



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:09 AM UTC

PDB ID : 4L0O / pdb_00004l0o
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 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
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

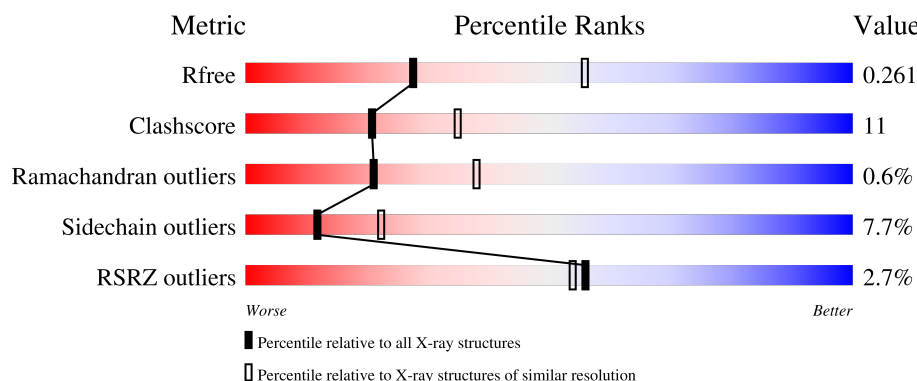
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	388	3% 66% 22% 5% 6%
1	C	388	2% 74% 18% 6%
1	E	388	4% 71% 21% 6%
1	G	388	3% 71% 20% 6%
1	H	388	0% 72% 22% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	388	
1	M	388	
1	O	388	

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	G	401	-	X	-	-
3	PO4	K	401	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22365 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	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

Continued on next page...

Continued from previous page...

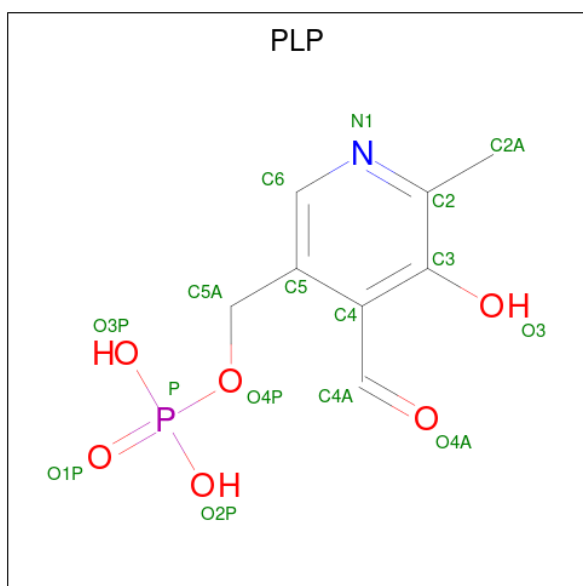
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	HIS	-	expression tag	UNP P56069
A	387	HIS	-	expression tag	UNP P56069
A	388	HIS	-	expression tag	UNP P56069
C	381	LEU	-	expression tag	UNP P56069
C	382	GLU	-	expression tag	UNP P56069
C	383	HIS	-	expression tag	UNP P56069
C	384	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

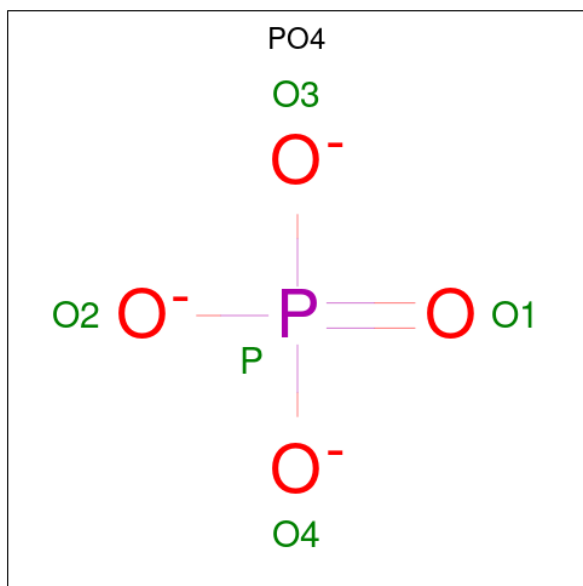
Chain	Residue	Modelled	Actual	Comment	Reference
M	388	HIS	-	expression tag	UNP P56069
O	381	LEU	-	expression tag	UNP P56069
O	382	GLU	-	expression tag	UNP P56069
O	383	HIS	-	expression tag	UNP P56069
O	384	HIS	-	expression tag	UNP P56069
O	385	HIS	-	expression tag	UNP P56069
O	386	HIS	-	expression tag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

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



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 (CCD ID: PO4) (formula: O_4P).

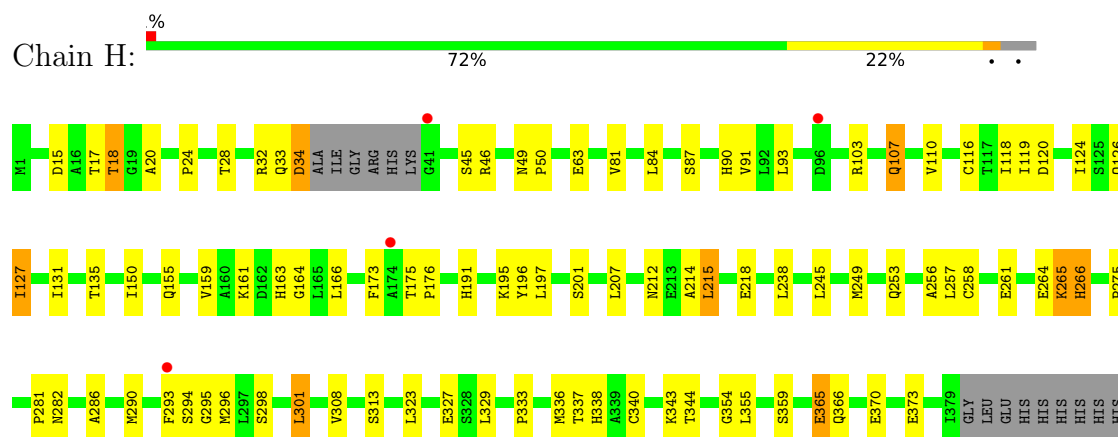


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	P	0	0
			5	4	1		

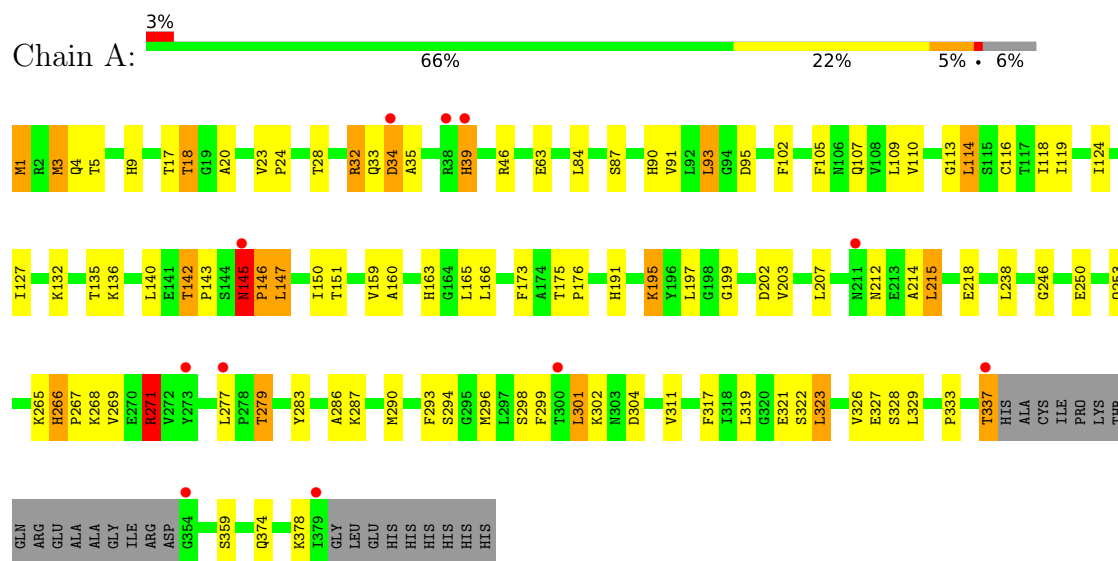
3 Residue-property plots [i](#)

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.

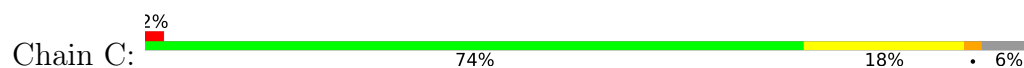
• Molecule 1: Cystathionine gamma-synthase

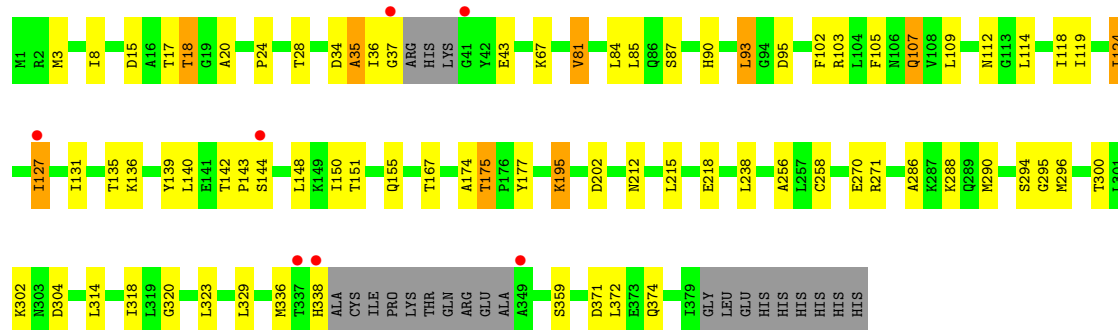


• Molecule 1: Cystathionine gamma-synthase

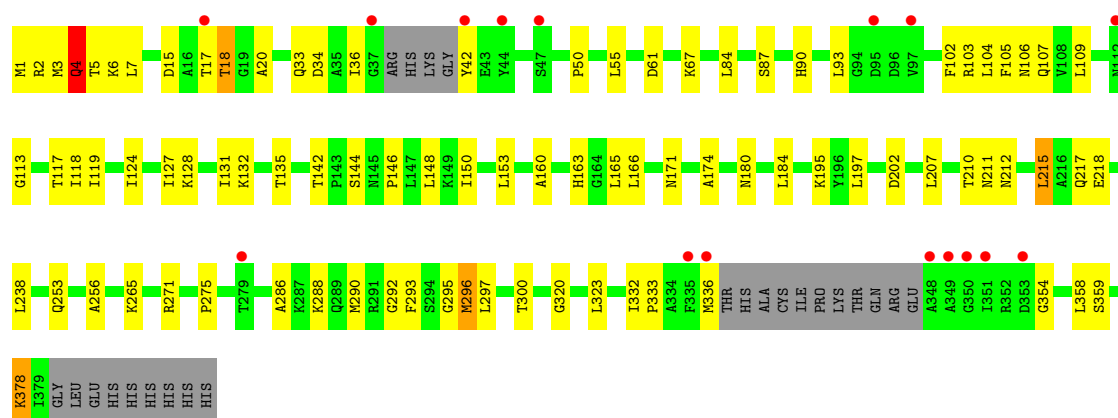


• Molecule 1: Cystathionine gamma-synthase

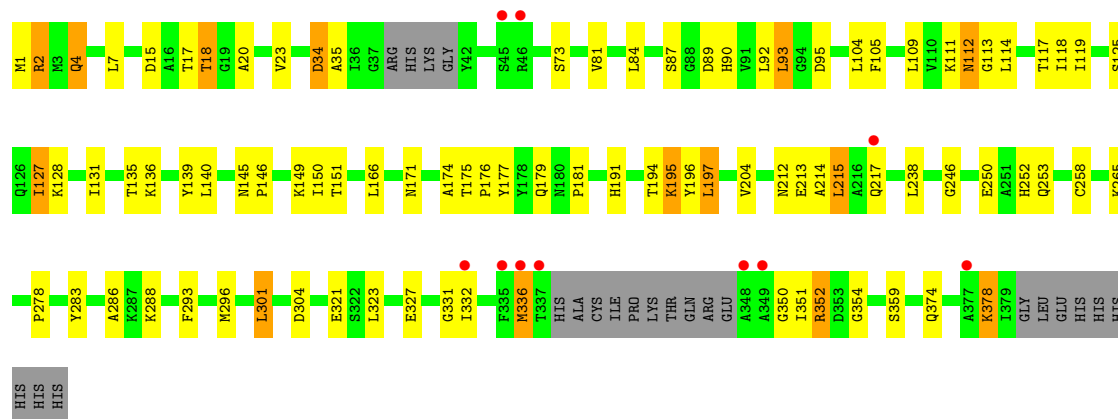




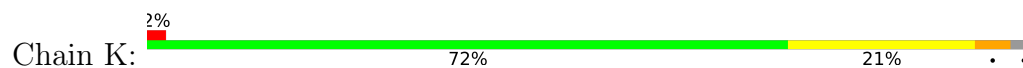
• Molecule 1: Cystathionine gamma-synthase

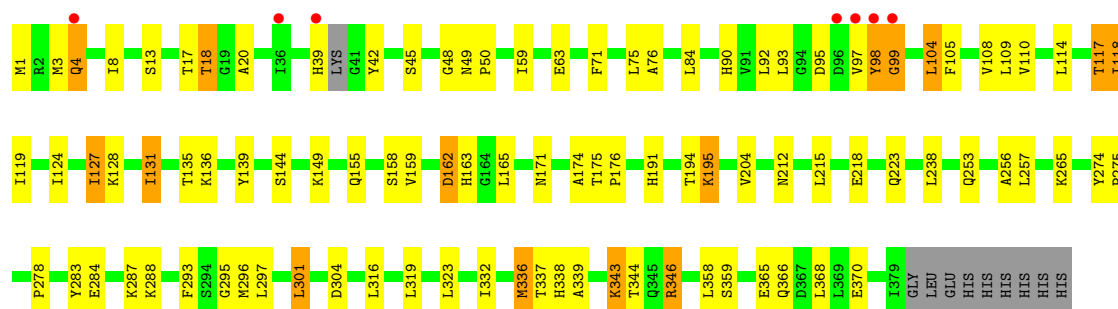


• Molecule 1: Cystathionine gamma-synthase

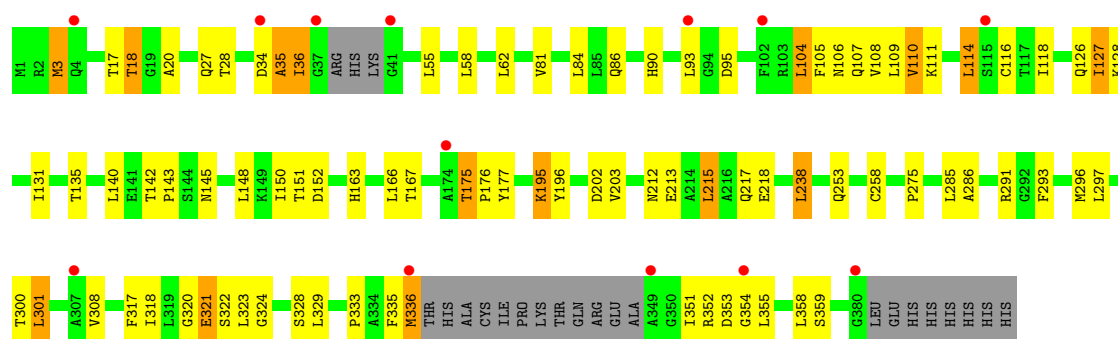


• Molecule 1: Cystathionine gamma-synthase

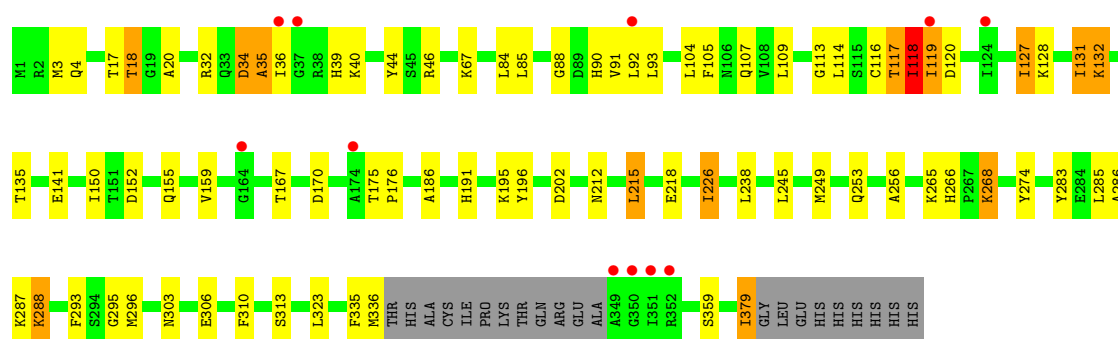
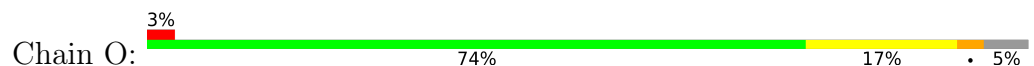




• Molecule 1: Cystathionine gamma-synthase



• Molecule 1: Cystathionine gamma-synthase



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 50.00 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.76) 99.9 (50.00-2.76)	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 , 0.261	Depositor DCC
R_{free} test set	4234 reflections (4.98%)	wwPDB-VP
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 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

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: 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	0.81	11/2808 (0.4%)	0.87	3/3804 (0.1%)
1	C	0.74	4/2829 (0.1%)	0.85	1/3832 (0.0%)
1	E	0.69	2/2777 (0.1%)	0.84	2/3764 (0.1%)
1	G	0.79	3/2812 (0.1%)	0.87	2/3811 (0.1%)
1	H	0.66	1/2881 (0.0%)	0.82	2/3904 (0.1%)
1	K	0.87	14/2919 (0.5%)	0.85	3/3954 (0.1%)
1	M	0.67	2/2815 (0.1%)	0.80	0/3812
1	O	0.92	8/2825 (0.3%)	0.87	5/3829 (0.1%)
All	All	0.77	45/22666 (0.2%)	0.85	18/30710 (0.1%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	338	HIS	CG-CD2	13.38	1.50	1.35
1	O	39	HIS	CE1-NE2	-13.35	1.19	1.32
1	K	39	HIS	C-O	10.76	1.45	1.23
1	C	338	HIS	CG-CD2	10.23	1.47	1.35
1	E	378	LYS	CE-NZ	9.20	1.76	1.49
1	H	34	ASP	C-O	8.65	1.40	1.23
1	K	338	HIS	ND1-CE1	8.47	1.41	1.32
1	A	145	ASN	CG-OD1	7.88	1.38	1.23
1	G	112	ASN	CG-OD1	-7.64	1.09	1.23
1	O	132	LYS	CE-NZ	7.52	1.72	1.49
1	O	379	ILE	C-O	7.37	1.38	1.23
1	G	336	MET	C-N	7.30	1.43	1.33
1	M	163	HIS	CE1-NE2	7.21	1.39	1.32
1	K	97	VAL	C-O	7.21	1.31	1.24
1	O	268	LYS	CE-NZ	7.11	1.70	1.49
1	A	39	HIS	CG-ND1	-6.82	1.30	1.38
1	E	4	GLN	CD-OE1	6.75	1.36	1.23
1	K	338	HIS	CD2-NE2	-6.49	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	ARG	C-N	6.37	1.41	1.33
1	A	39	HIS	CG-CD2	6.30	1.42	1.35
1	K	338	HIS	CE1-NE2	6.29	1.38	1.32
1	A	39	HIS	CD2-NE2	6.19	1.44	1.37
1	O	118	ILE	C-N	6.17	1.42	1.33
1	O	226	ILE	CA-CB	-6.13	1.47	1.54
1	A	146	PRO	N-CD	6.08	1.56	1.47
1	C	338	HIS	ND1-CE1	6.04	1.38	1.32
1	A	268	LYS	CG-CD	5.91	1.70	1.52
1	M	163	HIS	CG-CD2	5.86	1.42	1.35
1	K	337	THR	CB-OG1	5.86	1.53	1.43
1	K	39	HIS	ND1-CE1	5.51	1.38	1.32
1	K	39	HIS	CG-CD2	5.49	1.41	1.35
1	A	266	HIS	C-N	5.41	1.40	1.33
1	K	336	MET	SD-CE	5.41	1.93	1.79
1	K	4	GLN	CD-NE2	-5.40	1.22	1.33
1	A	271	ARG	C-O	5.39	1.30	1.23
1	O	226	ILE	C-O	-5.32	1.19	1.24
1	A	145	ASN	CB-CG	5.30	1.65	1.52
1	G	35	ALA	CA-CB	-5.29	1.45	1.53
1	O	265	LYS	CE-NZ	5.28	1.65	1.49
1	C	174	ALA	CA-CB	-5.24	1.44	1.53
1	C	175	THR	C-O	-5.13	1.17	1.24
1	K	39	HIS	CE1-NE2	5.13	1.37	1.32
1	K	346	ARG	NE-CZ	5.07	1.38	1.33
1	K	346	ARG	CZ-NH1	5.03	1.39	1.32
1	A	337	THR	CB-OG1	5.01	1.51	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	HIS	ND1-CE1-NE2	7.44	115.84	108.40
1	G	112	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	H	34	ASP	CA-C-O	-6.98	108.93	120.80
1	O	39	HIS	ND1-CE1-NE2	6.64	115.04	108.40
1	G	350	GLY	N-CA-C	-6.39	107.48	115.08
1	A	39	HIS	ND1-CG-CD2	6.07	112.17	106.10
1	A	39	HIS	CG-CD2-NE2	-5.76	101.44	107.20
1	K	4	GLN	CG-CD-NE2	5.69	124.94	116.40
1	H	266	HIS	N-CA-C	5.37	116.43	109.72
1	O	266	HIS	CA-C-N	5.34	125.41	119.32
1	O	266	HIS	C-N-CA	5.34	125.41	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	180	ASN	CA-C-N	5.31	125.63	119.47
1	E	180	ASN	C-N-CA	5.31	125.63	119.47
1	C	34	ASP	N-CA-C	-5.16	106.84	112.72
1	K	165	LEU	N-CA-C	5.15	118.15	110.52
1	K	4	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	O	274	TYR	CA-C-N	5.05	125.33	119.47
1	O	274	TYR	C-N-CA	5.05	125.33	119.47

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	2756	0	2762	77	0
1	C	2778	0	2775	51	0
1	E	2728	0	2708	57	0
1	G	2762	0	2748	66	0
1	H	2828	0	2824	57	0
1	K	2865	0	2858	62	0
1	M	2765	0	2764	65	0
1	O	2773	0	2762	80	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	494	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 11.

All (494) 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: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
1:H:164:GLY:HA3	1:A:132:LYS:HD3	1.35	1.06
1:O:35:ALA:CB	1:O:36:ILE:HA	1.86	1.04
1:O:35:ALA:HB1	1:O:36:ILE:HA	1.05	1.03
1:O:35:ALA:HB1	1:O:36:ILE:CA	1.89	1.01
1:C:35:ALA:HB1	1:C:36:ILE:HA	1.42	0.99
1:M:35:ALA:CB	1:M:36:ILE:HA	1.95	0.97
1:O:288:LYS:O	1:O:288:LYS:HD3	1.64	0.95
1:O:288:LYS:HD3	1:O:288:LYS:C	1.87	0.93
1:M:35:ALA:HB1	1:M:36:ILE:CA	1.99	0.92
1:M:321:GLU:HG3	1:M:321:GLU:O	1.66	0.92
1:H:150:ILE:HD13	1:H:286:ALA:HB2	1.54	0.89
1:C:35:ALA:CB	1:C:36:ILE:HA	2.02	0.89
1:E:217:GLN:HG3	1:G:217:GLN:HG2	1.53	0.88
1:C:35:ALA:HB1	1:C:36:ILE:CA	2.02	0.88
1:A:150:ILE:HD13	1:A:286:ALA:HB2	1.59	0.85
1:A:301:LEU:H	1:A:301:LEU:HD23	1.44	0.83
1:G:2:ARG:HG3	1:G:2:ARG:HH11	1.42	0.83
1:G:212:ASN:HD22	1:G:215:LEU:H	1.27	0.81
1:G:111:LYS:C	1:G:112:ASN:HD22	1.88	0.81
1:O:283:TYR:CE2	1:O:287:LYS:HE2	2.15	0.81
1:O:90:HIS:CD2	1:O:135:THR:HG22	2.17	0.80
1:M:106:ASN:O	1:M:110:VAL:HG11	1.82	0.79
1:O:288:LYS:C	1:O:288:LYS:CD	2.55	0.79
1:G:18:THR:HG22	1:G:20:ALA:H	1.46	0.78
1:O:288:LYS:O	1:O:288:LYS:CD	2.30	0.78
1:E:217:GLN:HG3	1:G:217:GLN:CG	2.14	0.78
1:E:84:LEU:HD22	1:E:218:GLU:HB3	1.65	0.78
1:A:146:PRO:O	1:A:147:LEU:HB2	1.82	0.78
1:H:124:ILE:HD13	1:H:155:GLN:HE21	1.49	0.77
1:A:279:THR:HB	1:K:287:LYS:HD2	1.67	0.77
1:H:366:GLN:O	1:H:370:GLU:HG3	1.84	0.77
1:O:92:LEU:HD23	1:O:117:THR:HG22	1.65	0.76
1:M:321:GLU:HG2	1:O:44:TYR:HB2	1.67	0.76
1:M:3:MET:HE1	1:M:62:LEU:HD22	1.66	0.76
1:E:150:ILE:HD13	1:E:286:ALA:HB2	1.68	0.75
1:A:110:VAL:HA	1:A:114:LEU:O	1.86	0.74
1:E:212:ASN:HD22	1:E:215:LEU:H	1.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:THR:HG22	1:C:20:ALA:H	1.53	0.72
1:O:253:GLN:NE2	1:O:293:PHE:H	1.88	0.72
1:H:175:THR:HB	1:H:176:PRO:HD2	1.69	0.72
1:A:253:GLN:NE2	1:A:293:PHE:H	1.88	0.72
1:H:253:GLN:NE2	1:H:293:PHE:H	1.87	0.72
1:A:90:HIS:HB3	1:A:135:THR:HA	1.72	0.71
1:O:132:LYS:NZ	1:O:132:LYS:CD	2.53	0.71
1:O:132:LYS:HB2	1:O:135:THR:HG23	1.71	0.71
1:O:84:LEU:HD22	1:O:218:GLU:HB3	1.70	0.71
1:G:93:LEU:HD12	1:G:139:TYR:HB3	1.72	0.71
1:M:296:MET:HE1	1:M:359:SER:OG	1.90	0.71
1:A:212:ASN:HD22	1:A:215:LEU:H	1.38	0.70
1:K:212:ASN:HB3	1:K:215:LEU:HB2	1.72	0.70
1:A:39:HIS:H	1:A:39:HIS:CD2	2.09	0.70
1:E:18:THR:HG22	1:E:20:ALA:H	1.56	0.70
1:K:175:THR:HB	1:K:176:PRO:HD2	1.73	0.70
1:O:286:ALA:C	1:O:288:LYS:H	1.99	0.69
1:A:145:ASN:HB2	1:A:173:PHE:CZ	2.27	0.69
1:C:296:MET:HE3	1:C:323:LEU:HD13	1.73	0.69
1:O:118:ILE:O	1:O:119:ILE:CG2	2.36	0.69
1:K:339:ALA:HA	1:K:346:ARG:NH2	2.08	0.68
1:G:4:GLN:HE21	1:G:7:LEU:HD12	1.58	0.68
1:H:212:ASN:HD22	1:H:215:LEU:H	1.42	0.68
1:K:339:ALA:HA	1:K:346:ARG:HH21	1.58	0.68
1:O:286:ALA:C	1:O:288:LYS:N	2.48	0.68
1:A:301:LEU:H	1:A:301:LEU:CD2	2.07	0.67
1:K:212:ASN:HD22	1:K:215:LEU:H	1.41	0.67
1:E:84:LEU:CD2	1:E:218:GLU:HB3	2.24	0.67
1:H:195:LYS:NZ	2:H:401:PLP:C4A	2.58	0.67
1:C:90:HIS:HB3	1:C:135:THR:HA	1.76	0.67
1:O:92:LEU:HB3	1:O:119:ILE:HD11	1.75	0.67
1:C:296:MET:HE1	1:C:359:SER:OG	1.95	0.67
1:O:84:LEU:CD2	1:O:218:GLU:HB3	2.24	0.67
1:O:119:ILE:HD12	1:O:127:ILE:HG22	1.75	0.67
1:C:84:LEU:C	1:C:85:LEU:HD23	2.20	0.66
1:M:301:LEU:H	1:M:301:LEU:HD23	1.60	0.66
1:A:95:ASP:HA	1:A:118:ILE:HG23	1.78	0.66
1:A:374:GLN:O	1:A:378:LYS:HD3	1.95	0.66
1:C:195:LYS:HZ1	2:C:401:PLP:C4A	2.09	0.65
1:A:286:ALA:HB1	1:A:290:MET:HE2	1.76	0.65
1:E:253:GLN:NE2	1:E:293:PHE:H	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:286:ALA:O	1:O:288:LYS:N	2.30	0.65
1:C:84:LEU:HD22	1:C:218:GLU:HB3	1.78	0.65
1:M:105:PHE:O	1:M:110:VAL:HG12	1.95	0.65
1:H:84:LEU:HD22	1:H:218:GLU:HB3	1.77	0.65
1:O:127:ILE:HG13	1:O:128:LYS:N	2.10	0.64
1:E:90:HIS:HE1	1:E:117:THR:OG1	1.81	0.64
1:E:378:LYS:NZ	1:E:378:LYS:CD	2.60	0.64
1:M:3:MET:CE	1:M:62:LEU:HD22	2.27	0.64
1:H:195:LYS:HZ1	2:H:401:PLP:C4A	2.11	0.64
1:E:105:PHE:HA	1:E:109:LEU:HB2	1.79	0.64
1:M:95:ASP:HA	1:M:118:ILE:HG23	1.80	0.63
1:O:212:ASN:HB3	1:O:215:LEU:HB2	1.81	0.63
1:A:102:PHE:HE1	1:A:118:ILE:HD11	1.64	0.63
1:A:212:ASN:HB3	1:A:215:LEU:HB2	1.81	0.63
1:H:120:ASP:HB3	1:H:126:GLN:NE2	2.14	0.63
1:O:109:LEU:HB3	1:O:114:LEU:HD12	1.79	0.63
1:E:87:SER:HB2	1:E:113:GLY:HA3	1.82	0.62
1:M:195:LYS:HD3	2:M:401:PLP:O4A	1.99	0.62
1:A:84:LEU:HD22	1:A:218:GLU:HB3	1.81	0.62
1:E:15:ASP:OD2	1:E:18:THR:HB	2.00	0.62
1:C:212:ASN:HB3	1:C:215:LEU:HB2	1.81	0.62
1:K:283:TYR:CE2	1:K:287:LYS:HD3	2.35	0.62
1:E:127:ILE:HG13	1:E:128:LYS:N	2.15	0.61
1:M:84:LEU:HD22	1:M:218:GLU:HB3	1.82	0.61
1:G:15:ASP:OD2	1:G:18:THR:HB	2.00	0.61
1:G:351:ILE:C	1:G:352:ARG:O	2.39	0.61
1:G:253:GLN:NE2	1:G:293:PHE:H	1.98	0.61
1:M:140:LEU:HD22	1:M:151:THR:HG21	1.81	0.61
1:K:284:GLU:HA	1:K:287:LYS:HE2	1.83	0.60
1:A:195:LYS:NZ	2:A:401:PLP:O4A	2.34	0.60
1:E:4:GLN:OE1	1:E:4:GLN:HA	2.01	0.60
1:K:296:MET:HE3	1:K:323:LEU:HD13	1.83	0.60
1:O:226:ILE:O	1:O:226:ILE:HG22	1.99	0.60
1:K:155:GLN:O	1:K:159:VAL:HG23	2.01	0.60
1:M:212:ASN:HD22	1:M:215:LEU:H	1.48	0.60
1:E:34:ASP:O	1:G:1:MET:N	2.33	0.60
1:G:296:MET:HE3	1:G:323:LEU:HD13	1.84	0.60
1:C:15:ASP:OD2	1:C:18:THR:HB	2.02	0.60
1:E:171:ASN:O	1:E:174:ALA:O	2.20	0.60
1:H:150:ILE:CD1	1:H:286:ALA:HB2	2.31	0.59
1:M:152:ASP:OD1	1:M:285:LEU:HD11	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ALA:CB	1:C:36:ILE:CA	2.70	0.59
1:O:84:LEU:C	1:O:85:LEU:HD23	2.27	0.59
1:C:150:ILE:HD13	1:C:286:ALA:HB2	1.83	0.59
1:A:195:LYS:HD3	2:A:401:PLP:O4A	2.02	0.59
1:C:35:ALA:HB1	1:C:36:ILE:C	2.26	0.59
1:A:197:LEU:HD13	1:A:207:LEU:HD12	1.85	0.59
1:E:142:THR:CG2	1:E:153:LEU:HD21	2.33	0.59
1:G:195:LYS:NZ	2:G:401:PLP:O3	2.30	0.59
1:C:270:GLU:HB3	1:C:300:THR:HG23	1.84	0.59
1:G:2:ARG:HH11	1:G:2:ARG:CG	2.15	0.58
1:M:90:HIS:HB3	1:M:135:THR:HA	1.86	0.58
1:A:18:THR:HG22	1:A:20:ALA:H	1.68	0.58
1:E:105:PHE:CD2	1:E:109:LEU:HD12	2.39	0.58
1:G:332:ILE:H	1:G:336:MET:HE2	1.68	0.58
1:M:3:MET:HE1	1:M:62:LEU:CD2	2.31	0.58
1:O:85:LEU:HD23	1:O:85:LEU:N	2.19	0.58
1:C:3:MET:HE2	1:C:177:TYR:HA	1.86	0.57
1:A:32:ARG:HB2	1:C:318:ILE:HG23	1.86	0.57
1:A:150:ILE:CD1	1:A:286:ALA:HB2	2.33	0.57
1:K:319:LEU:HD11	1:K:336:MET:HE3	1.85	0.57
1:E:256:ALA:HB2	1:E:295:GLY:HA2	1.87	0.57
1:A:160:ALA:O	1:A:165:LEU:HB2	2.04	0.57
1:G:331:GLY:HA2	1:G:336:MET:HE2	1.86	0.57
1:M:36:ILE:HG21	1:O:335:PHE:HB3	1.85	0.57
1:G:351:ILE:O	1:G:352:ARG:C	2.46	0.56
1:A:199:GLY:O	1:A:326:VAL:HG13	2.04	0.56
1:A:1:MET:HE2	1:A:5:THR:HG22	1.87	0.56
1:A:140:LEU:HD22	1:A:151:THR:HG21	1.87	0.56
1:C:85:LEU:HD23	1:C:85:LEU:N	2.20	0.56
1:C:296:MET:CE	1:C:323:LEU:HB2	2.36	0.56
1:G:95:ASP:HA	1:G:118:ILE:CG2	2.35	0.56
1:O:90:HIS:HB3	1:O:135:THR:HA	1.87	0.56
1:H:253:GLN:HE21	1:H:293:PHE:H	1.51	0.56
1:A:28:THR:HA	1:C:202:ASP:HA	1.88	0.56
1:C:35:ALA:HB1	1:C:37:GLY:N	2.21	0.56
1:H:212:ASN:HB3	1:H:215:LEU:HB2	1.86	0.55
1:C:195:LYS:HD2	1:C:195:LYS:N	2.21	0.55
1:K:343:LYS:HA	1:K:346:ARG:HD2	1.89	0.55
1:H:327:GLU:CD	1:H:327:GLU:H	2.14	0.55
1:C:296:MET:HE1	1:C:323:LEU:HB2	1.87	0.55
1:O:92:LEU:HD23	1:O:117:THR:CG2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:93:LEU:HD13	1:O:116:CYS:HB2	1.88	0.55
1:G:179:GLN:HG2	1:G:181:PRO:HD3	1.89	0.55
1:M:352:ARG:C	1:M:354:GLY:H	2.15	0.55
1:O:105:PHE:HA	1:O:109:LEU:HB2	1.88	0.55
1:C:212:ASN:HD22	1:C:215:LEU:H	1.53	0.55
1:G:327:GLU:CD	1:G:327:GLU:H	2.15	0.54
1:A:267:PRO:O	1:A:302:LYS:HD2	2.07	0.54
1:K:284:GLU:HA	1:K:287:LYS:CE	2.37	0.54
1:M:81:VAL:O	1:M:84:LEU:HG	2.06	0.54
1:M:318:ILE:HG23	1:O:32:ARG:HG3	1.89	0.54
1:H:103:ARG:HG3	1:H:107:GLN:HG3	1.89	0.54
1:C:124:ILE:HD12	1:C:155:GLN:HE21	1.71	0.54
1:E:42:TYR:CE1	1:E:50:PRO:HG3	2.43	0.54
1:M:351:ILE:HD12	1:M:351:ILE:H	1.73	0.54
1:C:102:PHE:HE1	1:C:118:ILE:HD11	1.72	0.53
1:E:148:LEU:HD11	1:E:297:LEU:HA	1.90	0.53
1:A:271:ARG:NH1	1:A:271:ARG:HG2	2.22	0.53
1:G:212:ASN:HD21	1:G:214:ALA:HB3	1.73	0.53
1:O:285:LEU:O	1:O:288:LYS:HB3	2.09	0.53
1:G:331:GLY:CA	1:G:336:MET:HE2	2.38	0.53
1:H:245:LEU:O	1:H:249:MET:HG2	2.07	0.53
1:G:212:ASN:ND2	1:G:215:LEU:H	2.02	0.53
1:O:132:LYS:HB2	1:O:135:THR:CG2	2.36	0.53
1:K:105:PHE:HA	1:K:109:LEU:HB2	1.90	0.53
1:M:213:GLU:O	1:M:217:GLN:HG2	2.09	0.53
1:O:18:THR:CG2	1:O:20:ALA:H	2.22	0.53
1:M:27:GLN:O	1:O:202:ASP:HB2	2.08	0.53
1:O:286:ALA:O	1:O:287:LYS:C	2.50	0.53
1:M:143:PRO:HB2	1:M:148:LEU:HD23	1.91	0.52
1:H:164:GLY:CA	1:A:132:LYS:HD3	2.24	0.52
1:A:173:PHE:CE2	1:A:296:MET:HG3	2.44	0.52
1:G:140:LEU:HD22	1:G:151:THR:HG21	1.89	0.52
1:H:333:PRO:O	1:H:338:HIS:HB2	2.10	0.52
1:C:140:LEU:HD22	1:C:151:THR:HG21	1.91	0.52
1:A:39:HIS:H	1:A:39:HIS:HD2	1.56	0.52
1:A:175:THR:HB	1:A:176:PRO:HD2	1.91	0.52
1:G:87:SER:HB2	1:G:113:GLY:HA3	1.91	0.52
1:A:279:THR:HB	1:K:287:LYS:CD	2.39	0.52
1:M:36:ILE:N	1:M:36:ILE:CD1	2.73	0.52
1:H:296:MET:HE1	1:H:323:LEU:HB2	1.92	0.52
1:A:333:PRO:HB3	1:A:337:THR:OG1	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:THR:CG2	1:G:20:ALA:HB2	2.40	0.51
1:M:297:LEU:HD11	1:M:358:LEU:HD12	1.93	0.51
1:O:196:TYR:OH	1:O:296:MET:HE2	2.10	0.51
1:K:90:HIS:HD2	1:K:135:THR:OG1	1.93	0.51
1:H:124:ILE:HD13	1:H:155:GLN:NE2	2.22	0.51
1:C:195:LYS:NZ	2:C:401:PLP:C4A	2.72	0.51
1:A:195:LYS:CE	2:A:401:PLP:O4A	2.59	0.51
1:A:283:TYR:CE2	1:A:287:LYS:HE2	2.45	0.51
1:A:159:VAL:O	1:A:163:HIS:HD2	1.93	0.51
1:C:256:ALA:HB2	1:C:295:GLY:HA2	1.93	0.51
1:O:131:ILE:CG2	1:O:132:LYS:N	2.73	0.51
1:O:118:ILE:HG23	1:O:119:ILE:N	2.26	0.51
1:O:131:ILE:HG22	1:O:132:LYS:N	2.24	0.51
1:M:109:LEU:O	1:M:114:LEU:HB2	2.11	0.51
1:A:271:ARG:HG2	1:A:271:ARG:HH11	1.76	0.51
1:E:297:LEU:HD11	1:E:358:LEU:HD12	1.92	0.51
1:M:3:MET:HA	1:M:3:MET:HE3	1.92	0.51
1:E:148:LEU:CD1	1:E:297:LEU:HA	2.41	0.50
1:H:195:LYS:HD2	1:H:195:LYS:N	2.26	0.50
1:A:95:ASP:HA	1:A:118:ILE:CG2	2.42	0.50
1:K:18:THR:HG23	1:K:20:ALA:H	1.75	0.50
1:O:127:ILE:O	1:O:131:ILE:HD12	2.11	0.50
1:A:301:LEU:CD2	1:A:301:LEU:N	2.71	0.50
1:C:212:ASN:ND2	1:C:215:LEU:H	2.08	0.50
1:C:296:MET:HE3	1:C:323:LEU:CD1	2.39	0.50
1:G:195:LYS:HD2	1:G:323:LEU:HG	1.93	0.50
1:G:321:GLU:O	1:G:321:GLU:HG3	2.12	0.50
1:K:278:PRO:HA	1:K:283:TYR:CD2	2.47	0.50
1:O:34:ASP:OD1	1:O:40:LYS:HE2	2.11	0.50
1:O:155:GLN:O	1:O:159:VAL:HG23	2.12	0.50
1:A:311:VAL:CG1	1:A:319:LEU:HD13	2.42	0.50
1:O:296:MET:HE1	1:O:359:SER:OG	2.12	0.50
1:A:3:MET:HA	1:A:3:MET:HE3	1.93	0.50
1:M:58:LEU:O	1:M:62:LEU:HG	2.12	0.50
1:G:109:LEU:HB3	1:G:114:LEU:HD12	1.94	0.50
1:G:351:ILE:O	1:G:352:ARG:O	2.29	0.50
1:G:95:ASP:HA	1:G:118:ILE:HG23	1.94	0.49
1:K:84:LEU:HD22	1:K:218:GLU:HB3	1.94	0.49
1:O:120:ASP:OD2	1:O:120:ASP:C	2.55	0.49
1:M:329:LEU:HB2	1:M:359:SER:HB3	1.93	0.49
1:G:90:HIS:HB3	1:G:135:THR:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ILE:HD11	1:E:275:PRO:HB3	1.94	0.49
1:H:159:VAL:O	1:H:163:HIS:HD2	1.95	0.49
1:H:301:LEU:H	1:H:301:LEU:HD23	1.78	0.49
1:E:153:LEU:HD12	1:E:184:LEU:HD12	1.94	0.49
1:H:296:MET:CE	1:H:323:LEU:HB2	2.43	0.49
1:A:93:LEU:CD2	1:A:116:CYS:HB2	2.43	0.49
1:M:150:ILE:HD11	1:M:275:PRO:HB3	1.95	0.49
1:H:18:THR:HG22	1:H:20:ALA:H	1.77	0.49
1:A:253:GLN:HE22	1:A:293:PHE:H	1.58	0.49
1:G:175:THR:HB	1:G:176:PRO:HD2	1.94	0.49
1:G:331:GLY:HA2	1:G:336:MET:CE	2.43	0.49
1:K:90:HIS:HB3	1:K:135:THR:HA	1.95	0.49
1:E:160:ALA:O	1:E:165:LEU:HB2	2.13	0.48
1:O:268:LYS:NZ	1:O:268:LYS:CD	2.65	0.48
1:H:308:VAL:HG13	1:E:36:ILE:HD12	1.96	0.48
1:M:142:THR:HA	1:M:143:PRO:C	2.39	0.48
1:O:175:THR:HB	1:O:176:PRO:HD2	1.95	0.48
1:E:90:HIS:HD2	1:E:135:THR:OG1	1.96	0.48
1:G:90:HIS:HD2	1:G:135:THR:OG1	1.96	0.48
1:M:202:ASP:OD2	1:M:203:VAL:HG23	2.14	0.48
1:A:1:MET:CE	1:A:9:HIS:HB2	2.44	0.47
1:E:103:ARG:HA	1:E:106:ASN:HB3	1.96	0.47
1:G:176:PRO:HD3	1:G:191:HIS:NE2	2.29	0.47
1:M:177:TYR:C	1:M:291:ARG:HH21	2.22	0.47
1:H:91:VAL:O	1:H:116:CYS:HA	2.14	0.47
1:H:197:LEU:HD13	1:H:207:LEU:HD12	1.96	0.47
1:M:106:ASN:O	1:M:110:VAL:CG1	2.59	0.47
1:M:308:VAL:HG22	1:O:36:ILE:HD13	1.96	0.47
1:M:317:PHE:CD2	1:M:328:SER:HB3	2.49	0.47
1:O:91:VAL:HG12	1:O:93:LEU:HD12	1.96	0.47
1:A:246:GLY:O	1:A:250:GLU:HG2	2.14	0.47
1:G:171:ASN:O	1:G:174:ALA:O	2.32	0.47
1:A:91:VAL:O	1:A:116:CYS:HA	2.14	0.47
1:M:18:THR:CG2	1:M:20:ALA:H	2.27	0.47
1:O:88:GLY:N	1:O:113:GLY:O	2.41	0.47
1:C:95:ASP:HA	1:C:118:ILE:HG23	1.96	0.47
1:M:212:ASN:HB3	1:M:215:LEU:HB2	1.96	0.47
1:G:112:ASN:HD22	1:G:112:ASN:N	2.13	0.47
1:G:331:GLY:CA	1:G:336:MET:CE	2.93	0.47
1:K:366:GLN:O	1:K:370:GLU:HG3	2.14	0.47
1:M:127:ILE:HG13	1:M:128:LYS:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:HB2	1:A:173:PHE:CE2	2.50	0.47
1:E:142:THR:HG21	1:E:153:LEU:HD21	1.97	0.47
1:E:160:ALA:O	1:E:163:HIS:O	2.33	0.47
1:A:63:GLU:OE1	1:A:191:HIS:CE1	2.68	0.47
1:A:142:THR:HA	1:A:143:PRO:C	2.39	0.47
1:K:253:GLN:NE2	1:K:293:PHE:H	2.13	0.47
1:K:332:ILE:H	1:K:336:MET:HE2	1.80	0.47
1:O:176:PRO:HD3	1:O:191:HIS:NE2	2.29	0.47
1:E:290:MET:HE3	1:E:292:GLY:O	2.14	0.46
1:A:105:PHE:HA	1:A:109:LEU:HB2	1.96	0.46
1:G:304:ASP:OD1	1:G:354:GLY:HA3	2.15	0.46
1:H:119:ILE:HD12	1:H:127:ILE:HG22	1.97	0.46
1:H:195:LYS:HZ2	2:H:401:PLP:C4A	2.28	0.46
1:G:119:ILE:HD12	1:G:127:ILE:HA	1.98	0.46
1:K:162:ASP:OD1	1:K:163:HIS:N	2.49	0.46
1:G:150:ILE:HD13	1:G:286:ALA:HB2	1.96	0.46
1:G:296:MET:HE1	1:G:323:LEU:HB2	1.97	0.46
1:K:109:LEU:HB3	1:K:114:LEU:HD12	1.97	0.46
1:M:196:TYR:OH	1:M:296:MET:HE2	2.16	0.46
1:A:33:GLN:C	1:A:34:ASP:O	2.57	0.46
1:G:128:LYS:HA	1:G:131:ILE:HD12	1.98	0.46
1:M:150:ILE:HD13	1:M:286:ALA:HB2	1.97	0.46
1:C:81:VAL:O	1:C:84:LEU:HG	2.16	0.46
1:E:296:MET:HE2	1:E:323:LEU:HD22	1.96	0.46
1:O:44:TYR:HE2	1:O:46:ARG:NH1	2.12	0.46
1:K:95:ASP:HB3	1:K:118:ILE:HG23	1.97	0.46
1:K:162:ASP:OD1	1:K:162:ASP:C	2.58	0.46
1:M:351:ILE:HD12	1:M:351:ILE:N	2.30	0.46
2:M:401:PLP:O3P	1:O:46:ARG:NH1	2.49	0.46
1:A:321:GLU:OE1	1:C:43:GLU:HB3	2.16	0.46
1:G:95:ASP:OD2	1:G:149:LYS:NZ	2.49	0.46
1:K:319:LEU:HD11	1:K:336:MET:CE	2.46	0.46
1:O:296:MET:CE	1:O:323:LEU:HB2	2.46	0.46
1:G:301:LEU:H	1:G:301:LEU:CD2	2.29	0.45
1:A:296:MET:HE1	1:A:359:SER:CB	2.46	0.45
1:E:320:GLY:O	1:E:336:MET:HE1	2.15	0.45
1:A:18:THR:CG2	1:A:20:ALA:H	2.29	0.45
1:C:286:ALA:HB1	1:C:290:MET:HE2	1.97	0.45
1:G:278:PRO:HA	1:G:283:TYR:CD2	2.51	0.45
1:A:1:MET:HE1	1:A:9:HIS:HB2	1.98	0.45
1:G:374:GLN:O	1:G:378:LYS:HD3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:18:THR:CG2	1:K:20:ALA:H	2.30	0.45
1:A:296:MET:HE1	1:A:359:SER:OG	2.16	0.45
1:E:197:LEU:HD13	1:E:207:LEU:HD12	1.97	0.45
1:G:81:VAL:O	1:G:84:LEU:HG	2.16	0.45
1:G:194:THR:HG23	1:G:204:VAL:HA	1.98	0.45
1:H:296:MET:HE3	1:H:323:LEU:HD13	1.97	0.45
1:A:317:PHE:CD2	1:A:328:SER:HB3	2.52	0.45
1:A:327:GLU:H	1:A:327:GLU:CD	2.24	0.45
1:C:320:GLY:O	1:C:336:MET:HE1	2.17	0.45
1:G:296:MET:CE	1:G:323:LEU:HB2	2.47	0.45
1:K:104:LEU:O	1:K:108:VAL:HB	2.17	0.45
1:E:90:HIS:CE1	1:E:117:THR:OG1	2.65	0.45
1:E:253:GLN:NE2	1:E:293:PHE:CD2	2.84	0.45
1:O:226:ILE:O	1:O:226:ILE:CG2	2.61	0.45
1:M:104:LEU:O	1:M:108:VAL:HB	2.16	0.45
1:H:81:VAL:O	1:H:84:LEU:HG	2.17	0.45
1:G:197:LEU:HD12	1:G:197:LEU:HA	1.62	0.45
1:M:93:LEU:HD13	1:M:116:CYS:HB2	1.98	0.45
1:M:195:LYS:NZ	2:M:401:PLP:O4A	2.49	0.45
1:O:310:PHE:HB2	1:O:379:ILE:HD13	1.98	0.45
1:M:175:THR:HB	1:M:176:PRO:HD2	1.98	0.44
1:C:127:ILE:O	1:C:131:ILE:HG13	2.17	0.44
1:K:256:ALA:HB2	1:K:295:GLY:HA2	1.99	0.44
1:K:274:TYR:CD1	1:K:275:PRO:HD2	2.52	0.44
1:M:110:VAL:HG13	1:M:111:LYS:H	1.82	0.44
1:M:195:LYS:HD2	1:M:195:LYS:N	2.31	0.44
1:M:335:PHE:HB3	1:O:36:ILE:HG21	2.00	0.44
1:E:4:GLN:OE1	1:E:7:LEU:HD12	2.18	0.44
1:G:89:ASP:OD1	1:G:136:LYS:HD3	2.17	0.44
1:O:256:ALA:HB2	1:O:295:GLY:HA2	2.00	0.44
1:H:32:ARG:HG2	1:H:33:GLN:N	2.33	0.44
1:K:71:PHE:CE2	1:K:223:GLN:HG3	2.53	0.44
1:O:268:LYS:NZ	1:O:268:LYS:CG	2.81	0.44
1:E:144:SER:O	1:E:148:LEU:HA	2.17	0.44
1:K:253:GLN:HE21	1:K:293:PHE:HD2	1.65	0.44
1:A:46:ARG:NH1	2:C:401:PLP:O3P	2.51	0.43
1:A:87:SER:HB2	1:A:113:GLY:HA3	1.99	0.43
1:M:55:LEU:HD21	1:M:238:LEU:HD12	2.00	0.43
1:E:102:PHE:HE1	1:E:118:ILE:HD11	1.83	0.43
1:E:148:LEU:HD21	1:E:296:MET:HB3	1.99	0.43
1:G:18:THR:CG2	1:G:20:ALA:H	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:CD	2:A:401:PLP:O4A	2.67	0.43
1:A:202:ASP:HA	1:C:28:THR:HA	2.00	0.43
1:O:18:THR:HG23	1:O:20:ALA:H	1.82	0.43
1:H:150:ILE:HD11	1:H:275:PRO:HB3	1.99	0.43
1:H:196:TYR:OH	1:H:296:MET:HE2	2.18	0.43
1:H:212:ASN:HD21	1:H:214:ALA:HB3	1.83	0.43
1:A:146:PRO:O	1:A:147:LEU:CB	2.60	0.43
1:G:125:SER:HA	1:G:128:LYS:HD2	2.00	0.43
1:H:90:HIS:HD2	1:H:135:THR:OG1	2.01	0.43
1:E:146:PRO:C	1:E:148:LEU:H	2.26	0.43
1:K:195:LYS:HG2	1:K:323:LEU:CD1	2.48	0.43
1:G:92:LEU:HD23	1:G:117:THR:HB	2.01	0.43
1:K:92:LEU:HB3	1:K:119:ILE:HD11	2.01	0.43
1:K:149:LYS:HB3	1:K:149:LYS:HE2	1.91	0.43
1:K:45:SER:HA	1:K:48:GLY:O	2.19	0.43
1:A:202:ASP:OD2	1:A:203:VAL:HG23	2.19	0.43
1:G:246:GLY:O	1:G:250:GLU:HG2	2.19	0.43
1:G:296:MET:HE3	1:G:323:LEU:CD1	2.49	0.43
1:K:92:LEU:HD11	1:K:131:ILE:HG13	2.01	0.43
1:O:283:TYR:CZ	1:O:287:LYS:HE2	2.51	0.43
1:O:303:ASN:HB3	1:O:306:GLU:OE1	2.19	0.43
1:G:196:TYR:HE1	1:G:252:HIS:CD2	2.37	0.42
1:M:148:LEU:CD1	1:M:297:LEU:HA	2.50	0.42
1:E:1:MET:HG3	1:E:5:THR:HB	2.00	0.42
1:K:3:MET:HE2	1:K:3:MET:HB2	1.94	0.42
1:K:59:ILE:HD12	1:K:59:ILE:HA	1.89	0.42
1:K:93:LEU:HD12	1:K:139:TYR:HB3	2.00	0.42
1:H:28:THR:HA	1:E:202:ASP:HA	2.01	0.42
1:A:3:MET:HA	1:A:3:MET:CE	2.49	0.42
1:K:63:GLU:OE1	1:K:191:HIS:HE1	2.03	0.42
1:K:98:TYR:O	1:K:99:GLY:C	2.62	0.42
1:K:124:ILE:O	1:K:127:ILE:HG12	2.19	0.42
1:O:141:GLU:HG3	1:O:170:ASP:HB3	2.01	0.42
1:H:365:GLU:HG2	1:H:366:GLN:N	2.34	0.42
1:C:93:LEU:HD12	1:C:139:TYR:HB3	2.01	0.42
1:M:253:GLN:HE21	1:M:293:PHE:HD2	1.68	0.42
1:O:40:LYS:HE3	1:O:40:LYS:HB2	1.87	0.42
1:H:298:SER:HB2	1:H:355:LEU:HD11	2.01	0.42
1:A:266:HIS:HA	1:A:267:PRO:HD3	1.91	0.42
1:E:253:GLN:HE21	1:E:293:PHE:HD2	1.67	0.42
1:K:127:ILE:HG13	1:K:128:LYS:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:TYR:CZ	1:E:50:PRO:HG3	2.54	0.42
1:K:124:ILE:HG22	1:K:128:LYS:HE2	2.02	0.42
1:M:195:LYS:HE2	1:M:322:SER:OG	2.20	0.42
1:M:196:TYR:CE2	1:M:324:GLY:HA2	2.55	0.42
1:O:167:THR:HB	1:O:186:ALA:HA	2.01	0.42
1:A:329:LEU:HB2	1:A:359:SER:HB3	2.01	0.42
1:C:329:LEU:HB2	1:C:359:SER:HB3	2.02	0.42
1:K:49:ASN:HA	1:K:50:PRO:HD3	1.95	0.42
1:K:63:GLU:OE1	1:K:191:HIS:CE1	2.73	0.42
1:M:35:ALA:CB	1:M:36:ILE:CA	2.72	0.42
1:H:46:ARG:NH1	2:E:401:PLP:O1P	2.53	0.42
1:K:316:LEU:HD23	1:K:368:LEU:HD23	2.02	0.42
1:M:128:LYS:HA	1:M:131:ILE:HD12	2.01	0.42
1:E:6:LYS:HD3	1:E:61:ASP:OD1	2.19	0.41
1:K:296:MET:HE1	1:K:323:LEU:HB2	2.01	0.41
1:M:28:THR:HA	1:O:202:ASP:HA	2.01	0.41
1:O:296:MET:HE1	1:O:323:LEU:HB2	2.01	0.41
1:C:143:PRO:HB2	1:C:148:LEU:HD23	2.01	0.41
1:K:283:TYR:O	1:K:287:LYS:HE2	2.19	0.41
1:M:320:GLY:O	1:M:336:MET:HE1	2.20	0.41
1:O:152:ASP:OD2	1:O:155:GLN:HG3	2.19	0.41
1:H:173:PHE:O	1:H:294:SER:OG	2.31	0.41
1:C:105:PHE:HA	1:C:109:LEU:HB2	2.02	0.41
1:C:112:ASN:HD22	1:C:112:ASN:HA	1.69	0.41
1:H:49:ASN:HA	1:H:50:PRO:HD3	1.90	0.41
1:O:117:THR:HG23	1:O:118:ILE:O	2.20	0.41
1:A:277:LEU:HB3	1:A:279:THR:HG23	2.02	0.41
1:C:314:LEU:HD21	1:C:372:LEU:HD23	2.03	0.41
1:E:332:ILE:HA	1:E:333:PRO:HD2	1.90	0.41
1:G:145:ASN:HA	1:G:146:PRO:HA	1.80	0.41
1:K:171:ASN:O	1:K:174:ALA:O	2.38	0.41
1:M:296:MET:CE	1:M:323:LEU:HB2	2.50	0.41
1:H:127:ILE:O	1:H:131:ILE:HG13	2.21	0.41
1:A:212:ASN:HD21	1:A:214:ALA:HB3	1.85	0.41
1:C:107:GLN:HE21	1:C:107:GLN:HA	1.85	0.41
1:C:142:THR:HA	1:C:143:PRO:C	2.46	0.41
1:K:301:LEU:H	1:K:301:LEU:HD23	1.85	0.41
1:O:288:LYS:HD3	1:O:288:LYS:HA	1.44	0.41
1:H:256:ALA:HB2	1:H:295:GLY:HA2	2.02	0.41
1:H:286:ALA:HB1	1:H:290:MET:HE2	2.01	0.41
1:A:277:LEU:C	1:A:279:THR:H	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:THR:OG1	1:E:211:ASN:N	2.53	0.41
1:K:127:ILE:CG1	1:K:128:LYS:N	2.83	0.41
1:O:195:LYS:HG3	1:O:323:LEU:O	2.21	0.41
1:H:63:GLU:OE1	1:H:191:HIS:HE1	2.04	0.41
1:H:264:GLU:C	1:H:266:HIS:H	2.29	0.41
1:C:103:ARG:HG3	1:C:107:GLN:HG3	2.03	0.41
1:C:271:ARG:HB2	1:C:300:THR:HG22	2.02	0.41
1:K:119:ILE:HD12	1:K:127:ILE:HG22	2.02	0.41
1:H:120:ASP:HB3	1:H:126:GLN:HE22	1.83	0.41
1:H:261:GLU:O	1:H:265:LYS:HG2	2.21	0.41
1:H:281:PRO:O	1:H:282:ASN:HB2	2.21	0.41
1:E:55:LEU:HD21	1:E:238:LEU:HD13	2.02	0.41
1:E:296:MET:HE2	1:E:323:LEU:CB	2.50	0.41
1:E:296:MET:HE2	1:E:323:LEU:HB2	2.01	0.41
1:G:73:SER:HB2	2:G:401:PLP:O3P	2.21	0.41
1:K:296:MET:HE1	1:K:359:SER:OG	2.21	0.41
1:K:297:LEU:HD11	1:K:358:LEU:HD12	2.03	0.41
1:M:333:PRO:HD2	1:M:355:LEU:O	2.21	0.41
1:O:245:LEU:O	1:O:249:MET:HG2	2.21	0.41
1:O:296:MET:HE1	1:O:359:SER:CB	2.51	0.41
1:A:23:VAL:HA	1:A:24:PRO:HD3	1.93	0.41
1:E:271:ARG:HB2	1:E:300:THR:HG22	2.03	0.41
1:K:194:THR:OG1	1:K:204:VAL:HA	2.21	0.41
1:M:175:THR:HB	1:M:176:PRO:CD	2.51	0.41
1:A:269:VAL:HG13	1:A:299:PHE:HD1	1.86	0.40
1:G:175:THR:C	1:G:177:TYR:N	2.79	0.40
1:K:42:TYR:CE1	1:K:50:PRO:HG3	2.57	0.40
1:K:75:LEU:O	1:K:76:ALA:C	2.63	0.40
1:H:15:ASP:HB2	1:H:24:PRO:HD3	2.03	0.40
1:H:161:LYS:O	1:H:163:HIS:O	2.40	0.40
1:H:329:LEU:HB2	1:H:359:SER:HB3	2.02	0.40
1:C:371:ASP:O	1:C:374:GLN:HG3	2.21	0.40
1:E:1:MET:HB3	1:G:34:ASP:O	2.22	0.40
1:G:4:GLN:HE21	1:G:7:LEU:CD1	2.30	0.40
1:K:90:HIS:CE1	1:K:117:THR:OG1	2.75	0.40
1:H:212:ASN:ND2	1:H:214:ALA:HB3	2.35	0.40
1:H:301:LEU:HD23	1:H:354:GLY:O	2.21	0.40
1:A:322:SER:OG	1:A:323:LEU:N	2.52	0.40
1:E:296:MET:SD	1:E:359:SER:HA	2.61	0.40
1:O:253:GLN:HE21	1:O:293:PHE:HD2	1.68	0.40
1:C:15:ASP:HB2	1:C:24:PRO:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:296:MET:HE1	1:G:359:SER:OG	2.21	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	359/388 (92%)	339 (94%)	17 (5%)	3 (1%)	16	30
1	C	360/388 (93%)	341 (95%)	15 (4%)	4 (1%)	11	22
1	E	358/388 (92%)	337 (94%)	20 (6%)	1 (0%)	36	56
1	G	359/388 (92%)	343 (96%)	15 (4%)	1 (0%)	36	56
1	H	369/388 (95%)	350 (95%)	18 (5%)	1 (0%)	36	56
1	K	374/388 (96%)	355 (95%)	17 (4%)	2 (0%)	24	43
1	M	359/388 (92%)	343 (96%)	14 (4%)	2 (1%)	21	38
1	O	363/388 (94%)	339 (93%)	22 (6%)	2 (1%)	21	38
All	All	2901/3104 (94%)	2747 (95%)	138 (5%)	16 (1%)	21	38

All (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
1	G	352	ARG
1	M	35	ALA
1	H	201	SER
1	A	34	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	302	LYS
1	E	354	GLY
1	A	35	ALA
1	C	175	THR
1	C	294	SER
1	K	343	LYS
1	O	119	ILE

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%)	8	17
1	C	295/316 (93%)	275 (93%)	20 (7%)	14	27
1	E	284/316 (90%)	264 (93%)	20 (7%)	14	26
1	G	292/316 (92%)	271 (93%)	21 (7%)	13	25
1	H	299/316 (95%)	274 (92%)	25 (8%)	10	19
1	K	302/316 (96%)	276 (91%)	26 (9%)	10	18
1	M	293/316 (93%)	269 (92%)	24 (8%)	10	20
1	O	293/316 (93%)	275 (94%)	18 (6%)	17	31
All	All	2351/2528 (93%)	2170 (92%)	181 (8%)	12	22

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	17	THR
1	H	18	THR
1	H	34	ASP
1	H	45	SER
1	H	87	SER
1	H	93	LEU
1	H	107	GLN
1	H	110	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	118	ILE
1	H	127	ILE
1	H	166	LEU
1	H	215	LEU
1	H	238	LEU
1	H	257	LEU
1	H	258	CYS
1	H	265	LYS
1	H	301	LEU
1	H	313	SER
1	H	336	MET
1	H	337	THR
1	H	340	CYS
1	H	343	LYS
1	H	344	THR
1	H	365	GLU
1	H	373	GLU
1	A	1	MET
1	A	3	MET
1	A	4	GLN
1	A	17	THR
1	A	18	THR
1	A	32	ARG
1	A	93	LEU
1	A	107	GLN
1	A	114	LEU
1	A	119	ILE
1	A	124	ILE
1	A	127	ILE
1	A	136	LYS
1	A	142	THR
1	A	145	ASN
1	A	147	LEU
1	A	166	LEU
1	A	195	LYS
1	A	215	LEU
1	A	238	LEU
1	A	265	LYS
1	A	271	ARG
1	A	279	THR
1	A	298	SER
1	A	301	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	304	ASP
1	A	323	LEU
1	C	8	ILE
1	C	17	THR
1	C	18	THR
1	C	67	LYS
1	C	81	VAL
1	C	87	SER
1	C	93	LEU
1	C	107	GLN
1	C	114	LEU
1	C	119	ILE
1	C	124	ILE
1	C	127	ILE
1	C	136	LYS
1	C	144	SER
1	C	167	THR
1	C	195	LYS
1	C	238	LEU
1	C	258	CYS
1	C	288	LYS
1	C	304	ASP
1	E	2	ARG
1	E	3	MET
1	E	4	GLN
1	E	17	THR
1	E	18	THR
1	E	33	GLN
1	E	67	LYS
1	E	93	LEU
1	E	104	LEU
1	E	107	GLN
1	E	119	ILE
1	E	124	ILE
1	E	131	ILE
1	E	132	LYS
1	E	166	LEU
1	E	195	LYS
1	E	215	LEU
1	E	265	LYS
1	E	288	LYS
1	E	296	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	2	ARG
1	G	4	GLN
1	G	17	THR
1	G	18	THR
1	G	23	VAL
1	G	34	ASP
1	G	93	LEU
1	G	104	LEU
1	G	105	PHE
1	G	127	ILE
1	G	166	LEU
1	G	195	LYS
1	G	197	LEU
1	G	213	GLU
1	G	215	LEU
1	G	238	LEU
1	G	258	CYS
1	G	265	LYS
1	G	288	LYS
1	G	301	LEU
1	G	378	LYS
1	K	1	MET
1	K	4	GLN
1	K	8	ILE
1	K	13	SER
1	K	17	THR
1	K	18	THR
1	K	98	TYR
1	K	104	LEU
1	K	110	VAL
1	K	117	THR
1	K	118	ILE
1	K	127	ILE
1	K	131	ILE
1	K	136	LYS
1	K	144	SER
1	K	158	SER
1	K	162	ASP
1	K	195	LYS
1	K	238	LEU
1	K	257	LEU
1	K	265	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	288	LYS
1	K	301	LEU
1	K	304	ASP
1	K	344	THR
1	K	365	GLU
1	M	3	MET
1	M	17	THR
1	M	18	THR
1	M	34	ASP
1	M	36	ILE
1	M	86	GLN
1	M	104	LEU
1	M	107	GLN
1	M	110	VAL
1	M	114	LEU
1	M	126	GLN
1	M	127	ILE
1	M	145	ASN
1	M	166	LEU
1	M	167	THR
1	M	175	THR
1	M	195	LYS
1	M	215	LEU
1	M	238	LEU
1	M	258	CYS
1	M	300	THR
1	M	301	LEU
1	M	321	GLU
1	M	336	MET
1	O	3	MET
1	O	4	GLN
1	O	17	THR
1	O	18	THR
1	O	34	ASP
1	O	67	LYS
1	O	104	LEU
1	O	107	GLN
1	O	117	THR
1	O	118	ILE
1	O	127	ILE
1	O	131	ILE
1	O	150	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	215	LEU
1	O	238	LEU
1	O	288	LYS
1	O	313	SER
1	O	336	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	90	HIS
1	H	112	ASN
1	H	126	GLN
1	H	155	GLN
1	H	163	HIS
1	H	179	GLN
1	H	212	ASN
1	H	253	GLN
1	H	345	GLN
1	A	39	HIS
1	A	90	HIS
1	A	106	ASN
1	A	107	GLN
1	A	112	ASN
1	A	163	HIS
1	A	212	ASN
1	A	217	GLN
1	A	253	GLN
1	C	9	HIS
1	C	107	GLN
1	C	112	ASN
1	C	155	GLN
1	C	212	ASN
1	C	253	GLN
1	C	280	HIS
1	E	33	GLN
1	E	90	HIS
1	E	212	ASN
1	E	239	GLN
1	E	253	GLN
1	G	4	GLN
1	G	90	HIS
1	G	112	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	163	HIS
1	G	212	ASN
1	G	233	GLN
1	G	253	GLN
1	G	280	HIS
1	K	27	GLN
1	K	90	HIS
1	K	107	GLN
1	K	112	ASN
1	K	179	GLN
1	K	191	HIS
1	K	212	ASN
1	K	224	ASN
1	K	253	GLN
1	K	345	GLN
1	M	27	GLN
1	M	79	HIS
1	M	86	GLN
1	M	107	GLN
1	M	155	GLN
1	M	212	ASN
1	M	217	GLN
1	M	253	GLN
1	M	282	ASN
1	O	4	GLN
1	O	9	HIS
1	O	79	HIS
1	O	90	HIS
1	O	163	HIS
1	O	179	GLN
1	O	212	ASN
1	O	253	GLN
1	O	282	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	PO4	K	401	-	4,4,4	3.12	4 (100%)	6,6,6	1.56	2 (33%)
2	PLP	A	401	-	14,15,16	2.22	2 (14%)	15,21,23	1.95	2 (13%)
2	PLP	M	401	-	14,15,16	2.15	2 (14%)	15,21,23	2.01	2 (13%)
2	PLP	O	401	-	14,15,16	2.38	2 (14%)	15,21,23	1.67	2 (13%)
2	PLP	E	401	-	14,15,16	2.32	2 (14%)	15,21,23	1.68	2 (13%)
2	PLP	H	401	-	14,15,16	2.41	2 (14%)	15,21,23	1.57	1 (6%)
2	PLP	G	401	1	15,15,16	2.91	7 (46%)	21,22,23	2.07	9 (42%)
2	PLP	C	401	-	14,15,16	2.38	2 (14%)	15,21,23	1.67	1 (6%)

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	-	-	2/8/8/8	0/1/1/1
2	PLP	M	401	-	-	2/8/8/8	0/1/1/1
2	PLP	O	401	-	-	2/8/8/8	0/1/1/1
2	PLP	E	401	-	-	0/8/8/8	0/1/1/1
2	PLP	H	401	-	-	1/8/8/8	0/1/1/1
2	PLP	G	401	1	-	2/6/6/8	0/1/1/1
2	PLP	C	401	-	-	2/8/8/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	PLP	O3-C3	-6.59	1.21	1.36
2	O	401	PLP	C4-C3	6.48	1.49	1.41
2	E	401	PLP	C4-C3	6.34	1.49	1.41
2	C	401	PLP	C4-C3	6.32	1.49	1.41
2	H	401	PLP	C4-C3	6.17	1.49	1.41
2	A	401	PLP	C4-C3	6.09	1.48	1.41
2	H	401	PLP	C4-C5	5.94	1.50	1.42
2	M	401	PLP	C4-C3	5.78	1.48	1.41
2	C	401	PLP	C4-C5	5.72	1.49	1.42
2	O	401	PLP	C4-C5	5.55	1.49	1.42
2	E	401	PLP	C4-C5	5.38	1.49	1.42
2	A	401	PLP	C4-C5	5.08	1.49	1.42
2	M	401	PLP	C4-C5	5.04	1.49	1.42
2	G	401	PLP	C3-C2	-4.59	1.36	1.41
2	G	401	PLP	P-O2P	-3.78	1.40	1.54
2	G	401	PLP	P-O3P	-3.70	1.41	1.54
3	K	401	PO4	P-O1	-3.42	1.42	1.50
3	K	401	PO4	P-O2	-3.12	1.45	1.54
2	G	401	PLP	P-O4P	-3.06	1.50	1.60
3	K	401	PO4	P-O4	-2.99	1.45	1.54
3	K	401	PO4	P-O3	-2.92	1.46	1.54
2	G	401	PLP	C5-C4	-2.65	1.37	1.40
2	G	401	PLP	P-O1P	-2.49	1.42	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C6-N1-C2	5.36	124.79	117.51
2	M	401	PLP	C6-N1-C2	5.27	124.68	117.51
2	C	401	PLP	C6-N1-C2	5.25	124.64	117.51
2	O	401	PLP	C6-N1-C2	5.02	124.33	117.51
2	E	401	PLP	C6-N1-C2	4.77	124.00	117.51
2	H	401	PLP	C6-N1-C2	4.53	123.66	117.51
2	M	401	PLP	O4A-C4A-C4	-4.27	114.67	124.80
2	G	401	PLP	O4P-C5A-C5	4.12	117.08	109.36
2	A	401	PLP	O4A-C4A-C4	-3.90	115.56	124.80
2	G	401	PLP	O2P-P-O4P	-3.89	96.52	106.67
2	G	401	PLP	C6-C5-C4	2.74	120.34	118.10
2	G	401	PLP	C5-C6-N1	-2.67	119.49	123.83
2	E	401	PLP	O4A-C4A-C4	-2.58	118.68	124.80
3	K	401	PO4	O4-P-O2	2.53	115.78	107.91
2	G	401	PLP	O3P-P-O4P	-2.46	100.25	106.67
2	G	401	PLP	O4P-P-O1P	-2.44	99.84	106.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	PLP	C4A-C4-C5	2.44	123.45	120.94
2	O	401	PLP	O4A-C4A-C4	-2.33	119.28	124.80
2	G	401	PLP	O3P-P-O1P	2.24	119.55	110.83
2	G	401	PLP	O2P-P-O1P	2.20	119.39	110.83
3	K	401	PO4	O4-P-O1	-2.04	103.75	110.95

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	401	PLP	C5A-O4P-P-O2P
2	G	401	PLP	C5A-O4P-P-O3P
2	M	401	PLP	C3-C4-C4A-O4A
2	O	401	PLP	C3-C4-C4A-O4A
2	A	401	PLP	C3-C4-C4A-O4A
2	C	401	PLP	C3-C4-C4A-O4A
2	A	401	PLP	C5-C4-C4A-O4A
2	M	401	PLP	C5-C4-C4A-O4A
2	O	401	PLP	C5-C4-C4A-O4A
2	H	401	PLP	C3-C4-C4A-O4A
2	C	401	PLP	C5-C4-C4A-O4A

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	4	0
2	M	401	PLP	3	0
2	E	401	PLP	1	0
2	H	401	PLP	3	0
2	G	401	PLP	2	0
2	C	401	PLP	3	0

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%)	0.18	11 (3%) 52 50	25, 43, 65, 81	0
1	C	366/388 (94%)	0.01	7 (1%) 66 64	23, 39, 62, 74	0
1	E	364/388 (93%)	0.26	16 (4%) 39 38	26, 42, 71, 88	0
1	G	365/388 (94%)	0.15	10 (2%) 56 54	22, 40, 68, 87	0
1	H	373/388 (96%)	0.05	4 (1%) 78 77	27, 39, 58, 79	0
1	K	378/388 (97%)	0.25	7 (1%) 66 64	27, 47, 71, 95	0
1	M	365/388 (94%)	0.30	13 (3%) 46 44	25, 47, 70, 96	0
1	O	367/388 (94%)	0.33	11 (2%) 52 50	28, 49, 75, 88	0
All	All	2941/3104 (94%)	0.19	79 (2%) 56 54	22, 43, 70, 96	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	GLY	5.6
1	O	349	ALA	5.3
1	M	37	GLY	5.1
1	G	45	SER	4.6
1	E	37	GLY	4.4
1	K	39	HIS	4.2
1	G	348	ALA	4.0
1	M	349	ALA	3.9
1	M	41	GLY	3.8
1	E	348	ALA	3.7
1	E	44	TYR	3.6
1	K	36	ILE	3.5
1	E	349	ALA	3.5
1	O	164	GLY	3.5
1	A	34	ASP	3.4
1	E	351	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	337	THR	3.3
1	E	42	TYR	3.3
1	C	349	ALA	3.1
1	A	273	TYR	3.1
1	K	96	ASP	3.1
1	E	353	ASP	3.0
1	G	337	THR	2.9
1	E	47	SER	2.9
1	K	98	TYR	2.9
1	O	351	ILE	2.9
1	O	119	ILE	2.9
1	G	335	PHE	2.9
1	C	41	GLY	2.8
1	H	174	ALA	2.8
1	A	277	LEU	2.8
1	O	36	ILE	2.7
1	M	380	GLY	2.6
1	G	349	ALA	2.6
1	E	95	ASP	2.6
1	G	377	ALA	2.6
1	K	97	VAL	2.6
1	O	174	ALA	2.6
1	A	38	ARG	2.6
1	E	112	ASN	2.5
1	M	307	ALA	2.5
1	K	99	GLY	2.4
1	O	352	ARG	2.4
1	M	102	PHE	2.4
1	C	338	HIS	2.3
1	E	350	GLY	2.3
1	M	354	GLY	2.3
1	M	174	ALA	2.3
1	A	145	ASN	2.3
1	O	37	GLY	2.3
1	A	211	ASN	2.3
1	O	350	GLY	2.3
1	C	337	THR	2.3
1	A	354	GLY	2.3
1	H	293	PHE	2.3
1	K	4	GLN	2.2
1	E	279	THR	2.2
1	E	335	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	92	LEU	2.2
1	M	115	SER	2.2
1	G	217	GLN	2.1
1	A	39	HIS	2.1
1	A	379	ILE	2.1
1	M	34	ASP	2.1
1	G	336	MET	2.1
1	G	332	ILE	2.1
1	G	46	ARG	2.1
1	O	124	ILE	2.1
1	E	336	MET	2.1
1	M	336	MET	2.1
1	H	96	ASP	2.0
1	M	93	LEU	2.0
1	H	41	GLY	2.0
1	C	127	ILE	2.0
1	E	97	VAL	2.0
1	C	144	SER	2.0
1	A	300	THR	2.0
1	E	17	THR	2.0
1	M	4	GLN	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 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	H	401	15/16	0.89	0.13	45,54,56,65	0
2	PLP	E	401	15/16	0.89	0.12	49,51,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	G	401	15/16	0.90	0.12	30,31,31,31	0
2	PLP	O	401	15/16	0.90	0.13	47,54,57,57	0
2	PLP	M	401	15/16	0.92	0.10	41,42,43,43	0
2	PLP	A	401	15/16	0.94	0.09	38,42,43,44	0
2	PLP	C	401	15/16	0.94	0.09	34,39,43,44	0
3	PO4	K	401	5/5	0.96	0.10	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.