WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 01:24 pm BST

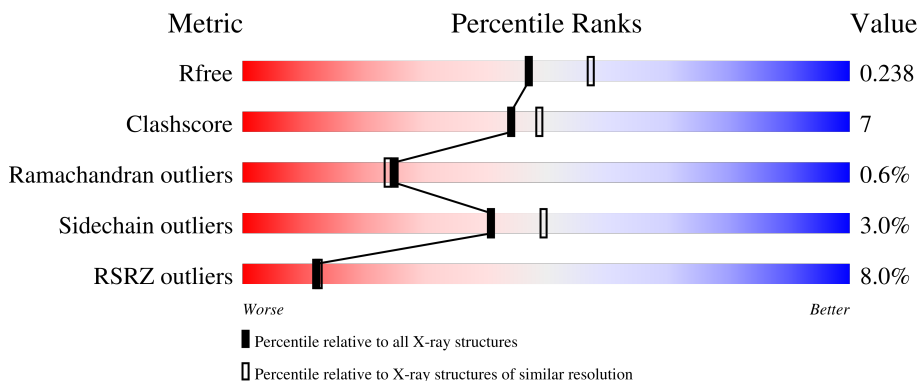|		
PDB ID	:	8OVH
Title	:	Crystal structure of O-acetyl-L-homoserine sulfhydrolase from Saccharomyces cerevisiae in complex with Pyridoxal-5'-phosphate
Authors	:	Saleem-Batcha, R.; Andexer, J.N.; Mohr, M.
Deposited on	:	2023-04-26
Resolution	:	2.17 Å(reported)

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	Percentile Ranks	Value
Rfree		0.238
Clashscore		7
Ramachandran outliers		0.6%
Sidechain outliers		3.0%
RSRZ outliers		8.0%

Worse — *Better*

▌ Percentile relative to all X-ray structures

◫ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (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 <=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	6% — 74% 11% • 14%
1	B	464	5% — 77% 8% 14%
1	C	464	7% — 74% 10% • 14%
1	D	464	9% — 74% 11% • 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 3095	C 1987	N 517	O 588	S 3	0	0	0
1	B	400	Total 3099	C 1989	N 518	O 589	S 3	0	1	0
1	C	400	Total 3095	C 1987	N 517	O 588	S 3	0	0	0
1	D	400	Total 3095	C 1987	N 517	O 588	S 3	0	0	0

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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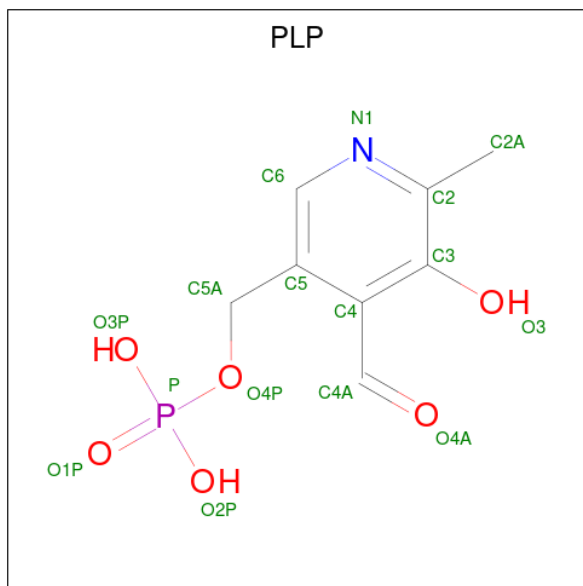
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P06106
B	-17	SER	-	expression tag	UNP P06106
B	-16	SER	-	expression tag	UNP P06106
B	-15	HIS	-	expression tag	UNP P06106
B	-14	HIS	-	expression tag	UNP P06106
B	-13	HIS	-	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 (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).

PLP

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 (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
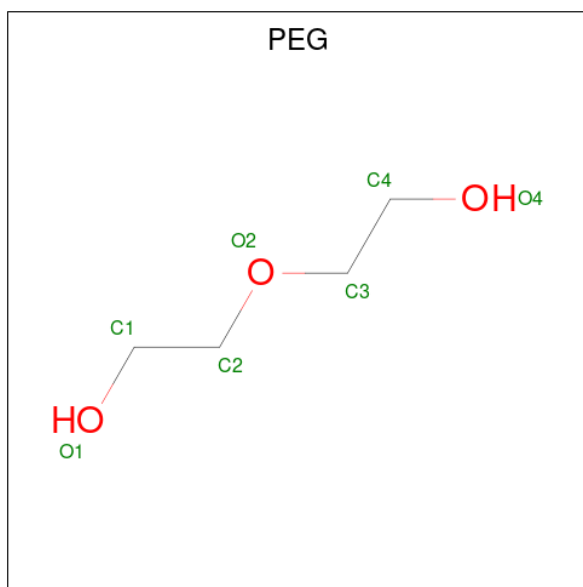
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- 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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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.
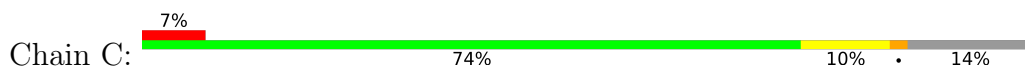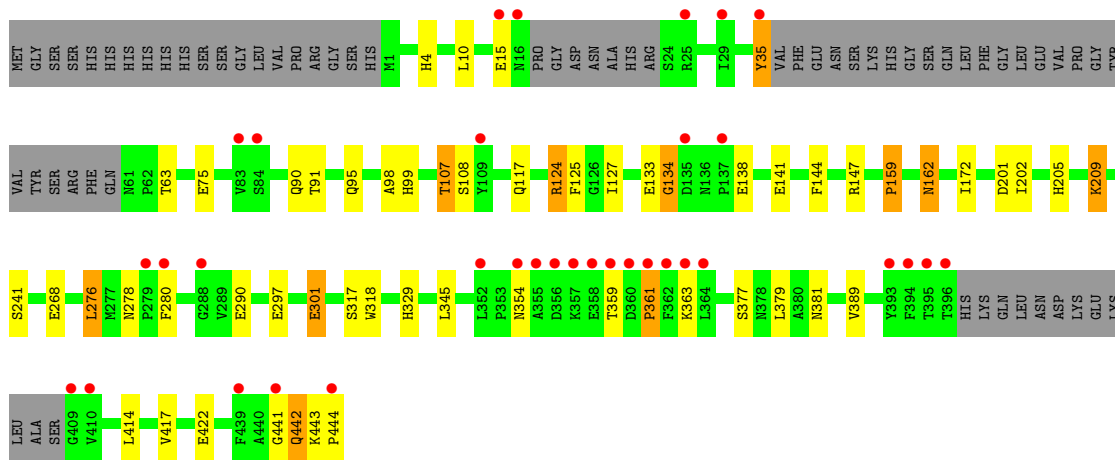
• Molecule 1: Homocysteine/cysteine synthase
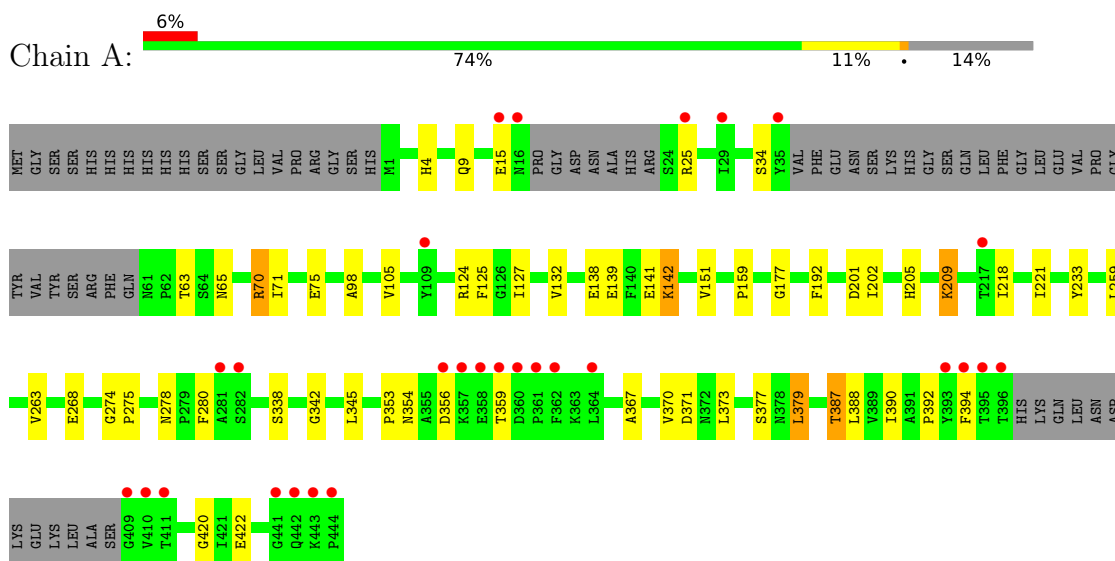
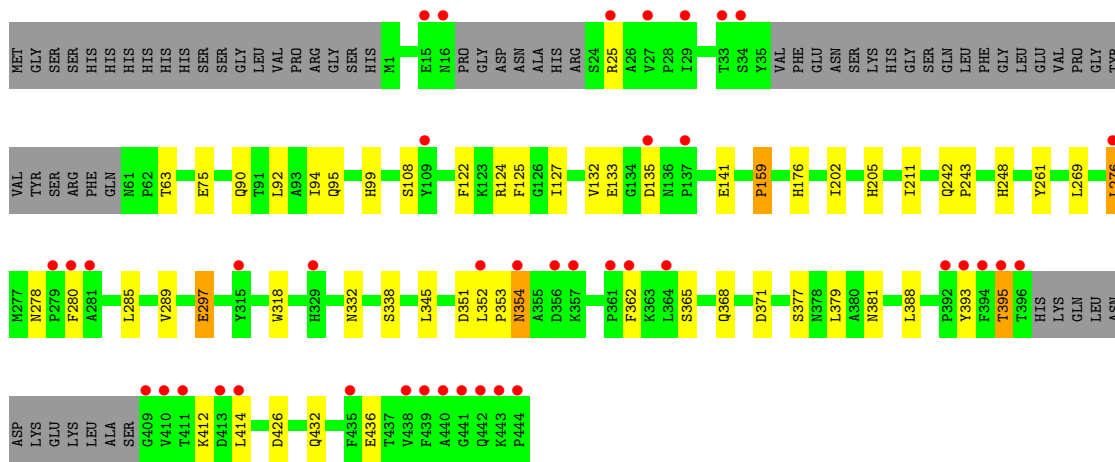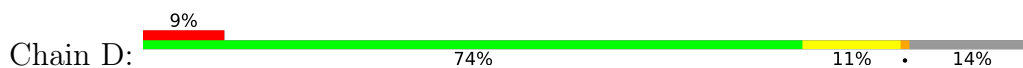• Molecule 1: Homocysteine/cysteine synthase
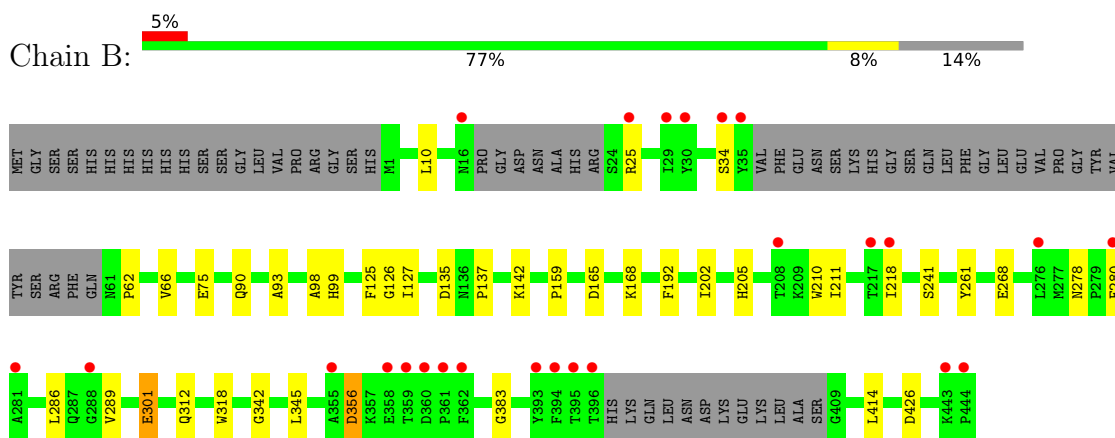
• Molecule 1: Homocysteine/cysteine synthase

• 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
$< I/\sigma(I) >$ [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)	0.31 , 36.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 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	0.44	0/3173	0.77	0/4308
1	B	0.47	0/3177	0.76	1/4313 (0.0%)
1	C	0.49	0/3173	0.80	3/4308 (0.1%)
1	D	0.46	1/3173 (0.0%)	0.77	1/4308 (0.0%)
All	All	0.47	1/12696 (0.0%)	0.77	5/17237 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	297	GLU	CD-OE1	5.26	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	159	PRO	N-CA-CB	-7.38	94.44	103.30
1	D	159	PRO	N-CA-CB	-5.86	96.15	102.60
1	C	124	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	301	GLU	CB-CA-C	5.44	121.27	110.40
1	C	301	GLU	CB-CA-C	5.32	121.04	110.40

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	37	0
1	C	3095	0	3010	50	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
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	161	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 (161) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:345:LEU:C	1:D:345:LEU:HD12	2.14	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:387:THR:HG23	1:A:422:GLU:CD	2.30	0.51
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
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: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:A:345:LEU:HD12	1:A:345:LEU:C	2.33	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:C:379:LEU:C	1:C:379:LEU:HD12	2.32	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:C:133:GLU:C	1:C:134:GLY:O	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:345:LEU:C	1:D:345:LEU:CD1	2.85	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:C:345:LEU:C	1:C:345:LEU:HD12	2.37	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
1:B:345:LEU:HD12	1:B:345:LEU:C	2.37	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:242:GLN:O	1:D:243:PRO:C	2.57	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: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:C:201:ASP:C	1:C:202:ILE:HD13	2.40	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
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:A:141:GLU:O	1:A:142:LYS:C	2.60	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%)	29	28
1	B	393/464 (85%)	379 (96%)	14 (4%)	0	100	100
1	C	392/464 (84%)	369 (94%)	18 (5%)	5 (1%)	12	8
1	D	392/464 (84%)	379 (97%)	11 (3%)	2 (0%)	29	28
All	All	1569/1856 (84%)	1501 (96%)	59 (4%)	9 (1%)	25	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	442	GLN
1	C	134	GLY
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%)	314 (97%)	11 (3%)	37	44
1	B	325/380 (86%)	321 (99%)	4 (1%)	71	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	325/380 (86%)	312 (96%)	13 (4%)	31	37
1	D	325/380 (86%)	314 (97%)	11 (3%)	37	44
All	All	1300/1520 (86%)	1261 (97%)	39 (3%)	41	49

All (39) 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	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	159	PRO
1	B	241	SER
1	B	301	GLU
1	B	356	ASP
1	C	35	TYR
1	C	63	THR
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

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Mol	Chain	Res	Type
1	D	276	LEU
1	D	297	GLU
1	D	338	SER
1	D	371	ASP
1	D	395	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	95	GLN
1	A	117	GLN
1	A	278	ASN
1	A	354	ASN
1	B	87	GLN
1	B	95	GLN
1	B	136	ASN
1	B	278	ASN
1	C	4	HIS
1	C	87	GLN
1	C	95	GLN
1	C	117	GLN
1	C	278	ASN
1	C	329	HIS
1	D	87	GLN
1	D	95	GLN
1	D	278	ASN
1	D	432	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	502	-	6,6,6	1.02	0	5,5,5	0.92	0
3	PEG	C	501	-	6,6,6	1.07	0	5,5,5	0.81	0
2	PLP	A	501	1	15,15,16	0.96	1 (6%)	20,22,23	1.36	2 (10%)
2	PLP	C	502	1	15,15,16	0.87	1 (6%)	20,22,23	1.42	3 (15%)
3	PEG	C	503	-	6,6,6	1.09	1 (16%)	5,5,5	0.72	0
2	PLP	B	501	1	15,15,16	0.86	1 (6%)	20,22,23	1.44	3 (15%)
2	PLP	D	501	1	15,15,16	0.77	0	20,22,23	1.10	1 (5%)
3	PEG	B	502	-	6,6,6	1.46	0	5,5,5	1.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	502	-	-	2/4/4/4	-
3	PEG	C	501	-	-	3/4/4/4	-
2	PLP	A	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	C	503	-	-	3/4/4/4	-
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
3	PEG	B	502	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C4A-C4	-2.37	1.46	1.51
3	C	503	PEG	O1-C1	2.32	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLP	C4A-C4	-2.17	1.47	1.51
2	C	502	PLP	C4A-C4	-2.17	1.47	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	502	PLP	O3-C3-C2	3.29	124.67	117.49
2	A	501	PLP	C4A-C4-C5	3.27	124.31	120.94
2	B	501	PLP	O3-C3-C2	-3.08	110.77	117.49
2	C	502	PLP	C4A-C4-C5	3.01	124.03	120.94
2	B	501	PLP	C4A-C4-C5	2.68	123.70	120.94
2	B	501	PLP	C6-C5-C4	-2.65	116.07	118.16
2	A	501	PLP	O4P-C5A-C5	2.47	114.06	109.35
2	D	501	PLP	O3P-P-O4P	-2.34	100.50	106.73
2	C	502	PLP	O2P-P-O4P	-2.01	101.38	106.73

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	D	502	PEG	11	0
3	C	501	PEG	11	0
2	A	501	PLP	1	0
2	C	502	PLP	2	0
3	C	503	PEG	10	0
2	B	501	PLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	PLP	1	0
3	B	502	PEG	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PLP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand PLP C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand PLP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand PLP D 501

Bond lengths

Bond angles

Torsions

Rings
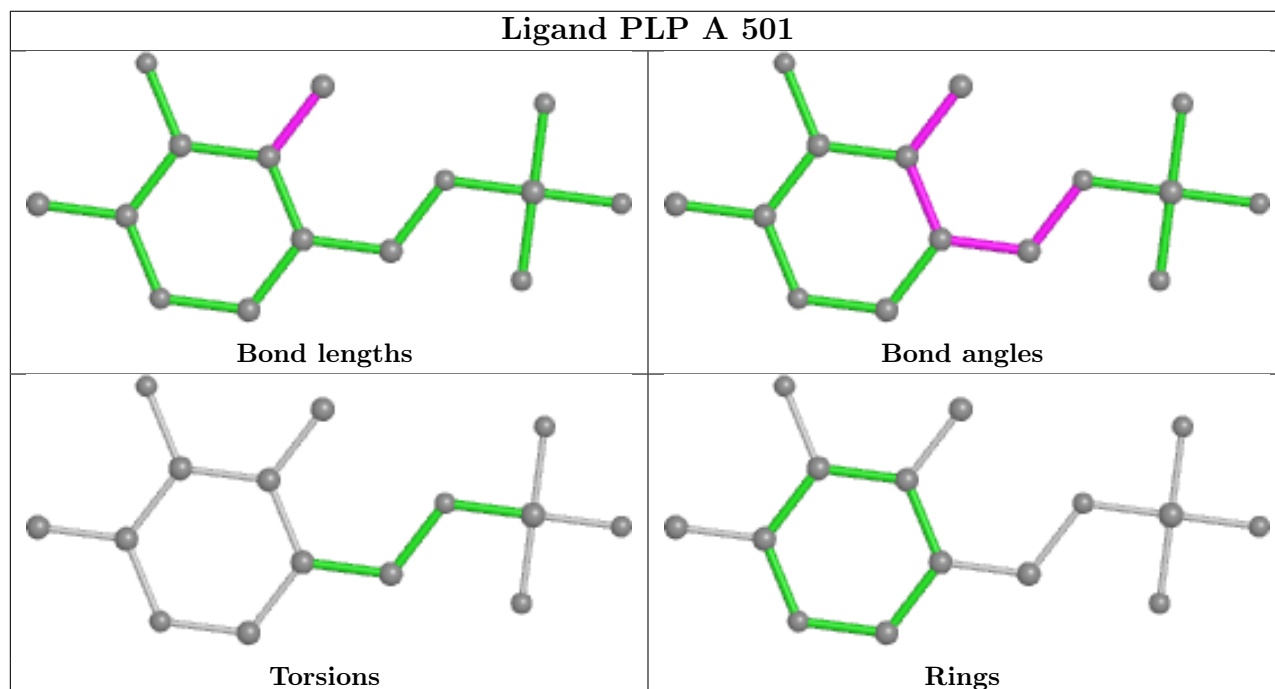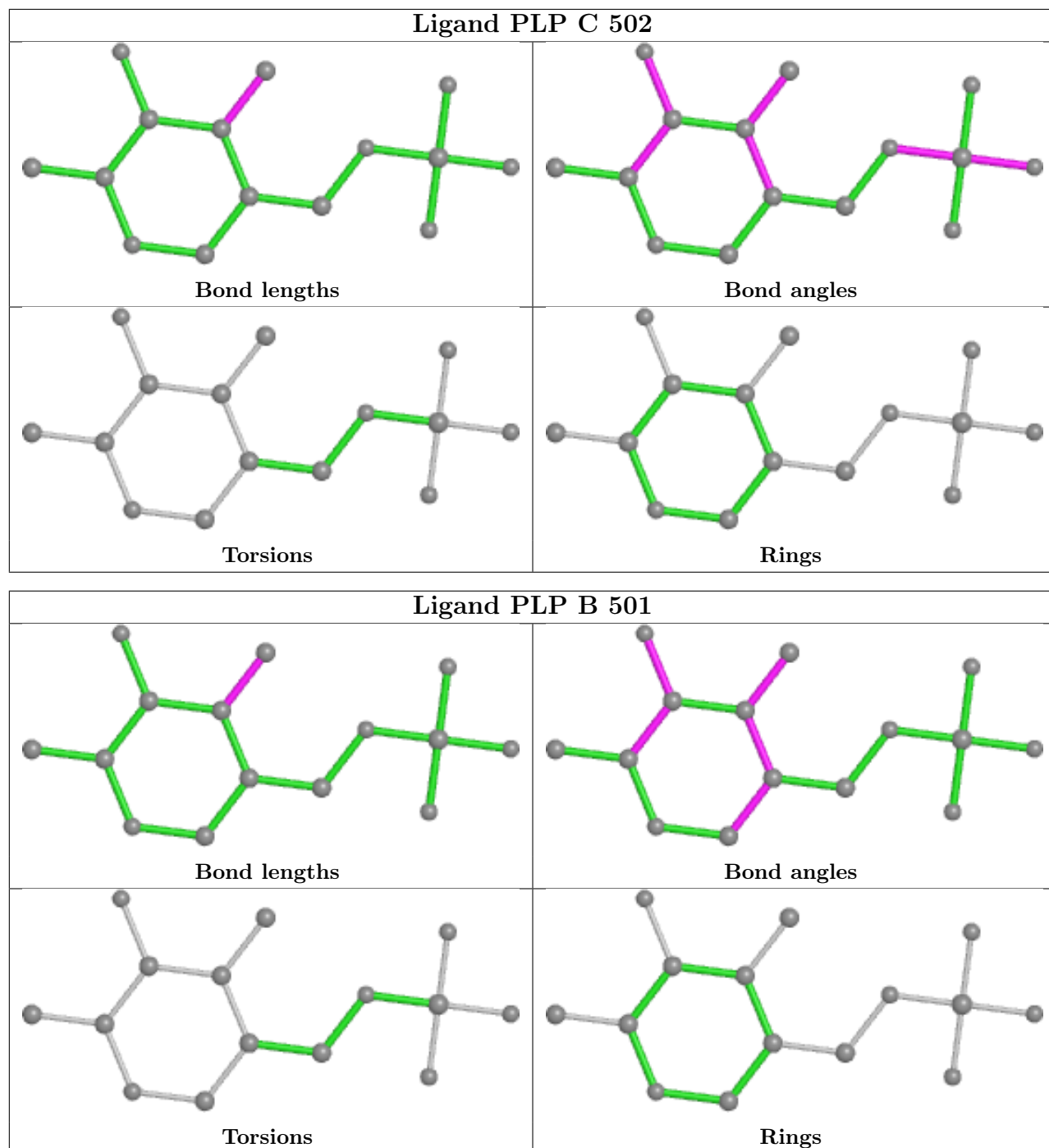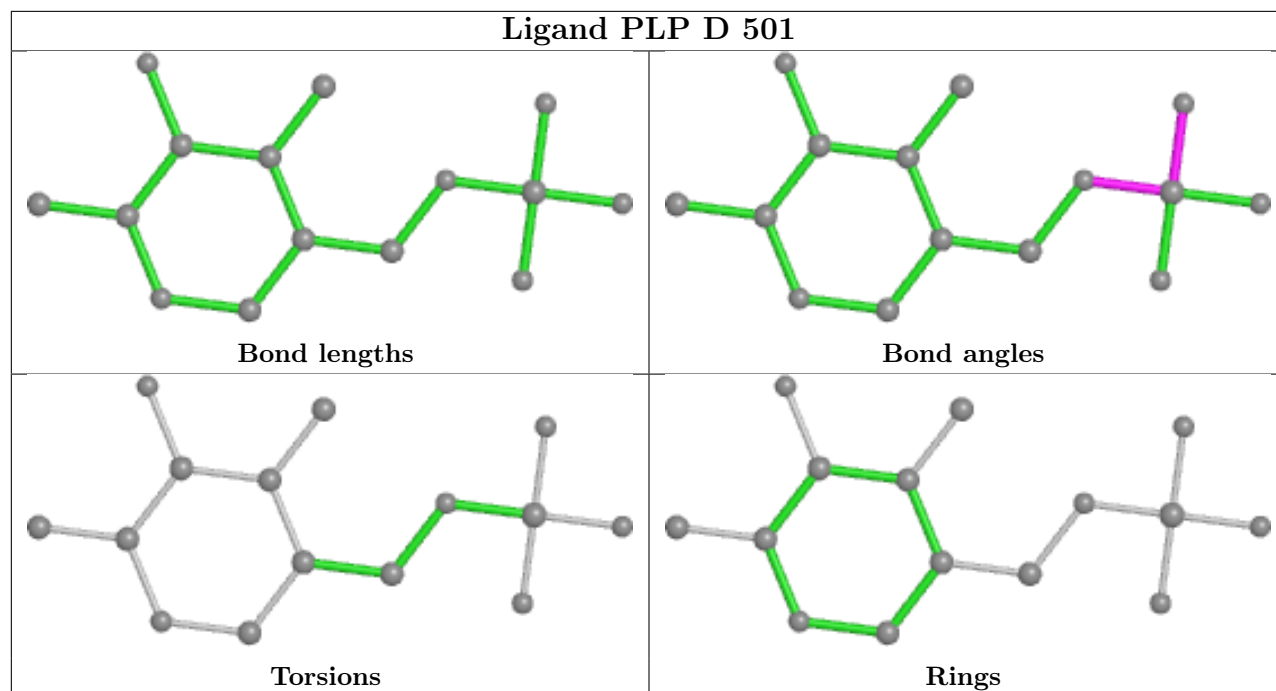
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	400/464 (86%)	0.19	28 (7%)	16	17	33, 48, 103, 145	0
1	B	400/464 (86%)	0.09	25 (6%)	20	21	31, 44, 93, 148	0
1	C	400/464 (86%)	0.24	34 (8%)	10	11	31, 45, 112, 154	0
1	D	400/464 (86%)	0.41	41 (10%)	6	7	33, 48, 111, 152	0
All	All	1600/1856 (86%)	0.23	128 (8%)	12	12	31, 46, 107, 154	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	GLY	9.5
1	D	396	THR	9.1
1	D	409	GLY	9.1
1	C	362	PHE	9.0
1	A	410	VAL	7.5
1	A	395	THR	7.3
1	D	443	LYS	7.3
1	A	444	PRO	6.7
1	A	394	PHE	6.6
1	B	444	PRO	6.5
1	D	438	VAL	6.4
1	A	396	THR	6.3
1	C	409	GLY	6.0
1	A	393	TYR	6.0
1	A	441	GLY	5.9
1	D	395	THR	5.8
1	D	393	TYR	5.8
1	C	16	ASN	5.7
1	A	362	PHE	5.7
1	C	396	THR	5.6
1	D	394	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	356	ASP	5.5
1	C	410	VAL	5.2
1	B	359	THR	5.1
1	B	396	THR	5.0
1	D	440	ALA	4.9
1	C	363	LYS	4.9
1	C	109	TYR	4.9
1	D	356	ASP	4.7
1	D	357	LYS	4.7
1	C	394	PHE	4.7
1	D	444	PRO	4.7
1	C	358	GLU	4.7
1	C	15	GLU	4.6
1	C	444	PRO	4.6
1	D	442	GLN	4.5
1	B	362	PHE	4.4
1	D	109	TYR	4.4
1	C	361	PRO	4.4
1	A	359	THR	4.3
1	A	442	GLN	4.2
1	C	395	THR	4.2
1	C	357	LYS	4.2
1	D	410	VAL	4.2
1	D	135	ASP	4.1
1	C	359	THR	4.1
1	C	354	ASN	4.1
1	C	360	ASP	4.0
1	A	16	ASN	3.9
1	B	35	TYR	3.9
1	D	439	PHE	3.8
1	B	395	THR	3.7
1	D	362	PHE	3.7
1	C	364	LEU	3.7
1	C	355	ALA	3.6
1	B	394	PHE	3.5
1	C	441	GLY	3.5
1	C	393	TYR	3.5
1	D	16	ASN	3.4
1	D	137	PRO	3.4
1	B	25	ARG	3.4
1	A	360	ASP	3.4
1	B	393	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	443	LYS	3.3
1	D	352	LEU	3.1
1	B	34	SER	3.1
1	D	411	THR	3.1
1	D	413	ASP	3.1
1	C	135	ASP	3.0
1	D	361	PRO	3.0
1	C	352	LEU	3.0
1	B	358	GLU	2.9
1	D	392	PRO	2.9
1	D	25	ARG	2.9
1	D	34	SER	2.9
1	A	358	GLU	2.9
1	A	356	ASP	2.8
1	A	361	PRO	2.8
1	D	364	LEU	2.8
1	B	29	ILE	2.8
1	A	109	TYR	2.8
1	D	441	GLY	2.8
1	B	443	LYS	2.8
1	C	29	ILE	2.8
1	A	411	THR	2.7
1	B	361	PRO	2.7
1	A	25	ARG	2.7
1	D	33	THR	2.7
1	B	280	PHE	2.6
1	D	27	VAL	2.6
1	C	439	PHE	2.6
1	B	360	ASP	2.5
1	D	329	HIS	2.5
1	C	137	PRO	2.5
1	B	355	ALA	2.5
1	C	35	TYR	2.5
1	C	280	PHE	2.4
1	B	16	ASN	2.4
1	D	354	ASN	2.4
1	C	279	PRO	2.4
1	A	281	ALA	2.4
1	B	281	ALA	2.4
1	C	83	VAL	2.3
1	A	217	THR	2.3
1	B	217	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	276	LEU	2.3
1	A	364	LEU	2.3
1	C	288	GLY	2.3
1	D	29	ILE	2.3
1	D	276	LEU	2.2
1	D	15	GLU	2.2
1	B	30	TYR	2.2
1	D	280	PHE	2.2
1	D	414	LEU	2.2
1	A	282	SER	2.2
1	A	35	TYR	2.2
1	D	435	PHE	2.2
1	B	218	ILE	2.1
1	C	84	SER	2.1
1	D	279	PRO	2.1
1	B	208	THR	2.1
1	D	281	ALA	2.1
1	C	25	ARG	2.1
1	D	315	TYR	2.1
1	A	29	ILE	2.0
1	A	15	GLU	2.0
1	A	357	LYS	2.0
1	B	288	GLY	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	B	502	7/7	0.80	0.38	29,34,48,51	7
3	PEG	C	501	7/7	0.85	0.37	33,39,51,53	7
3	PEG	C	503	7/7	0.85	0.25	34,40,46,51	7
3	PEG	D	502	7/7	0.87	0.28	34,39,54,57	7
2	PLP	D	501	15/16	0.96	0.11	43,49,53,54	0
2	PLP	A	501	15/16	0.97	0.11	35,45,53,54	0
2	PLP	C	502	15/16	0.98	0.10	39,48,53,55	0
2	PLP	B	501	15/16	0.98	0.10	35,43,50,53	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 D 501:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)
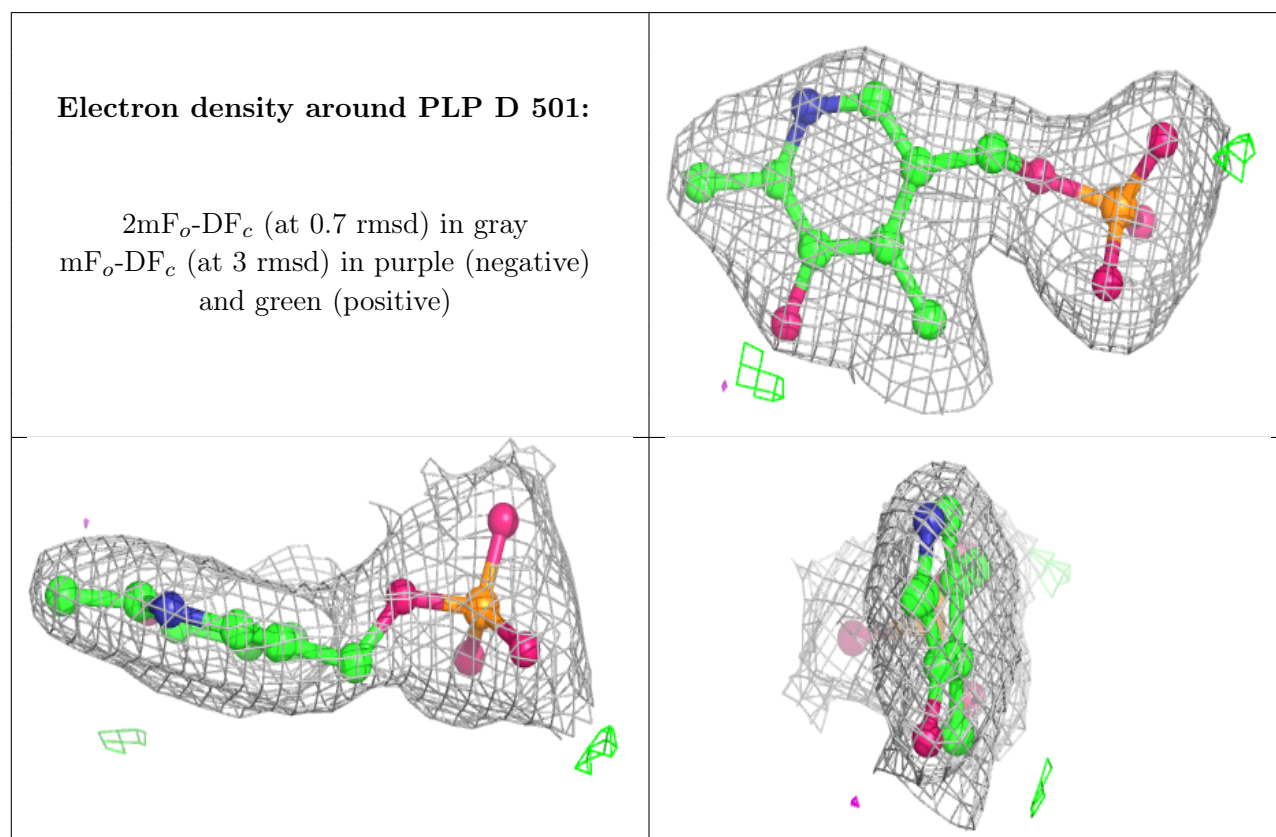
Electron density around PLP A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
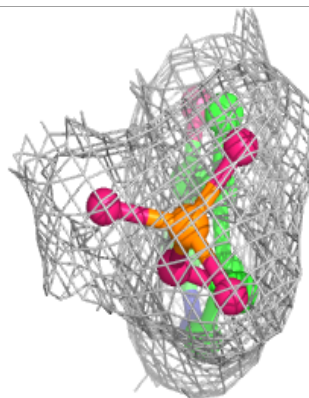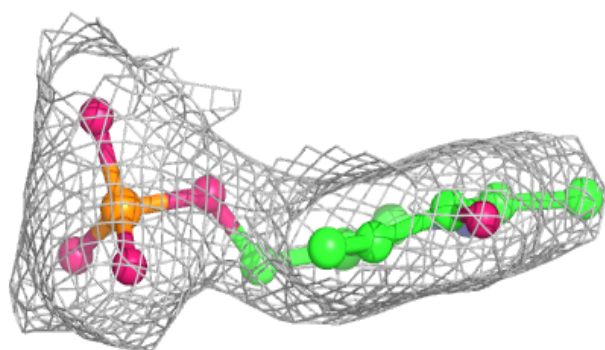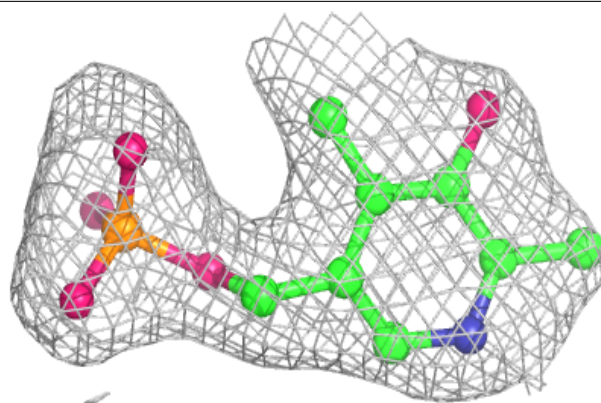
Electron density around PLP C 502:

$2mF_o$-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 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)
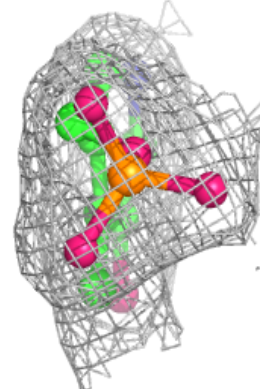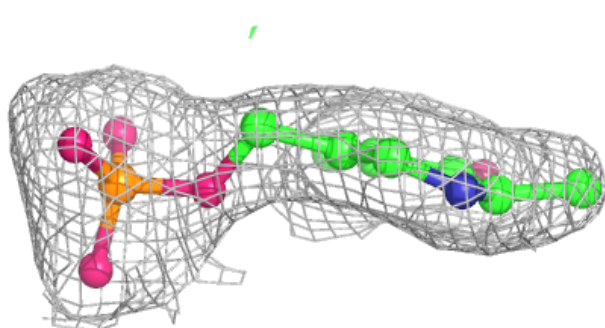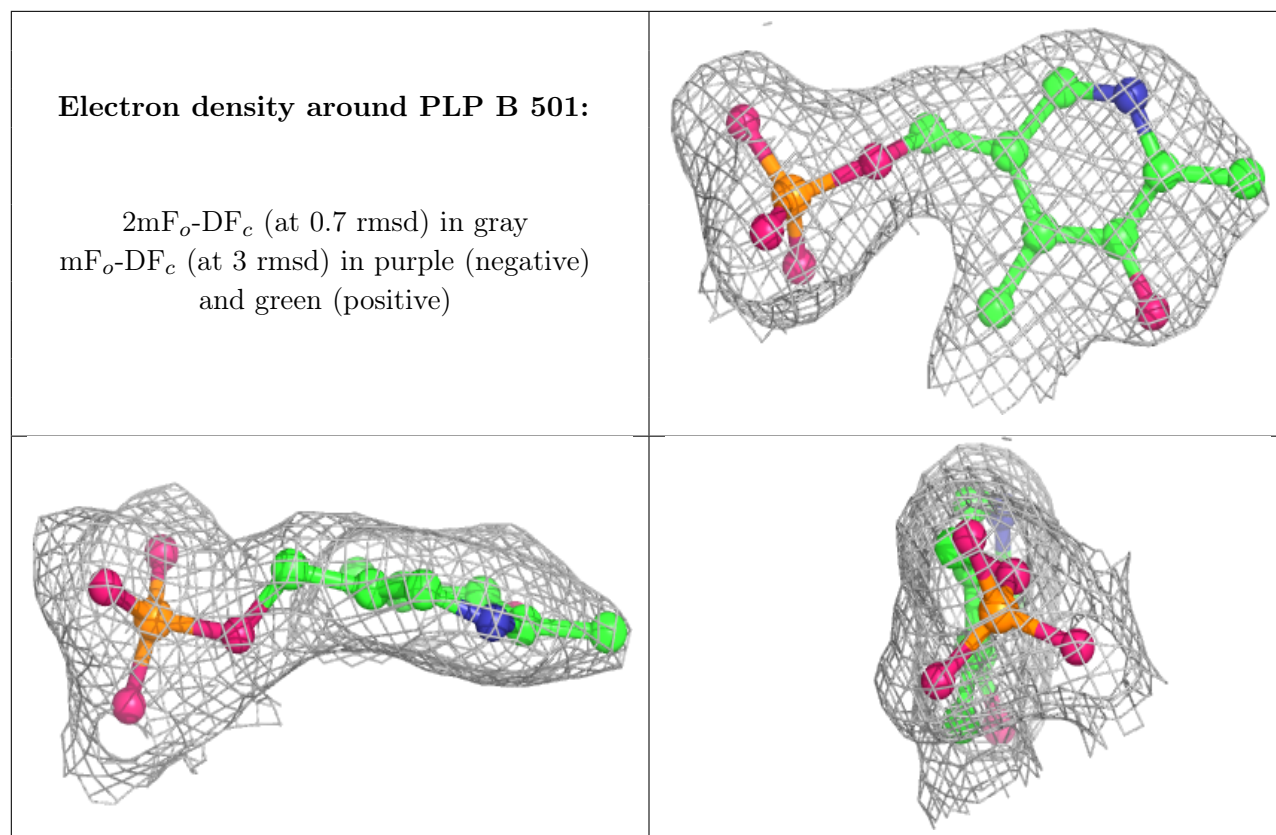
6.5 Other polymers (i)

There are no such residues in this entry.