Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 11:14 PM JST

PDB ID	:	7E13
Title	:	Caprylic acid targets a serine hydroxymethyltransferase to kill horseweed
Authors	:	Bai, L.Y.; Li, Z.R.
Deposited on	:	2021-01-29
Resolution	:	2.86 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 (i) 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 (i)) were used in the production of this report:

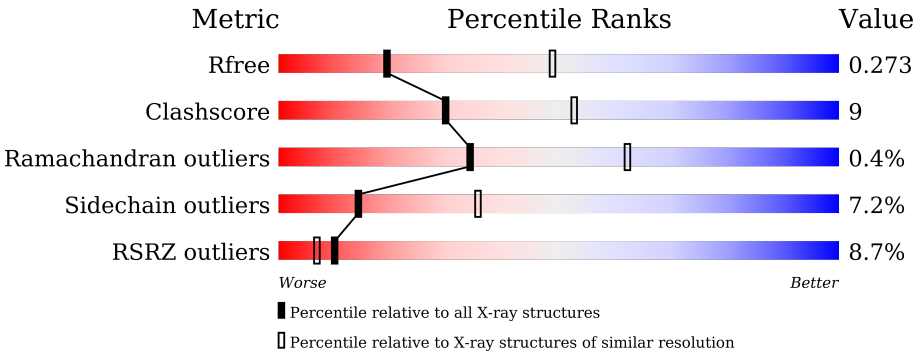
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	513	3% 73% 17% • 7%
1	B	513	3% 77% 14% • 7%
1	C	513	8% 69% 22% • 7%
1	D	513	18% 71% 19% • 7%

2 Entry composition

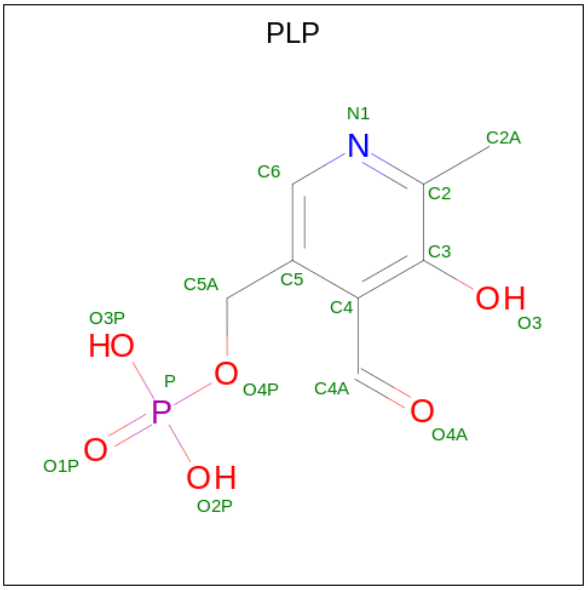
There are 2 unique types of molecules in this entry. The entry contains 14952 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	2	0
			3724	2366	637	703	18			
1	B	475	Total	C	N	O	S	14	3	0
			3732	2371	638	704	19			
1	C	475	Total	C	N	O	S	0	2	0
			3724	2366	637	703	18			
1	D	475	Total	C	N	O	S	0	2	0
			3724	2366	637	703	18			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: 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
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

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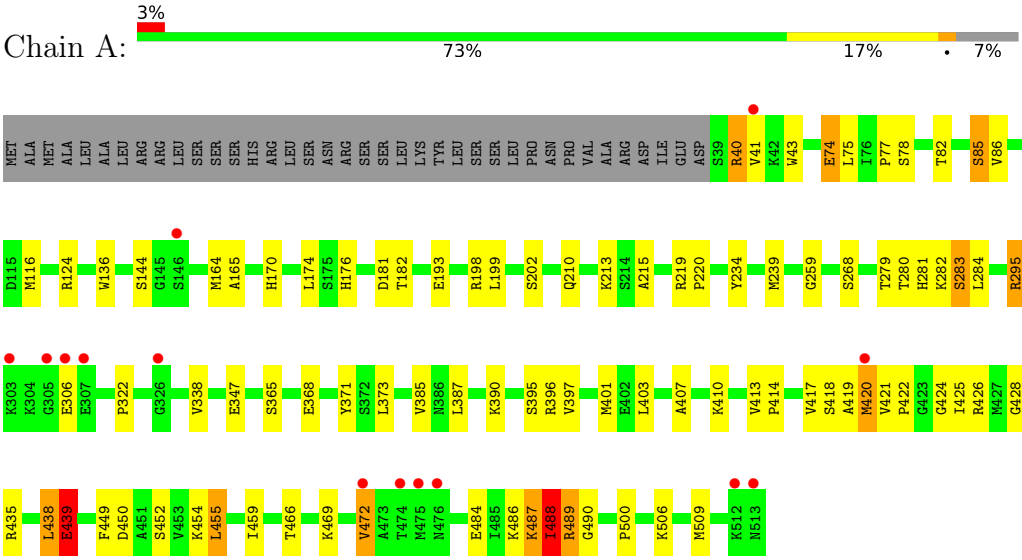
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

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.

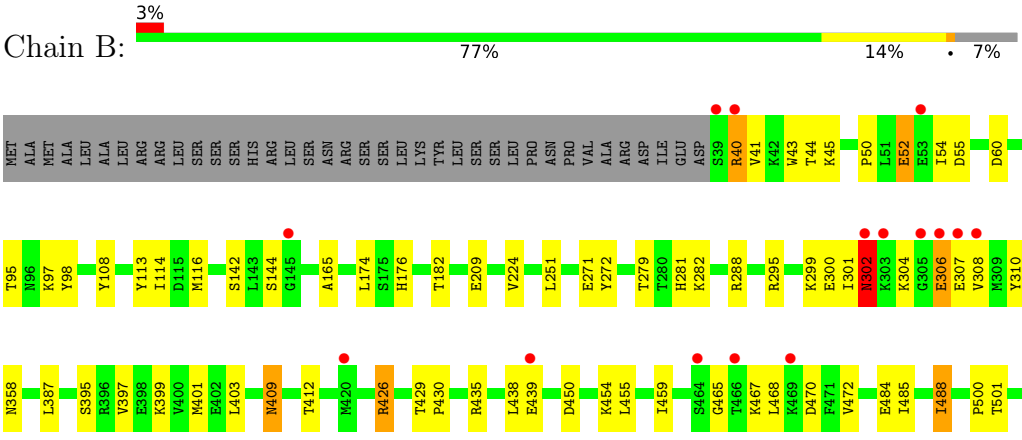
• Molecule 1: serine hydroxymethyltransferase

Chain A:



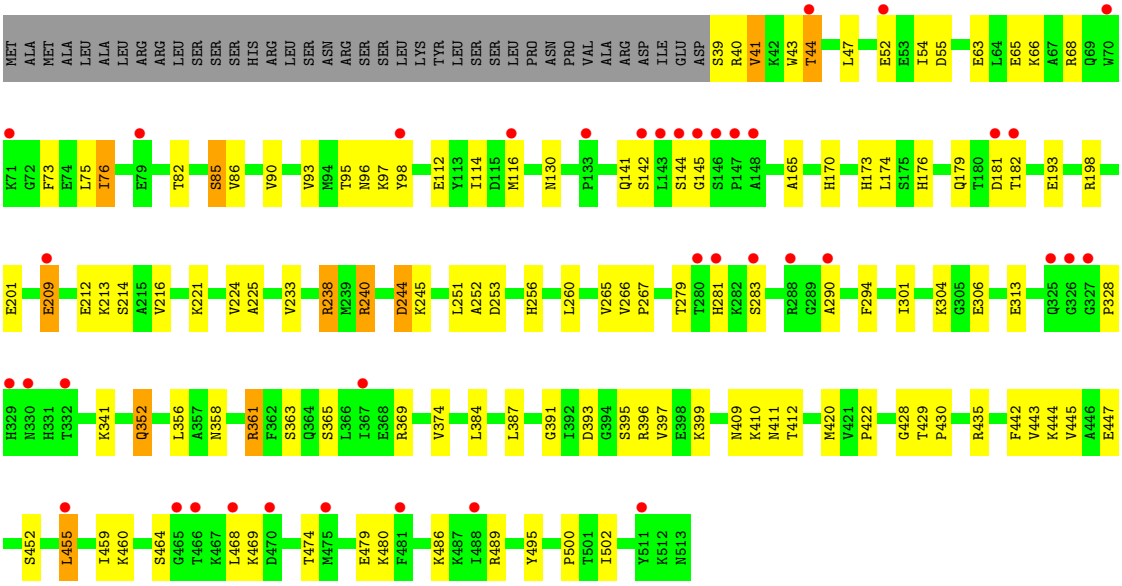
• Molecule 1: serine hydroxymethyltransferase

Chain B:



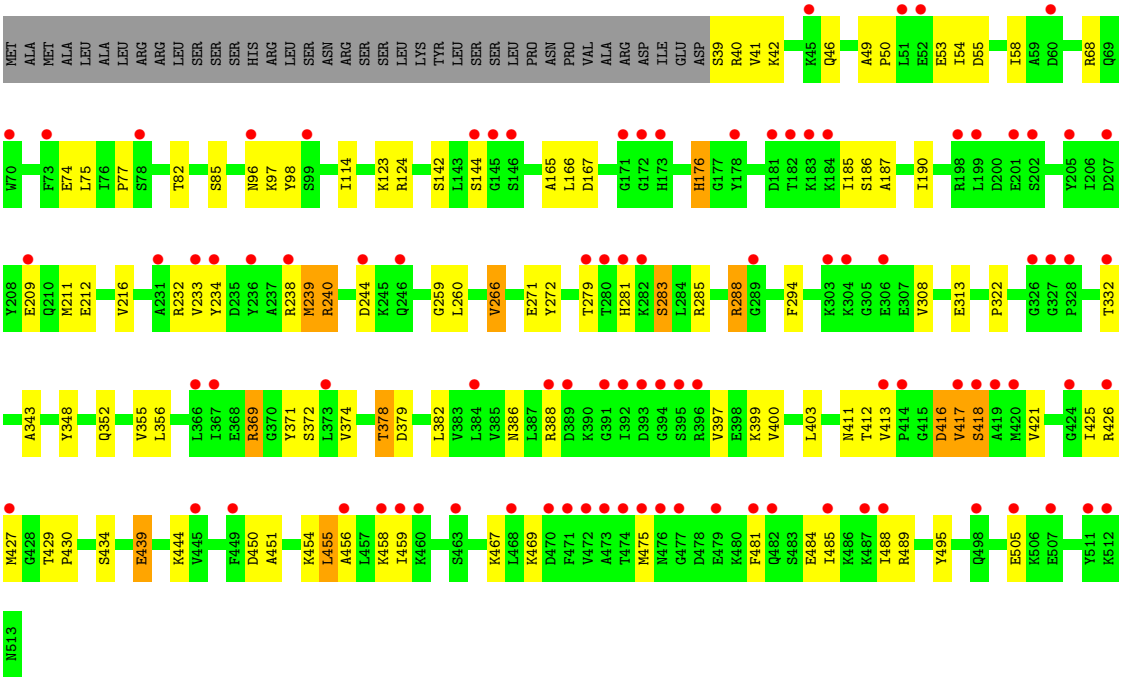
• Molecule 1: serine hydroxymethyltransferase

Chain C:



• Molecule 1: serine hydroxymethyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.87Å 121.87Å 306.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 2.86 43.09 – 2.86	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.12-2.86) 98.1 (43.09-2.86)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.270 0.225 , 0.273	Depositor DCC
R_{free} test set	2622 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	71.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14952	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 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 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	0.64	0/3799	0.77	0/5121
1	B	0.64	0/3807	0.77	0/5131
1	C	0.64	0/3799	0.75	0/5121
1	D	0.64	0/3799	0.72	0/5121
All	All	0.64	0/15204	0.75	0/20494

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3724	0	3731	77	0
1	B	3732	0	3740	60	7
1	C	3724	0	3731	82	8
1	D	3724	0	3733	80	1
2	A	16	0	7	5	0
2	B	16	0	7	5	0
2	C	16	0	7	5	0
All	All	14952	0	14956	280	8

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 9.

All (280) 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:484:GLU:OE2	1:A:487:LYS:CG	1.69	1.41
1:B:282:LYS:NZ	2:B:601:PLP:O4A	1.57	1.36
1:A:282:LYS:NZ	2:A:601:PLP:O4A	1.58	1.33
1:C:253:ASP:OD2	2:C:601:PLP:N1	1.60	1.32
1:A:484:GLU:O	1:A:487:LYS:HB3	1.20	1.25
1:D:369:ARG:HD3	1:D:450:ASP:CG	1.57	1.21
1:B:282:LYS:CE	2:B:601:PLP:O4A	1.87	1.21
1:D:369:ARG:HD3	1:D:450:ASP:CB	1.75	1.17
1:A:282:LYS:CE	2:A:601:PLP:O4A	1.97	1.13
1:D:369:ARG:HD3	1:D:450:ASP:OD2	1.50	1.09
1:D:369:ARG:CD	1:D:450:ASP:OD2	1.98	1.09
1:D:49:ALA:HB3	1:D:54:ILE:HD11	1.32	1.05
1:A:484:GLU:CD	1:A:487:LYS:HG2	1.79	1.03
1:A:282:LYS:NZ	2:A:601:PLP:C4A	2.23	1.02
1:A:484:GLU:OE2	1:A:487:LYS:HG2	0.83	1.01
1:A:484:GLU:O	1:A:487:LYS:CB	2.11	0.97
1:D:50:PRO:O	1:D:54:ILE:HG12	1.64	0.97
1:C:294:PHE:HE1	1:C:313:GLU:HG3	1.31	0.95
1:A:282:LYS:HE3	2:A:601:PLP:O4A	1.67	0.93
1:C:369:ARG:NH2	1:C:447:GLU:HB2	1.84	0.92
1:D:369:ARG:HD3	1:D:450:ASP:HB2	1.50	0.92
1:B:282:LYS:HE2	2:B:601:PLP:O4A	1.70	0.91
1:C:294:PHE:CE1	1:C:313:GLU:HG3	2.05	0.91
1:D:294:PHE:CE1	1:D:313:GLU:HG3	2.05	0.90
1:D:294:PHE:HE1	1:D:313:GLU:HG3	1.38	0.89
1:B:282:LYS:HZ2	2:B:601:PLP:C4A	1.91	0.82
1:B:50:PRO:HG2	1:B:52:GLU:HB2	1.60	0.81
1:C:369:ARG:HH22	1:C:447:GLU:HB2	1.46	0.80
1:A:488:ILE:O	1:A:490:GLY:N	2.14	0.80
1:C:464:SER:H	1:C:474:THR:HG21	1.49	0.77
1:B:506:LYS:H	1:B:506:LYS:HD2	1.50	0.76
1:C:253:ASP:OD2	2:C:601:PLP:C2	2.35	0.74
1:D:369:ARG:CD	1:D:450:ASP:CG	2.43	0.73
1:A:234:TYR:HD2	1:A:239:MET:HE1	1.54	0.73
1:B:409:ASN:OD1	1:B:426:ARG:NH2	2.23	0.72
1:A:234:TYR:CD2	1:A:239:MET:HE1	2.25	0.71
1:D:417:VAL:HG22	1:D:421:VAL:HG11	1.73	0.71
1:A:401:MET:HE3	1:A:449:PHE:HD1	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:GLU:O	1:C:213:LYS:HG3	1.93	0.69
1:D:53:GLU:HG2	1:D:53:GLU:O	1.93	0.69
1:A:164:MET:HE2	1:A:220:PRO:HG3	1.73	0.68
1:A:164:MET:CE	1:A:220:PRO:HG3	2.22	0.68
1:C:213:LYS:O	1:C:216:VAL:HG22	1.93	0.67
1:D:369:ARG:NE	1:D:450:ASP:OD2	2.28	0.67
1:D:369:ARG:CG	1:D:450:ASP:OD2	2.42	0.66
1:D:459:ILE:HG12	1:D:481:PHE:CD2	2.31	0.66
1:C:40:ARG:O	1:C:44:THR:HG23	1.96	0.66
1:C:260:LEU:HD23	1:C:352:GLN:HG2	1.78	0.65
1:D:369:ARG:CD	1:D:450:ASP:HB2	2.24	0.64
1:D:484:GLU:O	1:D:488:ILE:HG13	1.98	0.63
1:A:484:GLU:C	1:A:487:LYS:HB3	2.14	0.63
1:A:487:LYS:O	1:A:487:LYS:HD3	1.99	0.63
1:C:145:GLY:HA3	2:C:601:PLP:H5A2	1.81	0.62
1:B:484:GLU:O	1:B:488:ILE:HG23	2.00	0.62
1:C:455:LEU:O	1:C:455:LEU:HD22	1.99	0.62
1:B:282:LYS:NZ	2:B:601:PLP:C4A	2.55	0.61
1:C:85:SER:HB3	1:D:54:ILE:HG13	1.81	0.61
1:A:113:TYR:HD1	1:A:116:MET:HE2	1.63	0.61
1:C:304:LYS:HD2	1:C:306:GLU:OE1	1.99	0.61
1:C:97:LYS:HG2	1:C:114:ILE:HG13	1.83	0.61
1:D:403:LEU:O	1:D:489:ARG:NH2	2.33	0.61
1:A:97:LYS:HG2	1:A:114:ILE:HG13	1.83	0.60
1:D:49:ALA:CB	1:D:54:ILE:HD11	2.20	0.60
1:A:397:VAL:O	1:A:401:MET:HG3	2.02	0.60
1:C:399:LYS:HE2	1:C:468:LEU:HD21	1.84	0.60
1:D:68:ARG:NH2	1:D:74:GLU:OE2	2.33	0.59
1:D:55:ASP:OD2	1:D:58:ILE:CG1	2.50	0.59
1:C:361:ARG:NH1	1:C:365:SER:OG	2.36	0.59
1:B:302:ASN:ND2	1:B:306:GLU:O	2.36	0.58
1:D:400:VAL:HG21	1:D:456:ALA:HB2	1.85	0.58
1:A:219:ARG:NH2	1:C:181:ASP:HA	2.18	0.58
1:A:484:GLU:OE2	1:A:487:LYS:CB	2.47	0.58
1:D:234:TYR:HD2	1:D:239:MET:HE1	1.69	0.57
1:D:369:ARG:HG2	1:D:371:TYR:HE2	1.68	0.57
1:D:369:ARG:HG2	1:D:371:TYR:CE2	2.40	0.57
1:A:124:ARG:NH1	1:B:55:ASP:OD2	2.30	0.57
1:C:82:THR:HG22	1:D:96:ASN:OD1	2.05	0.57
1:D:451:ALA:HA	1:D:454:LYS:HD3	1.85	0.57
1:C:76:ILE:HD13	1:C:409:ASN:HD22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:GLY:O	1:C:460:LYS:NZ	2.36	0.56
1:D:77:PRO:HG3	1:D:426:ARG:HG2	1.87	0.56
1:C:464:SER:N	1:C:474:THR:HG21	2.19	0.56
1:C:55:ASP:OD2	1:D:124:ARG:NH1	2.33	0.56
1:B:304:LYS:HD2	1:B:304:LYS:O	2.06	0.56
1:C:95:THR:O	1:D:288:ARG:NH1	2.39	0.56
1:C:224:VAL:HG22	1:C:251:LEU:HD23	1.88	0.56
1:A:419:ALA:O	1:A:421:VAL:N	2.36	0.56
1:D:397:VAL:HG23	1:D:425:ILE:HD11	1.86	0.56
1:C:442:PHE:O	1:C:445:VAL:HG12	2.06	0.55
1:A:40:ARG:NE	1:A:40:ARG:H	2.05	0.55
1:A:450:ASP:OD1	1:A:454:LYS:HE3	2.07	0.55
1:C:253:ASP:OD2	2:C:601:PLP:C2A	2.54	0.55
1:B:41:VAL:HG13	1:B:45:LYS:NZ	2.21	0.55
1:B:43:TRP:O	1:B:45:LYS:N	2.34	0.54
1:C:240:ARG:HD3	1:C:244:ASP:OD2	2.07	0.54
1:D:279:THR:HB	1:D:281:HIS:CE1	2.43	0.54
1:A:174:LEU:HD13	1:B:322:PRO:HB2	1.89	0.54
1:C:369:ARG:CZ	1:C:447:GLU:HA	2.37	0.54
1:D:49:ALA:HB3	1:D:54:ILE:CD1	2.22	0.53
1:B:279:THR:HB	1:B:281:HIS:CE1	2.43	0.53
1:D:444:LYS:HG2	1:D:495:TYR:CD2	2.44	0.53
1:D:165:ALA:HB1	1:D:176:HIS:HB3	1.89	0.53
1:A:85:SER:HB2	1:A:338:VAL:HG11	1.91	0.53
1:D:371:TYR:OH	1:D:450:ASP:OD1	2.27	0.53
1:A:78:SER:HB2	1:A:282:LYS:HE2	1.91	0.52
1:C:73:PHE:CD2	1:C:445:VAL:HG23	2.43	0.52
1:C:369:ARG:NH2	1:C:447:GLU:CB	2.68	0.52
1:A:484:GLU:HA	1:A:487:LYS:HB2	1.91	0.52
1:C:374:VAL:HG22	1:C:384:LEU:HB3	1.91	0.52
1:A:484:GLU:CD	1:A:487:LYS:CB	2.78	0.51
1:B:50:PRO:C	1:B:52:GLU:H	2.12	0.51
1:B:455:LEU:HD12	1:B:455:LEU:O	2.09	0.51
1:D:374:VAL:HG11	1:D:413:VAL:HB	1.91	0.51
1:A:279:THR:HB	1:A:281:HIS:CE1	2.45	0.51
1:C:435:ARG:HA	1:C:502:ILE:HD11	1.92	0.51
1:C:212:GLU:OE1	1:C:238:ARG:NH1	2.44	0.51
1:C:486:LYS:HG3	1:C:489:ARG:HH21	1.76	0.51
1:B:41:VAL:HG22	1:B:43:TRP:H	1.75	0.51
1:B:450:ASP:OD2	1:B:454:LYS:HE2	2.10	0.51
1:C:65:GLU:OE2	1:C:68:ARG:NH1	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:SER:CB	1:D:54:ILE:HG13	2.40	0.51
1:A:219:ARG:NH2	1:C:181:ASP:OD1	2.42	0.51
1:D:444:LYS:HG2	1:D:495:TYR:CE2	2.46	0.51
1:A:387:LEU:HD13	1:A:397:VAL:HG21	1.93	0.50
1:C:165:ALA:CB	1:C:176:HIS:HB3	2.40	0.50
1:A:347:GLU:OE1	1:A:347:GLU:N	2.36	0.50
1:C:40:ARG:O	1:C:44:THR:CG2	2.59	0.50
1:B:165:ALA:CB	1:B:176:HIS:HB3	2.41	0.50
1:B:224:VAL:HG22	1:B:251:LEU:HD23	1.93	0.50
1:C:429:THR:H	1:C:430:PRO:HD3	1.77	0.50
1:D:459:ILE:HD13	1:D:475:MET:HG3	1.94	0.50
1:C:365:SER:O	1:C:369:ARG:HG3	2.12	0.50
1:C:279:THR:HB	1:C:281:HIS:CE1	2.46	0.50
1:B:397:VAL:HG12	1:B:401:MET:CE	2.42	0.50
1:C:435:ARG:HD2	1:C:502:ILE:HD13	1.94	0.50
1:D:75:LEU:HD23	1:D:427:MET:HG2	1.93	0.50
1:D:240:ARG:HD2	1:D:240:ARG:O	2.12	0.50
1:C:442:PHE:HA	1:C:445:VAL:HG12	1.95	0.49
1:D:388:ARG:NH1	1:D:416:ASP:HA	2.28	0.49
1:C:455:LEU:O	1:C:459:ILE:HG13	2.13	0.49
1:D:97:LYS:HG2	1:D:114:ILE:HG13	1.93	0.49
1:A:77:PRO:HB3	1:A:428:GLY:HA3	1.93	0.49
1:C:294:PHE:CE1	1:C:313:GLU:CG	2.87	0.48
1:D:55:ASP:OD2	1:D:58:ILE:HG12	2.12	0.48
1:A:170:HIS:CE1	1:A:198:ARG:HE	2.30	0.48
1:A:282:LYS:HZ3	2:A:601:PLP:C4A	2.18	0.48
1:D:212:GLU:O	1:D:216:VAL:HG13	2.12	0.48
1:B:295:ARG:HB3	1:B:310:TYR:CD2	2.49	0.48
1:A:165:ALA:CB	1:A:176:HIS:HB3	2.43	0.48
1:A:484:GLU:CD	1:A:487:LYS:CG	2.58	0.48
1:C:142[B]:SER:HB3	1:C:290:ALA:HB3	1.96	0.48
1:D:352:GLN:O	1:D:355:VAL:HG22	2.13	0.48
1:B:77:PRO:HG3	1:B:426:ARG:HD2	1.96	0.48
1:A:438:LEU:HG	1:B:40:ARG:HB3	1.94	0.48
1:D:166:LEU:HD23	1:D:167:ASP:O	2.14	0.48
1:D:397:VAL:O	1:D:400:VAL:HG22	2.13	0.48
1:A:302:ASN:HD21	1:A:306:GLU:HG2	1.77	0.47
1:D:185:ILE:HG23	1:D:186:SER:H	1.79	0.47
1:A:429:THR:H	1:A:430:PRO:HD3	1.80	0.47
1:A:484:GLU:O	1:A:487:LYS:N	2.45	0.47
1:B:77:PRO:CG	1:B:426:ARG:HD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:LYS:HB3	1:D:481:PHE:CZ	2.50	0.47
1:C:41:VAL:HA	1:C:44:THR:HG23	1.97	0.47
1:A:74:GLU:H	1:A:432:LEU:HD21	1.80	0.47
1:C:174:LEU:HD13	1:D:322:PRO:HB2	1.96	0.47
1:C:502:ILE:HD12	1:C:502:ILE:N	2.30	0.47
1:B:165:ALA:HB1	1:B:176:HIS:HB3	1.96	0.47
1:D:259:GLY:H	1:D:283:SER:HB3	1.80	0.47
1:B:281:HIS:ND1	1:B:288:ARG:HA	2.30	0.46
1:D:467:LYS:HD2	1:D:467:LYS:HA	1.82	0.46
1:B:301:ILE:HD12	1:B:301:ILE:H	1.80	0.46
1:B:429:THR:N	1:B:430:PRO:CD	2.79	0.46
1:C:170:HIS:CE1	1:C:198:ARG:HD2	2.50	0.46
1:D:187:ALA:HA	1:D:190:ILE:HD12	1.97	0.46
1:D:455:LEU:O	1:D:459:ILE:HG13	2.14	0.46
1:A:164:MET:HE1	1:A:220:PRO:HG3	1.97	0.46
1:A:506:LYS:HA	1:A:509:MET:HE2	1.96	0.46
1:A:426:ARG:NH2	1:B:108:TYR:OH	2.48	0.46
1:C:47:LEU:HD21	1:D:285:ARG:CZ	2.46	0.46
1:D:378:THR:OG1	1:D:382:LEU:O	2.32	0.46
1:B:50:PRO:C	1:B:52:GLU:N	2.69	0.46
1:B:455:LEU:O	1:B:459:ILE:HG13	2.15	0.46
1:A:371:TYR:CE1	1:A:390:LYS:HE3	2.51	0.45
1:C:444:LYS:HG2	1:C:495:TYR:CE2	2.52	0.45
1:B:41:VAL:HG13	1:B:45:LYS:HZ1	1.80	0.45
1:A:213:LYS:NZ	1:A:213:LYS:HB3	2.32	0.45
1:A:438:LEU:HD22	1:A:438:LEU:HA	1.66	0.45
1:A:469:LYS:O	1:A:472:VAL:HG23	2.17	0.45
1:B:501:THR:H	1:B:506:LYS:HE3	1.81	0.45
1:B:78:SER:HB2	1:B:282:LYS:HE3	1.98	0.45
1:B:97:LYS:HG2	1:B:114:ILE:HG13	1.98	0.45
1:C:387:LEU:HD13	1:C:397:VAL:HG21	1.99	0.45
1:C:429:THR:N	1:C:430:PRO:HD3	2.31	0.45
1:A:484:GLU:C	1:A:487:LYS:H	2.19	0.45
1:C:96:ASN:OD1	1:D:82:THR:HG22	2.16	0.45
1:C:265:VAL:HG23	1:C:266:VAL:HG13	1.99	0.45
1:A:401:MET:HE3	1:A:449:PHE:CD1	2.44	0.45
1:C:75:LEU:O	1:C:428:GLY:N	2.50	0.45
1:C:393:ASP:OD1	1:C:396:ARG:HD2	2.17	0.45
1:C:429:THR:N	1:C:430:PRO:CD	2.80	0.45
1:A:280:THR:HA	1:A:284:LEU:HD23	1.98	0.45
1:B:299:LYS:HG2	1:B:300:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LEU:HD13	1:B:397:VAL:HG21	1.99	0.45
1:B:397:VAL:HG12	1:B:401:MET:HE1	2.00	0.44
1:A:429:THR:N	1:A:430:PRO:CD	2.80	0.44
1:A:429:THR:N	1:A:430:PRO:HD3	2.33	0.44
1:A:410:LYS:HB2	1:A:422:PRO:HG2	1.98	0.44
1:C:233:VAL:HG21	1:C:267:PRO:HD2	1.99	0.44
1:B:41:VAL:HG21	1:B:44:THR:HB	1.98	0.44
1:B:403:LEU:HD23	1:B:485:ILE:HD13	1.99	0.44
1:A:488:ILE:HB	1:A:489:ARG:H	1.73	0.43
1:A:259:GLY:N	1:A:283:SER:OG	2.51	0.43
1:C:173:HIS:CE1	2:C:601:PLP:H5A1	2.53	0.43
1:C:361:ARG:O	1:C:361:ARG:HD3	2.18	0.43
1:A:396:ARG:NH2	1:A:466:THR:O	2.51	0.43
1:A:435:ARG:O	1:A:500:PRO:HD2	2.18	0.43
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.85	0.43
1:C:63:GLU:HA	1:C:66:LYS:HD3	2.00	0.43
1:C:420:MET:O	1:C:422:PRO:HD3	2.19	0.43
1:C:464:SER:H	1:C:474:THR:CG2	2.26	0.43
1:D:411:ASN:OD1	1:D:412:THR:N	2.52	0.43
1:B:354:GLN:NE2	1:B:358:ASN:OD1	2.46	0.43
1:B:435:ARG:O	1:B:500:PRO:HD2	2.19	0.43
1:C:361:ARG:HH11	1:C:443:VAL:HG22	1.84	0.43
1:D:271:GLU:HB3	1:D:272:TYR:CD2	2.54	0.43
1:A:193:GLU:HG3	1:C:193:GLU:HG3	2.00	0.43
1:B:429:THR:H	1:B:430:PRO:HD3	1.84	0.43
1:C:68:ARG:NH1	1:D:97:LYS:HD3	2.34	0.43
1:D:429:THR:N	1:D:430:PRO:CD	2.82	0.43
1:D:165:ALA:CB	1:D:176:HIS:HB3	2.49	0.42
1:D:403:LEU:HD12	1:D:485:ILE:HD13	2.01	0.42
1:A:455:LEU:HD13	1:A:459:ILE:HD11	2.01	0.42
1:D:39:SER:HA	1:D:42:LYS:HD2	2.01	0.42
1:D:343:ALA:HA	1:D:348:TYR:CD2	2.54	0.42
1:D:403:LEU:HD11	1:D:475:MET:SD	2.59	0.42
1:C:256:HIS:O	1:C:283:SER:HB2	2.19	0.42
1:C:435:ARG:O	1:C:500:PRO:HD2	2.18	0.42
1:B:41:VAL:HG22	1:B:43:TRP:N	2.34	0.42
1:B:43:TRP:C	1:B:45:LYS:N	2.73	0.42
1:A:85:SER:CB	1:B:54:ILE:HG21	2.50	0.42
1:B:113:TYR:HD1	1:B:116:MET:HE1	1.84	0.42
1:D:455:LEU:HD22	1:D:458:LYS:HD2	2.02	0.42
1:A:136:TRP:CE2	1:A:295:ARG:HD3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD12	1:A:414:PRO:HG3	2.01	0.42
1:A:484:GLU:HA	1:A:487:LYS:CB	2.50	0.42
1:B:484:GLU:O	1:B:488:ILE:CG2	2.66	0.42
1:B:271:GLU:HB3	1:B:272:TYR:CD2	2.55	0.42
1:D:260:LEU:HB3	1:D:266:VAL:CG2	2.50	0.42
1:A:373:LEU:HD22	1:A:385:VAL:HG22	2.02	0.42
1:B:399:LYS:HD2	1:B:472:VAL:HG22	2.02	0.42
1:B:465:GLY:HA3	1:B:470:ASP:OD2	2.20	0.41
1:C:245:LYS:HA	1:C:245:LYS:HD3	1.87	0.41
1:D:369:ARG:CD	1:D:450:ASP:CB	2.69	0.41
1:C:86:VAL:O	1:C:90:VAL:HG23	2.20	0.41
1:C:225:ALA:O	1:C:252:ALA:HA	2.19	0.41
1:D:232:ARG:HH21	1:D:379:ASP:CG	2.23	0.41
1:B:301:ILE:O	1:B:302:ASN:ND2	2.37	0.41
1:D:455:LEU:HD22	1:D:455:LEU:HA	1.80	0.41
1:A:75:LEU:HB2	1:A:407:ALA:O	2.21	0.41
1:A:113:TYR:CD1	1:A:116:MET:HE2	2.49	0.41
1:D:372:SER:HB2	1:D:386:ASN:HB3	2.03	0.41
1:A:322:PRO:HB2	1:B:174:LEU:HD13	2.02	0.41
1:A:413:VAL:HG13	1:A:424:GLY:HA3	2.02	0.41
1:C:358:ASN:HB3	1:C:442:PHE:CD2	2.56	0.41
1:D:418:SER:OG	1:D:421:VAL:HG12	2.21	0.41
1:A:82:THR:HG21	1:B:95:THR:HG21	2.02	0.41
1:A:164:MET:HE1	1:A:215:ALA:HB2	2.02	0.41
1:C:369:ARG:CZ	1:C:447:GLU:CA	2.98	0.41
1:C:141:GLN:HG2	1:C:328:PRO:HB3	2.02	0.41
1:D:343:ALA:HA	1:D:348:TYR:CG	2.56	0.41
1:A:438:LEU:O	1:A:439:GLU:HB2	2.21	0.40
1:C:165:ALA:HB1	1:C:176:HIS:HB3	2.04	0.40
1:B:468:LEU:O	1:B:472:VAL:HG23	2.20	0.40
1:A:403:LEU:HD23	1:A:403:LEU:HA	1.89	0.40
1:B:467:LYS:HD2	1:B:467:LYS:HA	1.76	0.40
1:C:112:GLU:O	1:C:116:MET:HG3	2.21	0.40
1:B:304:LYS:O	1:B:304:LYS:CG	2.70	0.40
1:C:455:LEU:HD23	1:C:455:LEU:HA	1.88	0.40
1:D:369:ARG:HB3	1:D:371:TYR:CE2	2.56	0.40
1:D:403:LEU:HD11	1:D:475:MET:HE3	2.01	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LYS:NZ	1:C:479:GLU:C[6_564]	1.07	1.13
1:B:304:LYS:CE	1:C:479:GLU:CB[6_564]	1.12	1.08
1:B:304:LYS:NZ	1:C:479:GLU:CA[6_564]	1.21	0.99
1:B:304:LYS:NZ	1:C:479:GLU:CB[6_564]	1.56	0.64
1:B:304:LYS:NZ	1:C:479:GLU:O[6_564]	1.70	0.50
1:B:304:LYS:NZ	1:C:480:LYS:N[6_564]	2.07	0.13
1:C:301:ILE:O	1:D:123:LYS:NZ[6_564]	2.12	0.08
1:B:304:LYS:CE	1:C:479:GLU:CA[6_564]	2.15	0.05

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	475/513 (93%)	445 (94%)	26 (6%)	4 (1%)	19	46
1	B	476/513 (93%)	447 (94%)	26 (6%)	3 (1%)	25	53
1	C	475/513 (93%)	455 (96%)	20 (4%)	0	100	100
1	D	475/513 (93%)	439 (92%)	35 (7%)	1 (0%)	47	75
All	All	1901/2052 (93%)	1786 (94%)	107 (6%)	8 (0%)	34	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	GLU
1	A	489	ARG
1	B	52	GLU
1	B	439	GLU
1	D	439	GLU
1	A	488	ILE
1	B	302	ASN
1	A	420	MET

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	396/428 (92%)	366 (92%)	30 (8%)	13	33
1	B	397/428 (93%)	376 (95%)	21 (5%)	22	50
1	C	396/428 (92%)	363 (92%)	33 (8%)	11	29
1	D	396/428 (92%)	364 (92%)	32 (8%)	11	30
All	All	1585/1712 (93%)	1469 (93%)	116 (7%)	14	35

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	41	VAL
1	A	43	TRP
1	A	74	GLU
1	A	85	SER
1	A	86	VAL
1	A	98	TYR
1	A	144	SER
1	A	181	ASP
1	A	182	THR
1	A	202	SER
1	A	210	GLN
1	A	268	SER
1	A	283	SER
1	A	295	ARG
1	A	365	SER
1	A	368	GLU
1	A	395	SER
1	A	417	VAL
1	A	418	SER
1	A	420	MET
1	A	425	ILE
1	A	438	LEU
1	A	439	GLU

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Mol	Chain	Res	Type
1	A	452	SER
1	A	455	LEU
1	A	472	VAL
1	A	486	LYS
1	A	487	LYS
1	A	488	ILE
1	B	40	ARG
1	B	60	ASP
1	B	82	THR
1	B	98	TYR
1	B	142[A]	SER
1	B	142[B]	SER
1	B	144	SER
1	B	182	THR
1	B	209	GLU
1	B	302	ASN
1	B	306	GLU
1	B	307	GLU
1	B	308	VAL
1	B	395	SER
1	B	409	ASN
1	B	412	THR
1	B	426	ARG
1	B	438	LEU
1	B	488	ILE
1	B	506	LYS
1	B	512	LYS
1	C	39	SER
1	C	41	VAL
1	C	43	TRP
1	C	44	THR
1	C	52	GLU
1	C	54	ILE
1	C	76	ILE
1	C	85	SER
1	C	93	VAL
1	C	98	TYR
1	C	130	ASN
1	C	144	SER
1	C	179	GLN
1	C	182	THR
1	C	201	GLU

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Mol	Chain	Res	Type
1	C	209	GLU
1	C	214	SER
1	C	221	LYS
1	C	238	ARG
1	C	240	ARG
1	C	244	ASP
1	C	341	LYS
1	C	352	GLN
1	C	356	LEU
1	C	361	ARG
1	C	363	SER
1	C	395	SER
1	C	410	LYS
1	C	411	ASN
1	C	412	THR
1	C	452	SER
1	C	455	LEU
1	C	469	LYS
1	D	40	ARG
1	D	41	VAL
1	D	46	GLN
1	D	85	SER
1	D	98	TYR
1	D	142[A]	SER
1	D	142[B]	SER
1	D	144	SER
1	D	176	HIS
1	D	209	GLU
1	D	211	MET
1	D	233	VAL
1	D	238	ARG
1	D	239	MET
1	D	240	ARG
1	D	244	ASP
1	D	266	VAL
1	D	283	SER
1	D	288	ARG
1	D	308	VAL
1	D	332	THR
1	D	369	ARG
1	D	378	THR
1	D	399	LYS

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Mol	Chain	Res	Type
1	D	416	ASP
1	D	417	VAL
1	D	418	SER
1	D	434	SER
1	D	439	GLU
1	D	455	LEU
1	D	469	LYS
1	D	505	GLU

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	411	ASN
1	D	256	HIS
1	D	330	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\|>2$
2	PLP	B	601	-	16,16,16	0.47	0	20,23,23	1.09	1 (5%)
2	PLP	A	601	-	16,16,16	0.76	0	20,23,23	1.29	1 (5%)
2	PLP	C	601	-	16,16,16	0.92	1 (6%)	20,23,23	1.53	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	B	601	-	-	2/8/8/8	0/1/1/1
2	PLP	A	601	-	-	7/8/8/8	0/1/1/1
2	PLP	C	601	-	-	7/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	PLP	P-O4P	2.61	1.68	1.60

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	PLP	O4P-C5A-C5	5.60	120.03	109.35
2	A	601	PLP	O4P-C5A-C5	4.66	118.22	109.35
2	B	601	PLP	O4P-C5A-C5	3.21	115.46	109.35
2	C	601	PLP	C3-C4-C5	2.36	120.07	118.26

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PLP	C5-C4-C4A-O4A
2	A	601	PLP	C4-C5-C5A-O4P
2	A	601	PLP	C6-C5-C5A-O4P
2	A	601	PLP	C5A-O4P-P-O2P
2	A	601	PLP	C5A-O4P-P-O3P
2	C	601	PLP	C3-C4-C4A-O4A
2	C	601	PLP	C5-C4-C4A-O4A
2	C	601	PLP	C4-C5-C5A-O4P
2	C	601	PLP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
2	C	601	PLP	C5A-O4P-P-O1P
2	C	601	PLP	C5A-O4P-P-O2P
2	C	601	PLP	C5A-O4P-P-O3P
2	A	601	PLP	C3-C4-C4A-O4A
2	B	601	PLP	C3-C4-C4A-O4A
2	B	601	PLP	C5-C4-C4A-O4A
2	A	601	PLP	C5A-O4P-P-O1P

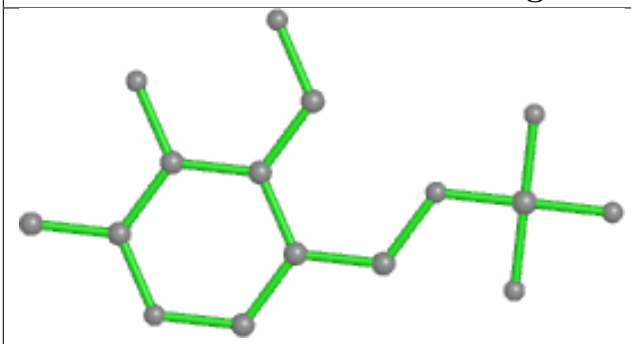
There are no ring outliers.

3 monomers are involved in 15 short contacts:

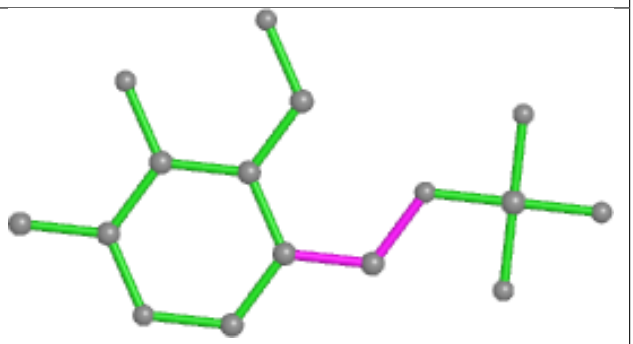
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PLP	5	0
2	A	601	PLP	5	0
2	C	601	PLP	5	0

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.

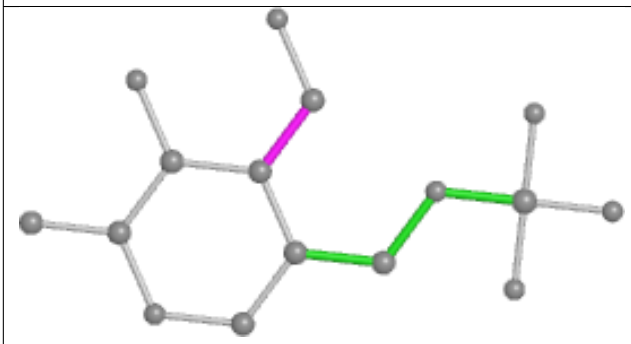
Ligand PLP B 601



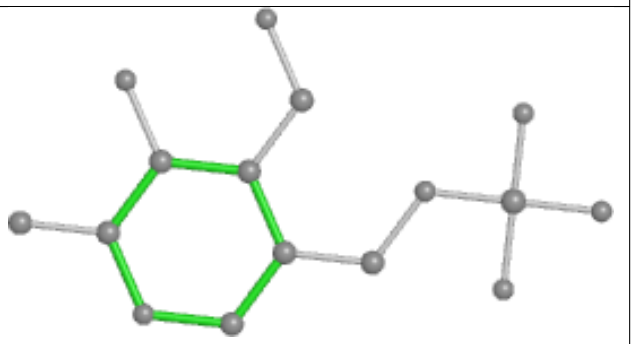
Bond lengths



Bond angles

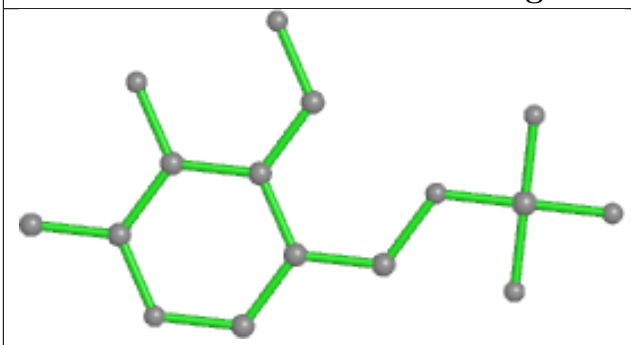


Torsions

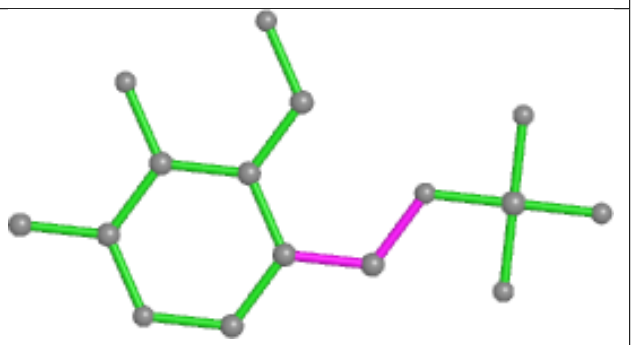


Rings

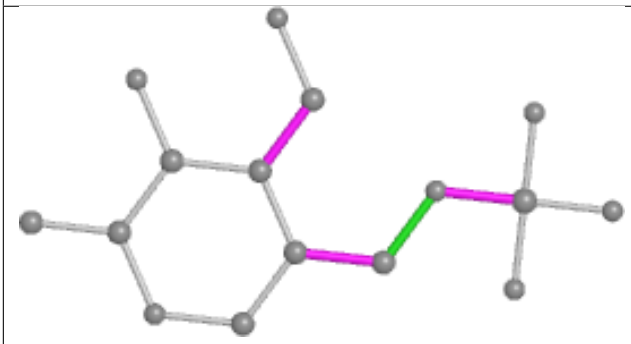
Ligand PLP A 601



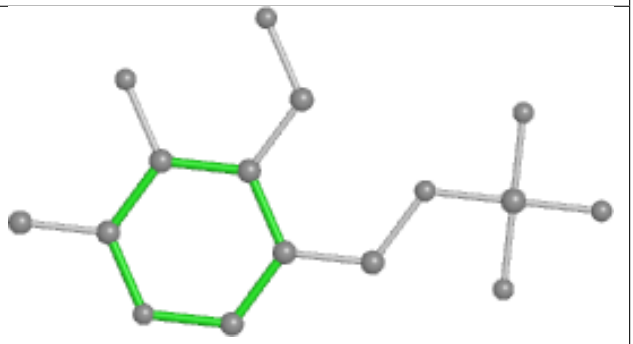
Bond lengths



Bond angles

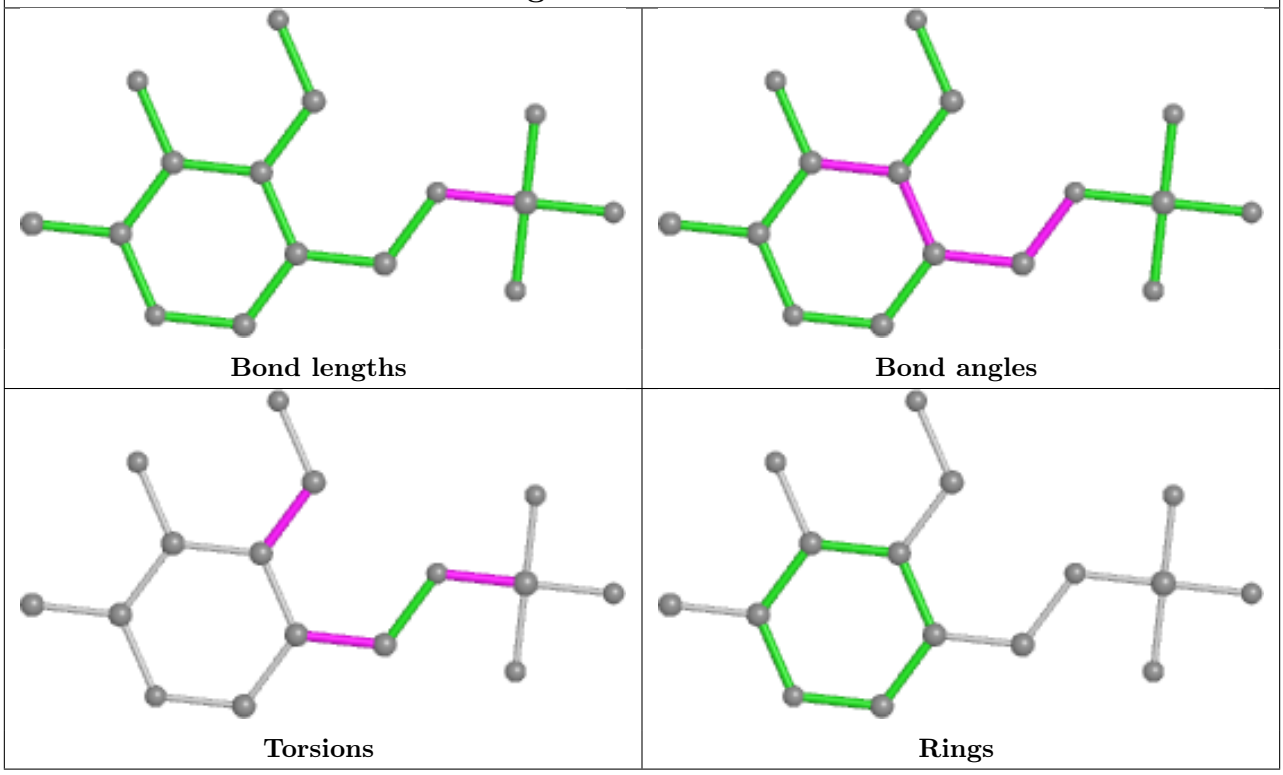


Torsions



Rings

Ligand PLP C 601



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, 95^{th} 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	475/513 (92%)	0.08	17 (3%) 42 37	40, 62, 109, 155	0
1	B	475/513 (92%)	0.07	15 (3%) 47 42	41, 63, 104, 181	0
1	C	475/513 (92%)	0.44	39 (8%) 11 8	46, 89, 128, 158	0
1	D	475/513 (92%)	0.93	94 (19%) 1 1	45, 102, 173, 212	0
All	All	1900/2052 (92%)	0.38	165 (8%) 10 7	40, 75, 147, 212	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	SER	14.3
1	D	414	PRO	11.8
1	B	40	ARG	8.3
1	D	424	GLY	5.6
1	D	393	ASP	5.6
1	D	281	HIS	5.5
1	C	181	ASP	5.3
1	D	472	VAL	5.2
1	D	471	PHE	4.9
1	D	183	LYS	4.9
1	C	466	THR	4.8
1	D	73	PHE	4.7
1	D	303	LYS	4.7
1	D	456	ALA	4.6
1	D	181	ASP	4.5
1	D	507	GLU	4.4
1	C	144	SER	4.3
1	D	389	ASP	4.3
1	D	184	LYS	4.3
1	D	182	THR	4.1
1	D	234	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	481	PHE	4.0
1	D	395	SER	4.0
1	D	326	GLY	4.0
1	C	70	TRP	4.0
1	A	475	MET	3.9
1	C	455	LEU	3.9
1	D	391	GLY	3.8
1	D	426	ARG	3.8
1	C	511	TYR	3.7
1	D	392	ILE	3.7
1	A	474	THR	3.7
1	D	144	SER	3.7
1	D	475	MET	3.5
1	A	307	GLU	3.4
1	B	306	GLU	3.3
1	B	466	THR	3.3
1	D	201	GLU	3.3
1	C	281	HIS	3.2
1	D	199	LEU	3.2
1	D	202	SER	3.2
1	A	303	LYS	3.2
1	C	146	SER	3.1
1	D	417	VAL	3.1
1	D	209	GLU	3.1
1	C	288	ARG	3.1
1	C	326	GLY	3.1
1	D	485	ILE	3.1
1	D	306	GLU	3.0
1	D	70	TRP	3.0
1	B	420	MET	3.0
1	D	205	TYR	3.0
1	D	498	GLN	3.0
1	D	146	SER	3.0
1	C	465	GLY	3.0
1	D	413	VAL	3.0
1	C	325	GLN	2.9
1	B	307	GLU	2.9
1	A	305	GLY	2.9
1	D	511	TYR	2.9
1	D	78	SER	2.9
1	D	463	SER	2.9
1	D	279	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	280	THR	2.9
1	C	367	ILE	2.9
1	C	209	GLU	2.8
1	C	182	THR	2.8
1	D	479	GLU	2.8
1	C	71	LYS	2.8
1	D	460	LYS	2.8
1	D	473	ALA	2.8
1	C	147	PRO	2.8
1	B	303	LYS	2.7
1	A	146	SER	2.7
1	A	476	ASN	2.7
1	C	143	LEU	2.7
1	D	384	LEU	2.7
1	D	474	THR	2.7
1	D	328	PRO	2.6
1	D	388	ARG	2.6
1	D	477	GLY	2.6
1	D	418	SER	2.6
1	D	373	LEU	2.6
1	D	470	ASP	2.6
1	A	512	LYS	2.5
1	A	302	ASN	2.5
1	D	459	ILE	2.5
1	D	198	ARG	2.5
1	D	45	LYS	2.5
1	D	171	GLY	2.5
1	B	308	VAL	2.5
1	B	53	GLU	2.5
1	C	332	THR	2.5
1	C	330	ASN	2.5
1	D	236	TYR	2.5
1	D	178	TYR	2.4
1	D	173	HIS	2.4
1	C	133	PRO	2.4
1	D	476	ASN	2.4
1	A	301	ILE	2.4
1	D	394	GLY	2.4
1	D	488	ILE	2.4
1	D	396	ARG	2.4
1	D	458	LYS	2.4
1	D	419	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	145	GLY	2.4
1	A	472	VAL	2.4
1	C	142[A]	SER	2.4
1	D	420	MET	2.3
1	D	366	LEU	2.3
1	D	233	VAL	2.3
1	D	238	ARG	2.3
1	A	326	GLY	2.3
1	D	427	MET	2.3
1	A	420	MET	2.3
1	D	304	LYS	2.3
1	D	367	ILE	2.3
1	C	44	THR	2.3
1	C	145	GLY	2.3
1	C	327	GLY	2.3
1	D	332	THR	2.3
1	C	468	LEU	2.3
1	D	246	GLN	2.3
1	D	505	GLU	2.3
1	A	298	LEU	2.3
1	D	449	PHE	2.3
1	A	306	GLU	2.3
1	D	60	ASP	2.2
1	D	172	GLY	2.2
1	D	327	GLY	2.2
1	C	52	GLU	2.2
1	D	231	ALA	2.2
1	B	302	ASN	2.2
1	D	482	GLN	2.2
1	D	512	LYS	2.2
1	B	305	GLY	2.2
1	D	52	GLU	2.2
1	A	513	ASN	2.2
1	C	283	SER	2.2
1	C	475	MET	2.2
1	C	116	MET	2.1
1	D	289	GLY	2.1
1	C	329	HIS	2.1
1	D	99	SER	2.1
1	B	469	LYS	2.1
1	C	98	TYR	2.1
1	C	290	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	51	LEU	2.1
1	C	470	ASP	2.1
1	A	41	VAL	2.1
1	B	464	SER	2.1
1	C	148	ALA	2.1
1	C	488	ILE	2.1
1	B	439	GLU	2.1
1	C	79	GLU	2.1
1	D	468	LEU	2.1
1	C	280	THR	2.1
1	D	282	LYS	2.1
1	D	445	VAL	2.0
1	D	244	ASP	2.0
1	D	481	PHE	2.0
1	B	145	GLY	2.0
1	D	207	ASP	2.0
1	D	487	LYS	2.0
1	D	96	ASN	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

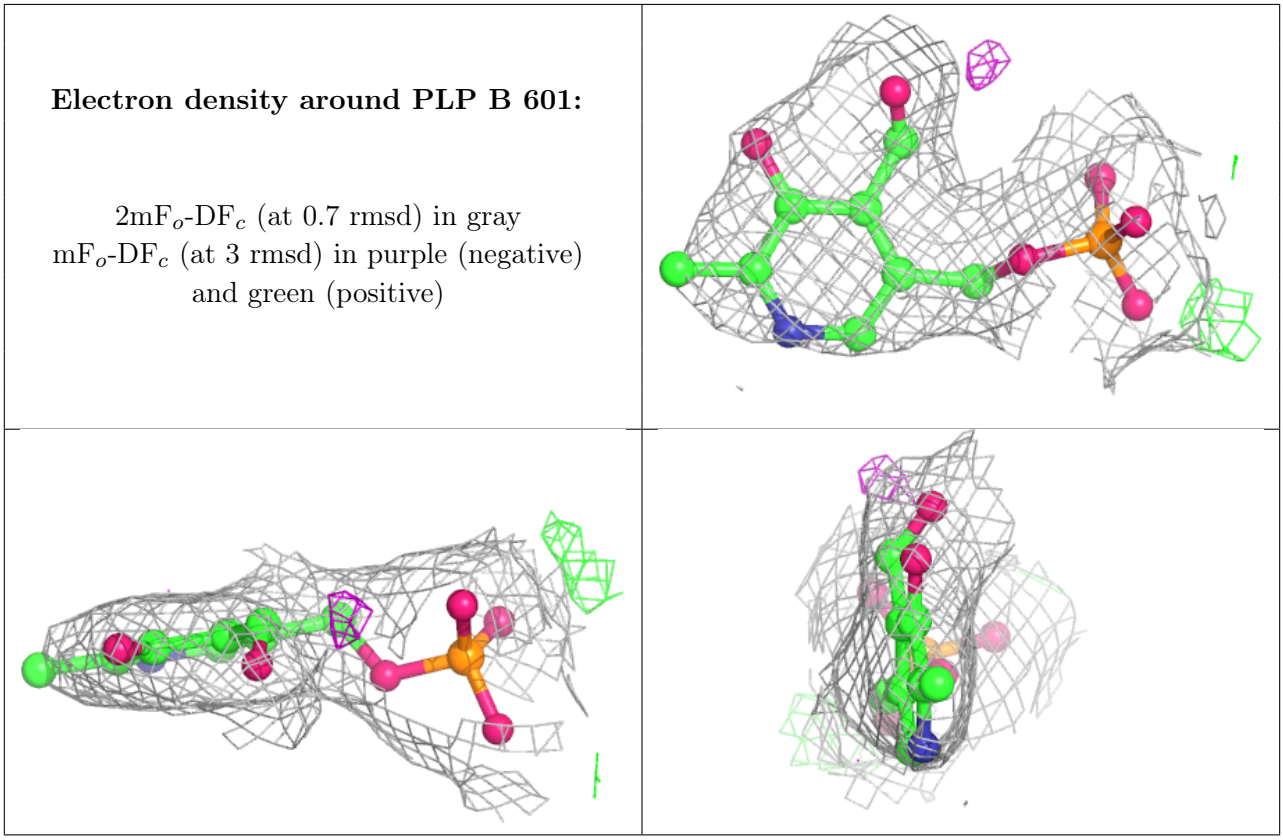
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	B	601	16/16	0.92	0.28	61,73,86,96	0
2	PLP	C	601	16/16	0.92	0.31	65,85,106,110	0
2	PLP	A	601	16/16	0.96	0.25	52,55,67,73	0

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.

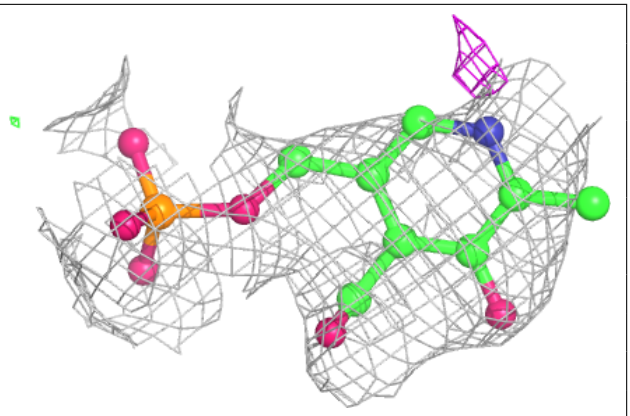
Electron density around PLP B 601:

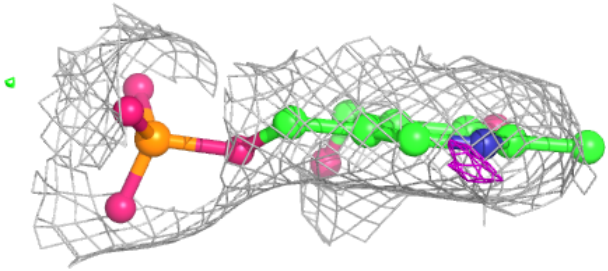
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

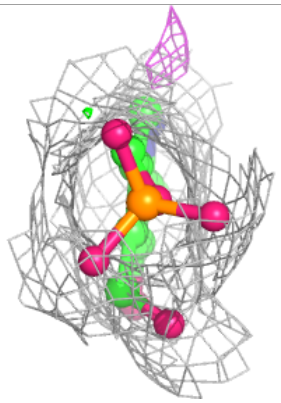


Electron density around PLP C 601:

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

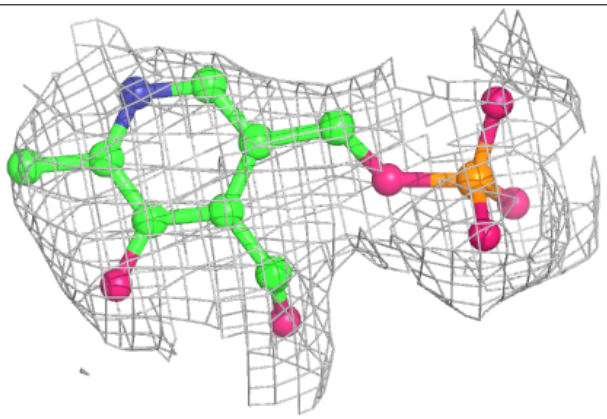


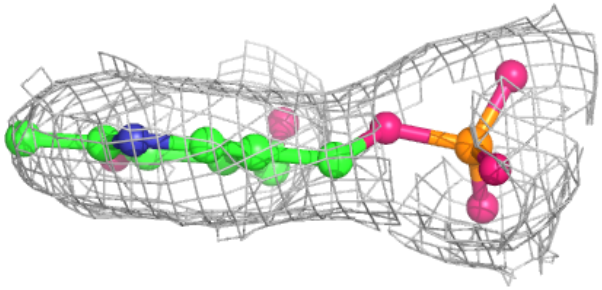


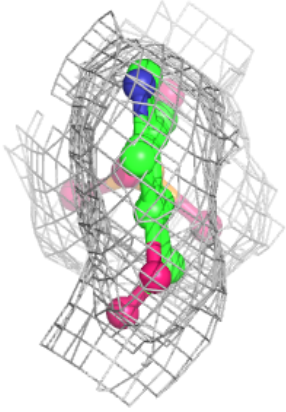


Electron density around PLP A 601:

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







6.5 Other polymers (i)

There are no such residues in this entry.