Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 09:21 PM JST

PDB ID	:	4ZM4
Title	:	Complex structure of PctV K276R mutant with PMP and 3-dehydroshkimate
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 (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:

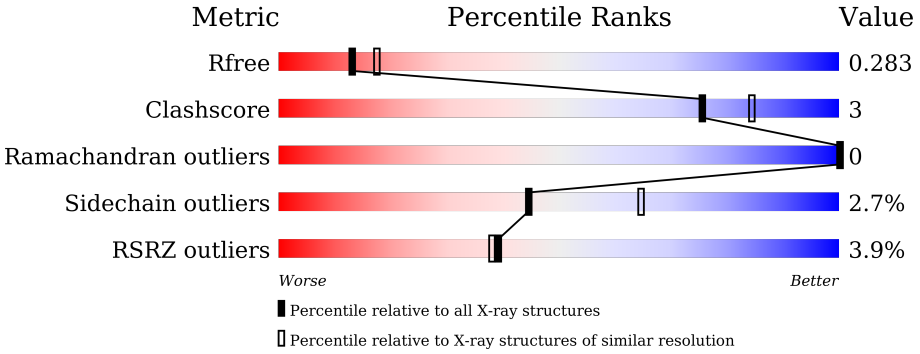
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	.% 85% 7% • 6%
1	B	447	2% 88% 6% • 5%
1	C	447	3% 86% 6% • 7%
1	D	447	12% 78% 7% • 13%
1	E	447	2% 87% 7% • 5%
1	F	447	2% 87% 6% 6%

2 Entry composition (i)

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

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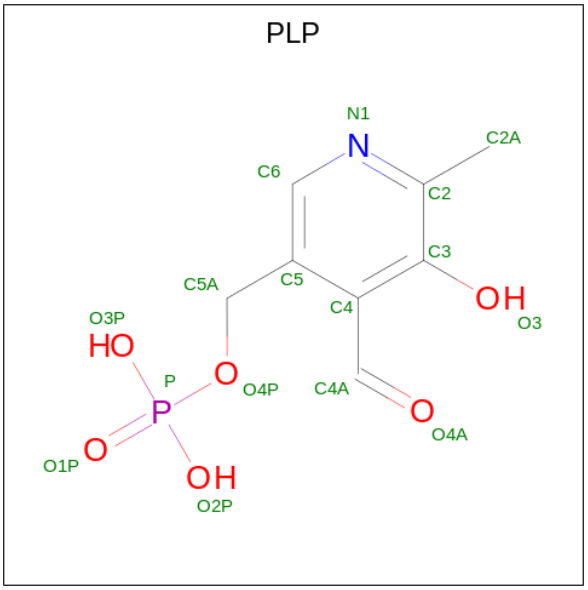
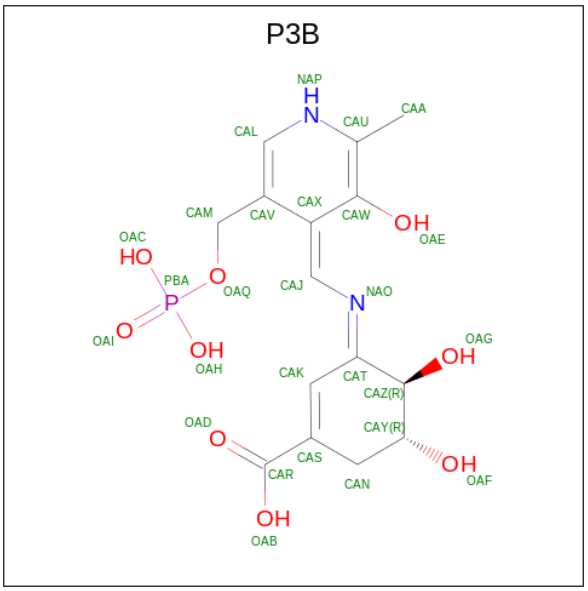
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP A8R0K5
E	0	HIS	-	expression tag	UNP A8R0K5
E	276	ARG	LYS	engineered mutation	UNP A8R0K5
F	-2	GLY	-	expression tag	UNP A8R0K5
F	-1	SER	-	expression tag	UNP A8R0K5
F	0	HIS	-	expression tag	UNP A8R0K5
F	276	ARG	LYS	engineered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

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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-[(phosphonooxy) methyl]pyridin-4(1H)-ylidene}methyl]imino}cyclohex-1-ene-1-carboxylic acid (three-letter code: P3B) (formula: $C_{15}H_{19}N_2O_9P$).



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

- Molecule 4 is water.

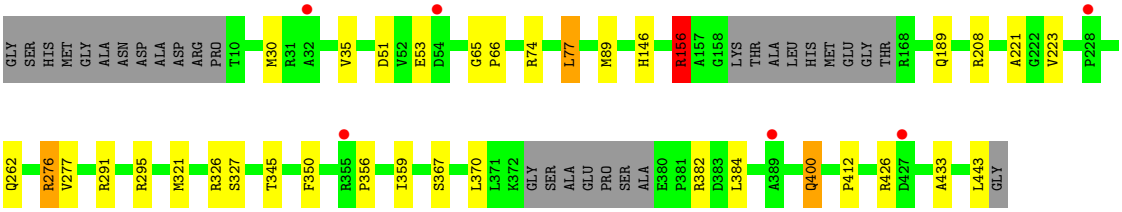
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	156	Total	O	0	0
			156	156		
4	C	117	Total	O	0	0
			117	117		
4	D	112	Total	O	0	0
			112	112		
4	E	150	Total	O	0	0
			150	150		
4	F	92	Total	O	0	0
			92	92		

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.

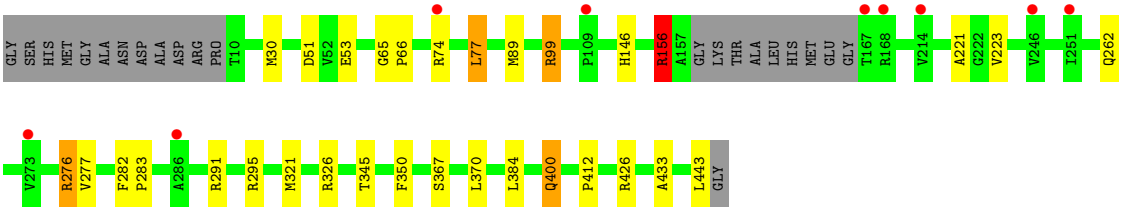
- Molecule 1: Aminotransferase

Chain A:



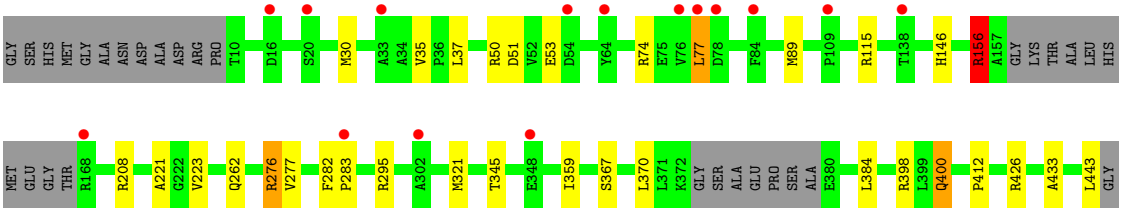
- Molecule 1: Aminotransferase

Chain B:



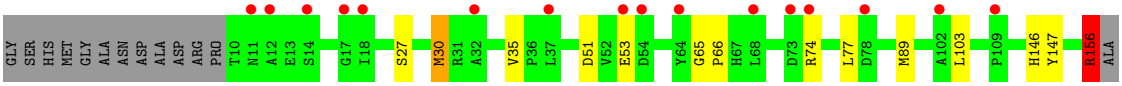
- Molecule 1: Aminotransferase

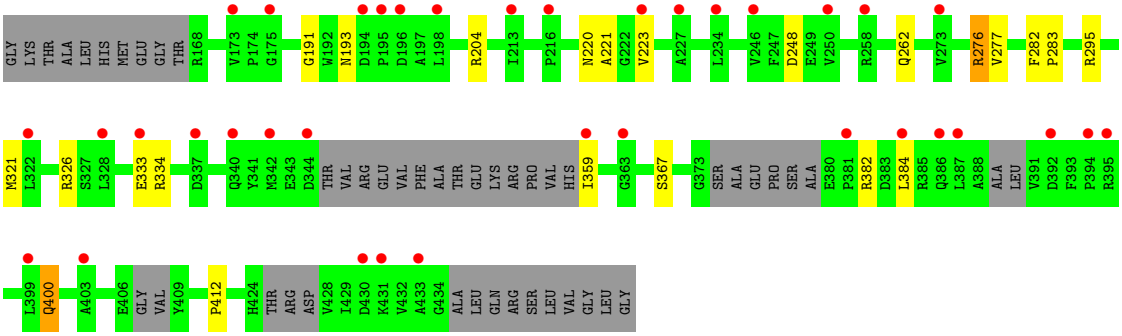
Chain C:



- Molecule 1: Aminotransferase

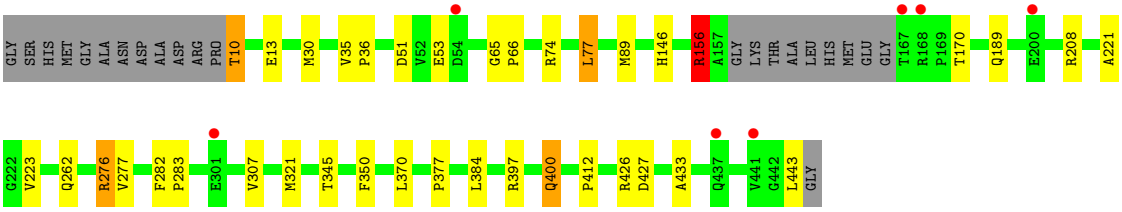
Chain D:





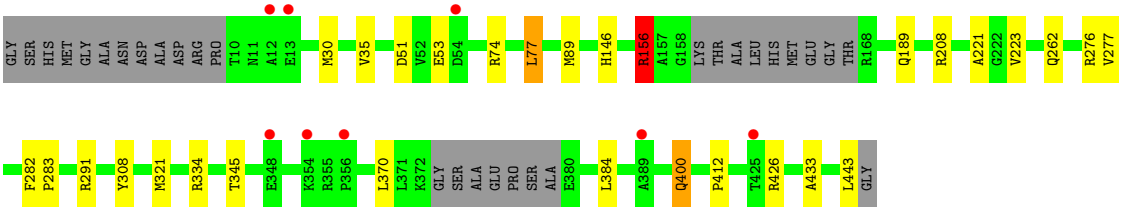
- Molecule 1: Aminotransferase

Chain E:



- Molecule 1: Aminotransferase

Chain F:



4 Data and refinement statistics (i)

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 29.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.98-2.40) 91.6 (29.84-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.39Å)	Xtriage
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 (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19717	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage'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.*

[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 (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	0.61	0/3224	0.77	7/4374 (0.2%)
1	B	0.58	0/3271	0.77	6/4441 (0.1%)
1	C	0.58	0/3220	0.74	4/4369 (0.1%)
1	D	0.63	0/2979	0.80	6/4035 (0.1%)
1	E	0.55	0/3271	0.74	3/4441 (0.1%)
1	F	0.52	0/3224	0.73	3/4374 (0.1%)
All	All	0.58	0/19189	0.76	29/26034 (0.1%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	334	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	D	156	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	B	156	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	C	156	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	326	ARG	CG-CD-NE	6.80	126.07	111.80
1	A	276	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	326	ARG	CG-CD-NE	6.50	125.44	111.80
1	B	276	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	D	276	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	334	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	276	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	F	208	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	276	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	B	276	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	291	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	E	208	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	367	SER	N-CA-CB	5.51	118.77	110.50
1	D	276	ARG	NE-CZ-NH1	5.49	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	276	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	276	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	382	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	208	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	99	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	208	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	F	156	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	156	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	156	ARG	CG-CD-NE	5.23	122.79	111.80
1	D	74	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	291	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3164	0	3179	21	0
1	B	3209	0	3220	16	0
1	C	3160	0	3176	18	0
1	D	2926	0	2922	27	0
1	E	3209	0	3220	20	0
1	F	3164	0	3179	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19717	0	18960	117	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 (117) 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
1:B:276:ARG:HH22	3:B:501:P3B:CAJ	2.04	0.70
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:A:35:VAL:HG13	1:A:35:VAL:O	2.00	0.62
1:F:400:GLN:HG2	1:F:412:PRO:HA	1.82	0.62
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:D:35:VAL:HG13	1:D:35:VAL:O	2.02	0.60
1:E:35:VAL:HG13	1:E:35:VAL:O	2.02	0.60
1:A:221:ALA:HB1	1:A:384:LEU:HD13	1.85	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:146:HIS:O	1:A:156:ARG:NH2	2.43	0.51
1:B:400:GLN:HG2	1:B:412:PRO:CA	2.40	0.51
1:F:74:ARG:HG2	1:F:77:LEU:HD23	1.92	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
1:C:370:LEU:HD21	1:C:443:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:223:VAL:HG12	1:D:223:VAL:O	2.20	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: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:E:276:ARG:H	1:F:308:TYR:HH	1.67	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%)	313 (98%)	8 (2%)	47	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	326/340 (96%)	317 (97%)	9 (3%)	43	63
1	C	321/340 (94%)	312 (97%)	9 (3%)	43	63
1	D	296/340 (87%)	289 (98%)	7 (2%)	49	68
1	E	326/340 (96%)	315 (97%)	11 (3%)	37	56
1	F	321/340 (94%)	314 (98%)	7 (2%)	52	71
All	All	1911/2040 (94%)	1860 (97%)	51 (3%)	44	65

All (51) 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	262	GLN
1	A	295	ARG
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	262	GLN
1	B	291	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	262	GLN
1	C	295	ARG
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

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Mol	Chain	Res	Type
1	D	262	GLN
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	262	GLN
1	E	377	PRO
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	262	GLN
1	F	400	GLN
1	F	426	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	$\#\|Z\| > 2$
3	P3B	B	501	-	25,28,28	4.00	13 (52%)	30,41,41	2.58	13 (43%)
2	PLP	C	501	-	16,16,16	2.42	3 (18%)	20,23,23	1.55	3 (15%)
2	PLP	A	501	-	16,16,16	3.20	3 (18%)	20,23,23	1.92	5 (25%)
2	PLP	D	501	-	16,16,16	3.01	4 (25%)	20,23,23	1.79	3 (15%)
2	PLP	F	501	-	16,16,16	3.02	3 (18%)	20,23,23	1.88	6 (30%)
3	P3B	E	501	-	25,28,28	3.22	11 (44%)	30,41,41	2.57	9 (30%)

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	P3B	B	501	-	-	0/12/31/31	0/2/2/2
2	PLP	C	501	-	-	0/8/8/8	0/1/1/1
2	PLP	A	501	-	-	1/8/8/8	0/1/1/1
2	PLP	D	501	-	-	2/8/8/8	0/1/1/1
2	PLP	F	501	-	-	0/8/8/8	0/1/1/1
3	P3B	E	501	-	-	1/12/31/31	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	P3B	CAN-CAS	-9.93	1.34	1.51
3	B	501	P3B	CAM-CAV	-9.28	1.37	1.50
3	E	501	P3B	CAN-CAS	-8.72	1.36	1.51
2	F	501	PLP	C3-C2	8.17	1.49	1.40
2	A	501	PLP	C3-C2	8.13	1.49	1.40
2	D	501	PLP	C4-C5	7.73	1.51	1.42
3	B	501	P3B	CAA-CAU	-7.54	1.37	1.49
2	A	501	PLP	C4-C5	6.92	1.50	1.42
3	E	501	P3B	CAM-CAV	-6.68	1.41	1.50
2	F	501	PLP	C4-C5	6.50	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	PLP	C3-C2	6.50	1.47	1.40
2	D	501	PLP	C3-C2	6.23	1.47	1.40
2	A	501	PLP	C4-C3	6.22	1.50	1.40
3	E	501	P3B	CAA-CAU	-6.17	1.39	1.49
3	B	501	P3B	CAY-CAZ	5.97	1.58	1.52
2	F	501	PLP	C4-C3	5.75	1.49	1.40
3	B	501	P3B	OAQ-CAM	5.42	1.46	1.43
2	D	501	PLP	C4-C3	4.81	1.48	1.40
2	C	501	PLP	C4-C5	4.65	1.47	1.42
2	C	501	PLP	C4-C3	4.63	1.47	1.40
3	E	501	P3B	CAY-CAZ	4.41	1.57	1.52
3	E	501	P3B	PBA-OAI	4.05	1.63	1.50
3	B	501	P3B	CAT-NAO	3.87	1.37	1.29
3	B	501	P3B	CAW-CAU	-3.47	1.32	1.37
3	B	501	P3B	CAU-NAP	3.42	1.38	1.34
3	B	501	P3B	CAR-CAS	-3.36	1.41	1.49
3	E	501	P3B	CAT-NAO	3.32	1.36	1.29
3	B	501	P3B	OAB-CAR	-3.24	1.21	1.30
3	E	501	P3B	CAL-NAP	2.95	1.41	1.36
3	B	501	P3B	OAG-CAZ	2.84	1.47	1.42
3	E	501	P3B	CAL-CAV	2.82	1.40	1.36
3	E	501	P3B	OAB-CAR	-2.62	1.23	1.30
2	D	501	PLP	C4-C4A	2.59	1.52	1.46
3	E	501	P3B	CAK-CAS	2.46	1.41	1.34
3	E	501	P3B	CAR-CAS	-2.34	1.43	1.49
3	B	501	P3B	PBA-OAQ	2.33	1.67	1.60
3	B	501	P3B	CAL-CAV	2.25	1.39	1.36

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	501	P3B	CAN-CAY-CAZ	7.68	118.80	109.24
3	E	501	P3B	CAX-CAW-CAU	5.97	123.74	118.36
2	A	501	PLP	C3-C4-C5	-5.71	113.88	118.26
3	B	501	P3B	CAN-CAY-CAZ	5.64	116.27	109.24
2	D	501	PLP	C3-C4-C5	-5.61	113.96	118.26
2	F	501	PLP	C4-C3-C2	-4.97	117.11	120.19
3	E	501	P3B	OAB-CAR-CAS	4.77	125.59	115.49
2	C	501	PLP	C3-C4-C5	-4.53	114.78	118.26
3	B	501	P3B	CAX-CAW-CAU	4.38	122.30	118.36
3	E	501	P3B	OAB-CAR-OAD	-4.20	114.00	123.61
3	B	501	P3B	CAY-CAN-CAS	3.85	119.29	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	P3B	CAL-NAP-CAU	-3.84	121.27	124.27
3	B	501	P3B	OAG-CAZ-CAY	3.76	116.68	110.28
3	B	501	P3B	OAB-CAR-OAD	-3.76	115.01	123.61
3	E	501	P3B	CAW-CAX-CAV	-3.66	117.19	119.26
3	B	501	P3B	CAW-CAX-CAV	-3.43	117.32	119.26
3	E	501	P3B	CAL-NAP-CAU	-3.41	121.61	124.27
3	B	501	P3B	OAB-CAR-CAS	3.30	122.50	115.49
3	B	501	P3B	OAF-CAY-CAN	-3.22	102.38	109.53
3	B	501	P3B	OAC-PBA-OAQ	3.21	115.29	106.73
2	D	501	PLP	C2A-C2-C3	-3.14	117.02	120.89
3	B	501	P3B	CAA-CAU-CAW	-3.06	118.57	122.34
3	E	501	P3B	CAY-CAN-CAS	2.94	117.52	111.78
3	E	501	P3B	OAG-CAZ-CAY	2.84	115.12	110.28
2	A	501	PLP	C4-C3-C2	-2.77	118.48	120.19
2	A	501	PLP	C5A-C5-C6	-2.73	114.88	119.37
2	F	501	PLP	O3P-P-O2P	2.73	118.06	107.64
2	D	501	PLP	C2A-C2-N1	2.54	122.63	117.67
2	F	501	PLP	C6-N1-C2	2.53	123.85	119.17
2	F	501	PLP	C3-C4-C5	-2.43	116.40	118.26
2	F	501	PLP	C2A-C2-C3	2.38	123.83	120.89
2	A	501	PLP	O4A-C4A-C4	-2.36	119.77	124.91
2	A	501	PLP	O3P-P-O2P	2.30	116.43	107.64
2	C	501	PLP	C4-C3-C2	-2.29	118.77	120.19
3	E	501	P3B	CAN-CAS-CAR	-2.27	112.66	116.91
3	B	501	P3B	OAF-CAY-CAZ	2.20	113.43	109.73
2	C	501	PLP	O3-C3-C2	2.17	122.22	117.49
3	B	501	P3B	CAV-CAL-NAP	-2.12	118.27	120.97
2	F	501	PLP	O3-C3-C2	2.11	122.08	117.49

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

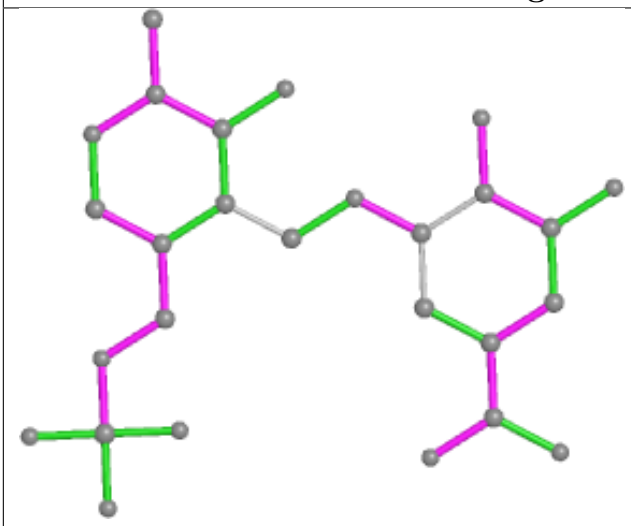
There are no ring outliers.

6 monomers are involved in 11 short contacts:

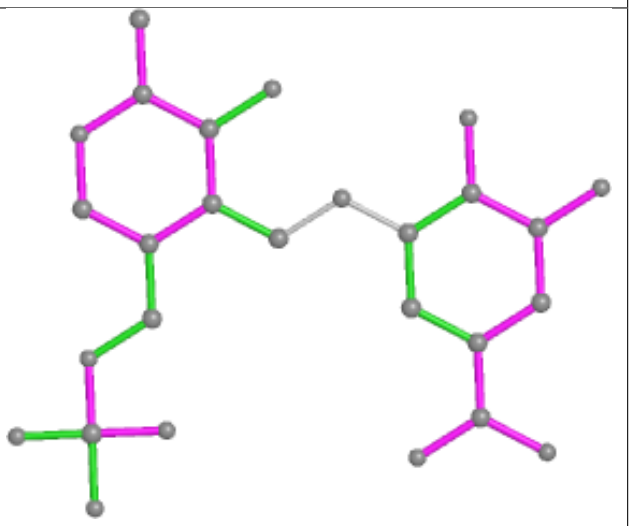
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	P3B	1	0
2	C	501	PLP	1	0
2	A	501	PLP	2	0
2	D	501	PLP	3	0
2	F	501	PLP	2	0
3	E	501	P3B	2	0

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 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.

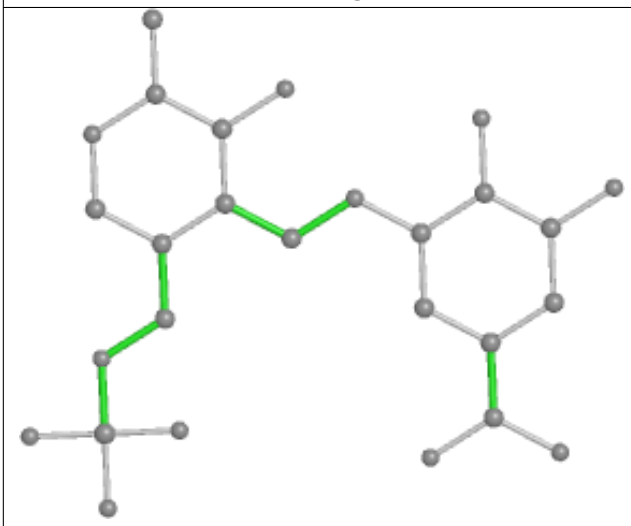
Ligand P3B B 501



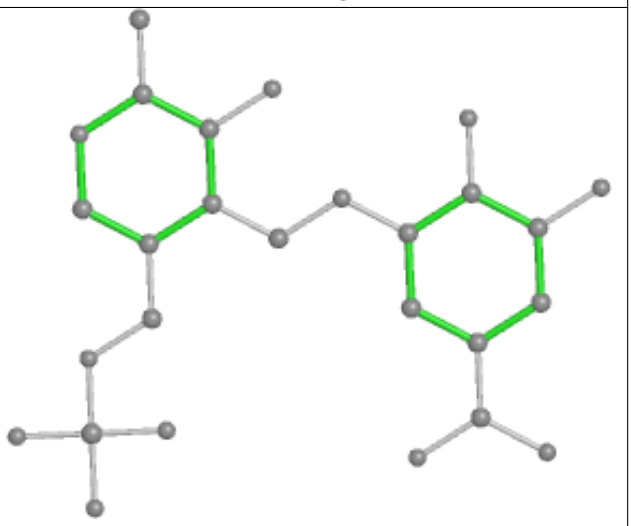
Bond lengths



Bond angles

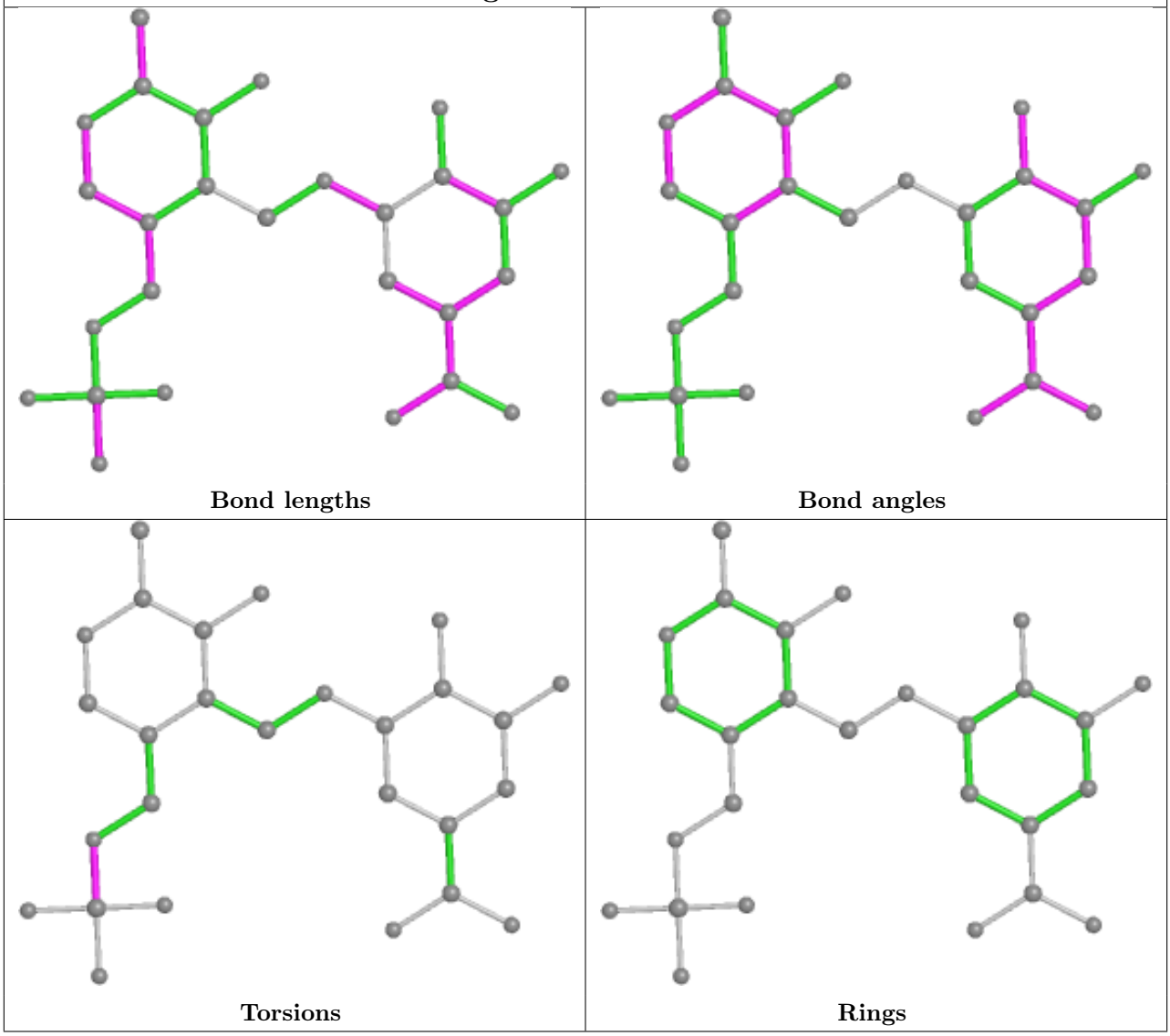


Torsions



Rings

Ligand P3B E 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.02	6 (1%)	75	73	13, 25, 42, 67	0
1	B	425/447 (95%)	-0.08	9 (2%)	63	61	13, 24, 41, 59	0
1	C	417/447 (93%)	0.31	15 (3%)	42	42	19, 31, 49, 64	0
1	D	387/447 (86%)	0.94	52 (13%)	3	2	18, 35, 50, 76	0
1	E	425/447 (95%)	0.01	7 (1%)	72	70	17, 29, 45, 64	0
1	F	418/447 (93%)	-0.02	8 (1%)	66	64	18, 31, 50, 72	0
All	All	2490/2682 (92%)	0.18	97 (3%)	39	38	13, 29, 48, 76	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	109	PRO	6.3
1	D	430	ASP	4.9
1	F	354	LYS	4.4
1	D	328	LEU	4.1
1	C	302	ALA	4.1
1	D	340	GLN	4.0
1	D	73	ASP	3.9
1	E	441	VAL	3.8
1	D	394	PRO	3.7
1	D	18	ILE	3.7
1	D	337	ASP	3.7
1	D	258	ARG	3.6
1	D	359	ILE	3.5
1	D	68	LEU	3.3
1	D	74	ARG	3.2
1	D	173	VAL	3.2
1	D	78	ASP	3.2
1	D	250	VAL	3.1
1	D	399	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	196	ASP	3.1
1	C	348	GLU	3.1
1	D	11	ASN	3.1
1	D	32	ALA	3.1
1	D	195	PRO	3.0
1	D	381	PRO	3.0
1	D	342	MET	3.0
1	A	355	ARG	2.9
1	B	273	VAL	2.9
1	C	283	PRO	2.8
1	C	138	THR	2.8
1	D	403	ALA	2.8
1	C	16	ASP	2.8
1	D	37	LEU	2.7
1	C	54	ASP	2.7
1	A	228	PRO	2.7
1	A	32	ALA	2.7
1	A	389	ALA	2.7
1	D	12	ALA	2.7
1	F	348	GLU	2.7
1	D	102	ALA	2.7
1	D	273	VAL	2.7
1	C	64	TYR	2.7
1	D	392	ASP	2.7
1	D	433	ALA	2.6
1	B	167	THR	2.6
1	E	167	THR	2.6
1	B	74	ARG	2.6
1	D	246	VAL	2.5
1	C	33	ALA	2.5
1	D	17	GLY	2.5
1	D	227	ALA	2.5
1	E	54	ASP	2.5
1	D	14	SER	2.5
1	B	286	ALA	2.4
1	D	54	ASP	2.4
1	F	12	ALA	2.4
1	C	77	LEU	2.4
1	E	301	GLU	2.4
1	D	216	PRO	2.4
1	D	53	GLU	2.4
1	D	194	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	200	GLU	2.3
1	D	431	LYS	2.3
1	C	78	ASP	2.3
1	D	223	VAL	2.3
1	D	213	ILE	2.3
1	A	54	ASP	2.3
1	E	168	ARG	2.3
1	D	322	LEU	2.3
1	C	109	PRO	2.2
1	D	363	GLY	2.2
1	B	168	ARG	2.2
1	C	76	VAL	2.2
1	E	437	GLN	2.2
1	C	20	SER	2.2
1	D	386	GLN	2.2
1	D	344	ASP	2.2
1	B	214	VAL	2.1
1	F	54	ASP	2.1
1	D	175	GLY	2.1
1	F	389	ALA	2.1
1	F	356	PRO	2.1
1	A	427	ASP	2.1
1	D	333	GLU	2.1
1	C	84	PHE	2.1
1	F	13	GLU	2.1
1	F	425	THR	2.1
1	D	198	LEU	2.0
1	D	234	LEU	2.0
1	C	168	ARG	2.0
1	D	64	TYR	2.0
1	D	387	LEU	2.0
1	D	395	ARG	2.0
1	B	109	PRO	2.0
1	B	246	VAL	2.0
1	B	251	ILE	2.0
1	D	384	LEU	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)

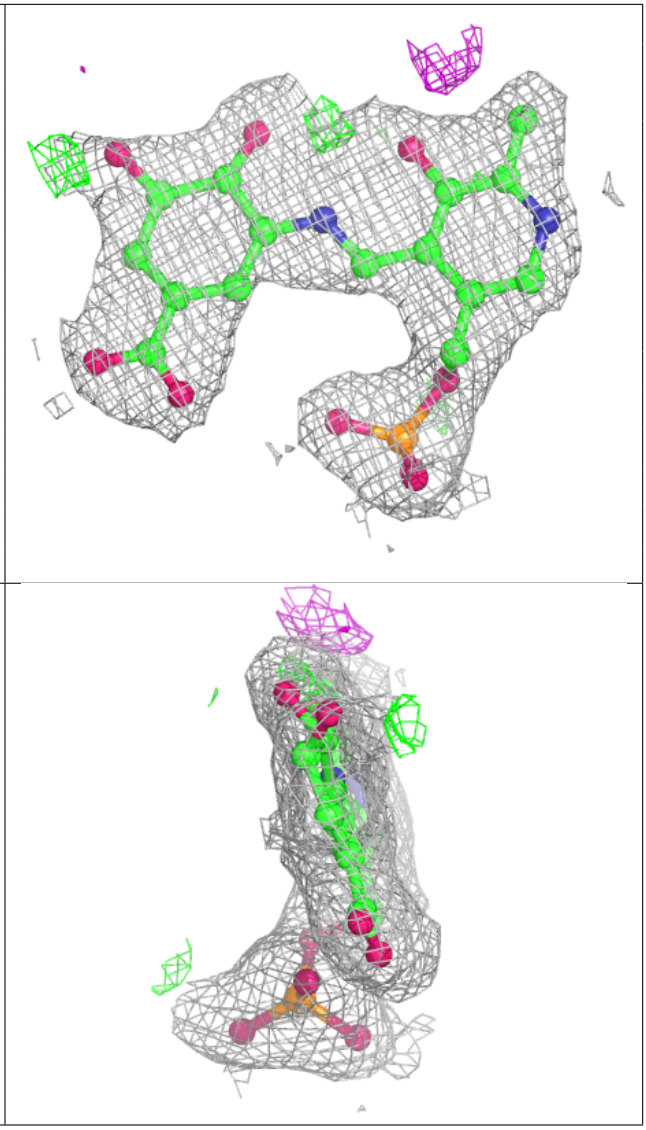
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLP	C	501	16/16	0.91	0.16	19,24,26,28	0
2	PLP	D	501	16/16	0.95	0.16	19,22,27,27	0
3	P3B	B	501	27/27	0.96	0.16	13,16,35,40	0
3	P3B	E	501	27/27	0.96	0.16	20,25,42,50	0
2	PLP	A	501	16/16	0.97	0.15	15,19,23,26	0
2	PLP	F	501	16/16	0.97	0.17	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.

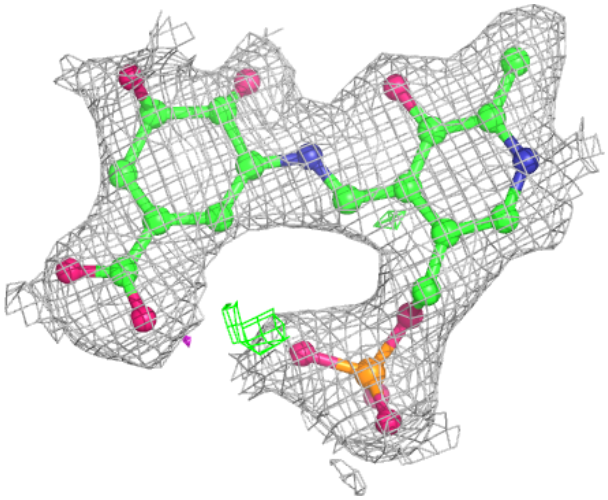
Electron density around P3B B 501:

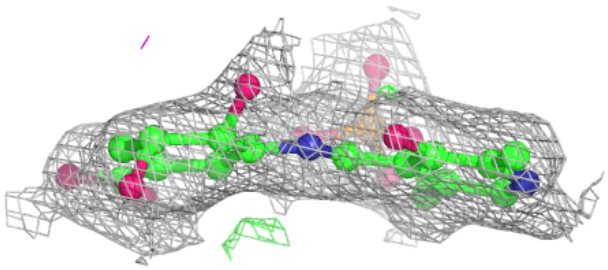
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

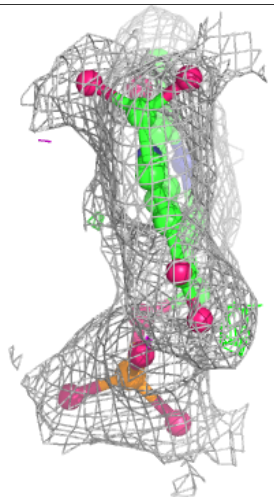


Electron density around P3B E 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.