



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:07 PM UTC

PDB ID : 9DZO / pdb_00009dzo
Title : Structure of ALAS bound to succinyl-CoA from *S. cerevisiae*
Authors : Tran, J.U.; Brown, B.L.
Deposited on : 2024-10-16
Resolution : 2.69 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

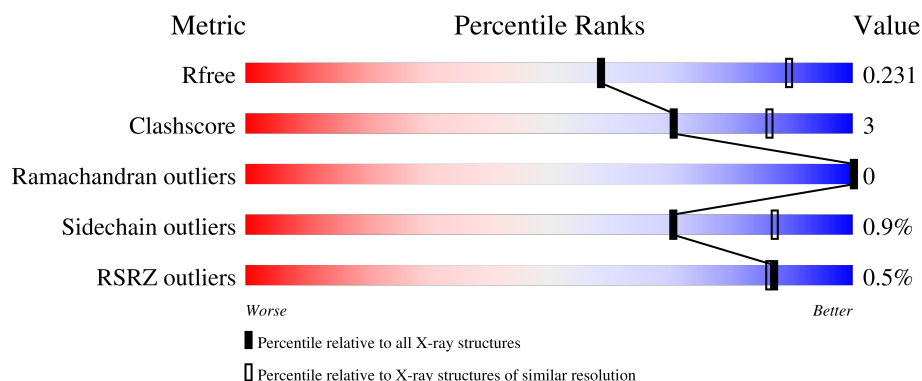
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	491	 89% 7% ..
1	B	491	 90% 7% .
1	C	491	 87% 8% . 5%
1	D	491	 89% 8% ..
1	E	491	 90% 7% .

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Mol	Chain	Length	Quality of chain
2	F	491	<div><div>%</div><div><div></div></div><div>90%</div><div>6% . .</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23215 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	468	Total	C	N	O	S	0	0	0
			3629	2293	637	685	14			
1	D	480	Total	C	N	O	S	0	0	0
			3723	2355	651	703	14			
1	A	479	Total	C	N	O	S	0	0	0
			3713	2349	648	702	14			
1	E	480	Total	C	N	O	S	0	0	0
			3723	2355	651	703	14			
1	B	480	Total	C	N	O	S	0	0	0
			3723	2355	651	703	14			

- Molecule 2 is a protein called 5-aminolevulinate synthase, mitochondrial.

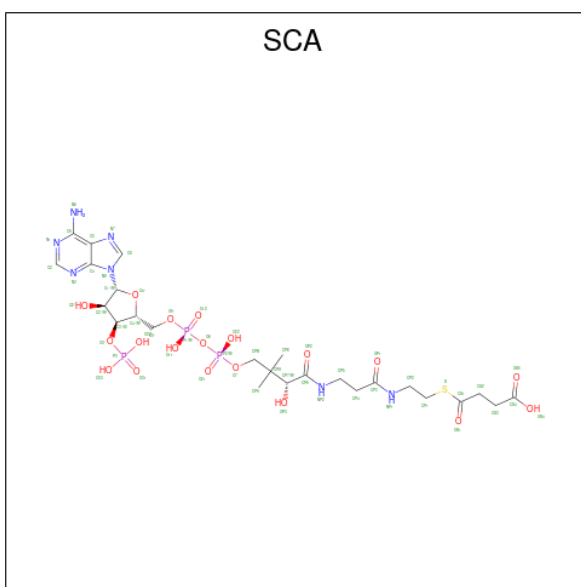
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	478	Total	C	N	O	P S	0	0	0
			3719	2352	648	704	1 14			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 4 is SUCCINYL-COENZYME A (CCD ID: SCA) (formula: $C_{25}H_{40}N_7O_{19}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		
4	A	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	136	Total	O	0	0
			136	136		
6	D	96	Total	O	0	0
			96	96		
6	A	122	Total	O	0	0
			122	122		

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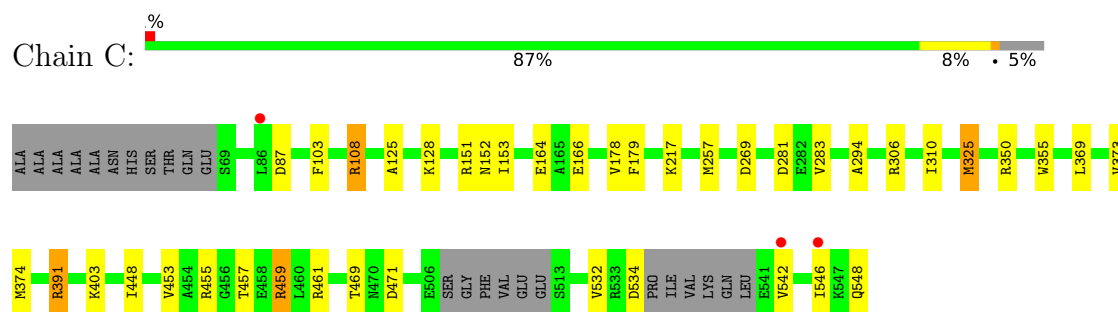
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	100	Total 100	O 100	0	0
6	B	91	Total 91	O 91	0	0
6	F	84	Total 84	O 84	0	0

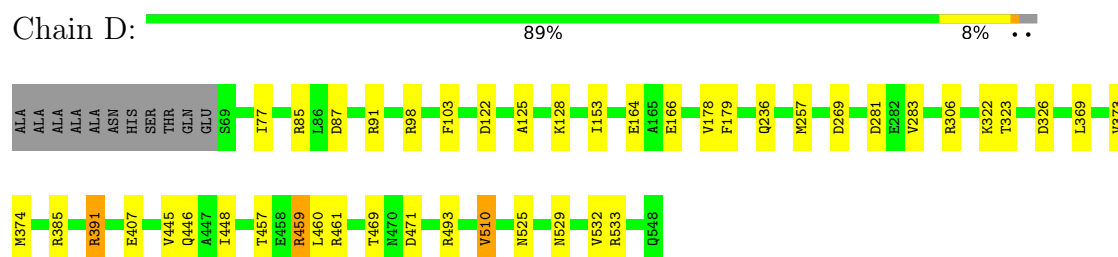
3 Residue-property plots

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.

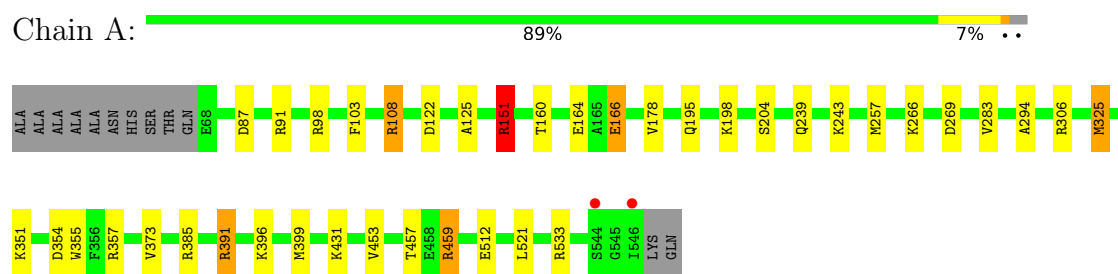
- Molecule 1: 5-aminolevulinate synthase, mitochondrial



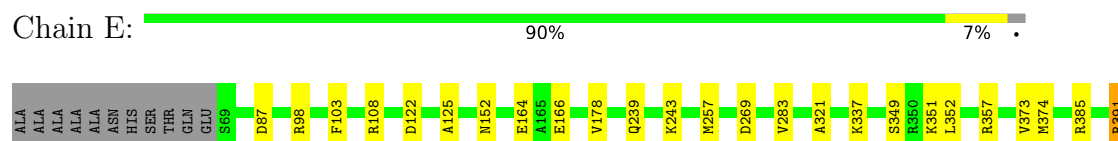
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- Molecule 1: 5-aminolevulinate synthase, mitochondrial

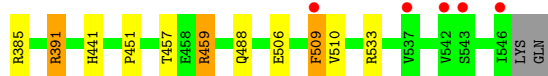
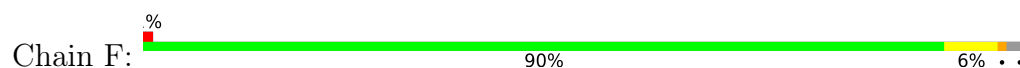




- Molecule 1: 5-aminolevulinate synthase, mitochondrial



- Molecule 2: 5-aminolevulinate synthase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.59Å 114.24Å 119.31Å 116.40° 97.51° 91.84°	Depositor
Resolution (Å)	48.77 – 2.69 48.77 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.77-2.69) 97.3 (48.77-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.105)	Depositor
R, R_{free}	0.180 , 0.227 0.186 , 0.231	Depositor DCC
R_{free} test set	3847 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23215	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LLP, PLP, SCA

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	0.57	0/3791	1.02	9/5137 (0.2%)
1	B	0.57	0/3801	1.00	7/5148 (0.1%)
1	C	0.58	0/3703	1.01	9/5012 (0.2%)
1	D	0.56	0/3801	1.00	6/5148 (0.1%)
1	E	0.56	0/3801	0.98	4/5148 (0.1%)
2	F	0.55	0/3772	0.99	7/5111 (0.1%)
All	All	0.57	0/22669	1.00	42/30704 (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	5
1	B	0	2
1	C	0	4
1	D	0	3
1	E	0	3
2	F	0	3
All	All	0	20

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	CG-CD-NE	-9.98	90.05	112.00
1	C	151	ARG	CA-CB-CG	-8.14	97.83	114.10
1	B	151	ARG	CA-CB-CG	-8.00	98.11	114.10
1	B	326	ASP	CA-CB-CG	6.55	119.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	269	ASP	CA-CB-CG	6.24	118.84	112.60
1	D	269	ASP	CA-CB-CG	6.23	118.83	112.60
2	F	509	PHE	CA-CB-CG	6.14	119.94	113.80
2	F	257	MET	CG-SD-CE	6.12	114.37	100.90
1	E	269	ASP	CA-CB-CG	6.10	118.70	112.60
2	F	87	ASP	CA-CB-CG	6.09	118.69	112.60
1	C	87	ASP	CA-CB-CG	6.06	118.66	112.60
1	E	87	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	325	MET	CG-SD-CE	-6.03	87.64	100.90
1	D	87	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	87	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	87	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	391	ARG	CG-CD-NE	-5.84	99.16	112.00
1	C	391	ARG	CG-CD-NE	-5.83	99.18	112.00
1	D	391	ARG	CG-CD-NE	-5.81	99.21	112.00
1	C	325	MET	CG-SD-CE	-5.78	88.17	100.90
1	E	391	ARG	CG-CD-NE	-5.75	99.35	112.00
1	A	269	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	151	ARG	CB-CG-CD	5.73	124.48	111.30
1	C	281	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	269	ASP	CA-CB-CG	5.67	118.27	112.60
2	F	269	ASP	CA-CB-CG	5.60	118.20	112.60
2	F	391	ARG	CG-CD-NE	-5.60	99.68	112.00
1	C	166	GLU	CB-CA-C	-5.58	101.53	110.79
1	D	407	GLU	CB-CG-CD	5.54	122.03	112.60
1	A	396	LYS	CG-CD-CE	5.47	123.88	111.30
2	F	281	ASP	CA-CB-CG	5.34	117.94	112.60
1	E	239	GLN	CB-CA-C	-5.27	100.88	110.63
1	D	281	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	179	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	281	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	179	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	239	GLN	CB-CA-C	-5.17	101.06	110.63
1	A	266	LYS	CB-CG-CD	5.12	123.09	111.30
2	F	179	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	239	GLN	CB-CA-C	-5.07	101.25	110.63
1	B	166	GLU	CB-CA-C	-5.07	102.37	110.79
1	A	166	GLU	CB-CA-C	-5.04	102.43	110.79

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	151	ARG	Sidechain
1	A	391	ARG	Sidechain
1	A	459	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	459	ARG	Sidechain
1	B	533	ARG	Sidechain
1	C	108	ARG	Sidechain
1	C	391	ARG	Sidechain
1	C	455	ARG	Sidechain
1	C	459	ARG	Sidechain
1	D	391	ARG	Sidechain
1	D	459	ARG	Sidechain
1	D	493	ARG	Sidechain
1	E	391	ARG	Sidechain
1	E	459	ARG	Sidechain
1	E	533	ARG	Sidechain
2	F	108	ARG	Sidechain
2	F	391	ARG	Sidechain
2	F	459	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	3713	0	3695	25	0
1	B	3723	0	3710	23	0
1	C	3629	0	3611	31	0
1	D	3723	0	3710	26	0
1	E	3723	0	3710	29	0
2	F	3719	0	3693	28	0
3	A	16	0	8	0	0
3	B	16	0	8	2	0
3	C	16	0	8	0	0
3	D	16	0	8	0	0
3	E	16	0	7	1	0
4	A	55	0	35	4	0
4	B	55	0	35	1	0
4	C	55	0	35	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	55	0	35	1	0
4	F	55	0	35	3	0
5	D	1	0	0	0	0
6	A	122	0	0	5	0
6	B	91	0	0	5	0
6	C	136	0	0	3	0
6	D	96	0	0	2	0
6	E	100	0	0	5	0
6	F	84	0	0	7	0
All	All	23215	0	22343	153	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 3.

All (153) 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)
4:F:601:SCA:H52	6:F:719:HOH:O	1.65	0.96
2:F:506:GLU:O	2:F:509:PHE:CD2	2.28	0.85
2:F:506:GLU:O	2:F:509:PHE:HD2	1.59	0.83
1:C:257:MET:HE2	1:C:448:ILE:HG21	1.62	0.81
1:E:152:ASN:OD1	2:F:91:ARG:HD2	1.82	0.79
1:D:257:MET:HE2	1:D:448:ILE:HG21	1.64	0.78
1:E:257:MET:HE2	1:E:448:ILE:HG21	1.67	0.77
2:F:488:GLN:HG3	6:F:774:HOH:O	1.84	0.76
1:E:357:ARG:NH2	2:F:91:ARG:O	2.22	0.73
1:C:534:ASP:C	6:C:758:HOH:O	2.35	0.70
2:F:231:LEU:CD2	2:F:267:ILE:HD11	2.22	0.70
1:C:355:TRP:CD2	1:D:77:ILE:HD12	2.27	0.70
1:B:399:MET:HE1	1:B:521:LEU:HD11	1.74	0.69
1:E:166:GLU:OE1	1:E:385:ARG:NH2	2.27	0.68
1:B:514:ASN:HB3	6:B:722:HOH:O	1.93	0.67
1:A:453:VAL:CG1	1:A:457:THR:OG1	2.43	0.67
1:D:166:GLU:OE1	1:D:385:ARG:NH2	2.28	0.67
1:B:166:GLU:OE1	1:B:385:ARG:NH2	2.28	0.67
2:F:166:GLU:OE1	2:F:385:ARG:NH2	2.28	0.67
1:A:166:GLU:OE1	1:A:385:ARG:NH2	2.28	0.66
1:C:453:VAL:CG1	1:C:457:THR:OG1	2.44	0.66
2:F:231:LEU:HD22	2:F:267:ILE:HD11	1.77	0.65
1:A:357:ARG:NH2	1:B:91:ARG:O	2.30	0.64
1:E:399:MET:HE1	1:E:521:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:MET:CE	6:E:734:HOH:O	2.45	0.64
2:F:209:HIS:CD2	4:F:601:SCA:H42	2.33	0.64
1:C:257:MET:HG2	6:C:801:HOH:O	1.98	0.63
1:E:349:SER:OG	1:E:352:LEU:HD13	2.01	0.61
1:B:150:THR:HB	6:B:716:HOH:O	2.01	0.60
1:A:399:MET:HE1	1:A:521:LEU:HD11	1.83	0.60
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.68	0.59
1:C:108:ARG:HG2	1:C:108:ARG:HH11	1.68	0.59
1:B:514:ASN:CG	6:B:722:HOH:O	2.47	0.57
2:F:291:PRO:HD3	2:F:302:PHE:CD1	2.40	0.57
1:A:354:ASP:OD1	1:A:357:ARG:NH1	2.39	0.56
1:E:374:MET:HE1	6:E:734:HOH:O	2.06	0.56
1:A:198:LYS:HG2	6:A:787:HOH:O	2.04	0.56
1:D:257:MET:HE1	1:D:461:ARG:HD2	1.86	0.56
2:F:108:ARG:HG2	2:F:108:ARG:HH11	1.68	0.56
1:C:453:VAL:HG12	1:C:457:THR:OG1	2.05	0.56
1:E:351:LYS:CE	2:F:78:ASP:OD1	2.54	0.55
1:C:542:VAL:CG1	1:C:546:ILE:HD11	2.36	0.55
1:E:374:MET:HE2	6:E:734:HOH:O	2.07	0.55
2:F:488:GLN:CG	6:F:774:HOH:O	2.47	0.55
1:E:321:ALA:N	6:E:705:HOH:O	2.40	0.55
1:C:350:ARG:CG	1:C:542:VAL:HG11	2.37	0.54
2:F:231:LEU:HD22	2:F:267:ILE:CD1	2.36	0.54
1:E:108:ARG:HH11	1:E:108:ARG:HG2	1.73	0.54
1:B:337:LYS:HZ1	3:B:601:PLP:C4A	2.21	0.54
1:E:257:MET:HE1	1:E:461:ARG:HD2	1.88	0.54
1:B:164:GLU:HG2	1:B:178:VAL:HG23	1.90	0.54
1:A:453:VAL:HG12	1:A:457:THR:OG1	2.06	0.54
1:C:350:ARG:HG2	1:C:542:VAL:HG11	1.90	0.53
1:E:257:MET:HE3	1:E:257:MET:HA	1.91	0.52
1:C:453:VAL:HG11	1:C:459:ARG:NH1	2.25	0.52
1:C:164:GLU:HG2	1:C:178:VAL:HG23	1.92	0.52
1:C:257:MET:HE1	1:C:461:ARG:HD2	1.90	0.52
1:C:294:ALA:HB1	1:C:325:MET:HE1	1.91	0.52
1:D:164:GLU:HG2	1:D:178:VAL:HG23	1.92	0.52
1:A:294:ALA:HB1	1:A:325:MET:HE1	1.92	0.51
1:A:306:ARG:HG2	1:A:306:ARG:HH11	1.75	0.51
2:F:231:LEU:HD21	2:F:267:ILE:HD11	1.91	0.51
1:C:306:ARG:HH11	1:C:306:ARG:HG2	1.76	0.51
1:A:257:MET:HG2	6:A:792:HOH:O	2.10	0.51
1:A:243:LYS:HD3	1:B:69:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:164:GLU:HG2	2:F:178:VAL:HG23	1.93	0.51
1:C:542:VAL:HG12	1:C:546:ILE:HD11	1.93	0.51
1:A:164:GLU:HG2	1:A:178:VAL:HG23	1.91	0.51
2:F:306:ARG:HG2	2:F:306:ARG:HH11	1.76	0.50
2:F:451:PRO:HG2	4:F:601:SCA:H82	1.93	0.50
1:A:453:VAL:HG11	1:A:459:ARG:NH1	2.27	0.50
1:E:164:GLU:HG2	1:E:178:VAL:HG23	1.94	0.50
1:C:152:ASN:OD1	1:D:91:ARG:HD2	2.11	0.49
1:B:306:ARG:HG2	1:B:306:ARG:HH11	1.78	0.49
1:B:514:ASN:CB	6:B:722:HOH:O	2.56	0.49
1:C:153:ILE:HG12	1:D:446:GLN:HG2	1.95	0.49
4:A:602:SCA:H42	4:A:602:SCA:CP1	2.42	0.49
1:A:533:ARG:NH2	6:A:706:HOH:O	2.40	0.49
1:A:195:GLN:HB3	6:A:810:HOH:O	2.11	0.49
1:D:306:ARG:HH11	1:D:306:ARG:HG2	1.78	0.48
1:D:457:THR:O	1:D:459:ARG:NH1	2.47	0.48
4:E:602:SCA:H5'2	4:E:602:SCA:P2	2.53	0.48
1:B:337:LYS:NZ	3:B:601:PLP:C4A	2.76	0.48
1:B:457:THR:O	1:B:459:ARG:NH1	2.47	0.48
1:E:457:THR:O	1:E:459:ARG:NH1	2.47	0.48
2:F:509:PHE:HB2	6:F:766:HOH:O	2.14	0.48
1:D:510:VAL:HG12	6:D:786:HOH:O	2.13	0.47
2:F:283:VAL:HG11	2:F:337:LLP:C3	2.44	0.47
1:A:351:LYS:CE	1:B:78:ASP:OD1	2.62	0.47
2:F:457:THR:O	2:F:459:ARG:NH1	2.47	0.46
1:D:525:ASN:HB3	1:D:533:ARG:HH22	1.79	0.46
1:B:469:THR:OG1	1:B:471:ASP:OD1	2.26	0.46
1:D:257:MET:CE	1:D:448:ILE:HG13	2.46	0.46
1:C:257:MET:HE3	1:C:257:MET:HA	1.98	0.46
1:C:453:VAL:HG12	1:C:457:THR:HG1	1.81	0.46
1:A:457:THR:O	1:A:459:ARG:NH1	2.47	0.45
1:D:257:MET:CE	1:D:461:ARG:HD2	2.46	0.45
1:E:103:PHE:CZ	1:E:125:ALA:HB2	2.51	0.45
1:C:457:THR:O	1:C:459:ARG:NH1	2.48	0.45
1:D:369:LEU:HB2	1:D:374:MET:HE3	1.98	0.45
1:E:351:LYS:HE3	2:F:78:ASP:OD1	2.16	0.45
1:D:98:ARG:NH2	1:D:122:ASP:OD2	2.47	0.45
1:D:469:THR:OG1	1:D:471:ASP:OD1	2.25	0.45
1:C:350:ARG:HG2	1:C:542:VAL:CG1	2.47	0.45
1:D:257:MET:HE3	1:D:257:MET:HA	1.97	0.45
1:D:153:ILE:HG23	1:D:153:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:LYS:NZ	1:D:326:ASP:OD2	2.43	0.44
1:D:323:THR:HB	6:D:727:HOH:O	2.17	0.44
1:B:103:PHE:CZ	1:B:125:ALA:HB2	2.52	0.44
1:E:243:LYS:HD3	2:F:69:SER:HB3	2.00	0.44
2:F:103:PHE:CZ	2:F:125:ALA:HB2	2.52	0.44
1:D:103:PHE:CZ	1:D:125:ALA:HB2	2.52	0.44
1:E:337:LYS:NZ	3:E:601:PLP:C4A	2.81	0.43
1:E:351:LYS:HE2	2:F:78:ASP:OD1	2.18	0.43
1:A:98:ARG:NH2	1:A:122:ASP:OD2	2.48	0.43
1:B:223:LYS:NZ	4:B:602:SCA:H1'	2.33	0.43
1:C:217:LYS:NZ	6:C:708:HOH:O	2.51	0.43
1:E:257:MET:CE	1:E:461:ARG:HD2	2.49	0.43
1:A:103:PHE:CZ	1:A:125:ALA:HB2	2.53	0.43
1:A:453:VAL:HG12	1:A:457:THR:HG1	1.82	0.43
1:E:349:SER:OG	1:E:352:LEU:CD1	2.66	0.43
2:F:441:HIS:HE1	6:F:716:HOH:O	2.01	0.43
1:C:350:ARG:CG	1:C:542:VAL:CG1	2.97	0.43
1:C:103:PHE:CZ	1:C:125:ALA:HB2	2.53	0.42
2:F:533:ARG:HG3	6:F:755:HOH:O	2.20	0.42
1:C:152:ASN:OD1	1:D:91:ARG:CD	2.67	0.42
4:A:602:SCA:CP1	4:A:602:SCA:CP4	2.97	0.42
1:E:257:MET:HG2	6:E:755:HOH:O	2.18	0.42
2:F:98:ARG:NH2	2:F:122:ASP:OD2	2.48	0.42
1:E:529:ASN:O	1:E:532:VAL:HG22	2.20	0.42
4:C:602:SCA:H93	4:C:602:SCA:O22	2.20	0.42
1:B:369:LEU:HB2	1:B:374:MET:HE3	2.02	0.42
4:A:602:SCA:H42	4:A:602:SCA:H12	2.02	0.42
1:C:257:MET:CE	1:C:461:ARG:HD2	2.49	0.41
1:B:351:LYS:HG3	6:B:748:HOH:O	2.19	0.41
1:D:445:VAL:HG11	1:D:460:LEU:HB3	2.02	0.41
1:E:352:LEU:HD11	6:F:778:HOH:O	2.20	0.41
1:E:431:LYS:HE3	1:E:449:ASN:ND2	2.36	0.41
1:D:529:ASN:O	1:D:532:VAL:HG22	2.21	0.41
1:A:355:TRP:HE1	1:B:80:GLU:HG2	1.85	0.41
1:D:445:VAL:CG1	1:D:460:LEU:HB3	2.51	0.41
1:E:257:MET:CE	1:E:448:ILE:HG13	2.50	0.41
1:B:98:ARG:NH2	1:B:122:ASP:OD2	2.47	0.41
1:B:529:ASN:O	1:B:532:VAL:HG22	2.21	0.41
1:C:310:ILE:HG12	1:C:532:VAL:HG12	2.03	0.41
1:A:151:ARG:NE	1:A:160:THR:HG21	2.36	0.41
1:C:469:THR:OG1	1:C:471:ASP:OD1	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ARG:NH2	1:E:122:ASP:OD2	2.48	0.40
1:C:369:LEU:HB2	1:C:374:MET:HE3	2.03	0.40
1:C:548:GLN:HB2	1:D:85:ARG:HD3	2.03	0.40
1:A:204:SER:OG	4:A:602:SCA:N1	2.51	0.40
1:A:431:LYS:NZ	6:A:714:HOH:O	2.55	0.40
1:B:399:MET:HE2	1:B:514:ASN:HD22	1.87	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	477/491 (97%)	463 (97%)	14 (3%)	0	100	100
1	B	478/491 (97%)	464 (97%)	14 (3%)	0	100	100
1	C	462/491 (94%)	448 (97%)	14 (3%)	0	100	100
1	D	478/491 (97%)	462 (97%)	16 (3%)	0	100	100
1	E	478/491 (97%)	463 (97%)	15 (3%)	0	100	100
2	F	475/491 (97%)	460 (97%)	15 (3%)	0	100	100
All	All	2848/2946 (97%)	2760 (97%)	88 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	404/411 (98%)	401 (99%)	3 (1%)	76	90
1	B	405/411 (98%)	402 (99%)	3 (1%)	76	90
1	C	394/411 (96%)	390 (99%)	4 (1%)	68	86
1	D	405/411 (98%)	400 (99%)	5 (1%)	63	84
1	E	405/411 (98%)	401 (99%)	4 (1%)	68	86
2	F	402/410 (98%)	399 (99%)	3 (1%)	76	90
All	All	2415/2465 (98%)	2393 (99%)	22 (1%)	70	87

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	128	LYS
1	C	283	VAL
1	C	373	VAL
1	C	403	LYS
1	D	128	LYS
1	D	236	GLN
1	D	283	VAL
1	D	373	VAL
1	D	510	VAL
1	A	283	VAL
1	A	373	VAL
1	A	512	GLU
1	E	283	VAL
1	E	373	VAL
1	E	493	ARG
1	E	510	VAL
1	B	283	VAL
1	B	373	VAL
1	B	510	VAL
2	F	128	LYS
2	F	283	VAL
2	F	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	397	HIS
1	C	442	GLN
1	C	446	GLN

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Mol	Chain	Res	Type
1	C	449	ASN
1	D	195	GLN
1	D	432	GLN
1	D	442	GLN
1	D	449	ASN
1	D	478	ASN
1	A	94	ASN
1	A	232	ASN
1	A	406	HIS
1	A	439	ASN
1	A	446	GLN
1	A	449	ASN
1	E	236	GLN
1	E	387	HIS
1	E	442	GLN
1	E	449	ASN
1	E	478	ASN
1	E	514	ASN
1	B	236	GLN
1	B	387	HIS
1	B	442	GLN
1	B	446	GLN
1	B	449	ASN
1	B	498	GLN
1	B	514	ASN
2	F	236	GLN
2	F	387	HIS
2	F	446	GLN
2	F	498	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	LLP	F	337	2	23,24,25	0.89	1 (4%)	25,32,34	1.35	4 (16%)

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	LLP	F	337	2	-	3/16/17/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	337	LLP	C4'-NZ	2.37	1.35	1.27

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	337	LLP	OP4-C5'-C5	2.73	114.47	109.36
2	F	337	LLP	C3-C4-C5	-2.43	116.33	118.28
2	F	337	LLP	CD-CG-CB	2.38	122.58	113.62
2	F	337	LLP	O3-C3-C2	2.08	121.89	117.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	337	LLP	O-C-CA-CB
2	F	337	LLP	C4-C4'-NZ-CE
2	F	337	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	337	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
4	SCA	B	602	-	55,57,57	0.90	3 (5%)	78,84,84	1.25	6 (7%)
3	PLP	A	601	-	16,16,16	0.65	0	20,23,23	0.92	1 (5%)
3	PLP	C	601	-	16,16,16	0.75	0	20,23,23	1.11	2 (10%)
4	SCA	F	601	-	55,57,57	1.00	3 (5%)	78,84,84	1.10	3 (3%)
4	SCA	E	602	-	55,57,57	0.94	3 (5%)	78,84,84	1.38	5 (6%)
3	PLP	E	601	-	16,16,16	0.60	0	20,23,23	1.32	3 (15%)
4	SCA	C	602	-	55,57,57	0.64	0	78,84,84	1.48	6 (7%)
4	SCA	A	602	-	55,57,57	0.95	3 (5%)	78,84,84	1.77	10 (12%)
3	PLP	D	601	-	16,16,16	0.74	0	20,23,23	1.05	1 (5%)
3	PLP	B	601	-	16,16,16	0.60	0	20,23,23	1.09	1 (5%)

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
4	SCA	B	602	-	-	23/56/72/72	0/3/3/3
3	PLP	A	601	-	-	1/8/8/8	0/1/1/1
3	PLP	C	601	-	-	2/8/8/8	0/1/1/1
4	SCA	F	601	-	-	18/56/72/72	0/3/3/3
4	SCA	E	602	-	-	26/56/72/72	0/3/3/3
3	PLP	E	601	-	-	1/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SCA	C	602	-	-	22/56/72/72	0/3/3/3
4	SCA	A	602	-	-	28/56/72/72	0/3/3/3
3	PLP	D	601	-	-	2/8/8/8	0/1/1/1
3	PLP	B	601	-	-	3/8/8/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	601	SCA	P2-O6	3.79	1.63	1.59
4	F	601	SCA	P1-O6	3.77	1.63	1.59
4	E	602	SCA	P2-O6	3.43	1.63	1.59
4	E	602	SCA	P1-O6	3.43	1.63	1.59
4	B	602	SCA	P3-O3'	3.25	1.65	1.59
4	A	602	SCA	P2-O6	3.07	1.62	1.59
4	A	602	SCA	P1-O6	2.82	1.62	1.59
4	B	602	SCA	P1-O6	2.67	1.62	1.59
4	F	601	SCA	P3-O3'	2.59	1.64	1.59
4	B	602	SCA	P2-O6	2.52	1.62	1.59
4	A	602	SCA	CS1-S	2.50	1.82	1.76
4	E	602	SCA	CS1-S	2.14	1.81	1.76

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	SCA	CP1-S-CS1	9.72	130.57	101.84
4	C	602	SCA	CP1-S-CS1	8.27	126.29	101.84
4	E	602	SCA	CP1-S-CS1	7.92	125.26	101.84
4	A	602	SCA	CS3-CS2-CS1	6.02	121.45	112.41
4	F	601	SCA	CP1-S-CS1	5.62	118.46	101.84
4	A	602	SCA	CS2-CS1-S	-5.43	106.93	113.40
4	B	602	SCA	CP5-CP4-CP3	5.07	120.83	112.39
4	E	602	SCA	CS2-CS1-S	4.62	118.91	113.40
4	B	602	SCA	CP1-S-CS1	4.62	115.49	101.84
3	E	601	PLP	O3-C3-C2	4.20	126.29	117.58
4	C	602	SCA	CS2-CS1-S	-4.11	108.51	113.40
4	C	602	SCA	P3-O3'-C3'	-3.80	113.27	123.43
4	B	602	SCA	CP5-NP2-CP6	3.67	129.13	122.55
3	B	601	PLP	O3-C3-C2	3.62	125.09	117.58
4	E	602	SCA	CS3-CS2-CS1	3.56	117.75	112.41
3	C	601	PLP	O3-C3-C2	3.50	124.84	117.58
4	C	602	SCA	OS1-CS1-S	3.40	127.02	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	SCA	CP2-NP1-CP3	3.27	128.91	122.82
4	E	602	SCA	OS1-CS1-S	-3.14	118.69	122.68
4	A	602	SCA	P3-O3'-C3'	-3.09	115.17	123.43
3	D	601	PLP	O3-C3-C2	2.91	123.62	117.58
4	F	601	SCA	CP5-CP4-CP3	2.60	116.72	112.39
4	A	602	SCA	OS1-CS1-S	2.57	125.96	122.68
4	A	602	SCA	CP4-CP3-NP1	2.57	121.02	116.34
4	C	602	SCA	CP5-CP4-CP3	2.50	116.55	112.39
4	C	602	SCA	O3'-P3-O31	-2.40	100.77	109.33
3	A	601	PLP	O3-C3-C2	2.37	122.49	117.58
4	B	602	SCA	C2'-C3'-C4'	-2.34	99.15	103.24
4	A	602	SCA	O3'-P3-O31	-2.26	101.28	109.33
4	E	602	SCA	P3-O3'-C3'	-2.24	117.44	123.43
4	B	602	SCA	CP7-CP6-NP2	2.16	120.58	116.48
3	E	601	PLP	O4P-P-O1P	-2.15	100.63	106.44
4	A	602	SCA	CP5-NP2-CP6	2.15	126.40	122.55
4	B	602	SCA	O2'-C2'-C3'	2.14	117.18	111.19
3	E	601	PLP	O3-C3-C4	-2.09	113.81	119.44
3	C	601	PLP	O4P-C5A-C5	2.06	113.21	109.36
4	A	602	SCA	OS1-CS1-CS2	2.04	126.33	123.98
4	F	601	SCA	O4'-C1'-N9	2.01	111.95	108.09

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	PLP	C5A-O4P-P-O2P
3	C	601	PLP	C5A-O4P-P-O3P
3	A	601	PLP	C5A-O4P-P-O3P
3	B	601	PLP	C5A-O4P-P-O2P
3	B	601	PLP	C5A-O4P-P-O3P
4	C	602	SCA	CP7-CPA-CPB-O7
4	C	602	SCA	CP9-CPA-CPB-O7
4	C	602	SCA	CP8-CPA-CPB-O7
4	C	602	SCA	CP6-CP7-CPA-CP9
4	C	602	SCA	OP2-CP6-CP7-CPA
4	C	602	SCA	NP2-CP6-CP7-CPA
4	C	602	SCA	OP2-CP6-CP7-OP3
4	C	602	SCA	NP2-CP6-CP7-OP3
4	A	602	SCA	C5'-O5'-P1-O11
4	A	602	SCA	C5'-O5'-P1-O12
4	A	602	SCA	CPB-O7-P2-O6

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Mol	Chain	Res	Type	Atoms
4	A	602	SCA	CPB-O7-P2-O21
4	A	602	SCA	CP9-CPA-CPB-O7
4	A	602	SCA	CP1-CP2-NP1-CP3
4	A	602	SCA	S-CP1-CP2-NP1
4	A	602	SCA	OS1-CS1-S-CP1
4	A	602	SCA	CS2-CS1-S-CP1
4	A	602	SCA	CS1-CS2-CS3-CS4
4	E	602	SCA	CPB-O7-P2-O6
4	E	602	SCA	CPB-O7-P2-O21
4	E	602	SCA	CPB-O7-P2-O22
4	E	602	SCA	CP7-CPA-CPB-O7
4	E	602	SCA	CP9-CPA-CPB-O7
4	E	602	SCA	CP8-CPA-CPB-O7
4	E	602	SCA	CP6-CP7-CPA-CPB
4	E	602	SCA	CP6-CP7-CPA-CP9
4	E	602	SCA	CP1-CP2-NP1-CP3
4	E	602	SCA	OS1-CS1-S-CP1
4	E	602	SCA	CS2-CS1-S-CP1
4	B	602	SCA	C5'-O5'-P1-O11
4	B	602	SCA	C5'-O5'-P1-O12
4	B	602	SCA	CPB-O7-P2-O6
4	B	602	SCA	CP7-CPA-CPB-O7
4	B	602	SCA	CP9-CPA-CPB-O7
4	B	602	SCA	CP8-CPA-CPB-O7
4	B	602	SCA	OP2-CP6-CP7-OP3
4	B	602	SCA	CP7-CP6-NP2-CP5
4	B	602	SCA	CP2-CP1-S-CS1
4	F	601	SCA	C5'-O5'-P1-O11
4	F	601	SCA	C5'-O5'-P1-O12
4	F	601	SCA	C5'-O5'-P1-O6
4	F	601	SCA	CPA-CPB-O7-P2
4	F	601	SCA	CP7-CPA-CPB-O7
4	F	601	SCA	CP9-CPA-CPB-O7
4	F	601	SCA	CP8-CPA-CPB-O7
4	F	601	SCA	OP2-CP6-CP7-OP3
4	F	601	SCA	NP2-CP6-CP7-OP3
4	F	601	SCA	CP2-CP1-S-CS1
4	A	602	SCA	CP4-CP3-NP1-CP2
4	A	602	SCA	OP1-CP3-NP1-CP2
4	B	602	SCA	OP2-CP6-NP2-CP5
4	C	602	SCA	C3'-C4'-C5'-O5'
4	C	602	SCA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	A	602	SCA	C3'-C4'-C5'-O5'
4	A	602	SCA	O4'-C4'-C5'-O5'
4	E	602	SCA	CS1-CS2-CS3-CS4
4	B	602	SCA	CS1-CS2-CS3-CS4
4	A	602	SCA	OP2-CP6-NP2-CP5
4	E	602	SCA	O4'-C4'-C5'-O5'
4	E	602	SCA	C3'-C4'-C5'-O5'
3	D	601	PLP	C3-C4-C4A-O4A
3	B	601	PLP	C5A-O4P-P-O1P
4	A	602	SCA	CP7-CP6-NP2-CP5
4	B	602	SCA	OP2-CP6-CP7-CPA
4	B	602	SCA	NP2-CP6-CP7-CPA
4	B	602	SCA	NP2-CP6-CP7-OP3
4	B	602	SCA	OP1-CP3-CP4-CP5
4	C	602	SCA	OS1-CS1-S-CP1
4	C	602	SCA	S-CS1-CS2-CS3
4	E	602	SCA	S-CS1-CS2-CS3
4	E	602	SCA	OS1-CS1-CS2-CS3
4	A	602	SCA	P1-O6-P2-O7
4	E	602	SCA	P1-O6-P2-O7
4	C	602	SCA	CS2-CS1-S-CP1
4	C	602	SCA	NP1-CP3-CP4-CP5
4	C	602	SCA	CP6-CP7-CPA-CP8
4	F	601	SCA	C3'-C4'-C5'-O5'
4	B	602	SCA	C2'-C1'-N9-C8
3	E	601	PLP	C4-C5-C5A-O4P
4	C	602	SCA	CPA-CPB-O7-P2
4	C	602	SCA	CP6-CP7-CPA-CPB
4	A	602	SCA	CP8-CPA-CPB-O7
4	C	602	SCA	C4'-C5'-O5'-P1
4	A	602	SCA	C5'-O5'-P1-O6
4	A	602	SCA	CPB-O7-P2-O22
4	E	602	SCA	C5'-O5'-P1-O12
4	E	602	SCA	OP3-CP7-CPA-CPB
4	B	602	SCA	C5'-O5'-P1-O6
4	B	602	SCA	CPB-O7-P2-O21
4	C	602	SCA	OP1-CP3-CP4-CP5
4	C	602	SCA	OP3-CP7-CPA-CP9
4	F	601	SCA	OP2-CP6-CP7-CPA
4	B	602	SCA	C4'-C5'-O5'-P1
4	B	602	SCA	S-CP1-CP2-NP1
4	F	601	SCA	NP2-CP6-CP7-CPA

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Mol	Chain	Res	Type	Atoms
4	F	601	SCA	CS2-CS3-CS4-OS5
4	F	601	SCA	CS2-CS3-CS4-OS4
3	D	601	PLP	C5-C4-C4A-O4A
4	A	602	SCA	C3'-O3'-P3-O31
4	B	602	SCA	C3'-O3'-P3-O31
4	C	602	SCA	OS1-CS1-CS2-CS3
4	F	601	SCA	P2-O6-P1-O12
4	B	602	SCA	O4'-C1'-N9-C8
4	E	602	SCA	CS2-CS3-CS4-OS5
4	E	602	SCA	CS2-CS3-CS4-OS4
4	B	602	SCA	NP1-CP3-CP4-CP5
4	F	601	SCA	CP1-CP2-NP1-CP3
4	E	602	SCA	CP6-CP7-CPA-CP8
4	E	602	SCA	OP3-CP7-CPA-CP9
4	E	602	SCA	OP3-CP7-CPA-CP8
4	E	602	SCA	C2'-C1'-N9-C8
4	E	602	SCA	P1-O6-P2-O22
4	A	602	SCA	C3'-O3'-P3-O32
4	A	602	SCA	CPA-CPB-O7-P2
4	A	602	SCA	NP2-CP6-CP7-OP3
4	A	602	SCA	C4'-C5'-O5'-P1
4	A	602	SCA	CP7-CPA-CPB-O7
4	C	602	SCA	P1-O6-P2-O21
4	A	602	SCA	P1-O6-P2-O21
4	A	602	SCA	P1-O6-P2-O22
4	F	601	SCA	P2-O6-P1-O11

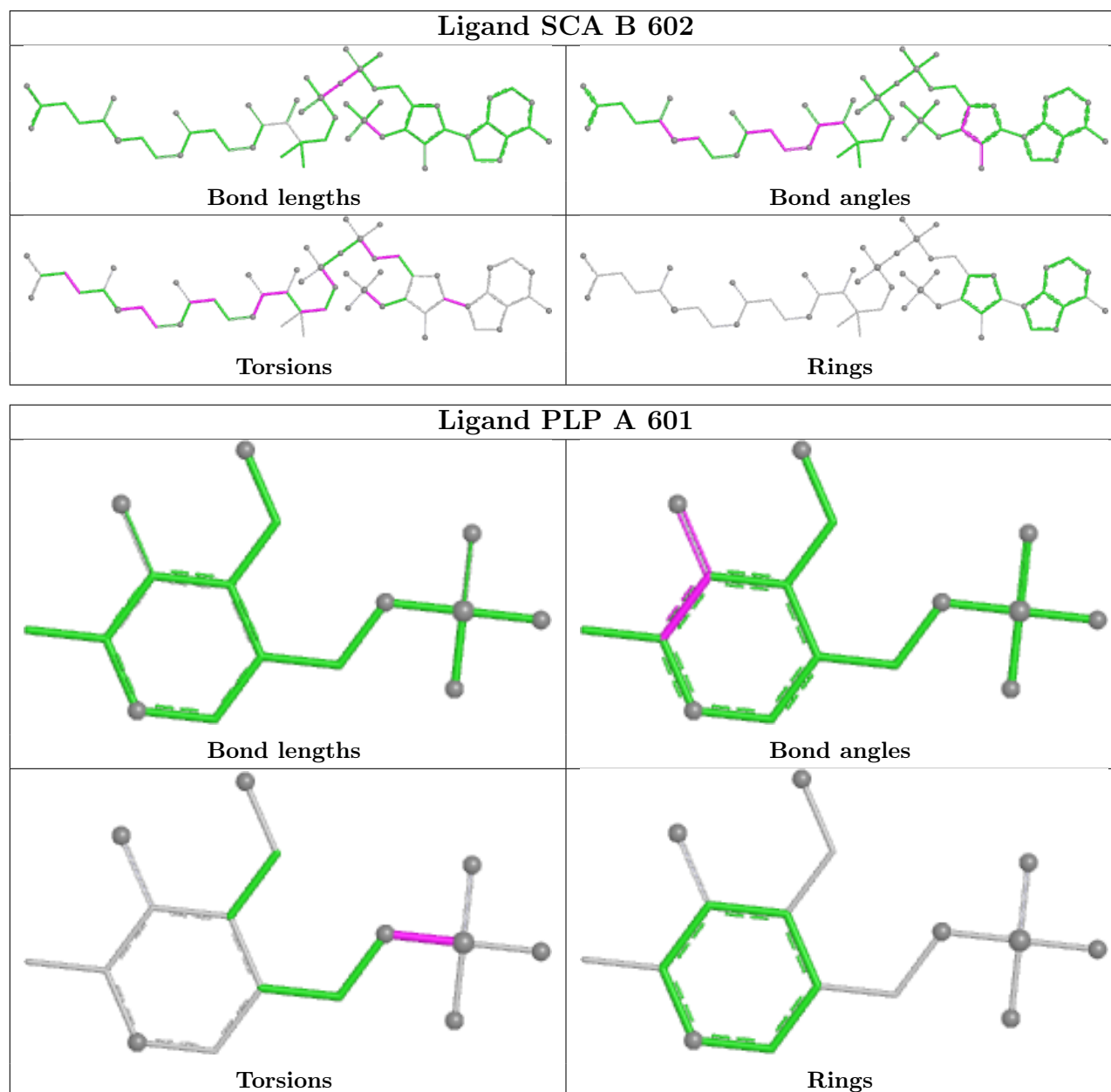
There are no ring outliers.

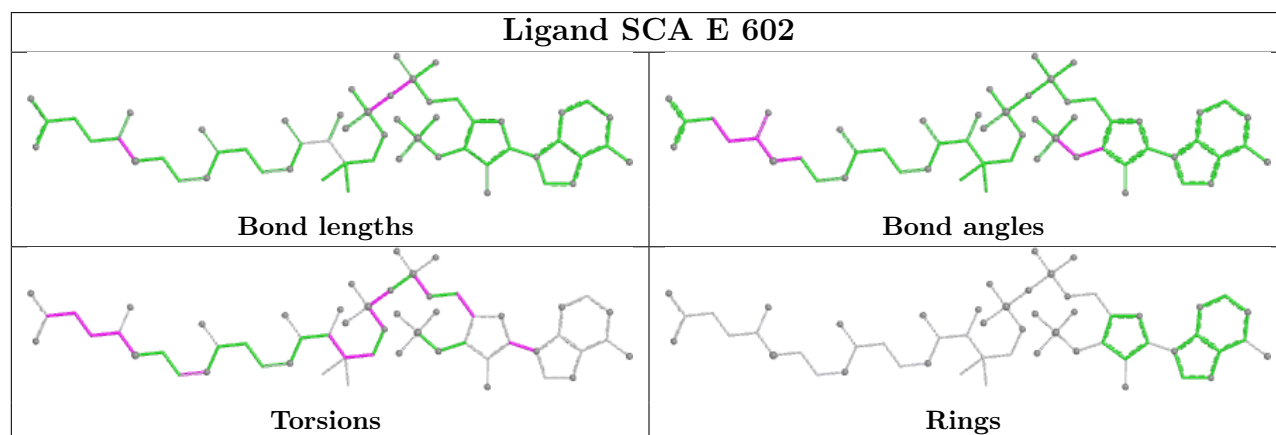
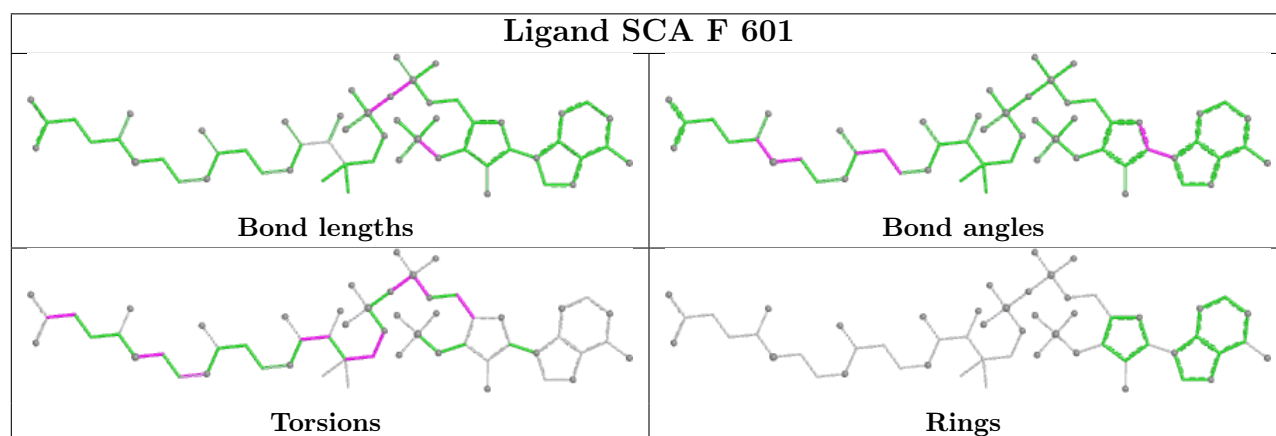
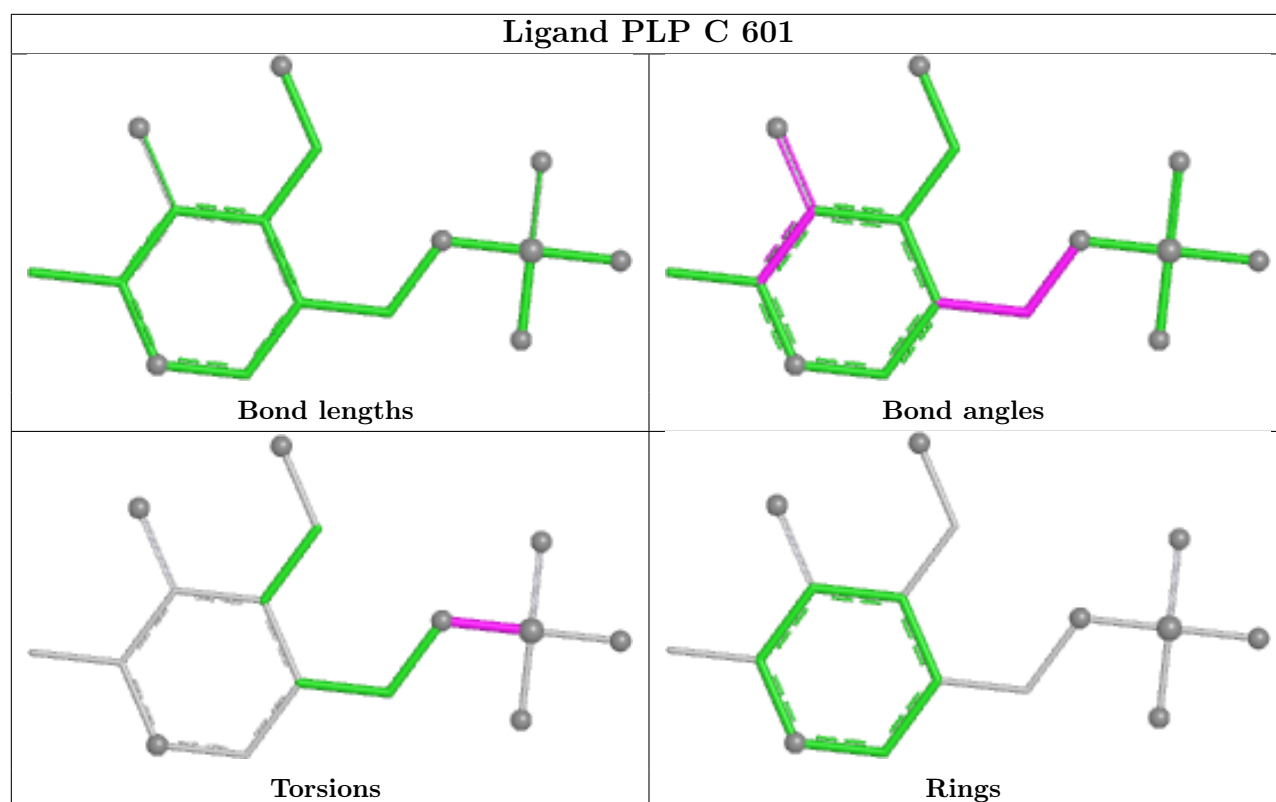
7 monomers are involved in 13 short contacts:

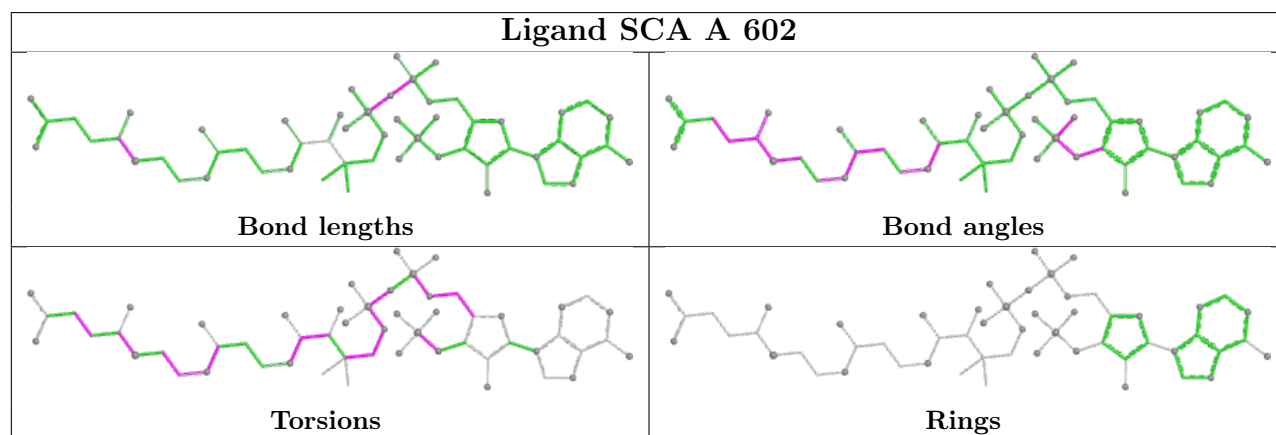
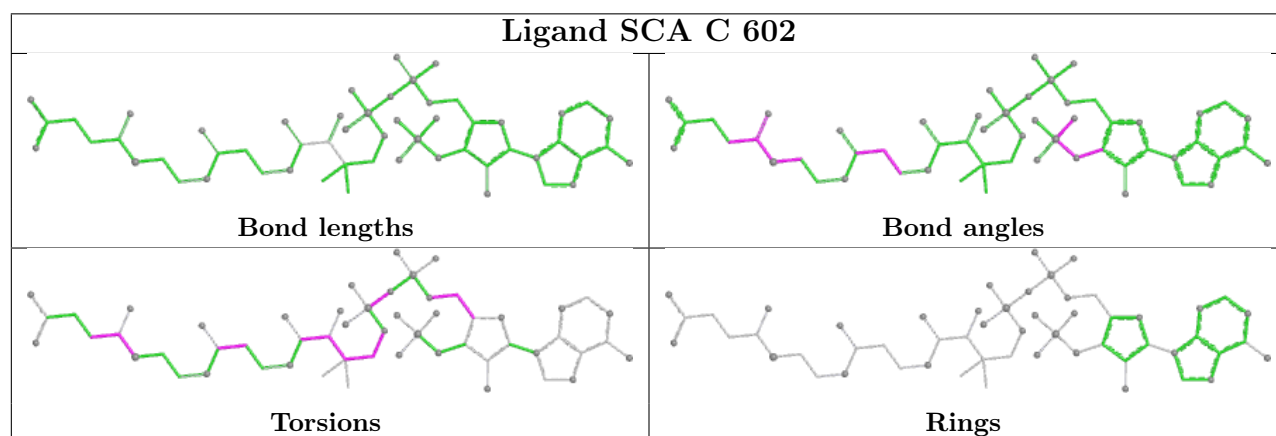
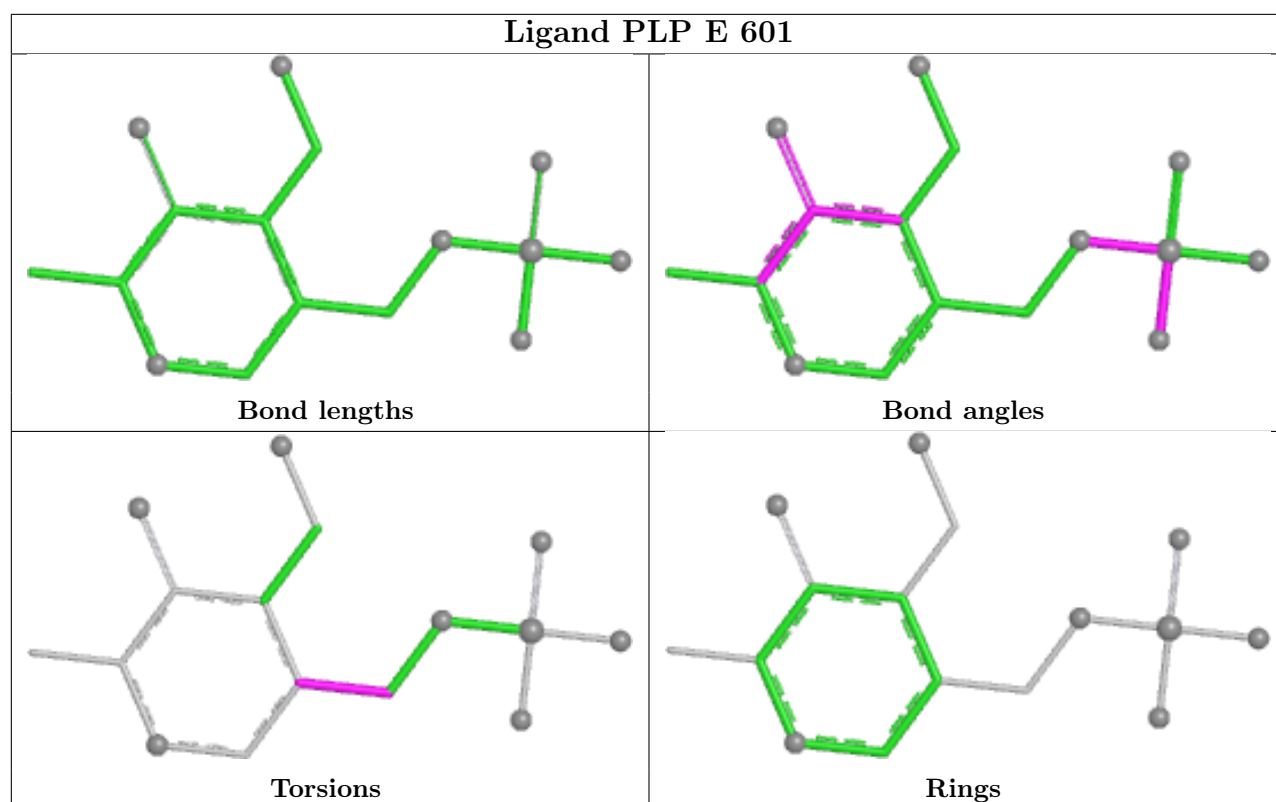
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	SCA	1	0
4	F	601	SCA	3	0
4	E	602	SCA	1	0
3	E	601	PLP	1	0
4	C	602	SCA	1	0
4	A	602	SCA	4	0
3	B	601	PLP	2	0

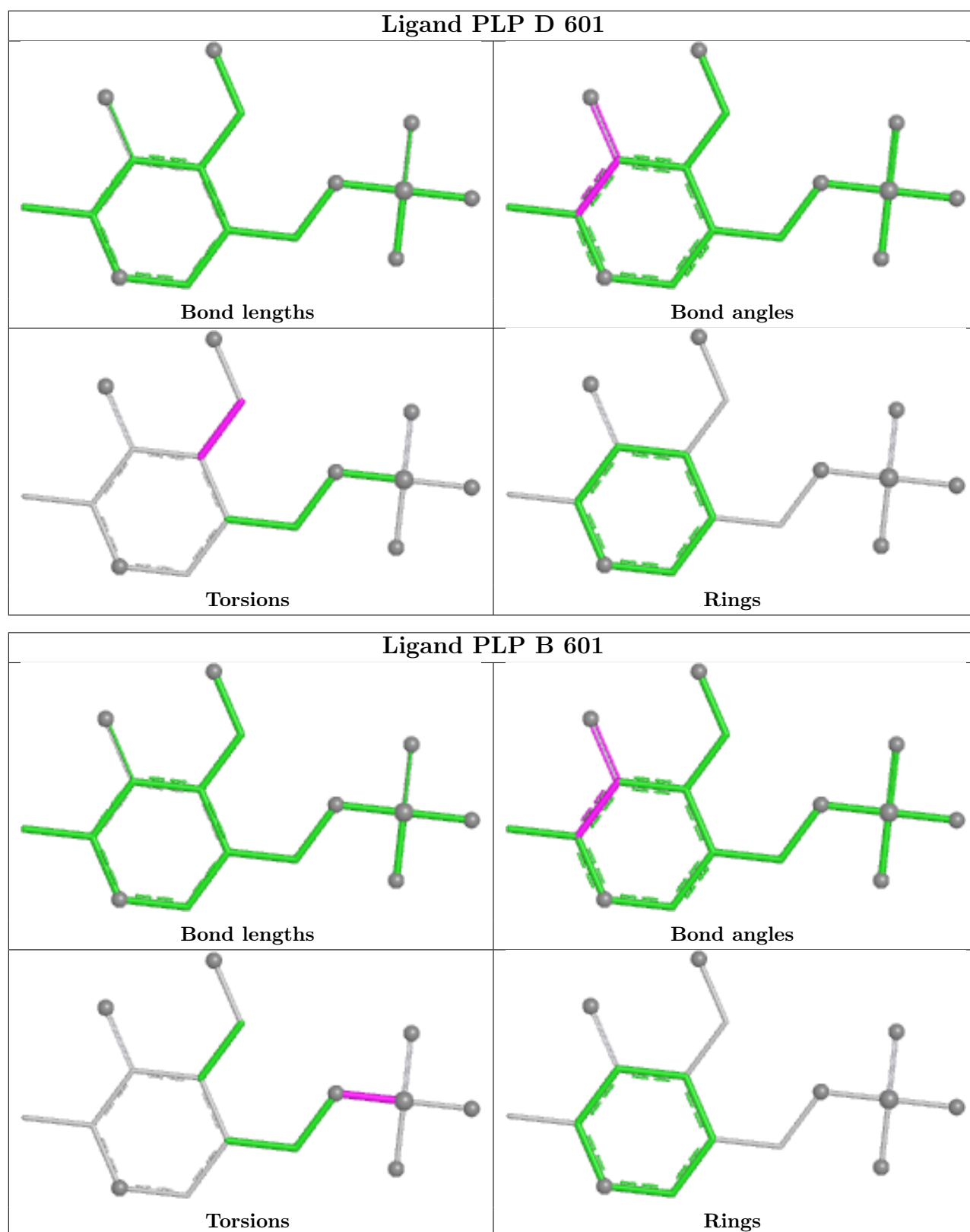
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	479/491 (97%)	-0.25	2 (0%) 88 87	29, 42, 70, 101	0
1	B	480/491 (97%)	-0.15	1 (0%) 91 90	32, 48, 81, 104	0
1	C	468/491 (95%)	-0.25	3 (0%) 85 85	28, 41, 67, 130	0
1	D	480/491 (97%)	-0.20	0 100 100	31, 45, 73, 112	0
1	E	480/491 (97%)	-0.06	2 (0%) 88 87	32, 51, 93, 107	0
2	F	477/491 (97%)	-0.09	5 (1%) 79 78	33, 50, 81, 114	0
All	All	2864/2946 (97%)	-0.17	13 (0%) 87 86	28, 46, 80, 130	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	543	SER	3.1
1	C	86	LEU	2.8
1	C	542	VAL	2.7
1	B	86	LEU	2.5
2	F	542	VAL	2.4
1	A	546	ILE	2.4
1	A	544	SER	2.3
2	F	546	ILE	2.2
1	C	546	ILE	2.1
2	F	509	PHE	2.1
2	F	537	VAL	2.1
1	E	510	VAL	2.1
1	E	507	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LLP	F	337	24/25	0.94	0.09	34,50,58,64	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

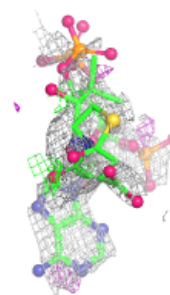
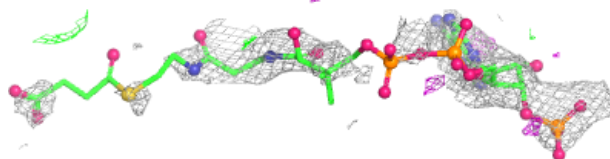
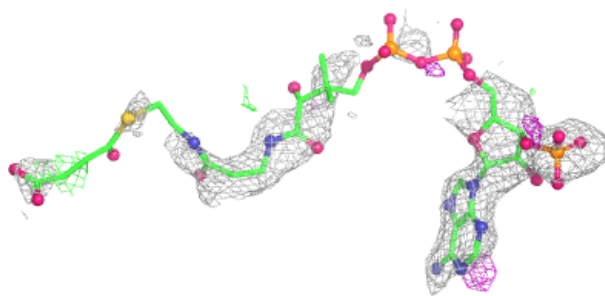
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SCA	F	601	55/55	0.70	0.17	81,111,162,179	0
4	SCA	B	602	55/55	0.73	0.14	61,105,150,170	0
4	SCA	A	602	55/55	0.77	0.15	46,99,164,178	0
4	SCA	C	602	55/55	0.78	0.14	61,101,152,161	0
4	SCA	E	602	55/55	0.78	0.15	61,104,162,171	0
5	MG	D	602	1/1	0.94	0.08	34,34,34,34	0
3	PLP	D	601	16/16	0.95	0.09	25,41,54,57	0
3	PLP	B	601	16/16	0.95	0.07	35,43,51,53	0
3	PLP	E	601	16/16	0.96	0.08	34,40,61,66	0
3	PLP	C	601	16/16	0.96	0.07	35,42,54,63	0
3	PLP	A	601	16/16	0.98	0.06	32,48,78,88	0

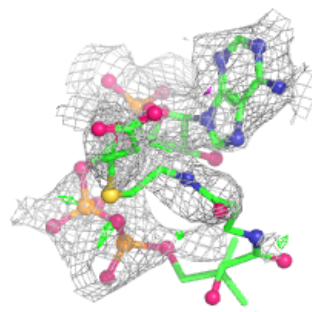
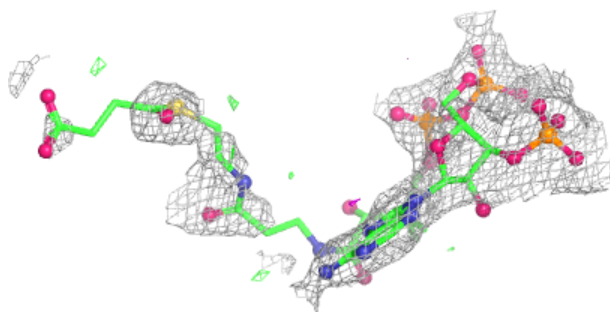
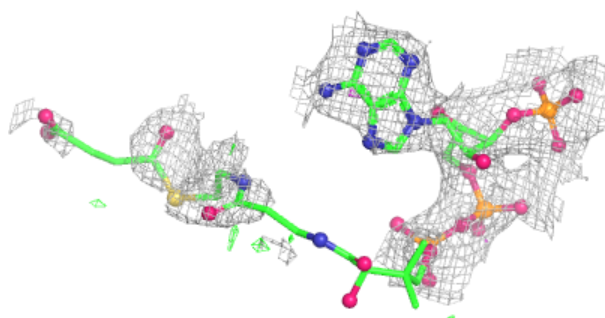
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SCA F 601:

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

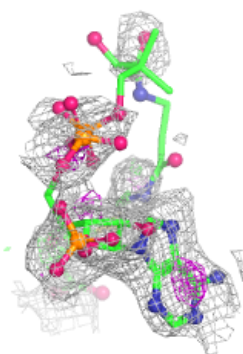
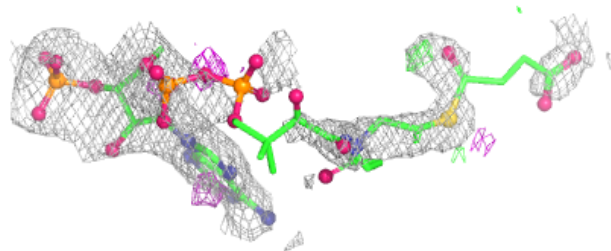
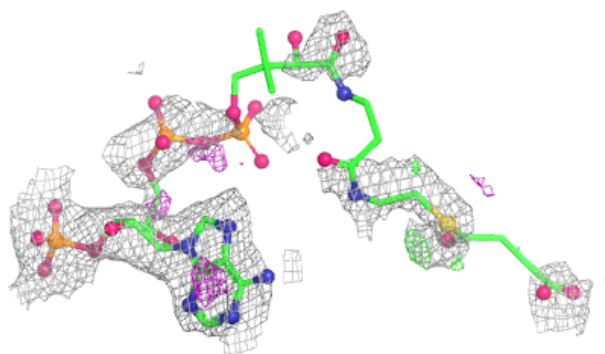
**Electron density around SCA B 602:**

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

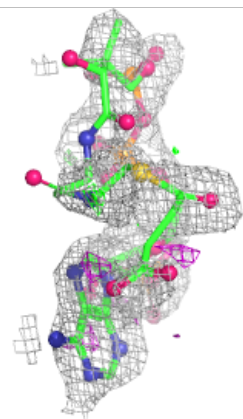
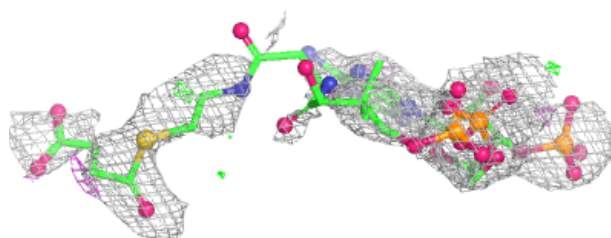
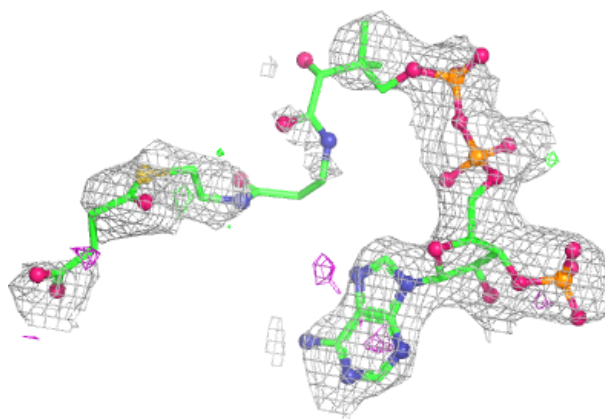


Electron density around SCA A 602:

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

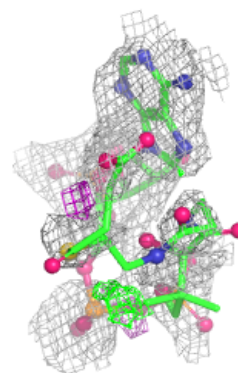
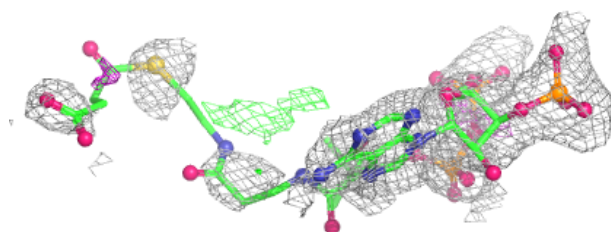
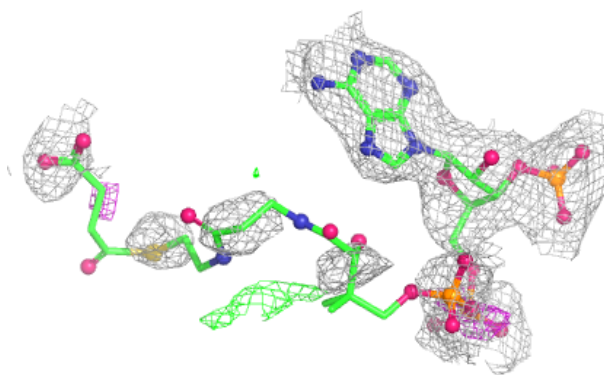
**Electron density around SCA C 602:**

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



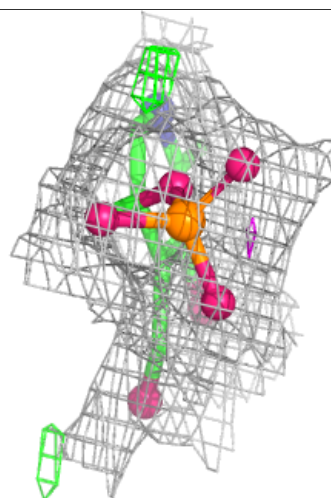
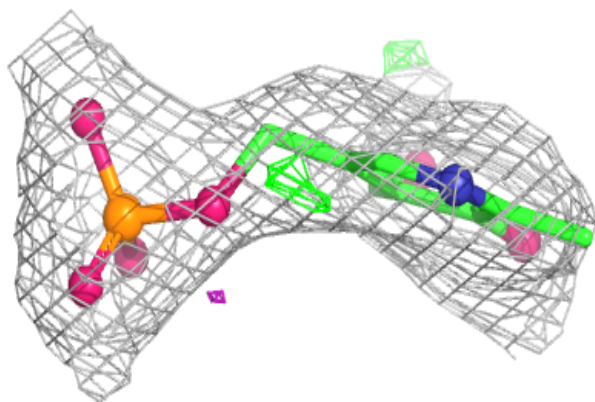
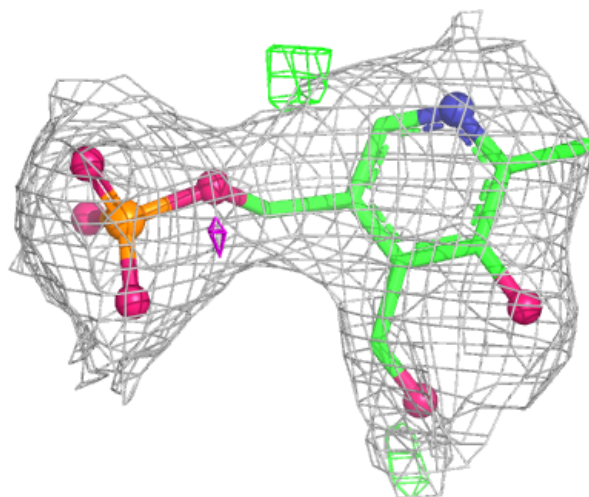
Electron density around SCA E 602:

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and green (positive)



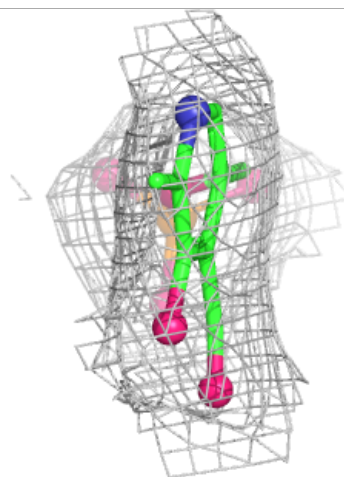
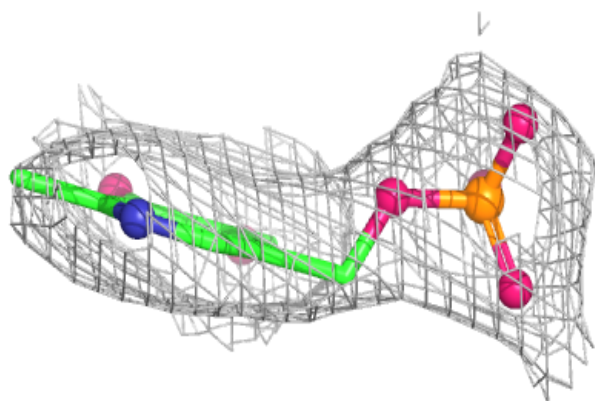
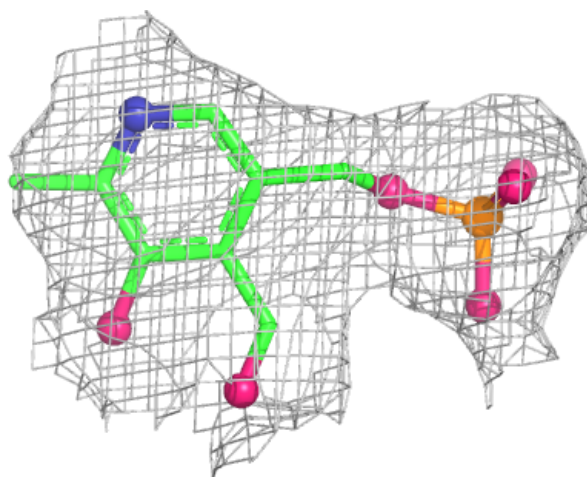
Electron density around PLP D 601:

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and green (positive)



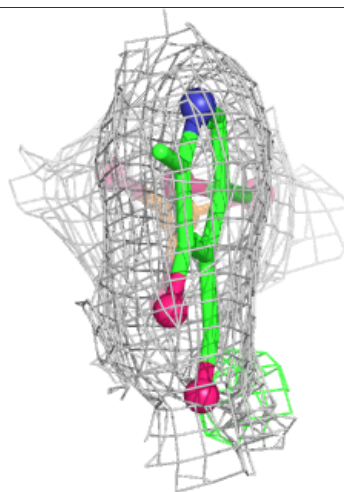
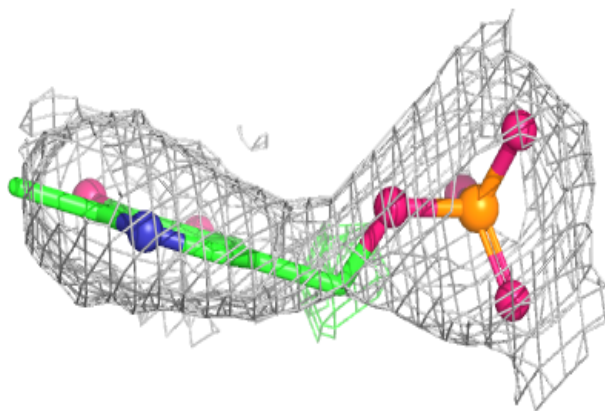
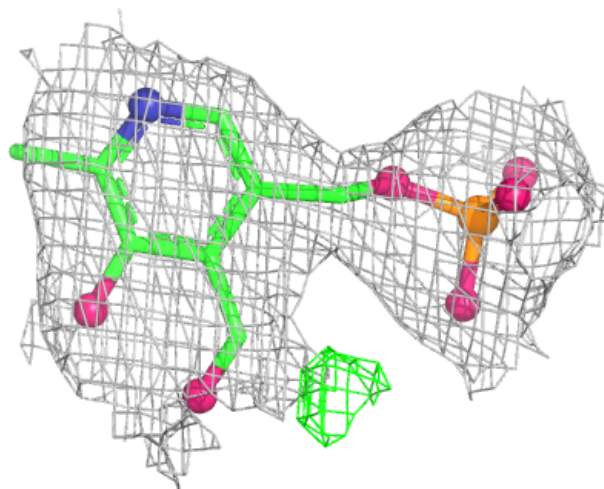
Electron density around PLP B 601:

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



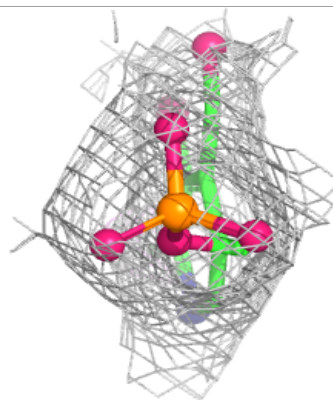
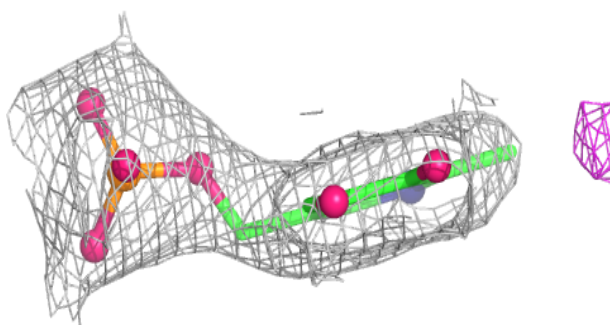
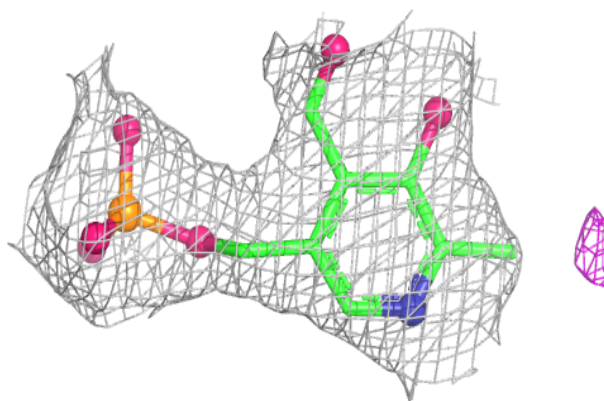
Electron density around PLP E 601:

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



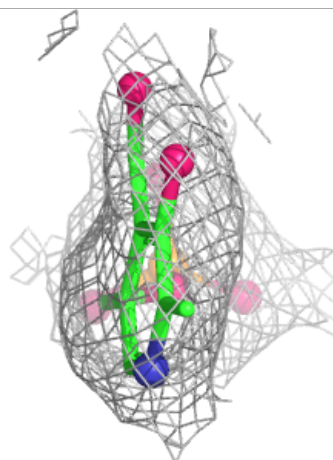
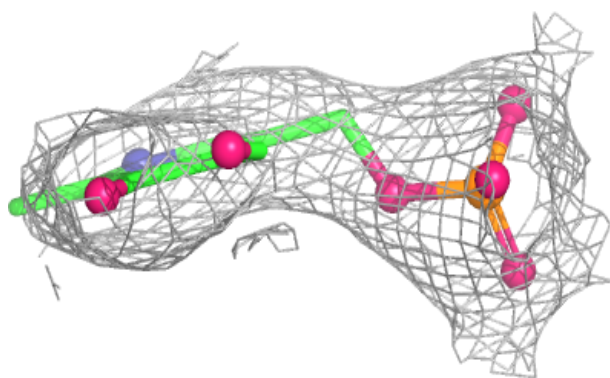
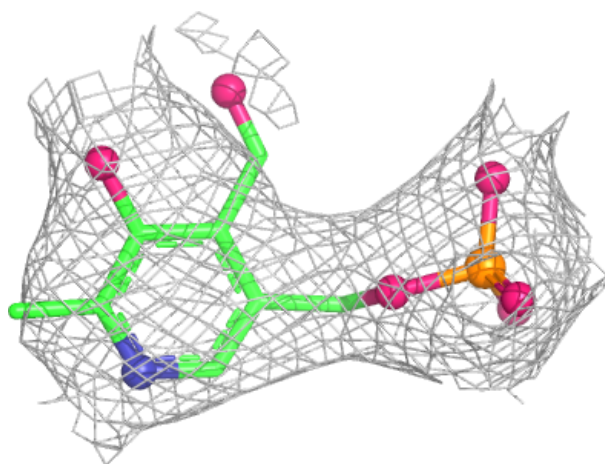
Electron density around PLP C 601:

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



Electron density around PLP A 601:

$2mF_o-DF_c$ (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.