



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:25 AM UTC

PDB ID : 4ZM4 / pdb_00004zm4
Title : Complex structure of PctV K276R mutant with PMP and 3-dehydroshikimate
Authors : Hirayama, A.; Miyanaga, A.; Kudo, F.; Eguchi, T.
Deposited on : 2015-05-02
Resolution : 2.40 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

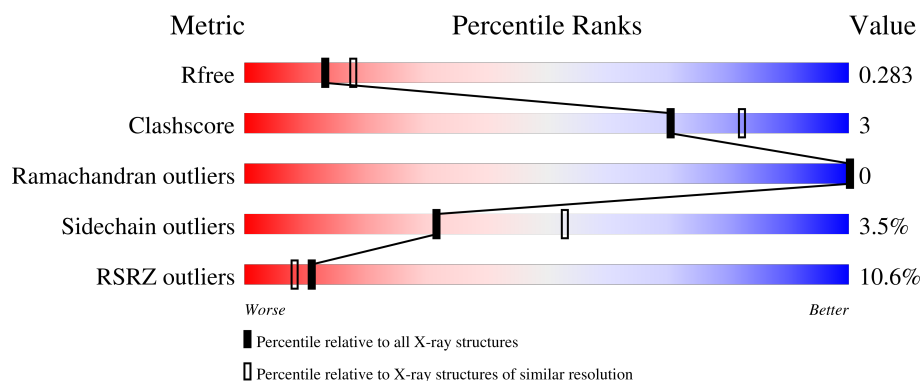
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	447	6% 85% 8% • 6%
1	B	447	2% 87% 7% • 5%
1	C	447	12% 84% 8% • 7%
1	D	447	34% 78% 7% • 13%
1	E	447	3% 86% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	F	447	3% 86% 7% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19717 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 Aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3164	1992	583	577	12			
1	B	425	Total	C	N	O	S	0	0	0
			3209	2018	590	589	12			
1	C	417	Total	C	N	O	S	0	0	0
			3160	1990	582	576	12			
1	D	387	Total	C	N	O	S	0	0	0
			2926	1843	536	535	12			
1	E	425	Total	C	N	O	S	0	0	0
			3209	2018	590	589	12			
1	F	418	Total	C	N	O	S	0	0	0
			3164	1992	583	577	12			

There are 24 discrepancies between the modelled and reference sequences:

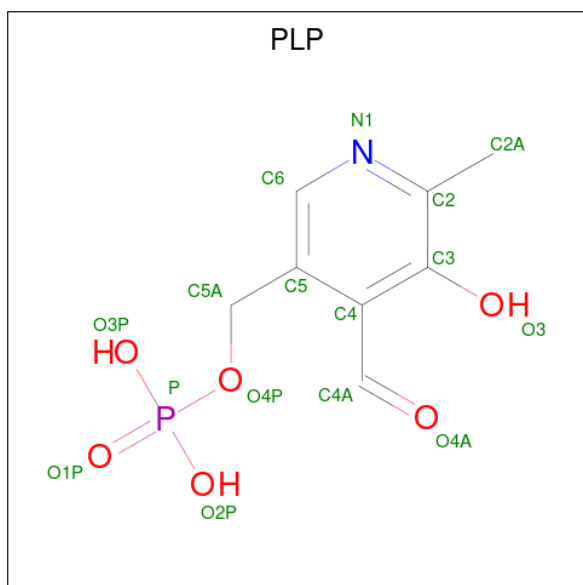
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A8R0K5
A	-1	SER	-	expression tag	UNP A8R0K5
A	0	HIS	-	expression tag	UNP A8R0K5
A	276	ARG	LYS	engineered mutation	UNP A8R0K5
B	-2	GLY	-	expression tag	UNP A8R0K5
B	-1	SER	-	expression tag	UNP A8R0K5
B	0	HIS	-	expression tag	UNP A8R0K5
B	276	ARG	LYS	engineered mutation	UNP A8R0K5
C	-2	GLY	-	expression tag	UNP A8R0K5
C	-1	SER	-	expression tag	UNP A8R0K5
C	0	HIS	-	expression tag	UNP A8R0K5
C	276	ARG	LYS	engineered mutation	UNP A8R0K5
D	-2	GLY	-	expression tag	UNP A8R0K5
D	-1	SER	-	expression tag	UNP A8R0K5
D	0	HIS	-	expression tag	UNP A8R0K5
D	276	ARG	LYS	engineered mutation	UNP A8R0K5
E	-2	GLY	-	expression tag	UNP A8R0K5

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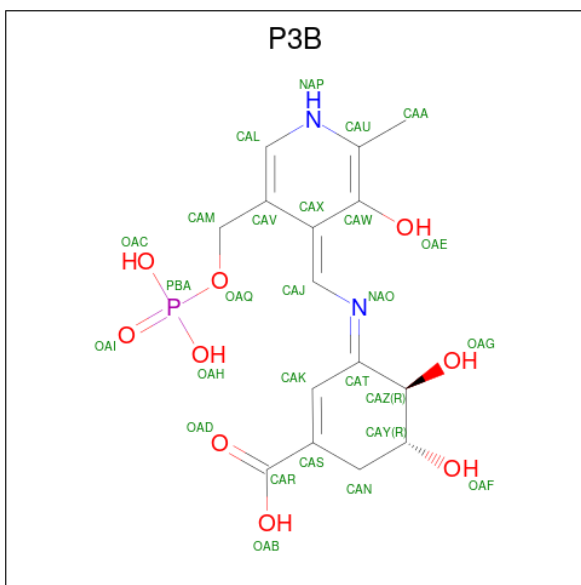
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP A8R0K5
E	0	HIS	-	expression tag	UNP A8R0K5
E	276	ARG	LYS	engineered mutation	UNP A8R0K5
F	-2	GLY	-	expression tag	UNP A8R0K5
F	-1	SER	-	expression tag	UNP A8R0K5
F	0	HIS	-	expression tag	UNP A8R0K5
F	276	ARG	LYS	engineered mutation	UNP A8R0K5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

- Molecule 3 is (3E,4R,5R)-4,5-dihydroxy-3-[(Z)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4(1H)-ylidene}methyl]imino}cyclohex-1-ene-1-carboxylic acid (CCD ID: P3B) (formula: C₁₅H₁₉N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 27	C 15	N 2	O 9	P 1	0	0
3	E	1	Total 27	C 15	N 2	O 9	P 1	0	0

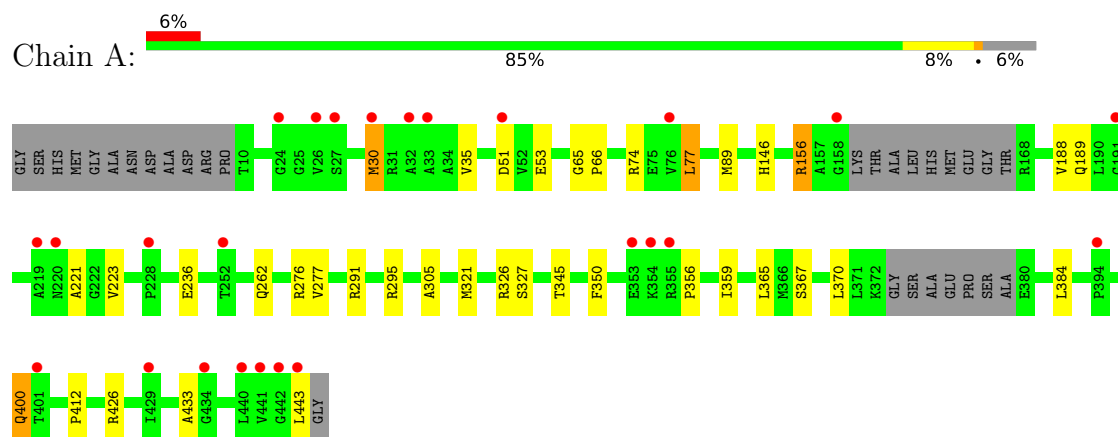
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	140	Total O 140 140	0	0
4	B	156	Total O 156 156	0	0
4	C	117	Total O 117 117	0	0
4	D	112	Total O 112 112	0	0
4	E	150	Total O 150 150	0	0
4	F	92	Total O 92 92	0	0

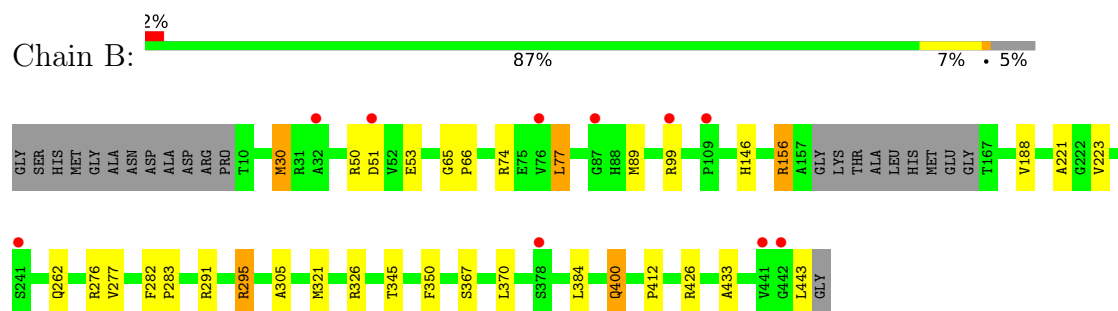
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

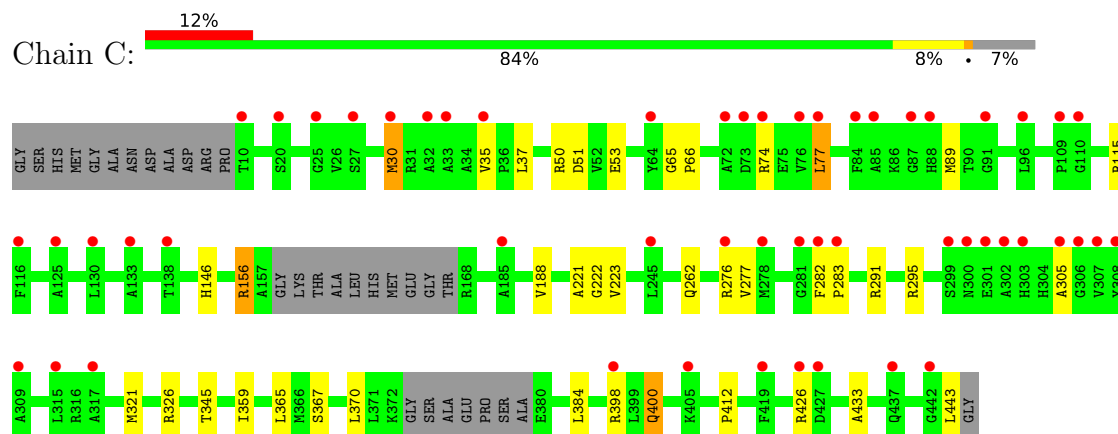
• Molecule 1: Aminotransferase



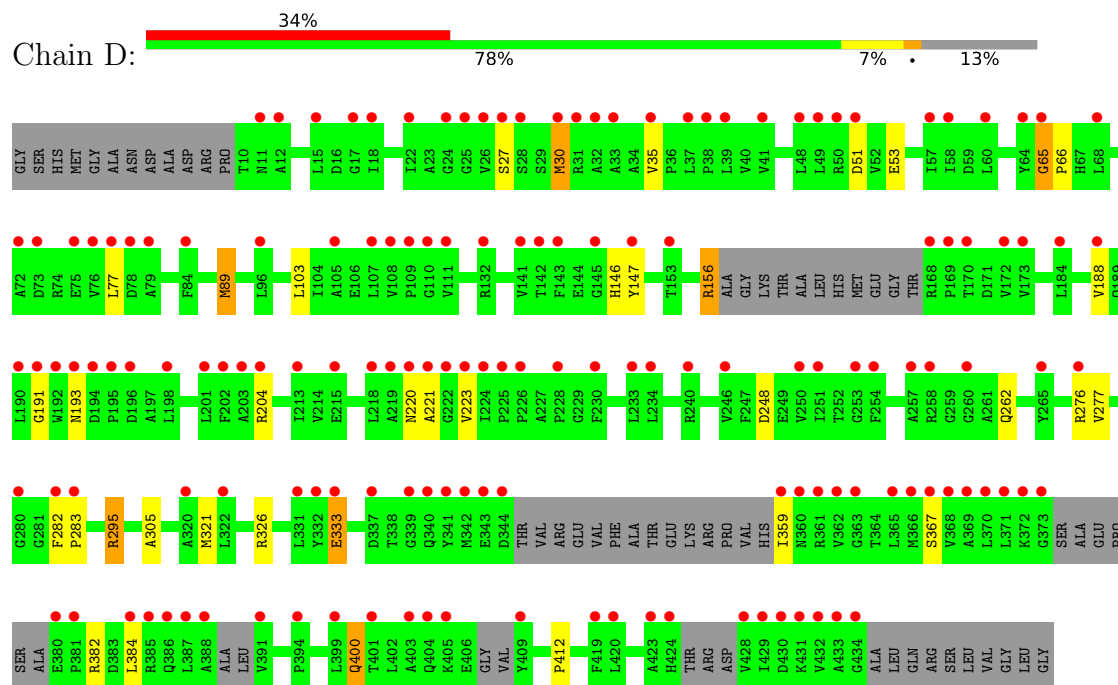
• Molecule 1: Aminotransferase



• Molecule 1: Aminotransferase



- Molecule 1: Aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	178.93Å 178.93Å 467.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.98 – 2.40 29.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.98-2.40) 91.5 (29.98-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.238 , 0.278 0.245 , 0.283	Depositor DCC
R_{free} test set	5134 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19717	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9455e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P3B, 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	0.84	0/3224	0.90	1/4374 (0.0%)
1	B	0.81	0/3271	0.90	3/4441 (0.1%)
1	C	0.82	0/3220	0.89	3/4369 (0.1%)
1	D	0.87	1/2979 (0.0%)	0.91	2/4035 (0.0%)
1	E	0.77	1/3271 (0.0%)	0.89	1/4441 (0.0%)
1	F	0.74	0/3224	0.87	2/4374 (0.0%)
All	All	0.81	2/19189 (0.0%)	0.89	12/26034 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	333	GLU	CA-C	7.03	1.61	1.52
1	E	236	GLU	CA-CB	5.55	1.62	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ARG	CG-CD-NE	6.40	126.07	112.00
1	A	326	ARG	CG-CD-NE	6.11	125.44	112.00
1	D	65	GLY	N-CA-C	5.79	124.15	112.34
1	C	65	GLY	N-CA-C	5.59	123.74	112.34
1	F	65	GLY	N-CA-C	5.53	123.63	112.34
1	B	50	ARG	N-CA-CB	5.49	119.22	110.65
1	C	222	GLY	N-CA-C	-5.49	102.70	112.58
1	D	333	GLU	CB-CA-C	5.30	119.86	110.85
1	C	326	ARG	CB-CG-CD	5.26	123.41	111.30
1	F	222	GLY	N-CA-C	-5.21	103.20	112.58
1	E	65	GLY	N-CA-C	5.20	122.94	112.34
1	B	367	SER	N-CA-CB	5.02	118.77	110.69

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	3164	0	3179	24	0
1	B	3209	0	3220	19	0
1	C	3160	0	3176	22	0
1	D	2926	0	2922	31	0
1	E	3209	0	3220	23	0
1	F	3164	0	3179	21	0
2	A	16	0	8	2	0
2	C	16	0	8	1	0
2	D	16	0	7	3	0
2	F	16	0	8	2	0
3	B	27	0	17	1	0
3	E	27	0	16	2	0
4	A	140	0	0	2	0
4	B	156	0	0	1	0
4	C	117	0	0	0	0
4	D	112	0	0	5	0
4	E	150	0	0	0	0
4	F	92	0	0	1	0
All	All	19717	0	18960	130	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 3.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ARG:HH22	2:D:501:PLP:C4A	1.85	0.89
1:E:276:ARG:HH22	3:E:501:P3B:CAJ	1.97	0.77
1:A:276:ARG:HH22	2:A:501:PLP:C4A	1.98	0.77
1:D:103:LEU:HD21	1:D:326:ARG:HH11	1.51	0.76
1:C:276:ARG:HH22	2:C:501:PLP:C4A	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:MET:HE1	1:B:305:ALA:HB2	1.72	0.71
1:B:276:ARG:HH22	3:B:501:P3B:CAJ	2.04	0.70
1:C:66:PRO:HG2	1:D:89:MET:HE3	1.78	0.65
1:E:400:GLN:HG2	1:E:412:PRO:HA	1.79	0.65
1:A:327:SER:O	1:C:74:ARG:NH1	2.30	0.64
1:A:400:GLN:HG2	1:A:412:PRO:HA	1.79	0.64
1:D:400:GLN:HG2	1:D:412:PRO:HA	1.81	0.63
1:C:400:GLN:HG2	1:C:412:PRO:HA	1.81	0.62
1:C:305:ALA:HB2	1:D:30:MET:HE1	1.81	0.62
1:F:400:GLN:HG2	1:F:412:PRO:HA	1.82	0.62
1:C:30:MET:HE1	1:D:305:ALA:HB2	1.82	0.62
1:A:35:VAL:HG13	1:A:35:VAL:O	2.00	0.61
1:B:400:GLN:HG2	1:B:412:PRO:HA	1.82	0.61
1:F:35:VAL:O	1:F:35:VAL:HG13	2.01	0.61
1:F:334:ARG:NH2	4:F:601:HOH:O	2.33	0.61
1:E:305:ALA:HB2	1:F:30:MET:HE1	1.82	0.60
1:E:121:THR:HG1	1:E:150:TRP:CD1	2.19	0.60
1:E:35:VAL:HG13	1:E:35:VAL:O	2.02	0.60
1:A:305:ALA:HB2	1:B:30:MET:HE1	1.83	0.59
1:A:221:ALA:HB1	1:A:384:LEU:HD13	1.85	0.59
1:D:35:VAL:HG13	1:D:35:VAL:O	2.02	0.59
1:D:221:ALA:HB1	1:D:384:LEU:HD13	1.84	0.59
1:E:221:ALA:HB1	1:E:384:LEU:HD13	1.83	0.59
1:E:10:THR:HG22	1:E:13:GLU:H	1.69	0.58
1:C:221:ALA:HB1	1:C:384:LEU:HD13	1.84	0.57
1:B:221:ALA:HB1	1:B:384:LEU:HD13	1.86	0.57
1:E:30:MET:HE1	1:F:305:ALA:HB2	1.87	0.56
1:F:221:ALA:HB1	1:F:384:LEU:HD13	1.85	0.56
1:E:36:PRO:HG3	1:E:397:ARG:HH12	1.71	0.56
1:A:400:GLN:HG2	1:A:412:PRO:CA	2.36	0.56
1:A:30:MET:HE3	1:A:30:MET:H	1.70	0.55
1:C:400:GLN:HG2	1:C:412:PRO:CA	2.36	0.55
1:F:400:GLN:HG2	1:F:412:PRO:CA	2.37	0.55
1:E:400:GLN:HG2	1:E:412:PRO:CA	2.37	0.54
1:D:193:ASN:O	1:D:382:ARG:NH1	2.40	0.54
1:D:30:MET:HE3	1:D:30:MET:H	1.74	0.53
1:D:400:GLN:HG2	1:D:412:PRO:CA	2.39	0.53
1:D:103:LEU:HD21	1:D:326:ARG:NH1	2.22	0.52
1:C:74:ARG:HG2	1:C:77:LEU:HD23	1.91	0.52
1:D:191:GLY:HA3	4:D:669:HOH:O	2.10	0.52
1:A:74:ARG:HG2	1:A:77:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:O	1:A:156:ARG:NH2	2.43	0.51
1:E:30:MET:HE3	1:E:30:MET:H	1.76	0.51
1:B:400:GLN:HG2	1:B:412:PRO:CA	2.40	0.51
1:B:30:MET:HE3	1:B:30:MET:H	1.76	0.50
1:C:30:MET:HE3	1:C:30:MET:H	1.76	0.50
1:F:74:ARG:HG2	1:F:77:LEU:HD23	1.92	0.50
1:F:30:MET:H	1:F:30:MET:HE3	1.75	0.50
1:B:74:ARG:HG2	1:B:77:LEU:HD23	1.93	0.50
1:D:51:ASP:HB3	1:D:53:GLU:H	1.77	0.50
1:D:146:HIS:O	1:D:156:ARG:NH2	2.44	0.50
1:F:146:HIS:O	1:F:156:ARG:NH2	2.44	0.49
4:A:714:HOH:O	1:C:50:ARG:HG3	2.12	0.49
1:B:51:ASP:HB3	1:B:53:GLU:H	1.77	0.49
1:D:276:ARG:NH2	2:D:501:PLP:C4A	2.67	0.49
1:A:51:ASP:HB3	1:A:53:GLU:H	1.77	0.49
1:D:295:ARG:NH2	4:D:604:HOH:O	2.45	0.49
1:E:74:ARG:HG2	1:E:77:LEU:HD23	1.93	0.49
1:E:51:ASP:HB3	1:E:53:GLU:H	1.78	0.49
1:A:276:ARG:HH22	2:A:501:PLP:H4A	1.77	0.48
1:F:276:ARG:NH2	2:F:501:PLP:C4A	2.76	0.48
1:C:345:THR:CG2	1:C:433:ALA:HB2	2.43	0.48
1:A:345:THR:CG2	1:A:433:ALA:HB2	2.44	0.47
1:C:51:ASP:HB3	1:C:53:GLU:H	1.79	0.47
1:F:51:ASP:HB3	1:F:53:GLU:H	1.80	0.47
1:E:345:THR:CG2	1:E:433:ALA:HB2	2.45	0.47
1:F:370:LEU:HD21	1:F:443:LEU:HD21	1.97	0.47
1:B:282:PHE:CD1	1:B:283:PRO:HD2	2.50	0.47
1:C:146:HIS:O	1:C:156:ARG:NH2	2.45	0.47
1:E:146:HIS:O	1:E:156:ARG:NH2	2.46	0.46
1:F:345:THR:CG2	1:F:433:ALA:HB2	2.45	0.46
1:D:277:VAL:O	1:D:321:MET:HG2	2.15	0.46
1:F:282:PHE:CD1	1:F:283:PRO:HD2	2.51	0.45
1:D:282:PHE:CD1	1:D:283:PRO:HD2	2.51	0.45
1:E:370:LEU:HD21	1:E:443:LEU:HD21	1.98	0.45
1:A:277:VAL:O	1:A:321:MET:HG2	2.17	0.45
1:C:277:VAL:O	1:C:321:MET:HG2	2.17	0.45
1:B:370:LEU:HD21	1:B:443:LEU:HD21	1.99	0.45
1:B:345:THR:CG2	1:B:433:ALA:HB2	2.46	0.45
1:A:370:LEU:HD21	1:A:443:LEU:HD21	1.99	0.45
1:B:277:VAL:O	1:B:321:MET:HG2	2.17	0.45
1:C:282:PHE:CD1	1:C:283:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:LEU:HD21	1:C:443:LEU:HD21	1.99	0.45
1:E:277:VAL:O	1:E:321:MET:HG2	2.17	0.44
1:B:65:GLY:N	1:B:66:PRO:CD	2.80	0.44
1:F:277:VAL:O	1:F:321:MET:HG2	2.18	0.44
1:B:295:ARG:NH2	4:B:608:HOH:O	2.51	0.44
1:D:248:ASP:OD2	2:D:501:PLP:N1	2.51	0.44
1:A:356:PRO:HA	4:A:699:HOH:O	2.18	0.43
1:B:146:HIS:O	1:B:156:ARG:NH2	2.45	0.43
1:D:147:TYR:HB3	1:D:220:ASN:HD22	1.83	0.43
1:E:350:PHE:HE2	1:E:370:LEU:HD13	1.83	0.43
1:A:223:VAL:HG12	1:A:223:VAL:O	2.18	0.43
1:B:65:GLY:N	1:B:66:PRO:HD3	2.34	0.43
1:D:359:ILE:HA	1:D:367:SER:O	2.19	0.43
1:F:223:VAL:HG12	1:F:223:VAL:O	2.19	0.43
1:E:282:PHE:CD1	1:E:283:PRO:HD2	2.54	0.43
1:B:223:VAL:O	1:B:223:VAL:HG12	2.19	0.42
1:C:223:VAL:HG12	1:C:223:VAL:O	2.19	0.42
1:B:350:PHE:HE2	1:B:370:LEU:HD13	1.84	0.42
1:D:276:ARG:HB2	4:D:618:HOH:O	2.19	0.42
1:E:156:ARG:NH1	1:E:189:GLN:OE1	2.53	0.42
1:E:223:VAL:O	1:E:223:VAL:HG12	2.19	0.42
1:A:65:GLY:N	1:A:66:PRO:CD	2.83	0.42
1:C:115:ARG:HD3	1:D:27:SER:O	2.20	0.42
1:D:30:MET:HG3	4:D:694:HOH:O	2.19	0.41
1:E:307:VAL:HG11	1:F:276:ARG:CZ	2.50	0.41
1:F:156:ARG:NH1	1:F:189:GLN:OE1	2.52	0.41
1:D:204:ARG:HG2	4:D:695:HOH:O	2.20	0.41
1:D:223:VAL:O	1:D:223:VAL:HG12	2.20	0.41
1:E:65:GLY:N	1:E:66:PRO:CD	2.83	0.41
1:F:276:ARG:HH21	2:F:501:PLP:C4A	2.33	0.41
1:A:35:VAL:O	1:A:35:VAL:CG1	2.68	0.41
1:C:115:ARG:HD3	1:D:27:SER:HA	2.01	0.41
1:C:359:ILE:HA	1:C:367:SER:O	2.21	0.41
1:F:35:VAL:O	1:F:35:VAL:CG1	2.68	0.41
1:A:65:GLY:N	1:A:66:PRO:HD3	2.36	0.40
1:A:156:ARG:NH1	1:A:189:GLN:OE1	2.54	0.40
1:A:359:ILE:HA	1:A:367:SER:O	2.21	0.40
1:D:35:VAL:O	1:D:35:VAL:CG1	2.69	0.40
1:C:35:VAL:HG12	1:C:37:LEU:O	2.22	0.40
1:D:65:GLY:N	1:D:66:PRO:CD	2.84	0.40
1:D:65:GLY:N	1:D:66:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:501:P3B:NAO	3:E:501:P3B:OAE	2.53	0.40
1:A:350:PHE:HE2	1:A:370:LEU:HD13	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/447 (92%)	401 (97%)	11 (3%)	0	100	100
1	B	421/447 (94%)	407 (97%)	14 (3%)	0	100	100
1	C	411/447 (92%)	402 (98%)	9 (2%)	0	100	100
1	D	373/447 (83%)	362 (97%)	11 (3%)	0	100	100
1	E	421/447 (94%)	408 (97%)	13 (3%)	0	100	100
1	F	412/447 (92%)	400 (97%)	12 (3%)	0	100	100
All	All	2450/2682 (91%)	2380 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/340 (94%)	309 (96%)	12 (4%)	30	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	326/340 (96%)	315 (97%)	11 (3%)	32	54
1	C	321/340 (94%)	309 (96%)	12 (4%)	30	51
1	D	296/340 (87%)	287 (97%)	9 (3%)	36	58
1	E	326/340 (96%)	315 (97%)	11 (3%)	32	54
1	F	321/340 (94%)	310 (97%)	11 (3%)	32	54
All	All	1911/2040 (94%)	1845 (96%)	66 (4%)	32	53

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	77	LEU
1	A	89	MET
1	A	156	ARG
1	A	188	VAL
1	A	236	GLU
1	A	262	GLN
1	A	291	ARG
1	A	295	ARG
1	A	365	LEU
1	A	400	GLN
1	A	426	ARG
1	B	30	MET
1	B	77	LEU
1	B	89	MET
1	B	99	ARG
1	B	156	ARG
1	B	188	VAL
1	B	262	GLN
1	B	291	ARG
1	B	295	ARG
1	B	400	GLN
1	B	426	ARG
1	C	30	MET
1	C	77	LEU
1	C	89	MET
1	C	156	ARG
1	C	188	VAL
1	C	262	GLN
1	C	291	ARG

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Mol	Chain	Res	Type
1	C	295	ARG
1	C	365	LEU
1	C	398	ARG
1	C	400	GLN
1	C	426	ARG
1	D	30	MET
1	D	77	LEU
1	D	89	MET
1	D	156	ARG
1	D	188	VAL
1	D	262	GLN
1	D	295	ARG
1	D	333	GLU
1	D	400	GLN
1	E	10	THR
1	E	30	MET
1	E	77	LEU
1	E	89	MET
1	E	156	ARG
1	E	170	THR
1	E	188	VAL
1	E	262	GLN
1	E	400	GLN
1	E	426	ARG
1	E	427	ASP
1	F	30	MET
1	F	77	LEU
1	F	89	MET
1	F	156	ARG
1	F	188	VAL
1	F	262	GLN
1	F	291	ARG
1	F	295	ARG
1	F	365	LEU
1	F	400	GLN
1	F	426	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	113	GLN

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Mol	Chain	Res	Type
1	B	67	HIS
1	B	360	ASN
1	C	113	GLN
1	C	358	HIS
1	D	113	GLN
1	D	360	ASN
1	E	67	HIS
1	E	113	GLN
1	F	220	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	D	501	-	16,16,16	2.80	4 (25%)	20,23,23	1.78	3 (15%)
3	P3B	B	501	-	26,28,28	3.96	12 (46%)	32,41,41	2.53	13 (40%)
2	PLP	A	501	-	16,16,16	2.98	3 (18%)	20,23,23	1.90	5 (25%)
2	PLP	F	501	-	16,16,16	2.80	3 (18%)	20,23,23	1.95	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	C	501	-	16,16,16	2.25	3 (18%)	20,23,23	1.53	3 (15%)
3	P3B	E	501	-	26,28,28	3.27	11 (42%)	32,41,41	2.51	9 (28%)

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	D	501	-	-	2/8/8/8	0/1/1/1
3	P3B	B	501	-	-	0/13/31/31	0/2/2/2
2	PLP	A	501	-	-	1/8/8/8	0/1/1/1
2	PLP	F	501	-	-	0/8/8/8	0/1/1/1
2	PLP	C	501	-	-	0/8/8/8	0/1/1/1
3	P3B	E	501	-	-	1/13/31/31	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	P3B	CAN-CAS	-10.39	1.34	1.51
3	B	501	P3B	CAM-CAV	-9.56	1.37	1.50
3	E	501	P3B	CAN-CAS	-9.13	1.36	1.51
2	F	501	PLP	C3-C2	7.81	1.49	1.41
2	A	501	PLP	C3-C2	7.77	1.49	1.41
3	B	501	P3B	CAA-CAU	-7.50	1.37	1.49
2	D	501	PLP	C4-C5	6.99	1.51	1.42
3	E	501	P3B	CAM-CAV	-6.88	1.41	1.50
2	A	501	PLP	C4-C5	6.26	1.50	1.42
2	C	501	PLP	C3-C2	6.20	1.47	1.41
3	E	501	P3B	CAA-CAU	-6.15	1.39	1.49
3	B	501	P3B	CAY-CAZ	5.98	1.58	1.52
2	D	501	PLP	C3-C2	5.94	1.47	1.41
2	F	501	PLP	C4-C5	5.88	1.50	1.42
2	A	501	PLP	C4-C3	5.51	1.50	1.41
2	F	501	PLP	C4-C3	5.08	1.49	1.41
3	B	501	P3B	CAT-NAO	4.64	1.37	1.29
3	E	501	P3B	CAY-CAZ	4.43	1.57	1.52
3	E	501	P3B	PBA-OAI	4.22	1.63	1.50
2	D	501	PLP	C4-C3	4.22	1.48	1.41
2	C	501	PLP	C4-C5	4.21	1.47	1.42
2	C	501	PLP	C4-C3	4.05	1.47	1.41
3	E	501	P3B	CAT-NAO	4.01	1.36	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	P3B	CAU-NAP	3.71	1.38	1.34
3	B	501	P3B	CAR-CAS	-3.53	1.41	1.49
3	B	501	P3B	OAQ-CAM	3.52	1.46	1.43
3	B	501	P3B	CAW-CAU	-3.47	1.32	1.37
3	B	501	P3B	OAB-CAR	-3.47	1.21	1.30
3	E	501	P3B	CAL-NAP	2.94	1.41	1.36
3	B	501	P3B	OAG-CAZ	2.94	1.47	1.42
3	E	501	P3B	OAB-CAR	-2.80	1.23	1.30
3	E	501	P3B	CAK-CAS	2.59	1.41	1.34
2	D	501	PLP	C4-C4A	2.56	1.52	1.46
3	E	501	P3B	CAL-CAV	2.51	1.40	1.36
3	E	501	P3B	CAR-CAS	-2.44	1.43	1.49
3	B	501	P3B	PBA-OAQ	2.34	1.67	1.60

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	P3B	CAN-CAY-CAZ	7.56	118.80	109.37
3	E	501	P3B	CAX-CAW-CAU	6.15	123.74	118.34
3	B	501	P3B	CAN-CAY-CAZ	5.53	116.27	109.37
2	A	501	PLP	C3-C4-C5	-5.48	113.88	118.28
2	F	501	PLP	C4-C3-C2	-5.39	117.11	120.14
2	D	501	PLP	C3-C4-C5	-5.38	113.96	118.28
3	E	501	P3B	OAB-CAR-CAS	4.81	125.59	115.43
3	B	501	P3B	CAX-CAW-CAU	4.51	122.30	118.34
2	C	501	PLP	C3-C4-C5	-4.35	114.78	118.28
3	E	501	P3B	OAB-CAR-OAD	-4.16	114.00	123.90
3	E	501	P3B	CAW-CAX-CAV	-3.96	117.19	119.28
3	B	501	P3B	CAY-CAN-CAS	3.90	119.29	111.77
3	B	501	P3B	OAG-CAZ-CAY	3.77	116.68	110.34
3	B	501	P3B	OAB-CAR-OAD	-3.73	115.01	123.90
3	B	501	P3B	CAW-CAX-CAV	-3.72	117.32	119.28
3	B	501	P3B	CAL-NAP-CAU	-3.54	121.27	124.20
3	B	501	P3B	OAB-CAR-CAS	3.34	122.50	115.43
3	B	501	P3B	OAC-PBA-OAQ	3.31	115.29	106.67
2	D	501	PLP	C2A-C2-C3	-3.23	117.02	120.80
3	B	501	P3B	OAF-CAY-CAN	-3.15	102.38	109.38
3	E	501	P3B	CAL-NAP-CAU	-3.13	121.61	124.20
3	B	501	P3B	CAA-CAU-CAW	-3.02	118.57	122.27
3	E	501	P3B	CAY-CAN-CAS	2.98	117.52	111.77
2	A	501	PLP	C4-C3-C2	-2.96	118.48	120.14
3	E	501	P3B	OAG-CAZ-CAY	2.84	115.12	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PLP	C5A-C5-C6	-2.75	114.88	119.36
2	F	501	PLP	O3P-P-O2P	2.73	118.06	107.80
2	D	501	PLP	C2A-C2-N1	2.65	122.63	117.64
2	F	501	PLP	C2A-C2-C3	2.59	123.83	120.80
2	F	501	PLP	C6-N1-C2	2.57	123.85	119.20
2	C	501	PLP	C4-C3-C2	-2.43	118.77	120.14
3	E	501	P3B	CAN-CAS-CAR	-2.36	112.66	116.99
2	F	501	PLP	C3-C4-C5	-2.34	116.40	118.28
2	A	501	PLP	O3P-P-O2P	2.30	116.43	107.80
2	C	501	PLP	O3-C3-C2	2.24	122.22	117.58
2	F	501	PLP	O3-C3-C2	2.17	122.08	117.58
3	B	501	P3B	OAF-CAY-CAZ	2.17	113.43	109.80
2	A	501	PLP	O4A-C4A-C4	-2.12	119.77	124.80
3	B	501	P3B	CAV-CAL-NAP	-2.11	118.27	120.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	PLP	C5A-O4P-P-O1P
2	D	501	PLP	C5A-O4P-P-O2P
3	E	501	P3B	CAM-OAQ-PBA-OAI
2	A	501	PLP	C4-C5-C5A-O4P

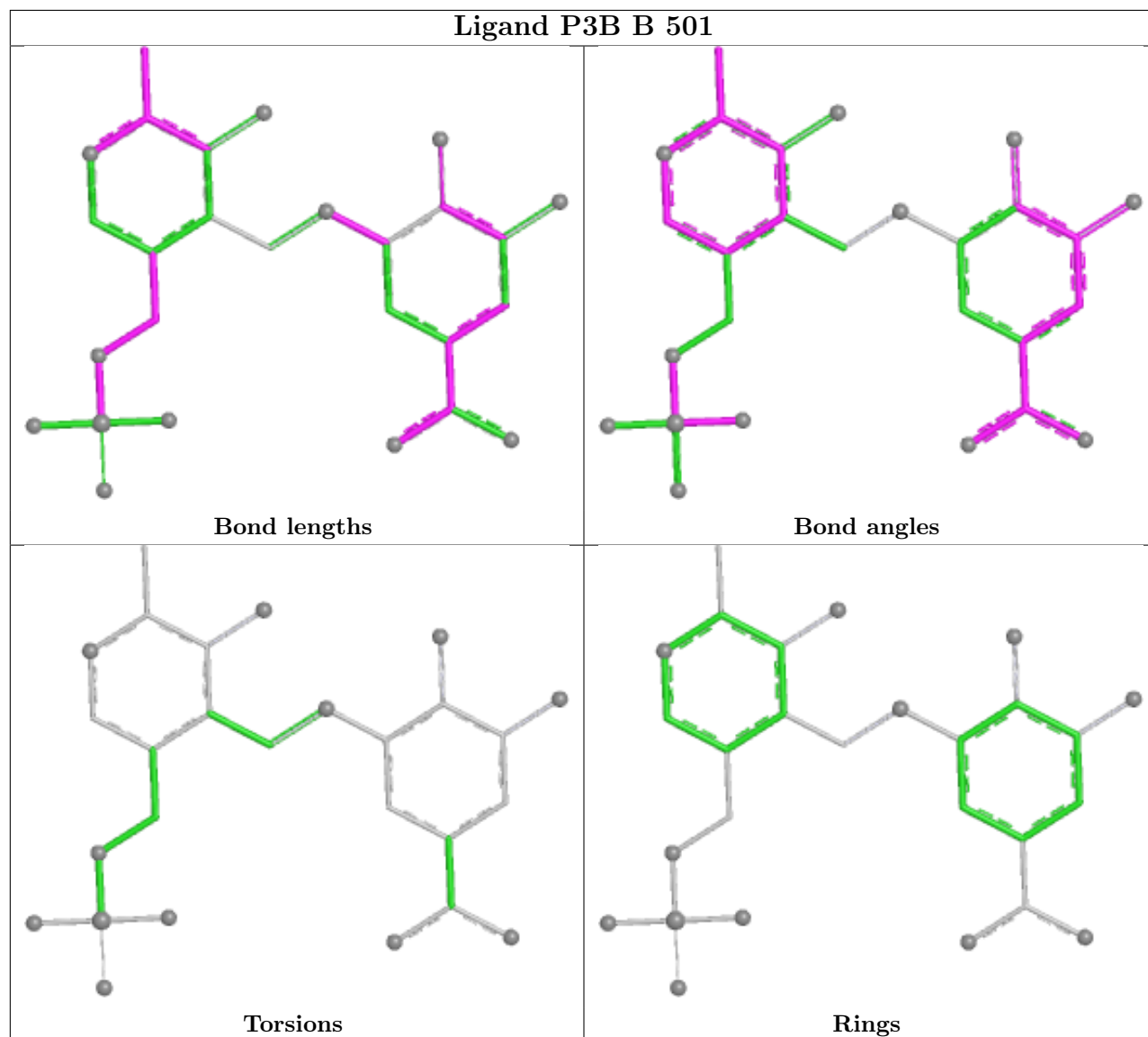
There are no ring outliers.

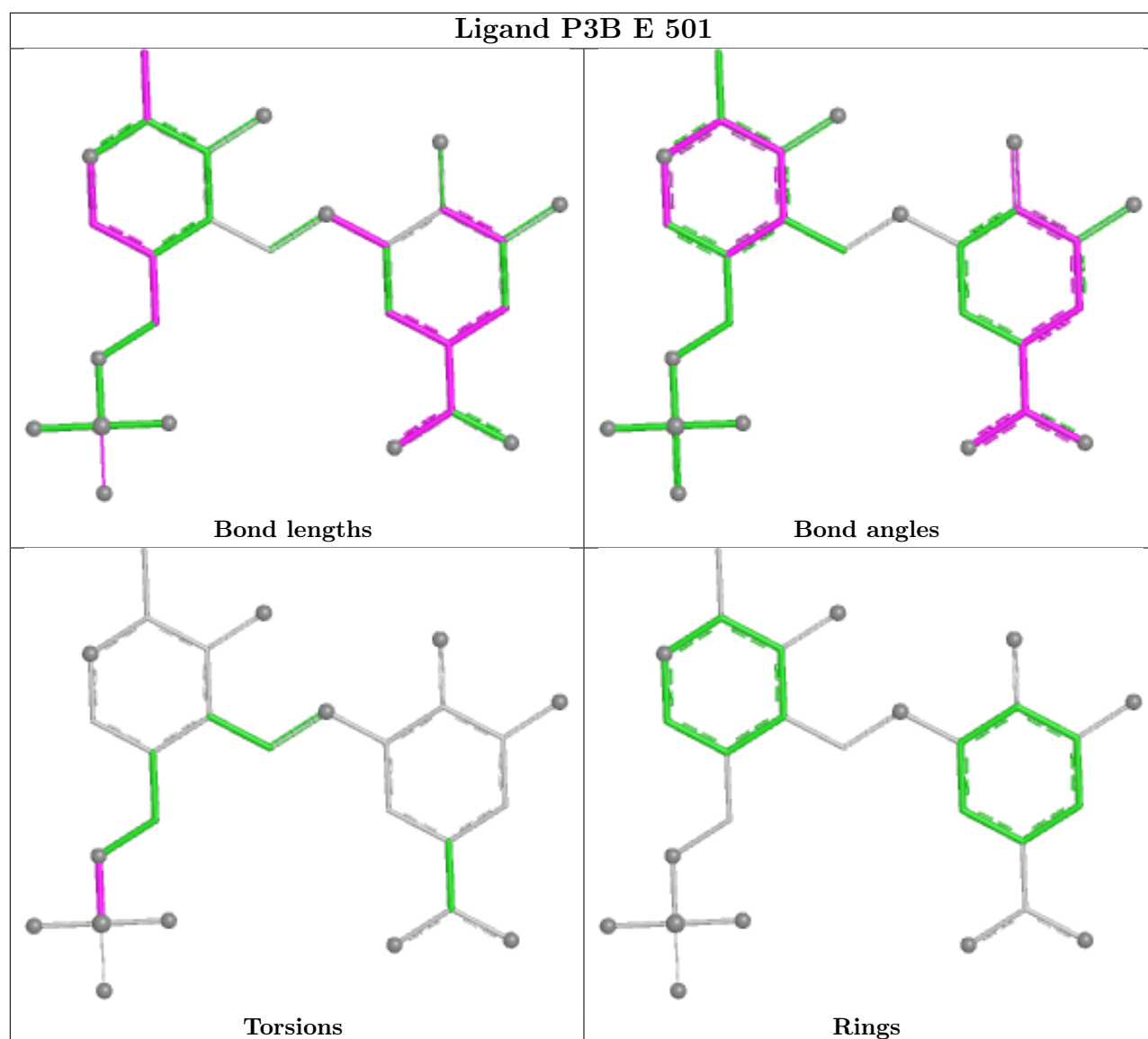
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	PLP	3	0
3	B	501	P3B	1	0
2	A	501	PLP	2	0
2	F	501	PLP	2	0
2	C	501	PLP	1	0
3	E	501	P3B	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	418/447 (93%)	0.56	25 (5%)	27 24	13, 25, 42, 67	0
1	B	425/447 (95%)	0.25	10 (2%)	59 55	13, 24, 41, 59	0
1	C	417/447 (93%)	0.98	53 (12%)	8 6	19, 31, 49, 64	0
1	D	387/447 (86%)	1.81	152 (39%)	1 0	18, 35, 50, 76	0
1	E	425/447 (95%)	0.40	13 (3%)	51 47	17, 29, 45, 64	0
1	F	418/447 (93%)	0.34	12 (2%)	53 50	18, 31, 50, 72	0
All	All	2490/2682 (92%)	0.71	265 (10%)	11 8	13, 29, 48, 76	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	302	ALA	5.2
1	D	246	VAL	5.1
1	D	76	VAL	5.1
1	D	373	GLY	5.1
1	D	359	ILE	5.0
1	D	433	ALA	4.9
1	D	68	LEU	4.7
1	D	109	PRO	4.5
1	D	25	GLY	4.5
1	D	399	LEU	4.4
1	D	362	VAL	4.3
1	D	337	ASP	4.2
1	D	32	ALA	4.2
1	D	77	LEU	4.2
1	A	354	LYS	4.1
1	D	57	ILE	4.1
1	D	110	GLY	4.0
1	D	225	PRO	4.0
1	D	381	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	430	ASP	3.9
1	C	138	THR	3.9
1	C	84	PHE	3.8
1	D	429	ILE	3.8
1	E	441	VAL	3.7
1	D	257	ALA	3.7
1	D	341	TYR	3.7
1	C	76	VAL	3.7
1	D	405	LYS	3.7
1	A	440	LEU	3.6
1	D	420	LEU	3.6
1	D	340	GLN	3.5
1	D	60	LEU	3.5
1	C	33	ALA	3.5
1	D	234	LEU	3.5
1	D	58	ILE	3.5
1	D	195	PRO	3.5
1	D	33	ALA	3.5
1	D	190	LEU	3.4
1	D	84	PHE	3.4
1	D	73	ASP	3.4
1	D	369	ALA	3.4
1	D	403	ALA	3.4
1	D	38	PRO	3.4
1	D	18	ILE	3.4
1	D	192	TRP	3.3
1	D	222	GLY	3.3
1	A	401	THR	3.2
1	F	354	LYS	3.2
1	D	367	SER	3.2
1	D	363	GLY	3.2
1	D	15	LEU	3.1
1	D	188	VAL	3.1
1	C	315	LEU	3.1
1	D	385	ARG	3.1
1	D	224	ILE	3.1
1	C	308	TYR	3.1
1	D	79	ALA	3.1
1	E	77	LEU	3.1
1	A	355	ARG	3.1
1	C	32	ALA	3.0
1	D	260	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	26	VAL	3.0
1	D	432	VAL	3.0
1	A	30	MET	3.0
1	D	219	ALA	3.0
1	D	226	PRO	3.0
1	D	419	PHE	3.0
1	D	387	LEU	3.0
1	D	213	ILE	2.9
1	E	377	PRO	2.9
1	C	130	LEU	2.9
1	D	145	GLY	2.9
1	D	360	ASN	2.9
1	D	258	ARG	2.9
1	F	219	ALA	2.9
1	C	64	TYR	2.9
1	E	437	GLN	2.9
1	D	223	VAL	2.9
1	D	331	LEU	2.9
1	D	386	GLN	2.9
1	D	105	ALA	2.9
1	C	73	ASP	2.9
1	A	434	GLY	2.9
1	C	306	GLY	2.9
1	C	30	MET	2.8
1	C	276	ARG	2.8
1	B	76	VAL	2.8
1	D	35	VAL	2.8
1	D	365	LEU	2.8
1	D	388	ALA	2.8
1	D	401	THR	2.8
1	D	168	ARG	2.8
1	D	17	GLY	2.7
1	D	322	LEU	2.7
1	D	31	ARG	2.7
1	B	109	PRO	2.7
1	D	11	ASN	2.7
1	A	27	SER	2.7
1	A	441	VAL	2.7
1	F	441	VAL	2.7
1	A	24	GLY	2.7
1	D	24	GLY	2.7
1	D	37	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	33	ALA	2.7
1	D	50	ARG	2.7
1	A	353	GLU	2.7
1	D	196	ASP	2.7
1	A	442	GLY	2.7
1	A	76	VAL	2.7
1	D	30	MET	2.7
1	C	283	PRO	2.6
1	E	109	PRO	2.6
1	C	74	ARG	2.6
1	D	132	ARG	2.6
1	D	198	LEU	2.6
1	D	371	LEU	2.6
1	D	170	THR	2.6
1	D	221	ALA	2.6
1	C	91	GLY	2.6
1	D	191	GLY	2.6
1	C	300	ASN	2.6
1	D	380	GLU	2.6
1	D	203	ALA	2.6
1	D	78	ASP	2.6
1	C	307	VAL	2.6
1	D	253	GLY	2.6
1	D	384	LEU	2.6
1	D	320	ALA	2.6
1	B	441	VAL	2.5
1	C	185	ALA	2.5
1	D	240	ARG	2.5
1	E	168	ARG	2.5
1	D	48	LEU	2.5
1	C	309	ALA	2.5
1	D	366	MET	2.5
1	A	158	GLY	2.5
1	C	281	GLY	2.5
1	D	193	ASN	2.5
1	C	110	GLY	2.5
1	D	22	ILE	2.5
1	D	282	PHE	2.5
1	B	32	ALA	2.5
1	C	317	ALA	2.5
1	D	12	ALA	2.5
1	A	394	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	169	PRO	2.4
1	D	343	GLU	2.4
1	D	194	ASP	2.4
1	E	354	LYS	2.4
1	F	51	ASP	2.4
1	D	107	LEU	2.4
1	A	26	VAL	2.4
1	C	27	SER	2.4
1	D	173	VAL	2.4
1	A	228	PRO	2.4
1	C	299	SER	2.4
1	D	434	GLY	2.4
1	C	437	GLN	2.4
1	D	49	LEU	2.4
1	D	332	TYR	2.4
1	D	143	PHE	2.4
1	D	41	VAL	2.4
1	D	220	ASN	2.4
1	D	333	GLU	2.4
1	B	241	SER	2.4
1	D	64	TYR	2.4
1	A	252	THR	2.3
1	D	153	THR	2.3
1	D	27	SER	2.3
1	C	77	LEU	2.3
1	D	39	LEU	2.3
1	D	218	LEU	2.3
1	F	77	LEU	2.3
1	D	147	TYR	2.3
1	D	409	TYR	2.3
1	C	405	LYS	2.3
1	D	215	GLU	2.3
1	E	167	THR	2.3
1	A	191	GLY	2.3
1	C	442	GLY	2.3
1	A	443	LEU	2.3
1	C	35	VAL	2.3
1	F	168	ARG	2.3
1	D	75	GLU	2.3
1	F	348	GLU	2.3
1	D	280	GLY	2.3
1	E	200	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	250	VAL	2.3
1	B	99	ARG	2.3
1	C	426	ARG	2.3
1	D	361	ARG	2.3
1	C	303	HIS	2.2
1	D	342	MET	2.2
1	D	72	ALA	2.2
1	E	10	THR	2.2
1	D	339	GLY	2.2
1	D	28	SER	2.2
1	F	75	GLU	2.2
1	D	276	ARG	2.2
1	D	202	PHE	2.2
1	D	254	PHE	2.2
1	D	111	VAL	2.2
1	D	404	GLN	2.2
1	D	431	LYS	2.2
1	D	142	THR	2.2
1	C	87	GLY	2.2
1	D	65	GLY	2.2
1	E	376	GLU	2.2
1	A	220	ASN	2.2
1	C	125	ALA	2.2
1	C	133	ALA	2.2
1	D	423	ALA	2.2
1	B	87	GLY	2.2
1	C	25	GLY	2.2
1	C	245	LEU	2.2
1	D	184	LEU	2.2
1	D	283	PRO	2.2
1	E	405	LYS	2.2
1	D	108	VAL	2.1
1	D	172	VAL	2.1
1	C	305	ALA	2.1
1	D	370	LEU	2.1
1	A	429	ILE	2.1
1	D	204	ARG	2.1
1	F	223	VAL	2.1
1	C	85	ALA	2.1
1	C	10	THR	2.1
1	D	228	PRO	2.1
1	C	278	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	32	ALA	2.1
1	A	219	ALA	2.1
1	C	72	ALA	2.1
1	D	265	TYR	2.1
1	C	427	ASP	2.1
1	D	394	PRO	2.1
1	C	419	PHE	2.1
1	C	96	LEU	2.1
1	D	251	ILE	2.1
1	D	372	LYS	2.1
1	A	51	ASP	2.1
1	C	20	SER	2.1
1	C	109	PRO	2.1
1	D	230	PHE	2.0
1	D	368	VAL	2.0
1	D	391	VAL	2.0
1	F	26	VAL	2.0
1	D	233	LEU	2.0
1	B	442	GLY	2.0
1	F	442	GLY	2.0
1	C	88	HIS	2.0
1	D	424	HIS	2.0
1	C	116	PHE	2.0
1	C	282	PHE	2.0
1	C	398	ARG	2.0
1	D	141	VAL	2.0
1	D	428	VAL	2.0
1	F	50	ARG	2.0
1	C	301	GLU	2.0
1	D	96	LEU	2.0
1	D	201	LEU	2.0
1	E	442	GLY	2.0
1	B	51	ASP	2.0
1	D	51	ASP	2.0
1	D	344	ASP	2.0
1	B	378	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

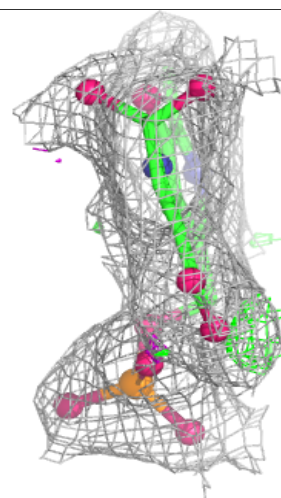
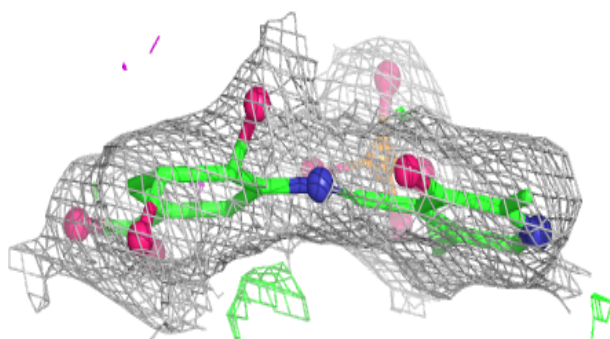
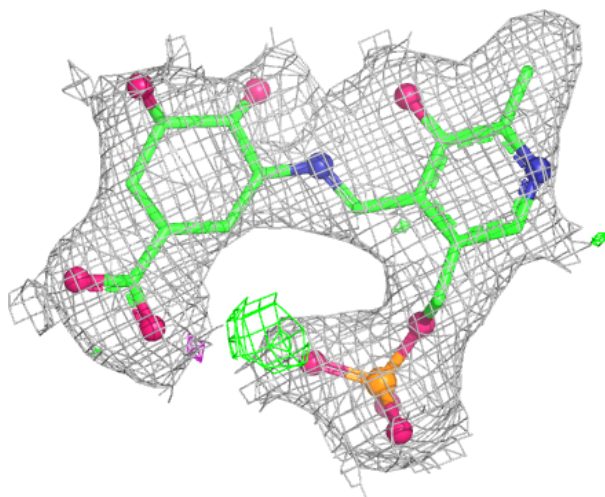
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	C	501	16/16	0.90	0.12	19,24,26,28	0
2	PLP	D	501	16/16	0.94	0.10	19,22,27,27	0
3	P3B	E	501	27/27	0.95	0.09	20,25,42,50	0
3	P3B	B	501	27/27	0.96	0.09	13,16,35,40	0
2	PLP	A	501	16/16	0.97	0.07	15,19,23,26	0
2	PLP	F	501	16/16	0.97	0.07	20,26,27,32	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.

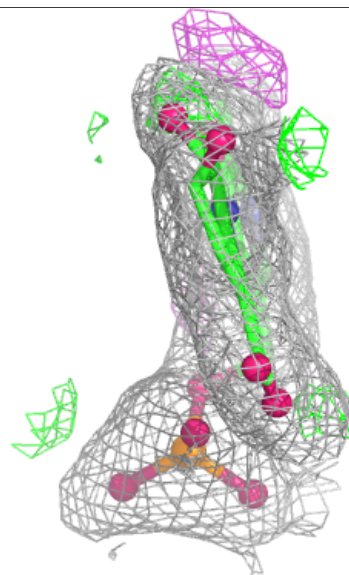
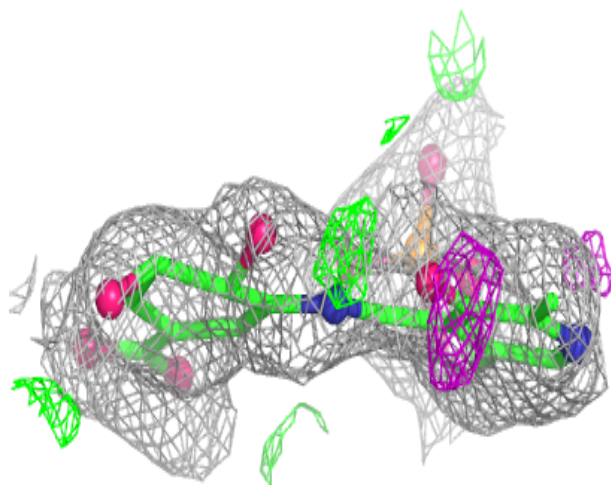
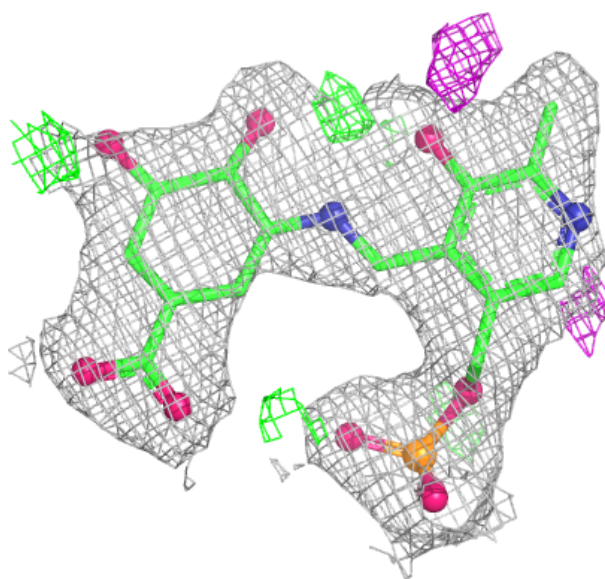
Electron density around P3B E 501:

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



Electron density around P3B 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.