



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 02:55 AM GMT

PDB ID : 4L0O
Title : Structure determination of cystathionine gamma-synthase from *Helicobacter pylori*
Authors : Tarique, K.F.; Rehman, S.A.A.; Gourinath, S.
Deposited on : 2013-05-31
Resolution : 2.76 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

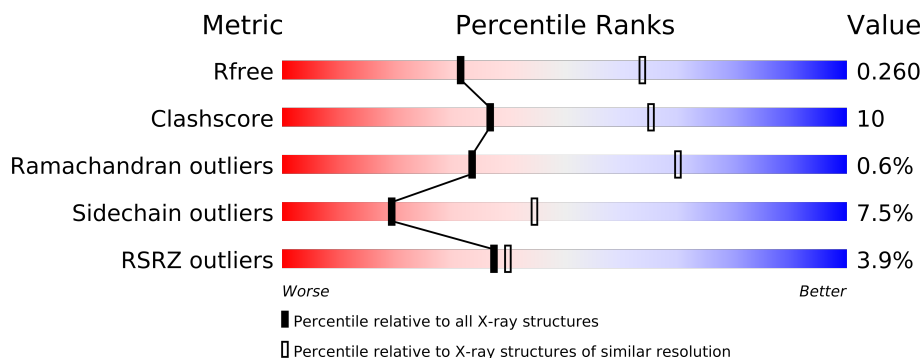
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.76 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}	66092	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	388	
1	C	388	
1	E	388	
1	G	388	
1	H	388	
1	K	388	
1	M	388	
1	O	388	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22365 atoms, of which 0 are hydrogen and 0 are deuterium.

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	H	373	Total	C	N	O	S	0	0	0
			2828	1801	480	537	10			
1	A	363	Total	C	N	O	S	0	0	0
			2756	1760	464	523	9			
1	C	366	Total	C	N	O	S	0	0	0
			2778	1771	468	530	9			
1	E	364	Total	C	N	O	S	0	0	0
			2728	1741	459	519	9			
1	G	365	Total	C	N	O	S	0	0	0
			2762	1760	464	529	9			
1	K	378	Total	C	N	O	S	0	0	0
			2865	1823	488	544	10			
1	M	365	Total	C	N	O	S	0	0	0
			2765	1763	465	528	9			
1	O	367	Total	C	N	O	S	0	0	0
			2773	1770	464	530	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	381	LEU	-	EXPRESSION TAG	UNP P56069
H	382	GLU	-	EXPRESSION TAG	UNP P56069
H	383	HIS	-	EXPRESSION TAG	UNP P56069
H	384	HIS	-	EXPRESSION TAG	UNP P56069
H	385	HIS	-	EXPRESSION TAG	UNP P56069
H	386	HIS	-	EXPRESSION TAG	UNP P56069
H	387	HIS	-	EXPRESSION TAG	UNP P56069
H	388	HIS	-	EXPRESSION TAG	UNP P56069
A	381	LEU	-	EXPRESSION TAG	UNP P56069
A	382	GLU	-	EXPRESSION TAG	UNP P56069
A	383	HIS	-	EXPRESSION TAG	UNP P56069
A	384	HIS	-	EXPRESSION TAG	UNP P56069
A	385	HIS	-	EXPRESSION TAG	UNP P56069

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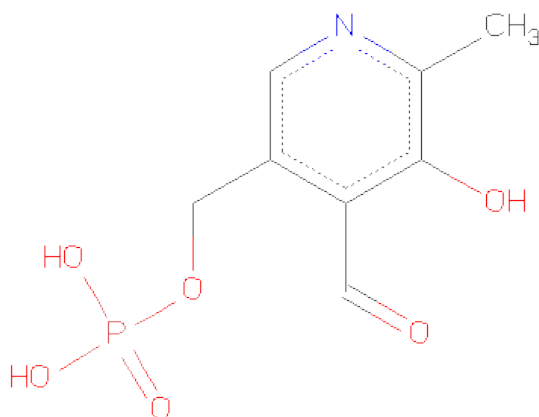
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	HIS	-	EXPRESSION TAG	UNP P56069
A	387	HIS	-	EXPRESSION TAG	UNP P56069
A	388	HIS	-	EXPRESSION TAG	UNP P56069
C	381	LEU	-	EXPRESSION TAG	UNP P56069
C	382	GLU	-	EXPRESSION TAG	UNP P56069
C	383	HIS	-	EXPRESSION TAG	UNP P56069
C	384	HIS	-	EXPRESSION TAG	UNP P56069
C	385	HIS	-	EXPRESSION TAG	UNP P56069
C	386	HIS	-	EXPRESSION TAG	UNP P56069
C	387	HIS	-	EXPRESSION TAG	UNP P56069
C	388	HIS	-	EXPRESSION TAG	UNP P56069
E	381	LEU	-	EXPRESSION TAG	UNP P56069
E	382	GLU	-	EXPRESSION TAG	UNP P56069
E	383	HIS	-	EXPRESSION TAG	UNP P56069
E	384	HIS	-	EXPRESSION TAG	UNP P56069
E	385	HIS	-	EXPRESSION TAG	UNP P56069
E	386	HIS	-	EXPRESSION TAG	UNP P56069
E	387	HIS	-	EXPRESSION TAG	UNP P56069
E	388	HIS	-	EXPRESSION TAG	UNP P56069
G	381	LEU	-	EXPRESSION TAG	UNP P56069
G	382	GLU	-	EXPRESSION TAG	UNP P56069
G	383	HIS	-	EXPRESSION TAG	UNP P56069
G	384	HIS	-	EXPRESSION TAG	UNP P56069
G	385	HIS	-	EXPRESSION TAG	UNP P56069
G	386	HIS	-	EXPRESSION TAG	UNP P56069
G	387	HIS	-	EXPRESSION TAG	UNP P56069
G	388	HIS	-	EXPRESSION TAG	UNP P56069
K	381	LEU	-	EXPRESSION TAG	UNP P56069
K	382	GLU	-	EXPRESSION TAG	UNP P56069
K	383	HIS	-	EXPRESSION TAG	UNP P56069
K	384	HIS	-	EXPRESSION TAG	UNP P56069
K	385	HIS	-	EXPRESSION TAG	UNP P56069
K	386	HIS	-	EXPRESSION TAG	UNP P56069
K	387	HIS	-	EXPRESSION TAG	UNP P56069
K	388	HIS	-	EXPRESSION TAG	UNP P56069
M	381	LEU	-	EXPRESSION TAG	UNP P56069
M	382	GLU	-	EXPRESSION TAG	UNP P56069
M	383	HIS	-	EXPRESSION TAG	UNP P56069
M	384	HIS	-	EXPRESSION TAG	UNP P56069
M	385	HIS	-	EXPRESSION TAG	UNP P56069
M	386	HIS	-	EXPRESSION TAG	UNP P56069
M	387	HIS	-	EXPRESSION TAG	UNP P56069

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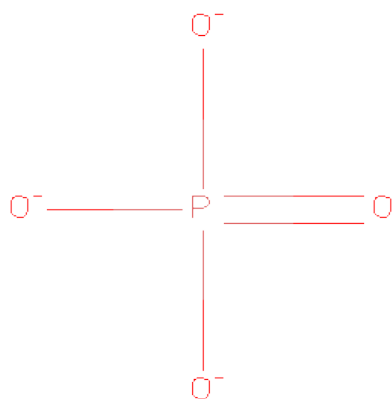
Chain	Residue	Modelled	Actual	Comment	Reference
M	388	HIS	-	EXPRESSION TAG	UNP P56069
O	381	LEU	-	EXPRESSION TAG	UNP P56069
O	382	GLU	-	EXPRESSION TAG	UNP P56069
O	383	HIS	-	EXPRESSION TAG	UNP P56069
O	384	HIS	-	EXPRESSION TAG	UNP P56069
O	385	HIS	-	EXPRESSION TAG	UNP P56069
O	386	HIS	-	EXPRESSION TAG	UNP P56069
O	387	HIS	-	EXPRESSION TAG	UNP P56069
O	388	HIS	-	EXPRESSION TAG	UNP P56069

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

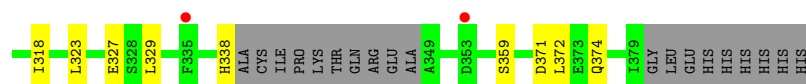


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	A	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	M	1	Total	C	N	O	P	0	0
			15	7	1	6	1		
2	O	1	Total	C	N	O	P	0	0
			15	7	1	6	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

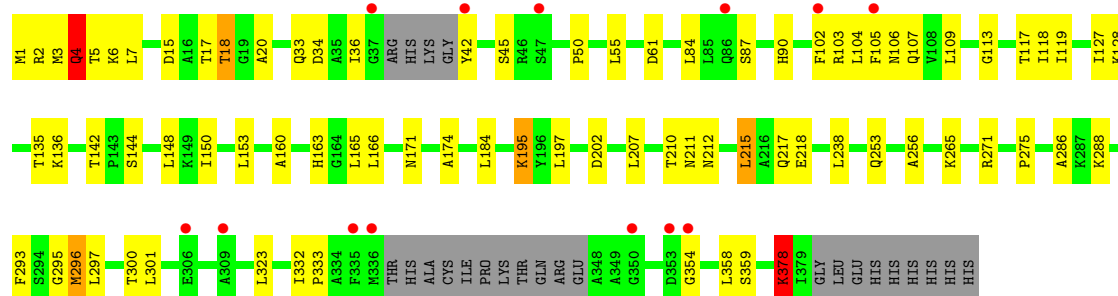


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	P	0	0
			5	4	1		



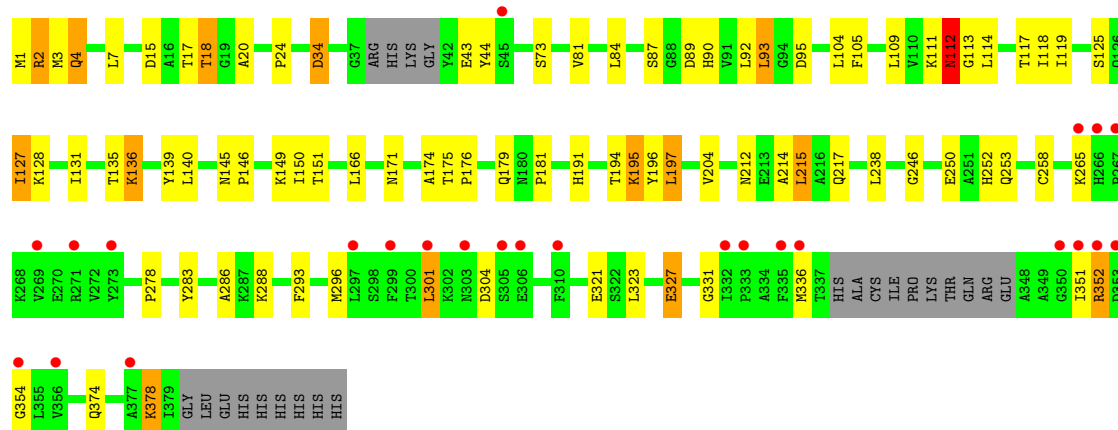
• Molecule 1: Cystathionine gamma-synthase

Chain E:



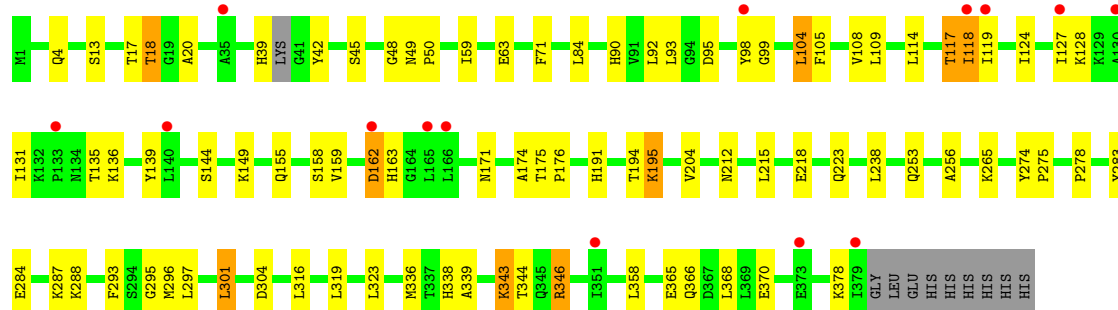
• Molecule 1: Cystathionine gamma-synthase

Chain G:



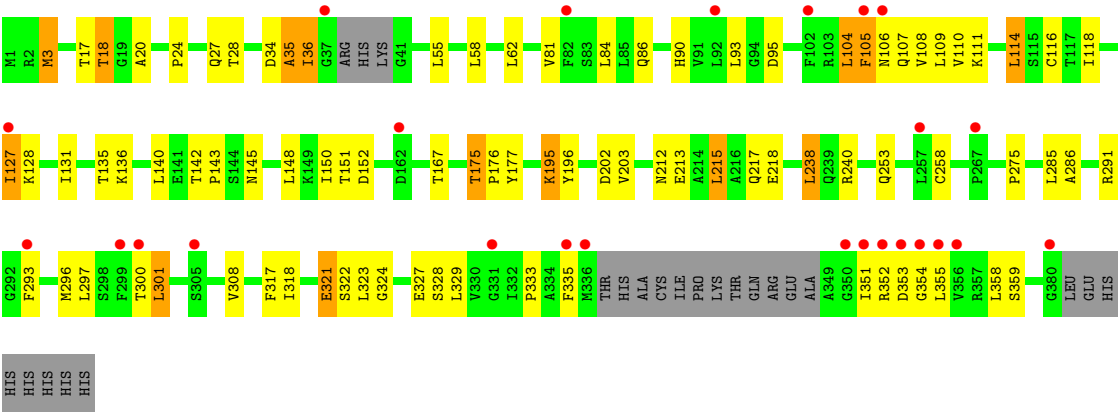
• Molecule 1: Cystathionine gamma-synthase

Chain K:



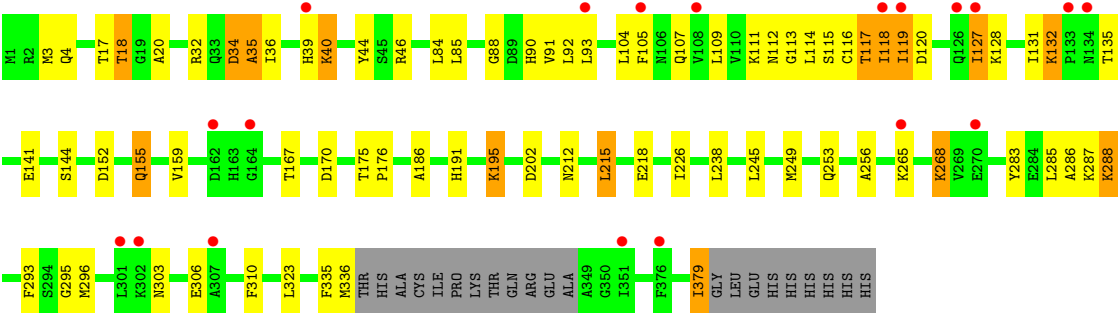
• Molecule 1: Cystathionine gamma-synthase

Chain M:



● Molecule 1: Cystathionine gamma-synthase

Chain O:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	115.81Å 174.89Å 324.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.76 48.28 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.76) 99.8 (48.28-2.76)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.234 , 0.278 0.221 , 0.260	Depositor DCC
R_{free} test set	4234 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84795 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22365	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.65	7/2808 (0.2%)	0.59	0/3804
1	C	0.57	1/2829 (0.0%)	0.57	0/3832
1	E	0.58	2/2777 (0.1%)	0.56	0/3764
1	G	0.64	4/2812 (0.1%)	0.59	0/3811
1	H	0.52	1/2881 (0.0%)	0.57	2/3904 (0.1%)
1	K	0.68	3/2919 (0.1%)	0.58	1/3954 (0.0%)
1	M	0.52	0/2815	0.55	0/3812
1	O	0.74	8/2825 (0.3%)	0.58	0/3829
All	All	0.62	26/22666 (0.1%)	0.57	3/30710 (0.0%)

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	39	HIS	C-O	11.43	1.45	1.23
1	E	378	LYS	CE-NZ	11.16	1.76	1.49
1	H	34	ASP	C-O	9.21	1.40	1.23
1	O	132	LYS	CE-NZ	9.14	1.72	1.49
1	K	338	HIS	CG-CD2	8.72	1.50	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	346	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	H	34	ASP	CA-C-O	-5.32	108.93	120.10
1	H	301	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2756	0	2762	72	0
1	C	2778	0	2775	44	0
1	E	2728	0	2708	53	0
1	G	2762	0	2748	59	0
1	H	2828	0	2824	52	0
1	K	2865	0	2858	55	0
1	M	2765	0	2764	64	0
1	O	2773	0	2762	76	0
2	A	15	0	5	4	0
2	C	15	0	5	3	0
2	E	15	0	4	1	0
2	G	15	0	6	2	0
2	H	15	0	5	3	0
2	M	15	0	5	3	0
2	O	15	0	5	0	0
3	K	5	0	0	0	0
All	All	22365	0	22236	454	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 454 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:132:LYS:CE	1:O:132:LYS:NZ	1.71	1.53
1:O:268:LYS:CE	1:O:268:LYS:NZ	1.70	1.51
1:E:378:LYS:CE	1:E:378:LYS:NZ	1.77	1.48
1:O:118:ILE:O	1:O:119:ILE:HG23	1.49	1.10
1:M:35:ALA:HB1	1:M:36:ILE:HA	1.16	1.10

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/388 (92%)	339 (94%)	17 (5%)	3 (1%)	27	63
1	C	360/388 (93%)	341 (95%)	15 (4%)	4 (1%)	21	53
1	E	358/388 (92%)	337 (94%)	20 (6%)	1 (0%)	50	83
1	G	359/388 (92%)	343 (96%)	15 (4%)	1 (0%)	50	83
1	H	369/388 (95%)	350 (95%)	18 (5%)	1 (0%)	50	83
1	K	374/388 (96%)	355 (95%)	17 (4%)	2 (0%)	38	74
1	M	359/388 (92%)	343 (96%)	14 (4%)	2 (1%)	33	70
1	O	363/388 (94%)	339 (93%)	22 (6%)	2 (1%)	33	70
All	All	2901/3104 (94%)	2747 (95%)	138 (5%)	16 (1%)	33	70

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	35	ALA
1	C	35	ALA
1	K	99	GLY
1	M	353	ASP
1	A	294	SER

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	293/316 (93%)	266 (91%)	27 (9%)	13	34
1	C	295/316 (93%)	276 (94%)	19 (6%)	25	55
1	E	284/316 (90%)	265 (93%)	19 (7%)	23	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	292/316 (92%)	268 (92%)	24 (8%)	17	40
1	H	299/316 (95%)	275 (92%)	24 (8%)	17	41
1	K	302/316 (96%)	281 (93%)	21 (7%)	21	49
1	M	293/316 (93%)	268 (92%)	25 (8%)	15	38
1	O	293/316 (93%)	275 (94%)	18 (6%)	26	58
All	All	2351/2528 (93%)	2174 (92%)	177 (8%)	19	45

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	136	LYS
1	G	112	ASN
1	O	34	ASP
1	E	195	LYS
1	G	2	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	90	HIS
1	G	90	HIS
1	O	112	ASN
1	E	163	HIS
1	E	212	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	A	401	-	13,15,16	2.00	3 (23%)	17,21,23	1.37	1 (5%)
2	PLP	C	401	-	13,15,16	2.15	3 (23%)	17,21,23	1.01	1 (5%)
2	PLP	E	401	-	13,15,16	2.09	3 (23%)	17,21,23	1.20	1 (5%)
2	PLP	G	401	1	14,15,16	3.04	6 (42%)	20,22,23	1.97	7 (35%)
2	PLP	H	401	-	13,15,16	2.21	3 (23%)	17,21,23	1.07	2 (11%)
3	PO4	K	401	-	4,4,4	1.74	0	6,6,6	0.38	0
2	PLP	M	401	-	13,15,16	1.98	3 (23%)	17,21,23	1.45	1 (5%)
2	PLP	O	401	-	13,15,16	2.15	3 (23%)	17,21,23	1.10	1 (5%)

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	A	401	-	-	0/8/8/8	0/1/1/1
2	PLP	C	401	-	-	0/8/8/8	0/1/1/1
2	PLP	E	401	-	-	0/8/8/8	0/1/1/1
2	PLP	G	401	1	-	0/6/6/8	0/1/1/1
2	PLP	H	401	-	-	0/8/8/8	0/1/1/1
3	PO4	K	401	-	-	0/0/0/0	0/0/0/0
2	PLP	M	401	-	-	0/8/8/8	0/1/1/1
2	PLP	O	401	-	-	0/8/8/8	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	PLP	C3-C2	-6.37	1.36	1.40
2	G	401	PLP	O3-C3	-6.29	1.21	1.37
2	H	401	PLP	C4-C5	6.21	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PLP	C4-C5	5.99	1.49	1.41
2	O	401	PLP	C4-C5	5.82	1.49	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	401	PLP	O4A-C4A-C4	-4.93	114.67	125.32
2	A	401	PLP	O4A-C4A-C4	-4.52	115.56	125.32
2	G	401	PLP	O4P-C5A-C5	3.85	117.08	109.26
2	G	401	PLP	O2P-P-O4P	-3.67	96.52	106.65
2	E	401	PLP	O4A-C4A-C4	-3.07	118.68	125.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/388 (93%)	0.23	10 (2%) 50 54	25, 43, 65, 81	0
1	C	366/388 (94%)	0.13	8 (2%) 59 62	23, 39, 62, 74	0
1	E	364/388 (93%)	0.32	13 (3%) 41 43	26, 42, 71, 88	0
1	G	365/388 (94%)	0.29	25 (6%) 17 17	22, 40, 68, 87	0
1	H	373/388 (96%)	0.08	0 100 100	27, 39, 58, 79	0
1	K	378/388 (97%)	0.33	14 (3%) 39 42	27, 47, 71, 95	0
1	M	365/388 (94%)	0.42	25 (6%) 17 17	25, 47, 70, 96	0
1	O	367/388 (94%)	0.43	19 (5%) 26 27	28, 49, 75, 88	0
All	All	2941/3104 (94%)	0.28	114 (3%) 37 40	22, 43, 70, 96	0

The worst 5 of 114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	335	PHE	6.4
1	O	164	GLY	5.8
1	O	119	ILE	5.1
1	M	102	PHE	4.5
1	A	273	TYR	4.4

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PLP	O	401	15/16	0.23	1.21	47,54,57,57	0
2	PLP	M	401	15/16	0.19	0.78	41,42,43,43	0
2	PLP	E	401	15/16	0.20	0.52	49,51,52,52	0
2	PLP	C	401	15/16	0.17	0.37	34,39,43,44	0
2	PLP	H	401	15/16	0.21	0.34	45,54,56,65	0
2	PLP	A	401	15/16	0.16	-0.50	38,42,43,44	0
3	PO4	K	401	5/5	0.10	-1.20	30,30,30,30	0
2	PLP	G	401	15/16	0.14	-2.06	30,31,31,31	0

6.5 Other polymers

There are no such residues in this entry.