Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 03:08 PM EDT

PDB ID	:	8ERB
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:

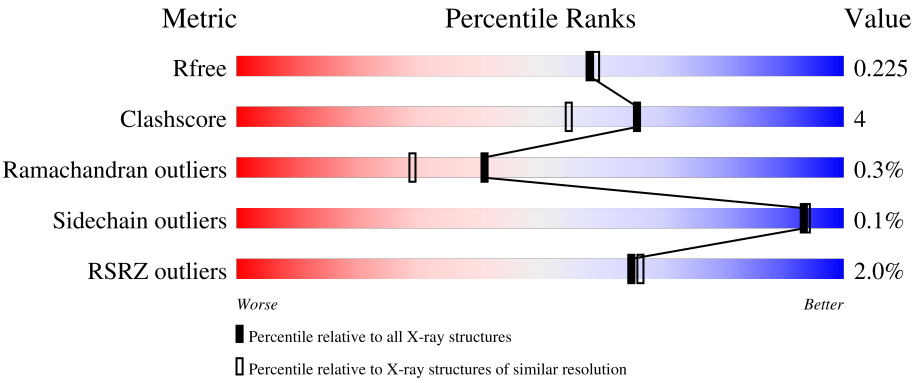
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	2% 88% 11%
1	B	433	2% 90% 9%
1	C	433	2% 89% 9%
1	D	433	2% 90% 8%
1	E	433	2% 85% 13%

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Mol	Chain	Length	Quality of chain
1	F	433	2% 86% 12%
1	G	433	2% 91% 8%
1	H	433	2% 89% 9%
1	I	433	3% 91% 7%
1	J	433	2% 91% 8%
1	K	433	2% 87% 11%
1	L	433	2% 91% 8%
1	M	433	2% 89% 9%
1	N	433	% 88% 9%
1	P	433	2% 88% 10%
1	Q	433	2% 89% 9%

2 Entry composition (i)

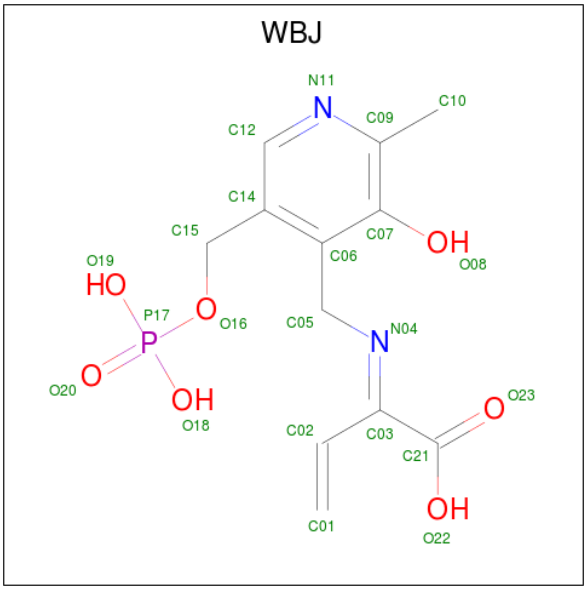
There are 3 unique types of molecules in this entry. The entry contains 55304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sulfhydrylase 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 (three-letter code: WBJ) (formula: $C_{12}H_{15}N_2O_7P$) (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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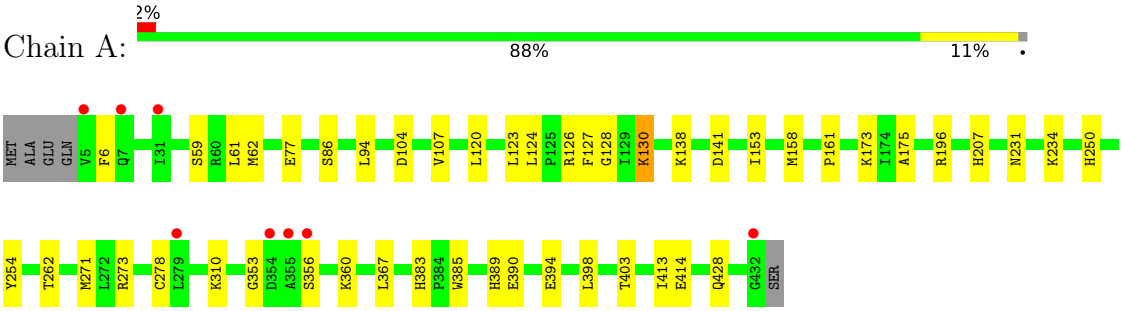
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	107	Total 107	O 107	0	0

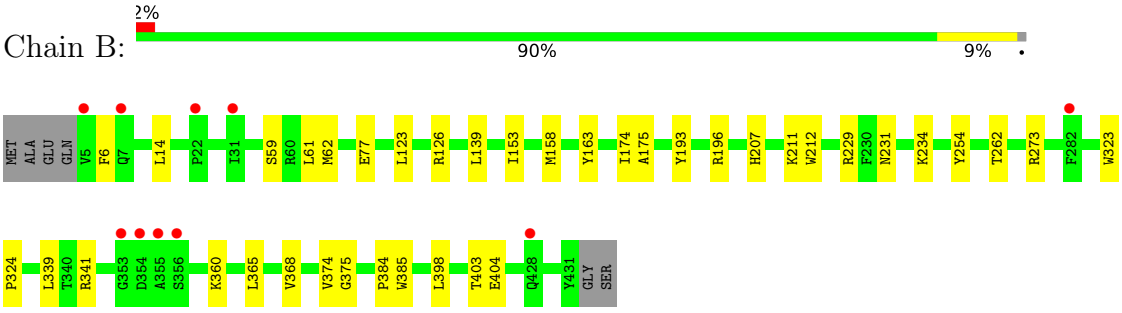
3 Residue-property plots (i)

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.

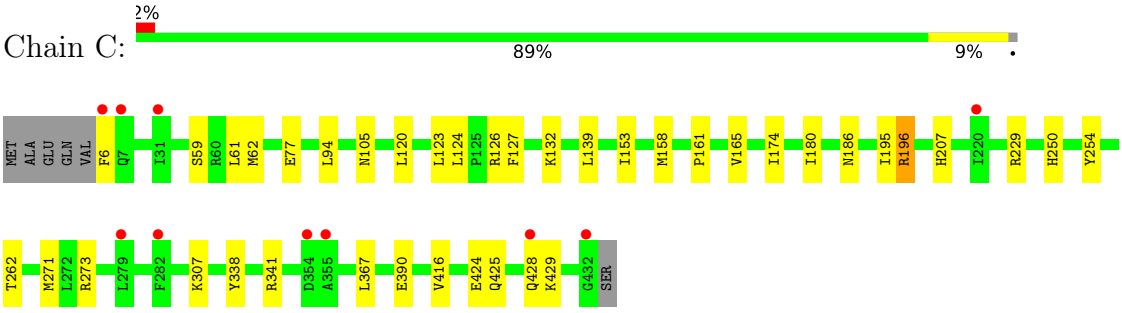
• Molecule 1: Sulfhydrylase FUB7



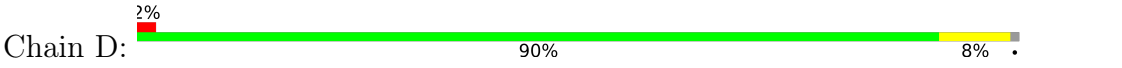
• Molecule 1: Sulfhydrylase FUB7

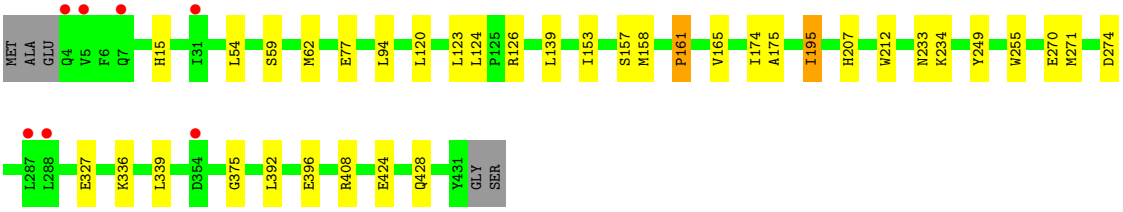


• Molecule 1: Sulfhydrylase FUB7



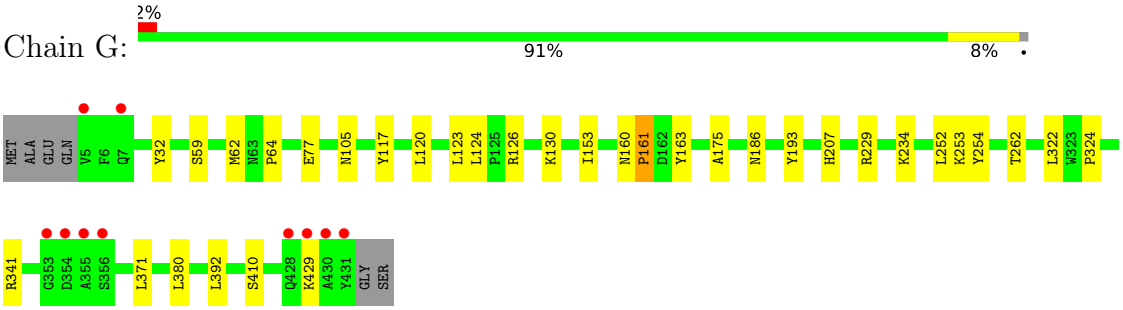
• Molecule 1: Sulfhydrylase FUB7





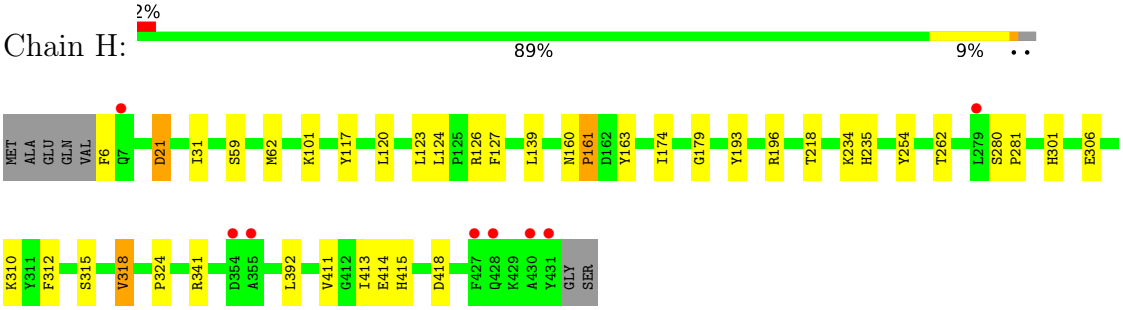
• Molecule 1: Sulfhydrylase FUB7

Chain G:



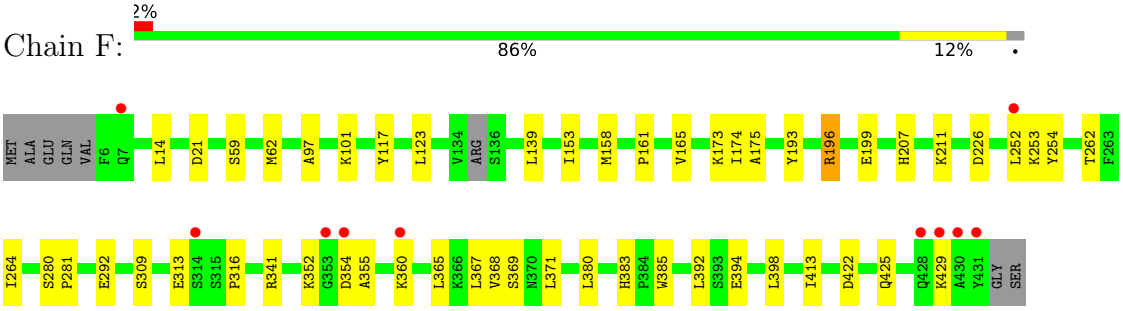
• Molecule 1: Sulfhydrylase FUB7

Chain H:



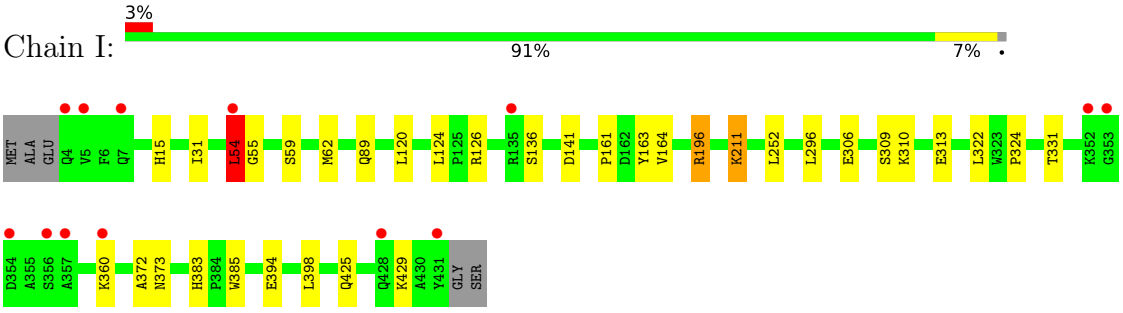
• Molecule 1: Sulfhydrylase FUB7

Chain F:



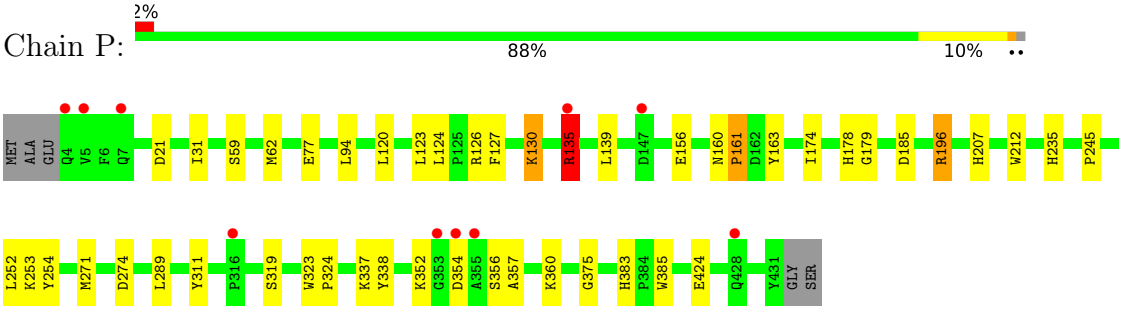
• Molecule 1: Sulfhydrylase FUB7

Chain I:



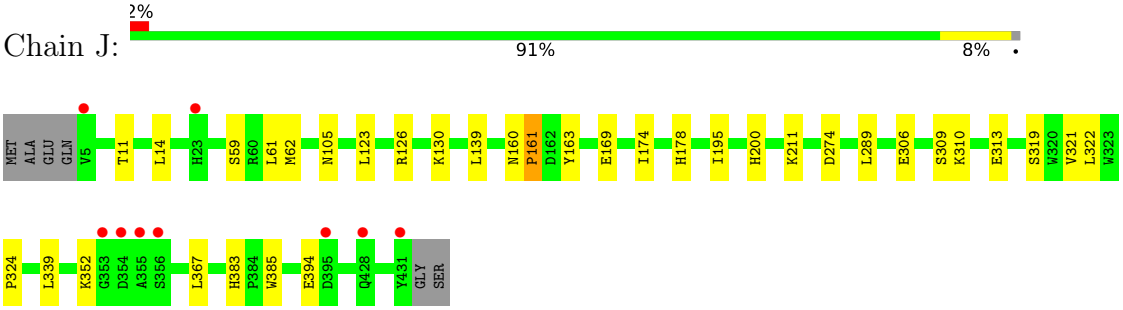
• Molecule 1: Sulfhydrylase FUB7

Chain P:



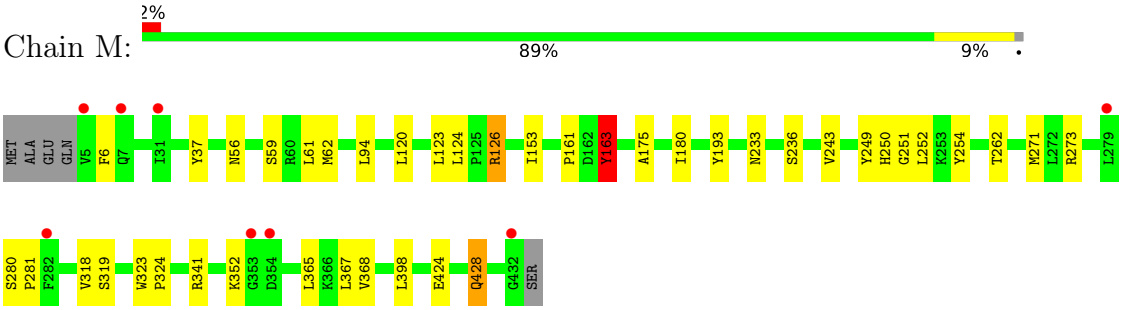
• Molecule 1: Sulfhydrylase FUB7

Chain J:



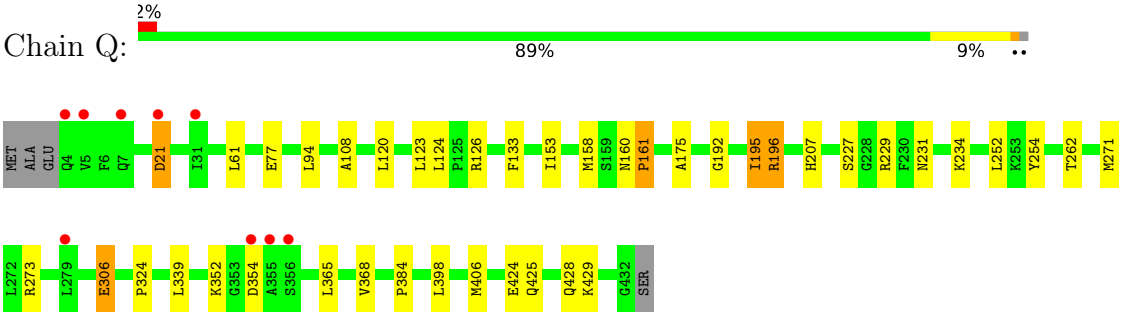
• Molecule 1: Sulfhydrylase FUB7

Chain M:



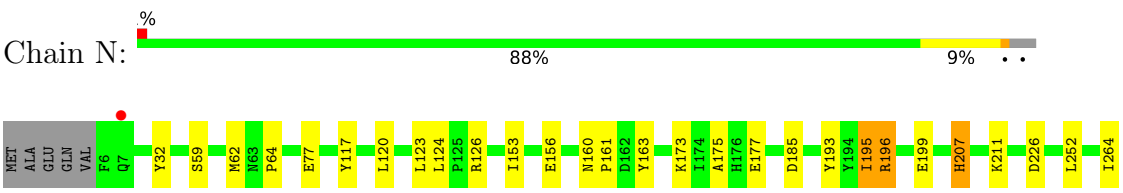
• Molecule 1: Sulfhydrylase FUB7

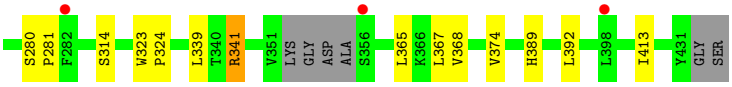
Chain Q:



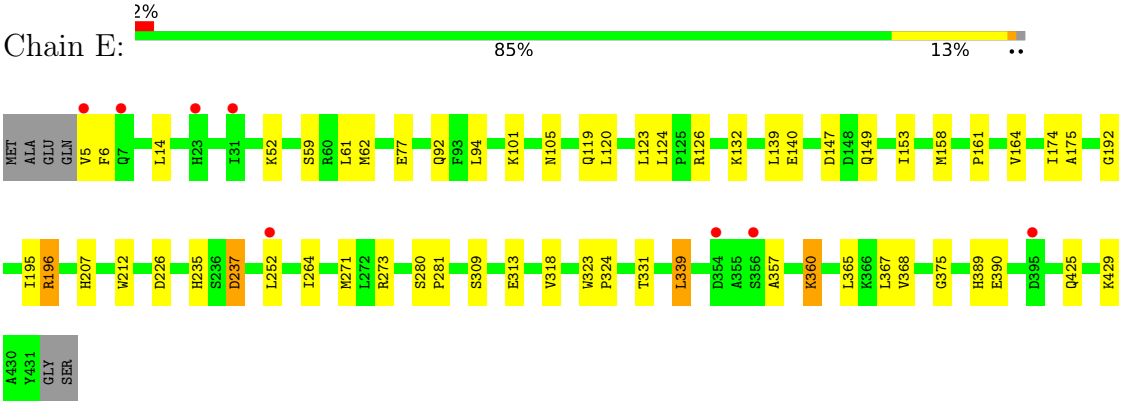
• Molecule 1: Sulfhydrylase FUB7

Chain N:

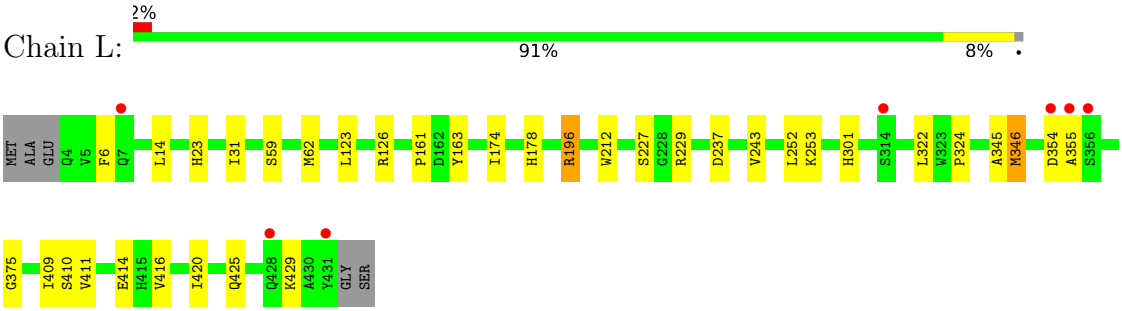




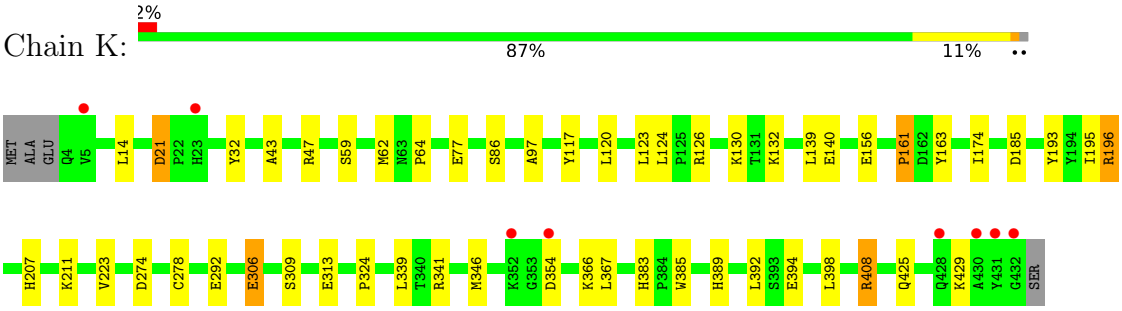
• Molecule 1: Sulfhydrylase FUB7



• Molecule 1: Sulfhydrylase FUB7



• Molecule 1: Sulfhydrylase FUB7



4 Data and refinement statistics (i)

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 48.27 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.75-1.98) 99.2 (48.27-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	28351 reflections (5.03%)	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)	0.39 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.47	0/3383	0.71	6/4595 (0.1%)
1	B	0.46	0/3386	0.66	0/4597
1	C	0.49	0/3376	0.67	0/4585
1	D	0.53	2/3377 (0.1%)	0.98	8/4587 (0.2%)
1	E	0.50	1/3379 (0.0%)	1.21	6/4590 (0.1%)
1	F	0.49	0/3360	0.68	3/4563 (0.1%)
1	G	0.48	1/3376 (0.0%)	0.67	2/4586 (0.0%)
1	H	0.45	0/3361	0.83	4/4565 (0.1%)
1	I	0.44	0/3377	0.72	7/4587 (0.2%)
1	J	0.45	0/3368	0.67	1/4575 (0.0%)
1	K	0.47	1/3381 (0.0%)	0.77	6/4592 (0.1%)
1	L	0.48	1/3377 (0.0%)	0.67	4/4587 (0.1%)
1	M	0.50	0/3372	0.73	6/4580 (0.1%)
1	N	0.46	0/3345	0.67	3/4543 (0.1%)
1	P	0.47	0/3388	0.75	5/4602 (0.1%)
1	Q	0.57	3/3381 (0.1%)	1.00	14/4592 (0.3%)
All	All	0.48	9/53987 (0.0%)	0.79	75/73326 (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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	306	GLU	CD-OE2	12.22	1.39	1.25
1	E	237	ASP	CG-OD2	11.35	1.51	1.25
1	D	327	GLU	CB-CG	7.84	1.67	1.52
1	Q	196	ARG	CG-CD	-6.90	1.34	1.51
1	Q	306	GLU	CD-OE1	-6.34	1.18	1.25
1	G	429	LYS	CG-CD	6.24	1.73	1.52
1	K	132	LYS	CE-NZ	-6.06	1.33	1.49
1	D	234	LYS	CE-NZ	5.65	1.63	1.49
1	L	346	MET	CG-SD	-5.33	1.67	1.81

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	237	ASP	CB-CG-OD1	45.50	159.25	118.30
1	E	237	ASP	CB-CG-OD2	-43.99	78.71	118.30
1	D	327	GLU	OE1-CD-OE2	-33.59	83.00	123.30
1	H	21	ASP	CB-CG-OD2	-25.77	95.11	118.30
1	Q	306	GLU	OE1-CD-OE2	-23.51	95.08	123.30
1	D	327	GLU	CG-CD-OE1	23.00	164.31	118.30
1	E	237	ASP	OD1-CG-OD2	-22.47	80.60	123.30
1	Q	21	ASP	CB-CG-OD2	-21.43	99.02	118.30
1	H	21	ASP	CB-CG-OD1	21.36	137.52	118.30
1	Q	21	ASP	CB-CG-OD1	20.08	136.37	118.30
1	D	327	GLU	CG-CD-OE2	-18.40	81.50	118.30
1	Q	306	GLU	CG-CD-OE1	16.92	152.14	118.30
1	P	135	ARG	NE-CZ-NH2	-16.03	112.29	120.30
1	K	21	ASP	CB-CG-OD2	-15.58	104.28	118.30
1	K	21	ASP	CB-CG-OD1	15.09	131.88	118.30
1	Q	306	GLU	CG-CD-OE2	-14.45	89.41	118.30
1	Q	196	ARG	NE-CZ-NH1	-14.01	113.29	120.30
1	I	126	ARG	NE-CZ-NH1	-9.45	115.58	120.30
1	P	135	ARG	CD-NE-CZ	9.29	136.60	123.60
1	P	135	ARG	CB-CG-CD	-8.35	89.89	111.60
1	A	158	MET	CA-CB-CG	8.31	127.43	113.30
1	N	252	LEU	CB-CG-CD2	8.30	125.11	111.00
1	I	54	LEU	CB-CG-CD1	8.22	124.98	111.00
1	I	126	ARG	NE-CZ-NH2	7.77	124.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	135	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	M	318	VAL	CG1-CB-CG2	7.34	122.65	110.90
1	D	195	ILE	CG1-CB-CG2	-7.10	95.78	111.40
1	Q	196	ARG	CD-NE-CZ	-7.09	113.68	123.60
1	E	360	LYS	CD-CE-NZ	-7.01	95.58	111.70
1	J	61	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	F	360	LYS	CD-CE-NZ	-6.87	95.90	111.70
1	H	21	ASP	OD1-CG-OD2	-6.84	110.31	123.30
1	L	346	MET	CA-CB-CG	-6.81	101.72	113.30
1	Q	398	LEU	CB-CG-CD1	6.72	122.43	111.00
1	G	252	LEU	CA-CB-CG	6.71	130.74	115.30
1	Q	195	ILE	CG1-CB-CG2	-6.69	96.69	111.40
1	D	336	LYS	CD-CE-NZ	-6.64	96.42	111.70
1	F	252	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	398	LEU	CB-CG-CD1	-6.38	100.16	111.00
1	F	429	LYS	CB-CG-CD	-6.29	95.25	111.60
1	Q	354	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	E	339	LEU	CB-CG-CD2	-6.13	100.58	111.00
1	I	54	LEU	CB-CG-CD2	5.99	121.18	111.00
1	Q	252	LEU	CA-CB-CG	5.94	128.97	115.30
1	D	54	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	N	195	ILE	CG1-CB-CG2	-5.93	98.36	111.40
1	K	306	GLU	CA-CB-CG	5.89	126.35	113.40
1	A	428	GLN	CA-CB-CG	5.81	126.18	113.40
1	D	234	LYS	CD-CE-NZ	5.80	125.03	111.70
1	Q	21	ASP	OD1-CG-OD2	-5.74	112.40	123.30
1	L	322	LEU	CA-CB-CG	5.63	128.25	115.30
1	I	252	LEU	CA-CB-CG	5.61	128.19	115.30
1	H	318	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	M	428	GLN	CA-CB-CG	-5.54	101.20	113.40
1	K	196	ARG	CD-NE-CZ	-5.54	115.85	123.60
1	A	310	LYS	CD-CE-NZ	5.46	124.26	111.70
1	M	318	VAL	CA-CB-CG1	5.41	119.02	110.90
1	I	322	LEU	CB-CG-CD1	-5.40	101.82	111.00
1	K	408	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	252	LEU	CA-CB-CG	5.37	127.65	115.30
1	Q	339	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	D	339	LEU	CB-CG-CD1	5.32	120.05	111.00
1	I	196	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	N	341	ARG	CG-CD-NE	5.24	122.80	111.80
1	A	130	LYS	CD-CE-NZ	5.21	123.69	111.70
1	M	126	ARG	NE-CZ-NH1	-5.20	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	196	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	K	306	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	M	163	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	L	252	LEU	CA-CB-CG	5.14	127.11	115.30
1	P	130	LYS	CB-CG-CD	-5.10	98.34	111.60
1	G	322	LEU	CA-CB-CG	5.09	127.01	115.30
1	M	251	GLY	C-N-CA	-5.06	109.05	121.70
1	L	196	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	A	173	LYS	CD-CE-NZ	-5.02	100.16	111.70

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
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3300	0	3228	33	0
1	B	3300	0	3238	32	0
1	C	3293	0	3219	29	0
1	D	3297	0	3220	19	0
1	E	3296	0	3225	39	0
1	F	3278	0	3202	30	0
1	G	3296	0	3217	20	0
1	H	3281	0	3203	32	0
1	I	3297	0	3220	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3288	0	3212	26	0
1	K	3301	0	3223	34	0
1	L	3297	0	3220	25	0
1	M	3292	0	3215	29	0
1	N	3263	0	3190	31	0
1	P	3305	0	3233	35	0
1	Q	3301	0	3223	23	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
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	421	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 (421) 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:A:130:LYS:NZ	3:A:601:HOH:O	2.03	0.90
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: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
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:E:158:MET:HE1	1:E:339:LEU:HD21	1.79	0.65
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:K:366:LYS:NZ	1:K:429:LYS:HZ3	2.05	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:354:ASP:OD2	1:L:355:ALA:N	2.42	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
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:Q:158:MET:CE	1:Q:324:PRO:HG3	2.41	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:235:HIS:C	1:E:237:ASP:H	2.13	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:K:425:GLN:HE22	1:K:429:LYS:NZ	2.09	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:J:139:LEU:HB3	1:J:174:ILE:HD11	1.93	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:Q:158:MET:HE1	1:Q:324:PRO:HG3	1.97	0.47
1:J:309:SER:O	1:J:313:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:E:365:LEU:HD13	1:E:368:VAL:HB	1.96	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: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:E:140:GLU:CD	1:E:140:GLU:H	2.18	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: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:B:231:ASN:CG	1:B:234:LYS:HG2	2.36	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:E:235:HIS:C	1:E:237:ASP:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:THR:HG21	1:H:234:LYS:HD2	1.97	0.45
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: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: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:C:126:ARG:HG3	1:C:126:ARG:NH1	2.33	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:160:ASN:HA	1:P:161:PRO:HA	1.89	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: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:J:59:SER:HA	1:J:62:MET:O	2.19	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:I:211:LYS:HZ3	1:I:373:ASN:HD22	1.67	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:105:ASN:CG	1:C:132:LYS:HE2	2.41	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: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: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:K:346:MET:HE1	1:K:408:ARG:CD	2.50	0.41
1:A:231:ASN:CG	1:A:234:LYS:HG2	2.41	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
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:K:140:GLU:H	1:K:140:GLU:CD	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:158:MET:HE1	1:B:339:LEU:HD21	2.02	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1	C	426/433 (98%)	416 (98%)	9 (2%)	1 (0%)	47	38
1	D	426/433 (98%)	416 (98%)	9 (2%)	1 (0%)	47	38
1	E	426/433 (98%)	415 (97%)	11 (3%)	0	100	100
1	F	422/433 (98%)	414 (98%)	6 (1%)	2 (0%)	29	16
1	G	426/433 (98%)	417 (98%)	8 (2%)	1 (0%)	47	38
1	H	424/433 (98%)	414 (98%)	9 (2%)	1 (0%)	47	38
1	I	426/433 (98%)	416 (98%)	8 (2%)	2 (0%)	29	16
1	J	425/433 (98%)	415 (98%)	8 (2%)	2 (0%)	29	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	427/433 (99%)	416 (97%)	8 (2%)	3 (1%)	22	11
1	L	426/433 (98%)	417 (98%)	8 (2%)	1 (0%)	47	38
1	M	426/433 (98%)	415 (97%)	10 (2%)	1 (0%)	47	38
1	N	419/433 (97%)	409 (98%)	10 (2%)	0	100	100
1	P	427/433 (99%)	416 (97%)	10 (2%)	1 (0%)	47	38
1	Q	427/433 (99%)	417 (98%)	9 (2%)	1 (0%)	47	38
All	All	6807/6928 (98%)	6647 (98%)	143 (2%)	17 (0%)	41	38

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 (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

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%)	86	85
1	D	347/350 (99%)	347 (100%)	0	100	100
1	E	347/350 (99%)	345 (99%)	2 (1%)	86	85
1	F	345/350 (99%)	343 (99%)	2 (1%)	86	85
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%)	92	92
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%)	346 (100%)	0	100	100
1	N	344/350 (98%)	342 (99%)	2 (1%)	86	85
1	P	348/350 (99%)	346 (99%)	2 (1%)	86	85
1	Q	347/350 (99%)	346 (100%)	1 (0%)	92	92
All	All	5544/5600 (99%)	5532 (100%)	12 (0%)	93	93

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	Q	352	LYS
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 (54)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	119	GLN
1	A	178	HIS
1	A	250	HIS
1	B	92	GLN
1	C	89	GLN
1	C	92	GLN
1	C	250	HIS
1	C	303	GLN
1	C	428	GLN
1	D	92	GLN
1	D	119	GLN
1	D	178	HIS
1	D	250	HIS
1	D	303	GLN
1	D	428	GLN
1	H	89	GLN
1	H	92	GLN
1	H	119	GLN
1	H	301	HIS
1	H	428	GLN
1	I	4	GLN
1	I	89	GLN
1	I	329	HIS
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	M	250	HIS
1	Q	4	GLN
1	Q	92	GLN
1	Q	178	HIS
1	Q	216	HIS
1	Q	235	HIS
1	Q	425	GLN
1	N	92	GLN
1	N	119	GLN
1	E	23	HIS
1	E	89	GLN

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Mol	Chain	Res	Type
1	E	92	GLN
1	E	105	ASN
1	E	119	GLN
1	E	149	GLN
1	L	23	HIS
1	L	178	HIS
1	L	301	HIS
1	L	303	GLN
1	L	428	GLN
1	K	119	GLN
1	K	178	HIS
1	K	425	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	M	501	-	21,22,22	2.12	3 (14%)	25,31,31	2.05	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	WBJ	D	501	-	21,22,22	1.89	3 (14%)	25,31,31	2.06	6 (24%)
2	WBJ	I	501	-	21,22,22	2.50	4 (19%)	25,31,31	2.05	7 (28%)
2	WBJ	Q	501	-	21,22,22	2.11	3 (14%)	25,31,31	1.95	6 (24%)
2	WBJ	N	501	-	21,22,22	2.14	4 (19%)	25,31,31	2.05	6 (24%)
2	WBJ	L	501	-	21,22,22	2.74	3 (14%)	25,31,31	2.01	7 (28%)
2	WBJ	A	501	-	21,22,22	2.23	3 (14%)	25,31,31	1.89	7 (28%)
2	WBJ	B	501	-	21,22,22	2.44	3 (14%)	25,31,31	1.84	7 (28%)
2	WBJ	P	501	-	21,22,22	2.74	4 (19%)	25,31,31	2.08	6 (24%)
2	WBJ	C	501	-	21,22,22	2.08	3 (14%)	25,31,31	1.97	5 (20%)
2	WBJ	K	501	-	21,22,22	2.90	3 (14%)	25,31,31	1.96	7 (28%)
2	WBJ	F	501	-	21,22,22	2.69	5 (23%)	25,31,31	2.04	7 (28%)
2	WBJ	H	501	-	21,22,22	2.88	3 (14%)	25,31,31	1.84	4 (16%)
2	WBJ	G	501	-	21,22,22	2.74	4 (19%)	25,31,31	1.93	8 (32%)
2	WBJ	E	501	-	21,22,22	1.90	4 (19%)	25,31,31	2.05	7 (28%)
2	WBJ	J	501	-	21,22,22	2.82	4 (19%)	25,31,31	2.00	7 (28%)

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	M	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	D	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	I	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	Q	501	-	-	5/14/17/17	0/1/1/1
2	WBJ	N	501	-	-	8/14/17/17	0/1/1/1
2	WBJ	L	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	A	501	-	-	6/14/17/17	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	C	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	K	501	-	-	3/14/17/17	0/1/1/1
2	WBJ	F	501	-	-	6/14/17/17	0/1/1/1
2	WBJ	H	501	-	-	5/14/17/17	0/1/1/1
2	WBJ	G	501	-	-	4/14/17/17	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WBJ	E	501	-	-	8/14/17/17	0/1/1/1
2	WBJ	J	501	-	-	6/14/17/17	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	WBJ	C03-C21	11.00	1.59	1.48
2	K	501	WBJ	C03-C21	10.92	1.59	1.48
2	J	501	WBJ	C03-C21	10.01	1.58	1.48
2	F	501	WBJ	C03-C21	9.97	1.58	1.48
2	P	501	WBJ	C03-C21	9.95	1.58	1.48
2	L	501	WBJ	C03-C21	9.95	1.58	1.48
2	G	501	WBJ	C03-C21	9.74	1.58	1.48
2	B	501	WBJ	C03-C21	9.20	1.57	1.48
2	I	501	WBJ	C03-C21	8.55	1.56	1.48
2	C	501	WBJ	C03-C21	7.99	1.56	1.48
2	A	501	WBJ	C03-C21	7.89	1.56	1.48
2	M	501	WBJ	C03-C21	7.37	1.55	1.48
2	N	501	WBJ	C03-C21	7.14	1.55	1.48
2	Q	501	WBJ	C03-C21	6.96	1.55	1.48
2	D	501	WBJ	C03-C21	6.31	1.54	1.48
2	J	501	WBJ	P17-O16	6.17	1.80	1.60
2	G	501	WBJ	P17-O16	6.14	1.80	1.60
2	L	501	WBJ	P17-O16	5.81	1.78	1.60
2	K	501	WBJ	P17-O16	5.78	1.78	1.60
2	H	501	WBJ	P17-O16	5.72	1.78	1.60
2	I	501	WBJ	P17-O16	5.68	1.78	1.60
2	E	501	WBJ	C03-C21	5.58	1.53	1.48
2	P	501	WBJ	P17-O16	5.30	1.77	1.60
2	F	501	WBJ	P17-O16	5.02	1.76	1.60
2	Q	501	WBJ	P17-O16	4.82	1.75	1.60
2	A	501	WBJ	P17-O16	4.71	1.75	1.60
2	B	501	WBJ	P17-O16	4.59	1.75	1.60
2	E	501	WBJ	P17-O16	4.37	1.74	1.60
2	N	501	WBJ	P17-O16	4.33	1.74	1.60
2	M	501	WBJ	P17-O16	4.13	1.73	1.60
2	D	501	WBJ	P17-O16	3.48	1.71	1.60
2	C	501	WBJ	P17-O16	2.94	1.69	1.60
2	G	501	WBJ	O16-C15	-2.69	1.35	1.45
2	J	501	WBJ	O16-C15	-2.68	1.35	1.45
2	I	501	WBJ	O16-C15	-2.66	1.35	1.45
2	P	501	WBJ	O16-C15	-2.54	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	501	WBJ	O16-C15	-2.52	1.35	1.45
2	H	501	WBJ	O16-C15	-2.52	1.35	1.45
2	G	501	WBJ	C07-C06	2.49	1.43	1.40
2	L	501	WBJ	O16-C15	-2.48	1.35	1.45
2	F	501	WBJ	C07-C06	2.42	1.43	1.40
2	F	501	WBJ	O16-C15	-2.38	1.36	1.45
2	A	501	WBJ	O16-C15	-2.33	1.36	1.45
2	E	501	WBJ	O16-C15	-2.22	1.36	1.45
2	M	501	WBJ	O22-C21	-2.21	1.24	1.30
2	E	501	WBJ	O22-C21	-2.21	1.24	1.30
2	D	501	WBJ	C12-C14	2.20	1.42	1.37
2	N	501	WBJ	O22-C21	-2.19	1.24	1.30
2	Q	501	WBJ	O16-C15	-2.17	1.36	1.45
2	I	501	WBJ	O22-C21	-2.15	1.24	1.30
2	J	501	WBJ	O22-C21	-2.15	1.24	1.30
2	B	501	WBJ	O16-C15	-2.11	1.37	1.45
2	F	501	WBJ	O22-C21	-2.08	1.24	1.30
2	P	501	WBJ	O22-C21	-2.08	1.24	1.30
2	N	501	WBJ	O16-C15	-2.04	1.37	1.45
2	C	501	WBJ	O16-C15	-2.03	1.37	1.45

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	WBJ	C21-C03-N04	-7.13	113.75	121.84
2	P	501	WBJ	C21-C03-N04	-6.94	113.96	121.84
2	C	501	WBJ	C21-C03-N04	-6.91	114.00	121.84
2	H	501	WBJ	C21-C03-N04	-6.84	114.08	121.84
2	J	501	WBJ	C21-C03-N04	-6.70	114.24	121.84
2	Q	501	WBJ	C21-C03-N04	-6.63	114.31	121.84
2	M	501	WBJ	C21-C03-N04	-6.60	114.35	121.84
2	L	501	WBJ	C21-C03-N04	-6.58	114.38	121.84
2	N	501	WBJ	C21-C03-N04	-6.55	114.41	121.84
2	F	501	WBJ	C21-C03-N04	-6.50	114.46	121.84
2	K	501	WBJ	C21-C03-N04	-6.39	114.59	121.84
2	E	501	WBJ	C21-C03-N04	-6.38	114.61	121.84
2	B	501	WBJ	C21-C03-N04	-6.18	114.83	121.84
2	A	501	WBJ	C21-C03-N04	-6.16	114.85	121.84
2	G	501	WBJ	C21-C03-N04	-6.01	115.02	121.84
2	I	501	WBJ	C21-C03-N04	-5.40	115.71	121.84
2	I	501	WBJ	O23-C21-C03	-4.12	115.47	121.99
2	E	501	WBJ	O23-C21-C03	-3.98	115.69	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	501	WBJ	O23-C21-C03	-3.73	116.08	121.99
2	I	501	WBJ	O22-C21-C03	3.50	119.18	113.42
2	P	501	WBJ	O23-C21-C03	-3.44	116.54	121.99
2	D	501	WBJ	O23-C21-C03	-3.34	116.71	121.99
2	F	501	WBJ	O23-C21-C03	-3.33	116.71	121.99
2	P	501	WBJ	O22-C21-C03	3.19	118.68	113.42
2	L	501	WBJ	O23-C21-C03	-3.12	117.06	121.99
2	E	501	WBJ	O22-C21-C03	3.11	118.55	113.42
2	I	501	WBJ	C07-C06-C14	-3.10	115.75	118.72
2	N	501	WBJ	O22-C21-C03	3.09	118.51	113.42
2	L	501	WBJ	O22-C21-C03	3.04	118.43	113.42
2	Q	501	WBJ	O23-C21-C03	-3.03	117.19	121.99
2	J	501	WBJ	O23-C21-C03	-3.02	117.21	121.99
2	K	501	WBJ	C07-C06-C14	-3.01	115.83	118.72
2	M	501	WBJ	C07-C06-C14	-2.95	115.89	118.72
2	F	501	WBJ	O22-C21-C03	2.94	118.27	113.42
2	D	501	WBJ	O22-C21-C03	2.93	118.25	113.42
2	M	501	WBJ	O23-C21-C03	-2.91	117.38	121.99
2	G	501	WBJ	C07-C06-C14	-2.89	115.95	118.72
2	M	501	WBJ	O16-P17-O20	-2.88	98.38	106.47
2	M	501	WBJ	O22-C21-C03	2.76	117.96	113.42
2	J	501	WBJ	O22-C21-C03	2.69	117.85	113.42
2	G	501	WBJ	O18-P17-O16	-2.67	99.63	106.73
2	A	501	WBJ	O23-C21-C03	-2.66	117.78	121.99
2	C	501	WBJ	O23-C21-C03	-2.57	117.92	121.99
2	G	501	WBJ	O23-C21-C03	-2.56	117.94	121.99
2	C	501	WBJ	C07-C06-C14	-2.55	116.27	118.72
2	C	501	WBJ	C10-C09-C07	2.55	124.04	120.89
2	I	501	WBJ	C10-C09-C07	2.52	124.00	120.89
2	A	501	WBJ	O19-P17-O18	2.52	117.27	107.64
2	F	501	WBJ	C10-C09-C07	2.52	124.00	120.89
2	N	501	WBJ	C07-C06-C14	-2.51	116.31	118.72
2	A	501	WBJ	C07-C06-C14	-2.50	116.32	118.72
2	I	501	WBJ	O19-P17-O18	2.48	117.12	107.64
2	B	501	WBJ	O23-C21-C03	-2.46	118.09	121.99
2	A	501	WBJ	O18-P17-O16	-2.44	100.24	106.73
2	F	501	WBJ	O16-P17-O20	-2.44	99.63	106.47
2	F	501	WBJ	C07-C06-C14	-2.43	116.38	118.72
2	L	501	WBJ	O19-P17-O18	2.42	116.87	107.64
2	M	501	WBJ	C10-C09-C07	2.41	123.86	120.89
2	A	501	WBJ	O22-C21-C03	2.41	117.39	113.42
2	D	501	WBJ	C07-C06-C14	-2.39	116.42	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	WBJ	C07-C06-C14	-2.38	116.43	118.72
2	E	501	WBJ	C10-C09-C07	2.38	123.82	120.89
2	L	501	WBJ	C07-C06-C14	-2.37	116.45	118.72
2	B	501	WBJ	O19-P17-O18	2.37	116.68	107.64
2	K	501	WBJ	O23-C21-C03	-2.35	118.27	121.99
2	P	501	WBJ	C07-C06-C14	-2.34	116.48	118.72
2	K	501	WBJ	O22-C21-C03	2.33	117.26	113.42
2	D	501	WBJ	O18-P17-O16	-2.33	100.53	106.73
2	E	501	WBJ	O19-P17-O16	-2.32	100.55	106.73
2	Q	501	WBJ	O18-P17-O16	-2.32	100.57	106.73
2	H	501	WBJ	C10-C09-C07	2.31	123.75	120.89
2	K	501	WBJ	O18-P17-O16	-2.31	100.58	106.73
2	N	501	WBJ	O18-P17-O16	-2.31	100.59	106.73
2	L	501	WBJ	O19-P17-O16	-2.29	100.64	106.73
2	J	501	WBJ	O19-P17-O18	2.27	116.33	107.64
2	G	501	WBJ	O22-C21-C03	2.27	117.15	113.42
2	Q	501	WBJ	O19-P17-O18	2.26	116.28	107.64
2	P	501	WBJ	O16-P17-O20	-2.26	100.14	106.47
2	N	501	WBJ	C10-C09-C07	2.26	123.67	120.89
2	J	501	WBJ	O16-P17-O20	-2.25	100.16	106.47
2	F	501	WBJ	O19-P17-O18	2.24	116.19	107.64
2	G	501	WBJ	O19-P17-O18	2.23	116.17	107.64
2	Q	501	WBJ	O22-C21-C03	2.23	117.09	113.42
2	K	501	WBJ	O19-P17-O16	-2.22	100.82	106.73
2	G	501	WBJ	C10-C09-C07	2.22	123.63	120.89
2	H	501	WBJ	O23-C21-C03	-2.21	118.48	121.99
2	A	501	WBJ	C10-C09-C07	2.21	123.61	120.89
2	E	501	WBJ	C07-C06-C14	-2.21	116.60	118.72
2	Q	501	WBJ	C07-C06-C14	-2.21	116.60	118.72
2	E	501	WBJ	O18-P17-O16	-2.19	100.89	106.73
2	P	501	WBJ	O19-P17-O18	2.19	116.01	107.64
2	D	501	WBJ	O19-P17-O18	2.19	116.00	107.64
2	B	501	WBJ	O18-P17-O16	-2.17	100.96	106.73
2	B	501	WBJ	O22-C21-C03	2.13	116.93	113.42
2	B	501	WBJ	C10-C09-C07	2.12	123.50	120.89
2	I	501	WBJ	O16-P17-O20	-2.11	100.54	106.47
2	J	501	WBJ	O18-P17-O16	-2.07	101.22	106.73
2	G	501	WBJ	O16-P17-O20	-2.06	100.70	106.47
2	J	501	WBJ	C07-C06-C14	-2.04	116.76	118.72
2	H	501	WBJ	O19-P17-O18	2.04	115.42	107.64
2	L	501	WBJ	C10-C09-C07	2.02	123.38	120.89
2	C	501	WBJ	O22-C21-C03	2.01	116.72	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	501	WBJ	O19-P17-O18	2.00	115.28	107.64

There are no chirality outliers.

All (91) 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-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-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-C05-C06-C07
2	D	501	WBJ	N04-C05-C06-C14
2	G	501	WBJ	C02-C03-C21-O22
2	G	501	WBJ	N04-C03-C21-O23
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-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

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Mol	Chain	Res	Type	Atoms
2	I	501	WBJ	N04-C05-C06-C07
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-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	B	501	WBJ	N04-C03-C21-O23
2	D	501	WBJ	N04-C03-C21-O23
2	L	501	WBJ	N04-C03-C21-O23
2	K	501	WBJ	N04-C03-C21-O23
2	H	501	WBJ	N04-C03-C21-O22
2	Q	501	WBJ	N04-C03-C21-O22
2	N	501	WBJ	C12-C14-C15-O16
2	E	501	WBJ	C12-C14-C15-O16
2	E	501	WBJ	C06-C14-C15-O16
2	A	501	WBJ	N04-C03-C21-O23
2	C	501	WBJ	N04-C03-C21-O23

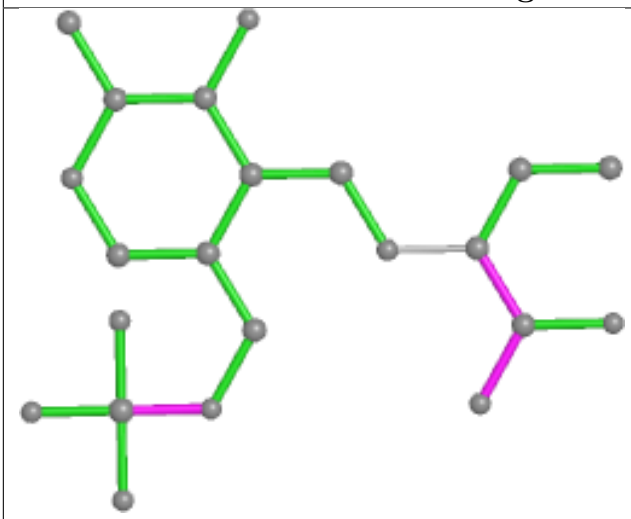
There are no ring outliers.

2 monomers are involved in 2 short contacts:

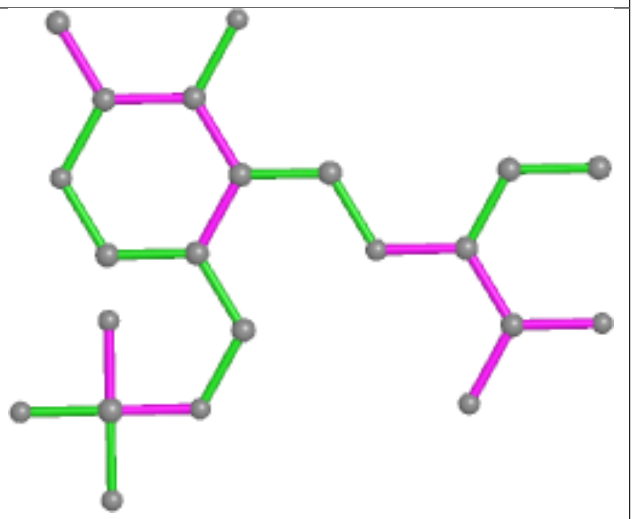
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	501	WBJ	1	0
2	B	501	WBJ	1	0

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 then 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.

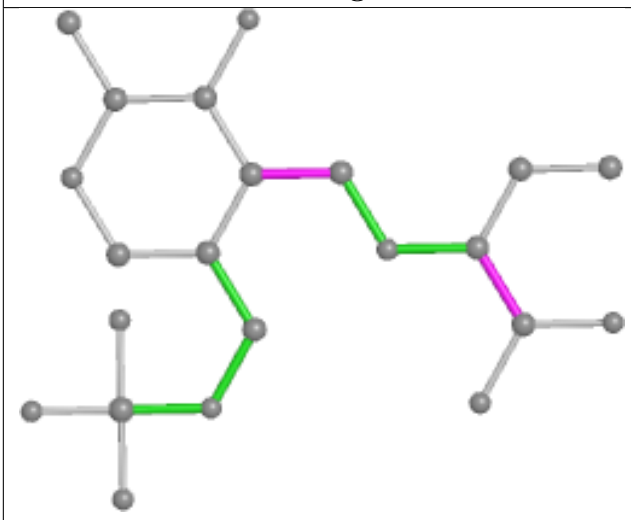
Ligand WBJ M 501



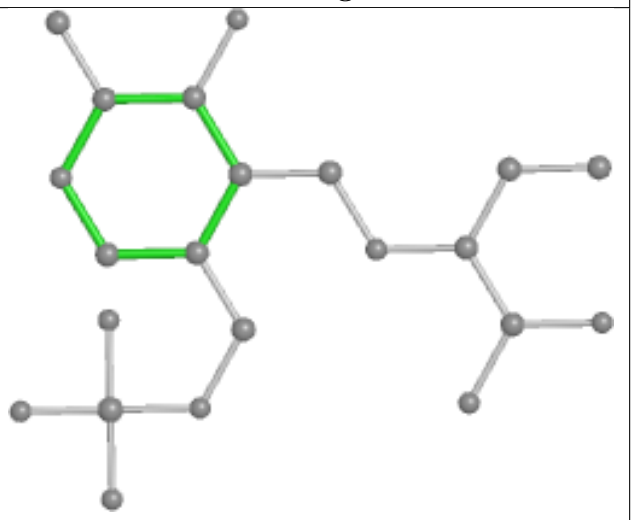
Bond lengths



Bond angles

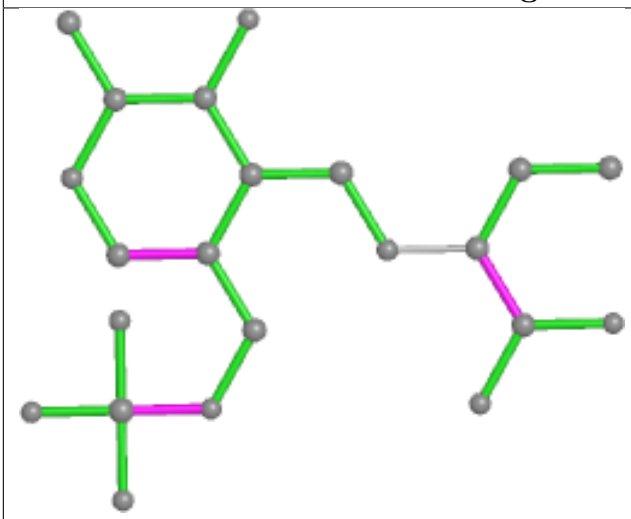


Torsions



Rings

Ligand WBJ D 501



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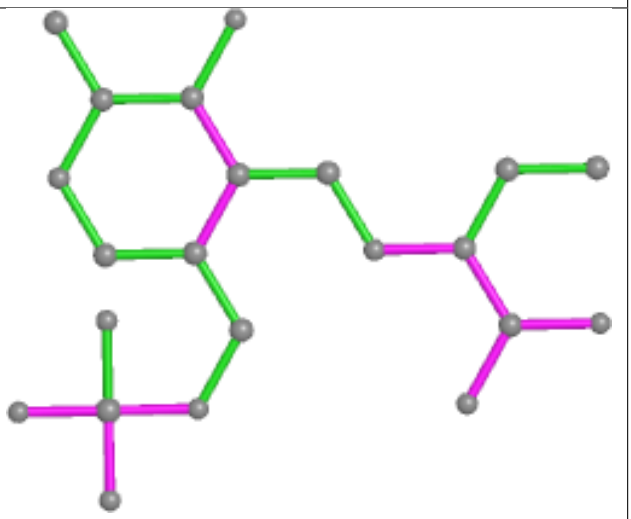
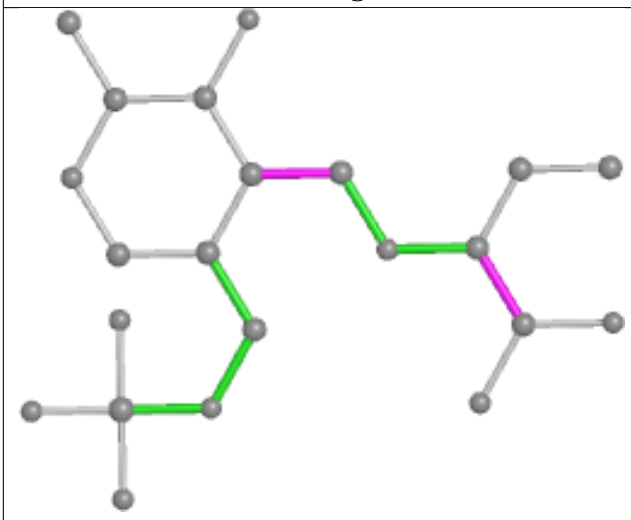


Bond angles



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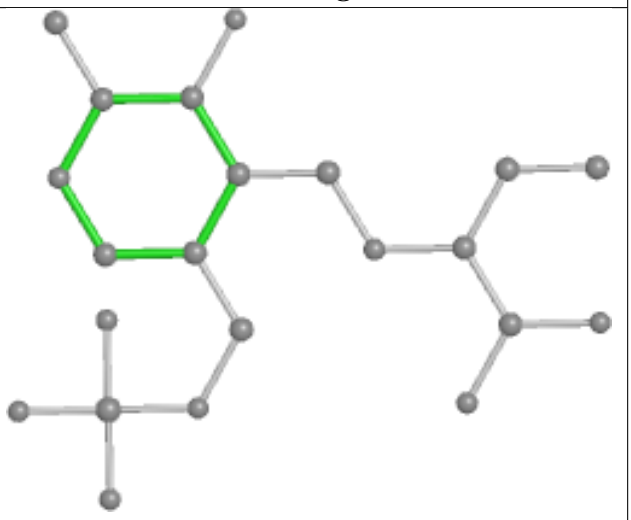
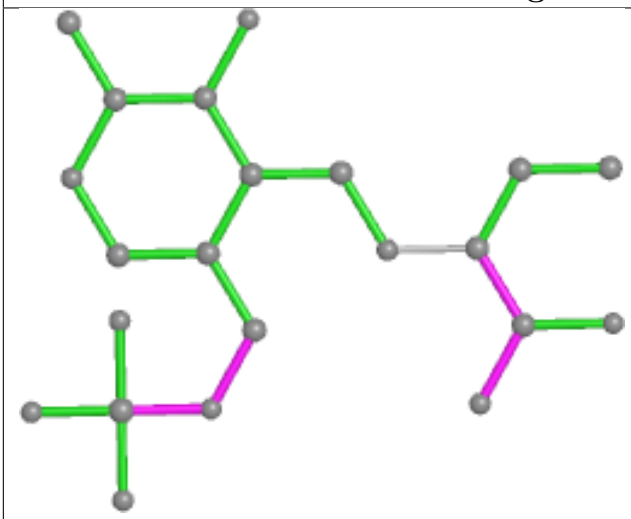
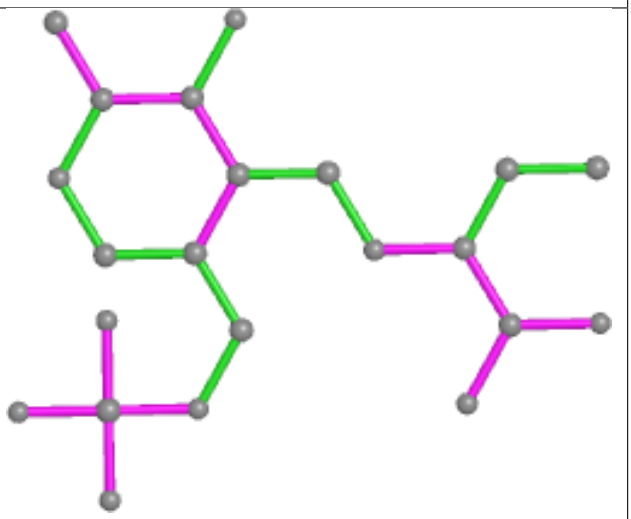


Rings

Ligand WBJ I 501



Bond lengths



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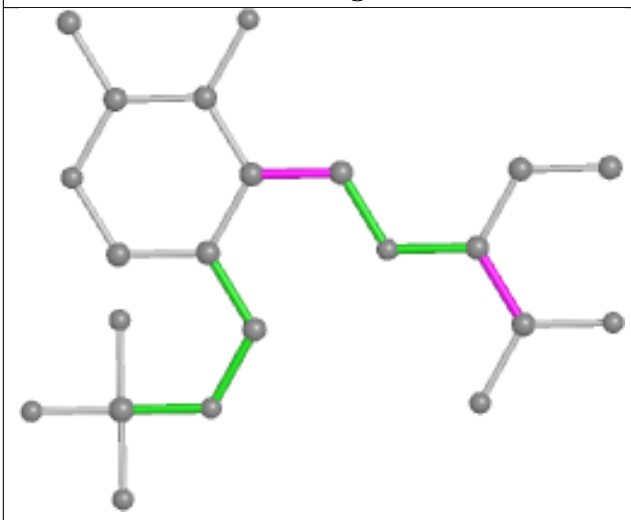

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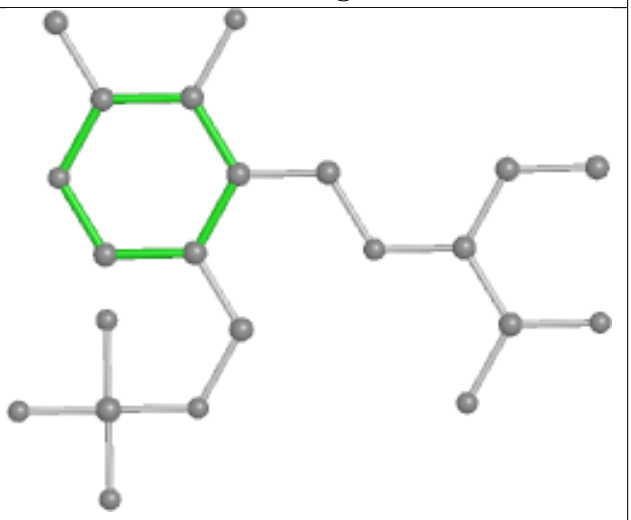
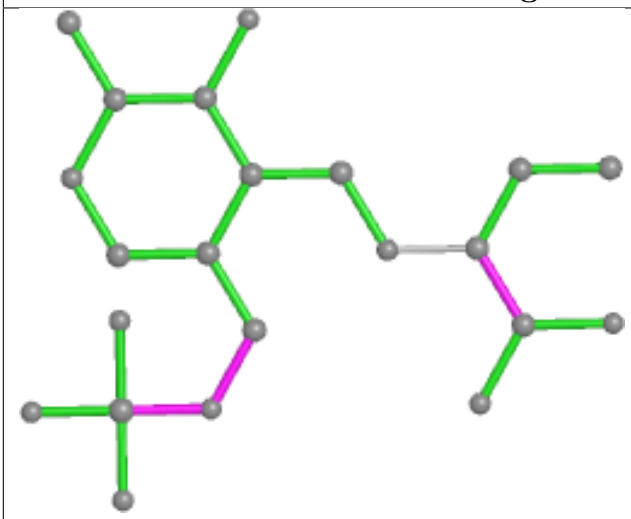


Rings

Ligand WBJ Q 501



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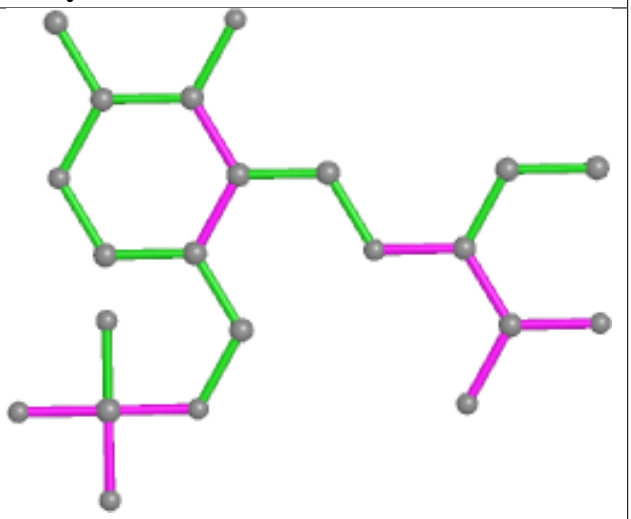
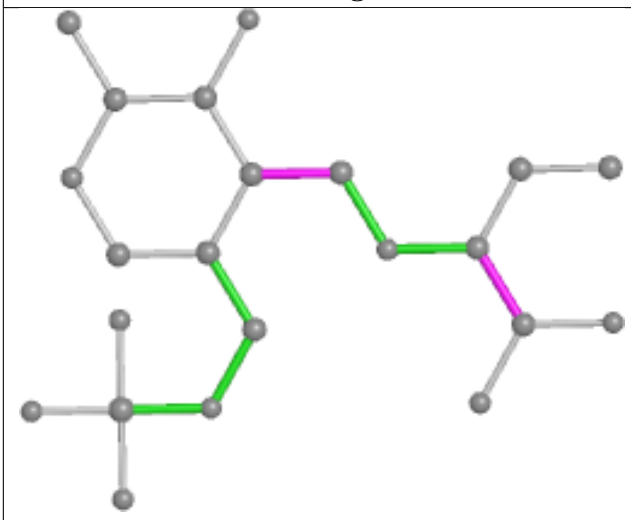
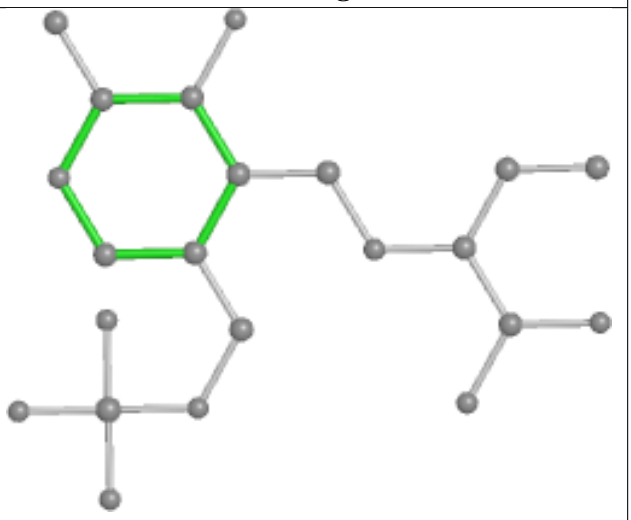


Bond angles

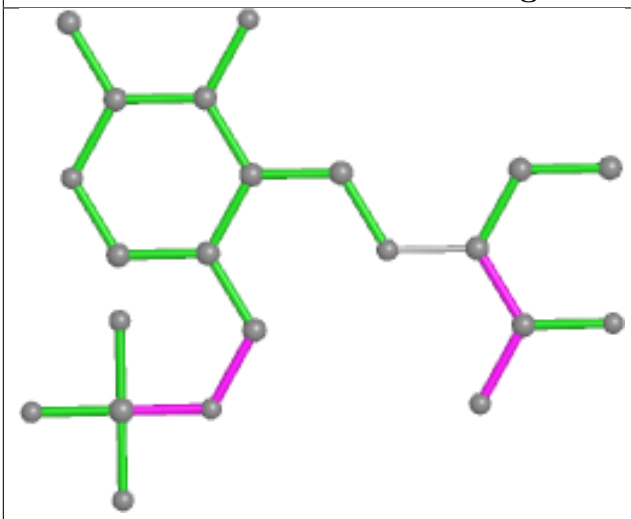


Torsions

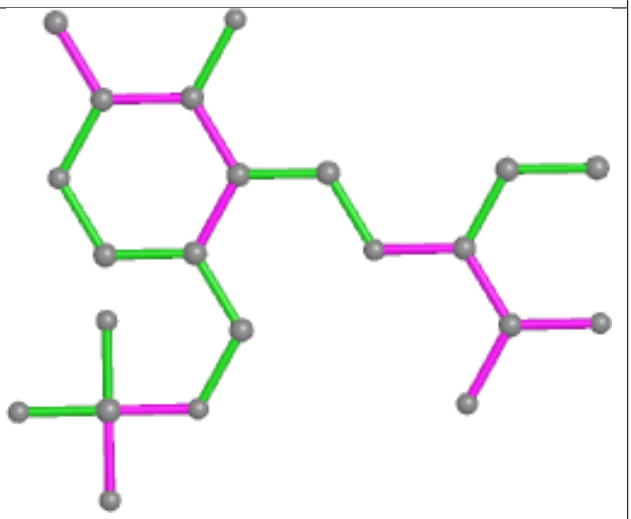


Rings

Ligand WBJ N 501



Bond lengths



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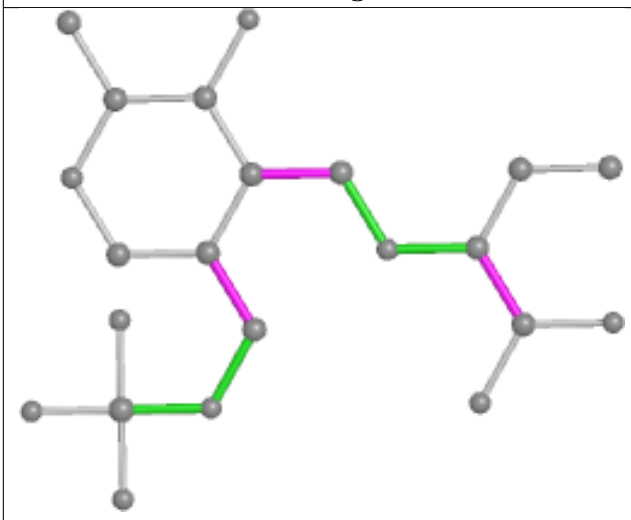

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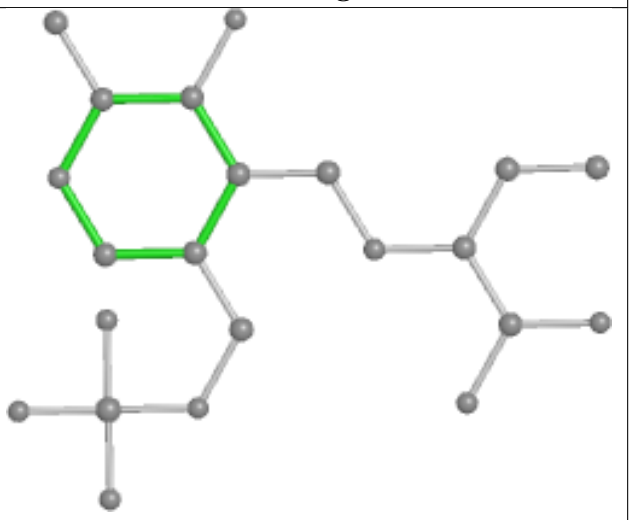
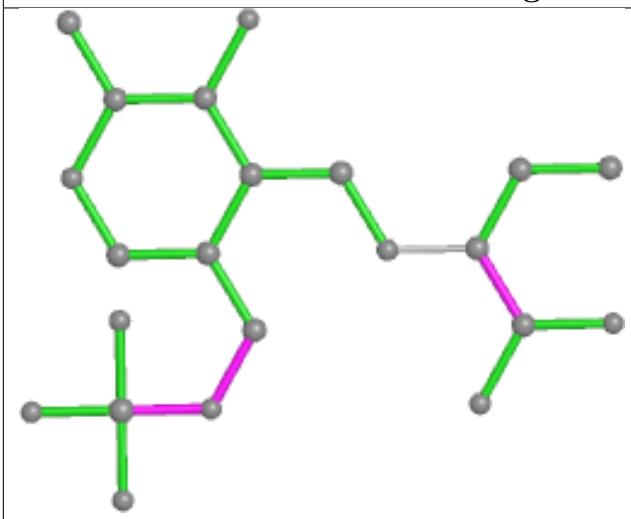


Rings

Ligand WBJ L 501



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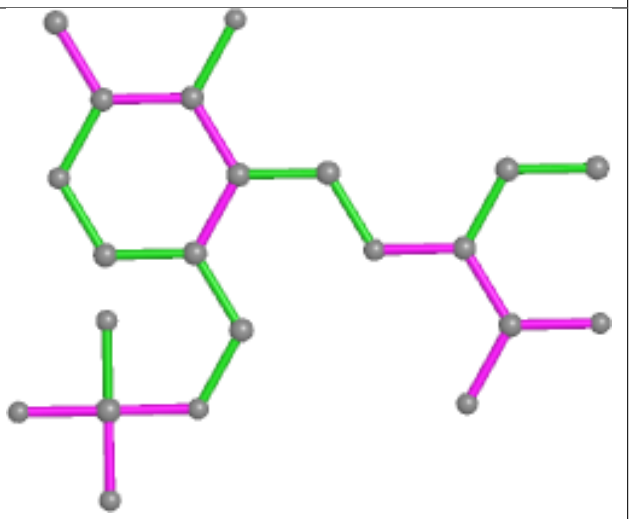
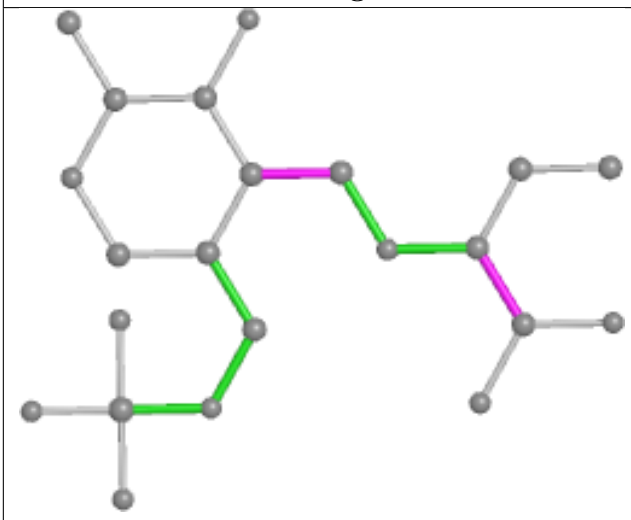


Bond angles



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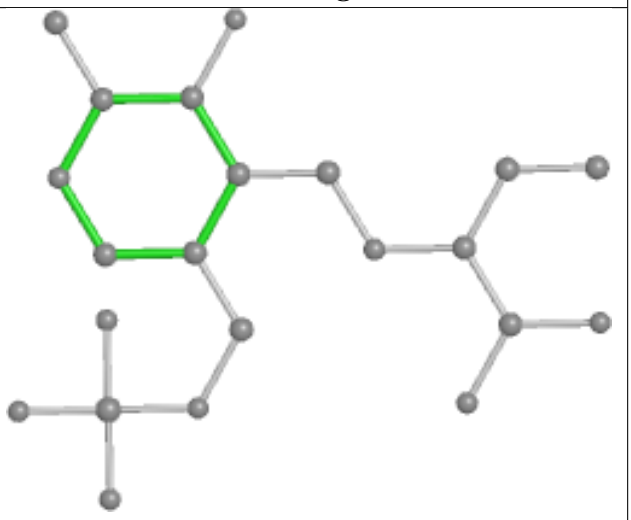
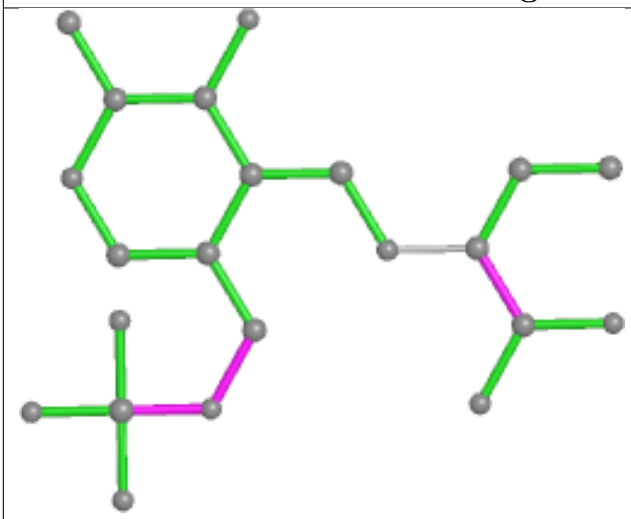
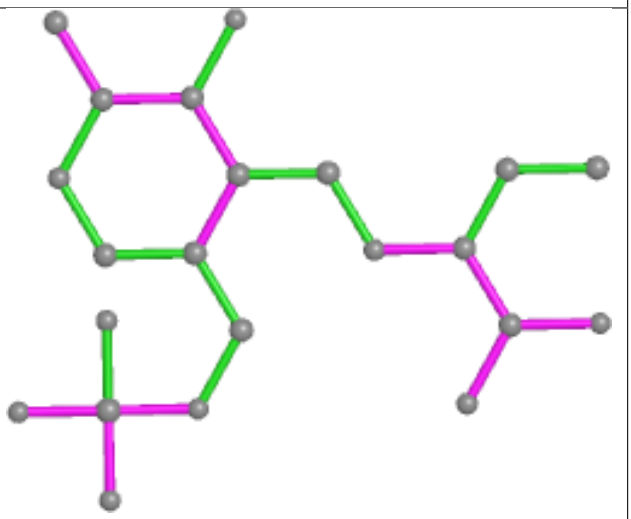


Rings

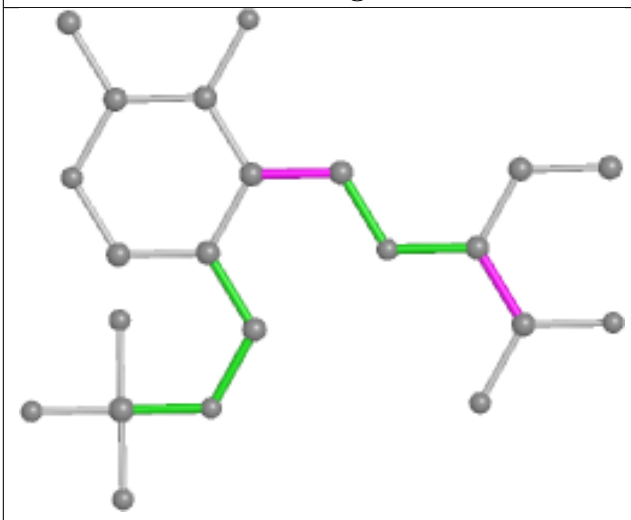
Ligand WBJ A 501



Bond lengths



Bond angles



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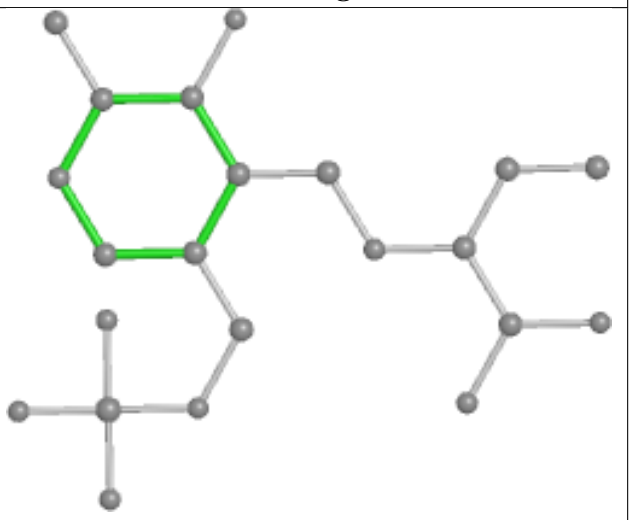
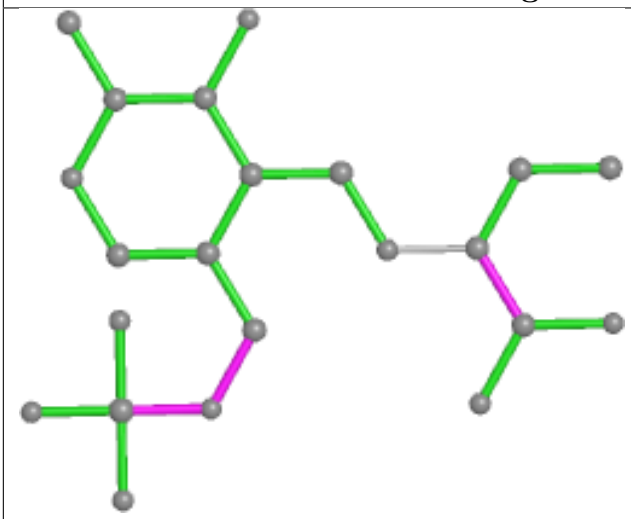


Rings

Ligand WBJ B 501



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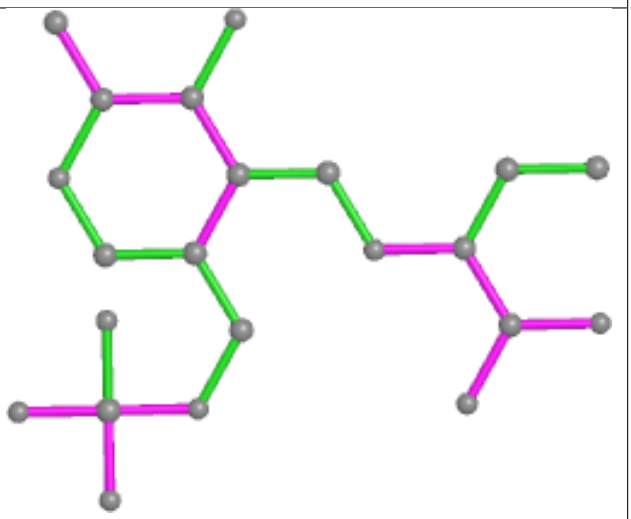
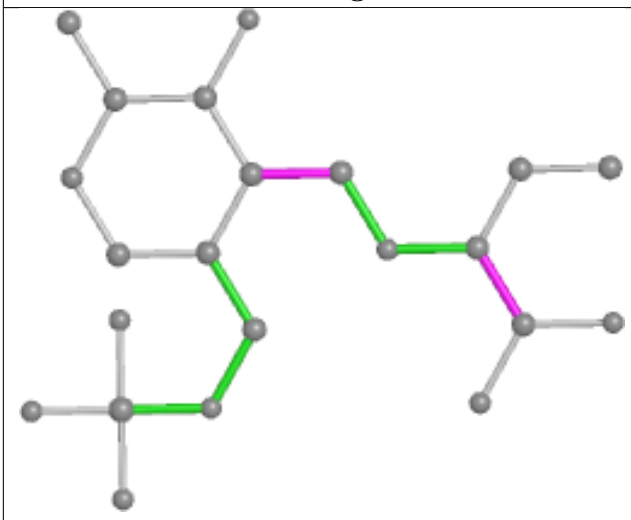
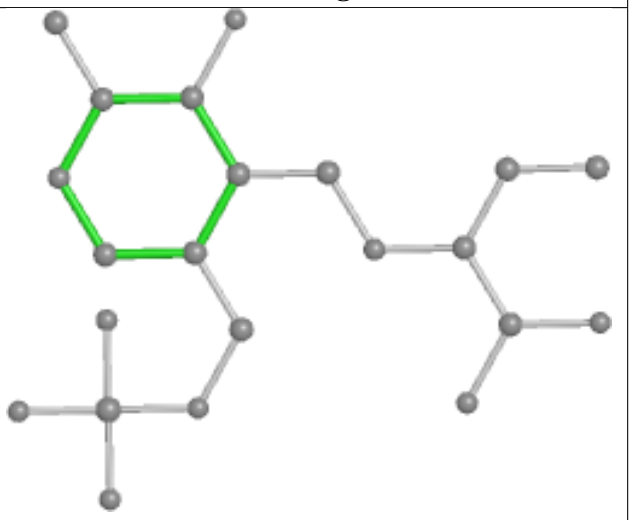


Bond angles

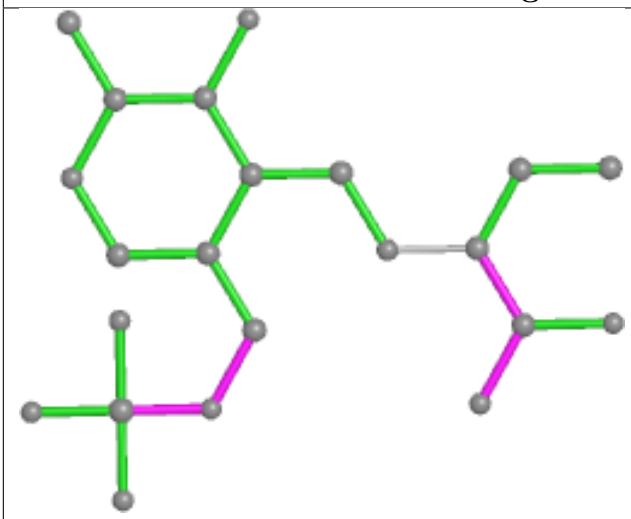


Torsions

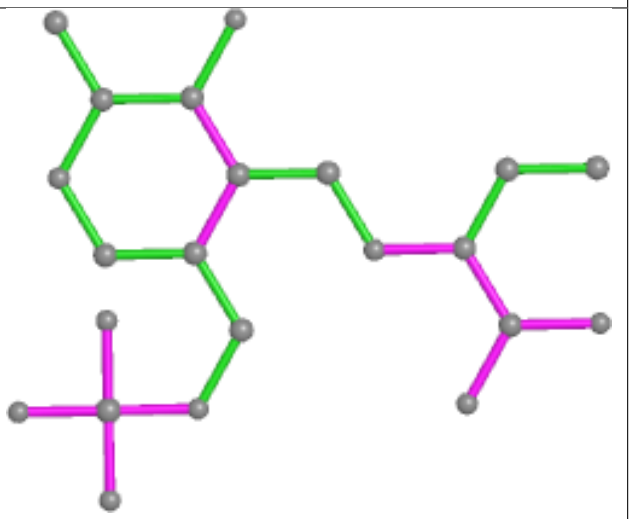


Rings

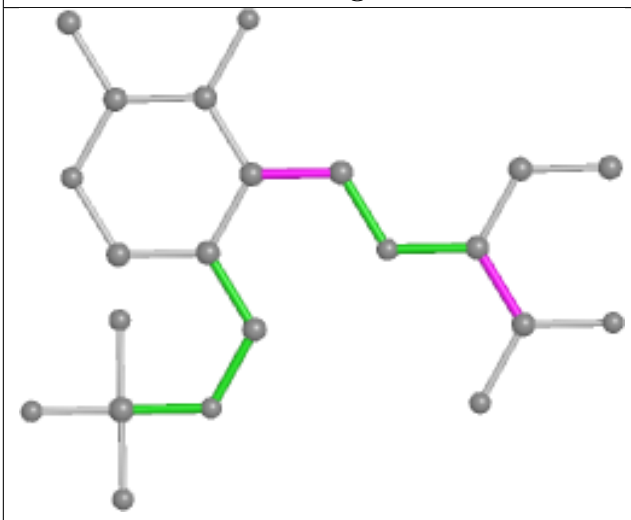
Ligand WBJ P 501



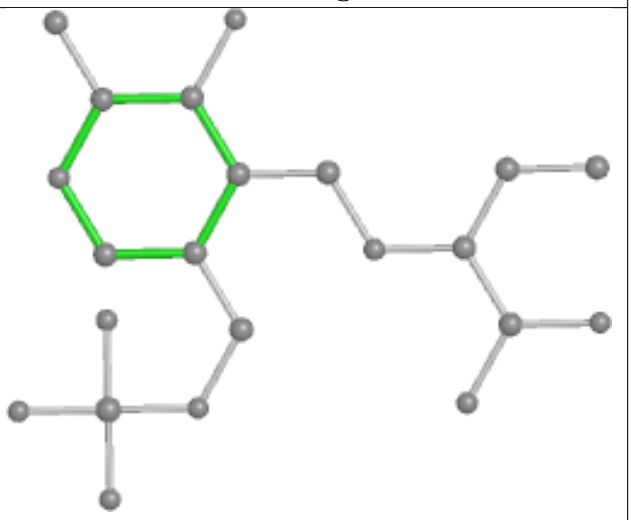
Bond lengths



Bond angles

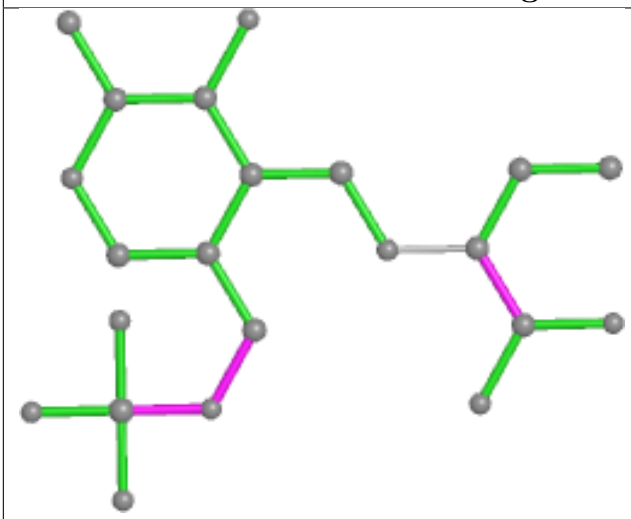


Torsions

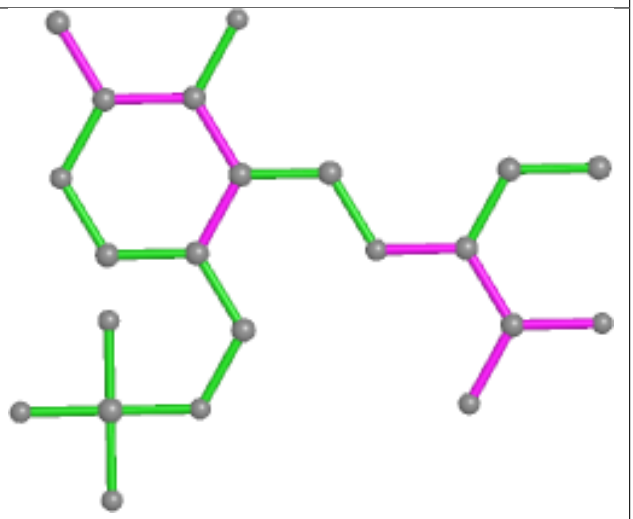


Rings

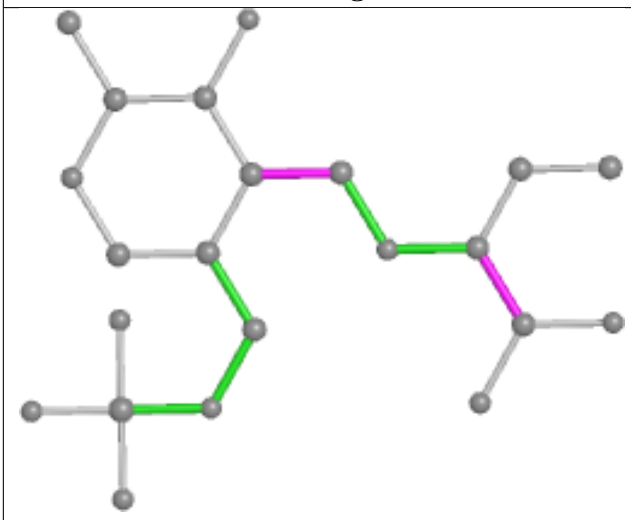
Ligand WBJ C 501



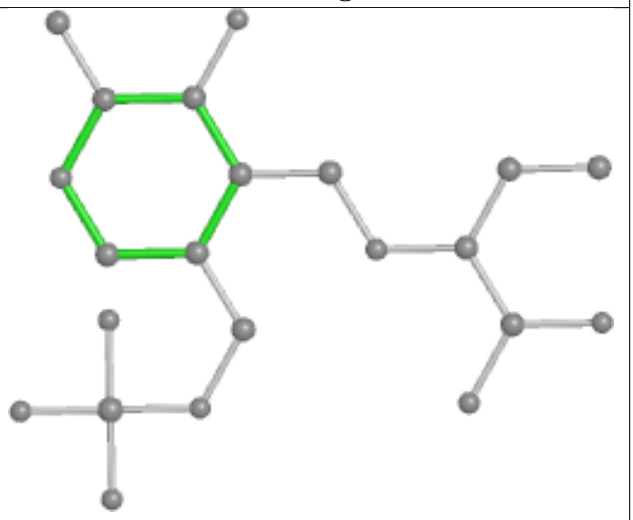
Bond lengths



Bond angles

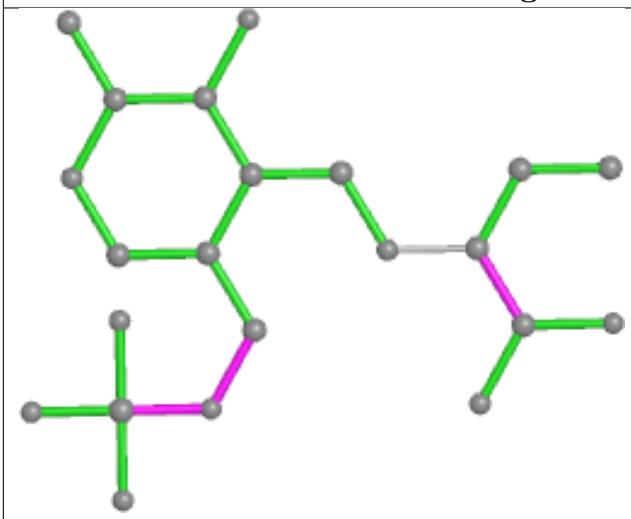


Torsions

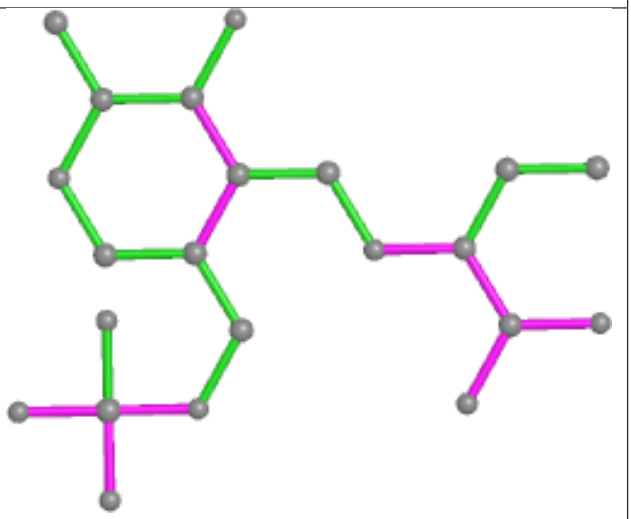


Rings

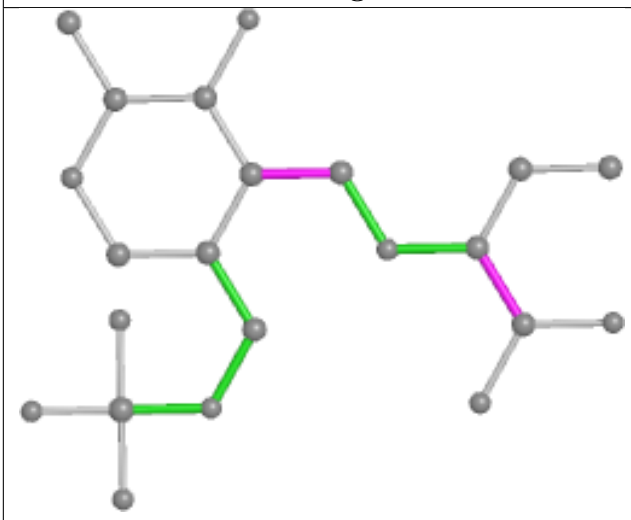
Ligand WBJ K 501



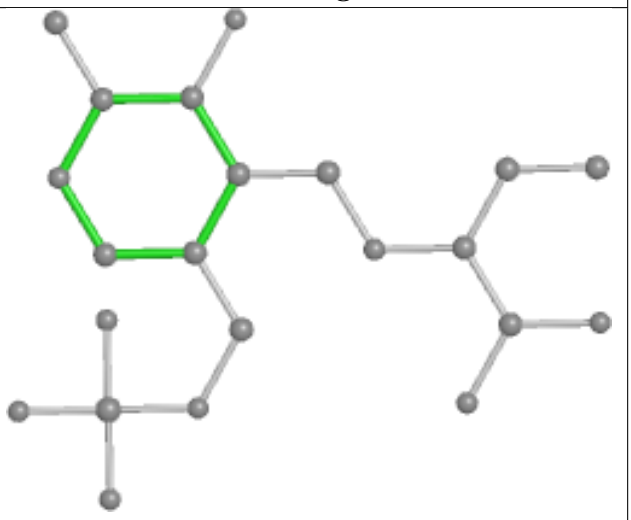
Bond lengths



Bond angles

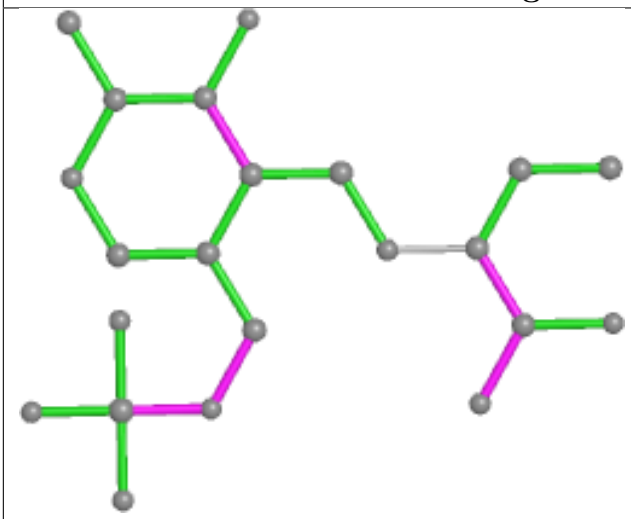


Torsions

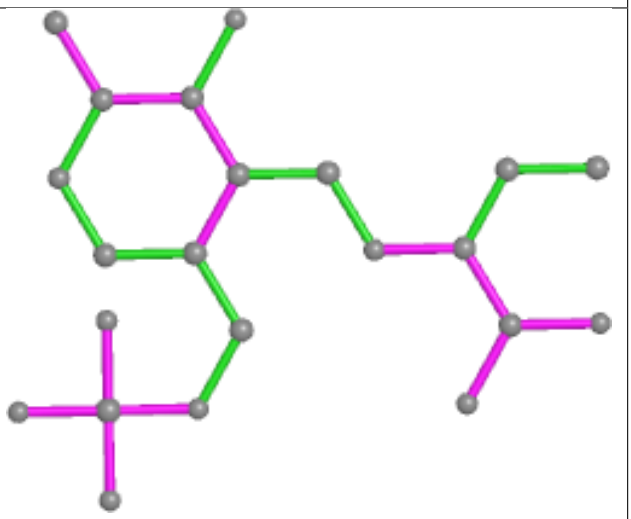


Rings

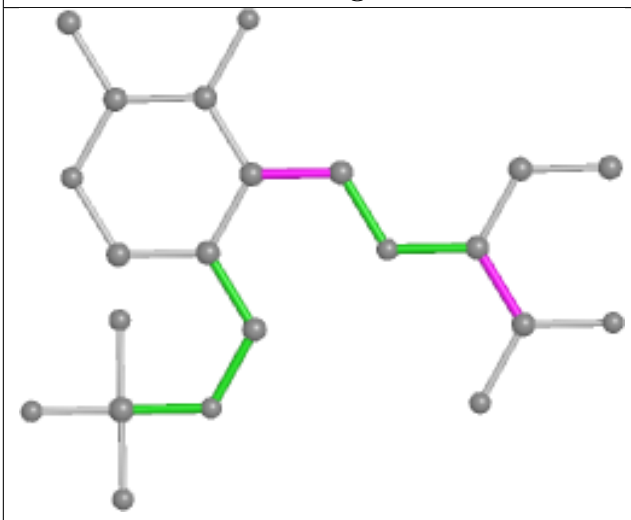
Ligand WBJ F 501



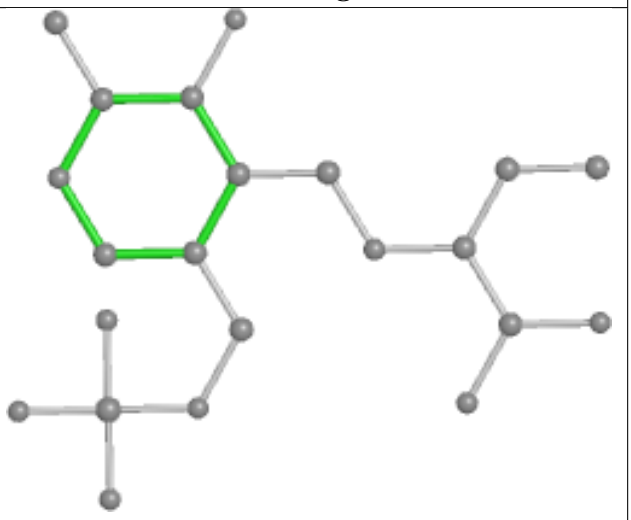
Bond lengths



Bond angles

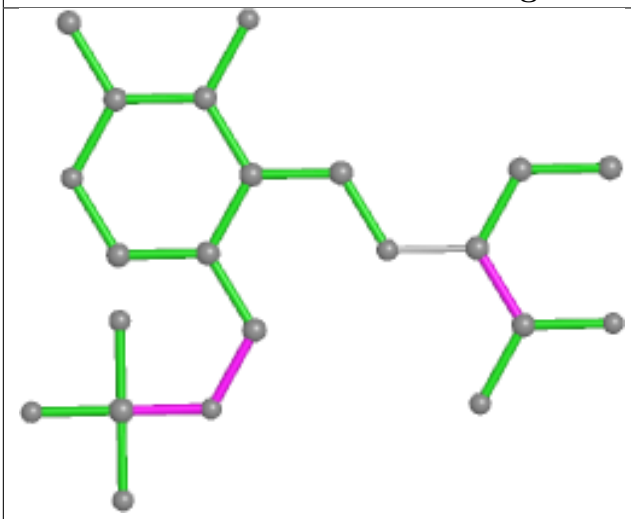


Torsions

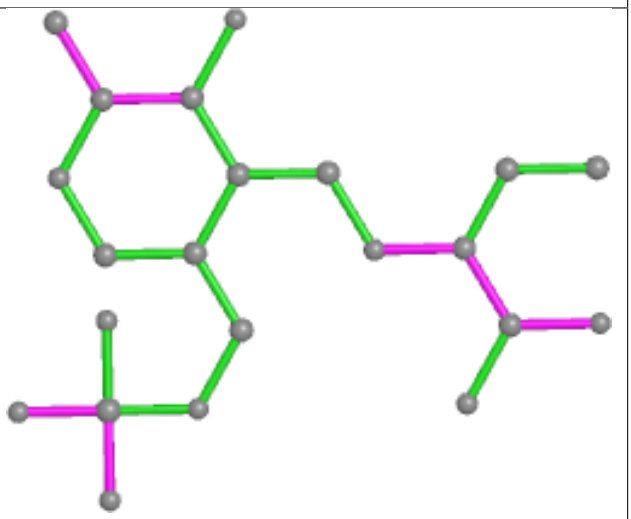


Rings

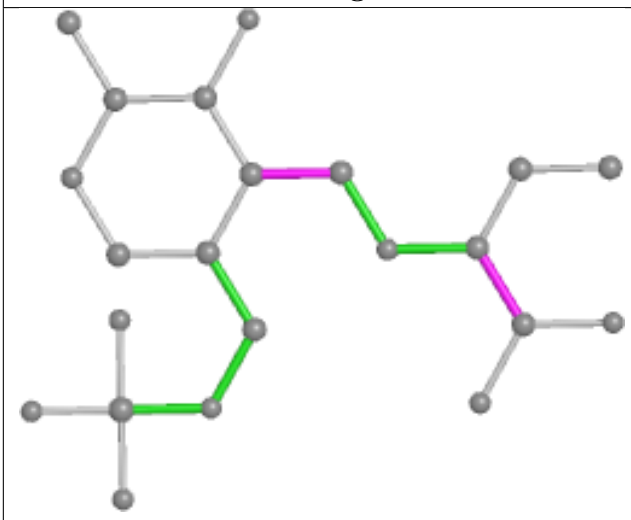
Ligand WBJ H 501



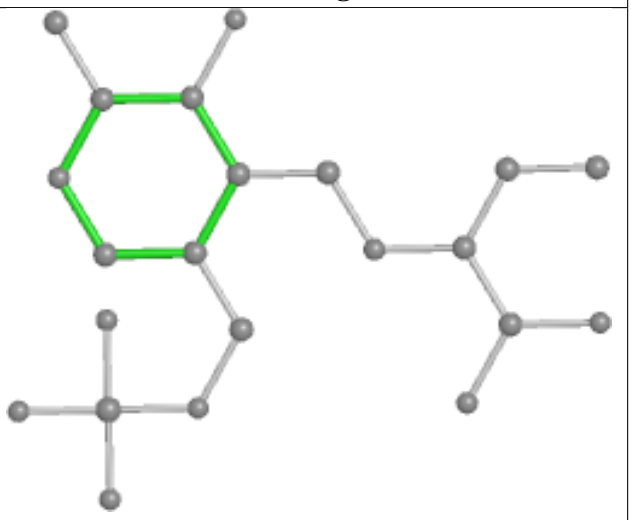
Bond lengths



Bond angles

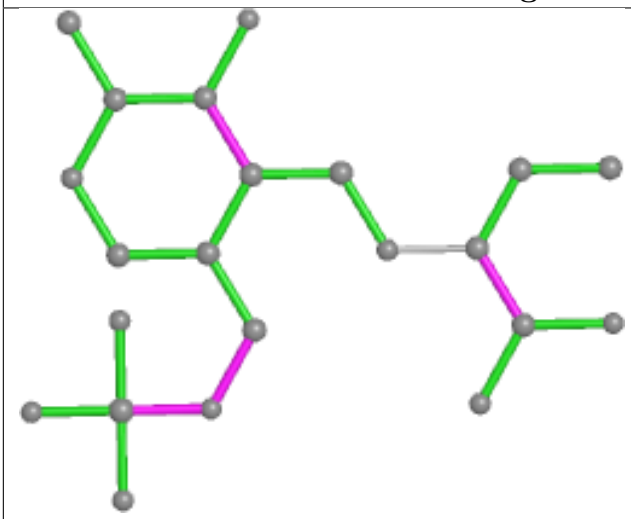


Torsions

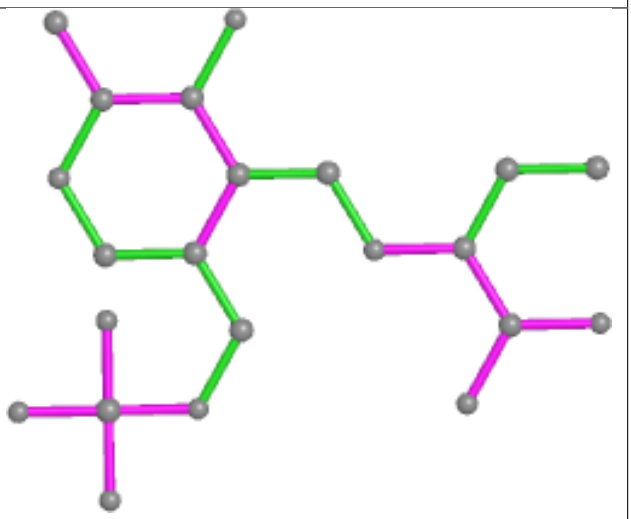


Rings

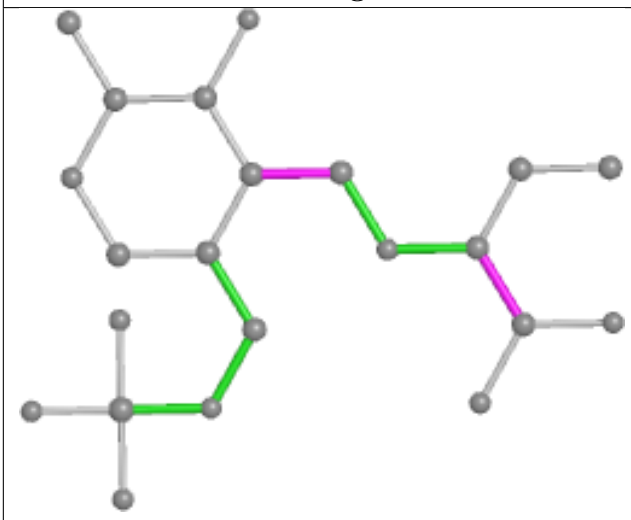
Ligand WBJ G 501



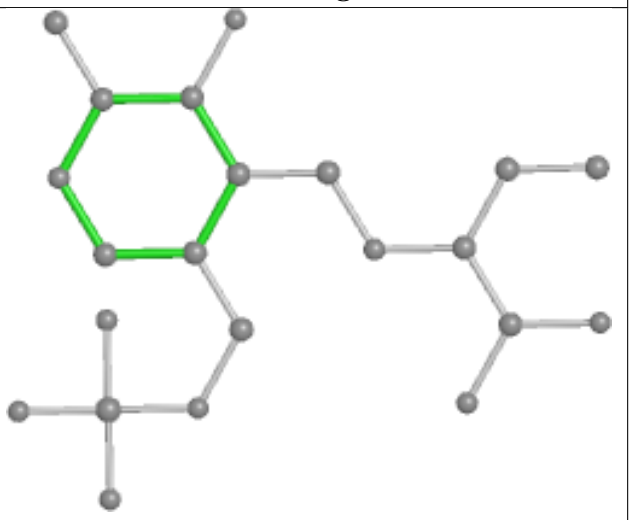
Bond lengths



Bond angles

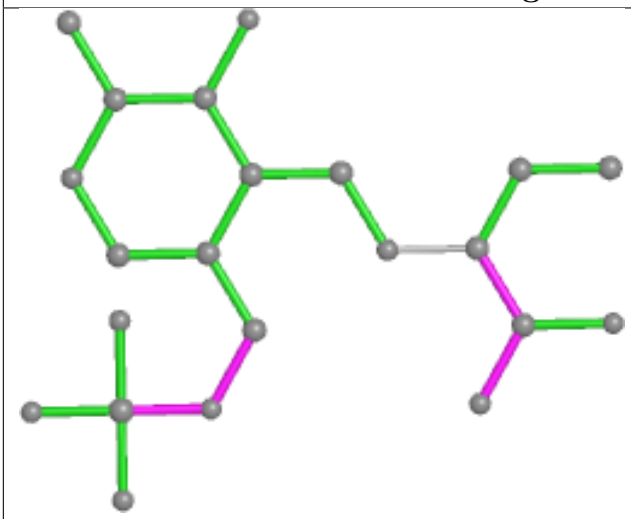


Torsions

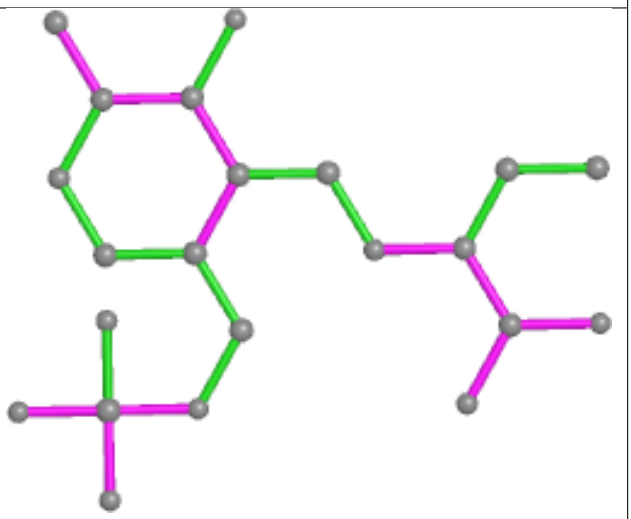


Rings

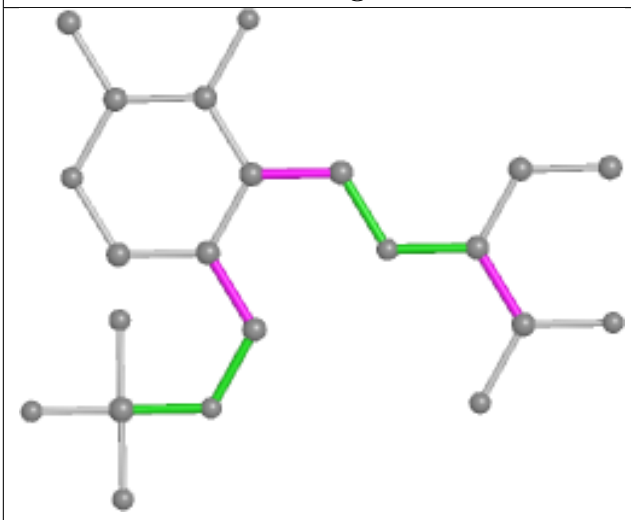
Ligand WBJ E 501



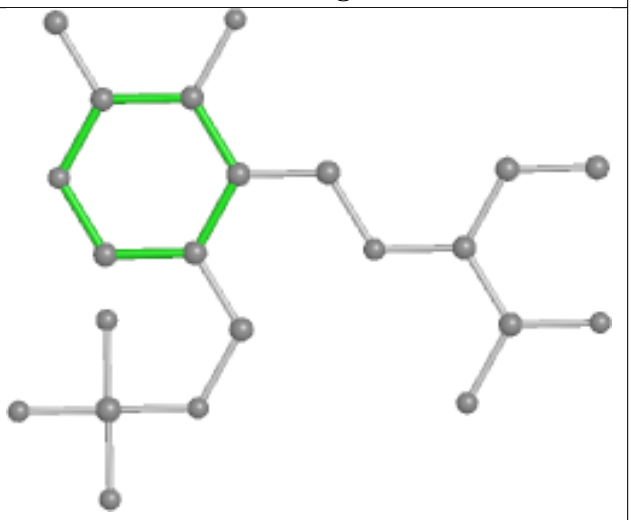
Bond lengths



Bond angles

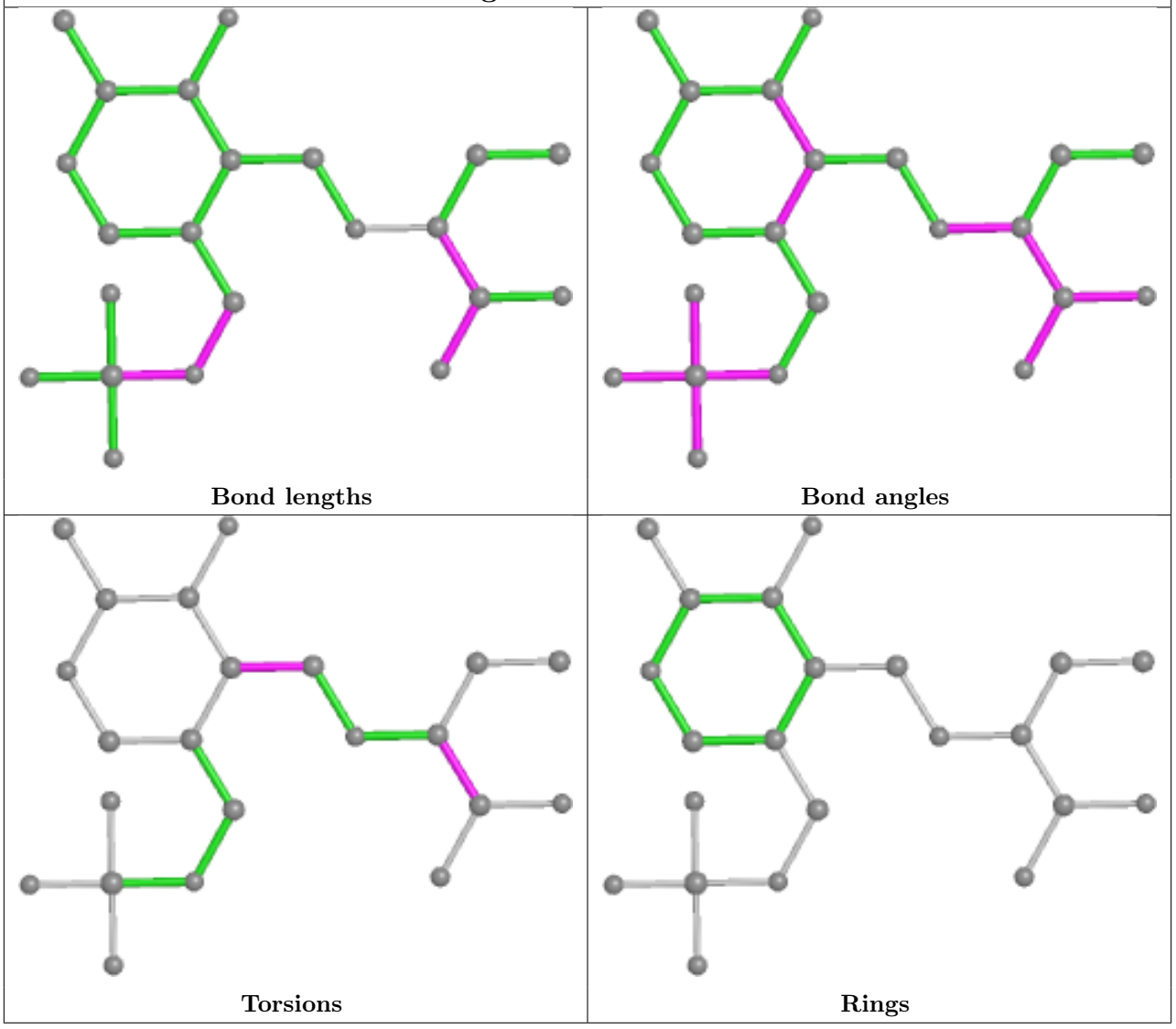


Torsions



Rings

Ligand WBJ J 501



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, 95^{th} 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%)	-0.03	8 (1%)	66	68	9, 20, 35, 57	1 (0%)
1	B	427/433 (98%)	0.02	10 (2%)	60	62	11, 21, 36, 64	0
1	C	427/433 (98%)	-0.15	10 (2%)	60	62	9, 17, 31, 60	0
1	D	428/433 (98%)	-0.07	7 (1%)	72	73	9, 18, 32, 54	0
1	E	427/433 (98%)	0.07	8 (1%)	66	68	10, 22, 38, 64	0
1	F	425/433 (98%)	0.00	10 (2%)	59	61	11, 21, 36, 55	0
1	G	427/433 (98%)	-0.04	10 (2%)	60	62	11, 21, 35, 55	0
1	H	426/433 (98%)	-0.00	8 (1%)	66	68	12, 23, 37, 55	0
1	I	428/433 (98%)	-0.01	13 (3%)	50	52	13, 23, 38, 56	0
1	J	427/433 (98%)	0.04	9 (2%)	63	65	12, 23, 38, 60	0
1	K	429/433 (99%)	0.02	8 (1%)	66	68	13, 22, 39, 62	0
1	L	428/433 (98%)	-0.06	7 (1%)	72	73	11, 21, 37, 51	0
1	M	428/433 (98%)	-0.07	8 (1%)	66	68	10, 19, 33, 60	0
1	N	422/433 (97%)	0.02	4 (0%)	84	85	10, 22, 35, 51	0
1	P	428/433 (98%)	-0.05	10 (2%)	60	62	11, 21, 36, 58	0
1	Q	429/433 (99%)	-0.08	9 (2%)	63	65	10, 18, 33, 56	0
All	All	6834/6928 (98%)	-0.02	139 (2%)	65	66	9, 21, 36, 64	1 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	5	VAL	5.6
1	N	7	GLN	5.4
1	E	354	ASP	5.1
1	K	354	ASP	5.0
1	C	354	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	7	GLN	4.7
1	B	5	VAL	4.6
1	E	356	SER	4.6
1	H	355	ALA	4.5
1	B	356	SER	4.5
1	H	431	TYR	4.5
1	K	432	GLY	4.2
1	B	354	ASP	4.2
1	P	354	ASP	4.0
1	I	354	ASP	4.0
1	J	354	ASP	3.9
1	Q	5	VAL	3.8
1	K	5	VAL	3.8
1	M	354	ASP	3.8
1	A	356	SER	3.7
1	D	4	GLN	3.7
1	G	5	VAL	3.6
1	F	353	GLY	3.6
1	M	5	VAL	3.5
1	I	5	VAL	3.5
1	C	355	ALA	3.4
1	A	354	ASP	3.4
1	G	354	ASP	3.4
1	M	7	GLN	3.3
1	F	428	GLN	3.3
1	K	431	TYR	3.2
1	F	354	ASP	3.2
1	A	7	GLN	3.2
1	K	352	LYS	3.2
1	C	432	GLY	3.1
1	P	428	GLN	3.1
1	I	428	GLN	3.1
1	J	428	GLN	3.0
1	H	7	GLN	3.0
1	H	430	ALA	3.0
1	J	431	TYR	3.0
1	I	360	LYS	2.9
1	N	398	LEU	2.9
1	Q	354	ASP	2.9
1	L	354	ASP	2.9
1	L	428	GLN	2.9
1	A	31	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	432	GLY	2.9
1	P	147	ASP	2.9
1	D	354	ASP	2.9
1	L	355	ALA	2.9
1	Q	7	GLN	2.9
1	D	7	GLN	2.8
1	A	5	VAL	2.8
1	Q	356	SER	2.8
1	E	7	GLN	2.8
1	G	355	ALA	2.7
1	D	5	VAL	2.7
1	F	360	LYS	2.7
1	M	282	PHE	2.7
1	I	431	TYR	2.7
1	J	355	ALA	2.7
1	Q	355	ALA	2.7
1	J	395	ASP	2.6
1	F	431	TYR	2.6
1	H	428	GLN	2.6
1	C	6	PHE	2.6
1	G	431	TYR	2.6
1	D	31	ILE	2.6
1	M	353	GLY	2.6
1	P	5	VAL	2.5
1	P	135	ARG	2.5
1	G	428	GLN	2.5
1	C	7	GLN	2.5
1	Q	4	GLN	2.5
1	N	356	SER	2.5
1	L	7	GLN	2.5
1	B	355	ALA	2.5
1	F	7	GLN	2.5
1	Q	31	ILE	2.5
1	E	252	LEU	2.4
1	I	7	GLN	2.4
1	I	353	GLY	2.4
1	H	427	PHE	2.4
1	G	353	GLY	2.4
1	G	7	GLN	2.4
1	L	356	SER	2.4
1	B	31	ILE	2.4
1	C	31	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	357	ALA	2.4
1	H	279	LEU	2.3
1	E	23	HIS	2.3
1	C	282	PHE	2.3
1	G	430	ALA	2.3
1	I	54	LEU	2.3
1	J	356	SER	2.3
1	M	31	ILE	2.3
1	F	314	SER	2.3
1	I	356	SER	2.3
1	G	429	LYS	2.3
1	J	353	GLY	2.2
1	A	279	LEU	2.2
1	A	432	GLY	2.2
1	F	430	ALA	2.2
1	F	252	LEU	2.2
1	B	282	PHE	2.2
1	K	428	GLN	2.2
1	B	22	PRO	2.2
1	G	356	SER	2.2
1	L	431	TYR	2.2
1	K	23	HIS	2.2
1	F	429	LYS	2.2
1	B	428	GLN	2.2
1	P	7	GLN	2.2
1	J	5	VAL	2.2
1	C	279	LEU	2.1
1	Q	21	ASP	2.1
1	E	395	ASP	2.1
1	A	355	ALA	2.1
1	D	287	LEU	2.1
1	M	279	LEU	2.1
1	Q	279	LEU	2.1
1	K	430	ALA	2.1
1	J	23	HIS	2.1
1	H	354	ASP	2.1
1	N	282	PHE	2.1
1	I	352	LYS	2.1
1	P	355	ALA	2.1
1	L	314	SER	2.1
1	P	4	GLN	2.1
1	P	316	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	4	GLN	2.1
1	B	353	GLY	2.0
1	P	353	GLY	2.0
1	C	428	GLN	2.0
1	C	220	ILE	2.0
1	D	288	LEU	2.0
1	E	31	ILE	2.0
1	I	135	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	0.96	0.12	13,19,26,29	0
2	WBJ	G	501	22/22	0.96	0.12	13,19,24,26	0
2	WBJ	H	501	22/22	0.97	0.11	14,19,31,33	0
2	WBJ	I	501	22/22	0.97	0.10	14,20,29,32	0
2	WBJ	J	501	22/22	0.97	0.10	13,23,29,35	0
2	WBJ	E	501	22/22	0.97	0.11	14,21,28,34	0
2	WBJ	L	501	22/22	0.97	0.11	13,21,27,30	0
2	WBJ	D	501	22/22	0.98	0.10	9,15,26,29	0
2	WBJ	P	501	22/22	0.98	0.10	13,17,27,31	0
2	WBJ	A	501	22/22	0.98	0.12	11,15,26,29	0
2	WBJ	M	501	22/22	0.98	0.10	11,15,26,29	0
2	WBJ	Q	501	22/22	0.98	0.10	13,18,26,29	0
2	WBJ	N	501	22/22	0.98	0.11	14,21,29,32	0
2	WBJ	C	501	22/22	0.98	0.10	9,15,25,29	0
2	WBJ	F	501	22/22	0.98	0.10	12,20,29,31	0

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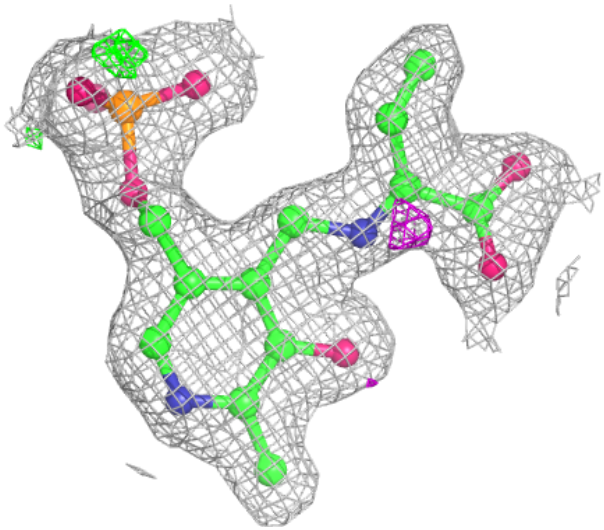
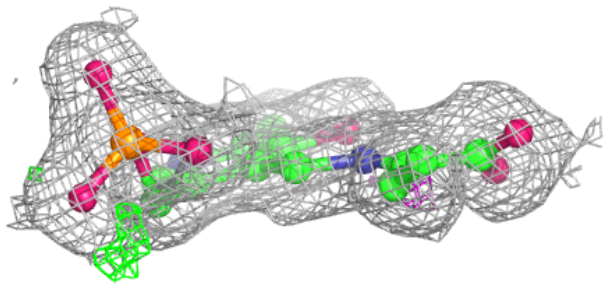
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	WBJ	K	501	22/22	0.98	0.10	14,20,30,34	0

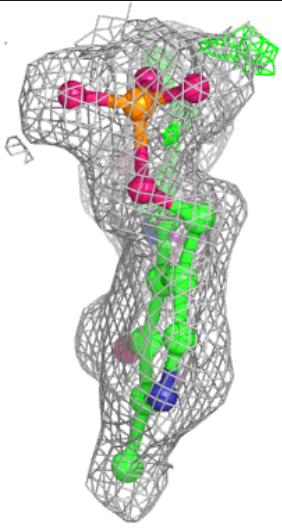
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

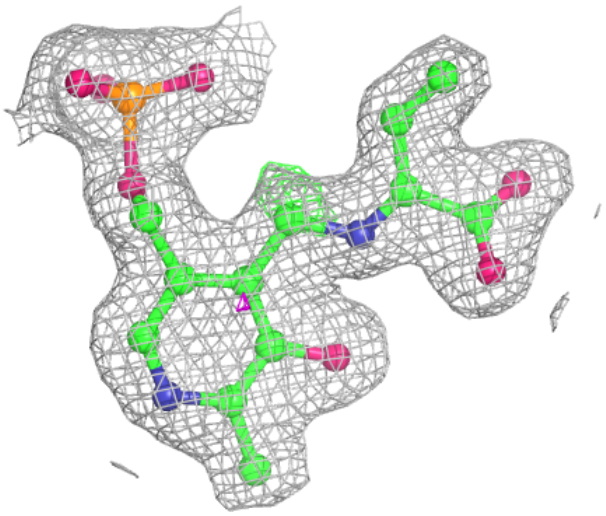


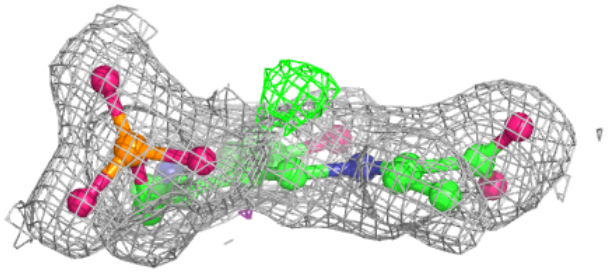


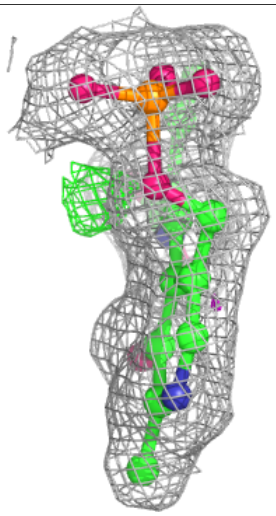


Electron density around WBJ G 501:

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

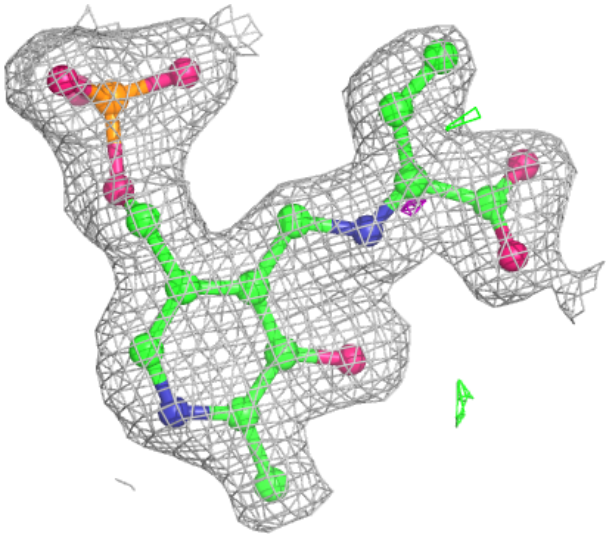


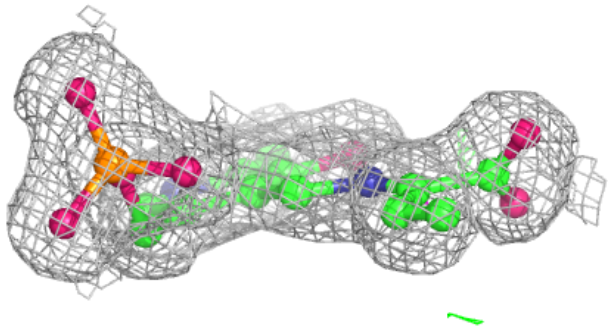


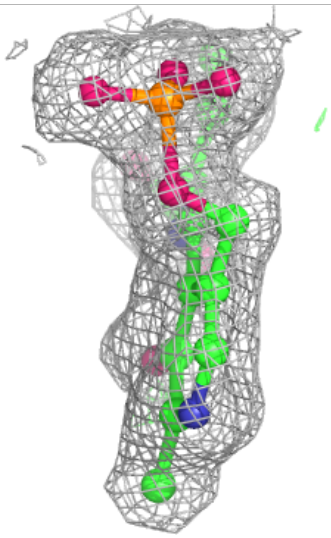


Electron density around WBJ H 501:

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

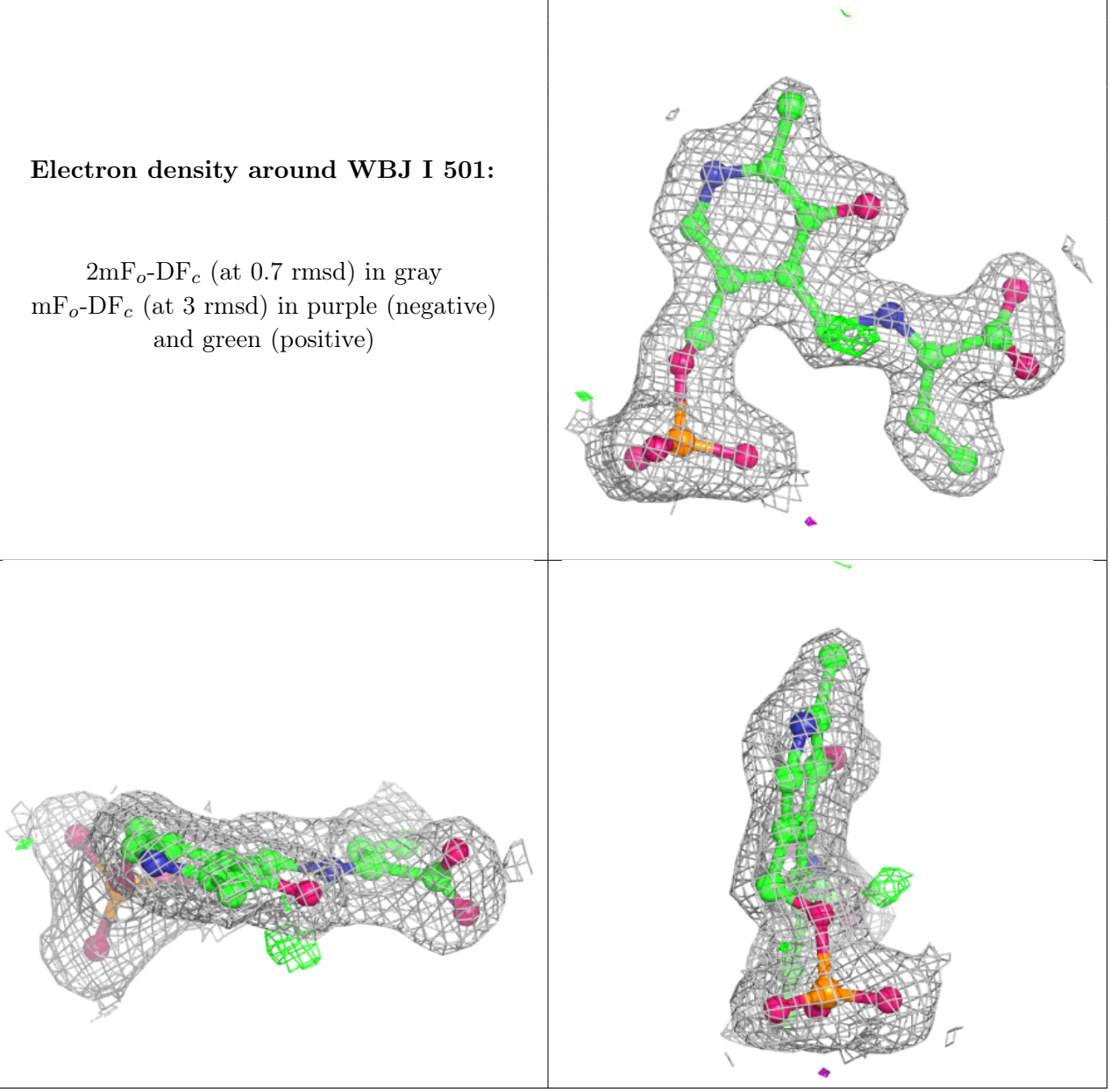






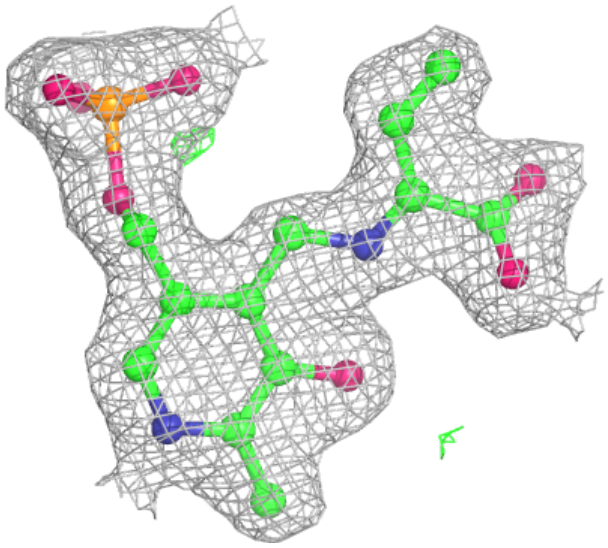
Electron density around WBJ I 501:

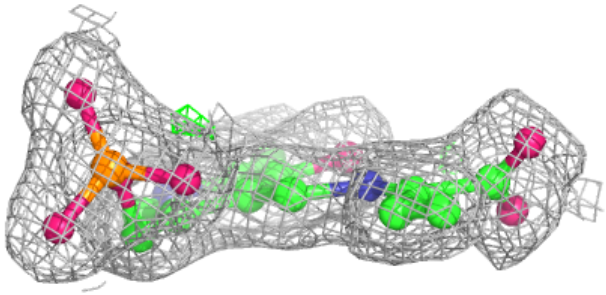
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

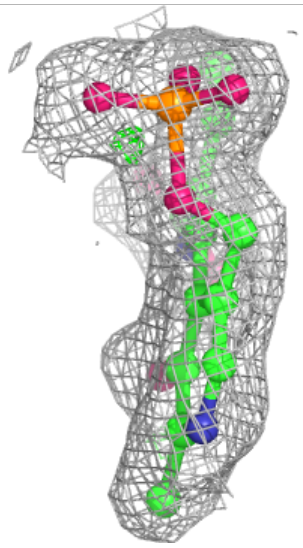


Electron density around WBJ J 501:

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

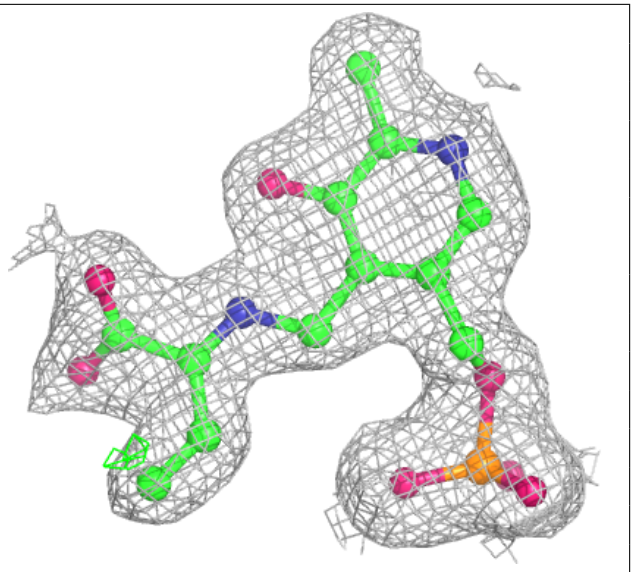


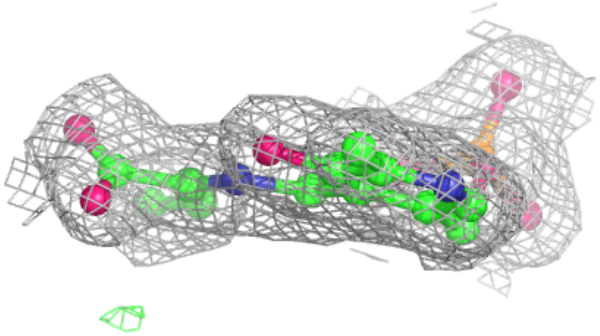


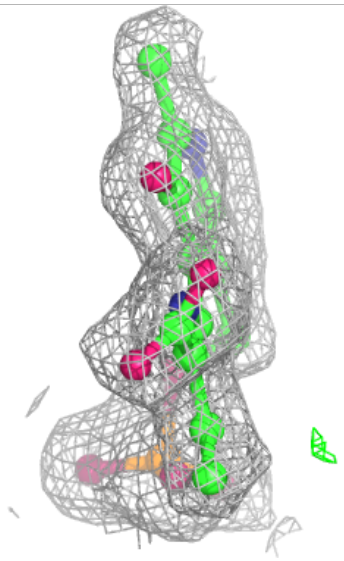


Electron density around WBJ E 501:

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

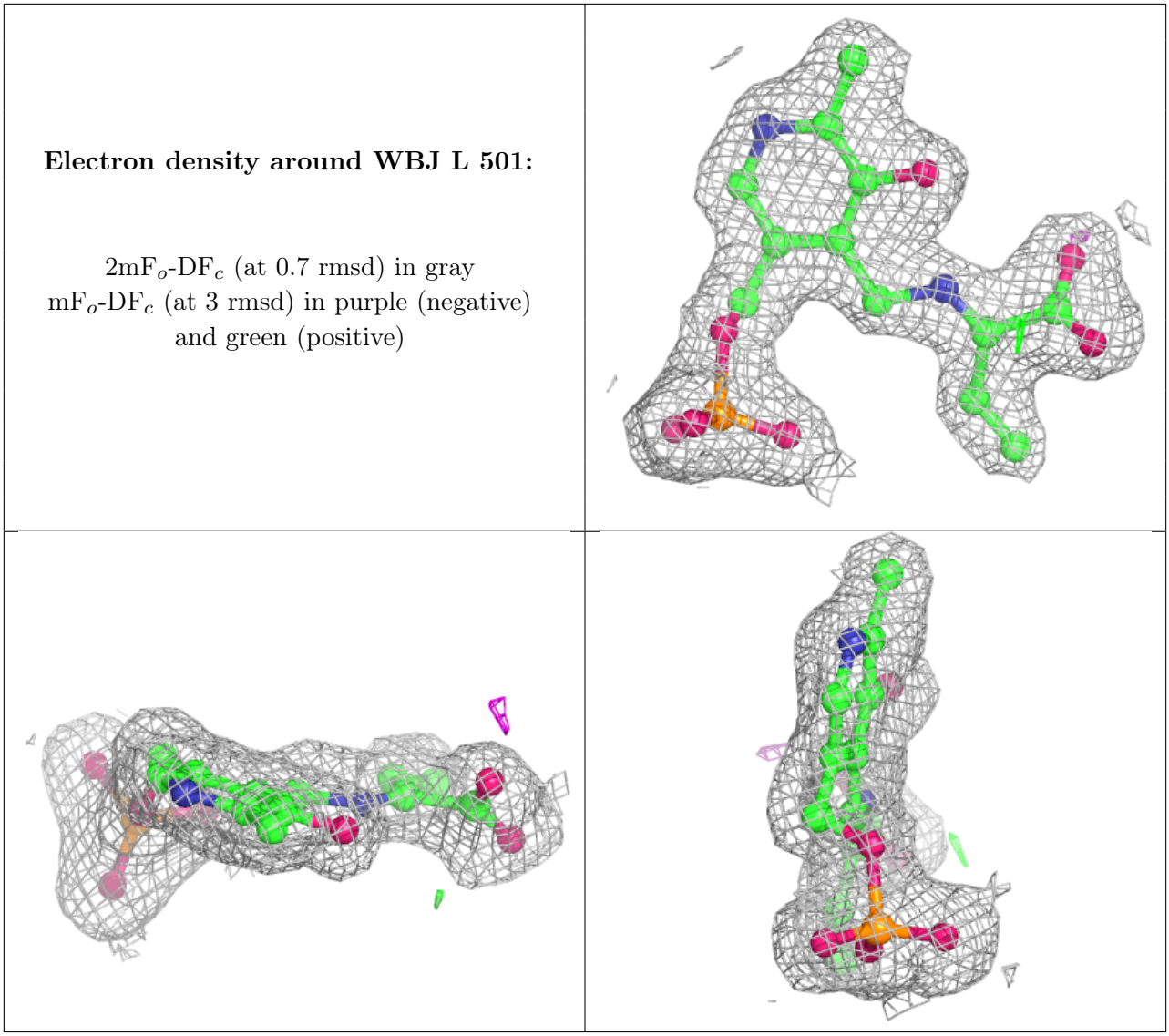






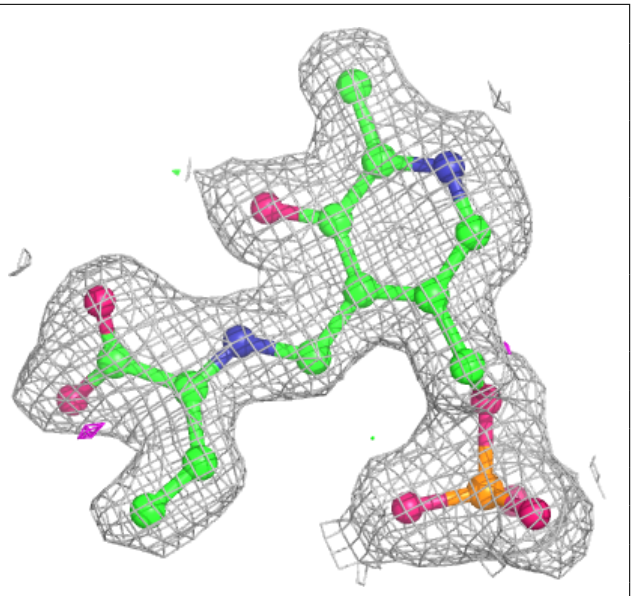
Electron density around WBJ L 501:

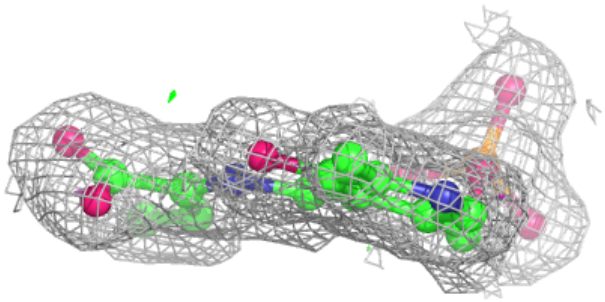
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

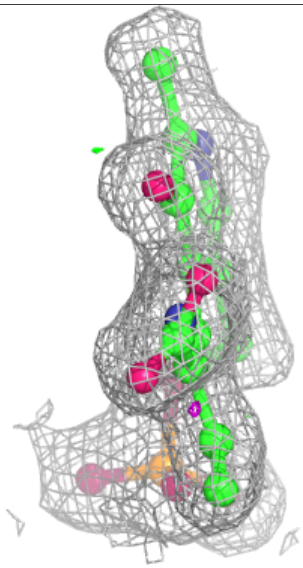


Electron density around WBJ D 501:

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

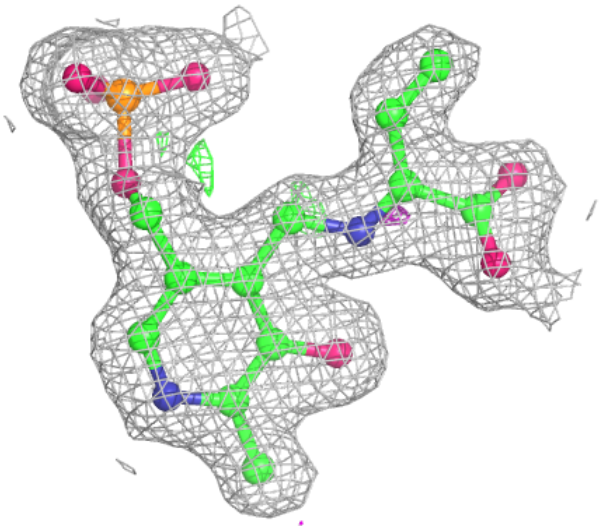


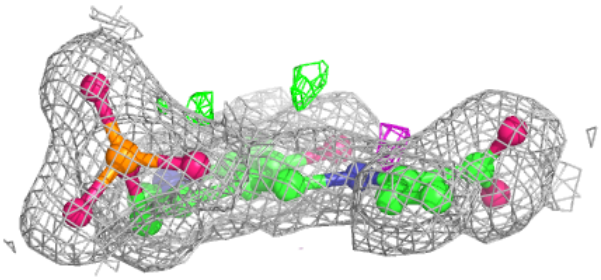


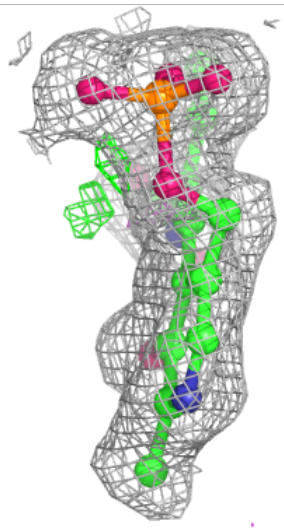


Electron density around WBJ P 501:

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

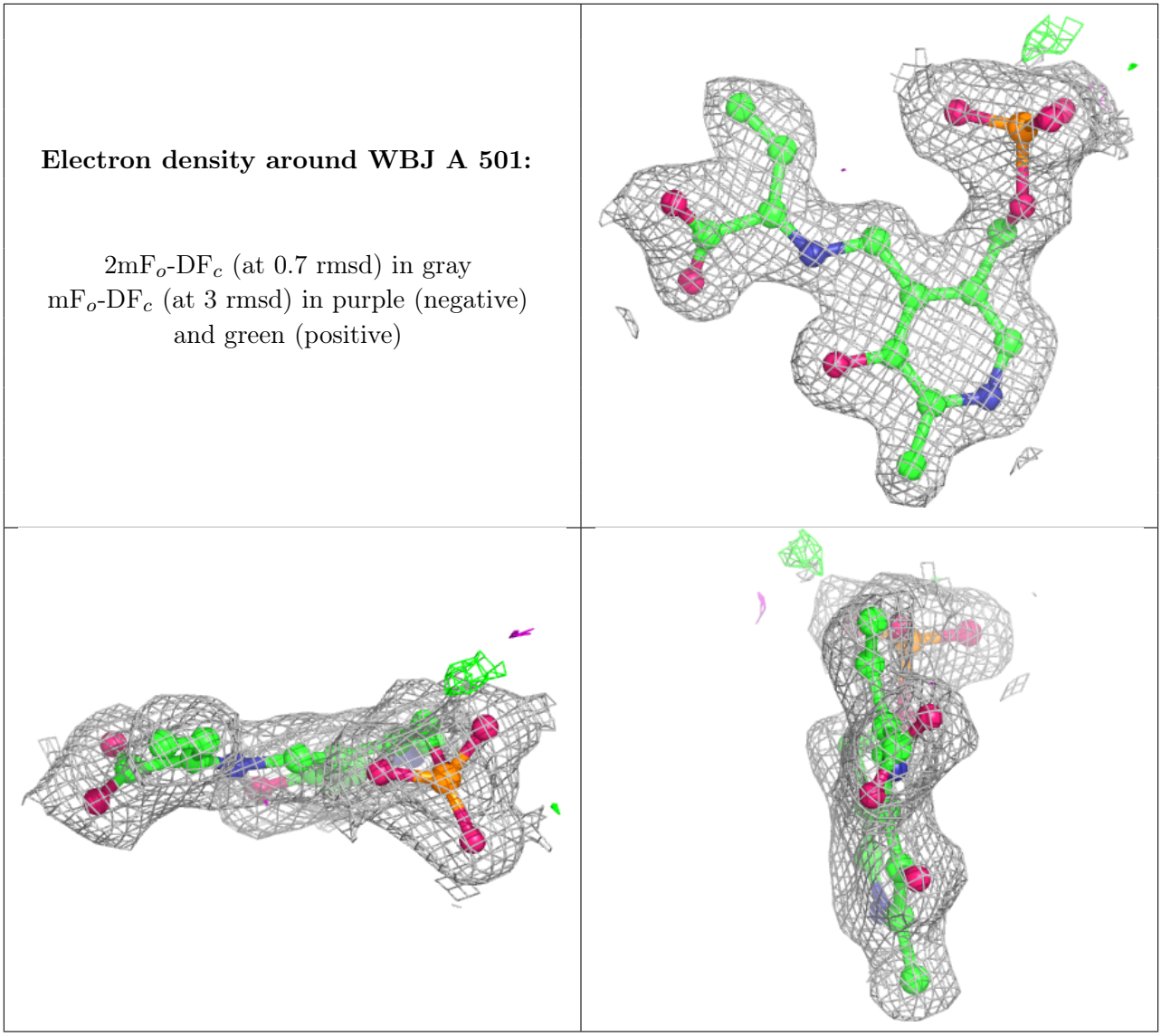






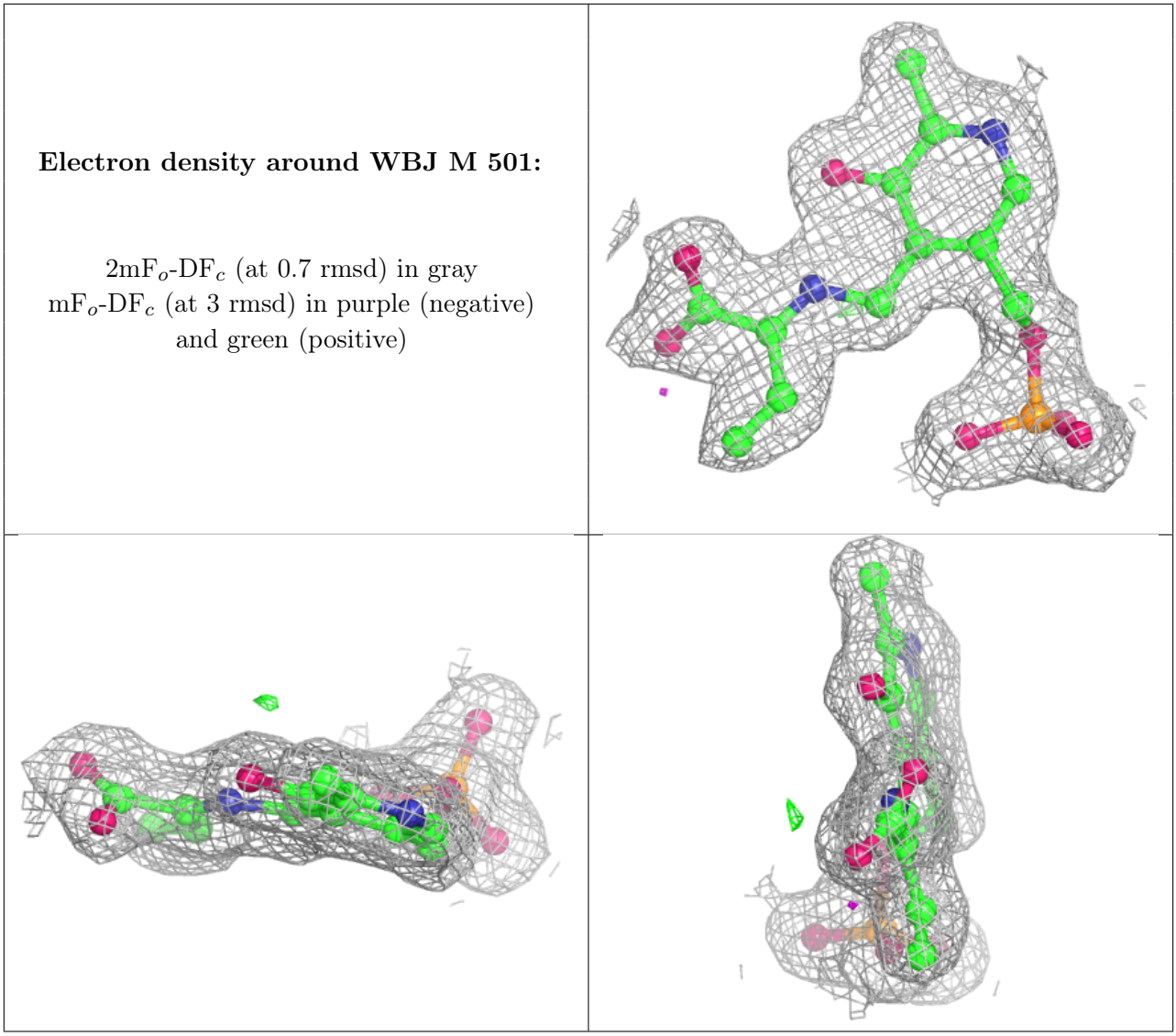
Electron density around WBJ A 501:

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



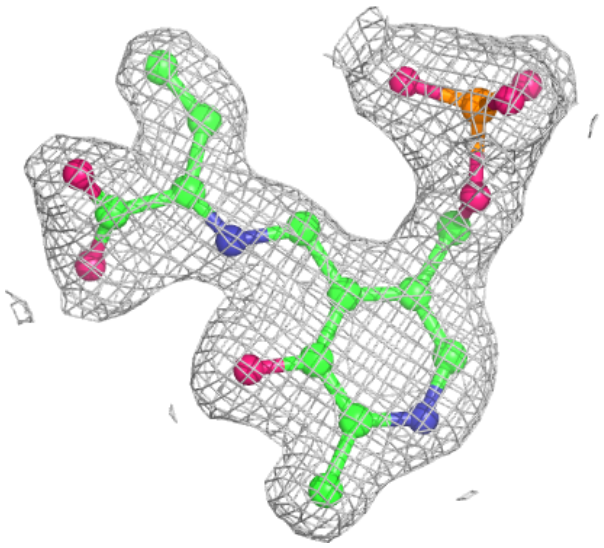
Electron density around WBJ M 501:

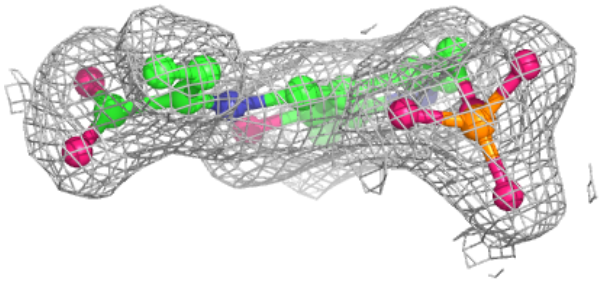
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

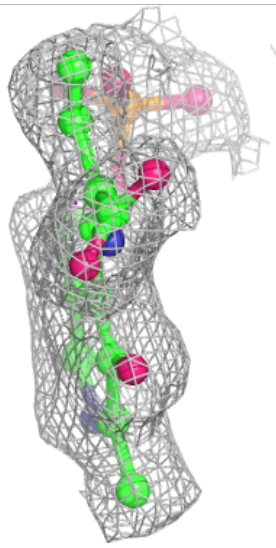


Electron density around WBJ Q 501:

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

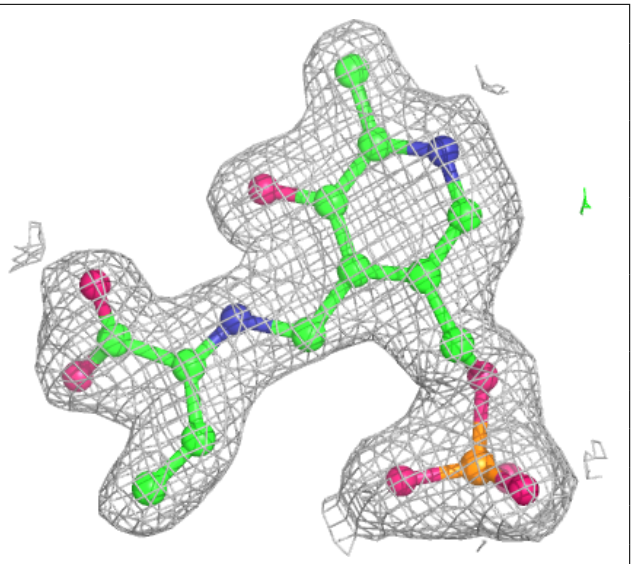


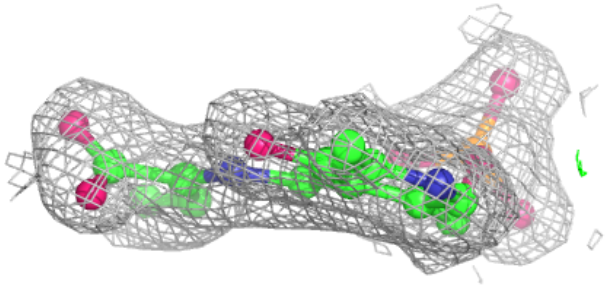


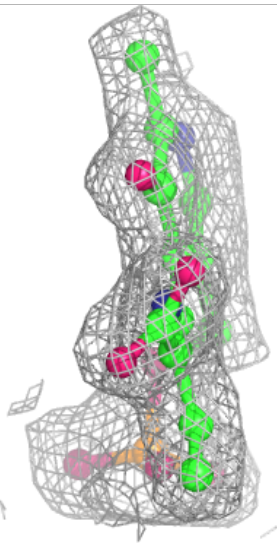


Electron density around WBJ N 501:

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

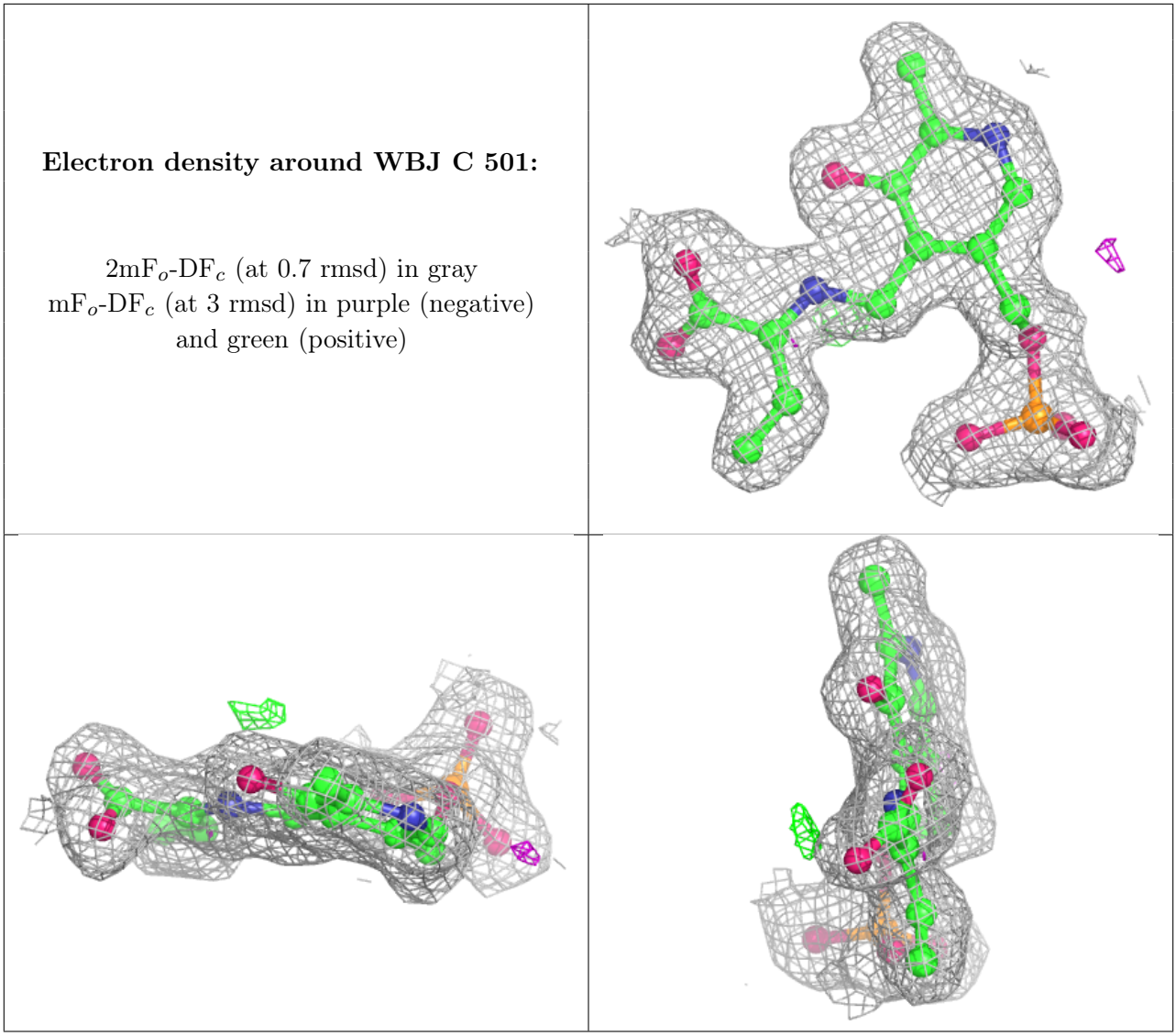






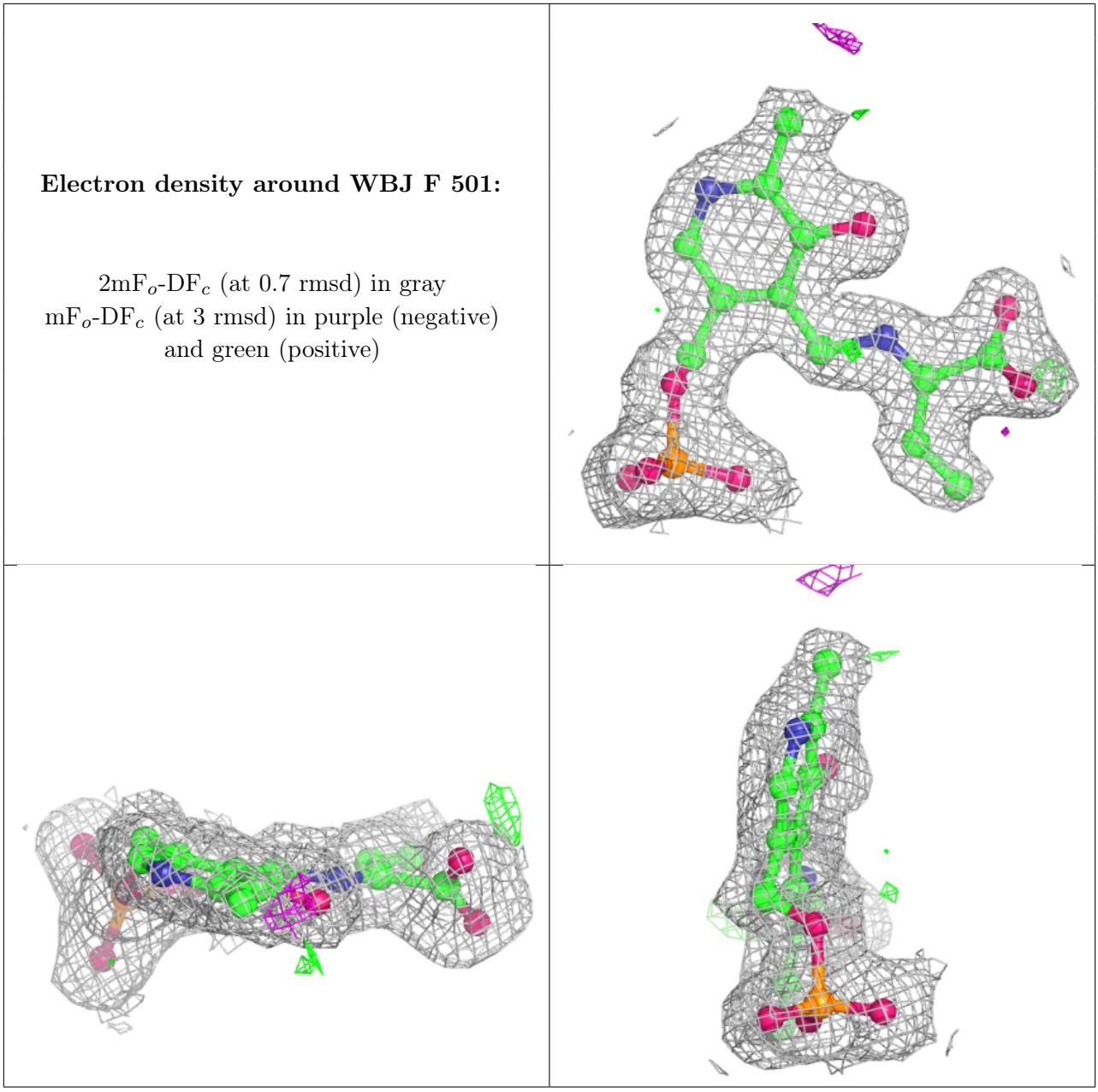
Electron density around WBJ C 501:

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



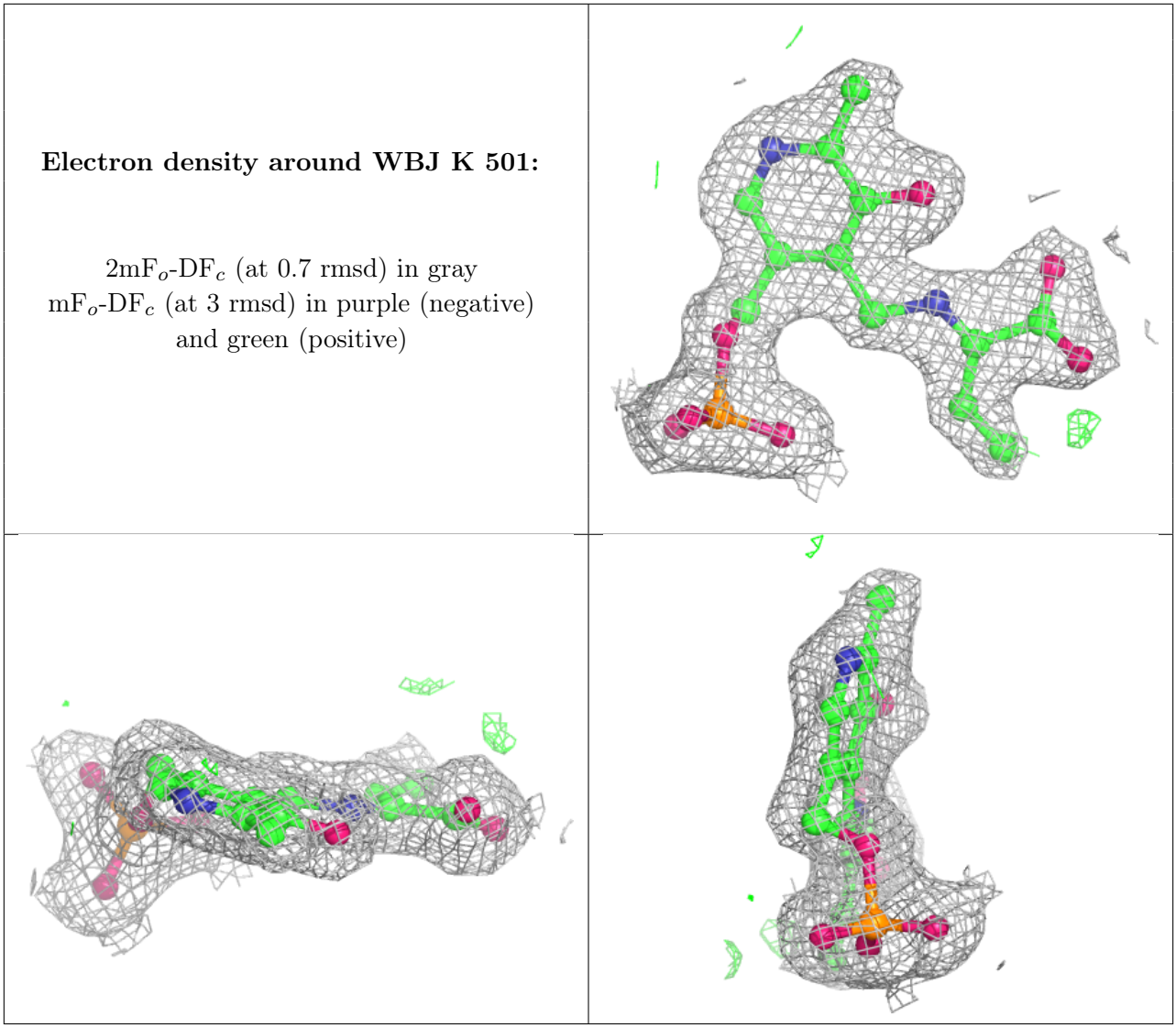
Electron density around WBJ F 501:

$2mF_o$-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 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.