



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:06 am GMT

PDB ID : 6YTJ  
Title : Magnesium chelatase H subunit (ChlH) E625K variant from *Synechocystis* sp.PCC6803  
Authors : Bisson, C.; Hunter, C.N.  
Deposited on : 2020-04-24  
Resolution : 2.79 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

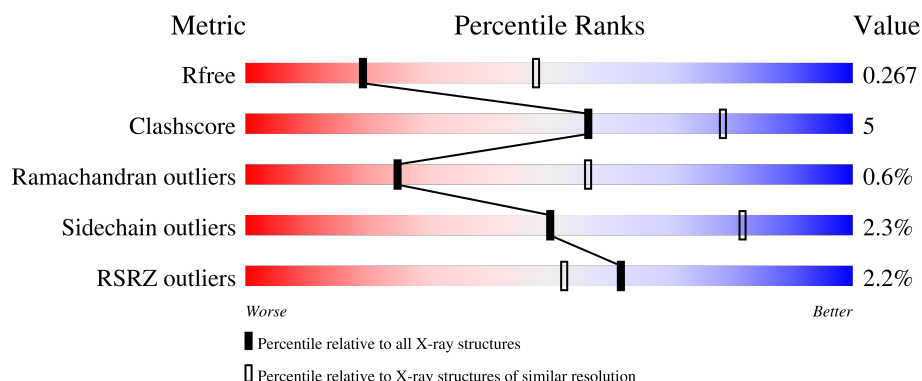
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	AAA	1351	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
1	BBB	1351	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19412 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 Mg-chelatase subunit ChlH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	1245	Total	C	N	O	S	0	0	0
			9808	6215	1665	1880	48			
1	BBB	1218	Total	C	N	O	S	0	0	0
			9585	6071	1624	1843	47			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-19	MET	-	initiating methionine	UNP P73020
AAA	-18	GLY	-	expression tag	UNP P73020
AAA	-17	SER	-	expression tag	UNP P73020
AAA	-16	SER	-	expression tag	UNP P73020
AAA	-15	HIS	-	expression tag	UNP P73020
AAA	-14	HIS	-	expression tag	UNP P73020
AAA	-13	HIS	-	expression tag	UNP P73020
AAA	-12	HIS	-	expression tag	UNP P73020
AAA	-11	HIS	-	expression tag	UNP P73020
AAA	-10	HIS	-	expression tag	UNP P73020
AAA	-9	SER	-	expression tag	UNP P73020
AAA	-8	SER	-	expression tag	UNP P73020
AAA	-7	GLY	-	expression tag	UNP P73020
AAA	-6	LEU	-	expression tag	UNP P73020
AAA	-5	VAL	-	expression tag	UNP P73020
AAA	-4	PRO	-	expression tag	UNP P73020
AAA	-3	ARG	-	expression tag	UNP P73020
AAA	-2	GLY	-	expression tag	UNP P73020
AAA	-1	SER	-	expression tag	UNP P73020
AAA	0	HIS	-	expression tag	UNP P73020
AAA	625	LYS	GLU	engineered mutation	UNP P73020
BBB	-19	MET	-	initiating methionine	UNP P73020
BBB	-18	GLY	-	expression tag	UNP P73020
BBB	-17	SER	-	expression tag	UNP P73020
BBB	-16	SER	-	expression tag	UNP P73020

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-15	HIS	-	expression tag	UNP P73020
BBB	-14	HIS	-	expression tag	UNP P73020
BBB	-13	HIS	-	expression tag	UNP P73020
BBB	-12	HIS	-	expression tag	UNP P73020
BBB	-11	HIS	-	expression tag	UNP P73020
BBB	-10	HIS	-	expression tag	UNP P73020
BBB	-9	SER	-	expression tag	UNP P73020
BBB	-8	SER	-	expression tag	UNP P73020
BBB	-7	GLY	-	expression tag	UNP P73020
BBB	-6	LEU	-	expression tag	UNP P73020
BBB	-5	VAL	-	expression tag	UNP P73020
BBB	-4	PRO	-	expression tag	UNP P73020
BBB	-3	ARG	-	expression tag	UNP P73020
BBB	-2	GLY	-	expression tag	UNP P73020
BBB	-1	SER	-	expression tag	UNP P73020
BBB	0	HIS	-	expression tag	UNP P73020
BBB	625	LYS	GLU	engineered mutation	UNP P73020

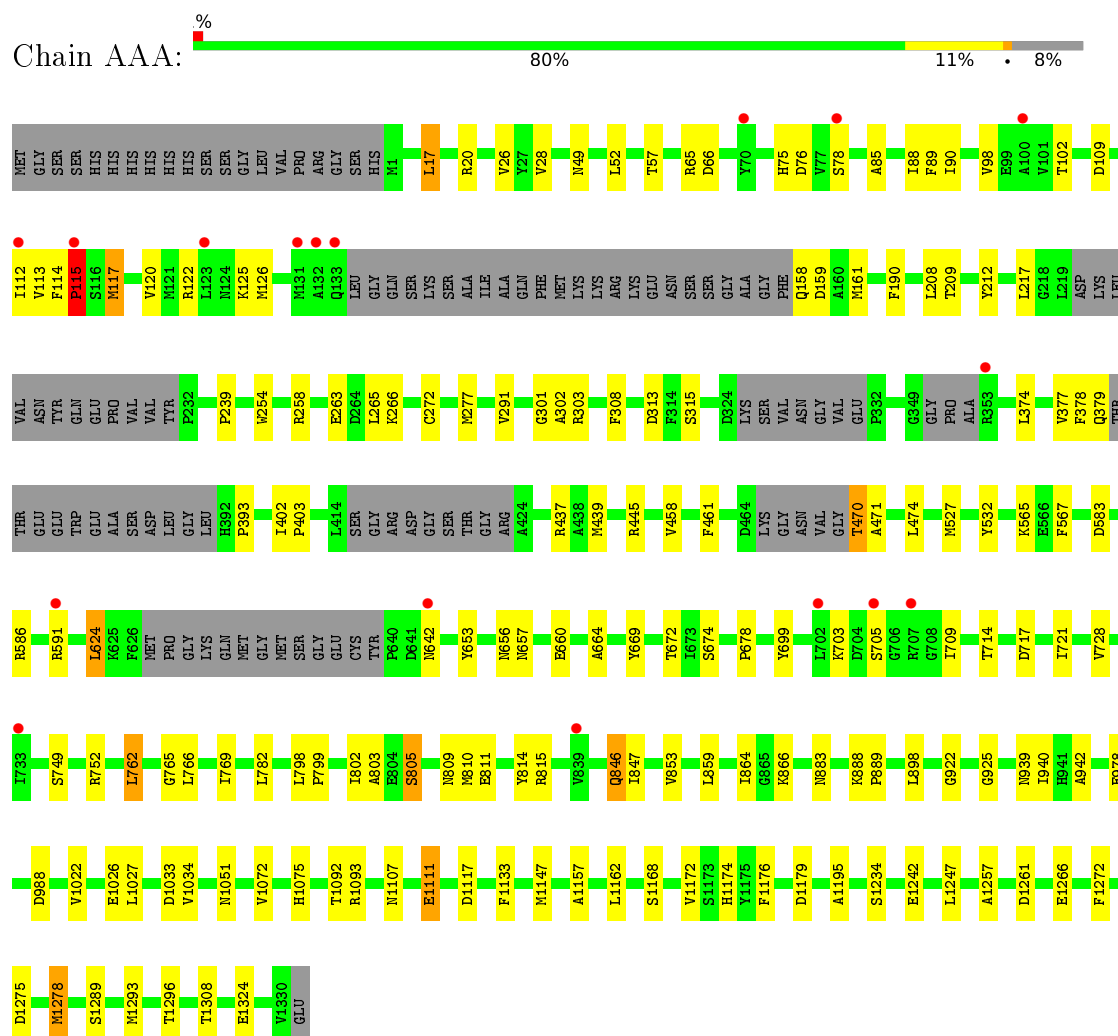
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	14	Total O 14 14	0	0
2	BBB	5	Total O 5 5	0	0

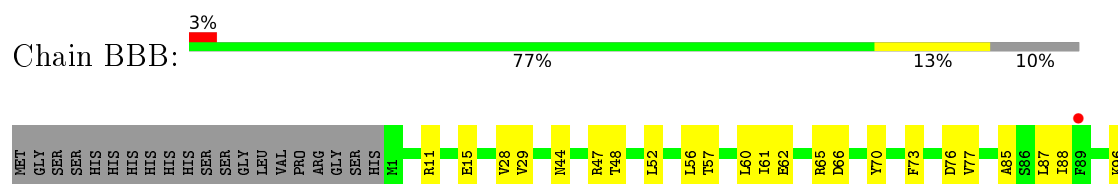
### 3 Residue-property plots [i](#)

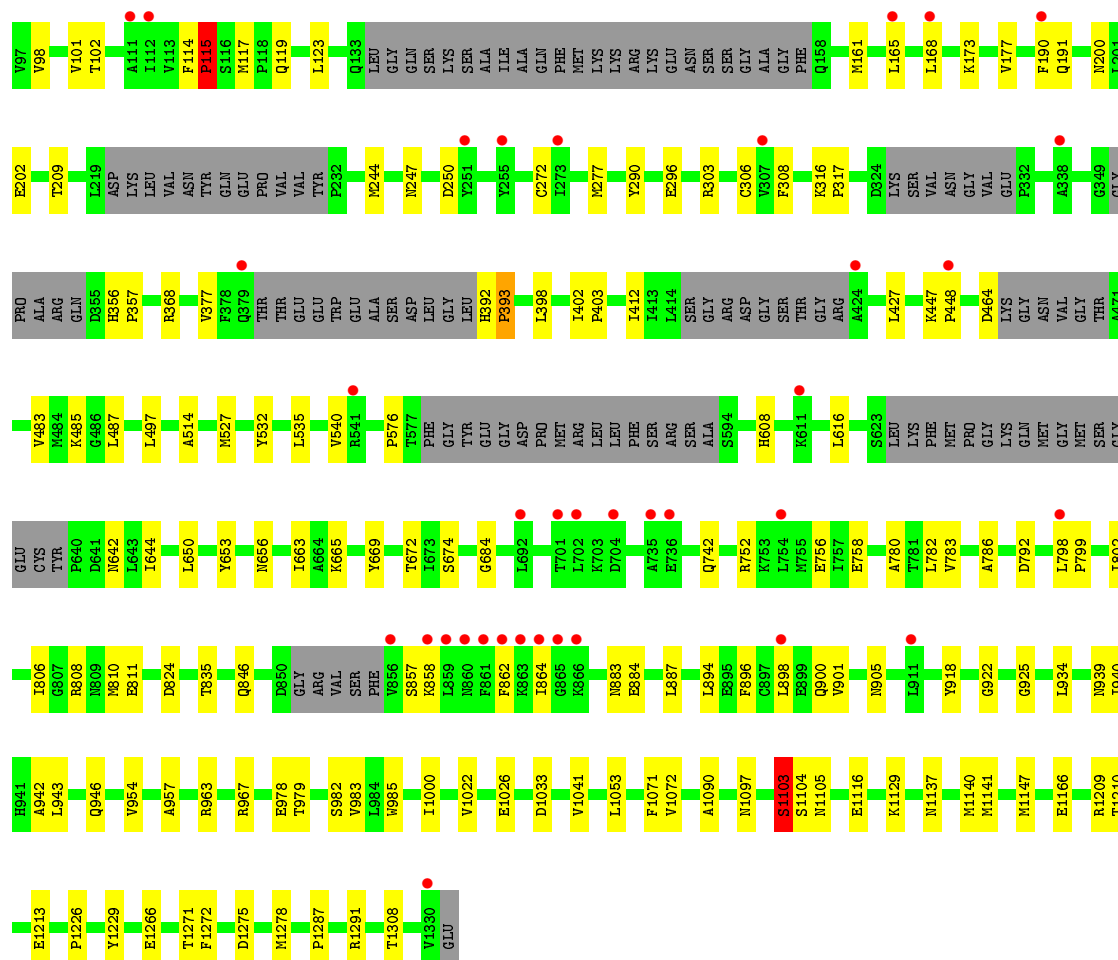
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Mg-chelatase subunit ChIH



#### • Molecule 1: Mg-chelatase subunit ChIH





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	320.42Å 320.42Å 104.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.11 – 2.79 80.11 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (80.11-2.79) 99.3 (80.11-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.209 , 0.268 0.212 , 0.267	Depositor DCC
$R_{free}$ test set	4926 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	AAA	0.66	0/10004	0.79	0/13567
1	BBB	0.67	0/9773	0.77	0/13256
All	All	0.66	0/19777	0.78	0/26823

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	9808	0	9684	106	0
1	BBB	9585	0	9460	90	0
2	AAA	14	0	0	0	0
2	BBB	5	0	0	0	0
All	All	19412	0	19144	194	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 5.

All (194) 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:AAA:88:ILE:O	1:AAA:117:MET:SD	1.90	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:89:PHE:N	1:AAA:117:MET:HE1	1.78	0.97
1:AAA:88:ILE:HG22	1:AAA:117:MET:SD	2.04	0.96
1:AAA:88:ILE:C	1:AAA:117:MET:SD	2.46	0.93
1:AAA:89:PHE:CA	1:AAA:117:MET:CE	2.49	0.89
1:AAA:89:PHE:HA	1:AAA:117:MET:HE3	1.53	0.89
1:AAA:89:PHE:HA	1:AAA:117:MET:CE	2.03	0.88
1:AAA:117:MET:N	1:AAA:117:MET:SD	2.51	0.83
1:AAA:90:ILE:H	1:AAA:117:MET:CE	1.93	0.82
1:AAA:90:ILE:H	1:AAA:117:MET:HE1	1.44	0.82
1:AAA:90:ILE:N	1:AAA:117:MET:CE	2.43	0.81
1:AAA:89:PHE:CA	1:AAA:117:MET:HE1	2.09	0.81
1:AAA:109:ASP:HB3	1:AAA:212:TYR:O	1.83	0.78
1:AAA:117:MET:HG2	1:AAA:120:VAL:HG23	1.70	0.74
1:AAA:803:ALA:HB2	1:AAA:810:MET:HE1	1.70	0.72
1:BBB:117:MET:HG2	1:BBB:119:GLN:HE22	1.56	0.70
1:AAA:89:PHE:N	1:AAA:117:MET:CE	2.55	0.69
1:AAA:89:PHE:CA	1:AAA:117:MET:HE3	2.17	0.69
1:AAA:161:MET:SD	1:AAA:190:PHE:HE1	2.16	0.69
1:BBB:402:ILE:HB	1:BBB:403:PRO:HD3	1.75	0.68
1:AAA:88:ILE:C	1:AAA:117:MET:HE1	2.13	0.68
1:AAA:90:ILE:N	1:AAA:117:MET:HE1	2.05	0.67
1:AAA:1034:VAL:O	1:AAA:1093:ARG:HD2	1.98	0.64
1:AAA:313:ASP:OD1	1:AAA:315:SER:OG	2.15	0.64
1:AAA:88:ILE:C	1:AAA:117:MET:CE	2.66	0.64
1:BBB:161:MET:SD	1:BBB:190:PHE:HE1	2.20	0.63
1:BBB:756:GLU:OE2	1:BBB:1209:ARG:NH2	2.31	0.63
1:AAA:672:THR:O	1:AAA:939:ASN:HA	2.01	0.61
1:BBB:808:ARG:NH2	1:BBB:824:ASP:OD1	2.34	0.60
1:AAA:762:LEU:O	1:AAA:762:LEU:HD12	2.01	0.60
1:BBB:101:VAL:HG12	1:BBB:123:LEU:HD22	1.84	0.60
1:BBB:798:LEU:HD23	1:BBB:835:THR:HG23	1.84	0.59
1:AAA:161:MET:SD	1:AAA:190:PHE:CE1	2.96	0.58
1:AAA:853:VAL:HG11	1:AAA:859:LEU:HD21	1.85	0.58
1:AAA:1162:LEU:HD11	1:AAA:1168:SER:HA	1.84	0.58
1:BBB:73:PHE:O	1:BBB:77:VAL:HG23	2.03	0.58
1:BBB:978:GLU:HA	1:BBB:1071:PHE:CD2	2.39	0.58
1:AAA:114:PHE:HB3	1:AAA:115:PRO:HD2	1.86	0.57
1:BBB:1033:ASP:HA	1:BBB:1072:VAL:HG22	1.87	0.56
1:BBB:247:ASN:ND2	1:BBB:250:ASP:OD2	2.36	0.56
1:BBB:247:ASN:HD21	1:BBB:250:ASP:CG	2.08	0.56
1:BBB:1104:SER:O	1:BBB:1105:ASN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:803:ALA:HB2	1:AAA:810:MET:CE	2.37	0.55
1:AAA:591:ARG:HD3	1:BBB:1116:GLU:HB3	1.89	0.54
1:AAA:1272:PHE:HA	1:AAA:1278:MET:HG2	1.89	0.54
1:AAA:657:ASN:ND2	1:AAA:660:GLU:HB2	2.22	0.54
1:AAA:1092:THR:HB	1:AAA:1147:MET:HG2	1.90	0.53
1:BBB:656:ASN:HD22	1:BBB:1166:GLU:HG3	1.73	0.53
1:BBB:161:MET:SD	1:BBB:190:PHE:CE1	3.02	0.52
1:BBB:28:VAL:O	1:BBB:85:ALA:HA	2.10	0.52
1:AAA:1022:VAL:CG1	1:AAA:1026:GLU:HB3	2.40	0.52
1:BBB:356:HIS:N	1:BBB:357:PRO:CD	2.73	0.52
1:AAA:98:VAL:O	1:AAA:102:THR:OG1	2.20	0.52
1:AAA:89:PHE:C	1:AAA:117:MET:CE	2.78	0.52
1:BBB:57:THR:HG21	1:BBB:76:ASP:OD2	2.10	0.51
1:BBB:114:PHE:O	1:BBB:115:PRO:C	2.48	0.51
1:BBB:277:MET:HE1	1:BBB:290:TYR:HB3	1.93	0.51
1:AAA:591:ARG:CD	1:BBB:1116:GLU:HB3	2.40	0.51
1:AAA:113:VAL:HG11	1:AAA:120:VAL:HG12	1.92	0.51
1:AAA:922:GLY:O	1:AAA:940:ILE:HA	2.10	0.51
1:BBB:669:TYR:CG	1:BBB:669:TYR:O	2.63	0.51
1:BBB:896:PHE:O	1:BBB:900:GLN:HG2	2.10	0.51
1:BBB:447:LYS:HG3	1:BBB:448:PRO:HD2	1.92	0.51
1:AAA:1157:ALA:HA	1:AAA:1195:ALA:O	2.10	0.50
1:AAA:126:MET:HG2	1:AAA:212:TYR:CZ	2.46	0.50
1:BBB:1266:GLU:OE2	1:BBB:1308:THR:OG1	2.20	0.50
1:AAA:1051:ASN:HA	1:AAA:1133:PHE:CE2	2.46	0.50
1:BBB:485:LYS:HG2	1:BBB:497:LEU:HD21	1.93	0.50
1:AAA:402:ILE:HB	1:AAA:403:PRO:HD3	1.92	0.50
1:BBB:663:ILE:HG13	1:BBB:1041:VAL:HG22	1.94	0.50
1:AAA:88:ILE:HG22	1:AAA:117:MET:CE	2.42	0.50
1:AAA:653:TYR:O	1:AAA:674:SER:HA	2.12	0.50
1:AAA:26:VAL:HA	1:AAA:57:THR:O	2.12	0.49
1:BBB:535:LEU:HD22	1:BBB:608:HIS:HB3	1.94	0.49
1:BBB:786:ALA:HB2	1:BBB:894:LEU:HD21	1.94	0.49
1:BBB:316:LYS:HB2	1:BBB:317:PRO:CD	2.43	0.49
1:AAA:1247:LEU:HG	1:AAA:1296:THR:HG21	1.95	0.49
1:AAA:678:PRO:HG2	1:AAA:765:GLY:O	2.12	0.49
1:AAA:1051:ASN:HA	1:AAA:1133:PHE:HE2	1.78	0.49
1:BBB:967:ARG:HH22	1:BBB:1213:GLU:CD	2.15	0.49
1:AAA:766:LEU:HD21	1:AAA:1242:GLU:HG3	1.94	0.49
1:AAA:57:THR:HG21	1:AAA:76:ASP:OD2	2.13	0.49
1:AAA:798:LEU:HB3	1:AAA:799:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:798:LEU:HB3	1:BBB:799:PRO:HD3	1.95	0.49
1:AAA:75:HIS:O	1:AAA:78:SER:HB3	2.12	0.48
1:AAA:1179:ASP:OD2	1:AAA:1257:ALA:HB2	2.13	0.48
1:BBB:799:PRO:HB3	1:BBB:810:MET:HE3	1.96	0.48
1:AAA:28:VAL:O	1:AAA:85:ALA:HA	2.12	0.48
1:BBB:29:VAL:O	1:BBB:60:LEU:HA	2.14	0.48
1:AAA:239:PRO:HB3	1:AAA:291:VAL:HG22	1.96	0.48
1:AAA:254:TRP:CZ3	1:AAA:258:ARG:HD2	2.49	0.48
1:AAA:117:MET:HG2	1:AAA:120:VAL:CG2	2.41	0.47
1:AAA:978:GLU:HB3	1:AAA:1075:HIS:CE1	2.49	0.47
1:BBB:1022:VAL:HG13	1:BBB:1026:GLU:HB3	1.95	0.47
1:AAA:717:ASP:O	1:AAA:721:ILE:HG12	2.14	0.47
1:BBB:1272:PHE:HA	1:BBB:1278:MET:HG2	1.97	0.47
1:BBB:11:ARG:HA	1:BBB:56:LEU:O	2.14	0.47
1:BBB:656:ASN:HA	1:BBB:925:GLY:O	2.14	0.47
1:BBB:377:VAL:HG11	1:BBB:412:ILE:HD13	1.96	0.47
1:AAA:89:PHE:C	1:AAA:117:MET:HE3	2.35	0.47
1:BBB:368:ARG:O	1:BBB:918:TYR:HB2	2.14	0.47
1:AAA:17:LEU:HD22	1:AAA:20:ARG:O	2.14	0.47
1:AAA:1275:ASP:C	1:AAA:1275:ASP:OD1	2.53	0.46
1:BBB:244:MET:HE3	1:BBB:308:PHE:CE2	2.51	0.46
1:AAA:474:LEU:HD11	1:AAA:769:ILE:CD1	2.45	0.46
1:AAA:888:LYS:HB3	1:AAA:889:PRO:HD3	1.97	0.46
1:BBB:665:LYS:NZ	1:BBB:940:ILE:O	2.49	0.46
1:AAA:1289:SER:O	1:AAA:1293:MET:HG3	2.16	0.46
1:BBB:173:LYS:NZ	1:BBB:296:GLU:OE2	2.45	0.46
1:AAA:699:TYR:CZ	1:AAA:703:LYS:HD2	2.50	0.46
1:BBB:1137:ASN:ND2	1:BBB:1140:MET:HG3	2.30	0.46
1:AAA:728:VAL:HG13	1:AAA:749:SER:HB3	1.99	0.45
1:BBB:272:CYS:HA	1:BBB:303:ARG:O	2.17	0.45
1:AAA:263:GLU:OE2	1:AAA:266:LYS:NZ	2.45	0.45
1:AAA:158:GLN:O	1:AAA:161:MET:HB2	2.16	0.45
1:BBB:672:THR:O	1:BBB:939:ASN:HA	2.16	0.45
1:AAA:846:GLN:HG3	1:AAA:847:ILE:N	2.32	0.45
1:BBB:114:PHE:CD1	1:BBB:190:PHE:CD1	3.05	0.45
1:AAA:1172:VAL:HG21	1:AAA:1174:HIS:NE2	2.32	0.44
1:BBB:392:HIS:N	1:BBB:393:PRO:CD	2.79	0.44
1:AAA:888:LYS:HB3	1:AAA:889:PRO:CD	2.47	0.44
1:BBB:967:ARG:NH2	1:BBB:1210:THR:HG23	2.32	0.44
1:AAA:811:GLU:OE2	1:AAA:815:ARG:CZ	2.66	0.44
1:AAA:88:ILE:HD12	1:AAA:88:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:302:ALA:HB2	1:AAA:439:MET:SD	2.57	0.44
1:BBB:1090:ALA:HA	1:BBB:1147:MET:CE	2.47	0.44
1:AAA:470:THR:OG1	1:AAA:471:ALA:N	2.51	0.44
1:BBB:177:VAL:CG1	1:BBB:427:LEU:HD21	2.47	0.44
1:BBB:277:MET:HE3	1:BBB:306:CYS:SG	2.58	0.44
1:AAA:52:LEU:HD22	1:AAA:209:THR:HG21	2.00	0.44
1:BBB:780:ALA:O	1:BBB:783:VAL:HB	2.18	0.44
1:AAA:437:ARG:HD3	1:AAA:669:TYR:CZ	2.53	0.43
1:BBB:684:GLY:HA2	1:BBB:758:GLU:HG2	2.00	0.43
1:AAA:565:LYS:HG3	1:AAA:567:PHE:CE1	2.54	0.43
1:AAA:378:PHE:O	1:AAA:379:GLN:C	2.57	0.43
1:AAA:799:PRO:O	1:AAA:810:MET:CE	2.67	0.43
1:BBB:1226:PRO:HA	1:BBB:1229:TYR:CE2	2.54	0.43
1:BBB:65:ARG:O	1:BBB:66:ASP:C	2.56	0.43
1:AAA:1033:ASP:HA	1:AAA:1072:VAL:HG22	2.00	0.43
1:BBB:47:ARG:HG3	1:BBB:48:THR:HG23	2.01	0.43
1:AAA:656:ASN:HA	1:AAA:925:GLY:O	2.18	0.43
1:BBB:1226:PRO:HA	1:BBB:1229:TYR:CZ	2.53	0.43
1:BBB:1097:ASN:ND2	1:BBB:1103:SER:O	2.44	0.43
1:BBB:884:GLU:HA	1:BBB:887:LEU:HB3	2.01	0.43
1:AAA:458:VAL:CG1	1:AAA:461:PHE:CD2	3.02	0.43
1:AAA:624:LEU:HD22	1:AAA:664:ALA:HA	2.01	0.43
1:AAA:782:LEU:HD11	1:AAA:898:LEU:HB2	2.01	0.43
1:BBB:514:ALA:HB3	1:BBB:1287:PRO:HG3	2.00	0.43
1:AAA:265:LEU:HD11	1:AAA:301:GLY:HA2	2.00	0.42
1:AAA:437:ARG:HD3	1:AAA:669:TYR:CE2	2.54	0.42
1:BBB:1000:ILE:HG22	1:BBB:1053:LEU:HD22	2.00	0.42
1:AAA:1266:GLU:OE2	1:AAA:1308:THR:OG1	2.20	0.42
1:AAA:810:MET:HG3	1:AAA:814:TYR:CE2	2.54	0.42
1:AAA:853:VAL:CG1	1:AAA:859:LEU:HD21	2.47	0.42
1:AAA:864:ILE:HG13	1:AAA:866:LYS:HG3	2.01	0.42
1:BBB:806:ILE:HG13	1:BBB:806:ILE:O	2.19	0.42
1:BBB:983:VAL:HG11	1:BBB:985:TRP:CZ2	2.54	0.42
1:AAA:527:MET:CE	1:AAA:532:TYR:HB2	2.50	0.42
1:BBB:464:ASP:OD1	1:BBB:1291:ARG:NH1	2.50	0.42
1:BBB:398:LEU:HD22	1:BBB:946:GLN:HG3	2.02	0.42
1:AAA:112:ILE:HD11	1:AAA:208:LEU:HD13	2.01	0.42
1:AAA:277:MET:O	1:AAA:308:PHE:HA	2.20	0.42
1:BBB:674:SER:HB3	1:BBB:940:ILE:HG23	2.01	0.42
1:BBB:901:VAL:HG23	1:BBB:934:LEU:HD13	2.02	0.42
1:AAA:374:LEU:O	1:AAA:377:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:200:ASN:HA	1:BBB:200:ASN:HD22	1.74	0.41
1:BBB:316:LYS:HB2	1:BBB:317:PRO:HD3	2.00	0.41
1:BBB:61:ILE:HD12	1:BBB:88:ILE:HG13	2.00	0.41
1:BBB:62:GLU:OE2	1:BBB:65:ARG:NH1	2.53	0.41
1:AAA:1027:LEU:HD12	1:AAA:1027:LEU:HA	1.89	0.41
1:BBB:527:MET:HE1	1:BBB:532:TYR:HD1	1.86	0.41
1:BBB:653:TYR:O	1:BBB:674:SER:HA	2.21	0.41
1:BBB:782:LEU:HD11	1:BBB:898:LEU:HB2	2.02	0.41
1:BBB:483:VAL:O	1:BBB:487:LEU:HG	2.21	0.41
1:BBB:954:VAL:O	1:BBB:957:ALA:HB3	2.21	0.41
1:AAA:1107:ASN:O	1:AAA:1111:GLU:HB2	2.21	0.41
1:BBB:44:ASN:HD22	1:BBB:202:GLU:CD	2.24	0.41
1:BBB:165:LEU:HD11	1:BBB:191:GLN:CG	2.50	0.41
1:BBB:922:GLY:O	1:BBB:940:ILE:HA	2.20	0.41
1:AAA:272:CYS:HA	1:AAA:303:ARG:O	2.21	0.41
1:BBB:943:LEU:O	1:BBB:943:LEU:HD12	2.21	0.41
1:BBB:117:MET:HG2	1:BBB:119:GLN:NE2	2.31	0.41
1:AAA:883:ASN:C	1:AAA:883:ASN:OD1	2.60	0.40
1:BBB:1271:THR:HG22	1:BBB:1272:PHE:CD1	2.56	0.40
1:AAA:1172:VAL:HG21	1:AAA:1174:HIS:CD2	2.57	0.40
1:AAA:802:ILE:O	1:AAA:805:SER:HB3	2.21	0.40
1:BBB:52:LEU:HD22	1:BBB:209:THR:HG21	2.04	0.40
1:BBB:616:LEU:HA	1:BBB:650:LEU:O	2.20	0.40
1:BBB:70:TYR:CE1	1:BBB:96:LYS:HB3	2.57	0.40
1:AAA:1034:VAL:O	1:AAA:1093:ARG:HB3	2.20	0.40
1:AAA:583:ASP:HB3	1:AAA:586:ARG:HB2	2.03	0.40
1:BBB:165:LEU:HA	1:BBB:168:LEU:HD12	2.04	0.40
1:BBB:98:VAL:O	1:BBB:102:THR:HB	2.21	0.40
1:BBB:979:THR:HA	1:BBB:1033:ASP:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	1227/1351 (91%)	1145 (93%)	77 (6%)	5 (0%)	34	66
1	BBB	1196/1351 (88%)	1100 (92%)	87 (7%)	9 (1%)	19	49
All	All	2423/2702 (90%)	2245 (93%)	164 (7%)	14 (1%)	25	56

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	65	ARG
1	AAA	217	LEU
1	AAA	942	ALA
1	BBB	115	PRO
1	BBB	942	ALA
1	AAA	115	PRO
1	BBB	393	PRO
1	BBB	1275	ASP
1	AAA	393	PRO
1	BBB	576	PRO
1	BBB	1103	SER
1	BBB	883	ASN
1	BBB	540	VAL
1	BBB	802	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	AAA	1063/1147 (93%)	1035 (97%)	28 (3%)	46	79
1	BBB	1040/1147 (91%)	1020 (98%)	20 (2%)	57	85
All	All	2103/2294 (92%)	2055 (98%)	48 (2%)	50	82

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	17	LEU
1	AAA	49	ASN

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Mol	Chain	Res	Type
1	AAA	66	ASP
1	AAA	115	PRO
1	AAA	117	MET
1	AAA	122	ARG
1	AAA	125	LYS
1	AAA	159	ASP
1	AAA	445	ARG
1	AAA	470	THR
1	AAA	624	LEU
1	AAA	642	ASN
1	AAA	705	SER
1	AAA	709	ILE
1	AAA	714	THR
1	AAA	752	ARG
1	AAA	762	LEU
1	AAA	805	SER
1	AAA	809	ASN
1	AAA	846	GLN
1	AAA	988	ASP
1	AAA	1111	GLU
1	AAA	1117	ASP
1	AAA	1176	PHE
1	AAA	1234	SER
1	AAA	1261	ASP
1	AAA	1278	MET
1	AAA	1324	GLU
1	BBB	15	GLU
1	BBB	87	LEU
1	BBB	115	PRO
1	BBB	642	ASN
1	BBB	644	ILE
1	BBB	742	GLN
1	BBB	752	ARG
1	BBB	792	ASP
1	BBB	811	GLU
1	BBB	846	GLN
1	BBB	857	SER
1	BBB	858	LYS
1	BBB	862	PHE
1	BBB	864	ILE
1	BBB	905	ASN
1	BBB	963	ARG

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Mol	Chain	Res	Type
1	BBB	982	SER
1	BBB	1103	SER
1	BBB	1129	LYS
1	BBB	1141	MET

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	AAA	1245/1351 (92%)	0.26	17 (1%)	75 70	27, 54, 99, 146	38 (3%)
1	BBB	1218/1351 (90%)	0.45	37 (3%)	50 40	37, 72, 108, 159	37 (3%)
All	All	2463/2702 (91%)	0.35	54 (2%)	62 52	27, 62, 105, 159	75 (3%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	863	LYS	8.5
1	BBB	862	PHE	6.3
1	BBB	424	ALA	4.7
1	AAA	132	ALA	3.9
1	BBB	255	TYR	3.8
1	BBB	860	ASN	3.3
1	BBB	702	LEU	3.3
1	BBB	859	LEU	3.2
1	AAA	705	SER	3.2
1	AAA	702	LEU	3.2
1	BBB	856	VAL	3.2
1	BBB	541	ARG	3.1
1	BBB	858	LYS	3.1
1	BBB	701	THR	2.9
1	BBB	798	LEU	2.9
1	BBB	911	LEU	2.9
1	BBB	379	GLN	2.6
1	AAA	131	MET	2.6
1	AAA	353	ARG	2.6
1	AAA	100	ALA	2.5
1	AAA	839	VAL	2.5
1	BBB	165	LEU	2.5
1	AAA	707	ARG	2.5
1	BBB	864	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	BBB	754	LEU	2.5
1	AAA	642	ASN	2.5
1	BBB	735	ALA	2.5
1	AAA	591	ARG	2.4
1	BBB	273	ILE	2.4
1	BBB	692	LEU	2.4
1	AAA	78	SER	2.4
1	AAA	123	LEU	2.4
1	BBB	251	TYR	2.3
1	BBB	704	ASP	2.3
1	AAA	115	PRO	2.3
1	AAA	133	GLN	2.3
1	AAA	70	TYR	2.2
1	BBB	861	PHE	2.2
1	BBB	865	GLY	2.2
1	BBB	898	LEU	2.2
1	BBB	1330	VAL	2.2
1	BBB	168	LEU	2.2
1	BBB	190	PHE	2.2
1	BBB	338	ALA	2.1
1	BBB	111	ALA	2.1
1	BBB	611	LYS	2.1
1	BBB	307	VAL	2.1
1	AAA	112	ILE	2.1
1	AAA	733	ILE	2.1
1	BBB	89	PHE	2.1
1	BBB	112	ILE	2.0
1	BBB	448	PRO	2.0
1	BBB	736	GLU	2.0
1	BBB	866	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.