



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:06 AM GMT

PDB ID : 6YTN  
Title : Magnesium chelatase H subunit (ChlH) E660W variant from *Synechocystis* sp.PCC6803  
Authors : Bisson, C.; Hunter, C.N.  
Deposited on : 2020-04-24  
Resolution : 2.70 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

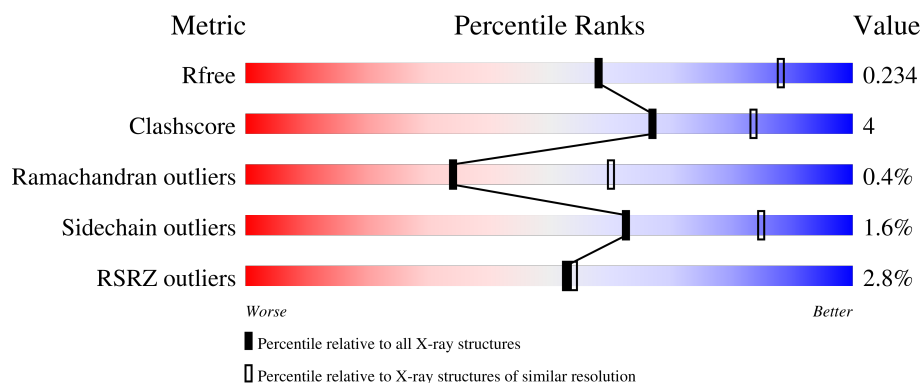
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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>2%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
1	BBB	1351	<div> <div>4%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19771 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	1258	Total	C	N	O	S	0	0	0
			9913	6285	1684	1894	50			
1	BBB	1251	Total	C	N	O	S	0	0	0
			9850	6240	1674	1886	50			

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	660	TRP	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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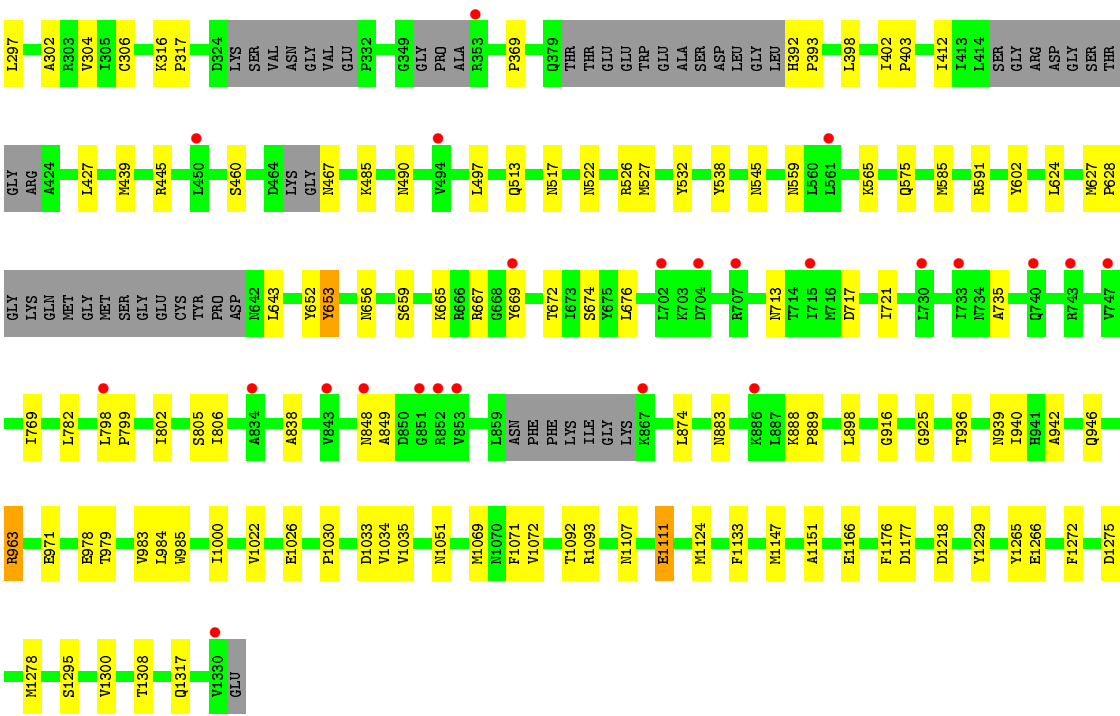
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-15	HIS	-	expression tag	UNP P73020
BBB	-14	HIS	-	expression tag	UNP P73020
BBB	-13	HIS	-	expression tag	UNP P73020
BBB	-12	HIS	-	expression tag	UNP P73020
BBB	-11	HIS	-	expression tag	UNP P73020
BBB	-10	HIS	-	expression tag	UNP P73020
BBB	-9	SER	-	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	660	TRP	GLU	engineered mutation	UNP P73020

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	5	Total O 5 5	0	0
2	BBB	3	Total O 3 3	0	0

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.

[illegible][illegible]



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	317.55Å 317.55Å 104.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.39 – 2.70 79.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (79.39-2.70) 99.9 (79.39-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.192 , 0.235 0.195 , 0.234	Depositor DCC
$R_{free}$ test set	5365 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.4	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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	0.65	0/10110	0.76	0/13707
1	BBB	0.66	0/10046	0.74	0/13623
All	All	0.65	0/20156	0.75	0/27330

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	9913	0	9804	76	0
1	BBB	9850	0	9727	79	0
2	AAA	5	0	0	0	0
2	BBB	3	0	0	0	0
All	All	19771	0	19531	154	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 4.

All (154) 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:109:ASP:HB3	1:AAA:212:TYR:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:644:ILE:HG23	1:AAA:649:ASN:HD22	1.53	0.73
1:BBB:526:ARG:HB3	1:BBB:559:ASN:HD22	1.61	0.65
1:AAA:538:TYR:OH	1:AAA:643:LEU:HD12	1.97	0.64
1:AAA:1022:VAL:HG13	1:AAA:1026:GLU:HB3	1.81	0.63
1:BBB:1266:GLU:OE2	1:BBB:1308:THR:OG1	2.13	0.61
1:AAA:538:TYR:OH	1:AAA:643:LEU:CD1	2.48	0.61
1:BBB:713:ASN:HD21	1:BBB:735:ALA:H	1.48	0.61
1:AAA:803:ALA:HB2	1:AAA:810:MET:CE	2.31	0.59
1:AAA:762:LEU:O	1:AAA:762:LEU:HD12	2.03	0.58
1:AAA:803:ALA:HB2	1:AAA:810:MET:HE2	1.85	0.58
1:AAA:678:PRO:HG2	1:AAA:765:GLY:O	2.03	0.58
1:AAA:1034:VAL:O	1:AAA:1093:ARG:HD2	2.05	0.57
1:BBB:1033:ASP:HA	1:BBB:1072:VAL:HG22	1.86	0.57
1:AAA:177:VAL:HG21	1:AAA:378:PHE:O	2.05	0.56
1:AAA:897:CYS:O	1:AAA:901:VAL:HG23	2.05	0.56
1:BBB:984:LEU:HD21	1:BBB:1000:ILE:HD12	1.88	0.56
1:AAA:1172:VAL:HG21	1:AAA:1174:HIS:CE1	2.42	0.55
1:BBB:527:MET:CE	1:BBB:532:TYR:HA	2.36	0.55
1:AAA:442:ALA:O	1:AAA:445:ARG:HB3	2.06	0.55
1:BBB:522:ASN:HD22	1:BBB:565:LYS:HB2	1.70	0.55
1:BBB:277:MET:HE2	1:BBB:290:TYR:CD1	2.43	0.54
1:BBB:277:MET:HE3	1:BBB:306:CYS:SG	2.48	0.54
1:AAA:1033:ASP:HA	1:AAA:1072:VAL:HG22	1.88	0.54
1:BBB:256:ASN:HA	1:BBB:266:LYS:HD3	1.88	0.54
1:AAA:782:LEU:HD11	1:AAA:898:LEU:HB2	1.91	0.53
1:BBB:665:LYS:NZ	1:BBB:940:ILE:O	2.41	0.52
1:BBB:545:ASN:HD21	1:BBB:591:ARG:HG2	1.75	0.52
1:BBB:888:LYS:HB3	1:BBB:889:PRO:HD3	1.92	0.52
1:AAA:734:ASN:HB3	1:AAA:736:GLU:OE2	2.10	0.52
1:AAA:114:PHE:HB3	1:AAA:115:PRO:HD2	1.92	0.51
1:BBB:782:LEU:HD11	1:BBB:898:LEU:HB2	1.92	0.51
1:BBB:277:MET:CE	1:BBB:306:CYS:SG	2.98	0.51
1:AAA:316:LYS:HB2	1:AAA:317:PRO:HD3	1.92	0.51
1:BBB:627:MET:HB3	1:BBB:628:PRO:HD2	1.93	0.51
1:AAA:316:LYS:HB2	1:AAA:317:PRO:CD	2.41	0.51
1:BBB:1092:THR:HB	1:BBB:1147:MET:HG2	1.92	0.51
1:BBB:316:LYS:HB2	1:BBB:317:PRO:CD	2.40	0.51
1:BBB:522:ASN:ND2	1:BBB:565:LYS:HD3	2.26	0.50
1:AAA:810:MET:HG3	1:AAA:814:TYR:CE2	2.46	0.50
1:BBB:114:PHE:O	1:BBB:115:PRO:C	2.50	0.50
1:BBB:545:ASN:HD21	1:BBB:591:ARG:CG	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:1272:PHE:HA	1:AAA:1278:MET:HG2	1.94	0.49
1:AAA:652:TYR:CD2	1:AAA:769:ILE:HD13	2.47	0.49
1:AAA:61:ILE:CD1	1:AAA:88:ILE:HG23	2.42	0.49
1:BBB:412:ILE:HD12	1:BBB:412:ILE:C	2.33	0.49
1:BBB:522:ASN:HD21	1:BBB:565:LYS:HD3	1.78	0.49
1:AAA:888:LYS:HB3	1:AAA:889:PRO:HD3	1.94	0.49
1:BBB:177:VAL:HG22	1:BBB:427:LEU:HD21	1.95	0.49
1:BBB:398:LEU:HD22	1:BBB:946:GLN:HG3	1.94	0.49
1:BBB:402:ILE:HB	1:BBB:403:PRO:HD3	1.95	0.48
1:BBB:672:THR:O	1:BBB:939:ASN:HA	2.13	0.48
1:BBB:1275:ASP:OD1	1:BBB:1275:ASP:C	2.52	0.48
1:BBB:979:THR:HA	1:BBB:1033:ASP:O	2.14	0.48
1:AAA:449:LYS:HA	1:AAA:452:LYS:HD2	1.96	0.48
1:AAA:798:LEU:HB3	1:AAA:799:PRO:HD3	1.96	0.48
1:AAA:26:VAL:HA	1:AAA:57:THR:O	2.14	0.48
1:BBB:28:VAL:O	1:BBB:85:ALA:HA	2.14	0.47
1:BBB:1022:VAL:HG13	1:BBB:1026:GLU:HB3	1.96	0.47
1:AAA:468:VAL:HG13	1:AAA:468:VAL:O	2.14	0.47
1:AAA:1157:ALA:HA	1:AAA:1195:ALA:O	2.15	0.47
1:AAA:674:SER:HB3	1:AAA:940:ILE:HG23	1.96	0.47
1:BBB:674:SER:HB3	1:BBB:940:ILE:HG23	1.96	0.47
1:AAA:644:ILE:CG2	1:AAA:649:ASN:HD22	2.24	0.47
1:BBB:460:SER:OG	1:BBB:467:ASN:ND2	2.47	0.47
1:BBB:1265:TYR:CE1	1:BBB:1300:VAL:HG11	2.50	0.46
1:BBB:44:ASN:HD22	1:BBB:198:GLN:HE21	1.64	0.46
1:AAA:114:PHE:CE2	1:AAA:193:TRP:CD2	3.04	0.46
1:BBB:369:PRO:HD3	1:BBB:916:GLY:O	2.15	0.46
1:AAA:369:PRO:HD3	1:AAA:916:GLY:O	2.15	0.46
1:BBB:717:ASP:O	1:BBB:721:ILE:HG12	2.15	0.46
1:AAA:484:MET:HE2	1:AAA:504:LEU:HD22	1.97	0.46
1:BBB:44:ASN:HD22	1:BBB:198:GLN:NE2	2.13	0.46
1:BBB:652:TYR:CD2	1:BBB:769:ILE:HD13	2.50	0.46
1:BBB:656:ASN:ND2	1:BBB:1166:GLU:HG3	2.30	0.46
1:AAA:398:LEU:HD22	1:AAA:946:GLN:HG3	1.98	0.46
1:AAA:726:GLN:NE2	1:AAA:1261:ASP:OD1	2.49	0.46
1:BBB:134:LEU:HB2	1:BBB:138:LYS:HB3	1.98	0.46
1:AAA:28:VAL:O	1:AAA:85:ALA:HA	2.16	0.46
1:BBB:27:TYR:HA	1:BBB:84:ILE:O	2.16	0.46
1:BBB:888:LYS:HB3	1:BBB:889:PRO:CD	2.45	0.46
1:AAA:853:VAL:HG11	1:AAA:859:LEU:HD21	1.98	0.45
1:AAA:983:VAL:HG11	1:AAA:985:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:102:THR:HB	1:AAA:103:PRO:HD3	1.99	0.45
1:AAA:61:ILE:HD13	1:AAA:88:ILE:HG23	1.97	0.45
1:AAA:808:ARG:NH1	1:AAA:812:GLU:OE1	2.49	0.45
1:AAA:1222:LYS:HA	1:AAA:1228:TRP:CG	2.52	0.45
1:AAA:486:GLY:O	1:AAA:490:ASN:HB2	2.16	0.45
1:AAA:896:PHE:O	1:AAA:900:GLN:HG2	2.17	0.45
1:BBB:1035:VAL:HG22	1:BBB:1151:ALA:HB1	1.99	0.45
1:BBB:676:LEU:HB2	1:BBB:936:THR:HG21	1.98	0.45
1:BBB:131:MET:HE1	1:BBB:141:ILE:HD11	1.99	0.44
1:AAA:27:TYR:CE2	1:AAA:58:GLY:HA3	2.53	0.44
1:AAA:302:ALA:HB2	1:AAA:439:MET:SD	2.57	0.44
1:BBB:1034:VAL:O	1:BBB:1093:ARG:HD2	2.18	0.44
1:AAA:1275:ASP:OD1	1:AAA:1275:ASP:C	2.55	0.44
1:AAA:587:LEU:H	1:BBB:1317:GLN:HE22	1.66	0.44
1:BBB:98:VAL:O	1:BBB:102:THR:HB	2.18	0.44
1:BBB:485:LYS:HG2	1:BBB:497:LEU:HD21	1.99	0.44
1:BBB:798:LEU:HB3	1:BBB:799:PRO:HD3	2.00	0.44
1:AAA:378:PHE:O	1:AAA:379:GLN:C	2.56	0.44
1:BBB:669:TYR:CG	1:BBB:669:TYR:O	2.71	0.44
1:BBB:294:VAL:HG22	1:BBB:304:VAL:HG11	1.99	0.43
1:BBB:316:LYS:HB2	1:BBB:317:PRO:HD3	1.99	0.43
1:BBB:848:ASN:OD1	1:BBB:849:ALA:N	2.50	0.43
1:BBB:117:MET:HB3	1:BBB:119:GLN:OE1	2.18	0.43
1:AAA:374:LEU:O	1:AAA:377:VAL:HB	2.19	0.43
1:BBB:302:ALA:HB2	1:BBB:439:MET:SD	2.59	0.43
1:AAA:624:LEU:HD21	1:AAA:643:LEU:HD23	2.00	0.43
1:BBB:585:MET:SD	1:BBB:1124:MET:HE2	2.59	0.43
1:AAA:69:ASN:N	1:AAA:69:ASN:HD22	2.16	0.43
1:BBB:624:LEU:HA	1:BBB:627:MET:HG3	2.01	0.42
1:AAA:313:ASP:OD2	1:AAA:358:ARG:NH2	2.52	0.42
1:AAA:113:VAL:HG11	1:AAA:120:VAL:HG12	2.01	0.42
1:AAA:27:TYR:HA	1:AAA:84:ILE:O	2.19	0.42
1:AAA:44:ASN:HD22	1:AAA:202:GLU:CD	2.23	0.42
1:AAA:669:TYR:CG	1:AAA:669:TYR:O	2.72	0.42
1:AAA:1029:ARG:HB2	1:AAA:1030:PRO:CD	2.50	0.42
1:AAA:809:ASN:OD1	1:AAA:811:GLU:HB3	2.19	0.42
1:AAA:656:ASN:HA	1:AAA:925:GLY:O	2.19	0.42
1:BBB:1272:PHE:HA	1:BBB:1278:MET:HG2	2.00	0.42
1:AAA:44:ASN:HA	1:AAA:47:ARG:NH1	2.34	0.42
1:AAA:62:GLU:O	1:AAA:65:ARG:HG3	2.19	0.42
1:BBB:1030:PRO:HA	1:BBB:1069:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:538:TYR:CZ	1:BBB:643:LEU:HB2	2.54	0.42
1:BBB:585:MET:SD	1:BBB:1124:MET:CE	3.08	0.42
1:AAA:85:ALA:HB1	1:AAA:88:ILE:HD12	2.02	0.42
1:BBB:656:ASN:HA	1:BBB:925:GLY:O	2.20	0.42
1:BBB:983:VAL:HG11	1:BBB:985:TRP:CZ2	2.54	0.42
1:BBB:297:LEU:O	1:BBB:302:ALA:HB3	2.19	0.42
1:AAA:114:PHE:O	1:AAA:115:PRO:C	2.57	0.41
1:AAA:405:LEU:HA	1:AAA:941:HIS:CD2	2.56	0.41
1:AAA:527:MET:CE	1:AAA:532:TYR:HA	2.51	0.41
1:AAA:712:VAL:HG21	1:AAA:743:ARG:HD2	2.02	0.41
1:BBB:575:GLN:NE2	1:BBB:602:TYR:HB3	2.36	0.41
1:BBB:963:ARG:HD2	1:BBB:963:ARG:O	2.21	0.41
1:BBB:165:LEU:HD11	1:BBB:191:GLN:CG	2.51	0.41
1:AAA:412:ILE:CD1	1:AAA:434:ILE:HD11	2.51	0.41
1:AAA:1200:ASP:OD2	1:AAA:1209:ARG:NH1	2.53	0.41
1:BBB:98:VAL:HG21	1:BBB:119:GLN:HB3	2.03	0.41
1:AAA:377:VAL:HG11	1:AAA:412:ILE:HD13	2.03	0.41
1:BBB:978:GLU:HA	1:BBB:1071:PHE:CD2	2.56	0.41
1:AAA:126:MET:HG2	1:AAA:212:TYR:CZ	2.55	0.40
1:AAA:782:LEU:HD23	1:AAA:782:LEU:HA	1.86	0.40
1:BBB:653:TYR:O	1:BBB:674:SER:HA	2.21	0.40
1:BBB:838:ALA:HB2	1:BBB:874:LEU:CD2	2.51	0.40
1:AAA:808:ARG:NH2	1:AAA:824:ASP:OD1	2.54	0.40
1:BBB:1034:VAL:O	1:BBB:1093:ARG:HB3	2.20	0.40
1:BBB:1107:ASN:O	1:BBB:1111:GLU:HB2	2.22	0.40
1:BBB:527:MET:HE1	1:BBB:532:TYR:HA	2.03	0.40
1:BBB:1051:ASN:HA	1:BBB:1133:PHE:CE2	2.55	0.40
1:BBB:392:HIS:N	1:BBB:393:PRO:CD	2.85	0.40
1:AAA:272:CYS:HA	1:AAA:303:ARG:O	2.21	0.40
1:BBB:141:ILE:HD12	1:BBB:141:ILE:C	2.42	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	1238/1351 (92%)	1173 (95%)	61 (5%)	4 (0%)	41	66
1	BBB	1231/1351 (91%)	1164 (95%)	62 (5%)	5 (0%)	34	60
All	All	2469/2702 (91%)	2337 (95%)	123 (5%)	9 (0%)	34	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	468	VAL
1	AAA	942	ALA
1	BBB	115	PRO
1	BBB	942	ALA
1	AAA	467	ASN
1	AAA	115	PRO
1	BBB	883	ASN
1	BBB	802	ILE
1	BBB	806	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	1075/1147 (94%)	1060 (99%)	15 (1%)	67	86
1	BBB	1067/1147 (93%)	1048 (98%)	19 (2%)	59	83
All	All	2142/2294 (93%)	2108 (98%)	34 (2%)	62	85

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	29	VAL
1	AAA	119	GLN
1	AAA	197	SER
1	AAA	199	GLU

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Mol	Chain	Res	Type
1	AAA	511	ASP
1	AAA	559	ASN
1	AAA	653	TYR
1	AAA	667	ARG
1	AAA	769	ILE
1	AAA	846	GLN
1	AAA	943	LEU
1	AAA	1022	VAL
1	AAA	1129	LYS
1	AAA	1218	ASP
1	AAA	1295	SER
1	BBB	102	THR
1	BBB	141	ILE
1	BBB	158	GLN
1	BBB	445	ARG
1	BBB	490	ASN
1	BBB	513	GLN
1	BBB	517	ASN
1	BBB	653	TYR
1	BBB	659	SER
1	BBB	667	ARG
1	BBB	805	SER
1	BBB	963	ARG
1	BBB	971	GLU
1	BBB	1111	GLU
1	BBB	1176	PHE
1	BBB	1177	ASP
1	BBB	1218	ASP
1	BBB	1229	TYR
1	BBB	1295	SER

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

### 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 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	1258/1351 (93%)	0.24	23 (1%) 68 70	37, 64, 110, 185	37 (2%)
1	BBB	1251/1351 (92%)	0.36	48 (3%) 40 39	45, 78, 116, 189	36 (2%)
All	All	2509/2702 (92%)	0.30	71 (2%) 53 54	37, 71, 113, 189	73 (2%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	145	MET	8.1
1	AAA	143	GLN	5.9
1	BBB	853	VAL	4.8
1	BBB	145	MET	4.7
1	BBB	139	SER	4.6
1	BBB	852	ARG	4.4
1	BBB	134	LEU	4.4
1	AAA	132	ALA	4.3
1	BBB	146	LYS	4.1
1	AAA	146	LYS	4.0
1	BBB	138	LYS	3.7
1	BBB	160	ALA	3.7
1	BBB	143	GLN	3.6
1	AAA	133	GLN	3.6
1	AAA	139	SER	3.5
1	AAA	144	PHE	3.4
1	BBB	97	VAL	3.4
1	BBB	144	PHE	3.3
1	BBB	240	LEU	3.3
1	BBB	159	ASP	3.2
1	BBB	135	GLY	3.2
1	AAA	138	LYS	3.1
1	AAA	702	LEU	3.0
1	BBB	730	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	AAA	140	ALA	2.9
1	BBB	140	ALA	2.9
1	BBB	669	TYR	2.9
1	BBB	141	ILE	2.8
1	BBB	848	ASN	2.7
1	BBB	561	LEU	2.7
1	AAA	707	ARG	2.6
1	AAA	733	ILE	2.6
1	BBB	733	ILE	2.5
1	BBB	743	ARG	2.5
1	AAA	141	ILE	2.5
1	AAA	147	LYS	2.5
1	BBB	115	PRO	2.5
1	BBB	798	LEU	2.5
1	BBB	707	ARG	2.5
1	AAA	540	VAL	2.5
1	BBB	147	LYS	2.5
1	BBB	132	ALA	2.4
1	BBB	494	VAL	2.4
1	BBB	133	GLN	2.4
1	BBB	851	GLY	2.4
1	BBB	353	ARG	2.3
1	BBB	702	LEU	2.3
1	BBB	1330	VAL	2.3
1	BBB	704	ASP	2.3
1	BBB	715	ILE	2.3
1	AAA	142	ALA	2.2
1	BBB	740	GLN	2.2
1	AAA	112	ILE	2.2
1	AAA	353	ARG	2.2
1	BBB	190	PHE	2.2
1	BBB	843	VAL	2.2
1	BBB	161	MET	2.1
1	BBB	886	LYS	2.1
1	BBB	747	VAL	2.1
1	BBB	867	LYS	2.1
1	AAA	134	LEU	2.1
1	AAA	862	PHE	2.1
1	AAA	709	ILE	2.1
1	BBB	136	GLN	2.1
1	BBB	68	GLU	2.1
1	AAA	269	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	BBB	834	ALA	2.0
1	AAA	131	MET	2.0
1	BBB	450	LEU	2.0
1	BBB	122	ARG	2.0
1	BBB	248	VAL	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 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.