



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:55 PM UTC

PDB ID : 6YT0 / pdb_00006yt0
Title : Magnesium chelatase H subunit (ChlH) E660D variant from *Synechocystis* sp.PCC6803
Authors : Bisson, C.; Hunter, C.N.
Deposited on : 2020-04-23
Resolution : 2.85 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

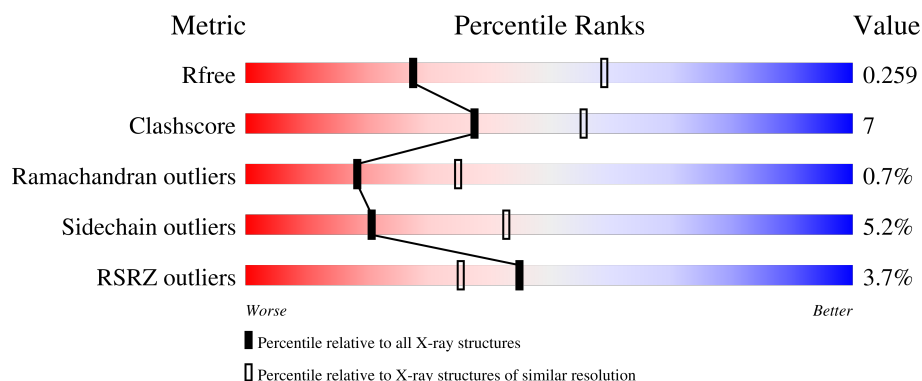
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	
1	B	1351	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19365 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	B	1207	Total	C	N	O	S	0	1	0
			9511	6023	1610	1831	47			
1	A	1248	Total	C	N	O	S	0	0	0
			9822	6221	1670	1882	49			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
B	660	ASP	GLU	engineered mutation	UNP P73020
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

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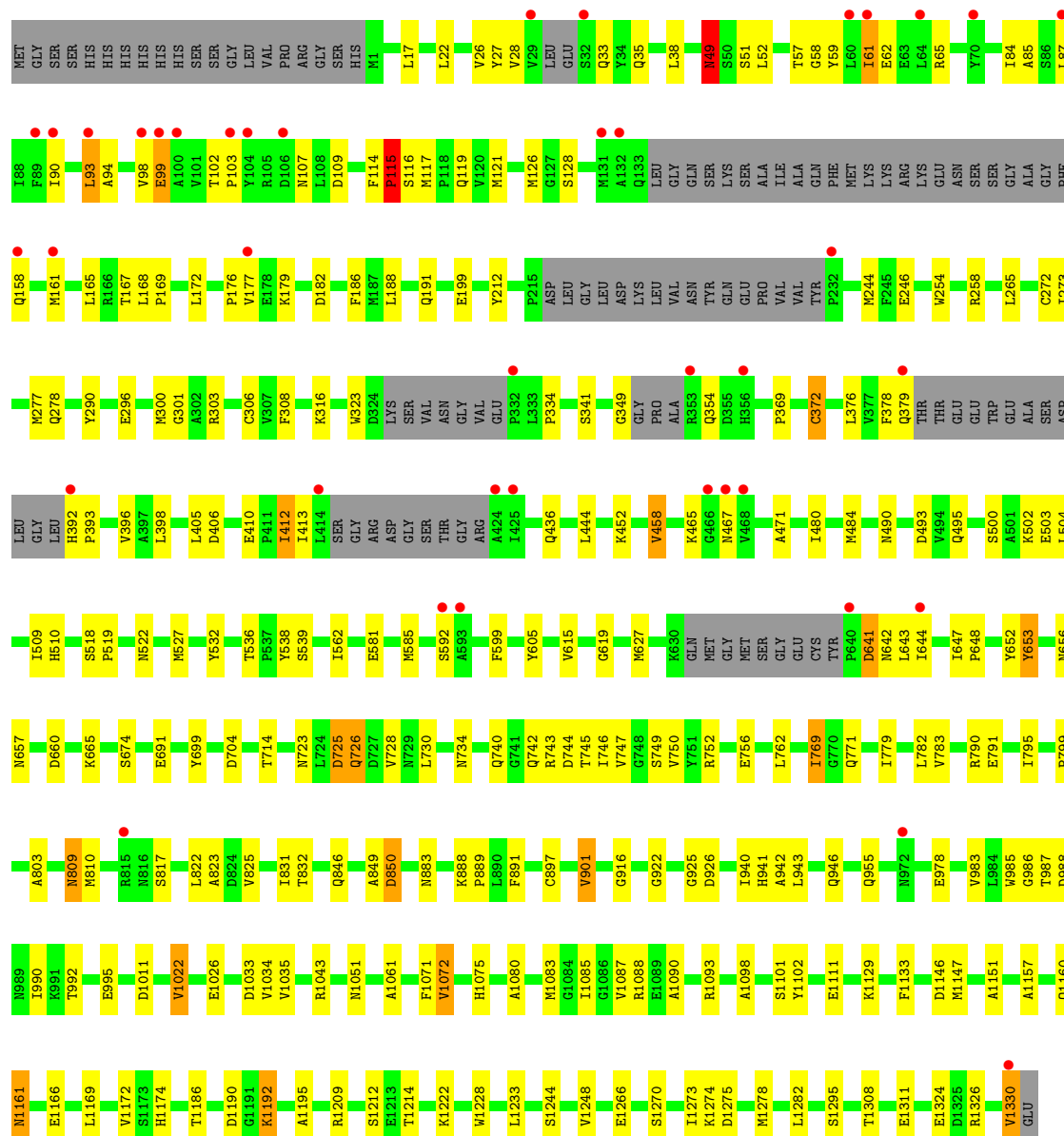
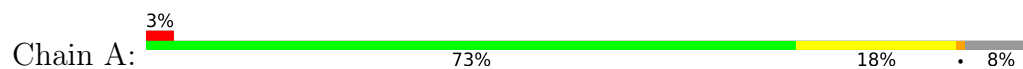
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP P73020
A	-14	HIS	-	expression tag	UNP P73020
A	-13	HIS	-	expression tag	UNP P73020
A	-12	HIS	-	expression tag	UNP P73020
A	-11	HIS	-	expression tag	UNP P73020
A	-10	HIS	-	expression tag	UNP P73020
A	-9	SER	-	expression tag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

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	8	Total O 8 8	0	0
2	A	24	Total O 24 24	0	0



• Molecule 1: Mg-chelatase subunit ChlH



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	321.79Å 321.79Å 104.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.60 – 2.85 54.60 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (54.60-2.85) 99.7 (54.60-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.209 , 0.260 0.213 , 0.259	Depositor DCC
R_{free} test set	4724 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19365	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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)

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	2/10019 (0.0%)	1.51	38/13586 (0.3%)
1	B	1.08	3/9700 (0.0%)	1.53	20/13157 (0.2%)
All	All	1.07	5/19719 (0.0%)	1.52	58/26743 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	488	GLN	C-O	-6.31	1.16	1.24
1	B	1150	ARG	C-O	5.36	1.30	1.24
1	A	316	LYS	N-CA	5.13	1.50	1.46
1	A	519	PRO	C-O	-5.08	1.17	1.23
1	B	844	GLN	C-O	5.07	1.30	1.24

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1186	THR	CA-CB-OG1	-7.37	98.55	109.60
1	A	61	ILE	CA-C-N	7.12	131.49	120.82
1	A	61	ILE	C-N-CA	7.12	131.49	120.82
1	A	926	ASP	CB-CA-C	6.61	117.38	109.85
1	A	742	GLN	CA-C-O	-6.57	113.58	120.55
1	A	809	ASN	CB-CA-C	6.47	120.90	110.16
1	B	406	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	61	ILE	O-C-N	6.25	128.02	121.89
1	B	1176	PHE	CA-CB-CG	6.18	119.98	113.80
1	B	1185	SER	CA-C-N	6.13	128.49	120.28
1	B	1185	SER	C-N-CA	6.13	128.49	120.28
1	A	1011	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	49	ASN	CB-CA-C	6.05	119.51	109.53
1	B	660	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	1133	PHE	CA-CB-CG	-5.96	107.84	113.80
1	A	747	VAL	CA-C-N	5.95	126.69	120.03
1	A	747	VAL	C-N-CA	5.95	126.69	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	ARG	CA-C-N	5.87	128.39	120.65
1	B	445	ARG	C-N-CA	5.87	128.39	120.65
1	A	406	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	488	GLN	CA-C-O	-5.78	113.32	119.97
1	A	410	GLU	CB-CA-C	5.78	115.89	110.17
1	A	704	ASP	CA-C-N	5.67	127.88	120.28
1	A	704	ASP	C-N-CA	5.67	127.88	120.28
1	A	115	PRO	N-CA-CB	-5.66	97.31	103.25
1	A	832	THR	CA-CB-OG1	-5.60	101.20	109.60
1	A	771	GLN	CB-CA-C	5.58	116.45	110.65
1	A	182	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	840	ALA	CA-C-O	-5.53	114.68	120.55
1	B	725	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	955	GLN	CB-CA-C	5.43	119.81	110.79
1	A	107	ASN	O-C-N	5.43	129.81	122.59
1	B	1011	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	725	ASP	N-CA-C	-5.37	106.58	113.23
1	B	106	ASP	CA-C-N	5.34	127.87	120.29
1	B	106	ASP	C-N-CA	5.34	127.87	120.29
1	A	471	ALA	CA-C-N	5.33	127.85	120.29
1	A	471	ALA	C-N-CA	5.33	127.85	120.29
1	A	244	MET	CA-C-O	-5.31	115.71	121.87
1	B	1099	SER	CA-C-O	-5.31	115.89	120.88
1	A	825	VAL	N-CA-C	-5.30	105.36	110.72
1	A	1273	ILE	CA-C-O	-5.30	116.08	120.80
1	B	1072	VAL	N-CA-C	-5.29	105.34	110.42
1	A	1072	VAL	N-CA-C	-5.29	105.45	110.42
1	A	742	GLN	N-CA-C	-5.26	105.55	111.28
1	A	107	ASN	CA-C-N	5.25	129.75	121.56
1	A	107	ASN	C-N-CA	5.25	129.75	121.56
1	A	1330	VAL	CA-C-O	5.15	129.56	120.80
1	A	1324	GLU	O-C-N	5.14	127.44	122.09
1	A	891	PHE	CB-CA-C	5.10	120.46	110.67
1	B	1142	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	1011	ASP	CA-C-N	5.06	127.38	120.54
1	A	1011	ASP	C-N-CA	5.06	127.38	120.54
1	A	1146	ASP	CB-CA-C	5.06	118.89	110.90
1	A	599	PHE	CA-C-N	5.06	127.32	120.44
1	A	599	PHE	C-N-CA	5.06	127.32	120.44
1	B	1307	GLU	CB-CA-C	5.05	117.97	109.48
1	B	177	VAL	CA-C-O	-5.04	115.51	120.85

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	9822	0	9695	145	0
1	B	9511	0	9371	125	0
2	A	24	0	0	0	0
2	B	8	0	0	0	0
All	All	19365	0	19066	269	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 7.

All (269) 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:527:MET:CE	1:A:532:TYR:HA	2.13	0.79
1:B:70:TYR:OH	1:B:96:LYS:O	2.01	0.76
1:A:1172:VAL:HG21	1:A:1174:HIS:CE1	2.20	0.76
1:A:392:HIS:O	1:A:396:VAL:HG23	1.85	0.76
1:A:109:ASP:HB3	1:A:212:TYR:O	1.87	0.74
1:A:49:ASN:HD22	1:A:49:ASN:C	1.97	0.72
1:A:493:ASP:OD1	1:A:495:GLN:NE2	2.24	0.71
1:B:256:ASN:O	1:B:266:LYS:HE2	1.91	0.69
1:B:806:ILE:HG22	1:B:806:ILE:O	1.91	0.69
1:A:803:ALA:HB2	1:A:810:MET:HE2	1.74	0.68
1:B:756:GLU:OE2	1:B:1209:ARG:NH2	2.27	0.68
1:A:49:ASN:ND2	1:A:52:LEU:H	1.93	0.67
1:B:367:ASN:OD1	1:B:917:GLU:HB3	1.97	0.65
1:B:402:ILE:HB	1:B:403:PRO:HD3	1.79	0.65
1:A:740:GLN:OE1	1:A:743:ARG:NH2	2.31	0.63
1:A:49:ASN:HD21	1:A:52:LEU:H	1.44	0.63
1:A:62:GLU:O	1:A:65:ARG:HG3	1.98	0.63
1:A:1090:ALA:HA	1:A:1147:MET:HE1	1.81	0.63
1:A:176:PRO:HG2	1:A:179:LYS:HD2	1.80	0.63
1:A:27:TYR:CE1	1:A:58:GLY:HA3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ASP:OD1	1:B:315:SER:OG	2.13	0.62
1:B:984:LEU:HD21	1:B:1000:ILE:HD12	1.82	0.61
1:B:811:GLU:OE2	1:B:815:ARG:NH1	2.33	0.61
1:B:1153:LYS:NZ	1:B:1189:ASP:OD2	2.34	0.61
1:A:467:ASN:HB2	1:A:1111:GLU:HB2	1.84	0.60
1:B:984:LEU:HD21	1:B:1000:ILE:CD1	2.32	0.60
1:B:98:VAL:O	1:B:102:THR:OG1	2.17	0.59
1:A:756:GLU:OE2	1:A:1209:ARG:NH2	2.33	0.59
1:B:1321:GLN:HE22	1:A:585:MET:HG2	1.68	0.59
1:B:762:LEU:O	1:B:762:LEU:HD12	2.03	0.58
1:B:165:LEU:HD11	1:B:191:GLN:HG2	1.86	0.58
1:B:527:MET:CE	1:B:532:TYR:HA	2.34	0.58
1:A:527:MET:HE3	1:A:532:TYR:HA	1.86	0.58
1:A:467:ASN:ND2	1:A:1248:VAL:HG12	2.19	0.57
1:B:735:ALA:HA	1:B:738:MET:HE2	1.85	0.57
1:A:117:MET:HB3	1:A:119:GLN:HE22	1.70	0.57
1:A:349:GLY:HA3	1:A:354:GLN:HA	1.87	0.57
1:A:723:ASN:O	1:A:726:GLN:NE2	2.37	0.57
1:B:782:LEU:HD11	1:B:898:LEU:HB2	1.85	0.57
1:B:810:MET:HE1	1:B:831:ILE:HG21	1.88	0.56
1:B:575:GLN:OE1	1:B:602:TYR:HB3	2.07	0.56
1:A:484:MET:HE1	1:A:504:LEU:HD13	1.87	0.56
1:B:1116:GLU:HB3	1:B:1120:GLU:OE2	2.07	0.55
1:A:165:LEU:HD11	1:A:191:GLN:CG	2.36	0.55
1:A:369:PRO:HD3	1:A:916:GLY:O	2.07	0.55
1:A:444:LEU:O	1:A:452:LYS:HE2	2.06	0.55
1:A:799:PRO:O	1:A:810:MET:CE	2.55	0.55
1:A:341:SER:HB3	1:A:372:CYS:SG	2.47	0.55
1:B:1034:VAL:O	1:B:1093:ARG:HD2	2.07	0.55
1:A:1275:ASP:OD1	1:A:1275:ASP:C	2.50	0.54
1:B:472:ALA:CB	1:B:620:THR:HG22	2.37	0.54
1:B:806:ILE:HD11	1:B:879:TYR:HE1	1.71	0.54
1:A:128:SER:HB2	1:A:179:LYS:HG2	1.88	0.54
1:A:810:MET:HE1	1:A:831:ILE:HG21	1.89	0.54
1:A:897:CYS:O	1:A:901:VAL:HG23	2.08	0.54
1:B:883:ASN:C	1:B:883:ASN:OD1	2.50	0.54
1:B:1019:ILE:HD13	1:B:1056:ALA:HB2	1.89	0.54
1:A:1157:ALA:HA	1:A:1195:ALA:O	2.08	0.54
1:A:762:LEU:HD12	1:A:762:LEU:O	2.08	0.54
1:B:181:GLN:HE21	1:B:185:ASN:HD21	1.55	0.54
1:A:1035:VAL:HG22	1:A:1151:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:TYR:CE2	1:B:35:GLN:HG3	2.44	0.53
1:B:44:ASN:HD22	1:B:47:ARG:HH11	1.54	0.53
1:B:806:ILE:HD11	1:B:879:TYR:CE1	2.43	0.53
1:A:1161:ASN:HD22	1:A:1161:ASN:N	2.06	0.53
1:A:527:MET:HE1	1:A:532:TYR:HA	1.87	0.53
1:B:946:GLN:OE1	1:B:1015:ARG:HD2	2.08	0.53
1:B:316:LYS:HB2	1:B:317:PRO:HD3	1.89	0.53
1:A:883:ASN:OD1	1:A:883:ASN:C	2.52	0.53
1:B:575:GLN:OE1	1:B:599:PHE:HA	2.09	0.53
1:B:766:LEU:HD21	1:B:1242:GLU:HG3	1.90	0.52
1:A:799:PRO:C	1:A:810:MET:HE3	2.33	0.52
1:B:173:LYS:NZ	1:B:296:GLU:OE2	2.36	0.52
1:A:28:VAL:O	1:A:85:ALA:HA	2.10	0.52
1:A:90:ILE:HB	1:A:93:LEU:HD12	1.91	0.52
1:B:483:VAL:O	1:B:487:LEU:HG	2.10	0.52
1:B:1033:ASP:HA	1:B:1072:VAL:HG22	1.91	0.52
1:A:725:ASP:HB3	1:A:730:LEU:HD12	1.92	0.52
1:A:656:ASN:HA	1:A:925:GLY:O	2.10	0.52
1:B:806:ILE:O	1:B:806:ILE:CG2	2.58	0.51
1:A:300:MET:HE1	1:A:436:GLN:HG3	1.92	0.51
1:A:265:LEU:HD11	1:A:301:GLY:HA2	1.92	0.51
1:B:1090:ALA:HA	1:B:1147:MET:HE1	1.92	0.51
1:A:656:ASN:ND2	1:A:1166:GLU:HG3	2.25	0.51
1:B:114:PHE:O	1:B:115:PRO:C	2.52	0.51
1:B:484:MET:HE2	1:B:504:LEU:HD22	1.93	0.51
1:B:707:ARG:O	1:B:709:ILE:N	2.44	0.51
1:A:458:VAL:CG2	1:A:480:ILE:HD11	2.40	0.51
1:A:444:LEU:HD22	1:A:648:PRO:HG2	1.93	0.50
1:A:699:TYR:OH	1:A:744:ASP:OD1	2.28	0.50
1:A:117:MET:HB3	1:A:119:GLN:NE2	2.27	0.50
1:B:656:ASN:HA	1:B:925:GLY:O	2.12	0.50
1:A:378:PHE:O	1:A:379:GLN:O	2.30	0.50
1:A:1022:VAL:HG13	1:A:1026:GLU:HB3	1.94	0.50
1:A:538:TYR:OH	1:A:643:LEU:HD12	2.12	0.50
1:A:992:THR:HB	1:A:995:GLU:HG3	1.94	0.50
1:B:485:LYS:HG2	1:B:497:LEU:HD21	1.94	0.49
1:A:27:TYR:OH	1:A:35:GLN:HG2	2.12	0.49
1:B:161:MET:HB3	1:B:194:LEU:HD21	1.94	0.49
1:B:27:TYR:CE1	1:B:58:GLY:HA3	2.48	0.49
1:B:888:LYS:HB3	1:B:889:PRO:HD3	1.94	0.49
1:B:114:PHE:CD1	1:B:190:PHE:CD1	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASN:C	1:A:49:ASN:ND2	2.67	0.49
1:A:158:GLN:O	1:A:161:MET:HB2	2.13	0.49
1:B:165:LEU:HD11	1:B:191:GLN:CG	2.41	0.49
1:B:674:SER:HB3	1:B:940:ILE:HG23	1.95	0.49
1:A:888:LYS:HB3	1:A:889:PRO:CD	2.42	0.49
1:A:27:TYR:HA	1:A:84:ILE:O	2.12	0.49
1:A:484:MET:HE1	1:A:504:LEU:CD1	2.43	0.49
1:B:799:PRO:CB	1:B:810:MET:HE3	2.42	0.48
1:A:465:LYS:HB3	1:A:1111:GLU:CD	2.37	0.48
1:B:798:LEU:HB3	1:B:799:PRO:HD3	1.95	0.48
1:A:26:VAL:HA	1:A:57:THR:O	2.13	0.48
1:A:1190:ASP:OD1	1:A:1192:LYS:HB3	2.13	0.48
1:B:28:VAL:O	1:B:85:ALA:HA	2.13	0.48
1:B:1266:GLU:OE2	1:B:1308:THR:OG1	2.22	0.48
1:A:510:HIS:CE1	1:A:522:ASN:HD22	2.31	0.48
1:B:1200:ASP:OD1	1:B:1202:THR:HG23	2.14	0.48
1:B:474:LEU:HD13	1:B:675:TYR:CZ	2.49	0.48
1:A:277:MET:HE3	1:A:306:CYS:HB3	1.95	0.47
1:A:277:MET:HB2	1:A:290:TYR:CE2	2.49	0.47
1:A:323:TRP:CZ3	1:A:334:PRO:HD3	2.49	0.47
1:A:1270:SER:HA	1:A:1274:LYS:HB2	1.96	0.47
1:B:94:ALA:O	1:B:98:VAL:HG23	2.14	0.47
1:A:1083:MET:HE1	1:A:1147:MET:HE2	1.97	0.47
1:A:376:LEU:HD13	1:A:396:VAL:HG22	1.97	0.47
1:A:728:VAL:HG13	1:A:749:SER:HB3	1.95	0.47
1:B:493:ASP:HB3	1:B:569:ASN:ND2	2.30	0.47
1:A:1033:ASP:HA	1:A:1072:VAL:HG22	1.97	0.47
1:B:239:PRO:HB3	1:B:291:VAL:HG22	1.97	0.47
1:A:126:MET:HG2	1:A:212:TYR:CZ	2.49	0.47
1:B:11:ARG:HA	1:B:56:LEU:O	2.15	0.47
1:B:854:SER:O	1:B:855:PHE:HB2	2.15	0.47
1:B:368:ARG:O	1:B:918:TYR:HB2	2.15	0.46
1:A:59:TYR:N	1:A:59:TYR:CD1	2.83	0.46
1:A:114:PHE:O	1:A:115:PRO:C	2.58	0.46
1:B:652:TYR:CG	1:B:769:ILE:CD1	2.98	0.46
1:B:799:PRO:HB3	1:B:810:MET:HE3	1.97	0.46
1:A:647:ILE:O	1:A:648:PRO:C	2.58	0.46
1:B:653:TYR:O	1:B:674:SER:HA	2.15	0.46
1:B:856:VAL:N	1:B:895:GLU:OE2	2.49	0.46
1:A:272:CYS:HA	1:A:303:ARG:O	2.16	0.46
1:A:165:LEU:HD11	1:A:191:GLN:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1222:LYS:HA	1:B:1228:TRP:CG	2.51	0.46
1:A:62:GLU:O	1:A:65:ARG:CG	2.64	0.46
1:A:126:MET:HG2	1:A:212:TYR:CE2	2.50	0.46
1:A:484:MET:CE	1:A:504:LEU:HD13	2.46	0.46
1:B:1272:PHE:HA	1:B:1278:MET:HG2	1.97	0.46
1:A:1034:VAL:O	1:A:1093:ARG:HD2	2.15	0.46
1:A:116:SER:O	1:A:121:MET:HG2	2.16	0.46
1:B:17:LEU:HD11	1:B:22:LEU:HB2	1.98	0.45
1:B:911:LEU:O	1:B:915:GLU:HG2	2.16	0.45
1:A:922:GLY:O	1:A:940:ILE:HA	2.15	0.45
1:B:447:LYS:HG3	1:B:448:PRO:HD2	1.99	0.45
1:B:740:GLN:OE1	1:B:740:GLN:HA	2.16	0.45
1:B:808:ARG:NH2	1:B:824:ASP:OD1	2.50	0.45
1:A:17:LEU:HD21	1:A:22:LEU:HB2	1.97	0.45
1:A:467:ASN:N	1:A:1111:GLU:OE2	2.43	0.45
1:A:398:LEU:HD22	1:A:946:GLN:HG3	1.97	0.45
1:A:799:PRO:CB	1:A:810:MET:HE3	2.46	0.45
1:A:1266:GLU:OE2	1:A:1308:THR:OG1	2.28	0.45
1:B:28:VAL:HA	1:B:59:TYR:O	2.17	0.45
1:B:265:LEU:HD11	1:B:301:GLY:HA2	1.98	0.45
1:A:277:MET:O	1:A:308:PHE:HA	2.16	0.45
1:A:799:PRO:O	1:A:810:MET:HE3	2.17	0.45
1:B:718:GLN:HA	1:B:718:GLN:OE1	2.16	0.45
1:B:764:CYS:O	1:B:1231:GLY:HA3	2.17	0.45
1:A:405:LEU:HA	1:A:941:HIS:CD2	2.52	0.44
1:B:356:HIS:N	1:B:357:PRO:CD	2.80	0.44
1:A:165:LEU:HA	1:A:168:LEU:HD12	1.98	0.44
1:B:983:VAL:HG11	1:B:985:TRP:CZ2	2.53	0.44
1:A:254:TRP:CZ3	1:A:258:ARG:HD2	2.52	0.44
1:B:238:HIS:ND1	1:B:239:PRO:HD2	2.33	0.44
1:B:11:ARG:HG3	1:B:57:THR:HG22	1.99	0.44
1:B:91:GLU:O	1:B:92:ASP:C	2.61	0.44
1:B:888:LYS:HB3	1:B:889:PRO:CD	2.47	0.44
1:A:99:GLU:O	1:A:103:PRO:HD2	2.17	0.44
1:A:186:PHE:CD1	1:A:186:PHE:C	2.96	0.44
1:A:746:ILE:O	1:A:750:VAL:HG23	2.18	0.44
1:B:87:LEU:HD21	1:B:161:MET:HE2	1.99	0.43
1:B:161:MET:SD	1:B:190:PHE:HE1	2.40	0.43
1:A:27:TYR:OH	1:A:35:GLN:CG	2.66	0.43
1:A:725:ASP:CB	1:A:730:LEU:HD12	2.48	0.43
1:B:267:ASP:OD1	1:B:268:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLN:NE2	1:B:285:GLY:O	2.49	0.43
1:B:978:GLU:HA	1:B:1071:PHE:CD2	2.53	0.43
1:B:982:SER:HA	1:B:1159:PHE:O	2.18	0.43
1:B:983:VAL:HB	1:B:1160:GLN:HG2	2.00	0.43
1:A:978:GLU:HB3	1:A:1075:HIS:CE1	2.53	0.43
1:A:1222:LYS:HA	1:A:1228:TRP:CG	2.54	0.43
1:B:184:ARG:HD2	1:B:184:ARG:O	2.19	0.43
1:A:300:MET:HE1	1:A:436:GLN:CG	2.48	0.43
1:A:392:HIS:N	1:A:393:PRO:CD	2.82	0.43
1:A:484:MET:CE	1:A:504:LEU:CD1	2.96	0.43
1:A:653:TYR:O	1:A:674:SER:HA	2.18	0.43
1:A:1043:ARG:NH1	1:A:1098:ALA:O	2.52	0.43
1:A:657:ASN:ND2	1:A:660:ASP:HB2	2.34	0.43
1:A:527:MET:CE	1:A:532:TYR:CA	2.90	0.43
1:A:641:ASP:O	1:A:643:LEU:N	2.51	0.43
1:A:779:ILE:O	1:A:783:VAL:HG23	2.18	0.43
1:B:1269:ASN:O	1:B:1273:ILE:HB	2.18	0.43
1:B:75:HIS:O	1:B:78:SER:OG	2.18	0.43
1:B:470:THR:OG1	1:B:620:THR:HA	2.19	0.43
1:A:1101:SER:C	1:A:1102:TYR:CD1	2.97	0.43
1:B:405:LEU:HD23	1:B:941:HIS:ND1	2.34	0.42
1:B:742:GLN:O	1:B:746:ILE:HG13	2.19	0.42
1:B:810:MET:HA	1:B:813:ILE:HD12	2.01	0.42
1:A:500:SER:OG	1:A:503:GLU:HG3	2.19	0.42
1:B:101:VAL:HG12	1:B:123:LEU:HD22	2.01	0.42
1:B:652:TYR:CD1	1:B:769:ILE:HD13	2.55	0.42
1:B:1001:MET:HE2	1:B:1019:ILE:HD12	2.01	0.42
1:A:986:GLY:O	1:A:990:ILE:HG13	2.19	0.42
1:A:723:ASN:C	1:A:725:ASP:H	2.27	0.42
1:A:1080:ALA:HB1	1:A:1085:ILE:O	2.18	0.42
1:B:369:PRO:HD3	1:B:916:GLY:O	2.19	0.42
1:B:170:THR:HG22	1:B:295:GLN:OE1	2.20	0.42
1:A:412:ILE:HG23	1:A:413:ILE:O	2.20	0.42
1:A:665:LYS:NZ	1:A:940:ILE:O	2.51	0.42
1:A:978:GLU:HA	1:A:1071:PHE:CD2	2.54	0.42
1:A:1169:LEU:CD1	1:A:1214:THR:HG22	2.50	0.42
1:B:315:SER:O	1:B:319:ASN:ND2	2.53	0.42
1:A:38:LEU:HA	1:A:38:LEU:HD23	1.84	0.42
1:B:14:PRO:HG3	1:B:53:ALA:HB1	2.01	0.42
1:B:39:SER:O	1:B:43:ARG:HG3	2.20	0.42
1:B:198:GLN:O	1:B:202:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:TYR:CD2	1:A:769:ILE:HD13	2.55	0.42
1:B:112:ILE:N	1:B:112:ILE:HD12	2.35	0.41
1:B:167:THR:O	1:B:170:THR:OG1	2.28	0.41
1:A:98:VAL:O	1:A:102:THR:OG1	2.37	0.41
1:B:484:MET:HE2	1:B:504:LEU:CD2	2.49	0.41
1:A:849:ALA:O	1:A:850:ASP:C	2.62	0.41
1:A:61:ILE:HG12	1:A:93:LEU:HD13	2.01	0.41
1:A:467:ASN:CG	1:A:1248:VAL:HG12	2.46	0.41
1:B:207:MET:HE2	1:B:208:LEU:N	2.36	0.41
1:B:472:ALA:HB2	1:B:620:THR:HG22	2.02	0.41
1:B:678:PRO:HG2	1:B:765:GLY:O	2.20	0.41
1:A:1061:ALA:HB2	1:A:1072:VAL:HG12	2.02	0.41
1:B:522:ASN:C	1:B:522:ASN:HD22	2.28	0.41
1:A:888:LYS:HB3	1:A:889:PRO:HD3	2.03	0.41
1:A:1278:MET:HE2	1:A:1282:LEU:HG	2.02	0.41
1:B:27:TYR:HA	1:B:84:ILE:O	2.21	0.41
1:B:698:SER:O	1:B:701:THR:HG22	2.20	0.41
1:A:102:THR:N	1:A:103:PRO:HD2	2.35	0.41
1:A:983:VAL:HG11	1:A:985:TRP:CZ2	2.55	0.41
1:A:1051:ASN:HA	1:A:1133:PHE:HE2	1.85	0.41
1:B:52:LEU:HD22	1:B:209:THR:HG21	2.01	0.41
1:A:657:ASN:CG	1:A:660:ASP:HB2	2.46	0.41
1:A:1244:SER:O	1:A:1248:VAL:HG23	2.20	0.41
1:B:495:GLN:HG3	1:B:568:GLY:CA	2.50	0.41
1:B:1167:ILE:O	1:B:1175:TYR:OH	2.33	0.41
1:A:126:MET:HE3	1:A:126:MET:HB2	1.87	0.41
1:A:527:MET:HE2	1:A:532:TYR:HB2	2.03	0.41
1:A:1090:ALA:HA	1:A:1147:MET:CE	2.48	0.41
1:B:762:LEU:HD12	1:B:762:LEU:C	2.45	0.41
1:B:900:GLN:OE1	1:B:935:PRO:HD3	2.20	0.41
1:B:1092:THR:HB	1:B:1147:MET:HG2	2.02	0.41
1:A:518:SER:OG	1:A:1326:ARG:O	2.35	0.41
1:A:790:ARG:HB2	1:A:795:ILE:HG13	2.03	0.41
1:A:562:ILE:HG21	1:A:605:TYR:CD2	2.56	0.41
1:B:1096:SER:O	1:B:1131:PHE:HB2	2.20	0.40
1:A:1088:ARG:HH11	1:A:1088:ARG:HG3	1.87	0.40
1:A:169:PRO:HA	1:A:172:LEU:HG	2.03	0.40
1:A:1233:LEU:HD13	1:A:1278:MET:HE1	2.03	0.40
1:B:885:GLU:O	1:B:889:PRO:HD2	2.21	0.40
1:A:822:LEU:O	1:A:823:ALA:C	2.64	0.40
1:A:987:THR:HG23	1:A:988:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:ASN:HA	1:A:1133:PHE:CE2	2.57	0.40
1:B:161:MET:SD	1:B:190:PHE:CE1	3.15	0.40
1:B:754:LEU:HD23	1:B:754:LEU:HA	1.95	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	1230/1351 (91%)	1161 (94%)	62 (5%)	7 (1%)	21	38
1	B	1184/1351 (88%)	1094 (92%)	81 (7%)	9 (1%)	16	31
All	All	2414/2702 (89%)	2255 (93%)	143 (6%)	16 (1%)	18	35

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	850	ASP
1	B	855	PHE
1	A	115	PRO
1	A	642	ASN
1	B	115	PRO
1	B	708	GLY
1	B	942	ALA
1	A	619	GLY
1	A	850	ASP
1	B	972	ASN
1	A	942	ALA
1	B	1113	SER
1	A	94	ALA
1	A	641	ASP
1	B	377	VAL

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Mol	Chain	Res	Type
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	1064/1147 (93%)	1010 (95%)	54 (5%)	21	43
1	B	1032/1147 (90%)	977 (95%)	55 (5%)	20	42
All	All	2096/2294 (91%)	1987 (95%)	109 (5%)	21	43

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	GLU
1	B	78	SER
1	B	102	THR
1	B	115	PRO
1	B	119	GLN
1	B	120	VAL
1	B	124	ASN
1	B	165	LEU
1	B	177	VAL
1	B	201	LEU
1	B	242	MET
1	B	246	GLU
1	B	249	LYS
1	B	273	ILE
1	B	318	VAL
1	B	324	ASP
1	B	361	GLU
1	B	425	ILE
1	B	445	ARG
1	B	495	GLN
1	B	518	SER
1	B	522	ASN

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Mol	Chain	Res	Type
1	B	575	GLN
1	B	604	THR
1	B	626	PHE
1	B	646	THR
1	B	659	SER
1	B	660	ASP
1	B	678	PRO
1	B	714	THR
1	B	721	ILE
1	B	736	GLU
1	B	745	THR
1	B	746	ILE
1	B	752	ARG
1	B	768	VAL
1	B	776	GLU
1	B	782	LEU
1	B	785	ILE
1	B	846	GLN
1	B	856	VAL
1	B	857	SER
1	B	894	LEU
1	B	905	ASN
1	B	920	LEU
1	B	982	SER
1	B	1018	LYS
1	B	1022	VAL
1	B	1045	LEU
1	B	1081	GLU
1	B	1103	SER
1	B	1113	SER
1	B	1176	PHE
1	B	1307	GLU
1	B	1314	GLU
1	A	33	GLN
1	A	49	ASN
1	A	51	SER
1	A	87	LEU
1	A	93	LEU
1	A	99	GLU
1	A	115	PRO
1	A	167	THR
1	A	177	VAL

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Mol	Chain	Res	Type
1	A	188	LEU
1	A	199	GLU
1	A	246	GLU
1	A	273	ILE
1	A	278	GLN
1	A	296	GLU
1	A	372	CYS
1	A	412	ILE
1	A	458	VAL
1	A	490	ASN
1	A	502	LYS
1	A	509	ILE
1	A	536	THR
1	A	539	SER
1	A	581	GLU
1	A	592	SER
1	A	615	VAL
1	A	627	MET
1	A	644	ILE
1	A	653	TYR
1	A	691	GLU
1	A	714	THR
1	A	726	GLN
1	A	734	ASN
1	A	745	THR
1	A	752	ARG
1	A	769	ILE
1	A	782	LEU
1	A	791	GLU
1	A	809	ASN
1	A	817	SER
1	A	846	GLN
1	A	901	VAL
1	A	943	LEU
1	A	1022	VAL
1	A	1087	VAL
1	A	1129	LYS
1	A	1160	GLN
1	A	1161	ASN
1	A	1186	THR
1	A	1192	LYS
1	A	1212	SER

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Mol	Chain	Res	Type
1	A	1295	SER
1	A	1311	GLU
1	A	1330	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	ASN
1	B	185	ASN
1	B	319	ASN
1	B	495	GLN
1	B	545	ASN
1	B	657	ASN
1	B	846	GLN
1	B	848	ASN
1	B	881	ASN
1	B	912	GLN
1	B	1097	ASN
1	B	1143	GLN
1	B	1301	ASN
1	B	1321	GLN
1	A	49	ASN
1	A	119	GLN
1	A	278	GLN
1	A	488	GLN
1	A	522	ASN
1	A	559	ASN
1	A	742	GLN
1	A	881	ASN
1	A	972	ASN
1	A	975	ASN
1	A	1107	ASN

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	A	1248/1351 (92%)	-0.07	40 (3%)	50 41	27, 50, 98, 134	35 (2%)
1	B	1207/1351 (89%)	0.32	50 (4%)	41 32	27, 72, 110, 155	36 (2%)
All	All	2455/2702 (90%)	0.12	90 (3%)	45 35	27, 60, 106, 155	71 (2%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	LEU	4.7
1	A	61	ILE	4.4
1	A	640	PRO	4.3
1	A	425	ILE	4.2
1	A	29	VAL	4.0
1	A	32	SER	4.0
1	A	64	LEU	4.0
1	B	132	ALA	3.9
1	B	332	PRO	3.8
1	A	392	HIS	3.8
1	B	859	LEU	3.6
1	A	644	ILE	3.6
1	B	853	VAL	3.6
1	B	626	PHE	3.5
1	A	1330	VAL	3.4
1	B	815	ARG	3.4
1	B	412	ILE	3.4
1	A	132	ALA	3.4
1	B	1330	VAL	3.1
1	A	592	SER	3.1
1	B	425	ILE	3.0
1	A	158	GLN	2.9
1	B	552	HIS	2.9
1	B	855	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	576	PRO	2.9
1	B	529	VAL	2.9
1	A	332	PRO	2.8
1	B	578	PHE	2.8
1	B	577	THR	2.8
1	A	353	ARG	2.8
1	A	103	PRO	2.8
1	B	232	PRO	2.7
1	B	244	MET	2.6
1	A	104	TYR	2.6
1	A	815	ARG	2.6
1	B	731	PRO	2.6
1	A	100	ALA	2.6
1	B	882	VAL	2.6
1	A	93	LEU	2.6
1	A	90	ILE	2.6
1	A	414	LEU	2.6
1	B	625	GLU	2.6
1	A	424	ALA	2.6
1	A	466	GLY	2.5
1	B	392	HIS	2.5
1	B	459	PHE	2.5
1	A	87	LEU	2.5
1	B	130	SER	2.4
1	B	353	ARG	2.4
1	A	379	GLN	2.4
1	A	356	HIS	2.4
1	B	365	LYS	2.4
1	A	161	MET	2.4
1	B	470	THR	2.4
1	A	177	VAL	2.3
1	B	645	GLY	2.3
1	B	160	ALA	2.3
1	B	546	TRP	2.3
1	B	90	ILE	2.3
1	B	354	GLN	2.3
1	A	70	TYR	2.3
1	B	159	ASP	2.3
1	B	269	LEU	2.3
1	B	858	LYS	2.2
1	B	324	ASP	2.2
1	A	99	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	467	ASN	2.2
1	B	248	VAL	2.2
1	B	513	GLN	2.2
1	B	89	PHE	2.2
1	B	575	GLN	2.2
1	B	356	HIS	2.2
1	B	538	TYR	2.2
1	B	561	LEU	2.2
1	B	31	GLU	2.2
1	A	106	ASP	2.1
1	B	885	GLU	2.1
1	A	972	ASN	2.1
1	A	131	MET	2.1
1	A	593	ALA	2.1
1	B	833	LEU	2.1
1	A	89	PHE	2.1
1	B	448	PRO	2.1
1	B	100	ALA	2.1
1	A	98	VAL	2.0
1	A	468	VAL	2.0
1	B	376	LEU	2.0
1	B	809	ASN	2.0
1	A	232	PRO	2.0
1	B	704	ASP	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.