Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2020 – 09:07 am GMT

PDB ID	:	6YSG
Title	:	Magnesium chelatase H subunit (ChlH) from Synechocystis sp.PCC6803 to 2.54 A resolution
Authors	:	Bisson, C.; Hunter, C.N.
Deposited on	:	2020-04-22
Resolution	:	2.54 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 following versions of software and data (see references ⓘ) were used in the production of this report:

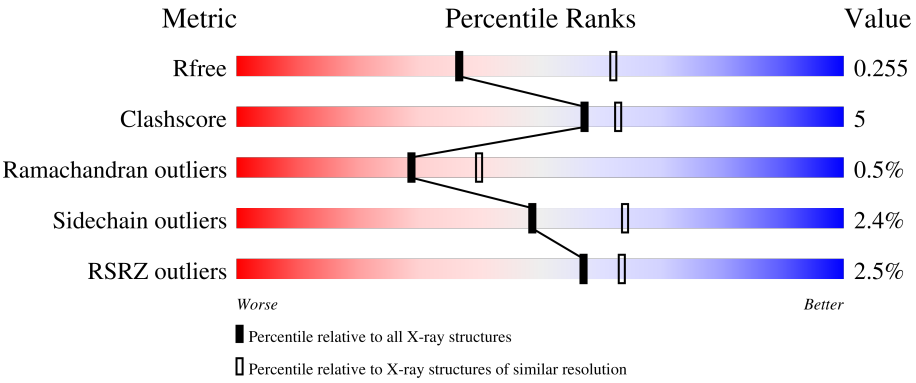
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

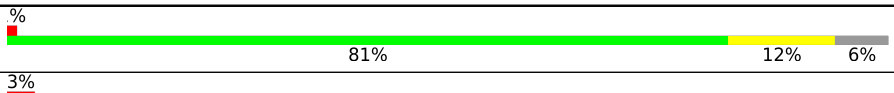
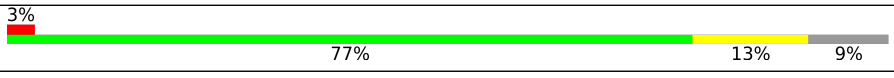
The reported resolution of this entry is 2.54 Å.

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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 >=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 <=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	1351	
1	B	1351	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19729 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	A	1264	Total	C	N	O	S	0	0	0
			9946	6301	1691	1904	50			
1	B	1225	Total	C	N	O	S	0	1	0
			9656	6116	1636	1856	48			

There are 40 discrepancies between the modelled and reference sequences:

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

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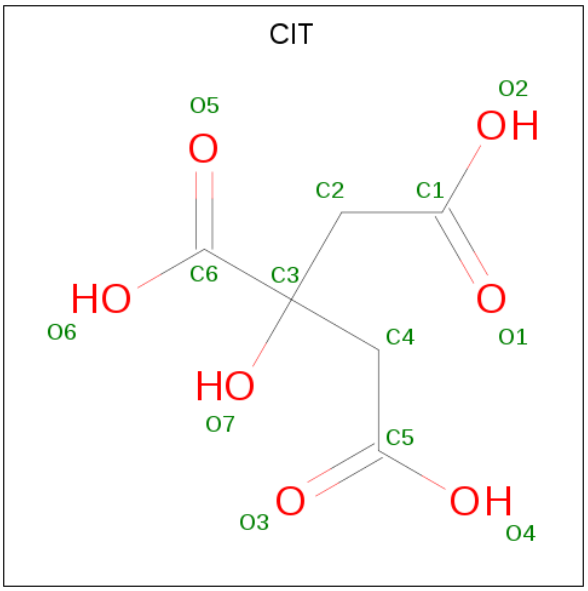
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P73020
B	-13	HIS	-	expression tag	UNP P73020
B	-12	HIS	-	expression tag	UNP P73020
B	-11	HIS	-	expression tag	UNP P73020
B	-10	HIS	-	expression tag	UNP P73020
B	-9	SER	-	expression tag	UNP P73020
B	-8	SER	-	expression tag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

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	85	Total O 85 85	0	0

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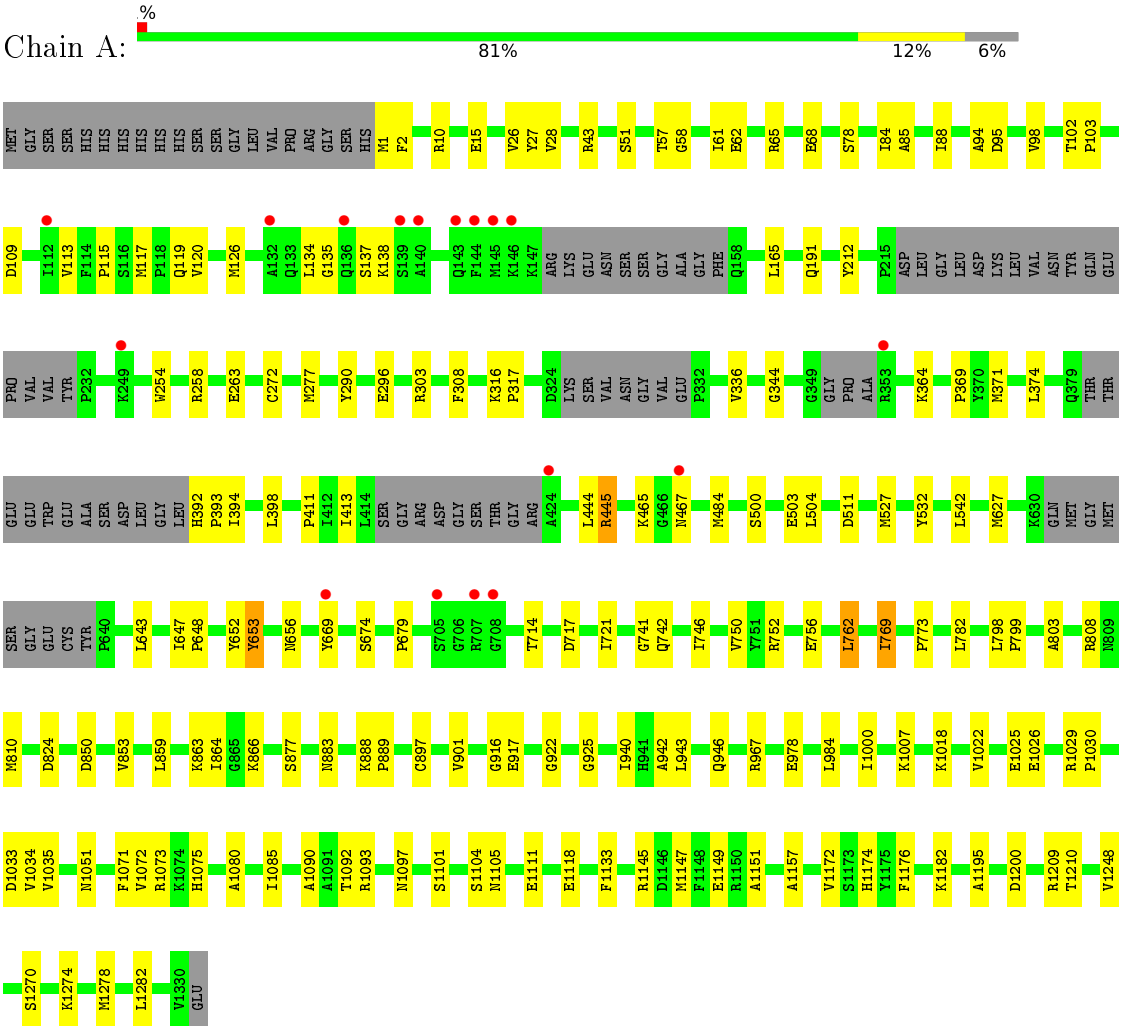
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	29	Total O 29 29	0	0

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.

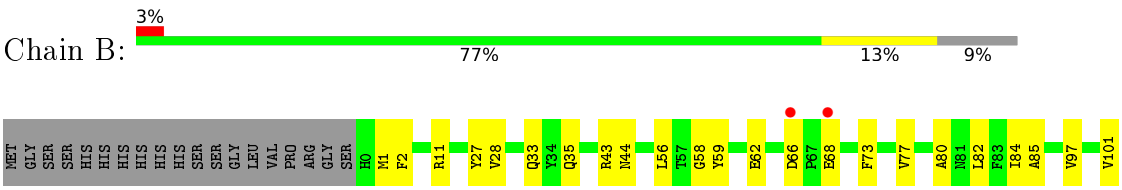
- Molecule 1: Mg-chelatase subunit ChlH

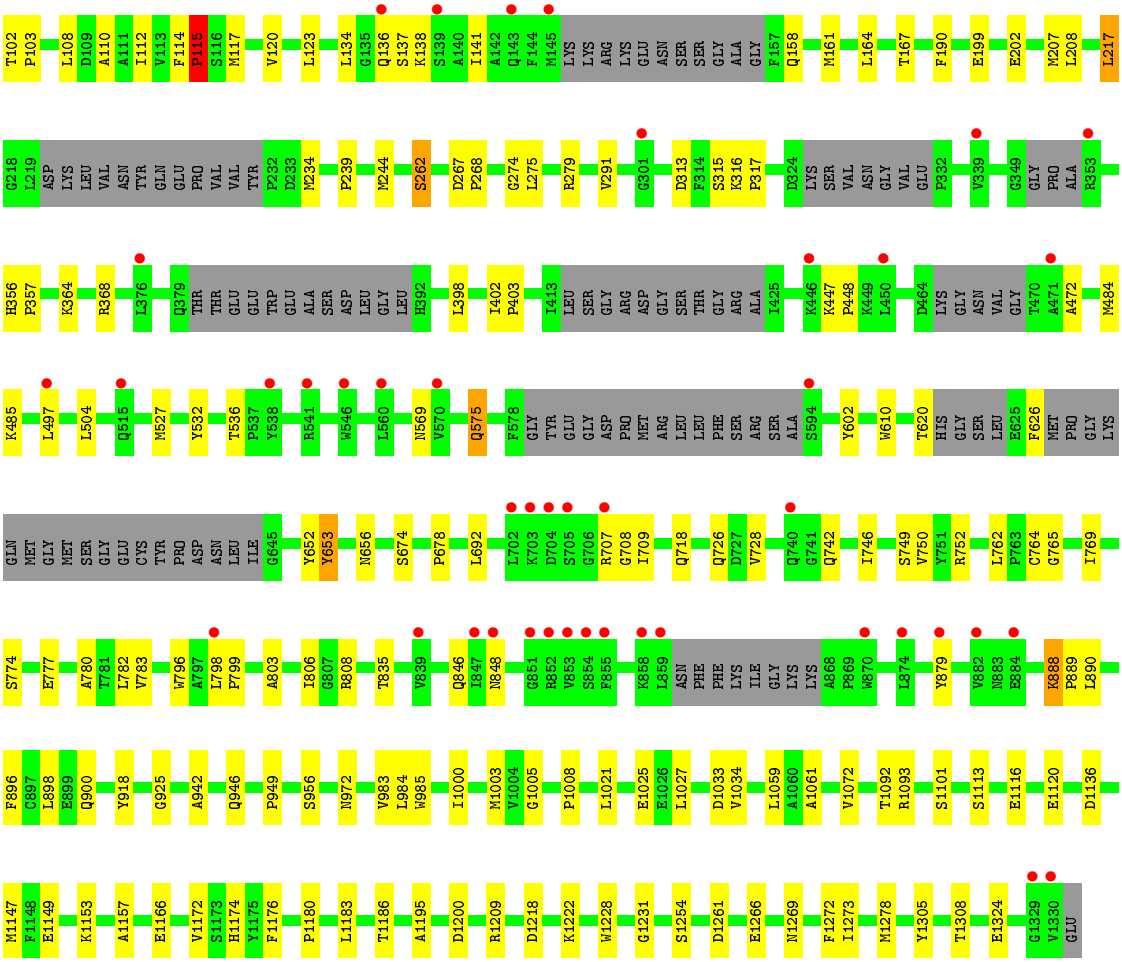
Chain A:



- Molecule 1: Mg-chelatase subunit ChlH

Chain B:




T102 P103 L108 D109 A110 A111 I112 V113 F114 P115 S116 M117 V120 L123 L134 G135 Q136 S137 K138 S139 A140 I141 A142 Q143 F144 M145 LYS LYS ARG LYS GLU ASN SER SER GLY ALA GLY F157 Q158 M161 L164 T167 F190 E199 E202 M207 L208 L217
G218 L219 ASP LYS LEU VAL ASN TYR GLN GLU PRO VAL VAL TYR P232 D233 M234 P239 M244 S262 D267 P268 G274 L275 R279 V291 G301 D313 F314 S315 K316 P317 D324 LYS SER VAL ASN GLY VAL GLU P332 V339 G349 GLY PRO ALA R353
H356 P357 K364 R368 L376 Q379 THR THR GLU GLU TRP GLU ALA SER ASP LEU GLY LEU H392 L398 I402 P403 I413 LEU SER GLY ARG ASP GLY SER THR GLY ARG ALA I425 K446 K447 P448 K449 L450 D464 LYS GLY ASN VAL GLY T470 A471 A472 M484
K485 L497 L504 Q515 M527 Y532 T536 P537 Y538 R541 W546 L560 N569 V570 Q575 F578 GLY TYR GLU GLY ASP PRO MET ARG LEU LEU PHE SER ARG SER ALA S594 Y602 W610 T620 HIS GLY SER LEU E625 F626 MET PRO GLY LYS
GLN MET GLY MET SER GLY GLU CYS TYR PRO ASP ASN LEU ILE G645 Y652 Y653 N656 S674 P678 L692 L702 K703 D704 S705 G706 R707 G708 I709 Q718 Q726 D727 V728 Q740 G741 Q742 I746 S749 V750 Y751 R752 L762 P763 C764 G765 I769
S774 E777 A780 T781 L782 V783 W796 A797 L798 P799 A803 I806 G807 R808 T835 V839 Q846 I847 N848 Q851 R852 V853 S854 F855 K858 L859 ASN PHE PHE LYS ILE GLY LYS LYS A868 P869 W870 L874 Y879 V882 N883 E884 K888 P889 L890
F896 C897 L898 E899 Q900 Y918 G925 A942 Q946 P949 S956 N972 V983 L984 W985 I1000 M1003 V1004 G1005 P1008 L1021 E1025 E1026 L1027 D1033 V1034 L1059 A1060 A1061 V1072 T1092 R1093 S1101 S1113 E1116 E1120 D1136
M1147 F1148 E1149 K1153 A1157 E1166 V1172 S1173 H1174 Y1175 F1176 P1180 L1183 T1186 A1195 D1200 R1209 D1218 K1222 W1228 G1231 S1254 D1261 E1266 N1269 F1272 I1273 M1278 Y1305 T1308 E1324 G1329 V1330 GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	321.12Å 321.12Å 104.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.78 – 2.54 83.78 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (83.78-2.54) 99.7 (83.78-2.54)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.202 , 0.255 0.207 , 0.255	Depositor DCC
R_{free} test set	6684 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19729	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CIT

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	0.72	3/10145 (0.0%)	0.86	0/13753
1	B	0.72	4/9848 (0.0%)	0.82	0/13354
All	All	0.72	7/19993 (0.0%)	0.84	0/27107

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	GLU	CD-OE1	9.11	1.35	1.25
1	B	68	GLU	CD-OE1	8.98	1.35	1.25
1	B	68	GLU	CD-OE2	7.62	1.34	1.25
1	A	68	GLU	CD-OE2	6.38	1.32	1.25
1	B	66	ASP	CG-OD2	5.97	1.39	1.25
1	A	1	MET	N-CA	5.20	1.56	1.46
1	B	66	ASP	CG-OD1	5.05	1.36	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9946	0	9833	95	0
1	B	9656	0	9516	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	5	1	0
3	A	85	0	0	0	0
3	B	29	0	0	1	0
All	All	19729	0	19354	189	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 (189) 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:B:1116:GLU:HB3	1:B:1120:GLU:OE2	1.80	0.81
1:A:803:ALA:HB2	1:A:810:MET:HE1	1.70	0.74
1:A:467:ASN:OD1	1:A:1111:GLU:HA	1.90	0.71
1:A:1172:VAL:HG21	1:A:1174:HIS:CE1	2.27	0.70
1:B:1034:VAL:O	1:B:1093:ARG:HD2	1.90	0.69
1:A:109:ASP:HB3	1:A:212:TYR:O	1.93	0.68
1:A:62:GLU:O	1:A:65:ARG:HG3	1.92	0.67
1:B:527:MET:HE3	1:B:532:TYR:HA	1.77	0.66
1:A:467:ASN:HB2	1:A:1111:GLU:HB2	1.77	0.65
1:B:141:ILE:HD11	1:B:167:THR:HG21	1.82	0.62
1:B:44:ASN:HD22	1:B:202:GLU:CD	2.03	0.61
1:B:984:LEU:HD21	1:B:1000:ILE:HD12	1.82	0.60
1:B:1003:MET:HE3	1:B:1034:VAL:HG12	1.84	0.60
1:B:402:ILE:HB	1:B:403:PRO:HD3	1.83	0.59
1:A:808:ARG:NH2	1:A:824:ASP:OD1	2.35	0.59
1:B:472:ALA:CB	1:B:620:THR:HG22	2.33	0.59
1:A:27:TYR:CE1	1:A:58:GLY:HA3	2.38	0.58
1:B:718:GLN:HA	1:B:718:GLN:OE1	2.03	0.58
1:A:717:ASP:O	1:A:721:ILE:HG12	2.04	0.58
1:B:806:ILE:HG22	1:B:806:ILE:O	2.03	0.58
1:B:207:MET:CE	1:B:208:LEU:HD23	2.33	0.58
1:A:799:PRO:O	1:A:810:MET:CE	2.52	0.57
1:B:316:LYS:HB2	1:B:317:PRO:HD3	1.85	0.57
1:A:527:MET:CE	1:A:532:TYR:HA	2.35	0.56
1:A:484:MET:HE2	1:A:504:LEU:CD1	2.34	0.56
1:B:1172:VAL:HG21	1:B:1174:HIS:CE1	2.41	0.56
1:B:472:ALA:HB2	1:B:620:THR:HG22	1.86	0.56
1:A:803:ALA:HB2	1:A:810:MET:CE	2.34	0.56
1:A:2:PHE:CE2	1:B:1025:GLU:HA	2.41	0.55
1:A:1092:THR:HB	1:A:1147:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ARG:HH12	1:A:917:GLU:HG2	1.71	0.55
1:A:465:LYS:HB3	1:A:1111:GLU:CD	2.27	0.55
1:A:762:LEU:HD12	1:A:762:LEU:O	2.07	0.54
1:B:575:GLN:OE1	1:B:602:TYR:HB3	2.06	0.54
1:A:1157:ALA:HA	1:A:1195:ALA:O	2.08	0.54
1:B:798:LEU:HB3	1:B:799:PRO:HD3	1.90	0.54
1:B:806:ILE:HD11	1:B:879:TYR:CE1	2.43	0.54
1:A:254:TRP:CH2	1:A:258:ARG:HD2	2.43	0.53
1:A:799:PRO:O	1:A:810:MET:HE2	2.08	0.53
1:A:1022:VAL:HG13	1:A:1026:GLU:HB3	1.91	0.53
1:B:652:TYR:CD2	1:B:769:ILE:HD13	2.43	0.53
1:B:267:ASP:OD1	1:B:268:PRO:HD2	2.09	0.53
1:A:1035:VAL:HG22	1:A:1151:ALA:HB1	1.91	0.53
1:A:316:LYS:HB2	1:A:317:PRO:HD3	1.91	0.53
1:A:444:LEU:HD22	1:A:648:PRO:HG2	1.91	0.53
1:A:978:GLU:HA	1:A:1071:PHE:CD2	2.43	0.53
1:B:97:VAL:O	1:B:101:VAL:HG23	2.09	0.53
1:A:134:LEU:HB2	1:A:138:LYS:HB3	1.90	0.53
1:B:484:MET:HE1	1:B:504:LEU:HD13	1.91	0.53
1:A:1029:ARG:HB2	1:A:1030:PRO:CD	2.39	0.52
1:A:467:ASN:ND2	1:A:1248:VAL:HG12	2.24	0.52
1:A:967:ARG:NH2	1:A:1210:THR:HG23	2.25	0.52
1:B:27:TYR:CE1	1:B:58:GLY:HA3	2.45	0.52
1:A:756:GLU:OE2	1:A:1209:ARG:NH2	2.42	0.52
1:A:484:MET:HE2	1:A:504:LEU:HD13	1.92	0.52
1:A:254:TRP:CZ3	1:A:258:ARG:HD2	2.44	0.52
1:A:1200:ASP:OD2	1:A:1209:ARG:NH1	2.44	0.51
1:B:678:PRO:HG2	1:B:765:GLY:O	2.10	0.51
1:A:277:MET:HB2	1:A:290:TYR:CE2	2.45	0.51
1:A:853:VAL:HG11	1:A:859:LEU:HD21	1.92	0.51
1:A:978:GLU:HB3	1:A:1075:HIS:CE1	2.45	0.51
1:A:1018:LYS:NZ	1:B:199:GLU:OE2	2.34	0.51
1:B:983:VAL:HG11	1:B:985:TRP:CZ2	2.46	0.51
1:A:165:LEU:HD11	1:A:191:GLN:CG	2.41	0.51
1:A:656:ASN:HA	1:A:925:GLY:O	2.10	0.51
1:A:984:LEU:HD21	1:A:1000:ILE:HD12	1.92	0.51
1:A:394:ILE:O	1:A:398:LEU:HG	2.11	0.51
1:A:484:MET:CE	1:A:504:LEU:HD13	2.41	0.51
1:A:1033:ASP:HA	1:A:1072:VAL:HG22	1.92	0.50
1:B:1003:MET:CE	1:B:1034:VAL:HG12	2.40	0.50
1:A:1025:GLU:HA	1:B:2:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:LYS:HG2	1:B:497:LEU:HD21	1.93	0.50
1:A:27:TYR:HA	1:A:84:ILE:O	2.11	0.50
1:A:28:VAL:O	1:A:85:ALA:HA	2.12	0.50
1:B:527:MET:CE	1:B:532:TYR:HA	2.39	0.50
1:A:413:ILE:HG13	1:A:669:TYR:CE1	2.47	0.50
1:B:28:VAL:O	1:B:85:ALA:HA	2.12	0.50
1:A:864:ILE:HG13	1:A:866:LYS:HG3	1.94	0.49
1:B:134:LEU:HB2	1:B:138:LYS:HB2	1.95	0.49
1:B:656:ASN:HA	1:B:925:GLY:O	2.12	0.49
1:A:1118:GLU:OE2	1:A:1182:LYS:NZ	2.43	0.49
1:A:94:ALA:O	1:A:98:VAL:HG23	2.13	0.49
1:B:1278:MET:HE3	1:B:1278:MET:HA	1.94	0.48
1:A:527:MET:HE1	1:A:532:TYR:HA	1.94	0.48
1:B:398:LEU:HD22	1:B:946:GLN:HG3	1.94	0.48
1:A:922:GLY:O	1:A:940:ILE:HA	2.12	0.48
1:B:114:PHE:CD1	1:B:190:PHE:CD1	3.01	0.48
1:B:114:PHE:O	1:B:115:PRO:C	2.52	0.48
1:A:316:LYS:HB2	1:A:317:PRO:CD	2.43	0.48
1:B:274:GLY:O	1:B:275:LEU:HD23	2.14	0.48
1:B:742:GLN:O	1:B:746:ILE:HG12	2.14	0.48
1:A:1278:MET:HE2	1:A:1282:LEU:HD21	1.95	0.47
1:B:11:ARG:HA	1:B:56:LEU:O	2.13	0.47
1:A:369:PRO:HD3	1:A:916:GLY:O	2.14	0.47
1:A:398:LEU:HD22	1:A:946:GLN:HG3	1.95	0.47
1:A:371:MET:CE	1:A:411:PRO:HB3	2.45	0.47
1:A:1029:ARG:HB2	1:A:1030:PRO:HD2	1.96	0.47
1:B:707:ARG:O	1:B:709:ILE:N	2.45	0.47
1:B:1005:GLY:HA3	1:B:1027:LEU:HD22	1.97	0.47
1:B:239:PRO:HB3	1:B:291:VAL:HG22	1.97	0.46
1:A:26:VAL:HA	1:A:57:THR:O	2.15	0.46
1:B:728:VAL:HG13	1:B:749:SER:HB3	1.98	0.46
1:B:368:ARG:O	1:B:918:TYR:HB2	2.15	0.46
1:A:883:ASN:OD1	1:A:883:ASN:C	2.54	0.46
1:B:653:TYR:O	1:B:674:SER:HA	2.16	0.46
1:A:117:MET:HB3	1:A:119:GLN:OE1	2.16	0.46
1:A:652:TYR:CD2	1:A:769:ILE:HD13	2.52	0.46
1:B:1021:LEU:HD11	1:B:1059:LEU:C	2.35	0.45
1:B:112:ILE:N	1:B:112:ILE:HD12	2.31	0.45
1:A:102:THR:HB	1:A:103:PRO:HD3	1.97	0.45
1:B:1272:PHE:HA	1:B:1278:MET:HG2	1.97	0.45
1:A:798:LEU:HB3	1:A:799:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:MET:O	1:A:308:PHE:HA	2.17	0.45
1:B:28:VAL:HA	1:B:59:TYR:O	2.18	0.45
1:A:1145:ARG:O	1:A:1149:GLU:HG3	2.17	0.44
1:B:949:PRO:HG2	1:B:1008:PRO:HG3	1.99	0.44
1:B:1183:LEU:O	1:B:1186:THR:HB	2.18	0.44
1:B:120:VAL:O	1:B:123:LEU:HB2	2.18	0.44
1:B:27:TYR:OH	1:B:35:GLN:HG3	2.17	0.44
1:A:272:CYS:HA	1:A:303:ARG:O	2.17	0.44
1:A:888:LYS:HB3	1:A:889:PRO:CD	2.47	0.44
1:B:1200:ASP:OD2	1:B:1209:ARG:NH1	2.51	0.44
1:B:983:VAL:HG11	1:B:985:TRP:CE2	2.52	0.44
1:B:896:PHE:O	1:B:900:GLN:HG2	2.17	0.44
1:B:115:PRO:HD3	1:B:164:LEU:HD23	2.00	0.44
1:B:115:PRO:HD3	1:B:164:LEU:CD2	2.47	0.44
1:B:569:ASN:O	1:B:610:TRP:HH2	2.00	0.44
1:B:80:ALA:O	1:B:108:LEU:HD23	2.18	0.44
1:A:113:VAL:HG11	1:A:120:VAL:HG12	1.99	0.43
1:B:762:LEU:O	1:B:762:LEU:HD12	2.18	0.43
1:B:1266:GLU:OE2	1:B:1308:THR:OG1	2.25	0.43
1:A:43:ARG:HD2	1:B:1136:ASP:OD1	2.18	0.43
1:A:10:ARG:HB3	1:A:58:GLY:O	2.18	0.43
1:B:82:LEU:CD2	1:B:110:ALA:HB3	2.47	0.43
1:B:764:CYS:O	1:B:1231:GLY:HA3	2.18	0.43
1:B:356:HIS:N	1:B:357:PRO:CD	2.81	0.43
1:B:806:ILE:HD11	1:B:879:TYR:HE1	1.83	0.43
1:A:1104:SER:O	1:A:1105:ASN:HB2	2.18	0.43
1:B:888:LYS:HB3	1:B:889:PRO:HD3	1.99	0.43
1:A:344:GLY:HA2	1:A:374:LEU:HD23	2.00	0.43
1:B:1033:ASP:HA	1:B:1072:VAL:HG22	2.01	0.43
1:A:742:GLN:O	1:A:746:ILE:HG12	2.18	0.43
1:B:798:LEU:HD23	1:B:835:THR:HG23	2.01	0.43
1:B:1222:LYS:HA	1:B:1228:TRP:CG	2.54	0.42
1:B:115:PRO:HG2	1:B:161:MET:HA	2.01	0.42
1:A:653:TYR:O	1:A:674:SER:HA	2.19	0.42
1:B:803:ALA:O	1:B:808:ARG:HB2	2.19	0.42
1:A:1090:ALA:HA	1:A:1147:MET:HE1	2.01	0.42
1:A:371:MET:HE3	1:A:411:PRO:HB3	2.02	0.42
1:B:43:ARG:NH1	3:B:1404:HOH:O	2.53	0.42
1:B:726:GLN:NE2	1:B:1261:ASP:OD1	2.52	0.42
1:B:888:LYS:HB3	1:B:889:PRO:CD	2.49	0.42
1:B:102:THR:N	1:B:103:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:CYS:O	1:A:901:VAL:HG23	2.20	0.42
1:B:447:LYS:HG3	1:B:448:PRO:HD2	2.01	0.42
1:B:692:LEU:HD21	1:B:750:VAL:CG1	2.50	0.42
1:A:126:MET:HG2	1:A:212:TYR:CZ	2.54	0.42
1:B:1254:SER:HB3	1:B:1305:TYR:CG	2.55	0.41
1:B:141:ILE:CD1	1:B:167:THR:HG21	2.48	0.41
1:B:780:ALA:O	1:B:783:VAL:HB	2.20	0.41
1:A:1051:ASN:HA	1:A:1133:PHE:CE2	2.55	0.41
1:A:1270:SER:HA	1:A:1274:LYS:HB2	2.02	0.41
1:A:500:SER:OG	1:A:503:GLU:HG3	2.19	0.41
1:B:1149:GLU:O	1:B:1153:LYS:HB2	2.20	0.41
1:B:316:LYS:HB2	1:B:317:PRO:CD	2.49	0.41
1:A:1034:VAL:O	1:A:1093:ARG:HD2	2.20	0.41
1:A:984:LEU:HD21	1:A:1000:ILE:CD1	2.50	0.41
1:B:656:ASN:HD22	1:B:1166:GLU:HG3	1.85	0.41
1:B:73:PHE:O	1:B:77:VAL:HG23	2.20	0.41
1:A:1097:ASN:HB3	1:A:1101:SER:HB2	2.01	0.41
1:A:679:PRO:HG3	1:A:773:PRO:HB3	2.01	0.41
1:B:782:LEU:HD11	1:B:898:LEU:HB2	2.02	0.41
1:B:1061:ALA:HB2	1:B:1072:VAL:HG12	2.03	0.41
1:B:1269:ASN:O	1:B:1273:ILE:HB	2.21	0.41
1:B:27:TYR:HA	1:B:84:ILE:O	2.20	0.41
1:A:61:ILE:HD12	1:A:88:ILE:HG12	2.03	0.41
1:A:647:ILE:O	1:A:648:PRO:C	2.59	0.41
1:A:1073:ARG:NH2	2:A:1401:CIT:H41	2.36	0.41
1:A:746:ILE:O	1:A:750:VAL:HG23	2.21	0.40
1:B:1092:THR:HB	1:B:1147:MET:HG2	2.03	0.40
1:B:796:TRP:O	1:B:890:LEU:HD12	2.21	0.40
1:B:82:LEU:HD23	1:B:110:ALA:HB3	2.03	0.40
1:B:1157:ALA:HA	1:B:1195:ALA:O	2.21	0.40
1:A:1080:ALA:HB1	1:A:1085:ILE:O	2.20	0.40
1:A:527:MET:HE3	1:A:532:TYR:HA	2.04	0.40
1:B:313:ASP:OD1	1:B:315:SER:OG	2.27	0.40
1:A:364:LYS:HD2	1:A:364:LYS:HA	1.91	0.40
1:A:392:HIS:N	1:A:393:PRO:CD	2.85	0.40
1:B:774:SER:OG	1:B:777:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1248/1351 (92%)	1182 (95%)	61 (5%)	5 (0%)	34 46
1	B	1202/1351 (89%)	1117 (93%)	77 (6%)	8 (1%)	22 30
All	All	2450/2702 (91%)	2299 (94%)	138 (6%)	13 (0%)	29 40

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	PRO
1	B	217	LEU
1	A	850	ASP
1	B	115	PRO
1	B	262	SER
1	B	708	GLY
1	B	942	ALA
1	B	972	ASN
1	A	135	GLY
1	A	942	ALA
1	B	1113	SER
1	A	741	GLY
1	B	888	LYS

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	A	1077/1147 (94%)	1053 (98%)	24 (2%)	52 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1047/1147 (91%)	1020 (97%)	27 (3%)	46 61
All	All	2124/2294 (93%)	2073 (98%)	51 (2%)	49 64

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	51	SER
1	A	78	SER
1	A	95	ASP
1	A	137	SER
1	A	263	GLU
1	A	296	GLU
1	A	336	VAL
1	A	445	ARG
1	A	511	ASP
1	A	542	LEU
1	A	627	MET
1	A	643	LEU
1	A	653	TYR
1	A	714	THR
1	A	752	ARG
1	A	762	LEU
1	A	769	ILE
1	A	782	LEU
1	A	863	LYS
1	A	877	SER
1	A	943	LEU
1	A	1007	LYS
1	A	1176	PHE
1	B	1	MET
1	B	33	GLN
1	B	62	GLU
1	B	115	PRO
1	B	117	MET
1	B	136	GLN
1	B	137	SER
1	B	158	GLN
1	B	217	LEU
1	B	234	MET
1	B	244	MET
1	B	262	SER

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Mol	Chain	Res	Type
1	B	279	ARG
1	B	364	LYS
1	B	536	THR
1	B	575	GLN
1	B	626	PHE
1	B	653	TYR
1	B	752	ARG
1	B	846	GLN
1	B	848	ASN
1	B	956	SER
1	B	1101	SER
1	B	1176	PHE
1	B	1180	PRO
1	B	1218	ASP
1	B	1324	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	ASN
1	B	734	ASN

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)

1 ligand is 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	CIT	A	1401	-	3,12,12	0.38	0	3,17,17	2.95	2 (66%)

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	CIT	A	1401	-	-	6/6/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1401	CIT	C3-C2-C1	3.62	120.77	114.98
2	A	1401	CIT	C3-C4-C5	3.51	120.60	114.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	CIT	C1-C2-C3-O7
2	A	1401	CIT	C1-C2-C3-C4
2	A	1401	CIT	C1-C2-C3-C6
2	A	1401	CIT	C2-C3-C4-C5
2	A	1401	CIT	O7-C3-C4-C5
2	A	1401	CIT	C6-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	CIT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1264/1351 (93%)	0.23	17 (1%)	77	82	26, 50, 94, 169	38 (3%)
1	B	1225/1351 (90%)	0.37	45 (3%)	41	48	34, 68, 110, 157	37 (3%)
All	All	2489/2702 (92%)	0.30	62 (2%)	57	63	26, 58, 105, 169	75 (3%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	855	PHE	7.5
1	A	145	MET	5.3
1	B	851	GLY	5.1
1	B	353	ARG	4.7
1	B	853	VAL	4.7
1	B	852	ARG	4.6
1	B	139	SER	4.4
1	A	143	GLN	4.2
1	B	854	SER	4.1
1	A	467	ASN	3.6
1	B	704	ASP	3.4
1	B	705	SER	3.4
1	A	140	ALA	3.3
1	A	424	ALA	3.3
1	A	146	LYS	3.1
1	A	132	ALA	3.0
1	B	702	LEU	2.9
1	B	848	ASN	2.9
1	A	139	SER	2.9
1	B	541	ARG	2.8
1	B	1330	VAL	2.8
1	B	882	VAL	2.7
1	B	143	GLN	2.7
1	B	594	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	858	LYS	2.6
1	B	497	LEU	2.6
1	A	353	ARG	2.6
1	A	136	GLN	2.5
1	B	471	ALA	2.5
1	B	538	TYR	2.5
1	A	705	SER	2.5
1	A	708	GLY	2.4
1	B	570	VAL	2.4
1	A	707	ARG	2.4
1	B	740	GLN	2.4
1	B	847	ILE	2.4
1	B	870	TRP	2.4
1	B	376	LEU	2.4
1	B	874	LEU	2.4
1	A	669	TYR	2.3
1	B	66	ASP	2.3
1	B	707	ARG	2.3
1	B	446	LYS	2.3
1	B	515	GLN	2.2
1	B	301	GLY	2.2
1	A	144	PHE	2.2
1	B	145	MET	2.2
1	A	112	ILE	2.2
1	B	560	LEU	2.1
1	B	546	TRP	2.1
1	B	1329	GLY	2.1
1	B	703	LYS	2.1
1	B	839	VAL	2.1
1	B	859	LEU	2.1
1	B	879	TYR	2.1
1	B	136	GLN	2.0
1	B	798	LEU	2.0
1	A	249	LYS	2.0
1	B	68	GLU	2.0
1	B	339	VAL	2.0
1	B	450	LEU	2.0
1	B	884	GLU	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	A	1401	13/13	0.58	0.35	66,92,116,118	0

6.5 Other polymers (i)

There are no such residues in this entry.