



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 10:15 AM EDT

PDB ID : 9XZ8 / pdb_00009xz8
Title : Mycobacterium tuberculosis Anthranilate phosphoribosyltransferase in complex with bi-substrate inhibitor 301f
Authors : Mittelstaedt, G.; Parker, E.J.
Deposited on : 2025-08-26
Resolution : 1.60 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

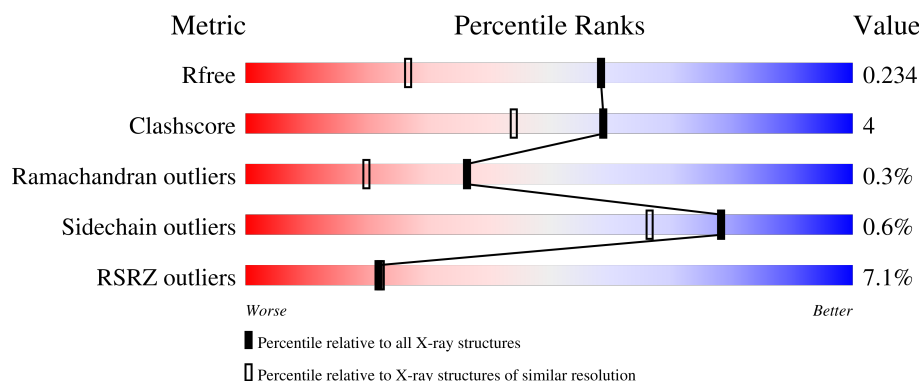
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	378	
1	B	378	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PEG	A	406	-	-	X	-
6	PEG	B	413	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5799 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 Anthranilate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	3	0
			2517	1575	468	465	9			
1	B	346	Total	C	N	O	S	0	5	0
			2544	1588	477	470	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	371	LEU	-	expression tag	UNP P9WFX5
A	372	GLU	-	expression tag	UNP P9WFX5
A	373	HIS	-	expression tag	UNP P9WFX5
A	374	HIS	-	expression tag	UNP P9WFX5
A	375	HIS	-	expression tag	UNP P9WFX5
A	376	HIS	-	expression tag	UNP P9WFX5
A	377	HIS	-	expression tag	UNP P9WFX5
A	378	HIS	-	expression tag	UNP P9WFX5
B	371	LEU	-	expression tag	UNP P9WFX5
B	372	GLU	-	expression tag	UNP P9WFX5
B	373	HIS	-	expression tag	UNP P9WFX5
B	374	HIS	-	expression tag	UNP P9WFX5
B	375	HIS	-	expression tag	UNP P9WFX5
B	376	HIS	-	expression tag	UNP P9WFX5
B	377	HIS	-	expression tag	UNP P9WFX5
B	378	HIS	-	expression tag	UNP P9WFX5

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

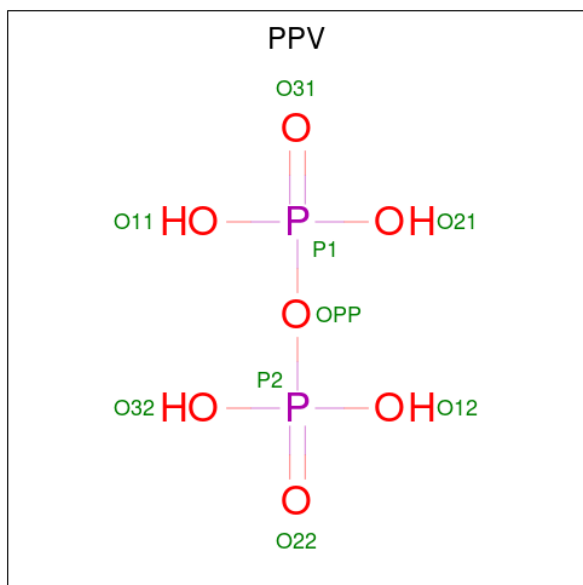
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

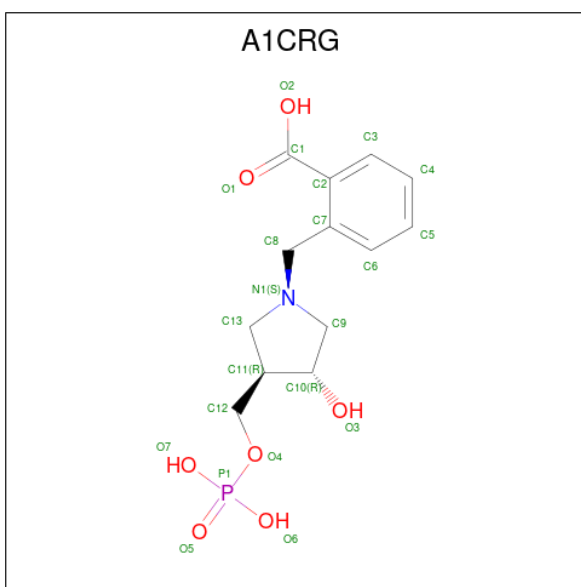
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PYROPHOSPHATE (CCD ID: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



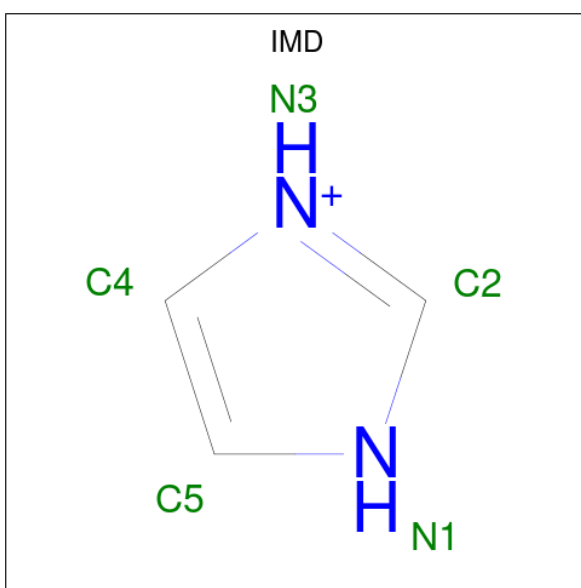
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is 2-((3R,4R)-3-hydroxy-4-[(phosphonooxy)methyl]pyrrolidin-1-yl)methylbenzoic acid (CCD ID: A1CRG) (formula: $\text{C}_{13}\text{H}_{18}\text{NO}_7\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	13	1	7	1		
4	B	1	Total	C	N	O	P	0	0
			22	13	1	7	1		

- Molecule 5 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



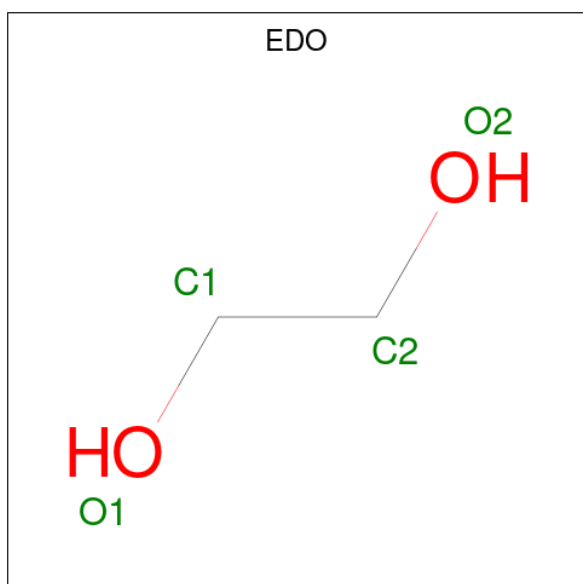
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		
5	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



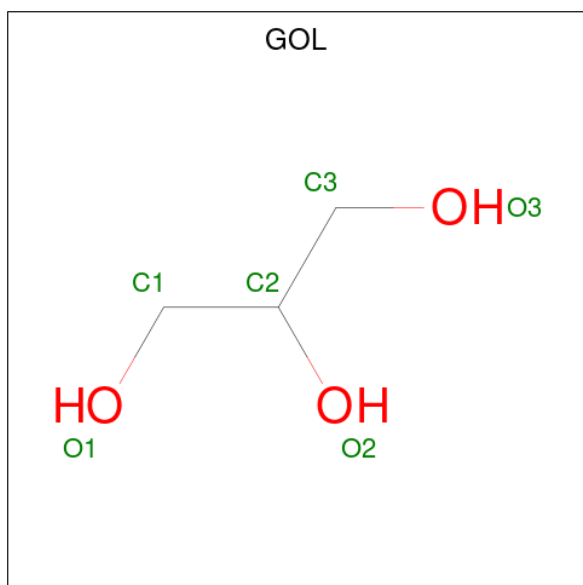
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cl	0	0
			1	1		

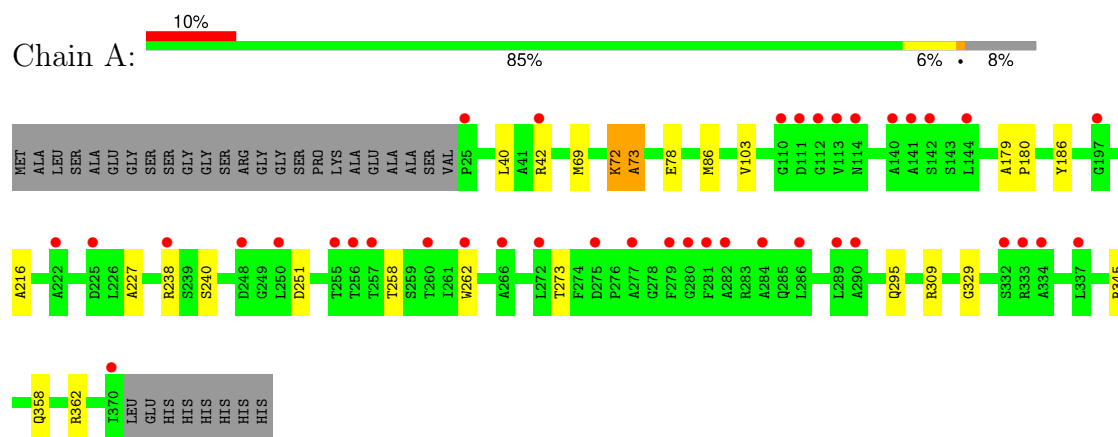
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	236	Total	O	0	0
			236	236		
10	B	329	Total	O	0	0
			329	329		

3 Residue-property plots

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: Anthranilate phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.04Å 80.69Å 110.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.72 – 1.60 45.72 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.72-1.60) 100.0 (45.72-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.186 , 0.225 0.196 , 0.234	Depositor DCC
R_{free} test set	4817 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5799	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 48.54 % 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 8.4799e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PPV, CL, MG, PEG, A1CRG, IMD, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	0/2565	1.12	4/3500 (0.1%)
1	B	0.73	0/2592	1.11	4/3535 (0.1%)
All	All	0.71	0/5157	1.12	8/7035 (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	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ARG	N-CA-CB	6.47	119.39	110.01
1	B	121	MET	CG-SD-CE	-6.15	87.36	100.90
1	B	104	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	237	ARG	CB-CA-C	5.78	120.66	110.37
1	A	72	LYS	CB-CA-C	5.76	120.36	110.79
1	A	251	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	258	THR	CA-CB-OG1	-5.33	101.61	109.60
1	B	69	MET	CG-SD-CE	-5.03	89.83	100.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238[A]	ARG	Sidechain
1	A	42[A]	ARG	Sidechain
1	B	238[A]	ARG	Sidechain
1	B	42[A]	ARG	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	2517	0	2500	17	0
1	B	2544	0	2528	22	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
4	A	22	0	0	0	0
4	B	22	0	0	0	0
5	A	5	0	5	2	0
5	B	5	0	5	1	0
6	A	14	0	20	6	0
6	B	14	0	20	6	0
7	A	12	0	18	1	0
7	B	32	0	48	2	0
8	A	6	0	8	0	0
8	B	18	0	24	5	0
9	B	1	0	0	0	0
10	A	236	0	0	5	0
10	B	329	0	0	7	0
All	All	5799	0	5176	46	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 (46) 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:78:GLU:HG3	6:A:406:PEG:H31	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:TRP:HA	8:B:407:GOL:H2	1.66	0.77
1:A:362:ARG:HE	6:A:410:PEG:H21	1.57	0.69
1:B:42[A]:ARG:HH11	1:B:42[A]:ARG:CG	2.06	0.68
1:B:263:ARG:NH1	1:B:270:ASP:OD2	2.27	0.68
5:A:405:IMD:H2	10:A:708:HOH:O	1.95	0.67
1:B:103:VAL:HG12	1:B:216:ALA:HB3	1.77	0.66
1:B:40:LEU:O	6:B:413:PEG:H32	1.95	0.65
1:B:346:ARG:HD2	8:B:417:GOL:H2	1.80	0.62
1:A:40:LEU:O	6:A:406:PEG:H41	2.01	0.60
7:B:416:EDO:H21	10:B:598:HOH:O	2.02	0.59
6:B:413:PEG:H42	10:B:626:HOH:O	2.02	0.58
1:B:42[A]:ARG:HH11	1:B:42[A]:ARG:HG2	1.68	0.58
1:A:103:VAL:HG12	1:A:216:ALA:HB3	1.85	0.58
6:B:412:PEG:H41	10:B:543:HOH:O	2.05	0.57
1:A:309:ARG:HD3	10:A:507:HOH:O	2.07	0.54
1:B:244:VAL:HG12	1:B:261:ILE:HG12	1.92	0.52
1:A:329:GLY:HA3	7:A:407:EDO:H12	1.91	0.52
1:A:78:GLU:CG	6:A:406:PEG:H31	2.39	0.52
1:B:229:VAL:HG23	10:B:504:HOH:O	2.10	0.50
1:B:81:GLU:N	6:B:412:PEG:H12	2.27	0.50
1:A:295:GLN:HG2	10:A:625:HOH:O	2.12	0.49
1:A:186:TYR:OH	10:A:501:HOH:O	2.19	0.49
7:B:415:EDO:H21	10:B:619:HOH:O	2.12	0.49
1:B:271:LYS:NZ	10:B:509:HOH:O	2.45	0.48
6:A:406:PEG:H42	10:A:574:HOH:O	2.13	0.48
1:A:86:MET:HE1	5:A:405:IMD:C4	2.44	0.46
1:B:86:MET:HE1	5:B:406:IMD:C4	2.46	0.46
1:B:346:ARG:CD	8:B:417:GOL:H2	2.46	0.46
1:B:158:ILE:O	1:B:178:PHE:HB2	2.16	0.45
1:B:42[A]:ARG:CG	1:B:42[A]:ARG:NH1	2.78	0.45
1:A:358:GLN:NE2	6:A:410:PEG:H12	2.32	0.44
1:B:46:ALA:CB	8:B:407:GOL:H31	2.48	0.44
1:B:40:LEU:O	6:B:413:PEG:C3	2.63	0.44
1:A:216:ALA:HA	1:A:240:SER:O	2.18	0.43
1:A:227:ALA:HB3	1:A:262:TRP:CH2	2.53	0.43
1:B:47:TRP:CA	8:B:407:GOL:H2	2.44	0.43
1:A:227:ALA:CB	1:A:262:TRP:CZ3	3.02	0.42
1:A:179:ALA:HB3	1:A:180:PRO:HD3	2.00	0.42
6:B:413:PEG:C4	10:B:626:HOH:O	2.66	0.42
1:A:72:LYS:O	1:A:73:ALA:CB	2.68	0.41
1:B:337:LEU:HB2	1:B:338:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:HB2	1:A:69:MET:HE2	1.90	0.41
1:B:295[B]:GLN:N	1:B:295[B]:GLN:CD	2.79	0.41
1:B:103:VAL:HG11	1:B:327:HIS:HB2	2.04	0.40
1:B:27:TRP:HB2	1:B:28:PRO:HD3	2.02	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	347/378 (92%)	339 (98%)	7 (2%)	1 (0%)	36	20
1	B	349/378 (92%)	342 (98%)	6 (2%)	1 (0%)	36	20
All	All	696/756 (92%)	681 (98%)	13 (2%)	2 (0%)	36	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ALA
1	B	73	ALA

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/265 (91%)	240 (100%)	1 (0%)	84	75
1	B	245/265 (92%)	241 (98%)	4 (2%)	55	33
All	All	486/530 (92%)	481 (99%)	5 (1%)	78	50

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	THR
1	B	42[A]	ARG
1	B	42[B]	ARG
1	B	238[A]	ARG
1	B	238[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	GLN
1	B	358	GLN
1	B	369	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 5 are monoatomic - leaving 25 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	PPV	B	404	2	6,8,8	1.32	0	12,13,13	1.17	1 (8%)
8	GOL	B	409	-	5,5,5	0.10	0	5,5,5	0.24	0
6	PEG	B	413	-	6,6,6	0.55	0	5,5,5	0.72	0
5	IMD	B	406	-	5,5,5	0.49	0	5,5,5	0.47	0
4	A1CRG	A	404	-	23,23,23	0.78	0	27,33,33	2.09	6 (22%)
6	PEG	A	406	-	6,6,6	0.56	0	5,5,5	0.37	0
6	PEG	B	412	-	6,6,6	0.25	0	5,5,5	0.20	0
7	EDO	A	411	-	3,3,3	0.14	0	2,2,2	0.29	0
7	EDO	B	416	-	3,3,3	0.52	0	2,2,2	0.35	0
3	PPV	A	403	2	6,8,8	0.75	0	12,13,13	0.86	0
7	EDO	B	408	-	3,3,3	0.07	0	2,2,2	0.28	0
7	EDO	B	415	-	3,3,3	0.37	0	2,2,2	0.37	0
8	GOL	B	407	-	5,5,5	0.09	0	5,5,5	0.54	0
8	GOL	A	408	-	5,5,5	0.08	0	5,5,5	0.26	0
8	GOL	B	417	-	5,5,5	0.22	0	5,5,5	0.61	0
7	EDO	B	419	-	3,3,3	0.23	0	2,2,2	0.09	0
6	PEG	A	410	-	6,6,6	0.28	0	5,5,5	0.31	0
7	EDO	B	410	-	3,3,3	0.33	0	2,2,2	0.04	0
7	EDO	B	418	-	3,3,3	0.35	0	2,2,2	0.55	0
7	EDO	A	407	-	3,3,3	0.19	0	2,2,2	0.07	0
7	EDO	B	414	-	3,3,3	0.70	0	2,2,2	0.85	0
4	A1CRG	B	405	-	23,23,23	0.83	0	27,33,33	2.31	6 (22%)
7	EDO	B	411	-	3,3,3	0.12	0	2,2,2	0.32	0
5	IMD	A	405	-	5,5,5	0.39	0	5,5,5	0.59	0
7	EDO	A	409	-	3,3,3	0.09	0	2,2,2	0.14	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	PPV	B	404	2	-	0/6/6/6	-
8	GOL	B	409	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	B	413	-	-	2/4/4/4	-
5	IMD	B	406	-	-	-	0/1/1/1
4	A1CRG	A	404	-	-	4/14/26/26	0/2/2/2
6	PEG	A	406	-	-	1/4/4/4	-
6	PEG	B	412	-	-	2/4/4/4	-
7	EDO	A	411	-	-	1/1/1/1	-
7	EDO	B	416	-	-	1/1/1/1	-
3	PPV	A	403	2	-	0/6/6/6	-
7	EDO	B	408	-	-	1/1/1/1	-
7	EDO	B	415	-	-	0/1/1/1	-
8	GOL	B	407	-	-	1/4/4/4	-
8	GOL	A	408	-	-	2/4/4/4	-
8	GOL	B	417	-	-	2/4/4/4	-
7	EDO	B	419	-	-	1/1/1/1	-
6	PEG	A	410	-	-	2/4/4/4	-
7	EDO	B	410	-	-	0/1/1/1	-
7	EDO	B	418	-	-	1/1/1/1	-
7	EDO	A	407	-	-	0/1/1/1	-
7	EDO	B	414	-	-	0/1/1/1	-
4	A1CRG	B	405	-	-	6/14/26/26	0/2/2/2
7	EDO	B	411	-	-	1/1/1/1	-
5	IMD	A	405	-	-	-	0/1/1/1
7	EDO	A	409	-	-	1/1/1/1	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	A1CRG	C8-N1-C9	8.44	129.65	113.39
4	A	404	A1CRG	C8-N1-C9	6.80	126.49	113.39
4	B	405	A1CRG	O6-P1-O4	-5.62	92.00	106.67
4	A	404	A1CRG	C13-N1-C9	3.98	109.91	104.12
4	A	404	A1CRG	O7-P1-O5	3.91	126.07	110.83
4	B	405	A1CRG	O3-C10-C9	3.01	117.99	110.94
4	B	405	A1CRG	C13-N1-C9	2.87	108.30	104.12
4	A	404	A1CRG	O1-C1-C2	-2.60	115.77	121.97
4	B	405	A1CRG	O7-P1-O6	2.56	117.41	107.80
4	A	404	A1CRG	O2-C1-C2	2.25	121.67	115.28
4	A	404	A1CRG	O4-P1-O5	-2.13	100.68	106.44
4	B	405	A1CRG	O7-P1-O5	2.09	118.97	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	404	PPV	O32-P2-O12	2.04	115.44	107.80

There are no chirality outliers.

All (31) torsion outliers are listed below:

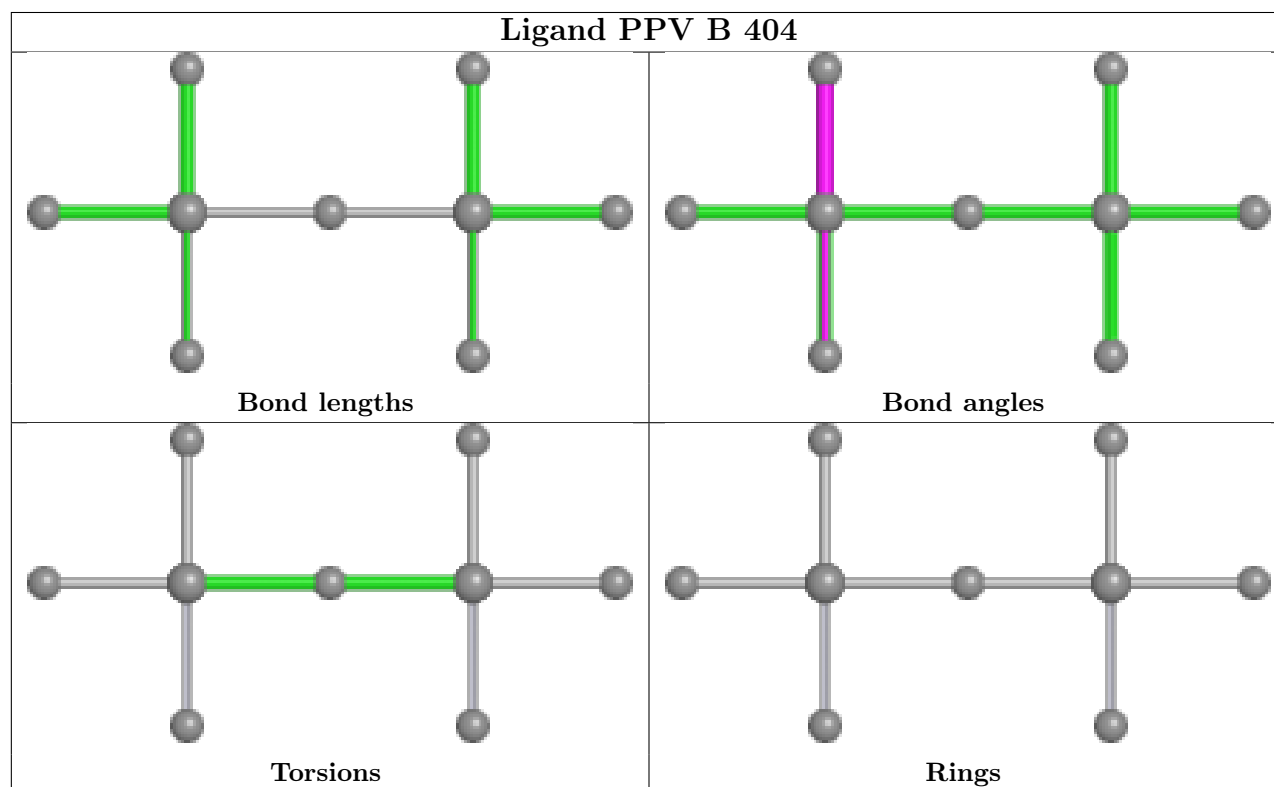
Mol	Chain	Res	Type	Atoms
4	A	404	A1CRG	C7-C8-N1-C9
4	A	404	A1CRG	C12-O4-P1-O6
4	A	404	A1CRG	C12-O4-P1-O7
4	B	405	A1CRG	C7-C8-N1-C9
4	B	405	A1CRG	C12-O4-P1-O5
4	B	405	A1CRG	C12-O4-P1-O6
4	B	405	A1CRG	C12-O4-P1-O7
8	A	408	GOL	C1-C2-C3-O3
8	B	417	GOL	O2-C2-C3-O3
6	B	413	PEG	C4-C3-O2-C2
6	B	412	PEG	O2-C3-C4-O4
6	B	413	PEG	O1-C1-C2-O2
8	B	409	GOL	O1-C1-C2-C3
8	B	417	GOL	C1-C2-C3-O3
8	B	409	GOL	O1-C1-C2-O2
7	B	411	EDO	O1-C1-C2-O2
6	B	412	PEG	O1-C1-C2-O2
7	B	418	EDO	O1-C1-C2-O2
7	B	419	EDO	O1-C1-C2-O2
4	A	404	A1CRG	C12-O4-P1-O5
8	A	408	GOL	O2-C2-C3-O3
8	B	407	GOL	O1-C1-C2-O2
6	A	406	PEG	O2-C3-C4-O4
7	A	409	EDO	O1-C1-C2-O2
6	A	410	PEG	C4-C3-O2-C2
7	B	408	EDO	O1-C1-C2-O2
7	B	416	EDO	O1-C1-C2-O2
4	B	405	A1CRG	O2-C1-C2-C3
4	B	405	A1CRG	O1-C1-C2-C3
7	A	411	EDO	O1-C1-C2-O2
6	A	410	PEG	O2-C3-C4-O4

There are no ring outliers.

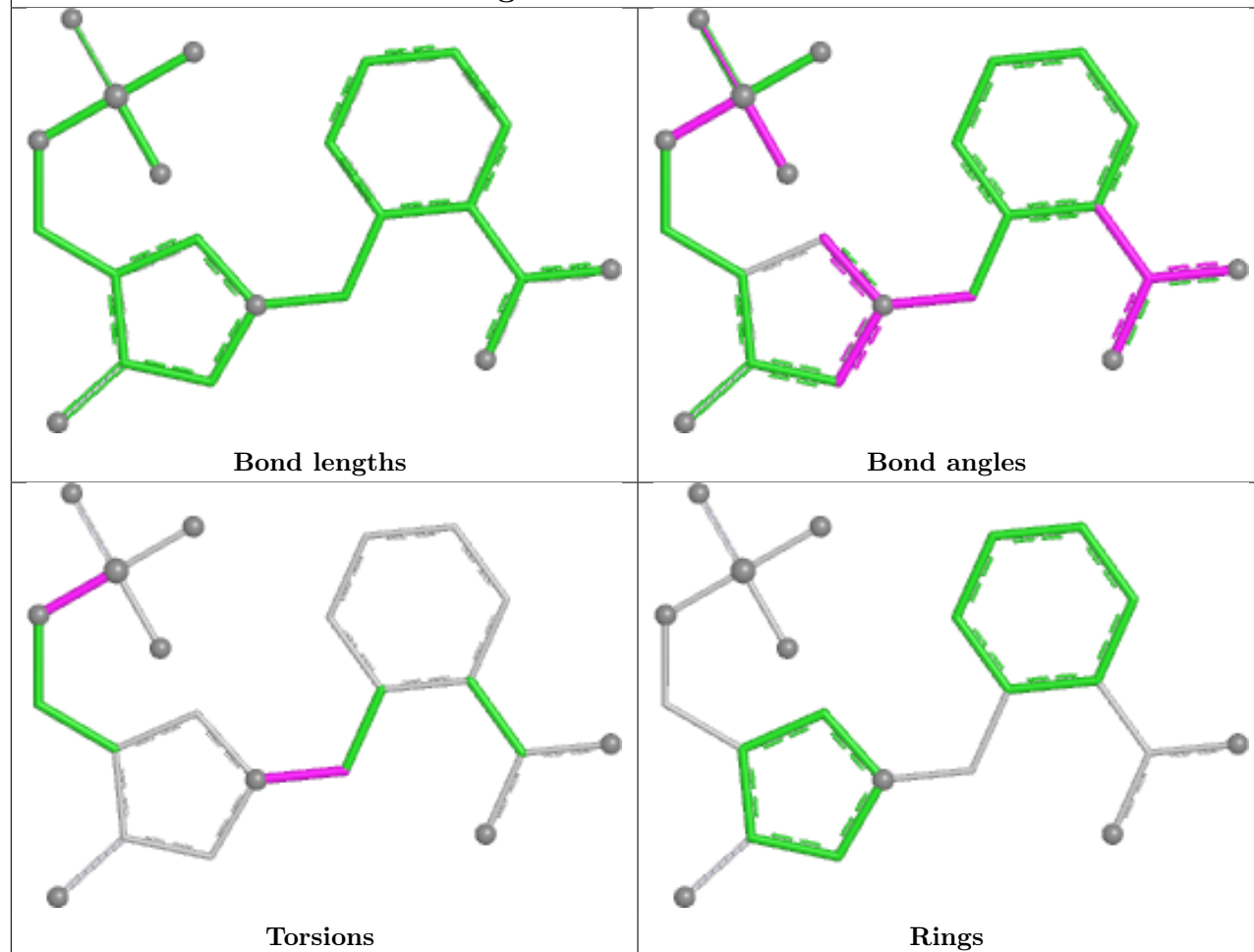
11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	413	PEG	4	0
5	B	406	IMD	1	0
6	A	406	PEG	4	0
6	B	412	PEG	2	0
7	B	416	EDO	1	0
7	B	415	EDO	1	0
8	B	407	GOL	3	0
8	B	417	GOL	2	0
6	A	410	PEG	2	0
7	A	407	EDO	1	0
5	A	405	IMD	2	0

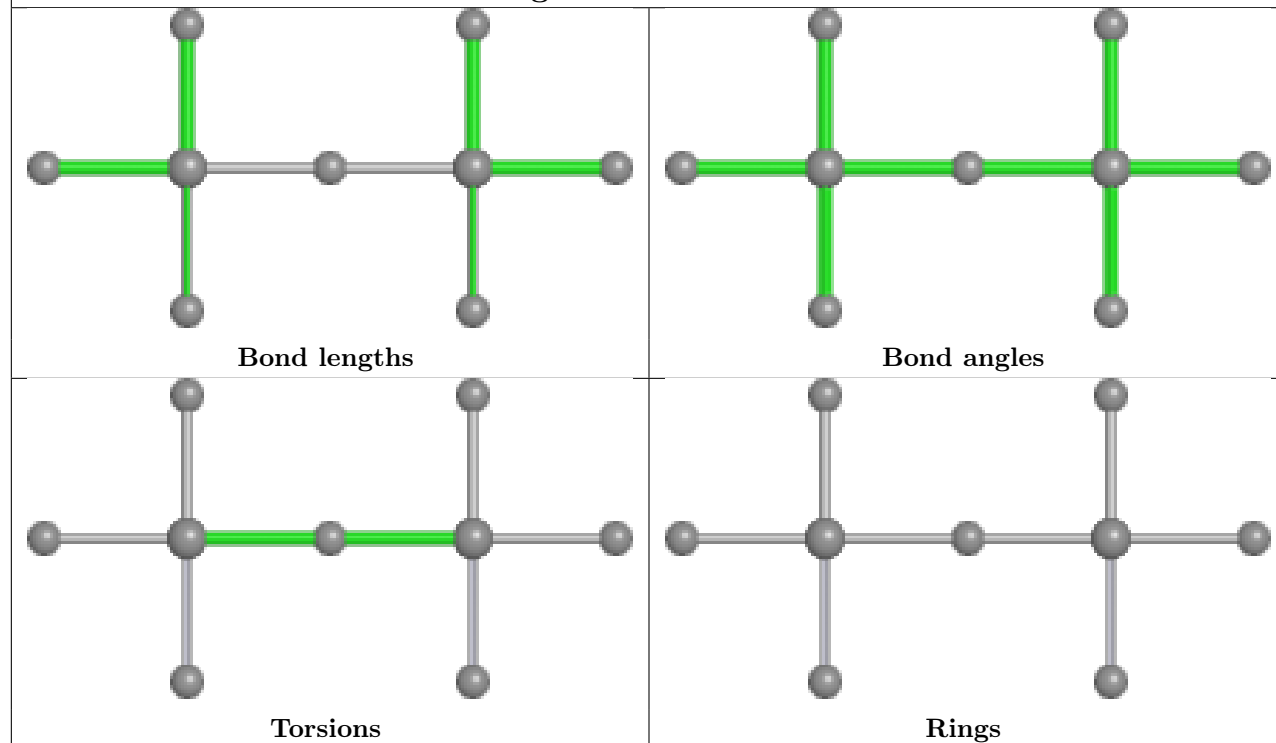
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

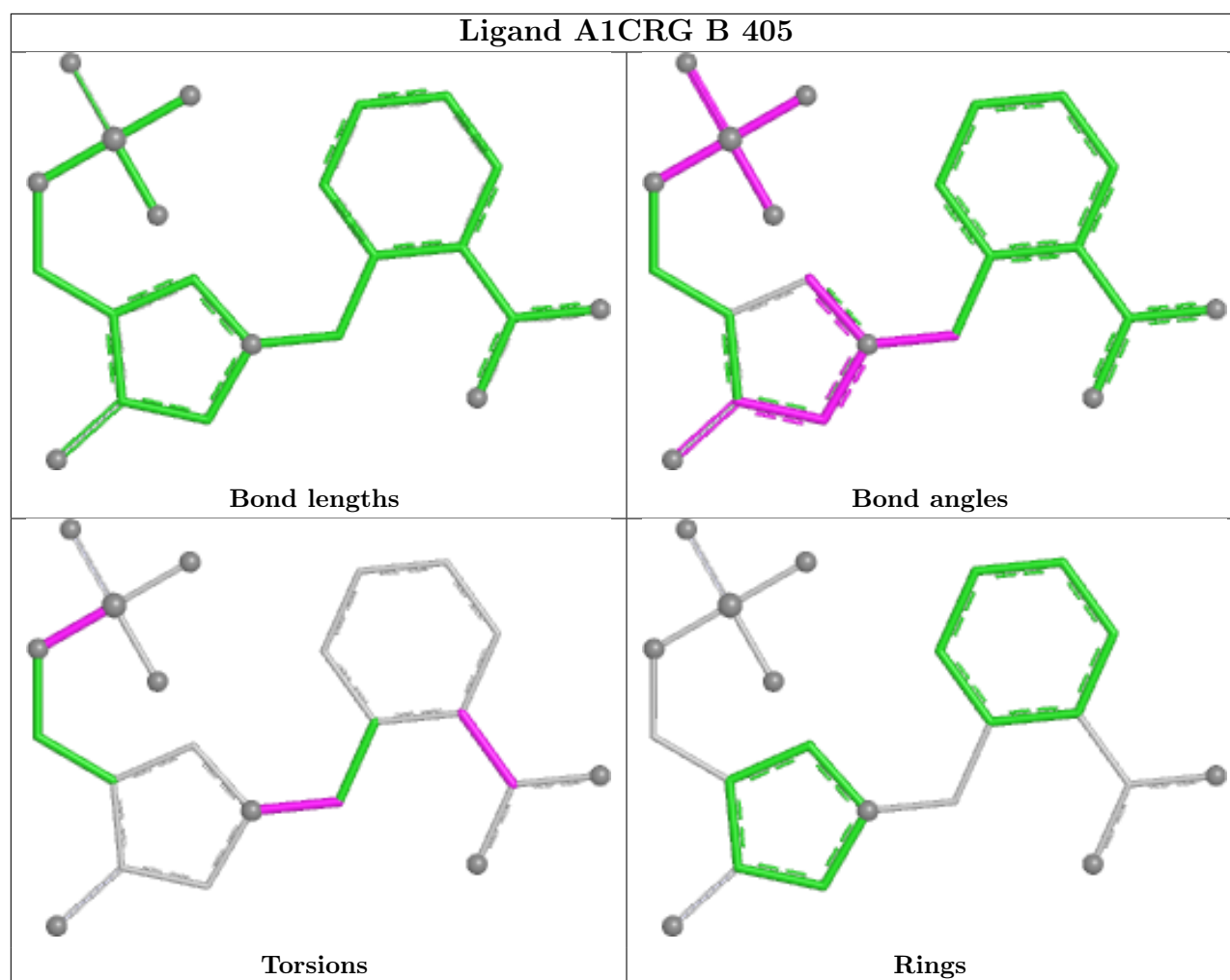


Ligand A1CRG A 404



Ligand PPV A 403





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	346/378 (91%)	0.59	39 (11%) 10 9	11, 26, 47, 87	3 (0%)
1	B	346/378 (91%)	0.05	10 (2%) 53 56	9, 20, 34, 69	5 (1%)
All	All	692/756 (91%)	0.32	49 (7%) 22 22	9, 23, 43, 87	8 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	ILE	5.4
1	B	370	ILE	5.0
1	B	334	ALA	4.6
1	A	286	LEU	3.9
1	A	238[A]	ARG	3.7
1	A	257	THR	3.6
1	A	113	VAL	3.6
1	A	272	LEU	3.4
1	B	332	SER	3.4
1	A	332	SER	3.3
1	A	334	ALA	3.3
1	A	256	THR	3.2
1	A	114	ASN	3.1
1	A	140	ALA	3.1
1	A	290	ALA	3.1
1	A	141	ALA	3.0
1	A	337	LEU	2.9
1	A	144	LEU	2.9
1	A	289	LEU	2.9
1	A	277	ALA	2.8
1	B	270	ASP	2.8
1	A	255	THR	2.8
1	A	282	ALA	2.8
1	B	331	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	225[A]	ASP	2.7
1	B	238[A]	ARG	2.6
1	A	25	PRO	2.6
1	A	248	ASP	2.5
1	A	110	GLY	2.5
1	A	142	SER	2.5
1	A	284	ALA	2.5
1	A	262	TRP	2.4
1	B	25	PRO	2.4
1	A	42[A]	ARG	2.4
1	B	114	ASN	2.3
1	A	266	ALA	2.3
1	A	281	PHE	2.3
1	B	333	ARG	2.2
1	A	250	LEU	2.2
1	B	335	GLU	2.2
1	A	112	GLY	2.2
1	A	333	ARG	2.1
1	A	111	ASP	2.1
1	A	279	PHE	2.1
1	A	260	THR	2.1
1	A	280	GLY	2.1
1	A	275	ASP	2.1
1	A	197	GLY	2.0
1	A	222	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 ⓘ

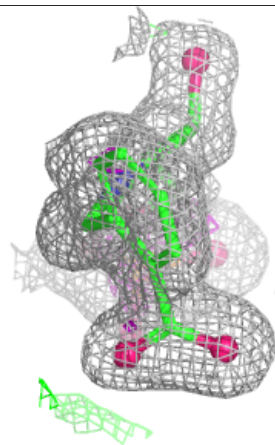
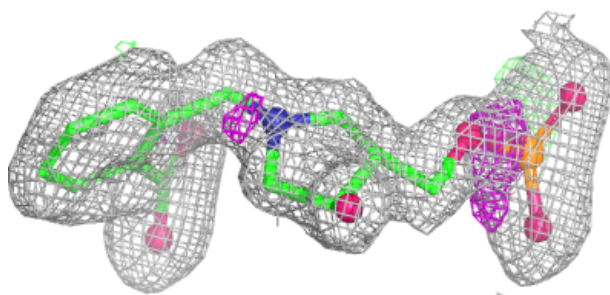
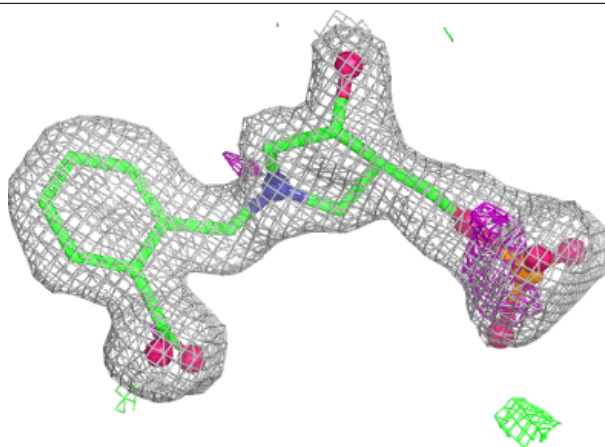
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	EDO	B	419	4/4	0.69	0.18	42,46,48,55	0
6	PEG	A	410	7/7	0.70	0.22	50,52,60,61	0
6	PEG	A	406	7/7	0.72	0.20	39,42,56,65	0
7	EDO	B	408	4/4	0.79	0.14	45,51,54,58	0
7	EDO	A	409	4/4	0.79	0.16	39,49,49,52	0
8	GOL	A	408	6/6	0.79	0.17	51,61,62,67	0
8	GOL	B	407	6/6	0.79	0.16	40,41,42,52	0
6	PEG	B	413	7/7	0.80	0.15	38,42,53,57	0
7	EDO	B	411	4/4	0.80	0.16	46,49,50,54	0
7	EDO	B	418	4/4	0.80	0.15	43,52,52,55	0
7	EDO	A	411	4/4	0.81	0.14	49,53,54,54	0
7	EDO	B	414	4/4	0.81	0.16	30,37,41,42	0
7	EDO	A	407	4/4	0.81	0.19	48,53,60,60	0
8	GOL	B	409	6/6	0.83	0.15	47,54,63,68	0
8	GOL	B	417	6/6	0.84	0.17	41,46,46,47	0
7	EDO	B	410	4/4	0.86	0.13	37,41,44,44	0
7	EDO	B	416	4/4	0.87	0.12	32,36,41,44	0
6	PEG	B	412	7/7	0.89	0.11	31,35,39,40	0
5	IMD	A	405	5/5	0.90	0.10	27,28,31,32	0
7	EDO	B	415	4/4	0.91	0.18	29,32,33,34	0
4	A1CRG	A	404	22/22	0.91	0.10	27,34,38,53	0
2	MG	A	402	1/1	0.93	0.06	28,28,28,28	0
5	IMD	B	406	5/5	0.94	0.12	24,24,25,25	0
4	A1CRG	B	405	22/22	0.95	0.07	19,21,25,32	0
3	PPV	A	403	9/9	0.97	0.07	20,24,26,29	0
2	MG	A	401	1/1	0.97	0.08	23,23,23,23	0
9	CL	B	403	1/1	0.97	0.23	37,37,37,37	0
2	MG	B	402	1/1	0.99	0.02	15,15,15,15	0
2	MG	B	401	1/1	0.99	0.03	15,15,15,15	0
3	PPV	B	404	9/9	0.99	0.04	14,15,17,18	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.

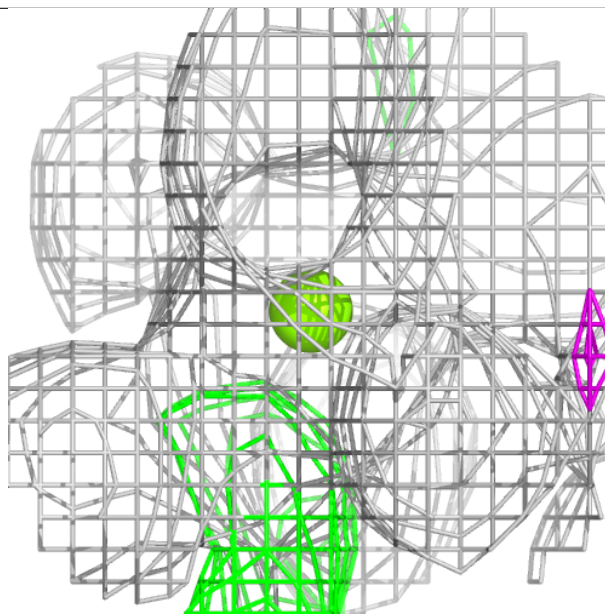
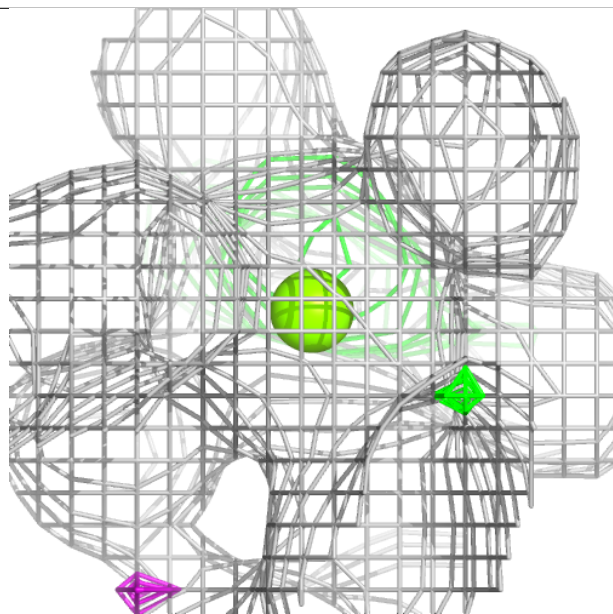
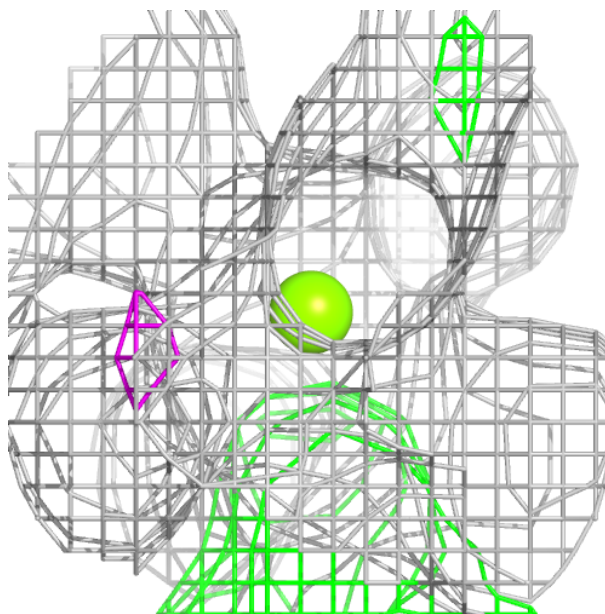
Electron density around A1CRG A 404:

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



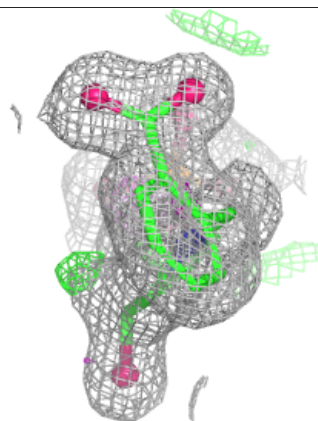
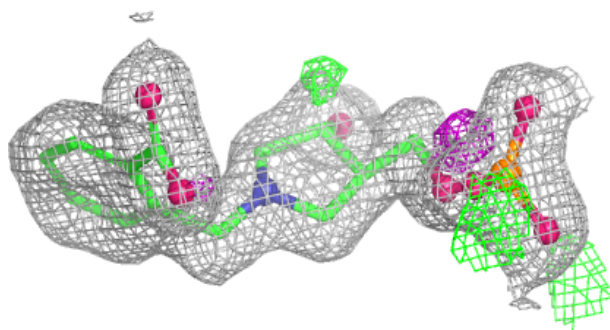
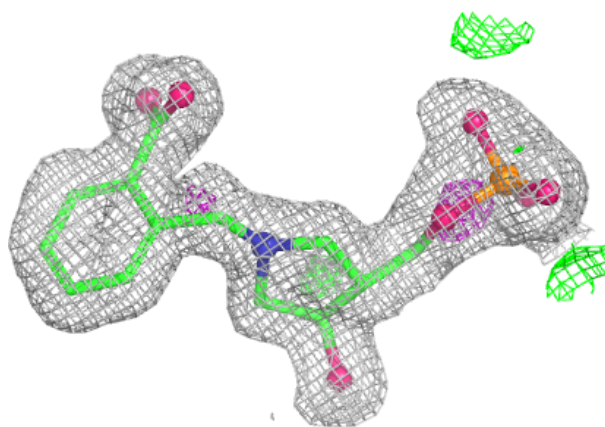
Electron density around MG A 402:

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



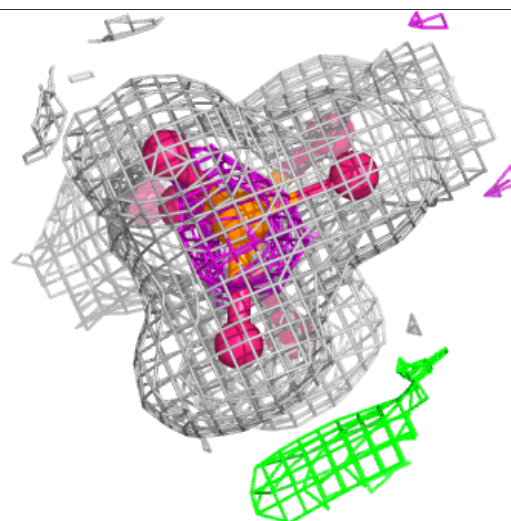
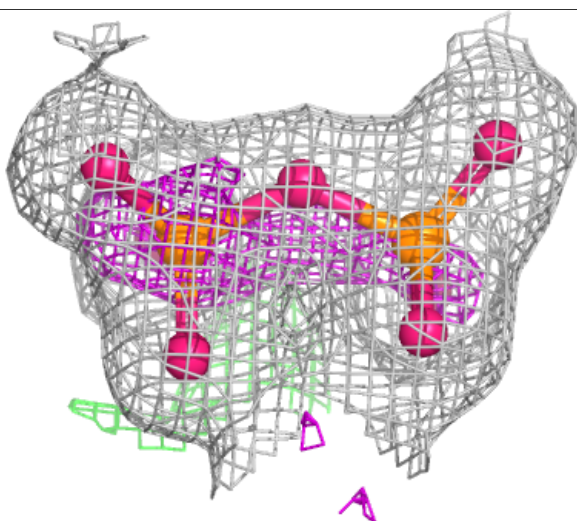
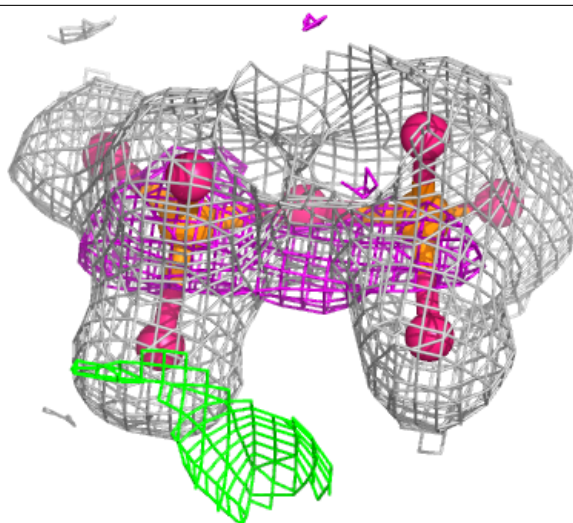
Electron density around A1CRG B 405:

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



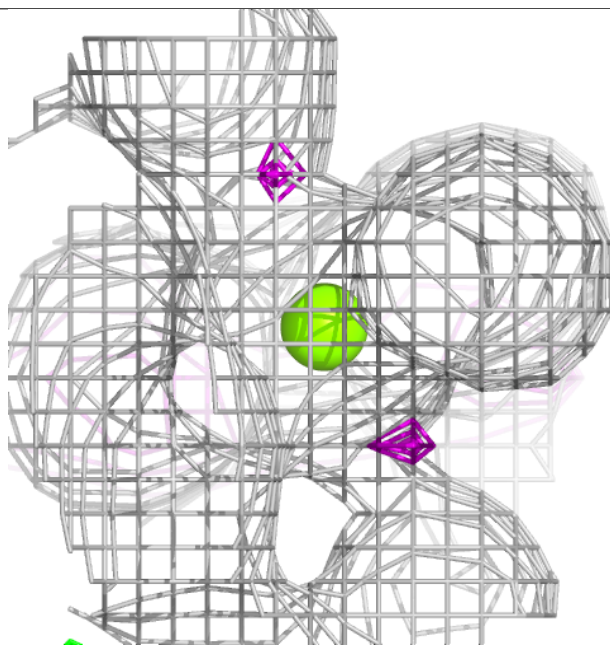
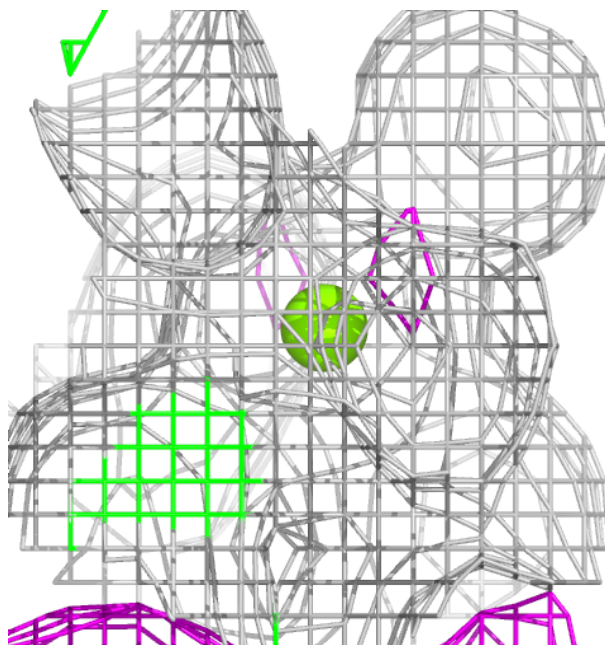
Electron density around PPV A 403:

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



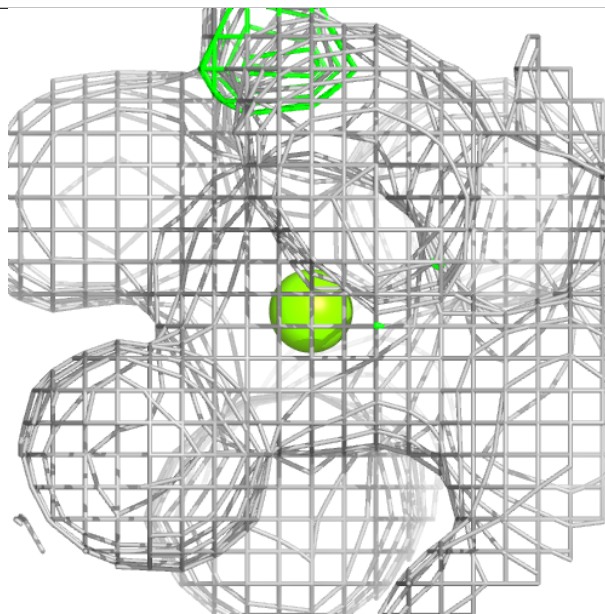
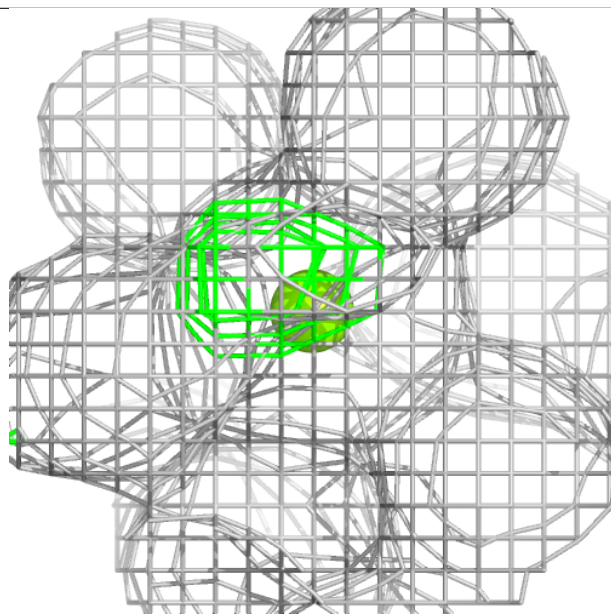
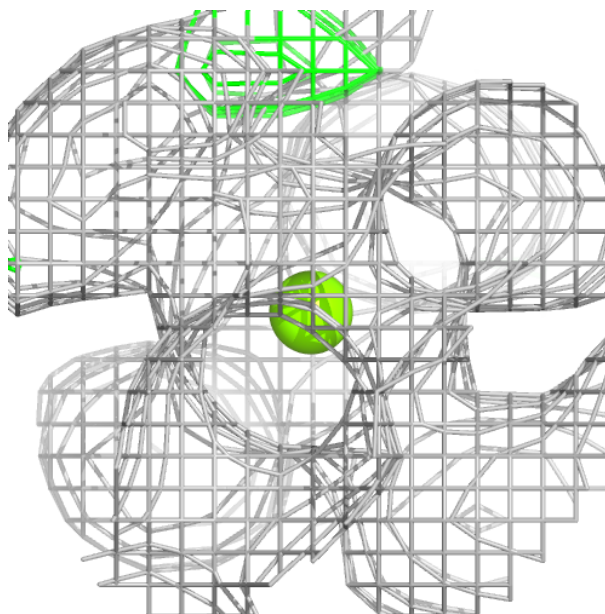
Electron density around MG A 401:

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



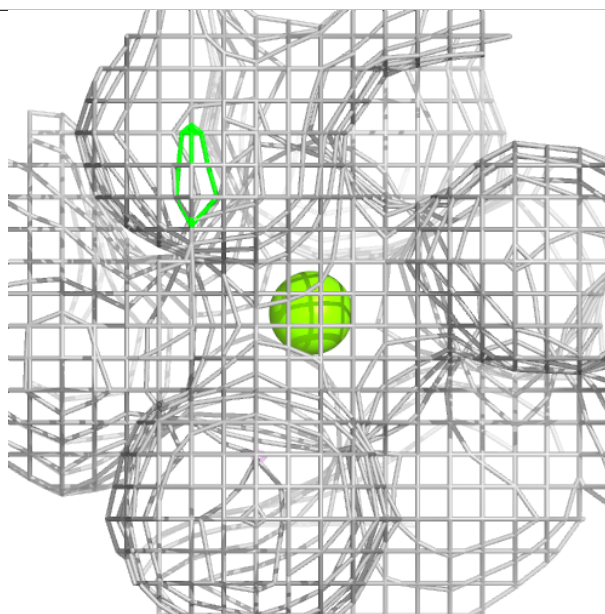
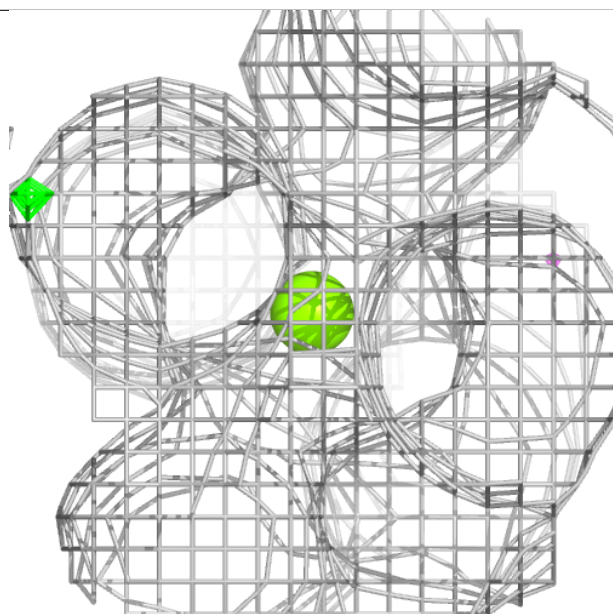
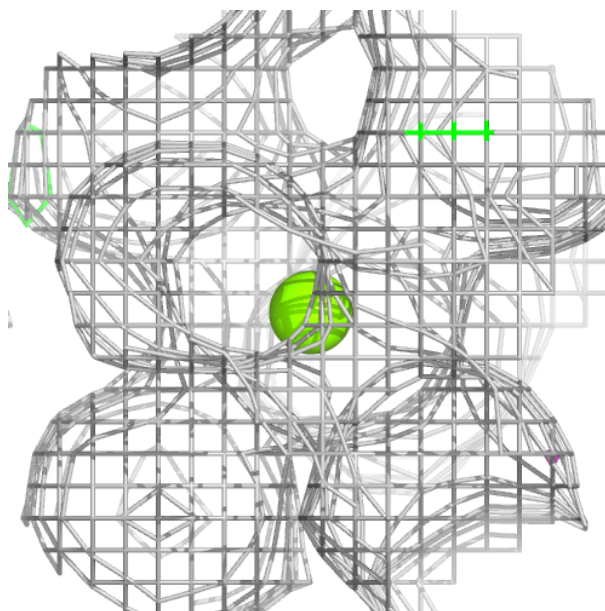
Electron density around MG B 402:

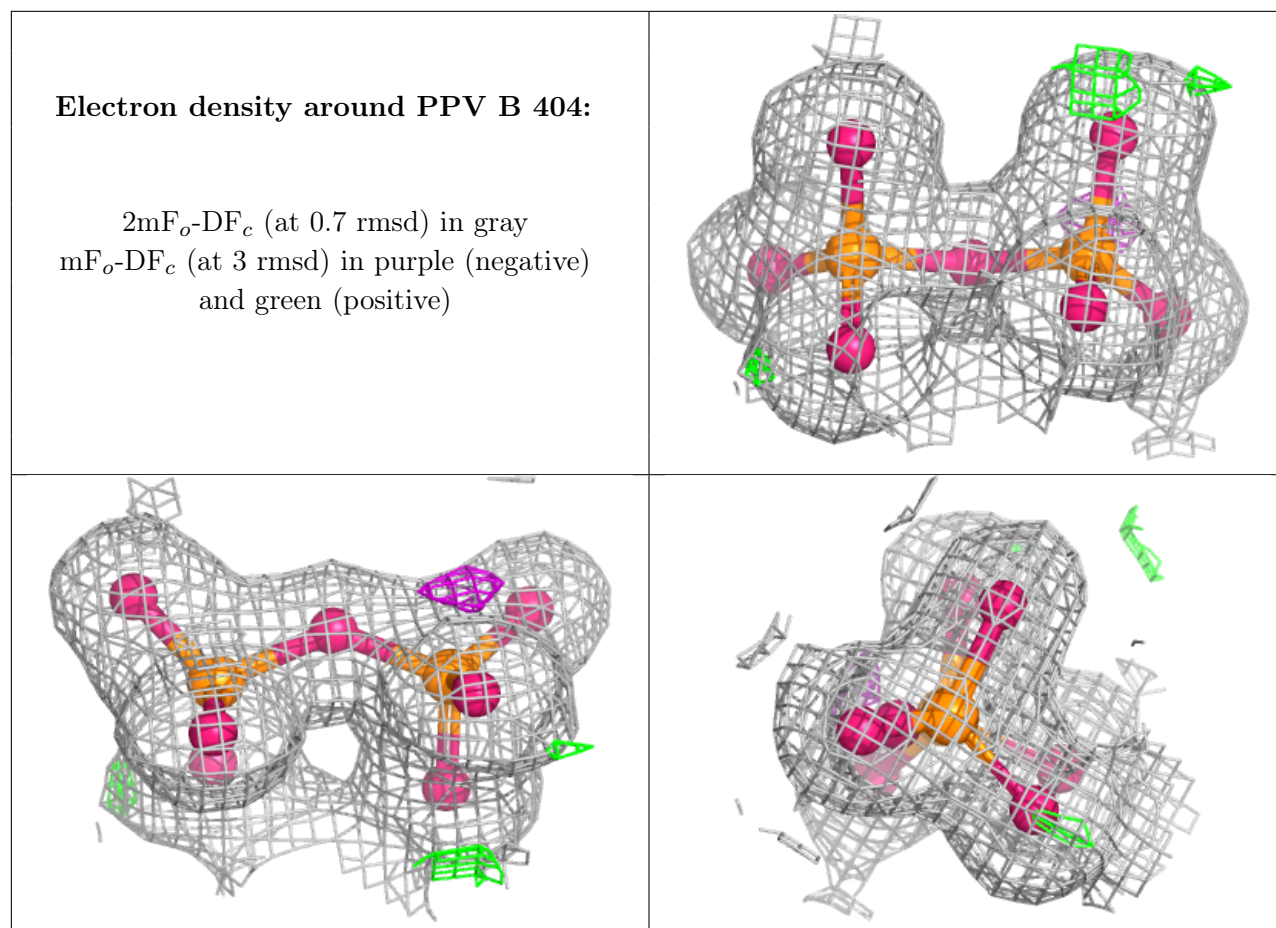
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.