



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:50 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

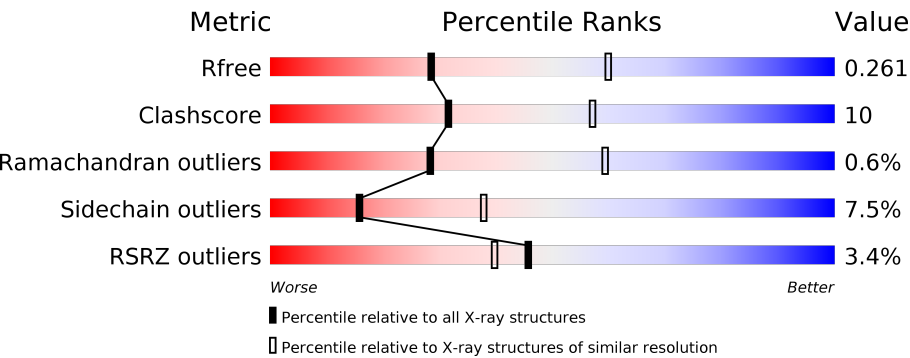
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

# 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 2.76 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 <sub>free</sub>	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div><div>%</div><div><div></div><div>67%</div><div>22%</div><div>•</div><div>6%</div></div></div>
1	C	388	<div><div>2%</div><div><div></div><div>76%</div><div>16%</div><div>•</div><div>6%</div></div></div>
1	E	388	<div><div>3%</div><div><div></div><div>73%</div><div>19%</div><div>••</div><div>6%</div></div></div>
1	G	388	<div><div>6%</div><div><div></div><div>72%</div><div>19%</div><div>•</div><div>6%</div></div></div>
1	H	388	<div><div></div><div><div></div><div>74%</div><div>20%</div><div>•</div><div>•</div></div></div>
1	K	388	<div><div>3%</div><div><div></div><div>75%</div><div>20%</div><div>•</div><div>•</div></div></div>

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Mol	Chain	Length	Quality of chain
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
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

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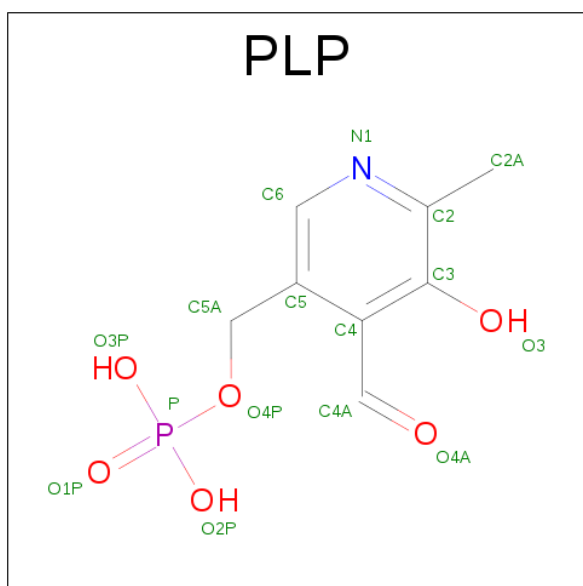
Chain	Residue	Modelled	Actual	Comment	Reference
A	386	HIS	-	EXPRESSION TAG	UNP P56069
A	387	HIS	-	EXPRESSION TAG	UNP P56069
A	388	HIS	-	EXPRESSION TAG	UNP P56069
C	381	LEU	-	EXPRESSION TAG	UNP P56069
C	382	GLU	-	EXPRESSION TAG	UNP P56069
C	383	HIS	-	EXPRESSION TAG	UNP P56069
C	384	HIS	-	EXPRESSION TAG	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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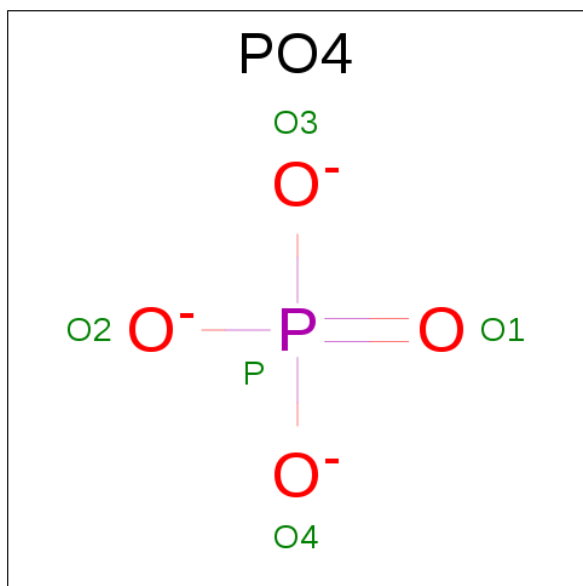
Chain	Residue	Modelled	Actual	Comment	Reference
M	388	HIS	-	EXPRESSION TAG	UNP P56069
O	381	LEU	-	EXPRESSION TAG	UNP P56069
O	382	GLU	-	EXPRESSION TAG	UNP P56069
O	383	HIS	-	EXPRESSION TAG	UNP P56069
O	384	HIS	-	EXPRESSION TAG	UNP P56069
O	385	HIS	-	EXPRESSION TAG	UNP P56069
O	386	HIS	-	EXPRESSION TAG	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: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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:  $\text{O}_4\text{P}$ ).

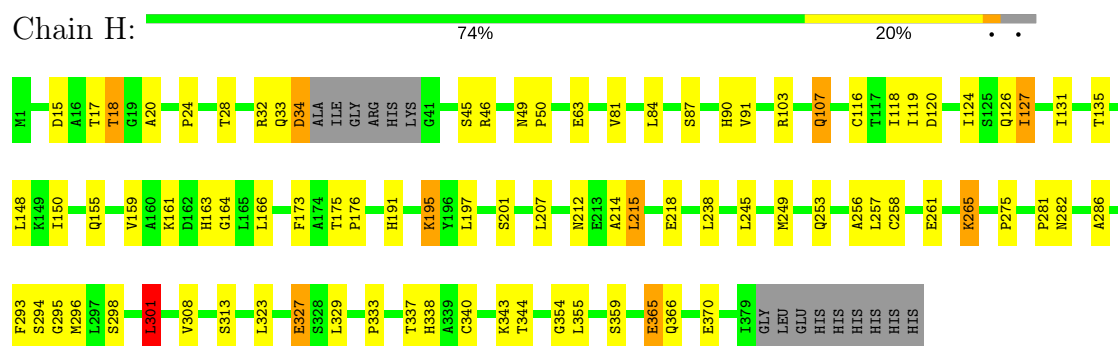


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	P	0	0
			5	4	1		

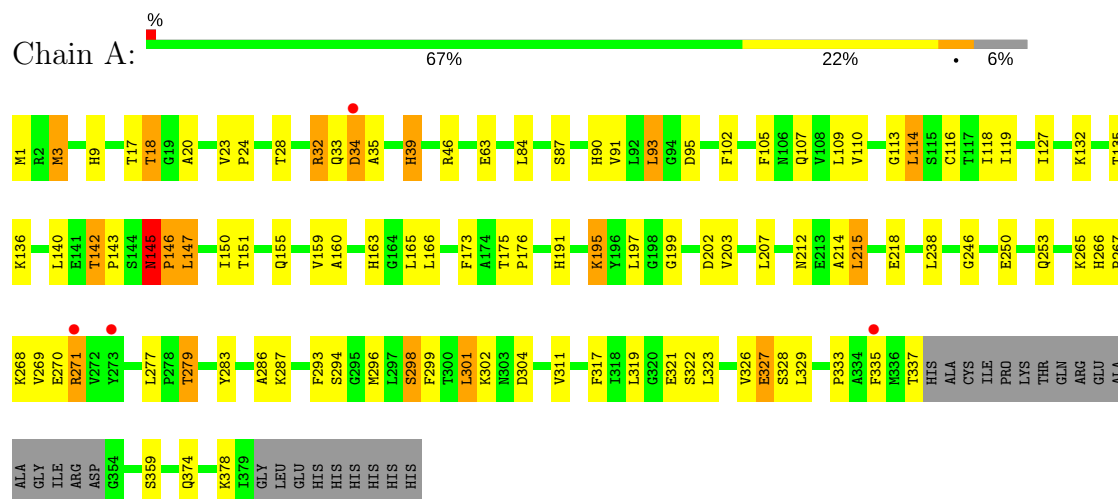
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

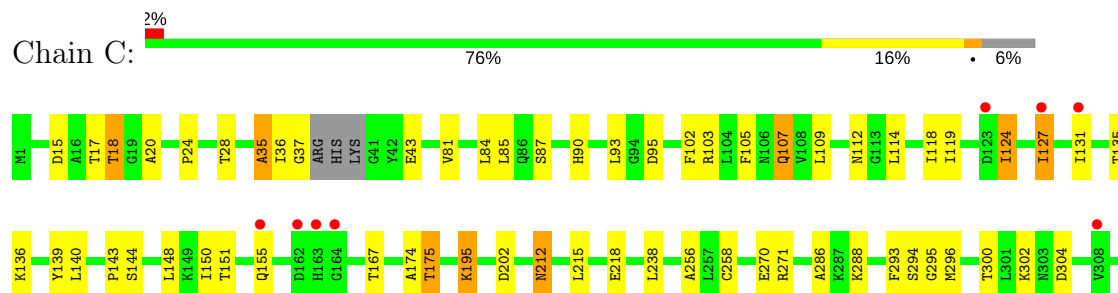
#### • Molecule 1: Cystathionine gamma-synthase



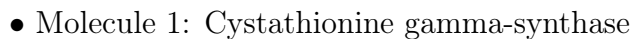
#### • Molecule 1: Cystathionine gamma-synthase

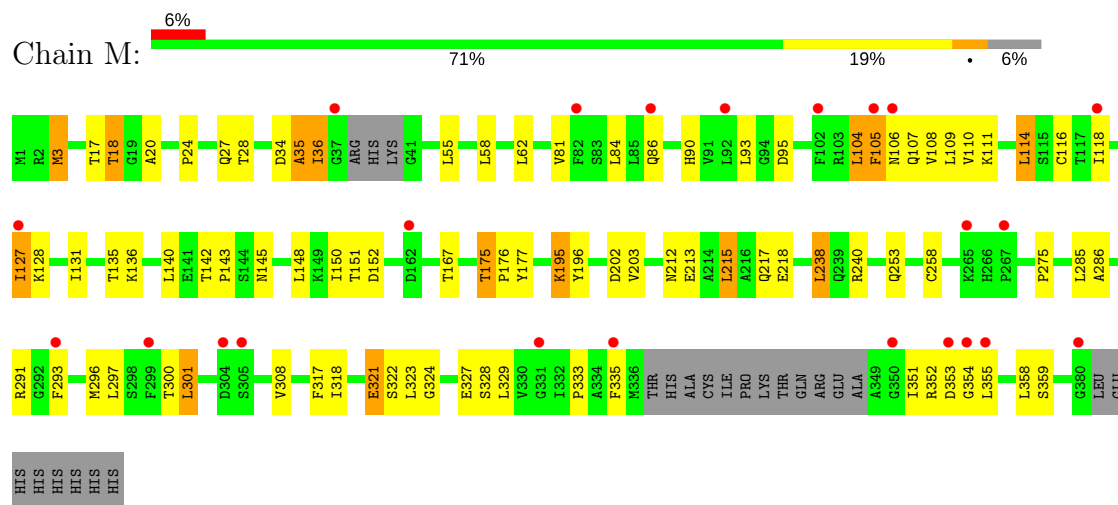


#### • Molecule 1: Cystathionine gamma-synthase

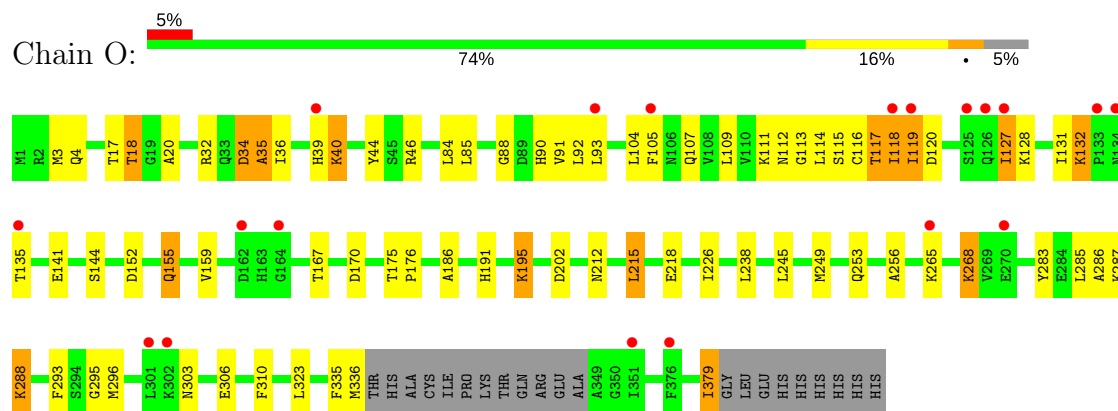








• Molecule 1: Cystathionine gamma-synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	4233 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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%)

All (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
1	O	268	LYS	CE-NZ	8.65	1.70	1.49
1	A	270	GLU	CD-OE1	8.32	1.34	1.25
1	O	379	ILE	C-O	7.86	1.38	1.23
1	A	270	GLU	CD-OE2	7.38	1.33	1.25
1	G	43	GLU	CD-OE2	7.06	1.33	1.25
1	G	112	ASN	CG-OD1	-6.78	1.09	1.24
1	C	338	HIS	CG-CD2	6.68	1.47	1.35
1	A	145	ASN	CG-OD1	6.62	1.38	1.24
1	O	265	LYS	CE-NZ	6.45	1.65	1.49
1	A	145	ASN	CB-CG	6.19	1.65	1.51
1	O	40	LYS	CD-CE	6.11	1.66	1.51
1	A	146	PRO	N-CD	6.08	1.56	1.47
1	G	44	TYR	CG-CD1	6.07	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	39	HIS	CE1-NE2	-5.85	1.19	1.32
1	E	4	GLN	CD-OE1	5.64	1.36	1.24
1	G	44	TYR	CE2-CZ	5.33	1.45	1.38
1	O	115	SER	CB-OG	5.31	1.49	1.42
1	A	268	LYS	CG-CD	5.22	1.70	1.52
1	K	346	ARG	CZ-NH1	5.18	1.39	1.33
1	A	298	SER	CB-OG	5.17	1.49	1.42
1	O	111	LYS	CB-CG	5.10	1.66	1.52

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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	15	0	5	0	0
3	K	5	0	0	0	0
All	All	22365	0	22236	454	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 10.

All (454) 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:C:296:MET:HE1	1:C:323:LEU:HB2	1.48	0.94
1:M:35:ALA:HB1	1:M:36:ILE:CA	1.99	0.92
1:M:321:GLU:O	1:M:321:GLU:HG3	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:H:296:MET:HE1	1:H:323:LEU:HB2	1.56	0.87
1:M:3:MET:HE1	1:M:62:LEU:HD22	1.54	0.86
1:A:150:ILE:HD13	1:A:286:ALA:HB2	1.59	0.85
1:A:301:LEU:HD23	1:A:301:LEU:H	1.44	0.83
1:G:2:ARG:HH11	1:G:2:ARG:HG3	1.42	0.83
1:G:331:GLY:HA2	1:G:336:MET:HE1	1.61	0.82
1:G:212:ASN:HD22	1:G:215:LEU:H	1.27	0.81
1:O:283:TYR:CE2	1:O:287:LYS:HE2	2.15	0.81
1:O:296:MET:HE1	1:O:323:LEU:HB2	1.63	0.80
1:G:296:MET:HE1	1:G:323:LEU:HB2	1.62	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:THR:HG22	1:G:20:ALA:H	1.46	0.78
1:O:288:LYS:CD	1:O:288:LYS:O	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:G:111:LYS:C	1:G:112:ASN:HD22	1.88	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: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
1:O:288:LYS:C	1:O:288:LYS:CD	2.55	0.73
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:HB2	1:O:135:THR:HG23	1.71	0.71
1:O:132:LYS:CD	1:O:132:LYS:NZ	2.53	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:K:296:MET:HE1	1:K:323:LEU:HB2	1.72	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:CD2	1:A:39:HIS:H	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:A:145:ASN:HB2	1:A:173:PHE:CZ	2.27	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:A:301:LEU:H	1:A:301:LEU:CD2	2.07	0.67
1:M:3:MET:HE1	1:M:62:LEU:CD2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:296:MET:HE1	1:M:323:LEU:HB2	1.77	0.67
1:C:90:HIS:HB3	1:C:135:THR:HA	1.76	0.67
1:H:195:LYS:NZ	2:H:401:PLP:C4A	2.58	0.67
1:O:92:LEU:HB3	1:O:119:ILE:HD11	1.75	0.67
1:O:119:ILE:HD12	1:O:127:ILE:HG22	1.75	0.67
1:O:84:LEU:CD2	1:O:218:GLU:HB3	2.24	0.67
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:O:288:LYS:C	1:O:288:LYS:HD3	1.87	0.66
1:C:195:LYS:HZ1	2:C:401:PLP:C4A	2.09	0.65
1:E:253:GLN:NE2	1:E:293:PHE:H	1.94	0.65
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:286:ALA:C	1:O:288:LYS:H	1.99	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:CD	1:E:378:LYS:NZ	2.60	0.64
1:O:286:ALA:C	1:O:288:LYS:N	2.48	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:C:84:LEU:C	1:C:85:LEU:HD23	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:226:ILE:O	1:O:226:ILE:HG22	1.99	0.60
1:M:3:MET:CE	1:M:62:LEU:HD22	2.27	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: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
1:C:35:ALA:CB	1:C:36:ILE:CA	2.70	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:G:331:GLY:CA	1:G:336:MET:HE1	2.32	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:O:85:LEU:HD23	1:O:85:LEU:N	2.19	0.58
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: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:M:36:ILE:HG21	1:O:335:PHE:HB3	1.85	0.57
1:A:199:GLY:O	1:A:326:VAL:HG13	2.04	0.56
1:G:351:ILE:C	1:G:352:ARG:O	2.39	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: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:C:195:LYS:HD2	1:C:195:LYS:N	2.21	0.55
1:H:212:ASN:HB3	1:H:215:LEU:HB2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:343:LYS:HA	1:K:346:ARG:HD2	1.89	0.55
1:O:92:LEU:HD23	1:O:117:THR:CG2	2.36	0.55
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:O:105:PHE:HA	1:O:109:LEU:HB2	1.88	0.55
1:O:84:LEU:C	1:O:85:LEU:HD23	2.27	0.55
1:C:212:ASN:HD22	1:C:215:LEU:H	1.53	0.55
1:A:267:PRO:O	1:A:302:LYS:HD2	2.07	0.54
1:C:35:ALA:HB1	1:C:36:ILE:C	2.26	0.54
1:K:284:GLU:HA	1:K:287:LYS:CE	2.37	0.54
1:M:318:ILE:HG23	1:O:32:ARG:HG3	1.89	0.54
1:M:81:VAL:O	1:M:84:LEU:HG	2.06	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:A:1:MET:HE2	1:A:9:HIS:HB2	1.90	0.53
1:G:212:ASN:ND2	1:G:215:LEU:H	2.02	0.53
1:H:245:LEU:O	1:H:249:MET:HG2	2.07	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: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:C:140:LEU:HD22	1:C:151:THR:HG21	1.91	0.52
1:H:333:PRO:O	1:H:338:HIS:HB2	2.10	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:G:351:ILE:O	1:G:352:ARG:C	2.46	0.52
1:M:36:ILE:N	1:M:36:ILE:CD1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:131:ILE:HG22	1:O:132:LYS:N	2.24	0.52
1:A:333:PRO:HB3	1:A:337:THR:OG1	2.09	0.52
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:131:ILE:CG2	1:O:132:LYS:N	2.73	0.51
1:K:90:HIS:HD2	1:K:135:THR:OG1	1.93	0.51
1:C:195:LYS:NZ	2:C:401:PLP:C4A	2.72	0.51
1:H:124:ILE:HD13	1:H:155:GLN:NE2	2.22	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:118:ILE:HG23	1:O:119:ILE:N	2.26	0.51
1:M:109:LEU:O	1:M:114:LEU:HB2	2.11	0.51
1:A:271:ARG:HH11	1:A:271:ARG:HG2	1.76	0.51
1:E:297:LEU:HD11	1:E:358:LEU:HD12	1.92	0.51
1:G:351:ILE:O	1:G:352:ARG:O	2.29	0.50
1:H:327:GLU:H	1:H:327:GLU:CD	2.14	0.50
1:E:148:LEU:CD1	1:E:297:LEU:HA	2.41	0.50
1:A:95:ASP:HA	1:A:118:ILE:CG2	2.42	0.50
1:H:195:LYS:HD2	1:H:195:LYS:N	2.26	0.50
1:K:18:THR:HG23	1:K:20:ALA:H	1.75	0.50
1:M:352:ARG:C	1:M:354:GLY:H	2.15	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: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:155:GLN:O	1:O:159:VAL:HG23	2.12	0.50
1:O:34:ASP:OD1	1:O:40:LYS:HE2	2.11	0.50
1:A:311:VAL:CG1	1:A:319:LEU:HD13	2.42	0.50
1:G:327:GLU:H	1:G:327:GLU:CD	2.15	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: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:E:296:MET:HE2	1:E:323:LEU:HD22	1.93	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
1:E:150:ILE:HD11	1:E:275:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LEU:HD12	1:E:184:LEU:HD12	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: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: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:H:18:THR:HG22	1:H:20:ALA:H	1.77	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:E:195:LYS:HZ2	1:E:323:LEU:HG	1.77	0.48
1:O:268:LYS:CD	1:O:268:LYS:NZ	2.65	0.48
1:H:308:VAL:HG13	1:E:36:ILE:HD12	1.96	0.48
1:O:175:THR:HB	1:O:176:PRO:HD2	1.95	0.48
1:O:286:ALA:O	1:O:287:LYS:C	2.50	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:OE1	1:A:191:HIS:CE1	2.68	0.47
1:K:253:GLN:NE2	1:K:293:PHE:H	2.13	0.47
1:O:176:PRO:HD3	1:O:191:HIS:NE2	2.29	0.47
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:G:119:ILE:HD12	1:G:127:ILE:HA	1.98	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:K:162:ASP:OD1	1:K:163:HIS:N	2.49	0.46
1:M:195:LYS:HZ3	1:M:323:LEU:HG	1.80	0.46
1:G:150:ILE:HD13	1:G:286:ALA:HB2	1.96	0.46
1:K:109:LEU:HB3	1:K:114:LEU:HD12	1.97	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: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:M:351:ILE:N	1:M:351:ILE:HD12	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:G:301:LEU:CD2	1:G:301:LEU:H	2.29	0.45
1:A:18:THR:CG2	1:A:20:ALA:H	2.29	0.45
1:G:278:PRO:HA	1:G:283:TYR:CD2	2.51	0.45
1:G:374:GLN:O	1:G:378:LYS:HD3	2.16	0.45
1:K:18:THR:CG2	1:K:20:ALA:H	2.30	0.45
1:E:197:LEU:HD13	1:E:207:LEU:HD12	1.97	0.45
1:G:194:THR:HG23	1:G:204:VAL:HA	1.98	0.45
1:G:81:VAL:O	1:G:84:LEU:HG	2.16	0.45
1:A:317:PHE:CD2	1:A:328:SER:HB3	2.52	0.45
1:K:104:LEU:O	1:K:108:VAL:HB	2.17	0.45
1:E:253:GLN:NE2	1:E:293:PHE:CD2	2.84	0.45
1:E:90:HIS:CE1	1:E:117:THR:OG1	2.65	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:O:120:ASP:C	1:O:120:ASP:OD2	2.55	0.45
1:G:197:LEU:HD12	1:G:197:LEU:HA	1.62	0.45
1:H:81:VAL:O	1:H:84:LEU:HG	2.17	0.45
1:M:93:LEU:HD13	1:M:116:CYS:HB2	1.98	0.45
1:O:310:PHE:HB2	1:O:379:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:195:LYS:NZ	2:M:401:PLP:O4A	2.49	0.44
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:N	1:M:195:LYS:HD2	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:C:174:ALA:O	1:C:175:THR:OG1	2.29	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:CG	1:O:268:LYS:NZ	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:87:SER:HB2	1:A:113:GLY:HA3	1.99	0.43
1:A:46:ARG:NH1	2:C:401:PLP:O3P	2.51	0.43
1:H:173:PHE:O	1:H:294:SER:OG	2.31	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
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:M:142:THR:HA	1:M:143:PRO:C	2.39	0.43
1:M:177:TYR:C	1:M:291:ARG:HH21	2.22	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: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:212:ASN:HD21	1:H:214:ALA:HB3	1.83	0.43
1:H:90:HIS:HD2	1:H:135:THR:OG1	2.01	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:149:LYS:HE2	1:K:149:LYS:HB3	1.91	0.43
1:K:92:LEU:HB3	1:K:119:ILE:HD11	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:LEU:HD12	1:K:139:TYR:HB3	2.00	0.42
1:K:59:ILE:HD12	1:K:59:ILE:HA	1.89	0.42
1:A:3:MET:CE	1:A:3:MET:HA	2.49	0.42
1:H:28:THR:HA	1:E:202:ASP:HA	2.01	0.42
1:K:124:ILE:O	1:K:127:ILE:HG12	2.19	0.42
1:K:63:GLU:OE1	1:K:191:HIS:HE1	2.03	0.42
1:O:141:GLU:HG3	1:O:170:ASP:HB3	2.01	0.42
1:C:93:LEU:HD12	1:C:139:TYR:HB3	2.01	0.42
1:H:365:GLU:HG2	1:H:366:GLN:N	2.34	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
1:A:142:THR:HA	1:A:143:PRO:C	2.39	0.42
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:A:296:MET:HE1	1:A:359:SER:OG	2.19	0.42
1:C:329:LEU:HB2	1:C:359:SER:HB3	2.02	0.42
1:K:162:ASP:C	1:K:162:ASP:OD1	2.58	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:M:28:THR:HA	1:O:202:ASP:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:152:ASP:OD2	1:O:155:GLN:HG3	2.19	0.41
1:A:33:GLN:C	1:A:34:ASP:O	2.57	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:HE1	1:M:359:SER:OG	2.20	0.41
1:A:212:ASN:HD21	1:A:214:ALA:HB3	1.85	0.41
1:A:327:GLU:H	1:A:327:GLU:CD	2.24	0.41
1:C:107:GLN:HA	1:C:107:GLN:HE21	1.85	0.41
1:H:127:ILE:O	1:H:131:ILE:HG13	2.21	0.41
1:K:301:LEU:H	1:K:301:LEU:HD23	1.85	0.41
1:O:288:LYS:HA	1:O:288:LYS:HD3	1.44	0.41
1:E:210:THR:OG1	1:E:211:ASN:N	2.53	0.41
1:H:256:ALA:HB2	1:H:295:GLY:HA2	2.02	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: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:H:63:GLU:OE1	1:H:191:HIS:HE1	2.04	0.41
1:K:119:ILE:HD12	1:K:127:ILE:HG22	2.02	0.41
1:E:55:LEU:HD21	1:E:238:LEU:HD13	2.02	0.41
1:G:73:SER:HB2	2:G:401:PLP:O3P	2.21	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:O:245:LEU:O	1:O:249:MET:HG2	2.21	0.41
1:H:281:PRO:O	1:H:282:ASN:HB2	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:M:3:MET:HE3	1:M:3:MET:HA	2.02	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:K:42:TYR:CE1	1:K:50:PRO:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:161:LYS:O	1:H:163:HIS:O	2.40	0.40
1:H:15:ASP:HB2	1:H:24:PRO:HD3	2.03	0.40
1:H:329:LEU:HB2	1:H:359:SER:HB3	2.02	0.40
1:K:90:HIS:CE1	1:K:117:THR:OG1	2.75	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: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: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

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%)	22	52
1	C	360/388 (93%)	341 (95%)	15 (4%)	4 (1%)	17	43
1	E	358/388 (92%)	337 (94%)	20 (6%)	1 (0%)	44	75
1	G	359/388 (92%)	343 (96%)	15 (4%)	1 (0%)	44	75
1	H	369/388 (95%)	350 (95%)	18 (5%)	1 (0%)	44	75
1	K	374/388 (96%)	355 (95%)	17 (4%)	2 (0%)	32	64
1	M	359/388 (92%)	343 (96%)	14 (4%)	2 (1%)	28	59
1	O	363/388 (94%)	339 (93%)	22 (6%)	2 (1%)	28	59
All	All	2901/3104 (94%)	2747 (95%)	138 (5%)	16 (1%)	28	59

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
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%)	11	28
1	C	295/316 (93%)	276 (94%)	19 (6%)	20	47
1	E	284/316 (90%)	265 (93%)	19 (7%)	19	44
1	G	292/316 (92%)	268 (92%)	24 (8%)	13	34
1	H	299/316 (95%)	275 (92%)	24 (8%)	14	35
1	K	302/316 (96%)	281 (93%)	21 (7%)	18	41
1	M	293/316 (93%)	268 (92%)	25 (8%)	12	32
1	O	293/316 (93%)	275 (94%)	18 (6%)	22	49
All	All	2351/2528 (93%)	2174 (92%)	177 (8%)	16	38

All (177) 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	107	GLN
1	H	118	ILE
1	H	127	ILE
1	H	148	LEU
1	H	166	LEU
1	H	195	LYS
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	327	GLU
1	H	337	THR
1	H	340	CYS
1	H	343	LYS
1	H	344	THR
1	H	365	GLU
1	A	3	MET
1	A	17	THR
1	A	18	THR
1	A	32	ARG
1	A	39	HIS
1	A	93	LEU
1	A	107	GLN
1	A	114	LEU
1	A	119	ILE
1	A	127	ILE
1	A	136	LYS
1	A	142	THR
1	A	145	ASN
1	A	147	LEU
1	A	155	GLN
1	A	166	LEU
1	A	195	LYS
1	A	215	LEU
1	A	238	LEU

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Mol	Chain	Res	Type
1	A	265	LYS
1	A	271	ARG
1	A	279	THR
1	A	298	SER
1	A	301	LEU
1	A	304	ASP
1	A	327	GLU
1	A	335	PHE
1	C	17	THR
1	C	18	THR
1	C	87	SER
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	212	ASN
1	C	238	LEU
1	C	258	CYS
1	C	288	LYS
1	C	293	PHE
1	C	304	ASP
1	C	327	GLU
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	45	SER
1	E	104	LEU
1	E	107	GLN
1	E	119	ILE
1	E	136	LYS
1	E	166	LEU
1	E	195	LYS
1	E	215	LEU
1	E	265	LYS

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Mol	Chain	Res	Type
1	E	288	LYS
1	E	296	MET
1	E	301	LEU
1	E	378	LYS
1	G	2	ARG
1	G	3	MET
1	G	4	GLN
1	G	17	THR
1	G	18	THR
1	G	24	PRO
1	G	34	ASP
1	G	93	LEU
1	G	104	LEU
1	G	105	PHE
1	G	112	ASN
1	G	127	ILE
1	G	136	LYS
1	G	166	LEU
1	G	195	LYS
1	G	197	LEU
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	327	GLU
1	G	378	LYS
1	K	4	GLN
1	K	13	SER
1	K	17	THR
1	K	18	THR
1	K	98	TYR
1	K	104	LEU
1	K	117	THR
1	K	118	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

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Mol	Chain	Res	Type
1	K	265	LYS
1	K	288	LYS
1	K	301	LEU
1	K	304	ASP
1	K	344	THR
1	K	365	GLU
1	K	378	LYS
1	M	3	MET
1	M	17	THR
1	M	18	THR
1	M	24	PRO
1	M	34	ASP
1	M	36	ILE
1	M	86	GLN
1	M	104	LEU
1	M	105	PHE
1	M	107	GLN
1	M	114	LEU
1	M	127	ILE
1	M	136	LYS
1	M	145	ASN
1	M	167	THR
1	M	175	THR
1	M	195	LYS
1	M	215	LEU
1	M	238	LEU
1	M	240	ARG
1	M	258	CYS
1	M	300	THR
1	M	301	LEU
1	M	321	GLU
1	M	327	GLU
1	O	3	MET
1	O	4	GLN
1	O	17	THR
1	O	18	THR
1	O	34	ASP
1	O	104	LEU
1	O	107	GLN
1	O	112	ASN
1	O	117	THR
1	O	118	ILE

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Mol	Chain	Res	Type
1	O	127	ILE
1	O	144	SER
1	O	155	GLN
1	O	195	LYS
1	O	215	LEU
1	O	238	LEU
1	O	288	LYS
1	O	336	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) 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	191	HIS
1	H	212	ASN
1	H	253	GLN
1	A	39	HIS
1	A	90	HIS
1	A	112	ASN
1	A	155	GLN
1	A	163	HIS
1	A	212	ASN
1	A	217	GLN
1	A	253	GLN
1	C	90	HIS
1	C	107	GLN
1	C	112	ASN
1	C	155	GLN
1	C	212	ASN
1	C	253	GLN
1	E	33	GLN
1	E	90	HIS
1	E	163	HIS
1	E	191	HIS
1	E	212	ASN
1	E	253	GLN
1	G	4	GLN
1	G	90	HIS

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Mol	Chain	Res	Type
1	G	112	ASN
1	G	163	HIS
1	G	212	ASN
1	G	253	GLN
1	G	280	HIS
1	K	90	HIS
1	K	112	ASN
1	K	191	HIS
1	K	212	ASN
1	K	253	GLN
1	K	345	GLN
1	M	107	GLN
1	M	155	GLN
1	M	212	ASN
1	M	253	GLN
1	O	4	GLN
1	O	9	HIS
1	O	90	HIS
1	O	112	ASN
1	O	163	HIS
1	O	212	ASN
1	O	253	GLN

### 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 carbohydrates 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	$\# Z  > 2$
2	PLP	A	401	-	15,15,16	3.27	3 (20%)	17,21,23	1.84	2 (11%)
2	PLP	C	401	-	15,15,16	3.36	3 (20%)	17,21,23	1.55	1 (5%)
2	PLP	E	401	-	15,15,16	3.37	3 (20%)	17,21,23	1.56	2 (11%)
2	PLP	G	401	1	15,15,16	3.06	7 (46%)	20,22,23	2.05	9 (45%)
2	PLP	H	401	-	15,15,16	3.52	3 (20%)	17,21,23	1.47	1 (5%)
3	PO4	K	401	-	4,4,4	2.71	4 (100%)	6,6,6	1.31	1 (16%)
2	PLP	M	401	-	15,15,16	3.16	3 (20%)	17,21,23	1.91	2 (11%)
2	PLP	O	401	-	15,15,16	3.38	3 (20%)	17,21,23	1.55	2 (11%)

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

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	PLP	O3-C3	-6.58	1.21	1.37
2	G	401	PLP	C3-C2	-6.54	1.36	1.40
3	K	401	PO4	P-O1	-3.46	1.42	1.50
2	G	401	PLP	P-O2P	-3.42	1.40	1.54
2	G	401	PLP	P-O3P	-3.35	1.41	1.54
2	G	401	PLP	P-O4P	-2.97	1.50	1.60
2	G	401	PLP	C5-C4	-2.57	1.37	1.40
3	K	401	PO4	P-O2	-2.50	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	401	PO4	P-O4	-2.39	1.45	1.54
2	G	401	PLP	P-O1P	-2.36	1.42	1.50
3	K	401	PO4	P-O3	-2.34	1.46	1.54
2	M	401	PLP	C4-C5	5.44	1.49	1.42
2	A	401	PLP	C4-C5	5.48	1.49	1.42
2	E	401	PLP	C4-C5	5.81	1.49	1.42
2	O	401	PLP	C4-C5	5.99	1.49	1.42
2	C	401	PLP	C4-C5	6.17	1.49	1.42
2	H	401	PLP	C4-C5	6.41	1.50	1.42
2	M	401	PLP	C4-C3	6.75	1.48	1.41
2	A	401	PLP	C4-C3	7.11	1.48	1.41
2	H	401	PLP	C4-C3	7.20	1.49	1.41
2	C	401	PLP	C4-C3	7.38	1.49	1.41
2	E	401	PLP	C4-C3	7.40	1.49	1.41
2	O	401	PLP	C4-C3	7.56	1.49	1.41
2	M	401	PLP	C2-C3	8.33	1.48	1.39
2	C	401	PLP	C2-C3	8.43	1.48	1.39
2	O	401	PLP	C2-C3	8.51	1.48	1.39
2	A	401	PLP	C2-C3	8.60	1.49	1.39
2	E	401	PLP	C2-C3	8.70	1.49	1.39
2	H	401	PLP	C2-C3	9.22	1.49	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	401	PLP	O4A-C4A-C4	-4.53	114.67	125.08
2	A	401	PLP	O4A-C4A-C4	-4.14	115.56	125.08
2	G	401	PLP	O2P-P-O4P	-3.84	96.52	106.73
2	E	401	PLP	O4A-C4A-C4	-2.78	118.68	125.08
2	G	401	PLP	C5-C6-N1	-2.59	119.49	123.87
2	O	401	PLP	O4A-C4A-C4	-2.52	119.28	125.08
2	G	401	PLP	O3P-P-O4P	-2.44	100.25	106.73
2	G	401	PLP	O4P-P-O1P	-2.37	99.84	106.47
3	K	401	PO4	O4-P-O2	2.14	115.78	107.90
2	G	401	PLP	O2P-P-O1P	2.27	119.39	110.50
2	G	401	PLP	O3P-P-O1P	2.31	119.55	110.50
2	G	401	PLP	C4A-C4-C5	2.57	123.45	120.86
2	G	401	PLP	C6-C5-C4	2.59	120.34	118.18
2	G	401	PLP	O4P-C5A-C5	3.86	117.08	109.32
2	H	401	PLP	C6-N1-C2	4.39	123.66	117.45
2	E	401	PLP	C6-N1-C2	4.63	124.00	117.45
2	O	401	PLP	C6-N1-C2	4.87	124.33	117.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	PLP	C6-N1-C2	5.09	124.64	117.45
2	M	401	PLP	C6-N1-C2	5.11	124.68	117.45
2	A	401	PLP	C6-N1-C2	5.19	124.79	117.45

There are no chirality outliers.

There are no torsion outliers.

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	C	401	PLP	3	0
2	E	401	PLP	1	0
2	G	401	PLP	2	0
2	H	401	PLP	3	0
2	M	401	PLP	3	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	363/388 (93%)	0.12	4 (1%) 80 78	25, 43, 65, 81	0
1	C	366/388 (94%)	0.08	9 (2%) 58 52	23, 39, 62, 74	0
1	E	364/388 (93%)	0.26	12 (3%) 47 41	26, 42, 71, 88	0
1	G	365/388 (94%)	0.23	23 (6%) 21 16	22, 40, 68, 87	0
1	H	373/388 (96%)	0.03	0 100 100	27, 39, 58, 79	0
1	K	378/388 (97%)	0.28	11 (2%) 52 46	27, 47, 71, 95	0
1	M	365/388 (94%)	0.34	23 (6%) 21 16	25, 47, 70, 96	0
1	O	367/388 (94%)	0.36	19 (5%) 28 22	28, 49, 75, 88	0
All	All	2941/3104 (94%)	0.21	101 (3%) 46 40	22, 43, 70, 96	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	164	GLY	5.6
1	O	133	PRO	4.6
1	G	335	PHE	4.6
1	O	119	ILE	4.5
1	A	273	TYR	4.2
1	O	105	PHE	4.2
1	E	350	GLY	4.0
1	G	353	ASP	3.9
1	G	332	ILE	3.9
1	M	350	GLY	3.8
1	C	127	ILE	3.6
1	M	102	PHE	3.6
1	K	98	TYR	3.5
1	G	301	LEU	3.5
1	K	119	ILE	3.4
1	G	350	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	269	VAL	3.3
1	E	306	GLU	3.3
1	G	351	ILE	3.3
1	G	273	TYR	3.2
1	G	45	SER	3.2
1	G	352	ARG	3.1
1	M	37	GLY	3.0
1	O	162	ASP	3.0
1	K	165	LEU	3.0
1	O	127	ILE	3.0
1	G	354	GLY	3.0
1	O	134	ASN	2.9
1	M	305	SER	2.9
1	G	310	PHE	2.9
1	M	293	PHE	2.8
1	M	354	GLY	2.8
1	G	265	LYS	2.8
1	C	353	ASP	2.8
1	M	92	LEU	2.8
1	G	303	ASN	2.8
1	M	106	ASN	2.7
1	M	335	PHE	2.7
1	O	351	ILE	2.7
1	A	34	ASP	2.6
1	K	379	ILE	2.6
1	C	131	ILE	2.6
1	E	309	ALA	2.6
1	C	155	GLN	2.6
1	K	373	GLU	2.6
1	K	127	ILE	2.6
1	K	118	ILE	2.6
1	E	86	GLN	2.6
1	E	335	PHE	2.6
1	G	377	ALA	2.5
1	O	118	ILE	2.5
1	C	162	ASP	2.5
1	C	164	GLY	2.5
1	K	162	ASP	2.5
1	O	302	LYS	2.5
1	G	305	SER	2.5
1	O	270	GLU	2.4
1	E	42	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	299	PHE	2.4
1	K	35	ALA	2.4
1	M	162	ASP	2.4
1	E	37	GLY	2.4
1	G	266	HIS	2.4
1	E	102	PHE	2.4
1	M	105	PHE	2.3
1	G	267	PRO	2.3
1	M	267	PRO	2.3
1	E	47	SER	2.3
1	K	133	PRO	2.3
1	G	271	ARG	2.3
1	C	123	ASP	2.3
1	K	130	ALA	2.3
1	G	306	GLU	2.2
1	C	308	VAL	2.2
1	G	336	MET	2.2
1	G	270	GLU	2.2
1	M	299	PHE	2.2
1	E	105	PHE	2.2
1	O	39	HIS	2.2
1	O	93	LEU	2.2
1	M	380	GLY	2.2
1	O	301	LEU	2.2
1	M	118	ILE	2.1
1	M	355	LEU	2.1
1	M	82	PHE	2.1
1	M	127	ILE	2.1
1	M	353	ASP	2.1
1	E	336	MET	2.1
1	A	335	PHE	2.1
1	E	267	PRO	2.1
1	O	135	THR	2.1
1	M	304	ASP	2.1
1	M	265	LYS	2.1
1	O	376	PHE	2.1
1	M	86	GLN	2.1
1	O	126	GLN	2.1
1	A	271	ARG	2.1
1	O	265	LYS	2.1
1	O	125	SER	2.1
1	M	331	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	163	HIS	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 carbohydrates 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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PLP	O	401	15/16	0.93	0.22	1.35	47,54,57,57	0
2	PLP	M	401	15/16	0.94	0.19	0.55	41,42,43,43	0
2	PLP	E	401	15/16	0.92	0.20	0.49	49,51,52,52	0
2	PLP	C	401	15/16	0.96	0.18	0.47	34,39,43,44	0
2	PLP	H	401	15/16	0.92	0.19	-0.02	45,54,56,65	0
2	PLP	A	401	15/16	0.95	0.16	-0.53	38,42,43,44	0
3	PO4	K	401	5/5	0.97	0.10	-1.14	30,30,30,30	0
2	PLP	G	401	15/16	0.94	0.13	-2.23	30,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.