



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:47 PM UTC

PDB ID : 8ERB / pdb_00008erb
Title : Crystal structure of Fub7 in complex with vinylglycine ketimine
Authors : Hai, Y.
Deposited on : 2022-10-11
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

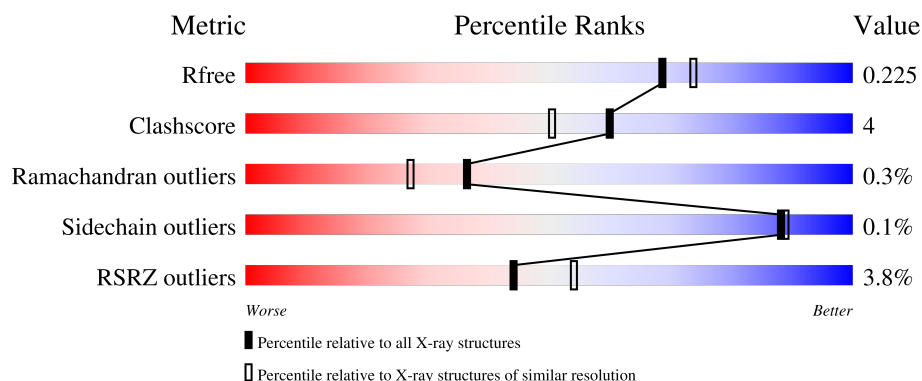
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

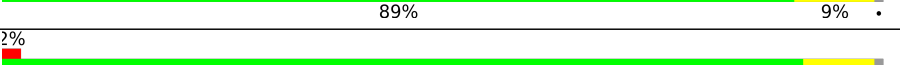
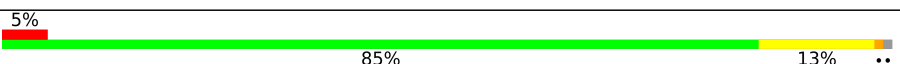
The reported resolution of this entry is 1.98 Å.

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.



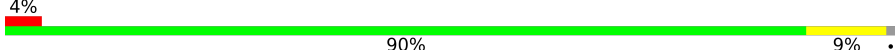
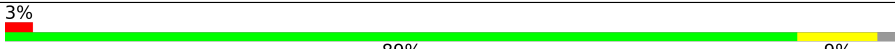
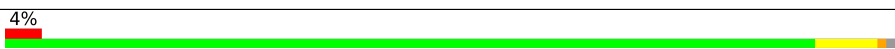
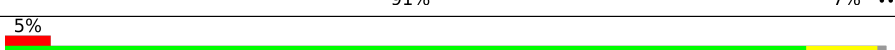
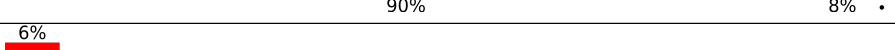
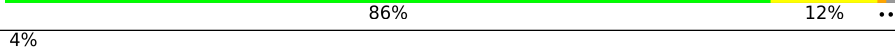
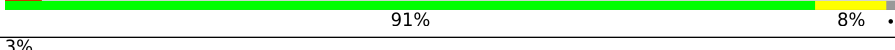
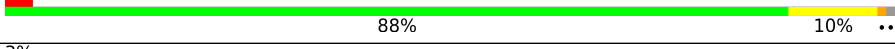
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	433	
1	B	433	
1	C	433	
1	D	433	
1	E	433	

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Mol	Chain	Length	Quality of chain
1	F	433	 4% 86% 12% .
1	G	433	 4% 90% 9% .
1	H	433	 3% 89% 9% .
1	I	433	 4% 91% 7% ..
1	J	433	 5% 90% 8% .
1	K	433	 6% 86% 12% ..
1	L	433	 4% 91% 8% .
1	M	433	 3% 88% 10% ..
1	N	433	 3% 87% 10% .
1	P	433	 4% 88% 10% ..
1	Q	433	 4% 90% 8% ..

2 Entry composition

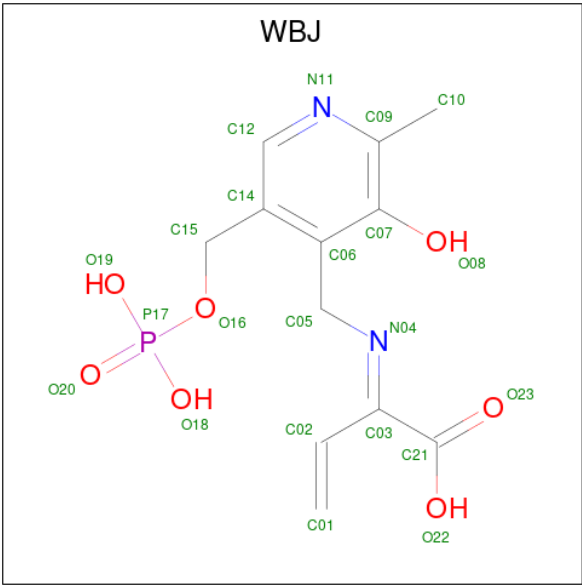
There are 3 unique types of molecules in this entry. The entry contains 55304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sulphydrylase FUB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	1	0
			3300	2096	570	627	7			
1	B	427	Total	C	N	O	S	0	1	0
			3300	2099	568	626	7			
1	C	427	Total	C	N	O	S	0	1	0
			3293	2091	569	626	7			
1	D	428	Total	C	N	O	S	0	0	0
			3297	2094	568	628	7			
1	G	427	Total	C	N	O	S	0	1	0
			3296	2093	568	628	7			
1	H	426	Total	C	N	O	S	0	0	0
			3281	2084	565	625	7			
1	F	425	Total	C	N	O	S	0	1	0
			3278	2083	564	624	7			
1	I	428	Total	C	N	O	S	0	0	0
			3297	2094	568	628	7			
1	P	428	Total	C	N	O	S	0	1	0
			3305	2099	571	628	7			
1	J	427	Total	C	N	O	S	0	0	0
			3288	2089	566	626	7			
1	M	428	Total	C	N	O	S	0	0	0
			3292	2091	567	627	7			
1	Q	429	Total	C	N	O	S	0	0	0
			3301	2096	569	629	7			
1	N	422	Total	C	N	O	S	0	1	0
			3263	2074	563	619	7			
1	E	427	Total	C	N	O	S	0	1	0
			3296	2094	569	626	7			
1	L	428	Total	C	N	O	S	0	0	0
			3297	2094	568	628	7			
1	K	429	Total	C	N	O	S	0	0	0
			3301	2096	569	629	7			

- Molecule 2 is (2E)-2-[(3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl)methyl]imino]but-3-enoic acid (CCD ID: WBJ) (formula: C₁₂H₁₅N₂O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	C	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	G	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	H	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	F	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	I	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	P	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	J	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	M	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	Q	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	N	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	E	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	L	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	K	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total	O	0	0
			224	224		
3	B	142	Total	O	0	0
			142	142		
3	C	206	Total	O	0	0
			206	206		
3	D	179	Total	O	0	0
			179	179		
3	G	144	Total	O	0	0
			144	144		
3	H	104	Total	O	0	0
			104	104		
3	F	132	Total	O	0	0
			132	132		
3	I	121	Total	O	0	0
			121	121		
3	P	119	Total	O	0	0
			119	119		
3	J	108	Total	O	0	0
			108	108		
3	M	148	Total	O	0	0
			148	148		
3	Q	151	Total	O	0	0
			151	151		
3	N	125	Total	O	0	0
			125	125		
3	E	137	Total	O	0	0
			137	137		
3	L	120	Total	O	0	0
			120	120		

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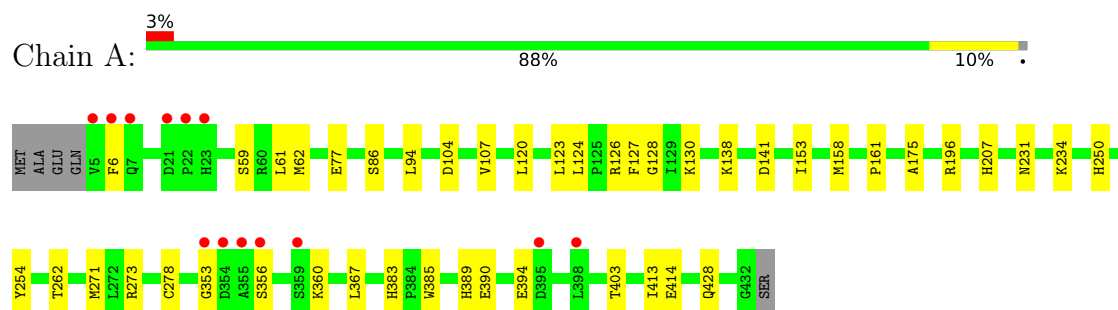
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	107	Total 107	O 107	0	0

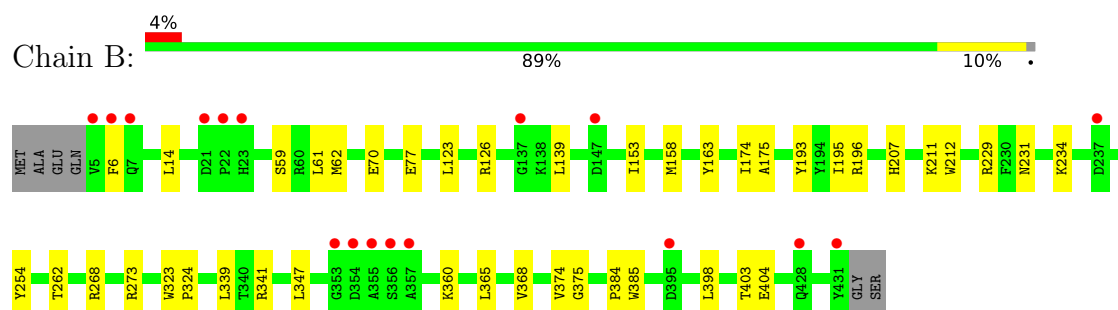
3 Residue-property plots [i](#)

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.

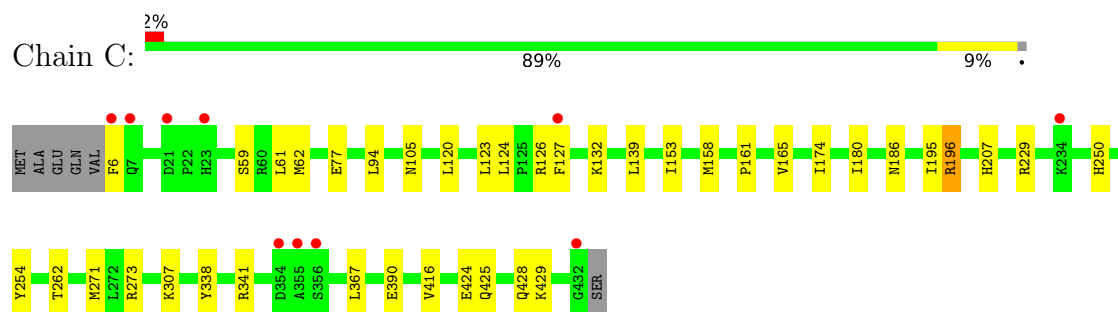
• Molecule 1: Sulfhydrylase FUB7



• Molecule 1: Sulfhydrylase FUB7

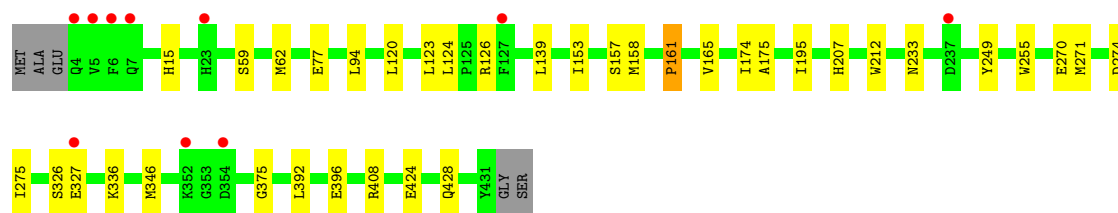


• Molecule 1: Sulfhydrylase FUB7

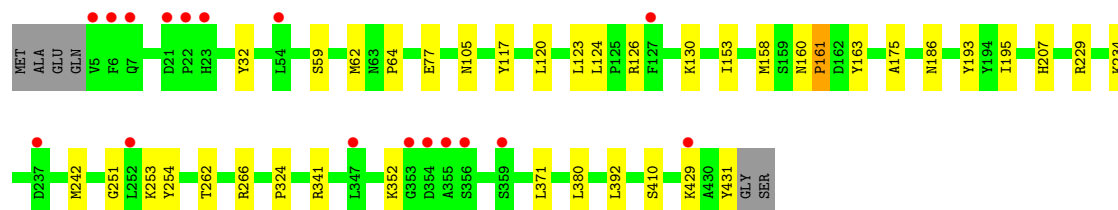
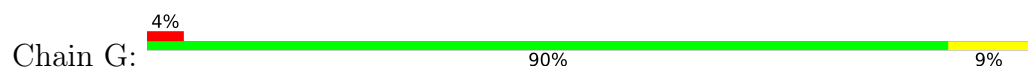


• Molecule 1: Sulfhydrylase FUB7

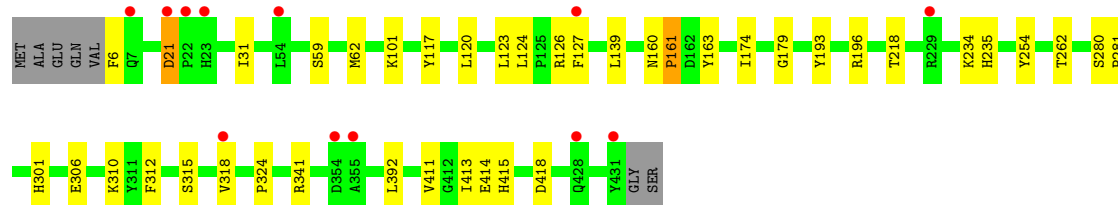
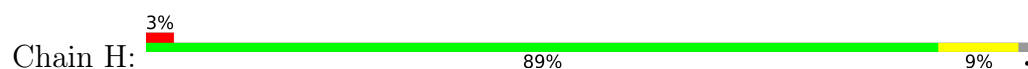




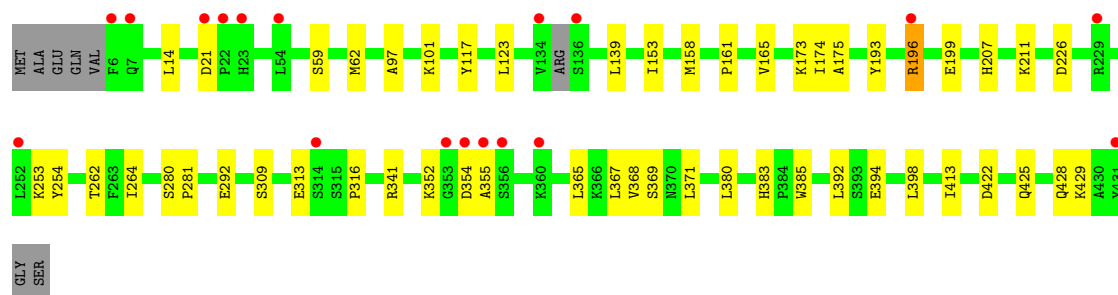
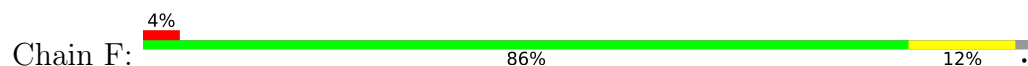
• Molecule 1: Sulfhydrylase FUB7



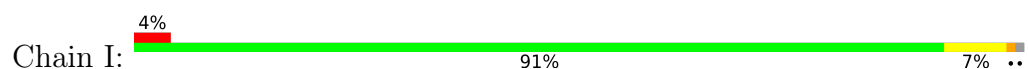
• Molecule 1: Sulfhydrylase FUB7



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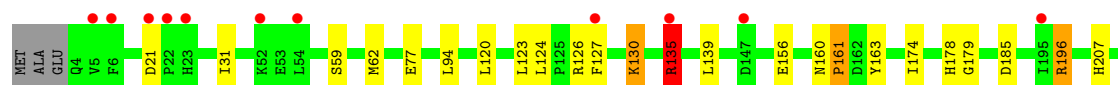
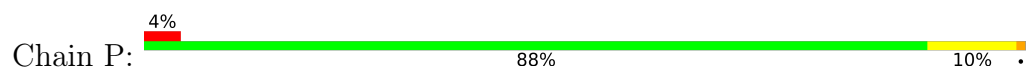


• Molecule 1: Sulfhydrylase FUB7

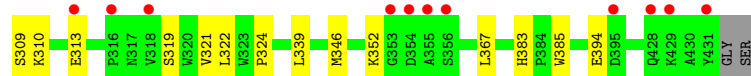
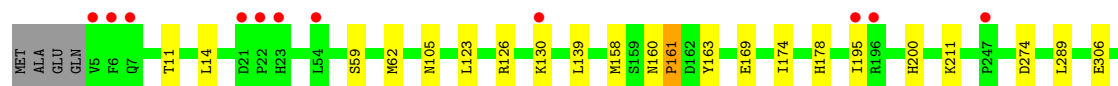
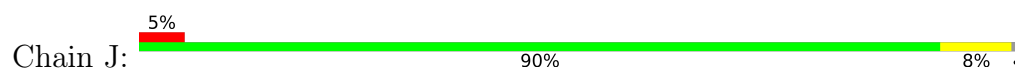




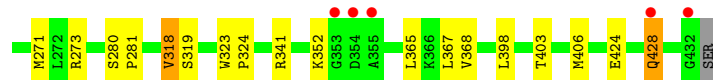
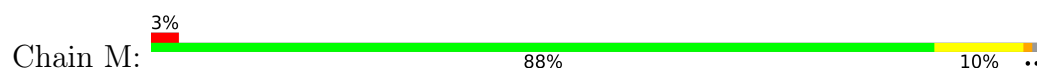
• Molecule 1: Sulfhydrylase FUB7



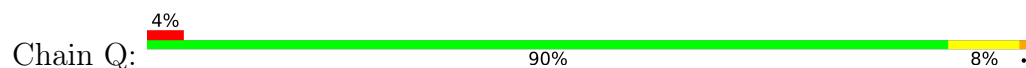
• Molecule 1: Sulfhydrylase FUB7



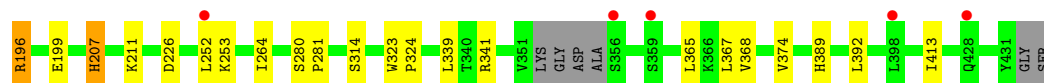
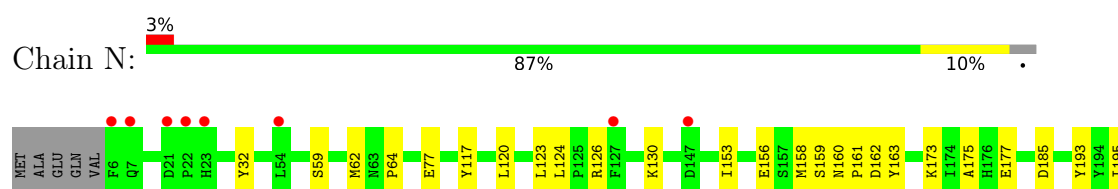
• Molecule 1: Sulfhydrylase FUB7



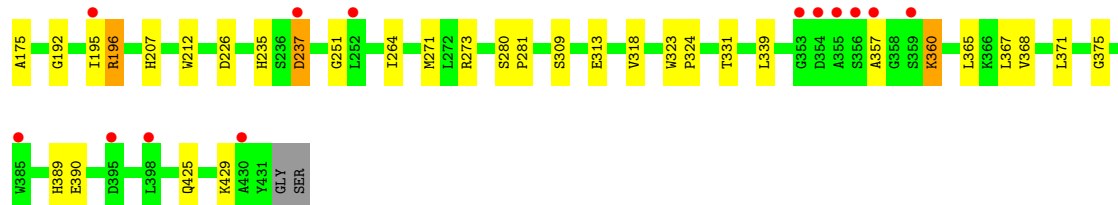
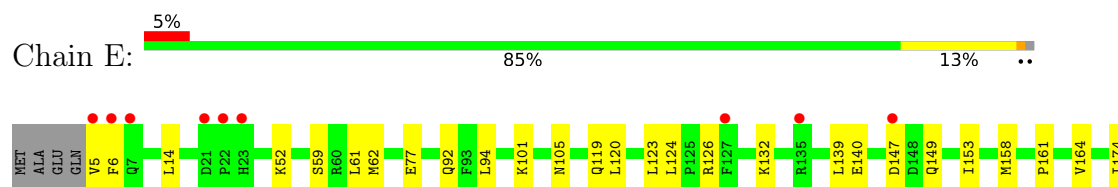
• Molecule 1: Sulfhydrylase FUB7



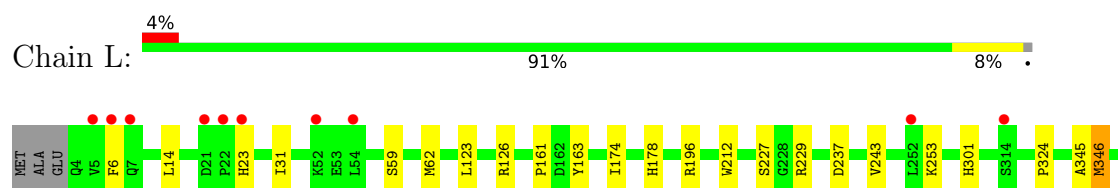
• Molecule 1: Sulfhydrylase FUB7



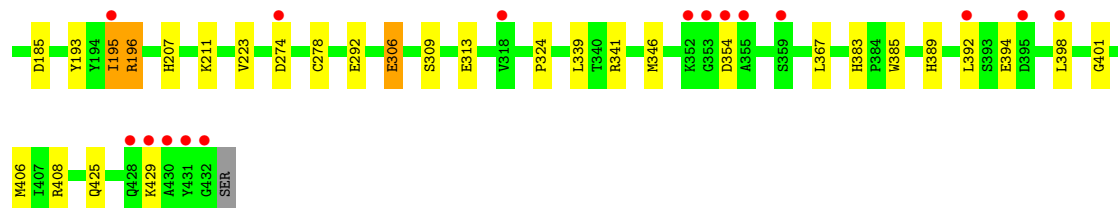
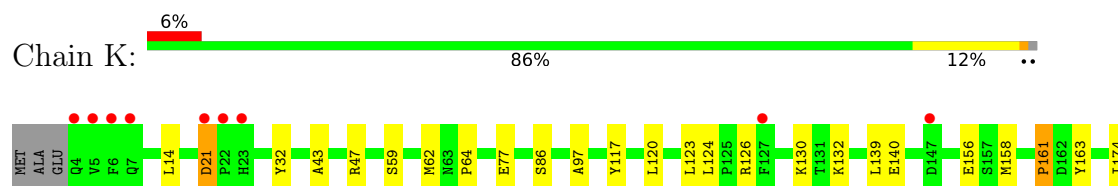
• Molecule 1: Sulfhydrylase FUB7



• Molecule 1: Sulfhydrylase FUB7



• Molecule 1: Sulfhydrylase FUB7



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.70Å 193.36Å 149.91Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	47.75 – 1.98 47.75 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.75-1.98) 99.2 (47.75-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.200 , 0.226 0.200 , 0.225	Depositor DCC
R_{free} test set	28453 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55304	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4422e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: WBJ

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	0.43	0/3383	0.67	3/4595 (0.1%)
1	B	0.40	0/3386	0.64	0/4597
1	C	0.45	0/3376	0.65	0/4585
1	D	0.48	1/3377 (0.0%)	0.84	6/4587 (0.1%)
1	E	0.48	1/3379 (0.0%)	0.82	8/4590 (0.2%)
1	F	0.45	0/3360	0.66	2/4563 (0.0%)
1	G	0.44	1/3376 (0.0%)	0.68	2/4586 (0.0%)
1	H	0.40	0/3361	0.66	3/4565 (0.1%)
1	I	0.40	0/3377	0.69	6/4587 (0.1%)
1	J	0.40	0/3368	0.63	0/4575
1	K	0.42	1/3381 (0.0%)	0.71	7/4592 (0.2%)
1	L	0.43	1/3377 (0.0%)	0.66	1/4587 (0.0%)
1	M	0.46	0/3372	0.73	7/4580 (0.2%)
1	N	0.41	0/3345	0.63	1/4543 (0.0%)
1	P	0.44	0/3388	0.70	4/4602 (0.1%)
1	Q	0.50	2/3381 (0.1%)	0.82	9/4592 (0.2%)
All	All	0.44	7/53987 (0.0%)	0.70	59/73326 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	H	0	1
1	K	0	2
1	M	0	1
1	N	0	1
1	P	0	1
1	Q	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	237	ASP	CG-OD2	13.74	1.51	1.25
1	Q	306	GLU	CD-OE2	7.23	1.39	1.25
1	G	429	LYS	CG-CD	7.07	1.73	1.52
1	Q	196	ARG	CG-CD	-5.92	1.34	1.52
1	L	346	MET	CG-SD	-5.38	1.67	1.80
1	K	132	LYS	CE-NZ	-5.15	1.33	1.49
1	D	336	LYS	CG-CD	5.11	1.67	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	327	GLU	CG-CD-OE1	19.96	164.31	118.40
1	E	237	ASP	CB-CG-OD1	17.76	159.25	118.40
1	E	237	ASP	OD1-CG-OD2	-17.62	80.60	122.90
1	E	237	ASP	CB-CG-OD2	-17.25	78.71	118.40
1	D	327	GLU	OE1-CD-OE2	-16.63	83.00	122.90
1	D	327	GLU	CG-CD-OE2	-16.05	81.50	118.40
1	Q	306	GLU	CG-CD-OE1	14.67	152.14	118.40
1	Q	306	GLU	CG-CD-OE2	-12.61	89.41	118.40
1	Q	306	GLU	OE1-CD-OE2	-11.59	95.08	122.90
1	H	21	ASP	CB-CG-OD2	-10.13	95.11	118.40
1	P	135	ARG	CB-CG-CD	-9.31	89.89	111.30
1	P	135	ARG	CD-NE-CZ	8.72	136.60	124.40
1	Q	21	ASP	CB-CG-OD2	-8.43	99.02	118.40
1	H	21	ASP	CB-CG-OD1	8.31	137.52	118.40
1	Q	196	ARG	NE-CZ-NH1	-8.21	113.29	121.50
1	Q	21	ASP	CB-CG-OD1	7.81	136.37	118.40
1	P	135	ARG	NE-CZ-NH2	-7.68	112.29	119.20
1	Q	196	ARG	CD-NE-CZ	-7.66	113.68	124.40
1	K	195	ILE	CA-C-N	-7.21	113.55	122.42
1	K	195	ILE	C-N-CA	-7.21	113.55	122.42
1	F	429	LYS	CB-CG-CD	-6.98	95.25	111.30
1	A	158	MET	CA-CB-CG	6.67	127.43	114.10
1	M	428	GLN	CA-CB-CG	-6.45	101.20	114.10
1	Q	353	GLY	CA-C-N	6.23	132.04	120.95
1	Q	353	GLY	C-N-CA	6.23	132.04	120.95
1	L	346	MET	CA-CB-CG	-6.19	101.72	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	21	ASP	CB-CG-OD2	-6.14	104.28	118.40
1	K	306	GLU	CA-CB-CG	6.13	126.35	114.10
1	K	196	ARG	CD-NE-CZ	-6.11	115.85	124.40
1	A	428	GLN	CA-CB-CG	6.04	126.18	114.10
1	I	126	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	K	21	ASP	CB-CG-OD1	5.86	131.88	118.40
1	M	251	GLY	CA-C-N	-5.84	109.05	121.32
1	M	251	GLY	C-N-CA	-5.84	109.05	121.32
1	P	130	LYS	CB-CG-CD	-5.63	98.34	111.30
1	E	237	ASP	CA-C-N	5.60	131.51	121.66
1	E	237	ASP	C-N-CA	5.60	131.51	121.66
1	D	326	SER	CA-C-N	-5.56	110.81	121.94
1	D	326	SER	C-N-CA	-5.56	110.81	121.94
1	I	126	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	M	318	VAL	CG1-CB-CG2	5.39	122.65	110.80
1	I	251	GLY	CA-C-N	-5.35	111.24	120.97
1	I	251	GLY	C-N-CA	-5.35	111.24	120.97
1	M	403	THR	CA-C-N	-5.32	111.31	121.94
1	M	403	THR	C-N-CA	-5.32	111.31	121.94
1	H	21	ASP	OD1-CG-OD2	-5.25	110.31	122.90
1	I	360	LYS	CB-CG-CD	5.19	123.24	111.30
1	D	336	LYS	CG-CD-CE	5.16	123.18	111.30
1	A	158	MET	CB-CA-C	5.16	117.54	110.94
1	G	251	GLY	CA-C-N	-5.13	112.89	120.94
1	G	251	GLY	C-N-CA	-5.13	112.89	120.94
1	E	360	LYS	CD-CE-NZ	-5.10	95.58	111.90
1	K	196	ARG	CB-CG-CD	-5.10	99.58	111.30
1	I	360	LYS	CA-CB-CG	-5.09	103.92	114.10
1	M	318	VAL	CA-CB-CG1	5.07	119.02	110.40
1	F	428	GLN	CB-CG-CD	-5.04	104.04	112.60
1	E	251	GLY	CA-C-N	-5.03	111.81	120.97
1	E	251	GLY	C-N-CA	-5.03	111.81	120.97
1	N	130	LYS	CB-CG-CD	-5.03	99.74	111.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	207	HIS	Peptide
1	H	21	ASP	Sidechain
1	K	21	ASP	Sidechain
1	K	306	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	M	163	TYR	Sidechain
1	N	207	HIS	Peptide
1	P	135	ARG	Sidechain
1	Q	21	ASP	Sidechain
1	Q	306	GLU	Sidechain

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	3300	0	3228	33	0
1	B	3300	0	3238	35	0
1	C	3293	0	3219	29	0
1	D	3297	0	3220	22	0
1	E	3296	0	3225	42	0
1	F	3278	0	3202	30	0
1	G	3296	0	3217	24	0
1	H	3281	0	3203	32	0
1	I	3297	0	3220	23	0
1	J	3288	0	3212	28	0
1	K	3301	0	3223	36	0
1	L	3297	0	3220	25	0
1	M	3292	0	3215	32	0
1	N	3263	0	3190	34	0
1	P	3305	0	3233	36	0
1	Q	3301	0	3223	25	0
2	A	22	0	0	0	0
2	B	22	0	0	1	0
2	C	22	0	0	0	0
2	D	22	0	0	0	0
2	E	22	0	0	0	0
2	F	22	0	0	0	0
2	G	22	0	0	0	0
2	H	22	0	0	0	0
2	I	22	0	0	0	0
2	J	22	0	0	0	0
2	K	22	0	0	0	0
2	L	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	22	0	0	0	0
2	N	22	0	0	0	0
2	P	22	0	0	0	0
2	Q	22	0	0	0	0
3	A	224	0	0	3	0
3	B	142	0	0	2	0
3	C	206	0	0	0	0
3	D	179	0	0	1	0
3	E	137	0	0	0	0
3	F	132	0	0	1	0
3	G	144	0	0	1	0
3	H	104	0	0	1	0
3	I	121	0	0	1	0
3	J	108	0	0	0	0
3	K	107	0	0	0	0
3	L	120	0	0	1	0
3	M	148	0	0	1	0
3	N	125	0	0	1	0
3	P	119	0	0	0	0
3	Q	151	0	0	2	0
All	All	55304	0	51488	446	0

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

All (446) 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:A:128:GLY:O	3:A:601:HOH:O	1.82	0.97
1:H:306:GLU:OE2	1:H:310:LYS:NZ	2.12	0.82
1:I:196:ARG:HG3	1:I:196:ARG:HH11	1.48	0.79
1:B:196:ARG:HG2	1:B:196:ARG:NH1	1.96	0.78
1:G:158:MET:HE2	1:G:195:ILE:HD11	1.65	0.78
1:B:196:ARG:HG2	1:B:196:ARG:HH11	1.51	0.76
1:A:385:TRP:CH2	1:A:394:GLU:HG2	2.22	0.74
1:H:196:ARG:HG3	1:H:196:ARG:HH11	1.52	0.72
1:N:193:TYR:CZ	1:N:341:ARG:HD3	2.24	0.72
1:H:301:HIS:HD2	1:H:411:VAL:O	1.72	0.72
1:J:123:LEU:O	1:J:126:ARG:HG2	1.90	0.72
1:E:92:GLN:HE21	1:E:119:GLN:HE22	1.38	0.72
1:A:61:LEU:HD11	1:A:273:ARG:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196[B]:ARG:HH21	1:A:196[B]:ARG:HG3	1.57	0.70
1:M:319:SER:HB3	1:M:352:LYS:HG3	1.72	0.70
1:M:163:TYR:HB3	1:M:324:PRO:HG3	1.73	0.69
1:H:196:ARG:HG3	1:H:196:ARG:NH1	2.05	0.69
1:I:196:ARG:HG3	1:I:196:ARG:NH1	2.06	0.69
1:H:415:HIS:H	1:J:11:THR:HG22	1.58	0.68
1:M:153:ILE:HD12	1:M:175:ALA:HB2	1.75	0.68
1:N:314:SER:OG	3:N:601:HOH:O	2.01	0.68
1:L:196:ARG:HH21	1:L:196:ARG:HG3	1.57	0.67
1:P:163:TYR:HB3	1:P:324:PRO:HG3	1.76	0.67
1:L:301:HIS:HD2	1:L:411:VAL:O	1.79	0.66
1:C:196[B]:ARG:HB2	1:C:196[B]:ARG:CZ	2.24	0.66
1:I:309:SER:O	1:I:313:GLU:HG2	1.96	0.66
1:M:319:SER:HA	1:M:352:LYS:HE3	1.79	0.65
1:E:61:LEU:HD21	1:E:273:ARG:HG3	1.79	0.65
1:E:158:MET:HE2	1:E:339:LEU:HD21	1.79	0.64
1:P:354:ASP:HB2	1:P:357:ALA:HB2	1.79	0.64
1:K:196:ARG:HB2	1:K:196:ARG:CZ	2.27	0.64
1:H:123:LEU:O	1:H:126:ARG:HG2	1.97	0.64
1:A:250:HIS:HE1	1:C:390:GLU:O	1.80	0.64
1:J:319:SER:HB3	1:J:352:LYS:HG3	1.79	0.64
1:P:135:ARG:HB2	1:P:135:ARG:CZ	2.28	0.64
1:K:163:TYR:HB3	1:K:324:PRO:HG3	1.80	0.64
1:K:425:GLN:HE22	1:K:429:LYS:HZ3	1.46	0.63
1:B:61:LEU:HD21	1:B:273:ARG:HA	1.80	0.63
1:E:158:MET:CE	1:E:339:LEU:HD21	2.29	0.63
1:H:163:TYR:HB3	1:H:324:PRO:HG3	1.78	0.63
1:Q:123:LEU:O	1:Q:126:ARG:HG2	1.99	0.63
1:B:77:GLU:OE2	1:B:207:HIS:NE2	2.29	0.63
1:P:135:ARG:HB2	1:P:135:ARG:NH1	2.14	0.63
1:Q:153:ILE:HD12	1:Q:175:ALA:HB2	1.80	0.63
1:M:123:LEU:HD11	1:E:271:MET:HE1	1.80	0.62
1:C:123:LEU:O	1:C:126:ARG:HG2	2.00	0.62
1:M:123:LEU:O	1:M:126:ARG:HG2	2.00	0.62
1:B:163:TYR:HB3	1:B:324:PRO:HG3	1.82	0.62
1:E:123:LEU:O	1:E:126:ARG:HG2	2.00	0.61
1:C:77:GLU:OE1	1:C:207:HIS:NE2	2.32	0.61
1:Q:425:GLN:NE2	1:Q:429:LYS:HE2	2.15	0.61
1:Q:158:MET:HE3	1:Q:324:PRO:HG3	1.83	0.61
1:B:123:LEU:HD22	1:D:274:ASP:HB3	1.82	0.61
1:C:425:GLN:OE1	1:C:429:LYS:HE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:123:LEU:O	1:P:126:ARG:HG2	2.01	0.60
1:B:123:LEU:O	1:B:126:ARG:HG2	2.01	0.60
1:I:163:TYR:HB3	1:I:324:PRO:HG3	1.82	0.60
1:F:316:PRO:O	1:F:352:LYS:HE2	2.02	0.60
1:K:120:LEU:HD23	1:K:124:LEU:HD12	1.84	0.60
1:I:425:GLN:O	1:I:429:LYS:HD3	2.02	0.60
1:A:390:GLU:O	1:C:250:HIS:HE1	1.85	0.59
1:N:163:TYR:HB3	1:N:324:PRO:HG3	1.84	0.59
1:G:123:LEU:O	1:G:126:ARG:HG2	2.02	0.59
1:P:135:ARG:HB2	1:P:135:ARG:HH11	1.66	0.59
1:Q:120:LEU:HD23	1:Q:124:LEU:HD12	1.84	0.59
1:L:163:TYR:HB3	1:L:324:PRO:HG3	1.84	0.59
1:K:123:LEU:O	1:K:126:ARG:HG2	2.01	0.59
1:A:127:PHE:HB3	1:C:127:PHE:HD1	1.67	0.59
1:L:123:LEU:O	1:L:126:ARG:HG2	2.02	0.59
1:E:425:GLN:O	1:E:429:LYS:HG3	2.03	0.59
1:B:139:LEU:HB3	1:B:174:ILE:HD11	1.85	0.58
1:D:123:LEU:O	1:D:126:ARG:HG2	2.04	0.58
1:G:163:TYR:HB3	1:G:324:PRO:HG3	1.84	0.58
1:N:123:LEU:O	1:N:126:ARG:HG2	2.04	0.58
1:E:196[A]:ARG:NH2	1:E:196[A]:ARG:HB2	2.18	0.58
1:N:193:TYR:CE1	1:N:341:ARG:HD3	2.38	0.58
1:K:117:TYR:CD1	1:K:392:LEU:HD11	2.38	0.58
1:L:345:ALA:O	1:L:346:MET:HG3	2.04	0.57
1:L:346:MET:HG2	1:L:409:ILE:O	2.04	0.57
1:D:424:GLU:O	1:D:428:GLN:HG3	2.03	0.57
1:H:139:LEU:HB3	1:H:174:ILE:HD11	1.86	0.57
1:C:139:LEU:HB3	1:C:174:ILE:HD11	1.87	0.57
1:C:120:LEU:HD23	1:C:124:LEU:HD12	1.87	0.57
1:A:94:LEU:HG	1:A:271:MET:HB3	1.85	0.57
1:A:138:LYS:HE2	1:A:141:ASP:OD2	2.04	0.57
1:M:193:TYR:O	1:M:341:ARG:HD2	2.04	0.57
1:J:313:GLU:OE2	1:J:321:VAL:HB	2.05	0.56
1:N:173:LYS:O	1:N:177:GLU:HG3	2.06	0.56
1:E:357:ALA:HA	1:E:360:LYS:HG2	1.86	0.56
1:G:254:TYR:HB3	1:G:262:THR:HG23	1.87	0.56
1:N:158:MET:HE2	1:N:195:ILE:HD11	1.86	0.56
1:M:341:ARG:O	1:M:341:ARG:HG2	2.06	0.56
1:A:127:PHE:HB3	1:C:127:PHE:CD1	2.39	0.56
1:D:139:LEU:HB3	1:D:174:ILE:HD11	1.88	0.56
1:J:306:GLU:OE2	1:J:310:LYS:HE3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:LEU:HD23	1:G:124:LEU:HD12	1.88	0.55
1:Q:192:GLY:O	1:Q:196:ARG:HD2	2.06	0.55
1:C:153:ILE:HG13	1:C:180:ILE:HD11	1.89	0.55
1:Q:94:LEU:HG	1:Q:271:MET:HB3	1.88	0.55
1:N:77:GLU:OE2	1:N:207:HIS:NE2	2.32	0.55
1:E:235:HIS:C	1:E:237:ASP:H	2.13	0.55
1:D:392:LEU:HB3	1:D:396:GLU:HB2	1.89	0.55
1:M:424:GLU:OE2	1:M:428:GLN:NE2	2.40	0.55
1:D:15:HIS:O	3:D:601:HOH:O	2.18	0.55
1:E:196[B]:ARG:HB3	1:E:196[B]:ARG:NH2	2.22	0.55
1:J:163:TYR:HB3	1:J:324:PRO:HG3	1.90	0.54
1:C:6:PHE:CZ	1:M:367:LEU:HD13	2.43	0.54
1:F:14:LEU:HD12	1:L:414:GLU:HG3	1.88	0.54
1:F:117:TYR:CD1	1:F:392:LEU:HD22	2.42	0.54
1:L:59:SER:HA	1:L:62:MET:O	2.07	0.54
1:A:356:SER:O	1:A:360:LYS:HG3	2.08	0.54
1:M:249:TYR:HB2	1:M:252:LEU:HD22	1.88	0.54
1:E:139:LEU:HB3	1:E:174:ILE:HD11	1.88	0.54
1:F:173:LYS:NZ	1:E:318:VAL:O	2.38	0.53
1:K:158:MET:HE2	1:K:195:ILE:HD11	1.90	0.53
1:F:385:TRP:CZ2	1:F:394:GLU:HG2	2.43	0.53
1:A:196[B]:ARG:HG3	1:A:196[B]:ARG:NH2	2.24	0.53
1:A:367:LEU:HD13	1:E:6:PHE:CZ	2.43	0.53
1:C:254:TYR:HB3	1:C:262:THR:HG23	1.91	0.53
1:M:59:SER:HA	1:M:62:MET:O	2.09	0.53
1:H:414:GLU:HB3	1:J:11:THR:HG22	1.90	0.52
1:F:394:GLU:O	1:F:398:LEU:HG	2.09	0.52
1:I:211:LYS:NZ	1:I:373:ASN:HD22	2.07	0.52
1:K:161:PRO:HD3	1:K:389:HIS:CE1	2.45	0.52
1:B:153:ILE:HD12	1:B:175:ALA:HB2	1.91	0.52
1:D:158:MET:HE2	1:D:195:ILE:HD11	1.92	0.52
1:E:105:ASN:ND2	1:E:132:LYS:HE2	2.25	0.52
1:M:254:TYR:HB3	1:M:262:THR:HG23	1.91	0.52
1:L:354:ASP:OD2	1:L:355:ALA:N	2.42	0.52
1:K:346:MET:HE1	1:K:408:ARG:HD2	1.92	0.52
1:M:120:LEU:HD23	1:M:124:LEU:HD12	1.92	0.52
1:E:161:PRO:HD3	1:E:389:HIS:CE1	2.44	0.52
1:K:130:LYS:N	1:K:130:LYS:HD3	2.25	0.52
1:I:306:GLU:OE2	1:I:310:LYS:HE3	2.10	0.52
1:P:139:LEU:HB3	1:P:174:ILE:HD11	1.91	0.51
1:E:92:GLN:HE21	1:E:119:GLN:NE2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:SER:HA	1:C:62:MET:O	2.10	0.51
1:I:59:SER:HA	1:I:62:MET:O	2.09	0.51
1:N:195:ILE:HG12	1:N:339:LEU:HD11	1.92	0.51
1:A:120:LEU:HD23	1:A:124:LEU:HD12	1.92	0.51
1:N:153:ILE:HD12	1:N:175:ALA:HB2	1.93	0.51
1:P:174:ILE:O	1:P:178:HIS:HD2	1.94	0.51
1:A:153:ILE:HD12	1:A:175:ALA:HB2	1.92	0.51
1:K:309:SER:O	1:K:313:GLU:HG2	2.10	0.51
1:A:77:GLU:OE2	1:A:207:HIS:NE2	2.41	0.51
1:E:140:GLU:CD	1:E:140:GLU:H	2.18	0.51
1:P:245:PRO:HG3	1:P:253:LYS:HE2	1.93	0.50
1:M:280:SER:HB2	1:M:281:PRO:HD2	1.94	0.50
1:F:21:ASP:OD1	1:F:21:ASP:N	2.45	0.50
1:E:77:GLU:OE2	1:E:207:HIS:NE2	2.40	0.50
1:A:414:GLU:HG3	1:E:14:LEU:HD12	1.94	0.50
1:B:231:ASN:CG	1:B:234:LYS:HG2	2.36	0.50
1:J:139:LEU:HB3	1:J:174:ILE:HD11	1.93	0.50
1:Q:158:MET:CE	1:Q:324:PRO:HG3	2.41	0.50
1:Q:229:ARG:HD2	3:Q:609:HOH:O	2.11	0.50
1:N:173:LYS:NZ	1:N:177:GLU:OE2	2.36	0.50
1:N:195:ILE:HG12	1:N:339:LEU:CD1	2.42	0.50
1:K:14:LEU:HD23	1:K:292:GLU:HG2	1.93	0.50
1:B:158:MET:HE2	1:B:339:LEU:HD21	1.93	0.50
1:I:394:GLU:O	1:I:398:LEU:HD22	2.12	0.50
1:I:429:LYS:HD2	1:I:429:LYS:N	2.27	0.50
1:J:174:ILE:O	1:J:178:HIS:HD2	1.94	0.50
1:F:383:HIS:CE1	1:F:385:TRP:HB3	2.47	0.50
1:J:158:MET:HE2	1:J:195:ILE:HD11	1.93	0.50
1:E:235:HIS:C	1:E:237:ASP:N	2.70	0.50
1:K:425:GLN:HE22	1:K:429:LYS:NZ	2.09	0.50
1:A:59:SER:HA	1:A:62:MET:O	2.12	0.49
1:H:6:PHE:CZ	1:J:367:LEU:HD13	2.47	0.49
1:H:312:PHE:O	1:H:318:VAL:HG11	2.12	0.49
1:F:158:MET:HG2	1:F:165:VAL:HG22	1.94	0.49
1:F:139:LEU:HB3	1:F:174:ILE:HD11	1.93	0.49
1:A:130:LYS:HD3	1:A:130:LYS:N	2.27	0.49
1:C:424:GLU:O	1:C:428:GLN:HG3	2.12	0.49
1:J:383:HIS:CE1	1:J:385:TRP:HB3	2.48	0.49
1:L:196:ARG:HG3	1:L:196:ARG:NH2	2.26	0.49
1:B:385:TRP:CE2	1:B:404:GLU:HB3	2.47	0.49
1:H:413:ILE:HG13	1:J:14:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:126:ARG:HG3	1:N:126:ARG:HH11	1.77	0.49
1:H:163:TYR:CB	1:H:324:PRO:HG3	2.42	0.49
1:P:120:LEU:HD23	1:P:124:LEU:HD12	1.95	0.49
1:Q:424:GLU:O	1:Q:428:GLN:HG2	2.13	0.49
1:K:59:SER:HA	1:K:62:MET:O	2.12	0.49
1:J:169:GLU:OE2	1:J:200:HIS:HD2	1.95	0.49
1:N:211:LYS:HD2	1:N:374:VAL:O	2.13	0.49
1:B:385:TRP:CD2	1:B:404:GLU:HB3	2.48	0.48
1:D:153:ILE:HD12	1:D:175:ALA:HB2	1.95	0.48
1:G:59:SER:HA	1:G:62:MET:O	2.12	0.48
1:N:193:TYR:O	1:N:341:ARG:HD2	2.11	0.48
1:L:416:VAL:O	1:L:420:ILE:HG13	2.13	0.48
1:H:120:LEU:HD23	1:H:124:LEU:HD12	1.95	0.48
1:F:367:LEU:HD13	1:L:6:PHE:CZ	2.48	0.48
1:M:250:HIS:HE1	1:E:390:GLU:O	1.97	0.48
1:G:126:ARG:HG3	1:G:126:ARG:HH11	1.78	0.48
1:F:59:SER:HA	1:F:62:MET:O	2.13	0.48
1:P:337:LYS:HD3	1:P:338:TYR:CZ	2.48	0.48
1:M:94:LEU:HG	1:M:271:MET:HB3	1.95	0.48
1:M:249:TYR:CB	1:M:252:LEU:HD22	2.44	0.48
1:N:126:ARG:HG3	1:N:126:ARG:NH1	2.29	0.48
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.77	0.48
1:G:371:LEU:HD11	1:G:380:LEU:HD22	1.94	0.48
1:E:164:VAL:HG13	1:E:331:THR:HG21	1.96	0.48
1:G:77:GLU:OE2	1:G:207:HIS:NE2	2.43	0.48
1:Q:77:GLU:OE2	1:Q:207:HIS:NE2	2.44	0.48
1:H:418:ASP:OD2	1:J:11:THR:HG21	2.14	0.48
1:F:253:LYS:HB3	3:F:674:HOH:O	2.13	0.48
1:K:207:HIS:HB2	1:K:223:VAL:HG12	1.96	0.48
1:B:6:PHE:CZ	1:N:367:LEU:HD13	2.50	0.47
1:D:270:GLU:O	1:D:274:ASP:HB2	2.14	0.47
1:A:6:PHE:CZ	1:E:367:LEU:HD13	2.50	0.47
1:B:126:ARG:HG3	1:B:126:ARG:HH11	1.79	0.47
1:P:94:LEU:HG	1:P:271:MET:HB3	1.96	0.47
1:H:415:HIS:N	1:J:11:THR:HG22	2.29	0.47
1:P:130:LYS:N	1:P:130:LYS:HD3	2.29	0.47
1:J:309:SER:O	1:J:313:GLU:HG2	2.15	0.47
1:M:233:ASN:HA	1:M:243:VAL:HG11	1.96	0.47
1:N:323:TRP:CD1	1:N:324:PRO:HD2	2.50	0.47
1:A:413:ILE:HG13	1:E:14:LEU:HD11	1.96	0.47
1:B:384:PRO:HD2	3:B:663:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ILE:HB	1:I:31:ILE:HB	1.97	0.47
1:H:59:SER:HA	1:H:62:MET:O	2.15	0.47
1:B:365:LEU:HD13	1:B:368:VAL:HB	1.96	0.47
1:H:415:HIS:H	1:J:11:THR:CG2	2.27	0.47
1:I:372:ALA:O	1:I:373:ASN:HB2	2.15	0.47
1:M:193:TYR:CZ	1:M:341:ARG:HD3	2.49	0.47
1:M:249:TYR:HB2	1:M:252:LEU:CD2	2.44	0.47
1:E:153:ILE:HD12	1:E:175:ALA:HB2	1.97	0.47
1:F:153:ILE:HD12	1:F:175:ALA:HB2	1.96	0.46
1:P:31:ILE:HB	1:L:31:ILE:HB	1.96	0.46
1:C:105:ASN:CG	1:C:132:LYS:HE2	2.41	0.46
1:K:383:HIS:CE1	1:K:385:TRP:HB3	2.50	0.46
1:C:196[B]:ARG:HH11	1:C:341:ARG:NH2	2.13	0.46
1:I:164:VAL:HG13	1:I:331:THR:HG21	1.96	0.46
1:N:159:SER:OG	1:N:162:ASP:OD1	2.28	0.46
1:E:365:LEU:HD13	1:E:368:VAL:HB	1.96	0.46
1:A:231:ASN:CG	1:A:234:LYS:HG2	2.41	0.46
1:D:120:LEU:HD23	1:D:124:LEU:HD12	1.97	0.46
1:Q:254:TYR:HB3	1:Q:262:THR:HG23	1.98	0.46
1:K:140:GLU:H	1:K:140:GLU:CD	2.21	0.46
1:F:354:ASP:OD1	1:F:355:ALA:N	2.48	0.46
1:N:341:ARG:O	1:N:341:ARG:HG2	2.16	0.46
1:M:61:LEU:HD21	1:M:273:ARG:HG3	1.98	0.46
1:A:130:LYS:NZ	3:A:601:HOH:O	2.03	0.46
1:B:158:MET:CE	1:B:339:LEU:HD21	2.45	0.46
1:C:158:MET:HG2	1:C:165:VAL:HG22	1.96	0.46
1:M:159:SER:OG	1:M:162:ASP:OD1	2.33	0.46
1:B:61:LEU:HD21	1:B:273:ARG:CA	2.45	0.46
1:C:94:LEU:HG	1:C:271:MET:HB3	1.98	0.46
1:A:161:PRO:HD3	1:A:389:HIS:CE1	2.50	0.46
1:K:394:GLU:O	1:K:398:LEU:HD23	2.16	0.45
1:F:309:SER:O	1:F:313:GLU:HG2	2.16	0.45
1:Q:384:PRO:HD2	3:Q:688:HOH:O	2.16	0.45
1:A:104:ASP:N	3:A:601:HOH:O	2.50	0.45
1:F:14:LEU:HD23	1:F:292:GLU:HG2	1.96	0.45
1:G:153:ILE:HD12	1:G:175:ALA:HB2	1.99	0.45
1:N:280:SER:HB2	1:N:281:PRO:HD2	1.97	0.45
1:L:301:HIS:HE1	3:L:647:HOH:O	1.98	0.45
1:F:413:ILE:HG13	1:L:14:LEU:HD11	1.98	0.45
1:P:252:LEU:HD11	1:P:254:TYR:CD1	2.51	0.45
1:B:403:THR:HG21	1:H:234:LYS:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:ALA:HB1	1:P:127:PHE:HZ	1.82	0.45
1:E:59:SER:HA	1:E:62:MET:O	2.16	0.45
1:E:309:SER:O	1:E:313:GLU:HG2	2.17	0.45
1:A:383:HIS:CE1	1:A:385:TRP:HB3	2.52	0.45
1:C:126:ARG:HG3	1:C:126:ARG:HH11	1.82	0.45
1:D:233:ASN:HB2	1:D:255:TRP:CE2	2.52	0.45
1:F:422:ASP:O	1:F:425:GLN:HG3	2.16	0.45
1:I:15:HIS:CD2	1:K:367:LEU:HD11	2.51	0.45
1:P:21:ASP:HB3	1:L:23:HIS:CD2	2.52	0.45
1:E:120:LEU:HD23	1:E:124:LEU:HD12	1.99	0.45
1:K:193:TYR:CE2	1:K:341:ARG:HG2	2.51	0.45
1:A:353:GLY:HA2	1:G:229:ARG:HH12	1.82	0.45
1:B:59:SER:HA	1:B:62:MET:O	2.17	0.45
1:C:196[A]:ARG:HG2	1:C:196[A]:ARG:HH11	1.81	0.45
1:G:242:MET:HE2	1:G:266:ARG:NH1	2.32	0.45
1:M:398:LEU:HD12	3:M:603:HOH:O	2.16	0.45
1:N:161:PRO:HD3	1:N:389:HIS:CE1	2.52	0.45
1:B:14:LEU:HD11	1:N:413:ILE:HG13	1.99	0.45
1:F:193:TYR:CE2	1:F:341:ARG:HG2	2.52	0.45
1:I:54:LEU:HD12	1:I:55:GLY:N	2.31	0.45
1:P:59:SER:HA	1:P:62:MET:O	2.17	0.45
1:Q:365:LEU:HD13	1:Q:368:VAL:HB	1.99	0.45
1:N:365:LEU:HD13	1:N:368:VAL:HB	1.99	0.45
1:I:296:LEU:HD12	3:I:706:HOH:O	2.16	0.45
1:C:367:LEU:HD13	1:M:6:PHE:CZ	2.52	0.44
1:F:365:LEU:HD13	1:F:368:VAL:HB	1.99	0.44
1:B:193:TYR:CE2	1:B:341:ARG:HG2	2.52	0.44
1:H:301:HIS:HE1	3:H:607:HOH:O	2.01	0.44
1:I:383:HIS:CE1	1:I:385:TRP:HB3	2.52	0.44
1:C:195:ILE:HD13	1:C:338:TYR:HB3	1.98	0.44
1:I:163:TYR:CB	1:I:324:PRO:HG3	2.47	0.44
1:K:86:SER:HB3	1:K:278:CYS:O	2.18	0.44
1:M:236:SER:HB2	1:M:243:VAL:HG21	2.00	0.44
1:L:212:TRP:CE2	1:L:375:GLY:HA2	2.52	0.44
1:D:271:MET:HE3	1:D:275:ILE:CD1	2.48	0.44
1:Q:61:LEU:HD21	1:Q:273:ARG:HA	1.98	0.44
1:L:346:MET:CG	1:L:410:SER:HA	2.48	0.44
1:H:193:TYR:CE2	1:H:341:ARG:HG2	2.53	0.44
1:A:403:THR:HG21	1:G:234:LYS:HD2	1.99	0.43
1:B:347:LEU:C	1:B:347:LEU:HD12	2.43	0.43
1:C:126:ARG:HG3	1:C:126:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLU:OE1	1:D:207:HIS:NE2	2.51	0.43
1:P:77:GLU:OE1	1:P:207:HIS:NE2	2.50	0.43
1:B:212:TRP:CE2	1:B:375:GLY:HA2	2.53	0.43
1:J:160:ASN:HA	1:J:161:PRO:HA	1.87	0.43
1:K:117:TYR:CD1	1:K:392:LEU:CD1	3.02	0.43
1:B:229:ARG:HG2	1:B:229:ARG:HH11	1.83	0.43
1:B:360:LYS:HE3	1:B:360:LYS:HB2	1.75	0.43
1:D:346:MET:HE3	1:D:346:MET:HB3	1.93	0.43
1:P:160:ASN:HA	1:P:161:PRO:HA	1.89	0.43
1:E:158:MET:HE3	1:E:195:ILE:HD11	2.01	0.43
1:L:346:MET:HG2	1:L:410:SER:HA	2.00	0.43
1:K:156:GLU:HG2	1:K:185:ASP:HB3	2.00	0.43
1:D:212:TRP:CE2	1:D:375:GLY:HA2	2.53	0.43
1:Q:231:ASN:OD1	1:Q:234:LYS:HG3	2.18	0.43
1:L:243:VAL:O	1:L:253:LYS:HB3	2.18	0.43
1:Q:371:LEU:HD12	1:Q:371:LEU:C	2.43	0.43
1:B:126:ARG:HG3	1:B:126:ARG:NH1	2.32	0.43
1:C:61:LEU:HD11	1:C:273:ARG:HG3	2.00	0.43
1:H:218:THR:HG21	1:J:289:LEU:HD21	2.00	0.43
1:F:280:SER:HB2	1:F:281:PRO:HD2	2.00	0.43
1:H:254:TYR:HB3	1:H:262:THR:HG23	2.00	0.43
1:P:356:SER:OG	1:P:360:LYS:HE3	2.18	0.43
1:N:117:TYR:HB3	1:N:392:LEU:HD21	2.01	0.43
1:K:195:ILE:HG12	1:K:339:LEU:CD2	2.48	0.43
1:K:196:ARG:CZ	1:K:196:ARG:CB	2.93	0.43
1:G:105:ASN:HA	1:G:130:LYS:O	2.19	0.43
1:F:101:LYS:HE3	1:P:126:ARG:HB2	2.00	0.43
1:G:160:ASN:HA	1:G:161:PRO:HA	1.89	0.43
1:P:346:MET:HE3	1:P:346:MET:HB3	1.90	0.43
1:J:59:SER:HA	1:J:62:MET:O	2.19	0.43
1:M:161:PRO:HB2	1:M:406:MET:HE2	1.99	0.43
1:G:117:TYR:CD1	1:G:392:LEU:HD22	2.54	0.42
1:H:315:SER:HB3	1:H:318:VAL:HG12	2.01	0.42
1:F:226:ASP:HB2	1:F:264:ILE:HB	2.00	0.42
1:J:105:ASN:HA	1:J:130:LYS:O	2.19	0.42
1:J:322:LEU:HD12	1:J:322:LEU:HA	1.93	0.42
1:N:226:ASP:HB2	1:N:264:ILE:HB	2.00	0.42
1:A:107:VAL:O	1:A:153:ILE:HA	2.19	0.42
1:C:229:ARG:HG2	1:C:229:ARG:NH1	2.35	0.42
1:D:94:LEU:HG	1:D:271:MET:HB3	2.00	0.42
1:D:157:SER:HB2	1:D:195:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:TYR:CE2	1:G:341:ARG:HG2	2.55	0.42
1:H:101:LYS:HB2	1:K:126:ARG:O	2.20	0.42
1:H:280:SER:HB2	1:H:281:PRO:HD2	2.02	0.42
1:F:369:SER:HB3	1:F:371:LEU:HD23	2.01	0.42
1:M:323:TRP:CD1	1:M:324:PRO:HD2	2.55	0.42
1:L:237:ASP:N	1:L:237:ASP:OD1	2.50	0.42
1:K:77:GLU:OE1	1:K:207:HIS:NE2	2.46	0.42
1:C:307:LYS:HD3	1:C:416:VAL:HG11	2.01	0.42
1:I:360:LYS:O	1:I:360:LYS:HG2	2.18	0.42
1:D:158:MET:HG2	1:D:165:VAL:HG22	2.01	0.42
1:P:383:HIS:CE1	1:P:385:TRP:HB3	2.54	0.42
1:K:130:LYS:HE2	1:K:130:LYS:HB2	1.67	0.42
1:H:179:GLY:HA2	1:H:235:HIS:CE1	2.55	0.42
1:J:346:MET:HE3	1:J:346:MET:HB3	1.87	0.42
1:N:252:LEU:HD23	1:N:253:LYS:C	2.45	0.42
1:P:135:ARG:HH11	1:P:135:ARG:CB	2.31	0.42
1:D:195:ILE:HD13	1:D:195:ILE:HG21	1.81	0.42
1:G:186:ASN:HB3	1:G:207:HIS:CE1	2.55	0.42
1:H:127:PHE:HZ	1:K:97:ALA:HB1	1.85	0.42
1:P:311:TYR:OH	1:P:424:GLU:HG2	2.20	0.42
1:A:123:LEU:O	1:A:126:ARG:HB2	2.20	0.42
1:D:161:PRO:HB3	1:D:408:ARG:HD3	2.02	0.42
1:P:196[A]:ARG:HH11	1:P:196[A]:ARG:HG2	1.85	0.42
1:Q:195:ILE:O	1:Q:196:ARG:HG3	2.20	0.42
1:E:212:TRP:NE1	1:E:375:GLY:HA2	2.35	0.42
1:L:301:HIS:CD2	1:L:411:VAL:O	2.67	0.42
2:B:501:WBJ:O08	2:B:501:WBJ:N04	2.53	0.41
1:J:195:ILE:HG12	1:J:339:LEU:CD2	2.50	0.41
1:Q:227:SER:OG	1:Q:229:ARG:HG2	2.20	0.41
1:Q:306:GLU:CD	1:Q:306:GLU:C	2.87	0.41
1:B:70:GLU:CD	1:B:268:ARG:HH22	2.27	0.41
1:B:254:TYR:HB3	1:B:262:THR:HG23	2.01	0.41
1:I:89:GLN:HE21	1:J:274:ASP:HA	1.86	0.41
1:N:59:SER:HA	1:N:62:MET:O	2.20	0.41
1:I:211:LYS:HZ3	1:I:373:ASN:HD22	1.68	0.41
1:P:156:GLU:HG2	1:P:185:ASP:HB3	2.01	0.41
1:P:179:GLY:HA2	1:P:235:HIS:CD2	2.55	0.41
1:N:32:TYR:CD2	1:N:64:PRO:HB2	2.55	0.41
1:L:227:SER:OG	1:L:229:ARG:HG2	2.20	0.41
1:A:254:TYR:HB3	1:A:262:THR:HG23	2.03	0.41
1:B:163:TYR:CB	1:B:324:PRO:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:LYS:O	1:G:431:TYR:OH	2.32	0.41
1:F:123:LEU:HD22	1:P:274:ASP:HB3	2.02	0.41
1:F:196[A]:ARG:NE	1:F:199:GLU:OE2	2.53	0.41
1:N:156:GLU:HG2	1:N:185:ASP:HB3	2.02	0.41
1:E:94:LEU:HG	1:E:271:MET:HB3	2.02	0.41
1:G:253:LYS:HB3	3:G:719:HOH:O	2.20	0.41
1:I:120:LEU:HD23	1:I:124:LEU:HD12	2.01	0.41
1:M:365:LEU:HD13	1:M:368:VAL:HB	2.02	0.41
1:Q:108:ALA:O	1:Q:133:PHE:HA	2.21	0.41
1:E:52:LYS:HE2	1:E:52:LYS:HA	2.03	0.41
1:K:401:GLY:O	1:K:406:MET:HE1	2.20	0.41
1:F:254:TYR:HB3	1:F:262:THR:HG23	2.01	0.41
1:M:37:TYR:CG	1:M:56:ASN:HB3	2.56	0.41
1:K:139:LEU:HB3	1:K:174:ILE:HD11	2.02	0.41
1:B:195:ILE:C	1:B:196:ARG:HG3	2.46	0.41
1:N:160:ASN:HA	1:N:161:PRO:HA	1.92	0.41
1:N:196[B]:ARG:HB2	1:N:196[B]:ARG:CZ	2.50	0.41
1:E:147:ASP:HB3	1:E:149:GLN:H	1.85	0.41
1:L:174:ILE:O	1:L:178:HIS:HD2	2.03	0.41
1:A:130:LYS:HE2	1:A:130:LYS:HB2	1.42	0.41
1:D:59:SER:HA	1:D:62:MET:O	2.21	0.41
1:G:380:LEU:HB2	1:G:410:SER:HB3	2.02	0.41
1:P:130:LYS:HE2	1:P:130:LYS:HB2	1.45	0.41
1:P:212:TRP:CE2	1:P:375:GLY:HA2	2.56	0.41
1:P:289:LEU:HD23	1:P:289:LEU:HA	1.88	0.41
1:P:319:SER:HB3	1:P:352:LYS:HG2	2.03	0.41
1:M:153:ILE:HG13	1:M:180:ILE:HD11	2.02	0.41
1:E:5:VAL:HG12	1:E:6:PHE:CD2	2.56	0.41
1:E:226:ASP:HB2	1:E:264:ILE:HB	2.03	0.41
1:K:32:TYR:CD2	1:K:64:PRO:HB2	2.56	0.41
1:H:117:TYR:CD1	1:H:392:LEU:HD22	2.56	0.41
1:F:371:LEU:HD11	1:F:380:LEU:HD22	2.02	0.41
1:P:21:ASP:OD2	1:P:21:ASP:N	2.53	0.41
1:M:126:ARG:O	1:E:101:LYS:HB2	2.21	0.41
1:E:371:LEU:C	1:E:371:LEU:HD12	2.46	0.41
1:K:126:ARG:HH11	1:K:126:ARG:HG3	1.86	0.41
1:A:86:SER:HB3	1:A:278:CYS:O	2.21	0.40
1:B:323:TRP:CD1	1:B:324:PRO:HD2	2.55	0.40
3:B:637:HOH:O	1:D:249:TYR:HA	2.21	0.40
1:J:130:LYS:HE2	1:J:130:LYS:HB2	1.79	0.40
2:L:501:WBJ:O08	2:L:501:WBJ:N04	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:MET:HE2	1:G:195:ILE:CD1	2.45	0.40
1:H:123:LEU:HD22	1:K:274:ASP:HB3	2.03	0.40
1:Q:161:PRO:HG2	1:Q:406:MET:SD	2.61	0.40
1:E:192:GLY:HA2	1:E:195:ILE:O	2.21	0.40
1:B:211[B]:LYS:HD2	1:B:374:VAL:O	2.21	0.40
1:G:32:TYR:CD2	1:G:64:PRO:HB2	2.57	0.40
1:I:136:SER:OG	1:I:141:ASP:OD2	2.28	0.40
1:Q:196:ARG:HH11	1:Q:196:ARG:HD3	1.28	0.40
1:N:120:LEU:HD23	1:N:124:LEU:HD12	2.02	0.40
1:E:323:TRP:CD1	1:E:324:PRO:HD2	2.57	0.40
1:L:425:GLN:OE1	1:L:429:LYS:HE2	2.21	0.40
1:C:186:ASN:HB3	1:C:207:HIS:CE1	2.56	0.40
1:G:126:ARG:HG3	1:G:126:ARG:NH1	2.36	0.40
1:H:160:ASN:HA	1:H:161:PRO:HA	1.90	0.40
1:E:280:SER:HB2	1:E:281:PRO:HD2	2.03	0.40
1:K:43:ALA:O	1:K:47:ARG:HG3	2.21	0.40
1:K:140:GLU:OE2	1:K:140:GLU:N	2.44	0.40
1:B:398:LEU:HD12	1:B:398:LEU:HA	1.86	0.40
1:P:323:TRP:CD1	1:P:324:PRO:HD2	2.57	0.40
1:J:385:TRP:CZ2	1:J:394:GLU:HG2	2.57	0.40
1:Q:126:ARG:HH11	1:Q:126:ARG:HG3	1.86	0.40
1:Q:160:ASN:HA	1:Q:161:PRO:HA	1.89	0.40
1:N:196[A]:ARG:NE	1:N:199:GLU:OE2	2.42	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	427/433 (99%)	418 (98%)	9 (2%)	0	100	100
1	B	427/433 (99%)	416 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	426/433 (98%)	416 (98%)	9 (2%)	1 (0%)	43	35
1	D	426/433 (98%)	416 (98%)	9 (2%)	1 (0%)	43	35
1	E	426/433 (98%)	415 (97%)	11 (3%)	0	100	100
1	F	422/433 (98%)	414 (98%)	6 (1%)	2 (0%)	24	14
1	G	426/433 (98%)	417 (98%)	8 (2%)	1 (0%)	43	35
1	H	424/433 (98%)	414 (98%)	9 (2%)	1 (0%)	43	35
1	I	426/433 (98%)	416 (98%)	8 (2%)	2 (0%)	24	14
1	J	425/433 (98%)	415 (98%)	8 (2%)	2 (0%)	24	14
1	K	427/433 (99%)	416 (97%)	8 (2%)	3 (1%)	18	9
1	L	426/433 (98%)	417 (98%)	8 (2%)	1 (0%)	43	35
1	M	426/433 (98%)	415 (97%)	10 (2%)	1 (0%)	43	35
1	N	419/433 (97%)	409 (98%)	10 (2%)	0	100	100
1	P	427/433 (99%)	416 (97%)	10 (2%)	1 (0%)	43	35
1	Q	427/433 (99%)	417 (98%)	9 (2%)	1 (0%)	43	35
All	All	6807/6928 (98%)	6647 (98%)	143 (2%)	17 (0%)	36	35

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	211	LYS
1	I	211	LYS
1	J	211	LYS
1	F	211	LYS
1	K	354	ASP
1	C	161	PRO
1	I	161	PRO
1	Q	161	PRO
1	D	161	PRO
1	H	161	PRO
1	F	161	PRO
1	P	161	PRO
1	M	161	PRO
1	L	161	PRO
1	K	161	PRO
1	J	161	PRO
1	G	161	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	347/350 (99%)	347 (100%)	0	100	100
1	B	348/350 (99%)	348 (100%)	0	100	100
1	C	346/350 (99%)	344 (99%)	2 (1%)	78	76
1	D	347/350 (99%)	347 (100%)	0	100	100
1	E	347/350 (99%)	345 (99%)	2 (1%)	78	76
1	F	345/350 (99%)	343 (99%)	2 (1%)	78	76
1	G	347/350 (99%)	347 (100%)	0	100	100
1	H	345/350 (99%)	345 (100%)	0	100	100
1	I	347/350 (99%)	346 (100%)	1 (0%)	86	86
1	J	346/350 (99%)	346 (100%)	0	100	100
1	K	347/350 (99%)	347 (100%)	0	100	100
1	L	347/350 (99%)	347 (100%)	0	100	100
1	M	346/350 (99%)	345 (100%)	1 (0%)	86	86
1	N	344/350 (98%)	342 (99%)	2 (1%)	78	76
1	P	348/350 (99%)	346 (99%)	2 (1%)	78	76
1	Q	347/350 (99%)	347 (100%)	0	100	100
All	All	5544/5600 (99%)	5532 (100%)	12 (0%)	88	88

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

Mol	Chain	Res	Type
1	C	196[A]	ARG
1	C	196[B]	ARG
1	F	196[A]	ARG
1	F	196[B]	ARG
1	I	54	LEU
1	P	196[A]	ARG
1	P	196[B]	ARG
1	M	318	VAL

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Mol	Chain	Res	Type
1	N	196[A]	ARG
1	N	196[B]	ARG
1	E	196[A]	ARG
1	E	196[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	105	ASN
1	A	119	GLN
1	A	178	HIS
1	A	235	HIS
1	A	250	HIS
1	A	334	GLN
1	B	92	GLN
1	B	235	HIS
1	B	317	ASN
1	C	89	GLN
1	C	92	GLN
1	C	200	HIS
1	C	250	HIS
1	C	303	GLN
1	C	428	GLN
1	D	119	GLN
1	D	250	HIS
1	D	428	GLN
1	G	89	GLN
1	G	200	HIS
1	G	250	HIS
1	H	92	GLN
1	H	105	ASN
1	H	119	GLN
1	H	301	HIS
1	H	428	GLN
1	F	7	GLN
1	F	92	GLN
1	F	118	ASN
1	F	200	HIS
1	I	4	GLN
1	I	89	GLN
1	I	92	GLN

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Mol	Chain	Res	Type
1	I	329	HIS
1	I	370	ASN
1	I	373	ASN
1	P	23	HIS
1	P	89	GLN
1	P	178	HIS
1	P	235	HIS
1	J	178	HIS
1	J	200	HIS
1	J	235	HIS
1	M	250	HIS
1	Q	118	ASN
1	Q	121	ASN
1	Q	178	HIS
1	Q	216	HIS
1	Q	235	HIS
1	Q	425	GLN
1	Q	428	GLN
1	N	118	ASN
1	N	149	GLN
1	N	200	HIS
1	N	317	ASN
1	N	334	GLN
1	N	373	ASN
1	E	23	HIS
1	E	89	GLN
1	E	105	ASN
1	E	119	GLN
1	E	235	HIS
1	E	389	HIS
1	E	391	GLN
1	L	23	HIS
1	L	92	GLN
1	L	118	ASN
1	L	178	HIS
1	L	235	HIS
1	L	250	HIS
1	L	301	HIS
1	L	303	GLN
1	L	428	GLN
1	K	4	GLN
1	K	23	HIS

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Mol	Chain	Res	Type
1	K	92	GLN
1	K	119	GLN
1	K	178	HIS
1	K	235	HIS
1	K	425	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
2	WBJ	K	501	-	21,22,22	2.99	5 (23%)	26,31,31	1.80	6 (23%)
2	WBJ	B	501	-	21,22,22	2.52	3 (14%)	26,31,31	1.67	7 (26%)
2	WBJ	P	501	-	21,22,22	2.82	4 (19%)	26,31,31	1.89	7 (26%)
2	WBJ	L	501	-	21,22,22	2.82	4 (19%)	26,31,31	1.84	7 (26%)
2	WBJ	G	501	-	21,22,22	2.82	4 (19%)	26,31,31	1.79	8 (30%)
2	WBJ	A	501	-	21,22,22	2.29	3 (14%)	26,31,31	1.74	7 (26%)
2	WBJ	N	501	-	21,22,22	2.21	5 (23%)	26,31,31	1.88	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	WBJ	H	501	-	21,22,22	2.97	3 (14%)	26,31,31	1.63	4 (15%)
2	WBJ	I	501	-	21,22,22	2.58	4 (19%)	26,31,31	1.95	7 (26%)
2	WBJ	C	501	-	21,22,22	2.15	3 (14%)	26,31,31	1.77	6 (23%)
2	WBJ	D	501	-	21,22,22	1.94	3 (14%)	26,31,31	1.85	6 (23%)
2	WBJ	Q	501	-	21,22,22	2.17	4 (19%)	26,31,31	1.76	6 (23%)
2	WBJ	F	501	-	21,22,22	2.77	5 (23%)	26,31,31	1.88	7 (26%)
2	WBJ	J	501	-	21,22,22	2.90	4 (19%)	26,31,31	1.82	7 (26%)
2	WBJ	M	501	-	21,22,22	2.18	3 (14%)	26,31,31	1.89	6 (23%)
2	WBJ	E	501	-	21,22,22	1.95	4 (19%)	26,31,31	1.88	7 (26%)

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	WBJ	K	501	-	-	2/14/17/17	0/1/1/1
2	WBJ	B	501	-	-	4/14/17/17	0/1/1/1
2	WBJ	P	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	L	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	G	501	-	-	4/14/17/17	0/1/1/1
2	WBJ	A	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	N	501	-	-	8/14/17/17	0/1/1/1
2	WBJ	H	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	I	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	C	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	D	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	Q	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	F	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	J	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	M	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	E	501	-	-	8/14/17/17	0/1/1/1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	WBJ	C03-C21	11.35	1.59	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	501	WBJ	C03-C21	11.26	1.59	1.48
2	J	501	WBJ	C03-C21	10.33	1.58	1.48
2	F	501	WBJ	C03-C21	10.29	1.58	1.48
2	P	501	WBJ	C03-C21	10.27	1.58	1.48
2	L	501	WBJ	C03-C21	10.26	1.58	1.48
2	G	501	WBJ	C03-C21	10.05	1.58	1.48
2	B	501	WBJ	C03-C21	9.49	1.57	1.48
2	I	501	WBJ	C03-C21	8.82	1.56	1.48
2	C	501	WBJ	C03-C21	8.25	1.56	1.48
2	A	501	WBJ	C03-C21	8.14	1.56	1.48
2	M	501	WBJ	C03-C21	7.61	1.55	1.48
2	N	501	WBJ	C03-C21	7.37	1.55	1.48
2	Q	501	WBJ	C03-C21	7.17	1.55	1.48
2	D	501	WBJ	C03-C21	6.52	1.54	1.48
2	J	501	WBJ	P17-O16	6.26	1.80	1.60
2	G	501	WBJ	P17-O16	6.23	1.80	1.60
2	L	501	WBJ	P17-O16	5.89	1.78	1.60
2	K	501	WBJ	P17-O16	5.86	1.78	1.60
2	H	501	WBJ	P17-O16	5.81	1.78	1.60
2	E	501	WBJ	C03-C21	5.76	1.53	1.48
2	I	501	WBJ	P17-O16	5.76	1.78	1.60
2	P	501	WBJ	P17-O16	5.37	1.77	1.60
2	F	501	WBJ	P17-O16	5.08	1.76	1.60
2	Q	501	WBJ	P17-O16	4.89	1.75	1.60
2	A	501	WBJ	P17-O16	4.77	1.75	1.60
2	B	501	WBJ	P17-O16	4.65	1.75	1.60
2	E	501	WBJ	P17-O16	4.43	1.74	1.60
2	N	501	WBJ	P17-O16	4.39	1.74	1.60
2	M	501	WBJ	P17-O16	4.18	1.73	1.60
2	D	501	WBJ	P17-O16	3.52	1.71	1.60
2	C	501	WBJ	P17-O16	2.97	1.69	1.60
2	G	501	WBJ	O16-C15	-2.69	1.35	1.44
2	J	501	WBJ	O16-C15	-2.68	1.35	1.44
2	I	501	WBJ	O16-C15	-2.66	1.35	1.44
2	G	501	WBJ	C07-C06	2.61	1.43	1.40
2	P	501	WBJ	O16-C15	-2.54	1.35	1.44
2	F	501	WBJ	C07-C06	2.54	1.43	1.40
2	K	501	WBJ	O16-C15	-2.52	1.35	1.44
2	H	501	WBJ	O16-C15	-2.51	1.35	1.44
2	L	501	WBJ	O16-C15	-2.48	1.35	1.44
2	F	501	WBJ	O16-C15	-2.37	1.36	1.44
2	M	501	WBJ	O22-C21	-2.36	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	WBJ	O22-C21	-2.36	1.24	1.30
2	N	501	WBJ	O22-C21	-2.34	1.24	1.30
2	A	501	WBJ	O16-C15	-2.32	1.36	1.44
2	D	501	WBJ	C12-C14	2.32	1.42	1.37
2	I	501	WBJ	O22-C21	-2.30	1.24	1.30
2	J	501	WBJ	O22-C21	-2.30	1.24	1.30
2	F	501	WBJ	O22-C21	-2.23	1.24	1.30
2	P	501	WBJ	O22-C21	-2.23	1.24	1.30
2	E	501	WBJ	O16-C15	-2.21	1.36	1.44
2	Q	501	WBJ	O16-C15	-2.16	1.36	1.44
2	B	501	WBJ	O16-C15	-2.11	1.37	1.44
2	K	501	WBJ	C12-C14	2.07	1.41	1.37
2	N	501	WBJ	C07-C06	2.06	1.43	1.40
2	Q	501	WBJ	C05-N04	-2.04	1.43	1.46
2	K	501	WBJ	C07-C06	2.03	1.43	1.40
2	N	501	WBJ	O16-C15	-2.03	1.37	1.44
2	L	501	WBJ	C12-C14	2.02	1.41	1.37
2	C	501	WBJ	O16-C15	-2.02	1.37	1.44

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	WBJ	C21-C03-N04	-5.61	113.75	122.12
2	P	501	WBJ	C21-C03-N04	-5.47	113.96	122.12
2	C	501	WBJ	C21-C03-N04	-5.44	114.00	122.12
2	H	501	WBJ	C21-C03-N04	-5.39	114.08	122.12
2	J	501	WBJ	C21-C03-N04	-5.28	114.24	122.12
2	Q	501	WBJ	C21-C03-N04	-5.23	114.31	122.12
2	M	501	WBJ	C21-C03-N04	-5.21	114.35	122.12
2	L	501	WBJ	C21-C03-N04	-5.19	114.38	122.12
2	N	501	WBJ	C21-C03-N04	-5.17	114.41	122.12
2	F	501	WBJ	C21-C03-N04	-5.13	114.46	122.12
2	K	501	WBJ	C21-C03-N04	-5.05	114.59	122.12
2	E	501	WBJ	C21-C03-N04	-5.04	114.61	122.12
2	B	501	WBJ	C21-C03-N04	-4.89	114.83	122.12
2	A	501	WBJ	C21-C03-N04	-4.87	114.85	122.12
2	G	501	WBJ	C21-C03-N04	-4.76	115.02	122.12
2	I	501	WBJ	C21-C03-N04	-4.29	115.71	122.12
2	I	501	WBJ	O23-C21-C03	-4.15	115.47	122.02
2	E	501	WBJ	O23-C21-C03	-4.01	115.69	122.02
2	N	501	WBJ	O23-C21-C03	-3.76	116.08	122.02
2	I	501	WBJ	O22-C21-C03	3.60	119.18	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	501	WBJ	O23-C21-C03	-3.47	116.54	122.02
2	F	501	WBJ	O23-C21-C03	-3.37	116.70	122.02
2	D	501	WBJ	O23-C21-C03	-3.37	116.71	122.02
2	I	501	WBJ	C07-C06-C14	-3.29	115.75	118.73
2	P	501	WBJ	O22-C21-C03	3.29	118.68	113.40
2	E	501	WBJ	O22-C21-C03	3.21	118.55	113.40
2	K	501	WBJ	C07-C06-C14	-3.20	115.83	118.73
2	N	501	WBJ	O22-C21-C03	3.19	118.51	113.40
2	L	501	WBJ	O23-C21-C03	-3.14	117.06	122.02
2	L	501	WBJ	O22-C21-C03	3.14	118.43	113.40
2	M	501	WBJ	C07-C06-C14	-3.13	115.89	118.73
2	G	501	WBJ	C07-C06-C14	-3.07	115.95	118.73
2	Q	501	WBJ	O23-C21-C03	-3.05	117.20	122.02
2	J	501	WBJ	O23-C21-C03	-3.04	117.21	122.02
2	F	501	WBJ	O22-C21-C03	3.03	118.27	113.40
2	D	501	WBJ	O22-C21-C03	3.02	118.25	113.40
2	M	501	WBJ	O16-P17-O20	-2.98	98.39	106.44
2	M	501	WBJ	O23-C21-C03	-2.94	117.38	122.02
2	M	501	WBJ	O22-C21-C03	2.84	117.96	113.40
2	J	501	WBJ	O22-C21-C03	2.78	117.85	113.40
2	C	501	WBJ	C10-C09-C07	2.77	124.04	120.80
2	I	501	WBJ	C10-C09-C07	2.74	124.00	120.80
2	F	501	WBJ	C10-C09-C07	2.73	124.00	120.80
2	C	501	WBJ	C07-C06-C14	-2.71	116.27	118.73
2	G	501	WBJ	O18-P17-O16	-2.70	99.63	106.67
2	A	501	WBJ	O23-C21-C03	-2.68	117.78	122.02
2	N	501	WBJ	C07-C06-C14	-2.66	116.31	118.73
2	A	501	WBJ	C07-C06-C14	-2.66	116.32	118.73
2	M	501	WBJ	C10-C09-C07	2.62	123.86	120.80
2	C	501	WBJ	O23-C21-C03	-2.60	117.92	122.02
2	E	501	WBJ	C10-C09-C07	2.59	123.83	120.80
2	F	501	WBJ	C07-C06-C14	-2.59	116.38	118.73
2	G	501	WBJ	O23-C21-C03	-2.58	117.94	122.02
2	D	501	WBJ	C07-C06-C14	-2.54	116.42	118.73
2	B	501	WBJ	C07-C06-C14	-2.53	116.43	118.73
2	A	501	WBJ	O19-P17-O18	2.52	117.27	107.80
2	H	501	WBJ	C10-C09-C07	2.52	123.75	120.80
2	F	501	WBJ	O16-P17-O20	-2.52	99.63	106.44
2	L	501	WBJ	C07-C06-C14	-2.51	116.45	118.73
2	B	501	WBJ	O23-C21-C03	-2.49	118.09	122.02
2	I	501	WBJ	O19-P17-O18	2.49	117.12	107.80
2	P	501	WBJ	C07-C06-C14	-2.48	116.48	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	WBJ	O22-C21-C03	2.48	117.39	113.40
2	A	501	WBJ	O18-P17-O16	-2.47	100.24	106.67
2	N	501	WBJ	C10-C09-C07	2.45	123.67	120.80
2	G	501	WBJ	C10-C09-C07	2.42	123.63	120.80
2	L	501	WBJ	O19-P17-O18	2.42	116.87	107.80
2	A	501	WBJ	C10-C09-C07	2.41	123.62	120.80
2	K	501	WBJ	O22-C21-C03	2.40	117.26	113.40
2	K	501	WBJ	O23-C21-C03	-2.37	118.27	122.02
2	B	501	WBJ	O19-P17-O18	2.37	116.69	107.80
2	D	501	WBJ	O18-P17-O16	-2.35	100.53	106.67
2	E	501	WBJ	C07-C06-C14	-2.35	116.60	118.73
2	Q	501	WBJ	C07-C06-C14	-2.35	116.60	118.73
2	E	501	WBJ	O19-P17-O16	-2.35	100.55	106.67
2	G	501	WBJ	O22-C21-C03	2.34	117.15	113.40
2	Q	501	WBJ	O18-P17-O16	-2.34	100.57	106.67
2	K	501	WBJ	O18-P17-O16	-2.34	100.58	106.67
2	N	501	WBJ	O18-P17-O16	-2.33	100.59	106.67
2	P	501	WBJ	O16-P17-O20	-2.33	100.14	106.44
2	J	501	WBJ	O16-P17-O20	-2.32	100.16	106.44
2	B	501	WBJ	C10-C09-C07	2.31	123.50	120.80
2	L	501	WBJ	O19-P17-O16	-2.31	100.64	106.67
2	Q	501	WBJ	O22-C21-C03	2.30	117.09	113.40
2	J	501	WBJ	O19-P17-O18	2.27	116.33	107.80
2	Q	501	WBJ	O19-P17-O18	2.26	116.28	107.80
2	K	501	WBJ	O19-P17-O16	-2.24	100.82	106.67
2	H	501	WBJ	O23-C21-C03	-2.24	118.48	122.02
2	F	501	WBJ	O19-P17-O18	2.24	116.19	107.80
2	G	501	WBJ	O19-P17-O18	2.23	116.17	107.80
2	E	501	WBJ	O18-P17-O16	-2.22	100.89	106.67
2	L	501	WBJ	C10-C09-C07	2.21	123.38	120.80
2	B	501	WBJ	O22-C21-C03	2.20	116.93	113.40
2	B	501	WBJ	O18-P17-O16	-2.19	100.96	106.67
2	P	501	WBJ	O19-P17-O18	2.19	116.01	107.80
2	D	501	WBJ	O19-P17-O18	2.19	116.00	107.80
2	I	501	WBJ	O16-P17-O20	-2.18	100.54	106.44
2	J	501	WBJ	C07-C06-C14	-2.18	116.76	118.73
2	G	501	WBJ	O16-P17-O20	-2.13	100.70	106.44
2	J	501	WBJ	O18-P17-O16	-2.09	101.22	106.67
2	C	501	WBJ	O22-C21-C03	2.07	116.72	113.40
2	P	501	WBJ	C10-C09-C07	2.06	123.20	120.80
2	H	501	WBJ	O19-P17-O18	2.03	115.42	107.80
2	C	501	WBJ	O18-P17-O16	-2.02	101.41	106.67

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	WBJ	C02-C03-C21-O22
2	A	501	WBJ	N04-C03-C21-O22
2	A	501	WBJ	C02-C03-C21-O23
2	A	501	WBJ	N04-C03-C21-O23
2	A	501	WBJ	N04-C05-C06-C07
2	A	501	WBJ	N04-C05-C06-C14
2	B	501	WBJ	C02-C03-C21-O22
2	B	501	WBJ	N04-C05-C06-C07
2	B	501	WBJ	N04-C05-C06-C14
2	C	501	WBJ	C02-C03-C21-O22
2	C	501	WBJ	N04-C03-C21-O22
2	C	501	WBJ	C02-C03-C21-O23
2	C	501	WBJ	N04-C03-C21-O23
2	C	501	WBJ	N04-C05-C06-C07
2	C	501	WBJ	N04-C05-C06-C14
2	D	501	WBJ	C02-C03-C21-O22
2	D	501	WBJ	N04-C03-C21-O22
2	D	501	WBJ	C02-C03-C21-O23
2	D	501	WBJ	N04-C03-C21-O23
2	D	501	WBJ	N04-C05-C06-C07
2	D	501	WBJ	N04-C05-C06-C14
2	G	501	WBJ	C02-C03-C21-O22
2	G	501	WBJ	N04-C05-C06-C07
2	G	501	WBJ	N04-C05-C06-C14
2	H	501	WBJ	C02-C03-C21-O22
2	H	501	WBJ	C02-C03-C21-O23
2	H	501	WBJ	N04-C03-C21-O23
2	H	501	WBJ	N04-C05-C06-C07
2	H	501	WBJ	N04-C05-C06-C14
2	F	501	WBJ	C02-C03-C21-O22
2	F	501	WBJ	N04-C03-C21-O22
2	F	501	WBJ	C02-C03-C21-O23
2	F	501	WBJ	N04-C03-C21-O23
2	F	501	WBJ	N04-C05-C06-C07
2	F	501	WBJ	N04-C05-C06-C14
2	I	501	WBJ	C02-C03-C21-O22
2	I	501	WBJ	N04-C03-C21-O22
2	I	501	WBJ	C02-C03-C21-O23
2	I	501	WBJ	N04-C03-C21-O23
2	I	501	WBJ	N04-C05-C06-C07

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Mol	Chain	Res	Type	Atoms
2	I	501	WBJ	N04-C05-C06-C14
2	P	501	WBJ	C02-C03-C21-O22
2	P	501	WBJ	N04-C03-C21-O22
2	P	501	WBJ	C02-C03-C21-O23
2	P	501	WBJ	N04-C03-C21-O23
2	P	501	WBJ	N04-C05-C06-C07
2	P	501	WBJ	N04-C05-C06-C14
2	J	501	WBJ	C02-C03-C21-O22
2	J	501	WBJ	N04-C03-C21-O22
2	J	501	WBJ	C02-C03-C21-O23
2	J	501	WBJ	N04-C03-C21-O23
2	J	501	WBJ	N04-C05-C06-C07
2	J	501	WBJ	N04-C05-C06-C14
2	M	501	WBJ	C02-C03-C21-O22
2	M	501	WBJ	N04-C03-C21-O22
2	M	501	WBJ	C02-C03-C21-O23
2	M	501	WBJ	N04-C03-C21-O23
2	M	501	WBJ	N04-C05-C06-C07
2	M	501	WBJ	N04-C05-C06-C14
2	Q	501	WBJ	C02-C03-C21-O22
2	Q	501	WBJ	C02-C03-C21-O23
2	Q	501	WBJ	N04-C05-C06-C07
2	Q	501	WBJ	N04-C05-C06-C14
2	N	501	WBJ	C02-C03-C21-O22
2	N	501	WBJ	N04-C03-C21-O22
2	N	501	WBJ	C02-C03-C21-O23
2	N	501	WBJ	N04-C03-C21-O23
2	N	501	WBJ	N04-C05-C06-C07
2	N	501	WBJ	N04-C05-C06-C14
2	E	501	WBJ	C02-C03-C21-O22
2	E	501	WBJ	N04-C03-C21-O22
2	E	501	WBJ	C02-C03-C21-O23
2	E	501	WBJ	N04-C03-C21-O23
2	E	501	WBJ	N04-C05-C06-C07
2	E	501	WBJ	N04-C05-C06-C14
2	L	501	WBJ	C02-C03-C21-O22
2	L	501	WBJ	N04-C03-C21-O22
2	L	501	WBJ	C02-C03-C21-O23
2	L	501	WBJ	N04-C03-C21-O23
2	L	501	WBJ	N04-C05-C06-C07
2	L	501	WBJ	N04-C05-C06-C14
2	K	501	WBJ	N04-C05-C06-C07

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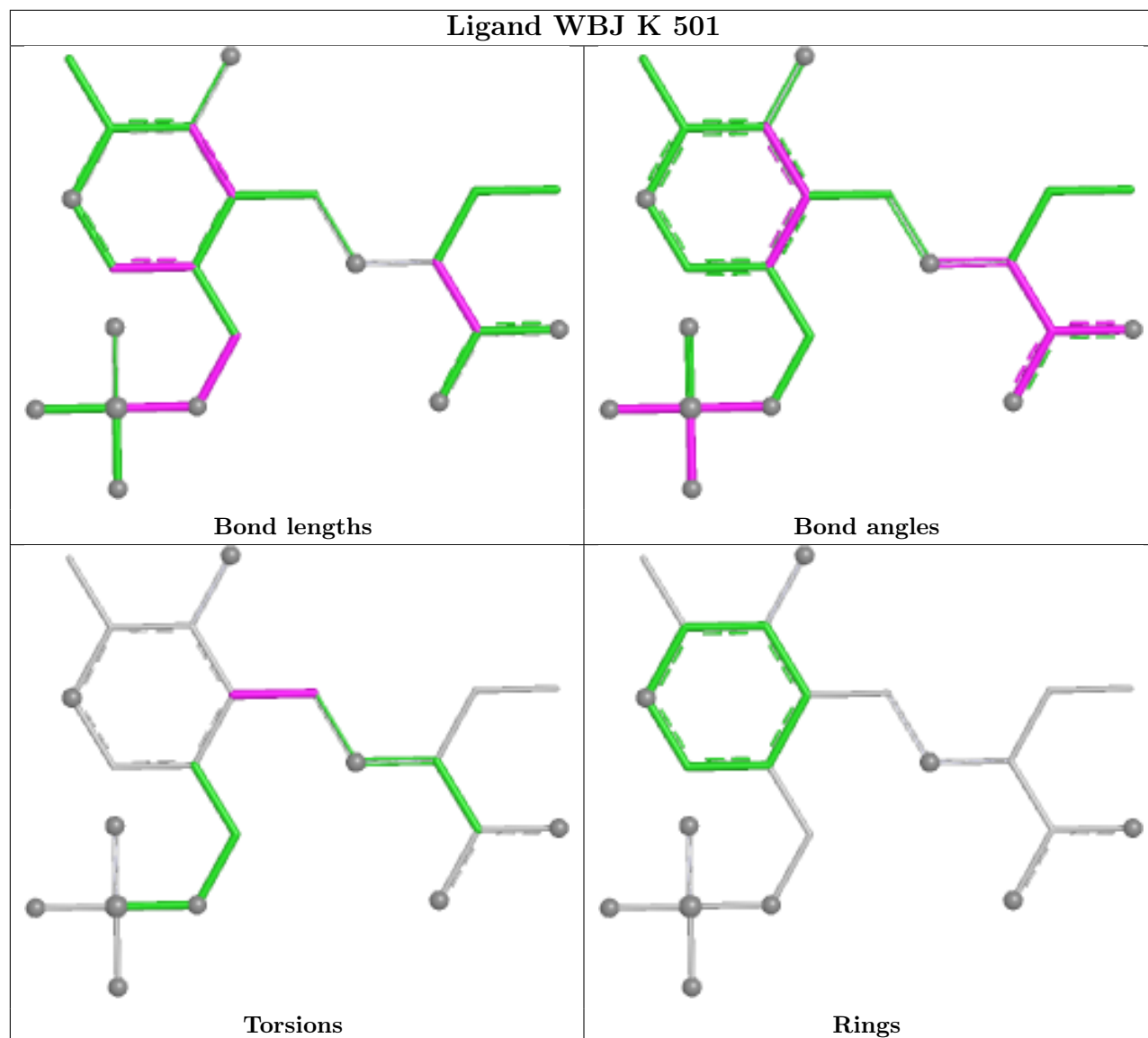
Mol	Chain	Res	Type	Atoms
2	K	501	WBJ	N04-C05-C06-C14
2	N	501	WBJ	C06-C14-C15-O16
2	H	501	WBJ	N04-C03-C21-O22
2	Q	501	WBJ	N04-C03-C21-O22
2	Q	501	WBJ	N04-C03-C21-O23
2	N	501	WBJ	C12-C14-C15-O16
2	E	501	WBJ	C12-C14-C15-O16
2	B	501	WBJ	C02-C03-C21-O23
2	G	501	WBJ	C02-C03-C21-O23
2	E	501	WBJ	C06-C14-C15-O16

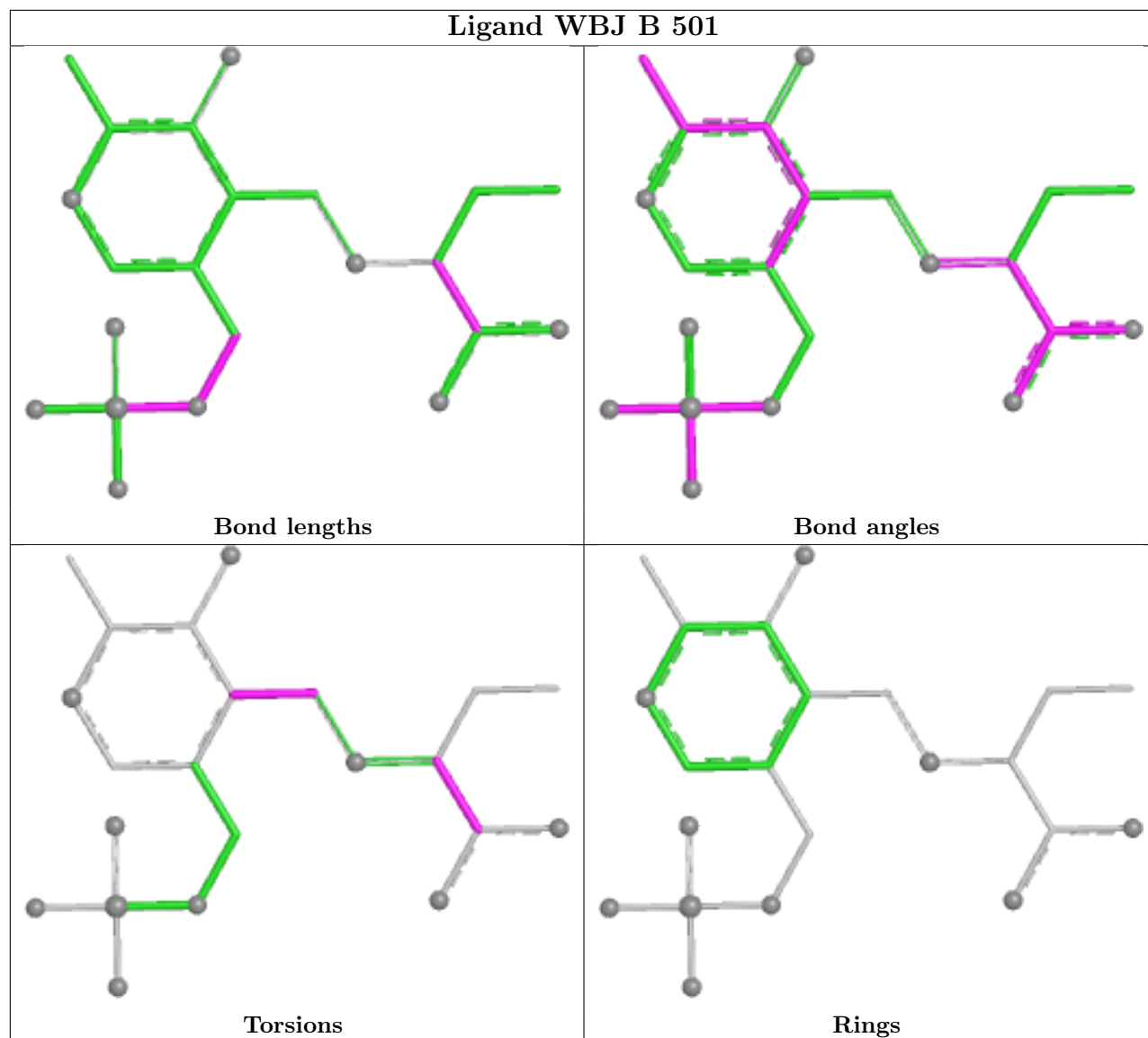
There are no ring outliers.

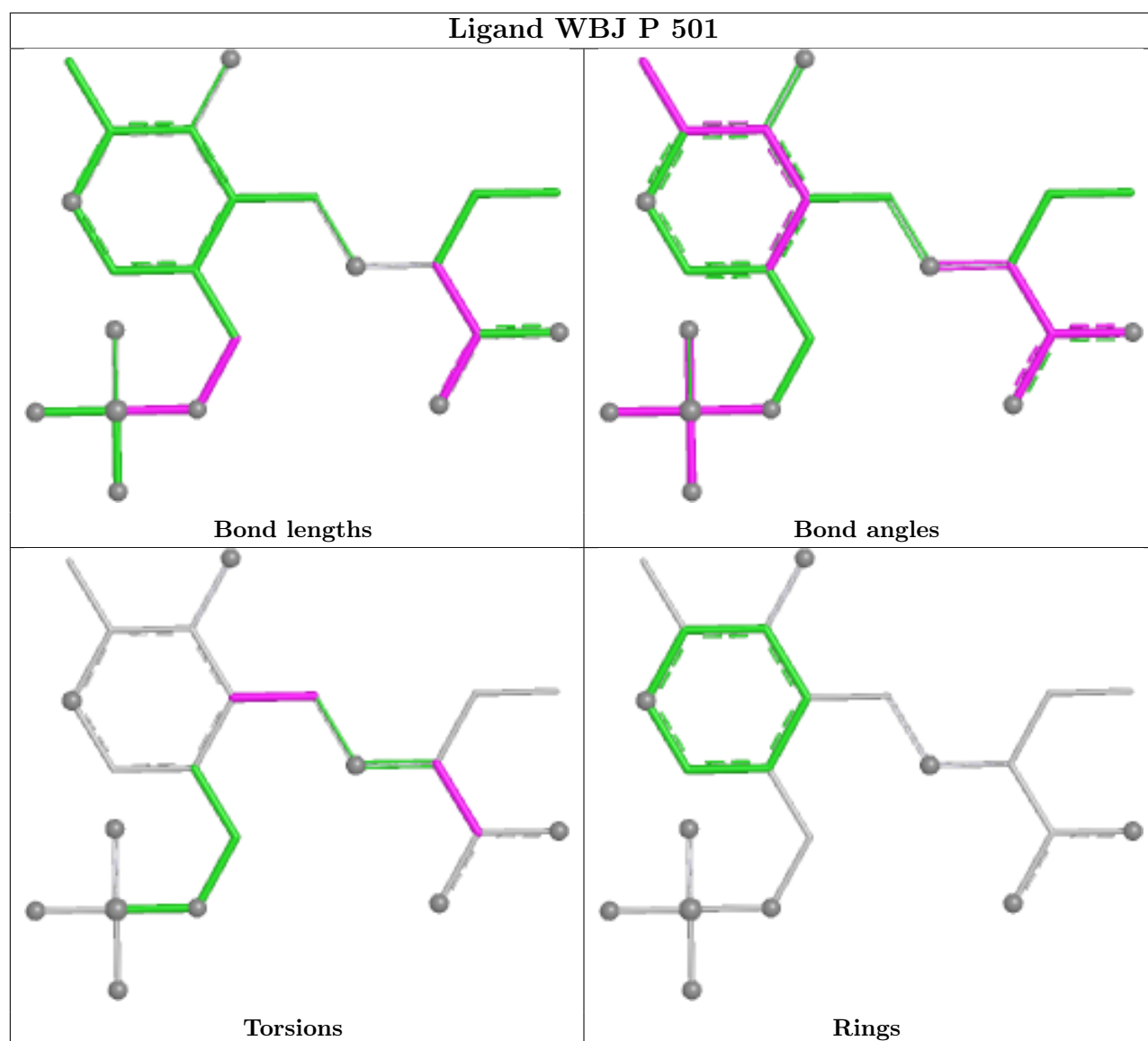
2 monomers are involved in 2 short contacts:

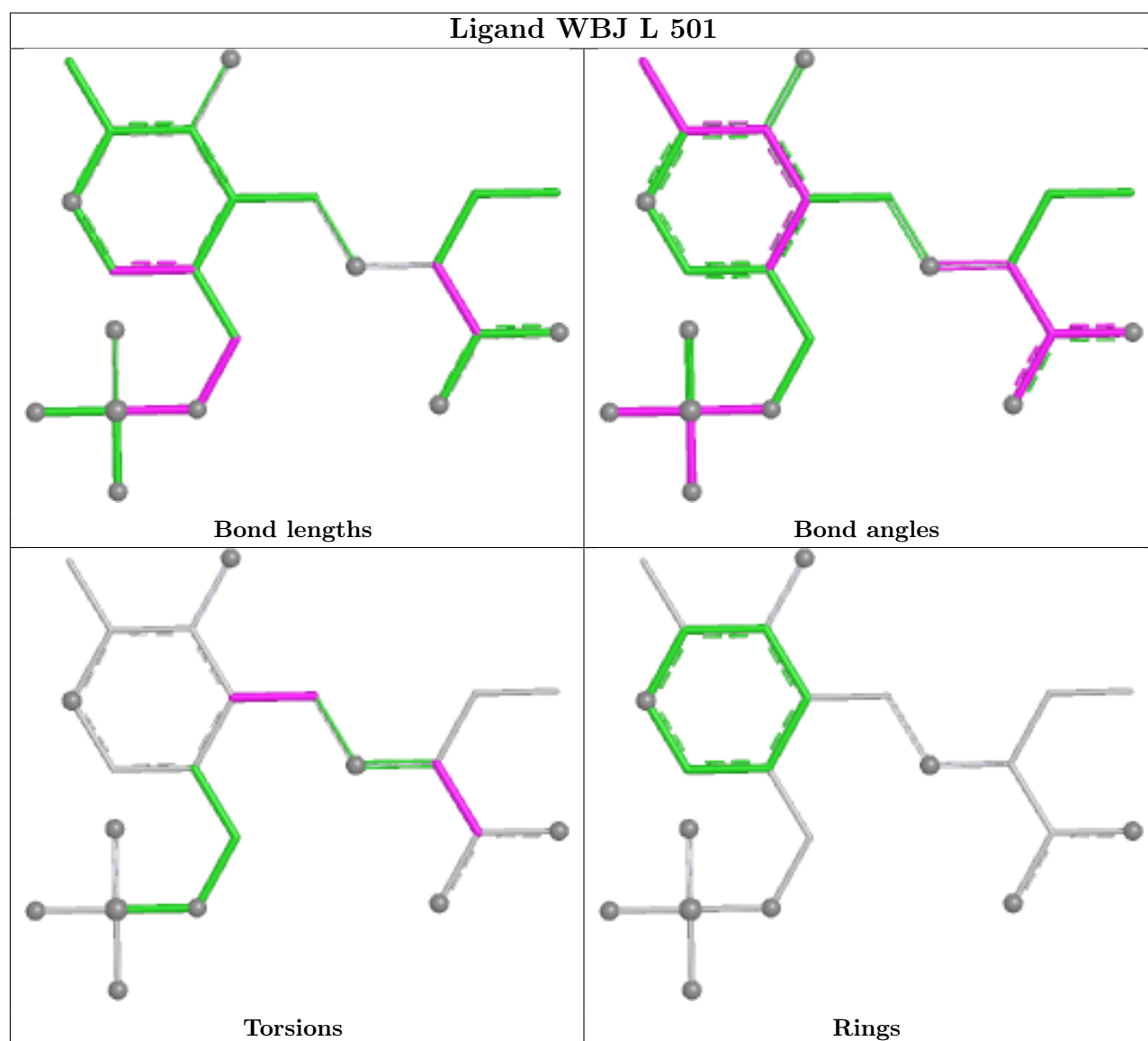
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	WBJ	1	0
2	L	501	WBJ	1	0

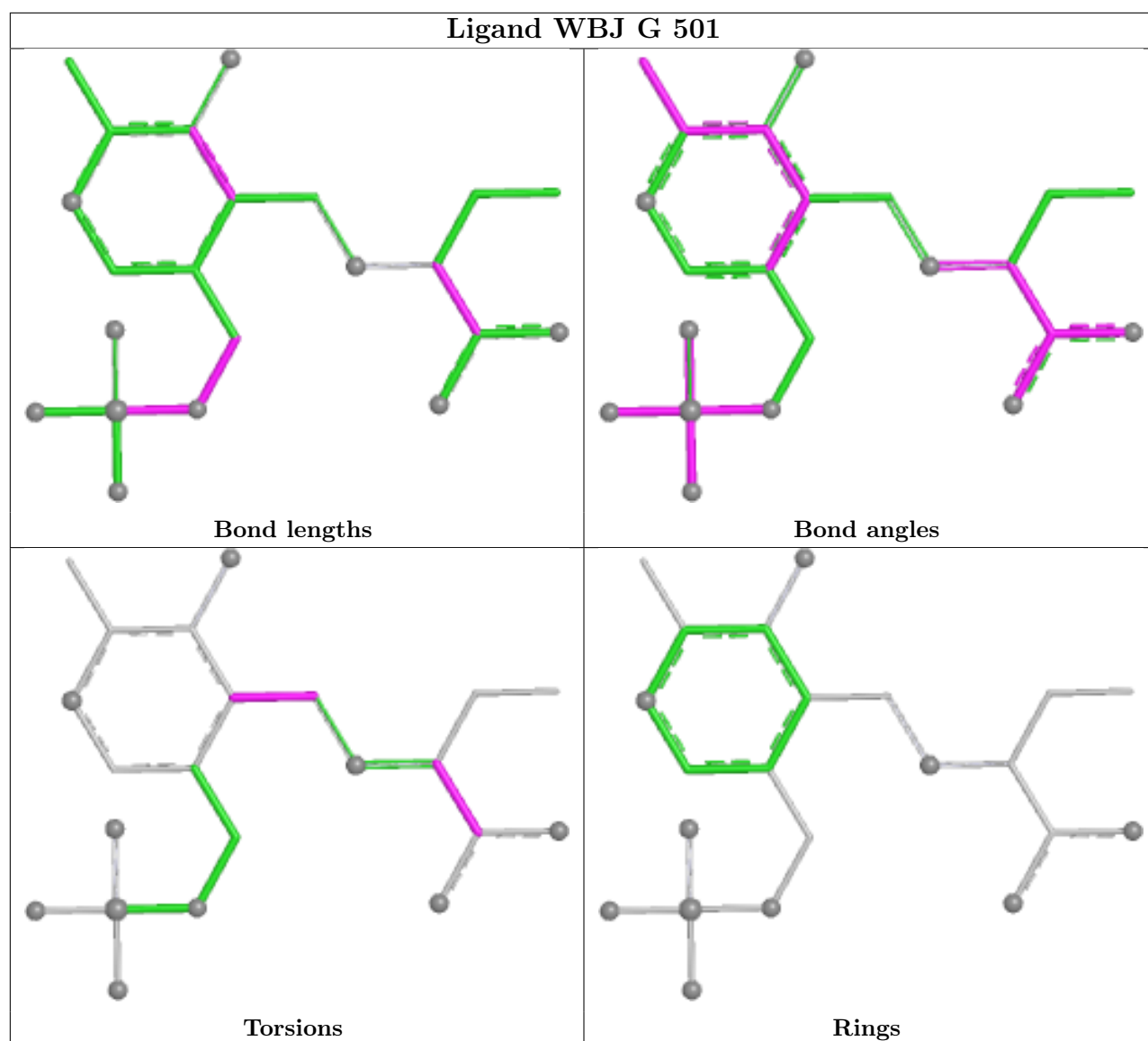
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

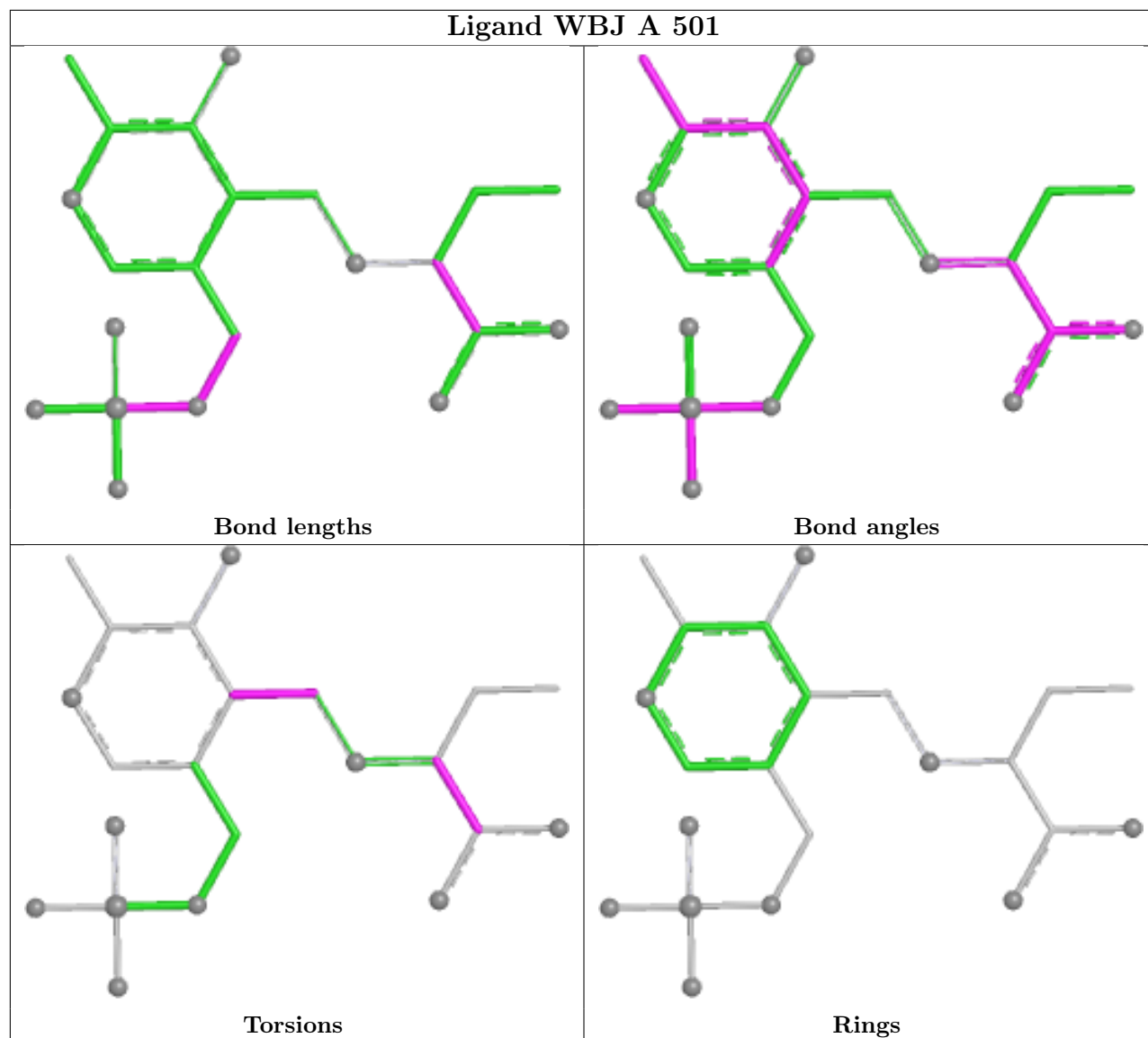


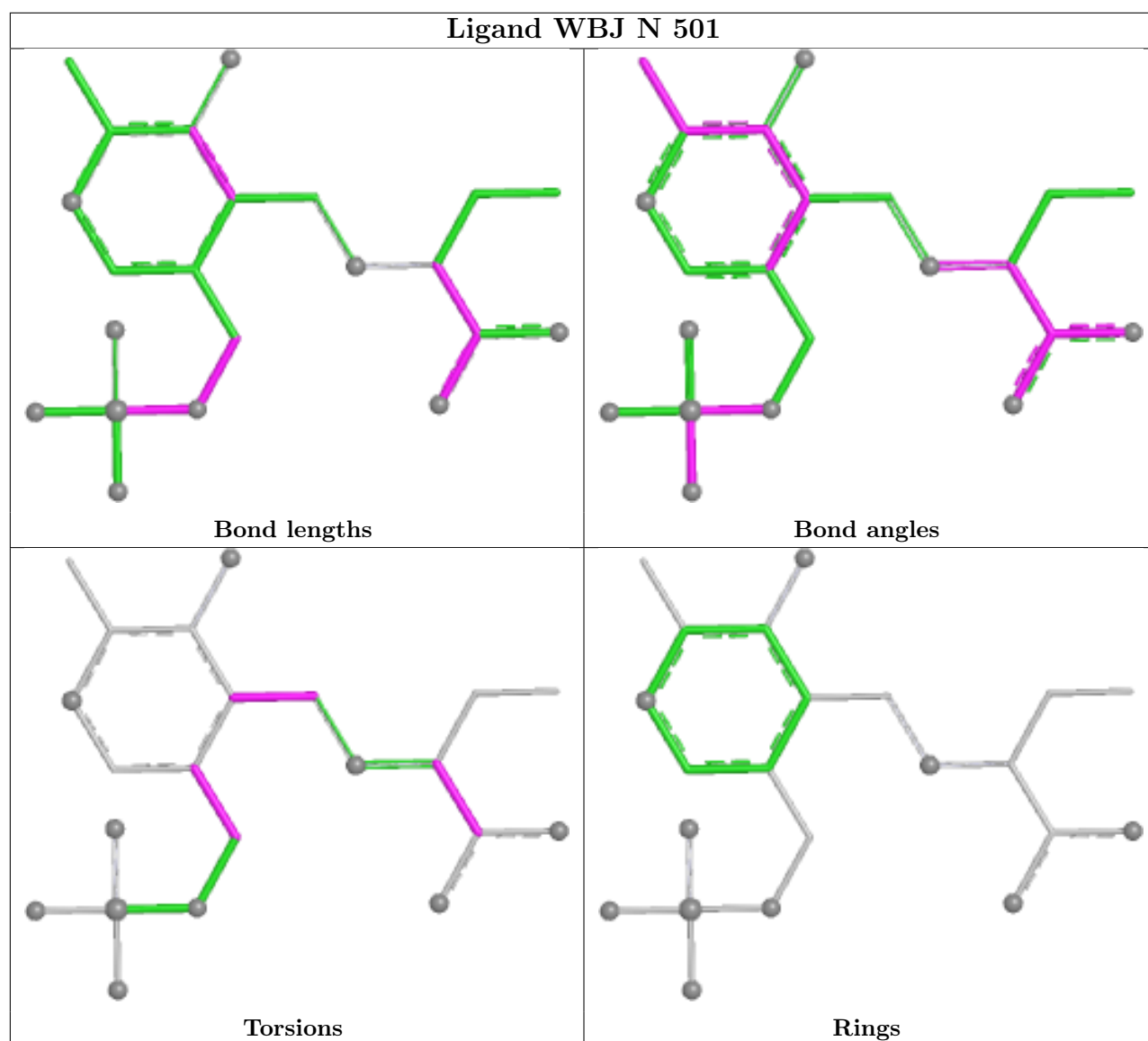


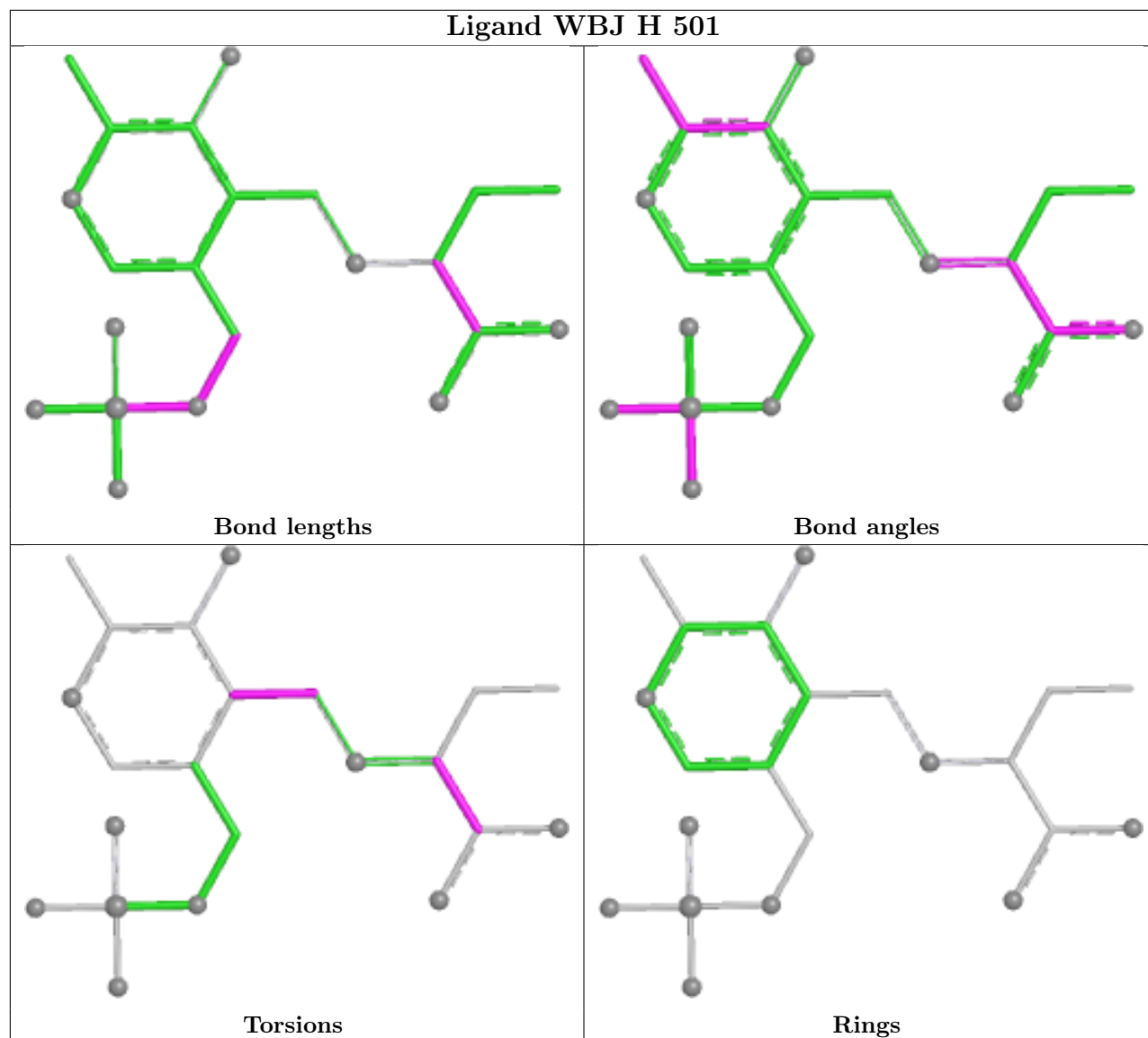




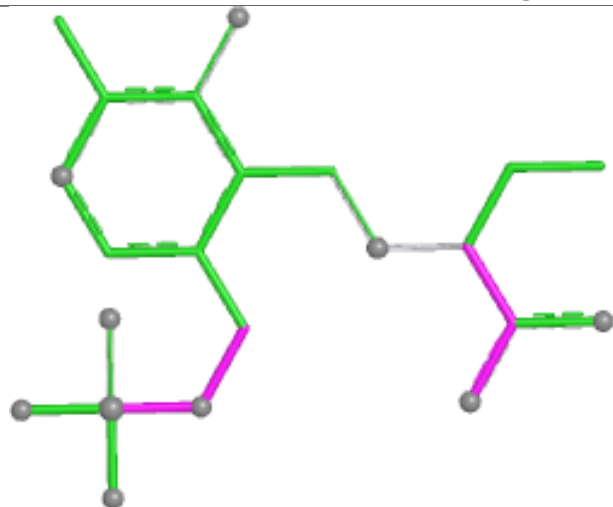




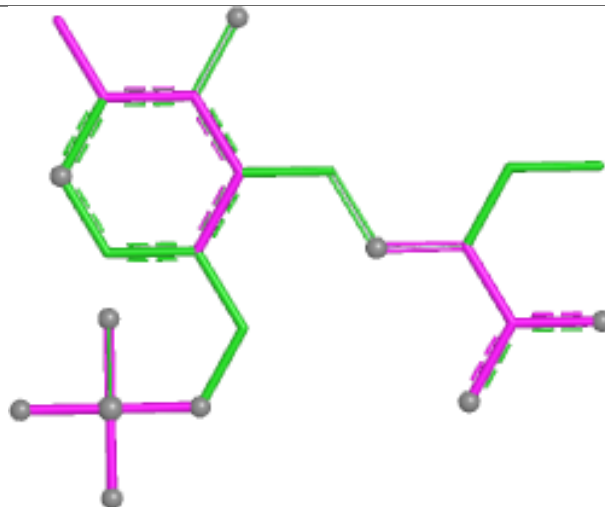




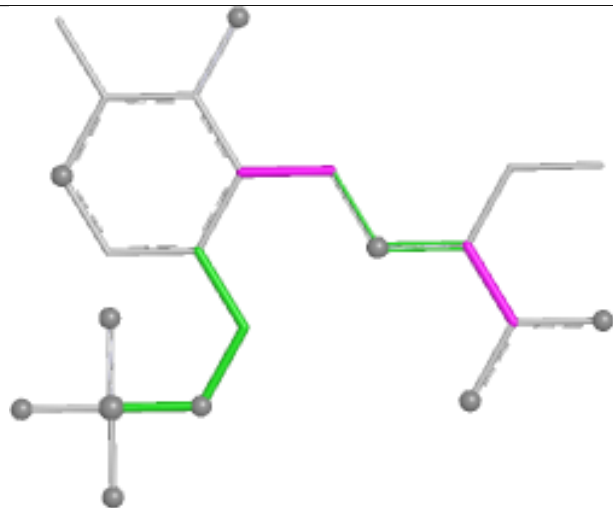
Ligand WBJ I 501



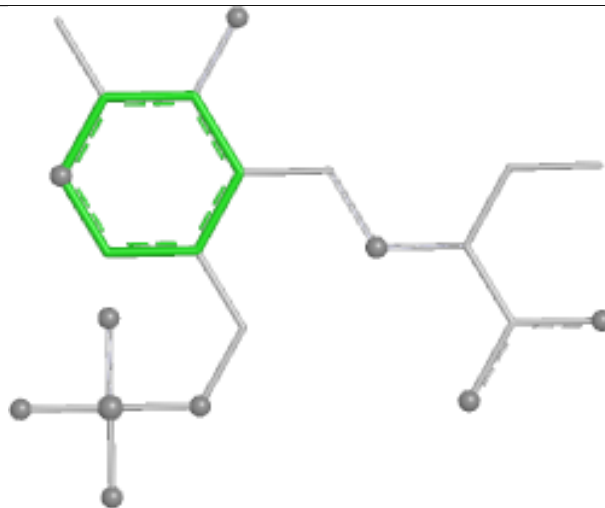
Bond lengths



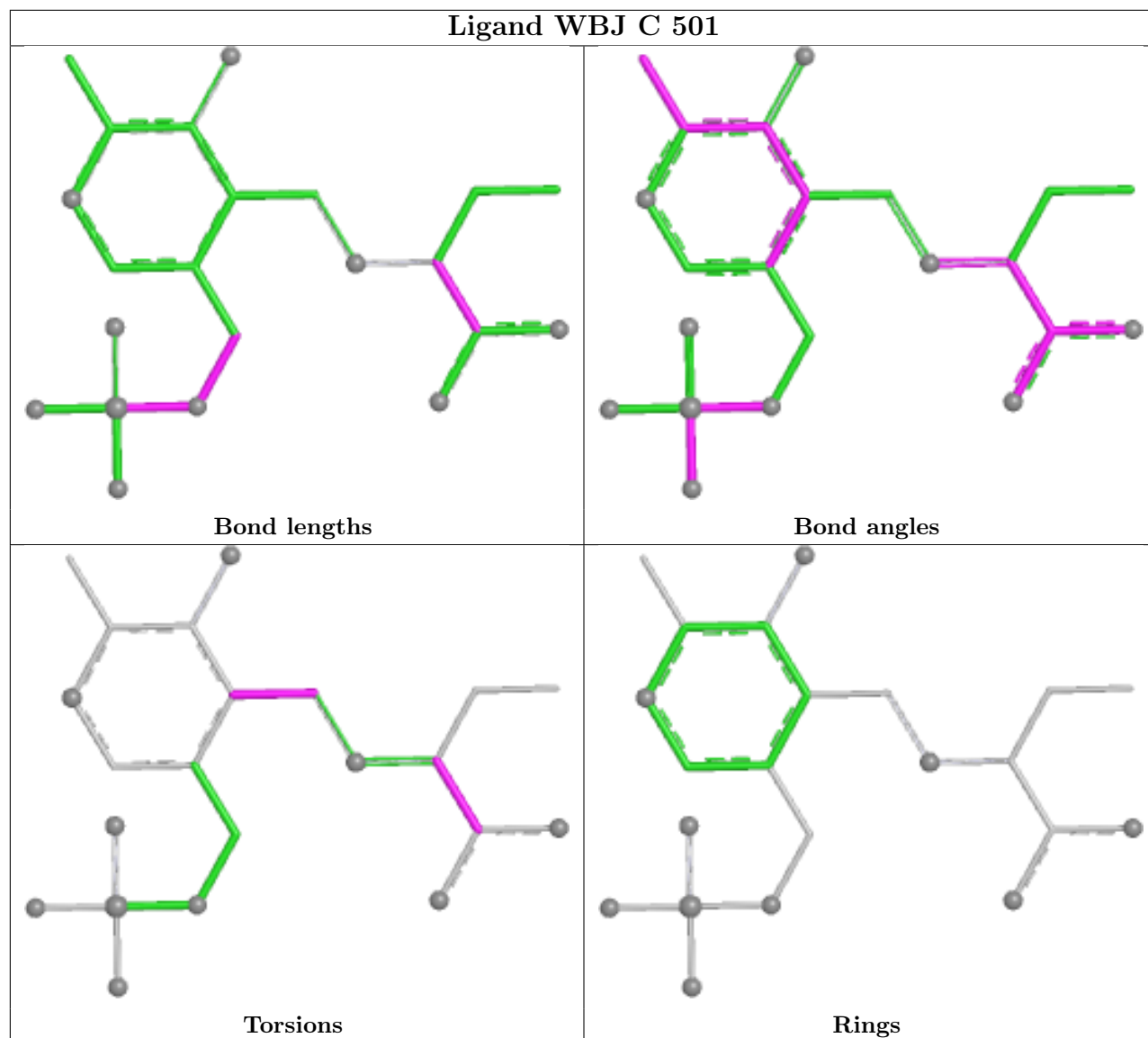
Bond angles

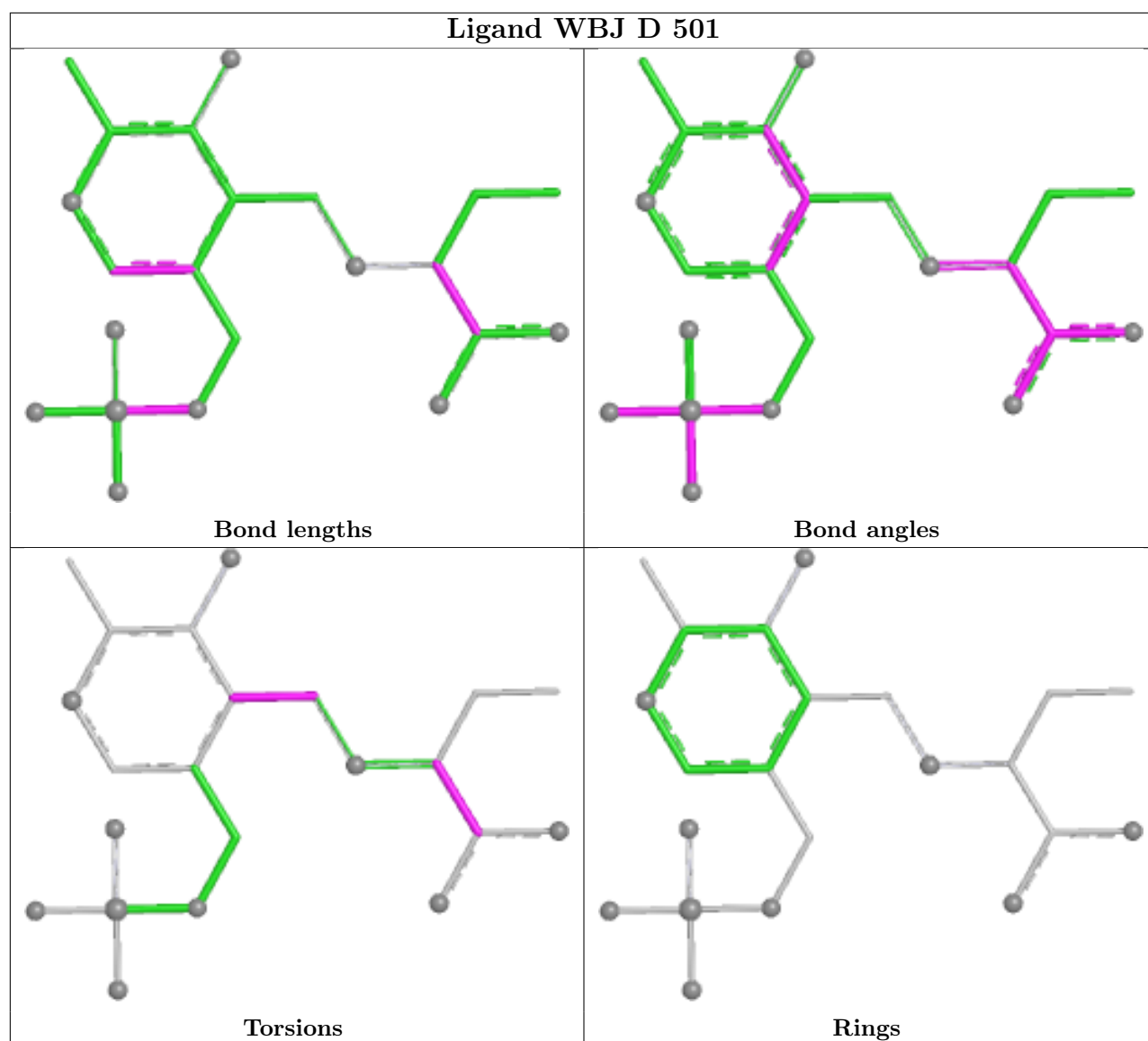


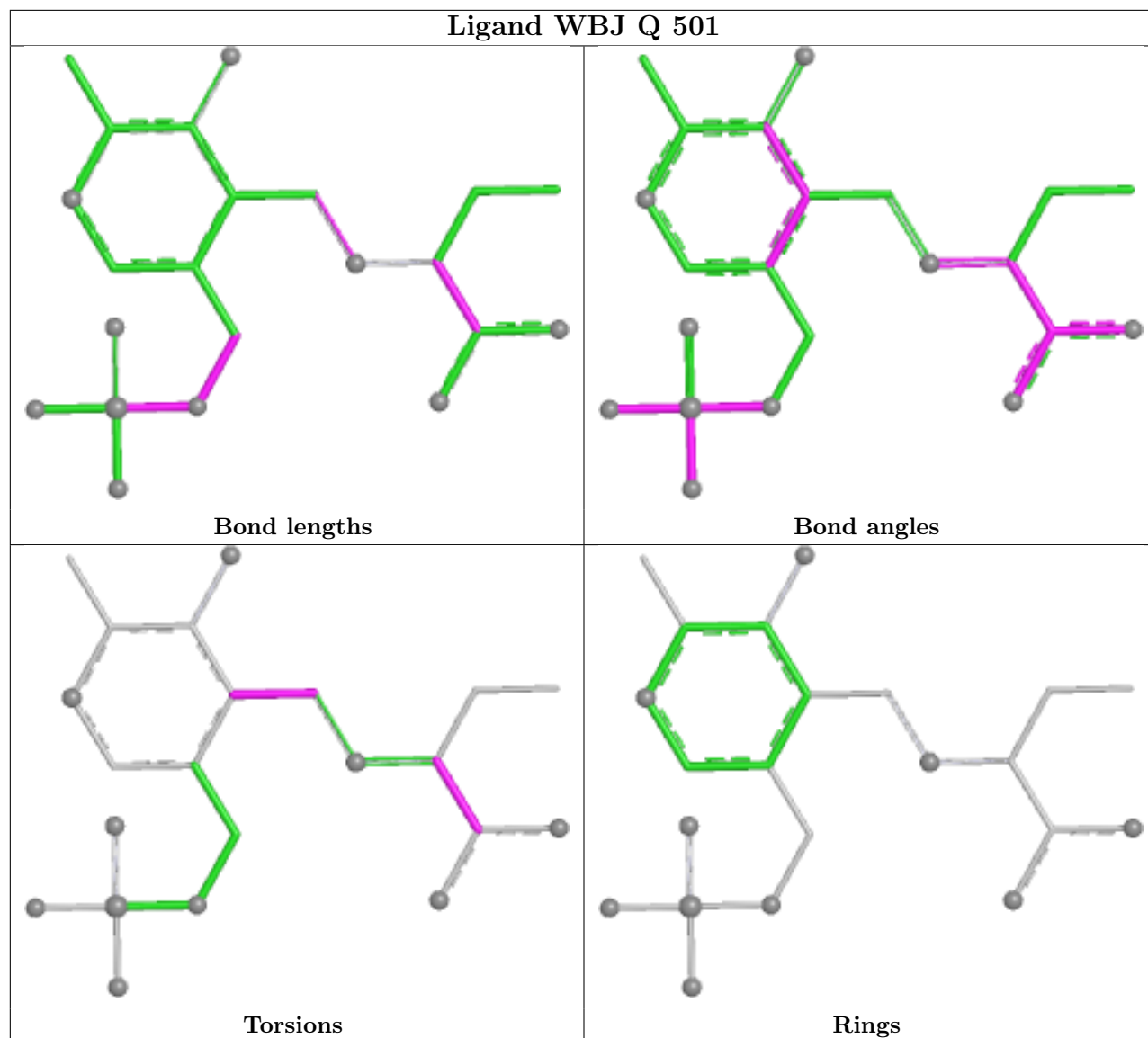
Torsions

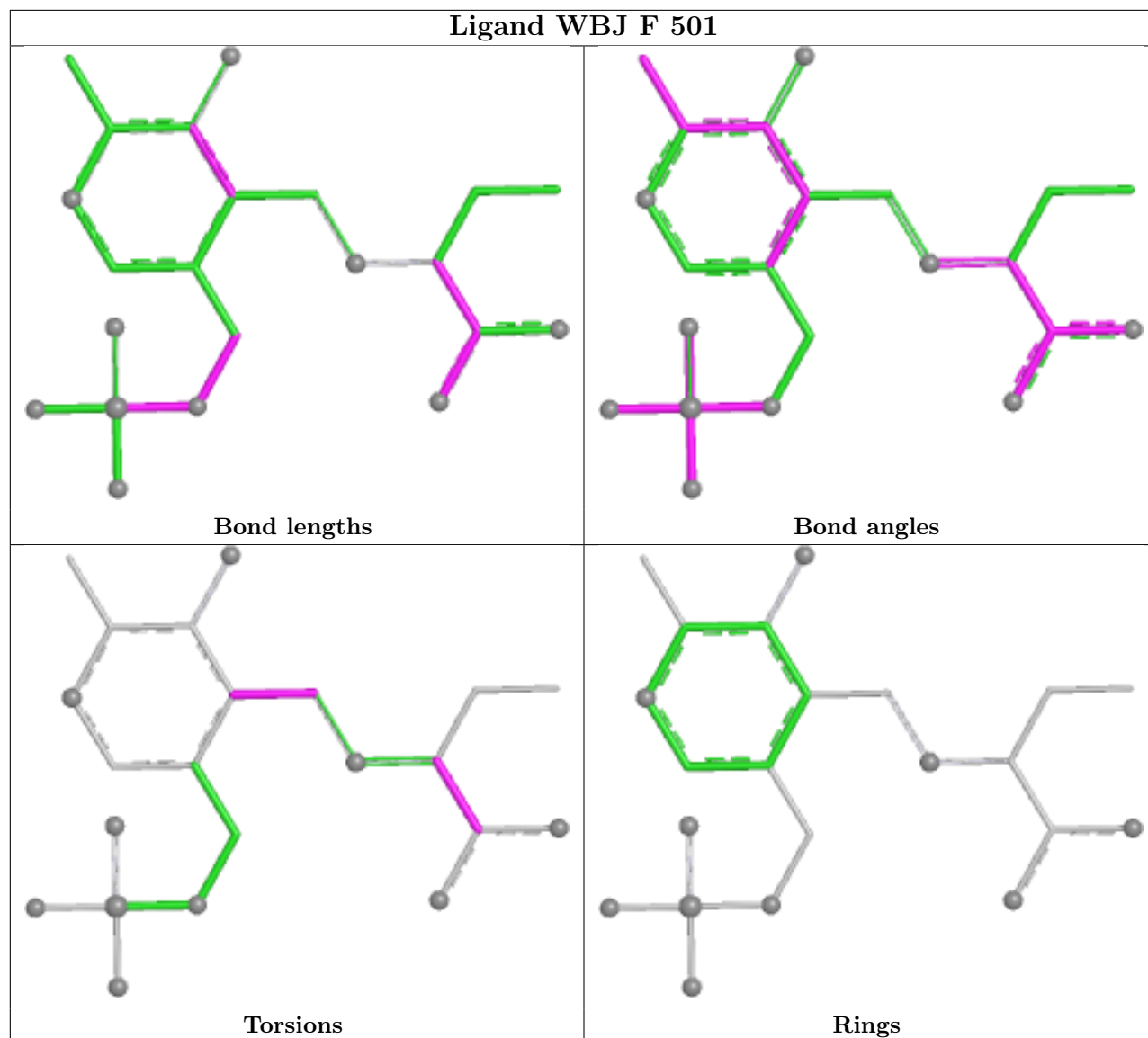


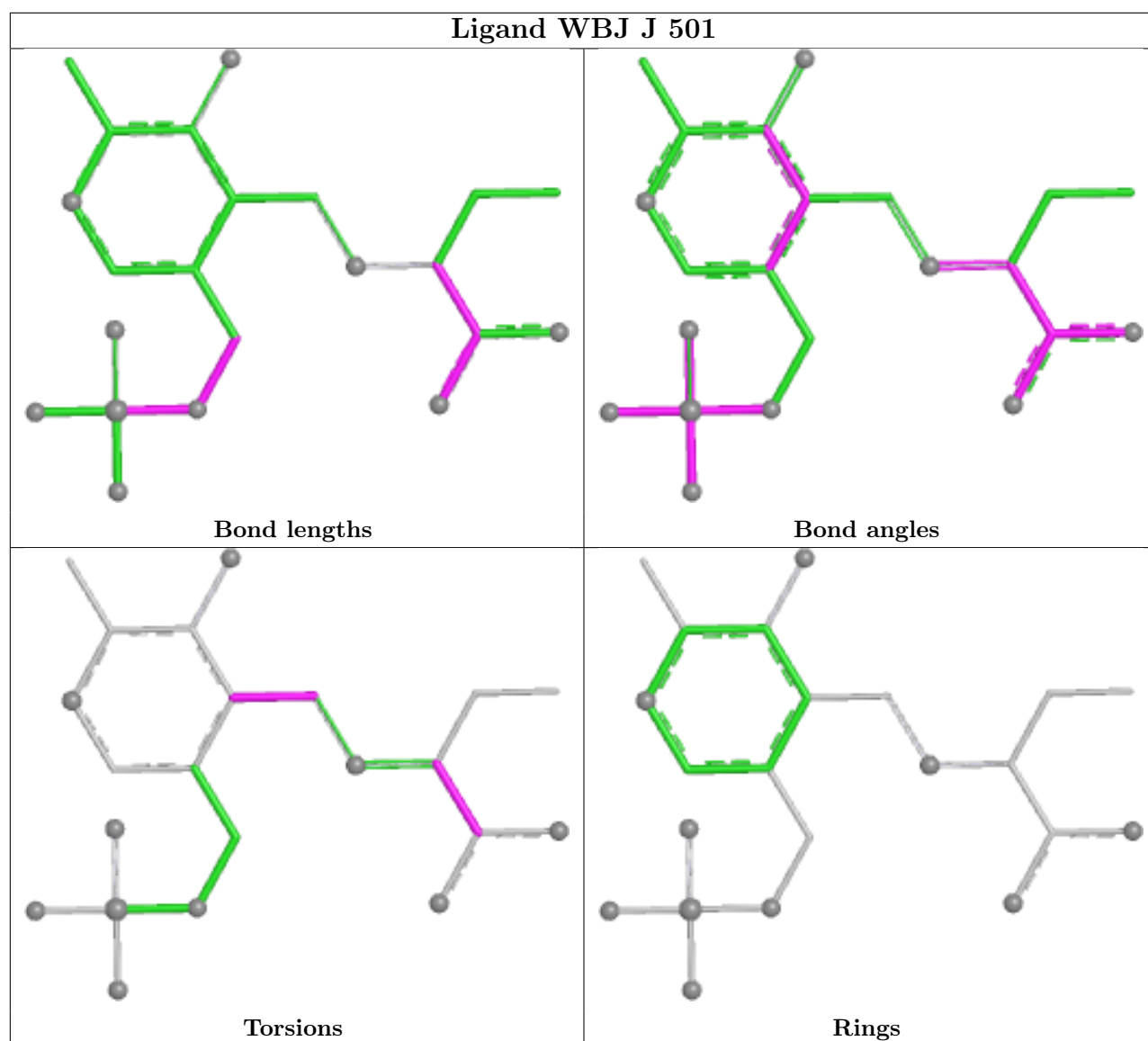
Rings

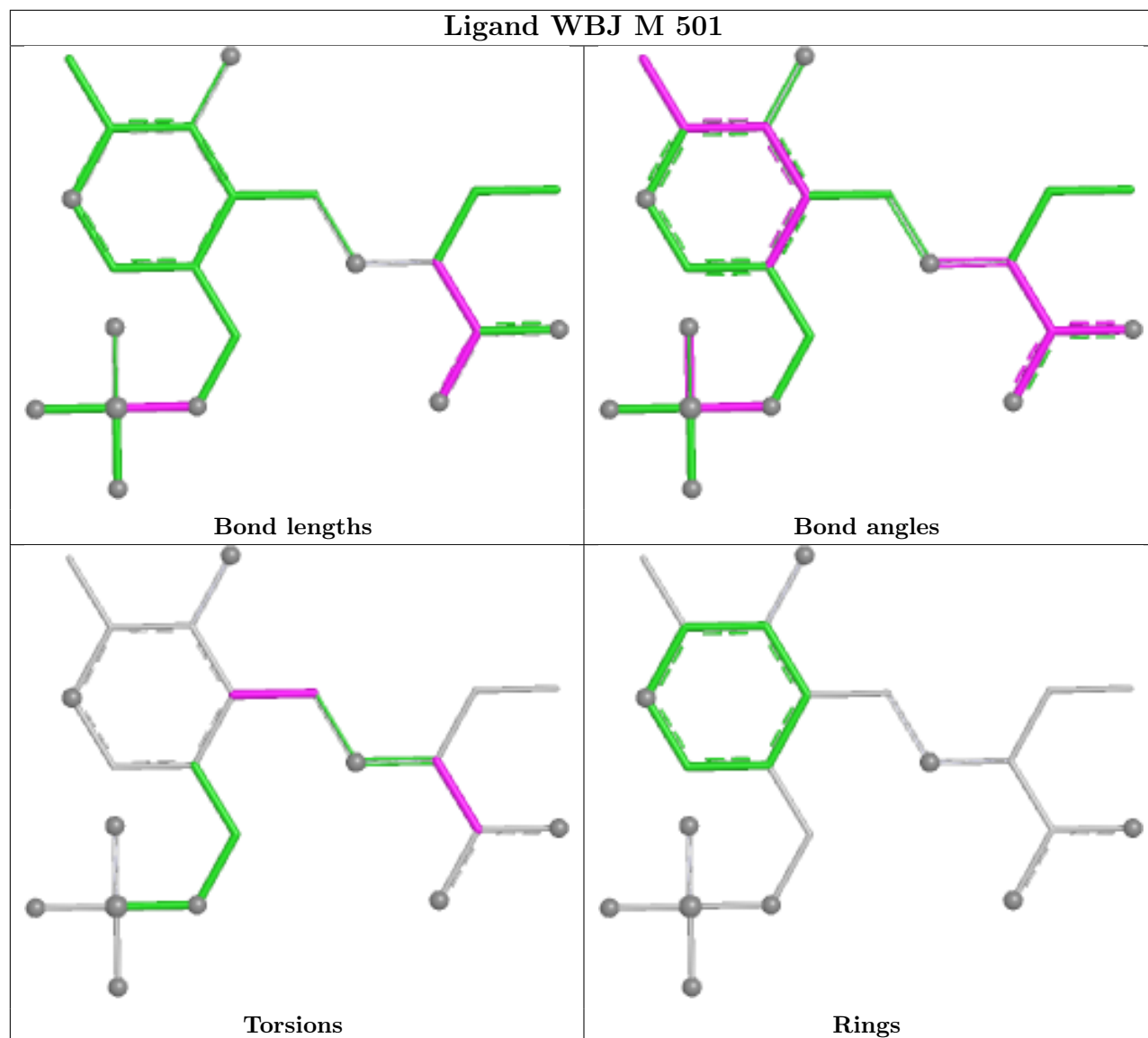


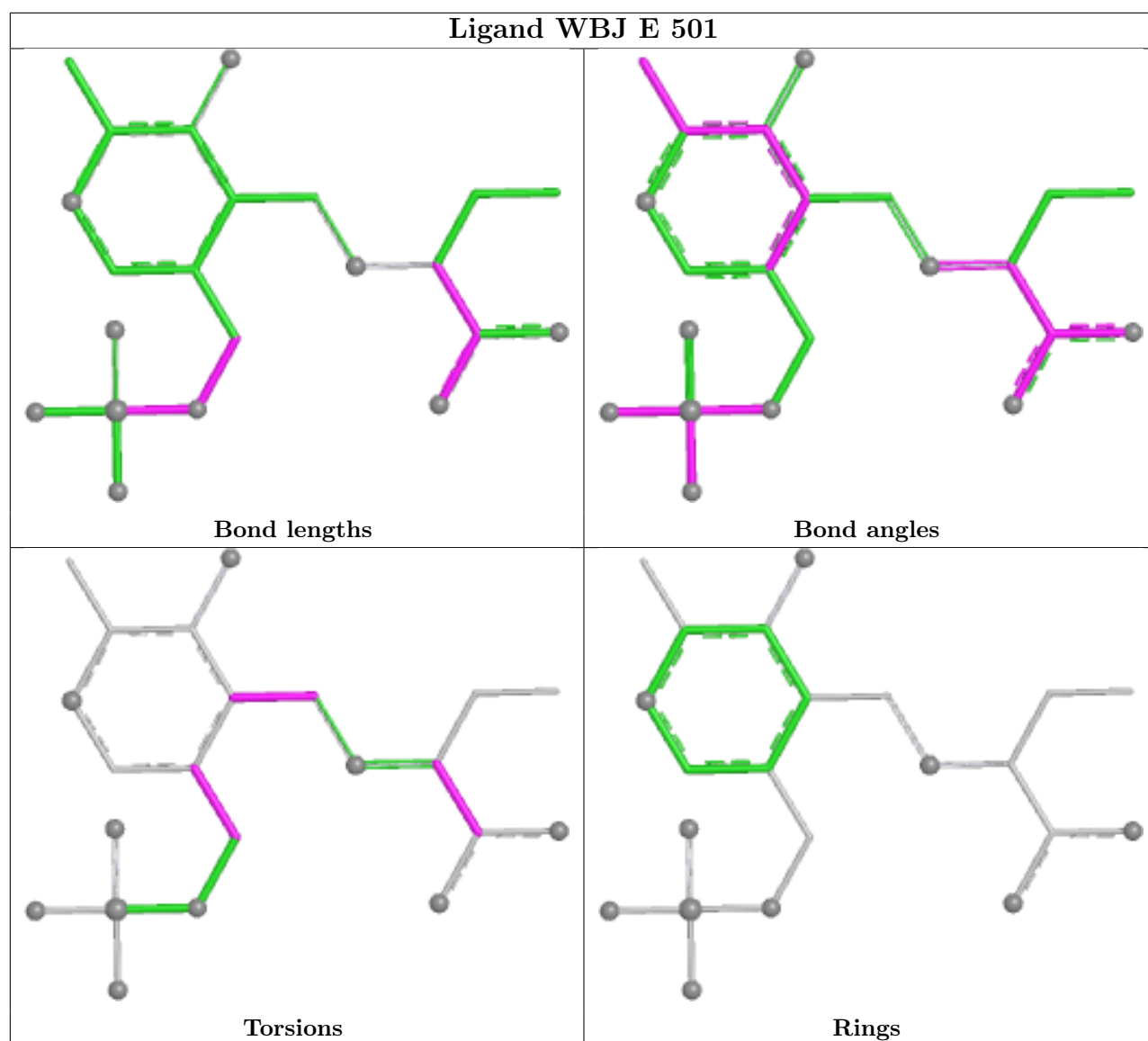












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	428/433 (98%)	-0.01	13 (3%)	52	62	9, 20, 35, 57	2 (0%)
1	B	427/433 (98%)	0.13	17 (3%)	42	52	7, 21, 36, 64	1 (0%)
1	C	427/433 (98%)	-0.20	10 (2%)	61	70	9, 17, 31, 60	1 (0%)
1	D	428/433 (98%)	-0.09	10 (2%)	61	70	9, 18, 32, 54	0
1	E	427/433 (98%)	0.19	22 (5%)	33	42	10, 22, 38, 64	1 (0%)
1	F	425/433 (98%)	0.10	18 (4%)	40	50	11, 21, 36, 55	1 (0%)
1	G	427/433 (98%)	0.05	17 (3%)	42	52	11, 21, 35, 55	1 (0%)
1	H	426/433 (98%)	0.17	12 (2%)	55	65	12, 23, 37, 55	0
1	I	428/433 (98%)	0.15	17 (3%)	42	52	13, 23, 38, 56	0
1	J	427/433 (98%)	0.25	22 (5%)	33	42	12, 23, 38, 60	0
1	K	429/433 (99%)	0.18	25 (5%)	29	37	13, 22, 39, 62	0
1	L	428/433 (98%)	0.05	17 (3%)	42	52	11, 21, 37, 51	0
1	M	428/433 (98%)	-0.03	13 (3%)	52	62	10, 19, 33, 60	0
1	N	422/433 (97%)	0.14	13 (3%)	51	61	10, 22, 35, 51	1 (0%)
1	P	428/433 (98%)	0.06	18 (4%)	40	50	11, 21, 36, 58	1 (0%)
1	Q	429/433 (99%)	-0.07	16 (3%)	45	55	10, 18, 33, 56	0
All	All	6834/6928 (98%)	0.07	260 (3%)	44	54	7, 21, 36, 64	9 (0%)

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	5	VAL	7.2
1	B	5	VAL	6.5
1	B	7	GLN	5.8
1	J	354	ASP	5.6
1	E	354	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	K	354	ASP	5.2
1	C	354	ASP	5.0
1	P	354	ASP	4.8
1	P	147	ASP	4.7
1	B	354	ASP	4.7
1	E	355	ALA	4.6
1	Q	355	ALA	4.6
1	F	353	GLY	4.6
1	C	6	PHE	4.4
1	A	354	ASP	4.4
1	Q	21	ASP	4.4
1	I	54	LEU	4.2
1	B	355	ALA	4.1
1	N	7	GLN	4.1
1	G	354	ASP	4.0
1	M	5	VAL	4.0
1	A	356	SER	4.0
1	D	4	GLN	4.0
1	H	21	ASP	4.0
1	P	135	ARG	3.9
1	J	395	ASP	3.9
1	P	355	ALA	3.9
1	M	7	GLN	3.9
1	D	5	VAL	3.9
1	J	5	VAL	3.9
1	D	6	PHE	3.9
1	Q	5	VAL	3.8
1	E	356	SER	3.8
1	J	428	GLN	3.8
1	M	353	GLY	3.7
1	Q	4	GLN	3.7
1	H	22	PRO	3.7
1	F	355	ALA	3.7
1	K	5	VAL	3.7
1	E	21	ASP	3.7
1	J	22	PRO	3.7
1	A	7	GLN	3.7
1	F	354	ASP	3.7
1	F	6	PHE	3.7
1	M	354	ASP	3.6
1	A	5	VAL	3.6
1	K	22	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	N	398	LEU	3.6
1	K	355	ALA	3.6
1	F	22	PRO	3.6
1	F	134	VAL	3.6
1	I	5	VAL	3.6
1	K	23	HIS	3.6
1	D	354	ASP	3.6
1	K	352	LYS	3.6
1	A	21	ASP	3.5
1	J	23	HIS	3.5
1	C	355	ALA	3.5
1	B	356	SER	3.5
1	I	147	ASP	3.5
1	I	353	GLY	3.4
1	F	252	LEU	3.4
1	K	147	ASP	3.4
1	I	354	ASP	3.4
1	I	355	ALA	3.4
1	A	23	HIS	3.3
1	N	147	ASP	3.3
1	G	355	ALA	3.3
1	Q	23	HIS	3.3
1	L	252	LEU	3.3
1	G	22	PRO	3.3
1	E	23	HIS	3.2
1	A	355	ALA	3.2
1	P	52	LYS	3.2
1	G	237	ASP	3.2
1	G	252	LEU	3.2
1	K	353	GLY	3.2
1	M	23	HIS	3.2
1	F	7	GLN	3.2
1	M	6	PHE	3.2
1	G	23	HIS	3.2
1	E	237	ASP	3.2
1	E	395	ASP	3.2
1	C	7	GLN	3.1
1	Q	7	GLN	3.1
1	E	7	GLN	3.1
1	N	356	SER	3.1
1	C	23	HIS	3.1
1	L	23	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	252	LEU	3.1
1	M	147	ASP	3.0
1	Q	354	ASP	3.0
1	J	21	ASP	3.0
1	P	5	VAL	2.9
1	H	431	TYR	2.9
1	B	147	ASP	2.9
1	A	6	PHE	2.9
1	B	22	PRO	2.9
1	G	54	LEU	2.9
1	F	360	LYS	2.9
1	P	22	PRO	2.9
1	B	6	PHE	2.9
1	H	23	HIS	2.9
1	L	354	ASP	2.9
1	Q	252	LEU	2.9
1	K	392	LEU	2.9
1	N	6	PHE	2.9
1	G	5	VAL	2.8
1	N	23	HIS	2.8
1	M	355	ALA	2.8
1	E	6	PHE	2.8
1	E	252	LEU	2.8
1	P	21	ASP	2.8
1	N	127	PHE	2.8
1	B	353	GLY	2.8
1	F	54	LEU	2.8
1	L	22	PRO	2.8
1	C	432	GLY	2.8
1	I	7	GLN	2.7
1	A	395	ASP	2.7
1	E	147	ASP	2.7
1	A	353	GLY	2.7
1	Q	432	GLY	2.7
1	L	353	GLY	2.7
1	E	398	LEU	2.7
1	I	22	PRO	2.7
1	P	23	HIS	2.7
1	J	355	ALA	2.7
1	P	353	GLY	2.6
1	D	327	GLU	2.6
1	K	359	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	54	LEU	2.6
1	I	23	HIS	2.6
1	H	7	GLN	2.6
1	Q	356	SER	2.6
1	B	428	GLN	2.6
1	D	23	HIS	2.6
1	K	6	PHE	2.6
1	A	398	LEU	2.6
1	K	21	ASP	2.6
1	F	356	SER	2.6
1	K	431	TYR	2.5
1	J	195	ILE	2.5
1	E	353	GLY	2.5
1	P	6	PHE	2.5
1	G	359	SER	2.5
1	H	355	ALA	2.5
1	G	21	ASP	2.5
1	Q	6	PHE	2.5
1	F	196[A]	ARG	2.5
1	J	196	ARG	2.5
1	F	23	HIS	2.5
1	E	359	SER	2.5
1	H	318	VAL	2.5
1	I	135	ARG	2.4
1	N	252	LEU	2.4
1	K	127	PHE	2.4
1	B	237	ASP	2.4
1	K	274	ASP	2.4
1	L	5	VAL	2.4
1	P	54	LEU	2.4
1	J	54	LEU	2.4
1	J	431	TYR	2.4
1	M	252	LEU	2.4
1	N	359	SER	2.4
1	C	234	LYS	2.4
1	E	195	ILE	2.4
1	H	428	GLN	2.4
1	L	428	GLN	2.4
1	B	137	GLY	2.4
1	C	356	SER	2.4
1	I	356	SER	2.4
1	K	429	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q	431	TYR	2.4
1	B	395	ASP	2.4
1	K	430	ALA	2.4
1	C	21	ASP	2.3
1	J	130	LYS	2.3
1	L	21	ASP	2.3
1	G	347	LEU	2.3
1	H	54	LEU	2.3
1	I	252	LEU	2.3
1	C	127	PHE	2.3
1	D	127	PHE	2.3
1	G	127	PHE	2.3
1	I	360	LYS	2.3
1	Q	234	LYS	2.3
1	J	318	VAL	2.3
1	J	313	GLU	2.3
1	I	4	GLN	2.3
1	F	431	TYR	2.3
1	N	22	PRO	2.3
1	E	357	ALA	2.3
1	Q	195	ILE	2.3
1	G	356	SER	2.3
1	D	237	ASP	2.3
1	P	428	GLN	2.3
1	K	4	GLN	2.3
1	K	7	GLN	2.3
1	P	431	TYR	2.2
1	M	432	GLY	2.2
1	K	395	ASP	2.2
1	N	428	GLN	2.2
1	B	23	HIS	2.2
1	N	21	ASP	2.2
1	E	22	PRO	2.2
1	B	431	TYR	2.2
1	K	195	ILE	2.2
1	M	428	GLN	2.2
1	L	398	LEU	2.2
1	B	21	ASP	2.2
1	J	356	SER	2.2
1	D	352	LYS	2.2
1	L	52	LYS	2.2
1	D	7	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	7	GLN	2.2
1	I	61	LEU	2.2
1	N	54	LEU	2.2
1	J	247	PRO	2.2
1	Q	22	PRO	2.2
1	L	355	ALA	2.2
1	L	7	GLN	2.1
1	M	237	ASP	2.1
1	L	359	SER	2.1
1	K	398	LEU	2.1
1	G	429	LYS	2.1
1	E	127	PHE	2.1
1	H	354	ASP	2.1
1	F	21	ASP	2.1
1	F	136	SER	2.1
1	H	229	ARG	2.1
1	Q	247	PRO	2.1
1	B	357	ALA	2.1
1	G	7	GLN	2.1
1	I	21	ASP	2.1
1	L	431	TYR	2.1
1	I	229	ARG	2.1
1	E	135	ARG	2.1
1	L	314	SER	2.1
1	G	353	GLY	2.1
1	K	432	GLY	2.1
1	E	385	TRP	2.1
1	K	318	VAL	2.1
1	A	22	PRO	2.1
1	K	428	GLN	2.1
1	E	430	ALA	2.1
1	H	127	PHE	2.0
1	P	127	PHE	2.0
1	A	359	SER	2.0
1	F	314	SER	2.0
1	P	352	LYS	2.0
1	J	6	PHE	2.0
1	J	429	LYS	2.0
1	L	6	PHE	2.0
1	F	229	ARG	2.0
1	M	234	LYS	2.0
1	G	6	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	195	ILE	2.0
1	J	353	GLY	2.0
1	J	316	PRO	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](#)

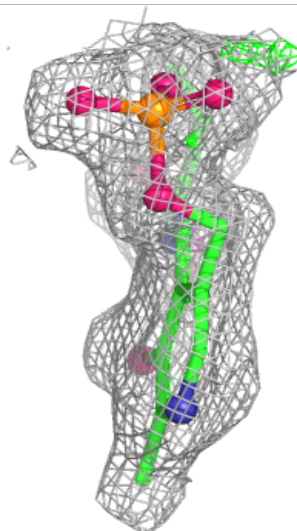
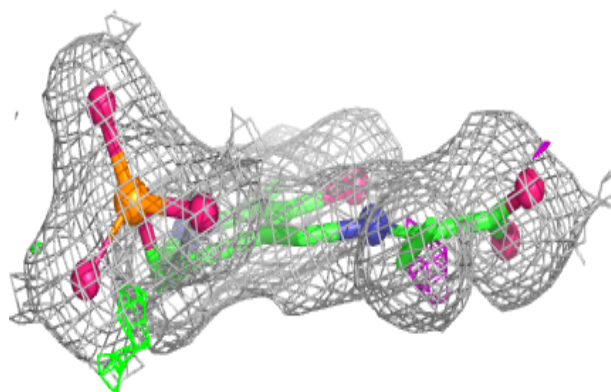
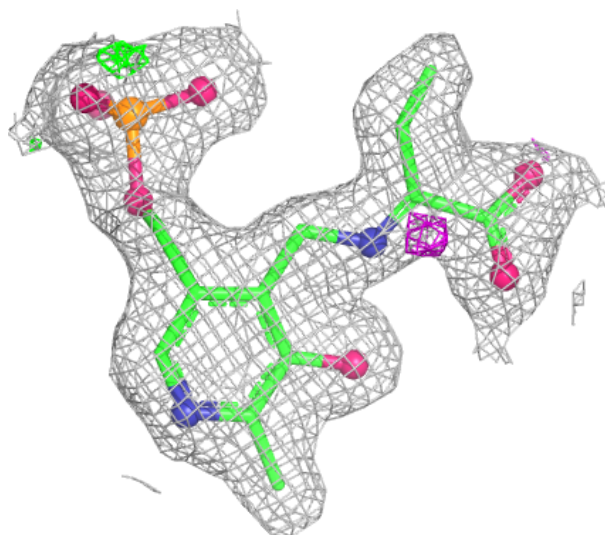
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	WBJ	B	501	22/22	0.97	0.07	13,19,26,29	0
2	WBJ	G	501	22/22	0.97	0.06	13,19,24,26	0
2	WBJ	H	501	22/22	0.97	0.07	14,19,31,33	0
2	WBJ	I	501	22/22	0.97	0.07	14,20,29,32	0
2	WBJ	J	501	22/22	0.97	0.07	13,23,29,35	0
2	WBJ	Q	501	22/22	0.97	0.06	13,18,26,29	0
2	WBJ	E	501	22/22	0.97	0.07	14,21,28,34	0
2	WBJ	D	501	22/22	0.98	0.06	9,15,26,29	0
2	WBJ	P	501	22/22	0.98	0.06	13,17,27,31	0
2	WBJ	A	501	22/22	0.98	0.06	11,15,26,29	0
2	WBJ	M	501	22/22	0.98	0.06	11,15,26,29	0
2	WBJ	C	501	22/22	0.98	0.06	9,15,25,29	0
2	WBJ	N	501	22/22	0.98	0.06	14,21,29,32	0
2	WBJ	F	501	22/22	0.98	0.06	12,20,29,31	0
2	WBJ	L	501	22/22	0.98	0.07	13,21,27,30	0
2	WBJ	K	501	22/22	0.98	0.06	14,20,30,34	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.

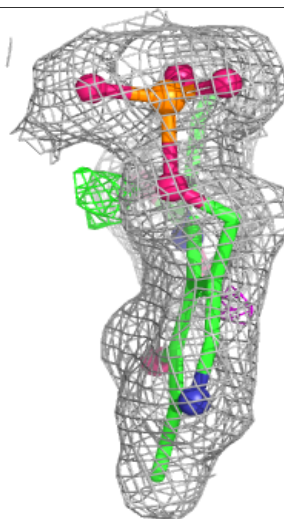
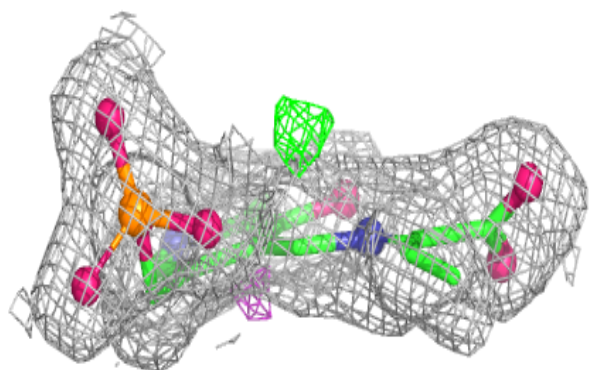
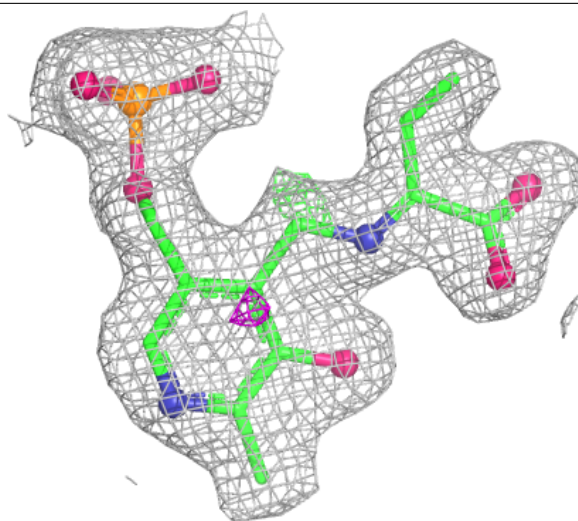
Electron density around WBJ B 501:

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



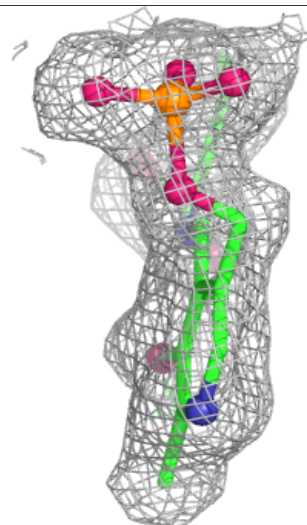
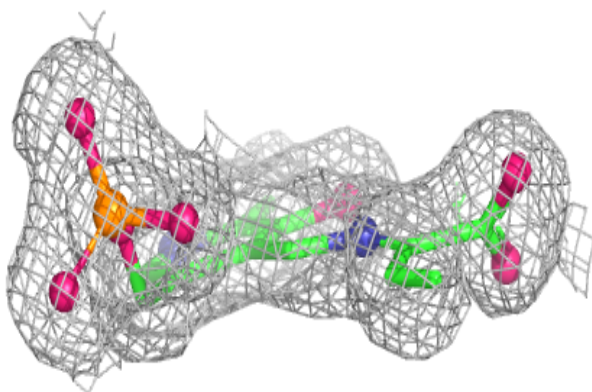
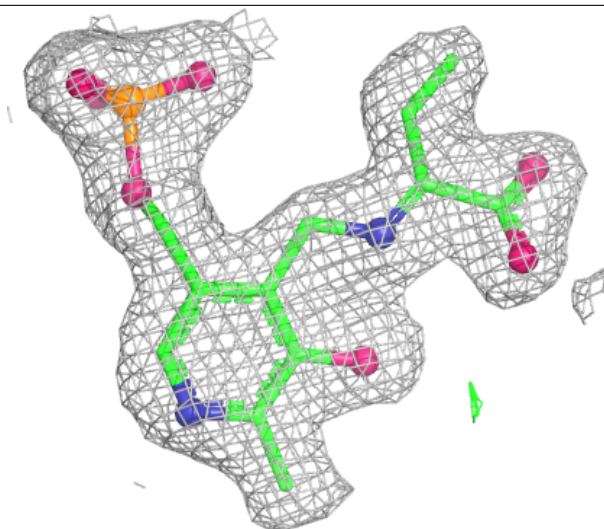
Electron density around WBJ G 501:

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



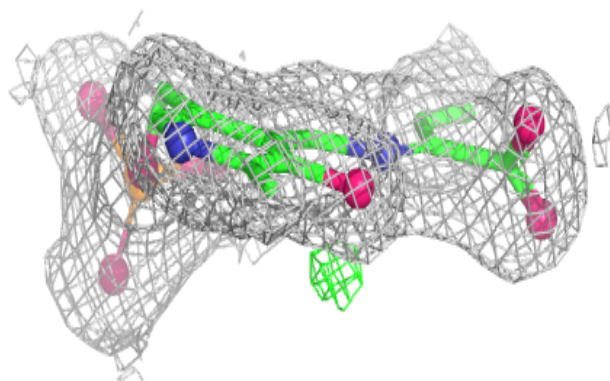
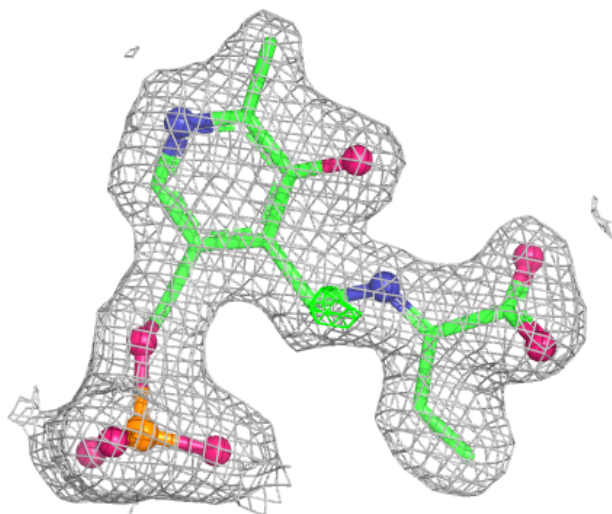
Electron density around WBJ H 501:

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



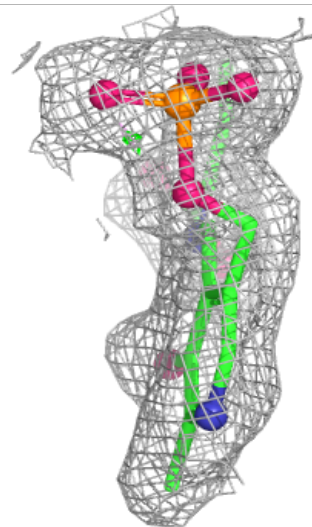
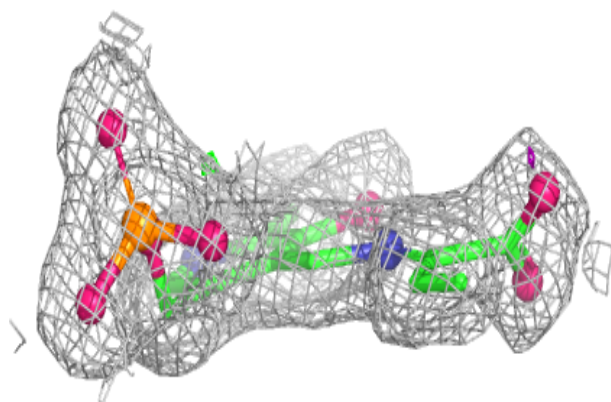
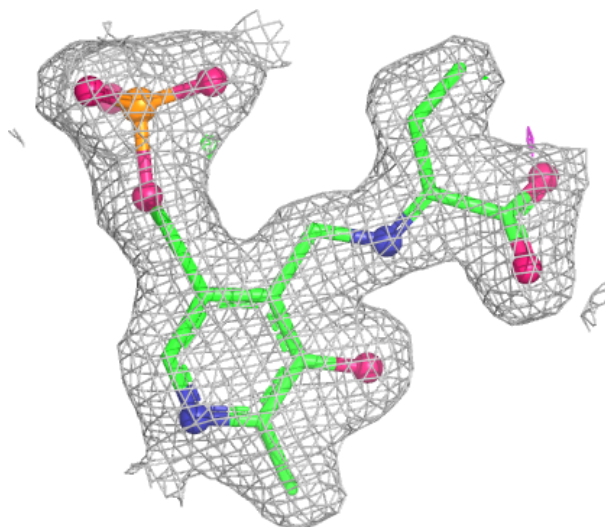
Electron density around WBJ I 501:

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



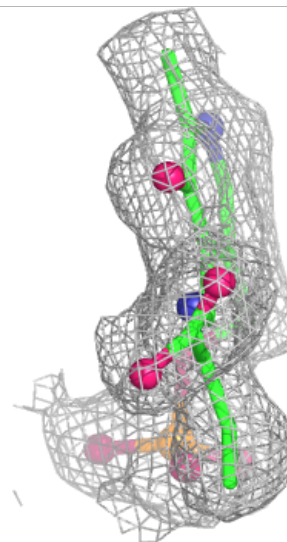
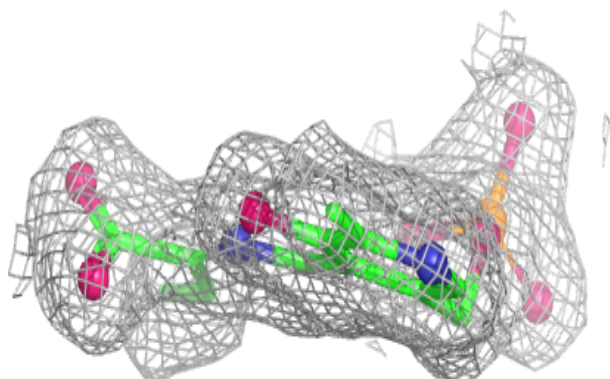
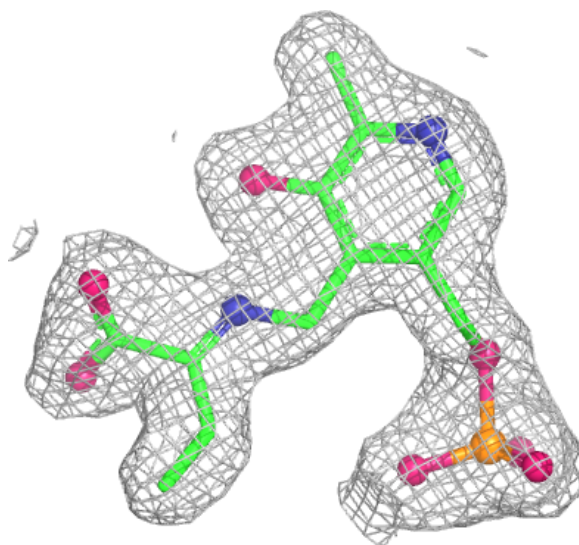
Electron density around WBJ J 501:

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



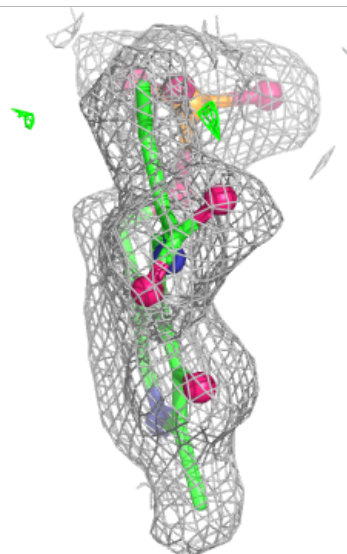
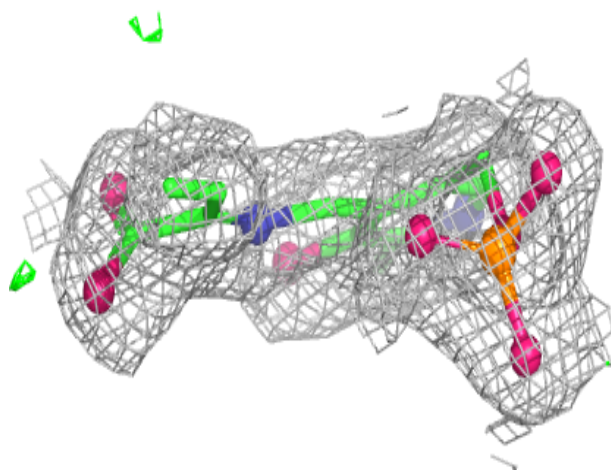
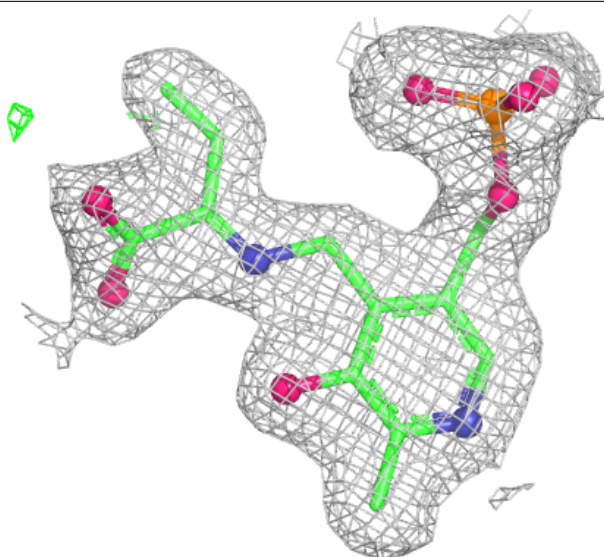
Electron density around WBJ Q 501:

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



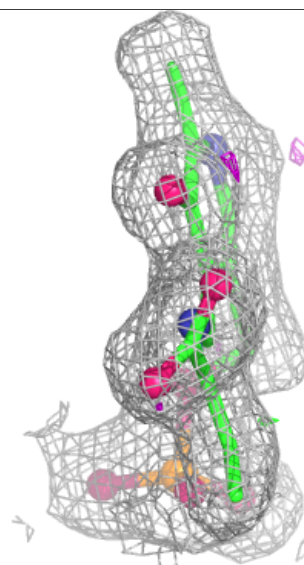
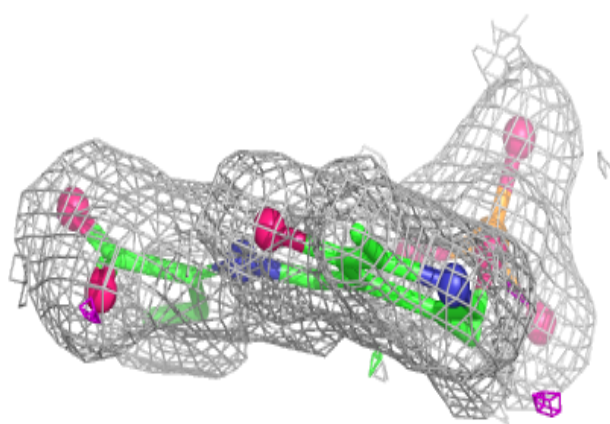
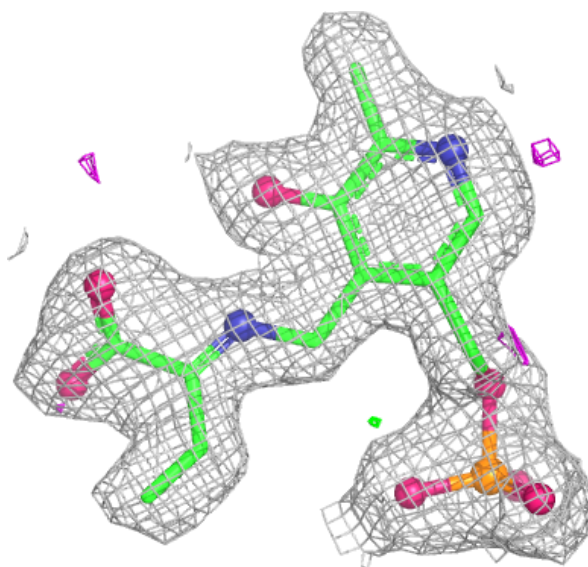
Electron density around WBJ E 501:

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



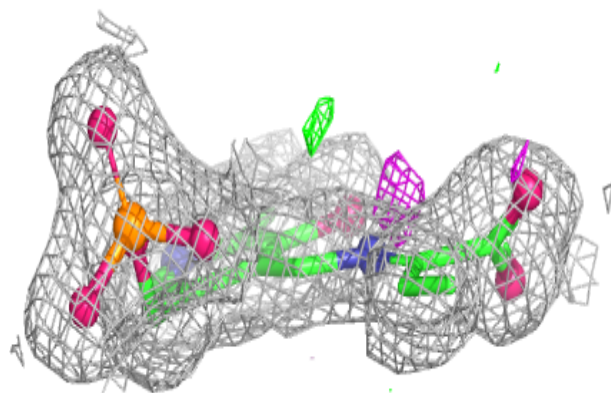
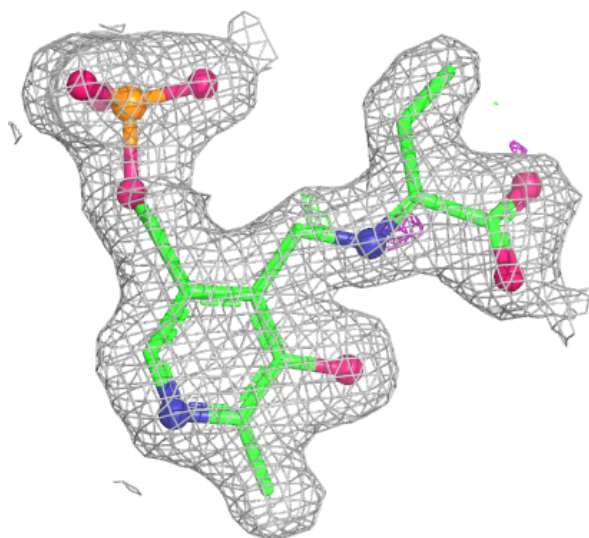
Electron density around WBJ D 501:

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



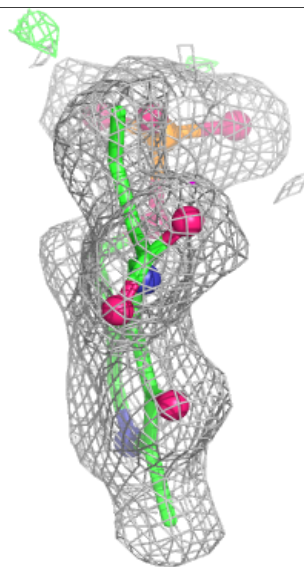
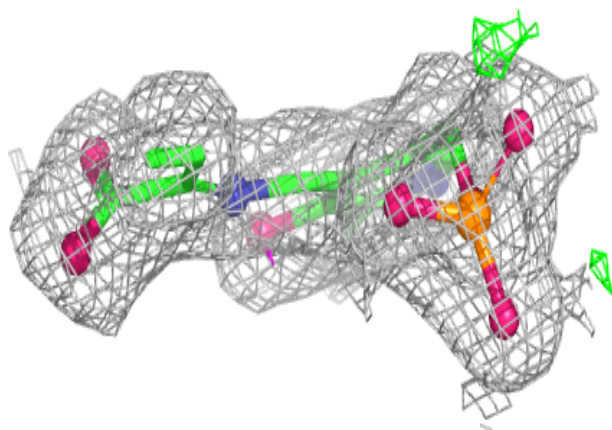
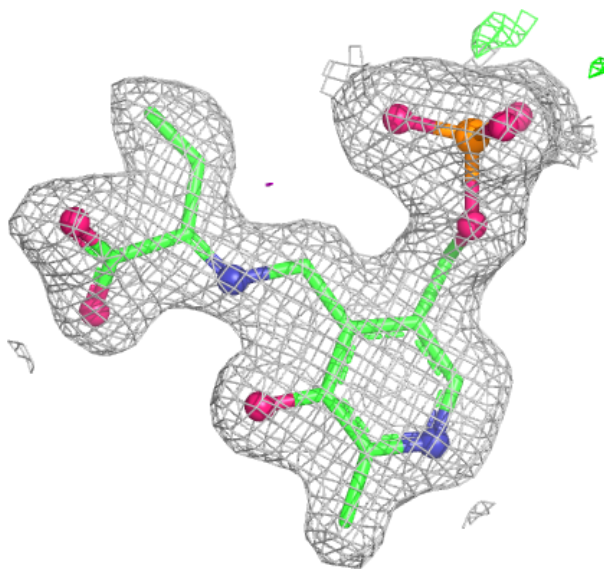
Electron density around WBJ P 501:

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



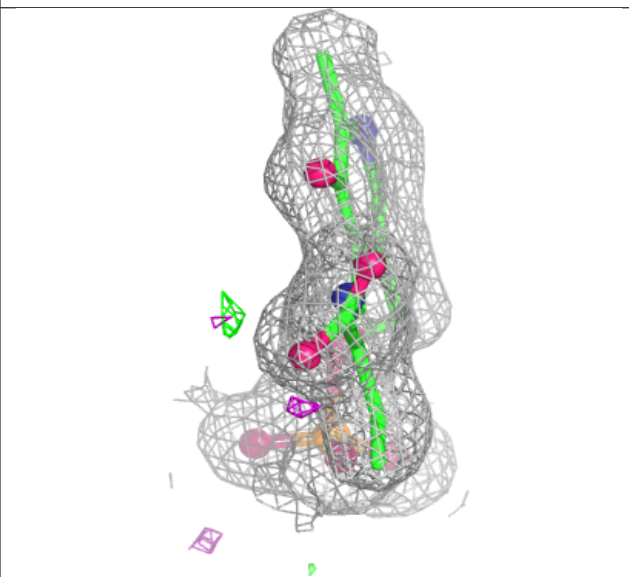
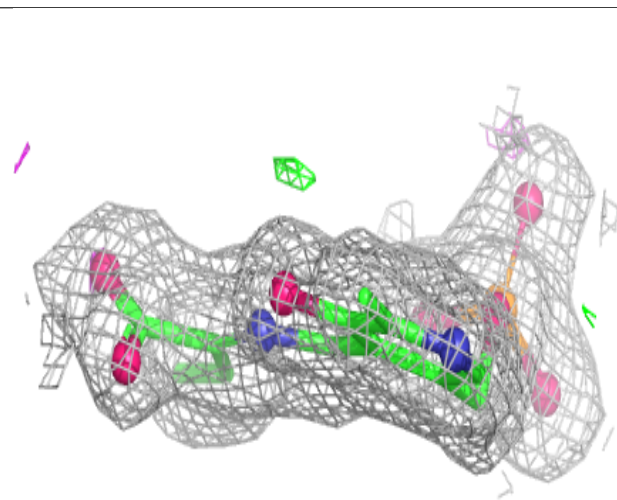
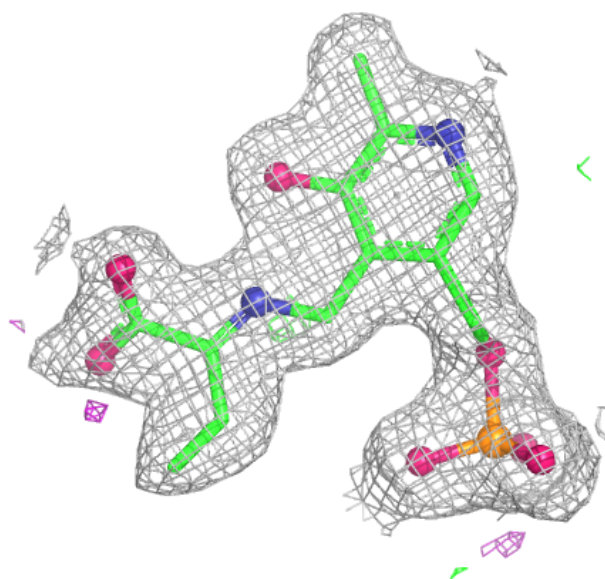
Electron density around WBJ A 501:

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



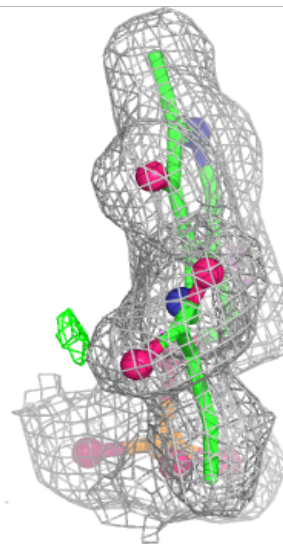
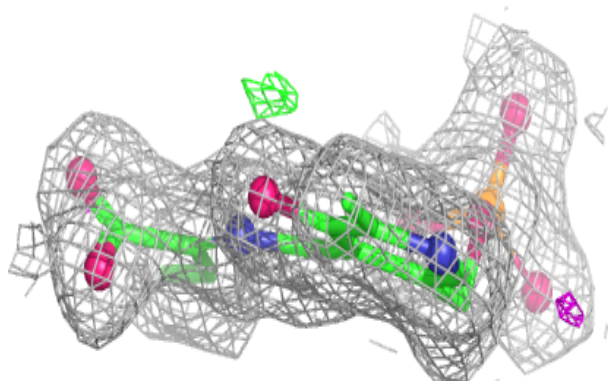
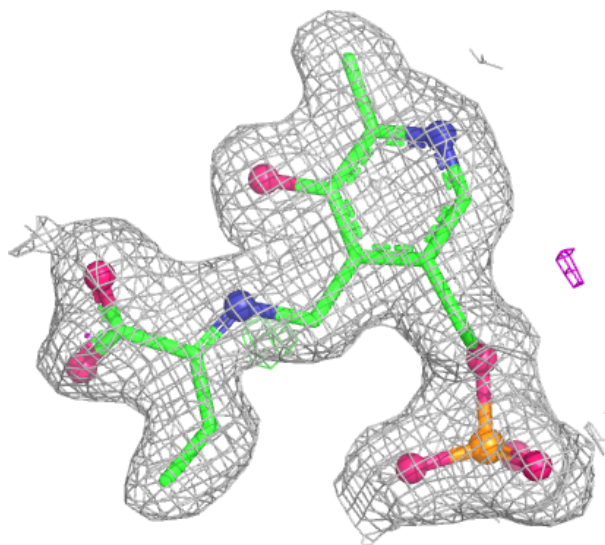
Electron density around WBJ M 501:

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



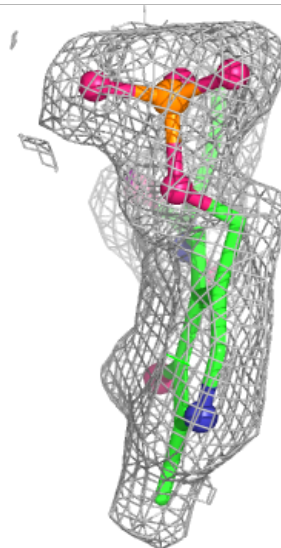
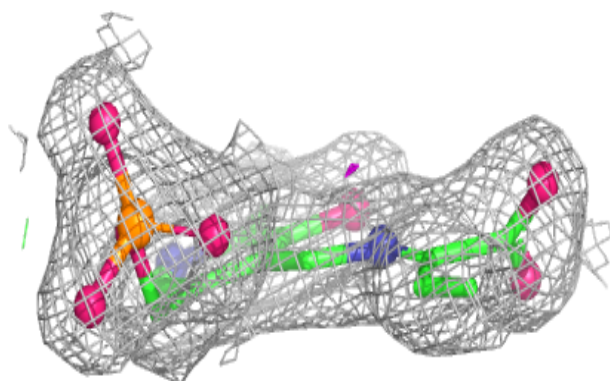
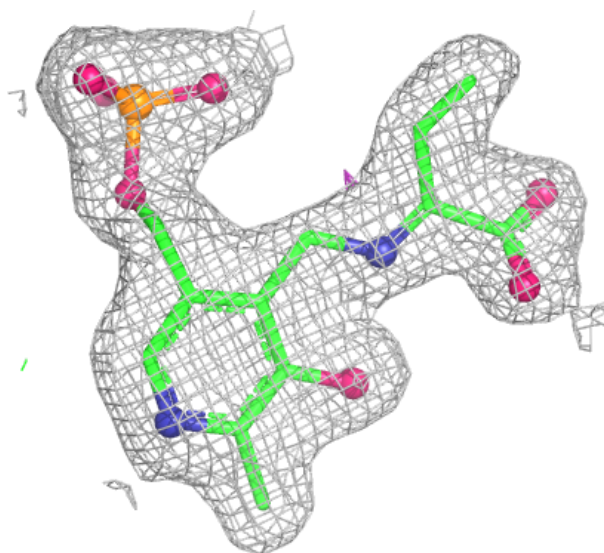
Electron density around WBJ C 501:

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



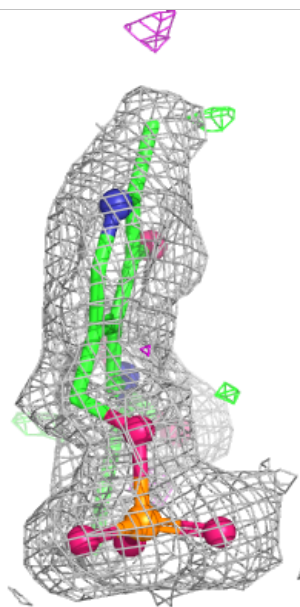
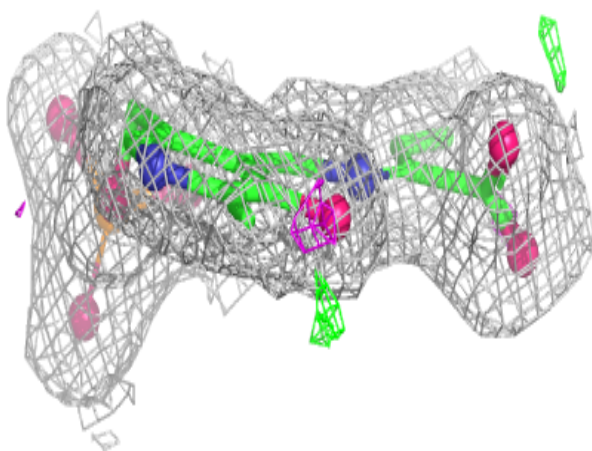
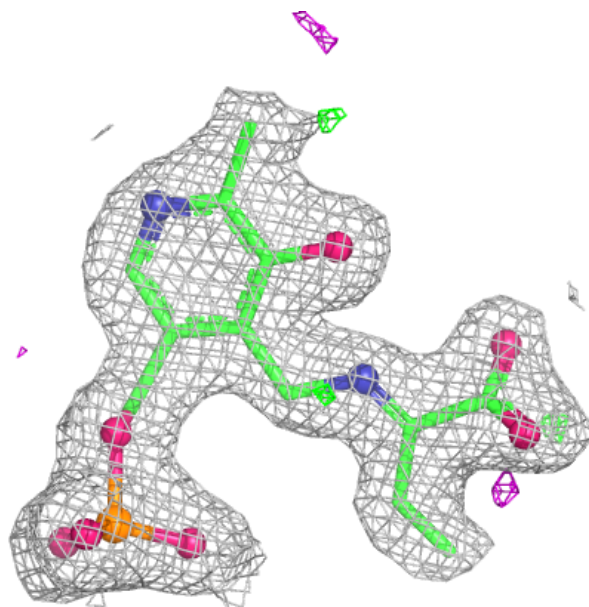
Electron density around WBJ N 501:

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and green (positive)



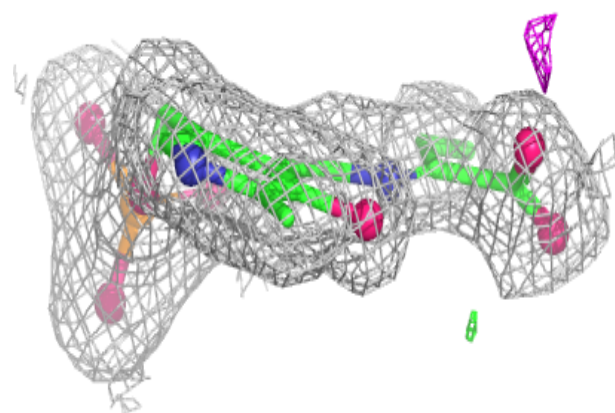
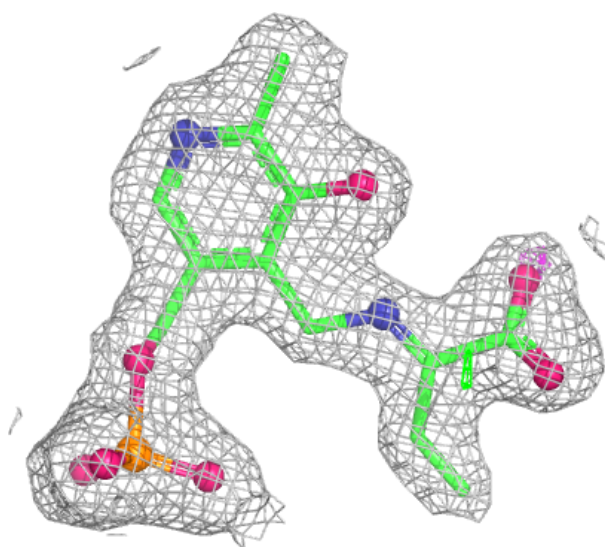
Electron density around WBJ F 501:

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



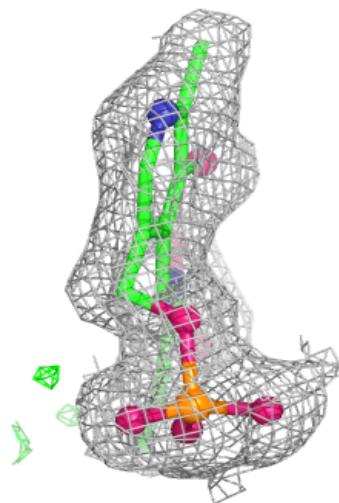
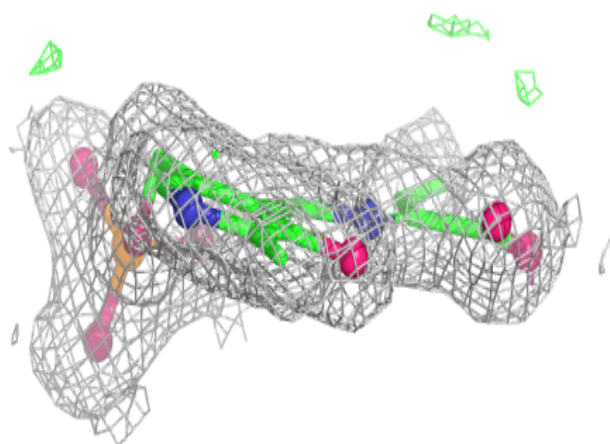
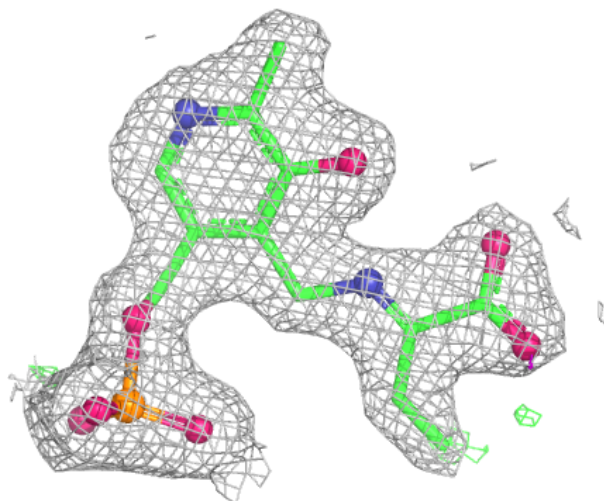
Electron density around WBJ L 501:

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



Electron density around WBJ K 501:

$2mF_o-DF_c$ (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.