



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 07:52 AM UTC

PDB ID : 7MK5 / pdb_00007mk5
Title : Crystal structure of Escherichia coli ClpP covalently inhibited by clipibicyclene
Authors : Culp, E.J.; Sychantha, D.; Hobson, C.; Pawlowski, A.J.; Prehna, G.; Wright, G.D.
Deposited on : 2021-04-21
Resolution : 2.95 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:

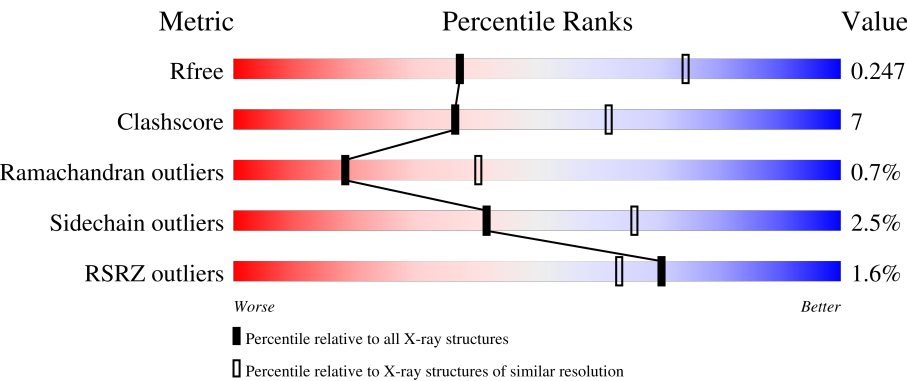
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.95 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.



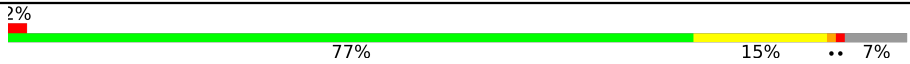
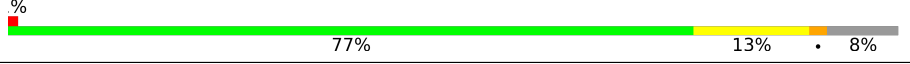
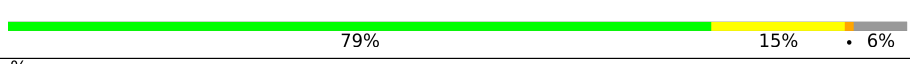
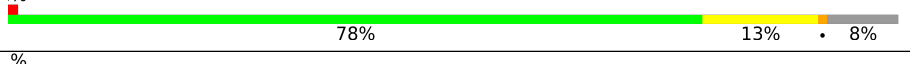
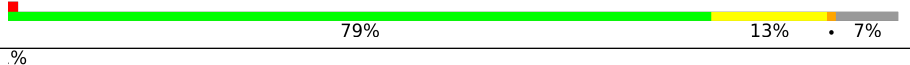
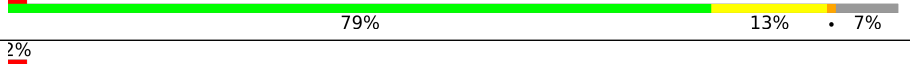
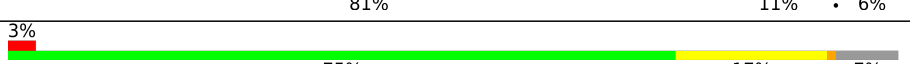
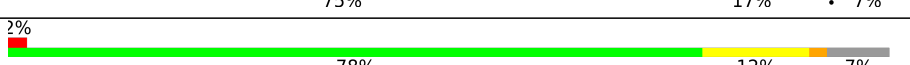
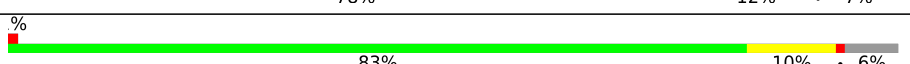
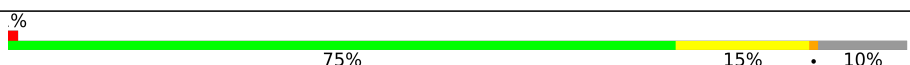
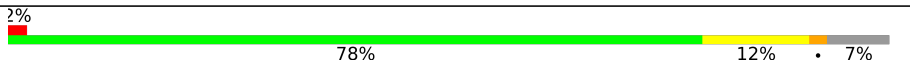
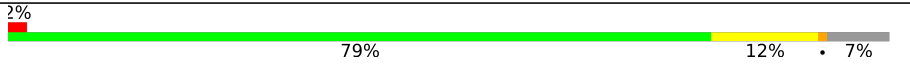
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	193	2% 81% 12% 6%
1	B	193	2% 79% 13% 6%
1	C	193	3% 80% 11% 7%
1	D	193	% 78% 16% 6%
1	E	193	% 77% 15% 6%

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Mol	Chain	Length	Quality of chain
1	F	193	
1	G	193	
1	H	193	
1	I	193	
1	J	193	
1	K	193	
1	L	193	
1	M	193	
1	N	193	
1	O	193	
1	P	193	
1	Q	193	
1	R	193	
1	S	193	
1	T	193	
1	U	193	
1	V	193	
1	W	193	
1	X	193	
1	Y	193	
1	Z	193	
1	a	193	
1	b	193	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 80695 atoms, of which 40496 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 ATP-dependent Clp protease proteolytic subunit.

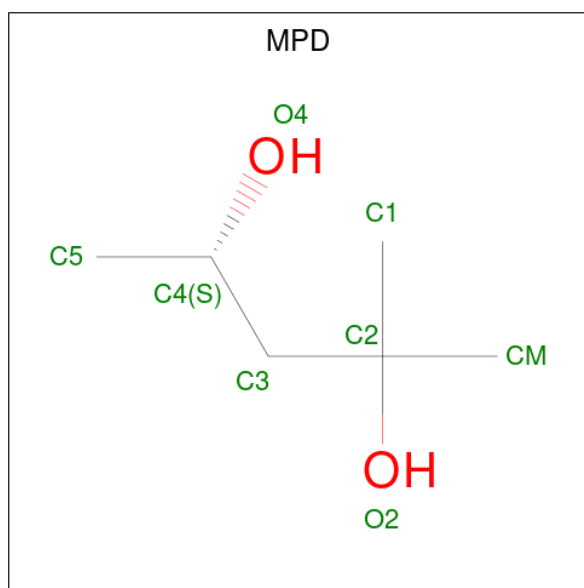
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	182	Total	C	H	N	O	S	0	0	0
			2857	902	1434	244	265	12			
1	B	181	Total	C	H	N	O	S	0	0	0
			2830	892	1421	242	263	12			
1	C	179	Total	C	H	N	O	S	0	0	0
			2800	886	1404	237	261	12			
1	D	181	Total	C	H	N	O	S	0	0	0
			2843	898	1428	242	263	12			
1	E	182	Total	C	H	N	O	S	0	0	0
			2858	902	1435	244	265	12			
1	F	180	Total	C	H	N	O	S	0	0	0
			2808	888	1404	241	263	12			
1	G	179	Total	C	H	N	O	S	0	0	0
			2779	878	1391	237	261	12			
1	H	177	Total	C	H	N	O	S	0	0	0
			2776	876	1390	239	260	11			
1	I	181	Total	C	H	N	O	S	0	0	0
			2838	893	1426	243	264	12			
1	J	181	Total	C	H	N	O	S	0	0	0
			2824	893	1413	242	264	12			
1	K	178	Total	C	H	N	O	S	0	0	0
			2790	878	1401	239	260	12			
1	L	179	Total	C	H	N	O	S	0	0	0
			2806	883	1410	240	261	12			
1	M	179	Total	C	H	N	O	S	0	0	0
			2808	887	1408	240	261	12			
1	N	180	Total	C	H	N	O	S	0	0	0
			2825	892	1418	241	262	12			
1	O	179	Total	C	H	N	O	S	0	0	0
			2786	880	1397	236	261	12			
1	P	181	Total	C	H	N	O	S	0	0	0
			2846	898	1431	242	263	12			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	182	Total	C	H	N	O	S	0	0	0
			2859	903	1435	243	266	12			
1	R	181	Total	C	H	N	O	S	0	0	0
			2836	895	1423	242	264	12			
1	S	181	Total	C	H	N	O	S	0	0	0
			2840	896	1425	243	264	12			
1	T	179	Total	C	H	N	O	S	0	0	0
			2806	883	1410	240	261	12			
1	U	179	Total	C	H	N	O	S	0	0	0
			2809	884	1412	240	261	12			
1	V	181	Total	C	H	N	O	S	0	0	0
			2825	890	1416	243	264	12			
1	W	174	Total	C	H	N	O	S	0	0	0
			2718	856	1363	232	256	11			
1	X	179	Total	C	H	N	O	S	0	0	0
			2788	880	1398	237	261	12			
1	Y	179	Total	C	H	N	O	S	0	0	0
			2806	883	1410	240	261	12			
1	Z	179	Total	C	H	N	O	S	0	0	0
			2806	883	1410	240	261	12			
1	a	177	Total	C	H	N	O	S	0	0	0
			2766	872	1388	235	259	12			
1	b	180	Total	C	H	N	O	S	0	0	0
			2825	892	1418	241	262	12			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	B	1	Total	C	H	O	0	0
			21	6	13	2		
2	B	1	Total	C	H	O	0	0
			22	6	14	2		
2	C	1	Total	C	H	O	0	0
			22	6	14	2		
2	D	1	Total	C	H	O	0	0
			22	6	14	2		
2	D	1	Total	C	H	O	0	0
			22	6	14	2		
2	D	1	Total	C	H	O	0	0
			22	6	14	2		
2	E	1	Total	C	H	O	0	0
			22	6	14	2		
2	F	1	Total	C	H	O	0	0
			22	6	14	2		
2	F	1	Total	C	H	O	0	0
			22	6	14	2		
2	F	1	Total	C	H	O	0	0
			22	6	14	2		
2	G	1	Total	C	H	O	0	0
			22	6	14	2		
2	H	1	Total	C	H	O	0	0
			22	6	14	2		
2	H	1	Total	C	H	O	0	0
			22	6	14	2		
2	I	1	Total	C	H	O	0	0
			22	6	14	2		
2	I	1	Total	C	H	O	0	0
			22	6	14	2		
2	J	1	Total	C	H	O	0	0
			22	6	14	2		
2	J	1	Total	C	H	O	0	0
			22	6	14	2		
2	K	1	Total	C	H	O	0	0
			22	6	14	2		
2	K	1	Total	C	H	O	0	0
			22	6	14	2		
2	L	1	Total	C	H	O	0	0
			22	6	14	2		

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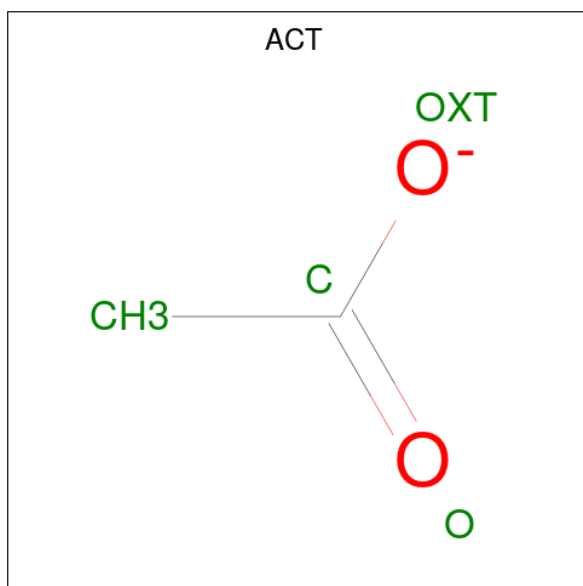
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	H	O	0	0
			22	6	14	2		
2	N	1	Total	C	H	O	0	0
			22	6	14	2		
2	N	1	Total	C	H	O	0	0
			22	6	14	2		
2	O	1	Total	C	H	O	0	0
			22	6	14	2		
2	O	1	Total	C	H	O	0	0
			22	6	14	2		
2	P	1	Total	C	H	O	0	0
			22	6	14	2		
2	P	1	Total	C	H	O	0	0
			22	6	14	2		
2	Q	1	Total	C	H	O	0	0
			22	6	14	2		
2	Q	1	Total	C	H	O	0	0
			22	6	14	2		
2	Q	1	Total	C	H	O	0	0
			22	6	14	2		
2	R	1	Total	C	H	O	0	0
			22	6	14	2		
2	S	1	Total	C	H	O	0	0
			22	6	14	2		
2	S	1	Total	C	H	O	0	0
			22	6	14	2		
2	T	1	Total	C	H	O	0	0
			22	6	14	2		
2	T	1	Total	C	H	O	0	0
			22	6	14	2		
2	U	1	Total	C	H	O	0	0
			22	6	14	2		
2	V	1	Total	C	H	O	0	0
			22	6	14	2		
2	W	1	Total	C	H	O	0	0
			22	6	14	2		
2	W	1	Total	C	H	O	0	0
			22	6	14	2		
2	X	1	Total	C	H	O	0	0
			22	6	14	2		
2	Y	1	Total	C	H	O	0	0
			22	6	14	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	Y	1	Total	C	H	O	0	0
			22	6	14	2		
2	Z	1	Total	C	H	O	0	0
			22	6	14	2		
2	Z	1	Total	C	H	O	0	0
			22	6	14	2		
2	a	1	Total	C	H	O	0	0
			22	6	14	2		
2	a	1	Total	C	H	O	0	0
			22	6	14	2		
2	b	1	Total	C	H	O	0	0
			22	6	14	2		
2	b	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



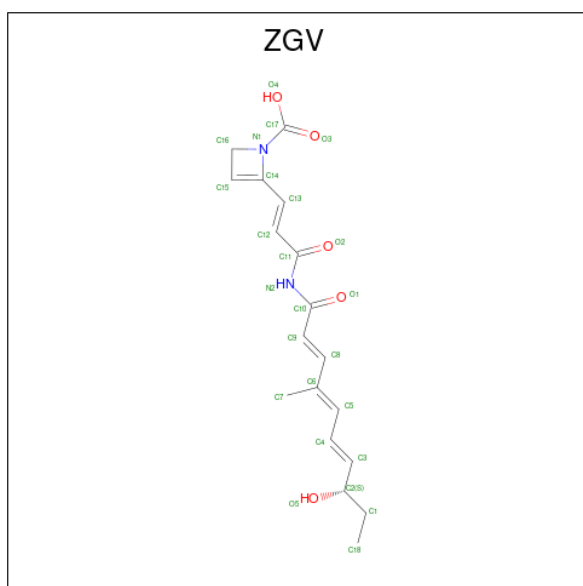
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	C	1	Total	C	H	O	0	0
			7	2	3	2		
3	F	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C H O 7 2 3 2	0	0
3	L	1	Total C H O 7 2 3 2	0	0
3	P	1	Total C H O 7 2 3 2	0	0
3	R	1	Total C H O 7 2 3 2	0	0
3	X	1	Total C H O 7 2 3 2	0	0
3	Z	1	Total C H O 7 2 3 2	0	0

- Molecule 4 is 4-[(1E)-3-{[(2E,4E,6E,8S)-8-hydroxy-4-methyldeca-2,4,6-trienoyl]amino}-3-oxoprop-1-en-1-yl]azete-1(2H)-carboxylic acid (CCD ID: ZGV) (formula: C₁₈H₂₂N₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 45	C 18	H 21	N 2	O 4	0	0
4	B	1	Total 21	C 9	H 7	N 2	O 3	0	0
4	C	1	Total 21	C 9	H 7	N 2	O 3	0	0
4	D	1	Total 21	C 9	H 7	N 2	O 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	F	1	Total	C	H	N	O	0	0
			24	11	8	2	3		
4	G	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	H	1	Total	C	H	N	O	0	0
			24	11	8	2	3		
4	I	1	Total	C	H	N	O	0	0
			23	10	8	2	3		
4	J	1	Total	C	H	N	O	0	0
			24	11	8	2	3		
4	K	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	L	1	Total	C	H	N	O	0	0
			32	14	13	2	3		
4	M	1	Total	C	H	N	O	0	0
			30	13	12	2	3		
4	N	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	O	1	Total	C	H	N	O	0	0
			45	18	21	2	4		
4	P	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	Q	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	R	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	S	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	T	1	Total	C	H	N	O	0	0
			24	11	8	2	3		
4	U	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	V	1	Total	C	H	N	O	0	0
			11	5	4	1	1		
4	W	1	Total	C	H	N	O	0	0
			45	18	21	2	4		
4	X	1	Total	C	H	N	O	0	0
			17	7	6	2	2		
4	Y	1	Total	C	H	N	O	0	0
			30	13	12	2	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	Z	1	Total	C	H	N	O	0	0
			11	5	4	1	1		
4	a	1	Total	C	H	N	O	0	0
			11	5	4	1	1		
4	b	1	Total	C	H	N	O	0	0
			17	7	6	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	4	Total	O	0	0
			4	4		
5	C	9	Total	O	0	0
			9	9		
5	D	4	Total	O	0	0
			4	4		
5	E	3	Total	O	0	0
			3	3		
5	F	3	Total	O	0	0
			3	3		
5	G	4	Total	O	0	0
			4	4		
5	H	5	Total	O	0	0
			5	5		
5	I	3	Total	O	0	0
			3	3		
5	J	5	Total	O	0	0
			5	5		
5	K	3	Total	O	0	0
			3	3		
5	L	4	Total	O	0	0
			4	4		
5	M	4	Total	O	0	0
			4	4		
5	N	3	Total	O	0	0
			3	3		
5	O	3	Total	O	0	0
			3	3		
5	P	2	Total	O	0	0
			2	2		

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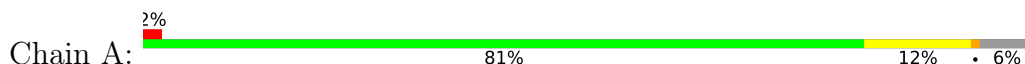
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Q	4	Total O 4 4	0	0
5	R	4	Total O 4 4	0	0
5	S	1	Total O 1 1	0	0
5	T	1	Total O 1 1	0	0
5	U	4	Total O 4 4	0	0
5	V	4	Total O 4 4	0	0
5	W	3	Total O 3 3	0	0
5	X	4	Total O 4 4	0	0
5	Y	4	Total O 4 4	0	0
5	Z	4	Total O 4 4	0	0
5	a	2	Total O 2 2	0	0
5	b	5	Total O 5 5	0	0

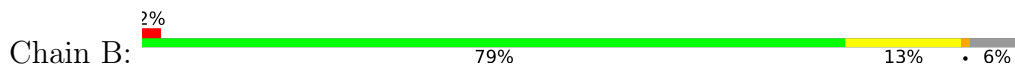
3 Residue-property plots [i](#)

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.

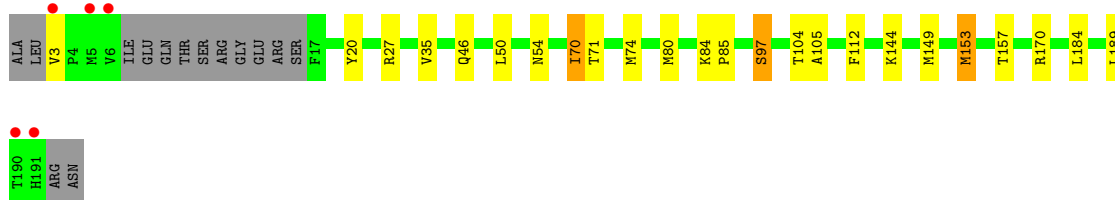
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



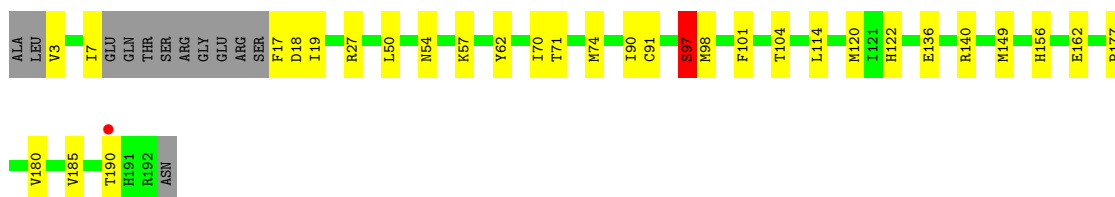
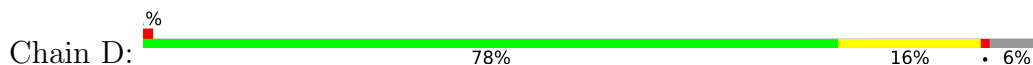
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



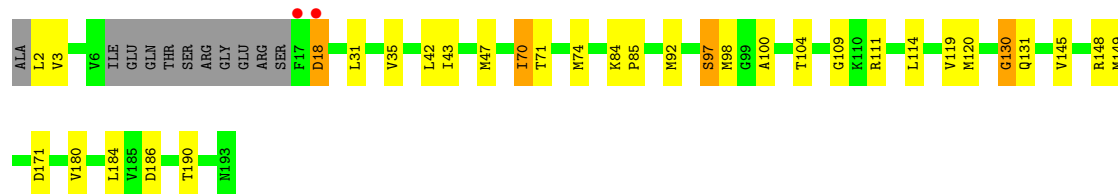
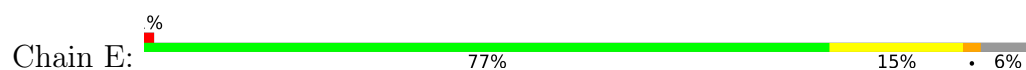
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



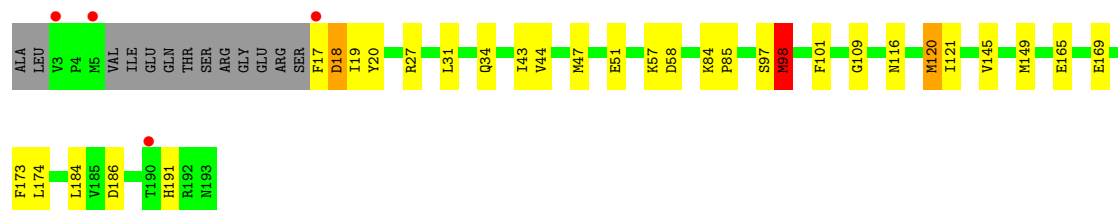
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



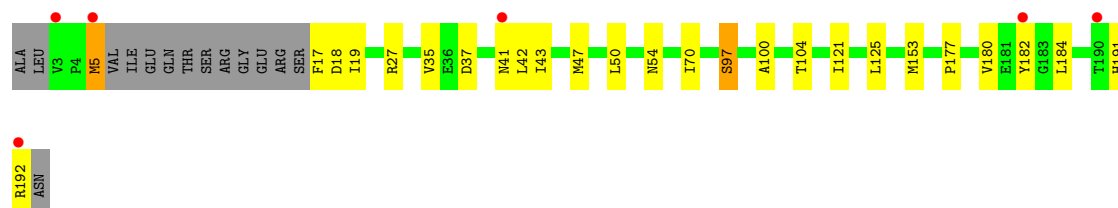
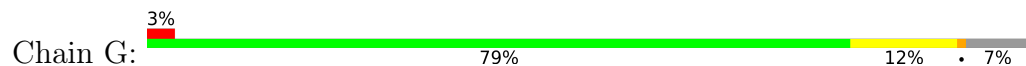
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



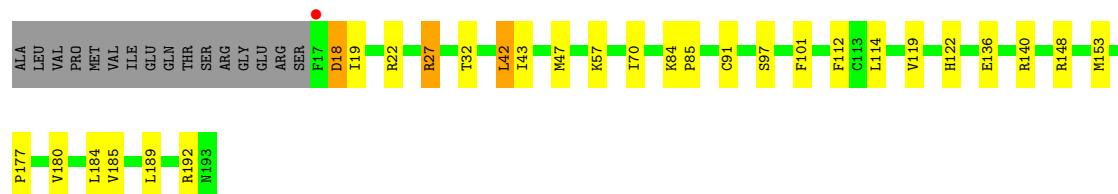
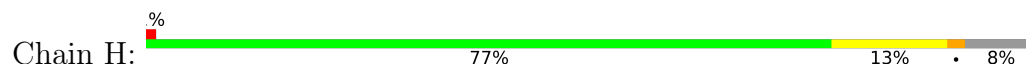
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



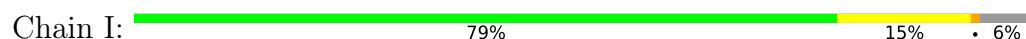
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



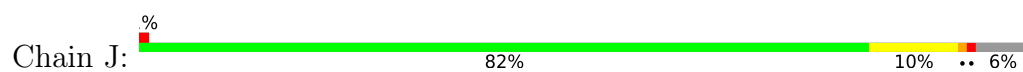
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



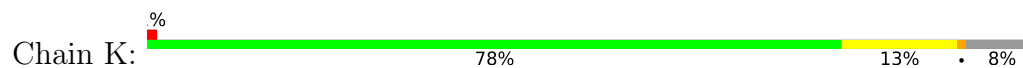
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



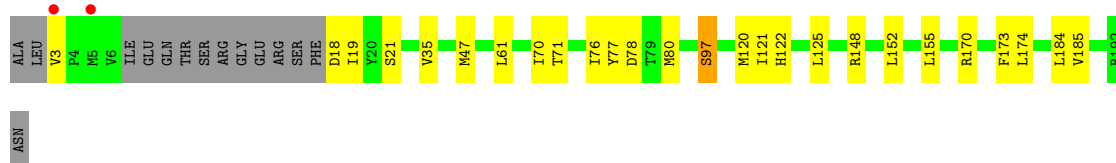
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



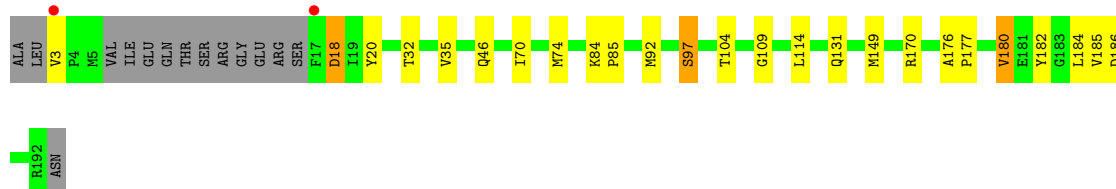
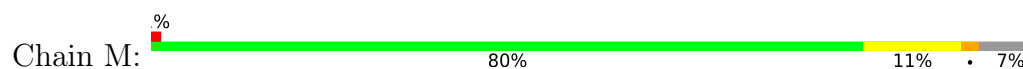
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



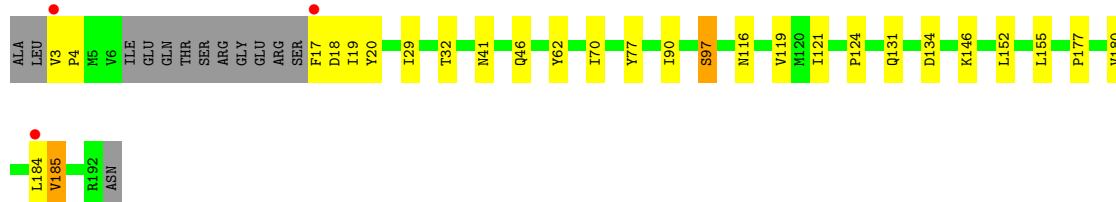
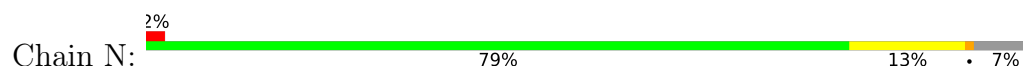
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



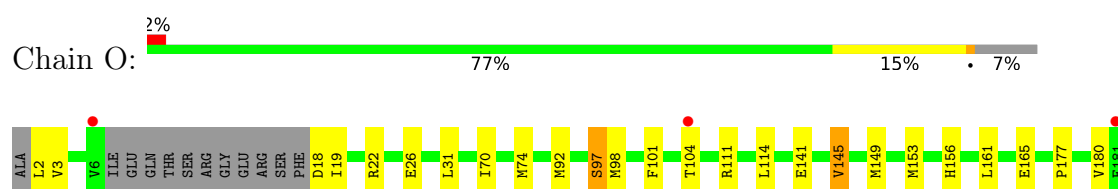
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



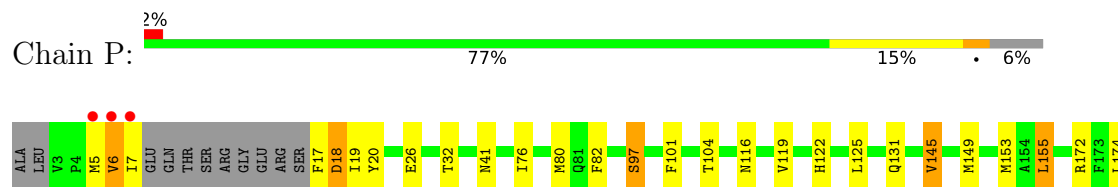
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



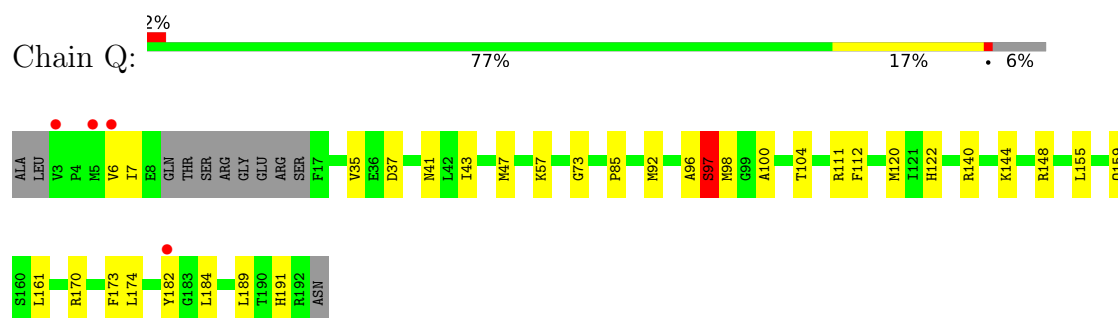
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



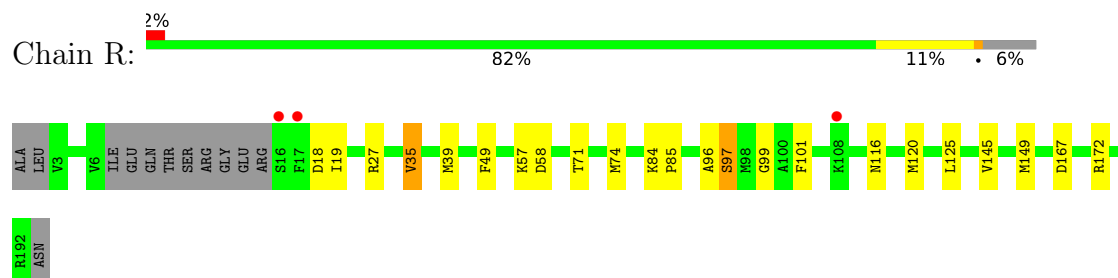
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



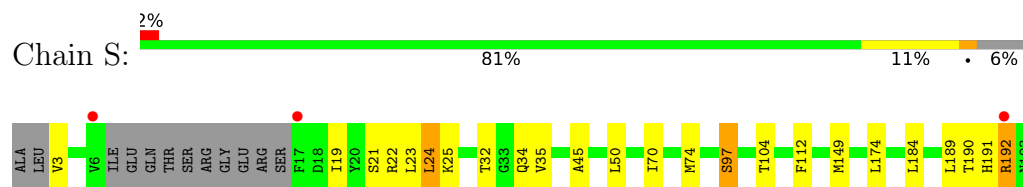
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



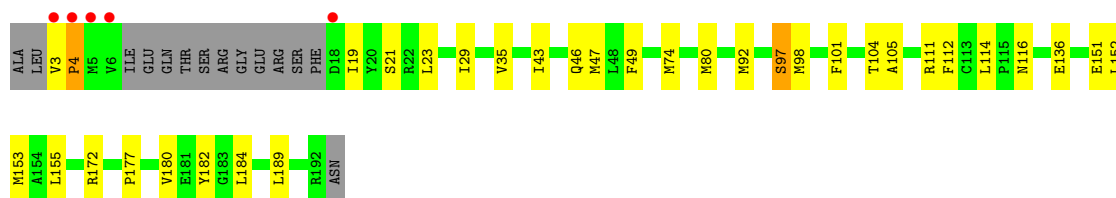
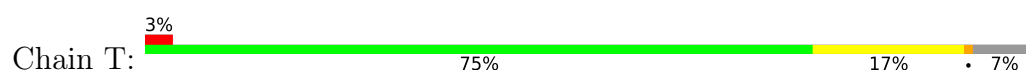
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



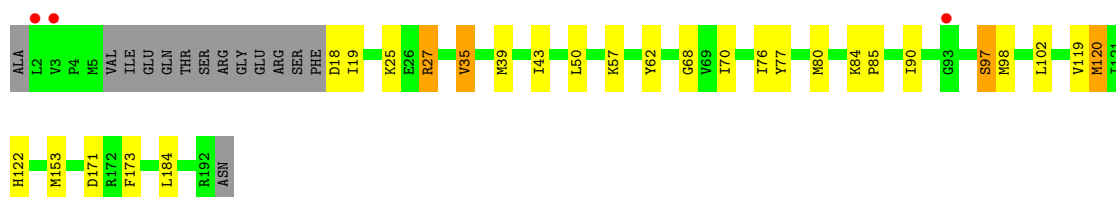
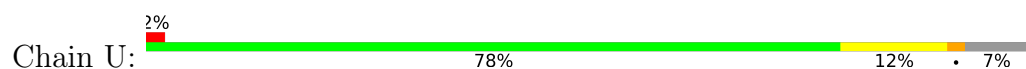
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



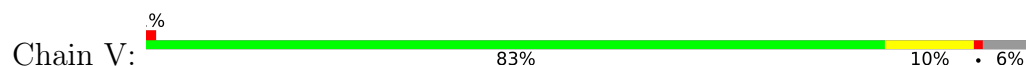
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



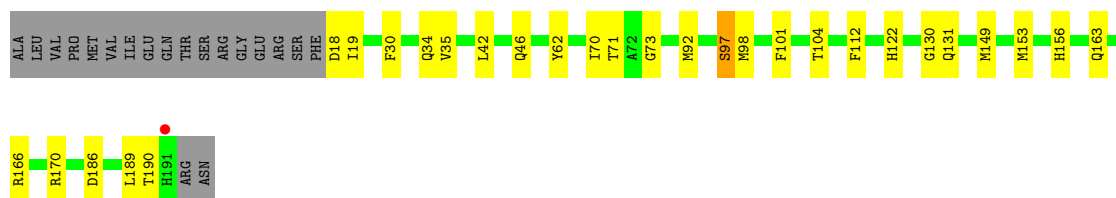
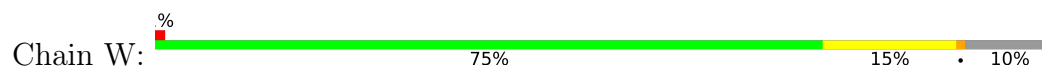
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



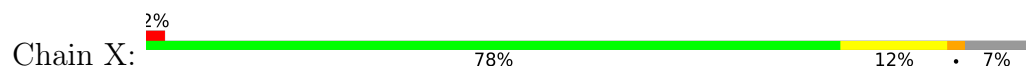
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



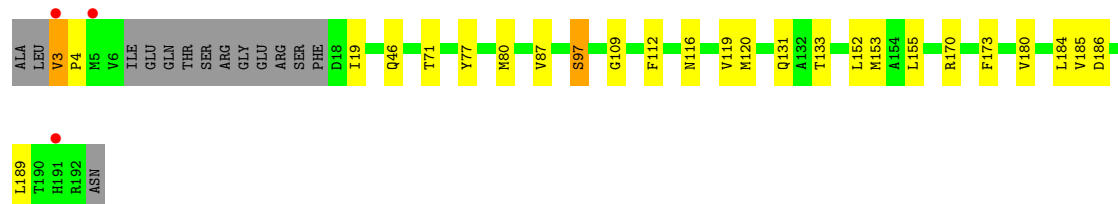
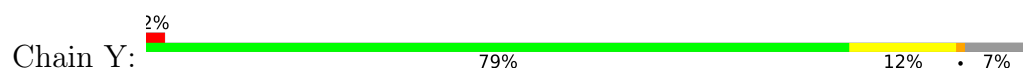
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



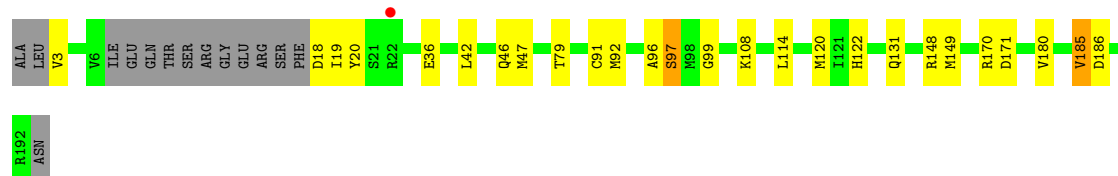
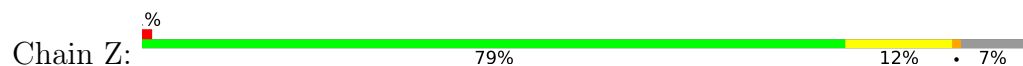
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



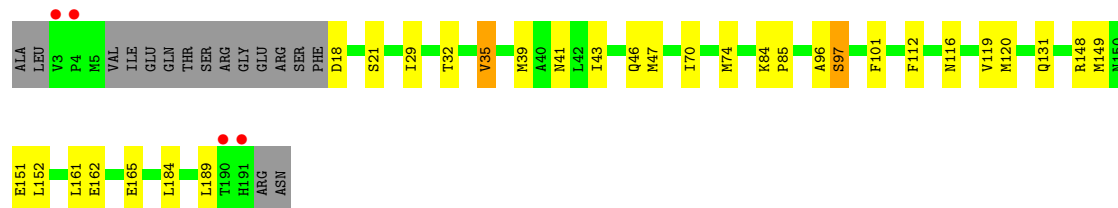
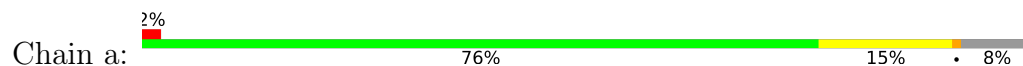
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



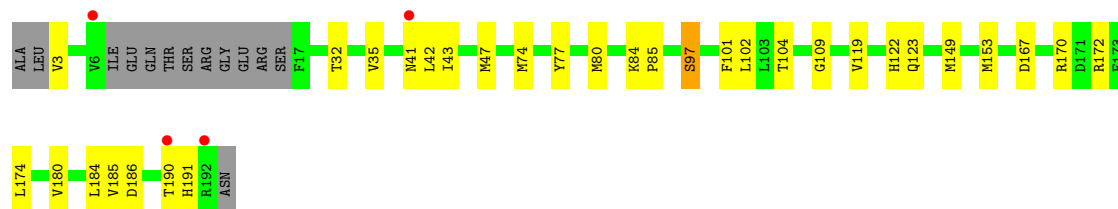
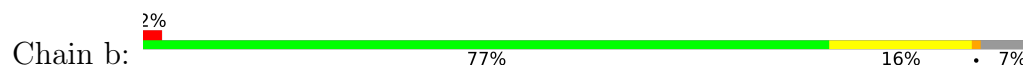
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.33Å 190.23Å 169.88Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	45.41 – 2.95 45.41 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.41-2.95) 99.8 (45.41-2.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.211 , 0.248 0.212 , 0.247	Depositor DCC
R_{free} test set	6043 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	80695	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, MPD, ZGV

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	0.28	0/1446	0.40	1/1949 (0.1%)
1	B	0.24	0/1431	0.37	1/1929 (0.1%)
1	C	0.20	0/1419	0.35	1/1913 (0.1%)
1	D	0.26	0/1438	0.44	1/1938 (0.1%)
1	E	0.35	2/1446 (0.1%)	0.45	2/1949 (0.1%)
1	F	0.67	1/1427 (0.1%)	0.58	2/1924 (0.1%)
1	G	0.22	0/1410	0.39	0/1901
1	H	0.30	0/1409	0.43	0/1899
1	I	0.21	0/1434	0.34	0/1933
1	J	0.38	1/1434 (0.1%)	0.43	1/1934 (0.1%)
1	K	0.30	0/1411	0.36	0/1901
1	L	0.20	0/1418	0.36	1/1911 (0.1%)
1	M	0.22	0/1423	0.38	1/1917 (0.1%)
1	N	0.27	0/1430	0.40	1/1927 (0.1%)
1	O	0.21	0/1411	0.38	1/1904 (0.1%)
1	P	0.17	0/1438	0.40	1/1938 (0.1%)
1	Q	0.34	0/1447	0.39	1/1950 (0.1%)
1	R	0.18	0/1436	0.36	1/1935 (0.1%)
1	S	0.69	1/1438 (0.1%)	0.61	0/1938
1	T	0.37	0/1418	0.49	2/1911 (0.1%)
1	U	0.37	0/1419	0.42	1/1912 (0.1%)
1	V	0.34	0/1431	0.40	1/1929 (0.1%)
1	W	0.26	0/1375	0.45	2/1852 (0.1%)
1	X	0.30	0/1412	0.40	1/1904 (0.1%)
1	Y	0.20	0/1418	0.36	1/1911 (0.1%)
1	Z	0.28	0/1418	0.44	2/1911 (0.1%)
1	a	0.33	0/1400	0.39	0/1887
1	b	0.21	0/1430	0.35	1/1927 (0.1%)
All	All	0.32	5/39867 (0.0%)	0.42	27/53734 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	131	GLN	CA-C	-7.76	1.42	1.52
1	F	97	SER	CA-C	6.80	1.61	1.52
1	S	97	SER	CA-C	5.43	1.60	1.52
1	E	130	GLY	C-N	5.41	1.41	1.33
1	J	97	SER	CA-C	5.22	1.59	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	108	LYS	O-C-N	-7.52	113.62	122.87
1	W	186	ASP	N-CA-C	7.29	120.66	111.69
1	P	97	SER	N-CA-CB	-7.27	98.20	110.49
1	F	98	MET	CA-C-N	6.74	128.56	120.14
1	F	98	MET	C-N-CA	6.74	128.56	120.14
1	W	97	SER	N-CA-CB	-6.71	99.15	110.49
1	O	97	SER	N-CA-CB	-6.38	99.72	110.49
1	B	97	SER	N-CA-CB	-6.33	99.80	110.49
1	Z	186	ASP	N-CA-C	6.24	117.88	111.14
1	L	97	SER	N-CA-CB	-6.11	100.17	110.49
1	V	97	SER	N-CA-CB	-6.10	100.18	110.49
1	Y	97	SER	N-CA-CB	-6.09	100.20	110.49
1	U	97	SER	N-CA-CB	-5.97	100.40	110.49
1	E	131	GLN	CA-C-O	-5.85	114.38	121.05
1	N	97	SER	N-CA-CB	-5.84	100.61	110.49
1	A	97	SER	N-CA-CB	-5.80	100.69	110.49
1	T	21	SER	N-CA-CB	5.60	119.17	110.44
1	X	97	SER	N-CA-CB	-5.57	101.07	110.49
1	M	97	SER	N-CA-CB	-5.55	101.10	110.49
1	D	97	SER	N-CA-CB	-5.54	101.12	110.49
1	C	97	SER	N-CA-CB	-5.41	101.35	110.49
1	E	97	SER	N-CA-CB	-5.40	101.37	110.49
1	J	97	SER	N-CA-CB	-5.24	101.63	110.49
1	T	97	SER	N-CA-CB	-5.20	101.71	110.49
1	Q	97	SER	N-CA-CB	-5.11	101.86	110.49
1	b	97	SER	N-CA-CB	-5.04	101.97	110.49
1	R	97	SER	N-CA-CB	-5.04	101.97	110.49

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	1423	1434	1434	18	0
1	B	1409	1421	1421	18	0
1	C	1396	1404	1404	18	0
1	D	1415	1428	1428	27	0
1	E	1423	1435	1434	21	0
1	F	1404	1404	1403	22	0
1	G	1388	1391	1390	20	0
1	H	1386	1390	1390	20	0
1	I	1412	1426	1425	21	0
1	J	1411	1413	1412	14	0
1	K	1389	1401	1399	25	0
1	L	1396	1410	1408	28	0
1	M	1400	1408	1408	16	0
1	N	1407	1418	1417	22	0
1	O	1389	1397	1395	30	0
1	P	1415	1431	1428	32	0
1	Q	1424	1435	1434	24	0
1	R	1413	1423	1422	16	0
1	S	1415	1425	1423	22	0
1	T	1396	1410	1408	33	0
1	U	1397	1412	1410	20	0
1	V	1409	1416	1416	15	0
1	W	1355	1363	1359	26	0
1	X	1390	1398	1397	24	0
1	Y	1396	1410	1408	17	0
1	Z	1396	1410	1408	19	0
1	a	1378	1388	1386	27	0
1	b	1407	1418	1417	24	0
2	A	16	28	28	0	0
2	B	16	27	28	1	0
2	C	8	14	14	2	0
2	D	24	42	42	4	0
2	E	8	14	14	1	0
2	F	24	42	42	2	0
2	G	8	14	14	1	0
2	H	16	28	28	3	0
2	I	16	28	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	16	28	28	2	0
2	K	16	28	28	2	0
2	L	8	14	14	1	0
2	M	8	14	14	0	0
2	N	16	28	28	3	0
2	O	16	28	28	3	0
2	P	16	28	28	2	0
2	Q	24	42	42	1	0
2	R	8	14	14	1	0
2	S	16	28	28	0	0
2	T	16	28	28	5	0
2	U	8	14	14	4	0
2	V	8	14	14	1	0
2	W	16	28	28	4	0
2	X	8	14	14	2	0
2	Y	16	28	28	2	0
2	Z	16	28	28	1	0
2	a	16	28	28	4	0
2	b	16	28	28	1	0
3	A	4	3	3	0	0
3	B	4	3	3	0	0
3	C	4	3	3	0	0
3	F	4	3	3	0	0
3	G	4	3	3	0	0
3	L	4	3	3	0	0
3	P	4	3	3	0	0
3	R	4	3	3	0	0
3	X	4	3	3	0	0
3	Z	4	3	3	0	0
4	A	24	21	0	0	0
4	B	14	7	0	0	0
4	C	14	7	0	0	0
4	D	14	7	0	0	0
4	E	14	7	0	0	0
4	F	16	8	0	0	0
4	G	14	7	0	0	0
4	H	16	8	0	0	0
4	I	15	8	0	0	0
4	J	16	8	0	0	0
4	K	14	7	0	0	0
4	L	19	13	0	0	0
4	M	18	12	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	14	7	0	0	0
4	O	24	21	0	0	0
4	P	14	7	0	0	0
4	Q	14	7	0	0	0
4	R	14	7	0	1	0
4	S	14	7	0	1	0
4	T	16	8	0	0	0
4	U	14	7	0	1	0
4	V	7	4	0	0	0
4	W	24	21	0	0	0
4	X	11	6	0	0	0
4	Y	18	12	0	0	0
4	Z	7	4	0	0	0
4	a	7	4	0	0	0
4	b	11	6	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	9	0	0	0	0
5	D	4	0	0	0	0
5	E	3	0	0	0	0
5	F	3	0	0	1	0
5	G	4	0	0	0	0
5	H	5	0	0	0	0
5	I	3	0	0	0	0
5	J	5	0	0	0	0
5	K	3	0	0	0	0
5	L	4	0	0	0	0
5	M	4	0	0	0	0
5	N	3	0	0	0	0
5	O	3	0	0	0	0
5	P	2	0	0	0	0
5	Q	4	0	0	0	0
5	R	4	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
5	U	4	0	0	0	0
5	V	4	0	0	0	0
5	W	3	0	0	0	0
5	X	4	0	0	0	0
5	Y	4	0	0	0	0
5	Z	4	0	0	0	0
5	a	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	b	5	0	0	0	0
All	All	40199	40496	40214	575	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (575) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:76:ILE:HG22	1:L:80:MET:HE3	1.45	0.99
1:K:5:MET:HA	1:K:18:ASP:HA	1.49	0.93
1:a:74:MET:HE3	1:a:149:MET:HE1	1.52	0.91
1:F:43:ILE:HG22	1:F:47:MET:HE2	1.53	0.90
1:P:125:LEU:HD13	1:W:130:GLY:C	1.97	0.89
1:Z:120:MET:HE3	1:Z:171:ASP:HB3	1.57	0.87
1:R:74:MET:SD	1:R:149:MET:HE1	2.15	0.86
1:K:74:MET:SD	1:K:149:MET:HE1	2.16	0.86
1:T:29:ILE:CG2	1:T:43:ILE:HD12	2.07	0.85
1:P:76:ILE:HG22	1:P:80:MET:HE3	1.62	0.81
1:L:76:ILE:CG2	1:L:80:MET:HE3	2.11	0.81
1:D:74:MET:HE3	1:D:98:MET:HE1	1.62	0.81
2:a:301:MPD:H53	2:a:301:MPD:HM2	1.63	0.80
1:T:104:THR:HG21	1:T:184:LEU:CD1	2.11	0.80
1:R:49:PHE:HB2	1:S:19:ILE:HD11	1.62	0.79
1:M:104:THR:OG1	1:M:184:LEU:HD23	1.82	0.79
1:O:104:THR:HG23	1:O:111:ARG:NH1	1.97	0.78
1:L:155:LEU:C	1:L:155:LEU:HD23	2.09	0.78
2:b:301:MPD:O2	2:b:301:MPD:O4	2.00	0.78
1:T:104:THR:HG21	1:T:184:LEU:HD13	1.67	0.76
1:K:5:MET:HG2	1:K:18:ASP:HA	1.68	0.76
1:H:101:PHE:CD1	1:H:153:MET:HE3	2.23	0.73
2:D:301:MPD:H11	2:D:301:MPD:H52	1.71	0.73
1:H:153:MET:HA	1:H:153:MET:HE2	1.71	0.72
1:R:18:ASP:OD1	1:R:19:ILE:N	2.22	0.72
1:E:130:GLY:C	1:L:125:LEU:HD13	2.13	0.72
1:P:101:PHE:CD1	1:P:153:MET:HE3	2.24	0.72
1:V:153:MET:HE2	1:V:153:MET:HA	1.72	0.72
2:N:301:MPD:O4	2:N:301:MPD:O2	2.06	0.71
1:Y:170:ARG:NH2	1:Z:131:GLN:OE1	2.23	0.71
1:L:173:PHE:C	1:L:174:LEU:HD12	2.15	0.71
1:H:180:VAL:HG12	1:H:185:VAL:HG23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:VAL:HG11	1:E:18:ASP:OD1	1.91	0.71
1:P:41:ASN:ND2	1:Q:92:MET:HE3	2.06	0.71
1:P:153:MET:HE2	1:P:153:MET:HA	1.71	0.71
1:G:18:ASP:OD1	1:G:19:ILE:N	2.24	0.70
2:W:402:MPD:O4	2:W:402:MPD:O2	1.98	0.70
1:V:131:GLN:OE1	1:b:170:ARG:NH2	2.24	0.70
1:W:73:GLY:HA3	1:W:98:MET:HE2	1.74	0.70
1:K:27:ARG:NH2	1:K:50:LEU:O	2.25	0.70
1:A:4:PRO:HD3	1:G:42:LEU:HD21	1.73	0.69
1:I:43:ILE:HG22	1:I:47:MET:HE3	1.75	0.69
1:W:18:ASP:OD1	1:W:19:ILE:N	2.26	0.68
1:Y:116:ASN:OD1	1:Z:148:ARG:NH1	2.26	0.68
1:H:43:ILE:HG22	1:H:47:MET:HE3	1.76	0.68
1:C:104:THR:OG1	1:C:184:LEU:HD22	1.93	0.67
1:I:104:THR:HG21	1:I:184:LEU:HD23	1.75	0.67
1:V:101:PHE:CD2	1:V:153:MET:HE3	2.29	0.67
1:D:27:ARG:NH2	1:D:50:LEU:O	2.27	0.67
1:Q:159:GLN:HG3	1:Q:182:TYR:CE1	2.28	0.67
1:W:112:PHE:HB3	1:W:189:LEU:CD1	2.24	0.67
1:F:18:ASP:OD1	1:F:19:ILE:N	2.27	0.67
1:N:62:TYR:CE1	1:N:90:ILE:HD12	2.30	0.67
1:S:149:MET:HE2	1:S:149:MET:HA	1.77	0.67
1:J:121:ILE:HG22	2:J:301:MPD:H51	1.77	0.67
1:T:43:ILE:HD13	1:T:46:GLN:OE1	1.95	0.67
1:O:18:ASP:OD1	1:O:19:ILE:N	2.28	0.67
1:B:42:LEU:HD12	1:C:20:TYR:OH	1.95	0.67
1:D:74:MET:HE1	1:D:101:PHE:CE1	2.29	0.66
1:N:119:VAL:HG11	1:N:184:LEU:HD22	1.76	0.66
1:U:18:ASP:OD1	1:U:19:ILE:N	2.29	0.66
1:K:18:ASP:OD1	1:K:19:ILE:N	2.28	0.66
1:Q:37:ASP:O	1:Q:41:ASN:ND2	2.28	0.66
1:N:119:VAL:HG11	1:N:184:LEU:CD2	2.26	0.66
1:a:74:MET:CE	1:a:149:MET:HE1	2.24	0.66
1:O:177:PRO:O	1:O:180:VAL:HG22	1.96	0.65
1:P:131:GLN:OE1	1:Q:170:ARG:NH2	2.29	0.65
1:L:3:VAL:O	1:L:3:VAL:HG13	1.96	0.65
1:I:27:ARG:NH2	1:I:54:ASN:O	2.30	0.65
1:b:101:PHE:CD2	1:b:153:MET:HE3	2.31	0.65
1:A:18:ASP:OD1	1:A:19:ILE:N	2.30	0.64
1:I:70:ILE:CG2	1:I:149:MET:HE3	2.27	0.64
2:O:301:MPD:H53	2:O:301:MPD:H13	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ASP:OD2	1:E:2:LEU:HD21	1.97	0.64
1:B:119:VAL:HG11	1:B:184:LEU:HD13	1.79	0.64
1:L:18:ASP:OD1	1:L:19:ILE:N	2.31	0.64
1:Y:155:LEU:HD23	1:Y:155:LEU:C	2.22	0.64
1:S:45:ALA:HB1	1:T:23:LEU:CD1	2.27	0.64
1:O:111:ARG:O	1:O:185:VAL:HG13	1.98	0.64
1:a:74:MET:HE3	1:a:149:MET:CE	2.27	0.64
1:H:136:GLU:OE2	1:H:140:ARG:NH1	2.31	0.63
1:V:18:ASP:OD1	1:V:19:ILE:N	2.30	0.63
1:D:18:ASP:OD1	1:D:19:ILE:N	2.32	0.63
1:P:125:LEU:CD1	1:W:130:GLY:C	2.71	0.63
1:G:177:PRO:O	1:G:180:VAL:HG22	1.98	0.63
1:J:170:ARG:NH2	1:K:131:GLN:OE1	2.32	0.63
1:W:34:GLN:N	1:W:34:GLN:OE1	2.31	0.63
1:C:27:ARG:NH2	1:C:50:LEU:O	2.32	0.63
1:A:4:PRO:HD2	1:G:42:LEU:HD11	1.80	0.62
1:R:49:PHE:CB	1:S:19:ILE:HD11	2.29	0.62
1:F:191:HIS:ND1	5:F:501:HOH:O	2.31	0.62
1:C:27:ARG:NH2	1:C:54:ASN:O	2.32	0.62
1:N:18:ASP:OD1	1:N:19:ILE:N	2.33	0.62
1:V:101:PHE:CE2	1:V:153:MET:HE3	2.34	0.62
1:b:174:LEU:HD22	1:b:184:LEU:HD12	1.82	0.62
1:P:104:THR:CG2	1:P:153:MET:HE1	2.30	0.62
1:S:21:SER:HA	1:S:24:LEU:HB2	1.82	0.62
1:C:153:MET:HE1	1:C:184:LEU:HD21	1.82	0.61
1:F:145:VAL:O	1:F:149:MET:HG2	2.00	0.61
1:J:19:ILE:HD11	1:K:49:PHE:CG	2.35	0.61
1:R:167:ASP:OD1	1:R:172:ARG:NH1	2.33	0.61
2:C:301:MPD:H12	2:C:301:MPD:O4	2.00	0.61
1:O:111:ARG:C	1:O:185:VAL:HG13	2.24	0.61
2:P:201:MPD:O4	2:P:201:MPD:O2	2.01	0.61
1:Q:155:LEU:C	1:Q:155:LEU:HD23	2.25	0.61
1:G:182:TYR:HD2	1:G:184:LEU:HD11	1.65	0.61
1:E:109:GLY:N	1:E:186:ASP:OD2	2.32	0.60
1:K:114:LEU:HD23	1:L:78:ASP:HB3	1.83	0.60
1:E:3:VAL:CG1	1:E:18:ASP:OD1	2.49	0.60
1:T:104:THR:HG21	1:T:184:LEU:HD12	1.82	0.60
1:O:74:MET:HE2	2:O:302:MPD:H51	1.83	0.60
2:Y:303:MPD:O4	2:Y:303:MPD:O2	2.16	0.60
1:L:47:MET:HE1	1:L:80:MET:HE2	1.83	0.60
1:U:120:MET:HE2	1:U:171:ASP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ARG:NH1	1:F:58:ASP:O	2.35	0.60
1:U:70:ILE:HG12	1:U:98:MET:HE3	1.83	0.60
1:I:190:THR:HG23	1:I:191:HIS:H	1.67	0.60
1:R:27:ARG:NH1	1:R:58:ASP:O	2.35	0.60
1:a:74:MET:HE1	1:a:101:PHE:CE1	2.36	0.60
2:K:301:MPD:H52	2:K:301:MPD:H12	1.83	0.60
1:O:101:PHE:CD2	1:O:153:MET:HE3	2.37	0.60
1:S:174:LEU:HD22	1:S:184:LEU:HD12	1.82	0.60
1:K:43:ILE:HG22	1:K:47:MET:HE3	1.83	0.60
2:U:301:MPD:H52	2:U:301:MPD:H11	1.84	0.60
1:a:70:ILE:HG23	1:a:149:MET:HE3	1.83	0.60
1:D:177:PRO:O	1:D:180:VAL:HG22	2.02	0.59
1:E:130:GLY:C	1:L:125:LEU:CD1	2.75	0.59
1:I:70:ILE:HG23	1:I:149:MET:HE3	1.85	0.59
1:L:174:LEU:HD22	1:L:184:LEU:CD1	2.32	0.59
1:I:43:ILE:CG2	1:I:47:MET:HE3	2.32	0.59
1:b:167:ASP:OD1	1:b:172:ARG:NH1	2.36	0.59
1:D:27:ARG:NH1	1:D:57:LYS:O	2.35	0.59
1:U:98:MET:HE2	2:U:301:MPD:O2	2.02	0.59
1:b:43:ILE:HG22	1:b:47:MET:HE3	1.84	0.59
1:b:104:THR:CG2	1:b:153:MET:HE1	2.32	0.59
1:Z:92:MET:HE3	1:a:41:ASN:OD1	2.02	0.59
1:O:104:THR:HG22	1:O:156:HIS:HB3	1.84	0.59
1:P:190:THR:O	1:P:191:HIS:ND1	2.35	0.59
1:S:45:ALA:HB1	1:T:23:LEU:HD11	1.84	0.59
1:B:3:VAL:N	1:B:4:PRO:CD	2.66	0.59
1:B:109:GLY:N	1:B:186:ASP:OD2	2.36	0.58
2:B:301:MPD:O4	2:B:301:MPD:H12	2.03	0.58
2:E:301:MPD:H12	2:E:301:MPD:O4	2.03	0.58
1:a:43:ILE:HG22	1:a:47:MET:HE3	1.85	0.58
1:F:44:VAL:HA	1:F:47:MET:HE3	1.85	0.58
1:a:29:ILE:HG23	1:a:46:GLN:OE1	2.04	0.58
1:X:170:ARG:NH2	1:Y:131:GLN:OE1	2.36	0.58
2:Q:301:MPD:H12	2:Q:301:MPD:O4	2.03	0.58
2:V:301:MPD:O2	2:V:301:MPD:O4	2.21	0.58
1:N:77:TYR:CZ	1:N:152:LEU:HD23	2.38	0.58
1:F:165:GLU:O	1:F:169:GLU:HG2	2.05	0.57
2:K:303:MPD:O4	2:K:303:MPD:O2	2.11	0.57
1:P:119:VAL:HG11	1:P:184:LEU:HD13	1.86	0.57
1:C:70:ILE:HG23	1:C:149:MET:HE3	1.86	0.57
1:P:180:VAL:HG12	1:P:185:VAL:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:3:VAL:O	1:V:3:VAL:HG13	2.03	0.57
1:Q:96:ALA:HB1	1:Q:120:MET:HE2	1.86	0.57
1:W:189:LEU:HD23	1:X:82:PHE:CE1	2.39	0.57
1:W:112:PHE:CG	1:W:189:LEU:HD11	2.39	0.57
1:D:27:ARG:NH2	1:D:54:ASN:O	2.37	0.56
1:K:5:MET:SD	1:K:18:ASP:N	2.78	0.56
1:K:177:PRO:O	1:K:180:VAL:HG22	2.03	0.56
1:X:19:ILE:HD11	1:Y:46:GLN:HA	1.87	0.56
1:B:120:MET:HE3	1:B:171:ASP:HB3	1.86	0.56
1:P:125:LEU:HD13	1:W:131:GLN:N	2.19	0.56
1:X:76:ILE:HG22	1:X:80:MET:HE2	1.88	0.56
1:K:5:MET:CG	1:K:18:ASP:HA	2.34	0.56
2:R:301:MPD:O4	2:R:301:MPD:HM1	2.05	0.56
1:J:112:PHE:CD1	1:J:189:LEU:HD13	2.40	0.56
1:A:119:VAL:HG11	1:A:184:LEU:HD13	1.87	0.56
1:E:119:VAL:HG11	1:E:184:LEU:HD22	1.87	0.56
1:L:18:ASP:HB3	1:L:21:SER:OG	2.06	0.56
1:T:112:PHE:HB3	1:T:189:LEU:HD13	1.88	0.56
1:B:173:PHE:C	1:B:174:LEU:HD22	2.31	0.56
1:A:101:PHE:CD2	1:A:153:MET:SD	3.00	0.55
1:b:42:LEU:O	1:b:42:LEU:HD23	2.06	0.55
1:O:104:THR:OG1	1:O:184:LEU:O	2.24	0.55
1:D:180:VAL:HG12	1:D:185:VAL:HG23	1.88	0.55
1:E:104:THR:HG22	1:E:184:LEU:HB3	1.89	0.55
2:I:303:MPD:H52	1:J:145:VAL:HG22	1.89	0.55
1:T:104:THR:CG2	1:T:184:LEU:HD12	2.36	0.55
1:G:100:ALA:O	1:G:104:THR:HG23	2.06	0.55
1:L:174:LEU:HD22	1:L:184:LEU:HD12	1.89	0.55
1:P:125:LEU:HD13	1:W:130:GLY:O	2.06	0.55
2:N:301:MPD:HO2	2:N:301:MPD:HO4	1.54	0.54
1:U:62:TYR:CE2	1:U:90:ILE:HG21	2.42	0.54
1:K:70:ILE:CG2	1:K:149:MET:HE3	2.37	0.54
1:G:37:ASP:O	1:G:41:ASN:OD1	2.24	0.54
1:Q:184:LEU:HD12	1:Q:184:LEU:N	2.22	0.54
1:E:145:VAL:O	1:E:149:MET:HG2	2.07	0.54
1:b:149:MET:HE2	1:b:149:MET:HA	1.89	0.54
1:F:51:GLU:OE2	1:G:192:ARG:NH1	2.41	0.54
1:D:149:MET:HE2	2:D:301:MPD:CM	2.38	0.54
1:R:27:ARG:NH1	1:R:57:LYS:O	2.41	0.54
1:H:43:ILE:CG2	1:H:47:MET:HE3	2.37	0.53
1:K:5:MET:HA	1:K:18:ASP:CA	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:62:TYR:CZ	1:N:90:ILE:HD12	2.43	0.53
1:M:32:THR:HG21	1:N:41:ASN:CG	2.34	0.53
1:W:163:GLN:OE1	1:W:166:ARG:NH2	2.41	0.53
1:D:162:GLU:OE1	1:D:162:GLU:N	2.40	0.53
1:W:112:PHE:CB	1:W:189:LEU:CD1	2.87	0.53
1:O:153:MET:HE2	1:O:153:MET:HA	1.90	0.53
1:K:70:ILE:HG23	1:K:149:MET:HE3	1.90	0.53
1:K:112:PHE:HB3	1:K:189:LEU:HD13	1.91	0.53
1:X:161:LEU:HD13	1:X:161:LEU:C	2.33	0.53
1:Y:112:PHE:HB3	1:Y:189:LEU:HD13	1.89	0.53
1:D:104:THR:HG22	1:D:156:HIS:HB3	1.91	0.53
1:O:104:THR:HG23	1:O:111:ARG:HH11	1.70	0.52
1:U:76:ILE:HG22	1:U:80:MET:HE2	1.90	0.52
1:D:149:MET:HE2	2:D:301:MPD:HM2	1.91	0.52
1:L:61:LEU:HD22	1:L:80:MET:HE2	1.91	0.52
1:D:101:PHE:CD2	1:D:149:MET:HE3	2.44	0.52
1:K:74:MET:CG	1:K:149:MET:HE1	2.39	0.52
1:Q:6:VAL:HG13	1:Q:6:VAL:O	2.09	0.52
1:O:101:PHE:CE2	1:O:153:MET:HE3	2.45	0.52
1:O:141:GLU:O	1:O:145:VAL:HG13	2.10	0.52
1:A:73:GLY:HA3	1:A:98:MET:HE2	1.92	0.52
1:X:149:MET:HE2	1:X:149:MET:HA	1.92	0.52
1:A:32:THR:HG1	1:G:41:ASN:CG	2.18	0.52
1:S:104:THR:HG21	1:S:184:LEU:CD2	2.39	0.52
1:Y:120:MET:HE2	1:Y:173:PHE:CZ	2.44	0.52
1:b:41:ASN:HD22	1:b:41:ASN:C	2.17	0.52
1:O:22:ARG:NH1	1:O:26:GLU:OE2	2.43	0.51
1:O:74:MET:CE	1:P:116:ASN:HB3	2.41	0.51
1:T:74:MET:HE1	1:T:101:PHE:CE1	2.45	0.51
1:W:112:PHE:HB3	1:W:189:LEU:HD13	1.91	0.51
1:R:74:MET:CE	1:R:149:MET:HE1	2.40	0.51
1:T:116:ASN:O	2:T:201:MPD:HM3	2.11	0.51
1:G:104:THR:HG22	1:G:184:LEU:HB3	1.93	0.51
1:M:74:MET:SD	1:M:149:MET:HE1	2.50	0.51
2:U:301:MPD:H52	2:U:301:MPD:C1	2.41	0.51
1:W:101:PHE:CD2	1:W:153:MET:HE3	2.45	0.51
1:I:119:VAL:HG11	1:I:184:LEU:HD13	1.93	0.51
1:Q:182:TYR:HD1	1:Q:182:TYR:O	1.93	0.51
1:N:180:VAL:HG12	1:N:185:VAL:HG12	1.93	0.51
1:P:101:PHE:HD1	1:P:153:MET:HE3	1.73	0.51
1:A:95:ALA:O	1:A:100:ALA:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:LEU:HD23	1:L:155:LEU:O	2.09	0.51
1:V:173:PHE:C	1:V:174:LEU:HD12	2.35	0.51
1:H:177:PRO:O	1:H:180:VAL:HG22	2.10	0.51
1:R:101:PHE:CE2	1:R:149:MET:SD	3.04	0.51
1:W:92:MET:HE3	1:X:41:ASN:ND2	2.26	0.51
1:E:148:ARG:NH1	1:F:116:ASN:OD1	2.42	0.50
1:H:18:ASP:OD1	1:H:19:ILE:N	2.43	0.50
2:H:301:MPD:C5	2:H:301:MPD:H12	2.41	0.50
1:K:153:MET:HE1	1:K:184:LEU:HD21	1.92	0.50
1:Y:19:ILE:HD11	1:Z:46:GLN:HA	1.93	0.50
1:W:122:HIS:O	2:W:402:MPD:H12	2.12	0.50
1:L:47:MET:HE1	1:L:80:MET:CE	2.40	0.50
1:Q:173:PHE:C	1:Q:174:LEU:HD12	2.36	0.50
1:E:100:ALA:O	1:E:104:THR:HG23	2.11	0.50
1:B:6:VAL:HG22	1:B:17:PHE:O	2.12	0.50
1:F:98:MET:O	1:F:101:PHE:HB3	2.11	0.50
1:S:45:ALA:HB1	1:T:23:LEU:HD12	1.93	0.49
1:U:62:TYR:CD2	1:U:90:ILE:HG21	2.47	0.49
1:W:19:ILE:HD11	1:X:46:GLN:HA	1.94	0.49
1:A:92:MET:HB3	1:A:114:LEU:HD12	1.94	0.49
1:B:131:GLN:OE1	1:C:170:ARG:NH2	2.40	0.49
1:L:77:TYR:CZ	1:L:152:LEU:HD23	2.47	0.49
1:V:27:ARG:NH2	1:V:50:LEU:O	2.45	0.49
1:a:74:MET:SD	1:a:149:MET:HE1	2.52	0.49
1:C:80:MET:HE1	1:C:105:ALA:HB3	1.94	0.49
1:L:61:LEU:CD2	1:L:80:MET:HE2	2.43	0.49
1:L:174:LEU:CD2	1:L:184:LEU:HD12	2.42	0.49
1:P:7:ILE:HD12	1:P:7:ILE:H	1.76	0.49
1:T:98:MET:HE1	2:T:202:MPD:HM2	1.95	0.49
1:Z:91:CYS:O	1:Z:114:LEU:HD23	2.12	0.49
1:a:116:ASN:O	2:a:303:MPD:H13	2.13	0.49
1:B:18:ASP:OD1	1:B:21:SER:OG	2.27	0.49
1:F:17:PHE:CZ	1:G:5:MET:HE3	2.47	0.49
1:F:27:ARG:NH1	1:F:57:LYS:O	2.45	0.49
1:Q:161:LEU:HD13	1:Q:161:LEU:O	2.12	0.49
1:S:191:HIS:O	1:S:192:ARG:HB2	2.12	0.49
1:K:114:LEU:HD23	1:L:78:ASP:CB	2.43	0.49
1:X:77:TYR:HA	1:X:80:MET:HE3	1.95	0.49
1:b:43:ILE:CG2	1:b:47:MET:HE3	2.42	0.49
1:L:120:MET:HE3	1:L:122:HIS:HD2	1.78	0.49
1:W:189:LEU:HD23	1:X:82:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MET:HE3	1:A:98:MET:HE1	1.93	0.49
1:O:2:LEU:HD13	1:O:3:VAL:N	2.28	0.49
1:W:112:PHE:CG	1:W:189:LEU:CD1	2.96	0.49
1:F:17:PHE:HZ	1:G:5:MET:HE3	1.77	0.48
1:J:120:MET:HE2	1:J:173:PHE:CZ	2.49	0.48
1:Q:112:PHE:HB3	1:Q:189:LEU:HD13	1.94	0.48
1:Z:47:MET:HE3	1:Z:79:THR:HG22	1.95	0.48
1:H:122:HIS:O	2:H:301:MPD:H11	2.14	0.48
1:N:29:ILE:HG23	1:N:46:GLN:OE1	2.13	0.48
1:M:92:MET:HB3	1:M:114:LEU:HD12	1.95	0.48
1:O:185:VAL:HG12	1:O:186:ASP:N	2.28	0.48
1:X:180:VAL:HG22	1:X:185:VAL:HG12	1.94	0.48
1:P:122:HIS:O	2:P:201:MPD:H12	2.14	0.48
1:X:91:CYS:O	1:X:114:LEU:HD23	2.13	0.48
1:a:162:GLU:OE1	1:a:162:GLU:N	2.44	0.48
1:H:101:PHE:CE1	1:H:153:MET:HE3	2.48	0.48
1:S:174:LEU:HD22	1:S:184:LEU:CD1	2.44	0.48
1:Z:3:VAL:HG22	1:Z:3:VAL:O	2.13	0.48
1:T:3:VAL:HB	1:T:4:PRO:HD3	1.96	0.48
1:b:119:VAL:HG11	1:b:184:LEU:HD13	1.94	0.48
1:A:177:PRO:O	1:A:180:VAL:HG22	2.14	0.48
1:D:3:VAL:HG22	1:D:3:VAL:O	2.12	0.48
1:D:136:GLU:OE2	1:D:140:ARG:NE	2.47	0.48
1:S:21:SER:O	1:S:24:LEU:N	2.47	0.48
1:T:104:THR:HA	1:T:111:ARG:HD2	1.95	0.48
1:I:2:LEU:HD23	1:I:3:VAL:N	2.29	0.48
1:Q:100:ALA:O	1:Q:104:THR:HG23	2.14	0.48
1:b:101:PHE:CG	1:b:153:MET:HE3	2.49	0.48
1:D:101:PHE:CD2	1:D:149:MET:CE	2.97	0.47
1:O:185:VAL:CG1	1:O:186:ASP:N	2.77	0.47
1:Q:73:GLY:HA3	1:Q:98:MET:HE2	1.96	0.47
1:D:122:HIS:O	2:D:301:MPD:H31	2.14	0.47
1:P:18:ASP:OD1	1:P:19:ILE:N	2.47	0.47
1:Z:42:LEU:HD23	1:Z:46:GLN:HE21	1.79	0.47
1:L:170:ARG:NH2	1:M:131:GLN:OE1	2.43	0.47
1:O:70:ILE:HA	1:O:98:MET:HE2	1.96	0.47
1:S:104:THR:HG21	1:S:184:LEU:HD23	1.95	0.47
1:C:157:THR:HG22	1:C:184:LEU:HD23	1.96	0.47
1:T:104:THR:CG2	1:T:184:LEU:CD1	2.88	0.47
1:a:70:ILE:CG2	1:a:149:MET:HE3	2.45	0.47
1:N:62:TYR:CE2	1:N:90:ILE:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:3:VAL:HG13	1:O:3:VAL:O	2.13	0.47
2:O:301:MPD:O4	2:O:301:MPD:O2	2.31	0.47
1:V:27:ARG:NH1	1:V:57:LYS:O	2.46	0.47
1:G:27:ARG:NH2	1:G:50:LEU:O	2.48	0.47
1:N:62:TYR:CZ	1:N:90:ILE:CD1	2.98	0.47
1:N:124:PRO:HD2	1:N:146:LYS:HG3	1.95	0.47
1:O:104:THR:HA	1:O:111:ARG:HD2	1.97	0.47
1:T:43:ILE:HG22	1:T:47:MET:HE3	1.97	0.47
1:T:182:TYR:CD1	1:T:184:LEU:CD2	2.98	0.47
1:U:27:ARG:NH1	1:U:57:LYS:O	2.48	0.47
1:A:46:GLN:HG2	1:B:19:ILE:HD12	1.96	0.47
1:D:120:MET:HE2	1:D:120:MET:HB3	1.85	0.47
1:b:77:TYR:HA	1:b:80:MET:HE3	1.97	0.47
1:M:18:ASP:OD1	1:M:20:TYR:N	2.48	0.47
1:O:74:MET:HE3	1:P:116:ASN:CB	2.44	0.47
1:S:191:HIS:O	1:S:192:ARG:CB	2.63	0.47
1:b:80:MET:HE2	1:b:102:LEU:HD22	1.97	0.47
1:P:104:THR:HG21	1:P:153:MET:HE1	1.97	0.47
1:Q:120:MET:HE3	1:Q:122:HIS:HD2	1.78	0.47
1:T:177:PRO:O	1:T:180:VAL:HG22	2.14	0.47
1:H:112:PHE:HB3	1:H:189:LEU:HD13	1.97	0.46
1:X:122:HIS:O	2:X:201:MPD:O4	2.32	0.46
1:b:80:MET:CE	1:b:102:LEU:HD22	2.46	0.46
1:A:74:MET:HE2	1:A:74:MET:HA	1.96	0.46
1:C:3:VAL:HG23	1:C:3:VAL:O	2.16	0.46
1:G:121:ILE:HG22	2:G:301:MPD:H51	1.96	0.46
1:K:27:ARG:NH2	1:K:54:ASN:O	2.48	0.46
1:H:180:VAL:CG1	1:H:185:VAL:HG23	2.43	0.46
1:R:35:VAL:HA	1:R:39:MET:SD	2.56	0.46
1:T:151:GLU:O	1:T:155:LEU:HG	2.16	0.46
1:I:42:LEU:C	1:I:42:LEU:HD23	2.41	0.46
1:G:191:HIS:O	1:G:192:ARG:CB	2.64	0.46
1:G:191:HIS:O	1:G:192:ARG:HB2	2.15	0.46
1:I:27:ARG:NH2	1:I:50:LEU:O	2.49	0.46
1:a:18:ASP:OD1	1:a:21:SER:N	2.44	0.46
1:C:70:ILE:CG2	1:C:149:MET:HE3	2.46	0.46
1:C:104:THR:HG23	1:C:184:LEU:HA	1.97	0.46
1:D:101:PHE:CE2	1:D:149:MET:HE3	2.50	0.46
1:J:107:ALA:HB3	1:J:110:LYS:HB2	1.97	0.46
1:M:3:VAL:HG23	1:M:3:VAL:O	2.16	0.46
1:A:29:ILE:HG23	1:A:46:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:MET:SD	1:E:149:MET:HE1	2.56	0.46
1:I:104:THR:HG22	1:I:184:LEU:HA	1.98	0.46
1:a:97:SER:O	2:a:301:MPD:H52	2.16	0.46
1:E:109:GLY:CA	1:E:186:ASP:OD2	2.65	0.45
1:T:80:MET:HE1	1:T:105:ALA:HB3	1.97	0.45
1:N:177:PRO:O	1:N:180:VAL:HG22	2.14	0.45
1:V:4:PRO:HD3	1:W:42:LEU:HD21	1.98	0.45
1:W:101:PHE:CE2	1:W:153:MET:HE3	2.51	0.45
1:a:161:LEU:C	1:a:161:LEU:HD13	2.41	0.45
1:L:148:ARG:NH1	1:L:152:LEU:CD1	2.79	0.45
1:I:177:PRO:O	1:I:180:VAL:HG22	2.16	0.45
1:L:155:LEU:C	1:L:155:LEU:CD2	2.81	0.45
1:Y:119:VAL:HG11	1:Y:184:LEU:HD13	1.98	0.45
1:a:112:PHE:HB3	1:a:189:LEU:HD13	1.98	0.45
1:A:101:PHE:CD1	1:A:101:PHE:C	2.95	0.45
1:B:109:GLY:CA	1:B:186:ASP:OD2	2.65	0.45
1:W:104:THR:HG22	1:W:156:HIS:HB3	1.99	0.45
1:Z:19:ILE:HD11	1:a:46:GLN:HA	1.99	0.45
2:a:301:MPD:H53	2:a:301:MPD:CM	2.41	0.45
1:B:3:VAL:HG12	1:B:3:VAL:O	2.17	0.45
1:P:177:PRO:O	1:P:180:VAL:HG22	2.16	0.45
1:S:104:THR:HG22	1:S:184:LEU:O	2.16	0.45
1:D:62:TYR:CE1	1:D:90:ILE:HG21	2.52	0.45
1:U:122:HIS:O	2:U:301:MPD:H31	2.17	0.45
1:Y:3:VAL:N	1:Y:4:PRO:CD	2.80	0.45
1:C:104:THR:HG23	1:C:184:LEU:O	2.17	0.45
1:F:19:ILE:HG23	1:F:20:TYR:N	2.32	0.45
1:N:17:PHE:O	1:N:18:ASP:HB3	2.16	0.45
1:Q:182:TYR:O	1:Q:182:TYR:CD1	2.70	0.45
1:W:170:ARG:NH2	1:X:131:GLN:OE1	2.50	0.45
1:D:17:PHE:O	1:D:18:ASP:HB3	2.17	0.44
1:U:39:MET:O	1:U:43:ILE:HG13	2.17	0.44
1:G:125:LEU:HD23	1:N:131:GLN:HA	1.99	0.44
1:M:180:VAL:HG12	1:M:185:VAL:HG23	1.98	0.44
1:B:155:LEU:CD2	1:V:162:GLU:HA	2.47	0.44
1:P:82:PHE:CE1	1:Q:189:LEU:HD23	2.52	0.44
1:S:24:LEU:HD22	1:S:50:LEU:HD21	1.99	0.44
1:B:155:LEU:HD21	1:V:162:GLU:HA	1.98	0.44
1:K:5:MET:CA	1:K:18:ASP:HA	2.34	0.44
1:L:174:LEU:HD12	1:L:174:LEU:N	2.32	0.44
1:P:155:LEU:HD23	1:P:155:LEU:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:96:ALA:HB1	1:R:120:MET:HE2	1.99	0.44
1:S:34:GLN:NE2	4:S:203:ZGV:O1	2.50	0.44
1:T:153:MET:CE	2:T:202:MPD:H52	2.47	0.44
1:H:18:ASP:O	1:H:22:ARG:HB2	2.17	0.44
1:K:43:ILE:CG2	1:K:47:MET:HE3	2.46	0.44
1:L:173:PHE:O	1:L:174:LEU:HD12	2.17	0.44
1:Z:170:ARG:NH2	1:a:131:GLN:OE1	2.49	0.44
1:D:74:MET:HE2	1:D:74:MET:HA	1.99	0.44
1:R:49:PHE:CG	1:S:19:ILE:HD11	2.52	0.44
1:I:84:LYS:N	1:I:85:PRO:HD2	2.33	0.44
1:R:84:LYS:N	1:R:85:PRO:HD2	2.33	0.44
1:X:170:ARG:NH1	1:Y:133:THR:HG21	2.32	0.44
1:Z:96:ALA:O	1:Z:99:GLY:N	2.50	0.44
1:a:35:VAL:HA	1:a:39:MET:SD	2.57	0.44
1:N:3:VAL:N	1:N:4:PRO:CD	2.81	0.44
1:R:125:LEU:HD12	4:R:303:ZGV:C13	2.48	0.44
1:W:30:PHE:CD1	1:W:62:TYR:HB2	2.53	0.44
1:M:182:TYR:HD2	1:M:184:LEU:CD1	2.31	0.44
1:O:74:MET:HE3	1:P:116:ASN:HB2	2.00	0.44
1:O:149:MET:HE2	1:O:149:MET:HA	1.99	0.44
1:S:74:MET:SD	1:S:149:MET:HE1	2.57	0.44
1:T:19:ILE:O	1:T:19:ILE:HG12	2.17	0.44
1:X:18:ASP:OD1	1:X:20:TYR:N	2.50	0.44
1:S:112:PHE:HB3	1:S:189:LEU:HD13	2.00	0.43
1:a:96:ALA:HB1	1:a:120:MET:HE2	2.00	0.43
1:C:46:GLN:HA	1:D:19:ILE:HD11	2.00	0.43
1:C:74:MET:SD	1:C:149:MET:HE1	2.58	0.43
1:D:101:PHE:CE2	1:D:149:MET:CE	3.01	0.43
1:G:43:ILE:CG2	1:G:47:MET:HE3	2.47	0.43
1:Q:57:LYS:O	1:Q:85:PRO:HB3	2.18	0.43
1:T:152:LEU:HD23	1:T:155:LEU:HD12	2.01	0.43
1:U:77:TYR:HA	1:U:80:MET:HE3	2.00	0.43
1:X:149:MET:HB3	2:X:201:MPD:HM3	2.00	0.43
1:A:92:MET:CB	1:A:114:LEU:HD12	2.48	0.43
1:Q:6:VAL:O	1:Q:6:VAL:CG1	2.65	0.43
1:T:182:TYR:HD1	1:T:184:LEU:CD2	2.32	0.43
1:Y:109:GLY:N	1:Y:186:ASP:OD2	2.51	0.43
1:G:5:MET:HA	1:G:17:PHE:O	2.18	0.43
1:K:29:ILE:HG23	1:K:46:GLN:OE1	2.18	0.43
1:Q:43:ILE:HG22	1:Q:47:MET:HE2	2.00	0.43
1:Q:161:LEU:HD13	1:Q:161:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:THR:HG23	1:D:190:THR:O	2.18	0.43
1:F:109:GLY:N	1:F:186:ASP:OD2	2.52	0.43
1:I:104:THR:HG21	1:I:184:LEU:CD2	2.48	0.43
1:J:3:VAL:N	1:J:4:PRO:CD	2.82	0.43
1:J:35:VAL:HA	1:J:39:MET:SD	2.59	0.43
1:O:74:MET:CE	1:P:116:ASN:CB	2.96	0.43
1:B:84:LYS:N	1:B:85:PRO:HD2	2.33	0.43
1:F:120:MET:HG3	1:F:173:PHE:CE1	2.54	0.43
1:G:27:ARG:NH2	1:G:54:ASN:O	2.52	0.43
1:Q:148:ARG:NH1	1:R:116:ASN:OD1	2.52	0.43
1:a:84:LYS:N	1:a:85:PRO:HD2	2.33	0.43
1:U:68:GLY:N	4:U:302:ZGV:O3	2.45	0.43
1:U:120:MET:HE3	1:U:173:PHE:CZ	2.54	0.43
1:X:170:ARG:HH11	1:Y:133:THR:HG21	1.83	0.43
1:X:182:TYR:HD1	1:X:184:LEU:CD1	2.31	0.43
1:a:96:ALA:O	1:a:97:SER:C	2.61	0.43
1:H:84:LYS:N	1:H:85:PRO:HD2	2.34	0.43
1:T:29:ILE:HG23	1:T:43:ILE:HD12	1.96	0.43
1:a:101:PHE:CE2	1:a:149:MET:SD	3.12	0.43
1:F:121:ILE:HG22	2:F:402:MPD:H51	2.01	0.43
1:H:119:VAL:HG11	1:H:184:LEU:HD22	2.00	0.43
1:b:180:VAL:HG22	1:b:185:VAL:HG23	2.00	0.43
1:E:84:LYS:N	1:E:85:PRO:HD2	2.34	0.43
1:X:190:THR:O	1:X:191:HIS:C	2.61	0.43
1:J:149:MET:HE2	2:J:301:MPD:HM1	2.00	0.42
1:S:45:ALA:CB	1:T:23:LEU:HD11	2.49	0.42
1:b:190:THR:HG23	1:b:191:HIS:N	2.33	0.42
1:F:43:ILE:HG22	1:F:47:MET:CE	2.38	0.42
1:H:148:ARG:NH2	1:N:116:ASN:OD1	2.53	0.42
1:Z:96:ALA:O	1:Z:97:SER:C	2.62	0.42
1:Q:140:ARG:HG2	1:Q:144:LYS:NZ	2.34	0.42
1:U:35:VAL:HA	1:U:39:MET:SD	2.59	0.42
1:U:84:LYS:N	1:U:85:PRO:HD2	2.34	0.42
2:W:401:MPD:H52	2:W:401:MPD:H11	2.00	0.42
1:X:84:LYS:N	1:X:85:PRO:HD2	2.34	0.42
1:X:161:LEU:HD13	1:X:161:LEU:O	2.19	0.42
1:I:70:ILE:HG21	1:I:149:MET:HE3	1.98	0.42
1:K:180:VAL:HG12	1:K:185:VAL:HG23	2.00	0.42
1:T:92:MET:HB3	1:T:114:LEU:HD12	2.01	0.42
1:a:161:LEU:HD11	1:a:165:GLU:OE2	2.19	0.42
1:H:27:ARG:NH1	1:H:57:LYS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:96:ALA:O	1:R:99:GLY:N	2.52	0.42
1:C:84:LYS:N	1:C:85:PRO:HD2	2.35	0.42
1:E:120:MET:HE3	1:E:171:ASP:HB3	2.01	0.42
1:J:19:ILE:HD11	1:K:49:PHE:CB	2.50	0.42
1:S:190:THR:HG22	1:S:191:HIS:CD2	2.55	0.42
1:X:182:TYR:CD1	1:X:184:LEU:CD1	3.03	0.42
1:H:91:CYS:O	1:H:114:LEU:HD23	2.20	0.42
2:H:301:MPD:H12	2:H:301:MPD:H52	2.01	0.42
1:I:121:ILE:HG22	2:I:301:MPD:H51	2.02	0.42
1:I:192:ARG:NH1	1:J:51:GLU:OE1	2.52	0.42
1:P:172:ARG:CZ	1:P:174:LEU:HD21	2.50	0.42
1:T:29:ILE:HG22	1:T:43:ILE:HD12	1.99	0.42
1:T:153:MET:HE2	2:T:202:MPD:H52	2.02	0.42
1:U:80:MET:CE	1:U:102:LEU:HD22	2.50	0.42
1:O:31:LEU:C	1:O:31:LEU:HD23	2.45	0.42
1:E:43:ILE:CG2	1:E:47:MET:HE3	2.50	0.42
1:H:42:LEU:HD21	1:N:4:PRO:HD3	2.01	0.42
1:N:77:TYR:OH	1:N:152:LEU:HD23	2.20	0.42
1:Z:120:MET:HE3	1:Z:171:ASP:CB	2.39	0.41
1:A:145:VAL:O	1:A:149:MET:HG2	2.20	0.41
1:H:192:ARG:NE	1:I:51:GLU:OE2	2.52	0.41
1:M:109:GLY:N	1:M:186:ASP:OD2	2.52	0.41
1:M:170:ARG:NH1	1:N:134:ASP:OD1	2.52	0.41
1:Y:77:TYR:CZ	1:Y:152:LEU:HD23	2.55	0.41
1:a:43:ILE:CG2	1:a:47:MET:HE3	2.50	0.41
1:N:19:ILE:HG23	1:N:20:TYR:N	2.35	0.41
1:B:19:ILE:HG23	1:B:20:TYR:N	2.35	0.41
1:P:18:ASP:OD1	1:P:20:TYR:N	2.53	0.41
1:X:120:MET:HE3	1:X:171:ASP:HB3	2.03	0.41
1:b:109:GLY:N	1:b:186:ASP:OD2	2.52	0.41
1:I:19:ILE:HD11	1:J:46:GLN:HA	2.03	0.41
1:M:149:MET:HA	1:M:149:MET:HE2	2.02	0.41
1:P:6:VAL:HG12	1:P:7:ILE:N	2.34	0.41
1:a:119:VAL:HG11	1:a:184:LEU:HD13	2.03	0.41
1:C:153:MET:HE3	1:C:153:MET:HB3	1.98	0.41
1:F:31:LEU:C	1:F:31:LEU:HD23	2.45	0.41
1:F:116:ASN:O	2:F:401:MPD:HM3	2.21	0.41
1:L:19:ILE:HD11	1:M:46:GLN:HA	2.02	0.41
1:L:121:ILE:HG22	2:L:502:MPD:HM3	2.03	0.41
1:O:101:PHE:CD1	1:O:101:PHE:C	2.98	0.41
1:O:190:THR:O	1:O:191:HIS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:153:MET:HE2	2:T:202:MPD:C5	2.50	0.41
1:Y:80:MET:HE3	1:Y:87:VAL:HG11	2.02	0.41
1:b:122:HIS:ND1	1:b:123:GLN:O	2.50	0.41
1:E:70:ILE:HG12	1:E:98:MET:HE3	2.02	0.41
1:U:119:VAL:HG11	1:U:184:LEU:HD13	2.01	0.41
2:Y:303:MPD:H11	1:Z:149:MET:HE3	2.03	0.41
1:a:148:ARG:HG3	1:a:152:LEU:HD13	2.03	0.41
1:D:91:CYS:O	1:D:114:LEU:HD23	2.21	0.41
1:M:176:ALA:O	1:M:180:VAL:HG13	2.20	0.41
1:O:161:LEU:HD21	1:O:165:GLU:OE2	2.21	0.41
1:U:50:LEU:HD23	1:U:50:LEU:HA	1.88	0.41
1:V:19:ILE:HD11	1:W:46:GLN:HA	2.03	0.41
1:V:96:ALA:O	1:V:97:SER:C	2.63	0.41
1:Z:122:HIS:O	2:Z:301:MPD:O2	2.23	0.41
1:b:74:MET:SD	1:b:149:MET:HE1	2.60	0.41
1:A:161:LEU:HD21	1:A:165:GLU:OE2	2.20	0.41
1:B:94:GLN:HA	1:B:118:ARG:O	2.20	0.41
1:J:101:PHE:HD1	1:J:153:MET:CE	2.33	0.41
1:N:121:ILE:HG22	2:N:301:MPD:H51	2.02	0.41
1:P:26:GLU:O	1:P:26:GLU:CG	2.69	0.41
1:Q:104:THR:HA	1:Q:111:ARG:HD2	2.02	0.41
1:T:49:PHE:CB	1:U:19:ILE:HD11	2.50	0.41
2:W:402:MPD:HO2	2:W:402:MPD:HO4	1.52	0.41
1:Z:18:ASP:OD1	1:Z:19:ILE:N	2.54	0.41
1:E:111:ARG:NH2	1:E:186:ASP:OD1	2.50	0.41
1:O:92:MET:HB3	1:O:114:LEU:HD12	2.03	0.41
1:P:19:ILE:HG23	1:P:20:TYR:N	2.36	0.41
1:T:49:PHE:HB2	1:U:19:ILE:HD11	2.02	0.41
1:Y:153:MET:HE1	1:Y:184:LEU:HD21	2.03	0.41
1:b:104:THR:HG21	1:b:153:MET:SD	2.61	0.41
1:b:41:ASN:C	1:b:41:ASN:ND2	2.79	0.40
2:C:301:MPD:O4	2:C:301:MPD:C1	2.69	0.40
1:F:84:LYS:HB2	1:F:85:PRO:HD3	2.03	0.40
1:P:5:MET:O	1:P:17:PHE:N	2.54	0.40
1:V:91:CYS:O	1:V:114:LEU:HD23	2.20	0.40
1:Z:18:ASP:OD1	1:Z:20:TYR:N	2.54	0.40
1:Z:180:VAL:HG22	1:Z:185:VAL:HG12	2.02	0.40
1:E:31:LEU:C	1:E:31:LEU:HD23	2.47	0.40
1:E:92:MET:HB3	1:E:114:LEU:HD12	2.03	0.40
1:W:70:ILE:HG23	1:W:149:MET:HE2	2.04	0.40
1:B:100:ALA:O	1:B:104:THR:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:PHE:HB3	1:C:189:LEU:HG	2.02	0.40
1:Y:155:LEU:HD23	1:Y:155:LEU:O	2.21	0.40
1:b:84:LYS:N	1:b:85:PRO:HD2	2.36	0.40
1:E:42:LEU:O	1:E:42:LEU:HD23	2.21	0.40
1:F:174:LEU:HD22	1:F:184:LEU:HD12	2.02	0.40
1:I:18:ASP:OD1	1:I:19:ILE:N	2.55	0.40
1:M:84:LYS:N	1:M:85:PRO:HD2	2.36	0.40
1:M:177:PRO:O	1:M:180:VAL:HG22	2.22	0.40
1:P:145:VAL:O	1:P:149:MET:HG2	2.22	0.40
1:b:42:LEU:HD23	1:b:42:LEU:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/193 (92%)	172 (97%)	5 (3%)	1 (1%)	21	45
1	B	177/193 (92%)	173 (98%)	3 (2%)	1 (1%)	21	45
1	C	175/193 (91%)	170 (97%)	4 (2%)	1 (1%)	21	45
1	D	177/193 (92%)	170 (96%)	6 (3%)	1 (1%)	21	45
1	E	178/193 (92%)	174 (98%)	3 (2%)	1 (1%)	21	45
1	F	176/193 (91%)	170 (97%)	5 (3%)	1 (1%)	21	45
1	G	175/193 (91%)	169 (97%)	5 (3%)	1 (1%)	21	45
1	H	175/193 (91%)	170 (97%)	3 (2%)	2 (1%)	11	29
1	I	177/193 (92%)	172 (97%)	4 (2%)	1 (1%)	21	45
1	J	177/193 (92%)	170 (96%)	5 (3%)	2 (1%)	11	29
1	K	174/193 (90%)	169 (97%)	4 (2%)	1 (1%)	21	45
1	L	175/193 (91%)	171 (98%)	3 (2%)	1 (1%)	21	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	175/193 (91%)	170 (97%)	3 (2%)	2 (1%)	11	29
1	N	176/193 (91%)	169 (96%)	6 (3%)	1 (1%)	21	45
1	O	175/193 (91%)	171 (98%)	3 (2%)	1 (1%)	21	45
1	P	177/193 (92%)	170 (96%)	4 (2%)	3 (2%)	7	20
1	Q	178/193 (92%)	173 (97%)	4 (2%)	1 (1%)	21	45
1	R	177/193 (92%)	173 (98%)	3 (2%)	1 (1%)	21	45
1	S	177/193 (92%)	171 (97%)	4 (2%)	2 (1%)	11	29
1	T	175/193 (91%)	169 (97%)	4 (2%)	2 (1%)	11	29
1	U	175/193 (91%)	169 (97%)	5 (3%)	1 (1%)	21	45
1	V	177/193 (92%)	171 (97%)	5 (3%)	1 (1%)	21	45
1	W	172/193 (89%)	167 (97%)	4 (2%)	1 (1%)	21	45
1	X	175/193 (91%)	169 (97%)	4 (2%)	2 (1%)	11	29
1	Y	175/193 (91%)	171 (98%)	3 (2%)	1 (1%)	21	45
1	Z	175/193 (91%)	168 (96%)	6 (3%)	1 (1%)	21	45
1	a	173/193 (90%)	169 (98%)	3 (2%)	1 (1%)	21	45
1	b	176/193 (91%)	169 (96%)	6 (3%)	1 (1%)	21	45
All	All	4922/5404 (91%)	4769 (97%)	117 (2%)	36 (1%)	18	40

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	SER
1	G	97	SER
1	H	97	SER
1	I	97	SER
1	J	97	SER
1	K	97	SER
1	M	97	SER
1	O	97	SER
1	P	6	VAL
1	Q	97	SER
1	R	97	SER
1	S	192	ARG
1	U	97	SER
1	V	97	SER
1	Z	97	SER

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Mol	Chain	Res	Type
1	a	97	SER
1	A	97	SER
1	E	97	SER
1	J	18	ASP
1	N	97	SER
1	P	97	SER
1	T	97	SER
1	W	97	SER
1	X	18	ASP
1	b	97	SER
1	L	97	SER
1	M	18	ASP
1	P	18	ASP
1	Y	97	SER
1	C	97	SER
1	D	97	SER
1	F	18	ASP
1	X	97	SER
1	H	18	ASP
1	S	97	SER
1	T	4	PRO

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	154/163 (94%)	152 (99%)	2 (1%)	61	78
1	B	152/163 (93%)	149 (98%)	3 (2%)	48	71
1	C	151/163 (93%)	146 (97%)	5 (3%)	33	58
1	D	153/163 (94%)	149 (97%)	4 (3%)	40	65
1	E	154/163 (94%)	148 (96%)	6 (4%)	28	54
1	F	151/163 (93%)	148 (98%)	3 (2%)	48	71
1	G	149/163 (91%)	144 (97%)	5 (3%)	32	58
1	H	149/163 (91%)	145 (97%)	4 (3%)	39	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	153/163 (94%)	148 (97%)	5 (3%)	33	58
1	J	152/163 (93%)	147 (97%)	5 (3%)	33	58
1	K	150/163 (92%)	146 (97%)	4 (3%)	39	64
1	L	151/163 (93%)	147 (97%)	4 (3%)	40	65
1	M	151/163 (93%)	148 (98%)	3 (2%)	48	71
1	N	152/163 (93%)	148 (97%)	4 (3%)	40	65
1	O	150/163 (92%)	149 (99%)	1 (1%)	76	87
1	P	153/163 (94%)	150 (98%)	3 (2%)	48	71
1	Q	154/163 (94%)	150 (97%)	4 (3%)	40	65
1	R	153/163 (94%)	150 (98%)	3 (2%)	48	71
1	S	153/163 (94%)	145 (95%)	8 (5%)	21	46
1	T	151/163 (93%)	148 (98%)	3 (2%)	48	71
1	U	151/163 (93%)	146 (97%)	5 (3%)	33	58
1	V	152/163 (93%)	149 (98%)	3 (2%)	48	71
1	W	145/163 (89%)	142 (98%)	3 (2%)	47	69
1	X	150/163 (92%)	147 (98%)	3 (2%)	48	71
1	Y	151/163 (93%)	147 (97%)	4 (3%)	40	65
1	Z	151/163 (93%)	149 (99%)	2 (1%)	61	78
1	a	149/163 (91%)	146 (98%)	3 (2%)	48	71
1	b	152/163 (93%)	149 (98%)	3 (2%)	48	71
All	All	4237/4564 (93%)	4132 (98%)	105 (2%)	42	66

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	32	THR
1	B	6	VAL
1	B	32	THR
1	B	71	THR
1	C	35	VAL
1	C	70	ILE
1	C	71	THR
1	C	144	LYS
1	C	153	MET

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Mol	Chain	Res	Type
1	D	7	ILE
1	D	70	ILE
1	D	71	THR
1	D	97	SER
1	E	18	ASP
1	E	35	VAL
1	E	70	ILE
1	E	71	THR
1	E	180	VAL
1	E	190	THR
1	F	34	GLN
1	F	98	MET
1	F	120	MET
1	G	5	MET
1	G	35	VAL
1	G	70	ILE
1	G	97	SER
1	G	153	MET
1	H	27	ARG
1	H	32	THR
1	H	42	LEU
1	H	70	ILE
1	I	6	VAL
1	I	34	GLN
1	I	35	VAL
1	I	70	ILE
1	I	181	GLU
1	J	35	VAL
1	J	71	THR
1	J	97	SER
1	J	108	LYS
1	J	189	LEU
1	K	3	VAL
1	K	5	MET
1	K	34	GLN
1	K	42	LEU
1	L	35	VAL
1	L	70	ILE
1	L	71	THR
1	L	185	VAL
1	M	35	VAL
1	M	70	ILE

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Mol	Chain	Res	Type
1	M	180	VAL
1	N	32	THR
1	N	70	ILE
1	N	155	LEU
1	N	185	VAL
1	O	145	VAL
1	P	32	THR
1	P	145	VAL
1	P	155	LEU
1	Q	7	ILE
1	Q	35	VAL
1	Q	97	SER
1	Q	191	HIS
1	R	35	VAL
1	R	71	THR
1	R	145	VAL
1	S	3	VAL
1	S	22	ARG
1	S	23	LEU
1	S	24	LEU
1	S	25	LYS
1	S	32	THR
1	S	35	VAL
1	S	70	ILE
1	T	35	VAL
1	T	136	GLU
1	T	172	ARG
1	U	25	LYS
1	U	27	ARG
1	U	35	VAL
1	U	120	MET
1	U	153	MET
1	V	32	THR
1	V	180	VAL
1	V	185	VAL
1	W	35	VAL
1	W	71	THR
1	W	190	THR
1	X	70	ILE
1	X	185	VAL
1	X	190	THR
1	Y	3	VAL

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Mol	Chain	Res	Type
1	Y	71	THR
1	Y	180	VAL
1	Y	185	VAL
1	Z	36	GLU
1	Z	185	VAL
1	a	32	THR
1	a	35	VAL
1	a	151	GLU
1	b	3	VAL
1	b	32	THR
1	b	35	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	163	GLN
1	E	193	ASN
1	F	54	ASN
1	F	94	GLN
1	H	163	GLN
1	H	193	ASN
1	J	38	HIS
1	J	163	GLN
1	K	64	ASN
1	K	163	GLN
1	R	81	GLN
1	R	163	GLN
1	S	163	GLN
1	X	81	GLN
1	Z	41	ASN
1	Z	191	HIS
1	a	116	ASN
1	a	122	HIS

5.3.3 RNA ⓘ

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](#)

88 ligands are modelled in this entry.

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	$\# Z > 2$
3	ACT	P	204	-	3,3,3	1.08	0	3,3,3	1.65	1 (33%)
2	MPD	B	302	-	7,7,7	0.31	0	9,10,10	0.23	0
2	MPD	B	301	-	7,7,7	1.03	0	9,10,10	0.76	0
2	MPD	J	303	-	7,7,7	0.31	0	9,10,10	0.25	0
2	MPD	A	302	-	7,7,7	0.32	0	9,10,10	0.27	0
2	MPD	Y	301	-	7,7,7	0.30	0	9,10,10	0.33	0
3	ACT	L	501	-	3,3,3	1.11	0	3,3,3	1.34	0
4	ZGV	W	403	1	20,24,25	0.43	0	22,30,32	0.67	1 (4%)
2	MPD	L	502	-	7,7,7	0.29	0	9,10,10	0.29	0
2	MPD	H	303	-	7,7,7	0.30	0	9,10,10	0.31	0
2	MPD	W	402	-	7,7,7	0.25	0	9,10,10	0.34	0
4	ZGV	P	203	1	11,14,25	0.63	0	10,18,32	0.97	1 (10%)
2	MPD	D	301	-	7,7,7	0.23	0	9,10,10	0.54	0
4	ZGV	I	302	1	12,15,25	0.69	1 (8%)	12,19,32	1.45	1 (8%)
4	ZGV	S	203	1	11,14,25	0.72	0	10,18,32	0.72	0
2	MPD	F	402	-	7,7,7	1.17	0	9,10,10	0.70	0
4	ZGV	B	304	1	11,14,25	0.76	1 (9%)	10,18,32	0.76	1 (10%)
2	MPD	Y	303	-	7,7,7	0.29	0	9,10,10	0.27	0
3	ACT	F	403	-	3,3,3	1.09	0	3,3,3	1.38	0
2	MPD	a	301	-	7,7,7	0.28	0	9,10,10	0.60	0
2	MPD	Q	304	-	7,7,7	0.31	0	9,10,10	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ZGV	a	302	1	2,7,25	1.75	1 (50%)	2,9,32	1.49	1 (50%)
2	MPD	P	201	-	7,7,7	0.23	0	9,10,10	0.43	0
2	MPD	K	301	-	7,7,7	0.30	0	9,10,10	0.47	0
3	ACT	B	303	-	3,3,3	1.15	0	3,3,3	1.38	0
2	MPD	I	303	-	7,7,7	0.31	0	9,10,10	0.35	0
4	ZGV	Q	303	1	11,14,25	0.80	1 (9%)	10,18,32	0.70	1 (10%)
2	MPD	P	202	-	7,7,7	0.29	0	9,10,10	0.42	0
4	ZGV	U	302	1	11,14,25	0.85	1 (9%)	10,18,32	0.71	0
2	MPD	Z	301	-	7,7,7	0.33	0	9,10,10	0.27	0
4	ZGV	O	303	1	20,24,25	0.58	1 (5%)	22,30,32	0.71	0
2	MPD	Z	302	-	7,7,7	0.31	0	9,10,10	0.46	0
4	ZGV	K	302	1	11,14,25	0.89	1 (9%)	10,18,32	0.59	0
2	MPD	C	301	-	7,7,7	0.99	1 (14%)	9,10,10	1.00	0
2	MPD	I	301	-	7,7,7	0.28	0	9,10,10	0.32	0
4	ZGV	R	303	1	11,14,25	0.69	0	10,18,32	0.80	1 (10%)
2	MPD	H	301	-	7,7,7	0.24	0	9,10,10	0.54	0
3	ACT	X	202	-	3,3,3	1.13	0	3,3,3	1.37	0
2	MPD	Q	301	-	7,7,7	0.99	1 (14%)	9,10,10	0.80	0
2	MPD	b	302	-	7,7,7	0.29	0	9,10,10	0.26	0
4	ZGV	J	302	1	13,16,25	0.71	1 (7%)	13,20,32	1.47	2 (15%)
2	MPD	b	301	-	7,7,7	0.30	0	9,10,10	0.39	0
4	ZGV	C	302	1	11,14,25	0.80	1 (9%)	10,18,32	0.71	1 (10%)
2	MPD	U	301	-	7,7,7	0.20	0	9,10,10	0.64	0
2	MPD	F	404	-	7,7,7	0.33	0	9,10,10	0.59	0
2	MPD	J	301	-	7,7,7	0.24	0	9,10,10	0.32	0
2	MPD	E	301	-	7,7,7	0.28	0	9,10,10	0.64	0
3	ACT	R	302	-	3,3,3	1.13	0	3,3,3	1.64	1 (33%)
4	ZGV	Y	302	1	15,18,25	0.57	0	16,23,32	0.79	1 (6%)
4	ZGV	E	302	1	11,14,25	0.81	1 (9%)	10,18,32	0.69	1 (10%)
4	ZGV	T	203	1	13,16,25	0.81	1 (7%)	13,20,32	1.20	1 (7%)
4	ZGV	H	302	1	13,16,25	0.58	0	13,20,32	2.04	3 (23%)
2	MPD	N	301	-	7,7,7	0.30	0	9,10,10	0.28	0
2	MPD	O	302	-	7,7,7	0.34	0	9,10,10	0.31	0
2	MPD	T	201	-	7,7,7	0.28	0	9,10,10	0.29	0
4	ZGV	N	303	1	11,14,25	0.82	1 (9%)	10,18,32	0.62	0
2	MPD	X	201	-	7,7,7	0.30	0	9,10,10	0.42	0
2	MPD	G	301	-	7,7,7	0.23	0	9,10,10	0.34	0
2	MPD	T	202	-	7,7,7	0.32	0	9,10,10	0.55	0
2	MPD	a	303	-	7,7,7	0.25	0	9,10,10	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MPD	M	301	-	7,7,7	0.35	0	9,10,10	0.25	0
4	ZGV	L	503	1	16,19,25	1.08	2 (12%)	17,24,32	0.84	1 (5%)
4	ZGV	G	303	1	11,14,25	0.74	0	10,18,32	0.65	0
4	ZGV	b	303	1	8,11,25	0.96	0	7,14,32	1.00	1 (14%)
2	MPD	O	301	-	7,7,7	0.31	0	9,10,10	0.29	0
2	MPD	A	301	-	7,7,7	0.32	0	9,10,10	0.27	0
2	MPD	D	303	-	7,7,7	0.32	0	9,10,10	0.25	0
2	MPD	S	201	-	7,7,7	0.31	0	9,10,10	0.28	0
3	ACT	A	303	-	3,3,3	1.17	0	3,3,3	1.34	0
4	ZGV	A	304	1	20,24,25	0.32	0	22,30,32	0.71	1 (4%)
4	ZGV	X	203	1	8,11,25	1.07	1 (12%)	7,14,32	0.92	0
2	MPD	R	301	-	7,7,7	0.98	0	9,10,10	0.80	0
2	MPD	V	301	-	7,7,7	0.85	0	9,10,10	0.76	0
3	ACT	C	303	-	3,3,3	1.04	0	3,3,3	1.34	0
3	ACT	G	302	-	3,3,3	1.23	0	3,3,3	1.62	1 (33%)
4	ZGV	M	302	1	15,18,25	0.64	1 (6%)	16,23,32	0.61	1 (6%)
4	ZGV	V	302	1	2,7,25	1.66	1 (50%)	2,9,32	1.58	1 (50%)
4	ZGV	Z	304	1	2,7,25	1.72	1 (50%)	2,9,32	1.55	1 (50%)
2	MPD	K	303	-	7,7,7	0.28	0	9,10,10	0.22	0
2	MPD	D	302	-	7,7,7	0.28	0	9,10,10	0.40	0
2	MPD	S	202	-	7,7,7	0.28	0	9,10,10	0.31	0
4	ZGV	F	405	1	13,16,25	0.59	0	13,20,32	1.38	1 (7%)
2	MPD	F	401	-	7,7,7	0.26	0	9,10,10	0.45	0
4	ZGV	D	304	1	11,14,25	0.81	1 (9%)	10,18,32	0.71	1 (10%)
2	MPD	N	302	-	7,7,7	0.25	0	9,10,10	0.35	0
2	MPD	Q	302	-	7,7,7	0.32	0	9,10,10	0.28	0
2	MPD	W	401	-	7,7,7	0.21	0	9,10,10	0.61	0
3	ACT	Z	303	-	3,3,3	1.19	0	3,3,3	1.34	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
2	MPD	B	302	-	-	0/5/5/5	-
2	MPD	B	301	-	-	2/5/5/5	-
2	MPD	J	303	-	-	2/5/5/5	-
2	MPD	A	302	-	-	1/5/5/5	-
2	MPD	Y	301	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ZGV	W	403	1	-	4/20/33/35	0/1/1/1
2	MPD	L	502	-	-	0/5/5/5	-
2	MPD	H	303	-	-	2/5/5/5	-
2	MPD	W	402	-	-	4/5/5/5	-
4	ZGV	P	203	1	-	2/7/20/35	0/1/1/1
2	MPD	D	301	-	-	2/5/5/5	-
4	ZGV	I	302	1	-	2/9/22/35	0/1/1/1
4	ZGV	S	203	1	-	2/7/20/35	0/1/1/1
2	MPD	F	402	-	-	1/5/5/5	-
4	ZGV	B	304	1	-	2/7/20/35	0/1/1/1
2	MPD	Y	303	-	-	4/5/5/5	-
2	MPD	a	301	-	-	3/5/5/5	-
2	MPD	Q	304	-	-	2/5/5/5	-
4	ZGV	a	302	1	-	0/0/11/35	0/1/1/1
2	MPD	P	201	-	-	4/5/5/5	-
2	MPD	K	301	-	-	2/5/5/5	-
2	MPD	I	303	-	-	0/5/5/5	-
4	ZGV	Q	303	1	-	2/7/20/35	0/1/1/1
2	MPD	P	202	-	-	2/5/5/5	-
4	ZGV	U	302	1	-	2/7/20/35	0/1/1/1
2	MPD	Z	301	-	-	3/5/5/5	-
4	ZGV	O	303	1	-	6/20/33/35	0/1/1/1
2	MPD	Z	302	-	-	0/5/5/5	-
4	ZGV	K	302	1	-	0/7/20/35	0/1/1/1
2	MPD	C	301	-	-	2/5/5/5	-
2	MPD	I	301	-	-	0/5/5/5	-
4	ZGV	R	303	1	-	0/7/20/35	0/1/1/1
2	MPD	H	301	-	-	4/5/5/5	-
2	MPD	Q	301	-	-	1/5/5/5	-
2	MPD	b	302	-	-	0/5/5/5	-
4	ZGV	J	302	1	-	0/10/23/35	0/1/1/1
2	MPD	b	301	-	-	5/5/5/5	-
4	ZGV	C	302	1	-	2/7/20/35	0/1/1/1
2	MPD	U	301	-	-	5/5/5/5	-
2	MPD	F	404	-	-	3/5/5/5	-
2	MPD	J	301	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	E	301	-	-	3/5/5/5	-
4	ZGV	Y	302	1	-	2/12/25/35	0/1/1/1
4	ZGV	E	302	1	-	2/7/20/35	0/1/1/1
4	ZGV	T	203	1	-	0/10/23/35	0/1/1/1
4	ZGV	H	302	1	-	2/10/23/35	0/1/1/1
2	MPD	N	301	-	-	4/5/5/5	-
2	MPD	O	302	-	-	0/5/5/5	-
2	MPD	T	201	-	-	1/5/5/5	-
4	ZGV	N	303	1	-	0/7/20/35	0/1/1/1
2	MPD	X	201	-	-	4/5/5/5	-
2	MPD	G	301	-	-	0/5/5/5	-
2	MPD	T	202	-	-	3/5/5/5	-
2	MPD	a	303	-	-	1/5/5/5	-
2	MPD	M	301	-	-	2/5/5/5	-
4	ZGV	L	503	1	-	2/14/27/35	0/1/1/1
4	ZGV	G	303	1	-	2/7/20/35	0/1/1/1
4	ZGV	b	303	1	-	0/3/16/35	0/1/1/1
2	MPD	O	301	-	-	2/5/5/5	-
2	MPD	A	301	-	-	0/5/5/5	-
2	MPD	D	303	-	-	1/5/5/5	-
2	MPD	S	201	-	-	0/5/5/5	-
4	ZGV	A	304	1	-	6/20/33/35	0/1/1/1
4	ZGV	X	203	1	-	0/3/16/35	0/1/1/1
2	MPD	R	301	-	-	0/5/5/5	-
2	MPD	V	301	-	-	1/5/5/5	-
4	ZGV	M	302	1	-	0/12/25/35	0/1/1/1
4	ZGV	V	302	1	-	0/0/11/35	0/1/1/1
4	ZGV	Z	304	1	-	0/0/11/35	0/1/1/1
2	MPD	K	303	-	-	5/5/5/5	-
2	MPD	D	302	-	-	2/5/5/5	-
2	MPD	S	202	-	-	0/5/5/5	-
4	ZGV	F	405	1	-	0/10/23/35	0/1/1/1
2	MPD	F	401	-	-	3/5/5/5	-
4	ZGV	D	304	1	-	0/7/20/35	0/1/1/1
2	MPD	N	302	-	-	3/5/5/5	-
2	MPD	Q	302	-	-	0/5/5/5	-
2	MPD	W	401	-	-	5/5/5/5	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	503	ZGV	C5-C6	3.25	1.36	1.33
4	K	302	ZGV	C15-C14	2.59	1.37	1.34
4	T	203	ZGV	C15-C14	2.56	1.37	1.34
4	a	302	ZGV	C13-C14	-2.44	1.45	1.49
4	Z	304	ZGV	C13-C14	-2.40	1.45	1.49
4	O	303	ZGV	C15-C14	2.37	1.37	1.34
4	U	302	ZGV	C15-C14	2.37	1.37	1.34
4	X	203	ZGV	C15-C14	2.32	1.37	1.34
4	N	303	ZGV	C15-C14	2.32	1.37	1.34
4	V	302	ZGV	C13-C14	-2.31	1.45	1.49
2	Q	301	MPD	O2-C2	-2.29	1.39	1.44
4	D	304	ZGV	C15-C14	2.27	1.37	1.34
4	I	302	ZGV	C15-C14	2.23	1.37	1.34
4	Q	303	ZGV	C15-C14	2.23	1.37	1.34
4	C	302	ZGV	C15-C14	2.23	1.37	1.34
4	E	302	ZGV	C15-C14	2.22	1.37	1.34
4	L	503	ZGV	C15-C14	2.20	1.37	1.34
2	C	301	MPD	O2-C2	-2.18	1.39	1.44
4	J	302	ZGV	C15-C14	2.16	1.37	1.34
4	B	304	ZGV	C15-C14	2.08	1.36	1.34
4	M	302	ZGV	C15-C14	2.02	1.36	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	302	ZGV	C8-C9-C10	6.01	128.73	120.98
4	J	302	ZGV	C8-C9-C10	4.71	127.05	120.98
4	F	405	ZGV	C8-C9-C10	4.42	126.67	120.98
4	I	302	ZGV	C8-C9-C10	4.32	126.97	122.22
4	T	203	ZGV	C8-C9-C10	3.70	125.75	120.98
4	H	302	ZGV	C13-C12-C11	2.67	136.18	125.43
4	P	203	ZGV	C16-N1-C14	-2.54	88.30	94.01
4	Y	302	ZGV	C16-N1-C14	-2.36	88.71	94.01
4	A	304	ZGV	C16-N1-C14	-2.34	88.76	94.01
4	R	303	ZGV	C16-N1-C14	-2.27	88.91	94.01
4	W	403	ZGV	C16-N1-C14	-2.27	88.92	94.01
4	V	302	ZGV	C16-N1-C14	-2.23	89.00	94.01
4	Z	304	ZGV	C16-N1-C14	-2.20	89.07	94.01
4	b	303	ZGV	C16-N1-C14	-2.16	89.16	94.01
4	J	302	ZGV	C16-N1-C14	-2.15	89.17	94.01
4	H	302	ZGV	C16-N1-C14	-2.13	89.22	94.01
4	a	302	ZGV	C16-N1-C14	-2.10	89.29	94.01
3	P	204	ACT	O-C-CH3	-2.07	114.03	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	302	ZGV	C16-N1-C14	-2.06	89.38	94.01
4	B	304	ZGV	C16-N1-C14	-2.06	89.39	94.01
4	Q	303	ZGV	C16-N1-C14	-2.05	89.41	94.01
3	R	302	ACT	O-C-CH3	-2.05	114.14	122.53
3	G	302	ACT	O-C-CH3	-2.03	114.20	122.53
4	D	304	ZGV	C16-N1-C14	-2.02	89.46	94.01
4	L	503	ZGV	C16-N1-C14	-2.02	89.47	94.01
4	M	302	ZGV	C16-N1-C14	-2.01	89.49	94.01
4	E	302	ZGV	C16-N1-C14	-2.01	89.50	94.01

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	MPD	C2-C3-C4-C5
2	C	301	MPD	C2-C3-C4-C5
2	D	301	MPD	C2-C3-C4-C5
2	F	404	MPD	C1-C2-C3-C4
2	F	404	MPD	O2-C2-C3-C4
2	H	301	MPD	C2-C3-C4-O4
2	K	301	MPD	C2-C3-C4-O4
2	K	301	MPD	C2-C3-C4-C5
2	K	303	MPD	C2-C3-C4-O4
2	O	301	MPD	C2-C3-C4-C5
2	U	301	MPD	C2-C3-C4-O4
2	U	301	MPD	C2-C3-C4-C5
2	W	401	MPD	C1-C2-C3-C4
2	W	401	MPD	C2-C3-C4-C5
2	X	201	MPD	C2-C3-C4-C5
2	Y	303	MPD	C2-C3-C4-O4
2	Y	303	MPD	C2-C3-C4-C5
2	Z	301	MPD	C2-C3-C4-C5
2	a	301	MPD	CM-C2-C3-C4
2	b	301	MPD	C2-C3-C4-O4
4	A	304	ZGV	C5-C6-C8-C9
4	A	304	ZGV	O1-C10-N2-C11
4	A	304	ZGV	C9-C10-N2-C11
4	B	304	ZGV	O1-C10-N2-C11
4	B	304	ZGV	C9-C10-N2-C11
4	C	302	ZGV	O1-C10-N2-C11
4	C	302	ZGV	C9-C10-N2-C11
4	E	302	ZGV	O1-C10-N2-C11

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Mol	Chain	Res	Type	Atoms
4	E	302	ZGV	C9-C10-N2-C11
4	G	303	ZGV	O1-C10-N2-C11
4	G	303	ZGV	C9-C10-N2-C11
4	H	302	ZGV	O1-C10-N2-C11
4	H	302	ZGV	C9-C10-N2-C11
4	I	302	ZGV	O1-C10-N2-C11
4	I	302	ZGV	C9-C10-N2-C11
4	L	503	ZGV	O1-C10-N2-C11
4	L	503	ZGV	C9-C10-N2-C11
4	O	303	ZGV	C18-C1-C2-C3
4	O	303	ZGV	C18-C1-C2-O5
4	O	303	ZGV	O1-C10-N2-C11
4	O	303	ZGV	C9-C10-N2-C11
4	P	203	ZGV	O1-C10-N2-C11
4	P	203	ZGV	C9-C10-N2-C11
4	Q	303	ZGV	O1-C10-N2-C11
4	Q	303	ZGV	C9-C10-N2-C11
4	S	203	ZGV	O1-C10-N2-C11
4	S	203	ZGV	C9-C10-N2-C11
4	U	302	ZGV	O1-C10-N2-C11
4	U	302	ZGV	C9-C10-N2-C11
4	W	403	ZGV	C5-C6-C8-C9
4	W	403	ZGV	O1-C10-N2-C11
4	W	403	ZGV	C9-C10-N2-C11
4	Y	302	ZGV	O1-C10-N2-C11
4	Y	302	ZGV	C9-C10-N2-C11
4	A	304	ZGV	C7-C6-C8-C9
4	W	403	ZGV	C7-C6-C8-C9
4	O	303	ZGV	C7-C6-C8-C9
4	A	304	ZGV	C1-C2-C3-C4
4	O	303	ZGV	C5-C6-C8-C9
2	U	301	MPD	O2-C2-C3-C4
2	N	301	MPD	C2-C3-C4-O4
2	P	201	MPD	C2-C3-C4-O4
2	T	202	MPD	C2-C3-C4-O4
2	W	402	MPD	C2-C3-C4-O4
2	Y	301	MPD	C2-C3-C4-O4
2	D	302	MPD	CM-C2-C3-C4
2	E	301	MPD	C1-C2-C3-C4
2	F	401	MPD	C1-C2-C3-C4
2	F	401	MPD	CM-C2-C3-C4
2	F	404	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	K	303	MPD	CM-C2-C3-C4
2	N	301	MPD	C1-C2-C3-C4
2	N	301	MPD	CM-C2-C3-C4
2	N	302	MPD	CM-C2-C3-C4
2	P	201	MPD	C1-C2-C3-C4
2	P	201	MPD	CM-C2-C3-C4
2	P	202	MPD	CM-C2-C3-C4
2	Q	304	MPD	C1-C2-C3-C4
2	Q	304	MPD	CM-C2-C3-C4
2	U	301	MPD	C1-C2-C3-C4
2	U	301	MPD	CM-C2-C3-C4
2	W	401	MPD	CM-C2-C3-C4
2	W	402	MPD	C1-C2-C3-C4
2	W	402	MPD	CM-C2-C3-C4
2	X	201	MPD	C1-C2-C3-C4
2	X	201	MPD	CM-C2-C3-C4
2	a	301	MPD	C1-C2-C3-C4
2	b	301	MPD	CM-C2-C3-C4
4	A	304	ZGV	O5-C2-C3-C4
2	H	301	MPD	C2-C3-C4-C5
2	K	303	MPD	C2-C3-C4-C5
2	M	301	MPD	C2-C3-C4-C5
2	T	202	MPD	C2-C3-C4-C5
2	Y	301	MPD	C2-C3-C4-C5
2	b	301	MPD	C2-C3-C4-C5
2	D	301	MPD	O2-C2-C3-C4
2	F	401	MPD	O2-C2-C3-C4
2	H	301	MPD	O2-C2-C3-C4
2	H	303	MPD	O2-C2-C3-C4
2	J	303	MPD	O2-C2-C3-C4
2	K	303	MPD	O2-C2-C3-C4
2	N	301	MPD	O2-C2-C3-C4
2	N	302	MPD	O2-C2-C3-C4
2	P	201	MPD	O2-C2-C3-C4
2	W	401	MPD	O2-C2-C3-C4
2	W	402	MPD	O2-C2-C3-C4
2	X	201	MPD	O2-C2-C3-C4
2	Y	303	MPD	O2-C2-C3-C4
2	Z	301	MPD	O2-C2-C3-C4
2	a	301	MPD	O2-C2-C3-C4
2	b	301	MPD	O2-C2-C3-C4
2	A	302	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	B	301	MPD	C2-C3-C4-O4
2	C	301	MPD	C2-C3-C4-O4
2	D	303	MPD	C2-C3-C4-O4
2	E	301	MPD	C2-C3-C4-O4
2	F	402	MPD	C2-C3-C4-O4
2	J	303	MPD	C2-C3-C4-O4
2	M	301	MPD	C2-C3-C4-O4
2	O	301	MPD	C2-C3-C4-O4
2	Q	301	MPD	C2-C3-C4-O4
2	T	201	MPD	C2-C3-C4-O4
2	V	301	MPD	C2-C3-C4-O4
2	W	401	MPD	C2-C3-C4-O4
2	a	303	MPD	C2-C3-C4-O4
2	D	302	MPD	C1-C2-C3-C4
2	E	301	MPD	CM-C2-C3-C4
2	H	301	MPD	C1-C2-C3-C4
2	H	303	MPD	CM-C2-C3-C4
2	K	303	MPD	C1-C2-C3-C4
2	N	302	MPD	C1-C2-C3-C4
2	P	202	MPD	C1-C2-C3-C4
2	T	202	MPD	C1-C2-C3-C4
2	Y	303	MPD	CM-C2-C3-C4
2	Z	301	MPD	C1-C2-C3-C4
2	b	301	MPD	C1-C2-C3-C4

There are no ring outliers.

35 monomers are involved in 58 short contacts:

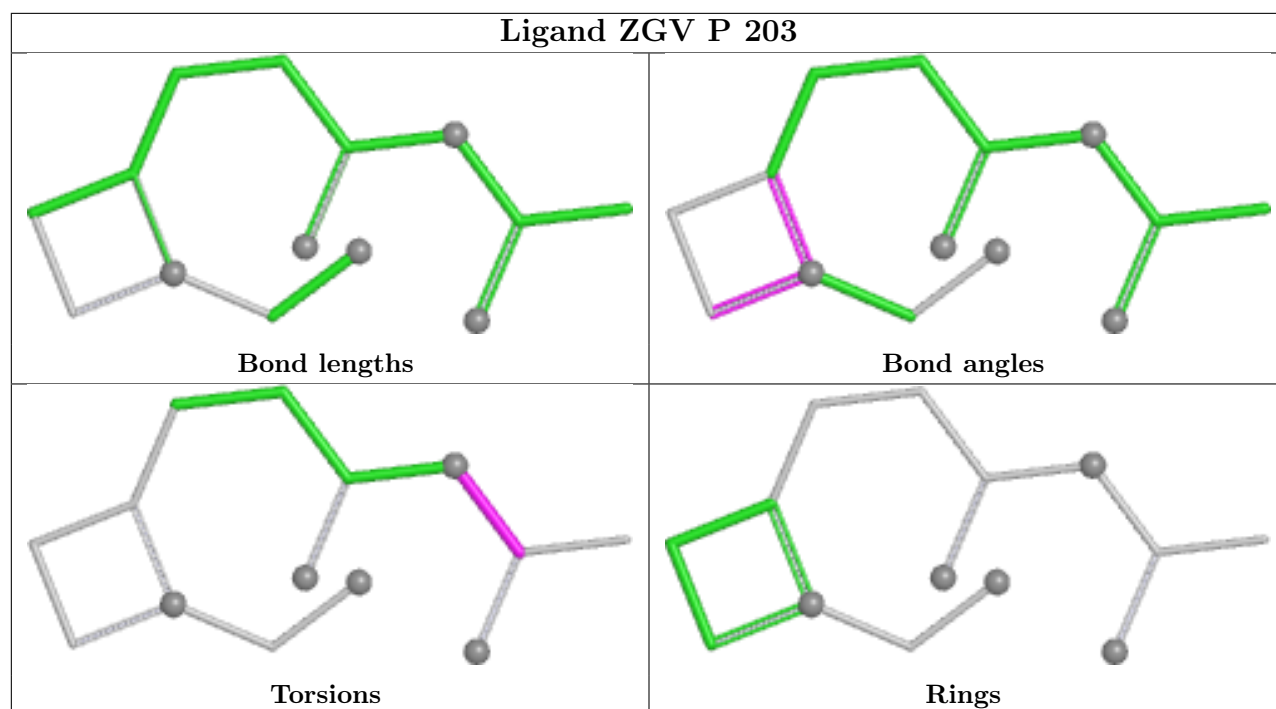
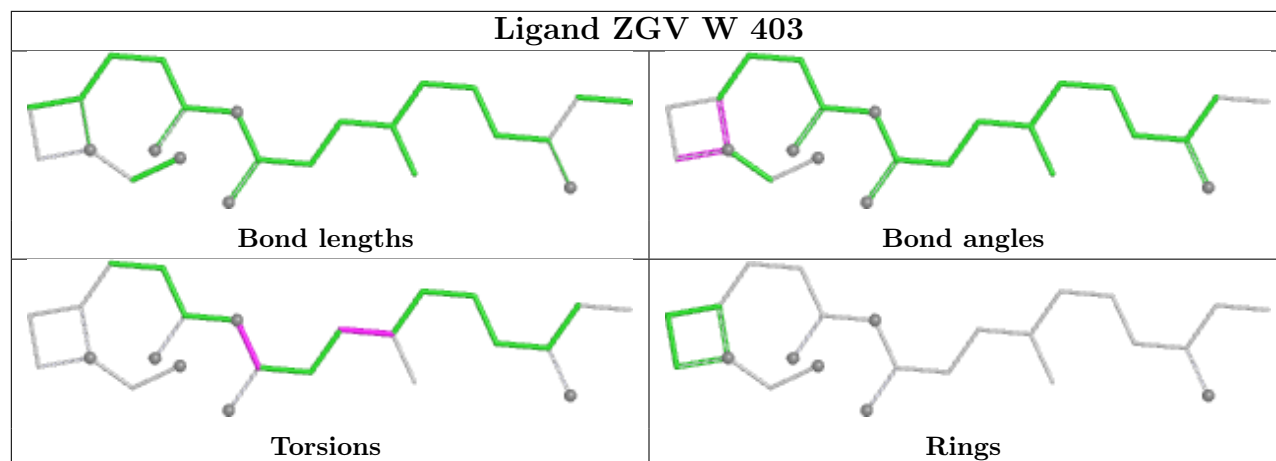
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	MPD	1	0
2	L	502	MPD	1	0
2	W	402	MPD	3	0
2	D	301	MPD	4	0
4	S	203	ZGV	1	0
2	F	402	MPD	1	0
2	Y	303	MPD	2	0
2	a	301	MPD	3	0
2	P	201	MPD	2	0
2	K	301	MPD	1	0
2	I	303	MPD	1	0
4	U	302	ZGV	1	0
2	Z	301	MPD	1	0

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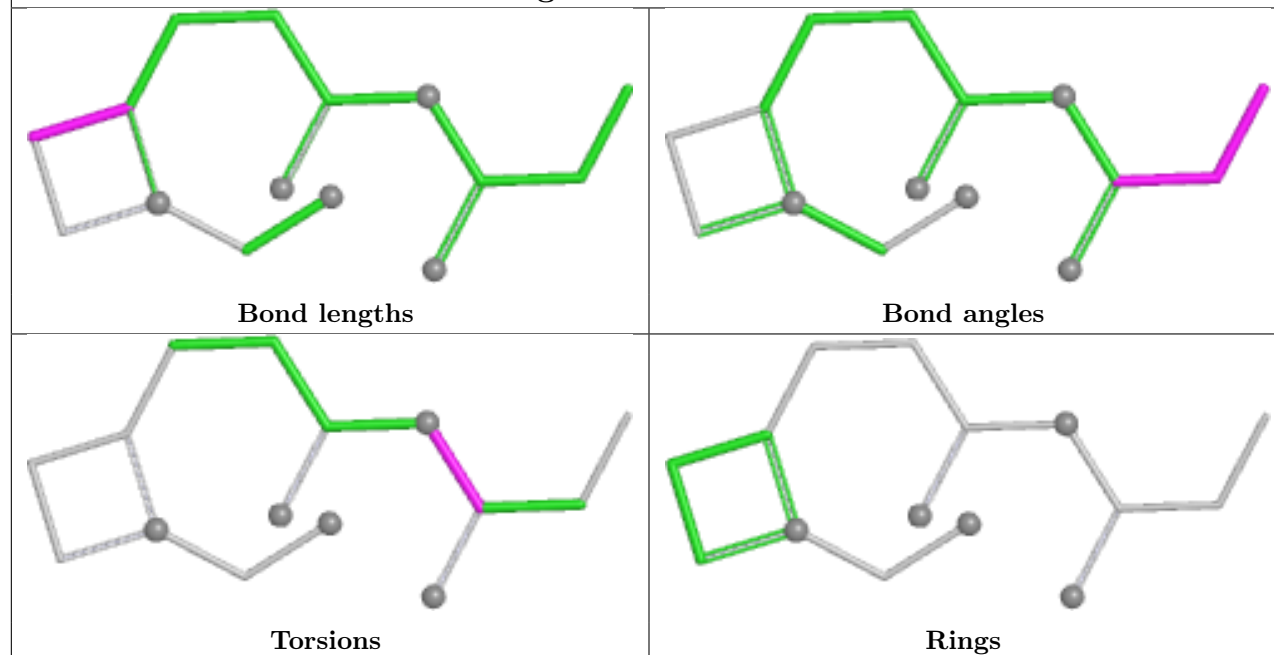
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	MPD	2	0
2	I	301	MPD	1	0
4	R	303	ZGV	1	0
2	H	301	MPD	3	0
2	Q	301	MPD	1	0
2	b	301	MPD	1	0
2	U	301	MPD	4	0
2	J	301	MPD	2	0
2	E	301	MPD	1	0
2	N	301	MPD	3	0
2	O	302	MPD	1	0
2	T	201	MPD	1	0
2	X	201	MPD	2	0
2	G	301	MPD	1	0
2	T	202	MPD	4	0
2	a	303	MPD	1	0
2	O	301	MPD	2	0
2	R	301	MPD	1	0
2	V	301	MPD	1	0
2	K	303	MPD	1	0
2	F	401	MPD	1	0
2	W	401	MPD	1	0

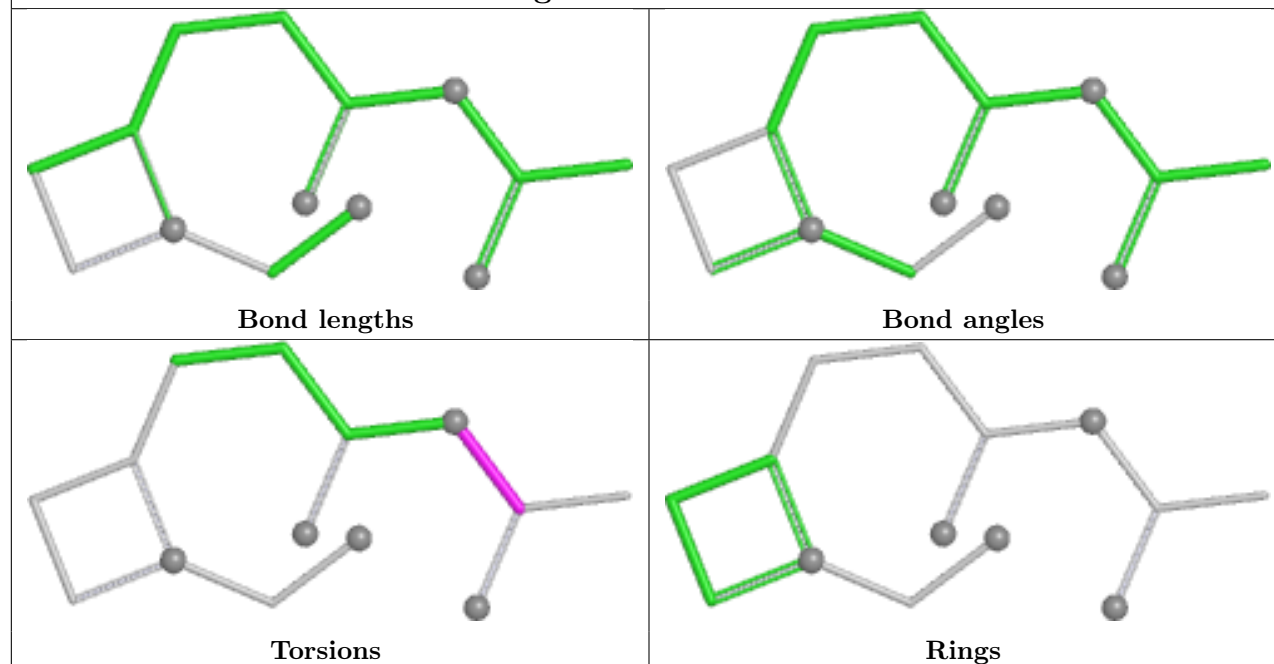
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



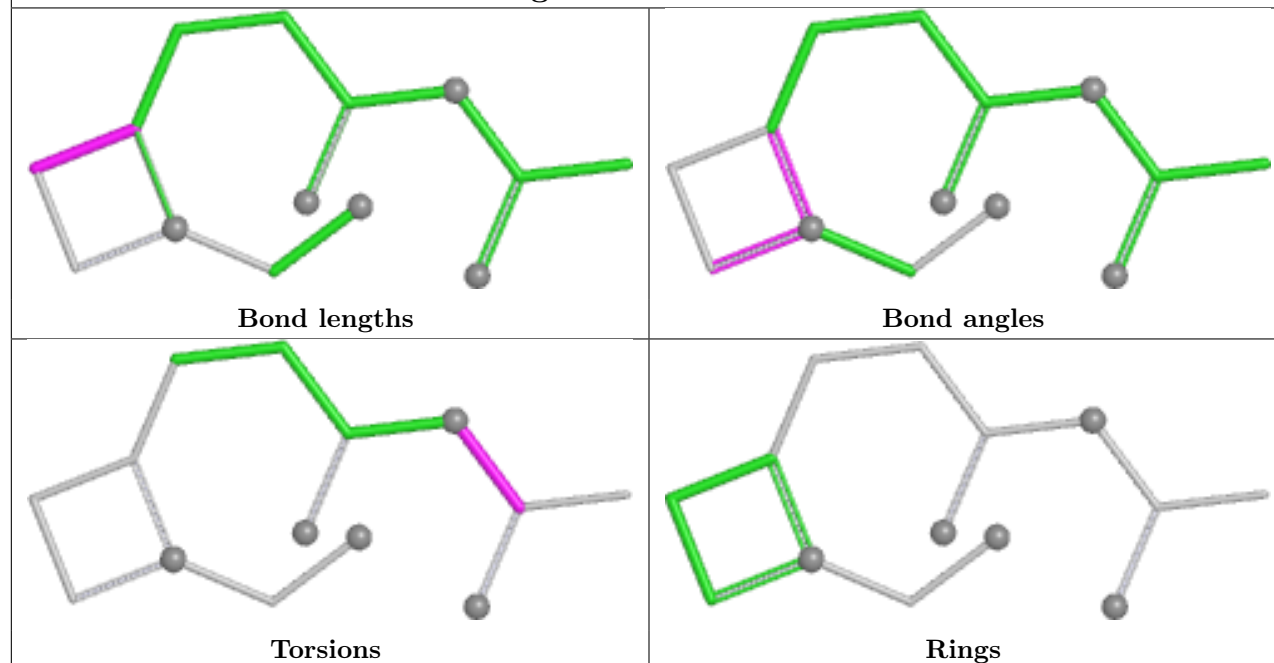
Ligand ZGV I 302



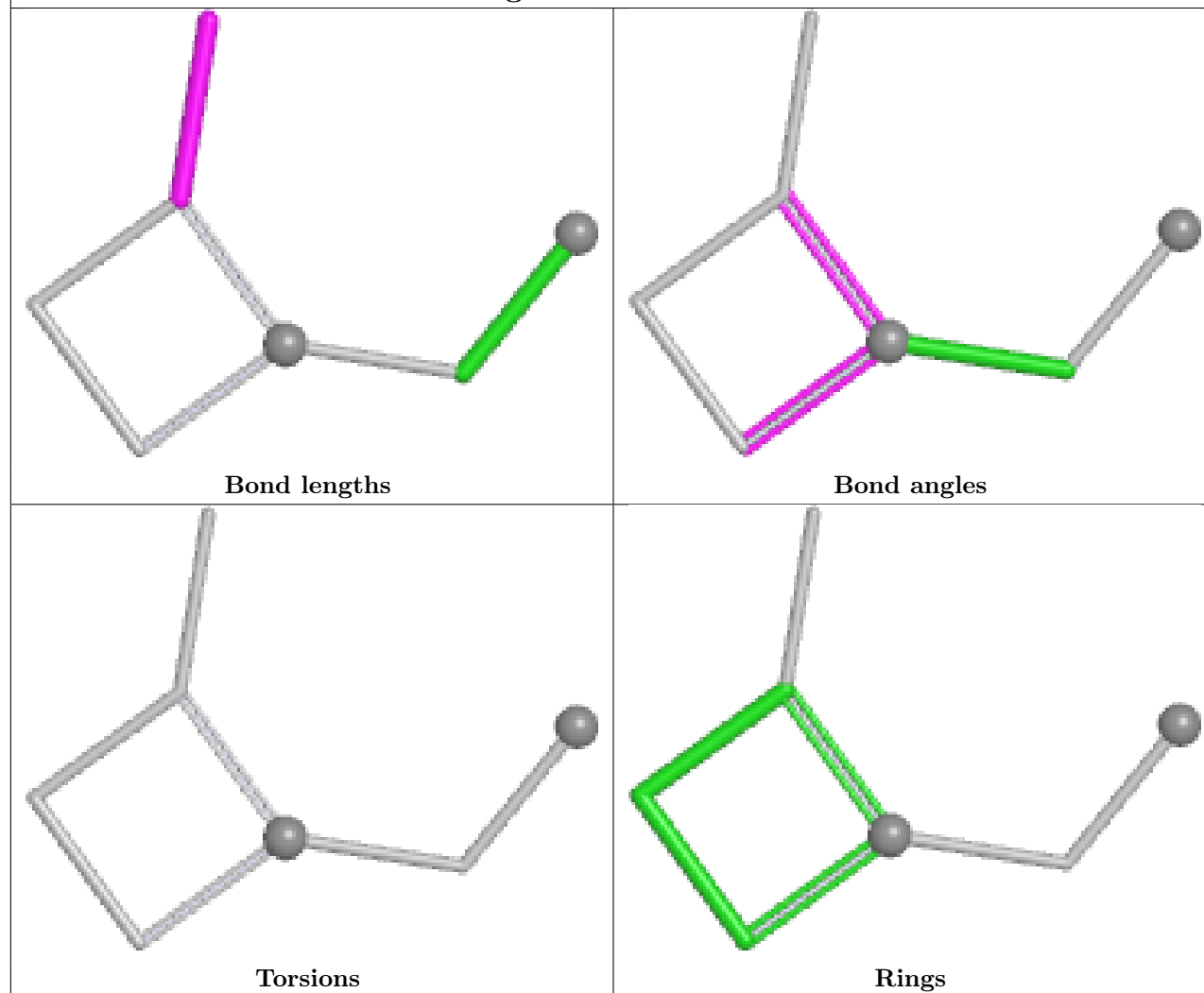
Ligand ZGV S 203



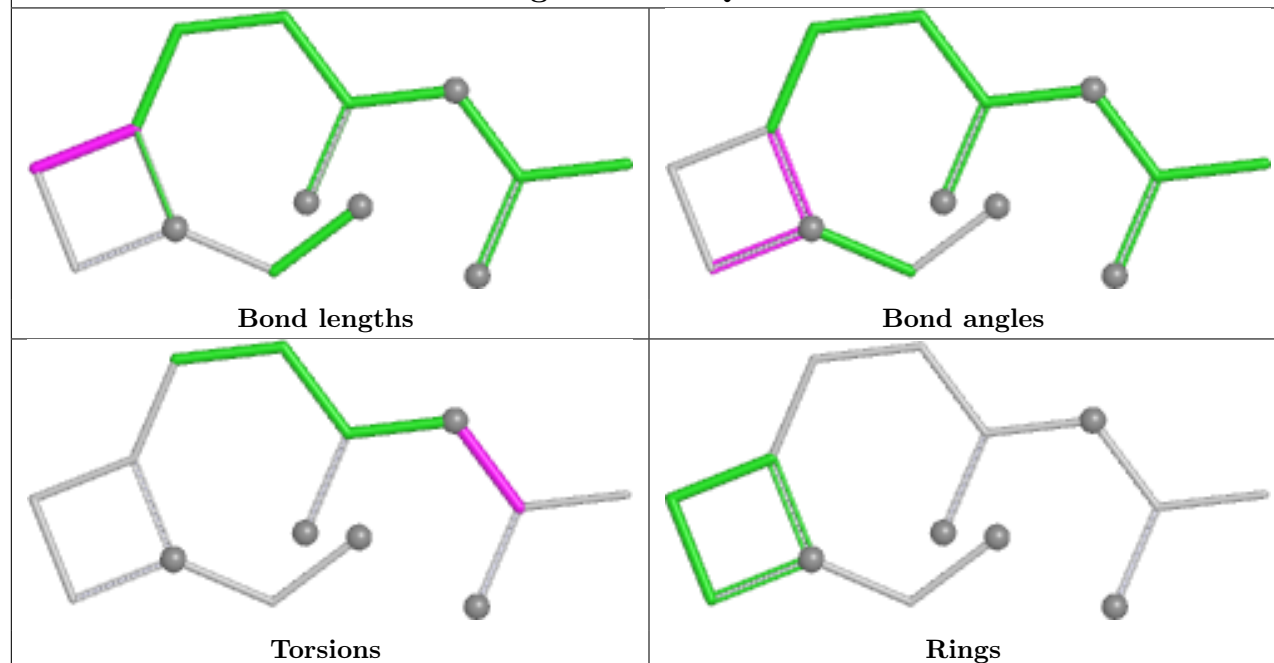
Ligand ZGV B 304



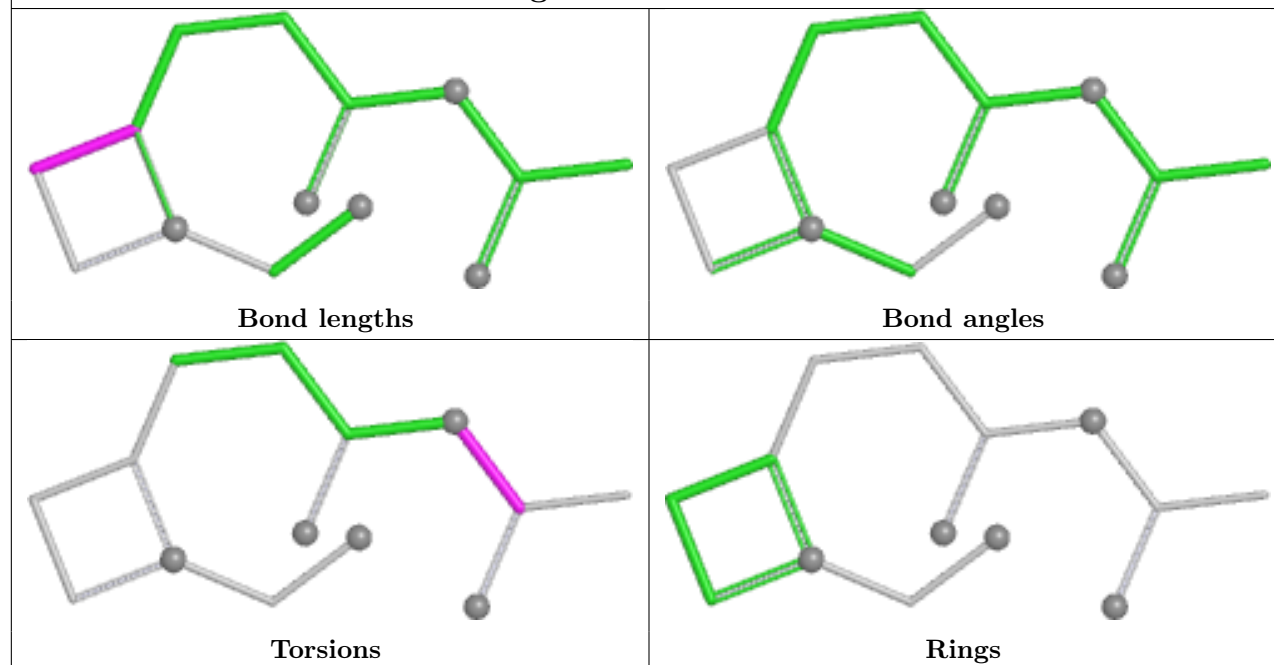
Ligand ZGV a 302

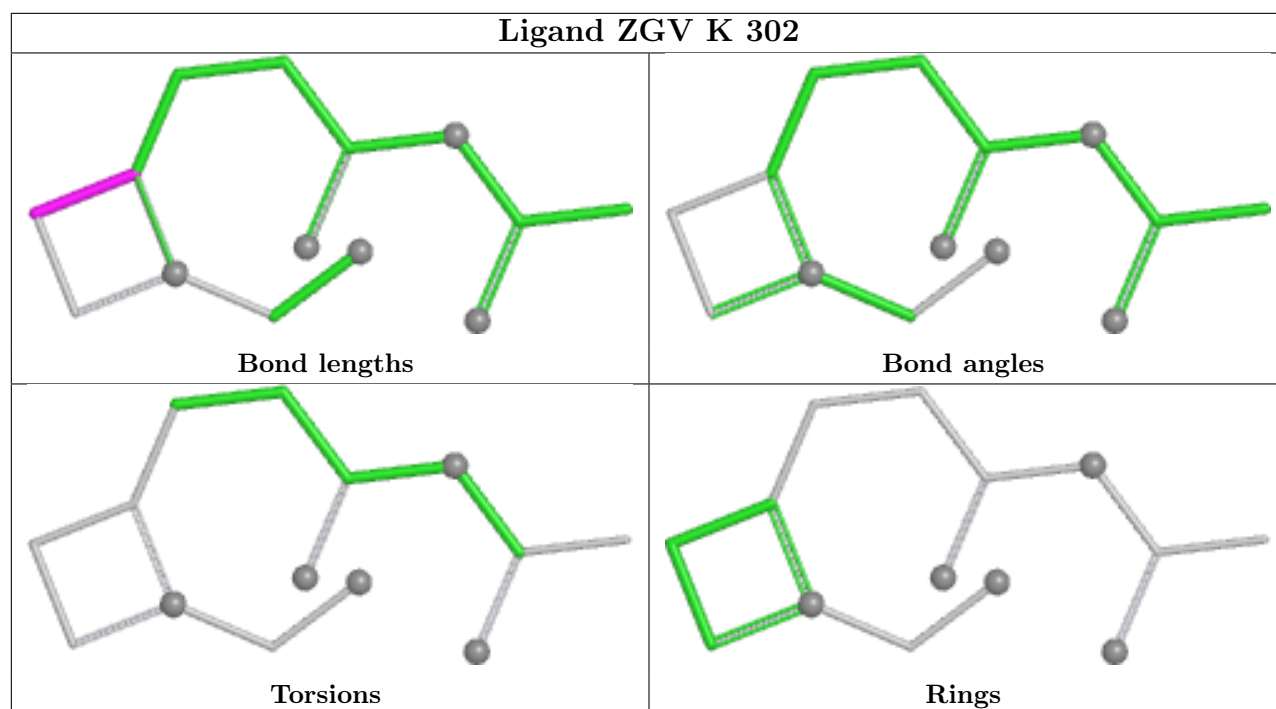
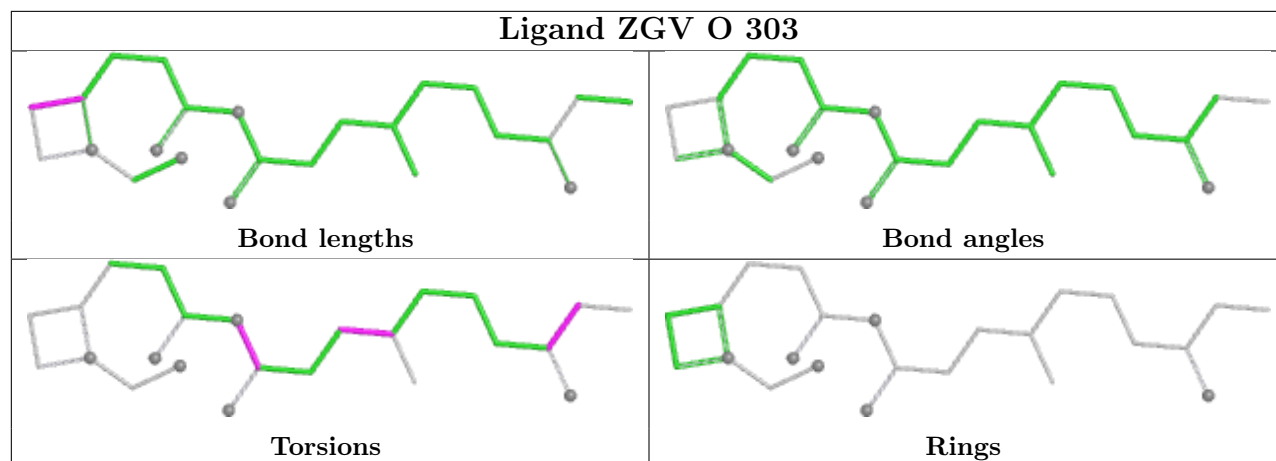


Ligand ZGV Q 303

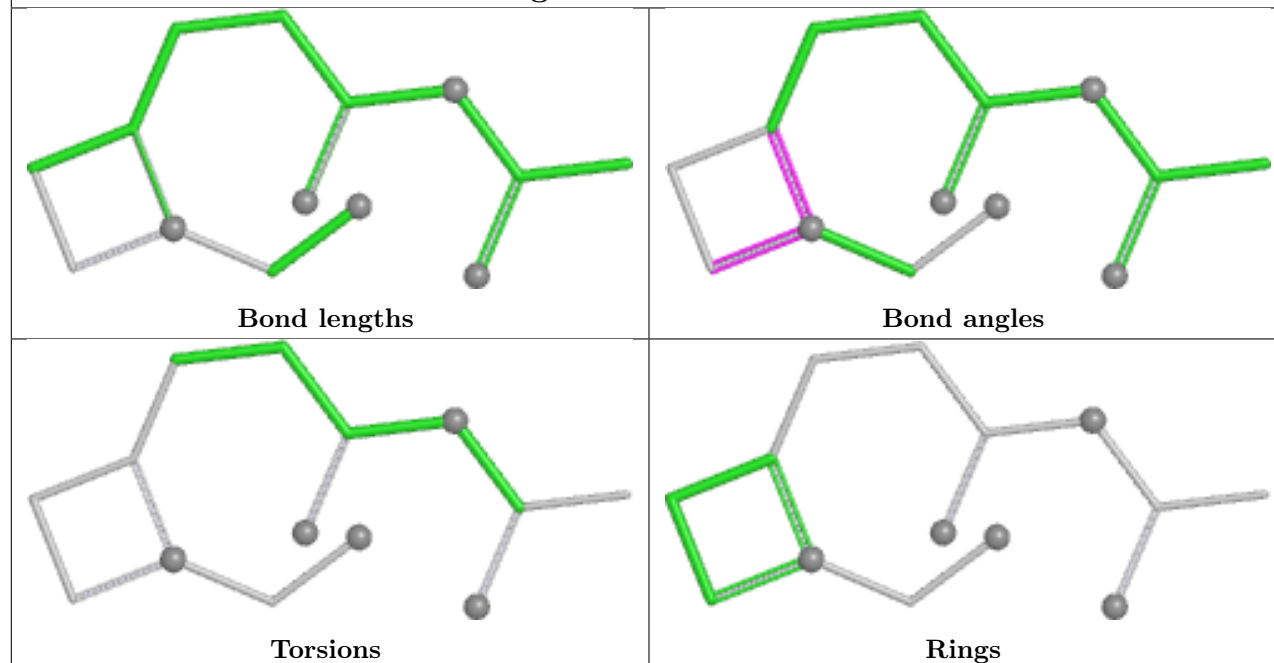


Ligand ZGV U 302

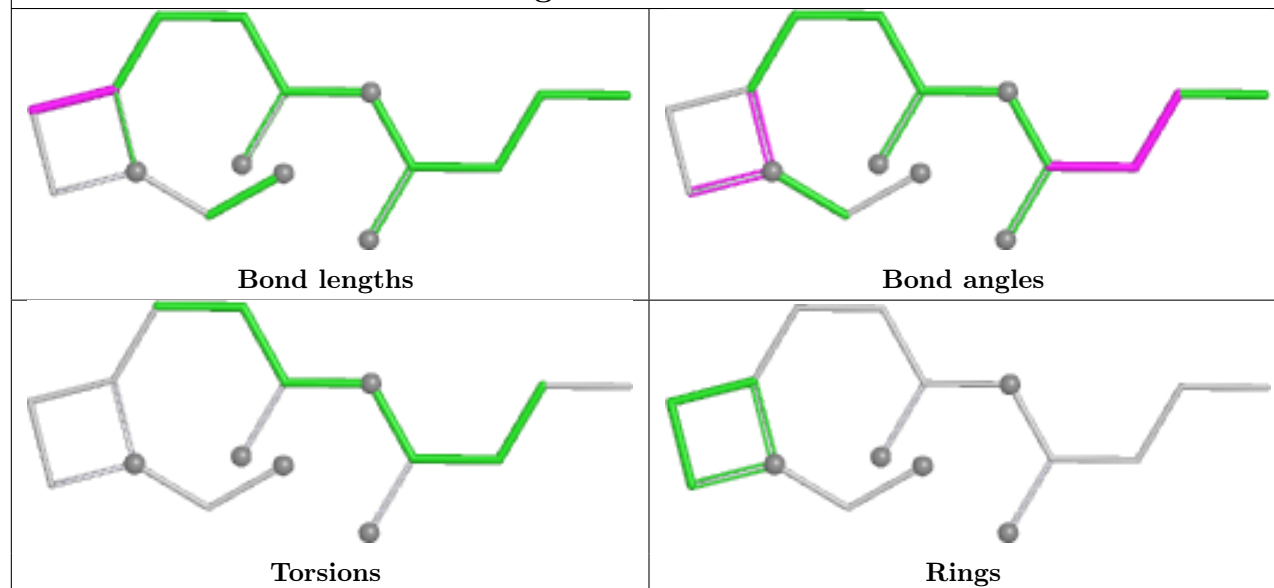




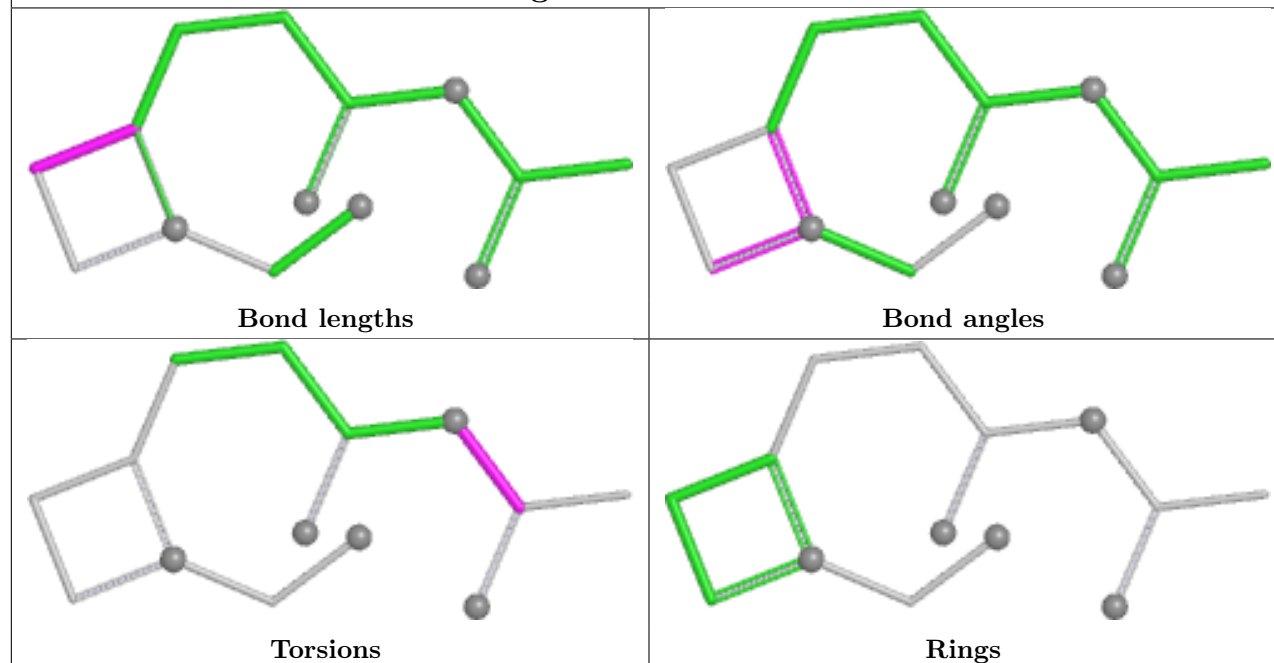
Ligand ZGV R 303



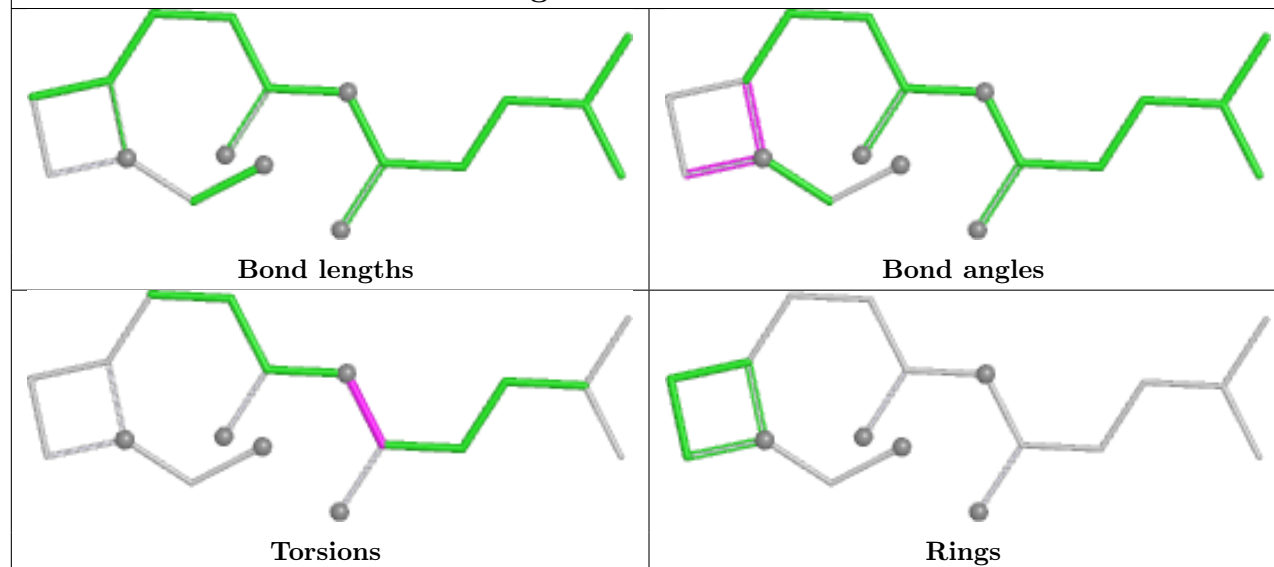
Ligand ZGV J 302



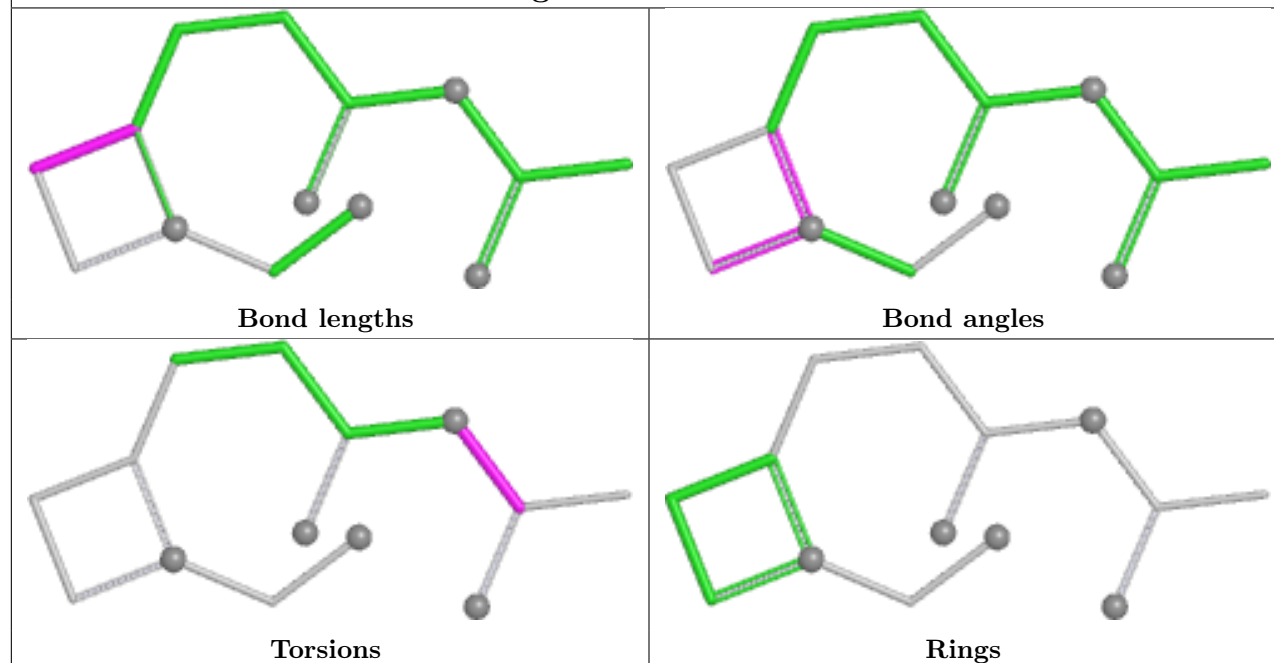
Ligand ZGV C 302



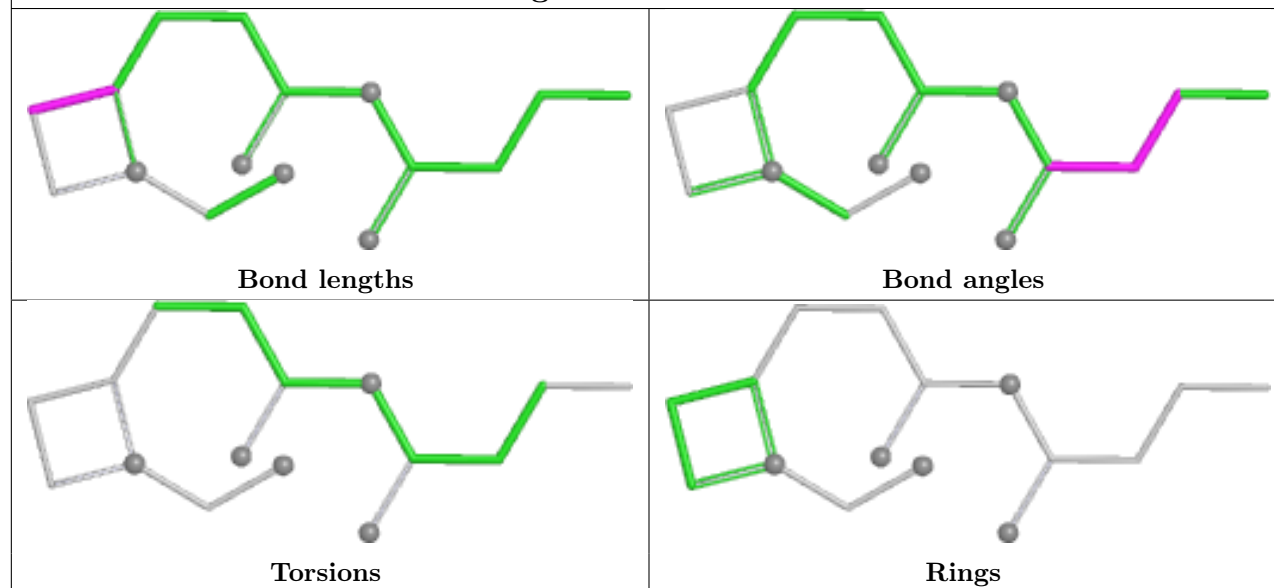
Ligand ZGV Y 302

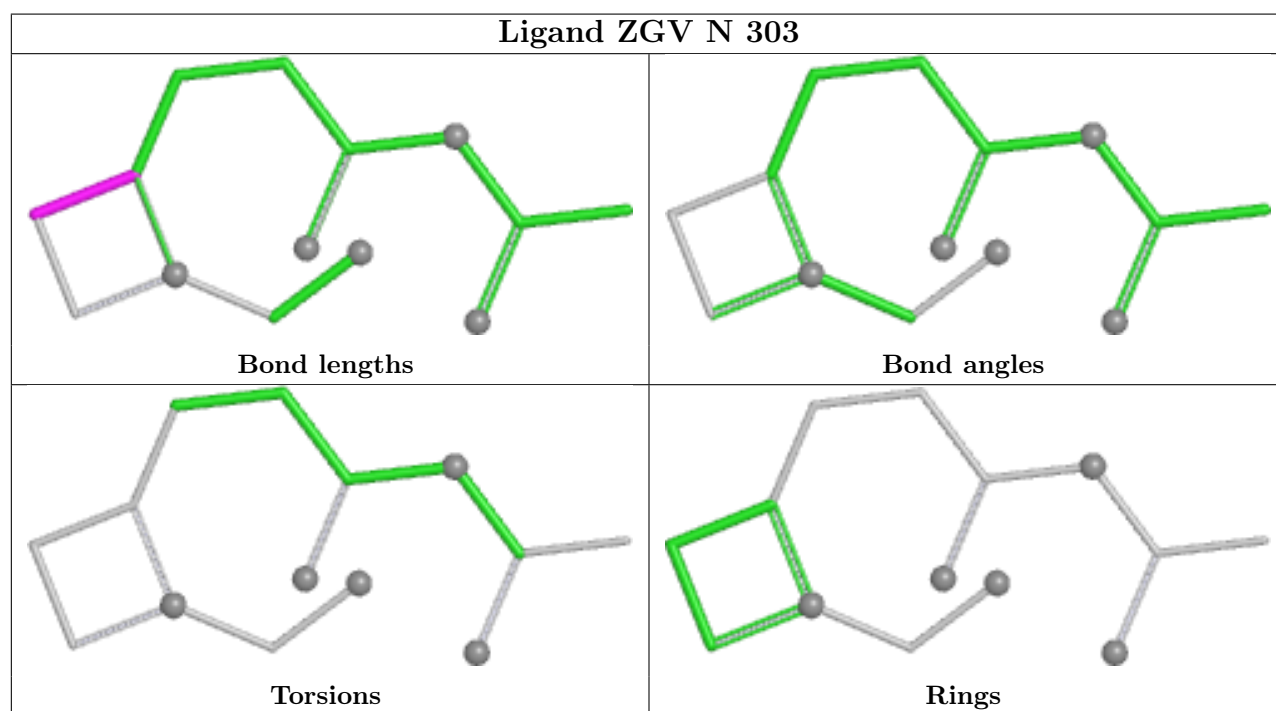
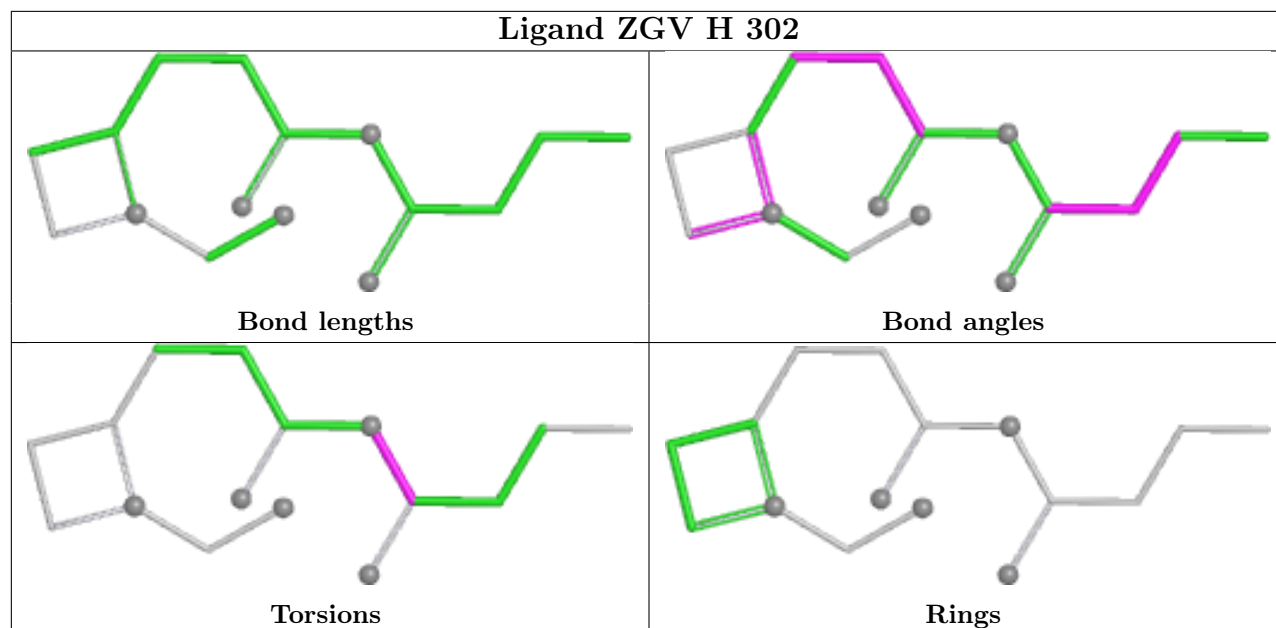


Ligand ZGV E 302

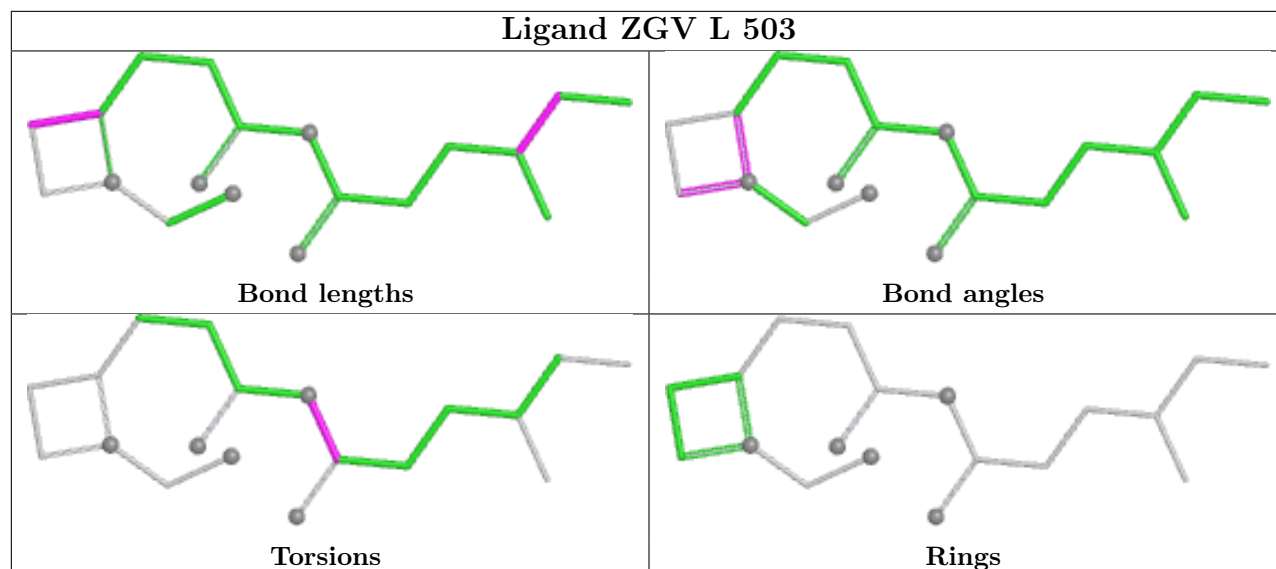


Ligand ZGV T 203

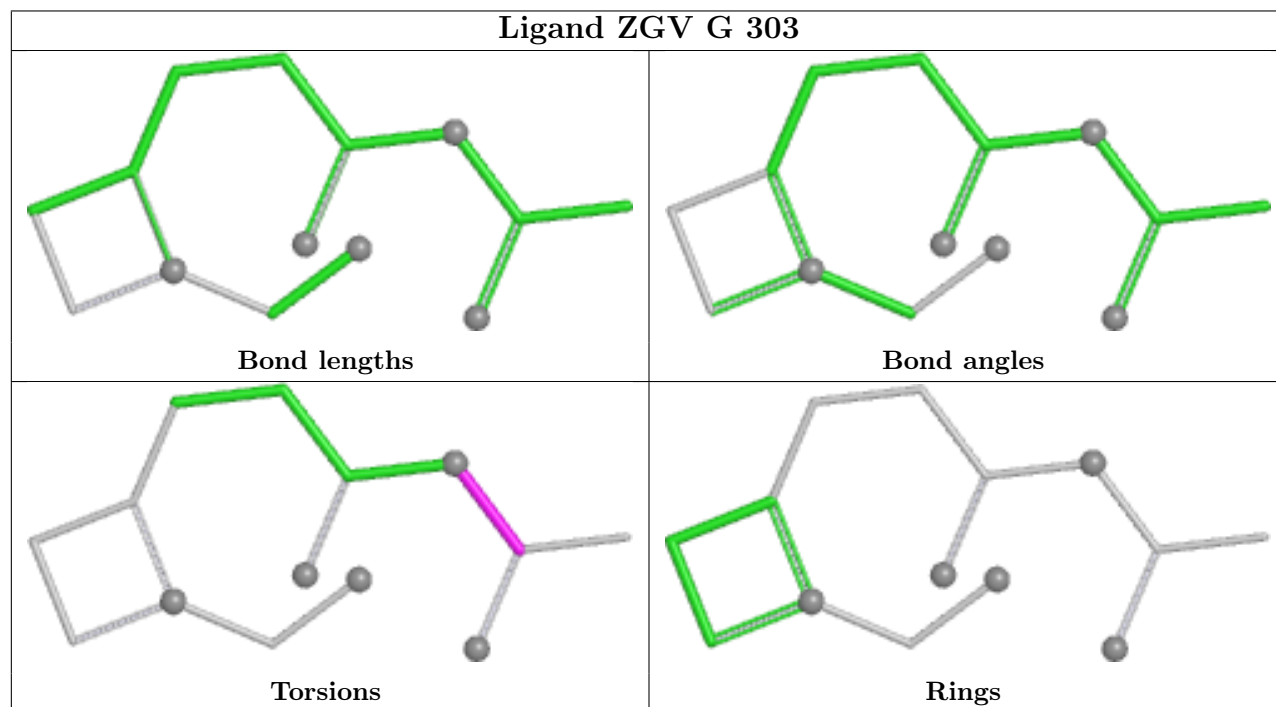




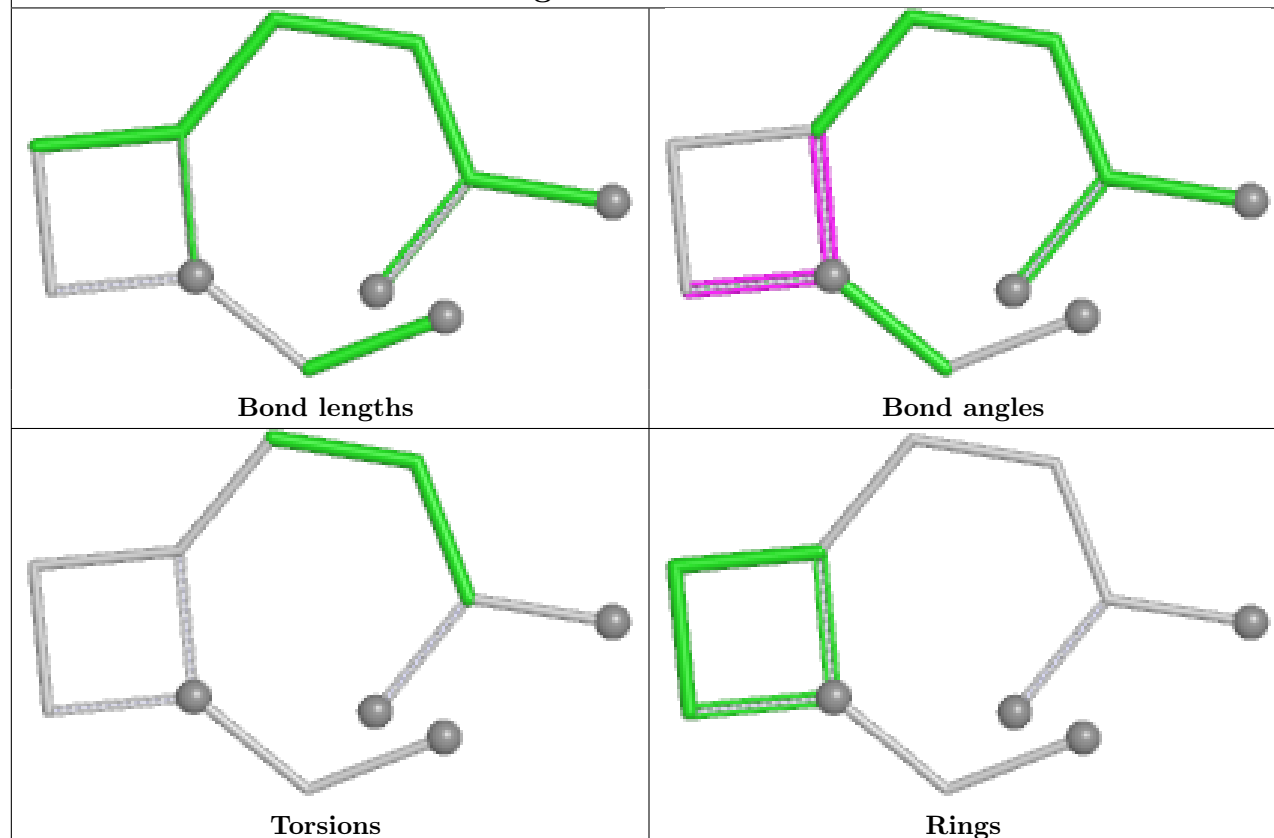
Ligand ZGV L 503



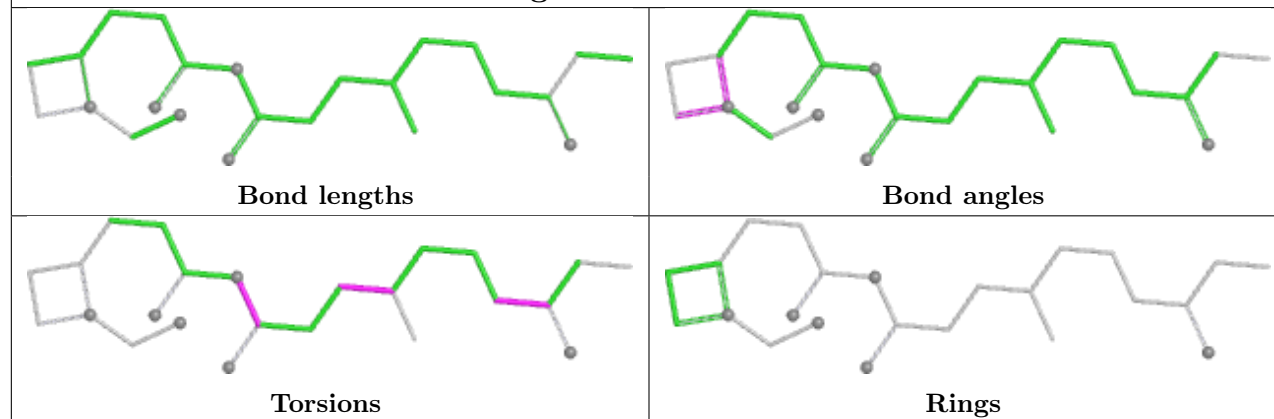
Ligand ZGV G 303



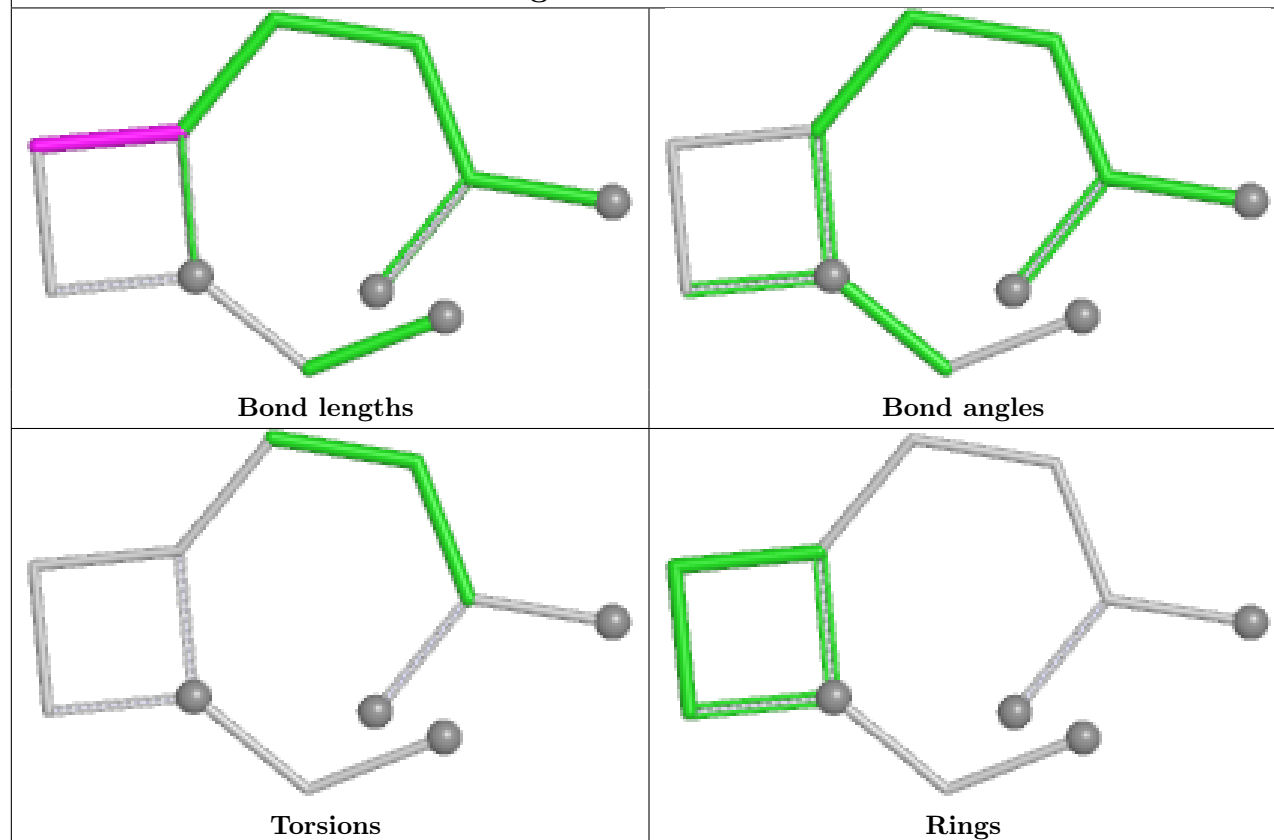
Ligand ZGV b 303



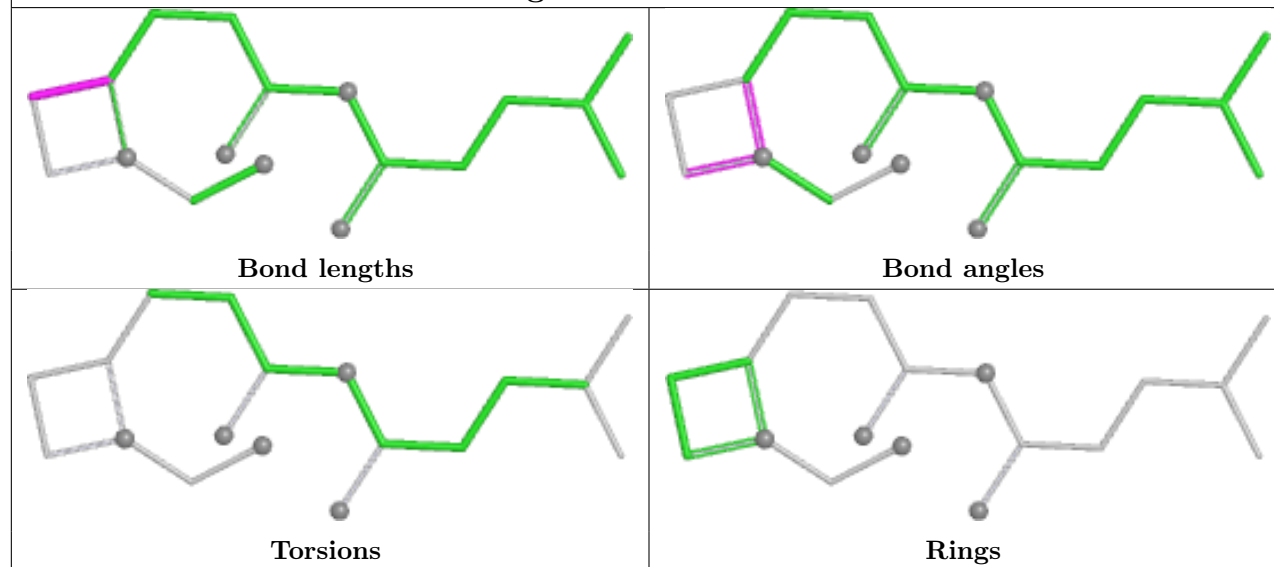
Ligand ZGV A 304

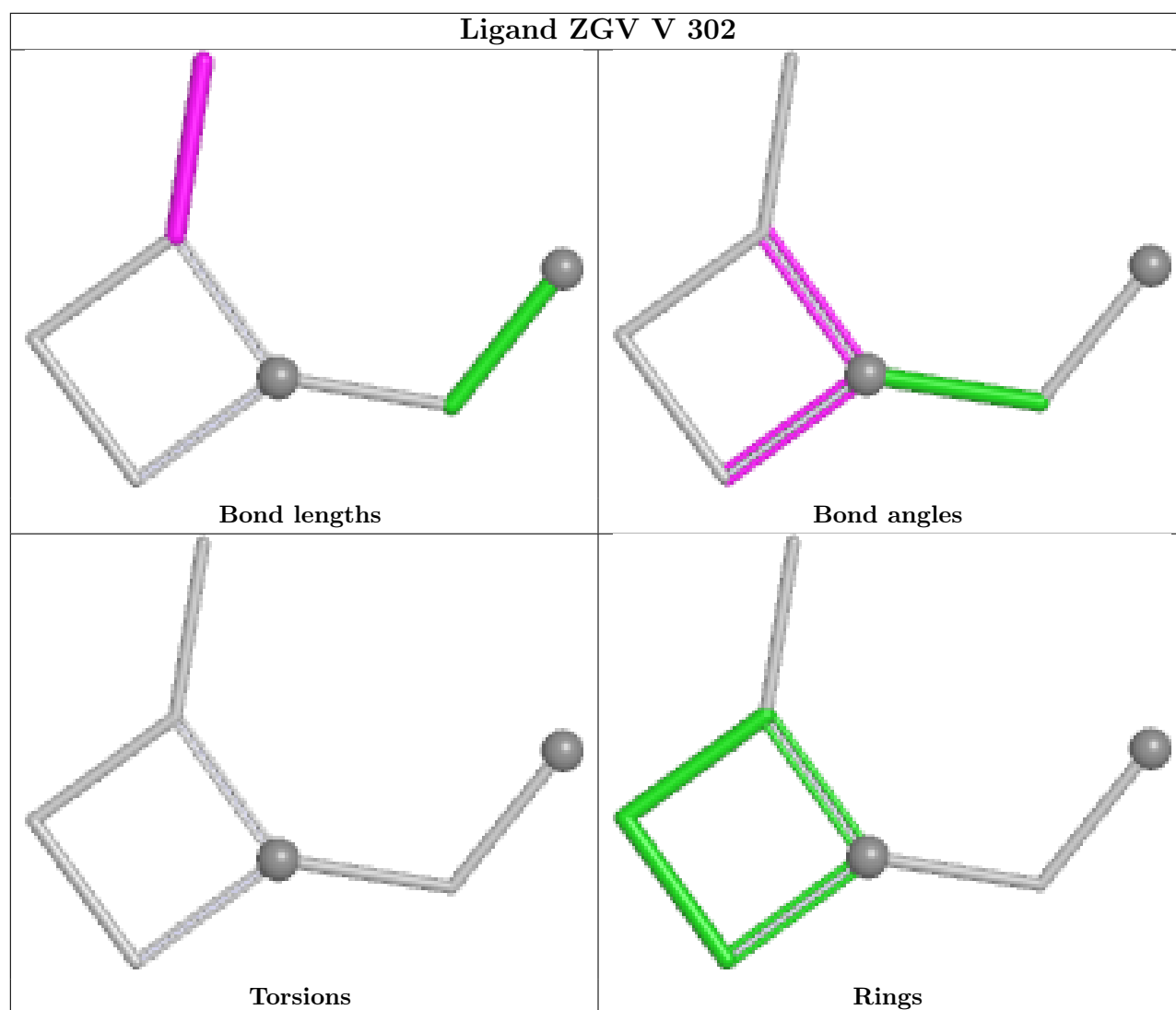


Ligand ZGV X 203

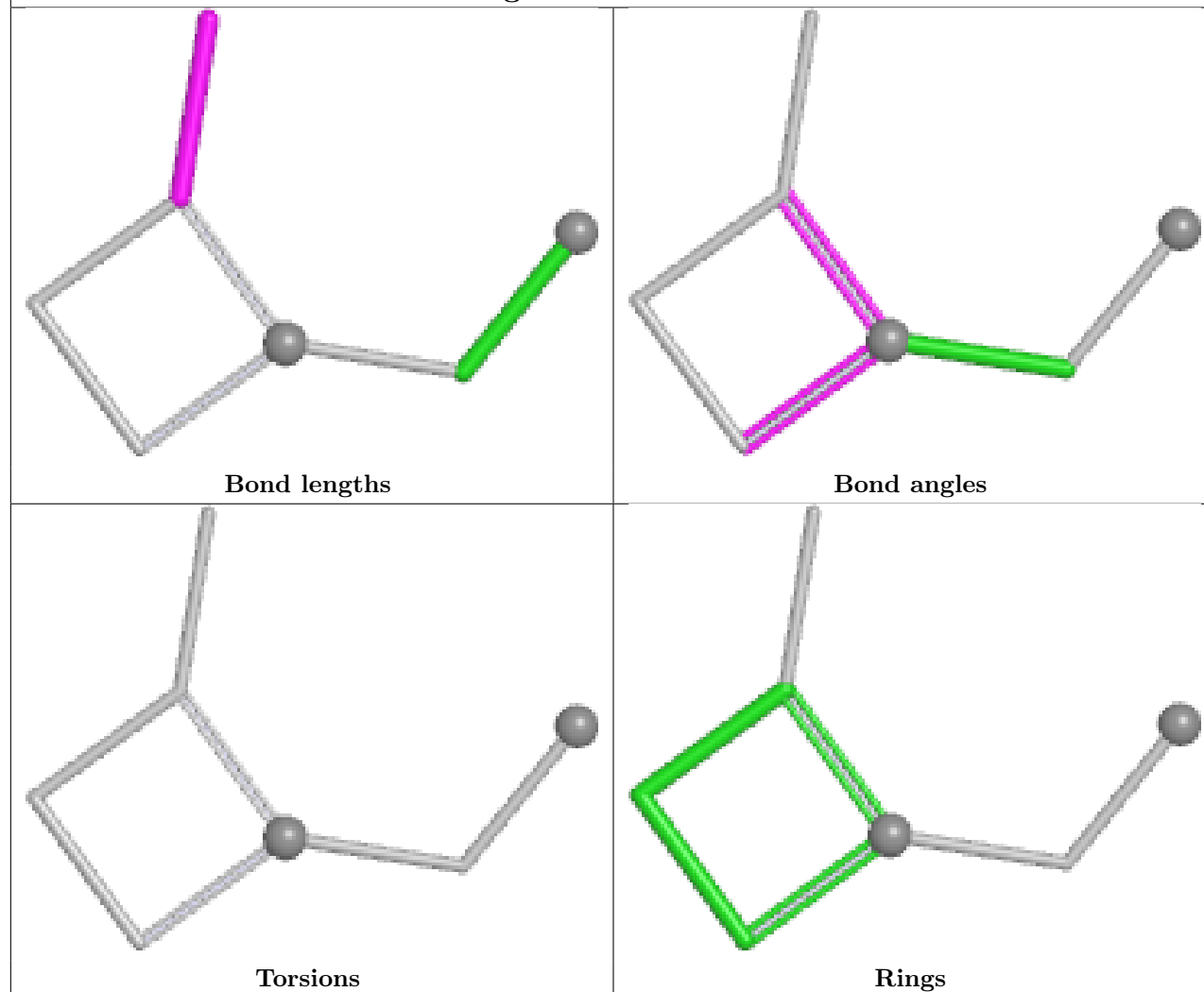


Ligand ZGV M 302

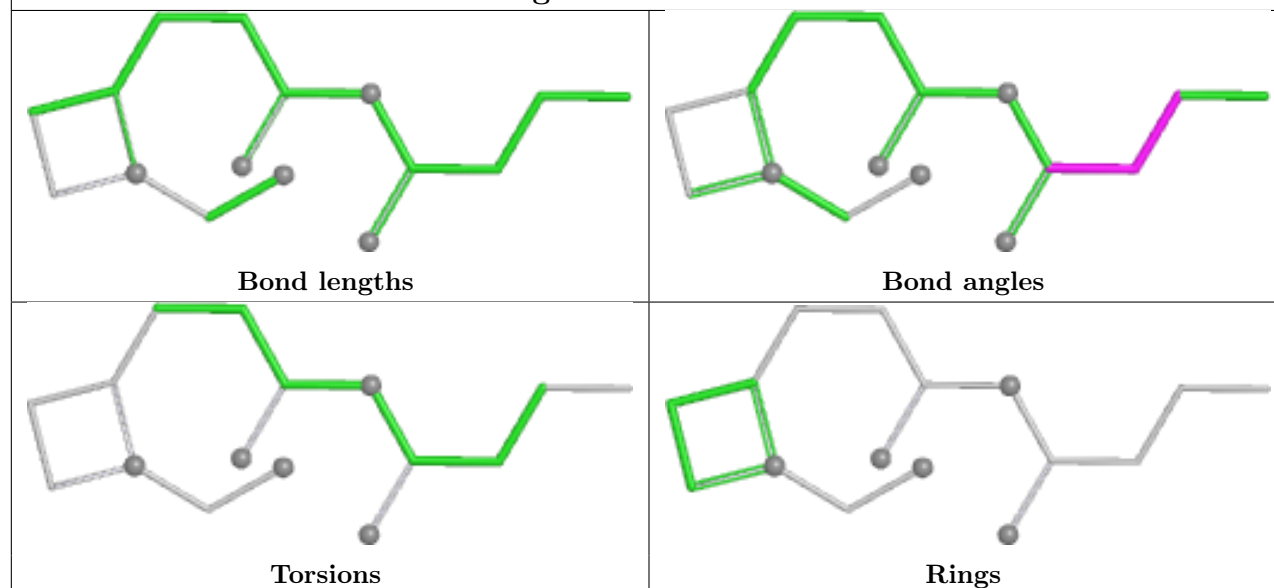


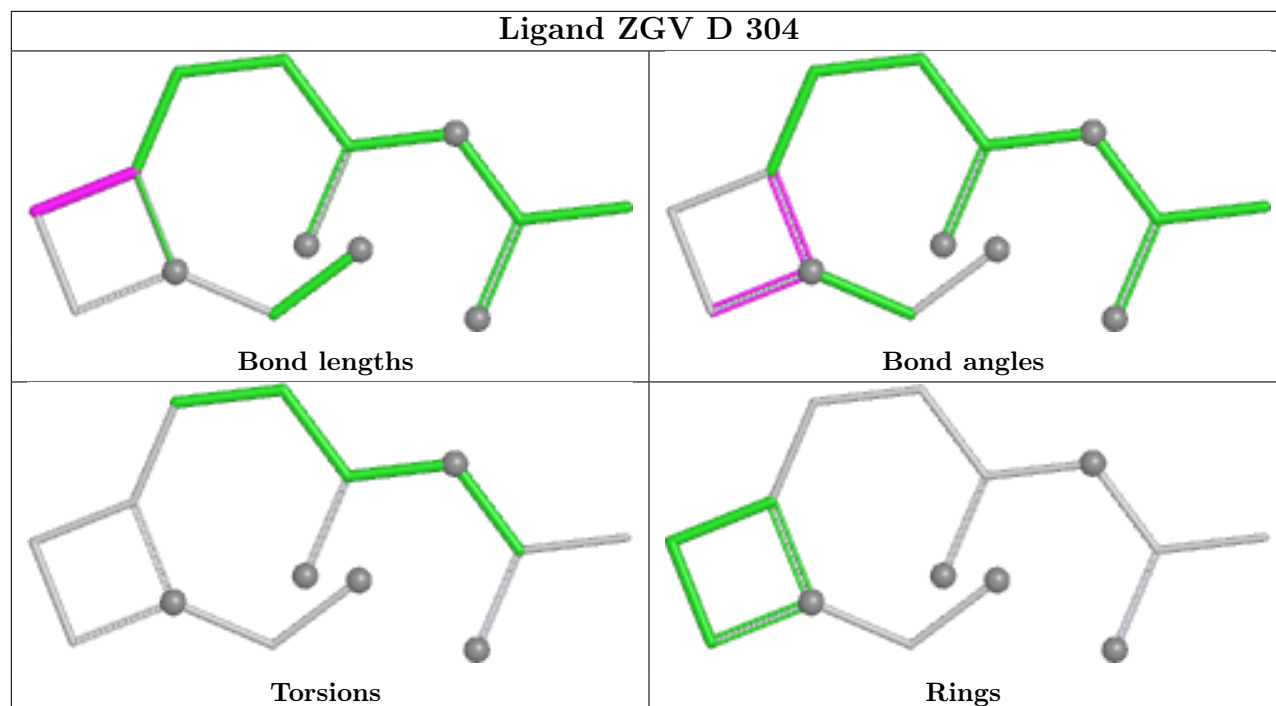


Ligand ZGV Z 304



Ligand ZGV F 405





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	182/193 (94%)	-0.00	3 (1%) 70 63	52, 63, 87, 111	0
1	B	181/193 (93%)	0.03	4 (2%) 62 54	52, 60, 86, 96	0
1	C	179/193 (92%)	-0.06	5 (2%) 55 47	48, 56, 87, 137	0
1	D	181/193 (93%)	-0.05	1 (0%) 85 82	48, 59, 80, 134	0
1	E	182/193 (94%)	0.03	2 (1%) 78 73	47, 58, 83, 153	0
1	F	180/193 (93%)	-0.03	4 (2%) 62 54	46, 58, 89, 134	0
1	G	179/193 (92%)	0.16	6 (3%) 48 41	51, 62, 90, 109	0
1	H	177/193 (91%)	-0.03	1 (0%) 85 82	50, 62, 81, 129	0
1	I	181/193 (93%)	0.02	0 100 100	50, 61, 90, 127	0
1	J	181/193 (93%)	-0.03	2 (1%) 78 73	47, 57, 84, 116	0
1	K	178/193 (92%)	0.01	2 (1%) 78 73	46, 58, 84, 131	0
1	L	179/193 (92%)	-0.05	2 (1%) 78 73	49, 57, 89, 150	0
1	M	179/193 (92%)	-0.01	2 (1%) 78 73	48, 59, 84, 141	0
1	N	180/193 (93%)	-0.05	3 (1%) 69 62	47, 60, 87, 114	0
1	O	179/193 (92%)	-0.02	4 (2%) 62 54	45, 56, 82, 112	0
1	P	181/193 (93%)	-0.01	4 (2%) 62 54	44, 54, 79, 112	0
1	Q	182/193 (94%)	-0.02	4 (2%) 62 54	44, 57, 87, 124	0
1	R	181/193 (93%)	0.03	3 (1%) 69 62	47, 59, 81, 128	0
1	S	181/193 (93%)	-0.09	3 (1%) 69 62	47, 56, 81, 152	0
1	T	179/193 (92%)	0.05	5 (2%) 55 47	49, 60, 89, 124	0
1	U	179/193 (92%)	-0.04	3 (1%) 69 62	47, 59, 84, 118	0
1	V	181/193 (93%)	-0.06	2 (1%) 78 73	44, 55, 80, 111	0
1	W	174/193 (90%)	-0.11	1 (0%) 85 82	45, 56, 78, 93	0
1	X	179/193 (92%)	-0.02	4 (2%) 62 54	47, 59, 82, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	179/193 (92%)	-0.14	3 (1%) 69 62	45, 55, 84, 126	0
1	Z	179/193 (92%)	-0.06	1 (0%) 85 82	47, 61, 89, 133	0
1	a	177/193 (91%)	0.09	4 (2%) 61 53	51, 62, 91, 120	0
1	b	180/193 (93%)	-0.03	4 (2%) 62 54	48, 57, 84, 109	0
All	All	5030/5404 (93%)	-0.02	82 (1%) 70 63	44, 59, 86, 153	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3	VAL	4.4
1	V	17	PHE	4.4
1	G	41	ASN	4.0
1	M	17	PHE	4.0
1	C	6	VAL	4.0
1	A	101	PHE	3.9
1	E	17	PHE	3.9
1	X	17	PHE	3.8
1	Q	6	VAL	3.7
1	N	3	VAL	3.7
1	C	191	HIS	3.7
1	B	17	PHE	3.6
1	E	18	ASP	3.5
1	P	6	VAL	3.4
1	Q	5	MET	3.4
1	Y	191	HIS	3.3
1	a	3	VAL	3.3
1	P	7	ILE	3.3
1	G	3	VAL	3.2
1	G	182	TYR	3.2
1	b	190	THR	3.2
1	C	3	VAL	3.2
1	R	17	PHE	3.1
1	K	5	MET	3.1
1	D	190	THR	3.0
1	B	5	MET	3.0
1	V	193	ASN	3.0
1	Y	3	VAL	3.0
1	P	5	MET	3.0
1	S	17	PHE	2.9
1	T	3	VAL	2.9
1	O	104	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	T	6	VAL	2.9
1	J	3	VAL	2.8
1	H	17	PHE	2.7
1	M	3	VAL	2.7
1	X	26	GLU	2.7
1	b	41	ASN	2.6
1	L	5	MET	2.6
1	T	5	MET	2.6
1	B	3	VAL	2.5
1	b	6	VAL	2.5
1	U	3	VAL	2.5
1	F	190	THR	2.5
1	A	2	LEU	2.5
1	B	6	VAL	2.5
1	C	5	MET	2.4
1	G	192	ARG	2.4
1	O	181	GLU	2.4
1	R	108	LYS	2.4
1	U	2	LEU	2.4
1	O	6	VAL	2.4
1	S	192	ARG	2.4
1	X	5	MET	2.4
1	T	18	ASP	2.4
1	a	191	HIS	2.4
1	Q	3	VAL	2.4
1	Z	22	ARG	2.3
1	J	17	PHE	2.3
1	U	93	GLY	2.3
1	R	16	SER	2.3
1	S	6	VAL	2.2
1	F	17	PHE	2.2
1	N	184	LEU	2.2
1	b	192	ARG	2.2
1	a	4	PRO	2.2
1	A	17	PHE	2.2
1	O	190	THR	2.2
1	F	5	MET	2.2
1	G	5	MET	2.2
1	K	149	MET	2.1
1	G	190	THR	2.1
1	Q	182	TYR	2.1
1	C	190	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	a	190	THR	2.1
1	W	191	HIS	2.1
1	T	4	PRO	2.0
1	N	17	PHE	2.0
1	X	191	HIS	2.0
1	P	190	THR	2.0
1	Y	5	MET	2.0
1	L	3	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
4	ZGV	U	302	14/25	0.58	0.24	67,77,87,93	0
4	ZGV	C	302	14/25	0.62	0.22	55,67,79,85	0
3	ACT	G	302	4/4	0.66	0.20	56,58,69,69	0
4	ZGV	I	302	15/25	0.66	0.23	64,72,85,87	0
3	ACT	Z	303	4/4	0.66	0.23	54,59,66,66	0
4	ZGV	W	403	24/25	0.67	0.20	61,81,104,105	0
4	ZGV	B	304	14/25	0.68	0.19	54,68,81,86	0
4	ZGV	N	303	14/25	0.68	0.20	53,65,77,82	0
4	ZGV	T	203	16/25	0.69	0.19	56,66,77,80	0
4	ZGV	L	503	19/25	0.70	0.22	54,72,90,93	0
4	ZGV	D	304	14/25	0.70	0.20	61,73,82,88	0
4	ZGV	S	203	14/25	0.70	0.19	58,71,81,89	0
4	ZGV	A	304	24/25	0.71	0.20	66,81,98,102	0
4	ZGV	G	303	14/25	0.72	0.22	61,70,83,87	0
4	ZGV	Q	303	14/25	0.72	0.17	52,63,73,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZGV	R	303	14/25	0.72	0.20	55,67,79,90	0
4	ZGV	E	302	14/25	0.72	0.18	58,64,74,78	0
4	ZGV	J	302	16/25	0.72	0.20	55,66,76,81	0
4	ZGV	K	302	14/25	0.72	0.17	61,68,80,82	0
4	ZGV	F	405	16/25	0.72	0.23	62,74,89,92	0
2	MPD	D	303	8/8	0.73	0.22	57,69,73,74	0
4	ZGV	O	303	24/25	0.73	0.21	56,75,91,100	0
4	ZGV	V	302	7/25	0.75	0.17	48,51,62,62	0
4	ZGV	M	302	18/25	0.76	0.19	66,79,89,93	0
3	ACT	A	303	4/4	0.77	0.12	55,58,66,66	0
2	MPD	Q	304	8/8	0.78	0.18	55,67,73,80	0
4	ZGV	H	302	16/25	0.78	0.18	52,67,83,84	0
4	ZGV	Y	302	18/25	0.78	0.17	49,61,74,75	0
2	MPD	Q	302	8/8	0.80	0.17	55,66,71,72	0
3	ACT	B	303	4/4	0.80	0.18	54,59,65,65	0
4	ZGV	X	203	11/25	0.80	0.14	48,57,69,81	0
2	MPD	Z	302	8/8	0.80	0.19	56,67,72,72	0
2	MPD	H	301	8/8	0.81	0.21	53,64,66,72	0
4	ZGV	P	203	14/25	0.82	0.15	51,61,71,79	0
2	MPD	H	303	8/8	0.82	0.21	59,71,76,79	0
4	ZGV	Z	304	7/25	0.82	0.15	51,56,64,68	0
3	ACT	R	302	4/4	0.83	0.18	55,61,67,67	0
4	ZGV	b	303	11/25	0.83	0.13	52,61,74,80	0
2	MPD	D	302	8/8	0.84	0.19	54,66,68,69	0
3	ACT	X	202	4/4	0.84	0.23	56,58,71,71	0
2	MPD	D	301	8/8	0.84	0.21	54,66,71,71	0
2	MPD	S	201	8/8	0.84	0.18	48,58,60,62	0
2	MPD	S	202	8/8	0.84	0.23	52,63,67,73	0
2	MPD	P	201	8/8	0.85	0.17	47,57,60,71	0
3	ACT	L	501	4/4	0.85	0.19	56,62,68,68	0
2	MPD	b	302	8/8	0.85	0.17	50,64,67,68	0
3	ACT	C	303	4/4	0.85	0.14	49,57,59,60	0
4	ZGV	a	302	7/25	0.86	0.12	50,52,63,63	0
2	MPD	K	303	8/8	0.86	0.17	51,62,65,67	0
2	MPD	a	301	8/8	0.87	0.18	53,65,68,69	0
2	MPD	U	301	8/8	0.87	0.18	56,68,72,73	0
2	MPD	I	303	8/8	0.88	0.16	51,62,65,71	0
2	MPD	F	402	8/8	0.88	0.16	49,61,65,67	0
2	MPD	M	301	8/8	0.88	0.17	49,61,63,66	0
2	MPD	O	302	8/8	0.88	0.14	49,59,64,64	0
2	MPD	C	301	8/8	0.88	0.15	49,60,63,63	0
2	MPD	B	302	8/8	0.88	0.15	56,68,72,75	0

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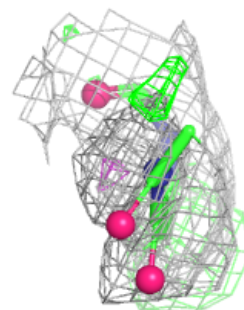
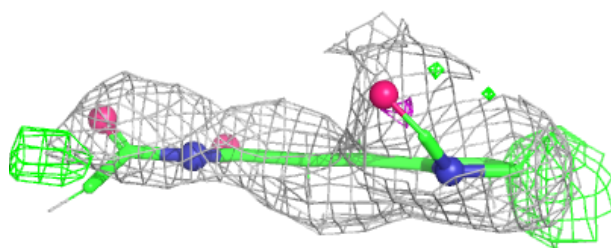
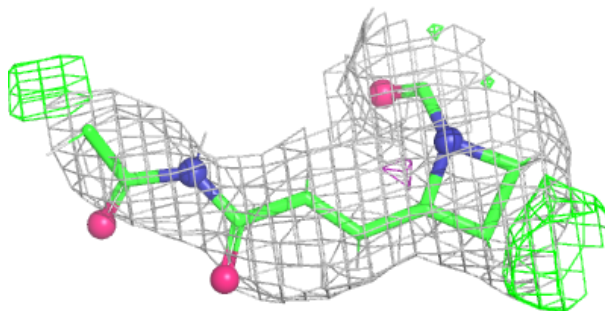
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MPD	I	301	8/8	0.88	0.16	53,64,69,70	0
2	MPD	Y	301	8/8	0.89	0.13	48,58,59,60	0
2	MPD	K	301	8/8	0.89	0.21	54,65,70,70	0
2	MPD	E	301	8/8	0.89	0.16	51,61,65,68	0
2	MPD	R	301	8/8	0.89	0.20	49,60,67,67	0
2	MPD	F	401	8/8	0.89	0.16	48,61,66,66	0
2	MPD	A	302	8/8	0.89	0.15	53,64,67,71	0
2	MPD	T	201	8/8	0.89	0.16	50,61,63,64	0
2	MPD	F	404	8/8	0.89	0.14	50,60,64,68	0
2	MPD	V	301	8/8	0.89	0.17	52,64,65,65	0
2	MPD	W	402	8/8	0.89	0.17	49,59,64,68	0
2	MPD	J	301	8/8	0.90	0.15	48,58,62,65	0
2	MPD	P	202	8/8	0.90	0.13	50,61,65,65	0
2	MPD	b	301	8/8	0.90	0.14	49,60,64,64	0
2	MPD	N	302	8/8	0.90	0.16	54,65,68,68	0
2	MPD	L	502	8/8	0.90	0.15	51,62,66,67	0
2	MPD	T	202	8/8	0.91	0.15	53,64,66,66	0
2	MPD	O	301	8/8	0.91	0.12	50,61,68,68	0
2	MPD	J	303	8/8	0.91	0.13	50,60,66,66	0
2	MPD	G	301	8/8	0.91	0.18	53,64,71,72	0
2	MPD	X	201	8/8	0.91	0.17	50,60,68,68	0
2	MPD	N	301	8/8	0.91	0.14	50,61,64,65	0
3	ACT	F	403	4/4	0.91	0.15	55,59,66,66	0
2	MPD	Y	303	8/8	0.91	0.15	47,57,63,63	0
2	MPD	Z	301	8/8	0.91	0.13	53,65,69,69	0
2	MPD	A	301	8/8	0.91	0.15	57,68,75,75	0
2	MPD	a	303	8/8	0.92	0.12	49,59,68,68	0
2	MPD	B	301	8/8	0.92	0.17	53,66,67,67	0
2	MPD	W	401	8/8	0.93	0.12	53,64,68,68	0
3	ACT	P	204	4/4	0.93	0.11	49,55,59,59	0
2	MPD	Q	301	8/8	0.93	0.15	48,60,62,62	0

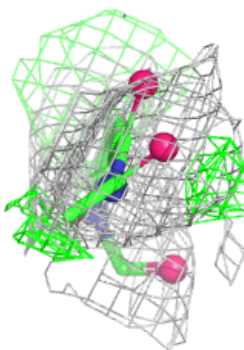
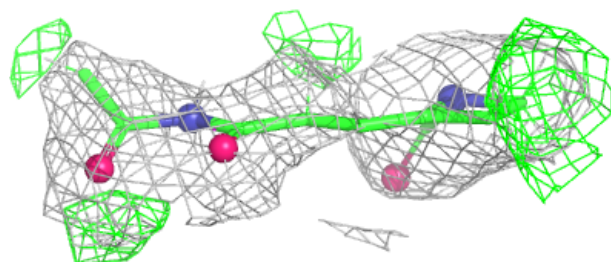
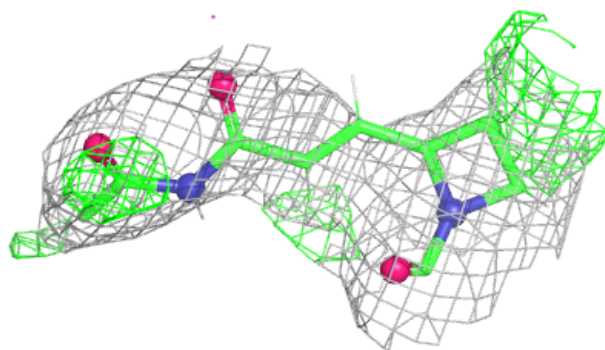
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZGV U 302:

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

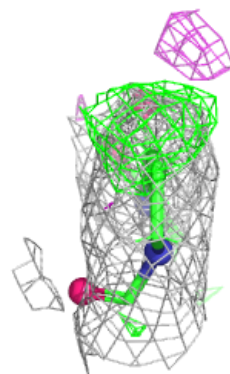
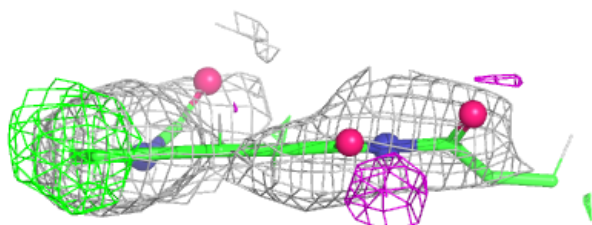
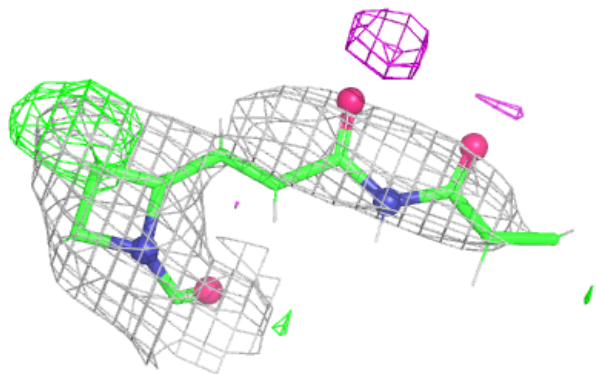
**Electron density around ZGV C 302:**

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

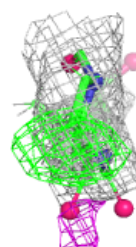
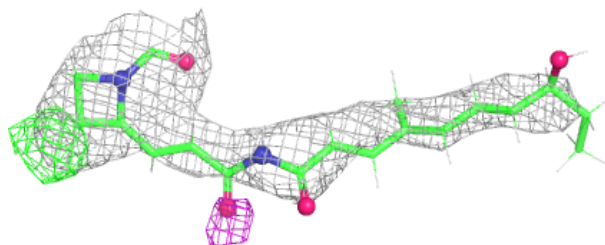


Electron density around ZGV I 302:

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

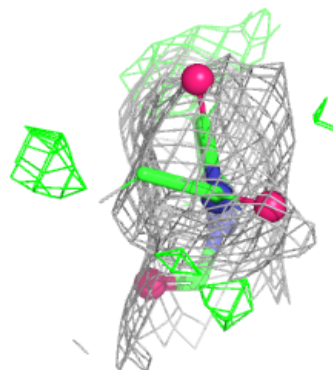
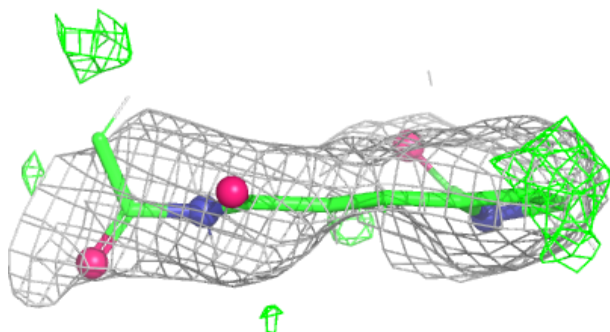
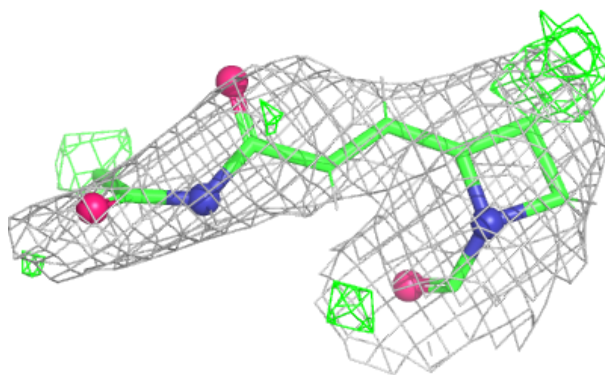
**Electron density around ZGV W 403:**

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

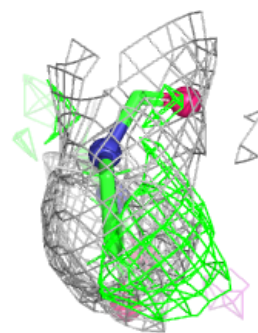
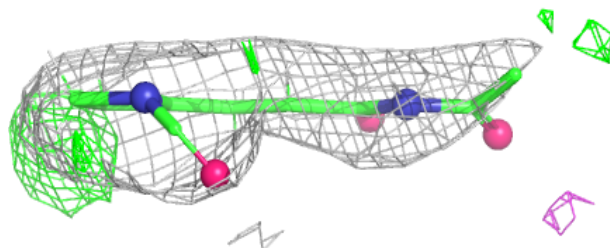
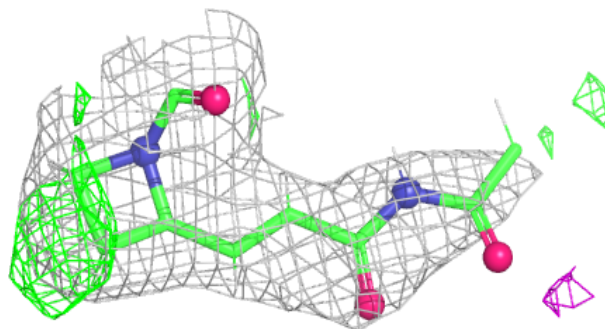


Electron density around ZGV B 304:

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

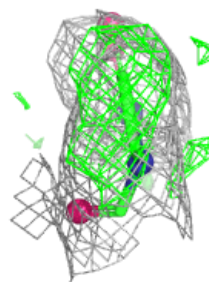
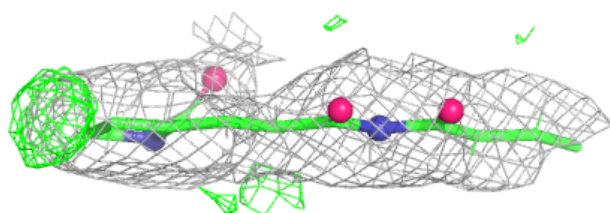
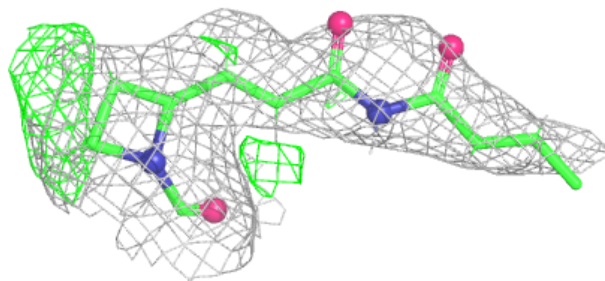
**Electron density around ZGV N 303:**

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

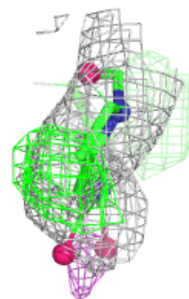
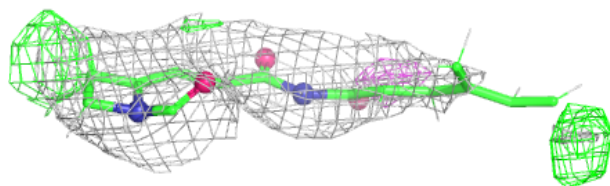
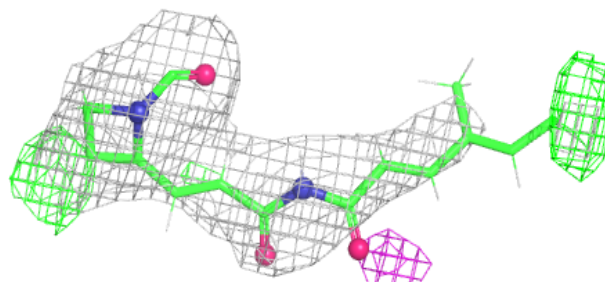


Electron density around ZGV T 203:

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

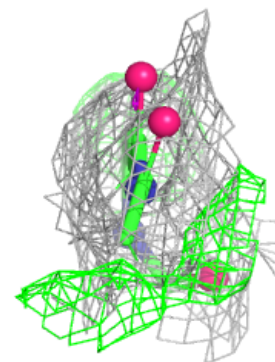
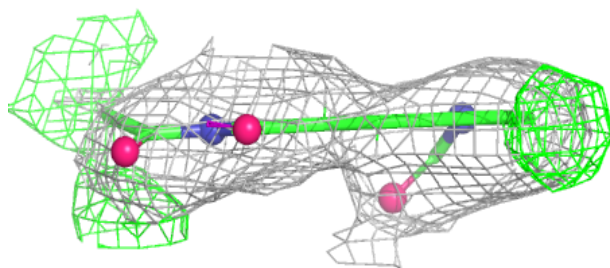
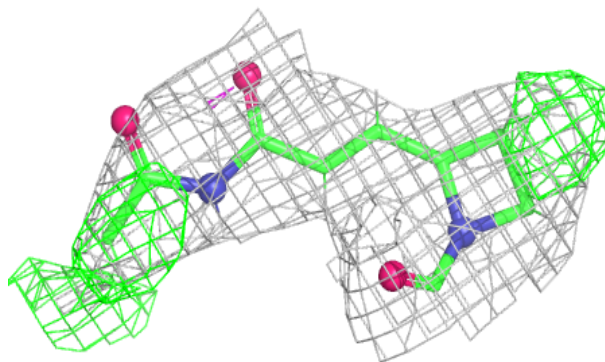
**Electron density around ZGV L 503:**

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

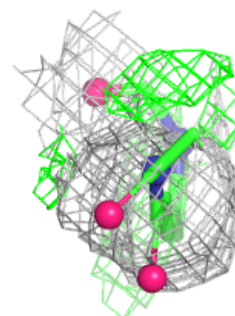
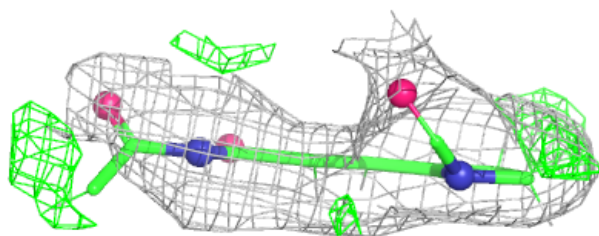
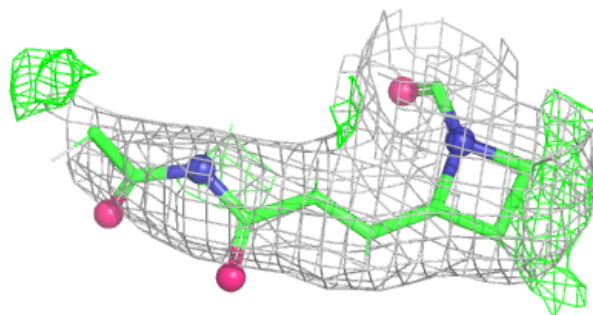


Electron density around ZGV D 304:

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

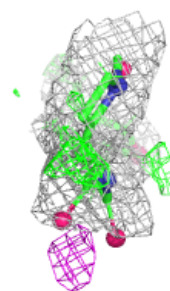
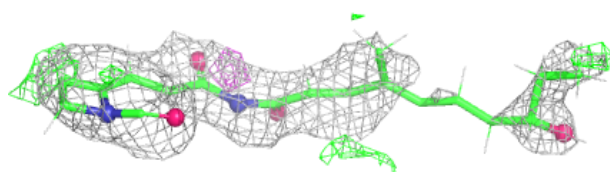
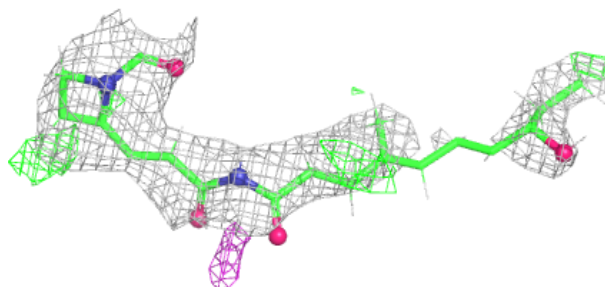
**Electron density around ZGV S 203:**

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

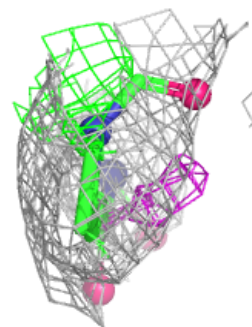
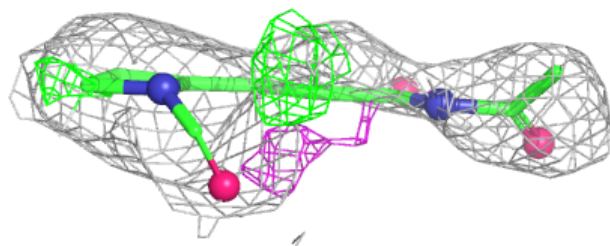
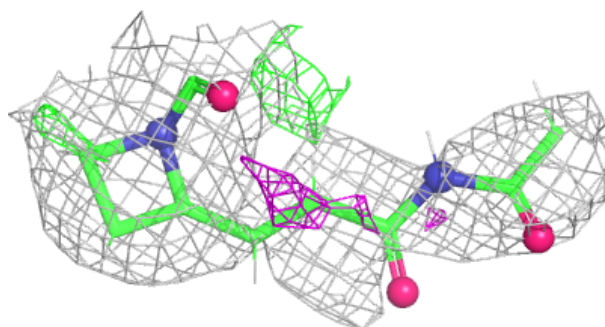


Electron density around ZGV A 304:

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

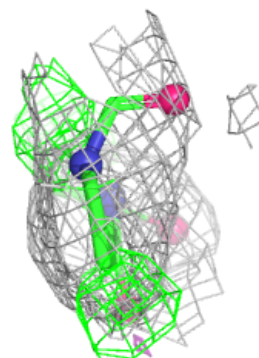
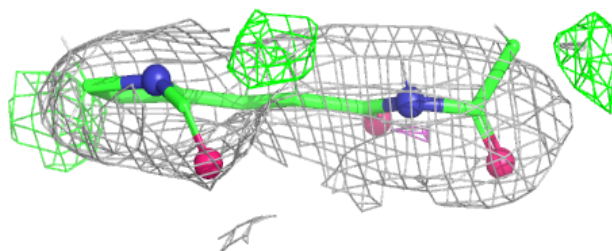
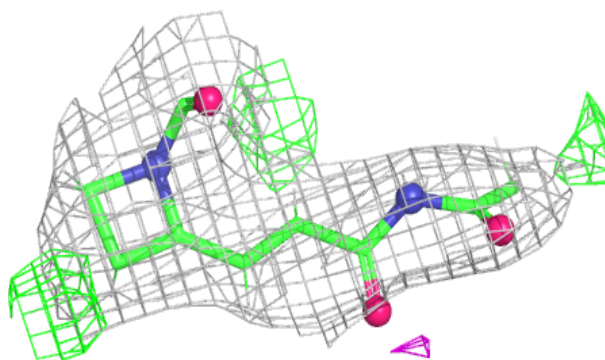
**Electron density around ZGV G 303:**

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

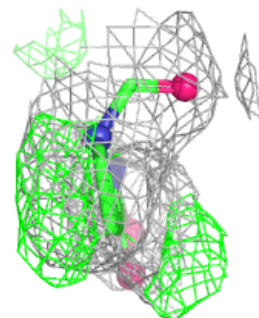
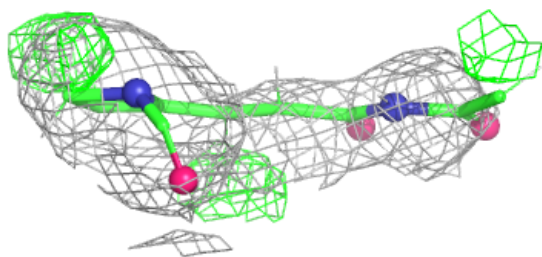
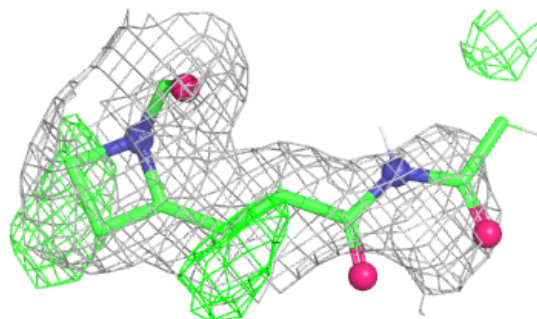


Electron density around ZGV Q 303:

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

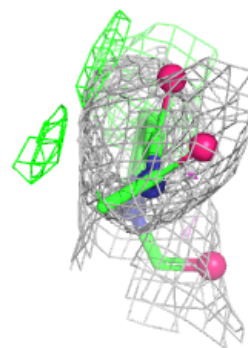
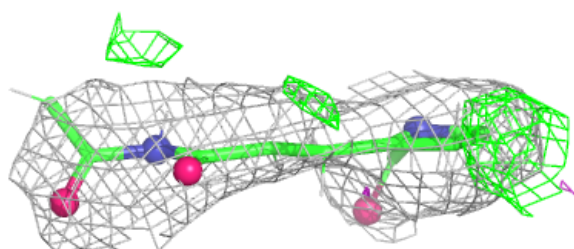
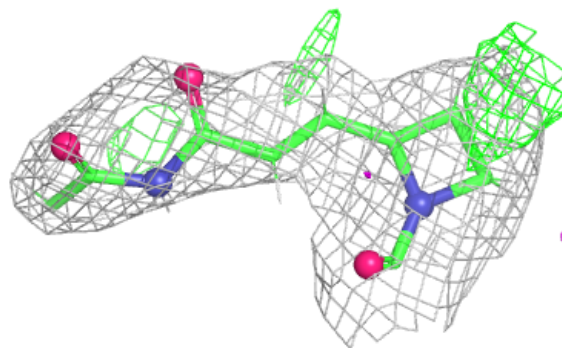
**Electron density around ZGV R 303:**

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

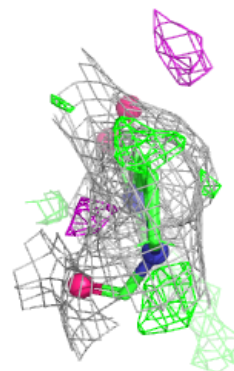
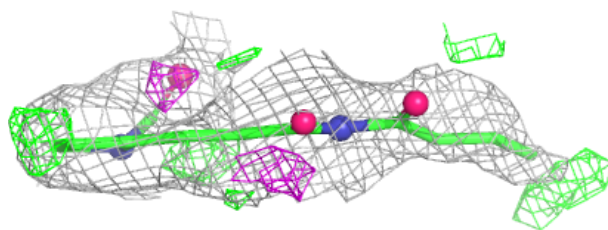
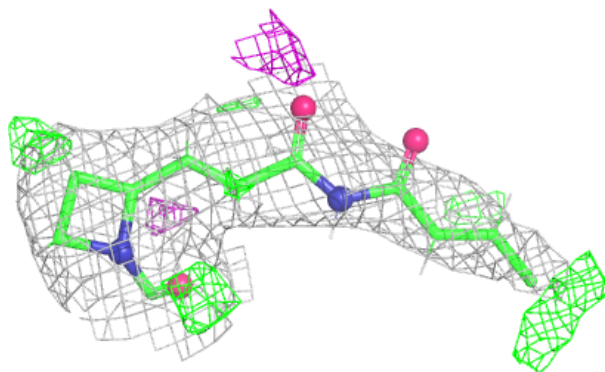


Electron density around ZGV E 302:

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

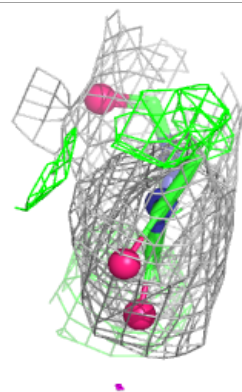
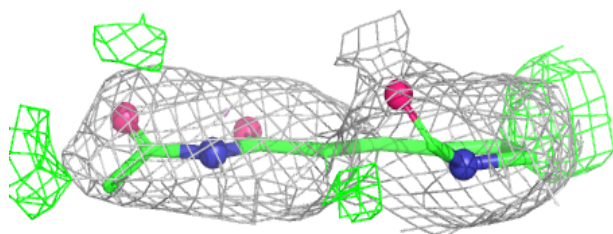
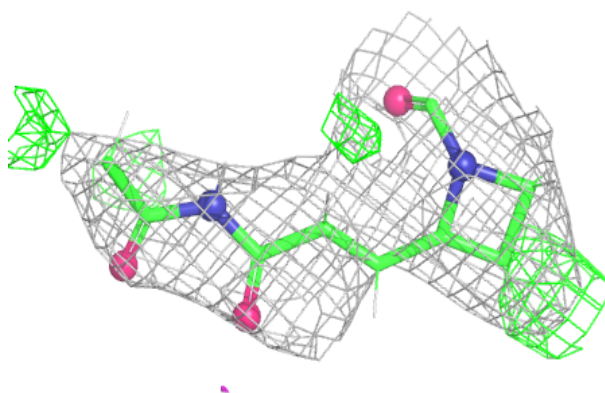
**Electron density around ZGV J 302:**

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

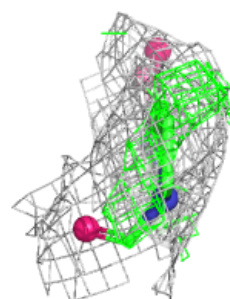
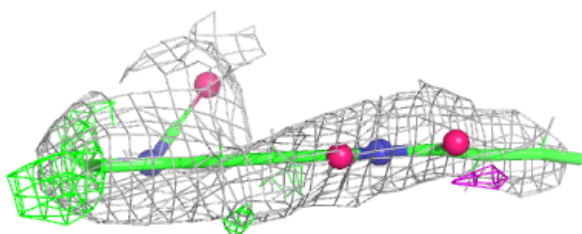
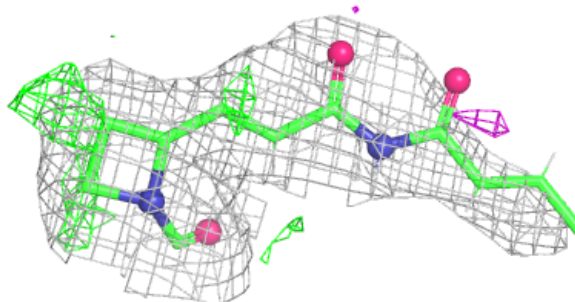


Electron density around ZGV K 302:

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

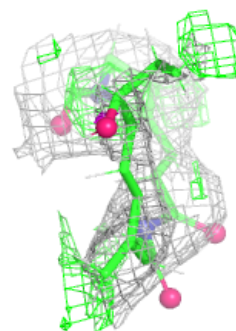
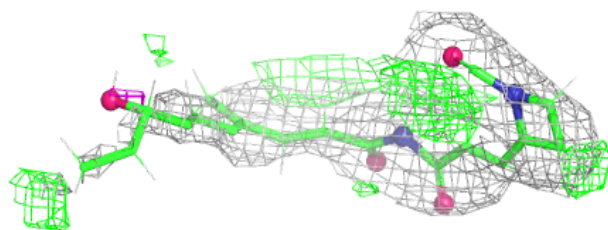
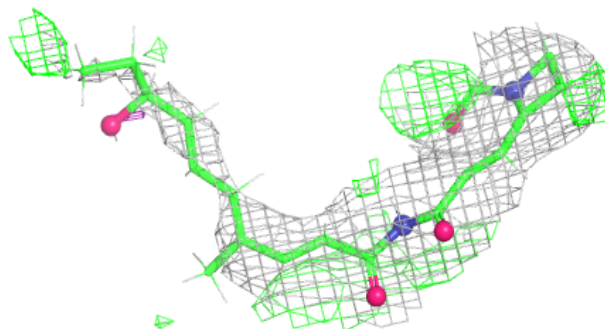
**Electron density around ZGV F 405:**

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



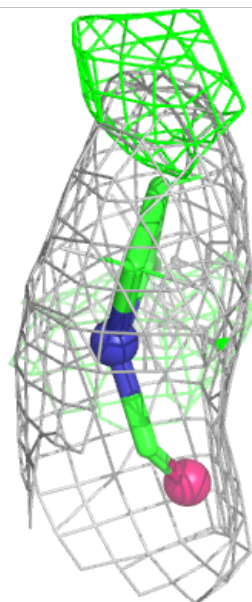
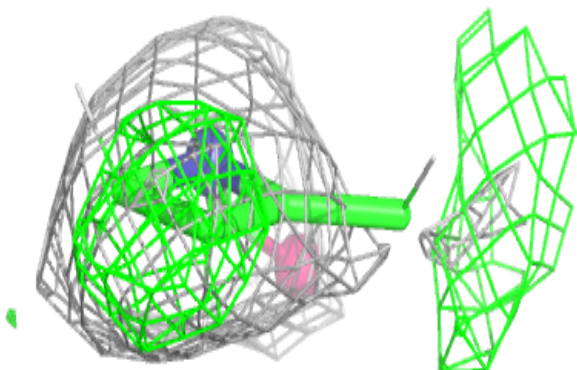
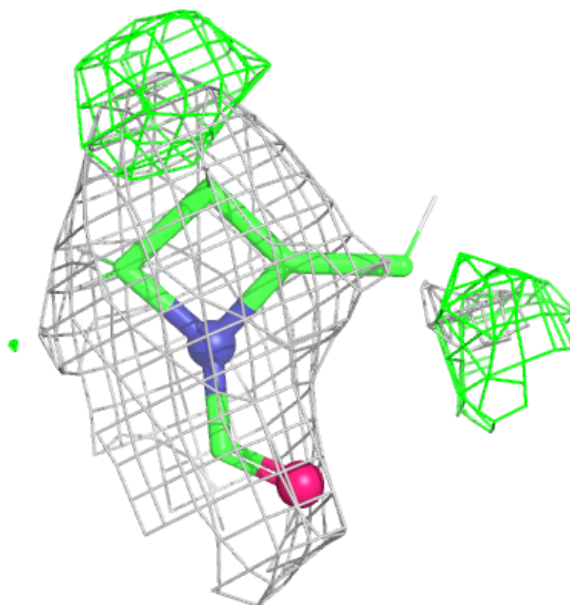
Electron density around ZGV O 303:

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



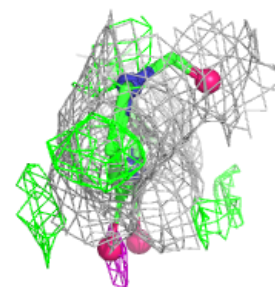
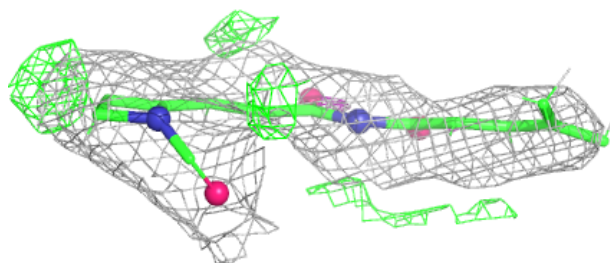
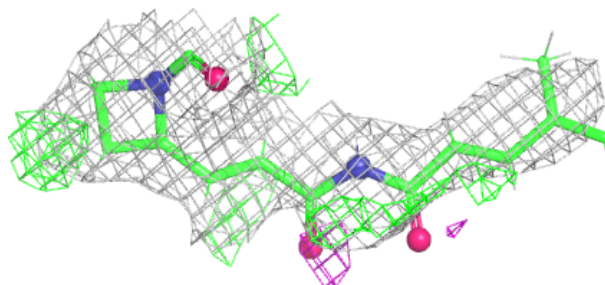
Electron density around ZGV V 302:

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

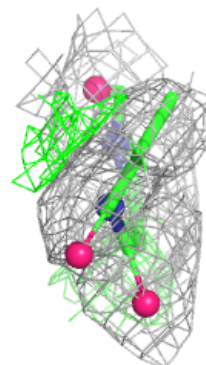
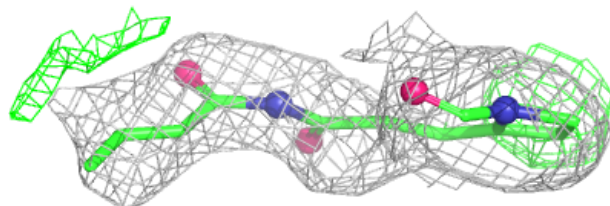
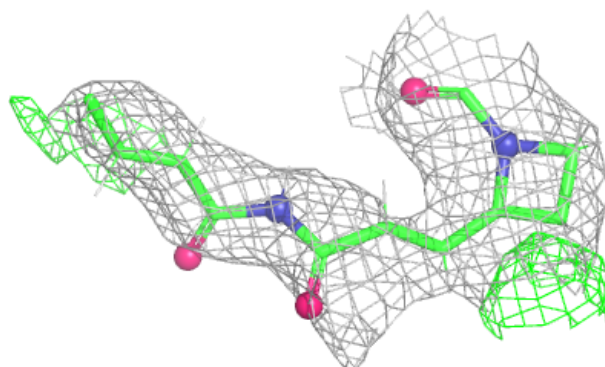


Electron density around ZGV M 302:

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

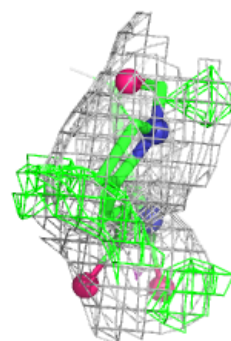
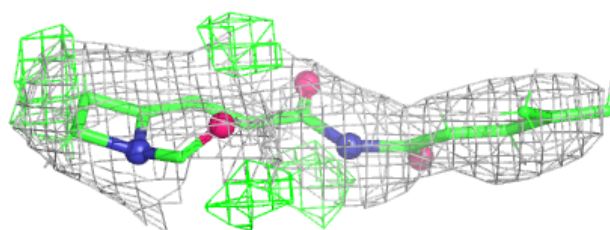
**Electron density around ZGV H 302:**

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

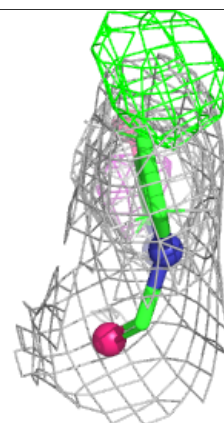
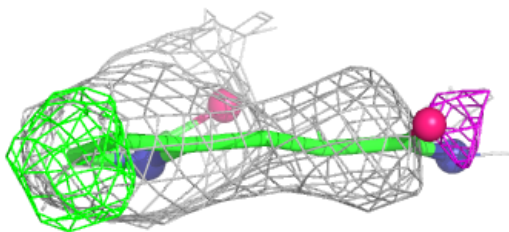
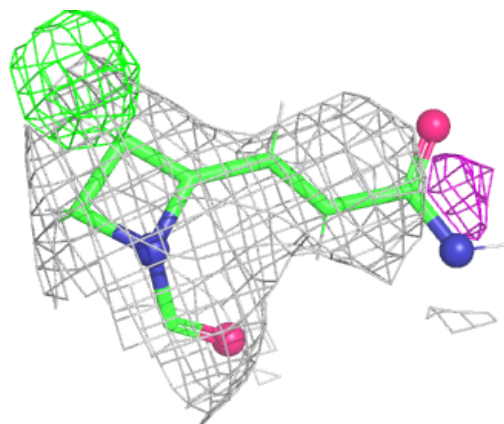


Electron density around ZGV Y 302:

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

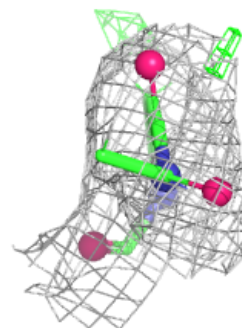
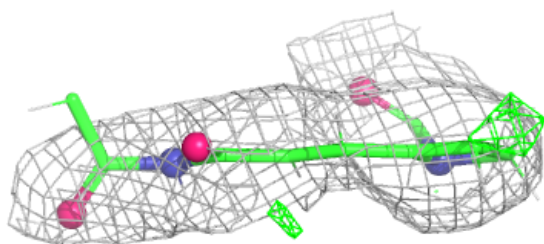
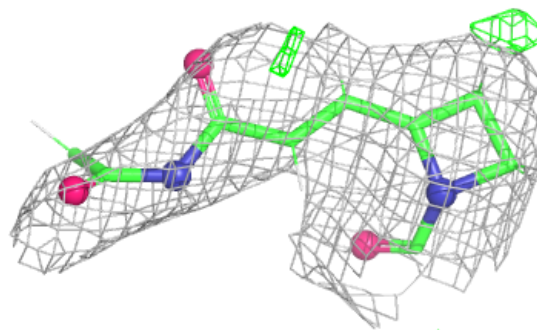
**Electron density around ZGV X 203:**

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



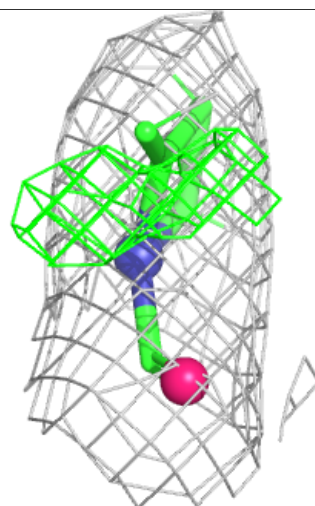
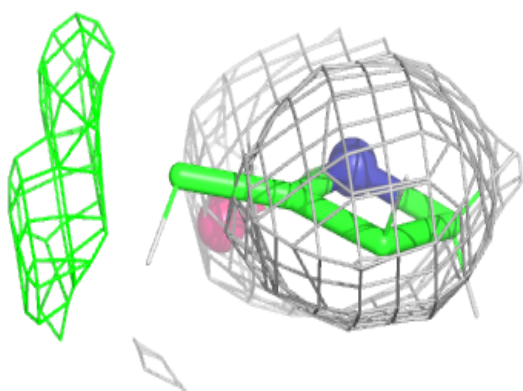
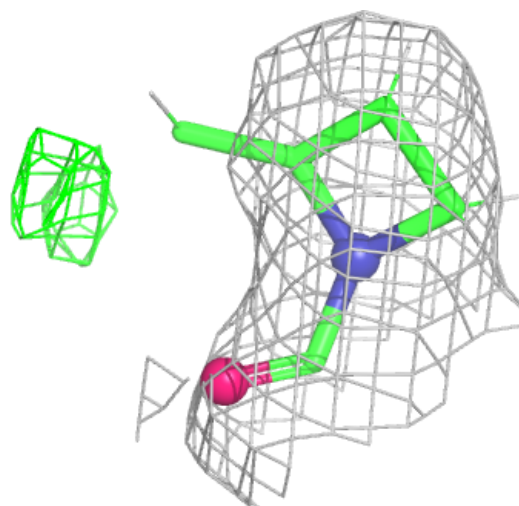
Electron density around ZGV P 203:

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



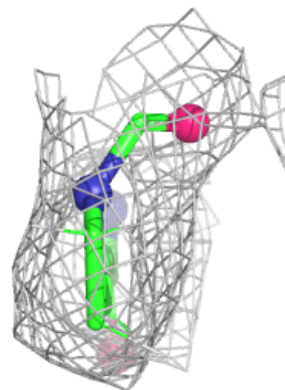
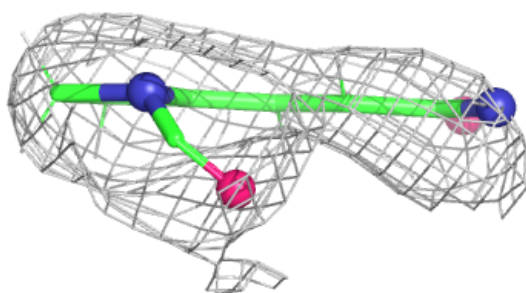
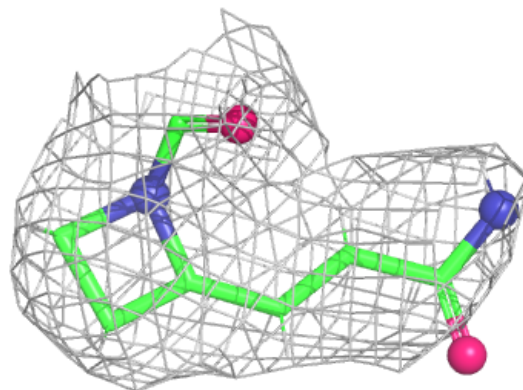
Electron density around ZGV Z 304:

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



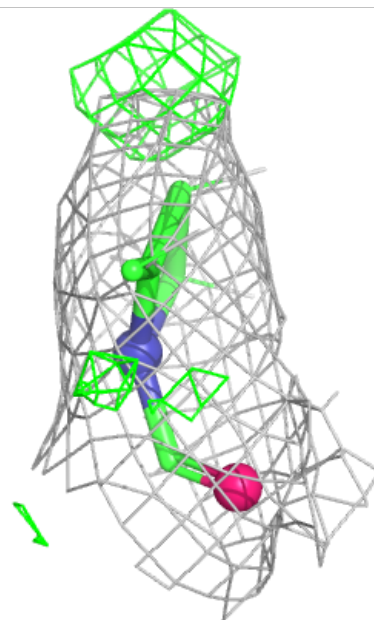
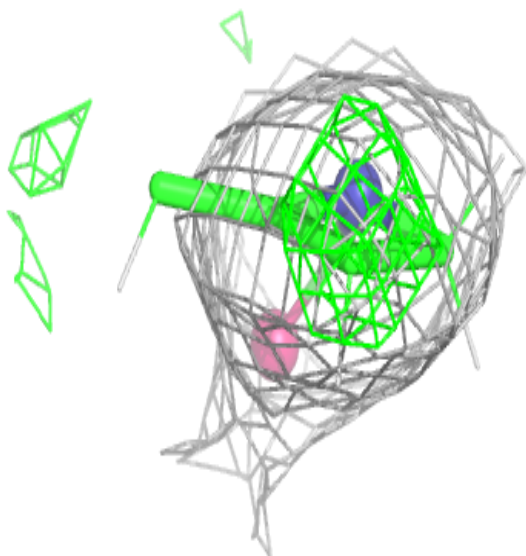
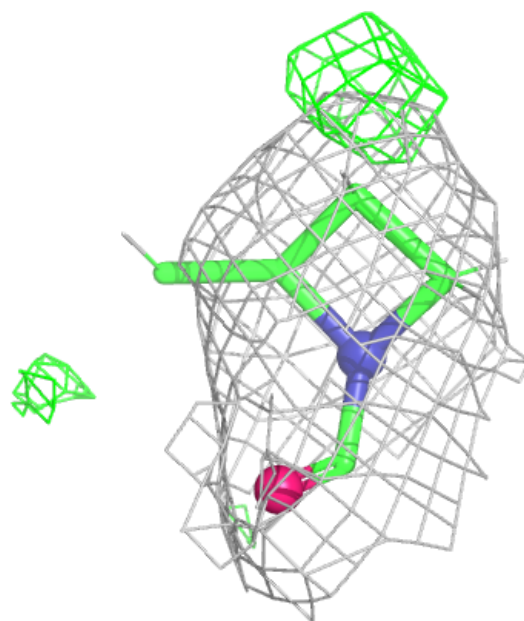
Electron density around ZGV b 303:

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



Electron density around ZGV a 302:

$2mF_o-DF_c$ (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.