



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:38 AM UTC

PDB ID : 8IS0 / pdb_00008is0
Title : Carbon Sulfoxide lyase - Y106F
Authors : Gong, W.M.; Wei, L.L.; Liu, L.
Deposited on : 2023-03-20
Resolution : 3.02 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

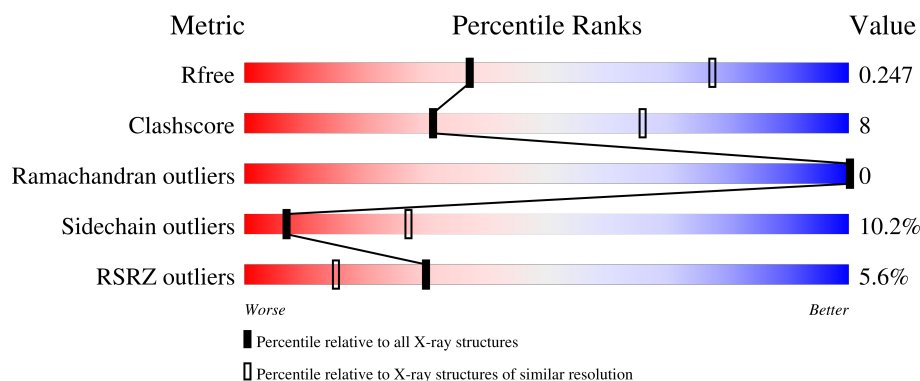
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	392	5% 72% 21% ...
1	B	392	5% 71% 21% 5%

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
3	DHA	A	402	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5604 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 Probable hercynylcysteine sulfoxide lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2774	1730	511	523	10			
1	B	373	Total	C	N	O	S	0	0	0
			2750	1715	504	521	10			

There are 46 discrepancies between the modelled and reference sequences:

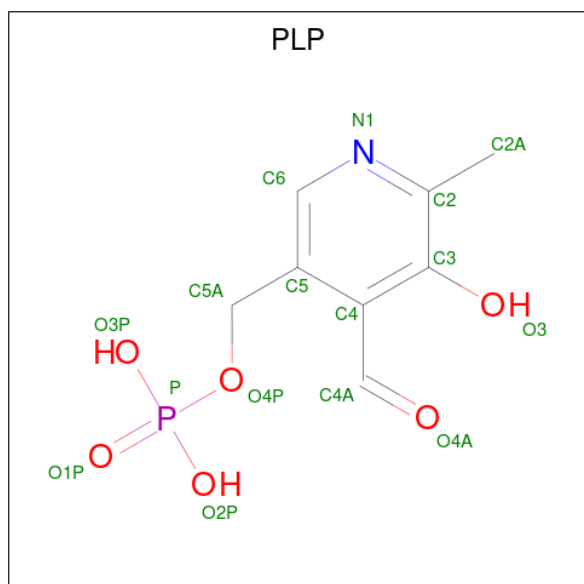
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0R5M7
A	-19	GLY	-	expression tag	UNP A0R5M7
A	-18	SER	-	expression tag	UNP A0R5M7
A	-17	SER	-	expression tag	UNP A0R5M7
A	-16	HIS	-	expression tag	UNP A0R5M7
A	-15	HIS	-	expression tag	UNP A0R5M7
A	-14	HIS	-	expression tag	UNP A0R5M7
A	-13	HIS	-	expression tag	UNP A0R5M7
A	-12	HIS	-	expression tag	UNP A0R5M7
A	-11	HIS	-	expression tag	UNP A0R5M7
A	-10	SER	-	expression tag	UNP A0R5M7
A	-9	SER	-	expression tag	UNP A0R5M7
A	-8	GLY	-	expression tag	UNP A0R5M7
A	-7	LEU	-	expression tag	UNP A0R5M7
A	-6	VAL	-	expression tag	UNP A0R5M7
A	-5	PRO	-	expression tag	UNP A0R5M7
A	-4	ARG	-	expression tag	UNP A0R5M7
A	-3	GLY	-	expression tag	UNP A0R5M7
A	-2	SER	-	expression tag	UNP A0R5M7
A	-1	HIS	-	expression tag	UNP A0R5M7
A	0	MET	-	expression tag	UNP A0R5M7
A	1	VAL	-	expression tag	UNP A0R5M7
A	106	PHE	TYR	engineered mutation	UNP A0R5M7
B	-20	MET	-	initiating methionine	UNP A0R5M7
B	-19	GLY	-	expression tag	UNP A0R5M7

Continued on next page...

Continued from previous page...

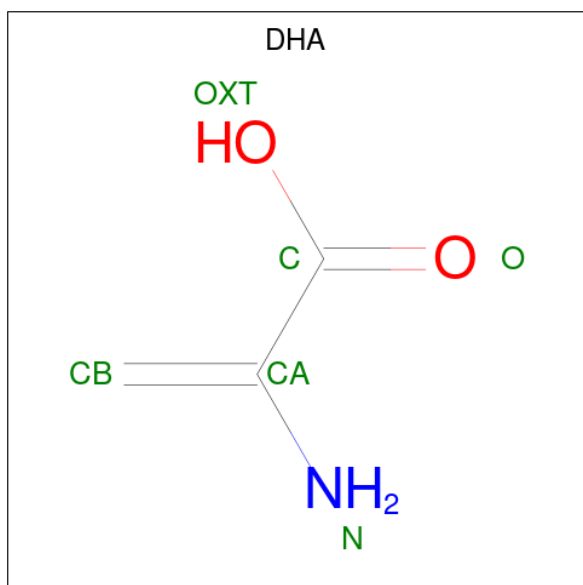
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	expression tag	UNP A0R5M7
B	-17	SER	-	expression tag	UNP A0R5M7
B	-16	HIS	-	expression tag	UNP A0R5M7
B	-15	HIS	-	expression tag	UNP A0R5M7
B	-14	HIS	-	expression tag	UNP A0R5M7
B	-13	HIS	-	expression tag	UNP A0R5M7
B	-12	HIS	-	expression tag	UNP A0R5M7
B	-11	HIS	-	expression tag	UNP A0R5M7
B	-10	SER	-	expression tag	UNP A0R5M7
B	-9	SER	-	expression tag	UNP A0R5M7
B	-8	GLY	-	expression tag	UNP A0R5M7
B	-7	LEU	-	expression tag	UNP A0R5M7
B	-6	VAL	-	expression tag	UNP A0R5M7
B	-5	PRO	-	expression tag	UNP A0R5M7
B	-4	ARG	-	expression tag	UNP A0R5M7
B	-3	GLY	-	expression tag	UNP A0R5M7
B	-2	SER	-	expression tag	UNP A0R5M7
B	-1	HIS	-	expression tag	UNP A0R5M7
B	0	MET	-	expression tag	UNP A0R5M7
B	1	VAL	-	expression tag	UNP A0R5M7
B	106	PHE	TYR	engineered mutation	UNP A0R5M7

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 2-AMINO-ACRYLIC ACID (CCD ID: DHA) (formula: $C_3H_5NO_2$) (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	B	1	Total	C	N	O	0	0
			6	3	1	2		

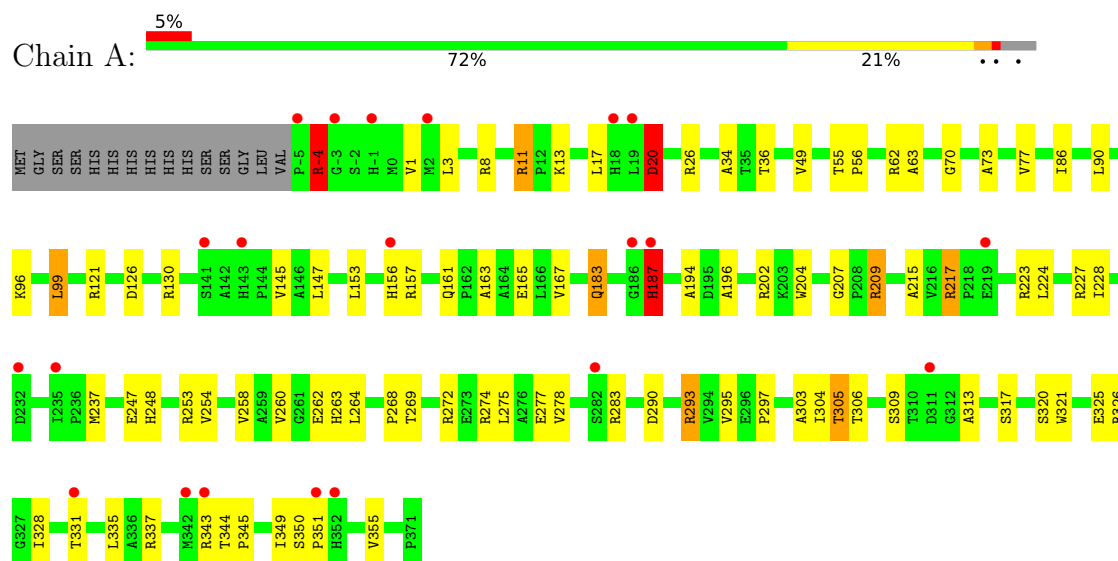
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	14	Total	O	0	0
			14	14		

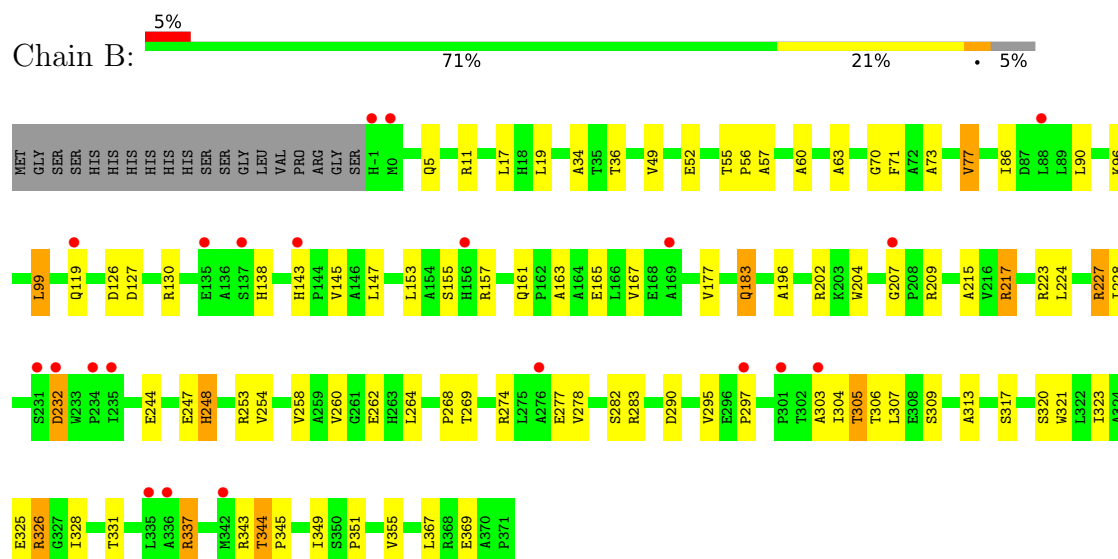
3 Residue-property plots

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: Probable hercynylcysteine sulfoxide lyase



- Molecule 1: Probable hercynylcysteine sulfoxide lyase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.52Å 173.28Å 82.86Å 90.00° 125.51° 90.00°	Depositor
Resolution (Å)	34.36 – 3.02 34.36 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.1 (34.36-3.02) 98.1 (34.36-3.02)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.197 , 0.240 0.205 , 0.247	Depositor DCC
R_{free} test set	1198 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5604	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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: PLP, DHA

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	0.63	2/2832 (0.1%)	1.07	3/3870 (0.1%)
1	B	0.63	1/2807 (0.0%)	1.07	1/3837 (0.0%)
All	All	0.63	3/5639 (0.1%)	1.07	4/7707 (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	12
1	B	0	8
All	All	0	20

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	HIS	CE1-NE2	5.46	1.38	1.32
1	A	263	HIS	CE1-NE2	5.23	1.37	1.32
1	A	156	HIS	CE1-NE2	5.04	1.37	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	HIS	CA-CB-CG	7.44	121.24	113.80
1	A	297	PRO	CB-CA-C	-6.06	103.86	111.56
1	A	20	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	297	PRO	CB-CA-C	-5.86	104.11	111.56

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-4	ARG	Sidechain
1	A	11	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	209	ARG	Sidechain
1	A	223	ARG	Sidechain
1	A	227	ARG	Sidechain
1	A	293	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	337	ARG	Sidechain
1	A	343	ARG	Sidechain
1	A	62	ARG	Sidechain
1	A	8	ARG	Sidechain
1	B	157	ARG	Sidechain
1	B	209	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	223	ARG	Sidechain
1	B	227	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	337	ARG	Sidechain
1	B	343	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2774	0	2744	47	0
1	B	2750	0	2721	45	0
2	A	15	0	7	3	0
2	B	15	0	7	1	0
3	A	6	0	2	0	0
3	B	6	0	2	1	0
4	A	24	0	0	1	0
4	B	14	0	0	1	0
All	All	5604	0	5483	91	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 8.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:HIS:HA	1:A:272:ARG:HG2	1.70	0.73
1:A:183:GLN:HE21	2:A:401:PLP:HO3	1.38	0.72
1:A:183:GLN:NE2	2:A:401:PLP:O3	2.23	0.71
1:B:183:GLN:HG3	1:B:304:ILE:HD11	1.78	0.66
1:A:163:ALA:O	1:A:167:VAL:HG23	1.98	0.63
1:A:70:GLY:O	1:A:217:ARG:NH2	2.32	0.62
1:A:187:HIS:HB3	1:A:275:LEU:CD1	2.28	0.62
1:B:99:LEU:C	1:B:99:LEU:HD23	2.25	0.61
1:B:163:ALA:O	1:B:167:VAL:HG23	2.00	0.61
1:A:99:LEU:HD23	1:A:99:LEU:C	2.26	0.61
1:A:187:HIS:HB3	1:A:275:LEU:HD13	1.81	0.61
1:B:183:GLN:NE2	2:B:401:PLP:O3	2.35	0.59
1:B:227:ARG:NH2	1:B:228:ILE:HD11	2.18	0.59
1:B:77:VAL:HG22	1:B:244:GLU:HB2	1.84	0.59
1:B:17:LEU:O	1:B:328:ILE:HA	2.05	0.57
1:A:183:GLN:HG3	1:A:304:ILE:HD11	1.86	0.57
1:A:17:LEU:O	1:A:328:ILE:HA	2.05	0.56
1:A:321:TRP:NE1	1:A:325:GLU:HG3	2.20	0.56
1:A:272:ARG:NH1	4:A:501:HOH:O	2.38	0.56
1:A:1:VAL:HG12	1:A:3:LEU:H	1.70	0.55
1:B:77:VAL:CG2	1:B:244:GLU:HB2	2.37	0.55
1:B:321:TRP:NE1	1:B:325:GLU:HG3	2.21	0.55
1:B:130:ARG:HA	1:B:161:GLN:HE22	1.72	0.55
1:B:34:ALA:CB	1:B:258:VAL:HG21	2.38	0.53
1:B:323:ILE:HG13	4:B:503:HOH:O	2.08	0.53
1:B:86:ILE:O	1:B:90:LEU:HG	2.10	0.52
1:A:202:ARG:HD3	1:A:209:ARG:HG2	1.91	0.51
1:B:196:ALA:HA	1:B:215:ALA:O	2.09	0.51
1:A:202:ARG:NH2	2:A:401:PLP:O3P	2.43	0.51
1:A:34:ALA:CB	1:A:258:VAL:HG21	2.40	0.51
1:A:86:ILE:O	1:A:90:LEU:HG	2.10	0.51
1:B:183:GLN:CG	1:B:304:ILE:HD11	2.40	0.51
1:B:258:VAL:O	1:B:262:GLU:HG3	2.10	0.50
1:A:130:ARG:HA	1:A:161:GLN:HE22	1.75	0.50
1:B:264:LEU:HA	1:B:268:PRO:HD3	1.93	0.50
1:A:258:VAL:O	1:A:262:GLU:HG3	2.12	0.49
1:B:70:GLY:O	1:B:217:ARG:NH2	2.43	0.49
1:A:196:ALA:HA	1:A:215:ALA:O	2.13	0.49
1:A:-4:ARG:HG3	1:A:-4:ARG:HH11	1.78	0.49
1:B:63:ALA:HA	1:B:73:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:HA	1:B:207:GLY:O	2.13	0.48
1:B:309:SER:OG	1:B:313:ALA:HB3	2.13	0.48
1:A:309:SER:OG	1:A:313:ALA:HB3	2.14	0.48
1:A:194:ALA:O	1:A:217:ARG:NH1	2.47	0.48
1:A:147:LEU:C	1:A:147:LEU:HD12	2.39	0.47
1:A:204:TRP:CH2	1:A:303:ALA:HB3	2.49	0.47
1:B:126:ASP:OD2	1:B:130:ARG:HB3	2.15	0.47
1:A:202:ARG:HA	1:A:207:GLY:O	2.15	0.47
1:B:204:TRP:CH2	1:B:303:ALA:HB3	2.50	0.47
1:A:126:ASP:OD2	1:A:130:ARG:HB3	2.15	0.47
1:A:349:ILE:HG22	1:A:351:PRO:HD3	1.96	0.47
1:B:147:LEU:C	1:B:147:LEU:HD12	2.39	0.46
1:A:283:ARG:HE	1:A:305:THR:HB	1.80	0.46
1:A:295:VAL:HG23	1:A:306:THR:O	2.14	0.46
1:B:349:ILE:HG22	1:B:351:PRO:HD3	1.98	0.46
1:B:283:ARG:HE	1:B:305:THR:HB	1.82	0.45
1:A:183:GLN:CG	1:A:304:ILE:HD11	2.46	0.45
1:A:248:HIS:CD2	1:A:253:ARG:CZ	3.00	0.45
1:B:337:ARG:HH12	3:B:402:DHA:C	2.30	0.45
1:A:63:ALA:HA	1:A:73:ALA:HB2	1.98	0.45
1:B:19:LEU:CD2	1:B:351:PRO:HB3	2.48	0.44
1:B:55:THR:N	1:B:56:PRO:HD2	2.32	0.44
1:A:-4:ARG:HB2	1:B:143:HIS:CD2	2.53	0.43
1:A:264:LEU:HA	1:A:268:PRO:HD3	2.00	0.43
1:A:55:THR:N	1:A:56:PRO:HD2	2.33	0.43
1:B:295:VAL:HG23	1:B:306:THR:O	2.18	0.43
1:B:326:ARG:NH1	1:B:369:GLU:OE1	2.47	0.43
1:A:153:LEU:HD21	1:A:304:ILE:HD12	2.01	0.43
1:A:187:HIS:NE2	1:A:204:TRP:CE2	2.87	0.43
1:B:71:PHE:CE2	1:B:217:ARG:HG2	2.54	0.43
1:B:130:ARG:HA	1:B:161:GLN:NE2	2.33	0.43
1:B:248:HIS:CD2	1:B:253:ARG:CZ	3.01	0.43
1:A:-4:ARG:HH11	1:A:-4:ARG:CG	2.33	0.42
1:B:344:THR:HG22	1:B:345:PRO:HD2	2.01	0.42
1:B:278:VAL:HG13	1:B:355:VAL:HG11	2.01	0.42
1:B:282:SER:HB3	1:B:305:THR:HG21	2.02	0.42
1:A:187:HIS:HB3	1:A:275:LEU:HD12	2.00	0.42
1:A:278:VAL:HG13	1:A:355:VAL:HG11	2.02	0.41
1:A:274:ARG:NH2	1:A:355:VAL:O	2.54	0.41
1:B:232:ASP:OD1	1:B:232:ASP:N	2.54	0.41
1:A:99:LEU:HA	1:A:147:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:GLU:HA	1:B:52:GLU:OE1	2.20	0.41
1:B:307:LEU:HD13	1:B:367:LEU:HD21	2.02	0.41
1:A:20:ASP:HA	1:A:350:SER:OG	2.21	0.41
1:A:130:ARG:HA	1:A:161:GLN:NE2	2.35	0.41
1:B:153:LEU:HD21	1:B:304:ILE:HD12	2.02	0.41
1:A:335:LEU:HD11	1:A:345:PRO:HD3	2.03	0.41
1:B:274:ARG:O	1:B:277:GLU:HB2	2.21	0.40
1:A:202:ARG:CD	1:A:209:ARG:HG2	2.52	0.40
1:B:57:ALA:O	1:B:60:ALA:HB3	2.21	0.40
1:B:167:VAL:HG22	1:B:177:VAL:HG11	2.04	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	375/392 (96%)	356 (95%)	19 (5%)	0	100	100
1	B	371/392 (95%)	351 (95%)	20 (5%)	0	100	100
All	All	746/784 (95%)	707 (95%)	39 (5%)	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	281/298 (94%)	250 (89%)	31 (11%)	6	24
1	B	280/298 (94%)	254 (91%)	26 (9%)	8	31
All	All	561/596 (94%)	504 (90%)	57 (10%)	7	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	ARG
1	A	11	ARG
1	A	13	LYS
1	A	20	ASP
1	A	26	ARG
1	A	36	THR
1	A	49	VAL
1	A	77	VAL
1	A	96	LYS
1	A	99	LEU
1	A	121	ARG
1	A	145	VAL
1	A	165	GLU
1	A	183	GLN
1	A	187	HIS
1	A	217	ARG
1	A	224	LEU
1	A	228	ILE
1	A	237	MET
1	A	247	GLU
1	A	254	VAL
1	A	260	VAL
1	A	269	THR
1	A	277	GLU
1	A	290	ASP
1	A	293	ARG
1	A	305	THR
1	A	317	SER
1	A	320	SER
1	A	331	THR
1	A	344	THR
1	B	5	GLN
1	B	11	ARG
1	B	36	THR
1	B	49	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	77	VAL
1	B	96	LYS
1	B	99	LEU
1	B	119	GLN
1	B	127	ASP
1	B	138	HIS
1	B	145	VAL
1	B	155	SER
1	B	165	GLU
1	B	183	GLN
1	B	224	LEU
1	B	232	ASP
1	B	247	GLU
1	B	254	VAL
1	B	260	VAL
1	B	269	THR
1	B	290	ASP
1	B	305	THR
1	B	317	SER
1	B	320	SER
1	B	331	THR
1	B	344	THR

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

Mol	Chain	Res	Type
1	A	5	GLN
1	A	38	HIS
1	A	248	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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$
3	DHA	B	402	2	4,5,5	1.54	2 (50%)	5,6,6	2.61	2 (40%)
3	DHA	A	402	2	4,5,5	1.70	2 (50%)	5,6,6	2.99	3 (60%)
2	PLP	A	401	3,1	15,15,16	0.85	1 (6%)	21,22,23	0.85	0
2	PLP	B	401	3,1	15,15,16	0.72	1 (6%)	21,22,23	1.04	1 (4%)

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	DHA	B	402	2	-	0/2/4/4	-
3	DHA	A	402	2	-	1/2/4/4	-
2	PLP	A	401	3,1	-	4/6/6/8	0/1/1/1
2	PLP	B	401	3,1	-	4/6/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	DHA	CA-C	2.62	1.57	1.50
2	B	401	PLP	C4A-C4	-2.28	1.47	1.51
3	B	402	DHA	OXT-C	-2.26	1.24	1.30
3	A	402	DHA	OXT-C	-2.06	1.25	1.30
2	A	401	PLP	C4A-C4	-2.03	1.47	1.51
3	B	402	DHA	CA-C	2.02	1.55	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	DHA	OXT-C-CA	5.52	120.49	112.44
3	B	402	DHA	OXT-C-CA	4.92	119.63	112.44
3	A	402	DHA	O-C-CA	-2.94	117.60	123.60
3	B	402	DHA	O-C-CA	-2.78	117.92	123.60
2	B	401	PLP	C4A-C4-C5	2.54	123.55	120.94
3	A	402	DHA	CB-CA-N	2.08	130.78	125.76

There are no chirality outliers.

All (9) torsion outliers are listed below:

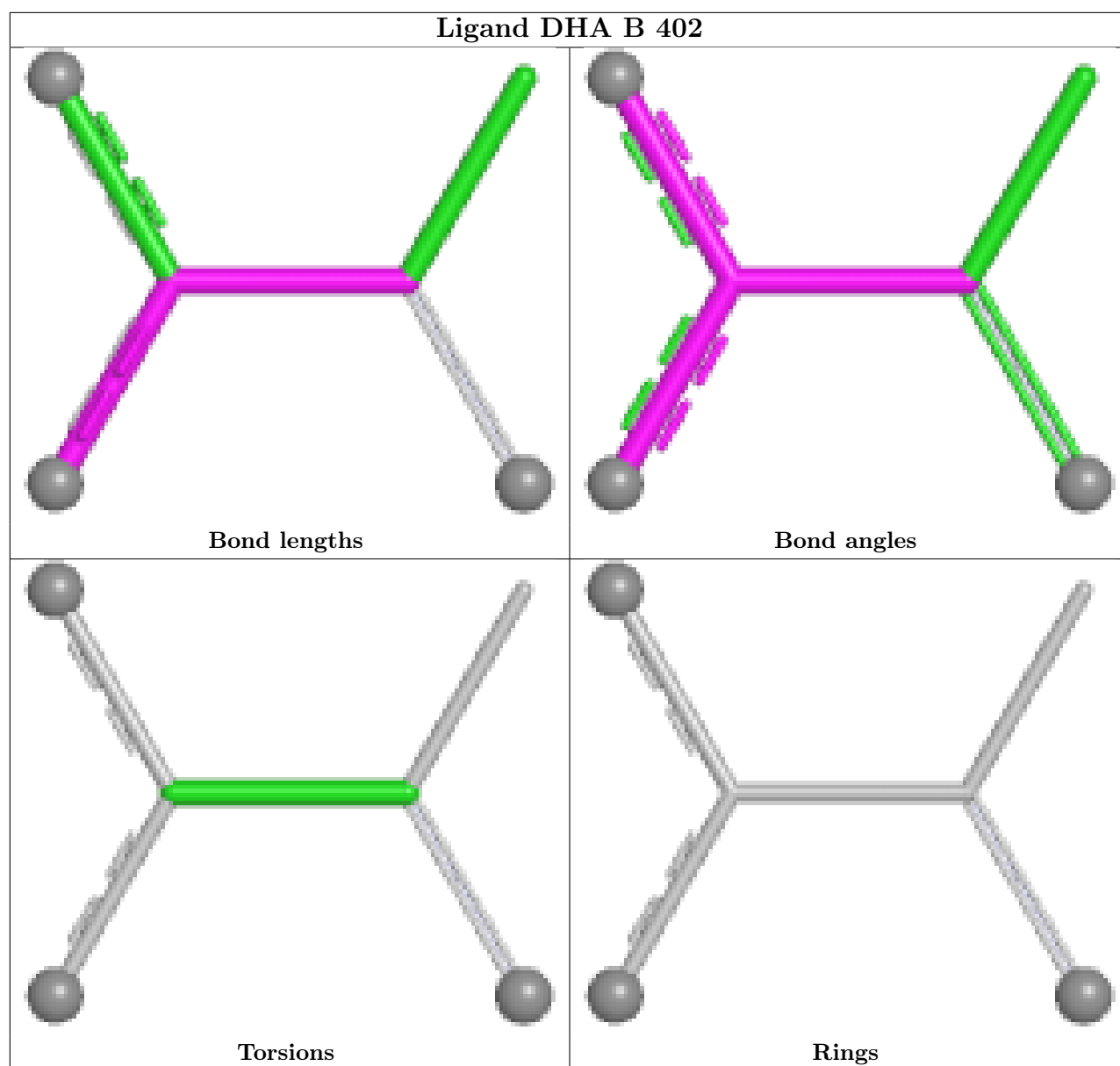
Mol	Chain	Res	Type	Atoms
2	A	401	PLP	C5A-O4P-P-O2P
2	A	401	PLP	C5A-O4P-P-O3P
2	B	401	PLP	C5A-O4P-P-O2P
2	B	401	PLP	C5A-O4P-P-O3P
2	A	401	PLP	C5A-O4P-P-O1P
3	A	402	DHA	OXT-C-CA-CB
2	A	401	PLP	C6-C5-C5A-O4P
2	B	401	PLP	C6-C5-C5A-O4P
2	B	401	PLP	C5A-O4P-P-O1P

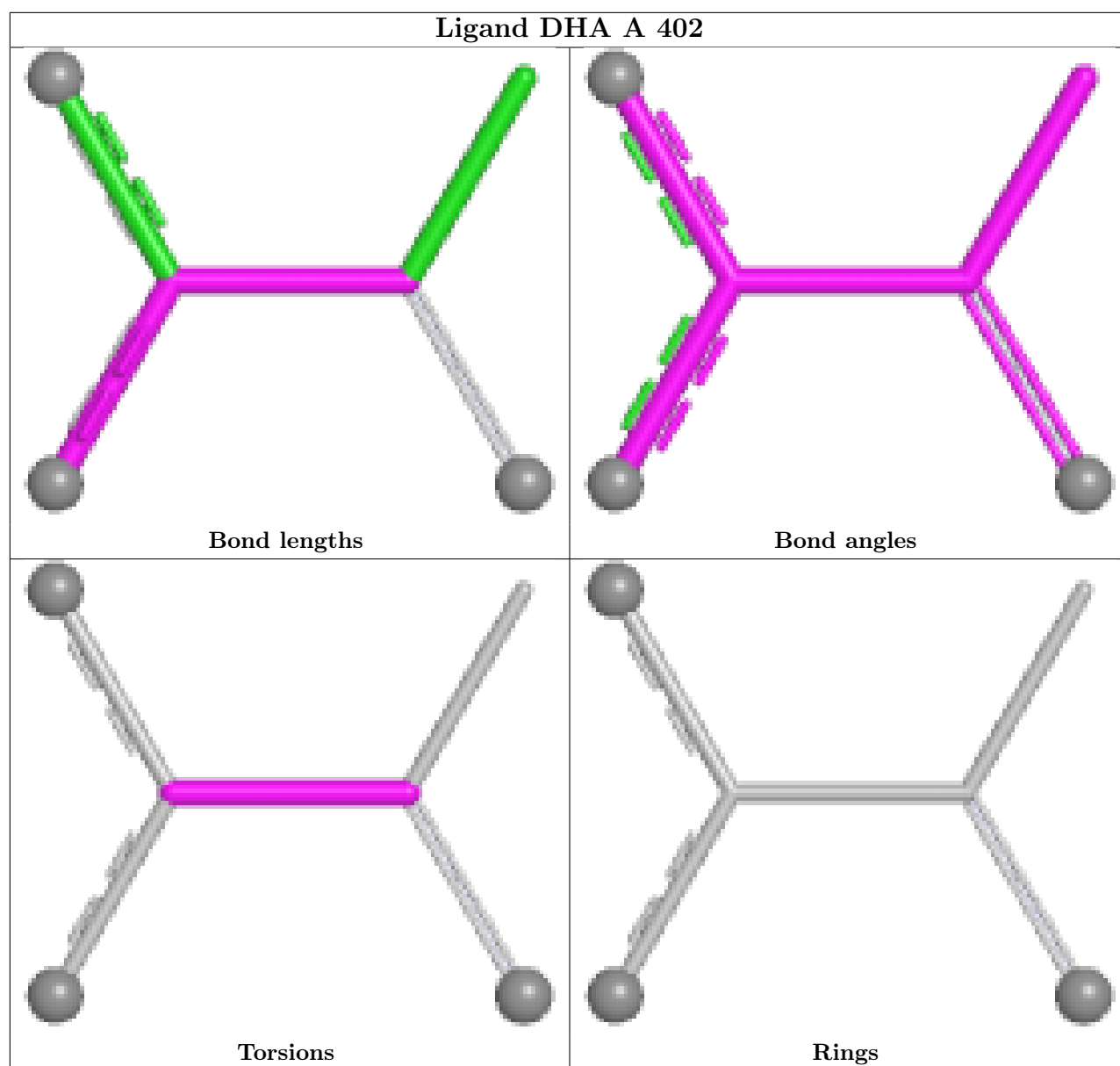
There are no ring outliers.

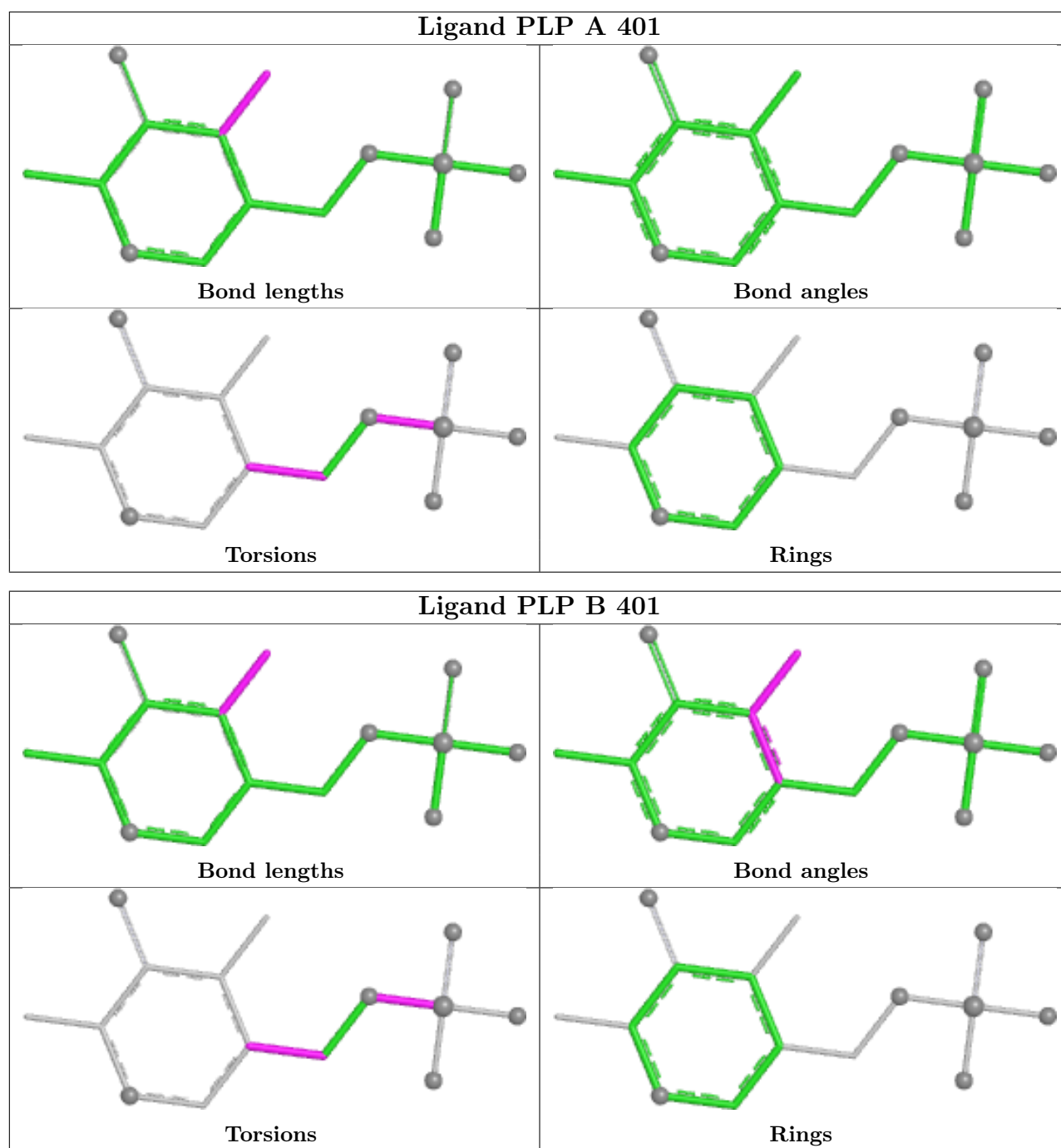
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	DHA	1	0
2	A	401	PLP	3	0
2	B	401	PLP	1	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	377/392 (96%)	0.47	21 (5%)	30 15	47, 79, 122, 162	0
1	B	373/392 (95%)	0.48	21 (5%)	30 15	50, 81, 114, 152	0
All	All	750/784 (95%)	0.48	42 (5%)	30 15	47, 80, 116, 162	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	PRO	4.1
1	B	235	ILE	4.0
1	A	-5	PRO	3.8
1	B	234	PRO	3.8
1	B	169	ALA	3.7
1	B	137	SER	3.6
1	B	231	SER	3.6
1	A	19	LEU	3.5
1	A	186	GLY	3.1
1	B	297	PRO	2.9
1	B	135	GLU	2.8
1	A	141	SER	2.8
1	A	235	ILE	2.8
1	A	232	ASP	2.7
1	B	342	MET	2.7
1	B	0	MET	2.6
1	A	331	THR	2.6
1	B	156	HIS	2.6
1	B	88	LEU	2.6
1	B	207	GLY	2.5
1	B	276	ALA	2.5
1	B	303	ALA	2.5
1	B	-1	HIS	2.5
1	A	2	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	311	ASP	2.4
1	A	352	HIS	2.4
1	A	282	SER	2.4
1	B	336	ALA	2.4
1	A	-1	HIS	2.4
1	A	18	HIS	2.4
1	A	156	HIS	2.4
1	B	335	LEU	2.3
1	A	187	HIS	2.2
1	B	143	HIS	2.2
1	B	119	GLN	2.2
1	A	342	MET	2.1
1	B	232	ASP	2.1
1	A	219	GLU	2.1
1	A	143	HIS	2.1
1	A	343	ARG	2.1
1	A	-3	GLY	2.0
1	B	301	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

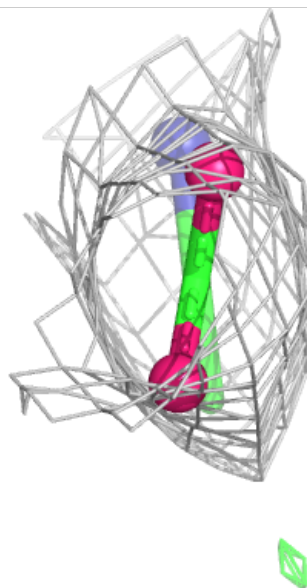
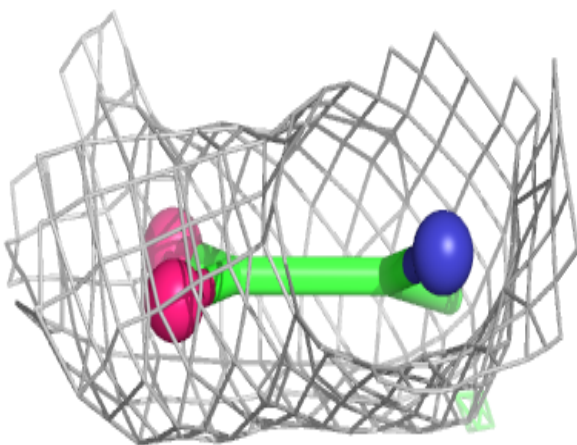
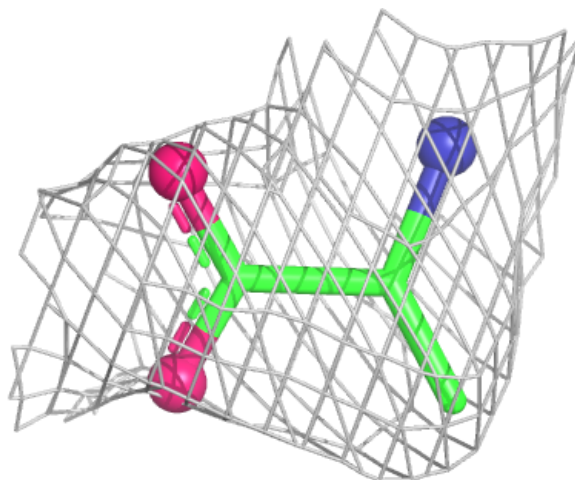
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DHA	A	402	6/6	0.91	0.15	68,80,87,99	0
3	DHA	B	402	6/6	0.95	0.16	70,81,88,122	0
2	PLP	A	401	15/16	0.96	0.07	55,58,71,71	0
2	PLP	B	401	15/16	0.97	0.07	51,56,69,77	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.

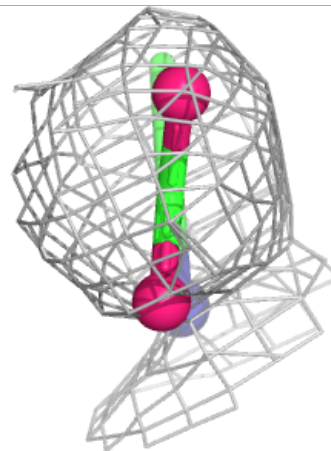
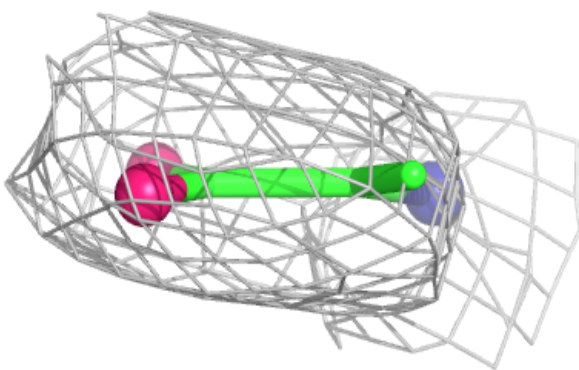
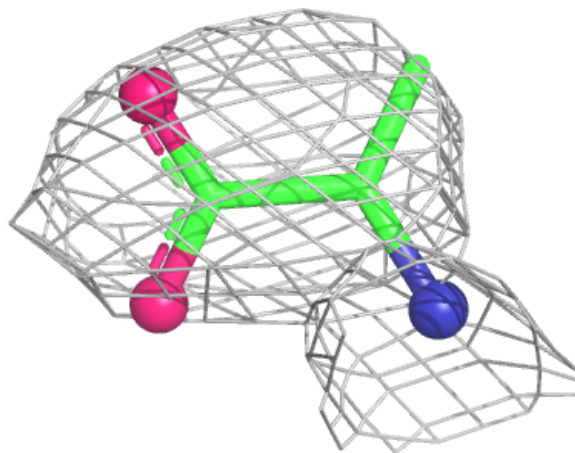
Electron density around DHA A 402:

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



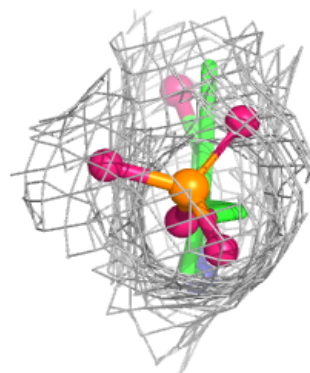
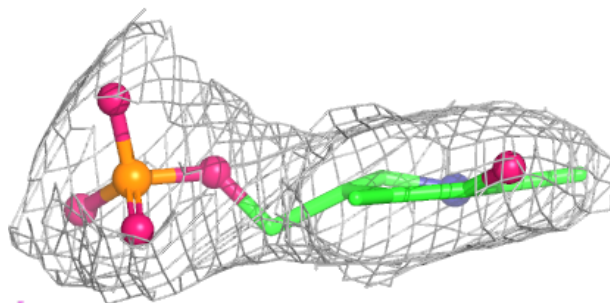
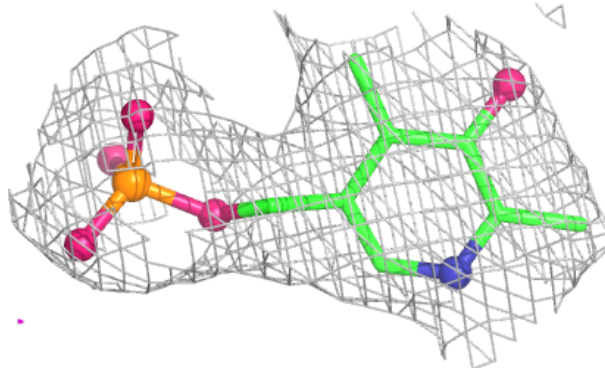
Electron density around DHA B 402:

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

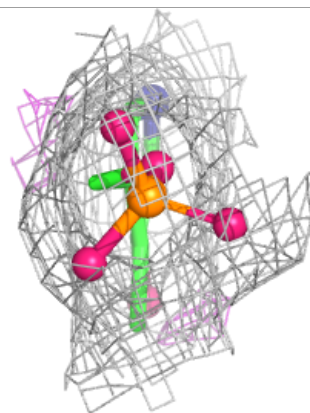
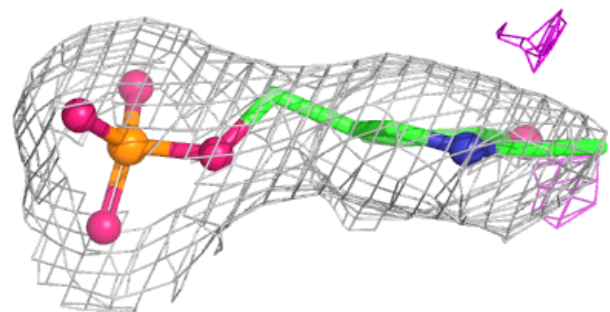
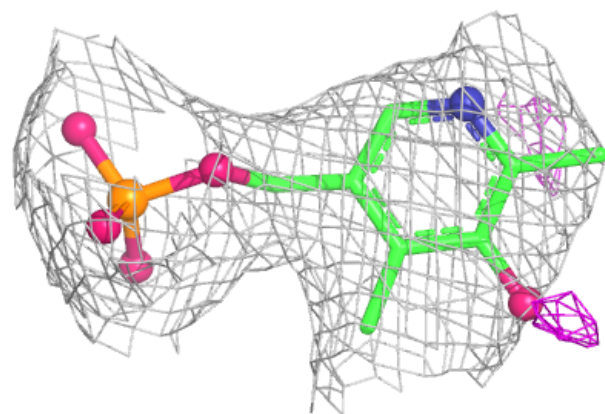


Electron density around PLP A 401:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.