



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 26, 2024 – 12:21 PM JST

PDB ID : 8ZPG
Title : SFX reaction state structure (20-40min) of alanine racemase
Authors : Kim, J.; Nam, K.H.; Cho, Y.
Deposited on : 2024-05-30
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

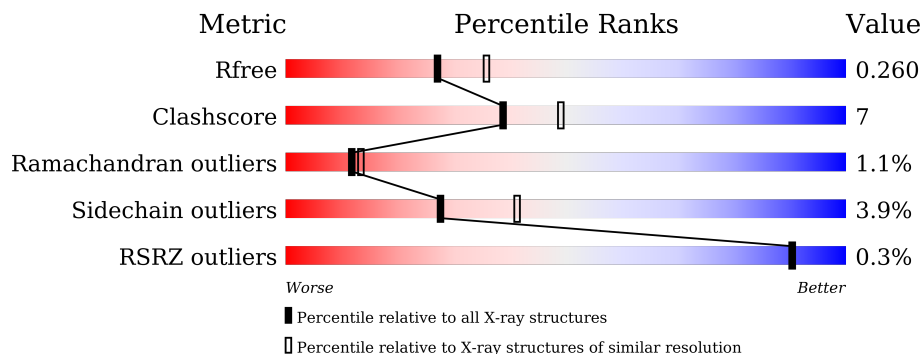
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	398	 % 83% 12% . .
1	B	398	 80% 14% . .
1	C	398	 79% 16% . .
1	D	398	 82% 14% . .

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12196 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.

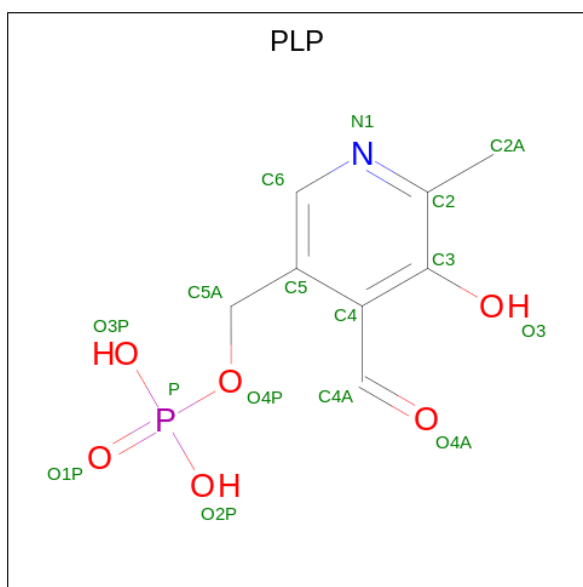
- Molecule 1 is a protein called Alanine racemase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3009	1924	527	544	14	0	0	0
1	B	386	3009	1924	527	544	14	0	0	0
1	C	386	3009	1924	527	544	14	0	0	0
1	D	386	3009	1924	527	544	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

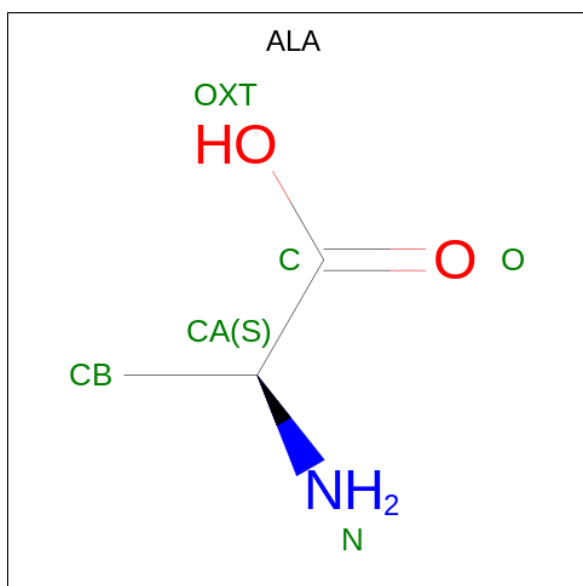
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P94494
A	-2	SER	-	expression tag	UNP P94494
A	-1	HIS	-	expression tag	UNP P94494
A	0	MET	-	expression tag	UNP P94494
B	-3	GLY	-	expression tag	UNP P94494
B	-2	SER	-	expression tag	UNP P94494
B	-1	HIS	-	expression tag	UNP P94494
B	0	MET	-	expression tag	UNP P94494
C	-3	GLY	-	expression tag	UNP P94494
C	-2	SER	-	expression tag	UNP P94494
C	-1	HIS	-	expression tag	UNP P94494
C	0	MET	-	expression tag	UNP P94494
D	-3	GLY	-	expression tag	UNP P94494
D	-2	SER	-	expression tag	UNP P94494
D	-1	HIS	-	expression tag	UNP P94494
D	0	MET	-	expression tag	UNP P94494

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
2	A	1	Total	15	8	1	5	1	0	0
2	B	1	Total	15	8	1	5	1	0	0
2	C	1	Total	15	8	1	5	1	0	0
2	D	1	Total	15	8	1	5	1	0	0

- Molecule 3 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	3	1	2		
3	C	1	Total	C	N	O	0	0
			6	3	1	2		
3	C	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

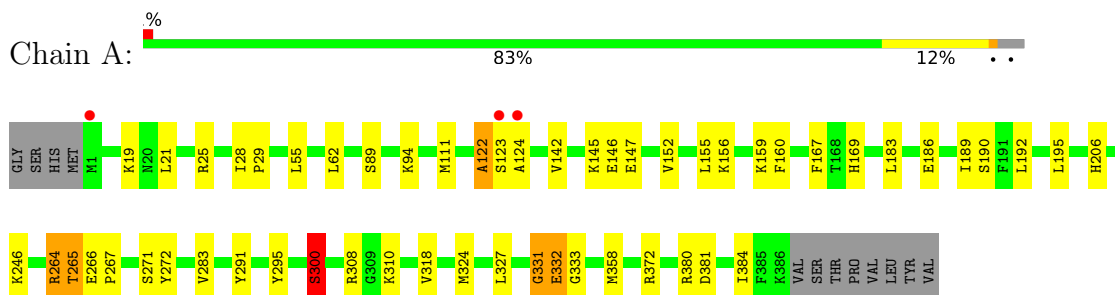
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	18	Total	O	0	0
			18	18		
5	C	21	Total	O	0	0
			21	21		
5	D	12	Total	O	0	0
			12	12		

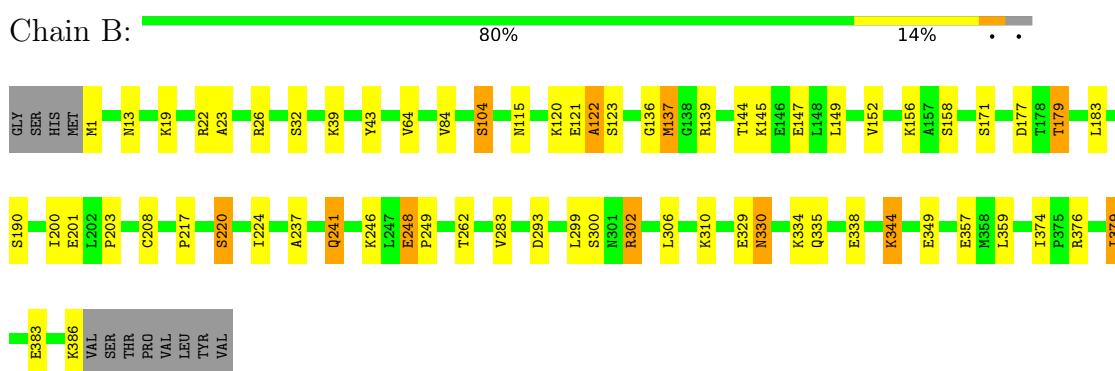
3 Residue-property plots [i](#)

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.

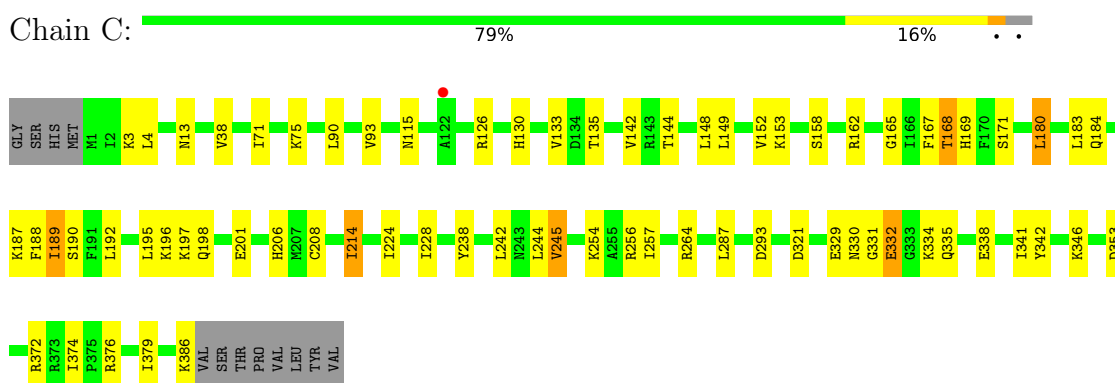
- Molecule 1: Alanine racemase 2




- Molecule 1: Alanine racemase 2

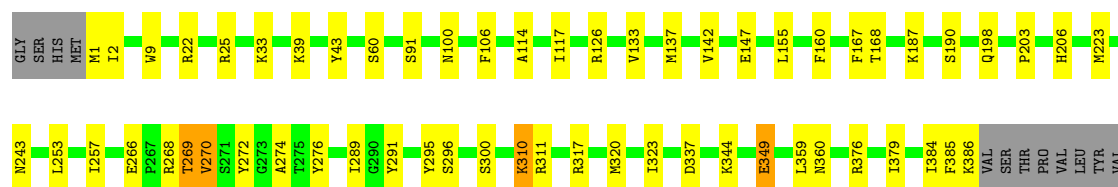


- Molecule 1: Alanine racemase 2



- Molecule 1: Alanine racemase 2

Chain D:  82% 14% ..



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.20Å 112.90Å 91.80Å 90.00° 114.00° 90.00°	Depositor
Resolution (Å)	67.32 – 2.30 67.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.32-2.30) 99.7 (67.32-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.205 , 0.259 0.205 , 0.260	Depositor DCC
R_{free} test set	74147 reflections (0.68%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.080 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12196	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.48	0/3063	0.66	0/4135
1	B	0.48	0/3063	0.66	0/4135
1	C	0.46	0/3063	0.65	0/4135
1	D	0.46	0/3063	0.65	1/4135 (0.0%)
All	All	0.47	0/12252	0.66	1/16540 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	155	LEU	CA-CB-CG	5.57	128.11	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3009	0	3113	45	0
1	B	3009	0	3113	40	0
1	C	3009	0	3113	49	0
1	D	3009	0	3113	36	0
2	A	15	0	7	2	0
2	B	15	0	7	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	7	4	0
2	D	15	0	7	0	0
3	A	6	0	4	2	0
3	C	12	0	8	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	27	0	0	0	0
5	B	18	0	0	1	0
5	C	21	0	0	0	0
5	D	12	0	0	0	0
All	All	12196	0	12492	165	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 7.

All (165) 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:310:LYS:HE3	1:D:311:ARG:H	1.12	1.14
1:D:1:MET:HG3	1:D:2:ILE:H	1.32	0.92
1:B:262:THR:HG22	1:B:283:VAL:HG22	1.54	0.88
1:A:122:ALA:O	1:A:124:ALA:N	2.08	0.85
1:C:180:LEU:HD12	1:C:180:LEU:O	1.76	0.84
1:B:329:GLU:O	1:B:330:ASN:HB2	1.79	0.81
3:A:402:ALA:HB3	2:B:401:PLP:C4A	2.12	0.80
1:A:272:TYR:HH	3:A:402:ALA:N	1.80	0.79
1:D:310:LYS:HE3	1:D:311:ARG:N	1.95	0.79
1:D:25:ARG:O	1:D:25:ARG:HD3	1.84	0.78
1:D:1:MET:HG3	1:D:2:ILE:N	1.99	0.78
1:A:331:GLY:O	1:A:332:GLU:HB2	1.85	0.76
1:C:376:ARG:O	1:C:386:LYS:HD2	1.87	0.75
1:C:331:GLY:O	1:C:332:GLU:HB2	1.86	0.74
1:A:152:VAL:O	1:A:156:LYS:HG3	1.89	0.73
1:D:379:ILE:HG12	1:D:384:ILE:HD13	1.69	0.73
1:B:237:ALA:O	1:B:241:GLN:HG2	1.88	0.73
1:C:334:LYS:HD3	1:C:335:GLN:N	2.06	0.71
1:A:266:GLU:HB2	1:A:267:PRO:HA	1.73	0.70
1:A:145:LYS:HZ3	1:A:146:GLU:HG3	1.56	0.70
1:B:379:ILE:HA	1:B:383:GLU:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:LYS:HA	1:C:346:LYS:HE2	1.75	0.67
1:A:384:ILE:O	1:A:384:ILE:HD12	1.95	0.66
1:A:264:ARG:HG2	1:A:264:ARG:HH11	1.60	0.66
1:D:33:LYS:HG3	1:D:223:MET:HG3	1.79	0.64
1:C:187:LYS:NZ	1:D:266:GLU:O	2.31	0.64
1:C:126:ARG:NH1	1:C:162:ARG:HD3	2.12	0.63
1:D:257:ILE:HD12	1:D:337:ASP:HB2	1.79	0.63
1:A:372:ARG:HG3	1:A:372:ARG:HH11	1.64	0.63
1:B:262:THR:CG2	1:B:283:VAL:HG22	2.28	0.62
1:C:188:PHE:O	1:C:192:LEU:HG	2.01	0.61
1:C:254:LYS:HE2	1:C:338:GLU:OE2	2.00	0.61
1:B:300:SER:O	1:B:302:ARG:HG2	2.02	0.59
1:D:376:ARG:O	1:D:386:LYS:HD3	2.03	0.59
1:C:3:LYS:O	1:C:4:LEU:HD23	2.02	0.59
1:B:177:ASP:OD1	1:B:179:THR:OG1	2.22	0.57
1:D:142:VAL:CG2	1:D:147:GLU:HG3	2.34	0.57
1:C:372:ARG:HH11	1:C:372:ARG:HG3	1.68	0.57
1:C:189:ILE:N	1:C:189:ILE:HD13	2.18	0.57
1:C:256:ARG:HH11	1:C:256:ARG:CG	2.17	0.57
1:D:266:GLU:HG2	1:D:268:ARG:NH1	2.20	0.56
1:D:22:ARG:HH11	1:D:22:ARG:HG3	1.70	0.56
1:C:167:PHE:HB3	1:C:206:HIS:CD2	2.41	0.56
1:C:115:ASN:OD1	1:C:158:SER:HB3	2.06	0.56
1:A:384:ILE:HD12	1:A:384:ILE:C	2.25	0.56
1:D:310:LYS:HG3	1:D:311:ARG:N	2.21	0.56
1:D:344:LYS:HG2	1:D:349:GLU:HB2	1.88	0.55
1:D:300:SER:HB3	1:D:317:ARG:HA	1.88	0.55
1:A:186:GLU:HA	1:A:189:ILE:HG12	1.89	0.54
1:B:344:LYS:NZ	1:B:349:GLU:OE2	2.41	0.54
1:A:142:VAL:HG23	1:A:147:GLU:CD	2.27	0.54
1:D:137:MET:O	1:D:137:MET:HG3	2.08	0.53
1:A:145:LYS:NZ	1:A:146:GLU:HG3	2.22	0.53
1:B:293:ASP:HB3	1:B:374:ILE:HD11	1.91	0.53
1:C:135:THR:O	1:C:184:GLN:HG2	2.09	0.53
1:B:217:PRO:O	1:B:220:SER:OG	2.28	0.52
1:C:208:CYS:HB2	1:C:224:ILE:HG22	1.91	0.52
1:C:264:ARG:O	1:C:264:ARG:HG3	2.08	0.52
1:A:265:THR:HG21	1:B:144:THR:HG22	1.91	0.52
1:B:329:GLU:O	1:B:330:ASN:CB	2.56	0.52
1:D:384:ILE:HG22	1:D:385:PHE:N	2.24	0.52
1:A:167:PHE:HB3	1:A:206:HIS:CE1	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:HD12	1:B:183:LEU:O	2.09	0.52
1:B:22:ARG:HG3	1:B:23:ALA:N	2.24	0.51
1:A:159:LYS:HG3	1:A:160:PHE:CD1	2.45	0.51
1:B:376:ARG:O	1:B:386:LYS:HD3	2.11	0.51
1:B:149:LEU:O	1:B:149:LEU:HG	2.09	0.51
1:C:256:ARG:HH11	1:C:256:ARG:HG2	1.75	0.50
1:C:228:ILE:N	2:C:401:PLP:O1P	2.40	0.50
1:B:306:LEU:HA	1:B:310:LYS:O	2.10	0.50
1:A:264:ARG:HG2	1:A:264:ARG:NH1	2.27	0.50
1:B:13:ASN:HA	1:B:379:ILE:HG23	1.92	0.50
1:C:329:GLU:O	1:C:330:ASN:HB2	2.11	0.50
1:A:291:TYR:HA	1:A:295:TYR:O	2.12	0.50
1:C:196:LYS:C	1:C:198:GLN:H	2.14	0.49
1:D:289:ILE:O	1:D:323:ILE:HG23	2.12	0.49
1:C:148:LEU:O	1:C:152:VAL:HG23	2.12	0.49
1:B:115:ASN:OD1	1:B:158:SER:HB3	2.12	0.49
1:B:208:CYS:HB2	1:B:224:ILE:HG22	1.95	0.49
1:A:186:GLU:HG3	1:A:189:ILE:HD11	1.93	0.49
1:C:257:ILE:HA	1:C:287:LEU:HD23	1.94	0.49
1:A:169:HIS:ND1	2:A:401:PLP:H2A2	2.27	0.48
1:B:386:LYS:HD2	1:B:386:LYS:C	2.33	0.48
1:B:152:VAL:O	1:B:156:LYS:HG3	2.14	0.48
1:A:358:MET:HE2	1:A:358:MET:HB2	1.70	0.48
1:C:341:ILE:O	1:C:342:TYR:HD1	1.96	0.48
1:A:380:ARG:O	1:A:381:ASP:HB2	2.14	0.48
1:C:183:LEU:O	1:C:183:LEU:HD23	2.13	0.48
1:D:359:LEU:O	1:D:360:ASN:HB2	2.13	0.48
1:A:372:ARG:HG3	1:A:372:ARG:NH1	2.27	0.48
1:C:180:LEU:HD12	1:C:180:LEU:C	2.31	0.48
1:C:169:HIS:CD2	2:C:401:PLP:H2A2	2.49	0.47
1:A:272:TYR:CZ	1:B:137:MET:HE3	2.48	0.47
1:C:214:ILE:HD11	1:C:245:VAL:HG21	1.95	0.47
1:C:334:LYS:HD3	1:C:335:GLN:H	1.79	0.47
1:C:321:ASP:OD2	1:D:39:LYS:HE3	2.14	0.47
1:C:142:VAL:HG21	1:C:148:LEU:HD13	1.97	0.47
1:D:291:TYR:HA	1:D:295:TYR:O	2.15	0.47
1:C:346:LYS:HE2	1:C:346:LYS:CA	2.45	0.47
1:B:19:LYS:HA	1:B:22:ARG:HG2	1.96	0.46
1:C:149:LEU:O	1:C:153:LYS:HG3	2.15	0.46
1:C:293:ASP:HB3	1:C:374:ILE:HD11	1.96	0.46
2:C:401:PLP:C4A	3:C:403:ALA:N	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:SER:HA	1:A:318:VAL:HG23	1.96	0.46
1:C:13:ASN:ND2	1:C:379:ILE:HG21	2.31	0.46
1:C:169:HIS:CG	2:C:401:PLP:H2A2	2.51	0.46
1:D:384:ILE:O	1:D:385:PHE:HB3	2.16	0.46
3:C:403:ALA:N	1:D:272:TYR:HH	2.14	0.46
1:A:169:HIS:CE1	2:A:401:PLP:C2	2.98	0.45
1:A:246:LYS:HA	1:A:246:LYS:HD3	1.61	0.45
1:C:130:HIS:HA	1:C:165:GLY:O	2.17	0.45
1:C:126:ARG:NH1	1:C:162:ARG:HH11	2.14	0.45
1:B:39:LYS:HB3	1:B:64:VAL:HA	1.99	0.45
1:D:114:ALA:HA	1:D:117:ILE:HD12	1.99	0.45
1:D:142:VAL:HG21	1:D:147:GLU:HG3	1.99	0.45
1:A:308:ARG:HH21	1:A:333:GLY:HA2	1.81	0.45
1:B:334:LYS:HE2	1:B:334:LYS:HB2	1.71	0.45
1:C:167:PHE:HB3	1:C:206:HIS:NE2	2.31	0.45
1:C:242:LEU:HB2	1:C:244:LEU:HD12	1.99	0.45
1:C:201:GLU:HA	1:C:201:GLU:OE1	2.16	0.44
1:A:186:GLU:CG	1:A:189:ILE:HD11	2.47	0.44
1:B:22:ARG:O	1:B:26:ARG:HG2	2.17	0.44
1:B:344:LYS:HG3	1:B:349:GLU:HG3	1.98	0.44
1:C:71:ILE:O	1:C:75:LYS:HG3	2.18	0.44
1:C:133:VAL:O	1:C:168:THR:HB	2.18	0.44
1:A:271:SER:HB2	1:A:324:MET:CE	2.48	0.44
1:A:264:ARG:HD2	1:A:264:ARG:HA	1.82	0.43
1:B:344:LYS:CG	1:B:349:GLU:HG3	2.48	0.43
1:A:111:MET:SD	1:A:155:LEU:HG	2.58	0.43
1:A:272:TYR:CZ	1:B:137:MET:CE	3.01	0.43
1:B:338:GLU:OE1	5:B:501:HOH:O	2.21	0.43
1:D:167:PHE:HB3	1:D:206:HIS:CE1	2.53	0.43
1:A:183:LEU:O	1:A:183:LEU:HD12	2.19	0.43
1:B:344:LYS:HZ2	1:B:349:GLU:HG3	1.84	0.43
1:B:121:GLU:O	1:B:122:ALA:HB3	2.19	0.42
1:D:133:VAL:O	1:D:168:THR:OG1	2.30	0.42
1:C:238:TYR:CD1	1:C:238:TYR:C	2.93	0.42
1:A:324:MET:SD	1:B:139:ARG:HG3	2.59	0.42
1:C:90:LEU:O	1:C:93:VAL:HG23	2.20	0.42
1:D:269:THR:HG22	1:D:274:ALA:HB1	2.01	0.42
1:B:299:LEU:CD2	1:B:359:LEU:HD21	2.50	0.42
1:C:256:ARG:CG	1:C:256:ARG:NH1	2.78	0.42
1:D:270:VAL:HG21	1:D:276:TYR:HD1	1.84	0.42
1:A:145:LYS:NZ	1:A:146:GLU:OE2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:HD11	1:A:62:LEU:HD11	2.02	0.41
1:A:189:ILE:HA	1:A:192:LEU:HD12	2.02	0.41
1:C:149:LEU:HD13	1:C:195:LEU:HD23	2.01	0.41
3:C:403:ALA:HB1	1:D:320:MET:CE	2.50	0.41
1:D:126:ARG:HG2	1:D:160:PHE:HA	2.01	0.41
1:B:248:GLU:HA	1:B:249:PRO:HD3	1.90	0.41
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.83	0.41
1:A:152:VAL:HG21	1:A:195:LEU:HD11	2.03	0.41
1:A:272:TYR:CE2	1:B:137:MET:HE3	2.56	0.41
1:A:142:VAL:CG2	1:A:147:GLU:HB3	2.51	0.41
1:A:167:PHE:HB3	1:A:206:HIS:NE2	2.35	0.41
1:B:84:VAL:O	1:B:104:SER:OG	2.38	0.41
1:D:9:TRP:O	1:D:253:LEU:HD12	2.21	0.41
1:D:320:MET:HB2	1:D:320:MET:HE3	1.70	0.41
1:A:28:ILE:HB	1:A:29:PRO:HD2	2.02	0.41
1:B:344:LYS:HG3	1:B:344:LYS:HZ3	1.48	0.40
1:A:283:VAL:CG1	1:A:327:LEU:HD12	2.51	0.40
1:D:206:HIS:HB3	1:D:223:MET:HB3	2.02	0.40
1:C:196:LYS:C	1:C:198:GLN:N	2.74	0.40
1:B:241:GLN:HG2	1:B:241:GLN:H	1.59	0.40
1:D:187:LYS:O	1:D:190:SER:HB3	2.22	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	384/398 (96%)	351 (91%)	28 (7%)	5 (1%)	10 11
1	B	384/398 (96%)	359 (94%)	17 (4%)	8 (2%)	5 5
1	C	384/398 (96%)	361 (94%)	22 (6%)	1 (0%)	37 47
1	D	384/398 (96%)	358 (93%)	23 (6%)	3 (1%)	16 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1536/1592 (96%)	1429 (93%)	90 (6%)	17 (1%)	12 13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	SER
1	A	300	SER
1	A	331	GLY
1	A	332	GLU
1	B	330	ASN
1	A	122	ALA
1	B	123	SER
1	B	43	TYR
1	D	203	PRO
1	C	332	GLU
1	D	43	TYR
1	D	106	PHE
1	B	120	LYS
1	B	335	GLN
1	B	122	ALA
1	B	136	GLY
1	B	203	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	320/331 (97%)	310 (97%)	10 (3%)	35 51
1	B	320/331 (97%)	301 (94%)	19 (6%)	16 23
1	C	320/331 (97%)	309 (97%)	11 (3%)	32 47
1	D	320/331 (97%)	310 (97%)	10 (3%)	35 51
All	All	1280/1324 (97%)	1230 (96%)	50 (4%)	27 41

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	21	LEU
1	A	25	ARG
1	A	89	SER
1	A	94	LYS
1	A	190	SER
1	A	264	ARG
1	A	265	THR
1	A	300	SER
1	A	310	LYS
1	B	1	MET
1	B	32	SER
1	B	104	SER
1	B	137	MET
1	B	145	LYS
1	B	147	GLU
1	B	171	SER
1	B	179	THR
1	B	190	SER
1	B	200	ILE
1	B	201	GLU
1	B	220	SER
1	B	241	GLN
1	B	246	LYS
1	B	248	GLU
1	B	302	ARG
1	B	344	LYS
1	B	357	GLU
1	B	379	ILE
1	C	38	VAL
1	C	144	THR
1	C	168	THR
1	C	171	SER
1	C	180	LEU
1	C	189	ILE
1	C	190	SER
1	C	197	LYS
1	C	214	ILE
1	C	245	VAL
1	C	353	ASP
1	D	60	SER
1	D	91	SER
1	D	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	198	GLN
1	D	243	ASN
1	D	269	THR
1	D	270	VAL
1	D	296	SER
1	D	310	LYS
1	D	349	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	ALA	C	402	2	5,5,5	0.86	0	6,6,6	1.19	0
2	PLP	B	401	-	15,15,16	1.08	1 (6%)	20,22,23	1.41	3 (15%)
3	ALA	A	402	-	5,5,5	0.75	0	6,6,6	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ALA	C	403	-	5,5,5	0.77	0	6,6,6	0.67	0
2	PLP	C	401	-	15,15,16	1.18	3 (20%)	20,22,23	1.61	4 (20%)
2	PLP	A	401	-	15,15,16	1.19	2 (13%)	20,22,23	1.81	5 (25%)
2	PLP	D	502	3	15,15,16	1.27	2 (13%)	20,22,23	1.50	4 (20%)

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	ALA	C	402	2	-	0/4/4/4	-
2	PLP	B	401	-	-	0/6/6/8	0/1/1/1
3	ALA	A	402	-	-	2/4/4/4	-
3	ALA	C	403	-	-	2/4/4/4	-
2	PLP	C	401	-	-	3/6/6/8	0/1/1/1
2	PLP	A	401	-	-	0/6/6/8	0/1/1/1
2	PLP	D	502	3	-	2/6/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	PLP	C2A-C2	3.32	1.56	1.50
2	A	401	PLP	C2A-C2	2.86	1.55	1.50
2	C	401	PLP	C2A-C2	2.70	1.55	1.50
2	A	401	PLP	O3-C3	2.39	1.42	1.37
2	D	502	PLP	O3-C3	2.34	1.42	1.37
2	B	401	PLP	C2A-C2	2.33	1.54	1.50
2	C	401	PLP	O3-C3	2.07	1.41	1.37
2	C	401	PLP	P-O4P	2.02	1.66	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	O4P-C5A-C5	-4.70	100.39	109.35
2	D	502	PLP	O4P-C5A-C5	-3.77	102.17	109.35
2	B	401	PLP	O4P-C5A-C5	-3.23	103.19	109.35
2	C	401	PLP	O4P-C5A-C5	-3.21	103.24	109.35
2	A	401	PLP	C5-C6-N1	-3.16	118.56	123.82
2	A	401	PLP	C6-C5-C4	3.06	120.57	118.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	PLP	C5-C6-N1	-2.69	119.34	123.82
2	D	502	PLP	C6-C5-C4	2.60	120.20	118.16
2	D	502	PLP	C5-C6-N1	-2.57	119.54	123.82
2	C	401	PLP	O3-C3-C2	2.52	122.98	117.49
2	A	401	PLP	O3-C3-C2	2.50	122.94	117.49
2	C	401	PLP	C6-N1-C2	2.43	123.67	119.17
2	B	401	PLP	O3-C3-C2	2.27	122.44	117.49
2	D	502	PLP	O3-C3-C2	2.25	122.40	117.49
2	B	401	PLP	C5-C6-N1	-2.14	120.25	123.82
2	A	401	PLP	C6-N1-C2	2.10	123.06	119.17

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	PLP	C5A-O4P-P-O1P
2	C	401	PLP	C5A-O4P-P-O3P
3	A	402	ALA	OXT-C-CA-N
3	A	402	ALA	O-C-CA-N
3	C	403	ALA	OXT-C-CA-CB
2	D	502	PLP	C5A-O4P-P-O1P
3	C	403	ALA	O-C-CA-CB
2	C	401	PLP	C5A-O4P-P-O2P
2	D	502	PLP	C5A-O4P-P-O3P

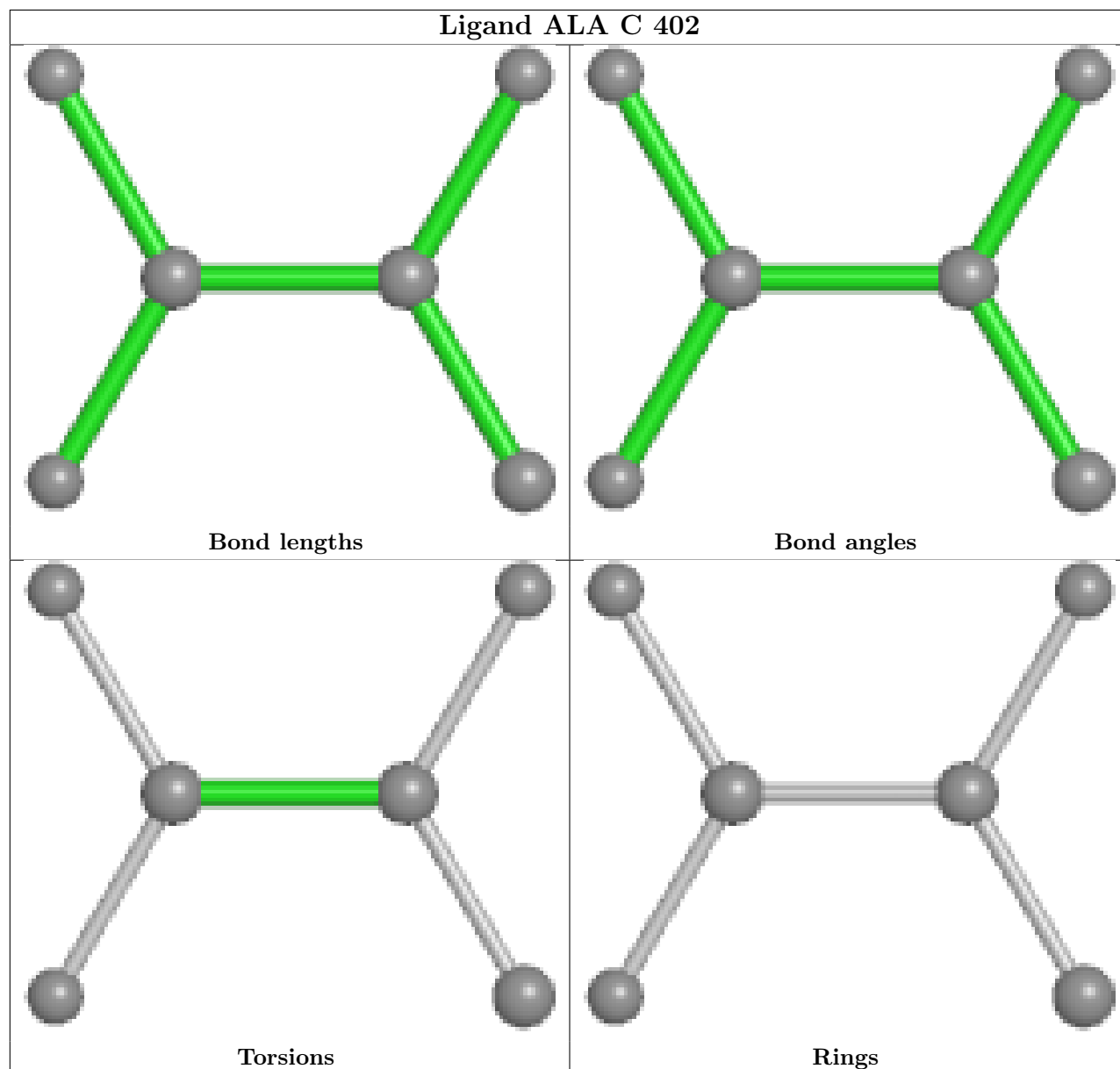
There are no ring outliers.

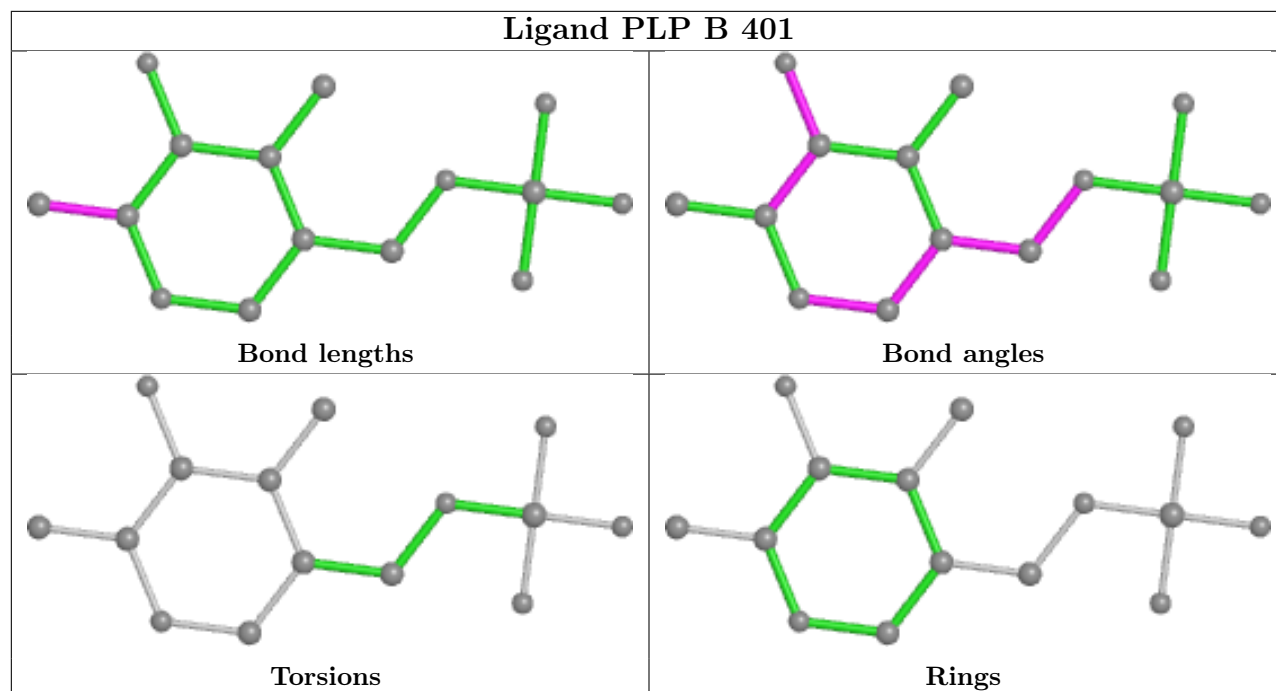
5 monomers are involved in 10 short contacts:

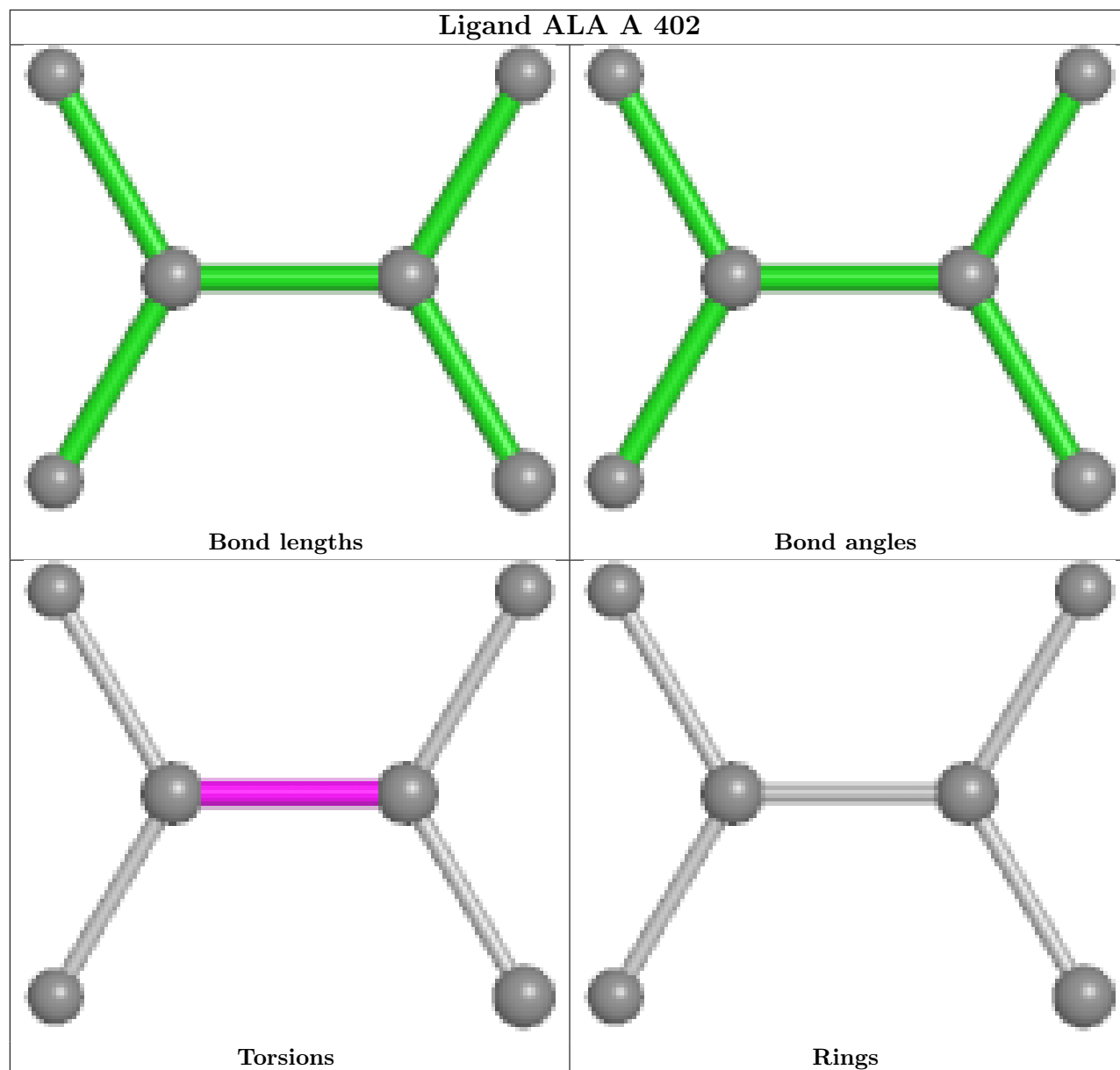
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PLP	1	0
3	A	402	ALA	2	0
3	C	403	ALA	3	0
2	C	401	PLP	4	0
2	A	401	PLP	2	0

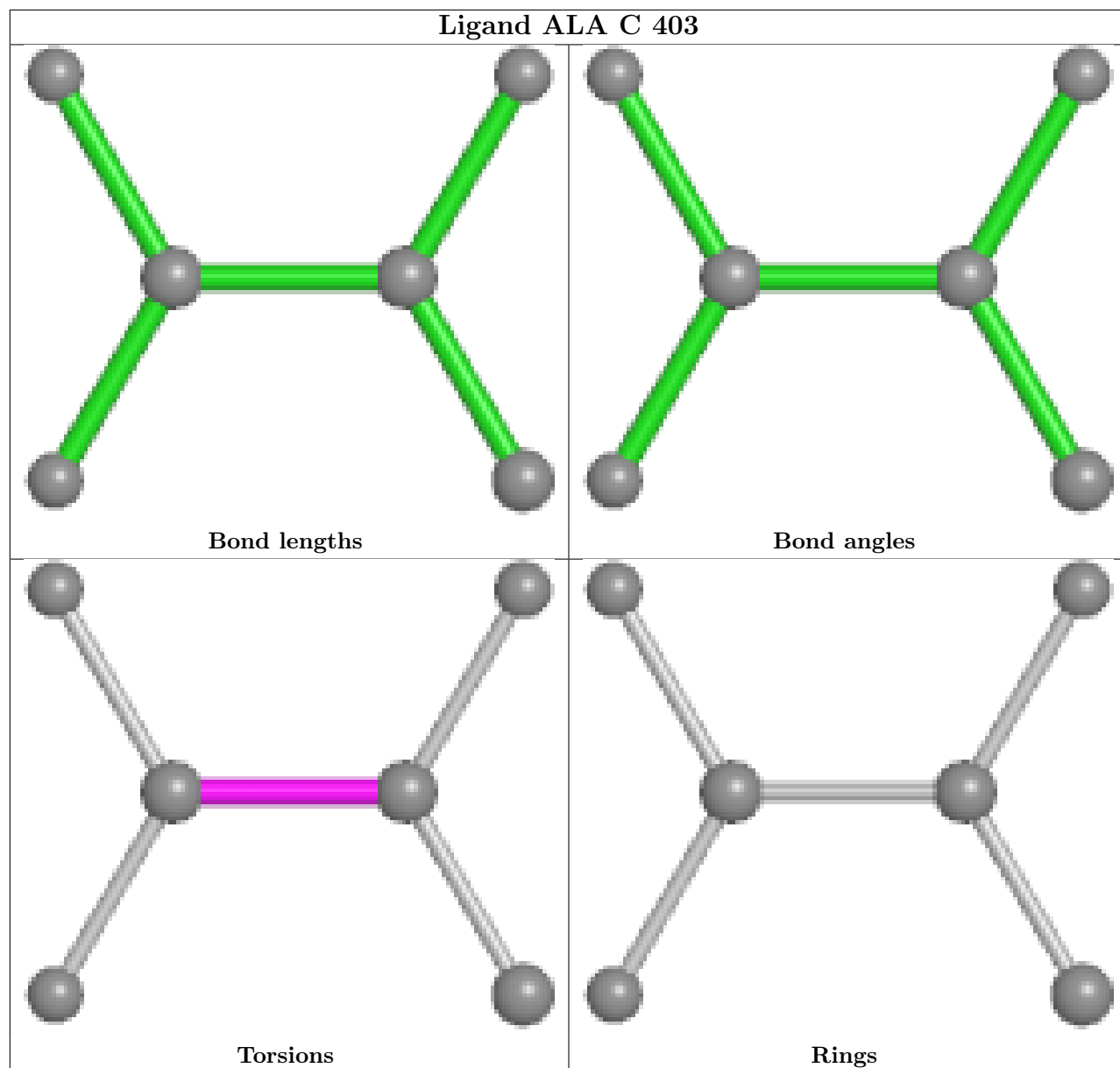
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

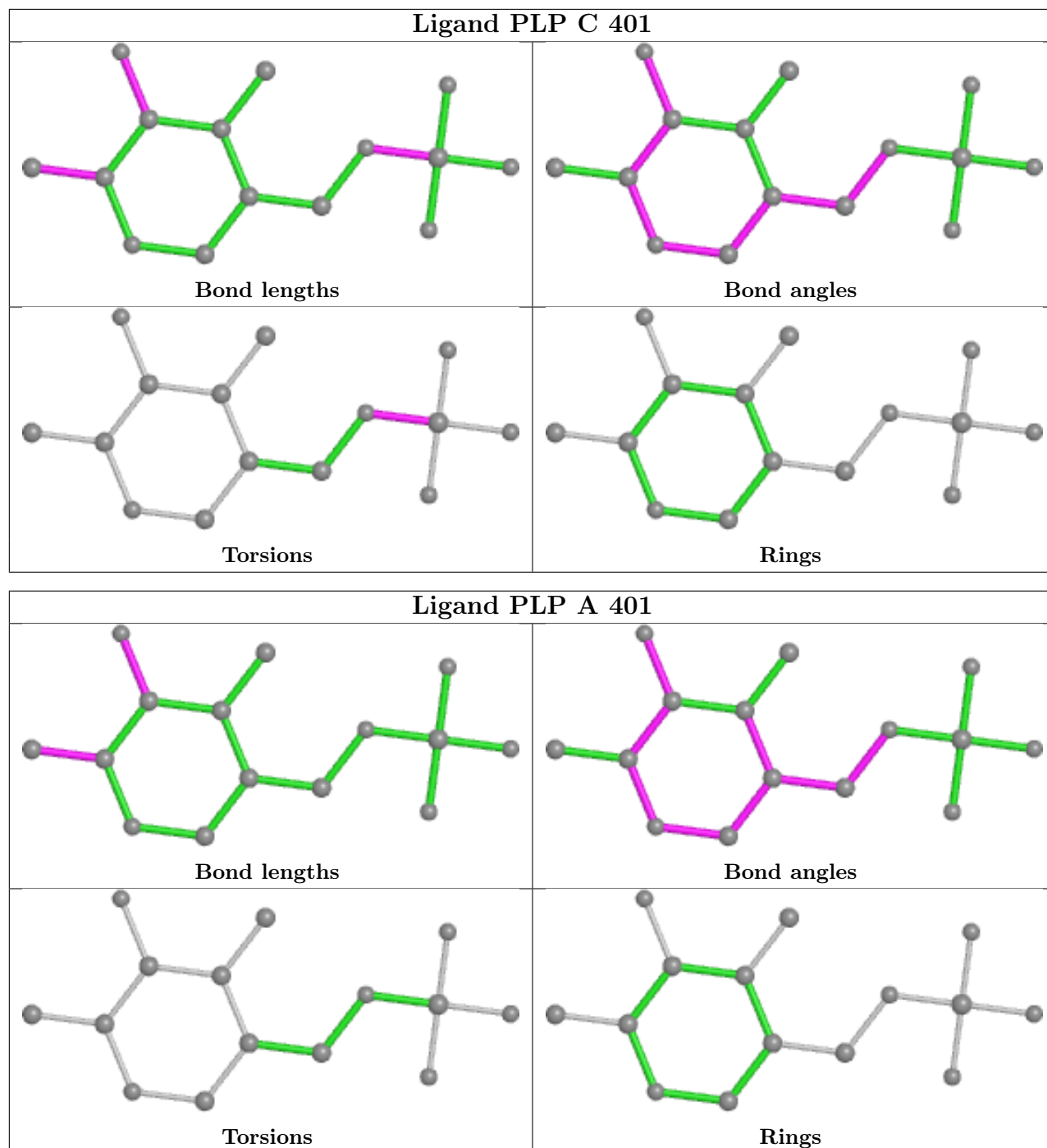
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

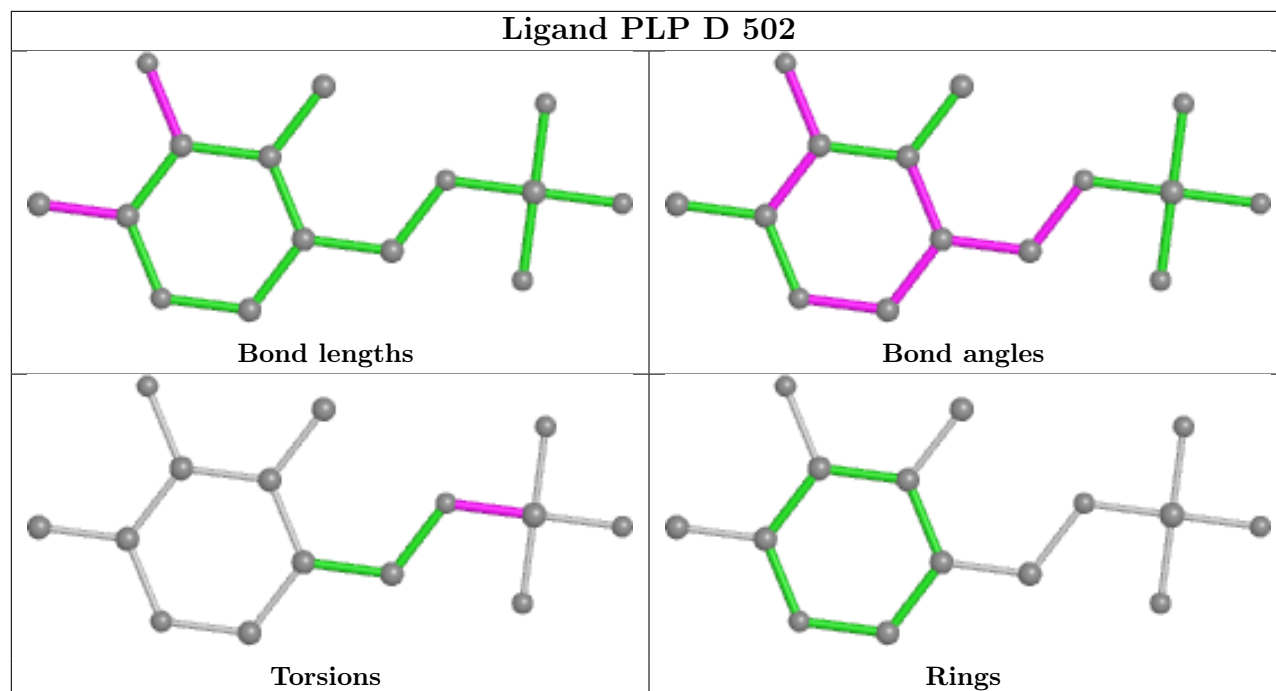












5.7 Other polymers [i](#)

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 [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	386/398 (96%)	-0.26	3 (0%) 82 83	36, 49, 72, 87	0
1	B	386/398 (96%)	-0.21	0 100 100	39, 51, 69, 85	0
1	C	386/398 (96%)	-0.08	1 (0%) 90 90	41, 55, 70, 87	0
1	D	386/398 (96%)	-0.26	0 100 100	38, 50, 69, 82	0
All	All	1544/1592 (96%)	-0.20	4 (0%) 90 90	36, 51, 70, 87	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	122	ALA	2.5
1	A	123	SER	2.1
1	A	124	ALA	2.1
1	A	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

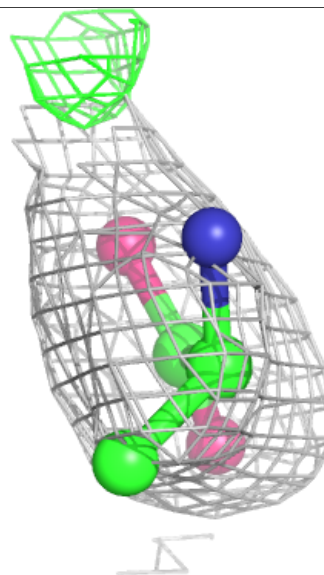
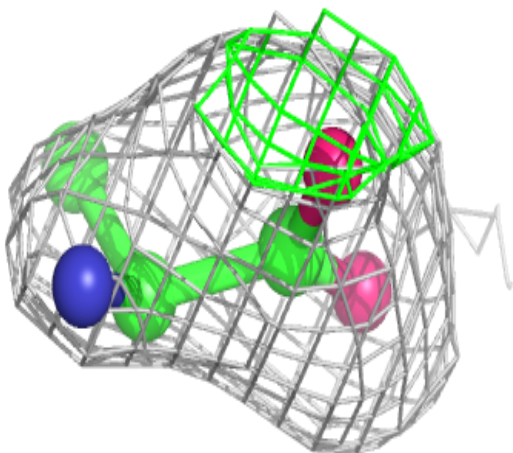
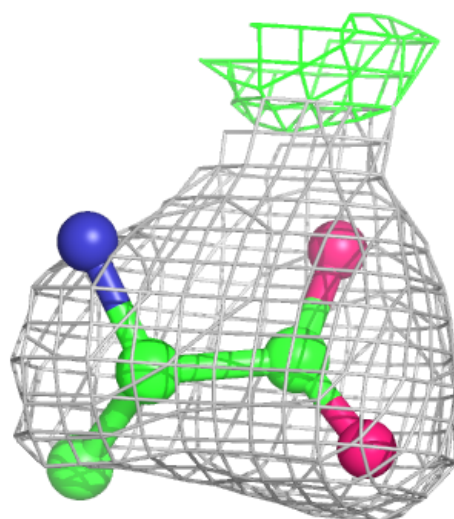
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ALA	C	403	6/6	0.87	0.10	54,58,62,67	0
3	ALA	C	402	6/6	0.90	0.10	44,47,53,54	0
2	PLP	C	401	15/16	0.91	0.09	49,58,64,65	0
2	PLP	D	502	15/16	0.92	0.10	46,52,60,63	0
3	ALA	A	402	6/6	0.93	0.09	51,56,58,61	0
2	PLP	B	401	15/16	0.95	0.09	45,54,58,58	0
2	PLP	A	401	15/16	0.95	0.09	40,48,56,59	0
4	CL	A	403	1/1	0.95	0.09	57,57,57,57	0
4	CL	B	402	1/1	0.96	0.10	56,56,56,56	0
4	CL	C	404	1/1	0.96	0.12	53,53,53,53	0
4	CL	D	503	1/1	0.98	0.05	51,51,51,51	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.

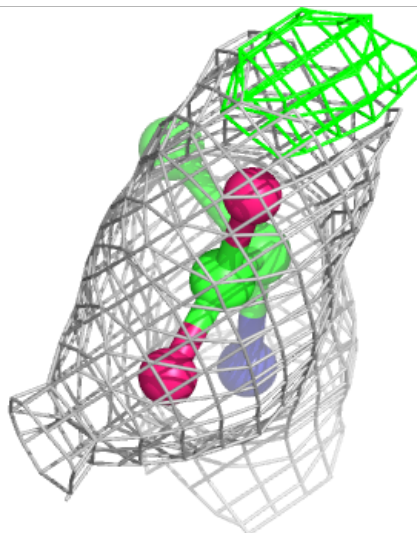
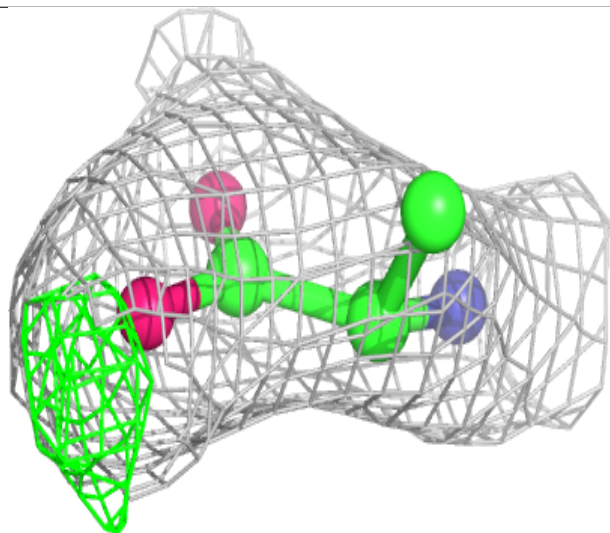
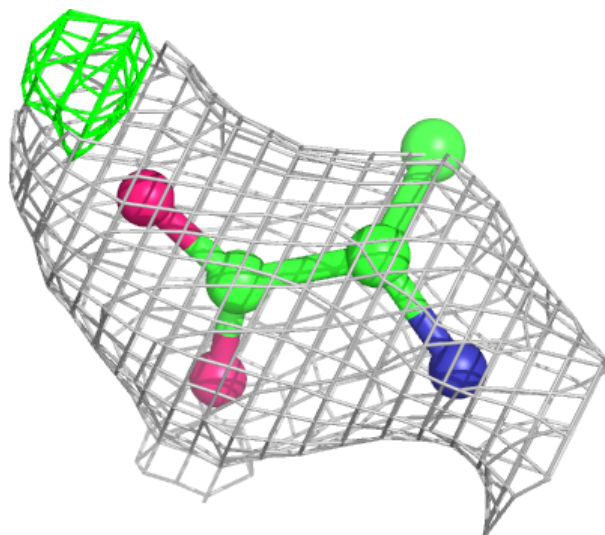
Electron density around ALA C 403:

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



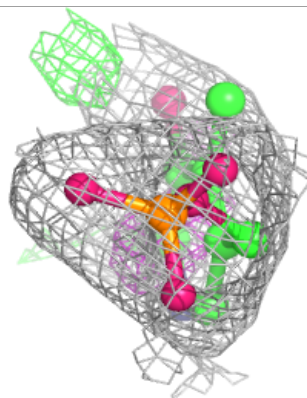
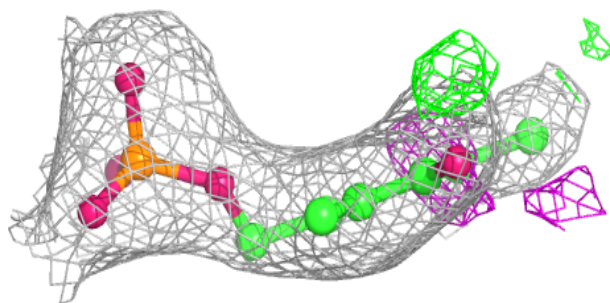
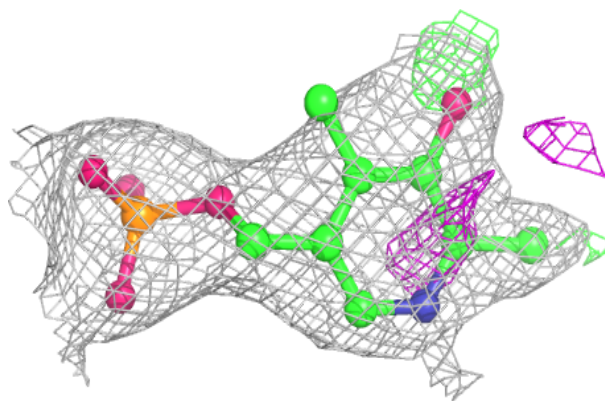
Electron density around ALA C 402:

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

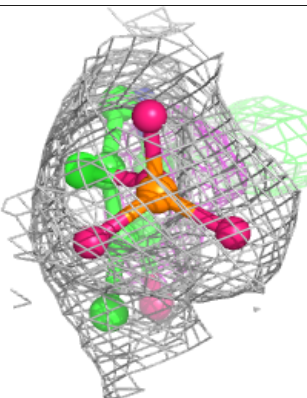
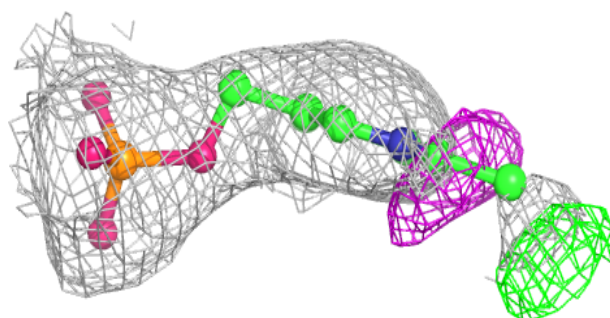
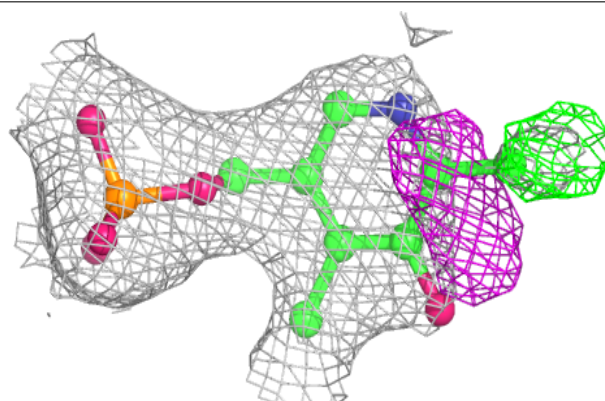


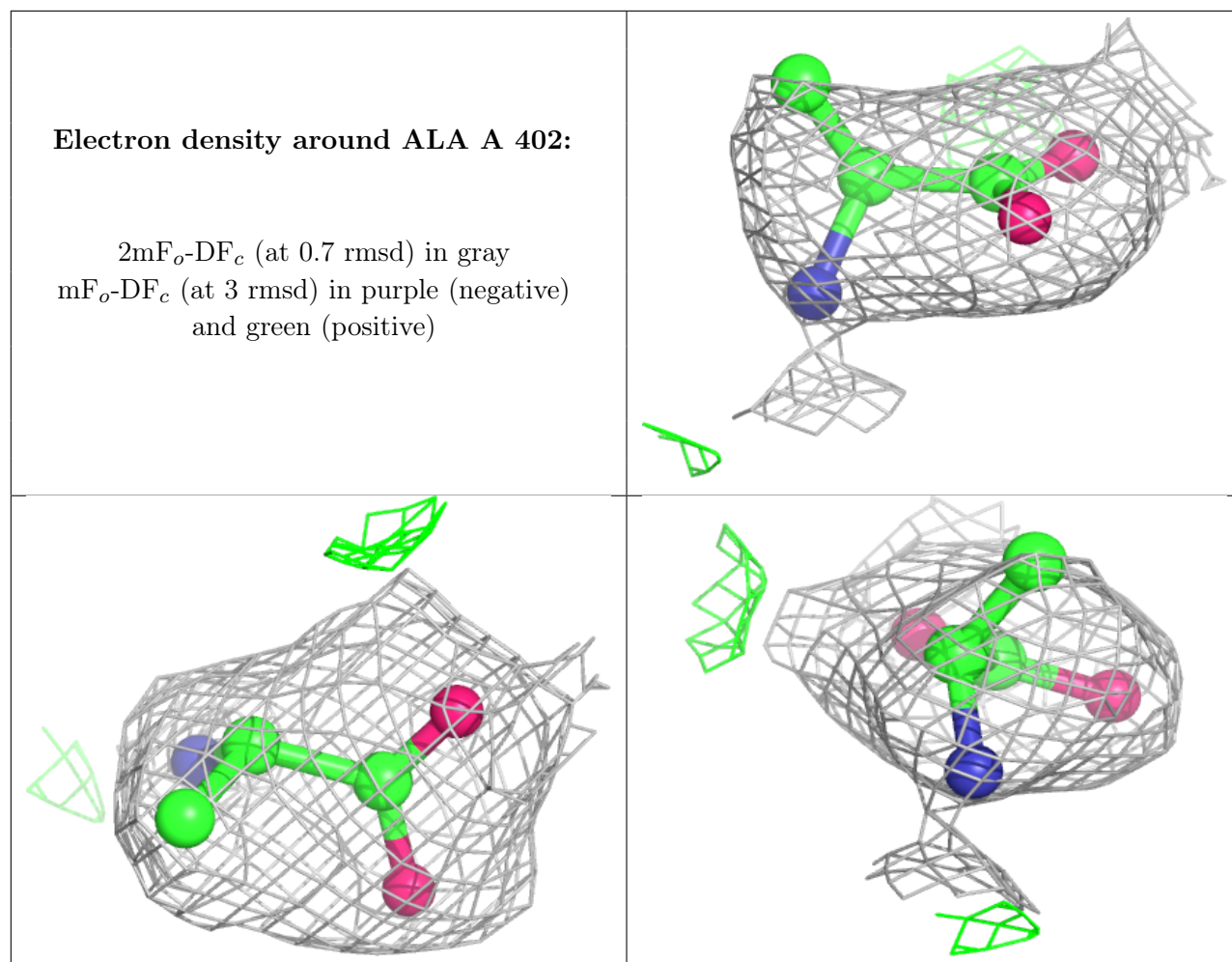
Electron density around PLP C 401:

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

**Electron density around PLP D 502:**

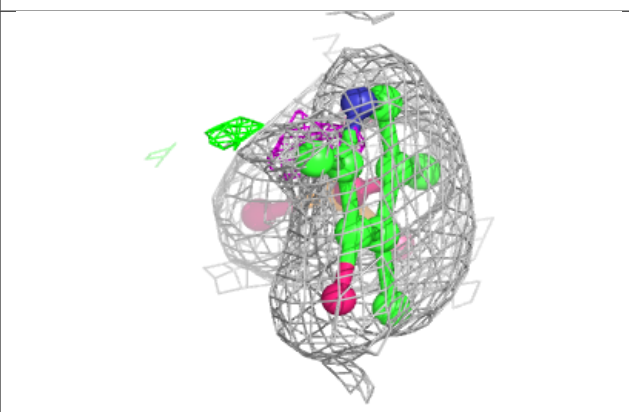
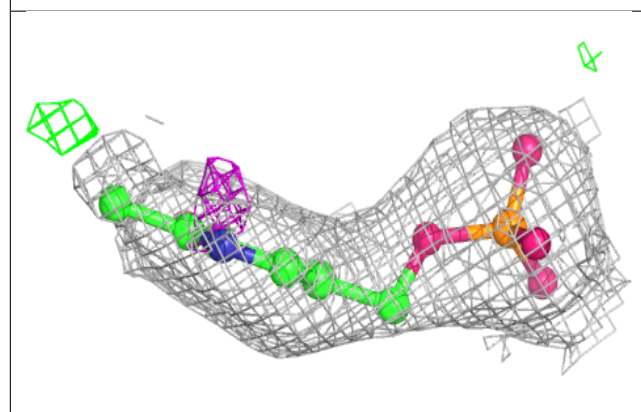
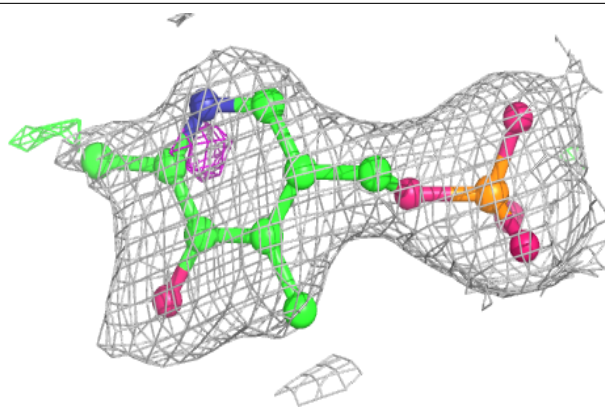
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



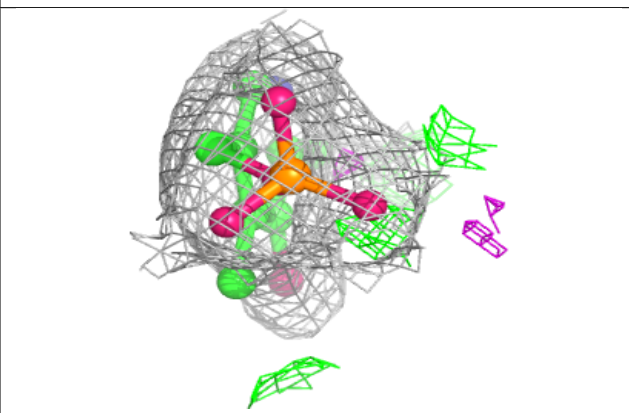
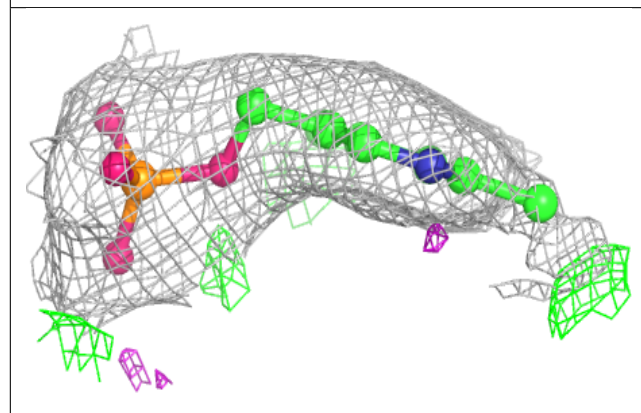
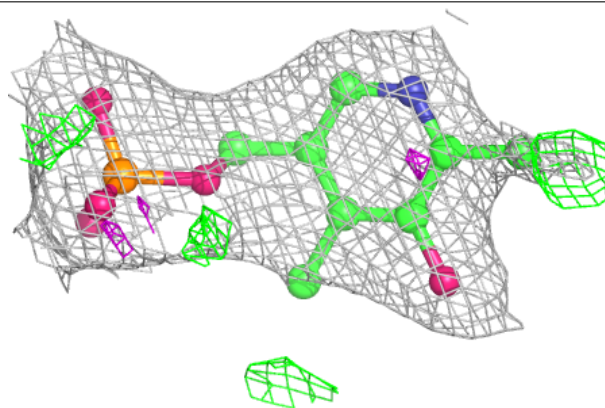


Electron density around PLP B 401:

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

**Electron density around PLP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.