



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:55 AM UTC

PDB ID : 8OVH / pdb_00008ovh
Title : Crystal structure of O-acetyl-L-homoserine sulphydrolase from *Saccharomyces cerevisiae* in complex with Pyridoxal-5'-phosphate
Authors : Saleem-Batcha, R.; Andexer, J.N.; Mohr, M.
Deposited on : 2023-04-26
Resolution : 2.17 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

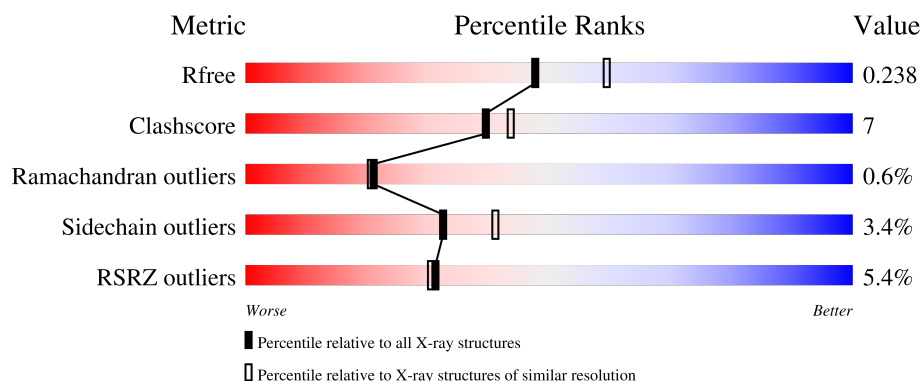
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	464	4% 73% 12% • 14%
1	B	464	5% 76% 10% • 14%
1	C	464	5% 72% 12% • 14%
1	D	464	5% 72% 13% • 14%

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	PEG	B	502	-	-	X	-
3	PEG	C	501	-	-	X	-
3	PEG	C	503	-	-	X	-
3	PEG	D	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12954 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 Homocysteine/cysteine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3095	1987	517	588	3			
1	B	400	Total	C	N	O	S	0	1	0
			3099	1989	518	589	3			
1	C	400	Total	C	N	O	S	0	0	0
			3095	1987	517	588	3			
1	D	400	Total	C	N	O	S	0	0	0
			3095	1987	517	588	3			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P06106
A	-18	GLY	-	expression tag	UNP P06106
A	-17	SER	-	expression tag	UNP P06106
A	-16	SER	-	expression tag	UNP P06106
A	-15	HIS	-	expression tag	UNP P06106
A	-14	HIS	-	expression tag	UNP P06106
A	-13	HIS	-	expression tag	UNP P06106
A	-12	HIS	-	expression tag	UNP P06106
A	-11	HIS	-	expression tag	UNP P06106
A	-10	HIS	-	expression tag	UNP P06106
A	-9	SER	-	expression tag	UNP P06106
A	-8	SER	-	expression tag	UNP P06106
A	-7	GLY	-	expression tag	UNP P06106
A	-6	LEU	-	expression tag	UNP P06106
A	-5	VAL	-	expression tag	UNP P06106
A	-4	PRO	-	expression tag	UNP P06106
A	-3	ARG	-	expression tag	UNP P06106
A	-2	GLY	-	expression tag	UNP P06106
A	-1	SER	-	expression tag	UNP P06106
A	0	HIS	-	expression tag	UNP P06106
B	-19	MET	-	initiating methionine	UNP P06106

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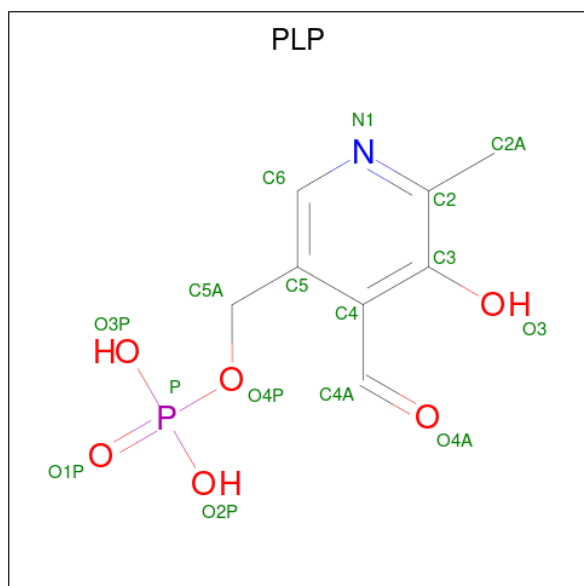
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P06106
B	-17	SER	-	expression tag	UNP P06106
B	-16	SER	-	expression tag	UNP P06106
B	-15	HIS	-	expression tag	UNP P06106
B	-14	HIS	-	expression tag	UNP P06106
B	-13	HIS	-	expression tag	UNP P06106
B	-12	HIS	-	expression tag	UNP P06106
B	-11	HIS	-	expression tag	UNP P06106
B	-10	HIS	-	expression tag	UNP P06106
B	-9	SER	-	expression tag	UNP P06106
B	-8	SER	-	expression tag	UNP P06106
B	-7	GLY	-	expression tag	UNP P06106
B	-6	LEU	-	expression tag	UNP P06106
B	-5	VAL	-	expression tag	UNP P06106
B	-4	PRO	-	expression tag	UNP P06106
B	-3	ARG	-	expression tag	UNP P06106
B	-2	GLY	-	expression tag	UNP P06106
B	-1	SER	-	expression tag	UNP P06106
B	0	HIS	-	expression tag	UNP P06106
C	-19	MET	-	initiating methionine	UNP P06106
C	-18	GLY	-	expression tag	UNP P06106
C	-17	SER	-	expression tag	UNP P06106
C	-16	SER	-	expression tag	UNP P06106
C	-15	HIS	-	expression tag	UNP P06106
C	-14	HIS	-	expression tag	UNP P06106
C	-13	HIS	-	expression tag	UNP P06106
C	-12	HIS	-	expression tag	UNP P06106
C	-11	HIS	-	expression tag	UNP P06106
C	-10	HIS	-	expression tag	UNP P06106
C	-9	SER	-	expression tag	UNP P06106
C	-8	SER	-	expression tag	UNP P06106
C	-7	GLY	-	expression tag	UNP P06106
C	-6	LEU	-	expression tag	UNP P06106
C	-5	VAL	-	expression tag	UNP P06106
C	-4	PRO	-	expression tag	UNP P06106
C	-3	ARG	-	expression tag	UNP P06106
C	-2	GLY	-	expression tag	UNP P06106
C	-1	SER	-	expression tag	UNP P06106
C	0	HIS	-	expression tag	UNP P06106
D	-19	MET	-	initiating methionine	UNP P06106
D	-18	GLY	-	expression tag	UNP P06106
D	-17	SER	-	expression tag	UNP P06106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P06106
D	-15	HIS	-	expression tag	UNP P06106
D	-14	HIS	-	expression tag	UNP P06106
D	-13	HIS	-	expression tag	UNP P06106
D	-12	HIS	-	expression tag	UNP P06106
D	-11	HIS	-	expression tag	UNP P06106
D	-10	HIS	-	expression tag	UNP P06106
D	-9	SER	-	expression tag	UNP P06106
D	-8	SER	-	expression tag	UNP P06106
D	-7	GLY	-	expression tag	UNP P06106
D	-6	LEU	-	expression tag	UNP P06106
D	-5	VAL	-	expression tag	UNP P06106
D	-4	PRO	-	expression tag	UNP P06106
D	-3	ARG	-	expression tag	UNP P06106
D	-2	GLY	-	expression tag	UNP P06106
D	-1	SER	-	expression tag	UNP P06106
D	0	HIS	-	expression tag	UNP P06106

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



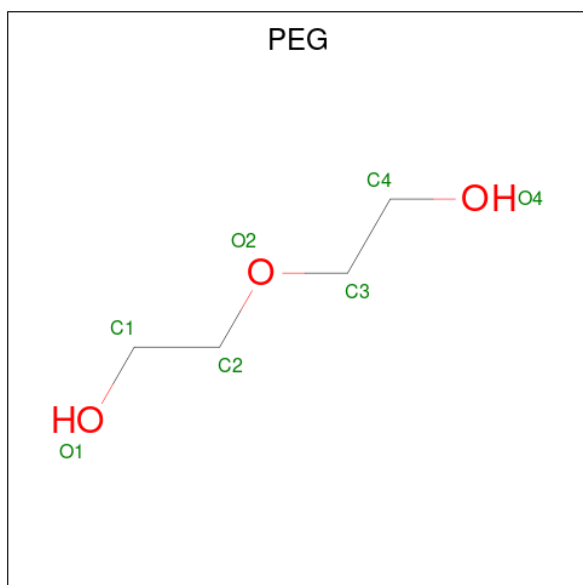
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		
4	B	133	Total	O	0	0
			133	133		
4	C	112	Total	O	0	0
			112	112		

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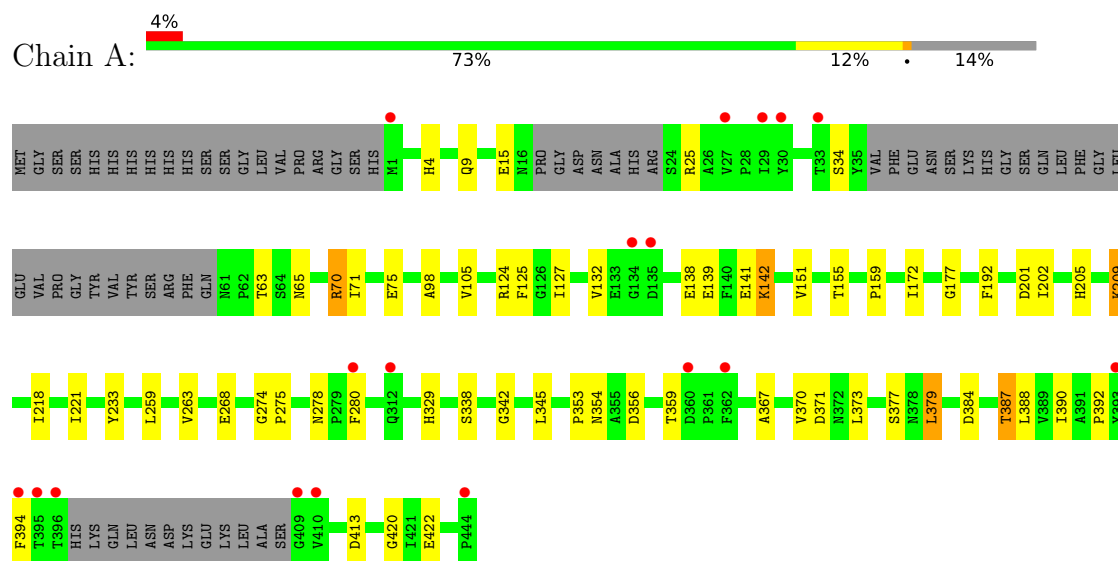
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	116	Total 116	O 116	0	0

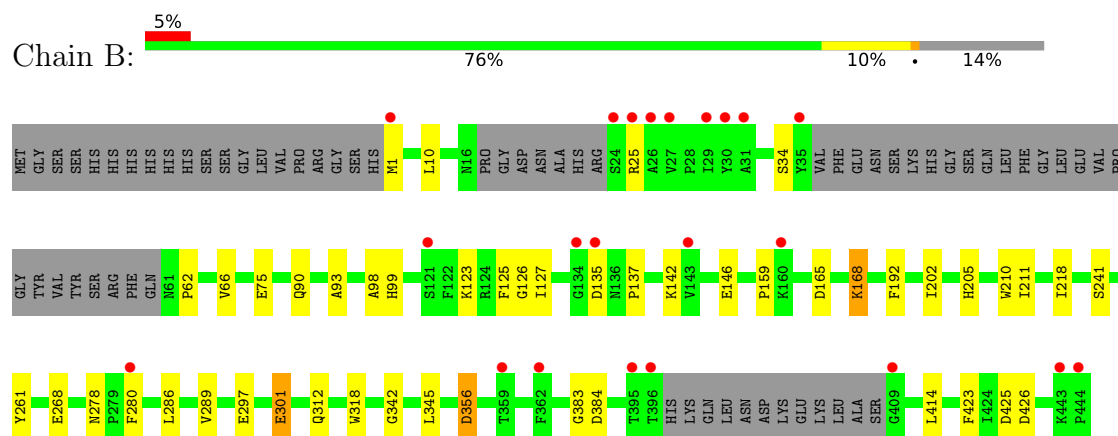
3 Residue-property plots

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.

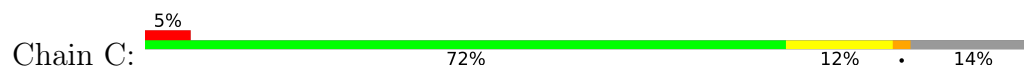
• Molecule 1: Homocysteine/cysteine synthase

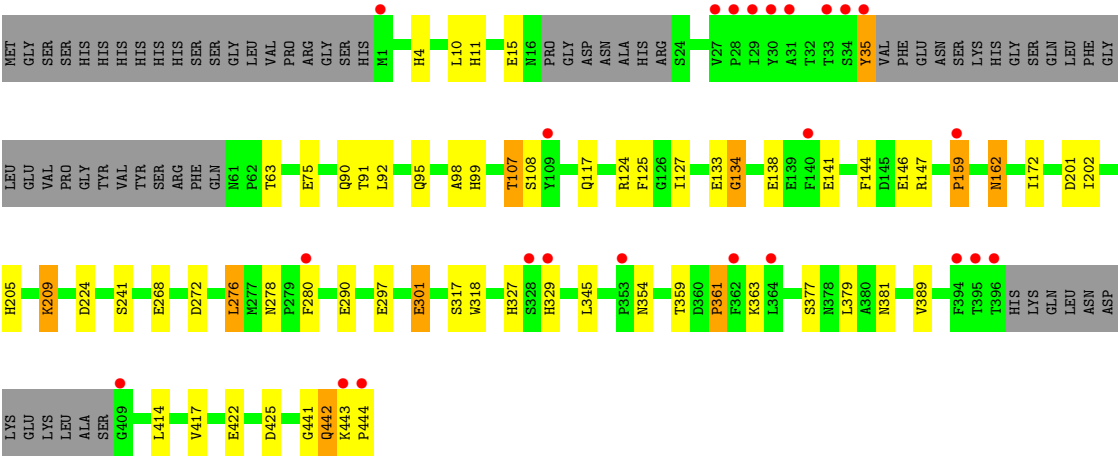


• Molecule 1: Homocysteine/cysteine synthase

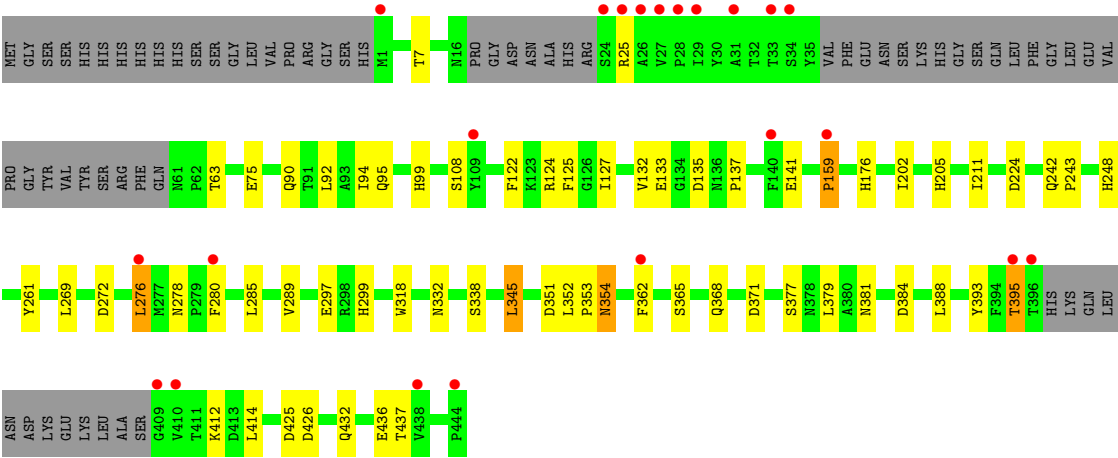


• Molecule 1: Homocysteine/cysteine synthase





● Molecule 1: Homocysteine/cysteine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.58Å 118.22Å 131.38Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	49.59 – 2.17 49.59 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.59-2.17) 97.5 (49.59-2.17)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.172 , 0.238 0.176 , 0.238	Depositor DCC
R_{free} test set	4833 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12954	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, PEG

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	0.65	0/3173	1.08	4/4308 (0.1%)
1	B	0.68	0/3177	1.08	4/4313 (0.1%)
1	C	0.67	0/3173	1.10	8/4308 (0.2%)
1	D	0.64	0/3173	1.07	9/4308 (0.2%)
All	All	0.66	0/12696	1.08	25/17237 (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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	PRO	N-CA-CB	-7.41	94.44	102.60
1	C	301	GLU	CB-CA-C	6.47	121.04	110.88
1	D	272	ASP	CA-CB-CG	6.39	119.00	112.60
1	D	7	THR	CA-CB-OG1	-6.38	100.03	109.60
1	C	425	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	224	ASP	CA-CB-CG	6.25	118.85	112.60
1	B	301	GLU	CB-CA-C	6.13	121.27	110.85
1	D	224	ASP	CA-CB-CG	6.04	118.64	112.60
1	D	299	HIS	CA-CB-CG	5.95	119.75	113.80
1	D	159	PRO	N-CA-CB	-5.86	96.15	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	ASP	CA-CB-CG	5.86	118.46	112.60
1	D	425	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	11	HIS	CA-CB-CG	-5.77	108.03	113.80
1	A	384	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	413	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	425	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	327	HIS	CB-CA-C	5.50	118.80	109.84
1	A	329	HIS	CB-CA-C	5.41	119.73	111.02
1	A	155	THR	CA-CB-OG1	-5.40	101.50	109.60
1	C	146	GLU	CB-CG-CD	5.29	121.60	112.60
1	D	384	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	137	PRO	N-CA-C	5.21	120.69	113.65
1	C	272	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	423	PHE	CA-CB-CG	5.10	118.90	113.80
1	D	437	THR	CA-CB-OG1	-5.06	102.01	109.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	ARG	Sidechain
1	C	147	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	3095	0	3010	50	0
1	B	3099	0	3012	39	0
1	C	3095	0	3010	51	0
1	D	3095	0	3010	46	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
2	C	15	0	7	2	0
2	D	15	0	7	1	0
3	B	7	0	10	9	0
3	C	14	0	20	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	10	11	0
4	A	121	0	0	2	0
4	B	133	0	0	4	0
4	C	112	0	0	5	0
4	D	116	0	0	1	0
All	All	12954	0	12108	164	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 (164) 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)
3:B:502:PEG:H11	1:D:99:HIS:HA	1.42	1.00
1:B:127:ILE:HD11	3:D:502:PEG:H12	1.61	0.82
1:A:65:ASN:HB2	4:A:712:HOH:O	1.82	0.80
1:A:387:THR:HG23	1:A:422:GLU:OE2	1.84	0.78
3:B:502:PEG:C1	1:D:99:HIS:HA	2.15	0.77
1:B:218:ILE:HG21	1:D:276:LEU:HD11	1.66	0.76
1:A:387:THR:CG2	1:A:422:GLU:OE2	2.33	0.76
1:C:127:ILE:HD11	3:C:501:PEG:C1	2.16	0.74
1:A:387:THR:HG22	1:A:420:GLY:H	1.53	0.73
1:C:127:ILE:HD11	3:C:501:PEG:H12	1.71	0.73
1:D:345:LEU:C	1:D:345:LEU:HD12	2.14	0.72
1:A:125:PHE:CE1	3:C:501:PEG:H42	2.26	0.70
1:C:124:ARG:HD3	3:C:503:PEG:H31	1.71	0.70
1:A:127:ILE:HD11	3:C:503:PEG:H12	1.71	0.70
1:A:280:PHE:HE1	1:D:280:PHE:HE1	1.40	0.69
1:B:135:ASP:HB3	4:B:606:HOH:O	1.92	0.69
1:B:125:PHE:CE1	3:B:502:PEG:H42	2.28	0.68
1:C:133:GLU:O	1:C:134:GLY:O	2.12	0.67
1:A:218:ILE:HG21	1:C:276:LEU:HD11	1.77	0.67
1:C:15:GLU:HA	4:C:613:HOH:O	1.94	0.67
1:A:15:GLU:HG3	4:A:631:HOH:O	1.95	0.66
1:D:141:GLU:OE1	1:D:176:HIS:NE2	2.21	0.66
1:B:127:ILE:HD11	3:D:502:PEG:C1	2.26	0.64
3:B:502:PEG:H41	1:D:269:LEU:HD22	1.79	0.63
1:B:426:ASP:OD2	1:C:4:HIS:HD2	1.81	0.62
1:A:71:ILE:HG13	1:A:221:ILE:HD13	1.82	0.62
1:A:387:THR:HG22	1:A:420:GLY:N	2.15	0.62
1:B:202:ILE:HD12	1:B:261:TYR:CE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PHE:CE1	1:D:280:PHE:HE1	2.19	0.60
1:C:107:THR:HG21	4:C:636:HOH:O	2.02	0.60
1:C:124:ARG:HD2	3:C:503:PEG:O4	2.01	0.60
1:A:75:GLU:OE1	1:A:205:HIS:NE2	2.32	0.60
1:B:280:PHE:HE1	1:C:280:PHE:HE1	1.48	0.60
1:C:125:PHE:CD1	3:C:503:PEG:H22	2.37	0.60
1:C:297:GLU:CG	4:C:657:HOH:O	2.50	0.59
1:C:201:ASP:O	1:C:202:ILE:HD13	2.03	0.59
1:A:98:ALA:O	3:C:503:PEG:H11	2.03	0.58
1:A:127:ILE:HD11	3:C:503:PEG:C1	2.33	0.58
1:A:387:THR:CG2	1:A:420:GLY:H	2.16	0.58
1:A:34:SER:HB3	1:C:379:LEU:HD13	1.86	0.57
1:A:25:ARG:NH1	1:D:377:SER:OG	2.38	0.57
1:C:124:ARG:CD	3:C:503:PEG:H31	2.35	0.57
1:A:387:THR:HG23	1:A:422:GLU:CD	2.30	0.56
1:A:124:ARG:NH2	1:C:268:GLU:OE2	2.38	0.56
1:A:387:THR:HG22	1:A:420:GLY:CA	2.35	0.56
1:B:137:PRO:HG3	1:B:168:LYS:HB3	1.88	0.56
1:B:142:LYS:HB3	4:B:730:HOH:O	2.06	0.56
1:B:25:ARG:NH1	1:C:377:SER:OG	2.39	0.56
3:B:502:PEG:H41	1:D:269:LEU:CD2	2.36	0.55
1:D:75:GLU:OE1	1:D:205:HIS:NE2	2.35	0.55
3:B:502:PEG:H32	1:D:95:GLN:HB3	1.88	0.55
1:A:345:LEU:HD12	1:A:345:LEU:C	2.33	0.54
1:D:125:PHE:CE1	3:D:502:PEG:C4	2.90	0.54
1:A:268:GLU:OE2	1:C:124:ARG:NH2	2.37	0.54
1:C:379:LEU:C	1:C:379:LEU:HD12	2.32	0.54
3:B:502:PEG:H12	1:D:127:ILE:HD11	1.89	0.54
1:C:99:HIS:HA	3:C:501:PEG:H11	1.90	0.53
1:C:125:PHE:CE1	3:C:503:PEG:H41	2.44	0.53
1:C:125:PHE:CE1	3:C:503:PEG:H22	2.43	0.53
1:C:133:GLU:C	1:C:134:GLY:O	2.51	0.52
1:A:34:SER:OG	1:C:381:ASN:HB2	2.09	0.52
1:B:75:GLU:OE1	1:B:205:HIS:NE2	2.39	0.52
1:B:218:ILE:CG2	1:D:276:LEU:HD11	2.39	0.52
1:C:127:ILE:HD11	3:C:501:PEG:H11	1.91	0.51
1:D:125:PHE:CE1	3:D:502:PEG:H41	2.46	0.51
1:A:377:SER:OG	1:D:25:ARG:NH1	2.44	0.51
1:B:268:GLU:OE2	1:D:124:ARG:NH2	2.41	0.51
1:C:127:ILE:CD1	3:C:501:PEG:H12	2.40	0.51
1:A:4:HIS:HD2	1:D:426:ASP:OD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:HG13	1:A:139:GLU:HB3	1.94	0.50
3:B:502:PEG:H32	1:D:95:GLN:O	2.11	0.50
1:D:345:LEU:C	1:D:345:LEU:CD1	2.85	0.50
1:B:34:SER:OG	1:D:381:ASN:HB2	2.12	0.50
1:D:125:PHE:CE1	3:D:502:PEG:H42	2.46	0.50
1:C:345:LEU:C	1:C:345:LEU:HD12	2.37	0.50
1:B:345:LEU:HD12	1:B:345:LEU:C	2.37	0.49
1:C:125:PHE:CE1	3:C:503:PEG:C4	2.95	0.49
1:D:278:ASN:ND2	1:D:280:PHE:H	2.10	0.49
1:A:105:VAL:O	1:A:151:VAL:HA	2.11	0.49
1:D:362:PHE:O	1:D:368:GLN:NE2	2.43	0.49
1:C:75:GLU:OE1	1:C:205:HIS:NE2	2.41	0.49
1:A:34:SER:CB	1:C:379:LEU:HD13	2.43	0.49
1:B:1:MET:HE3	1:B:297:GLU:OE1	2.13	0.49
1:B:192:PHE:CE2	1:B:342:GLY:HA2	2.48	0.49
1:B:99:HIS:HA	3:D:502:PEG:H11	1.94	0.48
1:C:90:GLN:HE22	2:C:502:PLP:H6	1.78	0.48
1:A:387:THR:HG22	1:A:420:GLY:HA3	1.95	0.48
1:D:432:GLN:HE21	1:D:436:GLU:HG3	1.78	0.48
1:A:367:ALA:HB2	1:A:394:PHE:CG	2.49	0.48
1:A:379:LEU:HD11	1:A:388:LEU:HD22	1.95	0.48
1:B:312:GLN:HG3	4:B:677:HOH:O	2.14	0.47
1:A:177:GLY:HA3	1:A:233:TYR:CE2	2.50	0.47
1:D:124:ARG:CD	3:D:502:PEG:H31	2.43	0.47
1:D:94:ILE:HG21	1:D:122:PHE:CE2	2.49	0.47
1:C:297:GLU:CB	4:C:657:HOH:O	2.63	0.47
1:D:242:GLN:O	1:D:243:PRO:C	2.57	0.47
1:C:318:TRP:HH2	1:C:414:LEU:HD12	1.80	0.47
1:A:387:THR:HG22	1:A:422:GLU:OE2	2.14	0.46
1:B:10:LEU:HD12	1:C:422:GLU:HG3	1.97	0.46
1:C:201:ASP:C	1:C:202:ILE:HD13	2.40	0.46
1:D:351:ASP:HA	4:D:625:HOH:O	2.16	0.46
1:A:390:ILE:HG23	1:A:392:PRO:HD3	1.98	0.46
1:B:280:PHE:CD2	1:D:280:PHE:HB2	2.51	0.46
1:C:209:LYS:NZ	2:C:502:PLP:O3	2.49	0.46
1:D:135:ASP:OD2	1:D:332:ASN:ND2	2.49	0.45
1:A:201:ASP:O	1:A:202:ILE:HD13	2.16	0.45
1:C:98:ALA:O	3:C:501:PEG:H11	2.16	0.45
1:A:141:GLU:O	1:A:142:LYS:C	2.60	0.45
1:A:274:GLY:N	1:A:275:PRO:CD	2.80	0.45
1:B:98:ALA:O	3:D:502:PEG:H11	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LEU:HD12	4:C:680:HOH:O	2.17	0.45
1:C:361:PRO:O	1:C:363:LYS:N	2.50	0.45
1:D:202:ILE:HD13	1:D:261:TYR:CZ	2.52	0.45
1:A:379:LEU:CD1	1:A:388:LEU:HD22	2.47	0.45
1:D:125:PHE:CE1	3:D:502:PEG:H21	2.52	0.45
1:D:352:LEU:HG	1:D:365:SER:HB3	1.98	0.44
1:A:125:PHE:CE1	3:C:501:PEG:H21	2.52	0.44
1:C:443:LYS:HB3	1:C:444:PRO:HD2	1.98	0.44
1:C:141:GLU:HA	1:C:144:PHE:CD2	2.52	0.44
1:C:278:ASN:ND2	1:C:280:PHE:H	2.15	0.44
1:C:95:GLN:O	3:C:501:PEG:H32	2.18	0.44
1:D:90:GLN:HE22	2:D:501:PLP:H6	1.82	0.44
1:D:353:PRO:O	1:D:354:ASN:HB2	2.18	0.44
1:A:367:ALA:HB2	1:A:394:PHE:CD1	2.52	0.44
1:D:211:ILE:HG23	1:D:289:VAL:HG22	2.00	0.44
1:A:124:ARG:CD	3:C:501:PEG:H31	2.48	0.44
1:B:93:ALA:HA	1:B:261:TYR:OH	2.17	0.44
1:B:146:GLU:H	1:B:146:GLU:CD	2.25	0.44
1:B:90:GLN:HE22	2:B:501:PLP:H6	1.82	0.43
1:B:210:TRP:NE1	1:B:383:GLY:HA2	2.34	0.43
1:C:389:VAL:HG12	1:C:417:VAL:HG22	2.00	0.43
1:B:125:PHE:HE1	3:B:502:PEG:H42	1.82	0.43
1:B:318:TRP:CH2	1:B:414:LEU:HD12	2.53	0.43
1:B:165:ASP:OD2	1:B:168:LYS:HD2	2.19	0.43
1:A:278:ASN:ND2	1:A:280:PHE:HB3	2.34	0.42
1:B:126:GLY:HA2	4:B:676:HOH:O	2.20	0.42
1:D:393:TYR:CZ	1:D:412:LYS:HG2	2.54	0.42
1:D:345:LEU:HD12	1:D:345:LEU:O	2.19	0.42
1:D:92:LEU:HD22	1:D:269:LEU:HB3	2.02	0.42
1:A:259:LEU:O	1:A:263:VAL:HG23	2.20	0.42
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.89	0.42
1:A:209:LYS:NZ	2:A:501:PLP:O3	2.51	0.41
1:C:162:ASN:HB3	1:C:329:HIS:CD2	2.55	0.41
1:D:124:ARG:HD2	3:D:502:PEG:H31	2.00	0.41
1:D:285:LEU:O	1:D:289:VAL:HG23	2.19	0.41
1:C:133:GLU:O	1:C:134:GLY:C	2.62	0.41
1:A:192:PHE:CE2	1:A:342:GLY:HA2	2.56	0.41
1:B:127:ILE:CD1	3:D:502:PEG:H12	2.43	0.41
1:A:9:GLN:O	1:A:70:ARG:HD3	2.20	0.41
1:C:441:GLY:O	1:C:442:GLN:HG3	2.21	0.41
1:B:356:ASP:OD1	1:B:356:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:TYR:CD1	1:C:35:TYR:N	2.88	0.41
1:A:370:VAL:HA	1:A:373:LEU:HD12	2.02	0.41
1:C:91:THR:OG1	1:C:117:GLN:NE2	2.53	0.41
1:A:124:ARG:HD2	3:C:501:PEG:O4	2.20	0.41
1:B:278:ASN:ND2	1:B:280:PHE:HB3	2.36	0.41
1:B:280:PHE:CD2	1:D:280:PHE:CB	3.04	0.41
1:C:10:LEU:HD23	1:C:290:GLU:HG2	2.01	0.40
1:D:318:TRP:HH2	1:D:414:LEU:HD12	1.86	0.40
1:D:379:LEU:HD11	1:D:388:LEU:HD22	2.02	0.40
1:B:62:PRO:O	1:B:66:VAL:HG23	2.20	0.40
1:B:210:TRP:CE2	1:B:383:GLY:HA2	2.56	0.40
1:A:280:PHE:CD2	1:C:280:PHE:CB	3.05	0.40
1:B:211:ILE:HG23	1:B:289:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	392/464 (84%)	374 (95%)	16 (4%)	2 (0%)	24	25
1	B	393/464 (85%)	379 (96%)	14 (4%)	0	100	100
1	C	392/464 (84%)	369 (94%)	18 (5%)	5 (1%)	9	7
1	D	392/464 (84%)	379 (97%)	11 (3%)	2 (0%)	24	25
All	All	1569/1856 (84%)	1501 (96%)	59 (4%)	9 (1%)	21	20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	442	GLN
1	C	134	GLY

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Mol	Chain	Res	Type
1	D	395	THR
1	A	354	ASN
1	D	354	ASN
1	A	209	LYS
1	C	209	LYS
1	C	354	ASN
1	C	361	PRO

5.3.2 Protein sidechains ⓘ

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	325/380 (86%)	313 (96%)	12 (4%)	30	38
1	B	325/380 (86%)	319 (98%)	6 (2%)	51	65
1	C	325/380 (86%)	311 (96%)	14 (4%)	26	32
1	D	325/380 (86%)	313 (96%)	12 (4%)	30	38
All	All	1300/1520 (86%)	1256 (97%)	44 (3%)	32	41

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	138	GLU
1	A	142	LYS
1	A	159	PRO
1	A	172	ILE
1	A	338	SER
1	A	353	PRO
1	A	356	ASP
1	A	359	THR
1	A	371	ASP
1	A	379	LEU
1	A	387	THR
1	B	123	LYS
1	B	159	PRO

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Mol	Chain	Res	Type
1	B	168	LYS
1	B	241	SER
1	B	301	GLU
1	B	356	ASP
1	C	35	TYR
1	C	63	THR
1	C	92	LEU
1	C	107	THR
1	C	108	SER
1	C	138	GLU
1	C	159	PRO
1	C	162	ASN
1	C	172	ILE
1	C	241	SER
1	C	276	LEU
1	C	301	GLU
1	C	317	SER
1	C	359	THR
1	D	63	THR
1	D	108	SER
1	D	132	VAL
1	D	133	GLU
1	D	159	PRO
1	D	248	HIS
1	D	276	LEU
1	D	297	GLU
1	D	338	SER
1	D	345	LEU
1	D	371	ASP
1	D	395	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	95	GLN
1	A	278	ASN
1	A	354	ASN
1	B	90	GLN
1	B	95	GLN
1	B	136	ASN
1	B	278	ASN

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Mol	Chain	Res	Type
1	B	329	HIS
1	B	368	GLN
1	C	4	HIS
1	C	65	ASN
1	C	90	GLN
1	C	95	GLN
1	C	194	GLN
1	C	278	ASN
1	C	329	HIS
1	D	90	GLN
1	D	95	GLN
1	D	264	HIS
1	D	278	ASN
1	D	329	HIS
1	D	381	ASN
1	D	432	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	PEG	B	502	-	6,6,6	1.48	0	5,5,5	1.24	0
2	PLP	B	501	1	15,15,16	0.89	1 (6%)	21,22,23	1.40	3 (14%)
2	PLP	D	501	1	15,15,16	0.79	0	21,22,23	1.07	1 (4%)
2	PLP	C	502	1	15,15,16	0.88	1 (6%)	21,22,23	1.40	3 (14%)
3	PEG	D	502	-	6,6,6	1.03	0	5,5,5	0.91	0
3	PEG	C	503	-	6,6,6	1.10	1 (16%)	5,5,5	0.71	0
3	PEG	C	501	-	6,6,6	1.08	0	5,5,5	0.80	0
2	PLP	A	501	1	15,15,16	0.98	1 (6%)	21,22,23	1.32	2 (9%)

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	PEG	B	502	-	-	2/4/4/4	-
2	PLP	B	501	1	-	0/6/6/8	0/1/1/1
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1
2	PLP	C	502	1	-	0/6/6/8	0/1/1/1
3	PEG	D	502	-	-	2/4/4/4	-
3	PEG	C	503	-	-	3/4/4/4	-
3	PEG	C	501	-	-	3/4/4/4	-
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C4A-C4	-2.46	1.46	1.51
3	C	503	PEG	O1-C1	2.35	1.54	1.42
2	B	501	PLP	C4A-C4	-2.24	1.47	1.51
2	C	502	PLP	C4A-C4	-2.24	1.47	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	PLP	O3-C3-C2	3.42	124.67	117.58
2	B	501	PLP	O3-C3-C2	-3.28	110.77	117.58
2	A	501	PLP	C4A-C4-C5	3.27	124.31	120.94
2	C	502	PLP	C4A-C4-C5	3.00	124.03	120.94
2	B	501	PLP	C4A-C4-C5	2.68	123.70	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	O4P-C5A-C5	2.51	114.06	109.36
2	B	501	PLP	C6-C5-C4	-2.47	116.07	118.10
2	D	501	PLP	O3P-P-O4P	-2.37	100.50	106.67
2	C	502	PLP	O2P-P-O4P	-2.03	101.38	106.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	PEG	C4-C3-O2-C2
3	C	503	PEG	C4-C3-O2-C2
3	C	501	PEG	C4-C3-O2-C2
3	C	503	PEG	O1-C1-C2-O2
3	C	501	PEG	O1-C1-C2-O2
3	C	501	PEG	O2-C3-C4-O4
3	C	503	PEG	O2-C3-C4-O4
3	D	502	PEG	O1-C1-C2-O2
3	B	502	PEG	C4-C3-O2-C2
3	B	502	PEG	O1-C1-C2-O2

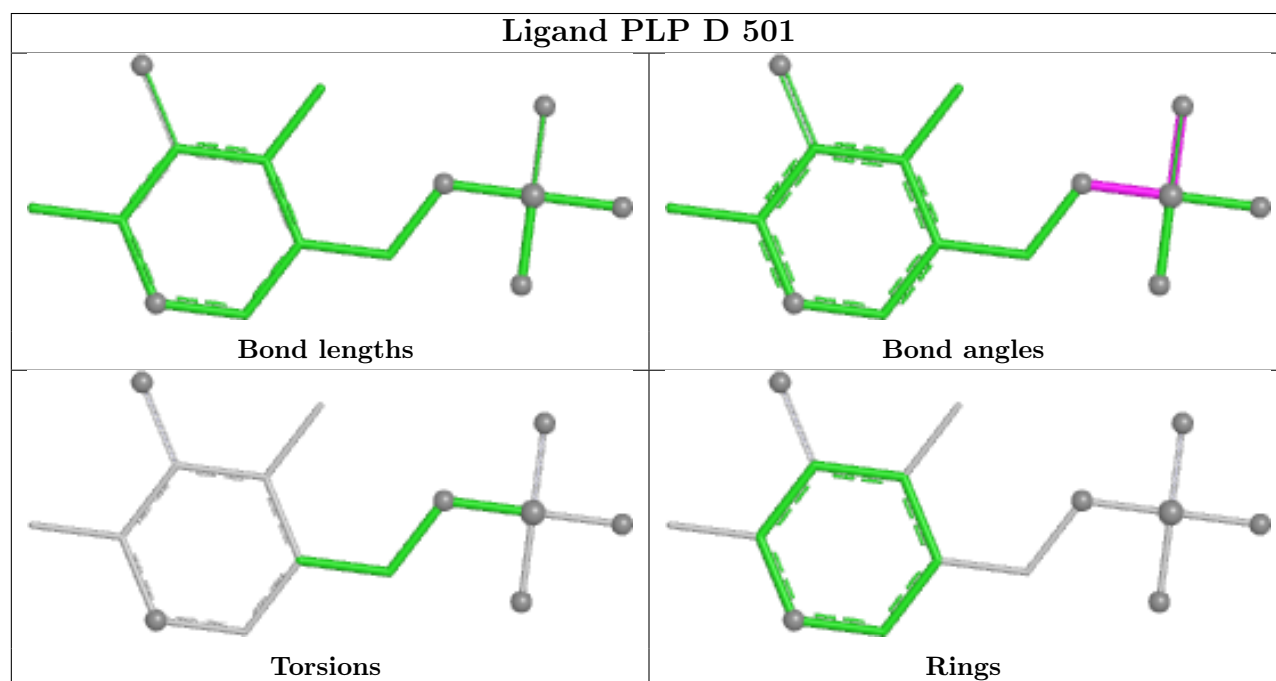
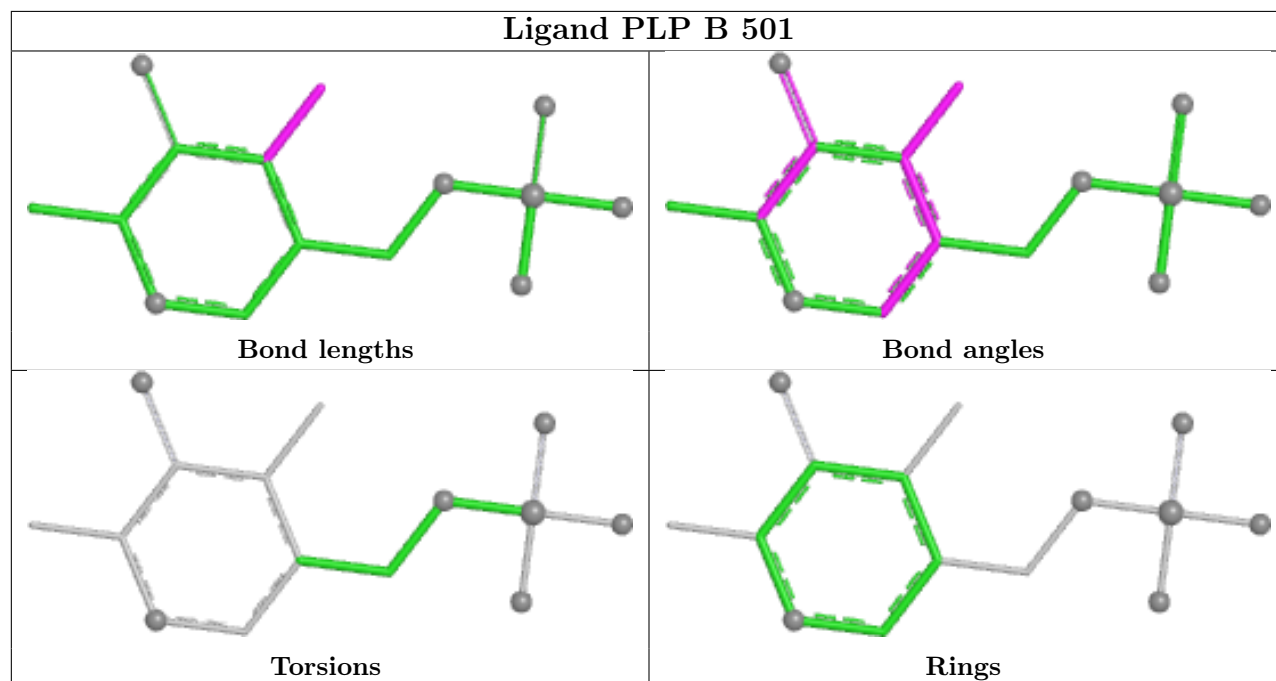
There are no ring outliers.

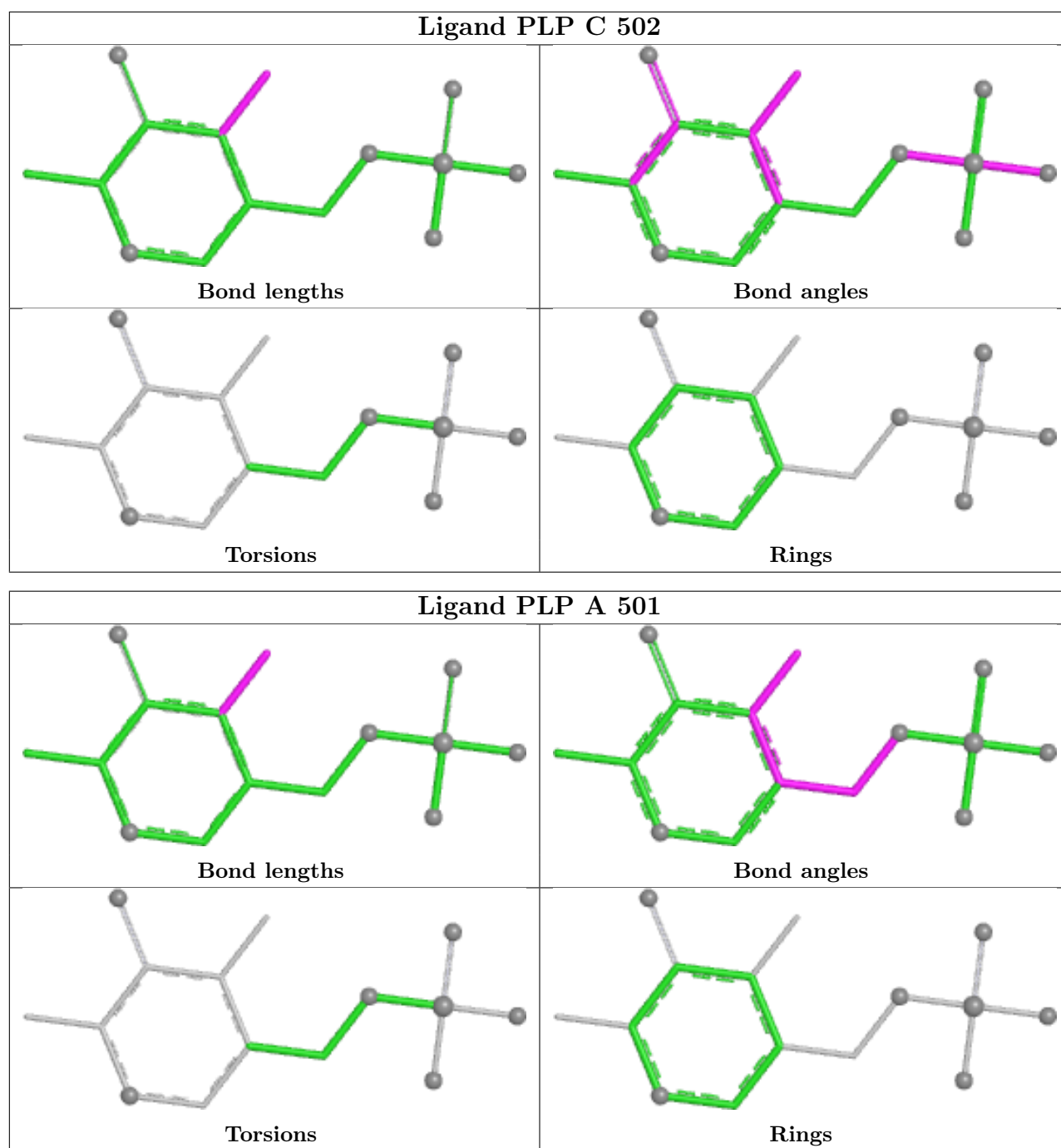
8 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	PEG	9	0
2	B	501	PLP	1	0
2	D	501	PLP	1	0
2	C	502	PLP	2	0
3	D	502	PEG	11	0
3	C	503	PEG	10	0
3	C	501	PEG	11	0
2	A	501	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	400/464 (86%)	0.07	18 (4%) 38 37	33, 48, 103, 145	0
1	B	400/464 (86%)	0.04	22 (5%) 30 30	17, 44, 93, 148	1 (0%)
1	C	400/464 (86%)	0.11	24 (6%) 27 27	31, 45, 112, 154	0
1	D	400/464 (86%)	0.13	22 (5%) 30 30	33, 48, 111, 152	0
All	All	1600/1856 (86%)	0.09	86 (5%) 31 30	17, 46, 107, 154	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	444	PRO	5.3
1	A	1	MET	5.0
1	A	444	PRO	5.0
1	B	135	ASP	4.6
1	D	27	VAL	4.5
1	D	1	MET	4.2
1	B	134	GLY	4.1
1	C	31	ALA	4.0
1	D	33	THR	3.9
1	B	27	VAL	3.8
1	C	1	MET	3.7
1	D	410	VAL	3.7
1	C	27	VAL	3.6
1	D	438	VAL	3.6
1	B	443	LYS	3.6
1	A	27	VAL	3.6
1	C	280	PHE	3.5
1	D	109	TYR	3.5
1	C	395	THR	3.5
1	A	394	PHE	3.4
1	A	362	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.3
1	D	396	THR	3.2
1	B	24	SER	3.2
1	A	396	THR	3.1
1	C	159	PRO	3.1
1	A	135	ASP	3.1
1	A	409	GLY	3.1
1	C	28	PRO	3.1
1	B	280	PHE	3.1
1	A	410	VAL	3.1
1	C	109	TYR	3.0
1	D	409	GLY	3.0
1	C	394	PHE	3.0
1	B	29	ILE	3.0
1	A	360	ASP	2.9
1	D	28	PRO	2.9
1	A	395	THR	2.9
1	D	29	ILE	2.9
1	D	25	ARG	2.8
1	B	409	GLY	2.8
1	A	29	ILE	2.8
1	C	329	HIS	2.8
1	C	396	THR	2.8
1	D	395	THR	2.7
1	D	140	PHE	2.7
1	C	362	PHE	2.6
1	C	444	PRO	2.6
1	B	31	ALA	2.6
1	B	359	THR	2.5
1	D	26	ALA	2.5
1	A	280	PHE	2.5
1	D	34	SER	2.5
1	C	140	PHE	2.4
1	D	24	SER	2.4
1	C	30	TYR	2.4
1	A	33	THR	2.4
1	A	393	TYR	2.3
1	C	409	GLY	2.3
1	C	33	THR	2.3
1	B	30	TYR	2.3
1	C	35	TYR	2.3
1	B	362	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	444	PRO	2.2
1	A	30	TYR	2.2
1	B	395	THR	2.2
1	C	353	PRO	2.2
1	D	31	ALA	2.2
1	D	280	PHE	2.2
1	A	134	GLY	2.2
1	B	121	SER	2.2
1	C	364	LEU	2.1
1	C	34	SER	2.1
1	C	328	SER	2.1
1	B	160	LYS	2.1
1	C	443	LYS	2.1
1	D	276	LEU	2.1
1	B	35	TYR	2.1
1	C	29	ILE	2.1
1	D	159	PRO	2.1
1	B	143	VAL	2.1
1	D	362	PHE	2.1
1	B	26	ALA	2.1
1	A	312	GLN	2.0
1	B	25	ARG	2.0
1	B	396	THR	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.

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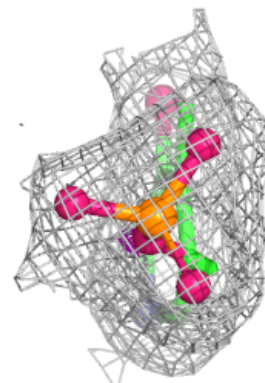
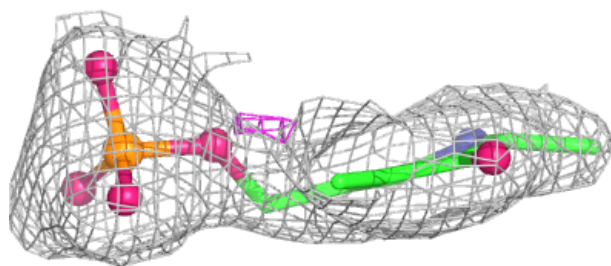
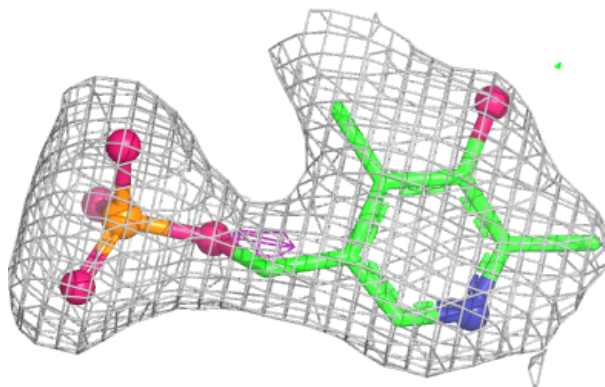
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	B	502	7/7	0.82	0.27	29,34,48,51	7
3	PEG	C	503	7/7	0.86	0.17	34,40,46,51	7
3	PEG	C	501	7/7	0.87	0.21	33,39,51,53	7
3	PEG	D	502	7/7	0.89	0.17	34,39,54,57	7
2	PLP	C	502	15/16	0.96	0.07	39,48,53,55	0
2	PLP	D	501	15/16	0.96	0.08	43,49,53,54	0
2	PLP	B	501	15/16	0.97	0.06	35,43,50,53	0
2	PLP	A	501	15/16	0.98	0.06	35,45,53,54	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.

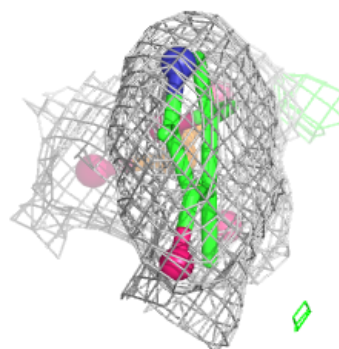
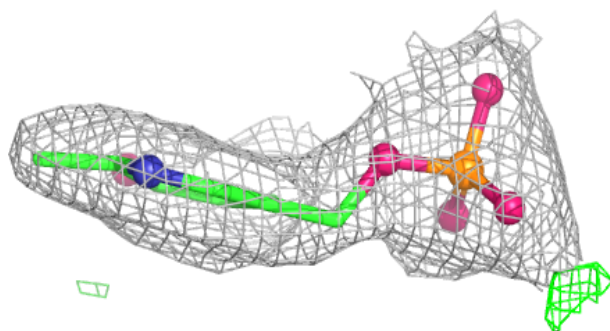
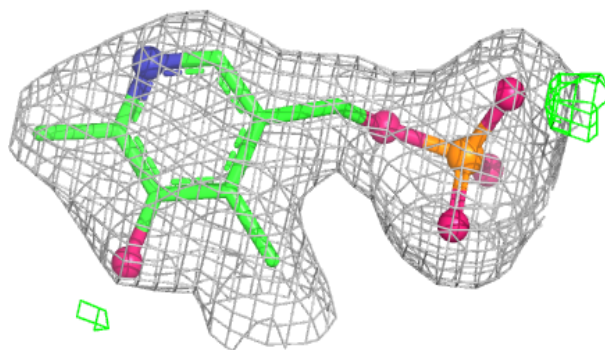
Electron density around PLP C 502:

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

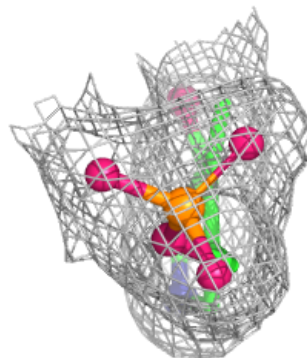
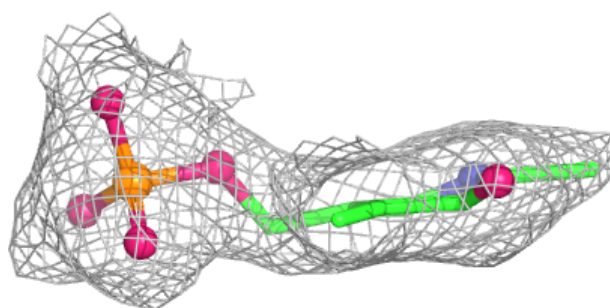
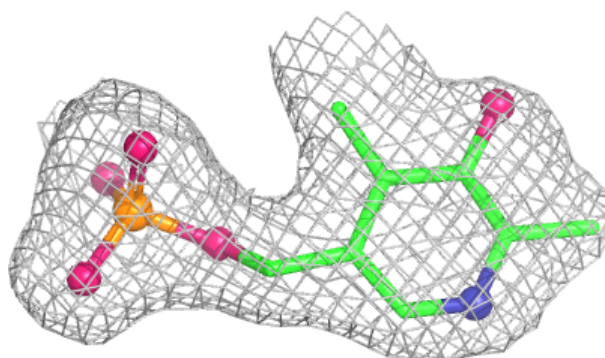


Electron density around PLP D 501:

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

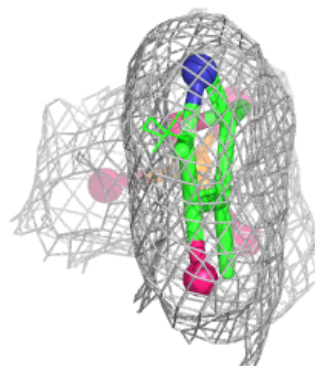
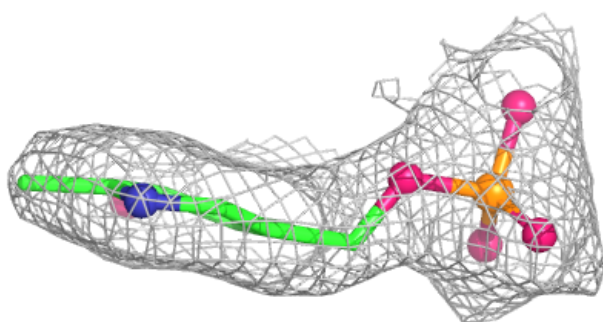
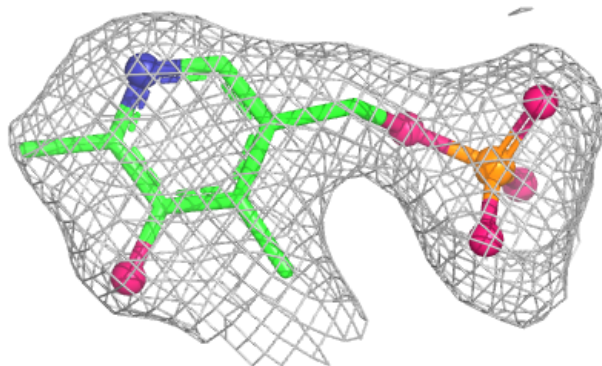
**Electron density around PLP B 501:**

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



Electron density around PLP A 501:

$2mF_o-DF_c$ (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.