Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 10:34 pm BST

PDB ID	:	2BWP
Title	:	5-Aminolevulinate Synthase from Rhodobacter capsulatus in complex with glycine
Authors	:	Astner, I.; Schulze, J.O.; Van Den Heuvel, J.J.; Jahn, D.; Schubert, W.-D.; Heinz, D.W.
Deposited on	:	2005-07-15
Resolution	:	2.70 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:

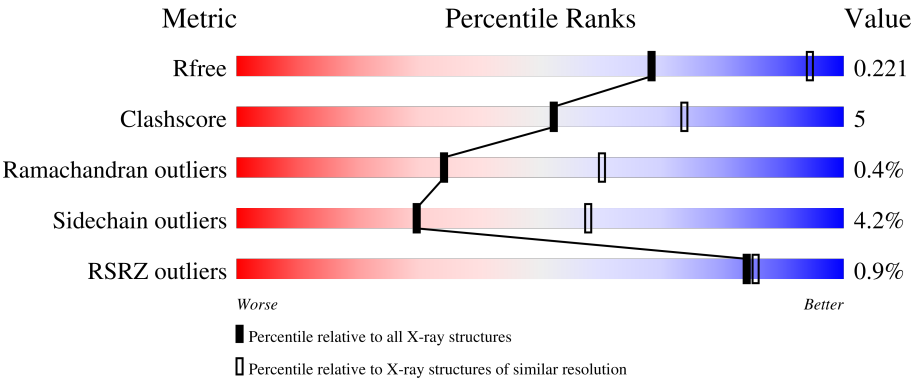
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	401	85% 13%
1	B	401	84% 14%
1	D	401	83% 15%
1	E	401	86% 13%

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
2	PLG	D	500	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12383 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 5-AMINOLEVULINATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3048	1936	539	558	15			
1	B	396	Total	C	N	O	S	0	0	0
			3029	1922	536	556	15			
1	D	398	Total	C	N	O	S	0	0	0
			3048	1936	539	558	15			
1	E	398	Total	C	N	O	S	0	0	0
			3048	1936	539	558	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	GLY	ASP	variant	UNP P18079
A	105	GLN	GLY	variant	UNP P18079
A	117	ASN	ILE	variant	UNP P18079
A	128	VAL	LEU	variant	UNP P18079
A	205	GLU	ASP	variant	UNP P18079
A	262	ARG	LYS	variant	UNP P18079
B	102	GLY	ASP	variant	UNP P18079
B	105	GLN	GLY	variant	UNP P18079
B	117	ASN	ILE	variant	UNP P18079
B	128	VAL	LEU	variant	UNP P18079
B	205	GLU	ASP	variant	UNP P18079
B	262	ARG	LYS	variant	UNP P18079
D	102	GLY	ASP	variant	UNP P18079
D	105	GLN	GLY	variant	UNP P18079
D	117	ASN	ILE	variant	UNP P18079
D	128	VAL	LEU	variant	UNP P18079
D	205	GLU	ASP	variant	UNP P18079
D	262	ARG	LYS	variant	UNP P18079
E	102	GLY	ASP	variant	UNP P18079
E	105	GLN	GLY	variant	UNP P18079
E	117	ASN	ILE	variant	UNP P18079

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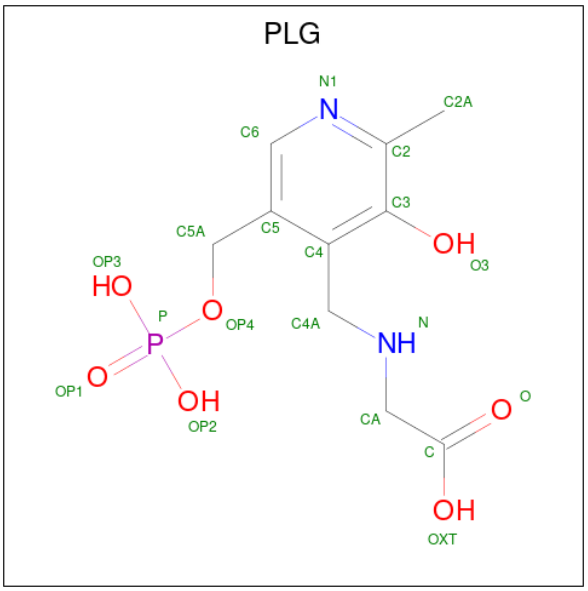
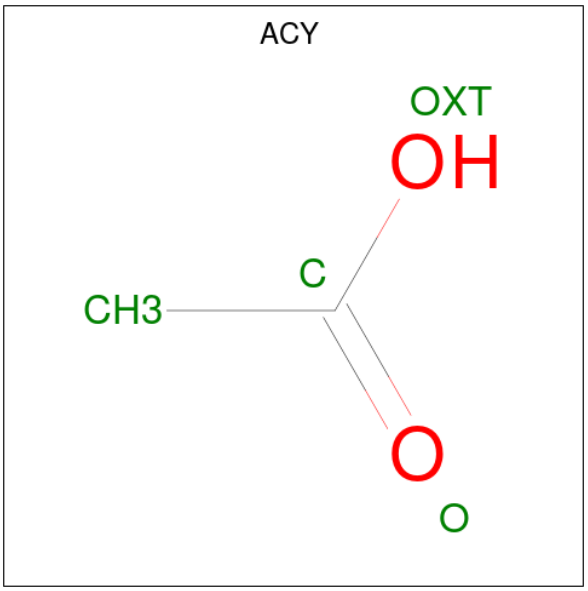
Chain	Residue	Modelled	Actual	Comment	Reference
E	128	VAL	LEU	variant	UNP P18079
E	205	GLU	ASP	variant	UNP P18079
E	262	ARG	LYS	variant	UNP P18079

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: $C_{10}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	E	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

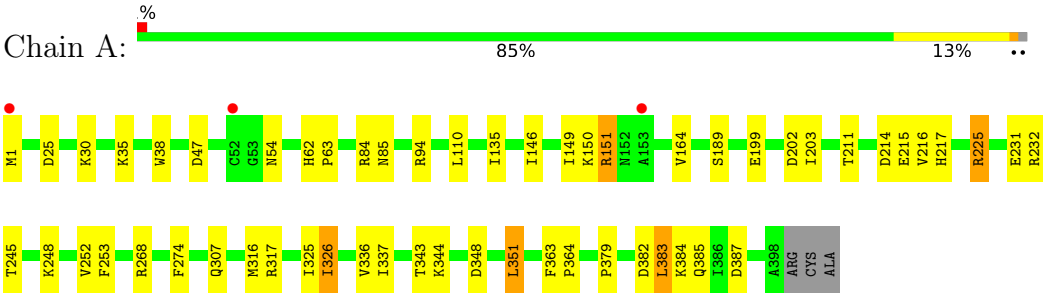
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total O 27 27	0	0
4	B	29	Total O 29 29	0	0
4	D	32	Total O 32 32	0	0
4	E	30	Total O 30 30	0	0

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.

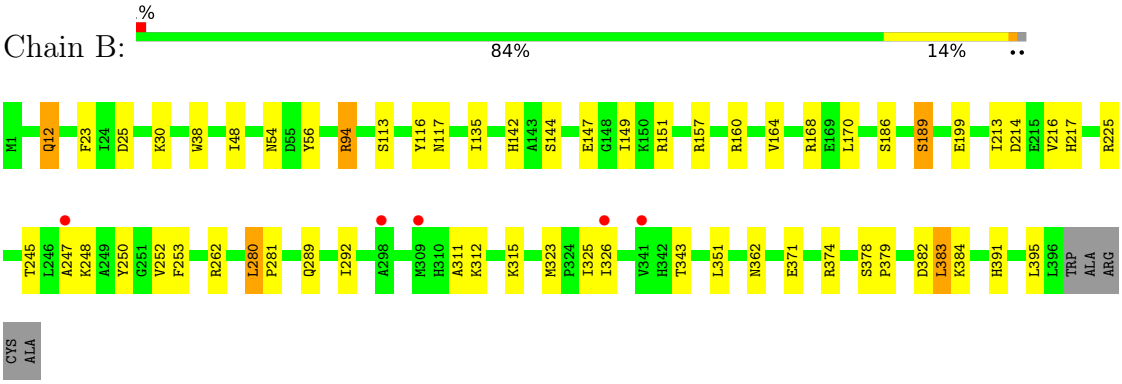
• Molecule 1: 5-AMINOLEVULINATE SYNTHASE

Chain A:



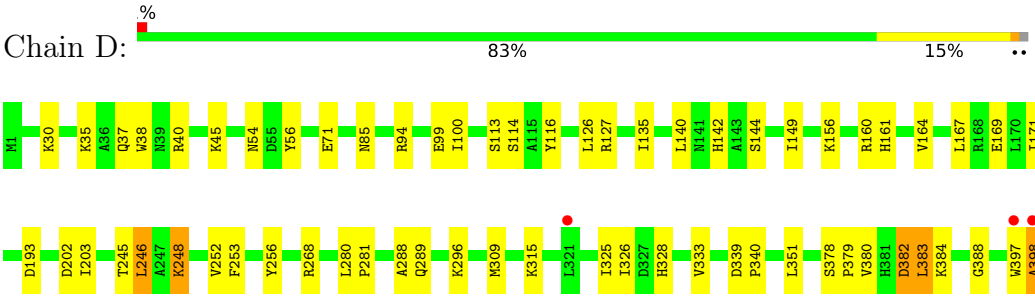
• Molecule 1: 5-AMINOLEVULINATE SYNTHASE

Chain B:



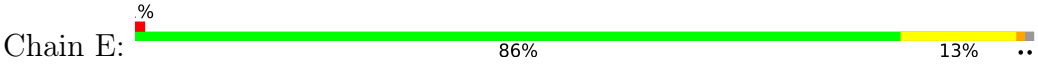
• Molecule 1: 5-AMINOLEVULINATE SYNTHASE

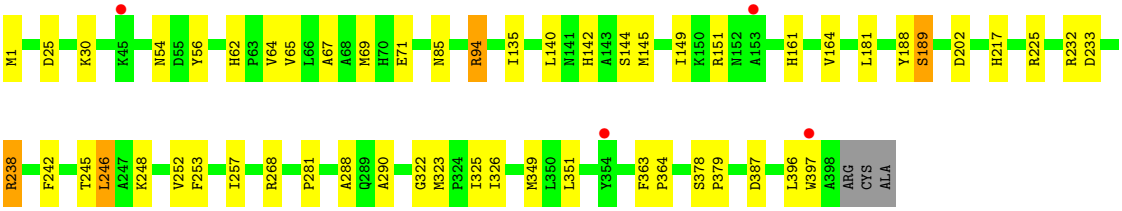
Chain D:



• Molecule 1: 5-AMINOLEVULINATE SYNTHASE

Chain E:




M1 D25 K30 K45 N54 D55 Y56 H62 P63 V64 V65 L66 A67 A68 M69 H70 E71 N85 R94 I135 L140 N141 H142 A143 S144 M145 I149 K150 R151 N152 A153 H161 V164 L181 Y188 S189 D202 H217 R225 R232 D233
R238 F242 T245 L246 A247 K248 V252 F253 I257 R268 P281 A288 Q289 A290 G322 M323 P324 I325 I326 M349 I350 L351 Y354 F363 P364 S378 P379 D387 L396 W397 A398 ARG CYS ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.00Å 92.02Å 248.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 29.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.70) 96.4 (29.83-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.220 0.169 , 0.221	Depositor DCC
R_{free} test set	2061 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12383	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PLG, ACY

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	0.88	1/3118 (0.0%)	0.79	2/4225 (0.0%)
1	B	0.87	1/3097 (0.0%)	0.79	2/4195 (0.0%)
1	D	1.01	4/3118 (0.1%)	0.81	2/4225 (0.0%)
1	E	0.92	3/3118 (0.1%)	0.81	4/4225 (0.1%)
All	All	0.92	9/12451 (0.1%)	0.80	10/16870 (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	E	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	398	ALA	C-O	21.17	1.63	1.23
1	B	12	GLN	CD-NE2	6.22	1.48	1.32
1	D	56	TYR	CE1-CZ	6.16	1.46	1.38
1	A	215	GLU	CB-CG	5.74	1.63	1.52
1	D	388	GLY	C-O	5.49	1.32	1.23
1	E	290	ALA	CA-CB	-5.46	1.41	1.52
1	E	56	TYR	CE2-CZ	5.37	1.45	1.38
1	E	233	ASP	CB-CG	5.01	1.62	1.51
1	D	71	GLU	CG-CD	5.00	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	E	225	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	D	268	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	348	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	232	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	E	323	MET	N-CA-C	-5.57	95.96	111.00
1	E	232	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	E	225	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	94	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	D	127	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	322	GLY	Peptide

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	3048	0	3030	36	0
1	B	3029	0	3015	33	0
1	D	3048	0	3030	40	0
1	E	3048	0	3030	35	0
2	A	20	0	12	3	0
2	B	20	0	12	2	0
2	D	20	0	11	7	0
2	E	20	0	12	4	0
3	A	4	0	3	0	0
3	D	4	0	3	1	0
3	E	4	0	3	0	0
4	A	27	0	0	1	0
4	B	29	0	0	0	0
4	D	32	0	0	1	0
4	E	30	0	0	1	0
All	All	12383	0	12161	133	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 5.

All (133) 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:D:398:ALA:C	1:D:398:ALA:O	1.63	1.36
1:D:383:LEU:H	1:D:383:LEU:HD23	1.22	1.02
1:D:383:LEU:H	1:D:383:LEU:CD2	1.74	1.00
1:A:248:LYS:NZ	2:A:500:PLG:H4A2	1.82	0.94
1:E:62:HIS:ND1	1:E:64:VAL:HG22	1.96	0.81
1:D:245:THR:HG21	1:D:248:LYS:HD3	1.63	0.80
1:E:67:ALA:O	1:E:71:GLU:HG2	1.84	0.78
1:A:248:LYS:HZ1	2:A:500:PLG:H4A2	1.47	0.77
1:E:238:ARG:HH11	1:E:238:ARG:HG2	1.49	0.77
1:B:113:SER:HB2	1:B:117:ASN:HD22	1.50	0.76
1:A:248:LYS:HZ3	2:A:500:PLG:H4A2	1.54	0.72
1:E:62:HIS:CE1	1:E:64:VAL:HG22	2.25	0.72
1:E:245:THR:HG21	1:E:248:LYS:HD2	1.73	0.71
1:D:248:LYS:HZ1	2:D:500:PLG:HA2	1.57	0.69
1:D:382:ASP:OD1	1:D:384:LYS:HB2	1.93	0.69
1:E:142:HIS:CE1	2:E:500:PLG:H	2.11	0.68
1:D:383:LEU:CD2	1:D:383:LEU:N	2.54	0.67
1:E:94:ARG:HG2	1:E:94:ARG:HH11	1.60	0.66
1:B:113:SER:HB2	1:B:117:ASN:ND2	2.12	0.64
1:A:225:ARG:HG3	1:A:231:GLU:OE2	1.98	0.64
1:E:142:HIS:HE1	2:E:500:PLG:H	1.47	0.63
1:E:202:ASP:OD1	1:E:238:ARG:NH2	2.32	0.62
1:E:248:LYS:NZ	2:E:500:PLG:H4A2	2.16	0.60
1:D:54:ASN:HB3	1:D:248:LYS:HG3	1.84	0.59
1:D:383:LEU:HD23	1:D:383:LEU:N	2.06	0.59
1:D:85:ASN:HB2	4:E:2001:HOH:O	2.02	0.58
1:A:151:ARG:NH2	1:B:147:GLU:O	2.37	0.57
1:B:378:SER:HB2	1:B:379:PRO:HD2	1.85	0.57
1:D:248:LYS:NZ	2:D:500:PLG:HA2	2.19	0.56
1:B:135:ILE:HG21	1:B:149:ILE:HG12	1.88	0.56
1:B:382:ASP:OD1	1:B:384:LYS:HB3	2.05	0.56
1:A:238:ARG:HH11	1:A:238:ARG:HG2	1.71	0.56
1:B:160:ARG:NH1	1:D:160:ARG:HD3	2.21	0.56
1:D:37:GLN:NE2	1:D:45:LYS:HD2	2.21	0.55
1:E:94:ARG:HG2	1:E:94:ARG:NH1	2.17	0.55
1:D:135:ILE:HG21	1:D:149:ILE:HG12	1.88	0.55
1:D:315:LYS:HG2	1:D:325:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TRP:HB2	1:B:48:ILE:HD13	1.90	0.53
1:D:164:VAL:HG13	1:D:203:ILE:HD11	1.90	0.53
1:A:110:LEU:HD11	1:A:274:PHE:CE2	2.43	0.52
1:D:339:ASP:OD1	1:D:340:PRO:HD2	2.10	0.52
1:E:135:ILE:HG21	1:E:149:ILE:HG12	1.90	0.52
1:B:54:ASN:HD21	1:B:374:ARG:HH12	1.56	0.52
1:E:142:HIS:CD2	1:E:144:SER:H	2.28	0.52
1:A:135:ILE:HG21	1:A:149:ILE:HG12	1.92	0.51
1:E:246:LEU:HG	1:E:288:ALA:HB1	1.91	0.51
1:D:167:LEU:O	1:D:171:ILE:HG22	2.11	0.50
1:D:378:SER:HB2	1:D:379:PRO:HD2	1.91	0.50
1:E:65:VAL:O	1:E:69:MET:HG3	2.11	0.50
1:B:54:ASN:HB3	1:B:248:LYS:HG2	1.93	0.50
1:A:326:ILE:HD11	1:A:336:VAL:CG2	2.41	0.49
1:A:151:ARG:HG2	1:B:151:ARG:NH1	2.27	0.49
1:B:157:ARG:HB3	1:B:170:LEU:HD13	1.94	0.49
1:A:317:ARG:NH2	1:A:387:ASP:OD1	2.46	0.49
1:D:248:LYS:HE2	2:D:500:PLG:H4A2	1.95	0.49
1:E:238:ARG:HG2	1:E:238:ARG:NH1	2.16	0.49
1:B:189:SER:HB3	1:B:217:HIS:NE2	2.28	0.49
1:B:247:ALA:HB2	1:B:253:PHE:HA	1.95	0.48
1:D:193:ASP:HB3	1:D:328:HIS:CG	2.48	0.48
1:E:378:SER:HB2	1:E:379:PRO:HD2	1.95	0.48
1:E:54:ASN:HB3	1:E:248:LYS:HG2	1.95	0.48
1:E:349:MET:HB3	1:E:396:LEU:HD11	1.96	0.48
1:A:164:VAL:HG11	1:A:199:GLU:HB3	1.96	0.47
1:B:391:HIS:CE1	1:B:395:LEU:HD11	2.49	0.47
1:D:140:LEU:HD12	1:D:161:HIS:CG	2.50	0.47
1:A:189:SER:HB3	1:A:217:HIS:CD2	2.50	0.47
1:B:362:ASN:HA	1:B:371:GLU:HG3	1.97	0.47
1:B:186:SER:HB3	1:B:213:ILE:HD11	1.97	0.46
1:E:189:SER:HB3	1:E:217:HIS:NE2	2.30	0.45
1:E:140:LEU:HD12	1:E:161:HIS:CG	2.52	0.45
1:D:248:LYS:NZ	2:D:500:PLG:H4A2	2.32	0.45
1:E:248:LYS:HZ3	2:E:500:PLG:H4A2	1.82	0.45
3:D:600:ACY:O	1:E:85:ASN:HB3	2.16	0.45
1:D:99:GLU:OE2	1:D:296:LYS:NZ	2.39	0.45
1:D:246:LEU:HG	1:D:288:ALA:HB1	1.98	0.45
1:A:214:ASP:OD1	1:A:214:ASP:C	2.56	0.44
1:D:325:ILE:HD11	1:D:333:VAL:HG13	2.00	0.44
1:A:35:LYS:HE3	1:A:47:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:NZ	2:B:500:PLG:H4A2	2.31	0.44
1:A:307:GLN:HB2	1:A:379:PRO:HD3	1.98	0.44
1:E:142:HIS:H	1:E:145:MET:CE	2.31	0.44
1:A:25:ASP:CG	1:B:94:ARG:HH11	2.21	0.44
1:B:383:LEU:H	1:B:383:LEU:HD22	1.82	0.44
1:D:248:LYS:CE	2:D:500:PLG:H4A2	2.48	0.44
1:D:114:SER:HB2	2:D:500:PLG:OP3	2.18	0.43
1:B:142:HIS:HB2	2:B:500:PLG:H2A3	2.00	0.43
1:A:253:PHE:HB2	1:B:281:PRO:HG3	2.01	0.43
1:D:38:TRP:CZ2	1:D:40:ARG:HG2	2.53	0.43
1:E:54:ASN:ND2	1:E:248:LYS:HE3	2.34	0.43
1:B:164:VAL:HG11	1:B:199:GLU:HB3	2.01	0.43
1:B:214:ASP:C	1:B:214:ASP:OD1	2.57	0.43
1:E:363:PHE:CD1	1:E:364:PRO:HA	2.53	0.43
1:A:211:THR:OG1	1:A:239:ILE:HA	2.19	0.43
1:A:164:VAL:HG13	1:A:203:ILE:HD12	2.00	0.43
1:B:113:SER:HA	1:B:280:LEU:HD13	1.99	0.43
1:A:326:ILE:HD11	1:A:336:VAL:HG21	2.00	0.43
1:A:363:PHE:CG	1:A:364:PRO:HA	2.54	0.42
1:A:84:ARG:HA	1:A:84:ARG:HD2	1.90	0.42
1:A:216:VAL:HG13	1:A:245:THR:CG2	2.49	0.42
1:A:146:ILE:O	1:A:150:LYS:HG2	2.20	0.42
1:B:250:TYR:CE1	1:B:292:ILE:HA	2.54	0.42
1:D:202:ASP:HB3	4:D:2019:HOH:O	2.20	0.42
1:D:281:PRO:HG3	1:E:253:PHE:HB2	2.02	0.42
1:E:94:ARG:NH1	1:E:94:ARG:CG	2.82	0.42
1:A:337:ILE:HB	1:A:343:THR:OG1	2.20	0.42
1:B:56:TYR:O	1:B:378:SER:HB2	2.18	0.42
1:D:253:PHE:CD1	1:E:281:PRO:HD3	2.54	0.42
1:D:126:LEU:HD13	1:D:181:LEU:HD13	2.02	0.42
1:E:142:HIS:HD2	1:E:144:SER:OG	2.03	0.42
1:A:54:ASN:HD22	1:A:248:LYS:HE3	1.85	0.42
1:A:62:HIS:HA	1:A:63:PRO:HD3	1.95	0.41
1:B:216:VAL:HG13	1:B:245:THR:CG2	2.49	0.41
1:D:100:ILE:HG21	1:D:256:TYR:CD1	2.56	0.41
1:E:161:HIS:HE1	1:E:188:TYR:CD2	2.38	0.41
1:A:344:LYS:HE3	4:A:2006:HOH:O	2.19	0.41
1:E:363:PHE:CG	1:E:364:PRO:HA	2.56	0.41
1:A:25:ASP:OD2	1:B:94:ARG:NH1	2.48	0.41
1:A:94:ARG:NE	1:B:25:ASP:OD2	2.53	0.41
1:E:242:PHE:O	1:E:257:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ALA:O	1:B:315:LYS:HG3	2.20	0.41
1:A:382:ASP:C	1:A:384:LYS:H	2.24	0.41
1:D:142:HIS:HB2	2:D:500:PLG:H2A3	2.02	0.41
1:B:116:TYR:CD2	1:B:144:SER:HB3	2.55	0.41
1:D:116:TYR:CD2	1:D:144:SER:HB3	2.55	0.41
1:D:378:SER:OG	1:D:380:VAL:HG22	2.21	0.41
1:A:85:ASN:HA	1:B:23:PHE:CD1	2.56	0.41
1:A:38:TRP:CE3	1:A:351:LEU:HD22	2.56	0.40
1:A:189:SER:HB3	1:A:217:HIS:NE2	2.36	0.40
1:D:309:MET:HE2	1:D:309:MET:C	2.42	0.40
1:A:202:ASP:OD1	1:A:238:ARG:NH2	2.55	0.40
1:D:38:TRP:CH2	1:D:40:ARG:HG2	2.56	0.40
1:D:94:ARG:NE	1:E:25:ASP:OD2	2.54	0.40
1:E:181:LEU:C	1:E:181:LEU:HD23	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	396/401 (99%)	383 (97%)	10 (2%)	3 (1%)	19	43
1	B	394/401 (98%)	384 (98%)	9 (2%)	1 (0%)	41	66
1	D	396/401 (99%)	387 (98%)	7 (2%)	2 (0%)	29	54
1	E	396/401 (99%)	385 (97%)	10 (2%)	1 (0%)	41	66
All	All	1582/1604 (99%)	1539 (97%)	36 (2%)	7 (0%)	34	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	LEU

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Mol	Chain	Res	Type
1	A	252	VAL
1	B	252	VAL
1	D	252	VAL
1	E	252	VAL
1	A	268	ARG
1	D	382	ASP

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/313 (99%)	301 (97%)	10 (3%)	39	68
1	B	310/313 (99%)	296 (96%)	14 (4%)	27	55
1	D	311/313 (99%)	297 (96%)	14 (4%)	27	55
1	E	311/313 (99%)	297 (96%)	14 (4%)	27	55
All	All	1243/1252 (99%)	1191 (96%)	52 (4%)	30	58

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	LYS
1	A	151	ARG
1	A	225	ARG
1	A	316	MET
1	A	325	ILE
1	A	326	ILE
1	A	351	LEU
1	A	383	LEU
1	A	385	GLN
1	B	12	GLN
1	B	30	LYS
1	B	168	ARG
1	B	189	SER
1	B	262	ARG

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Mol	Chain	Res	Type
1	B	280	LEU
1	B	289	GLN
1	B	312	LYS
1	B	323	MET
1	B	325	ILE
1	B	326	ILE
1	B	343	THR
1	B	351	LEU
1	B	383	LEU
1	D	30	LYS
1	D	35	LYS
1	D	113	SER
1	D	156	LYS
1	D	169	GLU
1	D	189	SER
1	D	246	LEU
1	D	248	LYS
1	D	280	LEU
1	D	289	GLN
1	D	326	ILE
1	D	351	LEU
1	D	383	LEU
1	D	397	TRP
1	E	1	MET
1	E	30	LYS
1	E	94	ARG
1	E	151	ARG
1	E	164	VAL
1	E	189	SER
1	E	238	ARG
1	E	246	LEU
1	E	268	ARG
1	E	325	ILE
1	E	326	ILE
1	E	351	LEU
1	E	387	ASP
1	E	397	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS

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Mol	Chain	Res	Type
1	A	105	GLN
1	A	117	ASN
1	A	307	GLN
1	B	117	ASN
1	B	237	HIS
1	B	307	GLN
1	B	359	GLN
1	D	4	ASN
1	D	12	GLN
1	D	37	GLN
1	D	54	ASN
1	D	105	GLN
1	D	342	HIS
1	E	85	ASN
1	E	142	HIS
1	E	307	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

7 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	PLG	D	500	-	20,20,20	1.74	3 (15%)	25,28,28	1.68	7 (28%)
3	ACY	A	600	-	3,3,3	0.60	0	3,3,3	1.00	0
3	ACY	D	600	-	3,3,3	0.90	0	3,3,3	0.57	0
2	PLG	B	500	-	20,20,20	2.00	6 (30%)	25,28,28	1.78	6 (24%)
2	PLG	A	500	-	20,20,20	1.85	6 (30%)	25,28,28	2.01	7 (28%)
2	PLG	E	500	-	20,20,20	1.46	2 (10%)	25,28,28	1.81	5 (20%)
3	ACY	E	600	-	3,3,3	0.70	0	3,3,3	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	D	500	-	-	6/12/12/12	0/1/1/1
2	PLG	A	500	-	-	7/12/12/12	0/1/1/1
2	PLG	E	500	-	-	7/12/12/12	0/1/1/1
2	PLG	B	500	-	-	7/12/12/12	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	PLG	C4A-C4	4.37	1.57	1.51
2	B	500	PLG	C4A-C4	4.28	1.57	1.51
2	B	500	PLG	C3-C2	3.83	1.44	1.40
2	E	500	PLG	P-OP1	3.74	1.62	1.50
2	A	500	PLG	C3-C2	3.69	1.44	1.40
2	D	500	PLG	P-OP1	3.50	1.61	1.50
2	B	500	PLG	P-OP1	3.26	1.61	1.50
2	A	500	PLG	C4A-C4	3.23	1.56	1.51
2	B	500	PLG	C5-C4	3.03	1.44	1.40
2	A	500	PLG	P-OP1	2.98	1.60	1.50
2	E	500	PLG	C4A-C4	2.97	1.55	1.51
2	D	500	PLG	C2A-C2	2.84	1.55	1.50
2	A	500	PLG	C2A-C2	2.79	1.55	1.50
2	B	500	PLG	C3-C4	2.63	1.44	1.40
2	A	500	PLG	P-OP2	2.56	1.64	1.54
2	A	500	PLG	OP4-C5A	-2.28	1.36	1.45
2	B	500	PLG	C6-C5	2.02	1.41	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	PLG	C4A-N-CA	-5.37	106.98	112.58
2	A	500	PLG	C6-C5-C4	4.50	121.30	118.12
2	E	500	PLG	C4A-C4-C5	4.49	124.70	119.71
2	B	500	PLG	C6-C5-C4	4.01	120.95	118.12
2	E	500	PLG	C6-C5-C4	3.95	120.91	118.12
2	D	500	PLG	C6-C5-C4	3.85	120.84	118.12
2	B	500	PLG	C5A-C5-C6	-3.73	113.23	119.37
2	E	500	PLG	O3-C3-C2	3.09	124.23	117.49
2	D	500	PLG	OP3-P-OP4	2.78	114.12	106.73
2	A	500	PLG	C5A-C5-C6	-2.76	114.83	119.37
2	A	500	PLG	C4A-C4-C3	2.73	122.97	120.04
2	B	500	PLG	C4A-N-CA	-2.65	109.82	112.58
2	A	500	PLG	C2A-C2-C3	2.62	124.13	120.89
2	B	500	PLG	OP3-P-OP4	2.55	113.51	106.73
2	D	500	PLG	C4A-C4-C5	2.51	122.50	119.71
2	B	500	PLG	C3-C4-C5	-2.50	116.32	118.72
2	A	500	PLG	C3-C4-C5	-2.41	116.41	118.72
2	D	500	PLG	OP2-P-OP1	-2.34	101.51	110.68
2	E	500	PLG	C5-C6-N1	-2.21	120.14	123.82
2	E	500	PLG	C5A-C5-C6	-2.12	115.88	119.37
2	D	500	PLG	C3-C4-C5	-2.10	116.70	118.72
2	B	500	PLG	C4A-C4-C5	2.09	122.03	119.71
2	D	500	PLG	C5A-C5-C6	-2.09	115.94	119.37
2	D	500	PLG	C4A-N-CA	-2.05	110.44	112.58
2	A	500	PLG	O3-C3-C2	2.01	121.88	117.49

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	PLG	C5A-OP4-P-OP2
2	A	500	PLG	C5A-OP4-P-OP3
2	B	500	PLG	C5A-OP4-P-OP1
2	B	500	PLG	C5A-OP4-P-OP2
2	B	500	PLG	C5A-OP4-P-OP3
2	D	500	PLG	C5-C4-C4A-N
2	D	500	PLG	C5A-OP4-P-OP2
2	D	500	PLG	C5A-OP4-P-OP3
2	E	500	PLG	C5A-OP4-P-OP2
2	E	500	PLG	C5A-OP4-P-OP3
2	A	500	PLG	C4-C4A-N-CA

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Mol	Chain	Res	Type	Atoms
2	A	500	PLG	C5-C4-C4A-N
2	B	500	PLG	C5-C4-C4A-N
2	B	500	PLG	OXT-C-CA-N
2	E	500	PLG	C5-C4-C4A-N
2	D	500	PLG	C4-C4A-N-CA
2	B	500	PLG	O-C-CA-N
2	D	500	PLG	C3-C4-C4A-N
2	A	500	PLG	C5A-OP4-P-OP1
2	E	500	PLG	O-C-CA-N
2	E	500	PLG	OXT-C-CA-N
2	A	500	PLG	C3-C4-C4A-N
2	B	500	PLG	C3-C4-C4A-N
2	E	500	PLG	C3-C4-C4A-N
2	A	500	PLG	C-CA-N-C4A
2	D	500	PLG	C5A-OP4-P-OP1
2	E	500	PLG	C4-C4A-N-CA

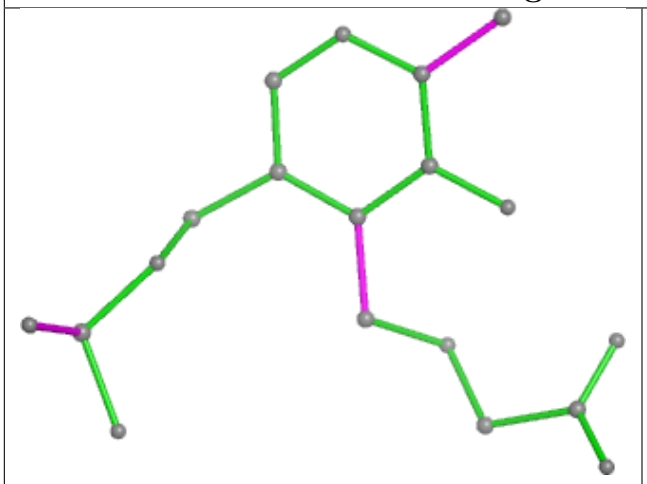
There are no ring outliers.

5 monomers are involved in 17 short contacts:

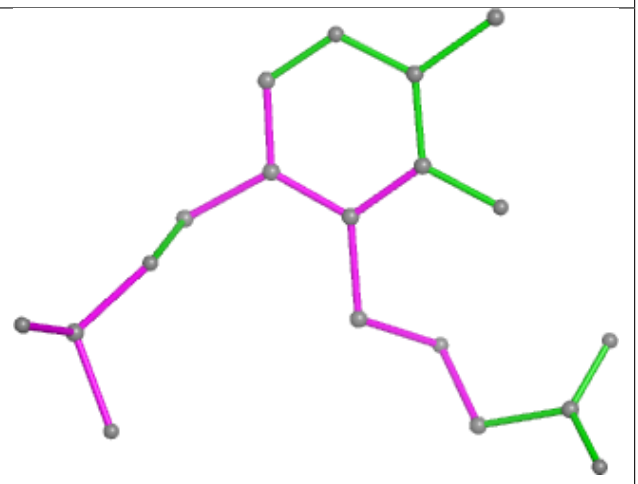
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	PLG	7	0
3	D	600	ACY	1	0
2	B	500	PLG	2	0
2	A	500	PLG	3	0
2	E	500	PLG	4	0

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.

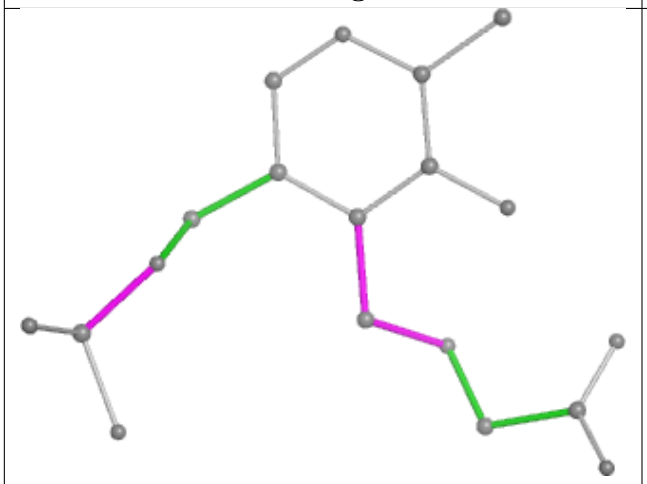
Ligand PLG D 500



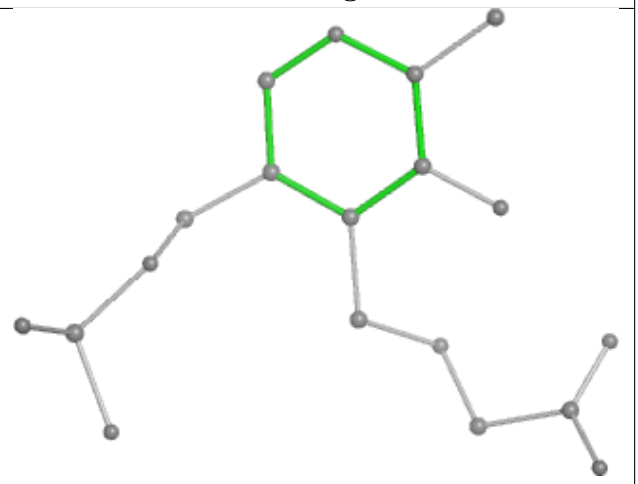
Bond lengths



Bond angles

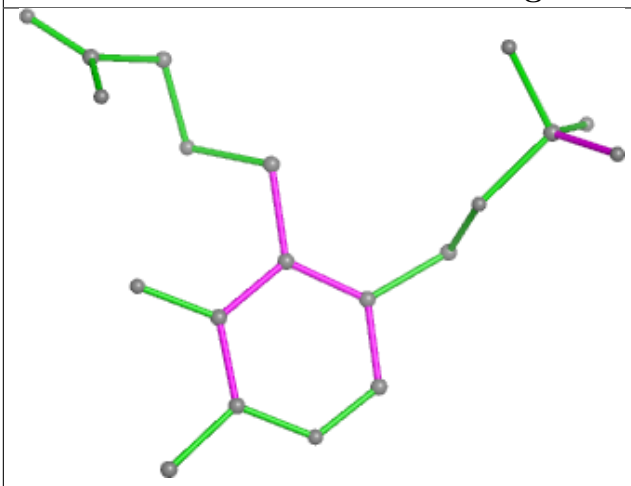


Torsions

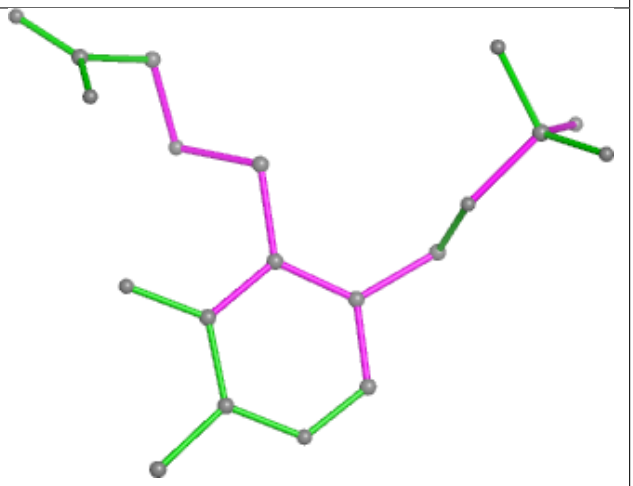


Rings

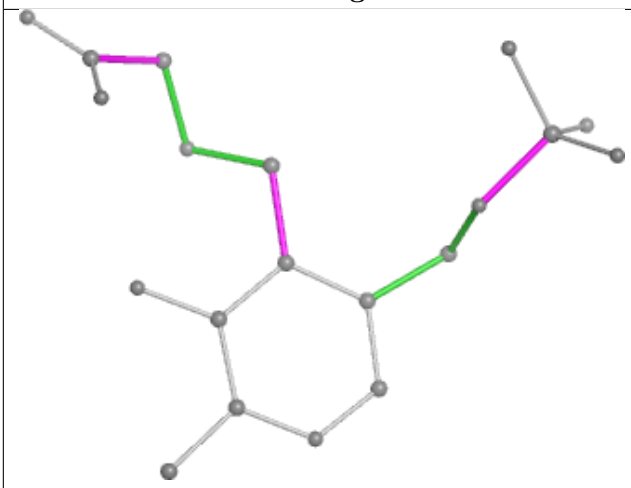
Ligand PLG B 500



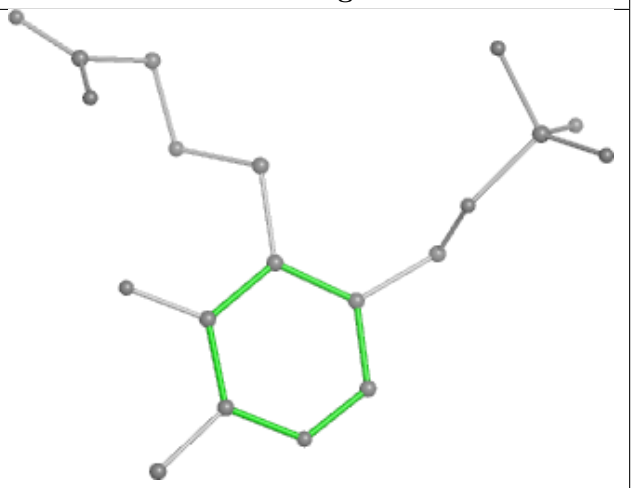
Bond lengths



Bond angles

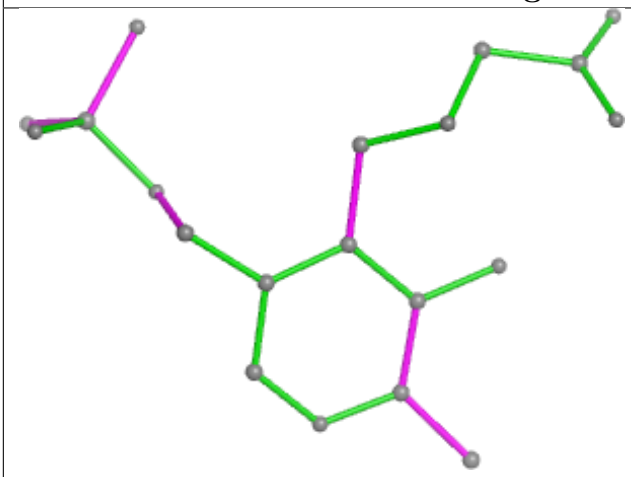


Torsions

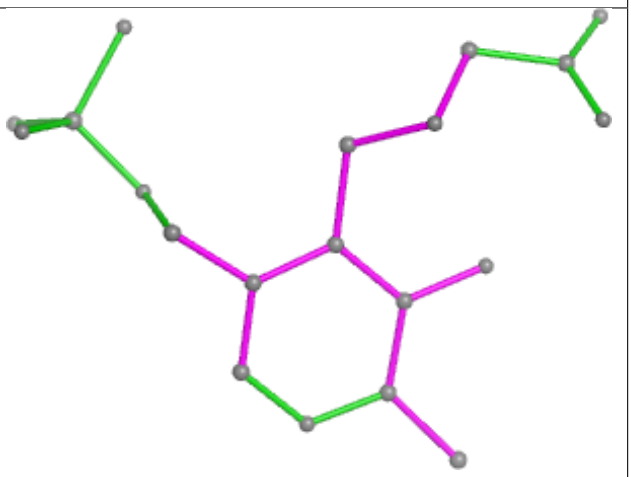


Rings

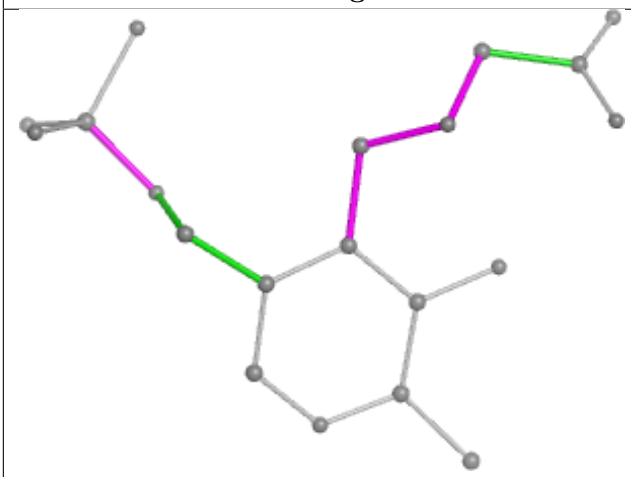
Ligand PLG A 500



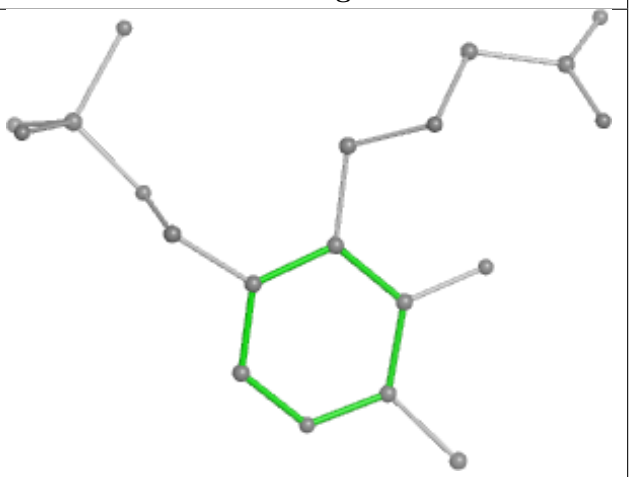
Bond lengths



Bond angles

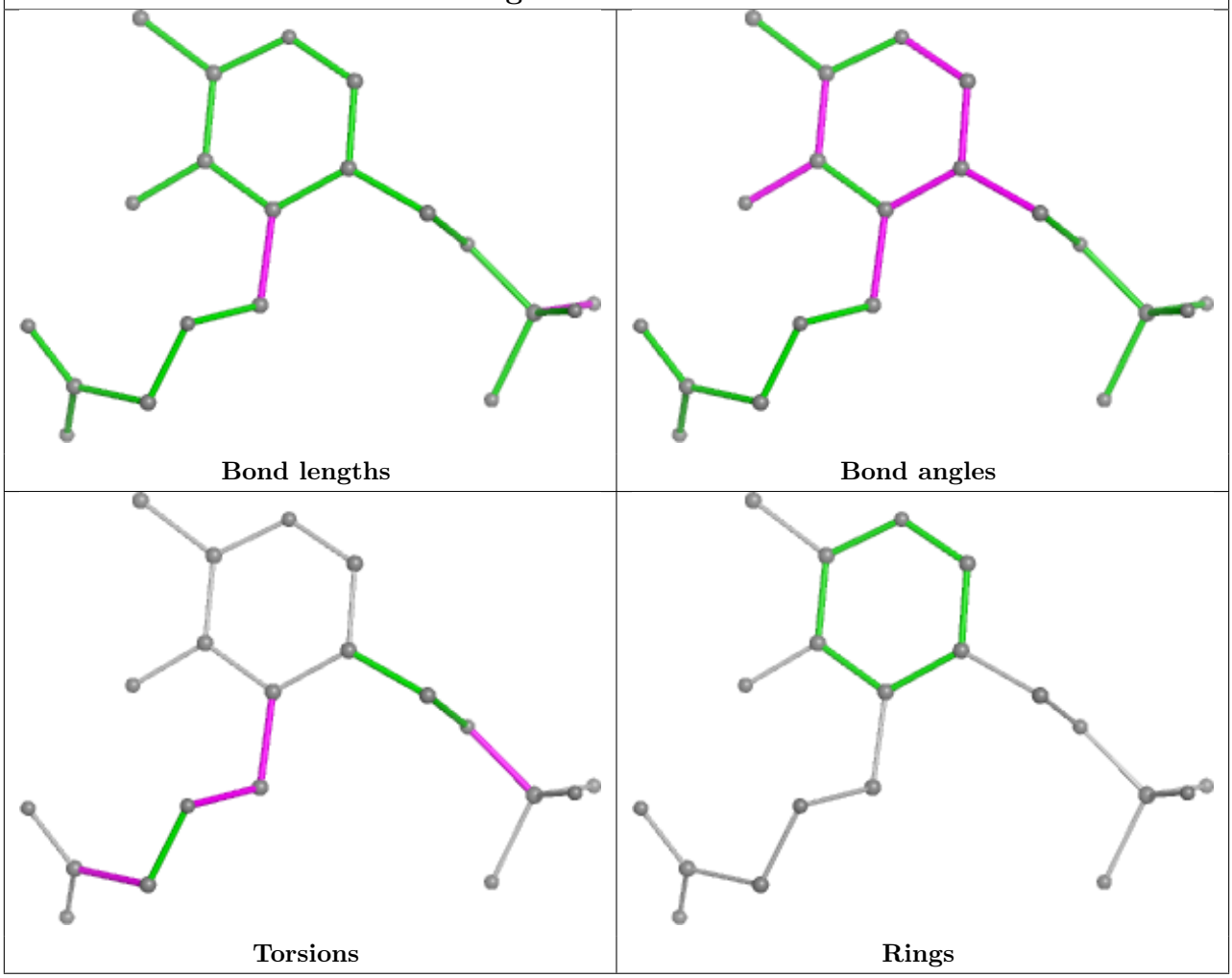


Torsions



Rings

Ligand PLG E 500



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	398/401 (99%)	-0.35	3 (0%) 86 87	18, 28, 45, 91	0
1	B	396/401 (98%)	-0.19	5 (1%) 77 78	18, 27, 45, 55	0
1	D	398/401 (99%)	-0.38	3 (0%) 86 87	18, 27, 45, 78	0
1	E	398/401 (99%)	-0.39	4 (1%) 82 83	18, 27, 45, 87	0
All	All	1590/1604 (99%)	-0.33	15 (0%) 84 85	18, 27, 45, 91	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	397	TRP	3.5
1	B	247	ALA	2.8
1	B	341	VAL	2.7
1	E	153	ALA	2.7
1	E	354	TYR	2.7
1	B	309	MET	2.6
1	A	1	MET	2.5
1	B	326	ILE	2.4
1	A	52	CYS	2.3
1	D	321	LEU	2.3
1	E	45	LYS	2.2
1	A	153	ALA	2.1
1	D	397	TRP	2.1
1	D	398	ALA	2.1
1	B	298	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

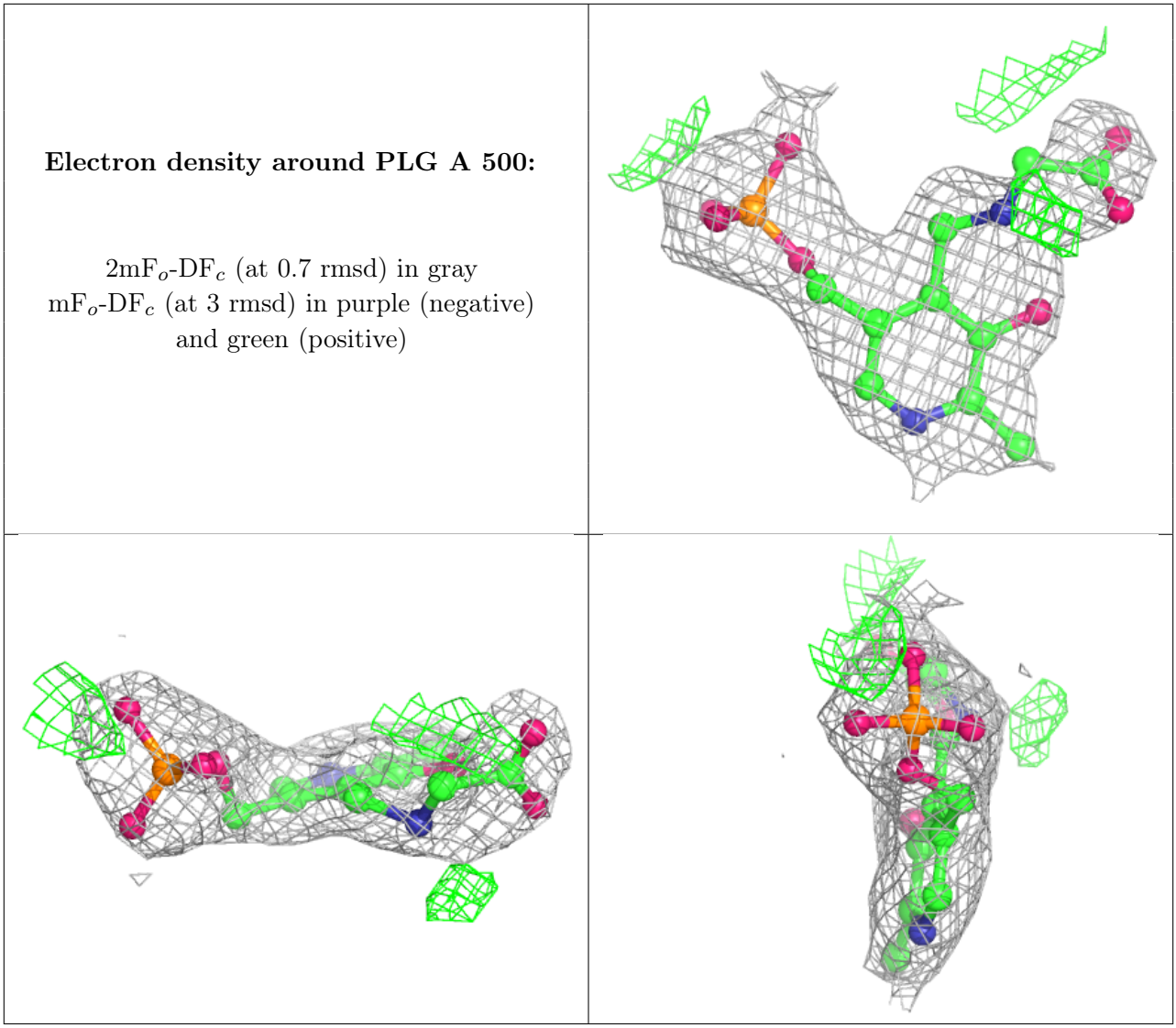
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	ACY	D	600	4/4	0.94	0.14	31,38,39,46	0
3	ACY	E	600	4/4	0.95	0.15	44,54,57,58	0
2	PLG	A	500	20/20	0.96	0.16	30,45,66,67	4
2	PLG	B	500	20/20	0.96	0.22	27,48,58,63	4
3	ACY	A	600	4/4	0.98	0.12	30,33,44,49	0
2	PLG	D	500	20/20	0.98	0.17	33,43,74,76	4
2	PLG	E	500	20/20	0.98	0.11	24,57,72,76	4

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.

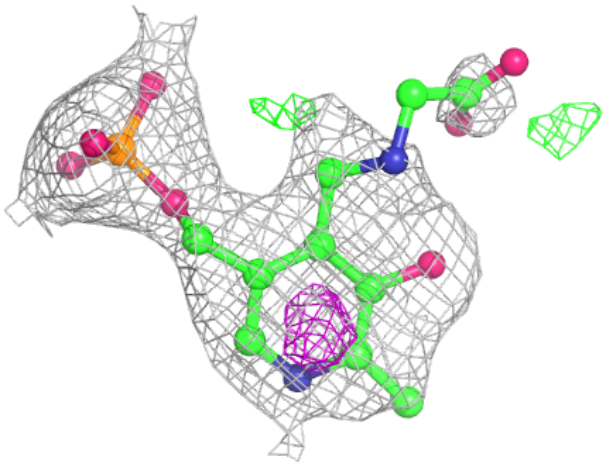
Electron density around PLG A 500:

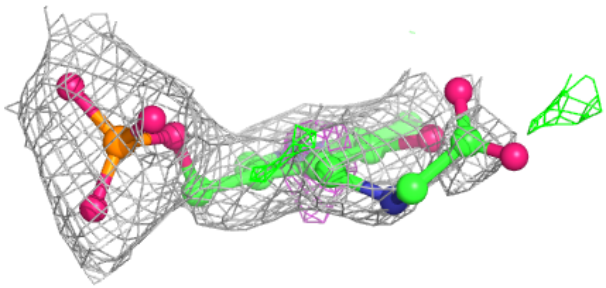
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

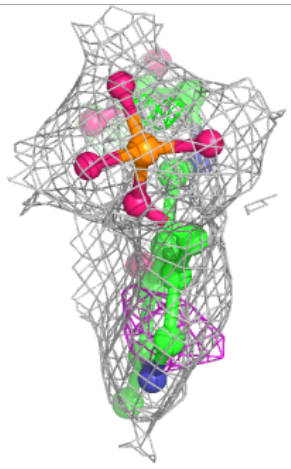


Electron density around PLG B 500:

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

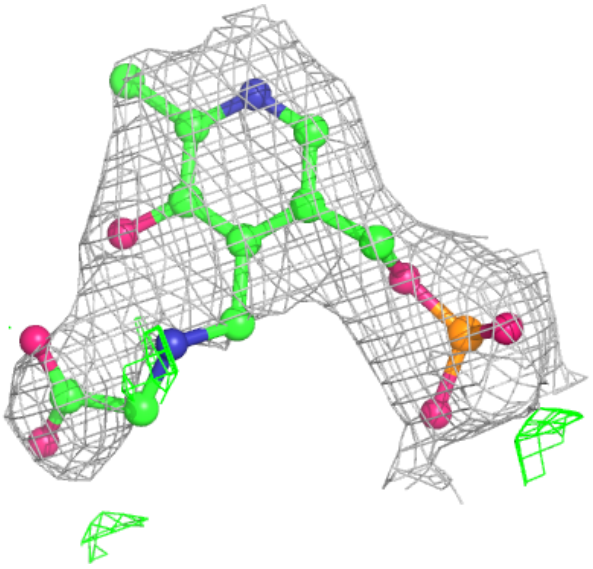


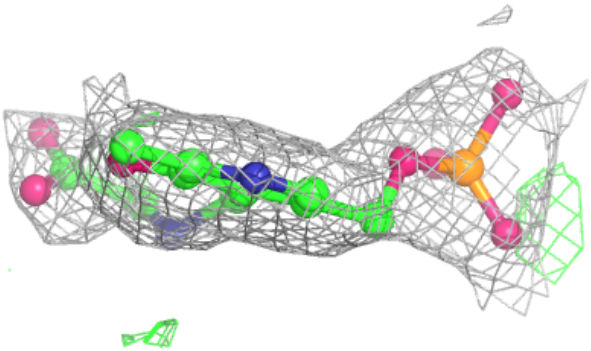


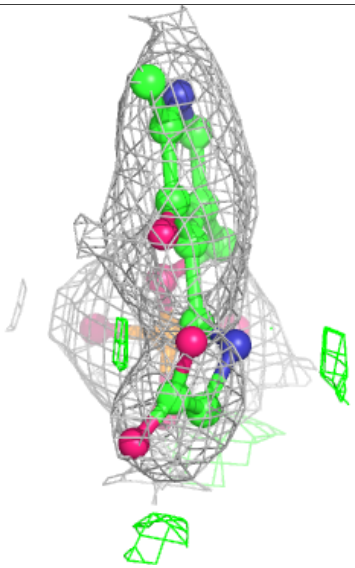


Electron density around PLG D 500:

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

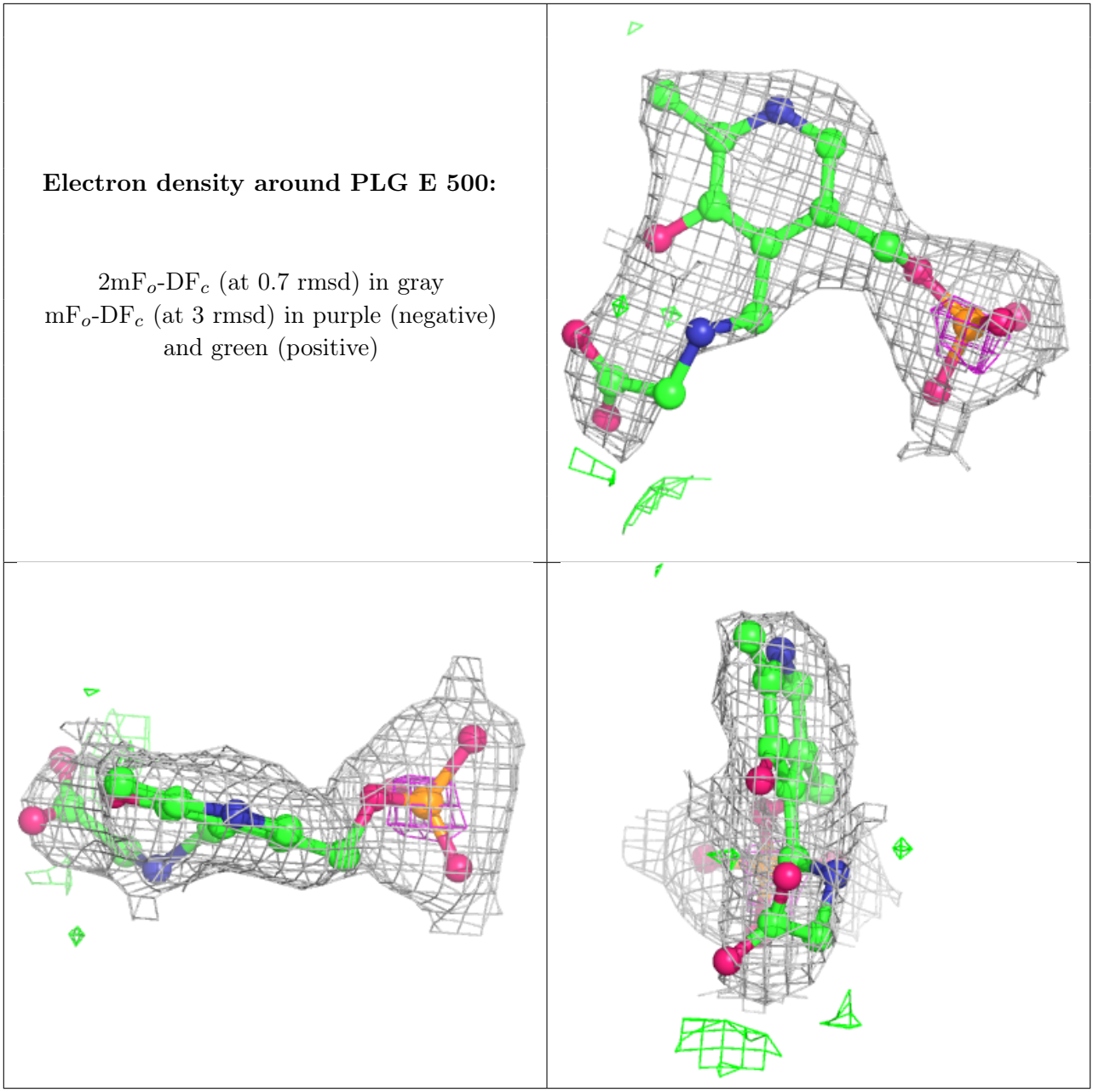






Electron density around PLG E 500:

$2mF_o$-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.