



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:02 PM UTC

PDB ID : 4ZY1 / pdb_00004zy1
Title : X-ray crystal structure of PfA-M17 in complex with hydroxamic acid-based inhibitor 10r
Authors : Drinkwater, N.; McGowan, S.
Deposited on : 2015-05-21
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

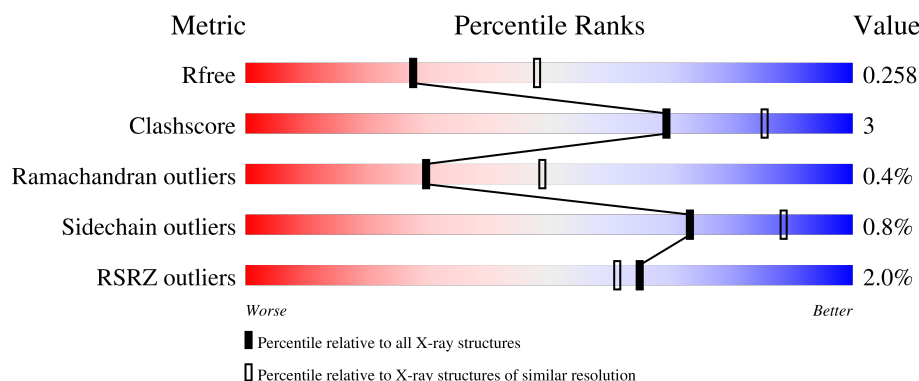
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



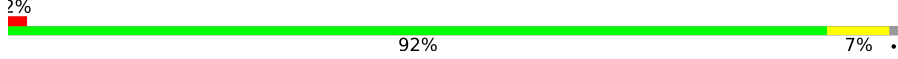
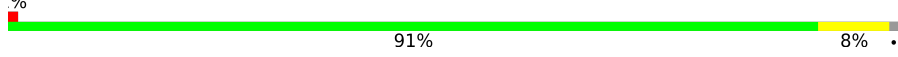
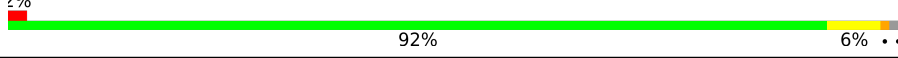
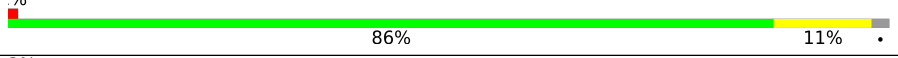
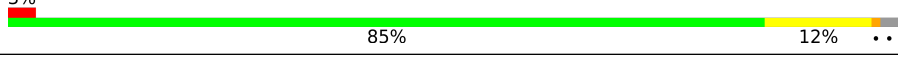
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	% 90% 8% .
1	B	522	3% 87% 11% ..
1	C	522	2% 90% 9% .
1	D	522	2% 88% 10% ..
1	E	522	% 92% 5% .

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Mol	Chain	Length	Quality of chain
1	F	522	
1	G	522	
1	H	522	
1	I	522	
1	J	522	
1	K	522	
1	L	522	

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
5	SO4	A	1007	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 49124 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	518	Total	C	N	O	S	0	0	0
			3970	2549	638	764	19			
1	B	516	Total	C	N	O	S	0	0	0
			3909	2513	634	743	19			
1	C	516	Total	C	N	O	S	0	0	0
			3946	2535	635	756	20			
1	D	514	Total	C	N	O	S	0	0	0
			3934	2532	635	747	20			
1	E	508	Total	C	N	O	S	0	0	0
			3890	2505	626	740	19			
1	F	511	Total	C	N	O	S	0	0	0
			3837	2468	620	730	19			
1	G	519	Total	C	N	O	S	0	0	0
			3971	2548	639	765	19			
1	H	517	Total	C	N	O	S	0	0	0
			3904	2507	634	744	19			
1	I	517	Total	C	N	O	S	0	0	0
			3944	2535	635	754	20			
1	J	514	Total	C	N	O	S	0	0	0
			3914	2517	633	744	20			
1	K	509	Total	C	N	O	S	0	0	0
			3890	2504	624	743	19			
1	L	510	Total	C	N	O	S	0	0	0
			3840	2468	618	735	19			

There are 36 discrepancies between the modelled and reference sequences:

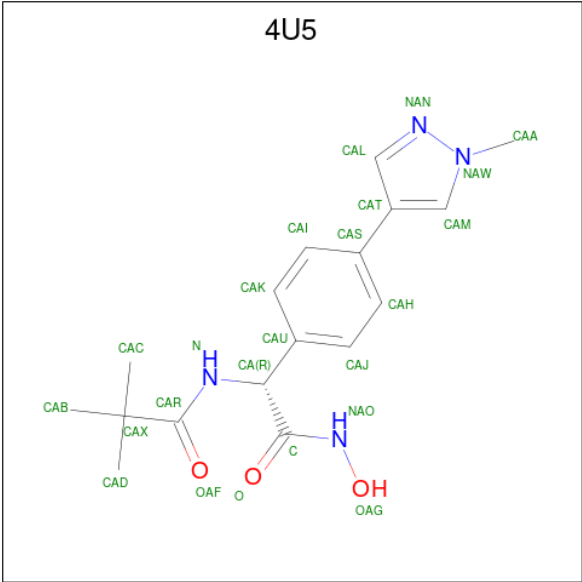
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	515	GLN	ASN	engineered mutation	UNP A0A024V0B1
A	546	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	152	GLN	ASN	engineered mutation	UNP A0A024V0B1
B	515	GLN	ASN	engineered mutation	UNP A0A024V0B1

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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-[4-(1-methyl-1H-pyrazol-4-yl)phenyl]-2-oxoethyl}-2,2-dimethylpropanamide (CCD ID: 4U5) (formula: C₁₇H₂₂N₄O₃).

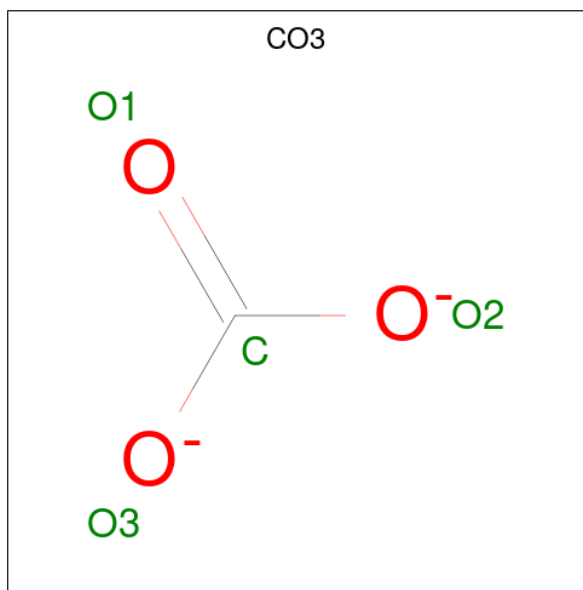


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	17	4	3		
2	B	1	Total	C	N	O	0	0
			24	17	4	3		
2	C	1	Total	C	N	O	0	0
			24	17	4	3		
2	D	1	Total	C	N	O	0	0
			24	17	4	3		
2	E	1	Total	C	N	O	0	0
			24	17	4	3		
2	F	1	Total	C	N	O	0	0
			24	17	4	3		
2	G	1	Total	C	N	O	0	0
			24	17	4	3		
2	H	1	Total	C	N	O	0	0
			24	17	4	3		
2	I	1	Total	C	N	O	0	0
			24	17	4	3		
2	J	1	Total	C	N	O	0	0
			24	17	4	3		
2	K	1	Total	C	N	O	0	0
			24	17	4	3		
2	L	1	Total	C	N	O	0	0
			24	17	4	3		

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

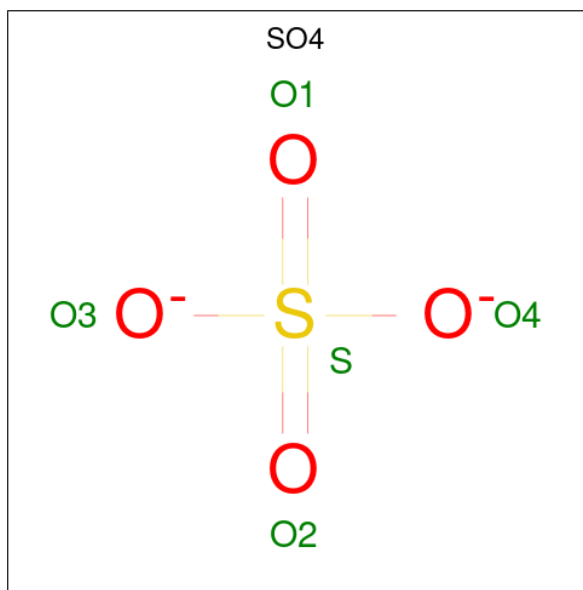
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	F	2	Total 2	Zn 2	0	0
3	G	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	J	2	Total 2	Zn 2	0	0
3	K	2	Total 2	Zn 2	0	0
3	L	2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

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



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



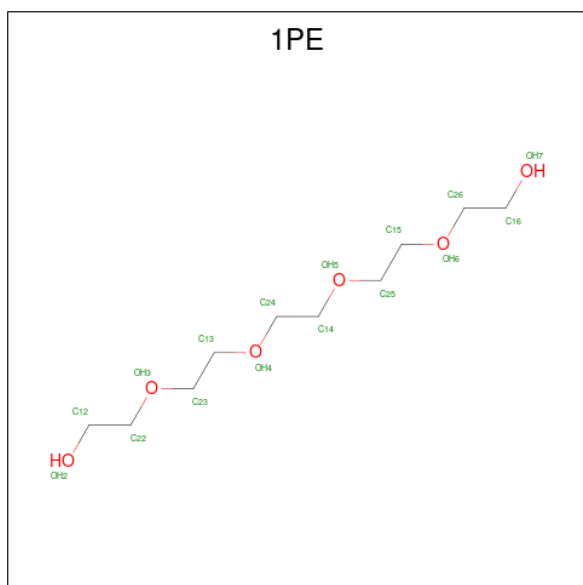
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
			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	J	1	Total	C	O	0	0
			10	6	4		
6	K	1	Total	C	O	0	0
			12	8	4		
6	K	1	Total	C	O	0	0
			12	8	4		
6	L	1	Total	C	O	0	0
			7	4	3		
6	L	1	Total	C	O	0	0
			10	6	4		
6	L	1	Total	C	O	0	0
			11	7	4		

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



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	110	Total	O	0	0
			110	110		
8	B	114	Total	O	0	0
			114	114		
8	C	121	Total	O	0	0
			121	121		
8	D	138	Total	O	0	0
			138	138		
8	E	129	Total	O	0	0
			129	129		
8	F	106	Total	O	0	0
			106	106		
8	G	116	Total	O	0	0
			116	116		
8	H	125	Total	O	0	0
			125	125		
8	I	138	Total	O	0	0
			138	138		
8	J	106	Total	O	0	0
			106	106		
8	K	140	Total	O	0	0
			140	140		

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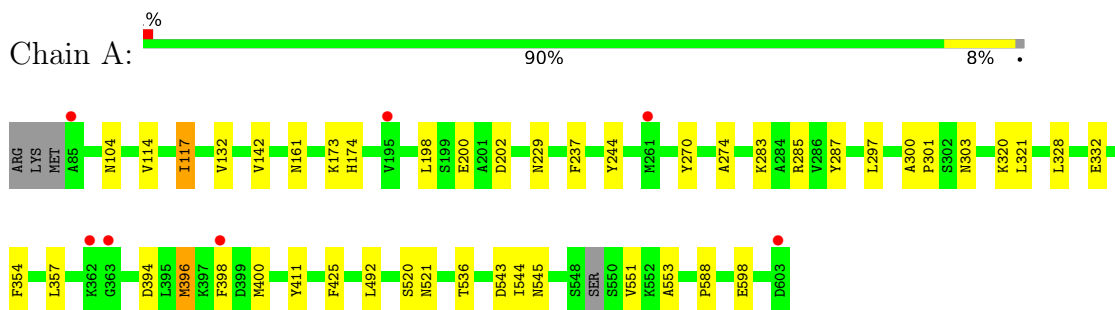
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	102	Total 102	O 102	0	0

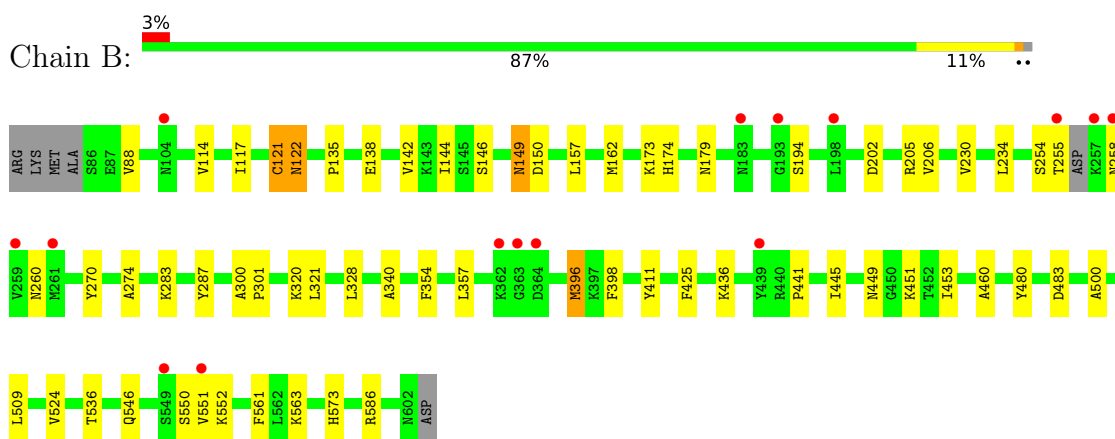
3 Residue-property plots [i](#)

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.

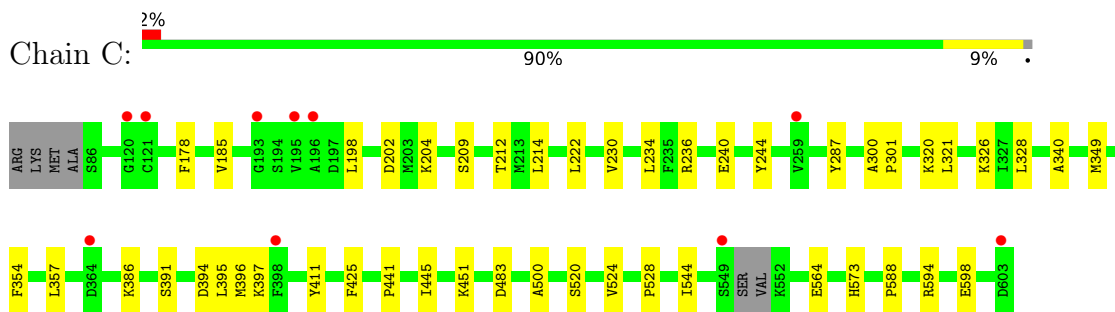
- Molecule 1: Probable M17 family aminopeptidase



- Molecule 1: Probable M17 family aminopeptidase

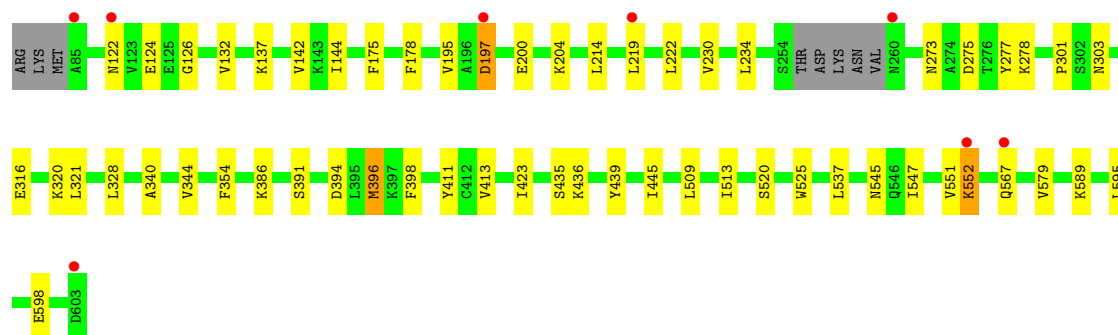


- Molecule 1: Probable M17 family aminopeptidase

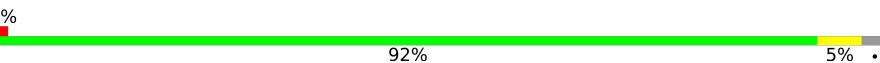


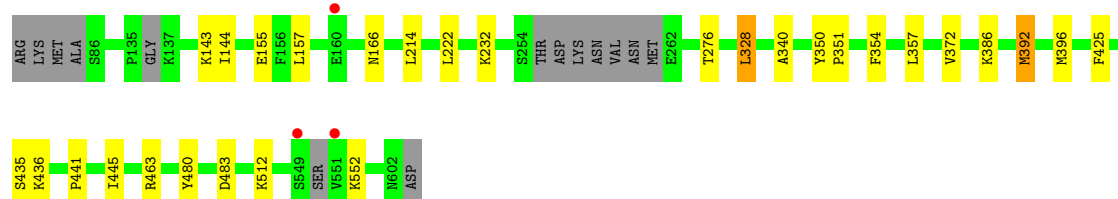
- Molecule 1: Probable M17 family aminopeptidase

Chain D: 



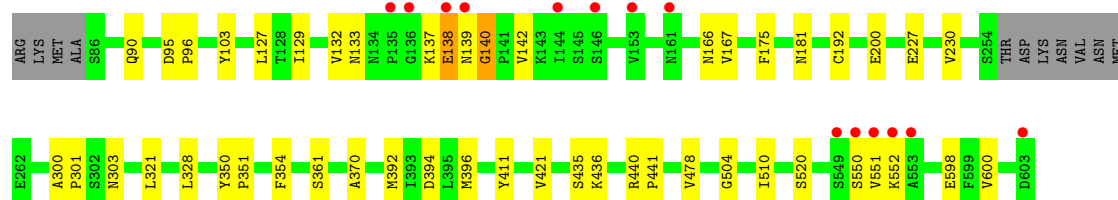
- Molecule 1: Probable M17 family aminopeptidase

Chain E: 

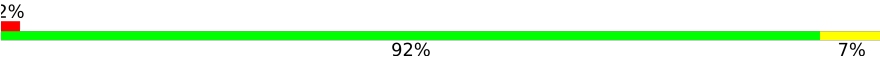


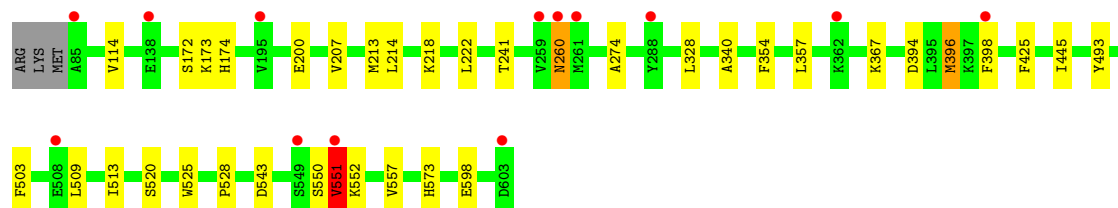
- Molecule 1: Probable M17 family aminopeptidase

Chain F: 



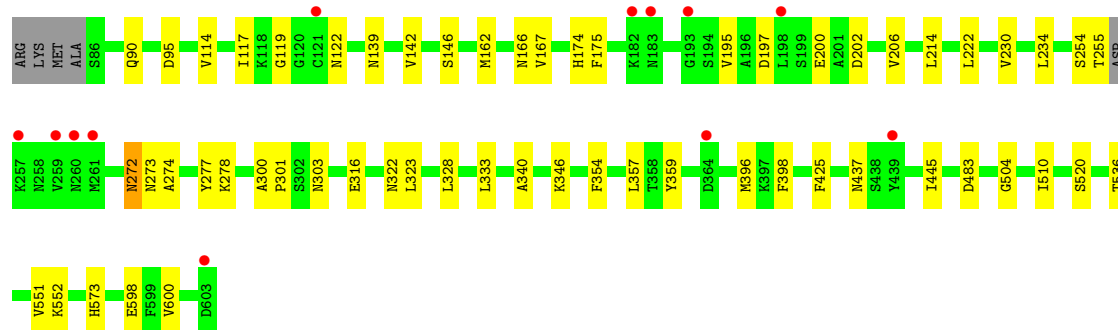
- Molecule 1: Probable M17 family aminopeptidase

Chain G: 

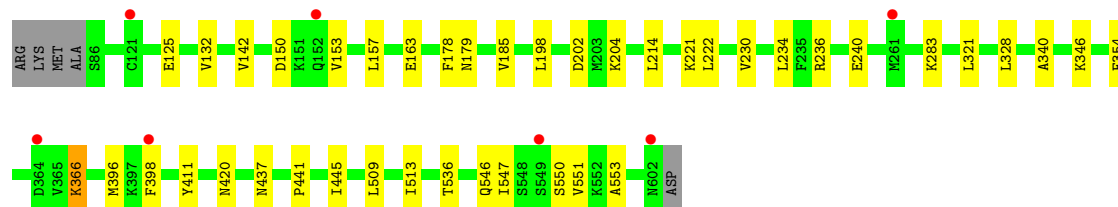
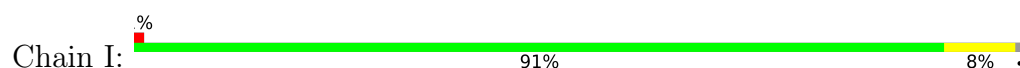


- Molecule 1: Probable M17 family aminopeptidase

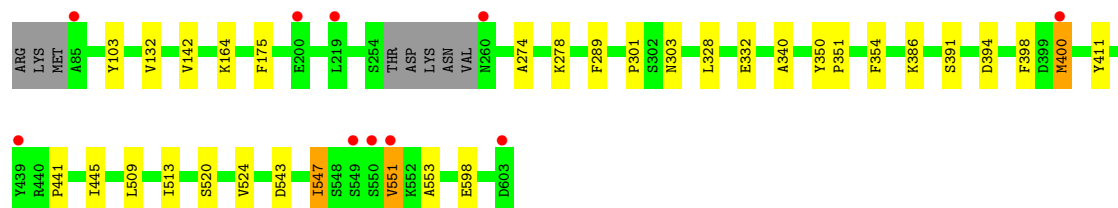
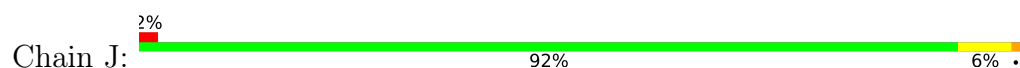
Chain H: 



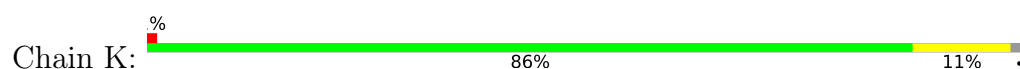
- Molecule 1: Probable M17 family aminopeptidase



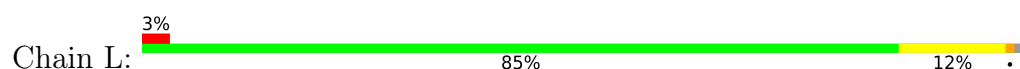
- Molecule 1: Probable M17 family aminopeptidase

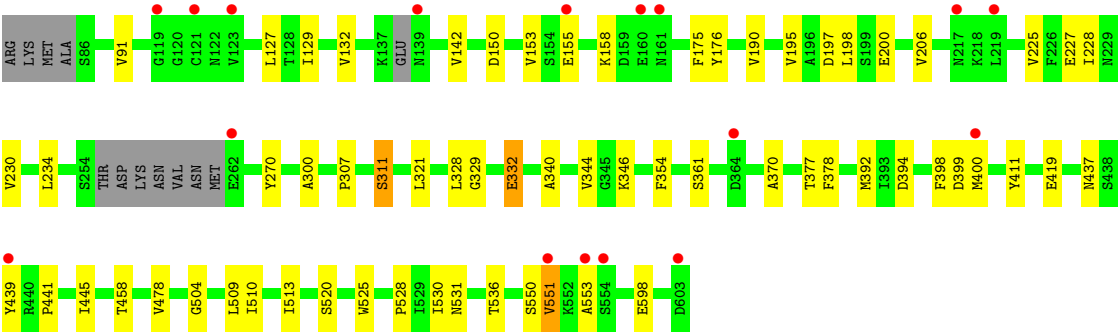


- Molecule 1: Probable M17 family aminopeptidase



- 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	174.10Å 177.32Å 229.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.50 48.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.90-2.50) 82.2 (48.90-2.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.203 , 0.257 0.206 , 0.258	Depositor DCC
R_{free} test set	11527 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49124	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 44.83 % 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 1.4421e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4U5, 1PE, CO3, SO4, ZN, GOL

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	0.26	0/4047	0.70	0/5491
1	B	0.28	0/3986	0.73	2/5414 (0.0%)
1	C	0.26	0/4023	0.69	0/5458
1	D	0.26	0/4011	0.70	0/5439
1	E	0.25	0/3965	0.68	0/5376
1	F	0.28	0/3914	0.73	5/5323 (0.1%)
1	G	0.27	0/4049	0.71	1/5497 (0.0%)
1	H	0.29	0/3981	0.72	0/5411
1	I	0.26	0/4022	0.69	0/5459
1	J	0.26	0/3991	0.71	1/5416 (0.0%)
1	K	0.26	0/3966	0.70	0/5381
1	L	0.29	0/3916	0.73	1/5327 (0.0%)
All	All	0.27	0/47871	0.71	10/64992 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	551	VAL	N-CA-C	-7.58	106.51	113.71
1	F	138	GLU	N-CA-C	6.91	121.88	113.17
1	B	121	CYS	CA-C-N	-6.44	114.11	123.00
1	B	121	CYS	C-N-CA	-6.44	114.11	123.00
1	J	551	VAL	N-CA-C	-6.11	107.30	113.47
1	F	140	GLY	CA-C-N	5.82	125.79	120.03
1	F	140	GLY	C-N-CA	5.82	125.79	120.03
1	F	103	TYR	CA-C-N	-5.44	114.52	122.19
1	F	103	TYR	C-N-CA	-5.44	114.52	122.19
1	G	551	VAL	N-CA-C	5.05	119.85	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3970	0	3881	29	0
1	B	3909	0	3794	40	0
1	C	3946	0	3853	25	0
1	D	3934	0	3873	34	0
1	E	3890	0	3817	16	0
1	F	3837	0	3692	23	0
1	G	3971	0	3876	25	0
1	H	3904	0	3773	34	0
1	I	3944	0	3857	21	0
1	J	3914	0	3833	19	0
1	K	3890	0	3807	42	0
1	L	3840	0	3699	42	0
2	A	24	0	0	0	0
2	B	24	0	0	0	0
2	C	24	0	0	0	0
2	D	24	0	0	1	0
2	E	24	0	0	0	0
2	F	24	0	0	0	0
2	G	24	0	0	0	0
2	H	24	0	0	0	0
2	I	24	0	0	0	0
2	J	24	0	0	0	0
2	K	24	0	0	0	0
2	L	24	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	1	0
4	E	4	0	0	1	0
4	F	4	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	4	0	0	0	0
5	A	15	0	0	3	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
5	H	10	0	0	0	0
5	I	10	0	0	0	0
5	J	10	0	0	0	0
5	K	20	0	0	1	0
5	L	15	0	0	0	0
6	A	21	0	22	1	0
6	B	20	0	20	2	0
6	C	22	0	24	1	0
6	D	20	0	20	2	0
6	E	24	0	28	0	0
6	F	10	0	13	0	0
6	G	21	0	20	1	0
6	H	10	0	10	1	0
6	I	23	0	26	0	0
6	J	21	0	26	1	0
6	K	24	0	28	2	0
6	L	28	0	34	3	0
7	G	6	0	8	0	0
8	A	110	0	0	3	1
8	B	114	0	0	2	0
8	C	121	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	138	0	0	1	0
8	E	129	0	0	1	0
8	F	106	0	0	2	0
8	G	116	0	0	2	1
8	H	125	0	0	3	0
8	I	138	0	0	0	0
8	J	106	0	0	0	0
8	K	140	0	0	1	0
8	L	102	0	0	1	0
All	All	49124	0	46034	323	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 3.

All (323) 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:328:LEU:HB2	1:K:354:PHE:HB3	1.62	0.80
1:G:551:VAL:HG21	1:G:557:VAL:HG21	1.65	0.79
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.70	0.73
1:L:531:ASN:H	6:L:1008:1PE:H251	1.55	0.72
1:H:117:ILE:HD11	1:H:146:SER:OG	1.90	0.71
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.73	0.69
1:L:329:GLY:N	1:L:332:GLU:OE1	2.25	0.69
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.74	0.67
1:H:139:ASN:HB3	1:H:166:ASN:HD22	1.60	0.67
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.77	0.66
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.79	0.65
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.78	0.65
1:A:200:GLU:HG3	1:A:521:ASN:HB3	1.79	0.64
1:H:322:ASN:ND2	8:H:1103:HOH:O	2.30	0.64
1:B:142:VAL:HG23	1:B:162:MET:HB3	1.80	0.64
1:A:396:MET:SD	1:A:398:PHE:HE2	2.21	0.64
1:B:122:ASN:N	1:B:122:ASN:HD22	1.95	0.63
5:A:1007:SO4:O2	1:B:586:ARG:NH1	2.32	0.63
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.80	0.63
1:B:157:LEU:HA	1:B:162:MET:HE3	1.81	0.62
1:F:520:SER:HB3	1:F:598:GLU:HG3	1.82	0.62
1:I:178:PHE:HZ	1:K:155:GLU:HG2	1.65	0.61
1:G:173:LYS:NZ	8:G:1103:HOH:O	2.32	0.61
1:L:155:GLU:O	1:L:158:LYS:HE3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.82	0.60
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.84	0.60
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.83	0.60
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.83	0.60
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.83	0.60
1:H:142:VAL:HG23	1:H:162:MET:HB3	1.82	0.60
1:I:546:GLN:HG2	1:I:547:ILE:HG23	1.84	0.59
1:A:104:ASN:ND2	5:A:1005:SO4:O1	2.35	0.58
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.84	0.58
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.84	0.58
1:B:563:LYS:NZ	8:B:1104:HOH:O	2.36	0.58
1:G:550:SER:O	1:G:552:LYS:N	2.36	0.58
1:J:543:ASP:OD2	1:K:254:SER:OG	2.21	0.58
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.85	0.58
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.86	0.58
1:I:125:GLU:HG3	1:I:221:LYS:HD3	1.86	0.57
1:L:150:ASP:HB3	1:L:153:VAL:HG22	1.87	0.57
1:L:307:PRO:O	1:L:311:SER:OG	2.23	0.57
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.85	0.56
1:C:230:VAL:HG12	1:C:234:LEU:HD23	1.87	0.56
1:E:480:TYR:OH	1:E:512:LYS:NZ	2.36	0.56
1:F:138:GLU:N	1:F:139:ASN:HA	2.21	0.56
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.86	0.56
1:E:232:LYS:NZ	1:E:276:THR:O	2.30	0.56
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.87	0.56
1:H:520:SER:HB3	1:H:598:GLU:HG3	1.87	0.56
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.88	0.55
1:L:377:THR:HA	1:L:400:MET:HE2	1.87	0.55
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.87	0.55
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.89	0.55
1:A:117:ILE:HD12	1:A:270:TYR:HB3	1.87	0.54
1:K:550:SER:O	1:K:550:SER:OG	2.19	0.54
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.71	0.54
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.89	0.54
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.88	0.54
1:B:500:ALA:HB3	1:B:524:VAL:HG22	1.89	0.54
1:C:321:LEU:HD11	1:C:411:TYR:HA	1.90	0.54
1:F:440:ARG:NH1	8:F:1105:HOH:O	2.41	0.54
1:K:552:LYS:HA	1:K:553:ALA:HB3	1.89	0.53
2:D:1001:4U5:NAO	4:D:1004:CO3:O1	2.41	0.53
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:ASN:ND2	8:H:1106:HOH:O	2.35	0.53
1:F:137:LYS:CB	1:F:140:GLY:H	2.22	0.53
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.90	0.53
1:C:209:SER:O	1:C:212:THR:OG1	2.27	0.53
1:H:90:GLN:HB3	1:H:95:ASP:HB2	1.90	0.53
1:B:396:MET:SD	1:B:398:PHE:HE2	2.32	0.53
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.91	0.52
1:D:413:VAL:HG11	1:D:423:ILE:HD12	1.89	0.52
1:K:214:LEU:HD21	1:K:222:LEU:HD22	1.90	0.52
1:K:549:SER:O	1:K:550:SER:HB3	2.08	0.52
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.91	0.52
1:K:232:LYS:NZ	1:K:276:THR:O	2.40	0.52
1:B:436:LYS:HG3	1:C:349:MET:HB3	1.91	0.52
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.90	0.52
1:A:173:LYS:NZ	8:A:1110:HOH:O	2.43	0.52
1:I:551:VAL:HG12	1:I:553:ALA:H	1.74	0.52
1:H:230:VAL:O	1:H:277:TYR:OH	2.25	0.51
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.92	0.51
1:G:218:LYS:O	1:J:164:LYS:NZ	2.42	0.51
1:K:398:PHE:C	1:K:400:MET:H	2.18	0.51
1:L:504:GLY:HA3	1:L:510:ILE:HD11	1.92	0.51
1:K:230:VAL:HG22	1:K:234:LEU:HD23	1.93	0.51
1:B:122:ASN:N	1:B:122:ASN:ND2	2.58	0.51
1:A:285:ARG:NH2	8:A:1106:HOH:O	2.38	0.51
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.92	0.51
1:B:121:CYS:HA	1:B:270:TYR:CE2	2.45	0.51
1:C:326:LYS:HE2	1:C:328:LEU:HD11	1.92	0.50
1:K:297:LEU:HB3	1:K:400:MET:HE1	1.94	0.50
1:E:166:ASN:ND2	8:E:1108:HOH:O	2.41	0.50
1:K:338:MET:HE3	1:K:468:ASP:HB3	1.93	0.50
1:K:158:LYS:HE2	1:K:161:ASN:HD21	1.75	0.50
1:A:545:ASN:ND2	5:A:1007:SO4:O4	2.45	0.50
1:B:122:ASN:ND2	1:B:149:ASN:HD22	2.10	0.50
1:G:509:LEU:O	1:G:513:ILE:HG12	2.12	0.50
1:K:207:VAL:HG11	1:K:241:THR:HG22	1.94	0.50
1:L:361:SER:OG	1:L:419:GLU:HA	2.12	0.50
1:D:396:MET:SD	1:D:398:PHE:HE2	2.35	0.49
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.93	0.49
1:I:132:VAL:HG21	1:I:142:VAL:HG13	1.94	0.49
1:K:114:VAL:HG12	1:K:274:ALA:HB1	1.95	0.49
1:G:396:MET:SD	1:G:398:PHE:HE2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HB3	1:A:400:MET:HE1	1.93	0.49
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.93	0.49
1:L:398:PHE:C	1:L:400:MET:H	2.21	0.49
1:A:520:SER:HB3	1:A:598:GLU:HG3	1.95	0.49
1:B:114:VAL:HG12	1:B:274:ALA:HB1	1.96	0.48
1:D:301:PRO:HB2	1:D:303:ASN:OD1	2.13	0.48
1:I:230:VAL:HG12	1:I:234:LEU:HD23	1.95	0.48
1:B:320:LYS:HB3	6:B:1006:1PE:H131	1.95	0.48
1:L:127:LEU:HD11	1:L:129:ILE:HD11	1.96	0.48
1:L:198:LEU:HD12	1:L:228:ILE:HD12	1.94	0.48
1:H:316:GLU:HG3	6:H:1007:1PE:H242	1.95	0.48
1:H:175:PHE:HD1	1:L:176:TYR:HB2	1.78	0.48
1:K:230:VAL:HG13	1:K:234:LEU:HB3	1.94	0.48
1:C:236:ARG:NE	1:C:240:GLU:OE2	2.46	0.48
1:C:520:SER:HB3	1:C:598:GLU:HG3	1.96	0.48
1:D:122:ASN:OD1	1:D:124:GLU:HG3	2.14	0.48
1:J:274:ALA:O	1:J:278:LYS:HG3	2.14	0.48
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.96	0.47
1:B:150:ASP:OD1	1:B:179:ASN:HB2	2.14	0.47
1:C:198:LEU:HD22	1:C:202:ASP:HB3	1.95	0.47
1:C:357:LEU:HB2	1:C:425:PHE:HB2	1.97	0.47
1:E:214:LEU:HD21	1:E:222:LEU:HD22	1.95	0.47
1:C:320:LYS:HZ1	6:C:1006:1PE:H142	1.79	0.47
1:D:394:ASP:HA	1:F:441:PRO:HB2	1.96	0.47
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.97	0.47
1:L:530:ILE:HG23	6:L:1008:1PE:H141	1.95	0.47
1:F:370:ALA:HB2	1:F:478:VAL:HG11	1.95	0.47
1:K:301:PRO:HB2	1:K:303:ASN:OD1	2.14	0.47
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.49	0.47
1:E:435:SER:OG	1:E:436:LYS:N	2.47	0.47
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.97	0.47
1:D:275:ASP:HA	1:D:278:LYS:HD2	1.96	0.47
1:D:316:GLU:HG3	6:D:1007:1PE:H221	1.97	0.47
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.97	0.47
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.97	0.47
1:K:392:MET:HE3	1:K:392:MET:HB3	1.83	0.46
1:L:536:THR:HG21	1:L:551:VAL:HG21	1.97	0.46
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.50	0.46
1:F:361:SER:HB2	1:F:421:VAL:H	1.80	0.46
1:B:449:ASN:HD21	1:B:451:LYS:HD2	1.81	0.46
1:H:504:GLY:HA3	1:H:510:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.96	0.46
1:A:320:LYS:HZ1	6:A:1009:1PE:H152	1.80	0.46
1:B:205:ARG:NH1	8:B:1106:HOH:O	2.42	0.46
1:F:435:SER:OG	1:F:436:LYS:N	2.49	0.46
1:G:503:PHE:O	1:G:573:HIS:N	2.42	0.46
1:G:114:VAL:HG12	1:G:274:ALA:HB1	1.97	0.46
1:H:272:ASN:H	1:H:272:ASN:HD22	1.63	0.46
1:D:230:VAL:HG12	1:D:234:LEU:HD23	1.98	0.45
1:F:90:GLN:NE2	1:F:95:ASP:O	2.46	0.45
1:H:122:ASN:ND2	8:H:1117:HOH:O	2.49	0.45
1:A:551:VAL:HG12	1:A:553:ALA:H	1.81	0.45
1:B:300:ALA:HA	1:B:301:PRO:HD3	1.85	0.45
1:C:386:LYS:HB3	1:C:391:SER:HB2	1.98	0.45
1:D:214:LEU:HD21	1:D:222:LEU:HD22	1.98	0.45
1:I:236:ARG:NE	1:I:240:GLU:OE2	2.37	0.45
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.97	0.45
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.98	0.45
1:B:144:ILE:HD13	1:B:162:MET:HG3	1.98	0.45
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.98	0.45
1:I:536:THR:HG21	1:I:551:VAL:HG23	1.98	0.45
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.98	0.45
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.98	0.45
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.98	0.45
1:G:207:VAL:HG11	1:G:241:THR:HG22	1.98	0.45
1:J:398:PHE:C	1:J:400:MET:H	2.25	0.45
1:B:453:ILE:HD13	1:B:561:PHE:HZ	1.81	0.45
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.99	0.45
1:F:133:ASN:HA	1:F:167:VAL:HG21	1.98	0.45
1:D:567:GLN:N	1:D:567:GLN:OE1	2.49	0.45
1:H:396:MET:SD	1:H:398:PHE:HE2	2.40	0.45
1:I:236:ARG:HD2	1:I:283:LYS:HG2	1.99	0.45
1:B:174:HIS:HB3	1:F:175:PHE:CD1	2.52	0.45
6:G:1007:1PE:H242	6:G:1007:1PE:H232	1.63	0.45
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.86	0.45
1:K:204:LYS:HB2	1:K:204:LYS:HE3	1.76	0.45
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.99	0.44
1:C:483:ASP:OD2	1:C:573:HIS:ND1	2.42	0.44
1:H:114:VAL:HG12	1:H:274:ALA:HB1	1.99	0.44
1:H:274:ALA:O	1:H:278:LYS:HG3	2.17	0.44
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.98	0.44
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:LYS:NZ	6:D:1007:1PE:H142	2.33	0.44
1:E:372:VAL:O	1:E:483:ASP:HA	2.18	0.44
1:J:520:SER:HB3	1:J:598:GLU:HG3	2.00	0.44
1:K:437:ASN:HD22	1:L:91:VAL:HG22	1.82	0.44
1:A:301:PRO:HB2	1:A:303:ASN:OD1	2.18	0.44
1:A:536:THR:HG21	1:A:551:VAL:HG23	2.00	0.44
1:K:161:ASN:HA	1:K:164:LYS:HE3	1.99	0.44
1:E:392:MET:HE3	1:E:392:MET:HB2	1.90	0.44
1:A:321:LEU:HD11	1:A:411:TYR:HA	2.00	0.43
1:B:135:PRO:HA	1:B:194:SER:O	2.18	0.43
1:H:333:LEU:HD21	1:H:354:PHE:HB2	2.00	0.43
1:K:208:LEU:HD23	1:K:208:LEU:HA	1.77	0.43
1:L:225:VAL:HG22	1:L:270:TYR:HB2	2.00	0.43
1:A:161:ASN:ND2	1:D:178:PHE:HZ	2.17	0.43
1:A:544:ILE:HG12	1:A:545:ASN:H	1.84	0.43
1:C:395:LEU:O	1:C:397:LYS:N	2.51	0.43
1:D:435:SER:OG	1:D:436:LYS:N	2.51	0.43
1:E:386:LYS:HE3	1:E:396:MET:SD	2.58	0.43
1:G:493:TYR:HA	1:L:553:ALA:H	1.83	0.43
1:I:198:LEU:HD22	1:I:202:ASP:HB3	2.00	0.43
1:J:551:VAL:C	1:J:553:ALA:H	2.27	0.43
1:K:221:LYS:HG3	1:K:266:HIS:HB2	1.99	0.43
1:F:504:GLY:HA3	1:F:510:ILE:HD11	2.00	0.43
1:K:104:ASN:ND2	5:K:1007:SO4:O3	2.51	0.43
1:K:441:PRO:HD2	1:L:378:PHE:CZ	2.54	0.43
1:B:283:LYS:HE2	1:B:287:TYR:CZ	2.53	0.43
1:H:300:ALA:HA	1:H:301:PRO:HD3	1.89	0.43
1:D:273:ASN:O	1:D:277:TYR:HD2	2.01	0.43
1:E:441:PRO:HB2	1:F:394:ASP:HA	2.01	0.43
1:E:463:ARG:NH2	4:E:1004:CO3:O2	2.44	0.43
1:C:500:ALA:HB3	1:C:524:VAL:HG22	2.00	0.43
1:G:543:ASP:CG	1:H:255:THR:H	2.27	0.43
1:K:320:LYS:HB3	6:K:1010:1PE:H252	2.01	0.43
1:C:300:ALA:HA	1:C:301:PRO:HD3	1.84	0.43
1:D:537:LEU:HA	1:D:545:ASN:HB2	2.01	0.43
1:J:301:PRO:HB2	1:J:303:ASN:OD1	2.19	0.43
1:D:204:LYS:HB2	1:D:204:LYS:HE3	1.74	0.42
1:K:204:LYS:NZ	8:K:1110:HOH:O	2.46	0.42
1:D:344:VAL:HA	1:D:439:TYR:CE2	2.54	0.42
1:L:332:GLU:H	1:L:332:GLU:CD	2.27	0.42
1:L:346:LYS:HB3	1:L:437:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:CYS:C	1:B:122:ASN:HD22	2.27	0.42
1:D:195:VAL:HG12	1:D:197:ASP:H	1.83	0.42
1:G:172:SER:HB2	1:G:213:MET:HE3	2.01	0.42
1:G:520:SER:HB3	1:G:598:GLU:HG3	2.01	0.42
1:K:441:PRO:HB2	1:L:394:ASP:HA	2.01	0.42
1:L:439:TYR:OH	1:L:458:THR:O	2.36	0.42
1:B:258:ASN:OD1	1:B:260:ASN:N	2.50	0.42
1:D:386:LYS:HE3	1:D:396:MET:SD	2.60	0.42
1:I:396:MET:SD	1:I:398:PHE:HE2	2.42	0.42
1:L:509:LEU:O	1:L:513:ILE:HG12	2.19	0.42
1:A:229:ASN:ND2	8:A:1115:HOH:O	2.50	0.42
1:F:133:ASN:HB3	1:F:192:CYS:HB2	2.01	0.42
1:L:344:VAL:HA	1:L:439:TYR:CE2	2.55	0.42
1:B:117:ILE:HD11	1:B:146:SER:OG	2.20	0.42
1:C:287:TYR:CD2	1:C:594:ARG:HG2	2.54	0.42
1:D:126:GLY:HA2	1:D:219:LEU:HD13	2.02	0.42
1:D:551:VAL:HG12	1:D:552:LYS:O	2.19	0.42
1:B:460:ALA:O	1:B:546:GLN:NE2	2.52	0.42
1:F:350:TYR:HA	1:F:351:PRO:HD3	1.94	0.42
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.01	0.42
1:I:346:LYS:HB3	1:I:437:ASN:O	2.19	0.42
1:A:244:TYR:OH	1:A:588:PRO:O	2.37	0.42
1:B:260:ASN:OD1	1:F:166:ASN:HB3	2.19	0.42
1:C:528:PRO:HB3	1:D:525:TRP:CZ3	2.54	0.42
1:L:195:VAL:HG12	1:L:197:ASP:H	1.85	0.42
1:L:230:VAL:HG12	1:L:234:LEU:HD23	2.02	0.42
1:I:509:LEU:O	1:I:513:ILE:HG12	2.20	0.42
1:K:320:LYS:HE2	6:K:1009:1PE:H252	2.02	0.41
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.36	0.41
1:D:321:LEU:HD11	1:D:411:TYR:HA	2.02	0.41
1:G:260:ASN:N	1:G:260:ASN:OD1	2.52	0.41
1:L:370:ALA:HB2	1:L:478:VAL:HG11	2.02	0.41
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.02	0.41
1:B:480:TYR:CD1	1:B:509:LEU:HD13	2.55	0.41
1:I:366:LYS:CG	1:I:420:ASN:HB3	2.50	0.41
1:D:132:VAL:HG11	1:D:144:ILE:HD13	2.03	0.41
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.55	0.41
1:G:367:LYS:NZ	8:G:1115:HOH:O	2.53	0.41
1:H:301:PRO:HB2	1:H:303:ASN:OD1	2.20	0.41
1:I:153:VAL:O	1:I:157:LEU:HG	2.21	0.41
1:K:152:GLN:HG2	1:K:180:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:198:LEU:HD22	1:K:202:ASP:HB3	2.02	0.41
1:B:173:LYS:HA	1:B:173:LYS:HD3	1.93	0.41
1:C:244:TYR:OH	1:C:588:PRO:O	2.38	0.41
1:F:127:LEU:HD11	1:F:129:ILE:HD11	2.02	0.41
1:H:323:LEU:HD22	1:H:359:TYR:HB2	2.02	0.41
1:L:411:TYR:HE1	6:L:1009:1PE:H261	1.85	0.41
1:A:283:LYS:HE2	1:A:287:TYR:CZ	2.56	0.41
1:E:357:LEU:HB2	1:E:425:PHE:HB2	2.03	0.41
1:F:300:ALA:HA	1:F:301:PRO:HD3	1.85	0.41
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.55	0.41
1:G:551:VAL:HG23	1:G:552:LYS:H	1.86	0.41
1:K:372:VAL:O	1:K:483:ASP:HA	2.21	0.41
1:D:509:LEU:O	1:D:513:ILE:HG12	2.21	0.41
1:E:350:TYR:HA	1:E:351:PRO:HD3	1.93	0.41
1:H:483:ASP:OD1	1:H:573:HIS:ND1	2.35	0.41
1:J:411:TYR:HE1	6:J:1008:1PE:H252	1.85	0.41
1:J:509:LEU:O	1:J:513:ILE:HG12	2.20	0.41
1:G:551:VAL:HG23	1:G:552:LYS:N	2.35	0.41
1:H:175:PHE:CD1	1:L:176:TYR:HB2	2.56	0.41
1:I:150:ASP:OD1	1:I:179:ASN:HB2	2.21	0.41
1:J:103:TYR:HA	1:J:289:PHE:CZ	2.55	0.41
1:L:132:VAL:HG12	1:L:227:GLU:HB2	2.03	0.41
1:L:300:ALA:O	8:L:1101:HOH:O	2.22	0.41
1:A:543:ASP:CG	1:B:255:THR:H	2.28	0.41
1:D:386:LYS:HB3	1:D:391:SER:HB2	2.03	0.41
1:G:528:PRO:HB3	1:L:525:TRP:CZ3	2.56	0.41
1:H:214:LEU:HD21	1:H:222:LEU:HD22	2.02	0.41
1:K:544:ILE:HD12	1:K:564:GLU:HG3	2.03	0.41
1:B:202:ASP:O	1:B:206:VAL:HG23	2.21	0.40
1:B:320:LYS:HE3	6:B:1007:1PE:H132	2.02	0.40
1:K:150:ASP:OD1	1:K:179:ASN:HB2	2.21	0.40
1:L:190:VAL:HG11	1:L:206:VAL:HG13	2.03	0.40
1:F:96:PRO:HG2	1:F:303:ASN:O	2.22	0.40
1:H:142:VAL:HG12	1:H:167:VAL:HG12	2.03	0.40
1:I:321:LEU:HD11	1:I:411:TYR:HA	2.03	0.40
1:J:350:TYR:HA	1:J:351:PRO:HD3	1.92	0.40
1:J:547:ILE:H	1:J:547:ILE:HG13	1.78	0.40
1:K:90:GLN:NE2	1:K:95:ASP:O	2.54	0.40
1:K:300:ALA:HA	1:K:301:PRO:HD3	1.87	0.40
1:H:346:LYS:HB3	1:H:437:ASN:O	2.21	0.40
1:J:386:LYS:HB3	1:J:391:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:395:LEU:HD11	1:K:581:TRP:CD1	2.55	0.40
1:L:392:MET:HE3	1:L:392:MET:HB3	2.00	0.40
1:A:200:GLU:HG2	1:A:237:PHE:CZ	2.56	0.40
1:C:451:LYS:NZ	1:C:564:GLU:O	2.45	0.40
1:D:137:LYS:N	8:D:1105:HOH:O	2.45	0.40
1:D:195:VAL:C	1:D:197:ASP:H	2.30	0.40
1:D:579:VAL:O	1:D:589:LYS:HD2	2.22	0.40
1:F:181:ASN:ND2	8:F:1115:HOH:O	2.55	0.40
1:H:195:VAL:HG12	1:H:197:ASP:H	1.87	0.40
1:H:202:ASP:O	1:H:206:VAL:HG23	2.21	0.40
1:K:274:ALA:O	1:K:278:LYS:HG3	2.22	0.40
1:K:395:LEU:HD23	1:K:398:PHE:CD2	2.56	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)
8:A:1106:HOH:O	8:G:1104:HOH:O[2_685]	2.18	0.02

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	514/522 (98%)	499 (97%)	14 (3%)	1 (0%)	43	63
1	B	512/522 (98%)	493 (96%)	13 (2%)	6 (1%)	10	20
1	C	512/522 (98%)	498 (97%)	13 (2%)	1 (0%)	43	63
1	D	510/522 (98%)	490 (96%)	18 (4%)	2 (0%)	30	49
1	E	500/522 (96%)	486 (97%)	13 (3%)	1 (0%)	43	63
1	F	507/522 (97%)	488 (96%)	15 (3%)	4 (1%)	16	31
1	G	517/522 (99%)	500 (97%)	15 (3%)	2 (0%)	30	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	513/522 (98%)	495 (96%)	14 (3%)	4 (1%)	16	31
1	I	515/522 (99%)	498 (97%)	16 (3%)	1 (0%)	43	63
1	J	510/522 (98%)	495 (97%)	15 (3%)	0	100	100
1	K	503/522 (96%)	486 (97%)	16 (3%)	1 (0%)	43	63
1	L	504/522 (97%)	480 (95%)	22 (4%)	2 (0%)	30	49
All	All	6117/6264 (98%)	5908 (97%)	184 (3%)	25 (0%)	30	49

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	550	SER
1	G	551	VAL
1	K	550	SER
1	B	550	SER
1	B	552	LYS
1	C	396	MET
1	H	273	ASN
1	I	550	SER
1	E	552	LYS
1	F	552	LYS
1	H	552	LYS
1	A	396	MET
1	D	396	MET
1	D	552	LYS
1	H	119	GLY
1	H	254	SER
1	B	138	GLU
1	B	149	ASN
1	B	254	SER
1	B	396	MET
1	F	396	MET
1	F	551	VAL
1	L	550	SER
1	G	396	MET
1	L	399	ASP

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/450 (94%)	419 (99%)	3 (1%)	76	89
1	B	408/450 (91%)	406 (100%)	2 (0%)	81	92
1	C	418/450 (93%)	415 (99%)	3 (1%)	76	89
1	D	418/450 (93%)	414 (99%)	4 (1%)	68	86
1	E	413/450 (92%)	410 (99%)	3 (1%)	76	89
1	F	396/450 (88%)	391 (99%)	5 (1%)	61	82
1	G	422/450 (94%)	420 (100%)	2 (0%)	81	92
1	H	407/450 (90%)	404 (99%)	3 (1%)	76	89
1	I	418/450 (93%)	414 (99%)	4 (1%)	68	86
1	J	414/450 (92%)	410 (99%)	4 (1%)	68	86
1	K	413/450 (92%)	409 (99%)	4 (1%)	68	86
1	L	401/450 (89%)	398 (99%)	3 (1%)	76	89
All	All	4950/5400 (92%)	4910 (99%)	40 (1%)	73	88

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ILE
1	A	332	GLU
1	A	492	LEU
1	B	88	VAL
1	B	122	ASN
1	C	185	VAL
1	C	204	LYS
1	C	544	ILE
1	D	197	ASP
1	D	200	GLU
1	D	547	ILE
1	D	595	LEU
1	E	143	LYS
1	E	328	LEU
1	E	392	MET
1	F	200	GLU
1	F	227	GLU
1	F	230	VAL

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Mol	Chain	Res	Type
1	F	392	MET
1	F	600	VAL
1	G	200	GLU
1	G	260	ASN
1	H	200	GLU
1	H	272	ASN
1	H	600	VAL
1	I	163	GLU
1	I	185	VAL
1	I	204	LYS
1	I	366	LYS
1	J	332	GLU
1	J	400	MET
1	J	524	VAL
1	J	547	ILE
1	K	230	VAL
1	K	547	ILE
1	K	550	SER
1	K	567	GLN
1	L	200	GLU
1	L	311	SER
1	L	332	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	272	ASN
1	A	273	ASN
1	A	424	HIS
1	A	437	ASN
1	B	122	ASN
1	B	179	ASN
1	C	139	ASN
1	C	174	HIS
1	C	233	ASN
1	C	272	ASN
1	C	515	GLN
1	D	104	ASN
1	E	166	ASN
1	F	104	ASN
1	F	322	ASN

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Mol	Chain	Res	Type
1	G	139	ASN
1	G	215	HIS
1	H	166	ASN
1	H	215	HIS
1	H	260	ASN
1	H	272	ASN
1	H	531	ASN
1	I	229	ASN
1	I	420	ASN
1	J	152	GLN
1	J	420	ASN
1	J	568	ASN
1	K	152	GLN
1	K	161	ASN
1	K	437	ASN
1	L	183	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 97 ligands modelled in this entry, 24 are monoatomic - leaving 73 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	1006	-	4,4,4	0.24	0	6,6,6	0.10	0
4	CO3	C	1004	-	3,3,3	0.83	0	2,3,3	0.16	0
4	CO3	L	1004	-	3,3,3	0.82	0	2,3,3	0.14	0
7	GOL	G	1006	-	5,5,5	0.35	0	5,5,5	0.39	0
5	SO4	L	1006	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	L	1007	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	F	1005	-	4,4,4	0.23	0	6,6,6	0.09	0
4	CO3	A	1004	-	3,3,3	0.81	0	2,3,3	0.15	0
6	1PE	E	1007	-	11,11,15	0.59	0	10,10,14	0.42	0
6	1PE	I	1008	-	10,10,15	0.56	0	9,9,14	0.37	0
6	1PE	E	1008	-	11,11,15	0.58	0	10,10,14	0.50	0
6	1PE	I	1007	-	11,11,15	0.58	0	10,10,14	0.42	0
4	CO3	I	1004	-	3,3,3	0.84	0	2,3,3	0.17	0
5	SO4	D	1005	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	H	1006	-	4,4,4	0.24	0	6,6,6	0.08	0
2	4U5	J	1001	3	24,25,25	3.25	5 (20%)	34,36,36	2.42	7 (20%)
2	4U5	E	1001	3	24,25,25	3.27	5 (20%)	34,36,36	2.48	6 (17%)
4	CO3	E	1004	-	3,3,3	0.83	0	2,3,3	0.14	0
5	SO4	L	1005	-	4,4,4	0.25	0	6,6,6	0.08	0
4	CO3	D	1004	-	3,3,3	0.83	0	2,3,3	0.17	0
5	SO4	I	1005	-	4,4,4	0.23	0	6,6,6	0.07	0
2	4U5	D	1001	3	24,25,25	3.27	5 (20%)	34,36,36	2.44	6 (17%)
5	SO4	A	1007	-	4,4,4	0.23	0	6,6,6	0.08	0
2	4U5	H	1001	3	24,25,25	3.22	6 (25%)	34,36,36	2.50	6 (17%)
5	SO4	K	1006	-	4,4,4	0.23	0	6,6,6	0.08	0
6	1PE	B	1006	-	9,9,15	0.53	0	8,8,14	0.37	0
6	1PE	B	1007	-	9,9,15	0.56	0	8,8,14	0.32	0
2	4U5	C	1001	3	24,25,25	3.30	5 (20%)	34,36,36	2.42	6 (17%)
6	1PE	C	1007	-	8,8,15	0.53	0	7,7,14	0.38	0
6	1PE	D	1008	-	9,9,15	0.54	0	8,8,14	0.36	0
2	4U5	G	1001	3	24,25,25	3.34	6 (25%)	34,36,36	2.48	6 (17%)
4	CO3	J	1004	-	3,3,3	0.85	0	2,3,3	0.15	0
6	1PE	G	1008	-	5,5,15	0.68	0	4,4,14	0.53	0
5	SO4	K	1005	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	E	1006	-	4,4,4	0.23	0	6,6,6	0.09	0
6	1PE	L	1008	-	6,6,15	0.61	0	5,5,14	0.50	0
6	1PE	L	1009	-	9,9,15	0.90	0	8,8,14	0.41	0
5	SO4	D	1006	-	4,4,4	0.25	0	6,6,6	0.07	0
4	CO3	K	1004	-	3,3,3	0.83	0	2,3,3	0.10	0
4	CO3	H	1004	-	3,3,3	0.83	0	2,3,3	0.13	0
5	SO4	A	1005	-	4,4,4	0.24	0	6,6,6	0.08	0
4	CO3	B	1004	-	3,3,3	0.82	0	2,3,3	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	K	1010	-	11,11,15	0.59	0	10,10,14	0.37	0
2	4U5	I	1001	3	24,25,25	3.32	6 (25%)	34,36,36	2.38	7 (20%)
4	CO3	G	1004	-	3,3,3	0.83	0	2,3,3	0.10	0
6	1PE	A	1008	-	8,8,15	0.52	0	7,7,14	0.39	0
2	4U5	B	1001	3	24,25,25	3.23	5 (20%)	34,36,36	2.48	6 (17%)
5	SO4	J	1005	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	J	1006	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	H	1005	-	4,4,4	0.23	0	6,6,6	0.08	0
2	4U5	A	1001	3	24,25,25	3.29	6 (25%)	34,36,36	2.41	7 (20%)
5	SO4	E	1005	-	4,4,4	0.23	0	6,6,6	0.11	0
6	1PE	G	1009	-	5,5,15	0.69	0	4,4,14	0.44	0
6	1PE	H	1007	-	9,9,15	0.54	0	8,8,14	0.41	0
5	SO4	K	1007	-	4,4,4	0.24	0	6,6,6	0.07	0
6	1PE	J	1007	-	10,10,15	0.87	0	9,9,14	0.34	0
6	1PE	L	1010	-	10,10,15	0.86	0	9,9,14	0.40	0
5	SO4	K	1008	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	C	1005	-	4,4,4	0.25	0	6,6,6	0.06	0
5	SO4	G	1005	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	B	1005	-	4,4,4	0.23	0	6,6,6	0.08	0
6	1PE	J	1008	-	9,9,15	0.89	0	8,8,14	0.42	0
6	1PE	D	1007	-	9,9,15	0.55	0	8,8,14	0.36	0
6	1PE	F	1006	-	9,9,15	0.90	0	8,8,14	0.41	0
2	4U5	F	1001	3	24,25,25	3.33	5 (20%)	34,36,36	2.38	6 (17%)
2	4U5	K	1001	3	24,25,25	3.25	5 (20%)	34,36,36	2.46	6 (17%)
4	CO3	F	1004	-	3,3,3	0.82	0	2,3,3	0.09	0
6	1PE	A	1009	-	11,11,15	0.64	0	10,10,14	0.40	0
6	1PE	G	1007	-	8,8,15	0.54	0	7,7,14	0.31	0
6	1PE	C	1006	-	12,12,15	0.65	0	11,11,14	0.40	0
2	4U5	L	1001	3	24,25,25	3.32	6 (25%)	34,36,36	2.38	6 (17%)
6	1PE	K	1009	-	11,11,15	0.59	0	10,10,14	0.45	0
5	SO4	I	1006	-	4,4,4	0.24	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	G	1006	-	-	2/4/4/4	-
6	1PE	E	1007	-	-	3/9/9/13	-
6	1PE	I	1008	-	-	3/8/8/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	E	1008	-	-	3/9/9/13	-
6	1PE	I	1007	-	-	6/9/9/13	-
2	4U5	J	1001	3	-	0/24/24/24	0/2/2/2
2	4U5	E	1001	3	-	1/24/24/24	0/2/2/2
2	4U5	D	1001	3	-	4/24/24/24	0/2/2/2
2	4U5	H	1001	3	-	2/24/24/24	0/2/2/2
6	1PE	B	1006	-	-	4/7/7/13	-
6	1PE	B	1007	-	-	4/7/7/13	-
2	4U5	C	1001	3	-	0/24/24/24	0/2/2/2
6	1PE	C	1007	-	-	3/6/6/13	-
6	1PE	D	1008	-	-	6/7/7/13	-
2	4U5	G	1001	3	-	0/24/24/24	0/2/2/2
6	1PE	G	1008	-	-	0/3/3/13	-
6	1PE	L	1008	-	-	2/4/4/13	-
6	1PE	L	1009	-	-	4/7/7/13	-
6	1PE	K	1010	-	-	5/9/9/13	-
2	4U5	I	1001	3	-	0/24/24/24	0/2/2/2
6	1PE	A	1008	-	-	5/6/6/13	-
2	4U5	B	1001	3	-	0/24/24/24	0/2/2/2
2	4U5	A	1001	3	-	0/24/24/24	0/2/2/2
6	1PE	G	1009	-	-	2/3/3/13	-
6	1PE	H	1007	-	-	3/7/7/13	-
6	1PE	J	1007	-	-	5/8/8/13	-
6	1PE	L	1010	-	-	2/8/8/13	-
6	1PE	J	1008	-	-	3/7/7/13	-
6	1PE	D	1007	-	-	2/7/7/13	-
6	1PE	F	1006	-	-	6/7/7/13	-
2	4U5	F	1001	3	-	4/24/24/24	0/2/2/2
2	4U5	K	1001	3	-	4/24/24/24	0/2/2/2
6	1PE	A	1009	-	-	5/9/9/13	-
6	1PE	G	1007	-	-	4/6/6/13	-
6	1PE	C	1006	-	-	4/10/10/13	-
2	4U5	L	1001	3	-	0/24/24/24	0/2/2/2
6	1PE	K	1009	-	-	4/9/9/13	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1001	4U5	NAW-NAN	-10.73	1.24	1.35
2	F	1001	4U5	NAW-NAN	-10.54	1.24	1.35
2	A	1001	4U5	NAW-NAN	-10.52	1.24	1.35
2	L	1001	4U5	NAW-NAN	-10.50	1.24	1.35
2	C	1001	4U5	NAW-NAN	-10.46	1.24	1.35
2	I	1001	4U5	NAW-NAN	-10.44	1.24	1.35
2	E	1001	4U5	NAW-NAN	-10.18	1.24	1.35
2	J	1001	4U5	NAW-NAN	-10.12	1.24	1.35
2	D	1001	4U5	NAW-NAN	-10.11	1.24	1.35
2	B	1001	4U5	NAW-NAN	-10.03	1.24	1.35
2	K	1001	4U5	NAW-NAN	-10.01	1.24	1.35
2	H	1001	4U5	NAW-NAN	-9.84	1.25	1.35
2	F	1001	4U5	CAU-CA	-8.16	1.40	1.52
2	D	1001	4U5	CAU-CA	-8.15	1.40	1.52
2	L	1001	4U5	CAU-CA	-8.14	1.40	1.52
2	K	1001	4U5	CAU-CA	-8.12	1.40	1.52
2	E	1001	4U5	CAU-CA	-8.12	1.40	1.52
2	I	1001	4U5	CAU-CA	-8.10	1.40	1.52
2	H	1001	4U5	CAU-CA	-8.09	1.40	1.52
2	J	1001	4U5	CAU-CA	-8.03	1.40	1.52
2	G	1001	4U5	CAU-CA	-8.01	1.40	1.52
2	C	1001	4U5	CAU-CA	-7.97	1.40	1.52
2	B	1001	4U5	CAU-CA	-7.91	1.40	1.52
2	A	1001	4U5	CAU-CA	-7.91	1.40	1.52
2	E	1001	4U5	CAS-CAT	-7.64	1.33	1.48
2	F	1001	4U5	CAS-CAT	-7.60	1.33	1.48
2	H	1001	4U5	CAS-CAT	-7.60	1.33	1.48
2	I	1001	4U5	CAS-CAT	-7.59	1.33	1.48
2	D	1001	4U5	CAS-CAT	-7.59	1.33	1.48
2	J	1001	4U5	CAS-CAT	-7.58	1.33	1.48
2	K	1001	4U5	CAS-CAT	-7.58	1.33	1.48
2	G	1001	4U5	CAS-CAT	-7.57	1.33	1.48
2	B	1001	4U5	CAS-CAT	-7.57	1.33	1.48
2	L	1001	4U5	CAS-CAT	-7.55	1.33	1.48
2	C	1001	4U5	CAS-CAT	-7.53	1.33	1.48
2	A	1001	4U5	CAS-CAT	-7.50	1.33	1.48
2	G	1001	4U5	CAL-CAT	-3.63	1.32	1.40
2	H	1001	4U5	CAL-CAT	-3.63	1.32	1.40
2	E	1001	4U5	CAL-CAT	-3.63	1.32	1.40
2	A	1001	4U5	CAL-CAT	-3.62	1.32	1.40
2	B	1001	4U5	CAL-CAT	-3.61	1.32	1.40
2	F	1001	4U5	CAL-CAT	-3.61	1.32	1.40
2	L	1001	4U5	CAL-CAT	-3.61	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1001	4U5	CAL-CAT	-3.60	1.32	1.40
2	C	1001	4U5	CAL-CAT	-3.60	1.32	1.40
2	K	1001	4U5	CAL-CAT	-3.59	1.32	1.40
2	J	1001	4U5	CAL-CAT	-3.58	1.32	1.40
2	D	1001	4U5	CAL-CAT	-3.57	1.32	1.40
2	E	1001	4U5	CAM-CAT	-3.02	1.32	1.38
2	G	1001	4U5	CAM-CAT	-3.01	1.32	1.38
2	D	1001	4U5	CAM-CAT	-3.00	1.32	1.38
2	L	1001	4U5	CAM-CAT	-3.00	1.32	1.38
2	K	1001	4U5	CAM-CAT	-2.98	1.32	1.38
2	J	1001	4U5	CAM-CAT	-2.97	1.32	1.38
2	C	1001	4U5	CAM-CAT	-2.96	1.32	1.38
2	I	1001	4U5	CAM-CAT	-2.96	1.32	1.38
2	F	1001	4U5	CAM-CAT	-2.96	1.32	1.38
2	B	1001	4U5	CAM-CAT	-2.96	1.32	1.38
2	A	1001	4U5	CAM-CAT	-2.94	1.32	1.38
2	H	1001	4U5	CAM-CAT	-2.92	1.33	1.38
2	A	1001	4U5	CAA-NAW	2.26	1.49	1.46
2	G	1001	4U5	CAA-NAW	2.10	1.48	1.46
2	I	1001	4U5	OAG-NAO	2.08	1.45	1.40
2	L	1001	4U5	OAG-NAO	2.03	1.44	1.40
2	H	1001	4U5	CAA-NAW	2.00	1.48	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1001	4U5	CAL-NAN-NAW	10.65	110.26	104.41
2	A	1001	4U5	CAL-NAN-NAW	10.45	110.15	104.41
2	B	1001	4U5	CAL-NAN-NAW	10.34	110.09	104.41
2	H	1001	4U5	CAL-NAN-NAW	10.32	110.08	104.41
2	I	1001	4U5	CAL-NAN-NAW	10.24	110.03	104.41
2	C	1001	4U5	CAL-NAN-NAW	10.21	110.02	104.41
2	L	1001	4U5	CAL-NAN-NAW	10.18	110.00	104.41
2	D	1001	4U5	CAL-NAN-NAW	10.18	110.00	104.41
2	J	1001	4U5	CAL-NAN-NAW	10.14	109.98	104.41
2	F	1001	4U5	CAL-NAN-NAW	10.13	109.97	104.41
2	E	1001	4U5	CAL-NAN-NAW	10.11	109.96	104.41
2	K	1001	4U5	CAL-NAN-NAW	10.10	109.96	104.41
2	E	1001	4U5	CAA-NAW-NAN	6.54	125.28	120.03
2	K	1001	4U5	CAA-NAW-NAN	6.47	125.22	120.03
2	H	1001	4U5	CAA-NAW-NAN	6.36	125.13	120.03
2	D	1001	4U5	CAA-NAW-NAN	6.35	125.12	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	4U5	CAA-NAW-NAN	6.30	125.08	120.03
2	J	1001	4U5	CAA-NAW-NAN	6.15	124.96	120.03
2	C	1001	4U5	CAA-NAW-NAN	6.12	124.94	120.03
2	G	1001	4U5	CAA-NAW-NAN	6.10	124.92	120.03
2	L	1001	4U5	CAA-NAW-NAN	5.88	124.74	120.03
2	F	1001	4U5	CAA-NAW-NAN	5.75	124.64	120.03
2	I	1001	4U5	CAA-NAW-NAN	5.64	124.55	120.03
2	A	1001	4U5	CAA-NAW-NAN	5.55	124.48	120.03
2	H	1001	4U5	CAM-NAW-NAN	-4.33	109.62	112.08
2	B	1001	4U5	CAM-NAW-NAN	-4.19	109.70	112.08
2	G	1001	4U5	CAM-NAW-NAN	-4.15	109.72	112.08
2	D	1001	4U5	CAM-NAW-NAN	-4.09	109.76	112.08
2	I	1001	4U5	CAM-NAW-NAN	-4.04	109.79	112.08
2	C	1001	4U5	CAM-NAW-NAN	-4.03	109.79	112.08
2	A	1001	4U5	CAM-NAW-NAN	-4.02	109.80	112.08
2	K	1001	4U5	CAM-NAW-NAN	-4.01	109.80	112.08
2	E	1001	4U5	CAM-NAW-NAN	-4.00	109.81	112.08
2	J	1001	4U5	CAM-NAW-NAN	-3.98	109.82	112.08
2	F	1001	4U5	CAM-NAW-NAN	-3.84	109.90	112.08
2	L	1001	4U5	CAM-NAW-NAN	-3.80	109.92	112.08
2	E	1001	4U5	CAA-NAW-CAM	-3.02	124.91	127.94
2	K	1001	4U5	CAA-NAW-CAM	-2.95	124.98	127.94
2	L	1001	4U5	CAT-CAM-NAW	-2.86	105.75	108.10
2	A	1001	4U5	CAT-CAM-NAW	-2.83	105.77	108.10
2	D	1001	4U5	CAA-NAW-CAM	-2.81	125.12	127.94
2	F	1001	4U5	CAT-CAM-NAW	-2.78	105.82	108.10
2	E	1001	4U5	CAT-CAM-NAW	-2.76	105.83	108.10
2	K	1001	4U5	CAT-CAM-NAW	-2.74	105.85	108.10
2	J	1001	4U5	CAA-NAW-CAM	-2.72	125.22	127.94
2	B	1001	4U5	CAA-NAW-CAM	-2.72	125.22	127.94
2	I	1001	4U5	CAT-CAM-NAW	-2.69	105.88	108.10
2	J	1001	4U5	CAT-CAM-NAW	-2.69	105.89	108.10
2	H	1001	4U5	CAA-NAW-CAM	-2.69	125.25	127.94
2	G	1001	4U5	CAT-CAM-NAW	-2.68	105.90	108.10
2	B	1001	4U5	CAT-CAM-NAW	-2.67	105.90	108.10
2	C	1001	4U5	CAA-NAW-CAM	-2.67	125.27	127.94
2	B	1001	4U5	CAT-CAL-NAN	-2.65	105.62	111.87
2	H	1001	4U5	CAT-CAM-NAW	-2.64	105.93	108.10
2	G	1001	4U5	CAT-CAL-NAN	-2.64	105.65	111.87
2	H	1001	4U5	CAT-CAL-NAN	-2.61	105.70	111.87
2	J	1001	4U5	CAT-CAL-NAN	-2.61	105.72	111.87
2	D	1001	4U5	CAT-CAL-NAN	-2.61	105.72	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1001	4U5	CAT-CAL-NAN	-2.60	105.73	111.87
2	A	1001	4U5	CAT-CAL-NAN	-2.60	105.74	111.87
2	D	1001	4U5	CAT-CAM-NAW	-2.60	105.96	108.10
2	L	1001	4U5	CAA-NAW-CAM	-2.60	125.33	127.94
2	E	1001	4U5	CAT-CAL-NAN	-2.60	105.74	111.87
2	C	1001	4U5	CAT-CAM-NAW	-2.59	105.97	108.10
2	L	1001	4U5	CAT-CAL-NAN	-2.58	105.78	111.87
2	G	1001	4U5	CAA-NAW-CAM	-2.58	125.35	127.94
2	C	1001	4U5	CAT-CAL-NAN	-2.57	105.81	111.87
2	F	1001	4U5	CAT-CAL-NAN	-2.55	105.84	111.87
2	I	1001	4U5	CAT-CAL-NAN	-2.54	105.87	111.87
2	F	1001	4U5	CAA-NAW-CAM	-2.48	125.45	127.94
2	I	1001	4U5	CAA-NAW-CAM	-2.27	125.66	127.94
2	A	1001	4U5	CAA-NAW-CAM	-2.21	125.72	127.94
2	I	1001	4U5	CAX-CAR-N	-2.13	114.59	117.49
2	J	1001	4U5	CAX-CAR-N	-2.11	114.62	117.49
2	A	1001	4U5	CAX-CAR-N	-2.08	114.66	117.49

There are no chirality outliers.

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1008	1PE	OH4-C13-C23-OH3
6	E	1007	1PE	OH5-C14-C24-OH4
6	G	1007	1PE	OH4-C13-C23-OH3
6	J	1007	1PE	OH5-C14-C24-OH4
6	L	1010	1PE	OH5-C14-C24-OH4
6	G	1007	1PE	C23-C13-OH4-C24
6	B	1006	1PE	OH5-C14-C24-OH4
6	A	1009	1PE	OH5-C14-C24-OH4
6	D	1007	1PE	OH5-C14-C24-OH4
6	C	1006	1PE	OH5-C14-C24-OH4
6	I	1007	1PE	OH5-C14-C24-OH4
6	L	1010	1PE	OH6-C15-C25-OH5
6	D	1007	1PE	OH4-C13-C23-OH3
6	A	1009	1PE	OH4-C13-C23-OH3
6	D	1008	1PE	OH5-C14-C24-OH4
6	B	1006	1PE	OH4-C13-C23-OH3
6	G	1009	1PE	OH6-C15-C25-OH5
6	A	1009	1PE	OH6-C15-C25-OH5
6	I	1008	1PE	OH4-C13-C23-OH3
6	G	1007	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
6	E	1007	1PE	OH6-C15-C25-OH5
6	F	1006	1PE	OH5-C14-C24-OH4
6	F	1006	1PE	OH6-C15-C25-OH5
6	K	1010	1PE	OH5-C14-C24-OH4
7	G	1006	GOL	O1-C1-C2-C3
7	G	1006	GOL	O1-C1-C2-O2
6	L	1008	1PE	OH5-C14-C24-OH4
6	E	1008	1PE	OH6-C15-C25-OH5
6	K	1010	1PE	OH6-C15-C25-OH5
6	D	1008	1PE	OH4-C13-C23-OH3
6	I	1007	1PE	OH4-C13-C23-OH3
6	A	1008	1PE	OH5-C14-C24-OH4
6	F	1006	1PE	OH7-C16-C26-OH6
6	J	1007	1PE	OH6-C15-C25-OH5
6	A	1008	1PE	C12-C22-OH3-C23
6	C	1007	1PE	OH5-C14-C24-OH4
6	I	1007	1PE	OH6-C15-C25-OH5
6	K	1009	1PE	OH6-C15-C25-OH5
6	G	1009	1PE	C24-C14-OH5-C25
6	D	1008	1PE	C12-C22-OH3-C23
6	D	1008	1PE	C24-C14-OH5-C25
6	G	1007	1PE	C24-C14-OH5-C25
6	L	1009	1PE	OH6-C15-C25-OH5
6	C	1006	1PE	OH6-C15-C25-OH5
6	A	1009	1PE	C13-C23-OH3-C22
6	B	1007	1PE	C24-C14-OH5-C25
6	C	1007	1PE	C12-C22-OH3-C23
6	I	1008	1PE	C12-C22-OH3-C23
6	K	1009	1PE	C14-C24-OH4-C13
6	B	1006	1PE	C14-C24-OH4-C13
6	K	1010	1PE	C23-C13-OH4-C24
6	C	1007	1PE	C23-C13-OH4-C24
6	J	1008	1PE	C25-C15-OH6-C26
6	E	1008	1PE	C24-C14-OH5-C25
6	E	1007	1PE	C15-C25-OH5-C14
6	F	1006	1PE	C15-C25-OH5-C14
6	K	1010	1PE	C15-C25-OH5-C14
6	H	1007	1PE	C14-C24-OH4-C13
6	H	1007	1PE	OH5-C14-C24-OH4
6	L	1008	1PE	C15-C25-OH5-C14
6	F	1006	1PE	C16-C26-OH6-C15
6	J	1008	1PE	C16-C26-OH6-C15

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Mol	Chain	Res	Type	Atoms
6	C	1006	1PE	C15-C25-OH5-C14
6	I	1007	1PE	C12-C22-OH3-C23
6	D	1008	1PE	C23-C13-OH4-C24
6	D	1008	1PE	C13-C23-OH3-C22
6	H	1007	1PE	C12-C22-OH3-C23
6	A	1008	1PE	C23-C13-OH4-C24
6	A	1009	1PE	C15-C25-OH5-C14
2	E	1001	4U5	NAO-C-CA-N
2	H	1001	4U5	NAO-C-CA-N
2	K	1001	4U5	O-C-CA-N
6	E	1008	1PE	C12-C22-OH3-C23
6	B	1006	1PE	C23-C13-OH4-C24
6	B	1007	1PE	C12-C22-OH3-C23
6	J	1007	1PE	C25-C15-OH6-C26
6	A	1008	1PE	C14-C24-OH4-C13
6	C	1006	1PE	C25-C15-OH6-C26
2	D	1001	4U5	O-C-CA-N
2	F	1001	4U5	O-C-CA-N
6	K	1009	1PE	C24-C14-OH5-C25
6	L	1009	1PE	C24-C14-OH5-C25
6	I	1007	1PE	C23-C13-OH4-C24
6	F	1006	1PE	C24-C14-OH5-C25
6	J	1008	1PE	OH6-C15-C25-OH5
6	K	1010	1PE	OH4-C13-C23-OH3
6	I	1007	1PE	C24-C14-OH5-C25
2	D	1001	4U5	O-C-CA-CAU
2	F	1001	4U5	O-C-CA-CAU
2	D	1001	4U5	NAO-C-CA-N
2	F	1001	4U5	NAO-C-CA-N
2	H	1001	4U5	O-C-CA-N
2	K	1001	4U5	NAO-C-CA-N
6	B	1007	1PE	OH4-C13-C23-OH3
6	J	1007	1PE	C24-C14-OH5-C25
6	J	1007	1PE	C16-C26-OH6-C15
6	L	1009	1PE	C16-C26-OH6-C15
6	L	1009	1PE	OH5-C14-C24-OH4
2	D	1001	4U5	NAO-C-CA-CAU
2	F	1001	4U5	NAO-C-CA-CAU
2	K	1001	4U5	O-C-CA-CAU
2	K	1001	4U5	NAO-C-CA-CAU
6	K	1009	1PE	OH4-C13-C23-OH3
6	B	1007	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
6	I	1008	1PE	OH5-C14-C24-OH4

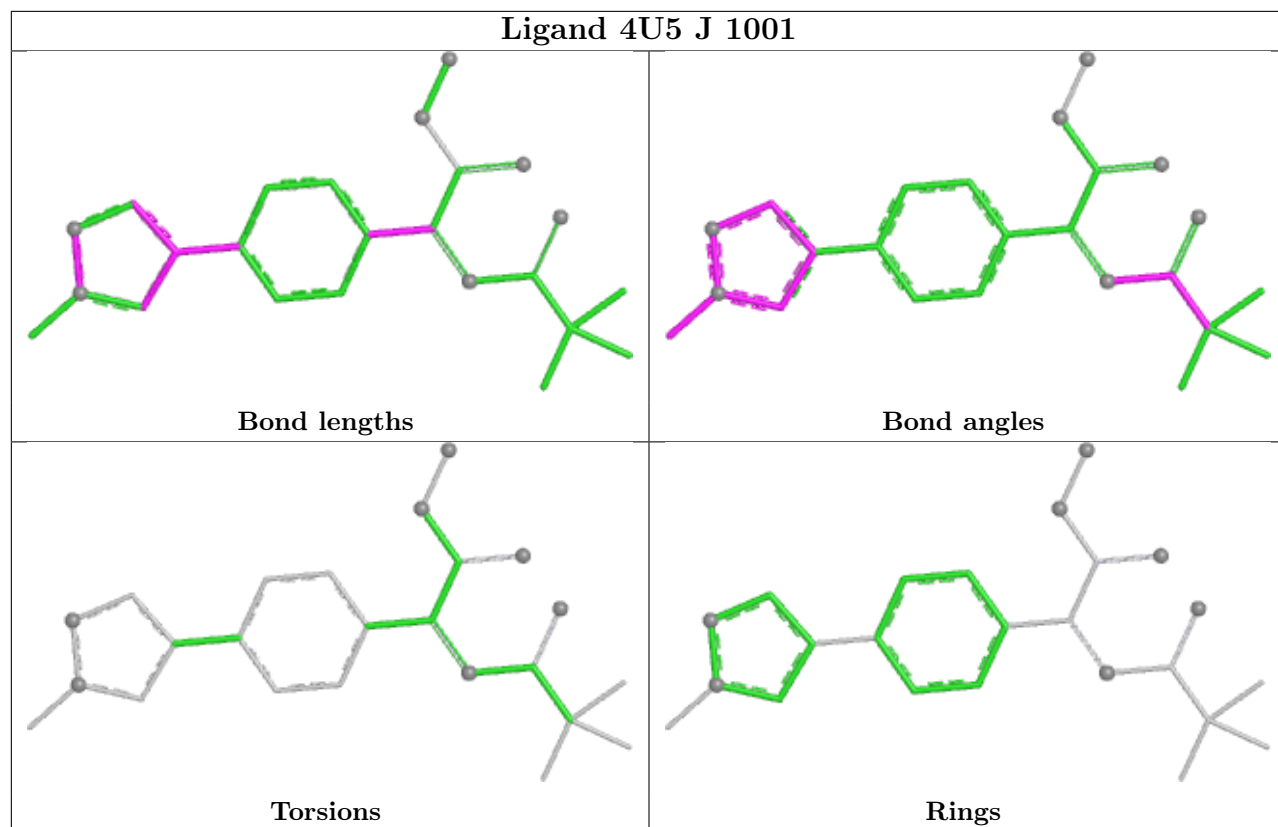
There are no ring outliers.

18 monomers are involved in 20 short contacts:

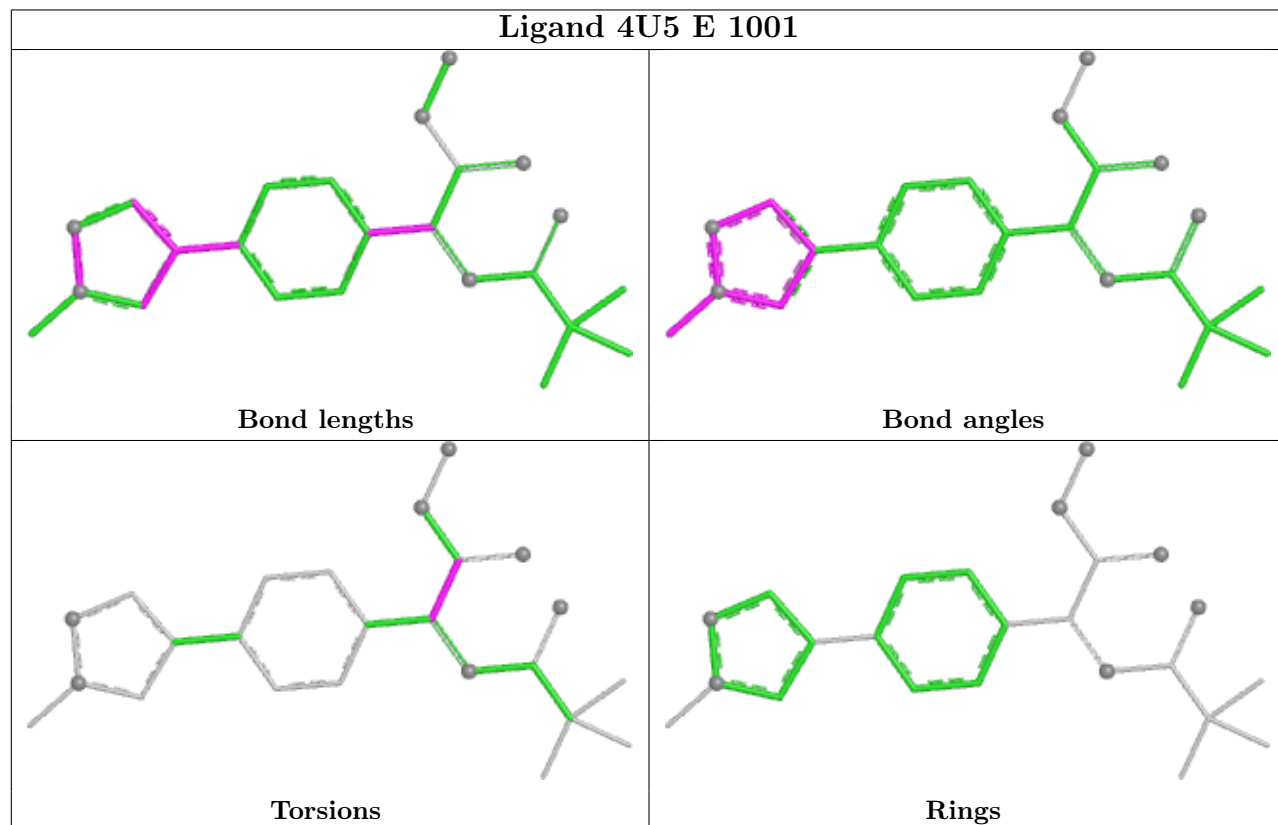
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1004	CO3	1	0
4	D	1004	CO3	1	0
2	D	1001	4U5	1	0
5	A	1007	SO4	2	0
6	B	1006	1PE	1	0
6	B	1007	1PE	1	0
6	L	1008	1PE	2	0
6	L	1009	1PE	1	0
5	A	1005	SO4	1	0
6	K	1010	1PE	1	0
6	H	1007	1PE	1	0
5	K	1007	SO4	1	0
6	J	1008	1PE	1	0
6	D	1007	1PE	2	0
6	A	1009	1PE	1	0
6	G	1007	1PE	1	0
6	C	1006	1PE	1	0
6	K	1009	1PE	1	0

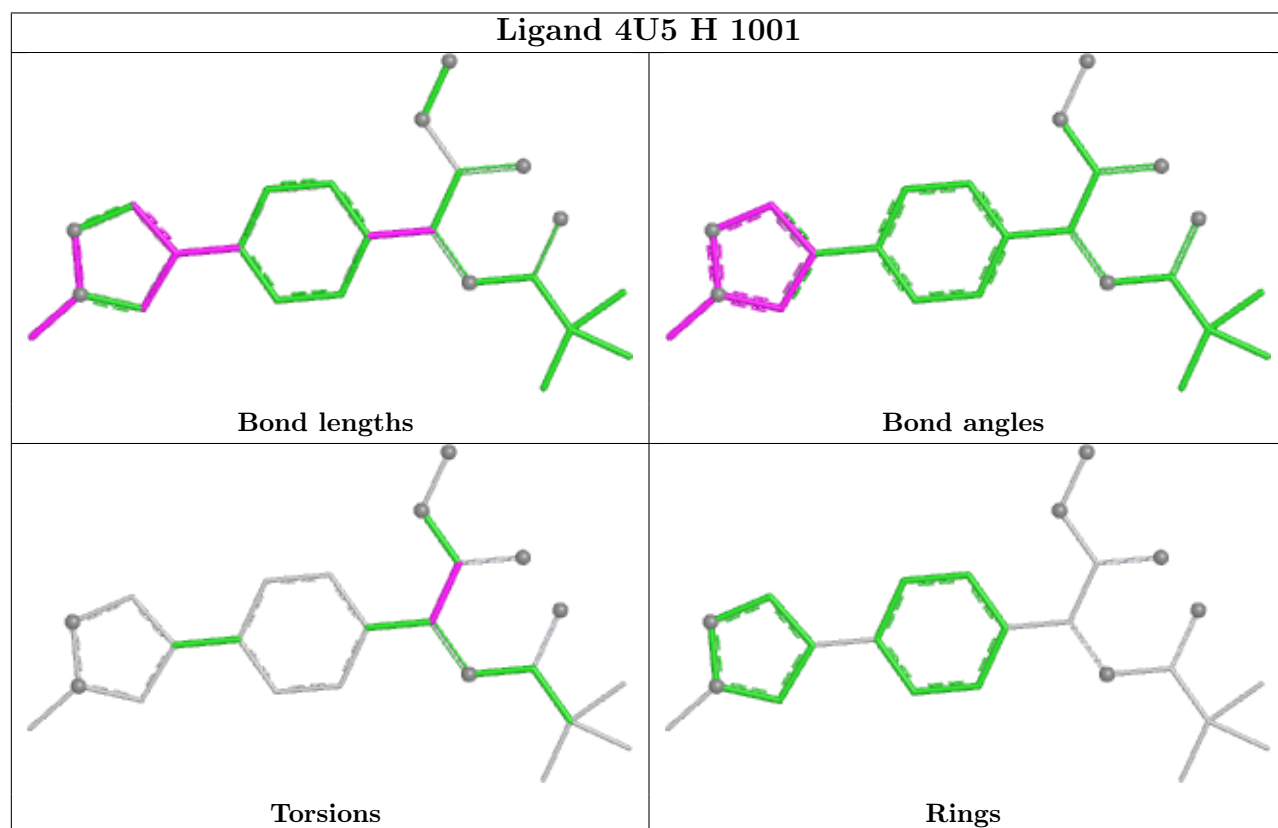
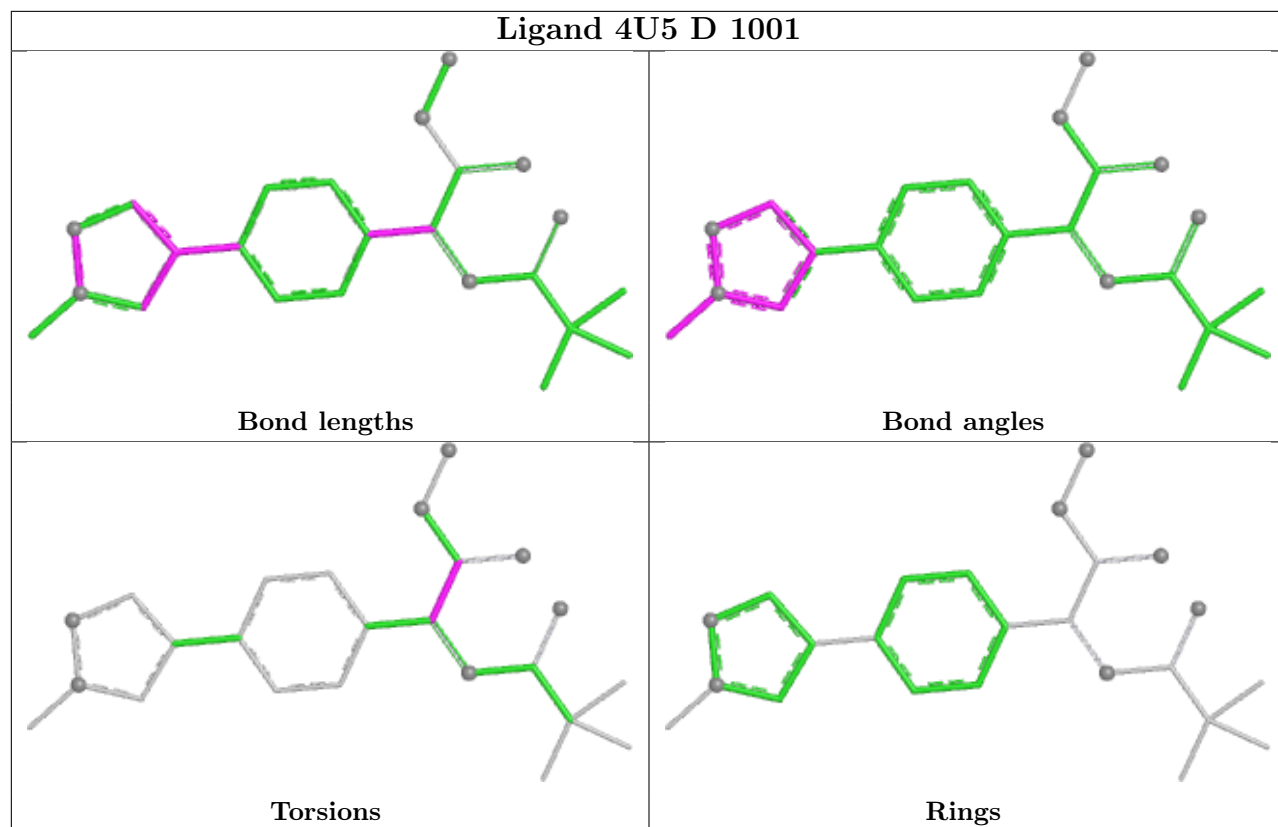
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

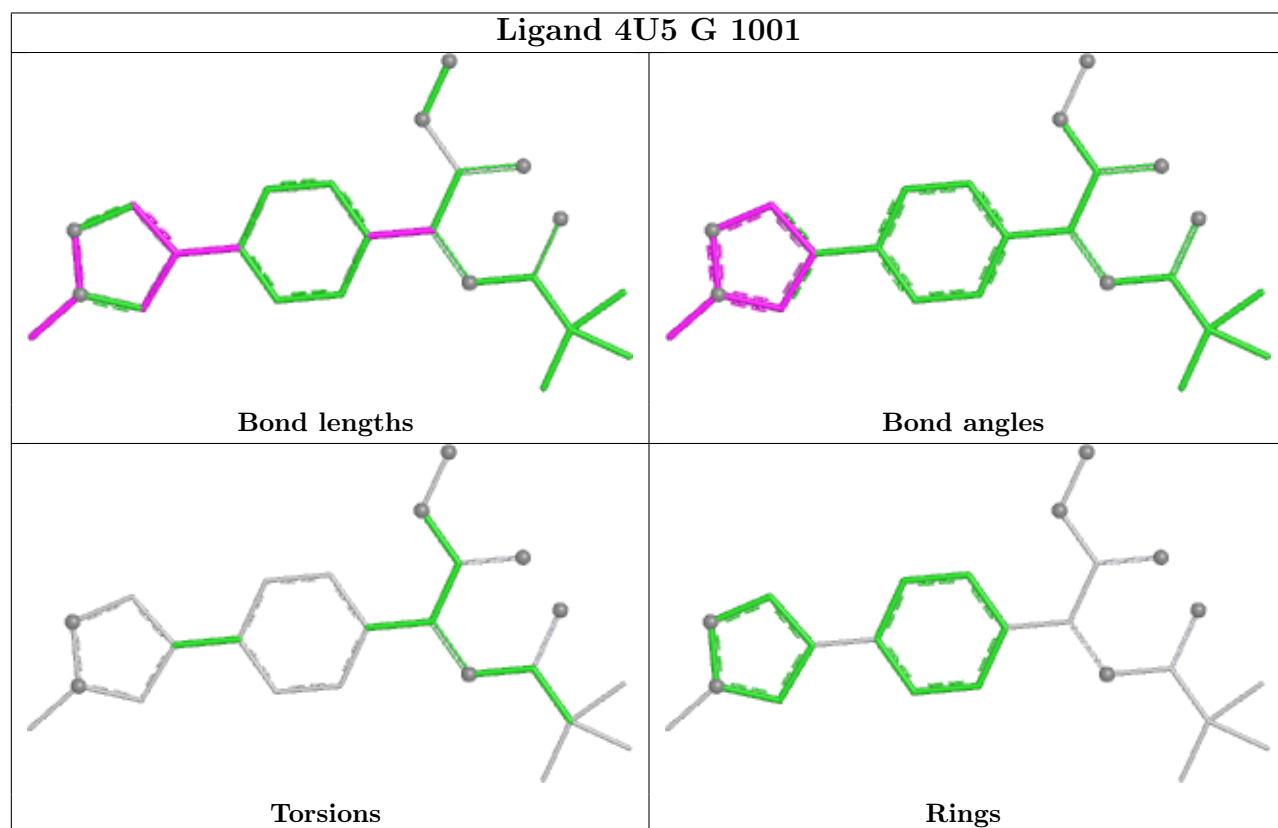
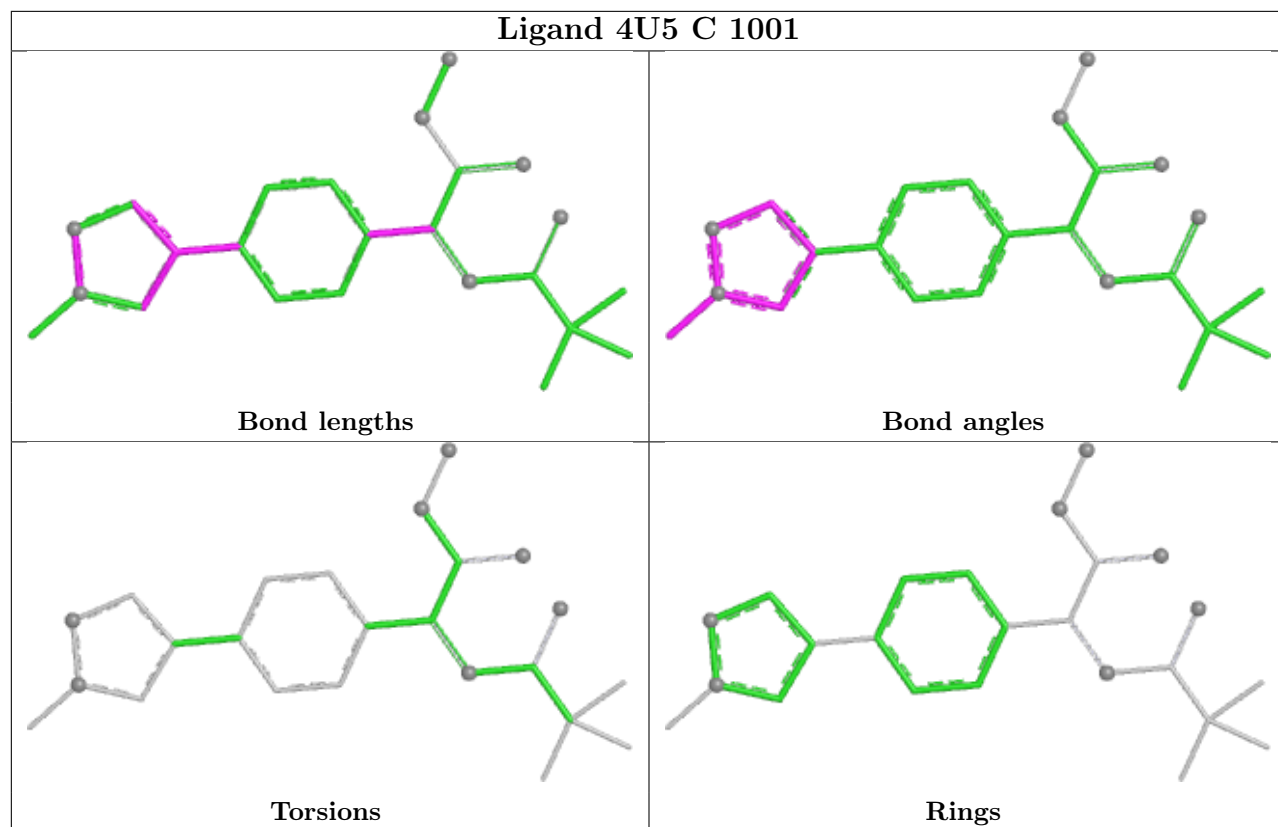
Ligand 4U5 J 1001



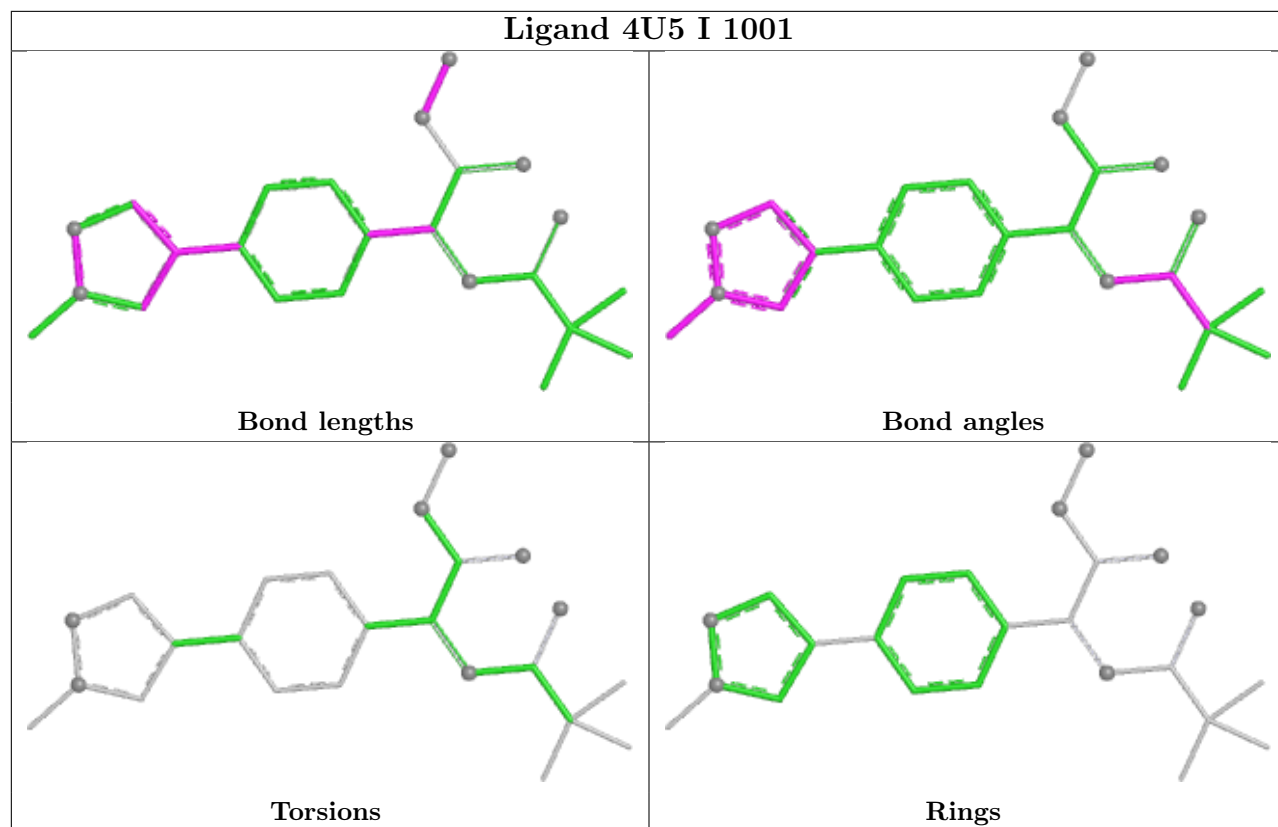
Ligand 4U5 E 1001



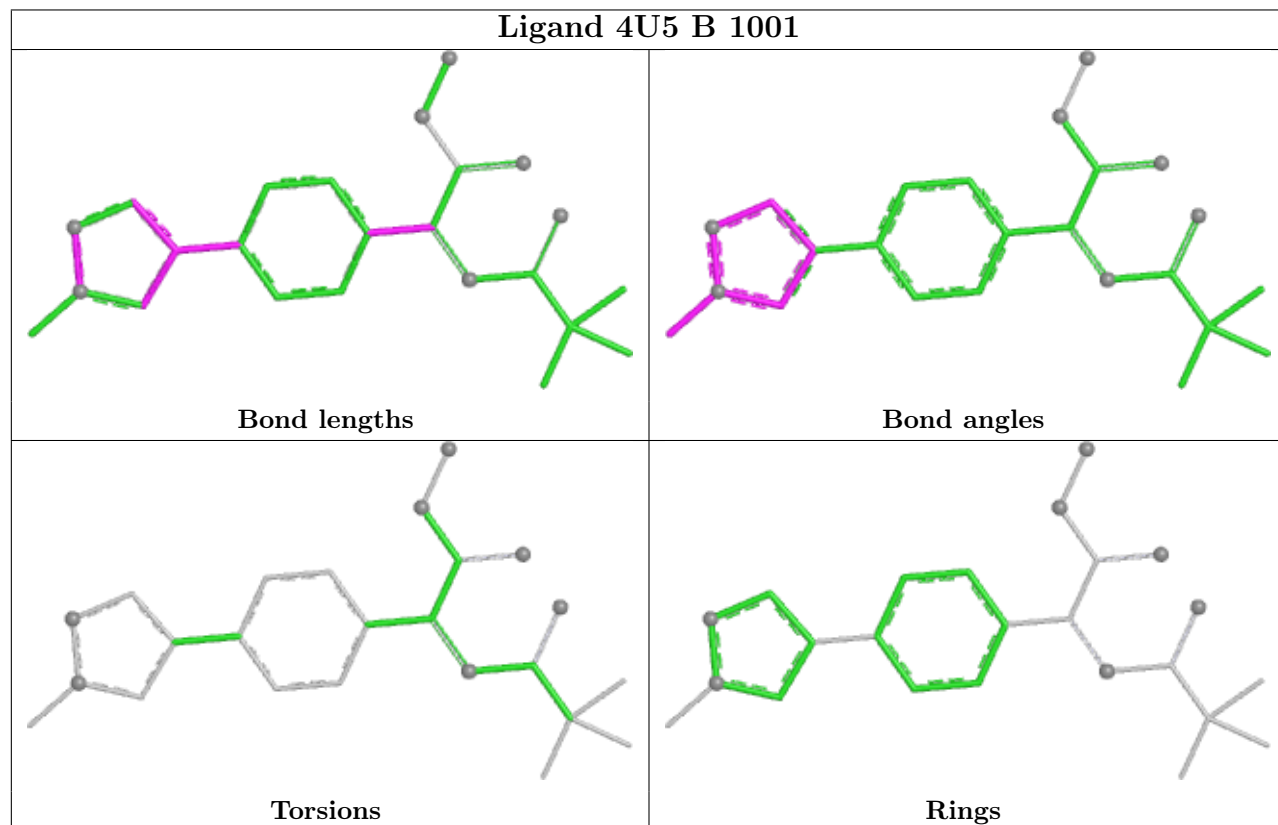


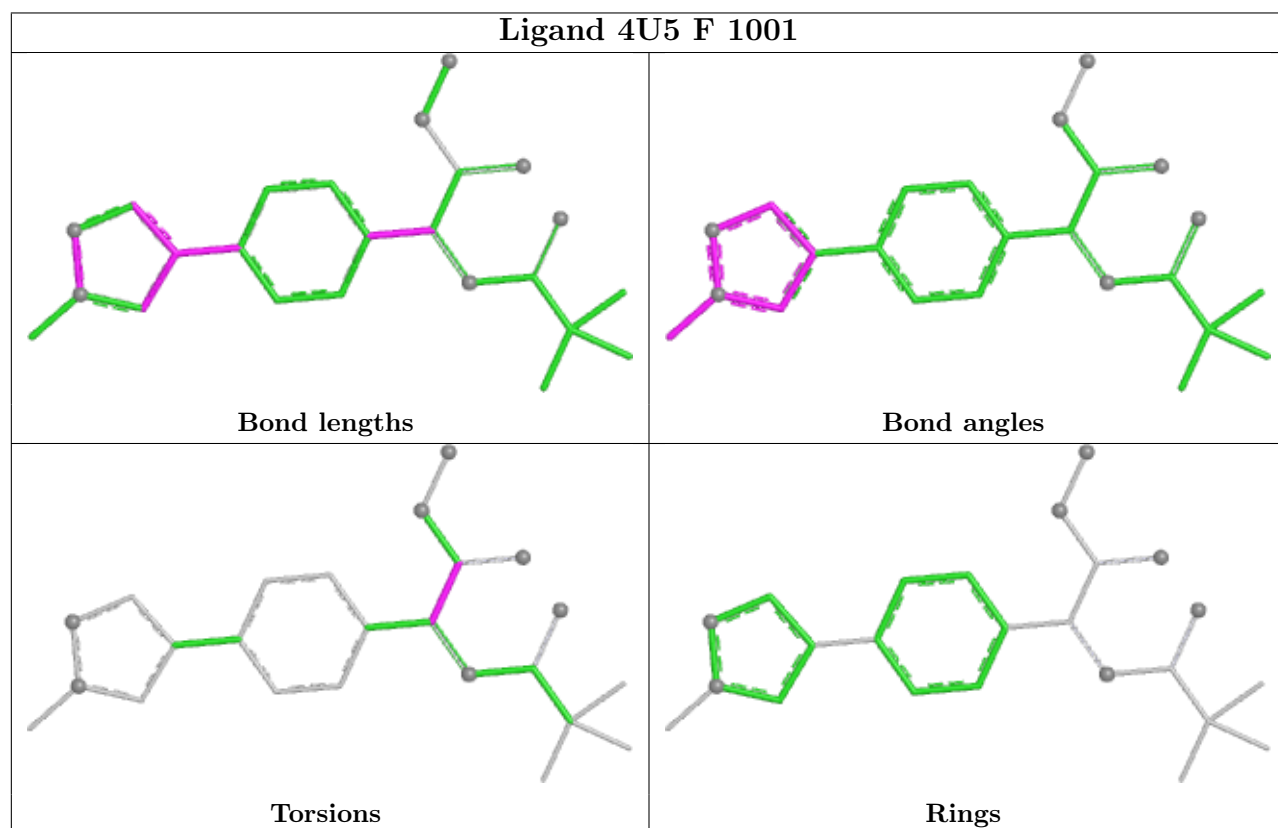
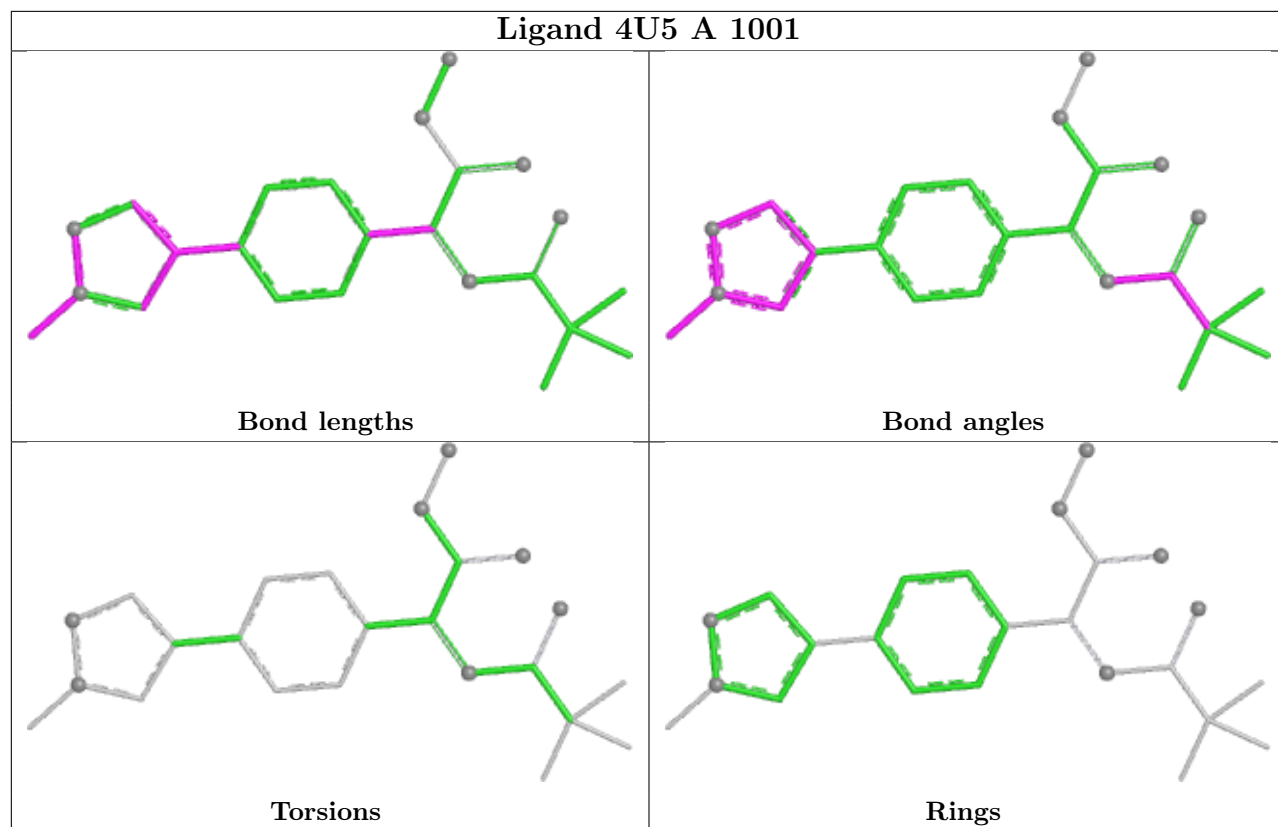


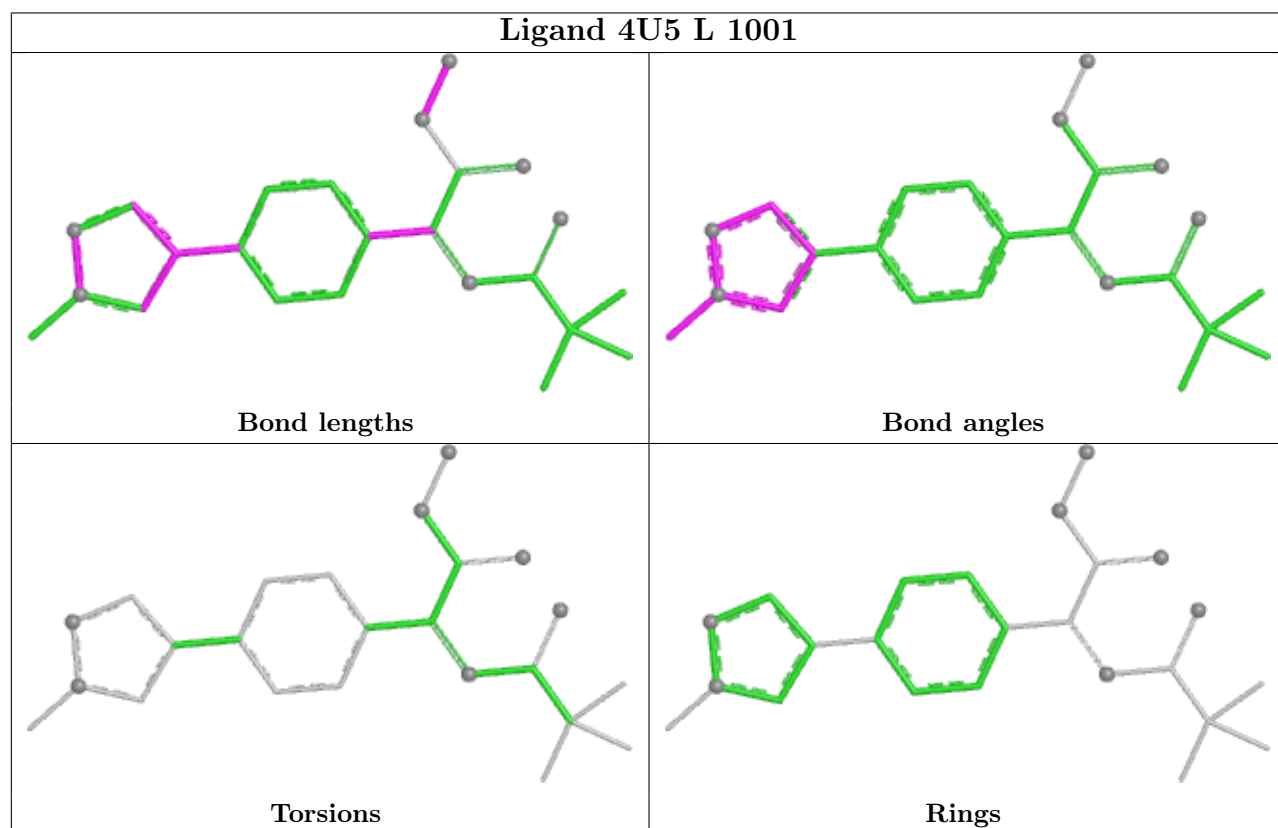
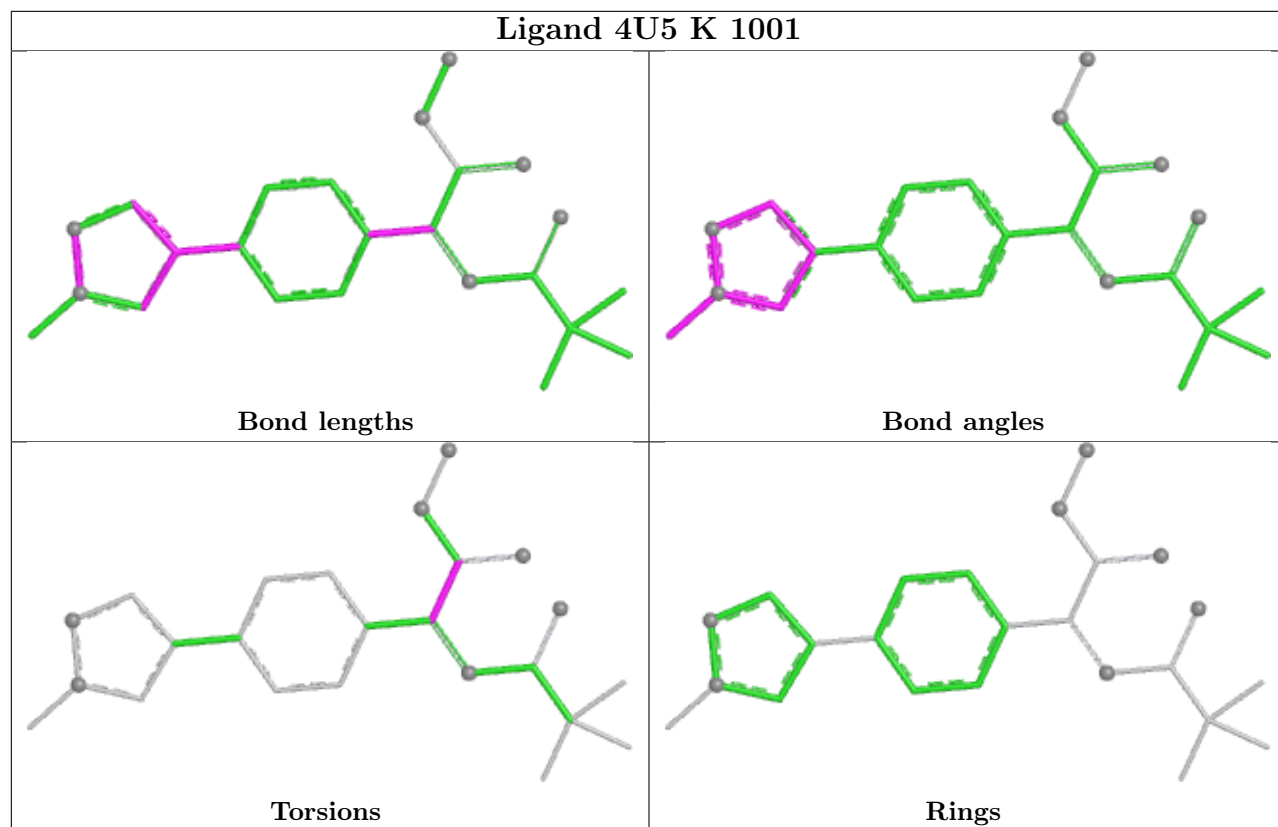
Ligand 4U5 I 1001



Ligand 4U5 B 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	518/522 (99%)	-0.06	7 (1%) 73 70	16, 32, 57, 96	1 (0%)
1	B	516/522 (98%)	0.13	15 (2%) 53 49	20, 35, 71, 104	0
1	C	516/522 (98%)	-0.02	10 (1%) 66 62	18, 33, 65, 106	4 (0%)
1	D	514/522 (98%)	-0.11	8 (1%) 70 67	19, 31, 54, 88	5 (0%)
1	E	508/522 (97%)	-0.17	3 (0%) 85 83	19, 32, 47, 80	2 (0%)
1	F	511/522 (97%)	0.12	14 (2%) 56 51	21, 35, 65, 97	3 (0%)
1	G	519/522 (99%)	-0.05	13 (2%) 58 54	19, 32, 61, 113	3 (0%)
1	H	517/522 (99%)	0.13	12 (2%) 61 57	18, 34, 75, 98	3 (0%)
1	I	517/522 (99%)	-0.05	7 (1%) 73 70	19, 32, 61, 77	2 (0%)
1	J	514/522 (98%)	-0.11	10 (1%) 66 62	17, 31, 52, 86	6 (1%)
1	K	509/522 (97%)	-0.18	6 (1%) 76 73	20, 30, 46, 88	3 (0%)
1	L	510/522 (97%)	0.21	17 (3%) 49 45	22, 39, 70, 88	5 (0%)
All	All	6169/6264 (98%)	-0.01	122 (1%) 65 61	16, 33, 64, 113	37 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	551	VAL	6.5
1	G	603	ASP	6.3
1	F	138	GLU	5.8
1	F	603	ASP	4.9
1	B	183	ASN	4.6
1	F	552	LYS	4.4
1	B	257	LYS	4.1
1	B	255	THR	4.0
1	D	260	ASN	4.0
1	H	257	LYS	4.0
1	C	549	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	J	551	VAL	4.0
1	A	603	ASP	3.9
1	C	364	ASP	3.8
1	E	549	SER	3.7
1	G	551	VAL	3.6
1	C	603	ASP	3.6
1	L	603	ASP	3.6
1	J	603	ASP	3.5
1	L	551	VAL	3.4
1	D	603	ASP	3.4
1	B	261	MET	3.4
1	L	219	LEU	3.4
1	H	261	MET	3.3
1	L	161	ASN	3.3
1	I	152	GLN	3.3
1	H	198	LEU	3.2
1	J	550	SER	3.2
1	J	400	MET	3.2
1	C	121	CYS	3.2
1	G	260	ASN	3.1
1	L	217	ASN	3.1
1	F	161	ASN	3.1
1	H	260	ASN	2.9
1	F	139	ASN	2.9
1	L	364	ASP	2.9
1	G	398	PHE	2.8
1	B	259	VAL	2.8
1	B	258	ASN	2.8
1	L	121	CYS	2.8
1	F	549	SER	2.8
1	C	195	VAL	2.8
1	K	602	ASN	2.7
1	L	439	TYR	2.7
1	A	362	LYS	2.7
1	H	193	GLY	2.7
1	G	549	SER	2.7
1	E	160	GLU	2.7
1	J	85	ALA	2.7
1	J	260	ASN	2.6
1	L	123	VAL	2.6
1	A	363	GLY	2.6
1	K	550	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	398	PHE	2.6
1	D	219	LEU	2.6
1	E	551	VAL	2.6
1	A	85	ALA	2.6
1	G	85	ALA	2.6
1	L	553	ALA	2.6
1	G	362	LYS	2.6
1	F	144	ILE	2.5
1	D	85	ALA	2.5
1	K	552	LYS	2.5
1	F	550	SER	2.5
1	G	259	VAL	2.5
1	I	398	PHE	2.4
1	F	136	GLY	2.4
1	I	121	CYS	2.4
1	H	603	ASP	2.4
1	B	549	SER	2.4
1	B	363	GLY	2.4
1	A	195	VAL	2.4
1	I	261	MET	2.4
1	K	549	SER	2.4
1	C	196	ALA	2.3
1	I	364	ASP	2.3
1	L	160	GLU	2.3
1	J	549	SER	2.3
1	L	262	GLU	2.3
1	F	553	ALA	2.3
1	F	153	VAL	2.3
1	H	259	VAL	2.3
1	L	554	SER	2.2
1	B	551	VAL	2.2
1	I	602	ASN	2.2
1	L	139	ASN	2.2
1	H	439	TYR	2.2
1	J	439	TYR	2.2
1	H	121	CYS	2.2
1	J	219	LEU	2.2
1	B	104	ASN	2.2
1	C	193	GLY	2.2
1	G	508	GLU	2.2
1	F	135	PRO	2.2
1	B	362	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	273	ASN	2.1
1	B	364	ASP	2.1
1	F	146	SER	2.1
1	H	364	ASP	2.1
1	D	552	LYS	2.1
1	A	398	PHE	2.1
1	L	400	MET	2.1
1	L	119	GLY	2.1
1	B	439	TYR	2.1
1	G	288	TYR	2.1
1	B	198	LEU	2.1
1	I	549	SER	2.1
1	H	183	ASN	2.1
1	G	261	MET	2.1
1	D	567	GLN	2.0
1	C	259	VAL	2.0
1	B	193	GLY	2.0
1	C	120	GLY	2.0
1	G	138	GLU	2.0
1	D	197	ASP	2.0
1	A	261	MET	2.0
1	G	195	VAL	2.0
1	H	182	LYS	2.0
1	J	200	GLU	2.0
1	L	155	GLU	2.0
1	D	122	ASN	2.0
1	K	254	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	L	1006	5/5	0.74	0.20	104,104,105,107	0
6	1PE	A	1009	12/16	0.76	0.19	52,56,62,62	0
6	1PE	G	1007	9/16	0.78	0.21	51,56,62,62	0
7	GOL	G	1006	6/6	0.78	0.25	58,61,64,66	0
5	SO4	H	1006	5/5	0.79	0.15	89,91,93,93	0
5	SO4	K	1006	5/5	0.80	0.15	87,89,90,90	0
5	SO4	I	1005	5/5	0.81	0.14	103,104,105,105	0
6	1PE	J	1007	11/16	0.81	0.16	41,55,63,63	0
6	1PE	L	1008	7/16	0.81	0.24	64,70,83,86	0
6	1PE	B	1007	10/16	0.81	0.19	55,70,76,76	0
5	SO4	L	1005	5/5	0.82	0.15	100,101,101,102	0
5	SO4	I	1006	5/5	0.82	0.14	92,92,93,93	0
6	1PE	A	1008	9/16	0.82	0.16	42,45,49,51	0
6	1PE	G	1009	6/16	0.83	0.17	45,48,49,53	0
6	1PE	C	1006	13/16	0.83	0.16	51,55,58,58	0
6	1PE	D	1007	10/16	0.83	0.15	36,49,56,58	0
6	1PE	L	1010	11/16	0.83	0.17	59,62,79,79	0
5	SO4	D	1006	5/5	0.83	0.14	93,94,94,95	0
5	SO4	D	1005	5/5	0.84	0.14	91,93,93,94	0
6	1PE	L	1009	10/16	0.84	0.15	50,56,73,75	0
6	1PE	H	1007	10/16	0.85	0.15	37,50,61,62	0
5	SO4	K	1008	5/5	0.85	0.15	93,96,97,97	0
5	SO4	J	1006	5/5	0.85	0.16	103,106,107,107	0
6	1PE	E	1007	12/16	0.85	0.12	45,50,57,59	0
6	1PE	B	1006	10/16	0.85	0.16	41,51,68,69	0
5	SO4	A	1007	5/5	0.85	0.14	81,82,83,87	0
6	1PE	G	1008	6/16	0.86	0.16	40,49,58,61	0
5	SO4	A	1006	5/5	0.86	0.14	71,75,78,79	0
6	1PE	D	1008	10/16	0.86	0.14	38,47,59,59	0
6	1PE	I	1007	12/16	0.86	0.13	37,53,55,61	0
6	1PE	I	1008	11/16	0.86	0.13	41,43,53,54	0
5	SO4	C	1005	5/5	0.87	0.19	71,71,72,74	0
5	SO4	G	1005	5/5	0.88	0.11	79,83,84,85	0
6	1PE	C	1007	9/16	0.88	0.14	42,45,49,50	0
6	1PE	J	1008	10/16	0.88	0.13	43,49,57,60	0
6	1PE	K	1009	12/16	0.88	0.13	47,49,52,52	0
5	SO4	F	1005	5/5	0.89	0.12	69,70,71,72	0
6	1PE	K	1010	12/16	0.89	0.12	33,38,58,60	0
5	SO4	J	1005	5/5	0.89	0.19	84,84,85,87	0
6	1PE	E	1008	12/16	0.90	0.13	24,39,58,58	0
6	1PE	F	1006	10/16	0.90	0.11	42,44,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	L	1007	5/5	0.90	0.12	72,72,73,78	0
5	SO4	K	1007	5/5	0.90	0.16	68,70,72,73	0
2	4U5	D	1001	24/24	0.91	0.12	25,37,44,47	0
5	SO4	E	1006	5/5	0.91	0.14	69,70,72,74	0
2	4U5	B	1001	24/24	0.92	0.12	28,38,43,48	0
2	4U5	A	1001	24/24	0.92	0.10	26,33,42,46	0
2	4U5	F	1001	24/24	0.92	0.11	30,36,45,52	0
5	SO4	A	1005	5/5	0.92	0.18	69,71,74,74	0
2	4U5	J	1001	24/24	0.93	0.10	24,36,46,48	0
2	4U5	K	1001	24/24	0.93	0.10	25,34,38,44	0
2	4U5	L	1001	24/24	0.93	0.11	29,38,45,48	0
2	4U5	C	1001	24/24	0.93	0.10	22,30,35,39	0
2	4U5	G	1001	24/24	0.94	0.10	25,36,39,41	0
2	4U5	H	1001	24/24	0.94	0.11	25,37,42,45	0
4	CO3	J	1004	4/4	0.94	0.09	32,32,33,36	0
2	4U5	E	1001	24/24	0.94	0.11	31,38,50,54	0
2	4U5	I	1001	24/24	0.95	0.09	22,34,40,45	0
4	CO3	K	1004	4/4	0.95	0.07	32,34,34,34	0
4	CO3	L	1004	4/4	0.95	0.07	27,32,34,34	0
4	CO3	A	1004	4/4	0.95	0.08	32,35,37,37	0
4	CO3	E	1004	4/4	0.95	0.11	33,35,36,39	0
4	CO3	G	1004	4/4	0.95	0.07	31,33,33,35	0
4	CO3	F	1004	4/4	0.96	0.08	21,24,26,27	0
4	CO3	D	1004	4/4	0.96	0.09	33,37,38,40	0
4	CO3	B	1004	4/4	0.97	0.04	23,26,26,29	0
4	CO3	C	1004	4/4	0.97	0.07	30,31,31,36	0
4	CO3	I	1004	4/4	0.97	0.06	29,35,36,37	0
4	CO3	H	1004	4/4	0.98	0.05	24,26,27,27	0
5	SO4	K	1005	5/5	0.98	0.06	31,32,33,33	0
5	SO4	B	1005	5/5	0.98	0.06	24,25,30,33	0
3	ZN	E	1002	1/1	0.99	0.03	32,32,32,32	0
3	ZN	F	1002	1/1	0.99	0.02	27,27,27,27	0
3	ZN	F	1003	1/1	0.99	0.01	30,30,30,30	0
3	ZN	G	1002	1/1	0.99	0.02	32,32,32,32	0
3	ZN	H	1002	1/1	0.99	0.03	30,30,30,30	0
3	ZN	J	1002	1/1	0.99	0.03	31,31,31,31	0
5	SO4	E	1005	5/5	0.99	0.05	30,30,32,32	0
3	ZN	K	1002	1/1	0.99	0.02	30,30,30,30	0
3	ZN	A	1002	1/1	0.99	0.02	31,31,31,31	0
3	ZN	B	1002	1/1	0.99	0.03	30,30,30,30	0
5	SO4	H	1005	5/5	0.99	0.06	24,27,29,30	0
3	ZN	D	1002	1/1	0.99	0.03	32,32,32,32	0

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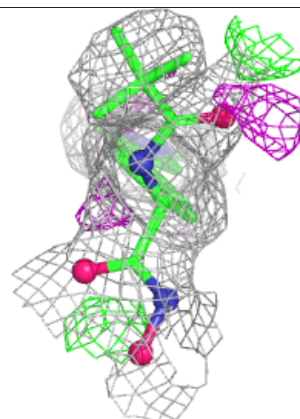
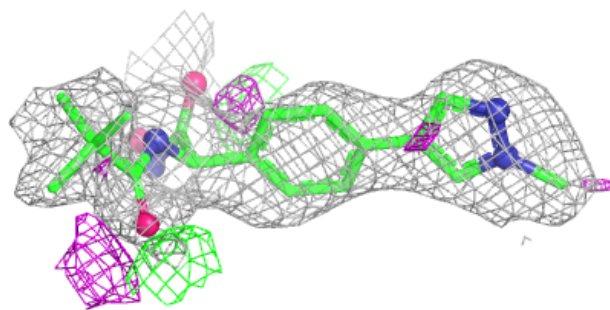
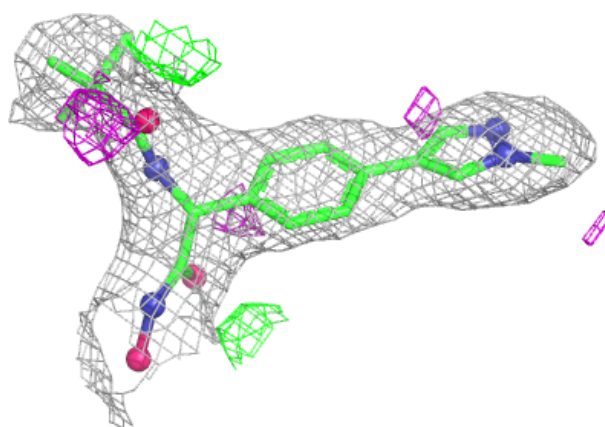
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	H	1003	1/1	1.00	0.01	23,23,23,23	0
3	ZN	I	1002	1/1	1.00	0.02	30,30,30,30	0
3	ZN	I	1003	1/1	1.00	0.01	25,25,25,25	0
3	ZN	B	1003	1/1	1.00	0.01	22,22,22,22	0
3	ZN	J	1003	1/1	1.00	0.01	25,25,25,25	0
3	ZN	E	1003	1/1	1.00	0.03	30,30,30,30	0
3	ZN	K	1003	1/1	1.00	0.02	31,31,31,31	0
3	ZN	L	1002	1/1	1.00	0.03	30,30,30,30	0
3	ZN	L	1003	1/1	1.00	0.03	33,33,33,33	0
3	ZN	C	1002	1/1	1.00	0.01	23,23,23,23	0
3	ZN	C	1003	1/1	1.00	0.01	28,28,28,28	0
3	ZN	A	1003	1/1	1.00	0.03	26,26,26,26	0
3	ZN	G	1003	1/1	1.00	0.03	27,27,27,27	0
3	ZN	D	1003	1/1	1.00	0.01	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.

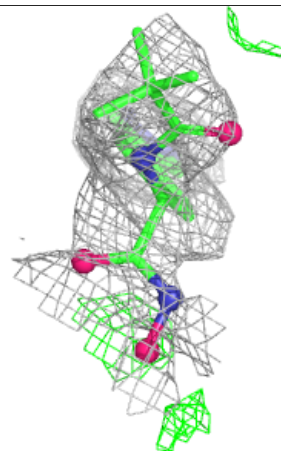
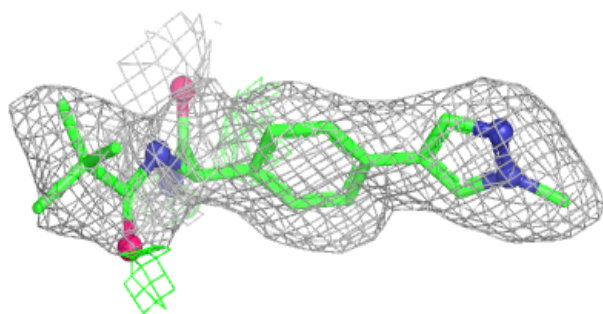
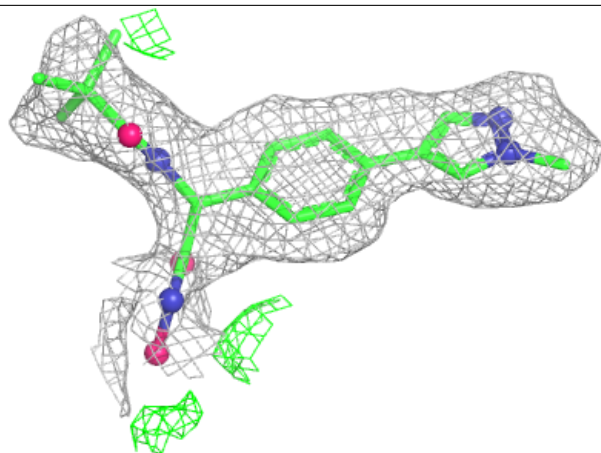
Electron density around 4U5 D 1001:

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



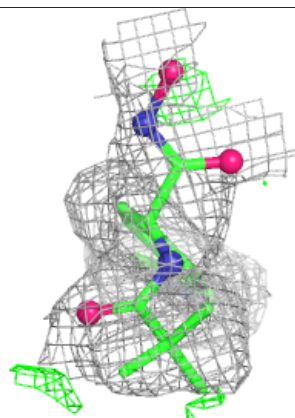
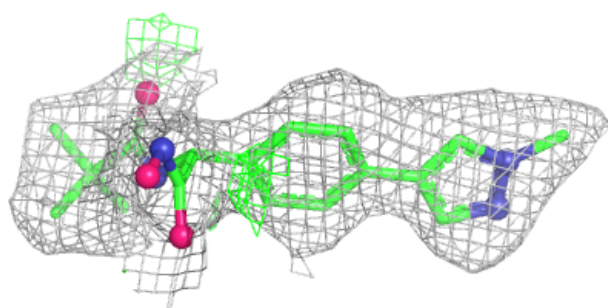
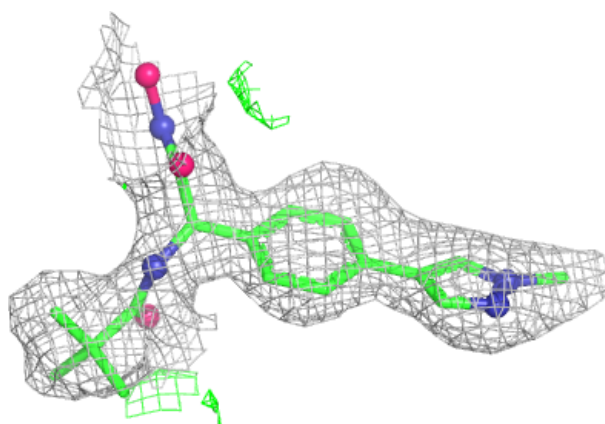
Electron density around 4U5 B 1001:

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and green (positive)

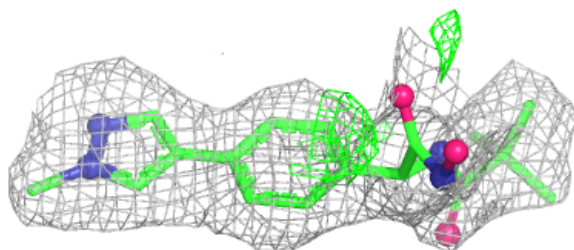
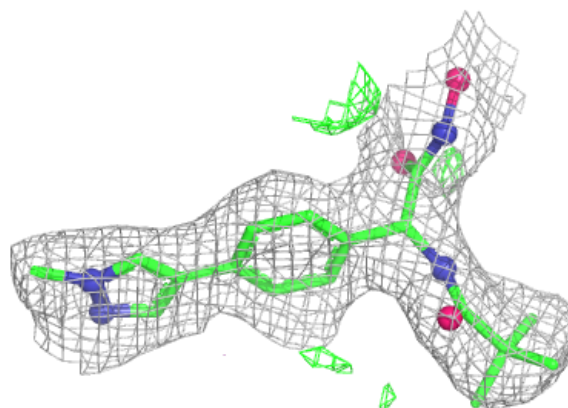


Electron density around 4U5 A 1001:

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

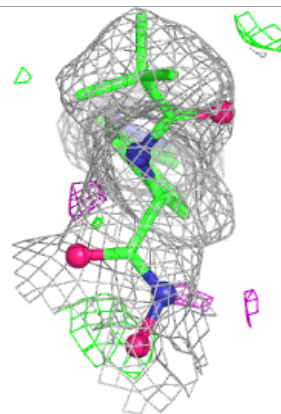
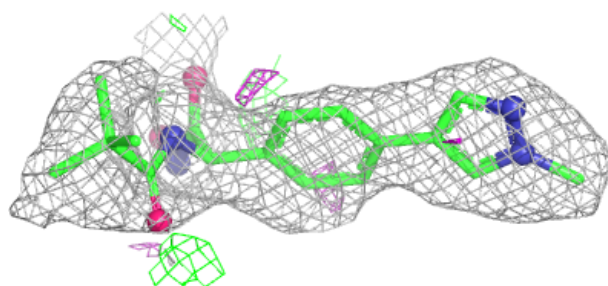
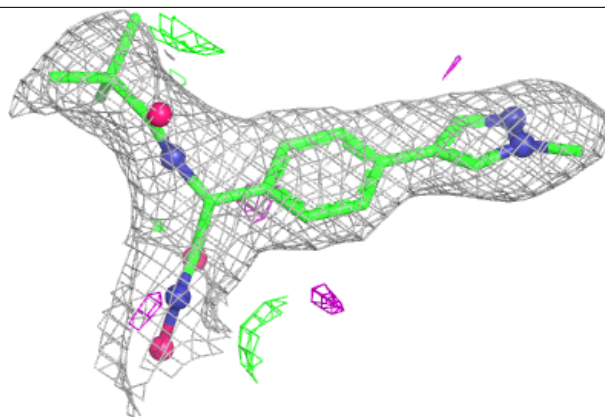
**Electron density around 4U5 F 1001:**

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

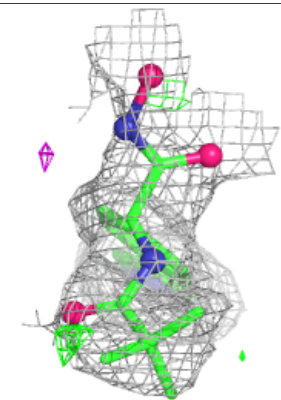
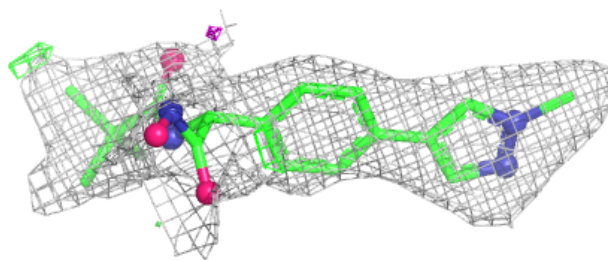
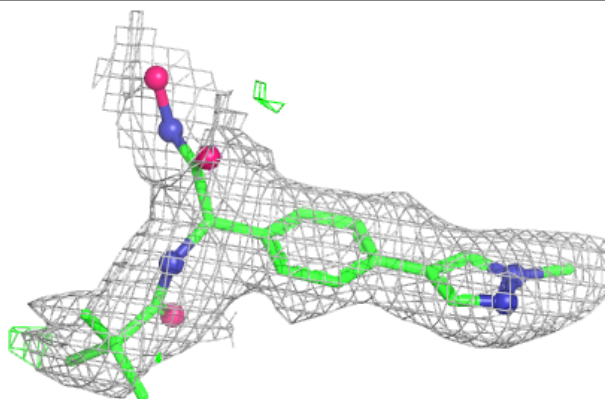


Electron density around 4U5 J 1001:

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

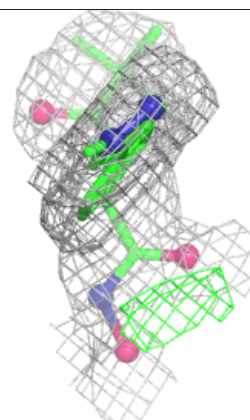
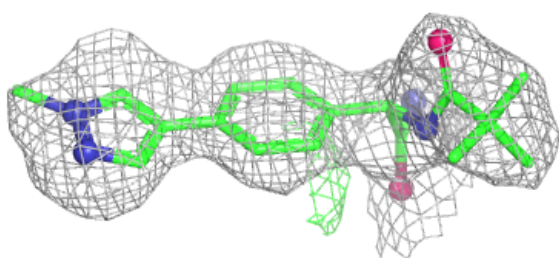
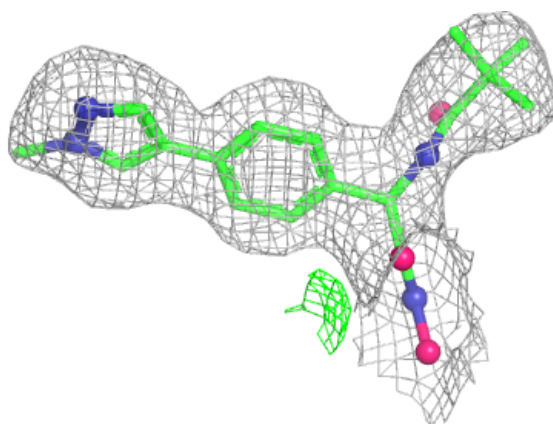
**Electron density around 4U5 K 1001:**

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



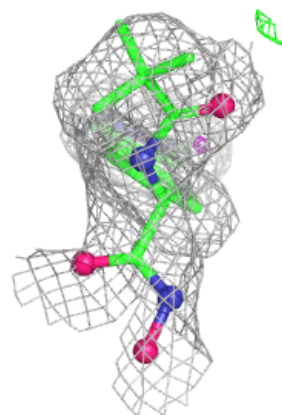
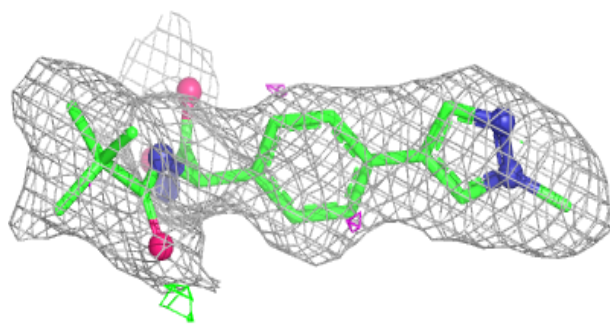
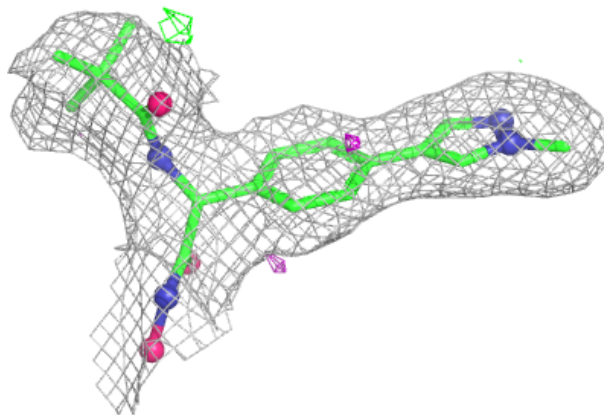
Electron density around 4U5 L 1001:

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



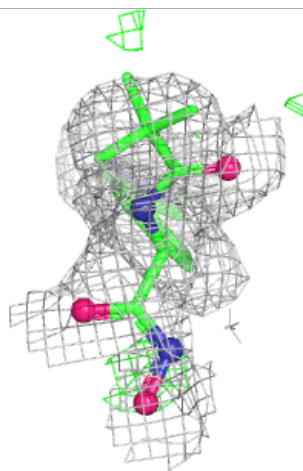
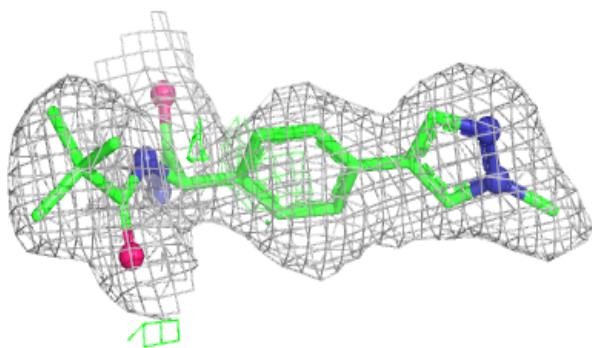
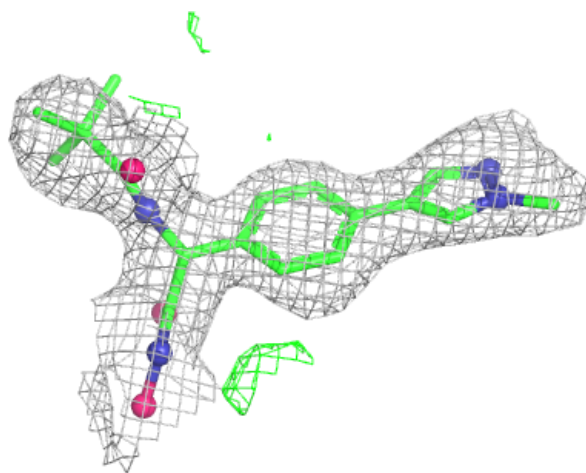
Electron density around 4U5 C 1001:

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



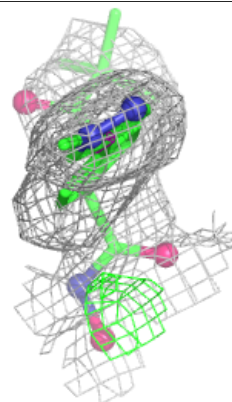
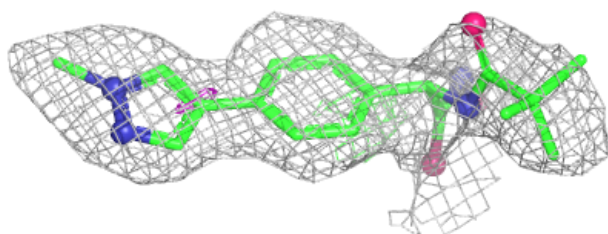
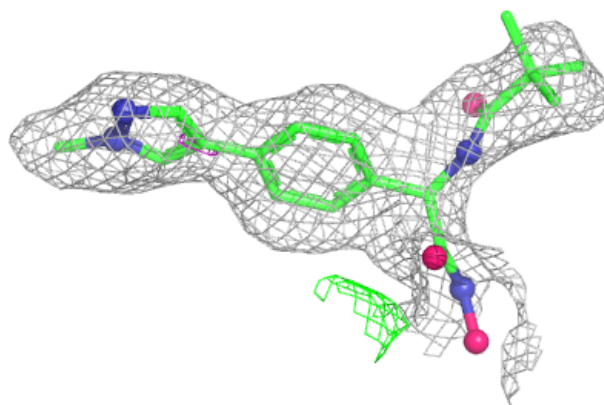
Electron density around 4U5 G 1001:

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

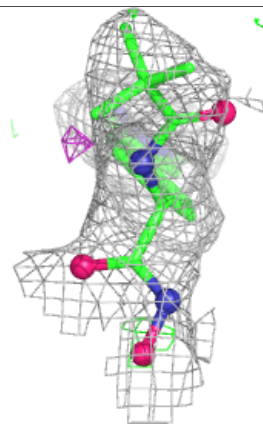
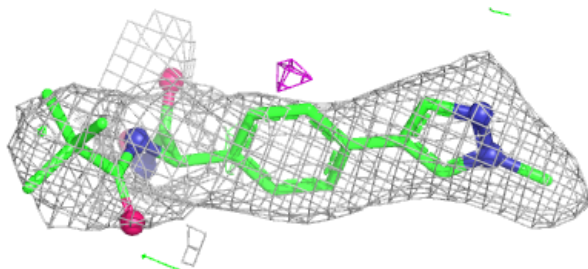
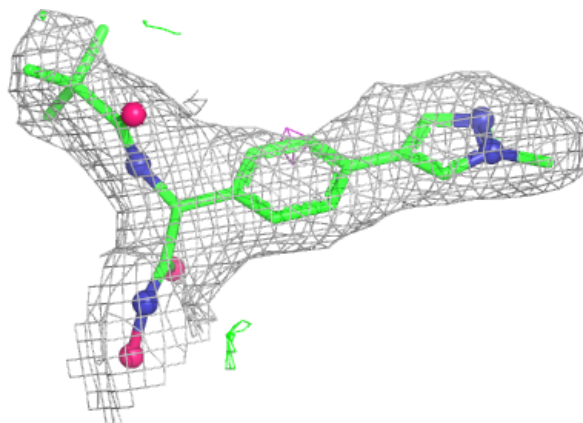


Electron density around 4U5 H 1001:

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

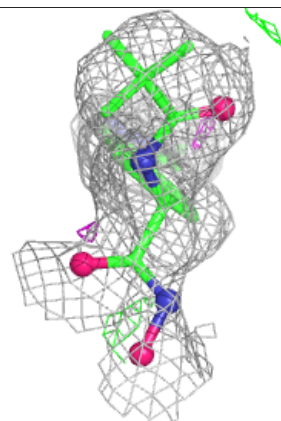
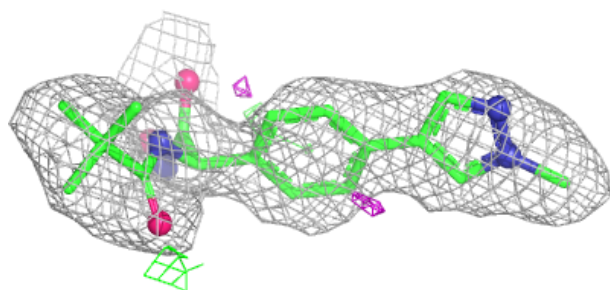
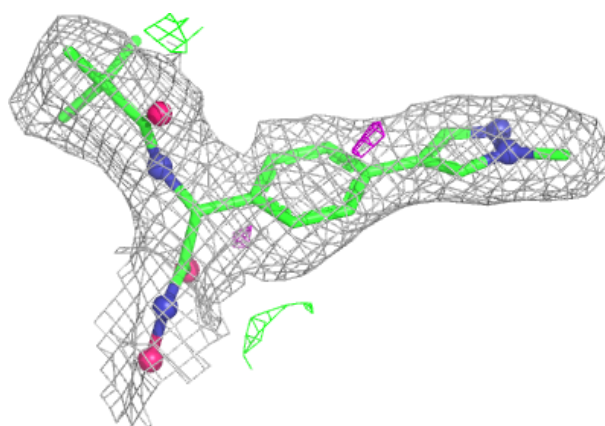
**Electron density around 4U5 E 1001:**

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



Electron density around 4U5 I 1001:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.