



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:10 PM UTC

PDB ID : 6YTJ / pdb_00006ytj
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

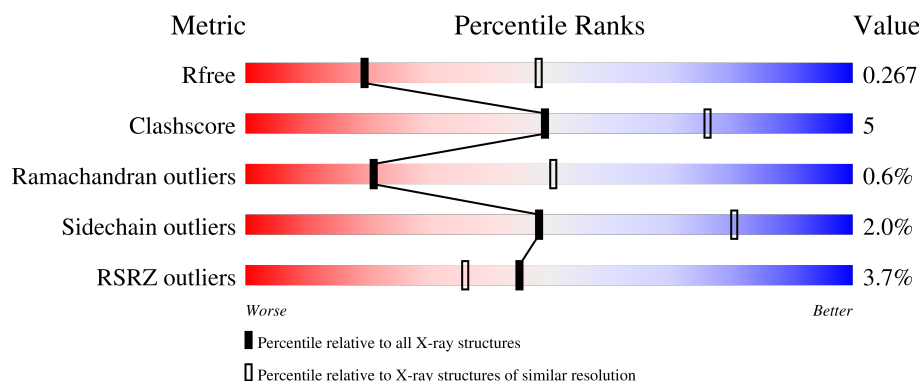
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	1351	4% 80% 11% 8%
1	BBB	1351	3% 77% 13% 10%

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

Continued on next page...

Continued from previous page...

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

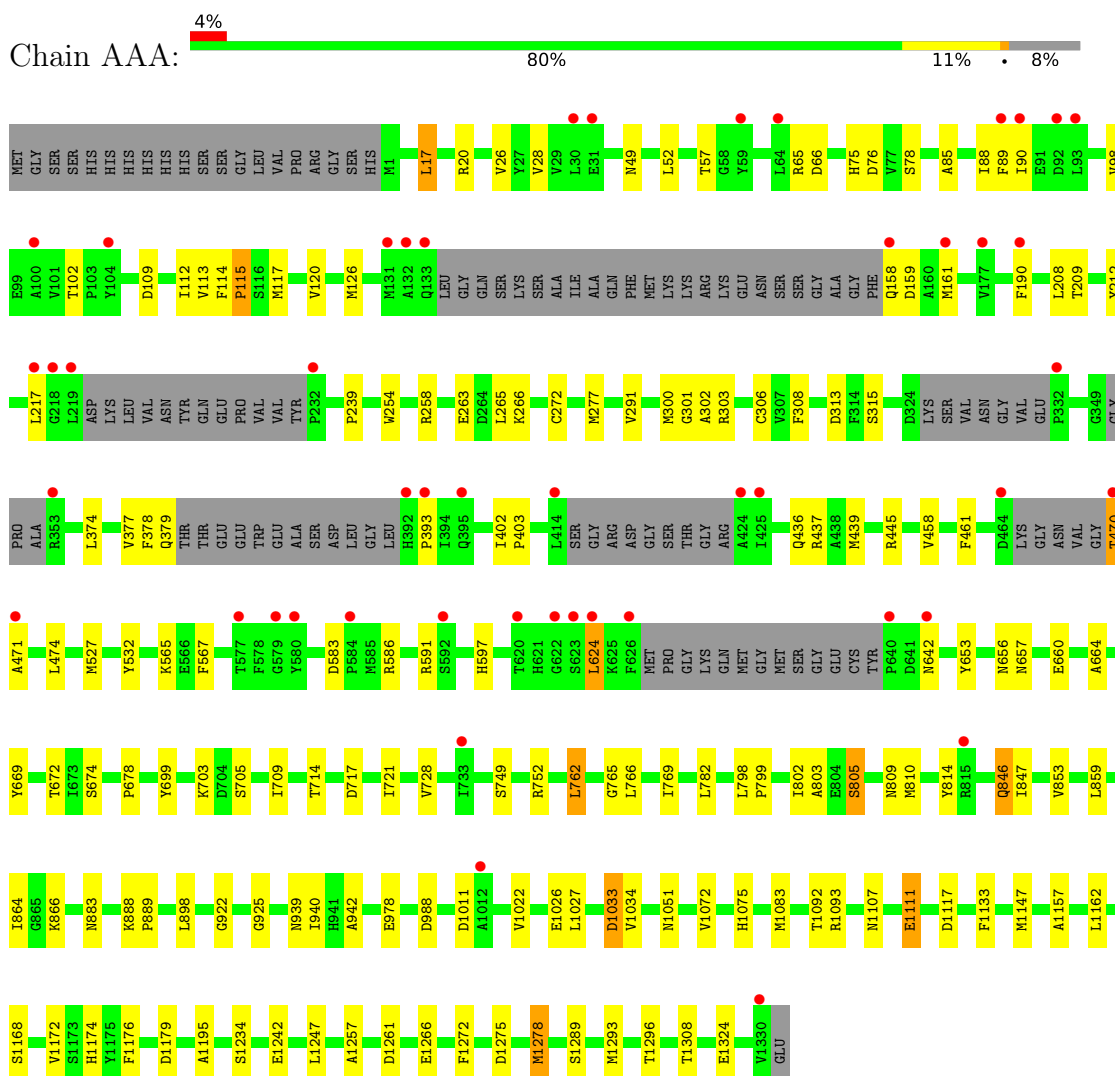
- Molecule 2 is water.

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

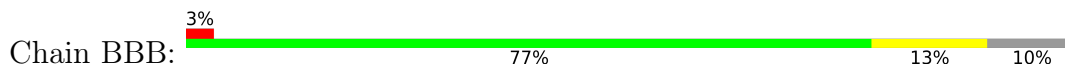
3 Residue-property plots [i](#)

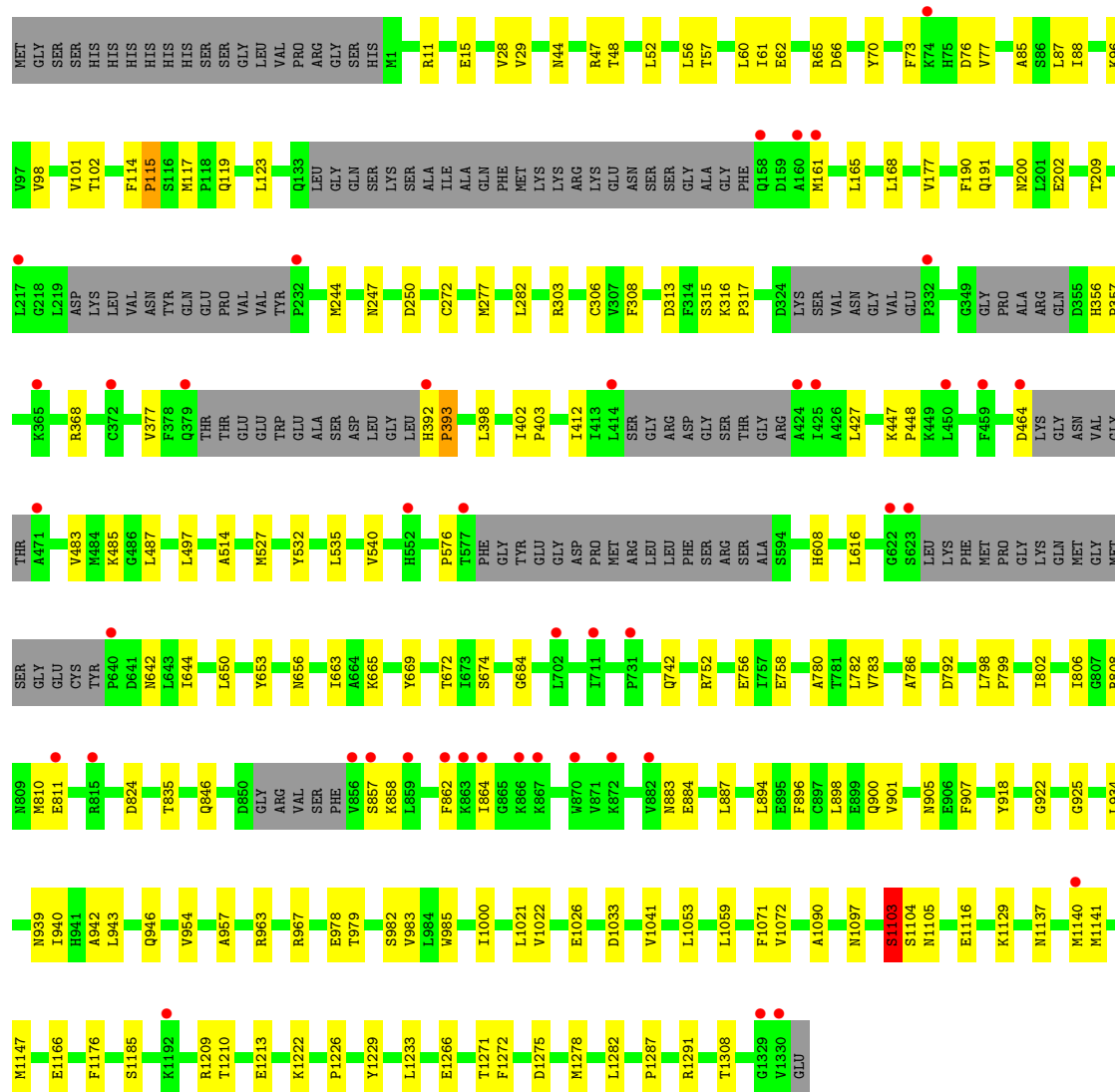
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	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) 99.2 (80.11-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	4970 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.00	0/10004	1.46	2/13567 (0.0%)
1	BBB	1.01	0/9773	1.47	9/13256 (0.1%)
All	All	1.01	0/19777	1.47	11/26823 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	1011	ASP	CA-CB-CG	5.62	118.22	112.60
1	BBB	1176	PHE	CA-CB-CG	5.54	119.34	113.80
1	BBB	282	LEU	CA-C-N	5.42	128.17	120.53
1	BBB	282	LEU	C-N-CA	5.42	128.17	120.53
1	BBB	1185	SER	CA-C-N	5.40	127.78	120.44
1	BBB	1185	SER	C-N-CA	5.40	127.78	120.44
1	BBB	1222	LYS	O-C-N	5.18	124.67	120.83
1	BBB	1222	LYS	CA-C-O	-5.13	116.85	119.77
1	BBB	907	PHE	CA-C-N	5.12	125.67	119.98
1	BBB	907	PHE	C-N-CA	5.12	125.67	119.98
1	AAA	1033	ASP	CA-CB-CG	5.10	117.70	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	9808	0	9684	115	0
1	BBB	9585	0	9460	95	0
2	AAA	14	0	0	0	0
2	BBB	5	0	0	0	0
All	All	19412	0	19144	208	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 (208) 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
1:AAA:89:PHE:CA	1:AAA:117:MET:HE1	1.76	1.15
1:AAA:89:PHE:N	1:AAA:117:MET:HE1	1.65	1.10
1:AAA:88:ILE:C	1:AAA:117:MET:SD	2.46	0.98
1:AAA:88:ILE:HG22	1:AAA:117:MET:SD	2.04	0.96
1:AAA:89:PHE:CA	1:AAA:117:MET:CE	2.49	0.89
1:AAA:89:PHE:HA	1:AAA:117:MET:CE	2.03	0.88
1:AAA:117:MET:SD	1:AAA:117:MET:N	2.51	0.83
1:BBB:1090:ALA:HA	1:BBB:1147:MET:HE1	1.58	0.83
1:AAA:90:ILE:H	1:AAA:117:MET:CE	1.93	0.82
1:AAA:90:ILE:N	1:AAA:117:MET:CE	2.43	0.81
1:AAA:109:ASP:HB3	1:AAA:212:TYR:O	1.83	0.78
1:AAA:90:ILE:N	1:AAA:117:MET:HE1	2.01	0.76
1:AAA:88:ILE:C	1:AAA:117:MET:HE1	2.11	0.75
1:AAA:117:MET:HG2	1:AAA:120:VAL:HG23	1.70	0.74
1:BBB:117:MET:HG2	1:BBB:119:GLN:HE22	1.56	0.70
1:AAA:89:PHE:C	1:AAA:117:MET:HE1	2.17	0.70
1:AAA:88:ILE:C	1:AAA:117:MET:CE	2.66	0.69
1:AAA:90:ILE:H	1:AAA:117:MET:HE1	1.53	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:803:ALA:HB2	1:AAA:810:MET:HE2	1.78	0.64
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: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:247:ASN:HD21	1:BBB:250:ASP:CG	2.08	0.61
1:BBB:808:ARG:NH2	1:BBB:824:ASP:OD1	2.34	0.60
1:AAA:762:LEU:HD12	1:AAA:762:LEU:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:799:PRO:C	1:AAA:810:MET:HE3	2.29	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:AAA:98:VAL:O	1:AAA:102:THR:OG1	2.20	0.56
1:BBB:247:ASN:ND2	1:BBB:250:ASP:OD2	2.36	0.56
1:BBB:114:PHE:O	1:BBB:115:PRO:C	2.48	0.56
1:BBB:1104:SER:O	1:BBB:1105:ASN:HB2	2.05	0.56
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:BBB:277:MET:HE3	1:BBB:306:CYS:SG	2.48	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:967:ARG:HH22	1:BBB:1213:GLU:CD	2.15	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:1266:GLU:OE2	1:BBB:1308:THR:OG1	2.20	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:BBB:57:THR:HG21	1:BBB:76:ASP:OD2	2.10	0.51
1:AAA:89:PHE:C	1:AAA:117:MET:CE	2.78	0.51
1:AAA:591:ARG:CD	1:BBB:1116:GLU:HB3	2.40	0.51
1:BBB:1278:MET:HE2	1:BBB:1282:LEU:HG	1.91	0.51
1:AAA:113:VAL:HG11	1:AAA:120:VAL:HG12	1.92	0.51
1:AAA:1275:ASP:OD1	1:AAA:1275:ASP:C	2.53	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:126:MET:HG2	1:AAA:212:TYR:CZ	2.46	0.50
1:AAA:1157:ALA:HA	1:AAA:1195:ALA:O	2.10	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:402:ILE:HB	1:AAA:403:PRO:HD3	1.92	0.50
1:BBB:244:MET:HE2	1:BBB:308:PHE:CZ	2.46	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:300:MET:HE1	1:AAA:436:GLN:HG3	1.94	0.49
1:AAA:26:VAL:HA	1:AAA:57:THR:O	2.12	0.49
1:BBB:313:ASP:OD1	1:BBB:315:SER:OG	2.27	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:678:PRO:HG2	1:AAA:765:GLY:O	2.12	0.49
1:AAA:1247:LEU:HG	1:AAA:1296:THR:HG21	1.95	0.49
1:AAA:89:PHE:HA	1:AAA:117:MET:HE3	1.89	0.49
1:AAA:1051:ASN:HA	1:AAA:1133:PHE:HE2	1.78	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
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:AAA:28:VAL:O	1:AAA:85:ALA:HA	2.12	0.48
1:BBB:527:MET:HE3	1:BBB:532:TYR:HA	1.95	0.48
1:AAA:277:MET:HE3	1:AAA:306:CYS:HB3	1.94	0.48
1:AAA:378:PHE:O	1:AAA:379:GLN:C	2.57	0.48
1:BBB:65:ARG:O	1:BBB:66:ASP:C	2.56	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:70:TYR:OH	1:BBB:96:LYS:O	2.27	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:527:MET:HE1	1:BBB:532:TYR:HD1	1.78	0.47
1:BBB:656:ASN:HA	1:BBB:925:GLY:O	2.14	0.47
1:BBB:799:PRO:CB	1:BBB:810:MET:HE3	2.44	0.47
1:BBB:377:VAL:HG11	1:BBB:412:ILE:HD13	1.96	0.47
1:BBB:368:ARG:O	1:BBB:918:TYR:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:17:LEU:HD22	1:AAA:20:ARG:O	2.14	0.47
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:AAA:1289:SER:O	1:AAA:1293:MET:HG3	2.16	0.46
1:AAA:532:TYR:OH	1:AAA:597:HIS:ND1	2.44	0.46
1:AAA:699:TYR:CZ	1:AAA:703:LYS:HD2	2.50	0.46
1:BBB:44:ASN:HD22	1:BBB:202:GLU:CD	2.24	0.46
1:BBB:1137:ASN:ND2	1:BBB:1140:MET:HG3	2.30	0.46
1:AAA:527:MET:HE3	1:AAA:532:TYR:HA	1.97	0.45
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:527:MET:HE1	1:AAA:532:TYR:HD1	1.82	0.45
1:AAA:846:GLN:HG3	1:AAA:847:ILE:N	2.32	0.45
1:AAA:883:ASN:OD1	1:AAA:883:ASN:C	2.60	0.45
1:BBB:114:PHE:CD1	1:BBB:190:PHE:CD1	3.05	0.45
1:AAA:1083:MET:HE1	1:AAA:1147:MET:HE2	1.99	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:88:ILE:HD12	1:AAA:88:ILE:N	2.33	0.44
1:AAA:302:ALA:HB2	1:AAA:439:MET:SD	2.57	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: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:90:ILE:H	1:AAA:117:MET:HE2	1.81	0.43
1:AAA:565:LYS:HG3	1:AAA:567:PHE:CE1	2.54	0.43
1:AAA:799:PRO:O	1:AAA:810:MET:CE	2.67	0.43
1:AAA:1266:GLU:OE2	1:AAA:1308:THR:OG1	2.20	0.43
1:BBB:1226:PRO:HA	1:BBB:1229:TYR:CE2	2.54	0.43
1:BBB:1233:LEU:HD13	1:BBB:1278:MET:HE1	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:527:MET:HE3	1:BBB:532:TYR:CA	2.49	0.43
1:BBB:884:GLU:HA	1:BBB:887:LEU:HB3	2.01	0.43
1:BBB:1097:ASN:ND2	1:BBB:1103:SER:O	2.44	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:762:LEU:HD12	1:AAA:762:LEU:C	2.42	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:300:MET:HE1	1:AAA:436:GLN:CG	2.49	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: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: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:398:LEU:HD22	1:BBB:946:GLN:HG3	2.02	0.42
1:BBB:464:ASP:OD1	1:BBB:1291:ARG:NH1	2.50	0.42
1:AAA:799:PRO:O	1:AAA:810:MET:HE3	2.19	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:806:ILE:O	1:BBB:806:ILE:HG13	2.19	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:BBB:1021:LEU:HD11	1:BBB:1059:LEU:C	2.45	0.42
1:BBB:665:LYS:NZ	1:BBB:940:ILE:O	2.49	0.41
1:AAA:374:LEU:O	1:AAA:377:VAL:HB	2.20	0.41
1:AAA:527:MET:HE3	1:AAA:532:TYR:CA	2.50	0.41
1:BBB:61:ILE:HD12	1:BBB:88:ILE:HG13	2.00	0.41
1:BBB:200:ASN:HD22	1:BBB:200:ASN:HA	1.74	0.41
1:BBB:316:LYS:HB2	1:BBB:317:PRO:HD3	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: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:AAA:272:CYS:HA	1:AAA:303:ARG:O	2.21	0.41
1:BBB:165:LEU:HD11	1:BBB:191:GLN:CG	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:922:GLY:O	1:BBB:940:ILE:HA	2.20	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:BBB:1271:THR:HG22	1:BBB:1272:PHE:CD1	2.56	0.40
1:AAA:802:ILE:O	1:AAA:805:SER:HB3	2.21	0.40
1:AAA:1172:VAL:HG21	1:AAA:1174:HIS:CD2	2.57	0.40
1:BBB:52:LEU:HD22	1:BBB:209:THR:HG21	2.04	0.40
1:BBB:70:TYR:CE1	1:BBB:96:LYS:HB3	2.57	0.40
1:BBB:616:LEU:HA	1:BBB:650:LEU:O	2.20	0.40
1:AAA:583:ASP:HB3	1:AAA:586:ARG:HB2	2.03	0.40
1:AAA:1034:VAL:O	1:AAA:1093:ARG:HB3	2.20	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 [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	AAA	1227/1351 (91%)	1145 (93%)	77 (6%)	5 (0%)	30 60
1	BBB	1196/1351 (88%)	1100 (92%)	87 (7%)	9 (1%)	16 44
All	All	2423/2702 (90%)	2245 (93%)	164 (7%)	14 (1%)	21 51

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [i](#)

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%)	1039 (98%)	24 (2%)	44	78
1	BBB	1040/1147 (91%)	1021 (98%)	19 (2%)	51	82
All	All	2103/2294 (92%)	2060 (98%)	43 (2%)	48	80

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	17	LEU
1	AAA	49	ASN
1	AAA	66	ASP
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

Continued on next page...

Continued from previous page...

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

Sometimes 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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	AAA	1245/1351 (92%)	-0.02	48 (3%)	43 34	27, 54, 99, 146	37 (2%)
1	BBB	1218/1351 (90%)	0.28	43 (3%)	47 38	34, 71, 108, 159	36 (2%)
All	All	2463/2702 (91%)	0.13	91 (3%)	45 36	27, 62, 105, 159	73 (2%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	219	LEU	5.1
1	BBB	862	PHE	5.0
1	AAA	640	PRO	4.7
1	BBB	332	PRO	4.6
1	AAA	470	THR	4.5
1	BBB	471	ALA	4.1
1	BBB	623	SER	4.0
1	BBB	864	ILE	4.0
1	AAA	425	ILE	3.9
1	AAA	580	TYR	3.8
1	BBB	424	ALA	3.8
1	BBB	425	ILE	3.7
1	BBB	392	HIS	3.7
1	BBB	856	VAL	3.7
1	AAA	392	HIS	3.6
1	BBB	640	PRO	3.6
1	AAA	464	ASP	3.6
1	AAA	177	VAL	3.5
1	BBB	815	ARG	3.5
1	BBB	1330	VAL	3.4
1	AAA	622	GLY	3.3
1	AAA	218	GLY	3.3
1	BBB	414	LEU	3.2
1	BBB	577	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BBB	459	PHE	3.2
1	AAA	424	ALA	3.1
1	AAA	158	GLN	3.1
1	BBB	161	MET	3.1
1	BBB	158	GLN	3.0
1	BBB	552	HIS	3.0
1	BBB	232	PRO	2.9
1	AAA	577	THR	2.9
1	BBB	217	LEU	2.9
1	BBB	450	LEU	2.9
1	AAA	623	SER	2.8
1	AAA	93	LEU	2.8
1	AAA	131	MET	2.8
1	AAA	815	ARG	2.8
1	BBB	863	LYS	2.7
1	BBB	859	LEU	2.7
1	BBB	365	LYS	2.7
1	BBB	1140	MET	2.7
1	BBB	464	ASP	2.7
1	BBB	711	ILE	2.6
1	AAA	1330	VAL	2.6
1	AAA	414	LEU	2.6
1	AAA	31	GLU	2.6
1	AAA	232	PRO	2.6
1	AAA	90	ILE	2.5
1	BBB	379	GLN	2.5
1	BBB	1192	LYS	2.4
1	AAA	30	LEU	2.4
1	BBB	74	LYS	2.4
1	AAA	332	PRO	2.4
1	BBB	857	SER	2.3
1	AAA	579	GLY	2.3
1	BBB	811	GLU	2.3
1	AAA	592	SER	2.3
1	AAA	217	LEU	2.3
1	AAA	626	PHE	2.3
1	AAA	1012	ALA	2.2
1	AAA	133	GLN	2.2
1	AAA	100	ALA	2.2
1	BBB	731	PRO	2.2
1	BBB	622	GLY	2.2
1	AAA	471	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	AAA	104	TYR	2.2
1	BBB	867	LYS	2.2
1	AAA	92	ASP	2.2
1	BBB	882	VAL	2.2
1	AAA	59	TYR	2.1
1	BBB	866	LYS	2.1
1	BBB	872	LYS	2.1
1	AAA	161	MET	2.1
1	AAA	395	GLN	2.1
1	BBB	372	CYS	2.1
1	AAA	624	LEU	2.1
1	AAA	132	ALA	2.1
1	AAA	620	THR	2.1
1	AAA	393	PRO	2.1
1	AAA	64	LEU	2.1
1	BBB	702	LEU	2.1
1	AAA	89	PHE	2.1
1	BBB	160	ALA	2.0
1	AAA	584	PRO	2.0
1	BBB	1329	GLY	2.0
1	AAA	190	PHE	2.0
1	BBB	870	TRP	2.0
1	AAA	642	ASN	2.0
1	AAA	733	ILE	2.0
1	AAA	353	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.