



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:23 PM UTC

PDB ID : 6YSG / pdb_00006ysg
Title : Magnesium chelatase H subunit (ChlH) from Synechocystis sp.PCC6803 to 2.54 Å 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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

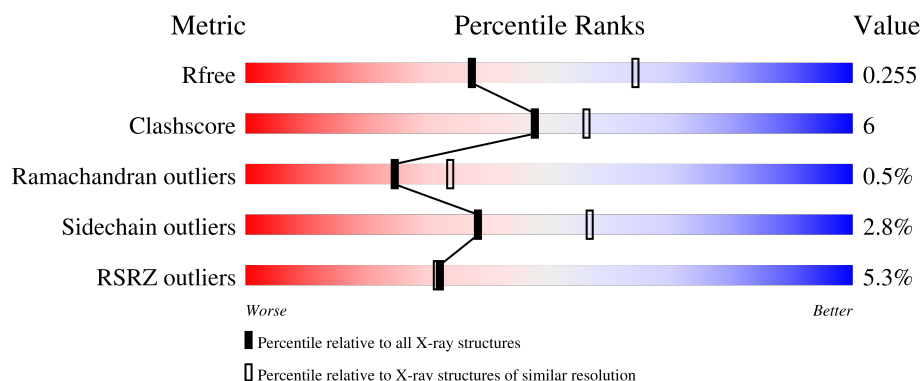
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	A	1351	 4% 78% 15% • 6%
1	B	1351	 6% 75% 15% • 9%

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:

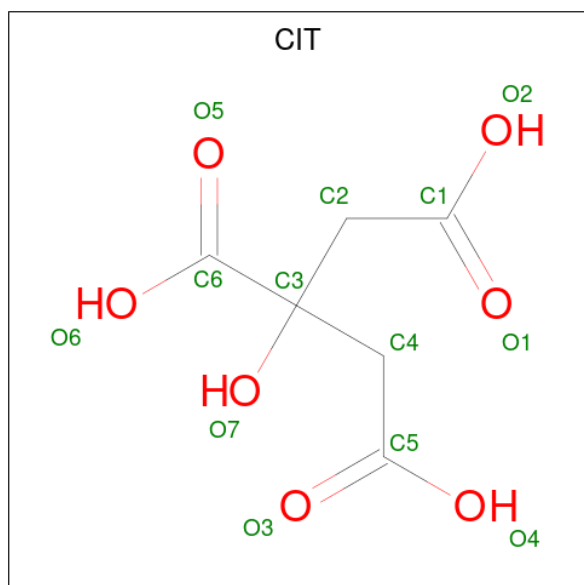
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P73020
A	-18	GLY	-	expression tag	UNP P73020
A	-17	SER	-	expression tag	UNP P73020
A	-16	SER	-	expression tag	UNP P73020
A	-15	HIS	-	expression tag	UNP P73020
A	-14	HIS	-	expression tag	UNP P73020
A	-13	HIS	-	expression 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 (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 3 is water.

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

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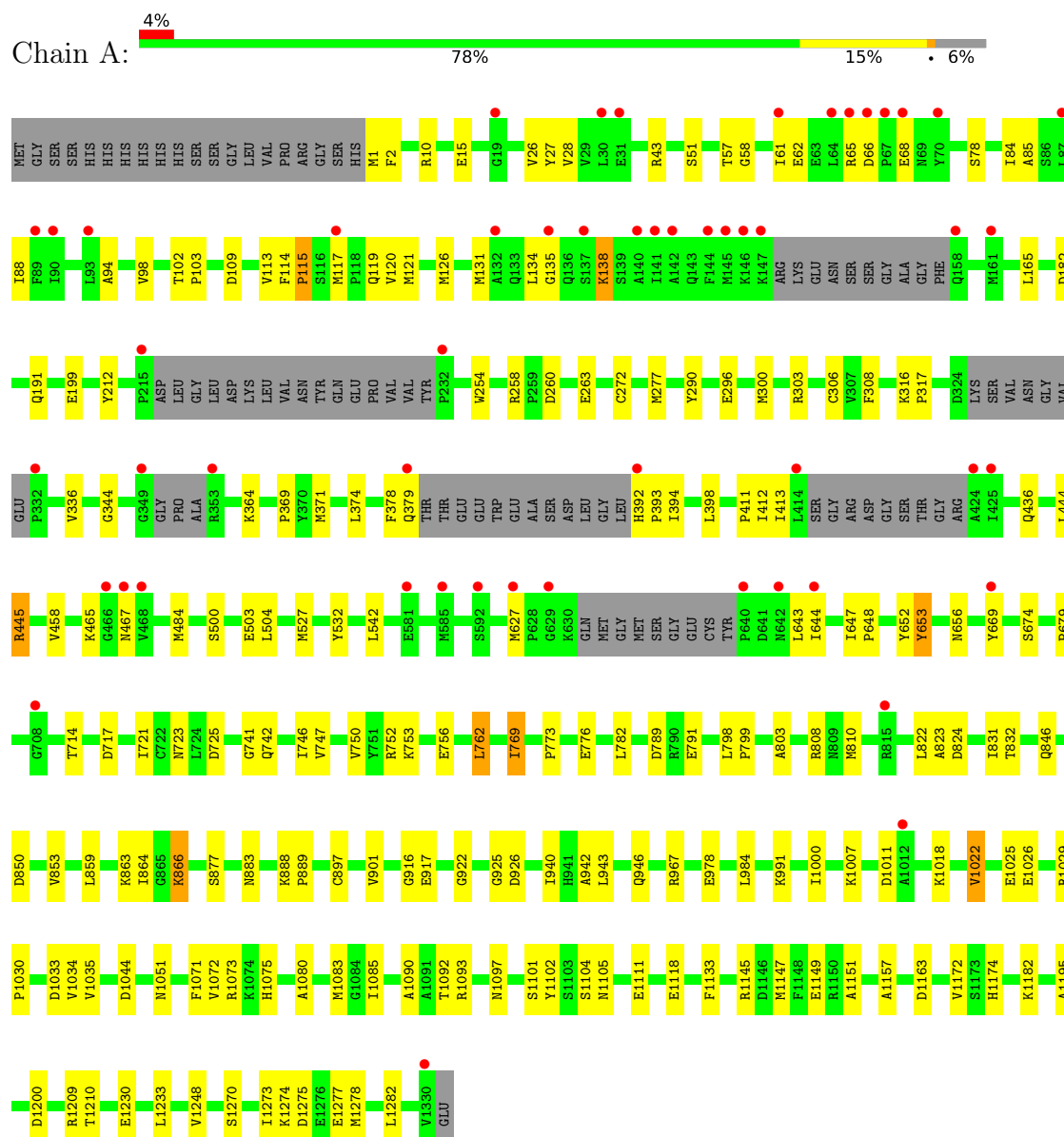
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	29	Total	O	0	0
			29	29		

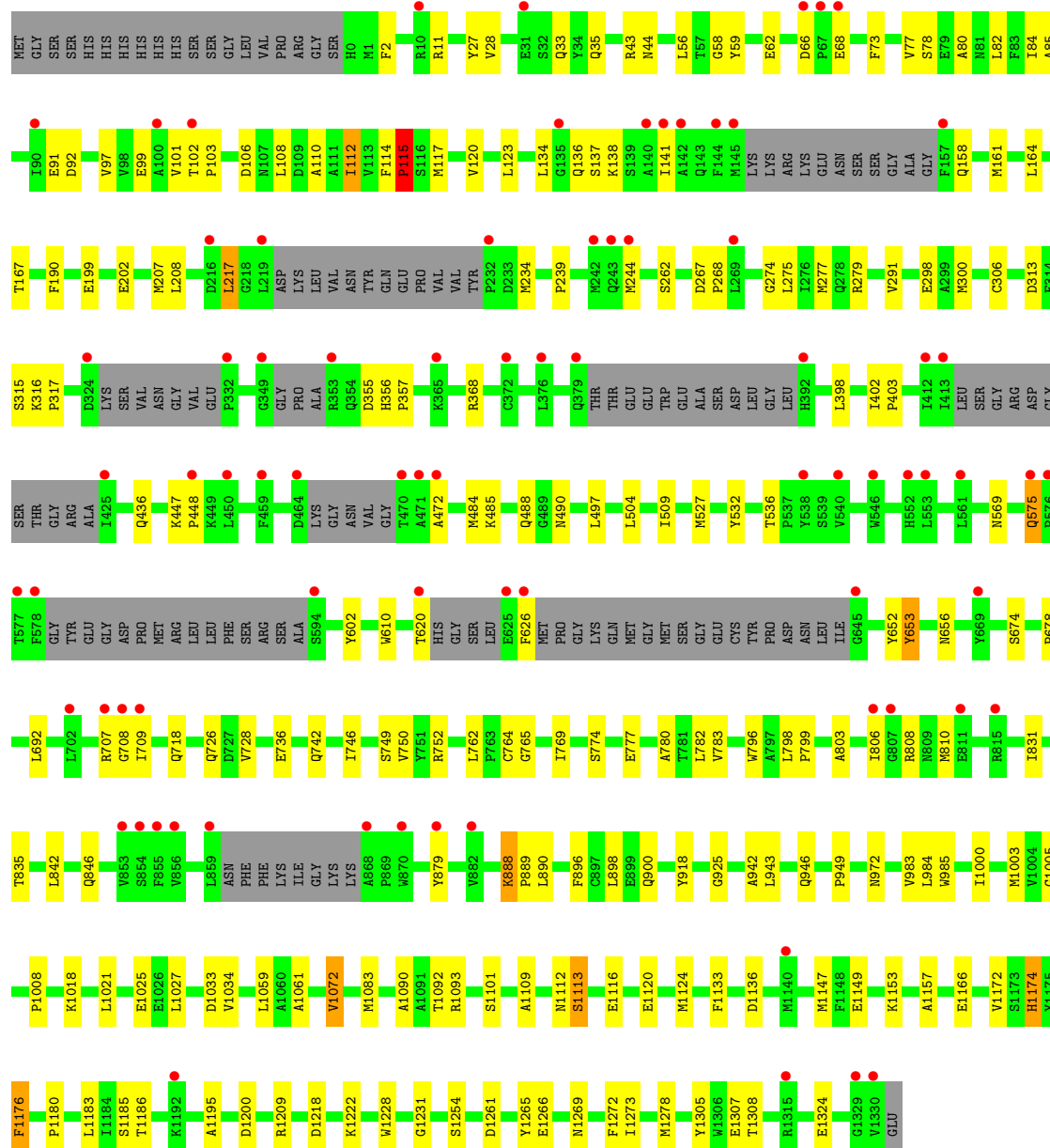
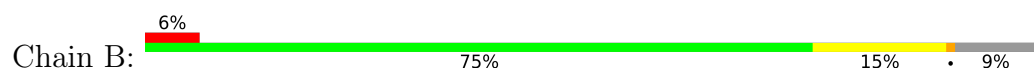
3 Residue-property plots [i](#)

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	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
$\langle I/\sigma(I) \rangle$ 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	6703 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 , 40.0	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	0.95	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	1.06	4/10145 (0.0%)	1.47	14/13753 (0.1%)
1	B	1.07	3/9848 (0.0%)	1.48	12/13354 (0.1%)
All	All	1.06	7/19993 (0.0%)	1.47	26/27107 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	ASP	CG-OD2	7.23	1.39	1.25
1	B	66	ASP	CG-OD1	6.12	1.36	1.25
1	A	66	ASP	CG-OD2	5.55	1.35	1.25
1	A	1	MET	N-CA	5.53	1.56	1.46
1	A	68	GLU	CD-OE1	5.43	1.35	1.25
1	B	68	GLU	CD-OE1	5.36	1.35	1.25
1	A	66	ASP	CG-OD1	5.34	1.35	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1011	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	1174	HIS	CA-CB-CG	6.51	120.31	113.80
1	A	1044	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	1185	SER	CA-C-N	6.31	128.74	120.28
1	B	1185	SER	C-N-CA	6.31	128.74	120.28
1	B	1133	PHE	CA-CB-CG	-5.98	107.82	113.80
1	A	926	ASP	CB-CA-C	5.91	116.59	109.85
1	A	747	VAL	CA-C-N	5.74	126.46	120.03
1	A	747	VAL	C-N-CA	5.74	126.46	120.03
1	B	106	ASP	CA-C-N	5.58	128.22	120.29
1	B	106	ASP	C-N-CA	5.58	128.22	120.29
1	A	260	ASP	CA-CB-CG	5.51	118.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1176	PHE	CA-CB-CG	5.40	119.20	113.80
1	B	1072	VAL	N-CA-C	-5.26	105.37	110.42
1	A	1277	GLU	CB-CA-C	5.21	118.98	110.96
1	A	182	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	1230	GLU	CB-CG-CD	5.18	121.41	112.60
1	B	355	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	789	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	1265	TYR	CA-C-O	-5.09	115.47	120.82
1	A	832	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	138	LYS	CA-C-N	5.07	127.03	120.44
1	A	138	LYS	C-N-CA	5.07	127.03	120.44
1	A	1273	ILE	CA-C-O	-5.05	116.31	120.80
1	B	298	GLU	CB-CG-CD	5.05	121.18	112.60
1	B	1307	GLU	CB-CA-C	5.03	118.04	109.75

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	111	0
1	B	9656	0	9516	112	0
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	219	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 6.

All (219) 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:A:803:ALA:HB2	1:A:810:MET:HE2	1.58	0.86

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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:B:527:MET:HE3	1:B:532:TYR:HA	1.69	0.74
1:A:467:ASN:OD1	1:A:1111:GLU:HA	1.90	0.71
1:A:484:MET:HE1	1:A:504:LEU:HD13	1.71	0.71
1:A:277:MET:HE3	1:A:306:CYS:HB3	1.73	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:B:277:MET:HE3	1:B:306:CYS:HB3	1.74	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:A:799:PRO:O	1:A:810:MET:HE3	1.94	0.67
1:B:44:ASN:HD22	1:B:202:GLU:CD	2.03	0.67
1:B:799:PRO:HB3	1:B:810:MET:HE3	1.78	0.66
1:A:467:ASN:HB2	1:A:1111:GLU:HB2	1.77	0.65
1:A:799:PRO:C	1:A:810:MET:HE3	2.23	0.64
1:B:141:ILE:HD11	1:B:167:THR:HG21	1.82	0.62
1:B:810:MET:HE1	1:B:831:ILE:HG21	1.81	0.61
1:B:984:LEU:HD21	1:B:1000:ILE:HD12	1.82	0.60
1:B:402:ILE:HB	1:B:403:PRO:HD3	1.83	0.59
1:A:300:MET:HE1	1:A:436:GLN:HG3	1.85	0.59
1:A:465:LYS:HB3	1:A:1111:GLU:CD	2.27	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:B:484:MET:HE2	1:B:504:LEU:HD22	1.84	0.58
1:A:1090:ALA:HA	1:A:1147:MET:HE1	1.86	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: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:484:MET:HE2	1:A:504:LEU:HD22	1.87	0.56
1:B:1003:MET:HE2	1:B:1034:VAL:HG12	1.87	0.56
1:A:2:PHE:CE2	1:B:1025:GLU:HA	2.41	0.55
1:A:445:ARG:HH12	1:A:917:GLU:HG2	1.71	0.55
1:A:1092:THR:HB	1:A:1147:MET:HG2	1.89	0.55
1:A:762:LEU:HD12	1:A:762:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:GLN:OE1	1:B:602:TYR:HB3	2.06	0.54
1:B:799:PRO:CB	1:B:810:MET:HE3	2.37	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: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:A:803:ALA:HB2	1:A:810:MET:CE	2.34	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:114:PHE:O	1:B:115:PRO:C	2.52	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: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:254:TRP:CZ3	1:A:258:ARG:HD2	2.44	0.52
1:A:527:MET:HE3	1:A:532:TYR:HA	1.91	0.51
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:300:MET:HE1	1:B:436:GLN:HG3	1.93	0.51
1:B:983:VAL:HG11	1:B:985:TRP:CZ2	2.46	0.51
1:A:1118:GLU:OE2	1:A:1182:LYS:NZ	2.43	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:394:ILE:O	1:A:398:LEU:HG	2.11	0.51
1:A:984:LEU:HD21	1:A:1000:ILE:HD12	1.92	0.51
1:A:883:ASN:OD1	1:A:883:ASN:C	2.54	0.50
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:A:121:MET:HE3	1:A:131:MET:HE2	1.94	0.50
1:B:485:LYS:HG2	1:B:497:LEU:HD21	1.93	0.50
1:B:1021:LEU:HD11	1:B:1059:LEU:C	2.35	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: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:B:1090:ALA:HA	1:B:1147:MET:HE1	1.93	0.50
1:B:527:MET:CE	1:B:532:TYR:HA	2.39	0.49
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:94:ALA:O	1:A:98:VAL:HG23	2.13	0.49
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:A:316:LYS:HB2	1:A:317:PRO:CD	2.43	0.48
1:B:1278:MET:HE3	1:B:1278:MET:HA	1.95	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: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:A:484:MET:HE1	1:A:504:LEU:CD1	2.43	0.47
1:B:1005:GLY:HA3	1:B:1027:LEU:HD22	1.97	0.47
1:A:484:MET:HE2	1:A:504:LEU:CD2	2.45	0.46
1:B:239:PRO:HB3	1:B:291:VAL:HG22	1.97	0.46
1:B:1003:MET:HE2	1:B:1034:VAL:CG1	2.45	0.46
1:A:26:VAL:HA	1:A:57:THR:O	2.15	0.46
1:B:368:ARG:O	1:B:918:TYR:HB2	2.15	0.46
1:B:728:VAL:HG13	1:B:749:SER:HB3	1.98	0.46
1:A:1278:MET:HE2	1:A:1282:LEU:HG	1.98	0.46
1:A:1083:MET:HE1	1:A:1147:MET:HE2	1.98	0.46
1:A:1233:LEU:HD13	1:A:1278:MET:HE1	1.98	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:112:ILE:N	1:B:112:ILE:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ILE:O	1:A:648:PRO:C	2.59	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:991:LYS:NZ	1:A:1163:ASP:OD2	2.49	0.45
1:A:798:LEU:HB3	1:A:799:PRO:HD3	1.99	0.45
1:B:1109:ALA:HB2	1:B:1124:MET:HE1	1.99	0.45
1:A:484:MET:CE	1:A:504:LEU:HD13	2.41	0.45
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:27:TYR:OH	1:B:35:GLN:HG3	2.17	0.44
1:B:120:VAL:O	1:B:123:LEU:HB2	2.18	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:A:272:CYS:HA	1:A:303:ARG:O	2.17	0.44
1:B:91:GLU:O	1:B:92:ASP:C	2.61	0.44
1:A:888:LYS:HB3	1:A:889:PRO:CD	2.47	0.44
1:B:983:VAL:HG11	1:B:985:TRP:CE2	2.52	0.44
1:B:1200:ASP:OD2	1:B:1209:ARG:NH1	2.51	0.44
1:B:313:ASP:OD1	1:B:315:SER:OG	2.27	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:80:ALA:O	1:B:108:LEU:HD23	2.18	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:A:113:VAL:HG11	1:A:120:VAL:HG12	1.99	0.43
1:A:1275:ASP:OD1	1:A:1275:ASP:C	2.61	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:356:HIS:N	1:B:357:PRO:CD	2.81	0.43
1:B:764:CYS:O	1:B:1231:GLY:HA3	2.18	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:A:723:ASN:C	1:A:725:ASP:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:798:LEU:HD23	1:B:835:THR:HG23	2.01	0.43
1:A:810:MET:HE1	1:A:831:ILE:HD13	2.00	0.42
1:B:115:PRO:HG2	1:B:161:MET:HA	2.01	0.42
1:B:1222:LYS:HA	1:B:1228:TRP:CG	2.54	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:B:1112:ASN:O	1:B:1113:SER:C	2.63	0.42
1:B:43:ARG:NH1	3:B:1404:HOH:O	2.53	0.42
1:B:656:ASN:OD1	1:B:656:ASN:C	2.62	0.42
1:B:726:GLN:NE2	1:B:1261:ASP:OD1	2.52	0.42
1:A:114:PHE:O	1:A:115:PRO:C	2.63	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
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:488:GLN:C	1:B:490:ASN:H	2.28	0.42
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:B:1254:SER:HB3	1:B:1305:TYR:CG	2.55	0.41
1:A:500:SER:OG	1:A:503:GLU:HG3	2.19	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: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:B:943:LEU:HD12	1:B:943:LEU:C	2.45	0.41
1:A:126:MET:HE3	1:A:126:MET:HB2	1.99	0.41
1:A:378:PHE:O	1:A:379:GLN:C	2.63	0.41
1:A:984:LEU:HD21	1:A:1000:ILE:CD1	2.50	0.41
1:A:1034:VAL:O	1:A:1093:ARG:HD2	2.20	0.41
1:B:73:PHE:O	1:B:77:VAL:HG23	2.20	0.41
1:B:656:ASN:HD22	1:B:1166:GLU:HG3	1.85	0.41
1:A:679:PRO:HG3	1:A:773:PRO:HB3	2.01	0.41
1:A:822:LEU:O	1:A:823:ALA:C	2.63	0.41
1:A:1097:ASN:HB3	1:A:1101:SER:HB2	2.01	0.41
1:A:1101:SER:C	1:A:1102:TYR:CD1	2.99	0.41
1:B:782:LEU:HD11	1:B:898:LEU:HB2	2.02	0.41
1:A:61:ILE:HD12	1:A:88:ILE:HG12	2.03	0.41
1:B:27:TYR:HA	1:B:84:ILE:O	2.20	0.41
1:B:1061:ALA:HB2	1:B:1072:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1269:ASN:O	1:B:1273:ILE:HB	2.21	0.41
1:A:1073:ARG:NH2	2:A:1401:CIT:H41	2.36	0.41
1:A:1278:MET:HE2	1:A:1282:LEU:CG	2.50	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:B:1083:MET:HE1	1:B:1147:MET:HE2	2.03	0.40
1:A:364:LYS:HA	1:A:364:LYS:HD2	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

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	A	1248/1351 (92%)	1182 (95%)	61 (5%)	5 (0%)	30	39
1	B	1202/1351 (89%)	1117 (93%)	77 (6%)	8 (1%)	18	25
All	All	2450/2702 (91%)	2299 (94%)	138 (6%)	13 (0%)	24	34

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	1047 (97%)	30 (3%)	38	57
1	B	1047/1147 (91%)	1018 (97%)	29 (3%)	38	57
All	All	2124/2294 (93%)	2065 (97%)	59 (3%)	38	57

All (59) 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	199	GLU
1	A	263	GLU
1	A	296	GLU
1	A	336	VAL
1	A	412	ILE
1	A	445	ARG
1	A	458	VAL
1	A	542	LEU
1	A	627	MET
1	A	643	LEU
1	A	644	ILE
1	A	653	TYR

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Mol	Chain	Res	Type
1	A	714	THR
1	A	752	ARG
1	A	753	LYS
1	A	762	LEU
1	A	769	ILE
1	A	776	GLU
1	A	782	LEU
1	A	791	GLU
1	A	846	GLN
1	A	863	LYS
1	A	866	LYS
1	A	877	SER
1	A	943	LEU
1	A	1007	LYS
1	A	1022	VAL
1	B	33	GLN
1	B	62	GLU
1	B	78	SER
1	B	99	GLU
1	B	112	ILE
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	279	ARG
1	B	509	ILE
1	B	536	THR
1	B	575	GLN
1	B	626	PHE
1	B	653	TYR
1	B	736	GLU
1	B	752	ARG
1	B	842	LEU
1	B	846	GLN
1	B	1018	LYS
1	B	1101	SER
1	B	1176	PHE
1	B	1180	PRO

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Mol	Chain	Res	Type
1	B	1218	ASP
1	B	1324	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	158	GLN
1	A	203	ASN
1	A	354	GLN
1	A	392	HIS
1	A	490	ASN
1	A	607	ASN
1	A	972	ASN
1	A	1051	ASN
1	A	1205	ASN
1	A	1301	ASN
1	B	44	ASN
1	B	495	GLN
1	B	848	ASN
1	B	1037	ASN
1	B	1055	GLN
1	B	1143	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	12,12,12	1.69	1 (8%)	17,17,17	1.51	4 (23%)

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	-	-	12/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	CIT	C3-C6	4.38	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1401	CIT	O6-C6-C3	3.33	119.54	113.14
2	A	1401	CIT	O5-C6-C3	-2.57	117.12	122.09
2	A	1401	CIT	C3-C2-C1	2.51	120.77	113.92
2	A	1401	CIT	C3-C4-C5	2.44	120.60	113.92

There are no chirality outliers.

All (12) 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	O7-C3-C4-C5
2	A	1401	CIT	O7-C3-C6-O6
2	A	1401	CIT	C2-C3-C4-C5
2	A	1401	CIT	C6-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	1401	CIT	C2-C3-C6-O6
2	A	1401	CIT	C1-C2-C3-C6
2	A	1401	CIT	C2-C3-C6-O5
2	A	1401	CIT	C4-C3-C6-O6
2	A	1401	CIT	O7-C3-C6-O5
2	A	1401	CIT	C4-C3-C6-O5

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	1264/1351 (93%)	0.02	53 (4%)	40	41	26, 49, 94, 169	37 (2%)
1	B	1225/1351 (90%)	0.44	79 (6%)	25	24	28, 68, 110, 157	37 (3%)
All	All	2489/2702 (92%)	0.23	132 (5%)	32	31	26, 58, 105, 169	74 (2%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ALA	6.6
1	B	413	ILE	5.9
1	A	392	HIS	5.4
1	B	157	PHE	5.2
1	B	332	PRO	5.1
1	A	467	ASN	5.0
1	B	578	PHE	4.9
1	A	135	GLY	4.7
1	B	141	ILE	4.7
1	A	425	ILE	4.6
1	A	640	PRO	4.6
1	B	626	PHE	4.5
1	A	141	ILE	4.3
1	A	414	LEU	4.2
1	B	425	ILE	4.0
1	B	620	THR	3.9
1	B	232	PRO	3.9
1	B	577	THR	3.8
1	A	815	ARG	3.7
1	A	144	PHE	3.7
1	B	856	VAL	3.5
1	A	142	ALA	3.5
1	B	859	LEU	3.5
1	B	68	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	815	ARG	3.5
1	A	30	LEU	3.5
1	A	424	ALA	3.4
1	A	132	ALA	3.4
1	A	158	GLN	3.3
1	A	161	MET	3.3
1	B	66	ASP	3.3
1	B	855	PHE	3.2
1	A	644	ILE	3.2
1	B	575	GLN	3.2
1	B	576	PRO	3.2
1	B	365	LYS	3.1
1	B	144	PHE	3.1
1	A	353	ARG	3.0
1	A	468	VAL	3.0
1	A	68	GLU	3.0
1	B	552	HIS	3.0
1	B	471	ALA	3.0
1	A	332	PRO	3.0
1	B	868	ALA	3.0
1	B	459	PHE	3.0
1	B	1330	VAL	2.9
1	B	379	GLN	2.9
1	B	470	THR	2.9
1	B	269	LEU	2.9
1	A	66	ASP	2.9
1	A	669	TYR	2.9
1	A	145	MET	2.9
1	A	585	MET	2.9
1	B	853	VAL	2.9
1	A	140	ALA	2.9
1	A	379	GLN	2.9
1	A	1330	VAL	2.8
1	B	392	HIS	2.8
1	A	232	PRO	2.8
1	B	145	MET	2.8
1	B	353	ARG	2.8
1	B	669	TYR	2.8
1	B	244	MET	2.8
1	A	31	GLU	2.8
1	B	464	ASP	2.8
1	A	592	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	645	GLY	2.7
1	A	147	LYS	2.7
1	B	879	TYR	2.7
1	A	87	LEU	2.6
1	B	594	SER	2.6
1	A	581	GLU	2.6
1	B	450	LEU	2.6
1	B	702	LEU	2.6
1	B	870	TRP	2.5
1	A	67	PRO	2.5
1	B	10	ARG	2.5
1	B	135	GLY	2.5
1	B	553	LEU	2.5
1	A	137	SER	2.5
1	B	324	ASP	2.5
1	A	708	GLY	2.5
1	B	1329	GLY	2.5
1	B	1192	LYS	2.5
1	A	64	LEU	2.4
1	B	882	VAL	2.4
1	A	61	ILE	2.4
1	A	349	GLY	2.3
1	A	90	ILE	2.3
1	B	90	ILE	2.3
1	B	412	ILE	2.3
1	B	372	CYS	2.3
1	A	146	LYS	2.3
1	A	70	TYR	2.3
1	A	215	PRO	2.3
1	B	561	LEU	2.3
1	B	625	GLU	2.3
1	B	1315	ARG	2.3
1	A	93	LEU	2.2
1	A	627	MET	2.2
1	B	709	ILE	2.2
1	B	216	ASP	2.2
1	B	811	GLU	2.2
1	B	448	PRO	2.2
1	B	243	GLN	2.2
1	A	466	GLY	2.2
1	A	642	ASN	2.2
1	B	140	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	19	GLY	2.2
1	B	376	LEU	2.1
1	B	67	PRO	2.1
1	A	89	PHE	2.1
1	B	349	GLY	2.1
1	B	708	GLY	2.1
1	B	540	VAL	2.1
1	A	1012	ALA	2.1
1	B	472	ALA	2.1
1	A	629	GLY	2.1
1	B	31	GLU	2.1
1	B	854	SER	2.1
1	B	100	ALA	2.1
1	B	807	GLY	2.1
1	B	806	ILE	2.1
1	B	242	MET	2.1
1	B	546	TRP	2.0
1	A	65	ARG	2.0
1	B	707	ARG	2.0
1	B	219	LEU	2.0
1	B	102	THR	2.0
1	A	117	MET	2.0
1	B	1140	MET	2.0
1	B	538	TYR	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](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	CIT	A	1401	13/13	0.73	0.17	66,92,116,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.