



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 AM UTC

PDB ID : 4ZHJ / pdb_00004zhj
Title : Crystal Structure of the Catalytic Subunit of Magnesium Chelatase
Authors : Chen, X.; Pu, H.; Fang, Y.; Liu, L.
Deposited on : 2015-04-25
Resolution : 2.50 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

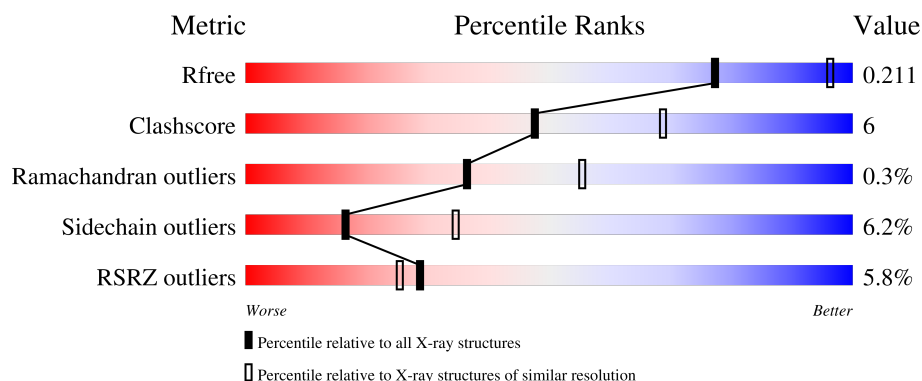
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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% 79% 13% • 7%
1	B	1351	6% 74% 15% • 9%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20168 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	1258	Total	C	N	O	S	0	3	0
			9817	6230	1664	1875	48			
1	B	1233	Total	C	N	O	S	0	5	0
			9471	6019	1614	1790	48			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	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	-	expression tag	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

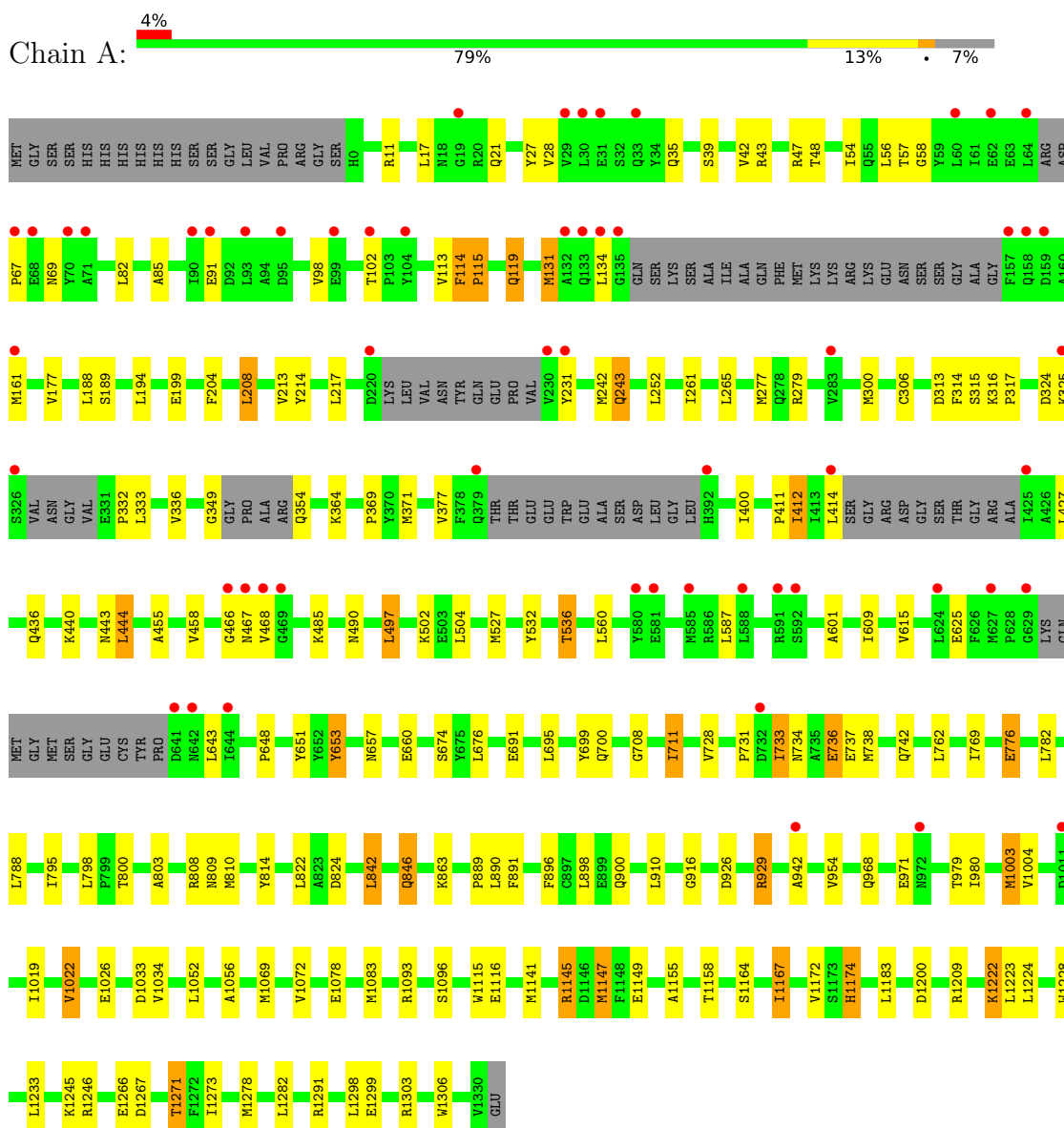
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	603	Total O 603 603	0	0
2	B	277	Total O 277 277	0	0

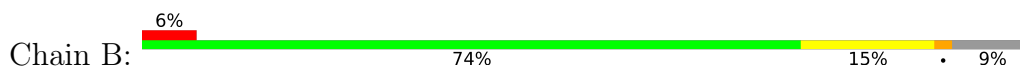
3 Residue-property plots

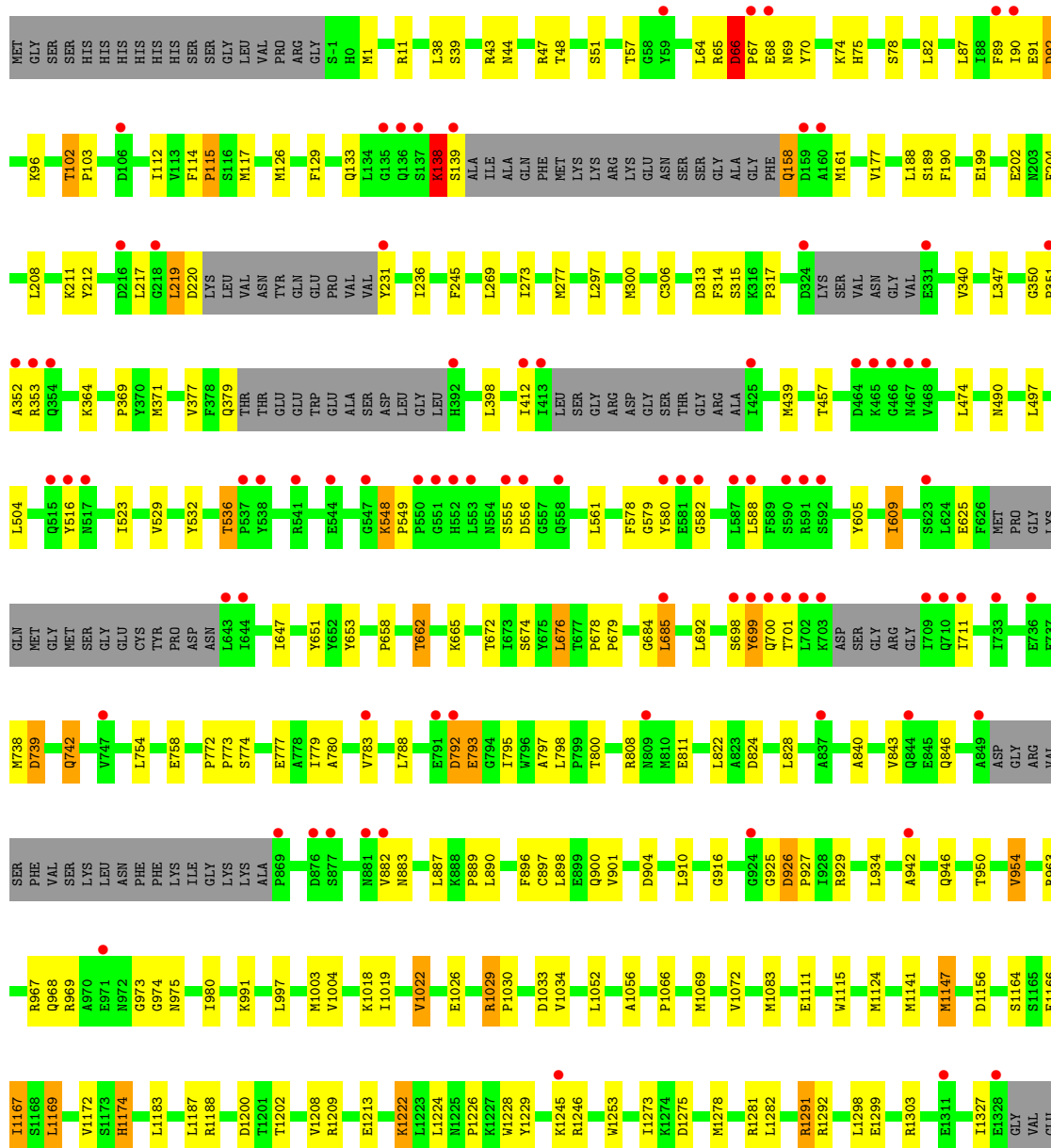
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	319.72Å 319.72Å 105.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.96 – 2.50 44.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.96-2.50) 97.1 (44.96-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.177 , 0.209 0.180 , 0.211	Depositor DCC
R_{free} test set	6735 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20168	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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	A	0.32	1/10021 (0.0%)	0.74	11/13604 (0.1%)
1	B	0.32	1/9675 (0.0%)	0.80	24/13164 (0.2%)
All	All	0.32	2/19696 (0.0%)	0.77	35/26768 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1174	HIS	CG-ND1	-5.65	1.32	1.38
1	A	1174	HIS	CG-ND1	-5.03	1.32	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	792	ASP	N-CA-C	12.98	128.80	111.28
1	B	1222	LYS	N-CA-C	10.43	126.10	112.12
1	B	793	GLU	N-CA-C	9.80	125.04	113.18
1	B	792	ASP	CB-CA-C	-8.59	99.57	112.11
1	B	609	ILE	CB-CA-C	-8.21	103.74	111.05
1	B	609	ILE	N-CA-C	7.52	117.56	111.62
1	A	609	ILE	CB-CA-C	-7.43	103.63	110.91
1	B	90	ILE	N-CA-C	7.20	118.02	107.37
1	A	1273	ILE	CB-CA-C	-7.15	103.90	110.91
1	B	138	LYS	CB-CA-C	7.08	124.51	110.42
1	B	1222	LYS	CB-CA-C	-6.95	99.73	111.26
1	A	91	GLU	N-CA-C	6.72	119.18	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1275	ASP	N-CA-C	-6.42	100.39	109.96
1	B	1167	ILE	N-CA-C	-6.31	97.89	106.85
1	B	942	ALA	N-CA-C	-6.13	97.73	110.80
1	B	1141	MET	N-CA-C	-6.07	95.67	107.62
1	B	1273	ILE	CB-CA-C	-6.00	105.03	110.91
1	A	213	VAL	CB-CA-C	-6.00	105.71	111.05
1	A	1167	ILE	N-CA-C	-5.97	97.23	106.72
1	A	1222	LYS	N-CA-C	5.93	123.44	110.80
1	B	1273	ILE	N-CA-C	5.90	117.08	112.12
1	B	516	TYR	CB-CA-C	-5.77	99.95	109.65
1	A	114	PHE	CA-C-N	5.64	126.90	119.84
1	A	114	PHE	C-N-CA	5.64	126.90	119.84
1	B	582	GLY	N-CA-C	5.58	126.41	113.18
1	B	114	PHE	CA-C-N	5.46	126.66	119.84
1	B	114	PHE	C-N-CA	5.46	126.66	119.84
1	B	548	LYS	CA-C-N	5.44	123.63	119.66
1	B	548	LYS	C-N-CA	5.44	123.63	119.66
1	A	1273	ILE	N-CA-C	5.41	116.67	112.12
1	A	942	ALA	N-CA-C	-5.34	99.42	110.80
1	A	609	ILE	N-CA-C	5.32	116.59	112.12
1	B	90	ILE	N-CA-CB	-5.11	105.23	111.67
1	B	926	ASP	CA-C-N	5.03	124.63	119.05
1	B	926	ASP	C-N-CA	5.03	124.63	119.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	138	LYS	Peptide
1	B	792	ASP	Peptide

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	9817	0	9630	92	0
1	B	9471	0	9182	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	603	0	0	10	0
2	B	277	0	0	5	0
All	All	20168	0	18812	214	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 (214) 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:1222:LYS:O	1:B:1228:TRP:CE3	2.11	1.02
1:B:66:ASP:CB	1:B:67:PRO:HA	2.00	0.90
1:B:66:ASP:CG	1:B:67:PRO:HA	2.00	0.87
1:B:67:PRO:O	1:B:69:ASN:N	2.13	0.81
1:B:883:ASN:O	1:B:887:LEU:HD23	1.80	0.80
1:A:1299:GLU:OE2	1:A:1303:ARG:NH1	2.16	0.78
1:A:1003:MET:SD	2:A:1958:HOH:O	2.43	0.77
1:B:679:PRO:HG3	1:B:773:PRO:HB3	1.68	0.76
1:B:1003:MET:SD	2:B:1657:HOH:O	2.44	0.75
1:B:67:PRO:C	1:B:69:ASN:H	1.97	0.71
1:B:126:MET:SD	2:B:1659:HOH:O	2.47	0.71
1:A:1115:TRP:O	1:A:1303:ARG:NH2	2.25	0.70
1:B:66:ASP:HB3	1:B:67:PRO:HA	1.73	0.69
1:B:1115:TRP:O	1:B:1303:ARG:NH2	2.26	0.69
1:B:340:VAL:HG22	1:B:371:MET:HE2	1.77	0.67
1:B:1003:MET:HE2	1:B:1034:VAL:HG12	1.74	0.67
1:A:467:ASN:HB2	1:A:1245:LYS:HG3	1.77	0.67
1:A:1116:GLU:O	2:A:1401:HOH:O	2.13	0.66
1:B:738:MET:HB3	1:B:742:GLN:HB3	1.77	0.66
1:B:973:GLY:HA3	1:B:975:ASN:H	1.61	0.65
1:B:883:ASN:O	1:B:887:LEU:CD2	2.46	0.64
1:A:300:MET:HE1	1:A:436:GLN:HG3	1.78	0.64
1:A:231:TYR:HB3	1:A:279:ARG:HE	1.61	0.64
1:A:808:ARG:NH2	1:A:824:ASP:OD1	2.29	0.64
1:A:131:MET:HE2	1:A:134:LEU:HD11	1.80	0.63
1:A:1222:LYS:O	1:A:1228:TRP:CE3	2.52	0.63
1:B:808:ARG:NH2	1:B:824:ASP:OD1	2.28	0.62
1:A:980:ILE:HB	1:A:1003:MET:HE3	1.80	0.62
1:A:261:ILE:HB	1:A:265:LEU:HD12	1.81	0.61
1:B:66:ASP:CB	1:B:67:PRO:CA	2.78	0.61
1:A:1164:SER:O	1:A:1167:ILE:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:ASP:OD1	1:A:1209:ARG:NH1	2.35	0.60
1:B:1222:LYS:O	1:B:1228:TRP:CD2	2.55	0.60
1:A:455:ALA:HB3	1:A:615[A]:VAL:HG22	1.85	0.59
1:B:1083:MET:HE1	1:B:1147:MET:HG2	1.84	0.59
1:B:926:ASP:HB2	1:B:991:LYS:HD3	1.85	0.59
1:B:89:PHE:HA	1:B:117:MET:HG3	1.85	0.59
1:B:1222:LYS:O	1:B:1228:TRP:HE3	1.80	0.58
1:B:1299:GLU:OE2	1:B:1303:ARG:NH1	2.36	0.57
1:B:1164:SER:O	1:B:1167:ILE:O	2.22	0.57
1:A:485:LYS:HG2	1:A:497:LEU:HD11	1.86	0.57
1:B:699:TYR:O	1:B:701:THR:N	2.37	0.57
1:B:1069:MET:HA	1:B:1069:MET:HE2	1.87	0.57
1:A:532:TYR:O	1:A:536:THR:HG23	2.05	0.56
1:A:1083:MET:HE1	1:A:1147:MET:HG2	1.86	0.56
1:B:1066:PRO:HG2	1:B:1069:MET:HG3	1.87	0.56
1:A:708:GLY:HA2	1:A:711:ILE:HD11	1.87	0.56
1:A:466:GLY:O	2:A:1402:HOH:O	2.18	0.56
1:B:588:LEU:HD21	1:B:1124:MET:HG3	1.88	0.56
1:B:1033:ASP:HA	1:B:1072:VAL:HG22	1.88	0.56
1:B:217:LEU:O	1:B:219:LEU:N	2.38	0.55
1:B:779:ILE:HG12	1:B:843:VAL:HG21	1.89	0.55
1:A:1278:MET:HE2	1:A:1282:LEU:HG	1.88	0.54
1:A:846:GLN:NE2	2:A:1431:HOH:O	2.40	0.54
1:B:797:ALA:HB3	1:B:800:THR:HG23	1.90	0.54
1:A:324:ASP:HB2	1:A:333:LEU:H	1.73	0.54
1:A:1267:ASP:O	1:A:1271:THR:HG23	2.08	0.54
1:B:980:ILE:HB	1:B:1003:MET:HE3	1.89	0.54
1:B:65:ARG:C	1:B:66:ASP:O	2.49	0.53
1:B:44:ASN:HD22	1:B:202:GLU:CD	2.16	0.53
1:A:803:ALA:HB2	1:A:810:MET:HE2	1.90	0.53
1:A:214:TYR:HB3	1:A:217:LEU:HD13	1.90	0.53
1:B:1299:GLU:O	1:B:1303:ARG:HG3	2.09	0.53
1:B:82:LEU:HD21	1:B:208:LEU:HD23	1.91	0.53
1:B:973:GLY:HA3	1:B:975:ASN:N	2.23	0.53
1:A:1003:MET:HE2	1:A:1034:VAL:HG12	1.91	0.52
1:B:1169:LEU:HG	1:B:1253:TRP:CZ2	2.45	0.52
1:A:1266:GLU:HG2	1:A:1306:TRP:HE1	1.74	0.51
1:A:11:ARG:HG3	1:A:57:THR:HG22	1.93	0.51
1:B:377:VAL:HG21	1:B:412:ILE:HG21	1.93	0.51
1:A:114:PHE:HB3	2:A:1957:HOH:O	2.10	0.51
1:B:658:PRO:O	1:B:662:THR:HG22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:HG3	1:B:48:THR:HG23	1.91	0.51
1:B:1003:MET:O	1:B:1029:ARG:NH2	2.44	0.51
1:A:377:VAL:HG21	1:A:412:ILE:HG21	1.92	0.51
1:A:653:TYR:O	1:A:674:SER:HA	2.11	0.51
1:B:579:GLY:H	1:B:580:TYR:HA	1.74	0.51
1:B:87:LEU:HD22	1:B:158:GLN:HG3	1.93	0.51
1:B:126:MET:HE2	1:B:212:TYR:CE2	2.46	0.51
1:A:731:PRO:HB2	1:A:733:ILE:HG23	1.93	0.50
1:B:126:MET:HE2	1:B:212:TYR:HE2	1.75	0.50
1:A:27:TYR:CZ	1:A:58:GLY:HA3	2.47	0.50
1:A:1022:VAL:HG13	1:A:1026:GLU:HB3	1.94	0.50
1:A:316:LYS:HB2	1:A:317:PRO:HD3	1.94	0.50
1:B:532:TYR:O	1:B:536:THR:HG23	2.12	0.50
1:A:115:PRO:HG2	1:A:161:MET:HG2	1.92	0.50
1:B:92:ASP:OD1	1:B:92:ASP:N	2.43	0.50
1:A:1145:ARG:HD3	1:A:1149:GLU:OE2	2.11	0.50
1:B:129:PHE:HA	1:B:133:GLN:HG3	1.92	0.50
1:B:555:SER:HB3	1:B:556:ASP:C	2.36	0.50
1:A:377:VAL:HG22	1:A:414:LEU:HD21	1.93	0.49
1:A:691:GLU:OE2	2:A:1403:HOH:O	2.20	0.49
1:B:82:LEU:HD11	1:B:112:ILE:HD13	1.94	0.49
1:B:698:SER:HA	1:B:699:TYR:C	2.36	0.49
1:B:277:MET:HE3	1:B:306:CYS:HB3	1.94	0.49
1:B:67:PRO:C	1:B:69:ASN:N	2.65	0.49
1:A:625:GLU:OE1	1:A:651:TYR:OH	2.21	0.49
1:B:1278:MET:HE2	1:B:1282:LEU:HG	1.94	0.48
1:B:161:MET:HE3	1:B:190:PHE:HE1	1.77	0.48
1:B:1022:VAL:HG13	1:B:1026:GLU:HB3	1.94	0.48
1:B:1172:VAL:HG21	1:B:1174:HIS:CE1	2.48	0.48
1:A:85:ALA:HB3	1:A:113:VAL:HG22	1.96	0.48
1:A:189:SER:HB2	1:A:204:PHE:CE1	2.48	0.48
1:B:625:GLU:OE2	1:B:651:TYR:OH	2.23	0.48
1:B:967:ARG:HH22	1:B:1213:GLU:CD	2.22	0.48
1:B:684:GLY:HA2	1:B:758:GLU:HG2	1.95	0.48
1:B:685:LEU:HD23	1:B:754:LEU:HD12	1.95	0.48
1:A:440:LYS:HB3	1:A:648:PRO:HD3	1.94	0.47
1:B:11:ARG:HG3	1:B:57:THR:HG22	1.95	0.47
1:A:926:ASP:HB3	1:A:929:ARG:HG2	1.97	0.47
1:A:1019:ILE:HD13	1:A:1056:ALA:HB2	1.96	0.47
1:A:277:MET:HE3	1:A:306:CYS:HB3	1.96	0.47
1:A:325:LYS:H	1:A:332:PRO:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:SER:HB3	1:A:1141:MET:HE1	1.96	0.47
1:B:653:TYR:O	1:B:674:SER:HA	2.15	0.47
1:A:738:MET:HB3	1:A:742:GLN:HG3	1.96	0.47
1:B:1164:SER:HA	1:B:1202:THR:HG21	1.97	0.47
1:B:1200:ASP:OD1	1:B:1209:ARG:NH1	2.48	0.47
1:B:138:LYS:HA	1:B:139:SER:HA	1.54	0.46
1:B:969:ARG:O	1:B:974:GLY:HA2	2.15	0.46
1:A:349:GLY:HA2	1:A:354:GLN:HA	1.97	0.46
2:A:2002:HOH:O	1:B:1:MET:HE1	2.15	0.46
1:A:657:ASN:HD21	1:A:660:GLU:HG3	1.81	0.46
1:A:810:MET:HG3	1:A:814:TYR:CE2	2.50	0.46
1:B:840:ALA:N	2:B:1404:HOH:O	2.26	0.46
1:B:739:ASP:OD1	1:B:739:ASP:N	2.47	0.45
1:B:51:SER:HB3	1:B:217:LEU:HD11	1.98	0.45
1:B:665:LYS:NZ	1:B:672:THR:OG1	2.49	0.45
1:A:314:PHE:C	1:A:317:PRO:HD2	2.42	0.45
1:B:75:HIS:O	1:B:78:SER:OG	2.32	0.45
1:B:102:THR:HG22	1:B:103:PRO:HD3	1.99	0.45
1:A:231:TYR:HB2	1:A:279:ARG:HH21	1.81	0.45
1:A:177:VAL:HG22	1:A:427:LEU:HD21	1.98	0.45
1:B:300:MET:HE2	1:B:439:MET:HG3	1.99	0.44
1:A:527:MET:HE3	1:A:532:TYR:HA	1.99	0.44
1:B:236:ILE:HB	1:B:245:PHE:HB2	1.98	0.44
1:B:678:PRO:HA	1:B:679:PRO:HD3	1.88	0.44
1:B:897:CYS:O	1:B:901:VAL:HG23	2.17	0.44
1:B:70:TYR:CE1	1:B:74:LYS:HE3	2.52	0.44
1:B:780:ALA:O	1:B:783:VAL:HG12	2.17	0.44
1:A:27:TYR:OH	1:A:35:GLN:HG3	2.18	0.44
1:B:189:SER:HB2	1:B:204:PHE:CE1	2.52	0.44
1:B:605:TYR:HA	1:B:609:ILE:HD13	2.00	0.44
1:A:369:PRO:HD3	1:A:916:GLY:O	2.17	0.44
1:B:350:GLY:O	1:B:352:ALA:HA	2.18	0.44
1:A:1222:LYS:O	1:A:1228:TRP:HB3	2.18	0.43
1:B:369:PRO:HD3	1:B:916:GLY:O	2.18	0.43
1:A:188:LEU:HD12	1:A:188:LEU:HA	1.87	0.43
1:B:379:GLN:NE2	2:B:1405:HOH:O	2.26	0.43
1:A:1033:ASP:HA	1:A:1072:VAL:HG22	1.98	0.43
1:B:1291:ARG:HD3	1:B:1327:ILE:HD12	1.99	0.43
1:A:21:GLN:HG3	1:A:217:LEU:HD11	1.99	0.43
1:A:560:LEU:HD13	1:A:601:ALA:HB2	2.01	0.43
1:B:523:ILE:HD13	1:B:561:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:LYS:HB2	1:B:1018:LYS:HE3	1.77	0.43
1:A:42:VAL:HG13	1:A:54:ILE:HB	2.00	0.43
1:A:82:LEU:HD21	1:A:208:LEU:HB3	2.00	0.43
1:B:211:LYS:HB3	1:B:212:TYR:CD2	2.54	0.43
1:A:896:PHE:O	1:A:900:GLN:HG2	2.19	0.42
1:B:1030:PRO:HG3	1:B:1069:MET:HE2	2.01	0.42
1:B:1156:ASP:OD2	1:B:1188:ARG:NH2	2.52	0.42
1:A:47:ARG:HG3	1:A:48:THR:HG23	2.01	0.42
1:B:676:LEU:HD23	1:B:676:LEU:HA	1.92	0.42
1:B:692:LEU:HD23	1:B:754:LEU:HD21	2.01	0.42
1:B:314:PHE:C	1:B:317:PRO:HD2	2.45	0.42
1:B:313:ASP:OD2	1:B:315:SER:OG	2.29	0.42
1:A:27:TYR:CE2	1:A:58:GLY:HA3	2.54	0.42
1:B:699:TYR:H	1:B:711:ILE:HD12	1.85	0.42
1:A:443:ASN:ND2	2:A:1414:HOH:O	2.31	0.42
1:B:70:TYR:OH	1:B:96:LYS:O	2.26	0.42
1:B:529:VAL:HG13	1:B:549:PRO:HB2	2.00	0.42
1:B:548:LYS:HA	1:B:549:PRO:HD3	1.91	0.42
1:B:950:THR:O	1:B:954:VAL:HG13	2.20	0.42
1:A:1003:MET:HE2	1:A:1034:VAL:CG1	2.49	0.42
1:A:1172:VAL:HG21	1:A:1174:HIS:CE1	2.55	0.42
1:B:795:ILE:HG22	1:B:889:PRO:HB2	2.01	0.42
1:B:39:SER:O	1:B:43:ARG:HG3	2.19	0.41
1:B:901:VAL:HG22	1:B:934:LEU:HD13	2.02	0.41
1:A:67:PRO:O	1:A:69:ASN:N	2.51	0.41
1:A:364:LYS:HA	1:A:364:LYS:HD2	1.88	0.41
1:B:973:GLY:CA	1:B:975:ASN:H	2.31	0.41
1:B:1226:PRO:HA	1:B:1229:TYR:CZ	2.55	0.41
1:A:131:MET:HE3	1:A:131:MET:HA	2.02	0.41
1:A:979:THR:HB	1:A:1155:ALA:HA	2.03	0.41
1:B:64:LEU:HD23	1:B:64:LEU:HA	1.82	0.41
1:B:679:PRO:HB3	1:B:777:GLU:O	2.19	0.41
1:B:774:SER:OG	1:B:777:GLU:HG2	2.20	0.41
1:A:699:TYR:HD1	1:A:711:ILE:HD13	1.85	0.41
1:A:776:GLU:HB2	2:A:1797:HOH:O	2.21	0.41
1:A:1034:VAL:O	1:A:1093:ARG:HD2	2.20	0.41
1:B:882:VAL:HB	1:B:887:LEU:HD21	2.00	0.41
1:B:273:ILE:HD12	1:B:297:LEU:HD22	2.03	0.41
1:B:398:LEU:HD22	1:B:946:GLN:HG3	2.03	0.41
1:A:119:GLN:H	1:A:119:GLN:HG3	1.52	0.41
1:A:313:ASP:OD2	1:A:315:SER:OG	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ILE:HD12	1:A:414:LEU:HD12	2.03	0.41
1:B:1298:LEU:HD12	1:B:1298:LEU:HA	1.90	0.41
1:A:243:GLN:NE2	2:A:1478:HOH:O	2.54	0.41
1:A:371:MET:CE	1:A:411:PRO:HB3	2.51	0.41
1:A:734:ASN:HB3	1:A:736:GLU:OE1	2.21	0.41
1:A:795:ILE:HG22	1:A:889:PRO:HB2	2.03	0.41
1:B:896:PHE:O	1:B:900:GLN:HG2	2.21	0.41
1:B:963:ARG:HD2	1:B:1208:VAL:HB	2.03	0.41
1:B:1019:ILE:HD13	1:B:1056:ALA:HB2	2.02	0.41
1:A:699:TYR:CD1	1:A:711:ILE:HD13	2.55	0.41
1:B:925:GLY:O	1:B:927:PRO:HD3	2.21	0.41
1:A:842:LEU:HG	1:A:891:PHE:HD1	1.85	0.40
1:A:27:TYR:HD2	1:A:56:LEU:HD11	1.87	0.40
1:A:39:SER:O	1:A:43:ARG:HG3	2.21	0.40
1:A:208:LEU:HD12	1:A:208:LEU:HA	1.88	0.40
1:B:231:TYR:N	2:B:1453:HOH:O	2.54	0.40
1:B:578:PHE:HD2	1:B:580:TYR:HE1	1.70	0.40
1:B:772:PRO:HG3	1:B:904:ASP:HB2	2.02	0.40
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.92	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	1242/1351 (92%)	1216 (98%)	25 (2%)	1 (0%)	48 68
1	B	1220/1351 (90%)	1159 (95%)	54 (4%)	7 (1%)	21 38
All	All	2462/2702 (91%)	2375 (96%)	79 (3%)	8 (0%)	36 55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	GLU
1	B	91	GLU
1	B	700	GLN
1	A	115	PRO
1	B	115	PRO
1	B	351	PRO
1	B	353	ARG
1	B	66	ASP

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	1050/1147 (92%)	981 (93%)	69 (7%)	15	32
1	B	988/1147 (86%)	931 (94%)	57 (6%)	18	38
All	All	2038/2294 (89%)	1912 (94%)	126 (6%)	16	34

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	28	VAL
1	A	98	VAL
1	A	102	THR
1	A	119	GLN
1	A	131	MET
1	A	194	LEU
1	A	199	GLU
1	A	208	LEU
1	A	242	MET
1	A	243	GLN
1	A	252	LEU
1	A	336	VAL
1	A	412	ILE
1	A	444	LEU
1	A	458	VAL

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Mol	Chain	Res	Type
1	A	468	VAL
1	A	490	ASN
1	A	497	LEU
1	A	502	LYS
1	A	504	LEU
1	A	536	THR
1	A	587	LEU
1	A	643	LEU
1	A	653	TYR
1	A	676	LEU
1	A	695	LEU
1	A	700	GLN
1	A	711	ILE
1	A	728	VAL
1	A	733	ILE
1	A	736	GLU
1	A	737	GLU
1	A	762	LEU
1	A	769	ILE
1	A	776	GLU
1	A	782	LEU
1	A	788	LEU
1	A	798	LEU
1	A	800	THR
1	A	809	ASN
1	A	822	LEU
1	A	842	LEU
1	A	846	GLN
1	A	863	LYS
1	A	890	LEU
1	A	898	LEU
1	A	910	LEU
1	A	929	ARG
1	A	954	VAL
1	A	968	GLN
1	A	971	GLU
1	A	1003	MET
1	A	1004	VAL
1	A	1022	VAL
1	A	1052	LEU
1	A	1069	MET
1	A	1078	GLU

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Mol	Chain	Res	Type
1	A	1145	ARG
1	A	1147	MET
1	A	1158	THR
1	A	1183	LEU
1	A	1223	LEU
1	A	1224	LEU
1	A	1233	LEU
1	A	1246	ARG
1	A	1271	THR
1	A	1291	ARG
1	A	1298	LEU
1	B	38	LEU
1	B	66	ASP
1	B	92	ASP
1	B	102	THR
1	B	115	PRO
1	B	158	GLN
1	B	177	VAL
1	B	188	LEU
1	B	199	GLU
1	B	219	LEU
1	B	220	ASP
1	B	269	LEU
1	B	347	LEU
1	B	364	LYS
1	B	457	THR
1	B	474	LEU
1	B	490	ASN
1	B	497	LEU
1	B	504	LEU
1	B	536	THR
1	B	647	ILE
1	B	662	THR
1	B	676	LEU
1	B	685	LEU
1	B	699	TYR
1	B	739	ASP
1	B	742	GLN
1	B	788	LEU
1	B	793	GLU
1	B	798	LEU
1	B	811	GLU

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Mol	Chain	Res	Type
1	B	822	LEU
1	B	828	LEU
1	B	846	GLN
1	B	890	LEU
1	B	898	LEU
1	B	910	LEU
1	B	929	ARG
1	B	954	VAL
1	B	968	GLN
1	B	997	LEU
1	B	1004	VAL
1	B	1022	VAL
1	B	1029	ARG
1	B	1052	LEU
1	B	1111	GLU
1	B	1147	MET
1	B	1166	GLU
1	B	1169	LEU
1	B	1183	LEU
1	B	1187	LEU
1	B	1224	LEU
1	B	1245	LYS
1	B	1246	ARG
1	B	1281	ARG
1	B	1291	ARG
1	B	1292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	522	ASN
1	A	596	HIS
1	A	607	ASN
1	A	649	ASN
1	A	912	GLN
1	A	1174	HIS
1	B	181	GLN
1	B	191	GLN
1	B	742	GLN
1	B	1055	GLN
1	B	1097	ASN

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Mol	Chain	Res	Type
1	B	1174	HIS
1	B	1269	ASN
1	B	1301	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 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	A	1258/1351 (93%)	-0.11	57 (4%)	38	33	17, 36, 76, 119	40 (3%)
1	B	1233/1351 (91%)	0.35	87 (7%)	22	19	21, 55, 95, 123	8 (0%)
All	All	2491/2702 (92%)	0.12	144 (5%)	29	25	17, 45, 88, 123	48 (1%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	849	ALA	6.4
1	A	326	SER	6.1
1	A	468	VAL	5.8
1	A	592	SER	5.4
1	B	136	GLN	5.1
1	A	467	ASN	5.1
1	A	135	GLY	5.0
1	A	67	PRO	5.0
1	A	230	VAL	5.0
1	A	392	HIS	4.9
1	B	809	ASN	4.8
1	A	325	LYS	4.7
1	B	468	VAL	4.7
1	A	629	GLY	4.6
1	B	703	LYS	4.3
1	A	157	PHE	4.3
1	B	581	GLU	4.3
1	A	64	LEU	4.2
1	B	465	LYS	4.2
1	B	331	GLU	4.1
1	B	971	GLU	4.1
1	B	709	ILE	4.0
1	B	700	GLN	3.9
1	B	352	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	161	MET	3.9
1	B	231	TYR	3.9
1	A	591	ARG	3.9
1	A	641	ASP	3.8
1	B	644	ILE	3.7
1	A	414	LEU	3.7
1	A	158	GLN	3.6
1	B	924	GLY	3.6
1	B	425	ILE	3.6
1	A	379	GLN	3.5
1	B	582	GLY	3.4
1	B	137	SER	3.4
1	A	93	LEU	3.4
1	B	580	TYR	3.4
1	B	544	GLU	3.4
1	B	139	SER	3.4
1	B	552	HIS	3.3
1	A	581	GLU	3.3
1	B	881[A]	ASN	3.3
1	A	624	LEU	3.3
1	B	701	THR	3.2
1	A	642	ASN	3.2
1	B	135	GLY	3.2
1	A	231	TYR	3.2
1	B	876	ASP	3.1
1	A	159	ASP	3.1
1	B	106	ASP	3.1
1	B	711	ILE	3.1
1	A	134	LEU	3.0
1	B	547	GLY	3.0
1	A	469	GLY	3.0
1	A	425	ILE	3.0
1	B	351	PRO	2.9
1	B	555	SER	2.9
1	B	710	GLN	2.9
1	A	972	ASN	2.9
1	B	218	GLY	2.9
1	A	644	ILE	2.9
1	A	588	LEU	2.9
1	B	588	LEU	2.9
1	B	517	ASN	2.9
1	B	783	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	216	ASP	2.8
1	A	1011	ASP	2.8
1	B	556	ASP	2.8
1	A	70	TYR	2.8
1	B	67	PRO	2.8
1	A	942	ALA	2.8
1	B	1328	GLU	2.8
1	A	466	GLY	2.7
1	A	90	ILE	2.7
1	A	31	GLU	2.7
1	B	160	ALA	2.7
1	B	558	GLN	2.7
1	B	733	ILE	2.7
1	B	590	SER	2.7
1	B	591	ARG	2.7
1	B	392	HIS	2.7
1	A	30	LEU	2.6
1	B	643	LEU	2.6
1	A	133	GLN	2.6
1	B	159	ASP	2.5
1	A	580	TYR	2.5
1	A	60	LEU	2.5
1	B	747	VAL	2.5
1	A	627	MET	2.5
1	B	516	TYR	2.5
1	B	464	ASP	2.5
1	A	283	VAL	2.5
1	B	592	SER	2.5
1	B	1311	GLU	2.5
1	B	90	ILE	2.5
1	B	354	GLN	2.5
1	B	942	ALA	2.5
1	A	33	GLN	2.4
1	B	353	ARG	2.4
1	A	91	GLU	2.4
1	B	702	LEU	2.4
1	B	467	ASN	2.4
1	B	68	GLU	2.4
1	B	551	GLY	2.4
1	A	99	GLU	2.4
1	B	550	PRO	2.3
1	B	413	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	324	ASP	2.3
1	B	882	VAL	2.3
1	B	736	GLU	2.3
1	A	585	MET	2.3
1	B	1245	LYS	2.3
1	A	71	ALA	2.3
1	A	102	THR	2.3
1	A	19	GLY	2.3
1	B	623	SER	2.3
1	B	791	GLU	2.3
1	A	29	VAL	2.3
1	A	132	ALA	2.2
1	B	466	GLY	2.2
1	B	877	SER	2.2
1	B	792	ASP	2.2
1	B	587	LEU	2.2
1	B	698	SER	2.2
1	A	732	ASP	2.2
1	A	68	GLU	2.2
1	B	537	PRO	2.2
1	B	844	GLN	2.1
1	B	412	ILE	2.1
1	B	699	TYR	2.1
1	B	541	ARG	2.1
1	B	89	PHE	2.1
1	A	62	GLU	2.1
1	A	104	TYR	2.1
1	A	95	ASP	2.1
1	B	553	LEU	2.1
1	B	59	TYR	2.1
1	B	515	GLN	2.1
1	B	837	ALA	2.1
1	B	685	LEU	2.1
1	B	538	TYR	2.1
1	B	869	PRO	2.1
1	A	220	ASP	2.0

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

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

6.3 Carbohydrates [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.