



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 08:56 am BST

PDB ID : 1I43
Title : CYSTATHIONINE GAMMA-SYNTHASE IN COMPLEX WITH THE INHIBITOR PPCA
Authors : Steegborn, C.; Laber, B.; Messerschmidt, A.; Huber, R.; Clausen, T.
Deposited on : 2001-02-19
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

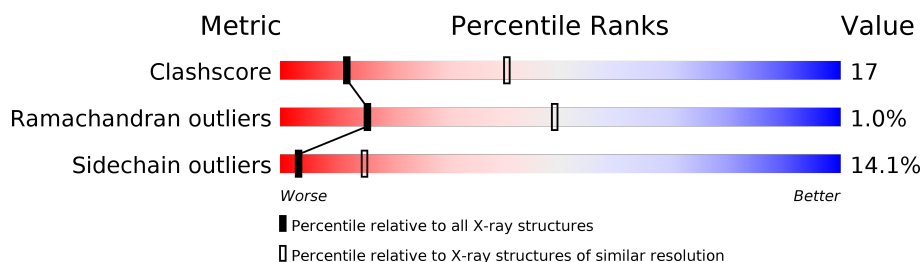
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)





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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	
1	B	445	
1	C	445	
1	D	445	
1	E	445	
1	F	445	
1	G	445	
1	H	445	

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Mol	Chain	Length	Quality of chain
1	I	445	
1	J	445	
1	K	445	
1	L	445	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	C	500	-	X	-	-
2	PLP	F	500	-	X	-	-
2	PLP	H	500	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36624 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 CYSTATHIONINE GAMMA-SYNTHASE.

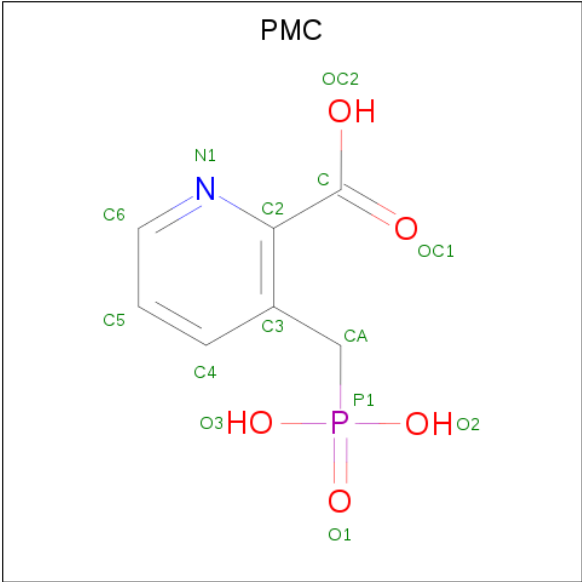
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	B	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	C	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	D	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	E	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	F	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	G	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	H	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	I	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	J	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	K	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			
1	L	396	Total	C	N	O	S	0	0	0
			3023	1928	513	566	16			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 3-(PHOSPHONOMETHYL)PYRIDINE-2-CARBOXYLIC ACID (three-letter code: PMC) (formula: C₇H₈NO₅P).



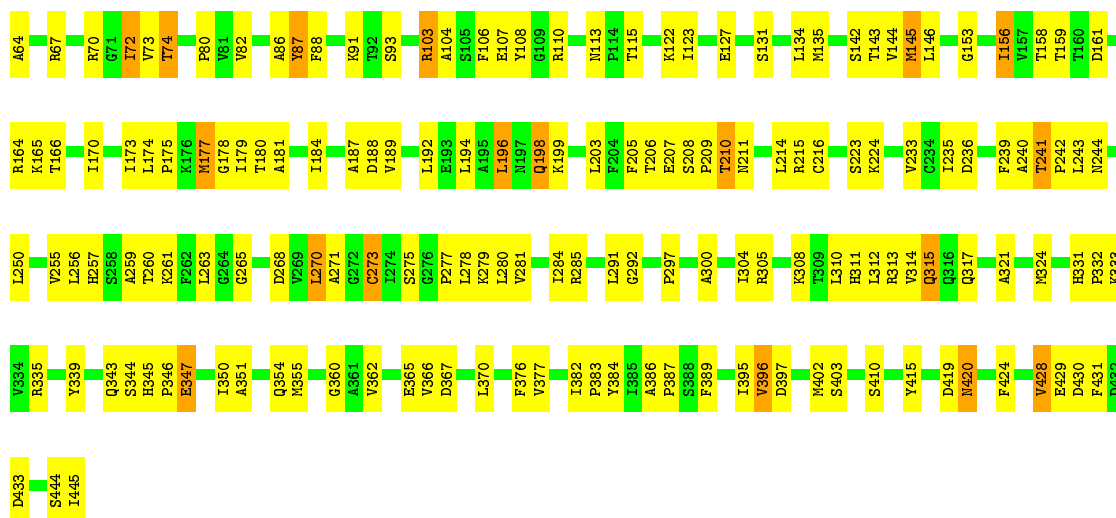
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	I	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	J	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	K	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
3	L	1	Total	C	N	O	P	0	0
			14	7	1	5	1		



- Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE

- Molecule 1: CYSTATHIONINE GAMMA-SYNTHASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	309.60Å 170.10Å 162.10Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.236 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36624	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

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: PLP, PMC

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	0.30	0/3082	0.51	0/4179
1	B	0.30	0/3082	0.51	0/4179
1	C	0.30	0/3082	0.51	0/4179
1	D	0.30	0/3082	0.51	0/4179
1	E	0.30	0/3082	0.51	0/4179
1	F	0.29	0/3082	0.50	0/4179
1	G	0.30	0/3082	0.50	0/4179
1	H	0.30	0/3082	0.50	0/4179
1	I	0.30	0/3082	0.51	0/4179
1	J	0.30	0/3082	0.51	0/4179
1	K	0.30	0/3082	0.51	0/4179
1	L	0.30	0/3082	0.50	0/4179
All	All	0.30	0/36984	0.51	0/50148

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 [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	3023	0	3052	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3023	0	3052	114	0
1	C	3023	0	3052	106	0
1	D	3023	0	3052	102	0
1	E	3023	0	3052	127	0
1	F	3023	0	3052	108	0
1	G	3023	0	3052	111	0
1	H	3023	0	3052	119	0
1	I	3023	0	3052	120	0
1	J	3023	0	3052	109	0
1	K	3023	0	3052	115	0
1	L	3023	0	3052	120	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
2	E	15	0	7	0	0
2	F	15	0	6	1	0
2	G	15	0	7	0	0
2	H	15	0	6	1	0
2	I	15	0	6	0	0
2	J	15	0	6	0	0
2	K	15	0	6	0	0
2	L	15	0	7	0	0
3	A	14	0	5	0	0
3	B	14	0	5	0	0
3	C	14	0	5	0	0
3	D	14	0	5	1	0
3	E	14	0	5	1	0
3	F	14	0	5	0	0
3	G	14	0	5	0	0
3	H	14	0	5	0	0
3	I	14	0	5	0	0
3	J	14	0	5	0	0
3	K	14	0	5	1	0
3	L	14	0	5	1	0
All	All	36624	0	36759	1268	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 17.

The worst 5 of 1268 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:I:376:PHE:HB2	1:I:445:ILE:HD11	1.21	1.12
1:C:376:PHE:HB2	1:C:445:ILE:HD11	1.40	1.03
1:F:241:THR:HG22	1:F:243:LEU:H	1.32	0.95
1:A:241:THR:HG22	1:A:243:LEU:H	1.32	0.94
1:K:241:THR:HG22	1:K:243:LEU:H	1.30	0.93

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	394/445 (88%)	355 (90%)	37 (9%)	2 (0%)	29	64
1	B	394/445 (88%)	364 (92%)	25 (6%)	5 (1%)	12	42
1	C	394/445 (88%)	353 (90%)	37 (9%)	4 (1%)	15	49
1	D	394/445 (88%)	363 (92%)	27 (7%)	4 (1%)	15	49
1	E	394/445 (88%)	354 (90%)	35 (9%)	5 (1%)	12	42
1	F	394/445 (88%)	356 (90%)	35 (9%)	3 (1%)	19	54
1	G	394/445 (88%)	357 (91%)	33 (8%)	4 (1%)	15	49
1	H	394/445 (88%)	363 (92%)	28 (7%)	3 (1%)	19	54
1	I	394/445 (88%)	354 (90%)	37 (9%)	3 (1%)	19	54
1	J	394/445 (88%)	354 (90%)	37 (9%)	3 (1%)	19	54
1	K	394/445 (88%)	359 (91%)	30 (8%)	5 (1%)	12	42
1	L	394/445 (88%)	356 (90%)	34 (9%)	4 (1%)	15	49
All	All	4728/5340 (88%)	4288 (91%)	395 (8%)	45 (1%)	15	49

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	ASP

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Mol	Chain	Res	Type
1	C	188	ASP
1	D	188	ASP
1	E	188	ASP
1	F	188	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	327/364 (90%)	278 (85%)	49 (15%)	3	12
1	B	327/364 (90%)	278 (85%)	49 (15%)	3	12
1	C	327/364 (90%)	284 (87%)	43 (13%)	4	17
1	D	327/364 (90%)	282 (86%)	45 (14%)	3	16
1	E	327/364 (90%)	281 (86%)	46 (14%)	3	15
1	F	327/364 (90%)	279 (85%)	48 (15%)	3	13
1	G	327/364 (90%)	281 (86%)	46 (14%)	3	15
1	H	327/364 (90%)	279 (85%)	48 (15%)	3	13
1	I	327/364 (90%)	281 (86%)	46 (14%)	3	15
1	J	327/364 (90%)	284 (87%)	43 (13%)	4	17
1	K	327/364 (90%)	281 (86%)	46 (14%)	3	15
1	L	327/364 (90%)	283 (86%)	44 (14%)	4	16
All	All	3924/4368 (90%)	3371 (86%)	553 (14%)	3	15

5 of 553 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	196	LEU
1	G	285	ARG
1	L	74	THR
1	F	245	GLN
1	G	72	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	63	HIS
1	G	343	GLN
1	K	420	ASN
1	F	343	GLN
1	G	63	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

24 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	G	500	1	15,15,16	3.74	6 (40%)	20,22,23	2.38	9 (45%)
3	PMC	A	600	-	11,14,14	2.22	5 (45%)	13,20,20	1.67	2 (15%)
3	PMC	C	602	-	11,14,14	2.21	5 (45%)	13,20,20	1.71	2 (15%)
2	PLP	K	500	1	15,15,16	4.24	4 (26%)	20,22,23	2.63	10 (50%)
2	PLP	E	500	1	15,15,16	3.65	5 (33%)	20,22,23	2.38	9 (45%)
3	PMC	E	604	-	11,14,14	2.17	4 (36%)	13,20,20	1.75	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PMC	G	606	-	11,14,14	1.93	5 (45%)	13,20,20	1.54	2 (15%)
2	PLP	L	500	1	15,15,16	3.36	5 (33%)	20,22,23	2.40	8 (40%)
3	PMC	K	610	-	11,14,14	2.13	5 (45%)	13,20,20	1.69	2 (15%)
3	PMC	B	601	-	11,14,14	2.10	6 (54%)	13,20,20	1.62	2 (15%)
2	PLP	I	500	1	15,15,16	4.00	5 (33%)	20,22,23	2.35	9 (45%)
2	PLP	D	500	1	15,15,16	4.51	5 (33%)	20,22,23	2.64	10 (50%)
3	PMC	D	603	-	11,14,14	1.96	5 (45%)	13,20,20	1.51	2 (15%)
2	PLP	J	500	1	15,15,16	3.71	5 (33%)	20,22,23	2.30	8 (40%)
3	PMC	L	611	-	11,14,14	1.98	5 (45%)	13,20,20	1.56	2 (15%)
3	PMC	I	608	-	11,14,14	2.01	4 (36%)	13,20,20	1.59	2 (15%)
3	PMC	F	605	-	11,14,14	2.11	4 (36%)	13,20,20	1.67	2 (15%)
2	PLP	A	500	1	15,15,16	3.98	5 (33%)	20,22,23	2.48	10 (50%)
2	PLP	C	500	1	15,15,16	3.73	5 (33%)	20,22,23	2.47	11 (55%)
2	PLP	H	500	1	15,15,16	4.35	7 (46%)	20,22,23	2.49	11 (55%)
2	PLP	F	500	1	15,15,16	4.27	5 (33%)	20,22,23	2.43	11 (55%)
2	PLP	B	500	1	15,15,16	4.37	4 (26%)	20,22,23	2.53	10 (50%)
3	PMC	J	609	-	11,14,14	1.97	5 (45%)	13,20,20	1.52	2 (15%)
3	PMC	H	607	-	11,14,14	2.05	6 (54%)	13,20,20	1.66	2 (15%)

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	G	500	1	-	2/6/6/8	0/1/1/1
3	PMC	A	600	-	-	3/5/9/9	0/1/1/1
3	PMC	C	602	-	-	3/5/9/9	0/1/1/1
2	PLP	K	500	1	-	2/6/6/8	0/1/1/1
2	PLP	E	500	1	-	2/6/6/8	0/1/1/1
3	PMC	E	604	-	-	3/5/9/9	0/1/1/1
3	PMC	G	606	-	-	3/5/9/9	0/1/1/1
2	PLP	L	500	1	-	2/6/6/8	0/1/1/1
3	PMC	K	610	-	-	3/5/9/9	0/1/1/1
3	PMC	B	601	-	-	3/5/9/9	0/1/1/1
2	PLP	I	500	1	-	2/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	D	500	1	-	2/6/6/8	0/1/1/1
3	PMC	D	603	-	-	4/5/9/9	0/1/1/1
2	PLP	J	500	1	-	2/6/6/8	0/1/1/1
3	PMC	L	611	-	-	3/5/9/9	0/1/1/1
3	PMC	I	608	-	-	3/5/9/9	0/1/1/1
3	PMC	F	605	-	-	3/5/9/9	0/1/1/1
2	PLP	A	500	1	-	2/6/6/8	0/1/1/1
2	PLP	C	500	1	-	2/6/6/8	0/1/1/1
2	PLP	H	500	1	-	2/6/6/8	0/1/1/1
2	PLP	F	500	1	-	2/6/6/8	0/1/1/1
2	PLP	B	500	1	-	2/6/6/8	0/1/1/1
3	PMC	J	609	-	-	3/5/9/9	0/1/1/1
3	PMC	H	607	-	-	3/5/9/9	0/1/1/1

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	PLP	C5-C4	13.96	1.55	1.40
2	D	500	PLP	C5-C4	13.59	1.55	1.40
2	F	500	PLP	C5-C4	13.49	1.55	1.40
2	I	500	PLP	C5-C4	13.45	1.55	1.40
2	H	500	PLP	C5-C4	13.31	1.55	1.40

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	500	PLP	C2A-C2-C3	5.93	128.22	120.89
2	L	500	PLP	C2A-C2-C3	5.84	128.10	120.89
2	E	500	PLP	C2A-C2-C3	5.82	128.08	120.89
2	F	500	PLP	C2A-C2-C3	5.81	128.07	120.89
2	A	500	PLP	C2A-C2-C3	5.81	128.06	120.89

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	500	PLP	C4-C5-C5A-O4P
2	G	500	PLP	C6-C5-C5A-O4P

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Mol	Chain	Res	Type	Atoms
3	A	600	PMC	C3-CA-P1-O3
3	A	600	PMC	C3-CA-P1-O2
3	A	600	PMC	C3-CA-P1-O1

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	604	PMC	1	0
3	K	610	PMC	1	0
3	D	603	PMC	1	0
3	L	611	PMC	1	0
2	H	500	PLP	1	0
2	F	500	PLP	1	0
2	B	500	PLP	1	0

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.