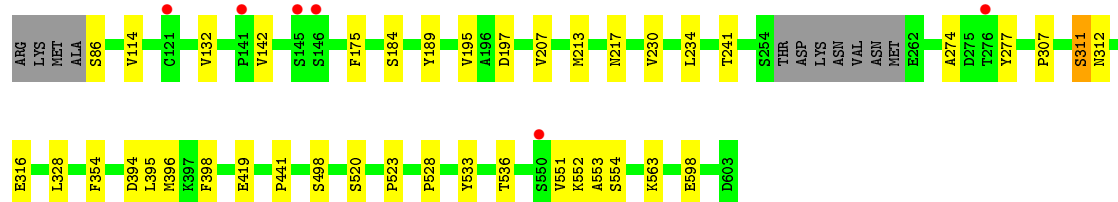
- Molecule 1: Probable M17 family aminopeptidase

Chain E: 89% 8% .



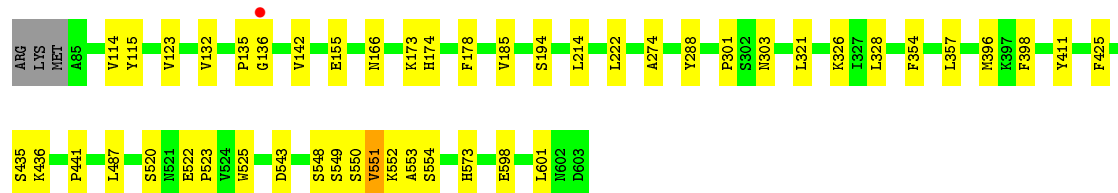
- Molecule 1: Probable M17 family aminopeptidase

Chain F: 90% 8% .



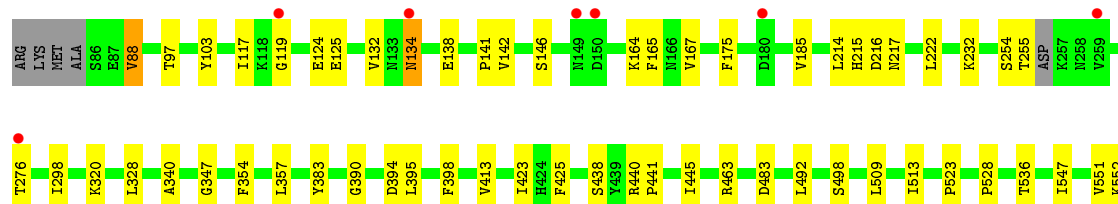
- Molecule 1: Probable M17 family aminopeptidase

Chain G: 90% 9% .



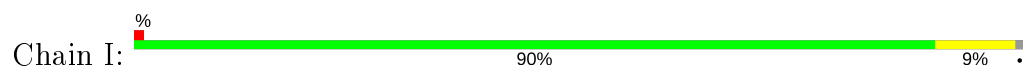
- Molecule 1: Probable M17 family aminopeptidase

Chain H: 87% 11% .

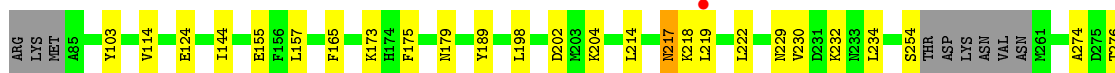
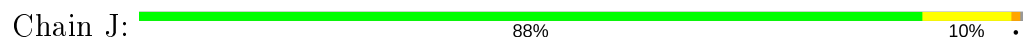




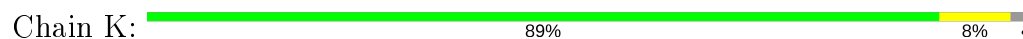
- Molecule 1: Probable M17 family aminopeptidase



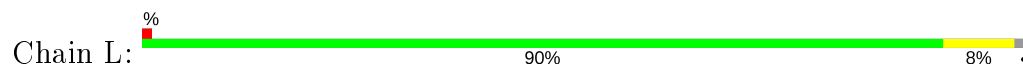
- Molecule 1: Probable M17 family aminopeptidase



- Molecule 1: Probable M17 family aminopeptidase



- Molecule 1: Probable M17 family aminopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.44Å 176.56Å 231.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.60 48.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.8 (48.56-2.60) 78.0 (48.56-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, R_{free}	0.192 , 0.244 0.195 , 0.245	Depositor DCC
R_{free} test set	9713 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49414	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 48.66 % 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 8.3349e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CO3, ZN, 4U6, 1PE

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	0.24	0/4018	0.44	0/5455
1	B	0.24	0/3970	0.43	0/5394
1	C	0.24	0/4012	0.40	0/5447
1	D	0.25	0/3988	0.44	0/5411
1	E	0.24	0/3960	0.43	0/5373
1	F	0.24	0/3920	0.42	0/5331
1	G	0.24	0/4048	0.43	0/5494
1	H	0.25	0/3967	0.43	0/5391
1	I	0.24	0/4017	0.41	0/5455
1	J	0.26	0/3999	0.45	0/5424
1	K	0.24	0/3966	0.41	0/5376
1	L	0.24	0/3904	0.43	0/5313
All	All	0.24	0/47769	0.43	0/64864

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

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	3942	0	3830	32	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3893	0	3777	32	0
1	C	3935	0	3843	30	0
1	D	3911	0	3832	39	0
1	E	3884	0	3801	24	0
1	F	3843	0	3703	27	0
1	G	3970	0	3883	31	1
1	H	3890	0	3771	39	0
1	I	3939	0	3843	28	0
1	J	3922	0	3851	42	0
1	K	3891	0	3824	28	0
1	L	3827	0	3671	26	0
2	A	28	0	0	1	0
2	B	28	0	0	1	0
2	C	28	0	0	0	0
2	D	28	0	0	2	0
2	E	28	0	0	0	0
2	F	28	0	0	0	0
2	G	28	0	0	0	0
2	H	28	0	0	1	0
2	I	28	0	0	0	0
2	J	28	0	0	2	0
2	K	28	0	0	0	0
2	L	28	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	2	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	21	0	22	2	0
5	B	10	0	10	0	0
5	C	22	0	24	2	0
5	D	20	0	20	2	0
5	E	24	0	28	0	0
5	F	22	0	25	1	0
5	G	21	0	20	0	0
5	H	10	0	10	2	0
5	I	23	0	26	0	0
5	J	11	0	13	2	0
5	K	12	0	14	2	0
5	L	10	0	13	0	0
6	A	5	0	0	0	0
6	B	5	0	0	2	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	G	5	0	0	1	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	0	0
7	A	162	0	0	5	0
7	B	148	0	0	1	0
7	C	168	0	0	1	0
7	D	196	0	0	1	0
7	E	204	0	0	1	0
7	F	126	0	0	1	0
7	G	167	0	0	2	0
7	H	127	0	0	1	0
7	I	144	0	0	3	0
7	J	148	0	0	2	0
7	K	189	0	0	3	0
7	L	134	0	0	2	0
All	All	49414	0	45854	346	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:GLN:C	1:D:568:ASN:HD22	1.74	0.89
1:H:134:ASN:ND2	1:H:141:PRO:O	2.12	0.83
1:J:217:ASN:ND2	1:J:219:LEU:H	1.78	0.81
1:I:143:LYS:NZ	1:I:159:ASP:OD2	2.14	0.80
1:D:390:GLY:O	2:D:1001:4U6:OAG	2.01	0.78
1:F:316:GLU:HG3	5:F:1006:1PE:H131	1.67	0.76
1:J:390:GLY:O	2:J:1001:4U6:OAG	2.04	0.76
1:J:217:ASN:HD22	1:J:219:LEU:H	1.33	0.74
1:I:232:LYS:NZ	1:I:276:THR:O	2.21	0.72
1:H:134:ASN:HB2	1:H:167:VAL:HG21	1.72	0.72
1:J:232:LYS:NZ	1:J:276:THR:O	2.23	0.72
1:B:173:LYS:NZ	1:F:217:ASN:OD1	2.23	0.71
1:G:550:SER:HA	1:G:552:LYS:H	1.53	0.71
1:G:123:VAL:HG12	1:G:185:VAL:HG21	1.71	0.71
1:K:232:LYS:NZ	1:K:276:THR:O	2.23	0.71
1:C:320:LYS:HZ1	5:C:1005:1PE:H142	1.55	0.70
1:H:492:LEU:HD22	1:K:552:LYS:HE3	1.74	0.70
1:A:320:LYS:HZ1	5:A:1006:1PE:H152	1.57	0.70
1:E:549:SER:N	1:E:550:SER:HA	2.07	0.70
1:D:357:LEU:HB2	1:D:425:PHE:HB2	1.74	0.69
1:A:552:LYS:O	1:A:554:SER:N	2.25	0.69
1:L:396:MET:SD	1:L:398:PHE:HE2	2.16	0.69
1:D:217:ASN:HD21	1:D:219:LEU:HB2	1.59	0.68
1:A:232:LYS:NZ	1:A:276:THR:O	2.26	0.68
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.76	0.68
1:D:549:SER:N	1:D:550:SER:HA	2.08	0.68
1:C:123:VAL:HG12	1:C:185:VAL:HG11	1.75	0.67
1:J:217:ASN:HD22	1:J:219:LEU:N	1.92	0.67
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.77	0.67
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.77	0.67
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.78	0.66
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.77	0.66
1:H:214:LEU:HD21	1:H:222:LEU:HD22	1.76	0.65
1:F:563:LYS:NZ	7:F:1103:HOH:O	2.28	0.65
1:J:552:LYS:O	1:J:554:SER:N	2.30	0.64
1:D:568:ASN:HD22	1:D:568:ASN:N	1.95	0.64
1:C:232:LYS:NZ	1:C:276:THR:O	2.30	0.64
1:B:390:GLY:O	2:B:1001:4U6:OAG	2.16	0.63
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.81	0.63
1:J:396:MET:SD	1:J:398:PHE:HE2	2.21	0.63
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.81	0.63
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.80	0.63
1:L:552:LYS:O	1:L:554:SER:N	2.32	0.63
1:H:164:LYS:NZ	1:L:184:SER:OG	2.32	0.62
1:K:118:LYS:NZ	1:K:272:ASN:OD1	2.31	0.62
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.81	0.62
1:J:217:ASN:ND2	1:J:219:LEU:N	2.45	0.62
1:K:411:TYR:HE1	5:K:1005:1PE:H132	1.64	0.62
1:F:307:PRO:O	1:F:311:SER:OG	2.19	0.61
1:D:135:PRO:O	1:D:137:LYS:N	2.33	0.60
1:E:232:LYS:NZ	1:E:276:THR:O	2.34	0.60
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.83	0.59
1:H:552:LYS:O	1:H:554:SER:N	2.34	0.59
1:I:552:LYS:O	1:I:554:SER:N	2.35	0.59
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.67	0.59
1:H:423:ILE:HD11	1:H:600:VAL:HG11	1.85	0.59
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.68	0.59
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.84	0.59
1:D:552:LYS:O	1:D:554:SER:N	2.35	0.59
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.84	0.58
1:B:395:LEU:O	1:B:398:PHE:HD2	1.87	0.58
1:E:552:LYS:O	1:E:554:SER:N	2.37	0.58
1:B:436:LYS:NZ	6:B:1006:SO4:O3	2.36	0.58
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.68	0.58
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.67	0.58
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.86	0.58
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.86	0.57
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.85	0.57
1:A:550:SER:HA	1:A:552:LYS:H	1.68	0.57
1:A:173:LYS:NZ	7:A:1105:HOH:O	2.38	0.57
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.86	0.57
1:D:320:LYS:HZ1	5:D:1005:1PE:H142	1.68	0.57
1:G:441:PRO:HB2	1:H:394:ASP:HA	1.88	0.56
2:J:1001:4U6:NAR	4:J:1004:CO3:O1	2.38	0.56
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.87	0.56
1:C:230:VAL:O	1:C:277:TYR:OH	2.19	0.56
1:G:173:LYS:NZ	7:G:1107:HOH:O	2.37	0.56
1:G:396:MET:SD	1:G:398:PHE:HE2	2.29	0.56
1:G:436:LYS:HG3	1:H:347:GLY:O	2.05	0.56
1:J:214:LEU:HD21	1:J:222:LEU:HD22	1.87	0.56
6:B:1006:SO4:O2	1:C:436:LYS:HG2	2.06	0.56
1:H:88:VAL:HG21	1:H:97:THR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:262:GLU:N	7:L:1104:HOH:O	2.38	0.56
1:I:440:ARG:NH2	7:I:1106:HOH:O	2.39	0.55
1:G:552:LYS:O	1:G:554:SER:N	2.39	0.55
1:K:440:ARG:NH2	7:K:1110:HOH:O	2.39	0.55
1:E:520:SER:HB3	1:E:598:GLU:HG3	1.88	0.55
1:G:326:LYS:HE3	1:G:328:LEU:HD11	1.88	0.55
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.88	0.55
1:F:396:MET:SD	1:F:398:PHE:HE2	2.30	0.55
1:C:395:LEU:O	1:C:398:PHE:HD2	1.90	0.54
1:A:204:LYS:NZ	7:A:1109:HOH:O	2.41	0.54
1:B:88:VAL:HG21	1:B:97:THR:HA	1.88	0.54
1:D:132:VAL:HG11	1:D:142:VAL:HG13	1.89	0.54
1:J:217:ASN:HD21	1:J:219:LEU:HB2	1.73	0.54
1:B:232:LYS:NZ	1:B:280:GLU:OE2	2.37	0.54
1:D:158:LYS:HE3	1:D:160:GLU:HB2	1.90	0.54
1:J:551:VAL:O	1:J:553:ALA:N	2.42	0.53
1:B:164:LYS:NZ	1:F:184:SER:OG	2.41	0.53
1:D:395:LEU:O	1:D:398:PHE:HD2	1.91	0.53
1:J:103:TYR:HB3	5:J:1005:1PE:H251	1.89	0.53
1:B:440:ARG:NH1	7:B:1114:HOH:O	2.41	0.53
1:F:213:MET:O	1:F:217:ASN:ND2	2.30	0.53
1:H:320:LYS:HE2	5:H:1005:1PE:H142	1.90	0.53
1:J:520:SER:HB3	1:J:598:GLU:HG3	1.89	0.53
1:D:391:SER:O	7:D:1101:HOH:O	2.19	0.53
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.91	0.53
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.91	0.53
1:H:413:VAL:HG11	1:H:423:ILE:HD12	1.91	0.53
1:J:217:ASN:HD21	1:J:219:LEU:CB	2.22	0.53
1:G:114:VAL:HG12	1:G:274:ALA:HB1	1.91	0.52
1:A:125:GLU:OE2	1:A:221:LYS:NZ	2.32	0.52
1:C:244:TYR:OH	1:C:588:PRO:O	2.28	0.52
1:A:520:SER:HB3	1:A:598:GLU:HG3	1.92	0.52
1:H:390:GLY:O	2:H:1001:4U6:OAG	2.27	0.52
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.75	0.52
1:F:230:VAL:HG12	1:F:234:LEU:HD23	1.92	0.52
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.92	0.52
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.92	0.51
1:B:254:SER:OG	1:B:255:THR:N	2.44	0.51
1:H:254:SER:OG	1:H:255:THR:N	2.44	0.51
1:L:236:ARG:NH1	7:L:1103:HOH:O	2.38	0.51
1:A:543:ASP:OD2	1:B:254:SER:OG	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:LYS:O	1:C:554:SER:N	2.43	0.51
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.93	0.51
1:D:366:LYS:HG3	1:D:420:ASN:HB3	1.92	0.51
1:E:567:GLN:NE2	7:E:1107:HOH:O	2.43	0.51
1:G:520:SER:HB3	1:G:598:GLU:HG3	1.93	0.51
1:E:198:LEU:HD22	1:E:202:ASP:HB3	1.93	0.51
1:K:220:SER:OG	7:K:1101:HOH:O	2.19	0.51
1:C:230:VAL:HG12	1:C:234:LEU:HD23	1.94	0.51
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.94	0.50
1:G:550:SER:HA	1:G:551:VAL:HB	1.92	0.50
1:I:436:LYS:NZ	7:I:1107:HOH:O	2.42	0.50
1:K:230:VAL:HG13	1:K:234:LEU:HB3	1.92	0.50
1:A:230:VAL:HG12	1:A:234:LEU:HD23	1.93	0.50
1:H:383:TYR:HE2	1:H:438:SER:HB2	1.76	0.50
1:J:165:PHE:HB3	1:J:189:TYR:OH	2.12	0.50
1:F:552:LYS:O	1:F:554:SER:N	2.45	0.50
1:K:165:PHE:HB3	1:K:189:TYR:OH	2.10	0.50
1:F:207:VAL:HG11	1:F:241:THR:HG22	1.94	0.50
1:H:395:LEU:O	1:H:398:PHE:HD2	1.94	0.50
1:I:114:VAL:HG12	1:I:274:ALA:HB1	1.94	0.50
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.94	0.50
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.93	0.49
1:D:200:GLU:OE1	1:D:200:GLU:N	2.45	0.49
1:B:413:VAL:HG11	1:B:423:ILE:HD13	1.94	0.49
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.94	0.49
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.93	0.49
1:D:439:TYR:H	1:D:439:TYR:HD2	1.61	0.49
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.94	0.49
1:K:475:LYS:NZ	7:K:1117:HOH:O	2.46	0.49
1:B:520:SER:HB3	1:B:598:GLU:HG3	1.94	0.49
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.95	0.48
1:E:230:VAL:HG13	1:E:234:LEU:HB3	1.94	0.48
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.95	0.48
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.94	0.48
1:G:543:ASP:OD2	1:H:254:SER:OG	2.29	0.48
1:J:602:ASN:O	1:J:603:ASP:HB2	2.13	0.48
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.95	0.48
1:I:125:GLU:N	1:I:125:GLU:OE1	2.45	0.48
1:J:114:VAL:HG12	1:J:274:ALA:HB1	1.94	0.48
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.48	0.48
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.94	0.48
1:L:359:TYR:HD2	1:L:423:ILE:HD12	1.78	0.48
1:B:138:GLU:O	1:B:194:SER:OG	2.30	0.48
1:G:436:LYS:HB2	6:G:1008:SO4:O1	2.14	0.48
1:C:331:LYS:HD3	1:C:334:GLU:OE1	2.13	0.48
1:H:124:GLU:O	1:H:185:VAL:HG12	2.13	0.48
1:I:274:ALA:O	1:I:278:LYS:HG3	2.14	0.47
1:I:520:SER:HB3	1:I:598:GLU:HG3	1.97	0.47
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.96	0.47
1:J:217:ASN:HD22	1:J:218:LYS:N	2.12	0.47
1:L:137:LYS:CB	1:L:140:GLY:H	2.26	0.47
1:C:195:VAL:HG12	1:C:197:ASP:H	1.78	0.47
1:F:395:LEU:O	1:F:398:PHE:HD2	1.96	0.47
1:J:217:ASN:ND2	1:J:219:LEU:HB2	2.28	0.47
1:A:85:ALA:N	7:A:1115:HOH:O	2.48	0.47
1:F:533:TYR:O	1:F:536:THR:HG22	2.14	0.47
1:L:138:GLU:N	1:L:139:ASN:HA	2.29	0.47
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.97	0.47
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.96	0.47
1:H:164:LYS:HE3	1:H:165:PHE:CZ	2.50	0.47
1:C:316:GLU:HG3	5:C:1005:1PE:H231	1.97	0.47
1:G:166:ASN:ND2	7:G:1113:HOH:O	2.48	0.47
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.97	0.47
1:K:520:SER:HB3	1:K:598:GLU:HG3	1.97	0.47
1:C:536:THR:HG21	1:C:551:VAL:HG21	1.97	0.46
1:K:198:LEU:HD22	1:K:202:ASP:HB3	1.96	0.46
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.97	0.46
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.97	0.46
1:A:440:ARG:NH1	7:A:1107:HOH:O	2.49	0.46
1:C:440:ARG:NH2	7:C:1114:HOH:O	2.47	0.46
1:H:509:LEU:O	1:H:513:ILE:HG12	2.15	0.46
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.98	0.46
1:E:118:LYS:NZ	1:E:272:ASN:OD1	2.42	0.46
1:H:440:ARG:NH1	7:H:1114:HOH:O	2.48	0.46
1:I:230:VAL:HG12	1:I:234:LEU:HD23	1.98	0.45
1:L:298:ILE:HG23	1:L:398:PHE:HA	1.98	0.45
1:D:533:TYR:O	1:D:536:THR:HG22	2.16	0.45
1:G:301:PRO:HB2	1:G:303:ASN:OD1	2.17	0.45
1:K:411:TYR:CE1	5:K:1005:1PE:H132	2.49	0.45
1:B:123:VAL:HG11	1:B:187:VAL:HG22	1.99	0.45
1:G:135:PRO:HA	1:G:194:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:435:SER:OG	1:G:436:LYS:N	2.50	0.45
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.98	0.45
1:K:567:GLN:O	1:K:568:ASN:ND2	2.49	0.45
1:D:274:ALA:O	1:D:278:LYS:HG3	2.16	0.45
1:G:132:VAL:HG21	1:G:142:VAL:HG13	1.99	0.45
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.99	0.45
1:A:586:ARG:NH1	7:A:1116:HOH:O	2.48	0.45
1:B:204:LYS:O	1:B:208:LEU:HD13	2.16	0.45
1:F:419:GLU:HG2	1:F:419:GLU:H	1.55	0.45
1:I:395:LEU:O	1:I:398:PHE:HD2	1.99	0.45
1:D:198:LEU:HD22	1:D:202:ASP:HB3	1.99	0.45
1:I:207:VAL:HG11	1:I:241:THR:HG22	1.99	0.45
1:H:175:PHE:CD1	1:L:176:TYR:HB2	2.52	0.45
1:A:361:SER:HB3	1:A:362:LYS:H	1.32	0.45
1:J:173:LYS:HB2	1:J:189:TYR:HE2	1.82	0.45
1:C:528:PRO:HB3	1:D:525:TRP:CZ3	2.52	0.44
1:J:124:GLU:OE1	1:J:179:ASN:ND2	2.50	0.44
1:L:498:SER:O	1:L:523:PRO:HG2	2.18	0.44
1:H:498:SER:O	1:H:523:PRO:HG2	2.17	0.44
1:I:124:GLU:O	1:I:185:VAL:HG12	2.17	0.44
1:A:214:LEU:HD21	1:A:222:LEU:HD22	1.98	0.44
1:D:230:VAL:HG12	1:D:234:LEU:HD23	1.98	0.44
1:L:230:VAL:HG12	1:L:234:LEU:HD23	1.99	0.44
1:J:198:LEU:HD22	1:J:202:ASP:HB3	1.99	0.44
1:K:137:LYS:O	1:K:194:SER:OG	2.26	0.44
1:F:114:VAL:HG12	1:F:274:ALA:HB1	1.99	0.44
1:H:132:VAL:HG21	1:H:142:VAL:HG13	1.99	0.44
1:H:483:ASP:OD1	1:H:573:HIS:ND1	2.37	0.44
1:H:463:ARG:NH1	1:H:547:ILE:HG22	2.32	0.44
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.99	0.44
1:D:320:LYS:NZ	5:D:1005:1PE:H142	2.32	0.44
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.52	0.44
1:I:300:ALA:HA	1:I:301:PRO:HD3	1.83	0.44
1:B:124:GLU:O	1:B:185:VAL:HG12	2.18	0.44
1:H:536:THR:HG21	1:H:551:VAL:HG23	2.00	0.44
1:B:274:ALA:O	1:B:278:LYS:HG3	2.18	0.43
1:H:103:TYR:CD2	5:H:1005:1PE:H222	2.52	0.43
1:K:338:MET:CE	1:K:468:ASP:HB3	2.48	0.43
1:B:165:PHE:HB3	1:B:189:TYR:OH	2.18	0.43
1:G:550:SER:HA	1:G:552:LYS:N	2.28	0.43
1:L:207:VAL:HG11	1:L:241:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLU:N	1:B:125:GLU:OE1	2.48	0.43
1:D:195:VAL:HG12	1:D:197:ASP:H	1.83	0.43
1:D:340:ALA:HA	1:D:445:ILE:HD12	2.00	0.43
1:J:340:ALA:HA	1:J:445:ILE:HD12	2.00	0.43
1:K:298:ILE:HG23	1:K:398:PHE:HA	2.00	0.43
1:B:195:VAL:HG12	1:B:197:ASP:H	1.83	0.43
1:L:176:TYR:OH	1:L:217:ASN:ND2	2.51	0.43
1:C:207:VAL:HG11	1:C:241:THR:HG22	2.00	0.43
1:A:301:PRO:HB2	1:A:303:ASN:OD1	2.19	0.43
1:H:215:HIS:O	1:H:217:ASN:N	2.52	0.43
1:A:150:ASP:OD2	1:A:179:ASN:HB2	2.19	0.43
1:A:386:LYS:HE3	1:A:396:MET:SD	2.59	0.43
1:F:195:VAL:HG12	1:F:197:ASP:H	1.84	0.43
1:G:522:GLU:HA	1:G:523:PRO:HD3	1.88	0.43
1:J:300:ALA:HA	1:J:301:PRO:HD3	1.90	0.43
1:D:454:GLU:OE1	1:D:539:SER:OG	2.34	0.43
1:H:528:PRO:HB3	1:K:525:TRP:CZ3	2.53	0.43
1:A:138:GLU:HA	1:A:194:SER:OG	2.18	0.42
1:B:169:LEU:HD22	1:B:202:ASP:OD1	2.18	0.42
1:D:383:TYR:HE2	1:D:438:SER:HB2	1.84	0.42
1:E:333:LEU:HD21	1:E:354:PHE:HB2	2.00	0.42
1:G:396:MET:SD	1:G:398:PHE:CE2	3.10	0.42
1:L:395:LEU:O	1:L:398:PHE:HD2	2.02	0.42
1:I:198:LEU:HA	1:I:198:LEU:HD12	1.91	0.42
1:B:174:HIS:HB3	1:F:175:PHE:CD2	2.54	0.42
1:B:169:LEU:HD23	1:B:205:ARG:NH1	2.35	0.42
1:G:548:SER:OG	1:G:549:SER:N	2.52	0.42
1:H:117:ILE:HD11	1:H:146:SER:OG	2.19	0.42
1:A:601:LEU:HD23	1:A:601:LEU:HA	1.89	0.42
1:F:142:VAL:HG21	1:F:189:TYR:CE2	2.55	0.42
1:J:229:ASN:ND2	7:J:1111:HOH:O	2.43	0.42
1:J:333:LEU:HD21	1:J:354:PHE:HB2	2.00	0.42
1:J:396:MET:SD	1:J:398:PHE:CE2	3.07	0.42
1:K:395:LEU:HD11	1:K:581:TRP:CG	2.55	0.42
1:A:195:VAL:HG12	1:A:197:ASP:H	1.84	0.42
1:A:198:LEU:HD22	1:A:202:ASP:HB3	2.01	0.42
1:A:525:TRP:CZ3	1:F:528:PRO:HB3	2.55	0.42
1:H:125:GLU:OE1	1:H:125:GLU:N	2.52	0.42
1:I:195:VAL:HG12	1:I:197:ASP:H	1.84	0.42
1:K:158:LYS:HE3	1:K:160:GLU:HB2	2.01	0.42
1:E:298:ILE:HG23	1:E:398:PHE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:LEU:HD11	1:E:222:LEU:HD22	2.02	0.42
1:E:338:MET:CE	1:E:468:ASP:HB3	2.50	0.42
1:B:207:VAL:HG11	1:B:241:THR:HG22	2.01	0.42
1:K:150:ASP:OD2	1:K:179:ASN:HB2	2.20	0.42
1:J:301:PRO:HB2	1:J:303:ASN:OD1	2.20	0.41
1:A:320:LYS:NZ	5:A:1006:1PE:H152	2.31	0.41
1:D:567:GLN:HB3	1:D:568:ASN:ND2	2.34	0.41
1:E:195:VAL:HG12	1:E:197:ASP:H	1.85	0.41
1:F:86:SER:HB2	1:F:312:ASN:OD1	2.20	0.41
1:G:321:LEU:HD11	1:G:411:TYR:HA	2.01	0.41
1:D:492:LEU:HD11	2:D:1001:4U6:CAJ	2.49	0.41
1:E:150:ASP:OD2	1:E:179:ASN:HB2	2.20	0.41
1:F:230:VAL:O	1:F:277:TYR:OH	2.19	0.41
1:I:214:LEU:HD21	1:I:222:LEU:HD22	2.02	0.41
1:A:394:ASP:HA	1:C:441:PRO:HB2	2.03	0.41
1:G:487:LEU:HD22	1:G:573:HIS:CE1	2.55	0.41
1:E:300:ALA:HA	1:E:301:PRO:HD3	1.86	0.41
1:F:498:SER:O	1:F:523:PRO:HG2	2.20	0.41
1:J:230:VAL:HG12	1:J:234:LEU:HD23	2.02	0.41
1:C:498:SER:O	1:C:523:PRO:HG2	2.20	0.41
1:D:301:PRO:HB2	1:D:303:ASN:OD1	2.20	0.41
1:J:376:ILE:HD11	1:J:465:THR:HG21	2.03	0.41
1:A:390:GLY:O	2:A:1001:4U6:OAG	2.38	0.41
1:C:357:LEU:HB2	1:C:425:PHE:HB2	2.03	0.41
1:J:463:ARG:N	4:J:1004:CO3:O3	2.46	0.41
1:J:487:LEU:HD22	1:J:573:HIS:CE1	2.56	0.41
1:L:375:GLY:O	1:L:429:VAL:HA	2.20	0.41
1:C:208:LEU:O	1:C:212:THR:HG23	2.21	0.41
1:C:383:TYR:HE2	1:C:438:SER:HB2	1.86	0.41
1:D:543:ASP:OD2	1:E:254:SER:OG	2.32	0.41
1:G:601:LEU:HA	1:G:601:LEU:HD23	1.91	0.41
1:H:232:LYS:HE3	1:H:276:THR:HG22	2.01	0.41
1:I:509:LEU:O	1:I:513:ILE:HG12	2.20	0.41
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.56	0.41
1:C:487:LEU:HD22	1:C:573:HIS:CE1	2.56	0.41
1:D:567:GLN:C	1:D:568:ASN:ND2	2.58	0.41
1:D:150:ASP:OD1	1:D:179:ASN:HB2	2.21	0.41
1:I:285:ARG:NH2	7:I:1119:HOH:O	2.53	0.41
1:I:321:LEU:HD11	1:I:411:TYR:HA	2.03	0.41
1:J:254:SER:OG	1:L:543:ASP:OD2	2.24	0.41
1:C:413:VAL:HG11	1:C:423:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:LYS:HE3	1:E:160:GLU:HB2	2.02	0.40
1:F:396:MET:SD	1:F:398:PHE:CE2	3.12	0.40
1:J:204:LYS:HB2	1:J:204:LYS:HE3	1.70	0.40
1:K:372:VAL:O	1:K:483:ASP:HA	2.21	0.40
1:L:127:LEU:HB2	1:L:219:LEU:HD21	2.03	0.40
1:C:198:LEU:HD22	1:C:202:ASP:HB3	2.03	0.40
1:C:520:SER:HB3	1:C:598:GLU:HG3	2.03	0.40
1:H:298:ILE:HG23	1:H:398:PHE:HA	2.02	0.40
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.56	0.40
1:L:341:TYR:CE1	1:L:428:ALA:HB1	2.56	0.40
1:C:321:LEU:HD11	1:C:411:TYR:HA	2.03	0.40
1:D:135:PRO:HA	1:D:194:SER:O	2.22	0.40
5:J:1005:1PE:H151	7:J:1197:HOH:O	2.22	0.40
1:A:393:ILE:HA	1:A:396:MET:HG2	2.02	0.40
1:E:302:SER:OG	1:E:378:PHE:HB2	2.21	0.40
1:I:525:TRP:CZ3	1:J:528:PRO:HB3	2.56	0.40
1:K:207:VAL:HG11	1:K:241:THR:HG22	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:OE2	1:G:115:TYR:OH[2_655]	2.05	0.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/522 (98%)	492 (96%)	15 (3%)	4 (1%)	19	39
1	B	512/522 (98%)	494 (96%)	14 (3%)	4 (1%)	19	39
1	C	512/522 (98%)	497 (97%)	13 (2%)	2 (0%)	34	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	510/522 (98%)	495 (97%)	12 (2%)	3 (1%)	25	47
1	E	503/522 (96%)	489 (97%)	12 (2%)	2 (0%)	34	57
1	F	507/522 (97%)	491 (97%)	14 (3%)	2 (0%)	34	57
1	G	517/522 (99%)	498 (96%)	16 (3%)	3 (1%)	25	47
1	H	512/522 (98%)	491 (96%)	17 (3%)	4 (1%)	19	39
1	I	516/522 (99%)	499 (97%)	13 (2%)	4 (1%)	19	39
1	J	509/522 (98%)	492 (97%)	14 (3%)	3 (1%)	25	47
1	K	500/522 (96%)	488 (98%)	12 (2%)	0	100	100
1	L	507/522 (97%)	494 (97%)	11 (2%)	2 (0%)	34	57
All	All	6116/6264 (98%)	5920 (97%)	163 (3%)	33 (0%)	29	52

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	LYS
1	A	553	ALA
1	B	138	GLU
1	C	553	ALA
1	D	136	GLY
1	D	553	ALA
1	E	553	ALA
1	F	553	ALA
1	G	553	ALA
1	H	216	ASP
1	H	553	ALA
1	I	553	ALA
1	J	550	SER
1	J	552	LYS
1	J	553	ALA
1	L	553	ALA
1	A	551	VAL
1	B	136	GLY
1	B	552	LYS
1	C	136	GLY
1	E	552	LYS
1	G	136	GLY
1	I	136	GLY
1	D	552	LYS
1	H	138	GLU

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Mol	Chain	Res	Type
1	I	139	ASN
1	L	552	LYS
1	F	551	VAL
1	A	550	SER
1	B	396	MET
1	G	551	VAL
1	I	552	LYS
1	H	119	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/450 (92%)	414 (100%)	2 (0%)	88	96
1	B	405/450 (90%)	404 (100%)	1 (0%)	93	98
1	C	416/450 (92%)	416 (100%)	0	100	100
1	D	411/450 (91%)	409 (100%)	2 (0%)	88	96
1	E	411/450 (91%)	411 (100%)	0	100	100
1	F	398/450 (88%)	397 (100%)	1 (0%)	92	98
1	G	421/450 (94%)	419 (100%)	2 (0%)	88	96
1	H	405/450 (90%)	403 (100%)	2 (0%)	88	96
1	I	415/450 (92%)	414 (100%)	1 (0%)	93	98
1	J	416/450 (92%)	415 (100%)	1 (0%)	93	98
1	K	414/450 (92%)	414 (100%)	0	100	100
1	L	394/450 (88%)	393 (100%)	1 (0%)	92	98
All	All	4922/5400 (91%)	4909 (100%)	13 (0%)	92	98

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	398	PHE
1	A	568	ASN

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Mol	Chain	Res	Type
1	B	88	VAL
1	D	439	TYR
1	D	568	ASN
1	F	311	SER
1	G	155	GLU
1	G	288	TYR
1	H	88	VAL
1	H	134	ASN
1	I	333	LEU
1	J	217	ASN
1	L	288	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	568	ASN
1	I	568	ASN
1	J	217	ASN
1	K	568	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 76 ligands modelled in this entry, 24 are monoatomic - leaving 52 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	4U6	K	1001	3	29,29,29	2.84	6 (20%)	40,41,41	1.60	2 (5%)
2	4U6	E	1001	3	29,29,29	2.80	4 (13%)	40,41,41	1.47	2 (5%)
5	1PE	I	1005	-	11,11,15	0.60	0	10,10,14	0.38	0
4	CO3	I	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	1PE	J	1005	-	10,10,15	0.84	0	9,9,14	0.37	0
2	4U6	C	1001	3	29,29,29	2.82	6 (20%)	40,41,41	1.57	2 (5%)
2	4U6	L	1001	3	29,29,29	2.78	5 (17%)	40,41,41	1.54	2 (5%)
5	1PE	E	1005	-	11,11,15	0.59	0	10,10,14	0.45	0
5	1PE	D	1005	-	9,9,15	0.58	0	8,8,14	0.38	0
5	1PE	F	1005	-	9,9,15	0.90	0	8,8,14	0.44	0
4	CO3	K	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	SO4	A	1007	-	4,4,4	0.12	0	6,6,6	0.09	0
4	CO3	L	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	B	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	SO4	B	1006	-	4,4,4	0.14	0	6,6,6	0.13	0
5	1PE	E	1006	-	11,11,15	0.59	0	10,10,14	0.39	0
2	4U6	I	1001	3	29,29,29	2.87	6 (20%)	40,41,41	1.58	2 (5%)
5	1PE	G	1007	-	5,5,15	0.71	0	4,4,14	0.40	0
6	SO4	J	1006	-	4,4,4	0.14	0	6,6,6	0.06	0
2	4U6	G	1001	3	29,29,29	2.79	4 (13%)	40,41,41	1.56	2 (5%)
5	1PE	F	1006	-	11,11,15	0.64	0	10,10,14	0.35	0
4	CO3	A	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	C	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	H	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	1PE	G	1005	-	8,8,15	0.56	0	7,7,14	0.28	0
5	1PE	C	1006	-	8,8,15	0.53	0	7,7,14	0.39	0
5	1PE	A	1006	-	11,11,15	0.65	0	10,10,14	0.37	0
4	CO3	D	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	SO4	D	1007	-	4,4,4	0.16	0	6,6,6	0.09	0
4	CO3	J	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
6	SO4	G	1008	-	4,4,4	0.13	0	6,6,6	0.13	0
2	4U6	A	1001	3	29,29,29	2.80	4 (13%)	40,41,41	1.47	1 (2%)
4	CO3	G	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	1PE	L	1005	-	9,9,15	0.89	0	8,8,14	0.42	0
6	SO4	F	1007	-	4,4,4	0.14	0	6,6,6	0.09	0
5	1PE	C	1005	-	12,12,15	0.67	0	11,11,14	0.32	0
5	1PE	I	1006	-	10,10,15	0.57	0	9,9,14	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4U6	J	1001	3	29,29,29	2.81	4 (13%)	40,41,41	1.53	3 (7%)
5	1PE	K	1005	-	11,11,15	0.61	0	10,10,14	0.41	0
2	4U6	F	1001	3	29,29,29	2.78	4 (13%)	40,41,41	1.48	2 (5%)
5	1PE	G	1006	-	5,5,15	0.69	0	4,4,14	0.55	0
5	1PE	H	1005	-	9,9,15	0.57	0	8,8,14	0.33	0
4	CO3	E	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
5	1PE	D	1006	-	9,9,15	0.55	0	8,8,14	0.36	0
5	1PE	A	1005	-	8,8,15	0.53	0	7,7,14	0.33	0
6	SO4	L	1006	-	4,4,4	0.13	0	6,6,6	0.07	0
5	1PE	B	1005	-	9,9,15	0.56	0	8,8,14	0.33	0
2	4U6	H	1001	3	29,29,29	2.76	5 (17%)	40,41,41	1.53	2 (5%)
4	CO3	F	1004	-	0,3,3	0.00	-	0,3,3	0.00	-
2	4U6	D	1001	3	29,29,29	2.76	4 (13%)	40,41,41	1.51	5 (12%)
6	SO4	K	1006	-	4,4,4	0.13	0	6,6,6	0.07	0
2	4U6	B	1001	3	29,29,29	2.77	4 (13%)	40,41,41	1.51	2 (5%)

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	4U6	K	1001	3	-	3/30/30/30	0/2/2/2
2	4U6	E	1001	3	-	3/30/30/30	0/2/2/2
5	1PE	I	1005	-	-	6/9/9/13	-
5	1PE	J	1005	-	-	4/8/8/13	-
2	4U6	C	1001	3	-	3/30/30/30	0/2/2/2
2	4U6	L	1001	3	-	4/30/30/30	0/2/2/2
5	1PE	E	1005	-	-	4/9/9/13	-
5	1PE	D	1005	-	-	3/7/7/13	-
5	1PE	F	1005	-	-	2/7/7/13	-
5	1PE	E	1006	-	-	3/9/9/13	-
2	4U6	I	1001	3	-	1/30/30/30	0/2/2/2
5	1PE	G	1007	-	-	2/3/3/13	-
2	4U6	G	1001	3	-	2/30/30/30	0/2/2/2
5	1PE	F	1006	-	-	5/9/9/13	-
5	1PE	G	1005	-	-	4/6/6/13	-
5	1PE	C	1006	-	-	5/6/6/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	A	1006	-	-	5/9/9/13	-
2	4U6	A	1001	3	-	0/30/30/30	0/2/2/2
5	1PE	L	1005	-	-	4/7/7/13	-
5	1PE	C	1005	-	-	6/10/10/13	-
5	1PE	I	1006	-	-	6/8/8/13	-
2	4U6	J	1001	3	-	3/30/30/30	0/2/2/2
2	4U6	F	1001	3	-	2/30/30/30	0/2/2/2
5	1PE	G	1006	-	-	1/3/3/13	-
5	1PE	H	1005	-	-	5/7/7/13	-
5	1PE	K	1005	-	-	7/9/9/13	-
5	1PE	D	1006	-	-	4/7/7/13	-
5	1PE	A	1005	-	-	3/6/6/13	-
5	1PE	B	1005	-	-	4/7/7/13	-
2	4U6	H	1001	3	-	0/30/30/30	0/2/2/2
2	4U6	D	1001	3	-	2/30/30/30	0/2/2/2
2	4U6	B	1001	3	-	0/30/30/30	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	4U6	CAW-CAT	-10.43	1.38	1.49
2	J	1001	4U6	CAW-CAT	-10.41	1.38	1.49
2	A	1001	4U6	CAW-CAT	-10.12	1.39	1.49
2	I	1001	4U6	CAW-CAT	-10.10	1.39	1.49
2	G	1001	4U6	CAW-CAT	-9.98	1.39	1.49
2	B	1001	4U6	CAW-CAT	-9.98	1.39	1.49
2	E	1001	4U6	CAW-CAT	-9.92	1.39	1.49
2	F	1001	4U6	CAW-CAT	-9.78	1.39	1.49
2	C	1001	4U6	CAW-CAT	-9.78	1.39	1.49
2	L	1001	4U6	CAW-CAT	-9.77	1.39	1.49
2	H	1001	4U6	CAW-CAT	-9.75	1.39	1.49
2	K	1001	4U6	CAW-CAT	-9.75	1.39	1.49
2	F	1001	4U6	CAZ-CA	-7.87	1.39	1.52
2	J	1001	4U6	CAZ-CA	-7.85	1.39	1.52
2	I	1001	4U6	CAZ-CA	-7.85	1.39	1.52
2	G	1001	4U6	CAZ-CA	-7.82	1.39	1.52
2	D	1001	4U6	CAZ-CA	-7.73	1.40	1.52
2	H	1001	4U6	CAZ-CA	-7.68	1.40	1.52
2	C	1001	4U6	CAZ-CA	-7.67	1.40	1.52
2	A	1001	4U6	CAZ-CA	-7.63	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1001	4U6	CAZ-CA	-7.60	1.40	1.52
2	E	1001	4U6	CAZ-CA	-7.59	1.40	1.52
2	B	1001	4U6	CAZ-CA	-7.49	1.40	1.52
2	K	1001	4U6	CAZ-CA	-7.46	1.40	1.52
2	K	1001	4U6	CAT-NAQ	7.38	1.34	1.29
2	I	1001	4U6	CAT-NAQ	7.05	1.34	1.29
2	A	1001	4U6	CAT-NAQ	6.93	1.34	1.29
2	E	1001	4U6	CAT-NAQ	6.88	1.34	1.29
2	C	1001	4U6	CAT-NAQ	6.84	1.34	1.29
2	L	1001	4U6	CAT-NAQ	6.81	1.34	1.29
2	B	1001	4U6	CAT-NAQ	6.69	1.34	1.29
2	G	1001	4U6	CAT-NAQ	6.65	1.34	1.29
2	F	1001	4U6	CAT-NAQ	6.61	1.34	1.29
2	H	1001	4U6	CAT-NAQ	6.60	1.34	1.29
2	J	1001	4U6	CAT-NAQ	6.21	1.33	1.29
2	D	1001	4U6	CAT-NAQ	5.75	1.33	1.29
2	G	1001	4U6	CAY-CAX	-3.92	1.39	1.49
2	F	1001	4U6	CAY-CAX	-3.89	1.39	1.49
2	D	1001	4U6	CAY-CAX	-3.83	1.39	1.49
2	H	1001	4U6	CAY-CAX	-3.81	1.39	1.49
2	E	1001	4U6	CAY-CAX	-3.81	1.39	1.49
2	J	1001	4U6	CAY-CAX	-3.78	1.39	1.49
2	B	1001	4U6	CAY-CAX	-3.77	1.39	1.49
2	L	1001	4U6	CAY-CAX	-3.74	1.39	1.49
2	A	1001	4U6	CAY-CAX	-3.72	1.39	1.49
2	K	1001	4U6	CAY-CAX	-3.72	1.39	1.49
2	I	1001	4U6	CAY-CAX	-3.71	1.39	1.49
2	C	1001	4U6	CAY-CAX	-3.68	1.39	1.49
2	C	1001	4U6	OAH-NAR	2.59	1.46	1.40
2	C	1001	4U6	OAG-NAQ	2.58	1.47	1.40
2	K	1001	4U6	OAG-NAQ	2.53	1.47	1.40
2	K	1001	4U6	OAH-NAR	2.41	1.46	1.40
2	I	1001	4U6	OAG-NAQ	2.25	1.47	1.40
2	H	1001	4U6	OAG-NAQ	2.21	1.46	1.40
2	L	1001	4U6	OAH-NAR	2.18	1.45	1.40
2	I	1001	4U6	OAH-NAR	2.13	1.45	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1001	4U6	OAG-NAQ-CAT	8.33	117.47	109.59
2	I	1001	4U6	OAG-NAQ-CAT	8.02	117.18	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1001	4U6	OAG-NAQ-CAT	7.90	117.06	109.59
2	L	1001	4U6	OAG-NAQ-CAT	7.88	117.04	109.59
2	A	1001	4U6	OAG-NAQ-CAT	7.68	116.86	109.59
2	F	1001	4U6	OAG-NAQ-CAT	7.65	116.83	109.59
2	E	1001	4U6	OAG-NAQ-CAT	7.54	116.72	109.59
2	C	1001	4U6	OAG-NAQ-CAT	7.52	116.70	109.59
2	B	1001	4U6	OAG-NAQ-CAT	7.37	116.56	109.59
2	H	1001	4U6	OAG-NAQ-CAT	7.36	116.55	109.59
2	J	1001	4U6	OAG-NAQ-CAT	6.99	116.20	109.59
2	D	1001	4U6	OAG-NAQ-CAT	5.83	115.10	109.59
2	J	1001	4U6	CBB-CAV-N	-2.72	113.92	117.66
2	D	1001	4U6	CBB-CAV-N	-2.68	113.97	117.66
2	K	1001	4U6	CBB-CAV-N	-2.54	114.17	117.66
2	L	1001	4U6	CBB-CAV-N	-2.51	114.20	117.66
2	D	1001	4U6	CAO-CAZ-CA	-2.36	116.93	120.80
2	J	1001	4U6	CAO-CAZ-CA	-2.32	116.99	120.80
2	C	1001	4U6	CAO-CAZ-CA	-2.27	117.07	120.80
2	D	1001	4U6	CAY-CAP-CAW	-2.20	118.70	121.09
2	D	1001	4U6	CAM-CAX-CAY	-2.20	117.55	121.36
2	H	1001	4U6	CBB-CAV-N	-2.15	114.70	117.66
2	I	1001	4U6	CBB-CAV-N	-2.15	114.70	117.66
2	B	1001	4U6	CAO-CAZ-CA	-2.14	117.28	120.80
2	E	1001	4U6	CBB-CAV-N	-2.14	114.72	117.66
2	F	1001	4U6	CBB-CAV-N	-2.09	114.79	117.66
2	G	1001	4U6	CAO-CAZ-CA	-2.04	117.45	120.80

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1005	1PE	OH4-C13-C23-OH3
5	E	1006	1PE	OH4-C13-C23-OH3
5	A	1006	1PE	OH5-C14-C24-OH4
5	I	1005	1PE	OH5-C14-C24-OH4
5	G	1005	1PE	OH5-C14-C24-OH4
5	I	1006	1PE	OH5-C14-C24-OH4
5	A	1006	1PE	OH6-C15-C25-OH5
5	I	1006	1PE	OH4-C13-C23-OH3
5	F	1006	1PE	OH6-C15-C25-OH5
5	H	1005	1PE	OH4-C13-C23-OH3
5	D	1005	1PE	OH5-C14-C24-OH4
5	C	1005	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
5	E	1005	1PE	OH4-C13-C23-OH3
5	C	1005	1PE	OH4-C13-C23-OH3
5	J	1005	1PE	OH5-C14-C24-OH4
5	I	1005	1PE	OH6-C15-C25-OH5
5	C	1005	1PE	OH6-C15-C25-OH5
5	B	1005	1PE	OH4-C13-C23-OH3
5	E	1005	1PE	OH5-C14-C24-OH4
5	A	1006	1PE	OH4-C13-C23-OH3
5	E	1006	1PE	OH5-C14-C24-OH4
5	F	1005	1PE	OH5-C14-C24-OH4
5	J	1005	1PE	C16-C26-OH6-C15
5	B	1005	1PE	C24-C14-OH5-C25
5	A	1005	1PE	OH5-C14-C24-OH4
5	C	1006	1PE	OH4-C13-C23-OH3
5	H	1005	1PE	OH5-C14-C24-OH4
5	I	1005	1PE	OH4-C13-C23-OH3
5	G	1007	1PE	OH6-C15-C25-OH5
5	A	1006	1PE	C15-C25-OH5-C14
5	C	1005	1PE	C14-C24-OH4-C13
5	D	1006	1PE	C12-C22-OH3-C23
5	K	1005	1PE	C23-C13-OH4-C24
5	J	1005	1PE	C15-C25-OH5-C14
5	C	1006	1PE	OH5-C14-C24-OH4
5	I	1005	1PE	C12-C22-OH3-C23
5	D	1006	1PE	OH5-C14-C24-OH4
5	L	1005	1PE	C25-C15-OH6-C26
5	K	1005	1PE	C12-C22-OH3-C23
5	B	1005	1PE	C12-C22-OH3-C23
5	C	1005	1PE	C25-C15-OH6-C26
5	E	1005	1PE	C12-C22-OH3-C23
5	L	1005	1PE	C24-C14-OH5-C25
5	C	1005	1PE	C15-C25-OH5-C14
5	G	1005	1PE	C14-C24-OH4-C13
5	G	1006	1PE	C15-C25-OH5-C14
5	I	1006	1PE	C12-C22-OH3-C23
5	I	1006	1PE	C13-C23-OH3-C22
5	E	1006	1PE	C23-C13-OH4-C24
5	I	1005	1PE	C24-C14-OH5-C25
5	K	1005	1PE	C14-C24-OH4-C13
5	C	1006	1PE	C13-C23-OH3-C22
5	I	1006	1PE	C24-C14-OH5-C25
2	L	1001	4U6	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
5	K	1005	1PE	C13-C23-OH3-C22
5	F	1005	1PE	OH6-C15-C25-OH5
5	J	1005	1PE	OH6-C15-C25-OH5
5	I	1006	1PE	C23-C13-OH4-C24
5	G	1005	1PE	OH4-C13-C23-OH3
5	F	1006	1PE	C25-C15-OH6-C26
5	I	1005	1PE	C23-C13-OH4-C24
5	C	1006	1PE	C14-C24-OH4-C13
5	H	1005	1PE	C12-C22-OH3-C23
5	G	1007	1PE	C24-C14-OH5-C25
5	H	1005	1PE	C23-C13-OH4-C24
5	G	1005	1PE	C13-C23-OH3-C22
2	L	1001	4U6	O-C-CA-CAZ
2	L	1001	4U6	NAR-C-CA-CAZ
2	K	1001	4U6	NAR-C-CA-N
2	C	1001	4U6	O-C-CA-N
2	I	1001	4U6	NAR-C-CA-N
2	G	1001	4U6	O-C-CA-N
2	G	1001	4U6	NAR-C-CA-N
2	D	1001	4U6	NAR-C-CA-N
5	F	1006	1PE	C15-C25-OH5-C14
5	D	1006	1PE	C14-C24-OH4-C13
5	A	1005	1PE	OH4-C13-C23-OH3
5	K	1005	1PE	C24-C14-OH5-C25
5	K	1005	1PE	OH4-C13-C23-OH3
5	C	1006	1PE	C12-C22-OH3-C23
5	K	1005	1PE	OH5-C14-C24-OH4
5	L	1005	1PE	C16-C26-OH6-C15
2	E	1001	4U6	O-C-CA-N
2	L	1001	4U6	NAR-C-CA-N
2	J	1001	4U6	O-C-CA-N
2	J	1001	4U6	NAR-C-CA-N
2	F	1001	4U6	O-C-CA-N
2	F	1001	4U6	NAR-C-CA-N
5	A	1005	1PE	C12-C22-OH3-C23
5	F	1006	1PE	C24-C14-OH5-C25
5	D	1005	1PE	C12-C22-OH3-C23
5	H	1005	1PE	C14-C24-OH4-C13
5	B	1005	1PE	OH5-C14-C24-OH4
5	D	1006	1PE	C24-C14-OH5-C25
5	E	1005	1PE	OH6-C15-C25-OH5
5	L	1005	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
2	K	1001	4U6	NAR-C-CA-CAZ
2	E	1001	4U6	O-C-CA-CAZ
2	C	1001	4U6	NAR-C-CA-CAZ
2	J	1001	4U6	NAR-C-CA-CAZ
2	K	1001	4U6	O-C-CA-N
2	E	1001	4U6	NAR-C-CA-N
2	C	1001	4U6	NAR-C-CA-N
2	D	1001	4U6	O-C-CA-N
5	F	1006	1PE	OH5-C14-C24-OH4
5	A	1006	1PE	C25-C15-OH6-C26

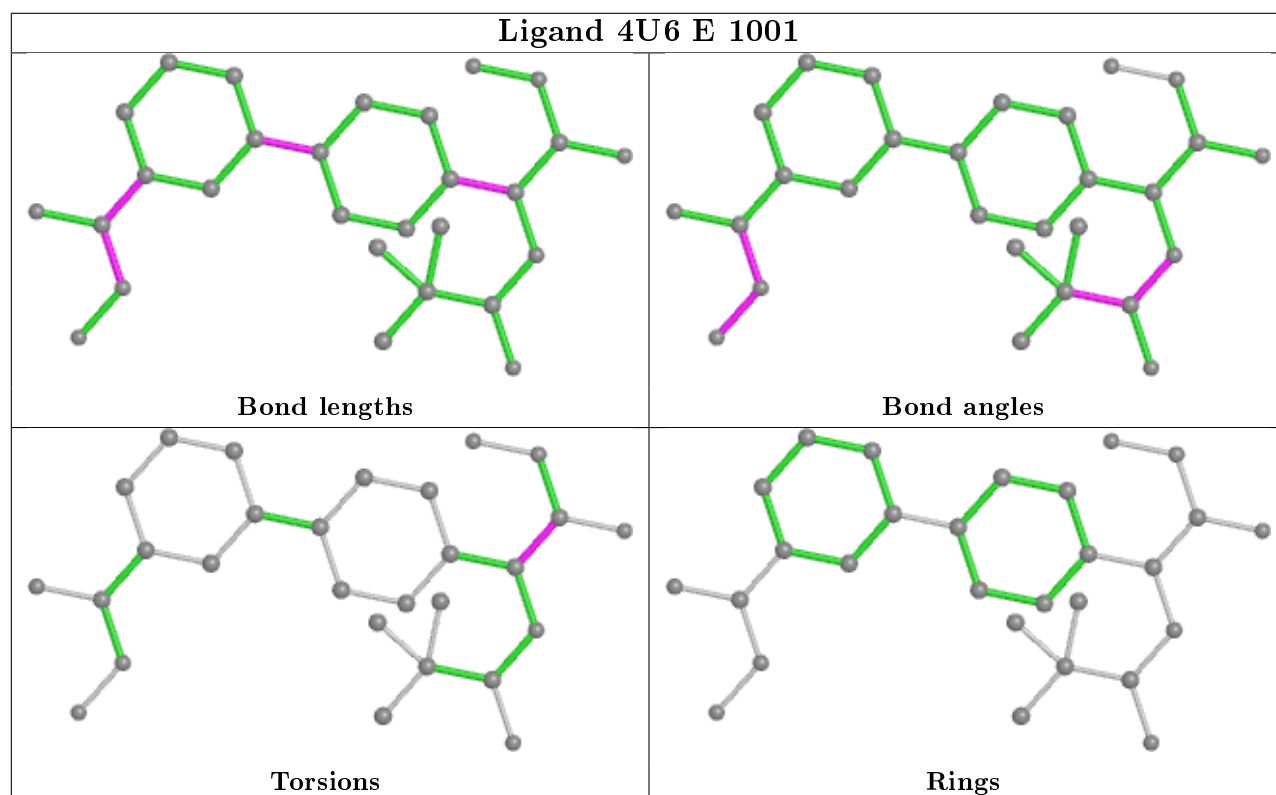
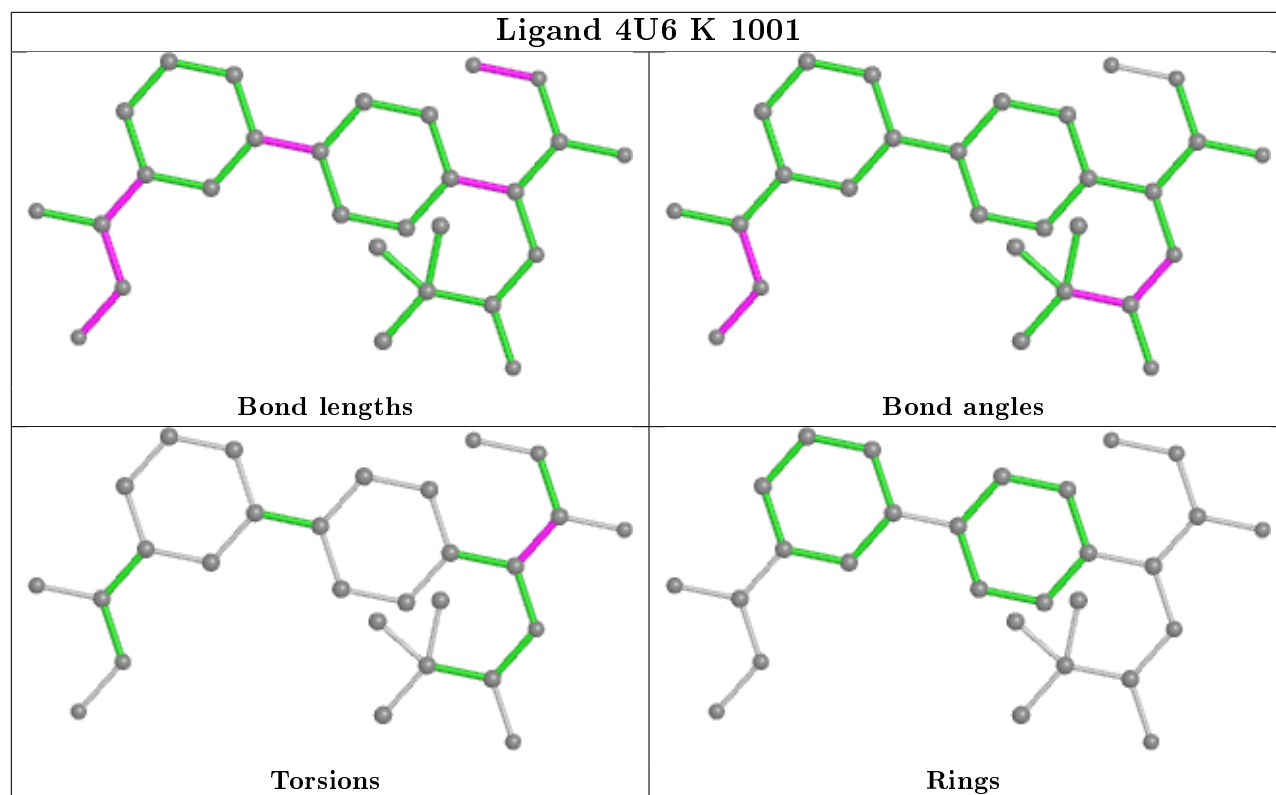
There are no ring outliers.

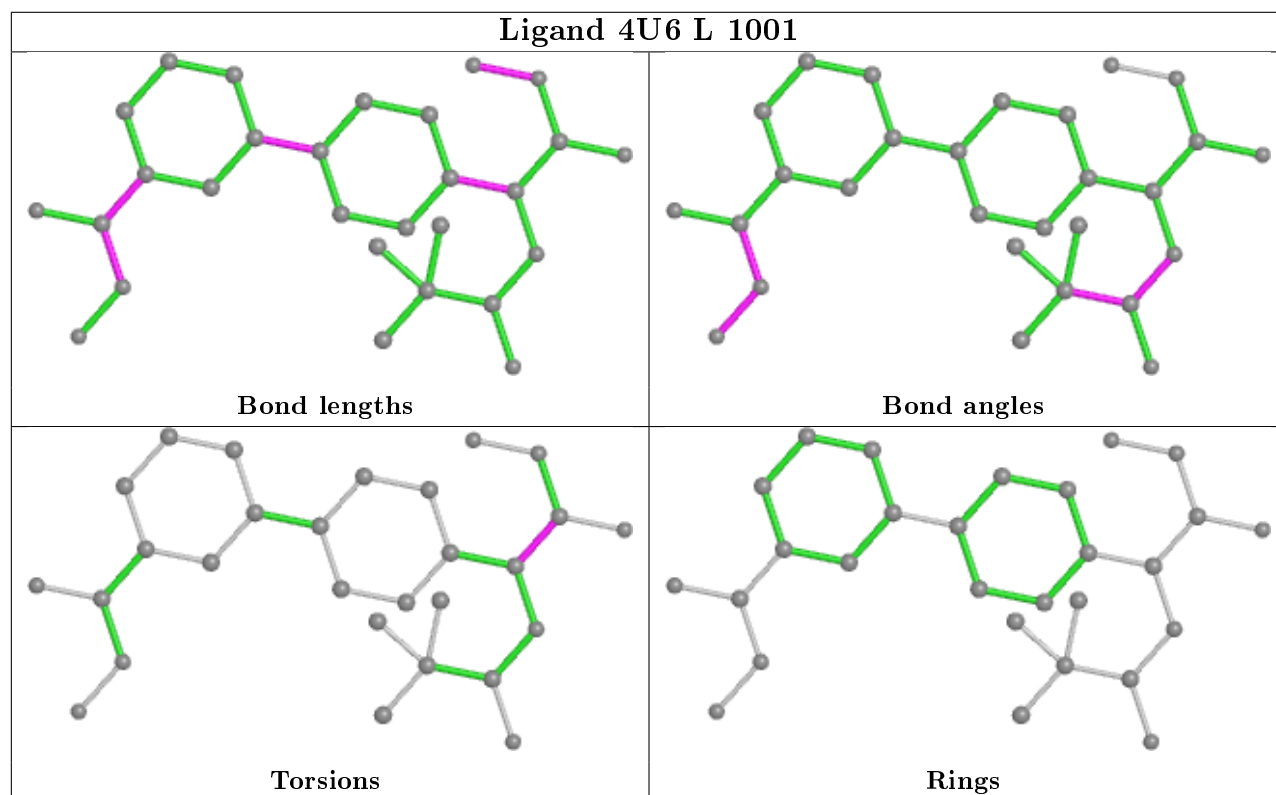
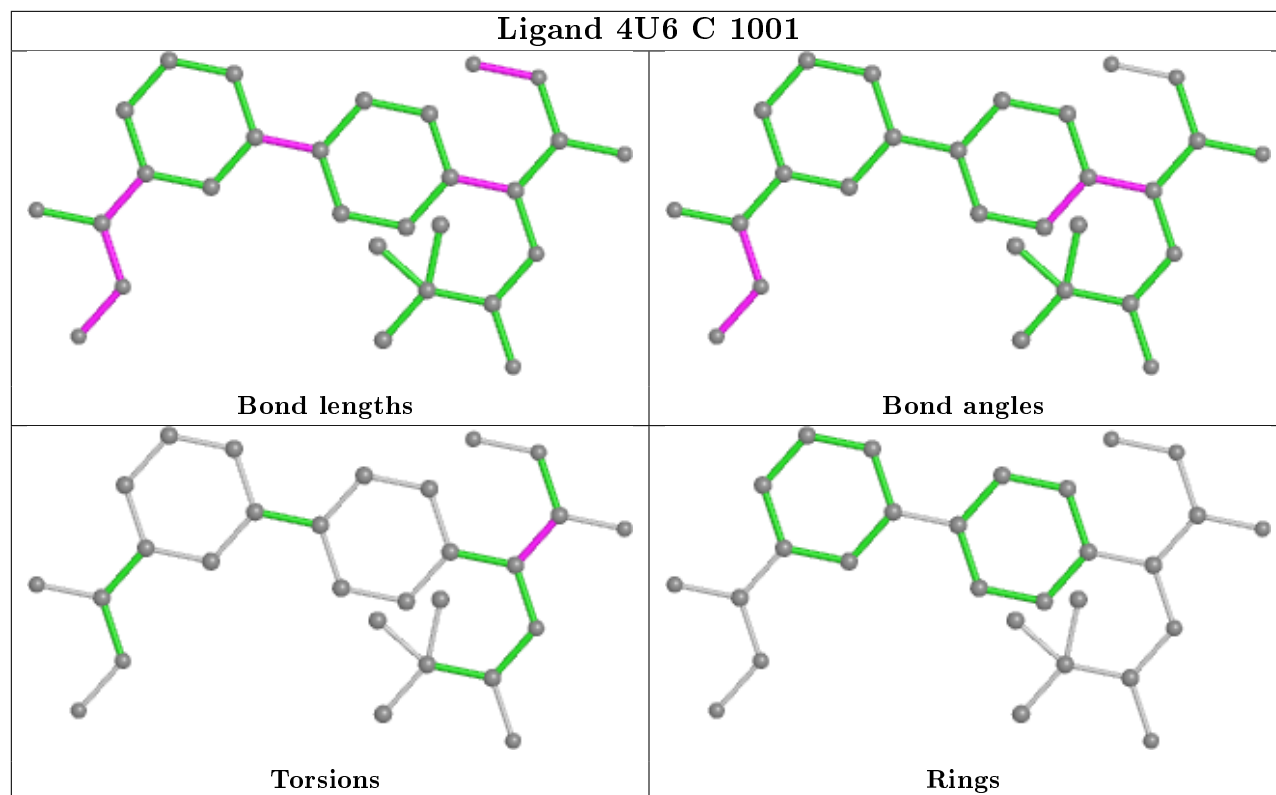
15 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1005	1PE	2	0
5	D	1005	1PE	2	0
6	B	1006	SO4	2	0
5	F	1006	1PE	1	0
5	A	1006	1PE	2	0
4	J	1004	CO3	2	0
6	G	1008	SO4	1	0
2	A	1001	4U6	1	0
5	C	1005	1PE	2	0
2	J	1001	4U6	2	0
5	K	1005	1PE	2	0
5	H	1005	1PE	2	0
2	H	1001	4U6	1	0
2	D	1001	4U6	2	0
2	B	1001	4U6	1	0

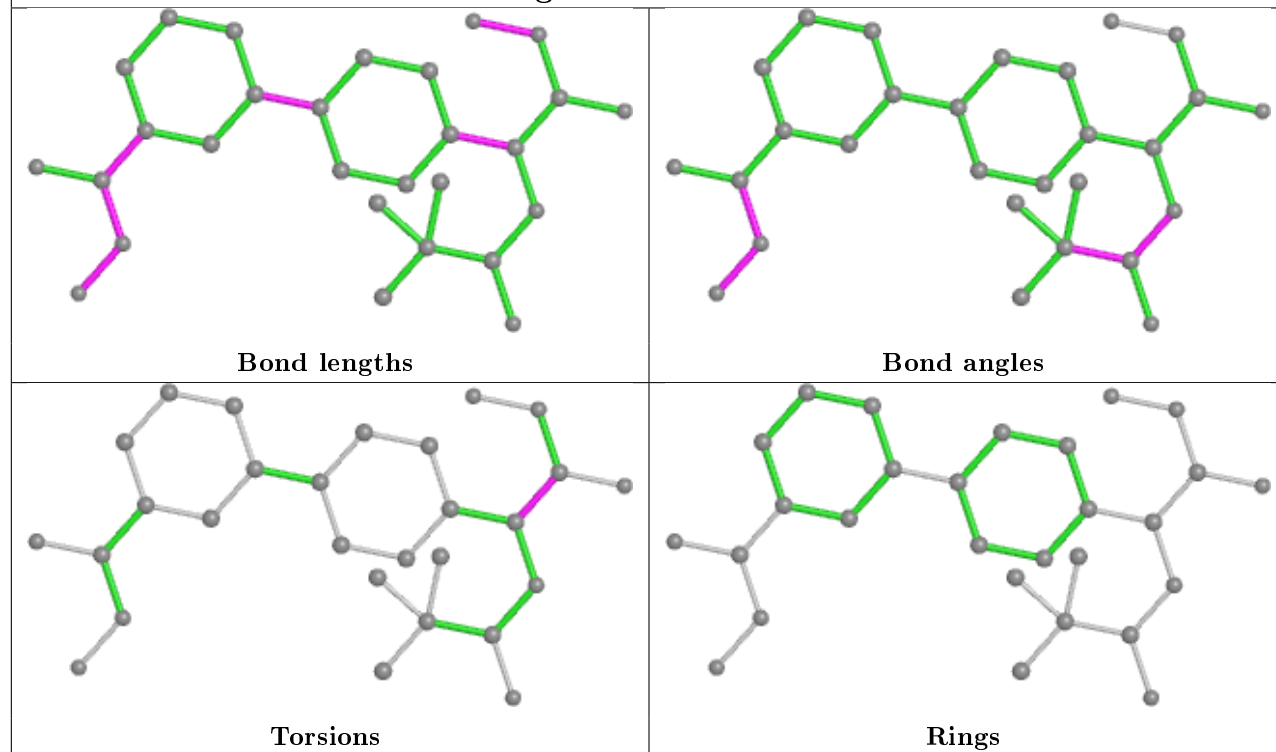
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

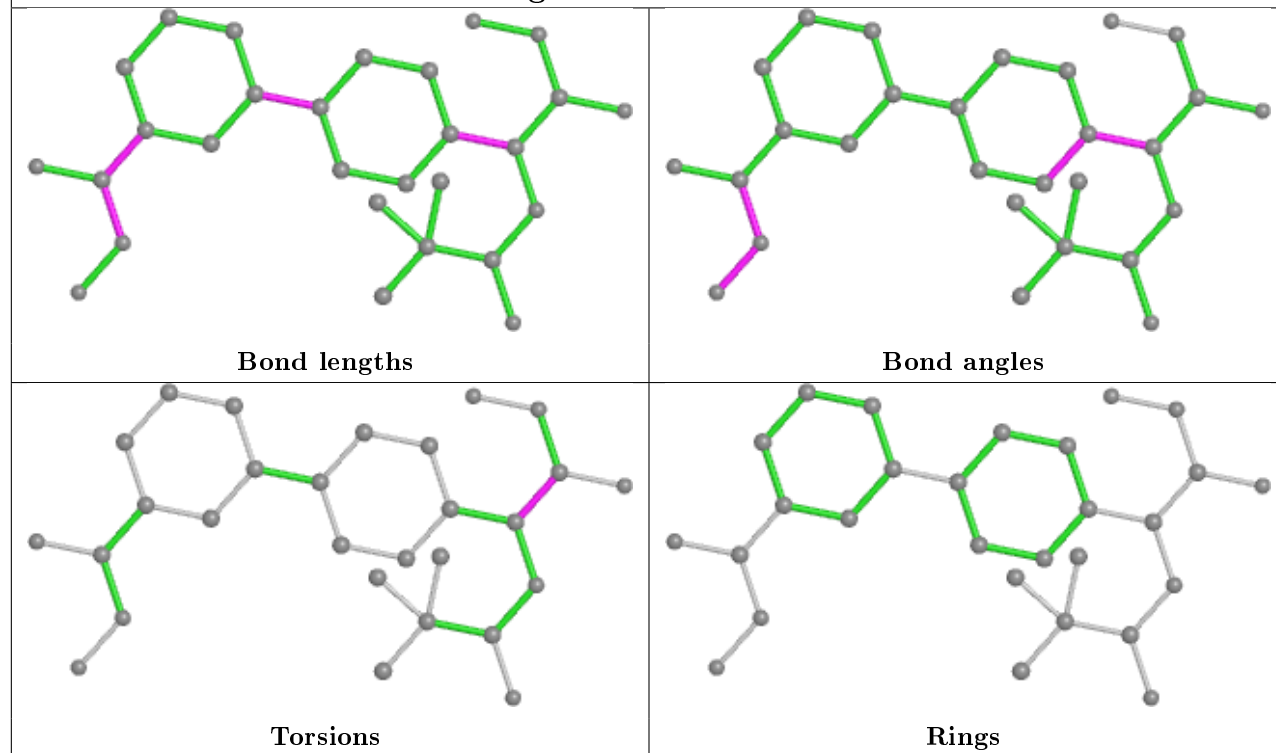


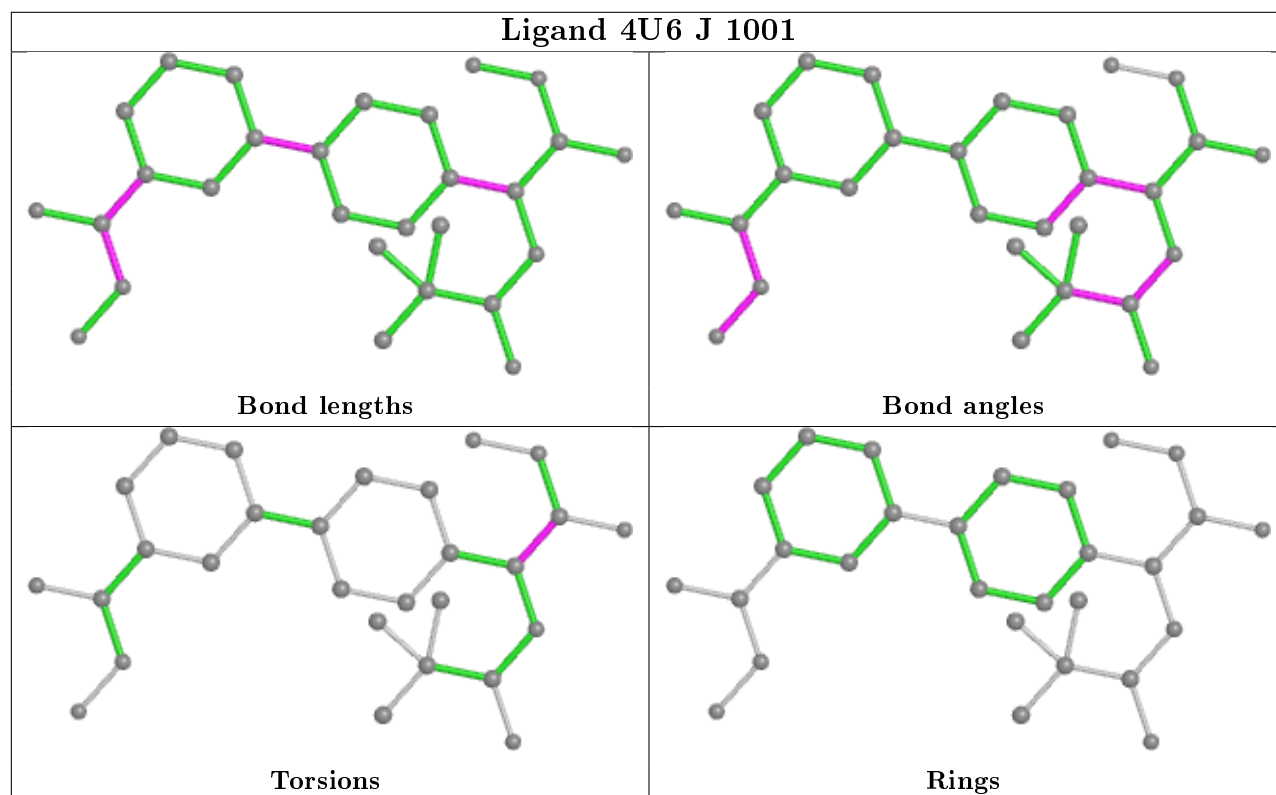
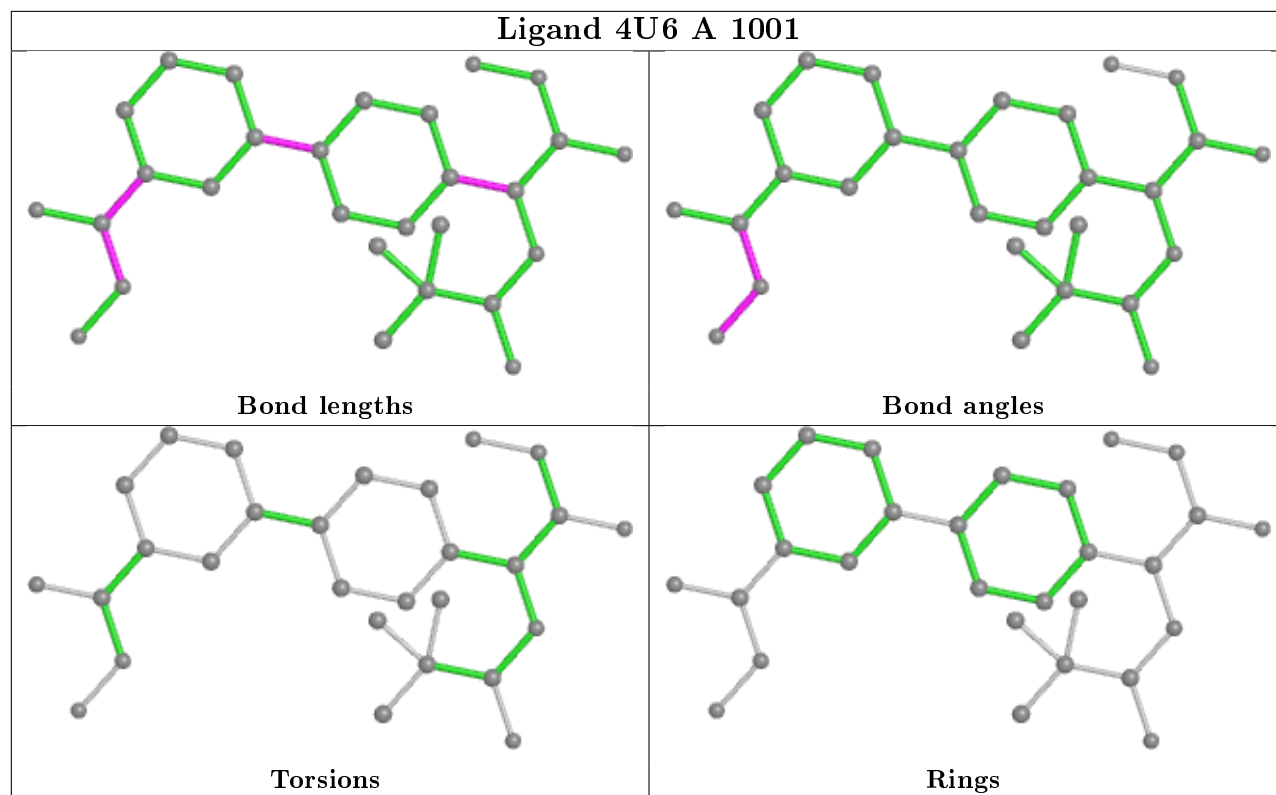


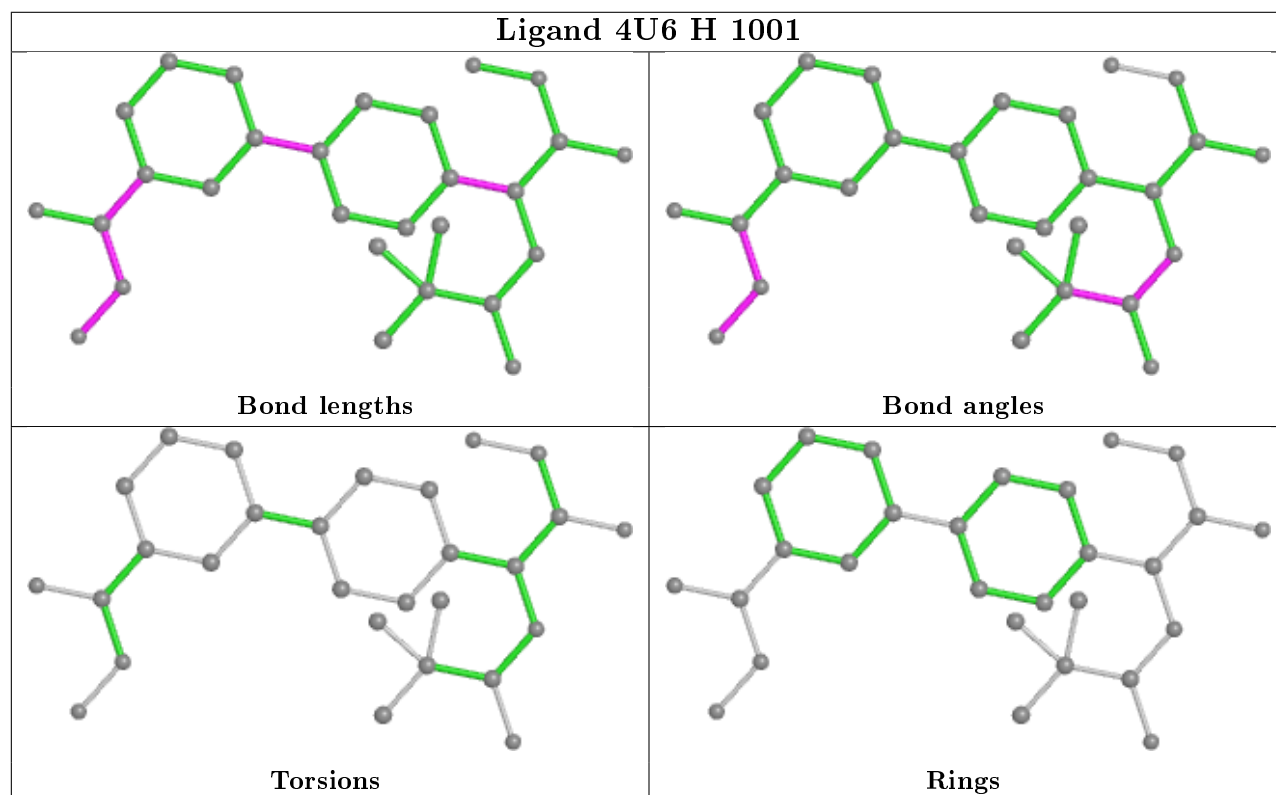
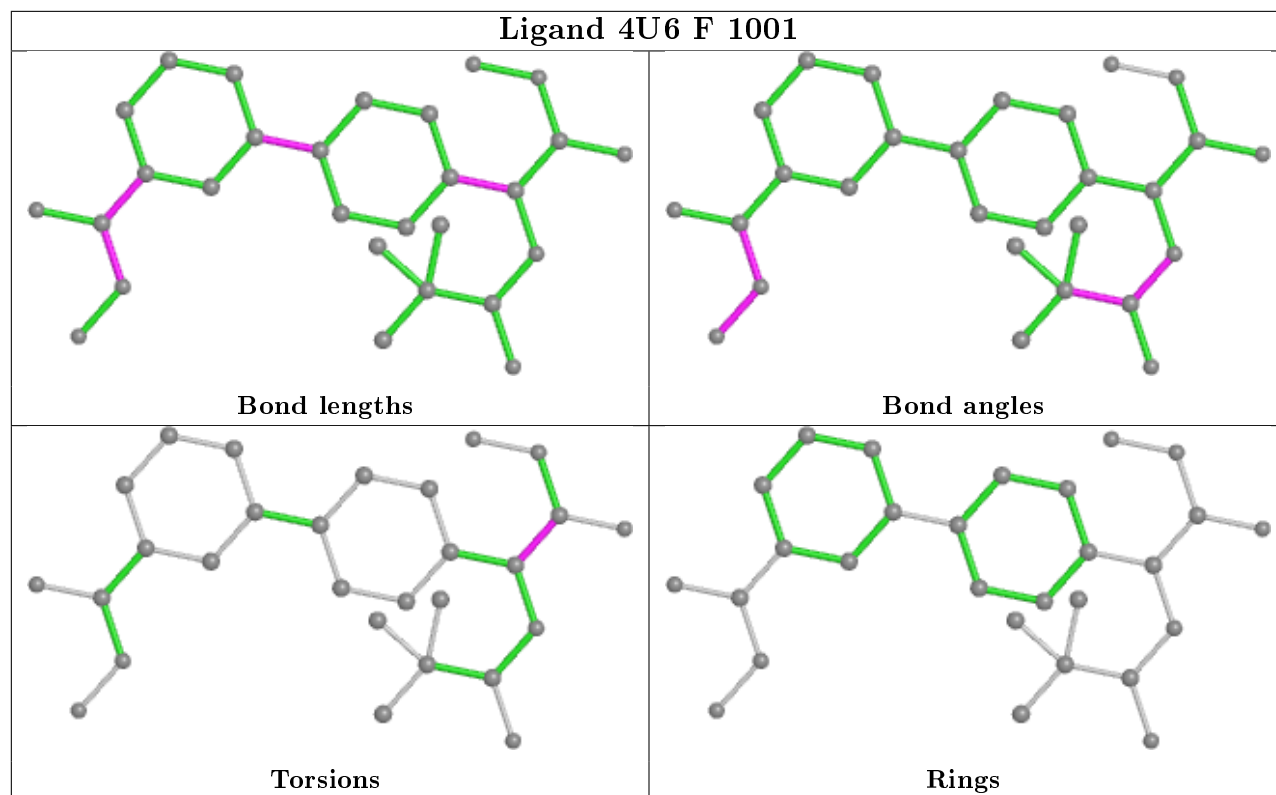
Ligand 4U6 I 1001

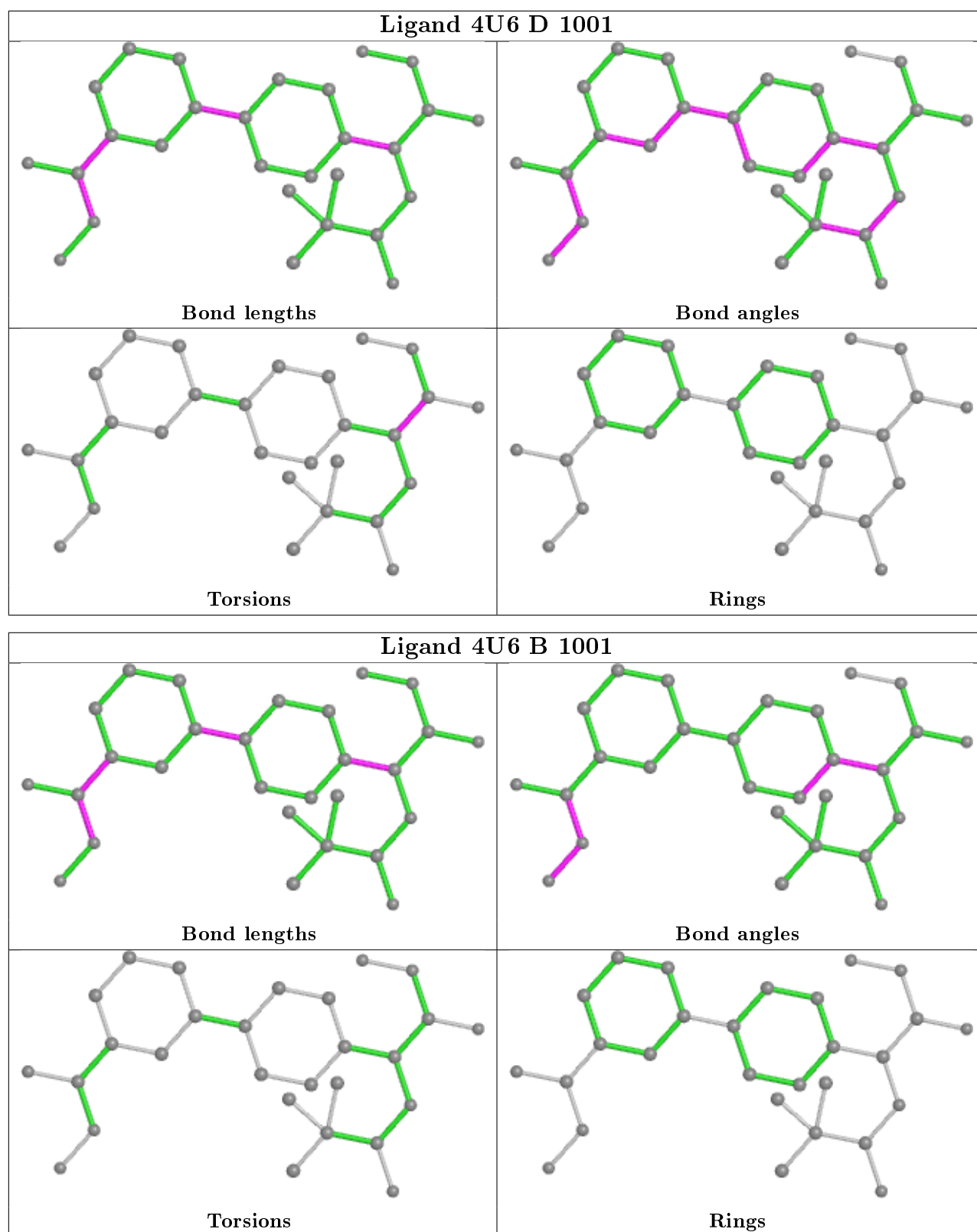


Ligand 4U6 G 1001









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	517/522 (99%)	-0.55	4 (0%) 86 84	11, 23, 46, 66	3 (0%)
1	B	516/522 (98%)	-0.35	9 (1%) 70 66	11, 25, 61, 78	2 (0%)
1	C	516/522 (98%)	-0.50	2 (0%) 92 91	12, 23, 50, 66	2 (0%)
1	D	514/522 (98%)	-0.64	1 (0%) 95 95	11, 21, 43, 61	0
1	E	509/522 (97%)	-0.68	0 100 100	11, 21, 39, 62	1 (0%)
1	F	511/522 (97%)	-0.37	6 (1%) 79 76	15, 29, 57, 84	0
1	G	519/522 (99%)	-0.57	1 (0%) 95 95	12, 21, 47, 68	0
1	H	516/522 (98%)	-0.32	7 (1%) 75 71	13, 26, 61, 84	1 (0%)
1	I	518/522 (99%)	-0.46	4 (0%) 86 84	12, 24, 53, 69	0
1	J	513/522 (98%)	-0.61	2 (0%) 92 91	13, 22, 44, 68	2 (0%)
1	K	508/522 (97%)	-0.65	0 100 100	11, 22, 39, 60	0
1	L	511/522 (97%)	-0.52	3 (0%) 89 88	12, 25, 53, 79	1 (0%)
All	All	6168/6264 (98%)	-0.52	39 (0%) 89 88	11, 23, 52, 84	12 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	274	ALA	4.2
1	B	136	GLY	4.1
1	L	138	GLU	4.0
1	J	603	ASP	3.2
1	A	603	ASP	3.2
1	C	274	ALA	3.2
1	H	259	VAL	2.9
1	B	197	ASP	2.7
1	G	136	GLY	2.6
1	B	154	SER	2.6
1	I	549	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	551	VAL	2.5
1	A	85	ALA	2.4
1	H	149	ASN	2.4
1	I	136	GLY	2.4
1	H	150	ASP	2.4
1	C	136	GLY	2.4
1	D	136	GLY	2.4
1	L	145	SER	2.3
1	F	276	THR	2.3
1	H	276	THR	2.3
1	F	146	SER	2.2
1	B	117	ILE	2.2
1	F	145	SER	2.2
1	J	219	LEU	2.2
1	B	196	ALA	2.1
1	L	146	SER	2.1
1	H	180	ASP	2.1
1	B	121	CYS	2.1
1	B	194	SER	2.1
1	F	121	CYS	2.1
1	H	134	ASN	2.1
1	A	196	ALA	2.1
1	F	550	SER	2.1
1	B	144	ILE	2.1
1	F	141	PRO	2.1
1	H	119	GLY	2.1
1	B	146	SER	2.0
1	I	120	GLY	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(\AA^2)	Q<0.9
5	1PE	F	1006	12/16	0.84	0.32	37,55,67,71	0
5	1PE	H	1005	10/16	0.87	0.18	22,42,52,52	0
5	1PE	B	1005	10/16	0.87	0.21	29,35,52,66	0
5	1PE	I	1006	11/16	0.89	0.21	28,36,43,45	0
5	1PE	D	1005	10/16	0.90	0.16	28,39,43,68	0
5	1PE	G	1005	9/16	0.90	0.18	21,29,37,45	0
5	1PE	A	1006	12/16	0.91	0.14	35,40,51,55	0
5	1PE	K	1005	12/16	0.91	0.17	18,27,52,55	0
5	1PE	G	1006	6/16	0.91	0.17	25,31,35,41	0
5	1PE	I	1005	12/16	0.92	0.21	31,41,46,47	0
5	1PE	G	1007	6/16	0.92	0.13	20,27,34,35	0
5	1PE	F	1005	10/16	0.92	0.16	28,34,55,56	0
5	1PE	E	1005	12/16	0.93	0.15	19,33,36,37	0
5	1PE	L	1005	10/16	0.93	0.13	24,31,44,49	0
2	4U6	H	1001	28/28	0.93	0.19	15,31,55,66	0
5	1PE	C	1005	13/16	0.93	0.21	19,35,43,44	0
5	1PE	D	1006	10/16	0.94	0.14	26,30,35,45	0
5	1PE	A	1005	9/16	0.94	0.15	18,28,36,40	0
5	1PE	E	1006	12/16	0.94	0.14	25,32,48,61	0
5	1PE	C	1006	9/16	0.94	0.14	21,32,39,43	0
2	4U6	C	1001	28/28	0.94	0.16	14,24,57,68	0
6	SO4	A	1007	5/5	0.94	0.15	44,56,69,78	0
2	4U6	I	1001	28/28	0.95	0.16	13,24,60,65	0
2	4U6	J	1001	28/28	0.95	0.15	15,25,47,53	0
5	1PE	J	1005	11/16	0.96	0.14	20,25,41,42	0
2	4U6	D	1001	28/28	0.96	0.14	14,22,44,55	0
2	4U6	E	1001	28/28	0.96	0.15	16,22,48,60	0
2	4U6	L	1001	28/28	0.96	0.13	17,27,37,69	0
6	SO4	J	1006	5/5	0.96	0.18	44,60,78,80	0
2	4U6	F	1001	28/28	0.96	0.14	16,24,44,72	0
2	4U6	A	1001	28/28	0.96	0.15	12,25,42,63	0
2	4U6	B	1001	28/28	0.96	0.16	10,23,49,65	0
4	CO3	D	1004	4/4	0.97	0.14	13,14,16,17	0
4	CO3	C	1004	4/4	0.97	0.14	14,16,17,22	0
4	CO3	H	1004	4/4	0.97	0.17	14,14,15,16	0
2	4U6	K	1001	28/28	0.97	0.14	16,23,50,63	0
2	4U6	G	1001	28/28	0.97	0.14	12,24,42,70	0
4	CO3	J	1004	4/4	0.97	0.10	17,19,24,26	0
6	SO4	F	1007	5/5	0.97	0.15	51,53,66,67	0
4	CO3	A	1004	4/4	0.97	0.13	15,16,16,19	0
4	CO3	K	1004	4/4	0.97	0.13	16,17,20,21	0

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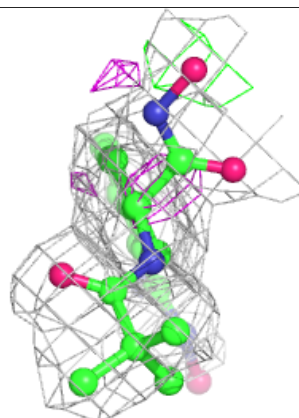
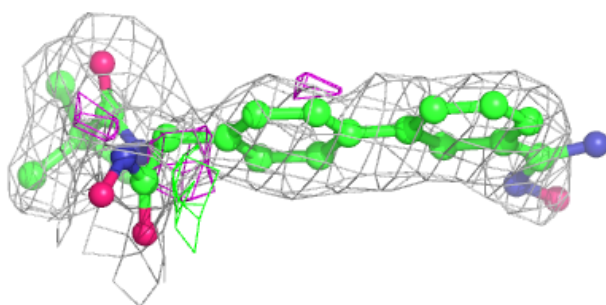
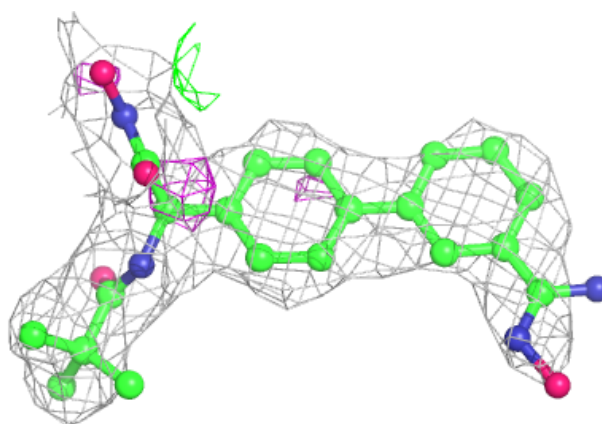
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CO3	L	1004	4/4	0.98	0.12	12,15,16,18	0
6	SO4	K	1006	5/5	0.98	0.29	34,54,56,65	0
4	CO3	B	1004	4/4	0.98	0.12	15,16,19,20	0
4	CO3	G	1004	4/4	0.98	0.12	14,17,18,19	0
4	CO3	I	1004	4/4	0.98	0.12	14,15,16,16	0
4	CO3	F	1004	4/4	0.98	0.10	14,19,20,22	0
6	SO4	B	1006	5/5	0.98	0.15	20,22,27,32	0
4	CO3	E	1004	4/4	0.98	0.12	17,19,19,20	0
3	ZN	I	1003	1/1	0.98	0.09	16,16,16,16	0
3	ZN	B	1003	1/1	0.99	0.07	16,16,16,16	0
3	ZN	E	1002	1/1	0.99	0.10	14,14,14,14	0
6	SO4	G	1008	5/5	0.99	0.09	17,19,21,28	0
3	ZN	F	1002	1/1	0.99	0.09	18,18,18,18	0
3	ZN	C	1003	1/1	0.99	0.07	11,11,11,11	0
3	ZN	L	1003	1/1	0.99	0.09	16,16,16,16	0
3	ZN	K	1002	1/1	0.99	0.11	17,17,17,17	0
3	ZN	B	1002	1/1	0.99	0.08	15,15,15,15	0
3	ZN	F	1003	1/1	0.99	0.09	16,16,16,16	0
6	SO4	L	1006	5/5	0.99	0.09	20,23,27,39	0
3	ZN	L	1002	1/1	0.99	0.07	17,17,17,17	0
6	SO4	D	1007	5/5	0.99	0.08	16,20,26,31	0
3	ZN	G	1002	1/1	0.99	0.08	17,17,17,17	0
3	ZN	C	1002	1/1	0.99	0.07	14,14,14,14	0
3	ZN	J	1002	1/1	0.99	0.07	19,19,19,19	0
3	ZN	H	1003	1/1	0.99	0.07	15,15,15,15	0
3	ZN	K	1003	1/1	0.99	0.09	14,14,14,14	0
3	ZN	D	1002	1/1	0.99	0.06	16,16,16,16	0
3	ZN	E	1003	1/1	1.00	0.08	19,19,19,19	0
3	ZN	I	1002	1/1	1.00	0.10	17,17,17,17	0
3	ZN	G	1003	1/1	1.00	0.08	12,12,12,12	0
3	ZN	A	1002	1/1	1.00	0.09	16,16,16,16	0
3	ZN	A	1003	1/1	1.00	0.08	10,10,10,10	0
3	ZN	H	1002	1/1	1.00	0.08	16,16,16,16	0
3	ZN	D	1003	1/1	1.00	0.06	13,13,13,13	0
3	ZN	J	1003	1/1	1.00	0.06	15,15,15,15	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.

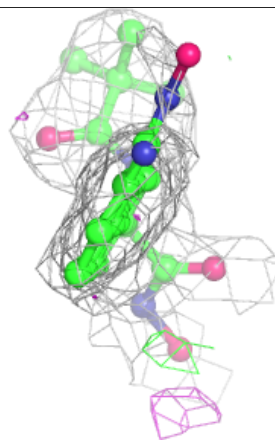
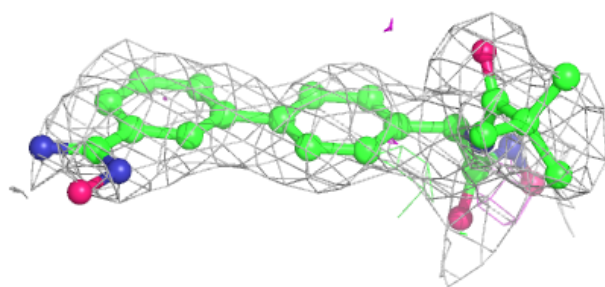
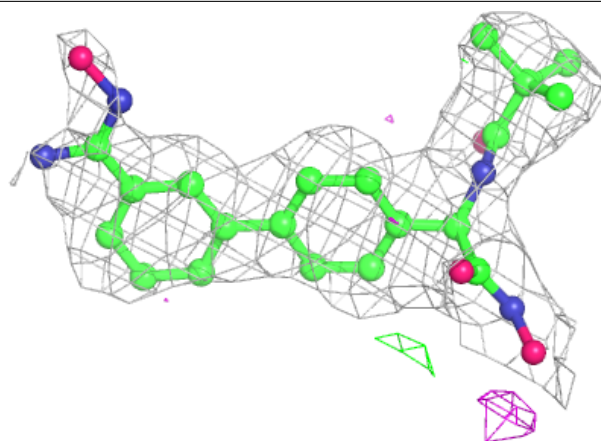
Electron density around 4U6 H 1001:

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

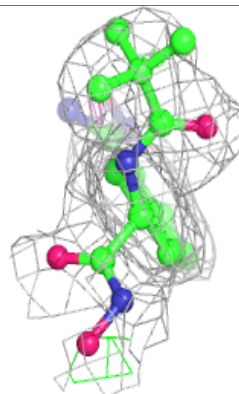
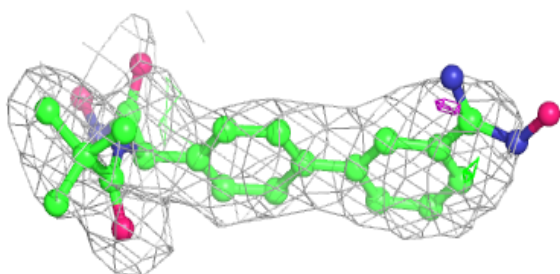
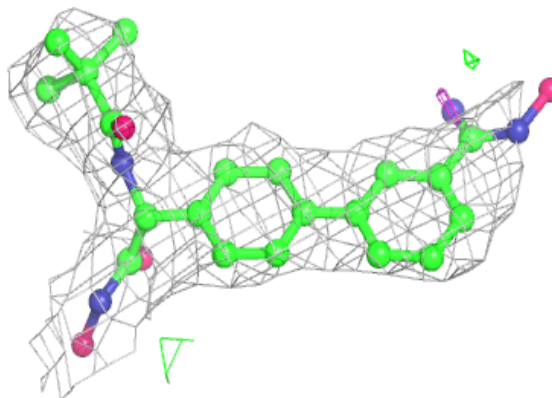


Electron density around 4U6 C 1001:

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

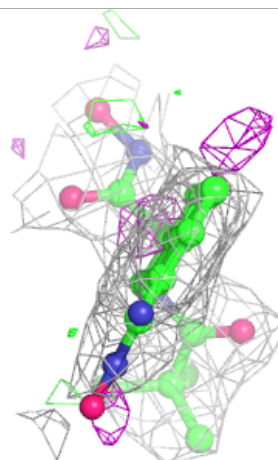
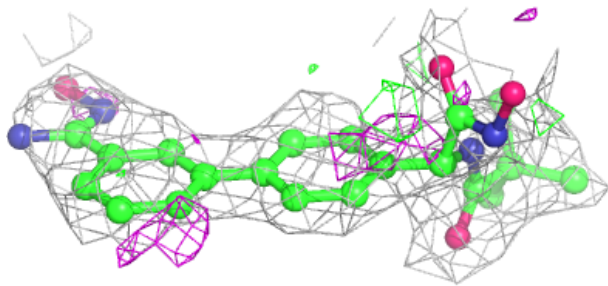
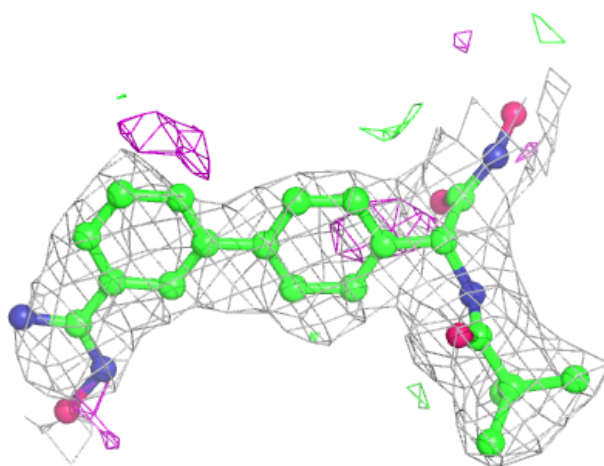
**Electron density around 4U6 I 1001:**

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



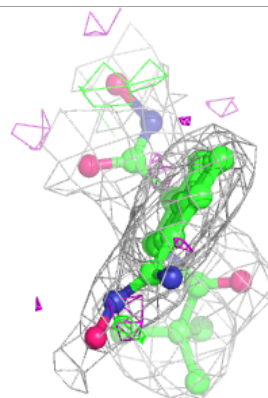
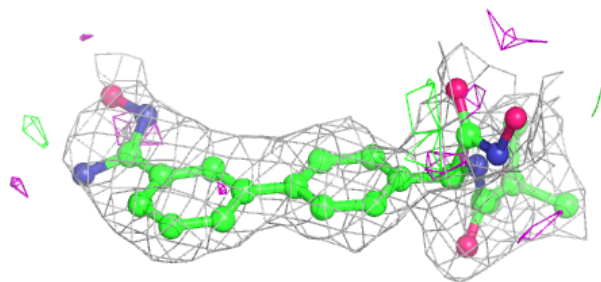
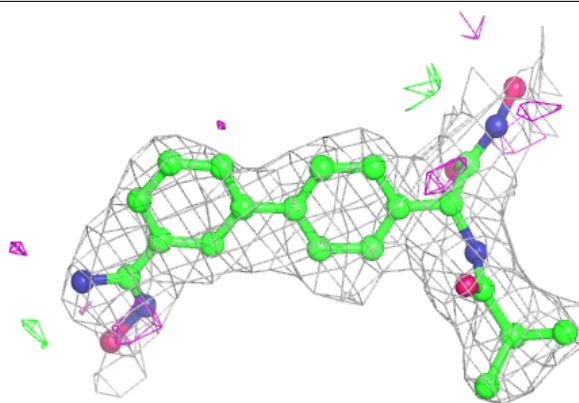
Electron density around 4U6 J 1001:

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and green (positive)

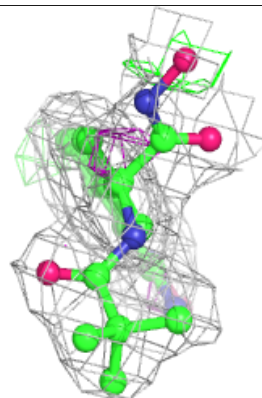
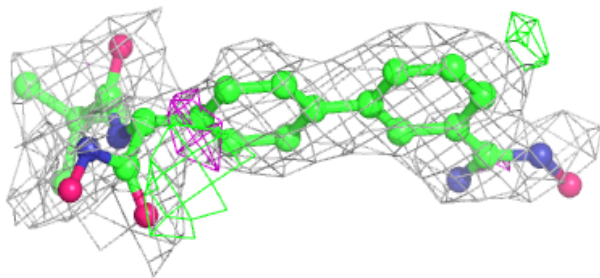
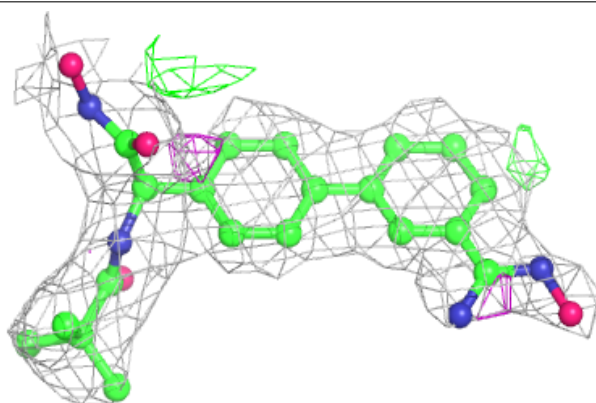


Electron density around 4U6 D 1001:

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

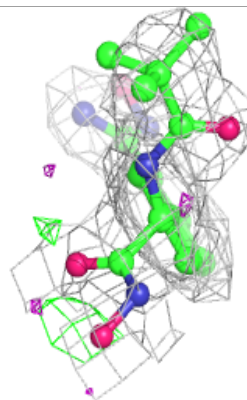
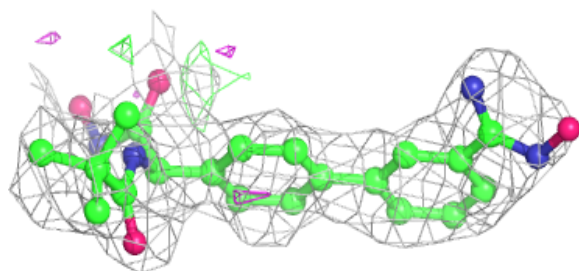
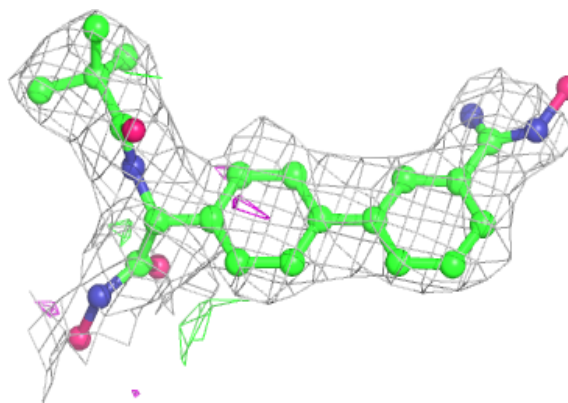
**Electron density around 4U6 E 1001:**

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

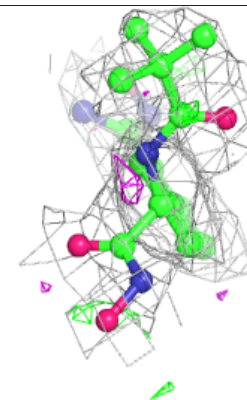
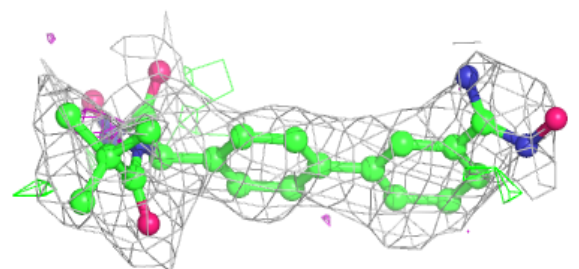
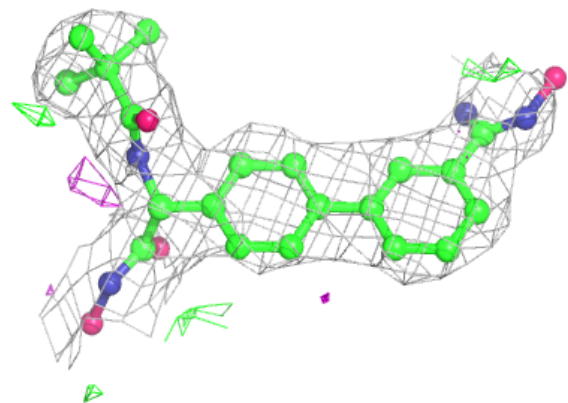


Electron density around 4U6 L 1001:

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

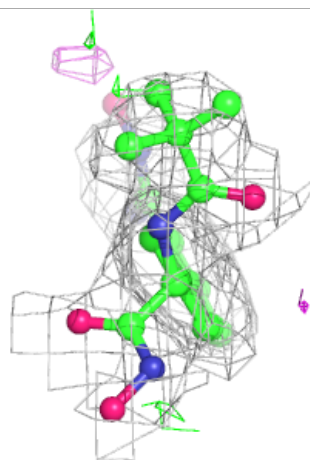
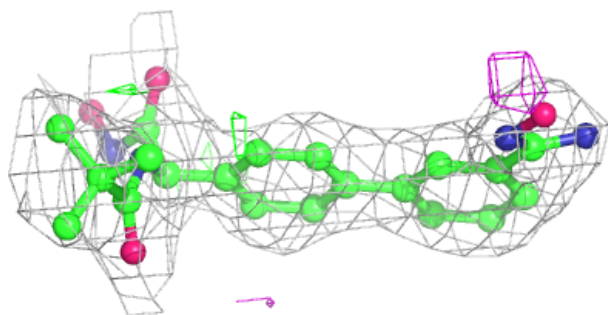
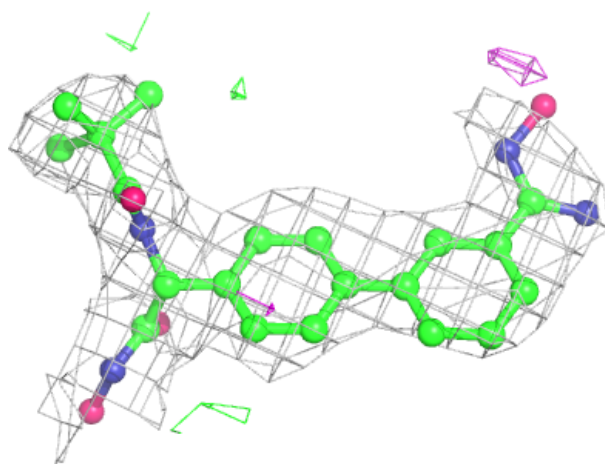
**Electron density around 4U6 F 1001:**

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



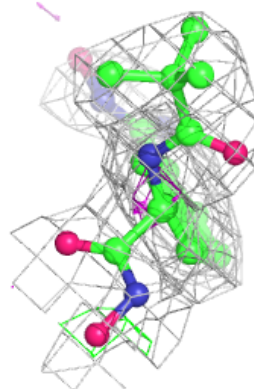
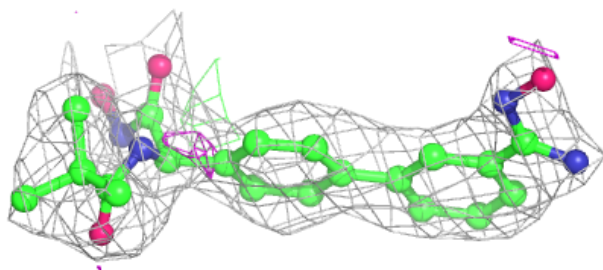
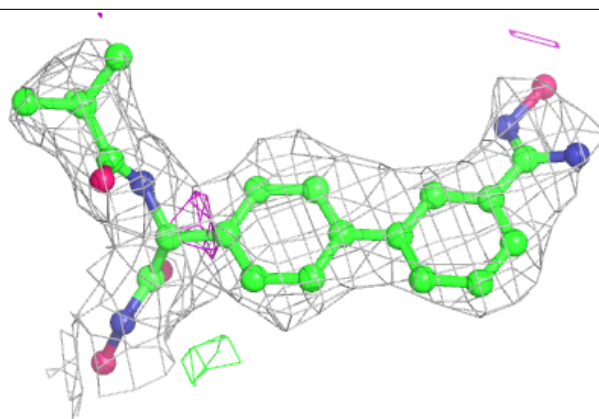
Electron density around 4U6 A 1001:

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

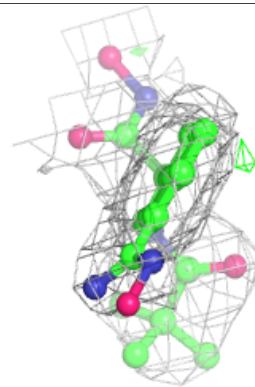
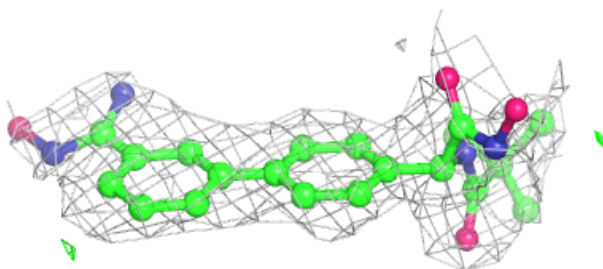
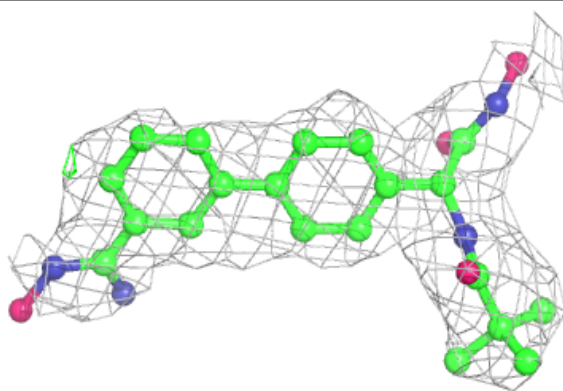


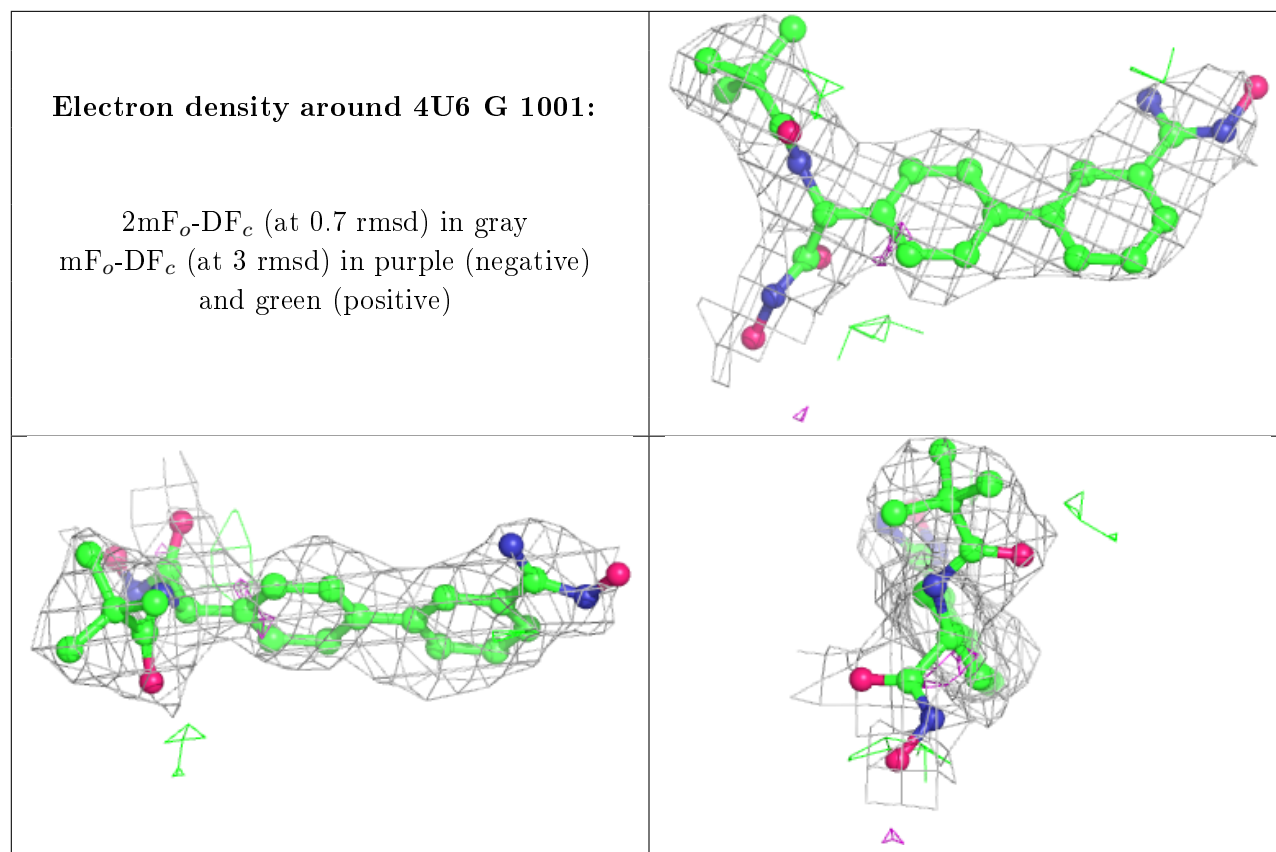
Electron density around 4U6 B 1001:

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

**Electron density around 4U6 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.