



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:35 AM UTC

PDB ID : 8H6U / pdb_00008h6u
Title : Class I sesquiterpene synthase BCBOT2 (complex)
Authors : Lou, T.T.; Ma, M.
Deposited on : 2022-10-18
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

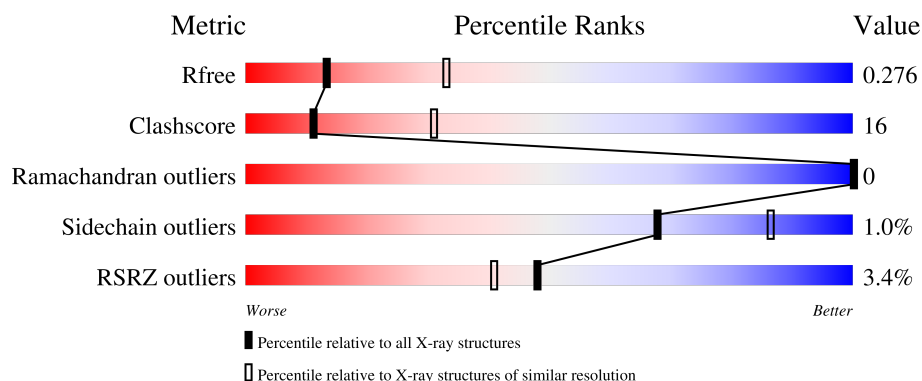
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	366	0% 70% 21% 8%
1	B	366	4% 68% 23% 8%
1	C	366	4% 66% 24% 8%
1	D	366	3% 61% 30% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11398 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 Presilphiperfolan-8-beta-ol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2719	1727	472	501	19			
1	B	337	Total	C	N	O	S	0	0	0
			2718	1727	472	500	19			
1	C	337	Total	C	N	O	S	0	0	0
			2718	1727	472	500	19			
1	D	337	Total	C	N	O	S	0	0	0
			2714	1724	471	500	19			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q6WP50
A	-4	SER	-	expression tag	UNP Q6WP50
A	-3	HIS	-	expression tag	UNP Q6WP50
A	-2	MET	-	expression tag	UNP Q6WP50
A	-1	ALA	-	expression tag	UNP Q6WP50
A	0	MET	-	expression tag	UNP Q6WP50
B	-5	GLY	-	expression tag	UNP Q6WP50
B	-4	SER	-	expression tag	UNP Q6WP50
B	-3	HIS	-	expression tag	UNP Q6WP50
B	-2	MET	-	expression tag	UNP Q6WP50
B	-1	ALA	-	expression tag	UNP Q6WP50
B	0	MET	-	expression tag	UNP Q6WP50
C	-5	GLY	-	expression tag	UNP Q6WP50
C	-4	SER	-	expression tag	UNP Q6WP50
C	-3	HIS	-	expression tag	UNP Q6WP50
C	-2	MET	-	expression tag	UNP Q6WP50
C	-1	ALA	-	expression tag	UNP Q6WP50
C	0	MET	-	expression tag	UNP Q6WP50
D	-5	GLY	-	expression tag	UNP Q6WP50
D	-4	SER	-	expression tag	UNP Q6WP50
D	-3	HIS	-	expression tag	UNP Q6WP50

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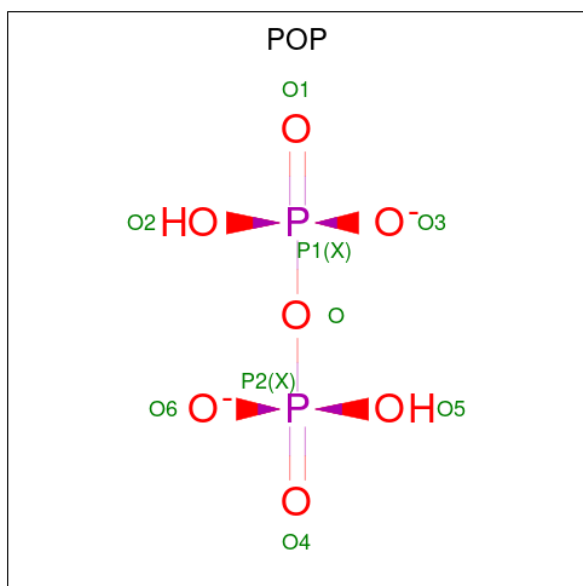
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP Q6WP50
D	-1	ALA	-	expression tag	UNP Q6WP50
D	0	MET	-	expression tag	UNP Q6WP50

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0
2	B	3	Total Mg 3 3	0	0
2	C	3	Total Mg 3 3	0	0
2	D	3	Total Mg 3 3	0	0

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂) (labeled as "Ligand of Interest" by depositor).



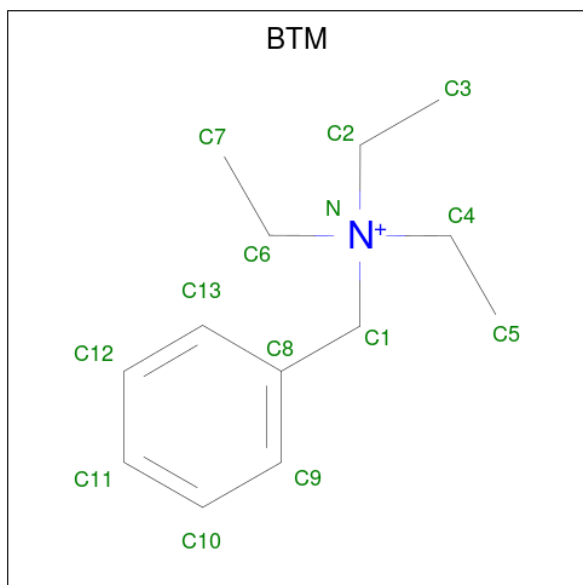
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	B	1	Total O P 9 7 2	0	0
3	C	1	Total O P 9 7 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is N-benzyl-N,N-diethylethanaminium (CCD ID: BTM) (formula: $C_{13}H_{22}N$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			14	13	1		
4	B	1	Total	C	N	0	0
			14	13	1		
4	C	1	Total	C	N	0	0
			14	13	1		
4	D	1	Total	C	N	0	0
			14	13	1		

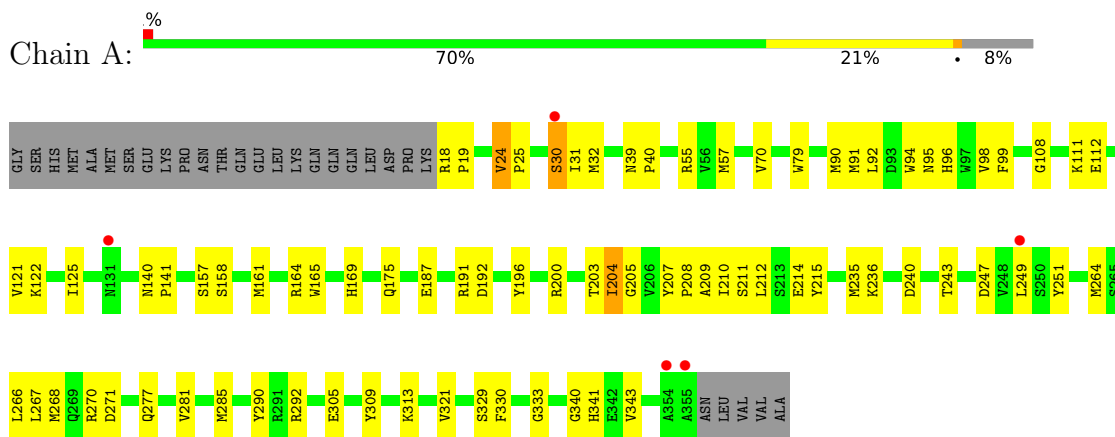
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	108	Total	O	0	0
			108	108		
5	C	104	Total	O	0	0
			104	104		
5	D	83	Total	O	0	0
			83	83		

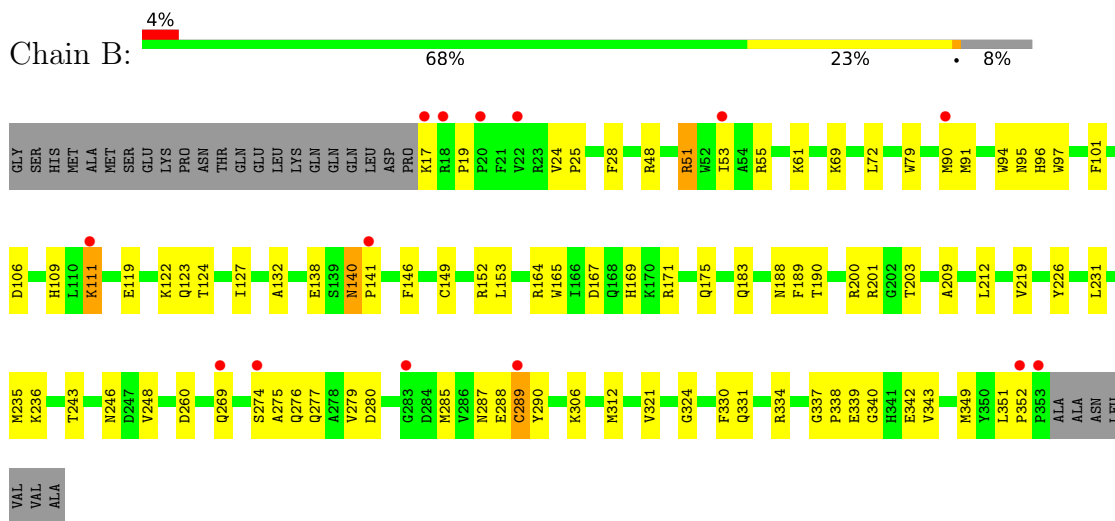
3 Residue-property plots [i](#)

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.

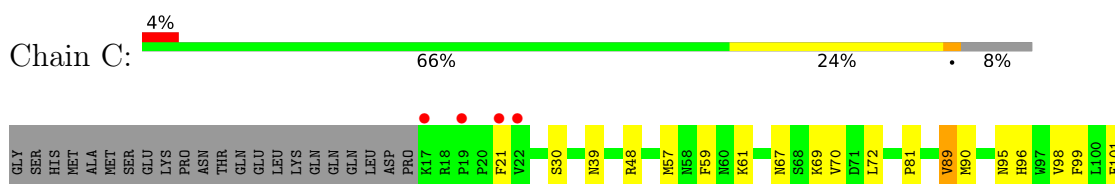
• Molecule 1: Presilphiperfolan-8-beta-ol synthase



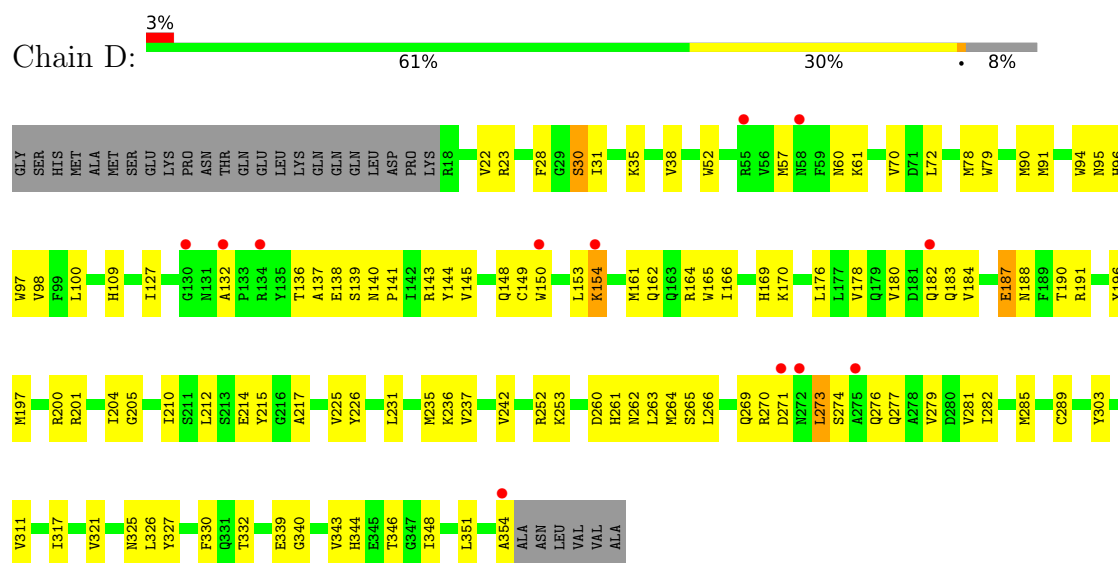
• Molecule 1: Presilphiperfolan-8-beta-ol synthase



• Molecule 1: Presilphiperfolan-8-beta-ol synthase



- Molecule 1: Presilphiperfolan-8-beta-ol synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.54Å 112.54Å 253.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.27 – 2.78 56.27 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.1 (56.27-2.78) 99.1 (56.27-2.78)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.215 , 0.271 0.224 , 0.276	Depositor DCC
R_{free} test set	2003 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11398	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BTM, POP, MG

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	0.60	1/2788 (0.0%)	0.74	8/3787 (0.2%)
1	B	0.58	3/2787 (0.1%)	0.68	7/3784 (0.2%)
1	C	0.61	3/2787 (0.1%)	0.74	8/3784 (0.2%)
1	D	0.66	1/2783 (0.0%)	0.68	7/3780 (0.2%)
All	All	0.61	8/11145 (0.1%)	0.71	30/15135 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	324	GLY	C-O	-6.04	1.16	1.23
1	D	23	ARG	C-O	-5.98	1.16	1.24
1	A	108	GLY	C-O	-5.83	1.18	1.23
1	B	219	VAL	C-O	-5.79	1.18	1.24
1	C	89	VAL	C-O	-5.57	1.17	1.24
1	C	248	VAL	C-O	-5.47	1.18	1.24
1	C	101	PHE	C-O	-5.39	1.17	1.24
1	B	122	LYS	C-O	-5.03	1.18	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	VAL	CA-C-N	10.74	130.85	119.78
1	A	24	VAL	C-N-CA	10.74	130.85	119.78
1	A	70	VAL	N-CA-C	-7.51	103.13	110.72
1	C	333	GLY	N-CA-C	-7.41	106.52	114.67
1	B	140	ASN	CA-C-N	7.15	128.78	119.84
1	B	140	ASN	C-N-CA	7.15	128.78	119.84
1	C	140	ASN	CA-C-N	6.93	126.45	119.24
1	C	140	ASN	C-N-CA	6.93	126.45	119.24
1	C	70	VAL	N-CA-C	-6.75	103.91	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	344	HIS	N-CA-C	-6.39	102.84	112.04
1	A	333	GLY	N-CA-C	-6.34	107.02	115.32
1	D	30	SER	CB-CA-C	-6.12	109.50	116.54
1	D	351	LEU	CA-C-N	6.03	126.59	120.38
1	D	351	LEU	C-N-CA	6.03	126.59	120.38
1	B	111	LYS	N-CA-C	6.00	117.82	111.28
1	A	140	ASN	CA-C-N	5.63	125.30	119.05
1	A	140	ASN	C-N-CA	5.63	125.30	119.05
1	B	109	HIS	N-CA-C	5.63	122.80	110.80
1	B	190	THR	N-CA-C	-5.59	106.13	113.12
1	C	30	SER	CB-CA-C	-5.54	110.17	116.54
1	C	332	THR	N-CA-C	5.51	118.06	110.35
1	D	109	HIS	N-CA-C	5.50	117.36	111.36
1	D	273	LEU	N-CA-C	5.41	119.04	109.96
1	A	30	SER	CB-CA-C	-5.33	110.41	116.54
1	D	344	HIS	N-CA-C	-5.32	105.93	112.90
1	A	341	HIS	N-CA-C	-5.30	105.58	111.36
1	D	214	GLU	N-CA-C	-5.27	105.53	111.28
1	C	138	GLU	N-CA-C	5.26	117.02	111.28
1	B	269	GLN	N-CA-C	5.12	117.60	111.71
1	B	289	CYS	N-CA-C	-5.01	105.52	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2719	0	2627	77	2
1	B	2718	0	2630	85	1
1	C	2718	0	2631	96	2
1	D	2714	0	2623	92	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	0	0	0
3	B	9	0	0	1	0
3	C	9	0	0	1	0
3	D	9	0	0	1	0
4	A	14	0	22	3	0
4	B	14	0	22	2	0
4	C	14	0	22	5	0
4	D	14	0	22	4	0
5	A	130	0	0	4	0
5	B	108	0	0	3	0
5	C	104	0	0	5	0
5	D	83	0	0	4	0
All	All	11398	0	10599	352	3

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 16.

All (352) 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:B:53:ILE:HD12	1:B:96:HIS:CG	1.74	1.21
1:A:249:LEU:CD1	1:A:329:SER:HB3	1.72	1.19
1:C:90:MET:HE3	1:C:215:TYR:CE2	1.77	1.18
1:B:153:LEU:CD1	1:B:165:TRP:CE3	2.28	1.15
1:B:53:ILE:CD1	1:B:96:HIS:CG	2.30	1.15
1:B:53:ILE:HD12	1:B:96:HIS:CB	1.79	1.12
1:B:48:ARG:HA	1:B:51:ARG:HH21	1.11	1.12
1:C:249:LEU:HD22	1:C:329:SER:HB3	1.29	1.08
1:A:249:LEU:HD13	1:A:329:SER:HB3	1.38	1.05
1:D:354:ALA:HB2	5:D:560:HOH:O	1.56	1.04
1:C:96:HIS:HD2	5:C:517:HOH:O	1.43	1.02
1:A:249:LEU:CD1	1:A:329:SER:CB	2.40	0.98
1:B:153:LEU:HD13	1:B:165:TRP:CD2	2.00	0.97
1:B:340:GLY:O	1:B:343:VAL:HG12	1.64	0.97
1:A:340:GLY:O	1:A:343:VAL:HG12	1.65	0.96
1:C:249:LEU:CD2	1:C:329:SER:HB3	1.96	0.96
1:D:136:THR:CG2	1:D:139:SER:H	1.78	0.96
1:B:53:ILE:HD12	1:B:96:HIS:HB3	1.44	0.95
1:D:197:MET:O	1:D:201:ARG:HG3	1.66	0.94
1:A:249:LEU:HD12	1:A:329:SER:HB3	1.45	0.94
1:D:340:GLY:O	1:D:343:VAL:HG12	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:CD1	1:B:96:HIS:HB3	1.98	0.92
1:C:150:TRP:CZ3	1:C:165:TRP:CD1	2.59	0.90
1:B:90:MET:SD	1:B:149:CYS:SG	2.71	0.89
1:D:330:PHE:CE2	1:D:343:VAL:HG13	2.08	0.89
1:B:48:ARG:CA	1:B:51:ARG:HH21	1.85	0.88
1:D:330:PHE:HE2	1:D:343:VAL:HG13	1.36	0.86
1:B:153:LEU:HD13	1:B:165:TRP:CE3	2.08	0.86
1:B:53:ILE:HD13	1:B:96:HIS:CD2	2.11	0.86
1:A:266:LEU:HD11	1:A:270:ARG:HD2	1.57	0.85
1:A:305:GLU:HG3	1:B:28:PHE:HB3	1.57	0.85
1:D:281:VAL:HG12	1:D:285:MET:HE2	1.60	0.84
1:B:153:LEU:HD11	1:B:165:TRP:CE3	2.12	0.83
1:D:136:THR:HG23	1:D:139:SER:H	1.43	0.82
1:B:106:ASP:O	1:B:111:LYS:HD3	1.79	0.81
1:B:25:PRO:HD3	1:B:279:VAL:HG22	1.62	0.81
1:C:150:TRP:HZ3	1:C:165:TRP:CD1	1.98	0.80
1:C:340:GLY:O	1:C:343:VAL:HG12	1.81	0.80
1:A:249:LEU:HD13	1:A:329:SER:CB	2.08	0.80
1:D:136:THR:HG22	1:D:139:SER:OG	1.82	0.79
1:A:249:LEU:HD12	1:A:329:SER:CB	2.09	0.79
1:B:53:ILE:HD13	1:B:96:HIS:CG	2.17	0.79
1:C:150:TRP:CZ3	1:C:165:TRP:HD1	2.00	0.77
1:C:150:TRP:CE3	1:C:165:TRP:CD1	2.75	0.75
1:B:153:LEU:HD12	1:B:165:TRP:CZ3	2.23	0.74
1:B:53:ILE:CD1	1:B:96:HIS:CB	2.53	0.73
1:B:53:ILE:CD1	1:B:96:HIS:CD2	2.69	0.73
1:D:162:GLN:O	1:D:166:ILE:HG13	1.88	0.73
1:A:205:GLY:C	1:A:208:PRO:HD2	2.13	0.73
1:A:207:TYR:N	1:A:208:PRO:HD2	2.04	0.73
1:C:249:LEU:HD22	1:C:329:SER:CB	2.15	0.73
1:A:305:GLU:HG3	1:B:28:PHE:CB	2.19	0.72
1:D:95:ASN:O	1:D:98:VAL:HG12	1.89	0.72
1:D:90:MET:HE3	1:D:212:LEU:HD11	1.70	0.72
1:D:90:MET:HE3	1:D:212:LEU:CD1	2.20	0.72
1:D:273:LEU:HA	1:D:277:GLN:HE21	1.55	0.71
1:A:330:PHE:CE2	1:A:343:VAL:HG13	2.25	0.71
1:B:17:LYS:O	1:B:275:ALA:HB2	1.89	0.71
1:B:153:LEU:CD1	1:B:165:TRP:CZ3	2.73	0.70
1:D:210:ILE:HD13	1:D:235:MET:HG2	1.72	0.70
1:D:91:MET:HG2	1:D:212:LEU:HG	1.74	0.70
1:C:95:ASN:HA	1:C:98:VAL:HG12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:TYR:OH	1:C:268:MET:HE1	1.92	0.70
1:C:90:MET:HE3	1:C:215:TYR:CD2	2.28	0.69
1:C:150:TRP:HE3	1:C:165:TRP:NE1	1.91	0.69
1:D:190:THR:O	1:D:270:ARG:NH1	2.25	0.69
1:D:136:THR:HG22	1:D:139:SER:H	1.58	0.68
1:D:90:MET:HG2	1:D:215:TYR:CE2	2.28	0.68
1:B:276:GLN:O	1:B:279:VAL:HG12	1.94	0.68
1:C:330:PHE:CE2	1:C:343:VAL:HG13	2.29	0.68
1:B:153:LEU:HD12	1:B:165:TRP:CE3	2.27	0.67
1:D:266:LEU:HD21	1:D:270:ARG:HD3	1.75	0.67
1:B:330:PHE:CE2	1:B:343:VAL:HG13	2.29	0.67
1:C:336:LEU:HB3	1:C:339:GLU:HG2	1.78	0.66
1:C:95:ASN:O	1:C:98:VAL:HG12	1.96	0.66
1:C:161:MET:HE3	1:C:220:ASN:HB3	1.79	0.65
1:D:346:THR:HB	1:D:348:ILE:HD12	1.79	0.64
1:B:90:MET:HE3	1:B:90:MET:C	2.22	0.64
1:A:30:SER:HB2	1:A:290:TYR:CD2	2.32	0.64
1:B:48:ARG:HA	1:B:51:ARG:NH2	1.97	0.63
1:C:161:MET:HE1	1:C:164:ARG:NH1	2.12	0.63
1:A:192:ASP:HB3	1:A:270:ARG:NH2	2.14	0.63
1:A:205:GLY:O	1:A:208:PRO:HG2	1.98	0.63
1:A:18:ARG:NH1	1:A:18:ARG:HB2	2.13	0.63
1:B:248:VAL:O	1:B:349:MET:HE1	1.99	0.63
1:B:53:ILE:HD11	1:B:96:HIS:HB3	1.82	0.62
1:D:262:ASN:OD1	1:D:264:MET:HB2	2.00	0.62
1:A:249:LEU:CD1	1:A:329:SER:HB2	2.26	0.61
1:C:137:ALA:O	1:C:141:PRO:HG3	1.99	0.61
1:C:150:TRP:HZ3	1:C:165:TRP:HD1	1.40	0.61
1:D:72:LEU:HD12	1:D:96:HIS:CD2	2.35	0.61
1:A:157:SER:HA	5:A:517:HOH:O	2.00	0.61
1:B:209:ALA:HB2	4:B:405:BTM:H12	1.81	0.61
1:B:90:MET:HG2	1:B:152:ARG:NE	2.16	0.61
1:C:111:LYS:HG3	5:C:551:HOH:O	1.99	0.61
1:A:192:ASP:HA	1:A:270:ARG:NE	2.16	0.61
1:C:252:ARG:NH1	1:C:339:GLU:OE2	2.31	0.61
1:D:178:VAL:O	1:D:182:GLN:HG3	2.00	0.60
1:D:94:TRP:CE3	1:D:212:LEU:HD22	2.37	0.60
1:D:79:TRP:CD1	1:D:321:VAL:HA	2.36	0.60
1:D:191:ARG:O	1:D:270:ARG:HD2	2.02	0.60
1:B:153:LEU:CD1	1:B:165:TRP:CD2	2.68	0.60
1:B:72:LEU:HD12	1:B:96:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:THR:HG23	1:D:138:GLU:N	2.17	0.59
1:C:164:ARG:HD3	1:C:226:TYR:CE2	2.38	0.59
1:D:277:GLN:O	1:D:281:VAL:HG23	2.02	0.59
1:B:25:PRO:CD	1:B:279:VAL:HG22	2.30	0.59
1:D:165:TRP:CE2	1:D:169:HIS:CE1	2.91	0.59
1:A:240:ASP:OD2	1:A:292:ARG:NH2	2.34	0.59
1:C:150:TRP:CE3	1:C:165:TRP:NE1	2.71	0.58
1:A:207:TYR:N	1:A:208:PRO:CD	2.65	0.58
1:D:330:PHE:CE2	1:D:343:VAL:CG1	2.86	0.58
1:A:18:ARG:HB3	1:A:19:PRO:HD3	1.84	0.58
1:B:175:GLN:HB3	1:B:203:THR:HG23	1.86	0.58
1:A:281:VAL:O	1:A:285:MET:HG3	2.04	0.58
1:B:331:GLN:NE2	5:B:503:HOH:O	2.34	0.58
1:B:330:PHE:HE2	1:B:343:VAL:HG13	1.69	0.57
1:C:332:THR:HG23	1:C:335:TYR:H	1.69	0.57
1:D:57:MET:HE2	1:D:100:LEU:HD22	1.85	0.57
1:A:30:SER:CB	1:A:290:TYR:CD2	2.87	0.57
1:D:164:ARG:HD3	1:D:226:TYR:CE2	2.40	0.57
1:A:79:TRP:CD1	1:A:321:VAL:HA	2.39	0.57
1:B:340:GLY:O	1:B:343:VAL:CG1	2.46	0.57
1:D:38:VAL:HG22	1:D:78:MET:HG2	1.86	0.57
1:D:90:MET:CG	1:D:215:TYR:CE2	2.88	0.57
1:C:106:ASP:O	1:C:111:LYS:HD3	2.04	0.57
1:A:330:PHE:HE2	1:A:343:VAL:HG13	1.68	0.56
1:B:340:GLY:C	1:B:343:VAL:HG12	2.30	0.56
1:A:90:MET:HE3	1:A:215:TYR:CE2	2.41	0.55
1:A:270:ARG:HG2	1:A:270:ARG:HH11	1.70	0.55
1:A:95:ASN:HA	1:A:98:VAL:HG12	1.87	0.55
1:D:276:GLN:O	1:D:279:VAL:HG12	2.06	0.55
1:D:282:ILE:HA	1:D:285:MET:HE3	1.87	0.55
1:B:164:ARG:HD3	1:B:226:TYR:CE2	2.42	0.55
1:C:330:PHE:CD2	1:C:343:VAL:HG13	2.42	0.55
1:A:330:PHE:CD2	1:A:343:VAL:HG13	2.42	0.54
1:C:248:VAL:HG12	1:C:249:LEU:HD12	1.89	0.54
1:D:263:LEU:HD21	1:D:285:MET:HE1	1.88	0.54
1:A:204:ILE:HG12	1:A:243:THR:CG2	2.37	0.54
1:B:246:ASN:HB2	5:B:533:HOH:O	2.07	0.54
1:D:266:LEU:CD2	1:D:270:ARG:HD3	2.37	0.54
1:C:209:ALA:HB2	4:C:405:BTM:H10	1.90	0.54
1:D:150:TRP:CE2	1:D:154:LYS:HG3	2.42	0.54
1:D:166:ILE:HG22	1:D:170:LYS:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LEU:HB3	1:C:339:GLU:CG	2.37	0.54
1:A:55:ARG:NH2	5:A:509:HOH:O	2.40	0.53
1:C:135:TYR:CD1	1:C:140:ASN:HB3	2.44	0.53
1:B:17:LYS:C	1:B:19:PRO:HD3	2.34	0.53
1:C:106:ASP:O	1:C:111:LYS:CD	2.57	0.53
1:A:111:LYS:HG3	1:A:112:GLU:HG3	1.91	0.52
1:B:48:ARG:CA	1:B:51:ARG:NH2	2.67	0.52
1:D:90:MET:HG2	1:D:215:TYR:CZ	2.45	0.52
1:C:90:MET:CE	1:C:215:TYR:CE2	2.71	0.52
1:B:79:TRP:CD1	1:B:321:VAL:HA	2.45	0.52
1:D:30:SER:OG	1:D:31:ILE:N	2.43	0.52
1:C:263:LEU:O	1:C:267:LEU:HG	2.09	0.52
1:D:200:ARG:NH1	5:D:501:HOH:O	2.42	0.52
1:B:51:ARG:HH11	1:B:55:ARG:HH12	1.56	0.52
1:B:183:GLN:OE1	1:B:188:ASN:ND2	2.31	0.52
1:C:95:ASN:HA	1:C:98:VAL:CG1	2.41	0.51
1:D:136:THR:HG23	1:D:139:SER:N	2.20	0.51
1:C:95:ASN:CA	1:C:98:VAL:HG12	2.40	0.51
1:C:264:MET:O	1:C:268:MET:HG3	2.11	0.51
1:D:226:TYR:OH	1:D:235:MET:HE1	2.11	0.51
1:D:136:THR:HG22	1:D:139:SER:CB	2.40	0.51
1:C:153:LEU:HG	1:C:165:TRP:CD2	2.46	0.51
1:D:97:TRP:HB2	1:D:145:VAL:HG12	1.92	0.51
1:A:18:ARG:HB2	1:A:18:ARG:CZ	2.39	0.51
1:C:330:PHE:HE2	1:C:343:VAL:HG13	1.76	0.51
1:B:90:MET:HG2	1:B:152:ARG:CZ	2.41	0.51
1:D:78:MET:HE1	1:D:327:TYR:HB2	1.93	0.51
1:A:209:ALA:HB2	4:A:405:BTM:H12	1.93	0.50
1:C:266:LEU:HD12	1:C:270:ARG:HB2	1.92	0.50
1:B:24:VAL:HG12	1:B:25:PRO:O	2.11	0.50
1:D:182:GLN:HA	1:D:187:GLU:HG3	1.93	0.50
1:A:264:MET:HE3	1:A:268:MET:HE2	1.94	0.50
1:C:72:LEU:HD12	1:C:96:HIS:ND1	2.27	0.50
1:C:110:LEU:HD13	1:C:117:ALA:HA	1.94	0.50
1:C:162:GLN:O	1:C:165:TRP:HB3	2.11	0.50
1:A:204:ILE:CG1	1:A:243:THR:HG22	2.41	0.50
1:C:249:LEU:HD21	1:C:330:PHE:CD1	2.47	0.50
1:A:277:GLN:O	1:A:281:VAL:HG23	2.12	0.50
1:C:249:LEU:HD23	1:C:329:SER:C	2.37	0.50
1:C:48:ARG:CZ	1:C:89:VAL:HG21	2.42	0.49
1:C:90:MET:HE3	1:C:215:TYR:CZ	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD11	1:A:96:HIS:CE1	2.47	0.49
1:B:106:ASP:O	1:B:111:LYS:CD	2.55	0.49
1:B:334:ARG:HH21	3:B:404:POP:P2	2.35	0.49
1:A:340:GLY:C	1:A:343:VAL:HG12	2.34	0.49
1:C:90:MET:HG2	1:C:152:ARG:CZ	2.43	0.49
1:D:237:VAL:HG13	1:D:289:CYS:HB3	1.94	0.49
1:A:204:ILE:HG12	1:A:243:THR:HG22	1.95	0.49
1:A:309:TYR:CZ	1:A:313:LYS:HE3	2.47	0.49
1:C:150:TRP:HE3	1:C:165:TRP:HE1	1.60	0.49
1:D:205:GLY:O	4:D:405:BTM:H10	2.12	0.49
1:A:205:GLY:O	1:A:208:PRO:HD2	2.12	0.48
1:D:153:LEU:HG	1:D:165:TRP:CE3	2.48	0.48
1:B:91:MET:HA	1:B:212:LEU:HD11	1.95	0.48
1:C:48:ARG:NH1	1:C:89:VAL:HG21	2.28	0.48
1:D:231:LEU:HD11	1:D:311:VAL:HG13	1.96	0.48
1:D:253:LYS:N	5:D:507:HOH:O	2.35	0.48
1:A:330:PHE:CD2	1:A:343:VAL:CG1	2.97	0.48
1:A:57:MET:SD	1:A:141:PRO:HB2	2.54	0.47
1:D:60:ASN:O	1:D:61:LYS:C	2.54	0.47
1:C:340:GLY:HA2	1:C:343:VAL:HG12	1.96	0.47
1:B:94:TRP:CE3	1:B:212:LEU:HD22	2.49	0.47
1:D:265:SER:O	1:D:269:GLN:HG2	2.14	0.47
1:C:204:ILE:O	4:C:405:BTM:H6	2.15	0.47
1:B:17:LYS:HA	1:B:275:ALA:H	1.79	0.47
1:A:31:ILE:HG13	1:A:32:MET:HE2	1.96	0.47
1:B:287:ASN:HA	1:B:290:TYR:CD2	2.49	0.47
1:D:150:TRP:CZ2	1:D:154:LYS:HD2	2.50	0.47
1:D:150:TRP:CZ2	1:D:154:LYS:CD	2.98	0.47
1:C:95:ASN:C	1:C:98:VAL:HG12	2.40	0.46
1:C:21:PHE:CD1	1:C:21:PHE:C	2.93	0.46
1:C:302:SER:OG	1:C:308:ASP:OD2	2.27	0.46
1:B:51:ARG:HH11	1:B:55:ARG:NH1	2.13	0.46
1:C:124:THR:HA	1:C:127:ILE:HD12	1.98	0.46
1:C:252:ARG:HH12	1:C:339:GLU:CD	2.23	0.46
1:D:176:LEU:O	1:D:180:VAL:HG23	2.15	0.46
1:C:98:VAL:HG13	1:C:99:PHE:CD1	2.50	0.46
4:D:405:BTM:H2	4:D:405:BTM:H7A	1.53	0.46
1:B:111:LYS:HE2	1:B:111:LYS:HB3	1.75	0.46
1:C:161:MET:HE3	1:C:220:ASN:CA	2.45	0.46
1:A:121:VAL:O	1:A:125:ILE:HG13	2.16	0.46
1:A:251:TYR:OH	1:A:268:MET:HE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:MET:O	1:A:268:MET:HG3	2.16	0.46
1:A:266:LEU:HD12	1:A:270:ARG:HB2	1.96	0.46
1:B:97:TRP:CD1	1:B:146:PHE:HB2	2.50	0.46
1:C:253:LYS:HB2	5:C:521:HOH:O	2.15	0.46
1:D:150:TRP:CZ2	1:D:154:LYS:HG3	2.51	0.46
1:B:91:MET:HG2	1:B:212:LEU:HG	1.98	0.45
1:C:277:GLN:O	1:C:281:VAL:HG23	2.16	0.45
1:A:161:MET:SD	1:A:164:ARG:NH1	2.89	0.45
1:C:136:THR:O	1:C:137:ALA:C	2.57	0.45
1:C:335:TYR:HB2	5:C:510:HOH:O	2.15	0.45
1:D:271:ASP:HB2	1:D:273:LEU:HG	1.98	0.45
1:A:196:TYR:CZ	1:A:200:ARG:HG3	2.52	0.45
1:C:99:PHE:HA	4:C:405:BTM:H5	1.98	0.45
1:D:70:VAL:O	1:D:332:THR:OG1	2.26	0.45
1:C:254:ASP:OD2	1:C:262:ASN:HB2	2.16	0.45
1:D:183:GLN:OE1	1:D:188:ASN:ND2	2.49	0.45
1:B:312:MET:HE2	1:B:312:MET:HA	1.98	0.45
1:A:264:MET:HE3	1:A:264:MET:HB3	1.83	0.45
1:B:189:PHE:CZ	1:B:260:ASP:HB3	2.52	0.45
1:A:32:MET:O	5:A:501:HOH:O	2.21	0.45
1:A:94:TRP:CE3	1:A:212:LEU:HD22	2.52	0.45
1:A:175:GLN:HB3	1:A:203:THR:HG23	1.99	0.45
1:C:99:PHE:CD1	4:C:405:BTM:H5B	2.52	0.45
3:D:404:POP:O	4:D:405:BTM:H6A	2.17	0.45
1:A:24:VAL:O	1:A:24:VAL:HG23	2.16	0.44
1:B:231:LEU:O	1:B:235:MET:HG3	2.17	0.44
1:D:22:VAL:CG1	1:D:279:VAL:HG11	2.47	0.44
1:D:217:ALA:HB3	1:D:317:ILE:HD11	1.99	0.44
1:D:252:ARG:NH1	1:D:339:GLU:OE1	2.50	0.44
1:A:165:TRP:CD1	1:A:165:TRP:C	2.95	0.44
1:A:330:PHE:CE2	1:A:343:VAL:CG1	3.00	0.44
1:C:95:ASN:O	1:C:98:VAL:CG1	2.64	0.44
1:B:165:TRP:CE2	1:B:169:HIS:CE1	3.06	0.44
1:C:286:VAL:O	1:C:289:CYS:HB2	2.16	0.44
1:D:136:THR:HG21	5:D:577:HOH:O	2.17	0.44
1:A:270:ARG:HG2	1:A:270:ARG:NH1	2.32	0.44
1:D:150:TRP:CZ2	1:D:154:LYS:CG	3.01	0.44
1:A:24:VAL:HA	1:A:25:PRO:HD2	1.60	0.44
1:C:264:MET:CE	1:C:279:VAL:HG13	2.47	0.44
1:D:127:ILE:HA	1:D:132:ALA:HB3	2.00	0.44
1:C:340:GLY:C	1:C:343:VAL:HG12	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:CZ	4:A:405:BTM:H1	2.53	0.44
1:A:165:TRP:CE2	1:A:169:HIS:CE1	3.05	0.44
1:A:204:ILE:HB	1:A:243:THR:HG22	2.00	0.44
1:B:201:ARG:CZ	1:B:236:LYS:HE3	2.47	0.44
1:D:141:PRO:O	1:D:144:TYR:HB3	2.18	0.44
1:C:21:PHE:CD1	1:C:21:PHE:O	2.71	0.43
1:B:119:GLU:O	1:B:123:GLN:HG2	2.17	0.43
1:B:53:ILE:HD12	1:B:96:HIS:ND1	2.26	0.43
1:B:140:ASN:HA	1:B:141:PRO:HD2	1.79	0.43
1:B:200:ARG:HB3	1:B:243:THR:HG21	2.00	0.43
1:D:136:THR:O	1:D:137:ALA:C	2.60	0.43
1:B:337:GLY:HA3	1:B:338:PRO:HD2	1.84	0.43
1:D:136:THR:HG23	1:D:138:GLU:H	1.81	0.43
1:D:236:LYS:HB2	1:D:236:LYS:HE2	1.83	0.43
1:A:211:SER:HA	1:A:214:GLU:OE1	2.18	0.43
1:C:39:ASN:HA	1:C:81:PRO:O	2.18	0.43
1:D:140:ASN:ND2	1:D:143:ARG:HG3	2.33	0.43
1:D:196:TYR:CZ	1:D:200:ARG:HG3	2.54	0.43
1:D:242:VAL:HG13	1:D:325:ASN:CG	2.43	0.43
1:C:96:HIS:CD2	5:C:517:HOH:O	2.33	0.43
1:C:339:GLU:O	1:C:339:GLU:HG3	2.15	0.43
1:D:346:THR:CB	1:D:348:ILE:HD12	2.45	0.43
1:B:91:MET:O	1:B:95:ASN:ND2	2.40	0.43
1:B:279:VAL:HG13	1:B:280:ASP:N	2.33	0.43
1:C:98:VAL:HG13	1:C:99:PHE:HD1	1.83	0.43
1:B:274:SER:HB3	1:B:277:GLN:HG3	2.00	0.43
1:D:274:SER:OG	1:D:277:GLN:HG2	2.19	0.42
1:C:334:ARG:HH21	3:C:404:POP:P1	2.42	0.42
1:D:225:VAL:HG13	1:D:303:TYR:CE1	2.54	0.42
1:B:351:LEU:HB3	1:B:352:PRO:HD2	2.01	0.42
1:D:90:MET:HE1	1:D:149:CYS:HB3	2.00	0.42
1:D:144:TYR:O	1:D:148:GLN:HG2	2.18	0.42
1:B:167:ASP:O	1:B:171:ARG:HG3	2.19	0.42
1:B:306:LYS:HA	1:B:306:LYS:HD3	1.70	0.42
1:D:188:ASN:ND2	1:D:260:ASP:HB2	2.34	0.42
1:C:128:MET:HA	1:C:150:TRP:CE2	2.55	0.42
1:C:342:GLU:O	1:C:346:THR:HG23	2.18	0.42
1:A:39:ASN:HA	1:A:40:PRO:HD2	1.94	0.42
1:A:200:ARG:O	1:A:204:ILE:HB	2.20	0.42
4:B:405:BTM:H4	4:B:405:BTM:C13	2.49	0.42
1:C:273:LEU:HD13	1:C:277:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:SER:O	1:B:275:ALA:C	2.62	0.42
1:B:339:GLU:HA	1:B:342:GLU:OE2	2.19	0.42
1:B:124:THR:HA	1:B:127:ILE:HD12	2.02	0.42
1:C:161:MET:HE3	1:C:220:ASN:CB	2.46	0.42
1:D:150:TRP:NE1	1:D:154:LYS:HD3	2.35	0.42
1:B:51:ARG:HD2	1:B:55:ARG:NH1	2.35	0.42
1:A:91:MET:HG2	1:A:212:LEU:HG	2.01	0.42
1:C:98:VAL:O	1:C:102:ASP:HB2	2.19	0.42
1:C:300:LEU:HD21	1:C:311:VAL:HG11	2.02	0.42
1:D:52:TRP:CH2	1:D:145:VAL:HG22	2.55	0.42
1:C:230:SER:OG	1:C:296:ALA:O	2.32	0.41
1:C:21:PHE:HB3	1:C:350:TYR:CD1	2.55	0.41
1:C:249:LEU:HD23	1:C:329:SER:O	2.20	0.41
1:C:306:LYS:HA	1:C:306:LYS:HD3	1.74	0.41
1:C:161:MET:HE3	1:C:220:ASN:HA	2.02	0.41
1:A:18:ARG:HB3	1:A:19:PRO:CD	2.50	0.41
1:D:57:MET:SD	1:D:141:PRO:HB2	2.61	0.41
1:A:187:GLU:O	1:A:191:ARG:HG2	2.20	0.41
1:D:28:PHE:CD2	1:D:326:LEU:HD21	2.55	0.41
1:A:158:SER:N	5:A:517:HOH:O	2.47	0.41
1:A:210:ILE:HD13	1:A:235:MET:HG2	2.03	0.41
1:B:97:TRP:O	1:B:101:PHE:N	2.45	0.41
1:D:90:MET:O	1:D:90:MET:SD	2.79	0.41
4:D:405:BTM:H3B	4:D:405:BTM:H1A	1.85	0.41
1:C:57:MET:HB2	1:C:59:PHE:CE1	2.56	0.41
1:C:67:ASN:HD21	1:C:96:HIS:CE1	2.39	0.41
1:D:188:ASN:OD1	1:D:261:HIS:HE1	2.04	0.41
1:B:138:GLU:OE2	1:B:138:GLU:N	2.51	0.41
1:C:99:PHE:CZ	4:C:405:BTM:H1	2.56	0.41
1:D:204:ILE:HD12	1:D:204:ILE:HA	1.96	0.41
1:B:61:LYS:CD	5:B:555:HOH:O	2.69	0.41
1:C:204:ILE:HG23	1:C:206:VAL:HG23	2.03	0.41
1:C:225:VAL:HG13	1:C:303:TYR:CE2	2.56	0.41
1:A:267:LEU:O	1:A:271:ASP:O	2.39	0.40
1:B:285:MET:O	1:B:289:CYS:SG	2.65	0.40
1:C:161:MET:HE1	1:C:164:ARG:CZ	2.51	0.40
1:C:183:GLN:OE1	1:C:188:ASN:ND2	2.49	0.40
1:A:94:TRP:HZ2	1:A:208:PRO:HB2	1.87	0.40
1:D:161:MET:HE3	1:D:161:MET:HB3	1.88	0.40
1:A:204:ILE:O	4:A:405:BTM:H4	2.21	0.40
1:A:247:ASP:O	1:A:251:TYR:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLU:O	1:B:288:GLU:HG3	2.21	0.40
1:C:206:VAL:HG21	1:C:239:ALA:HA	2.04	0.40
1:D:180:VAL:O	1:D:184:VAL:HG23	2.20	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LYS:NZ	1:C:256:GLU:O[3_544]	1.78	0.42
1:C:134:ARG:NH1	1:D:138:GLU:OE1[5_544]	1.99	0.21
1:A:55:ARG:NH1	1:B:132:ALA:O[5_544]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/366 (92%)	320 (95%)	16 (5%)	0	100	100
1	B	335/366 (92%)	324 (97%)	11 (3%)	0	100	100
1	C	335/366 (92%)	318 (95%)	17 (5%)	0	100	100
1	D	335/366 (92%)	320 (96%)	15 (4%)	0	100	100
All	All	1341/1464 (92%)	1282 (96%)	59 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/314 (92%)	287 (99%)	2 (1%)	76	90
1	B	290/314 (92%)	288 (99%)	2 (1%)	76	90
1	C	290/314 (92%)	285 (98%)	5 (2%)	53	80
1	D	289/314 (92%)	286 (99%)	3 (1%)	68	86
All	All	1158/1256 (92%)	1146 (99%)	12 (1%)	68	86

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

Mol	Chain	Res	Type
1	A	204	ILE
1	A	236	LYS
1	B	51	ARG
1	B	69	LYS
1	C	61	LYS
1	C	69	LYS
1	C	159	GLN
1	C	220	ASN
1	C	339	GLU
1	D	35	LYS
1	D	154	LYS
1	D	187	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	96	HIS
1	A	175	GLN
1	A	220	ASN
1	A	224	HIS
1	A	287	ASN
1	A	323	GLN
1	A	341	HIS
1	B	41	ASN
1	B	67	ASN
1	B	96	HIS
1	C	96	HIS
1	C	287	ASN

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Mol	Chain	Res	Type
1	C	331	GLN
1	C	341	HIS
1	C	344	HIS
1	D	67	ASN
1	D	96	HIS
1	D	148	GLN
1	D	175	GLN
1	D	277	GLN
1	D	287	ASN
1	D	341	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	POP	B	404	2	6,8,8	0.71	0	12,13,13	0.78	0
4	BTM	D	405	-	14,14,14	1.09	1 (7%)	18,18,18	0.81	1 (5%)
4	BTM	A	405	-	14,14,14	0.95	1 (7%)	18,18,18	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POP	A	404	2	6,8,8	0.85	0	12,13,13	1.12	1 (8%)
3	POP	C	404	2	6,8,8	0.62	0	12,13,13	0.83	0
3	POP	D	404	2	6,8,8	0.69	0	12,13,13	0.76	0
4	BTM	B	405	-	14,14,14	0.91	1 (7%)	18,18,18	0.79	0
4	BTM	C	405	-	14,14,14	1.25	1 (7%)	18,18,18	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POP	B	404	2	-	0/6/6/6	-
4	BTM	D	405	-	-	9/14/14/14	0/1/1/1
4	BTM	A	405	-	-	0/14/14/14	0/1/1/1
3	POP	A	404	2	-	0/6/6/6	-
3	POP	C	404	2	-	0/6/6/6	-
3	POP	D	404	2	-	0/6/6/6	-
4	BTM	B	405	-	-	3/14/14/14	0/1/1/1
4	BTM	C	405	-	-	9/14/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	405	BTM	C1-C8	3.62	1.59	1.51
4	D	405	BTM	C1-C8	3.01	1.58	1.51
4	B	405	BTM	C1-C8	2.37	1.56	1.51
4	A	405	BTM	C1-C8	2.32	1.56	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	POP	O5-P2-O	2.91	114.38	104.64
4	D	405	BTM	C8-C1-N	2.35	119.28	115.56

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	405	BTM	C8-C1-N-C2

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Mol	Chain	Res	Type	Atoms
4	C	405	BTM	C3-C2-N-C6
4	D	405	BTM	C3-C2-N-C1
4	C	405	BTM	C7-C6-N-C2
4	D	405	BTM	C8-C1-N-C6
4	C	405	BTM	C7-C6-N-C4
4	C	405	BTM	C3-C2-N-C1
4	C	405	BTM	C7-C6-N-C1
4	D	405	BTM	C8-C1-N-C4
4	C	405	BTM	C3-C2-N-C4
4	D	405	BTM	C5-C4-N-C2
4	D	405	BTM	C3-C2-N-C6
4	D	405	BTM	C3-C2-N-C4
4	D	405	BTM	C5-C4-N-C6
4	C	405	BTM	C5-C4-N-C2
4	D	405	BTM	C5-C4-N-C1
4	B	405	BTM	C3-C2-N-C1
4	C	405	BTM	C5-C4-N-C1
4	C	405	BTM	C5-C4-N-C6
4	B	405	BTM	C3-C2-N-C4
4	B	405	BTM	C3-C2-N-C6

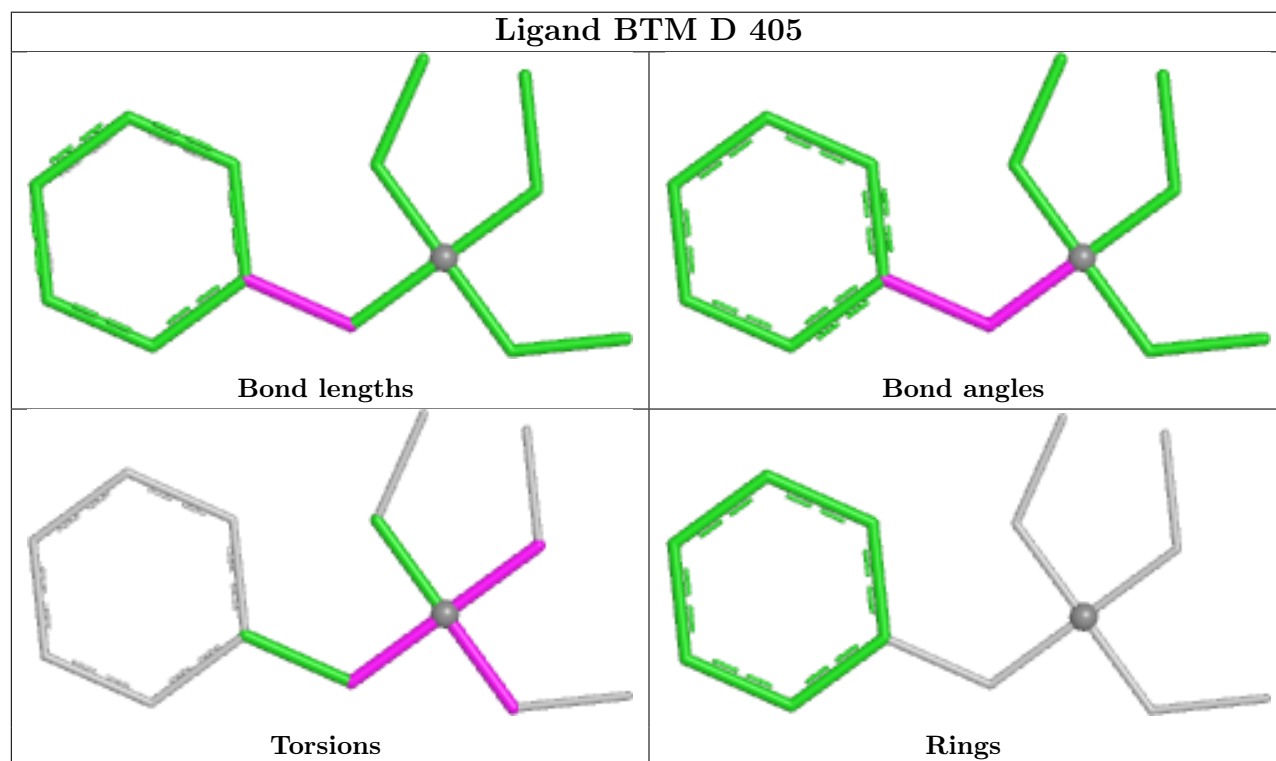
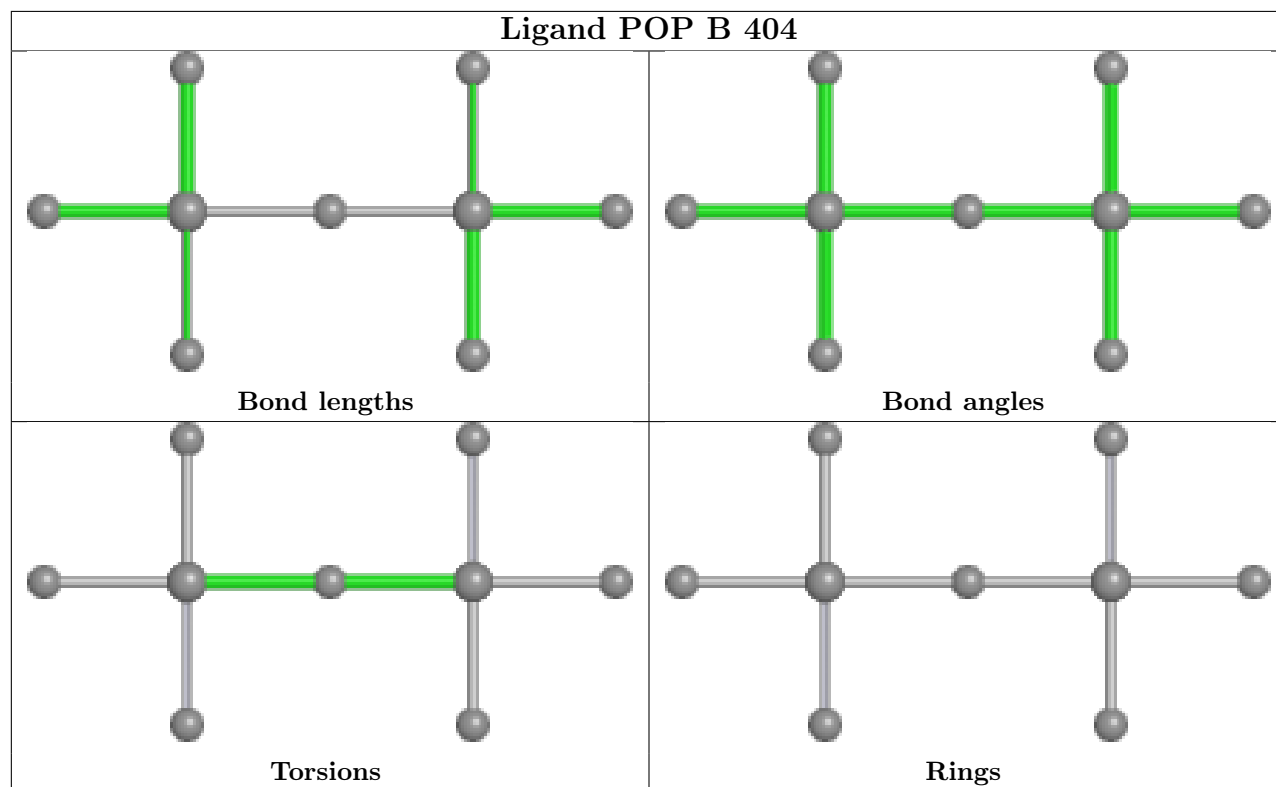
There are no ring outliers.

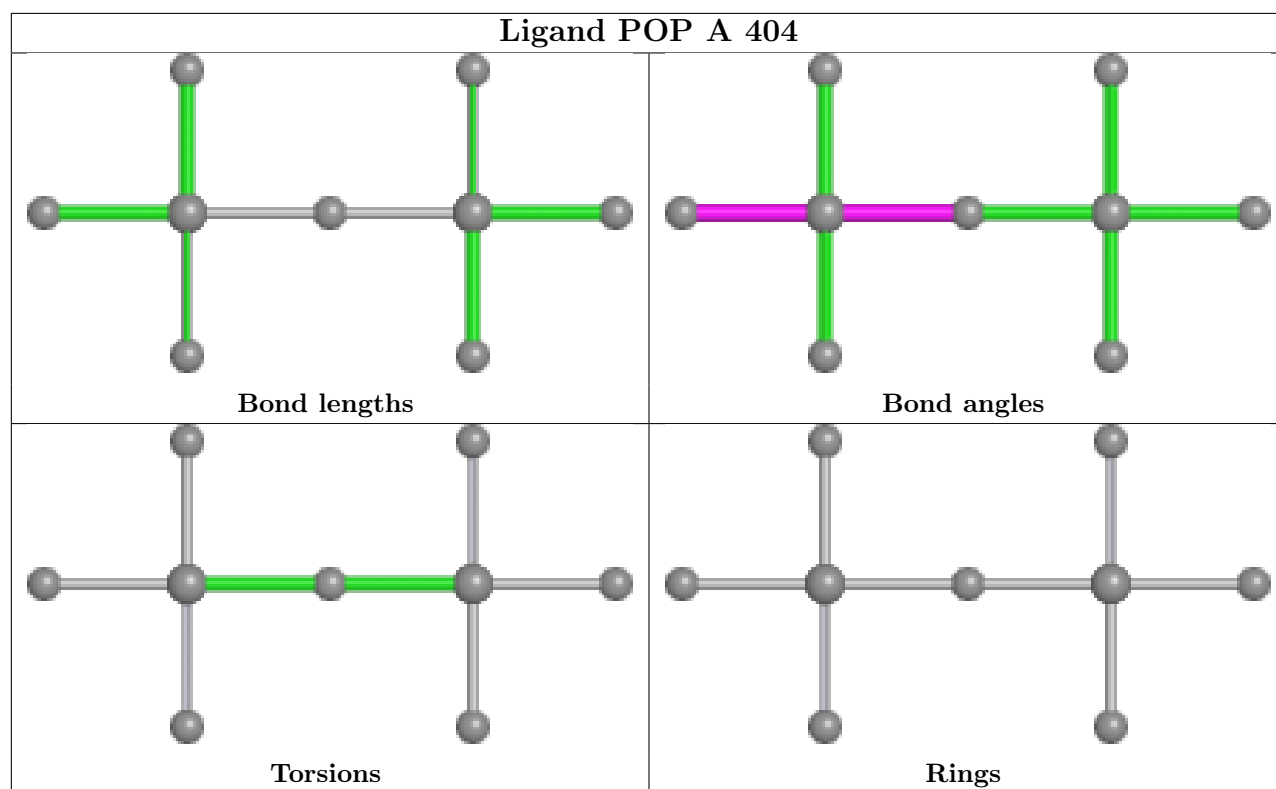
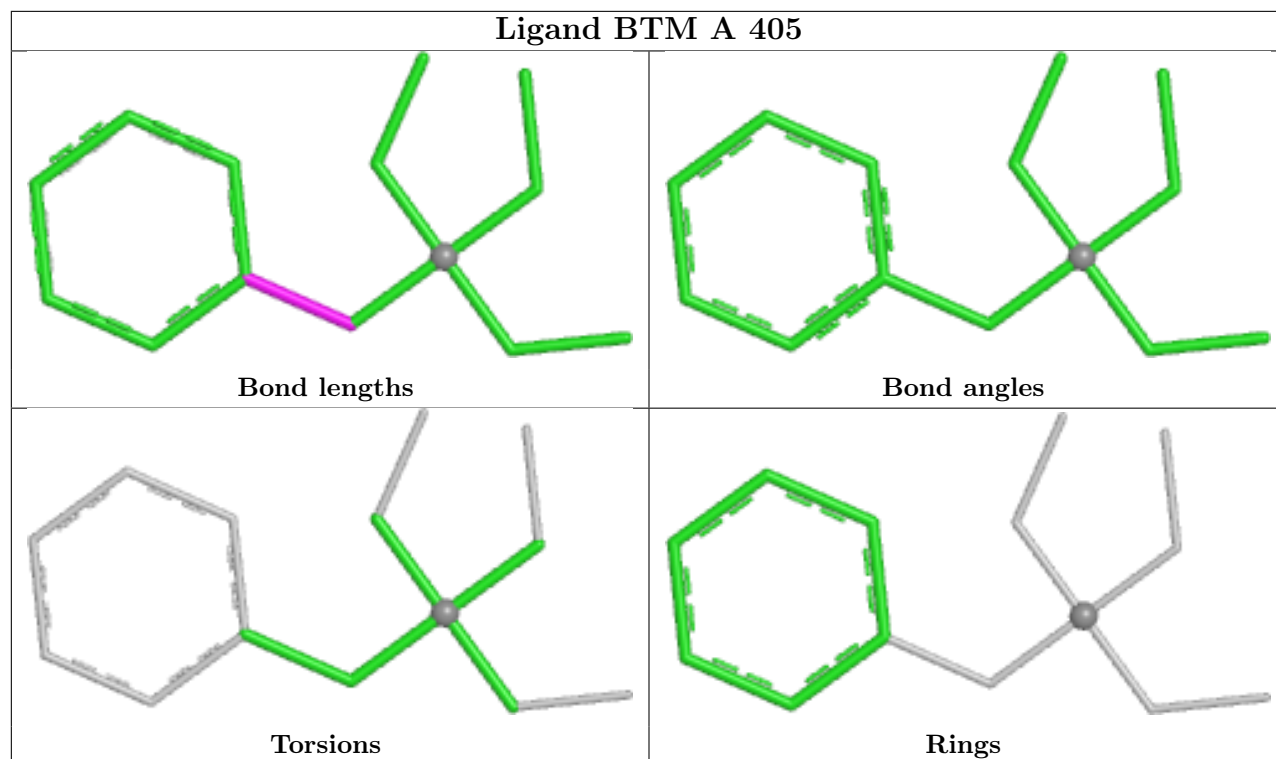
7 monomers are involved in 16 short contacts:

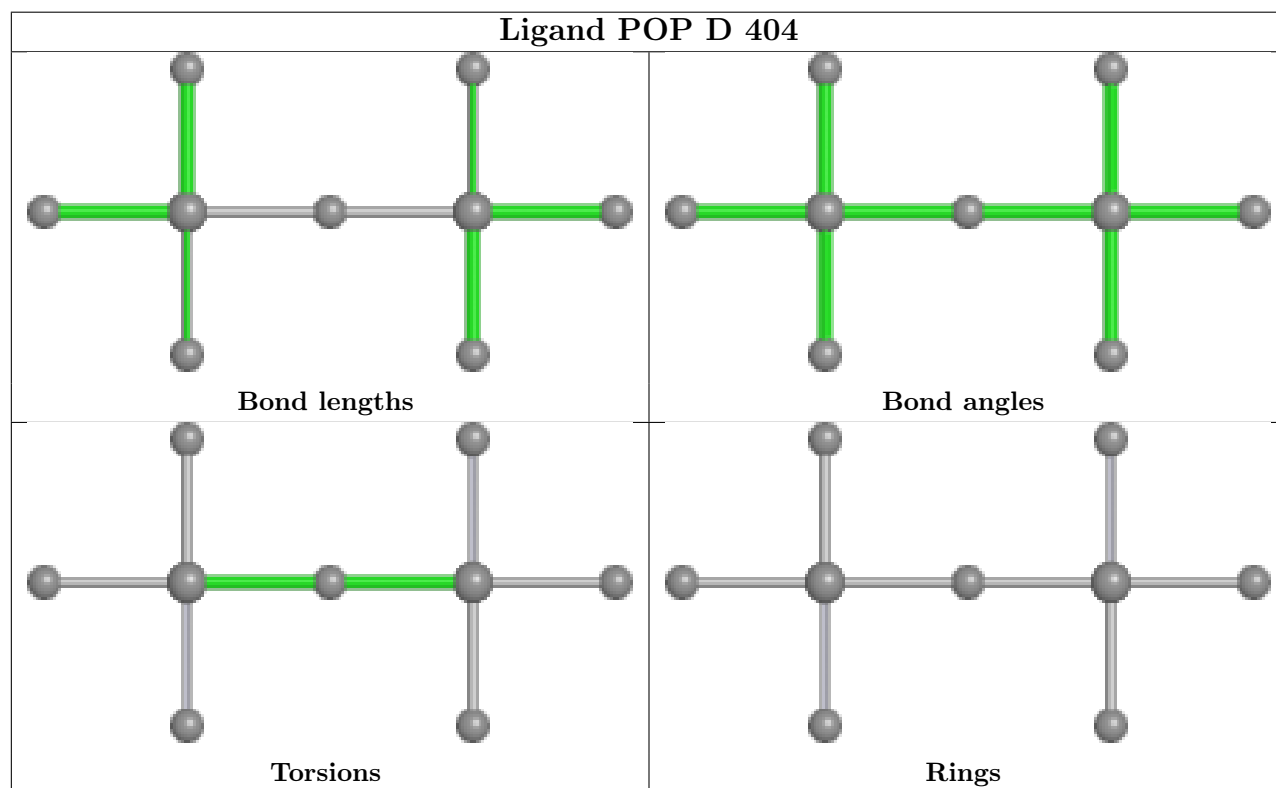
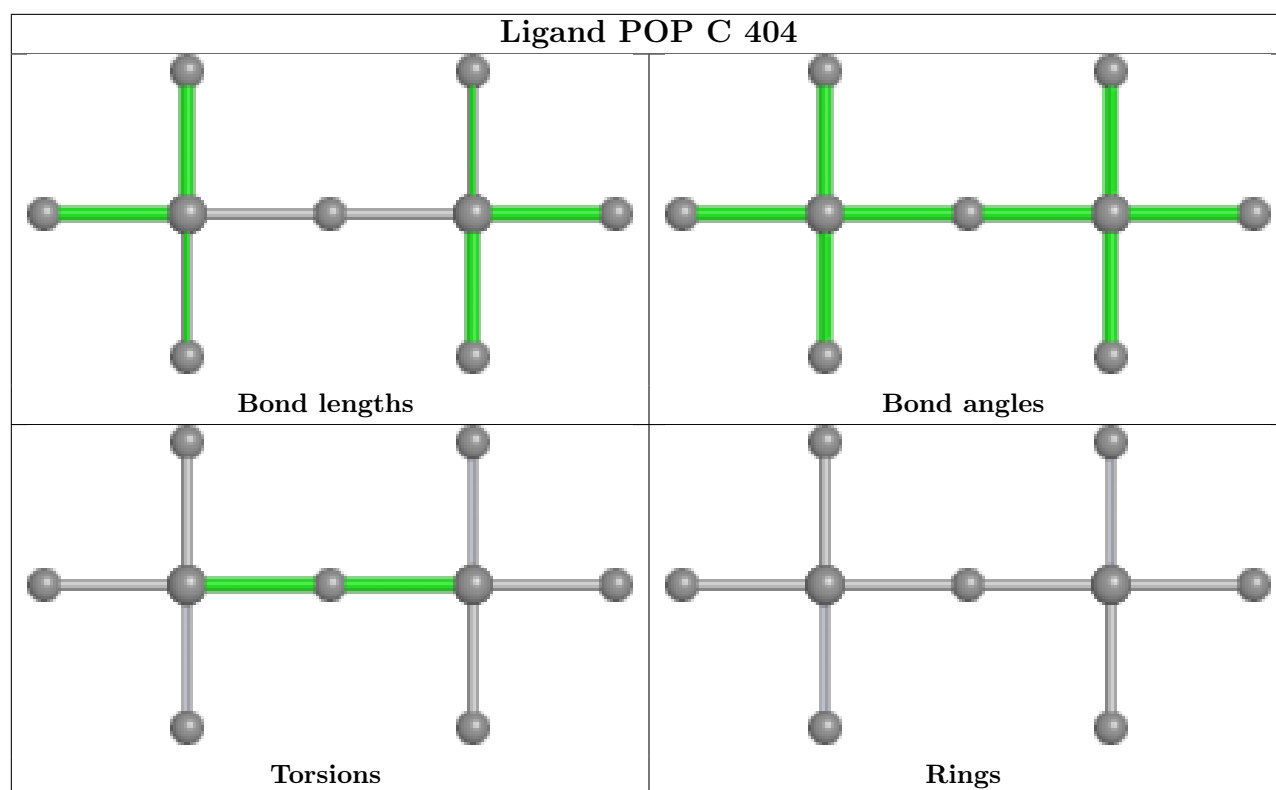
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	POP	1	0
4	D	405	BTM	4	0
4	A	405	BTM	3	0
3	C	404	POP	1	0
3	D	404	POP	1	0
4	B	405	BTM	2	0
4	C	405	BTM	5	0

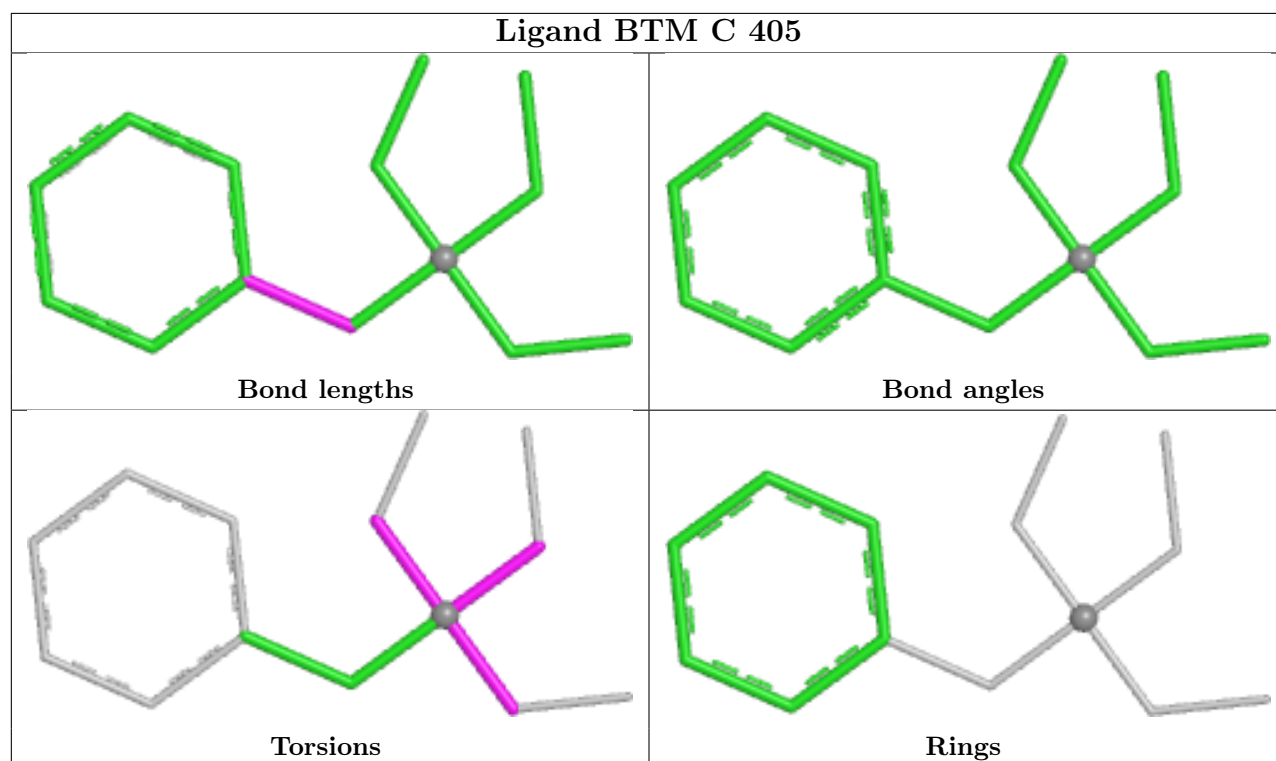
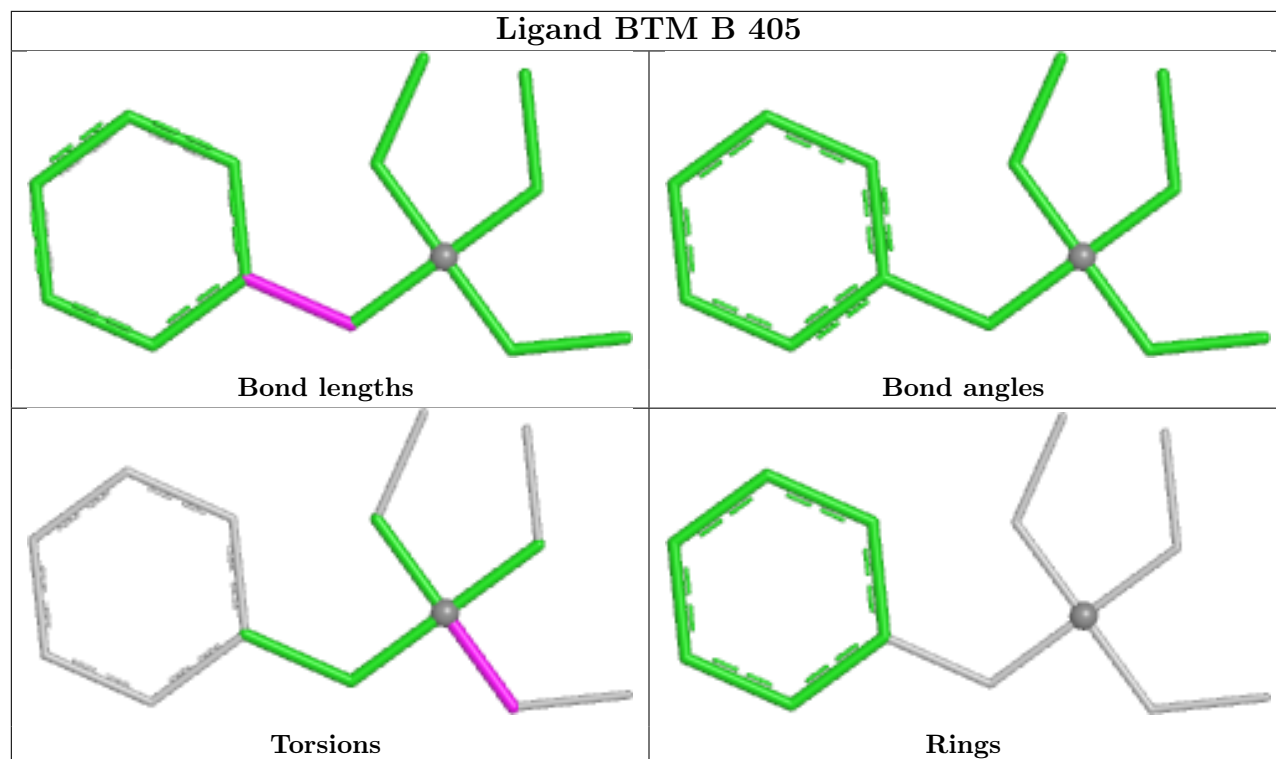
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/366 (92%)	0.17	5 (1%) 72 65	19, 29, 41, 68	0
1	B	337/366 (92%)	0.31	14 (4%) 40 34	20, 31, 51, 75	0
1	C	337/366 (92%)	0.30	15 (4%) 38 32	18, 29, 50, 73	0
1	D	337/366 (92%)	0.45	12 (3%) 46 39	23, 35, 55, 76	0
All	All	1349/1464 (92%)	0.31	46 (3%) 48 41	18, 31, 51, 76	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	272	ASN	5.9
1	D	354	ALA	4.0
1	B	17	LYS	4.0
1	B	90	MET	3.8
1	A	355	ALA	3.7
1	D	130	GLY	3.7
1	D	272	ASN	3.6
1	B	353	PRO	3.6
1	C	21	PHE	3.6
1	C	353	PRO	3.3
1	B	141	PRO	3.2
1	B	111	LYS	3.1
1	C	138	GLU	3.0
1	C	277	GLN	3.0
1	C	102	ASP	2.9
1	D	132	ALA	2.9
1	C	341	HIS	2.9
1	D	134	ARG	2.8
1	C	111	LYS	2.7
1	B	53	ILE	2.6
1	B	274	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	271	ASP	2.5
1	A	354	ALA	2.5
1	B	289	CYS	2.5
1	B	18	ARG	2.5
1	B	283	GLY	2.4
1	A	30	SER	2.3
1	B	269	GLN	2.3
1	D	154	LYS	2.2
1	C	165	TRP	2.2
1	C	349	MET	2.2
1	B	352	PRO	2.2
1	D	150	TRP	2.2
1	A	131	ASN	2.2
1	D	275	ALA	2.1
1	D	55	ARG	2.1
1	C	109	HIS	2.1
1	A	249	LEU	2.1
1	D	58	ASN	2.1
1	C	22	VAL	2.1
1	B	20	PRO	2.1
1	D	182	GLN	2.1
1	C	17	LYS	2.0
1	C	19	PRO	2.0
1	B	22	VAL	2.0
1	C	278	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

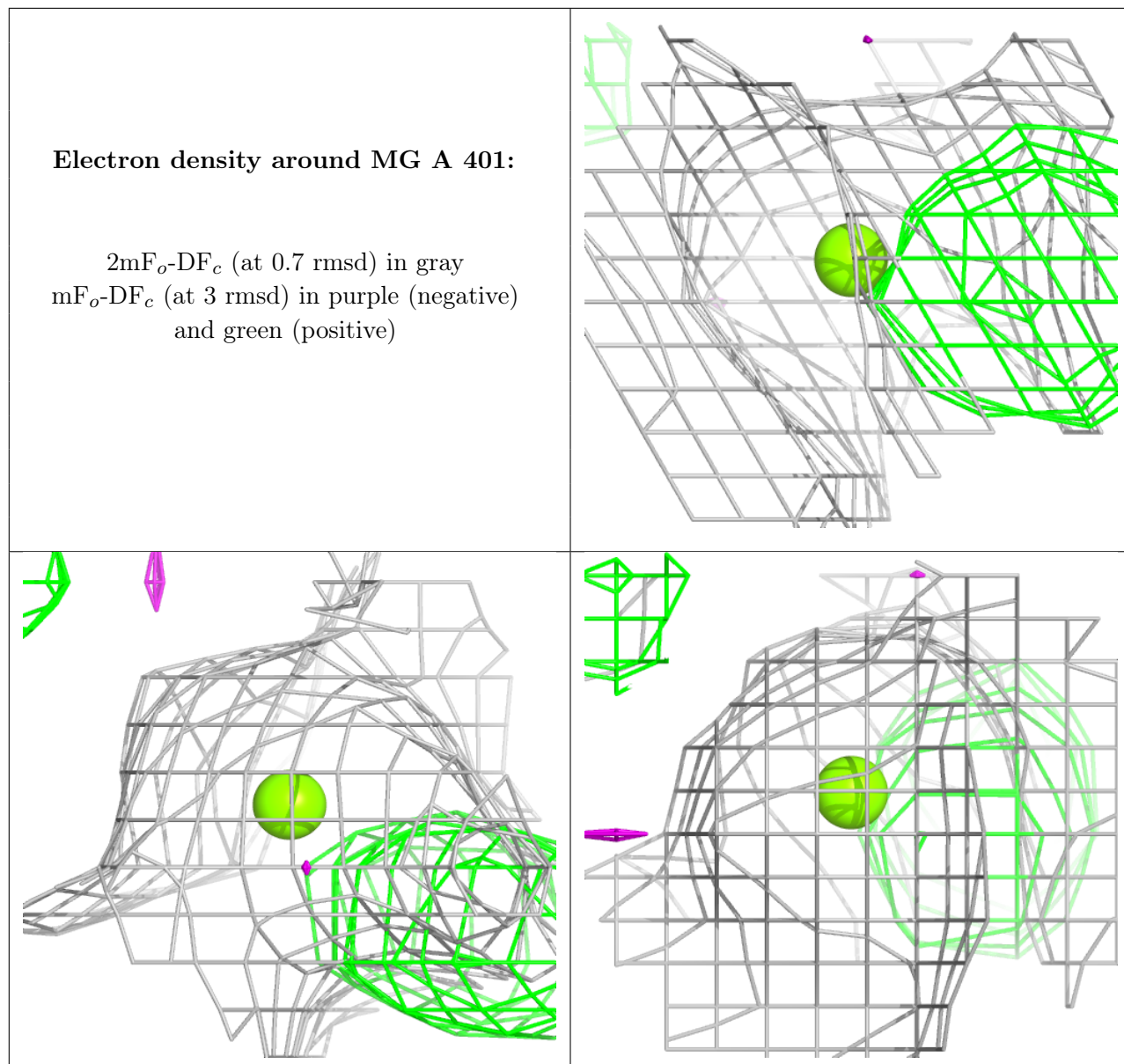
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	401	1/1	0.64	0.14	26,26,26,26	0
2	MG	B	403	1/1	0.81	0.12	37,37,37,37	0
2	MG	B	401	1/1	0.87	0.09	30,30,30,30	0
2	MG	A	402	1/1	0.89	0.08	17,17,17,17	0
4	BTM	A	405	14/14	0.89	0.16	20,26,30,31	0
4	BTM	C	405	14/14	0.90	0.15	22,28,32,37	0
2	MG	C	402	1/1	0.91	0.07	30,30,30,30	0
2	MG	D	403	1/1	0.91	0.09	31,31,31,31	0
4	BTM	D	405	14/14	0.92	0.15	30,35,37,37	0
4	BTM	B	405	14/14	0.93	0.13	25,30,38,43	0
2	MG	C	403	1/1	0.93	0.08	32,32,32,32	0
2	MG	D	401	1/1	0.93	0.10	37,37,37,37	0
3	POP	B	404	9/9	0.95	0.08	25,34,40,42	0
2	MG	D	402	1/1	0.96	0.04	39,39,39,39	0
3	POP	D	404	9/9	0.96	0.07	31,33,36,37	0
2	MG	B	402	1/1	0.96	0.05	38,38,38,38	0
3	POP	C	404	9/9	0.97	0.06	23,26,32,34	0
3	POP	A	404	9/9	0.97	0.06	17,23,24,24	0
2	MG	C	401	1/1	0.97	0.07	29,29,29,29	0
2	MG	A	403	1/1	1.00	0.05	23,23,23,23	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.

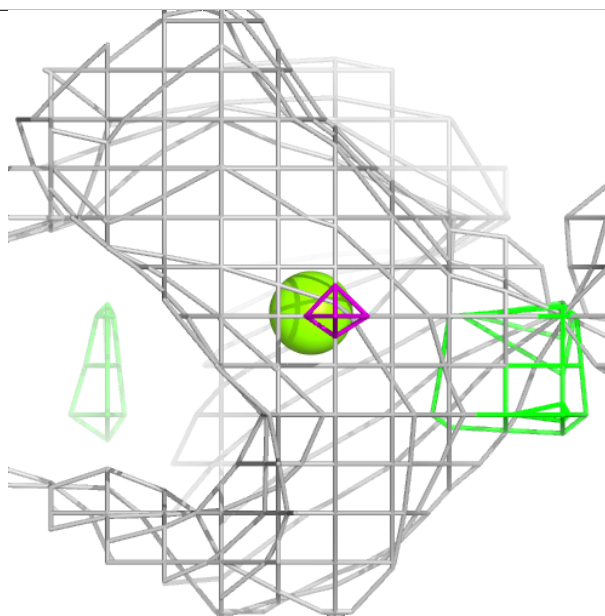
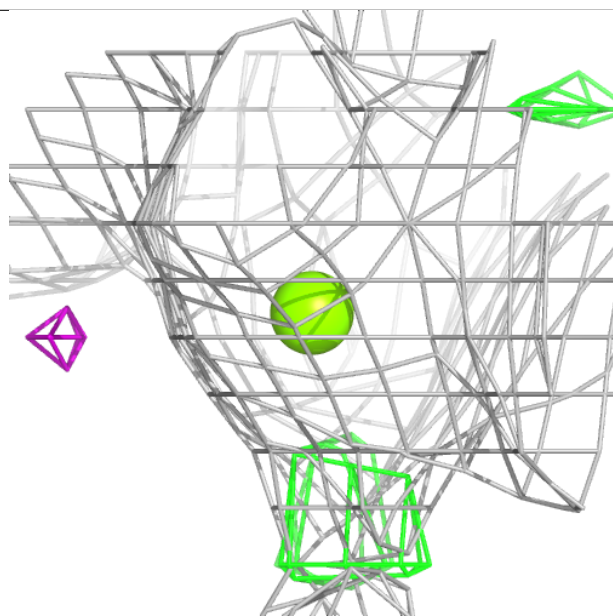
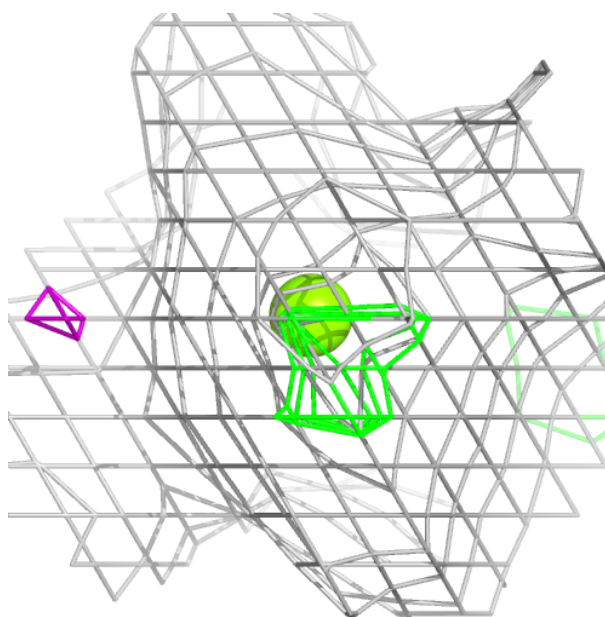
Electron density around MG A 401:

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



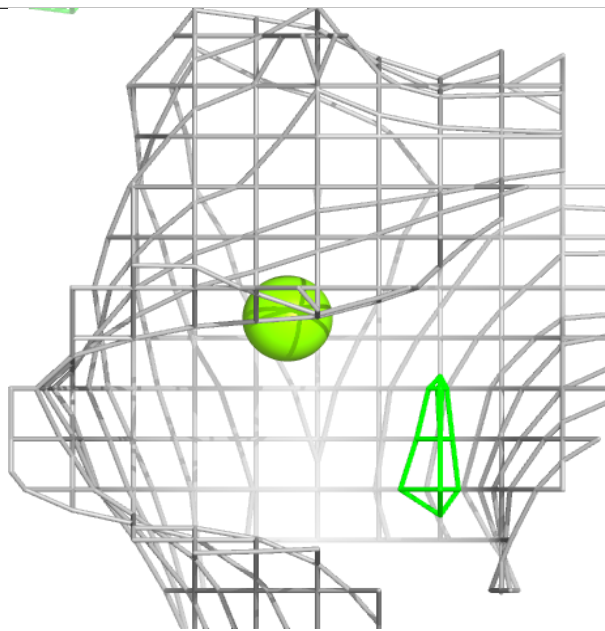
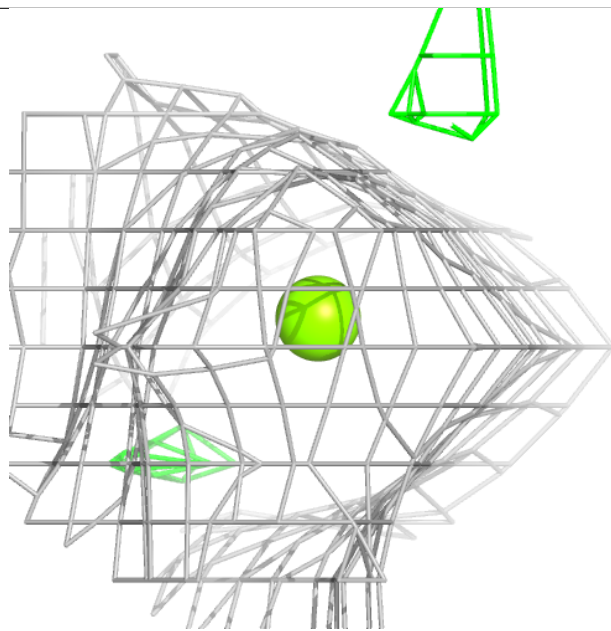
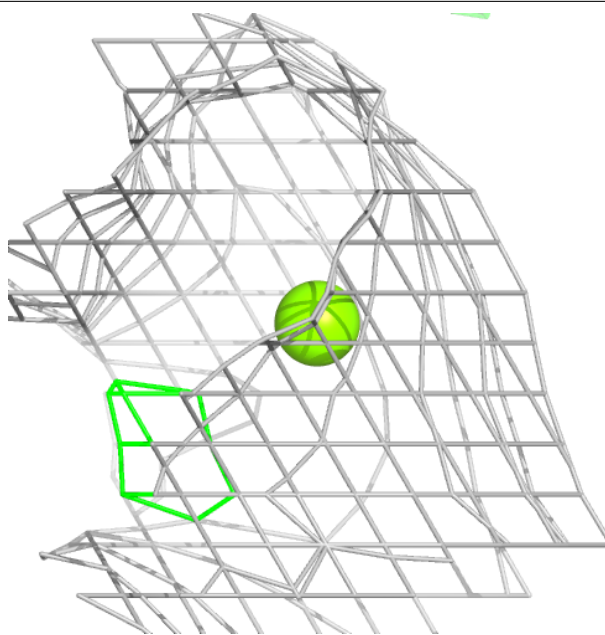
Electron density around MG B 403:

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



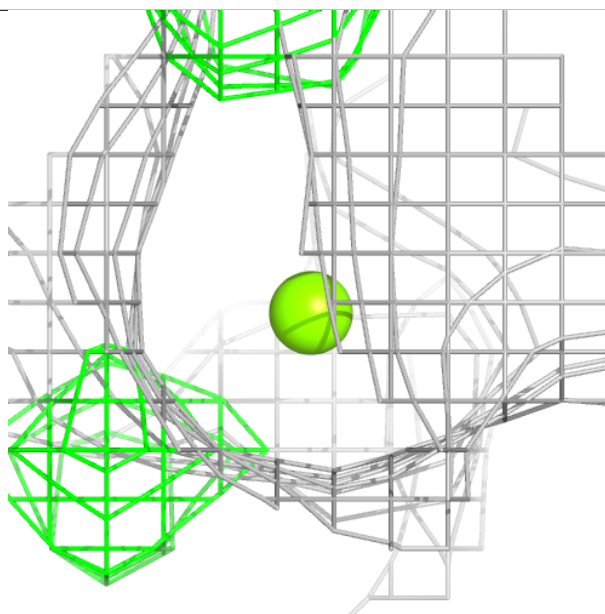
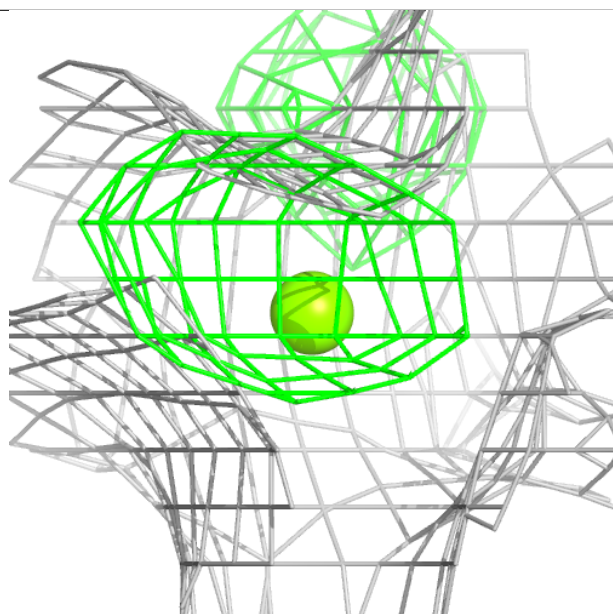
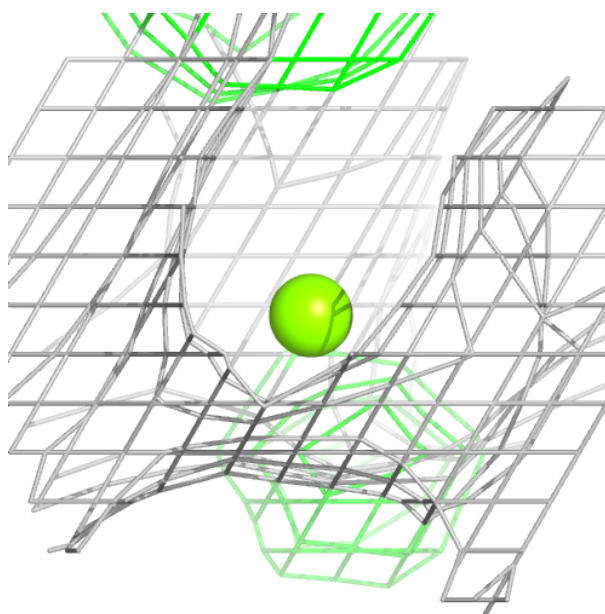
Electron density around MG B 401:

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



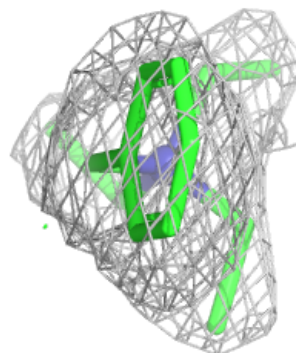
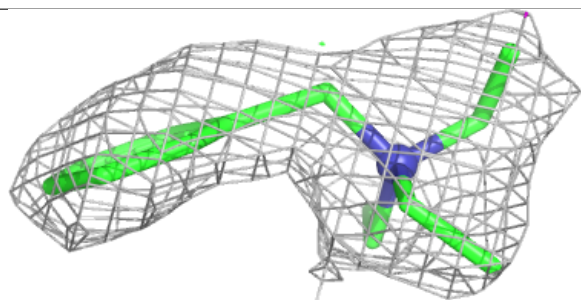
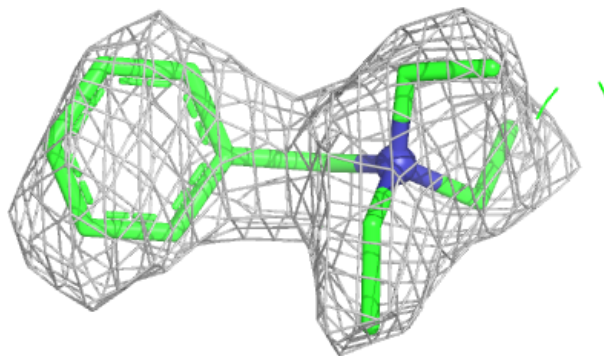
Electron density around MG A 402:

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

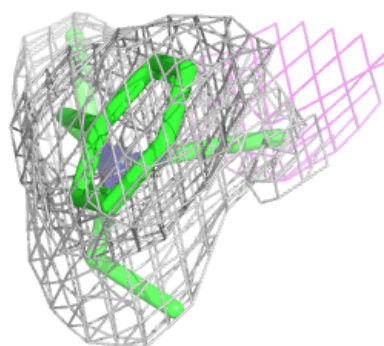
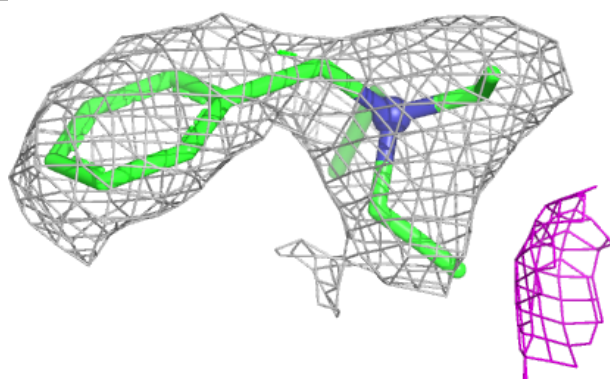
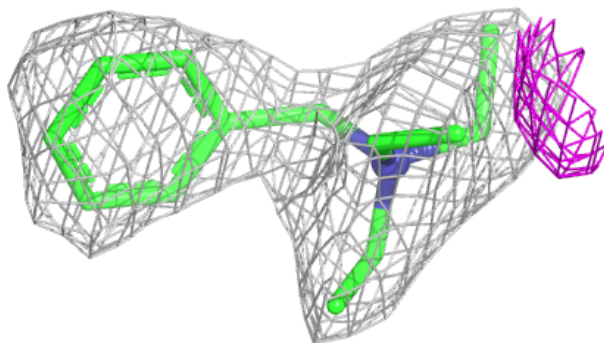


Electron density around BTM A 405:

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

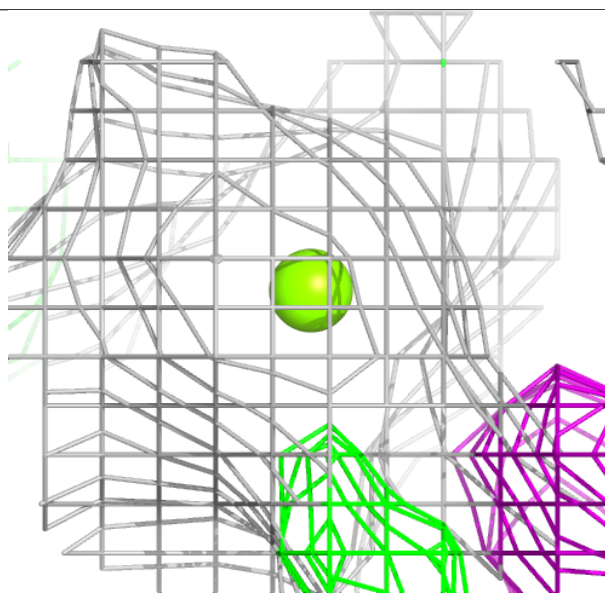
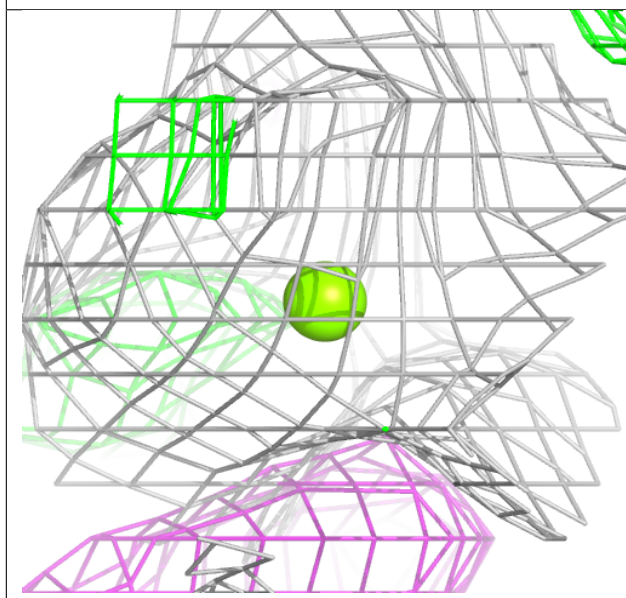
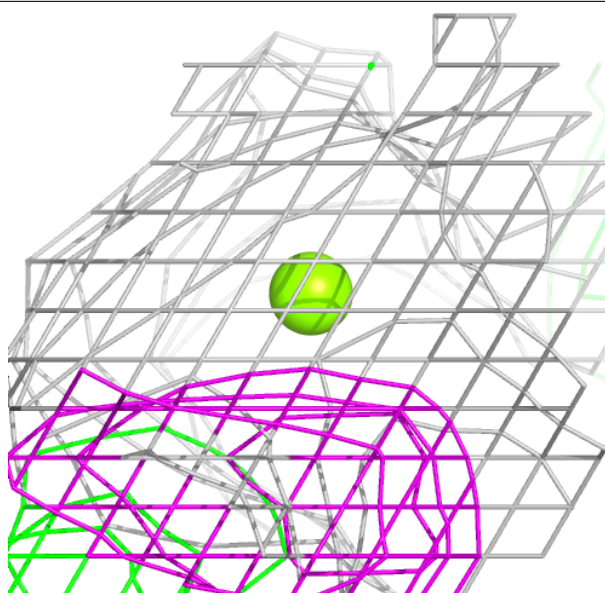
**Electron density around BTM C 405:**

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



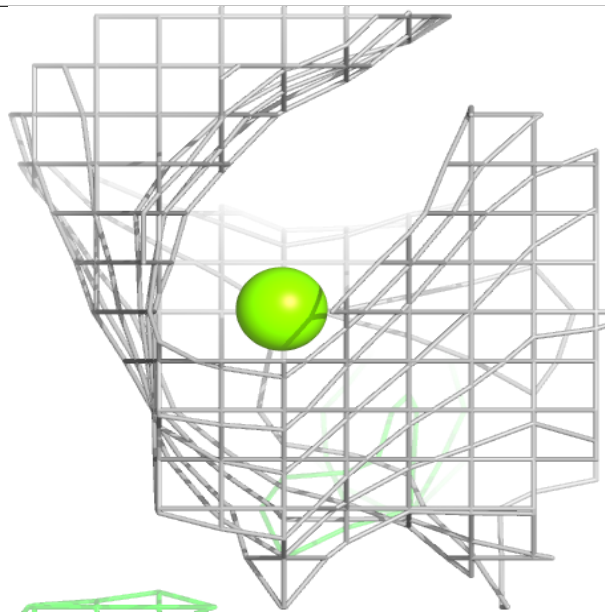
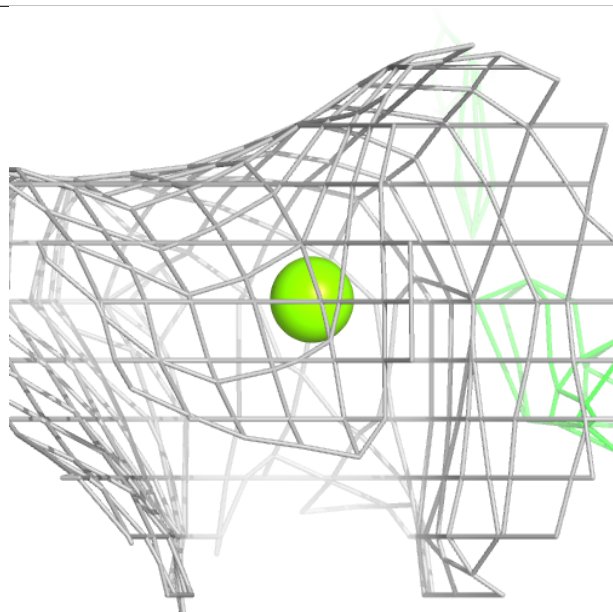
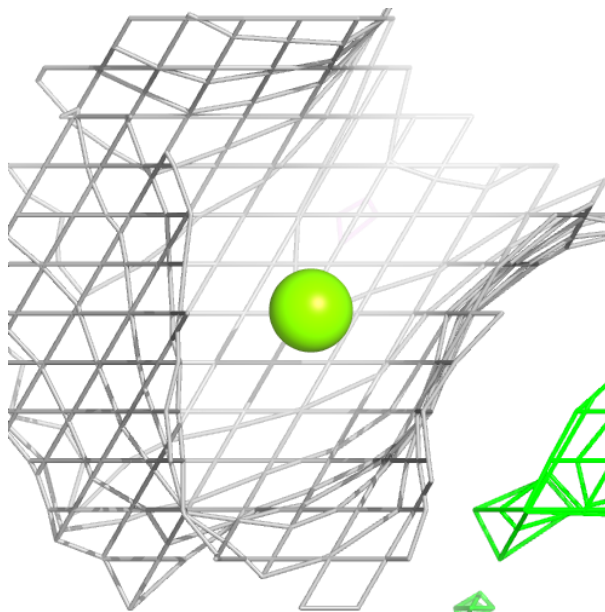
Electron density around MG C 402:

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



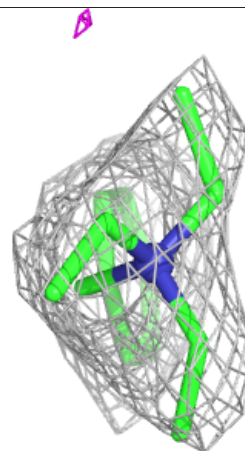
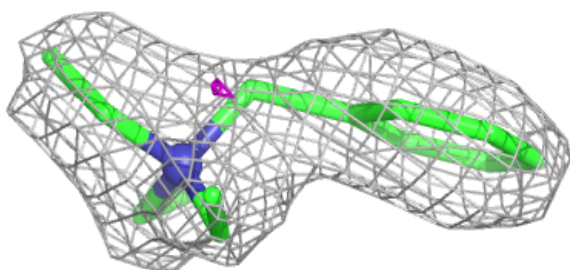
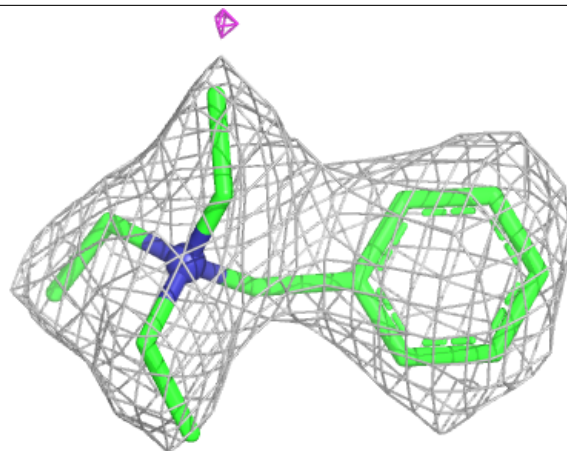
Electron density around MG D 403:

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

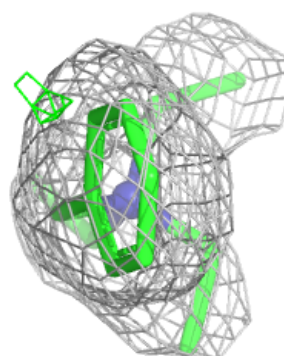
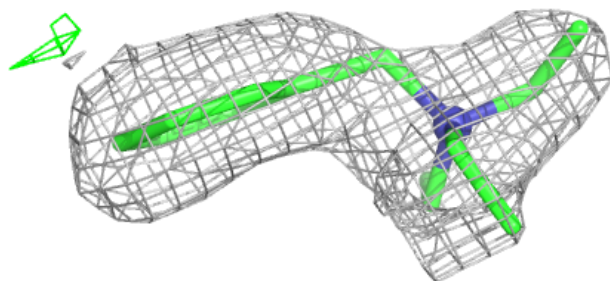
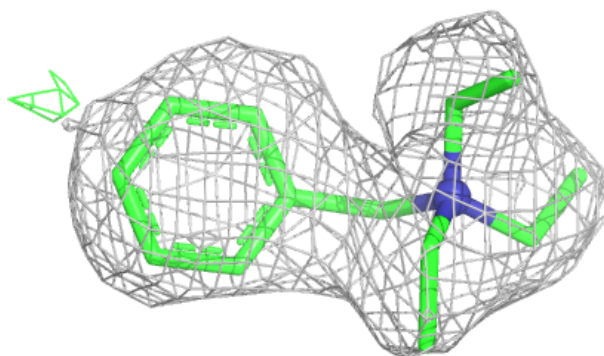


Electron density around BTM D 405:

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

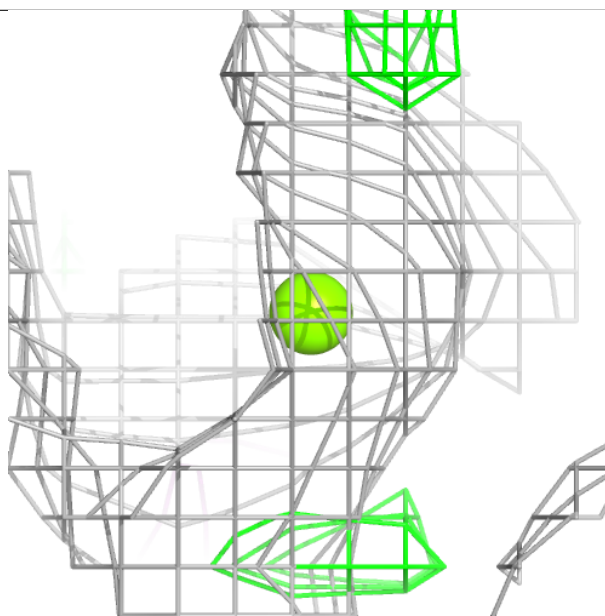
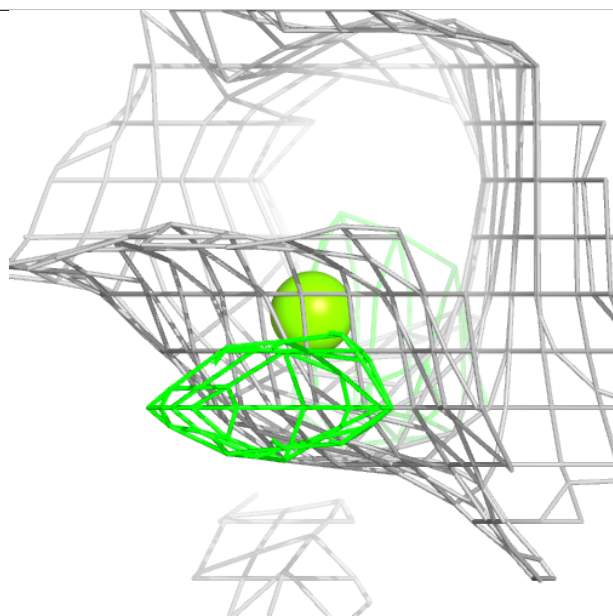
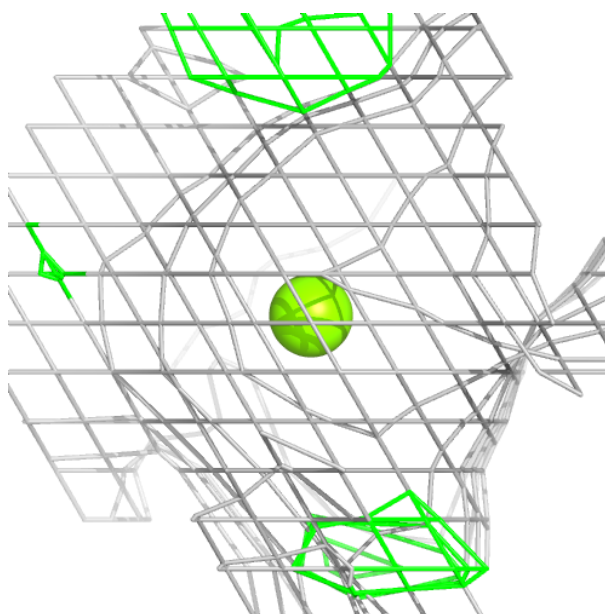
**Electron density around BTM B 405:**

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



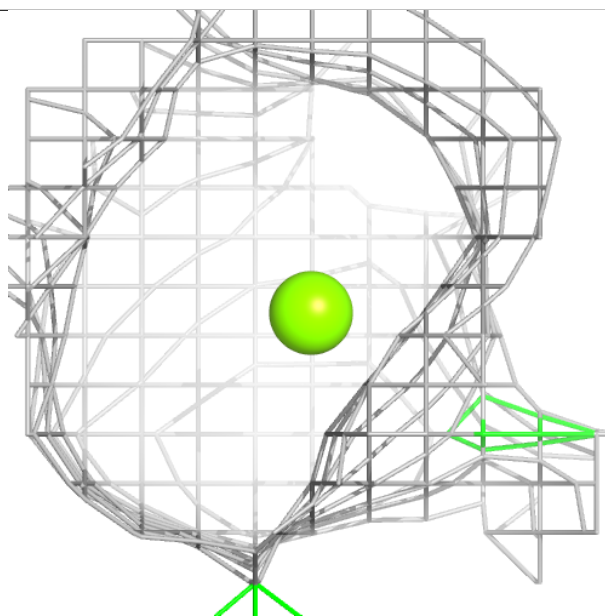
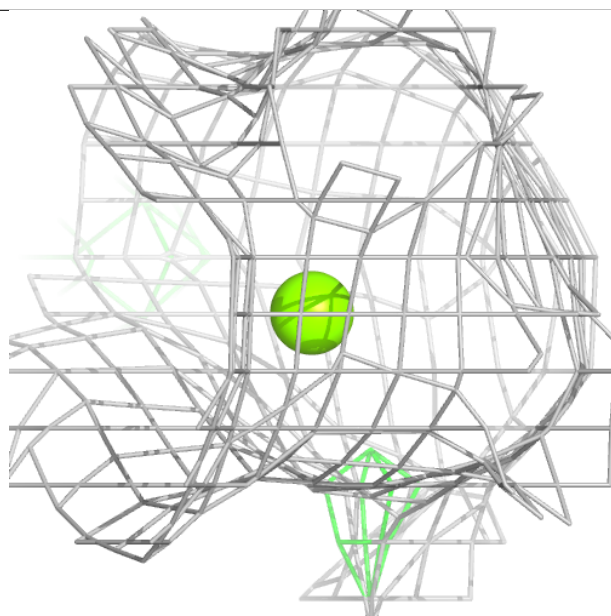
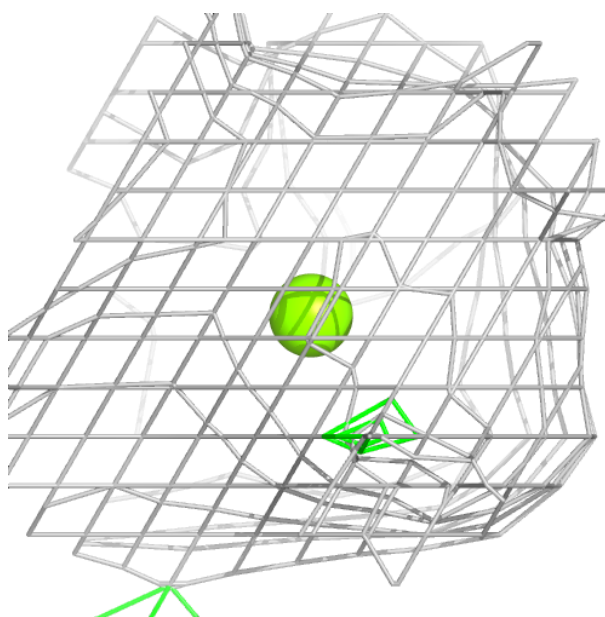
Electron density around MG C 403:

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



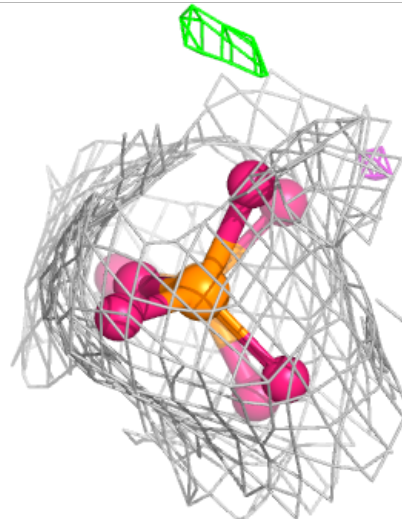
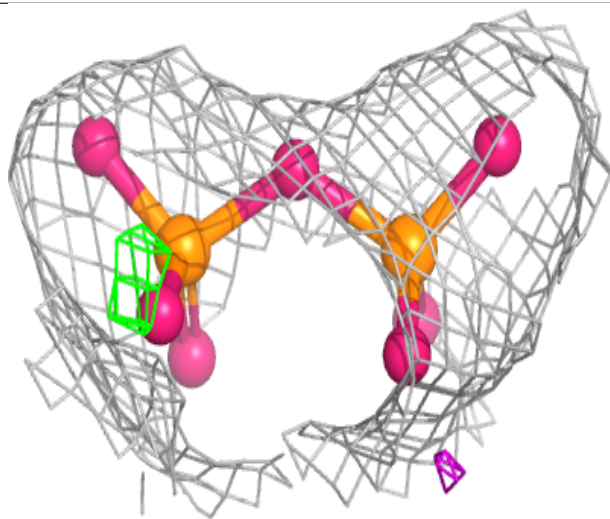
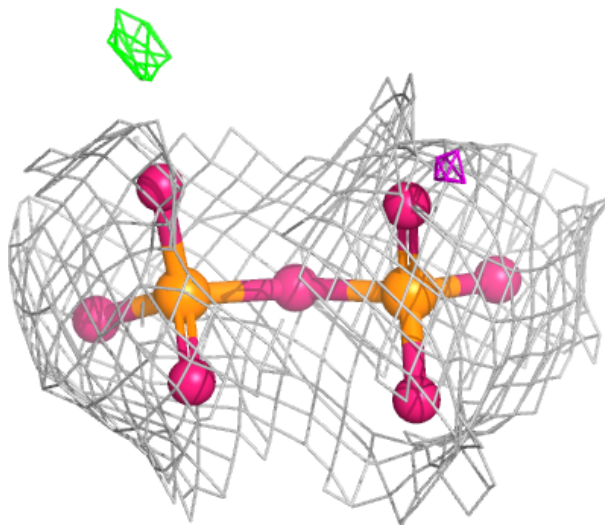
Electron density around MG D 401:

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



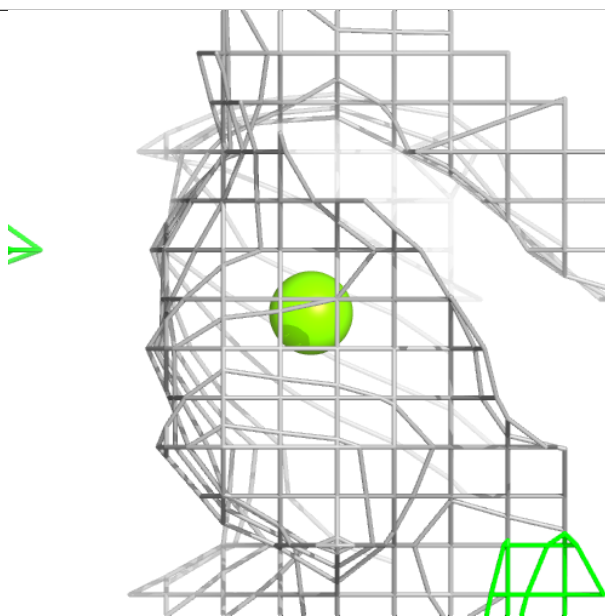
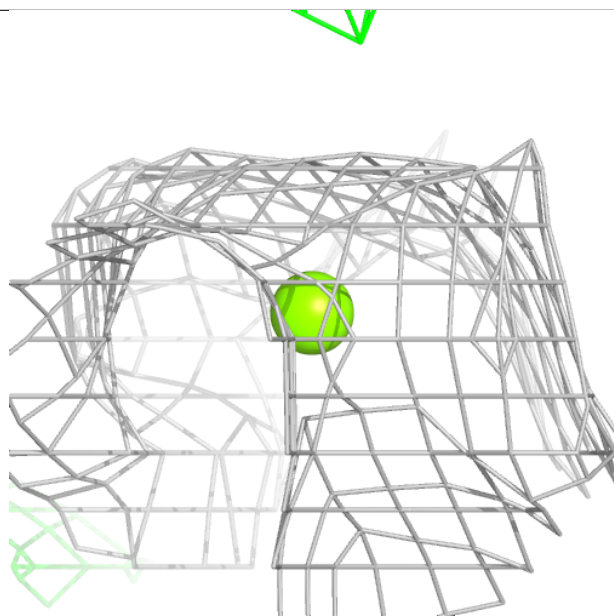
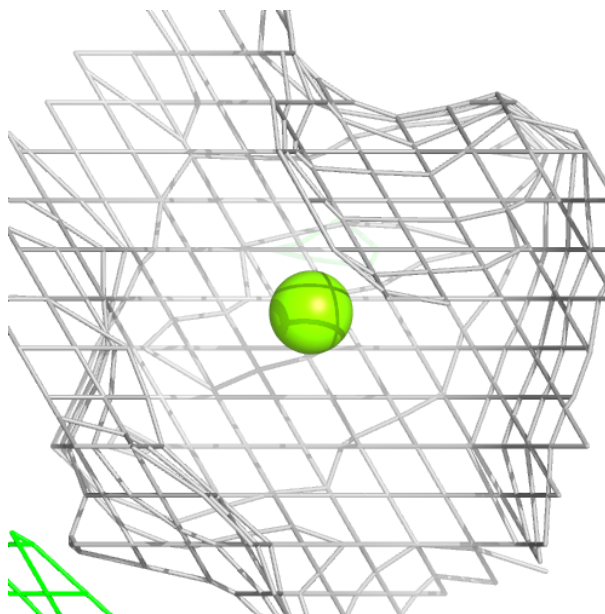
Electron density around POP B 404:

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



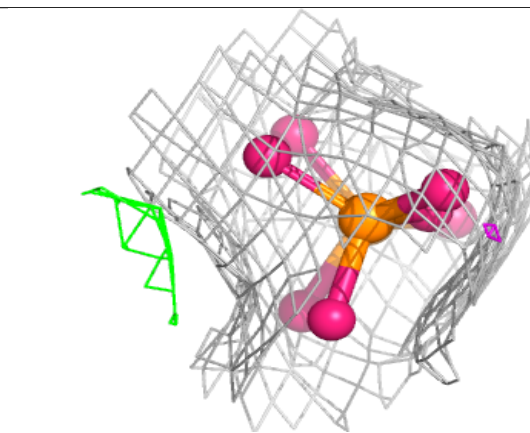
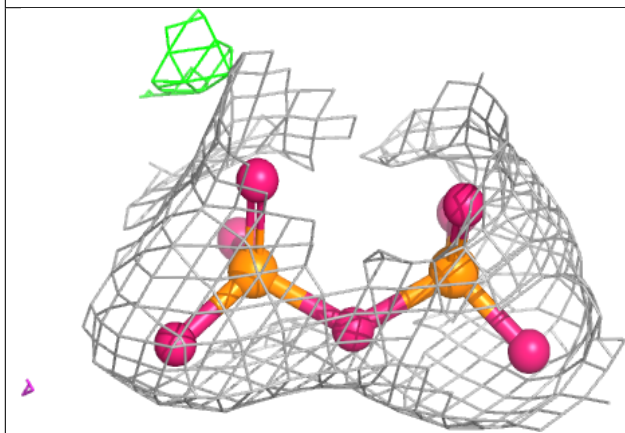
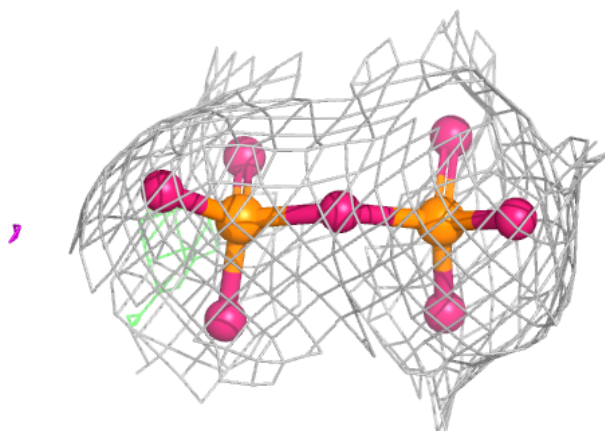
Electron density around MG D 402:

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



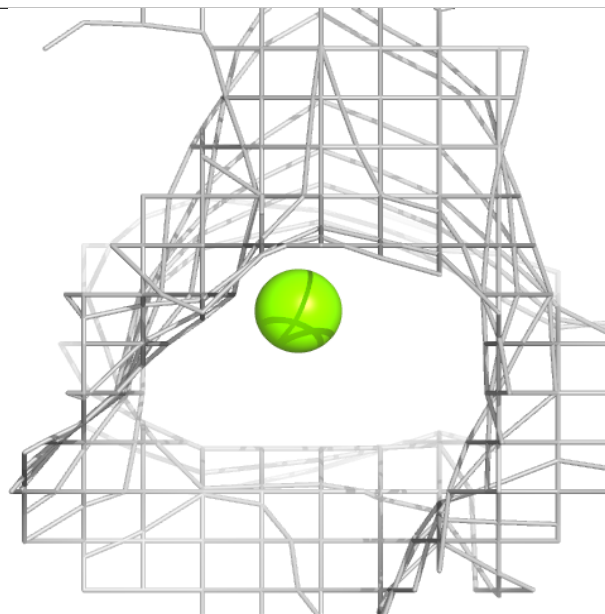
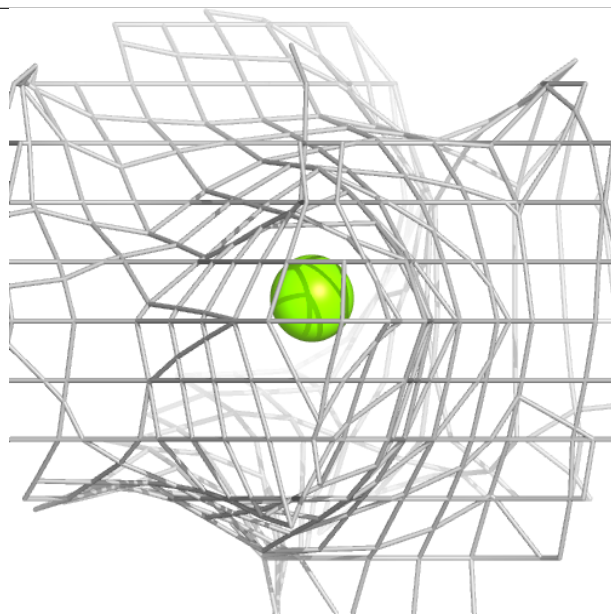
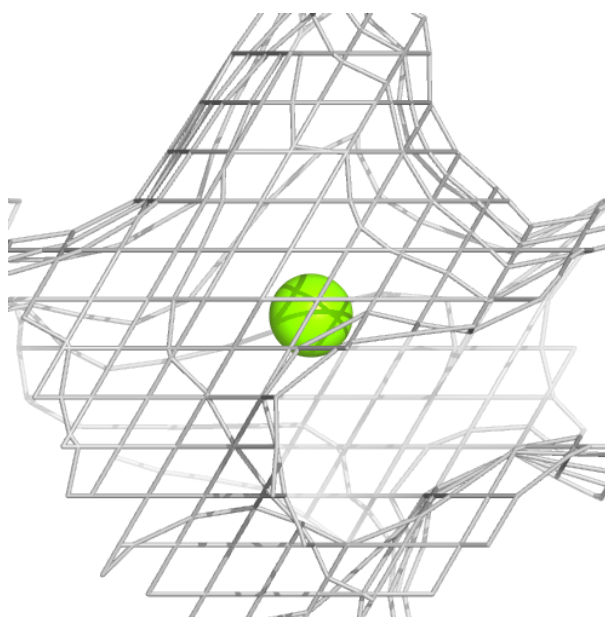
Electron density around POP D 404:

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



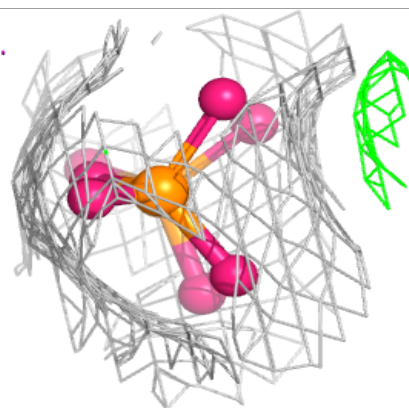
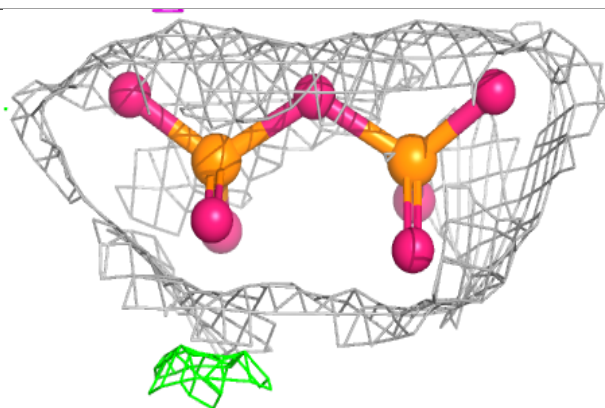
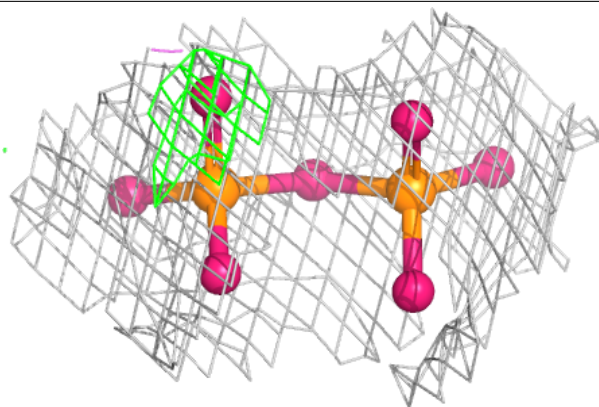
Electron density around MG B 402:

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



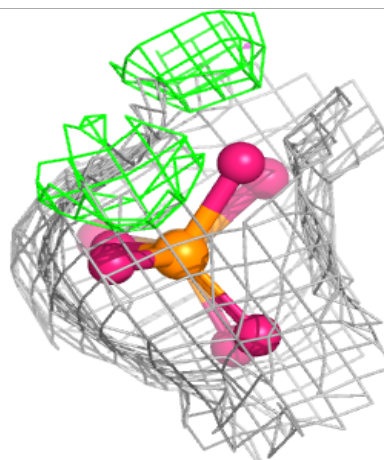
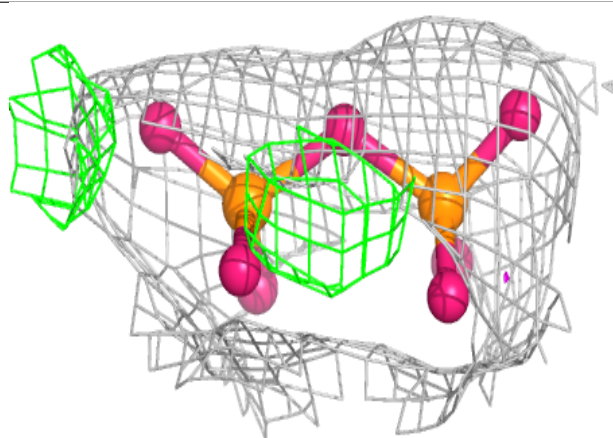
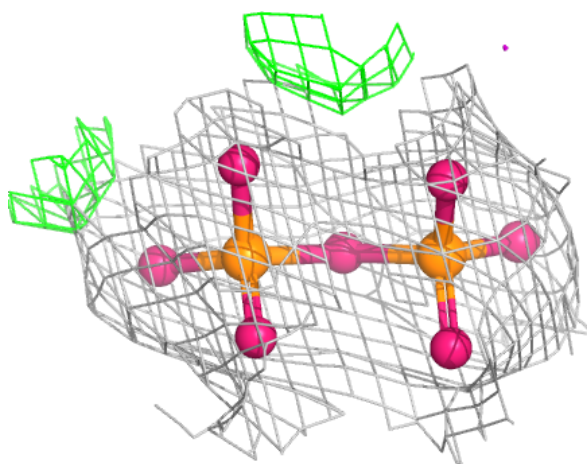
Electron density around POP C 404:

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



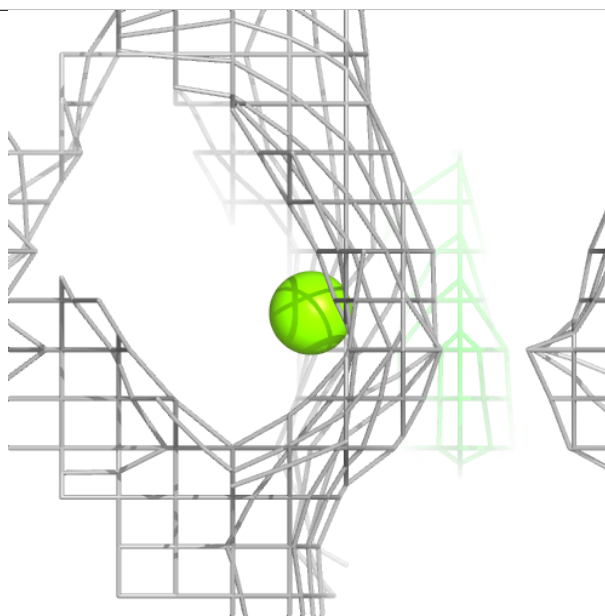
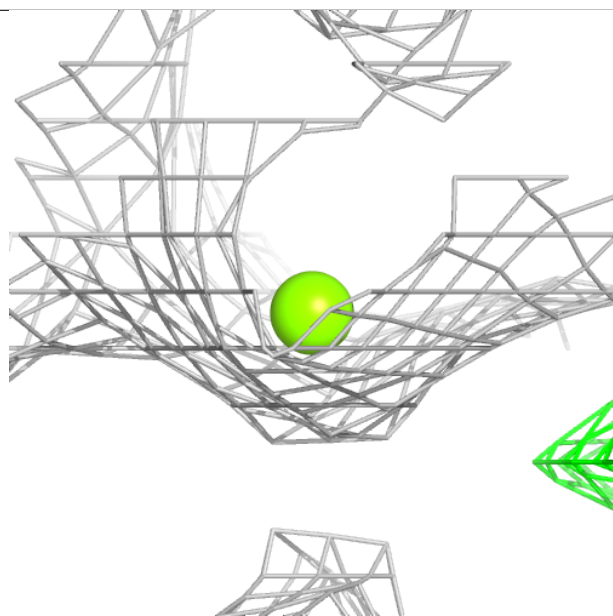
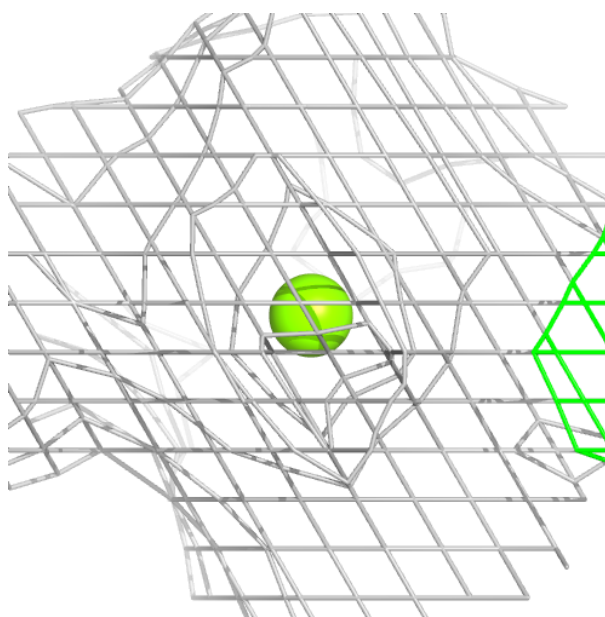
Electron density around POP A 404:

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



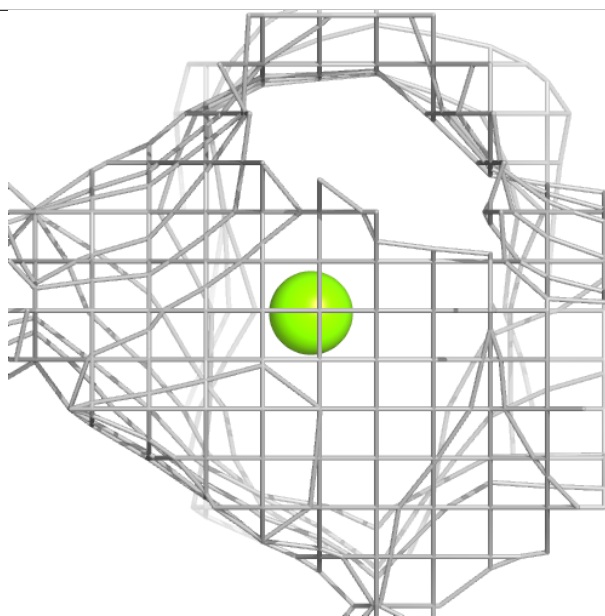
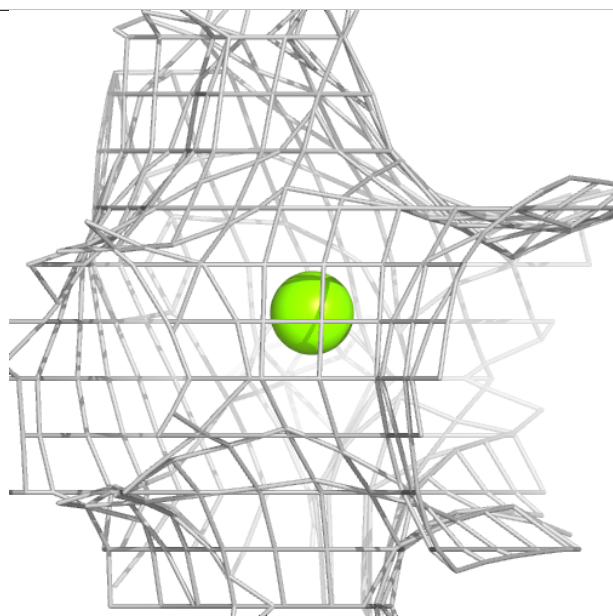
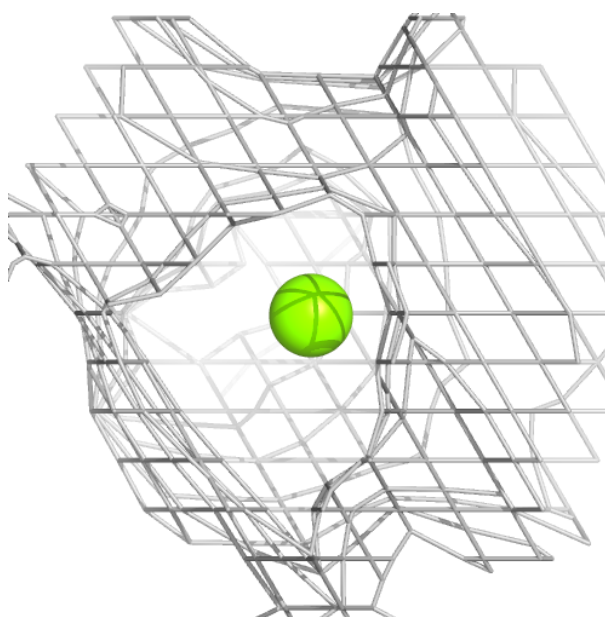
Electron density around MG C 401:

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



Electron density around MG A 403:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.