



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:21 pm BST

PDB ID : 1LBQ
Title : The crystal structure of *Saccharomyces cerevisiae* ferrochelatase
Authors : Karlberg, T.; Lecerof, D.; Gora, M.; Silvegren, G.; Labbe-Bois, R.; Hansson, M.; Al-Karadaghi, S.
Deposited on : 2002-04-04
Resolution : 2.40 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

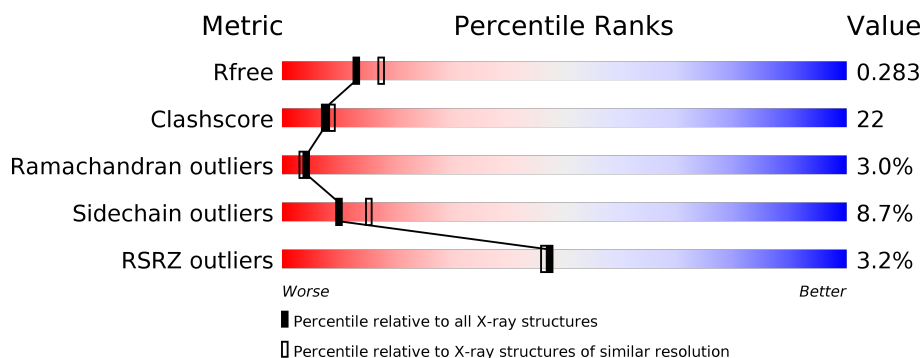
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	362	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>• • •</div> </div> </div>
1	B	362	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>7%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5797 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 Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2846	1834	472	530	10			
1	B	354	Total	C	N	O	S	0	0	0
			2829	1825	467	527	10			

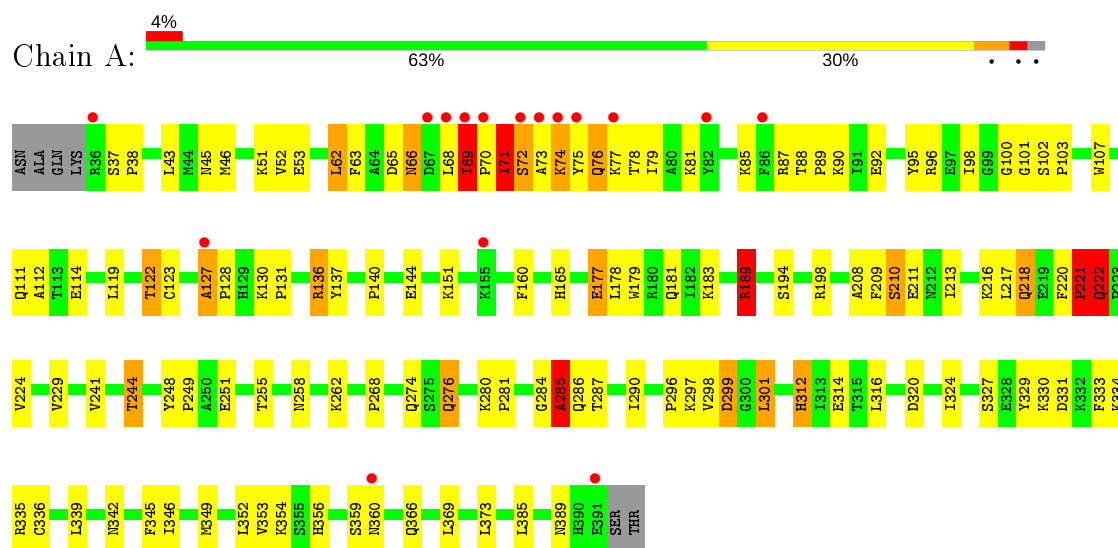
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	58	Total	O	0	0
			58	58		

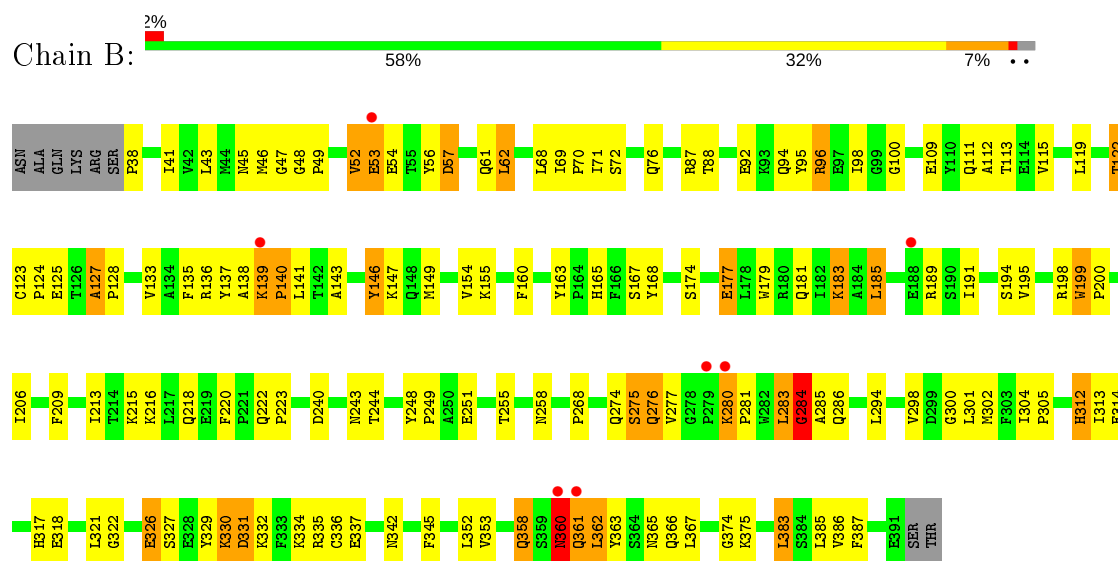
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Ferrochelatase



• Molecule 1: Ferrochelatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.61Å 97.17Å 121.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.40 19.84 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.80-2.40) 97.8 (19.84-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.282 0.256 , 0.283	Depositor DCC
R_{free} test set	2348 reflections (6.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5797	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	0.40	0/2919	0.71	3/3955 (0.1%)
1	B	0.40	0/2902	0.67	4/3932 (0.1%)
All	All	0.40	0/5821	0.69	7/7887 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	GLY	N-CA-C	7.71	132.37	113.10
1	B	54	GLU	N-CA-C	-7.34	91.17	111.00
1	A	285	ALA	N-CA-C	-6.93	92.28	111.00
1	B	62	LEU	CA-CB-CG	6.69	130.68	115.30
1	A	210	SER	N-CA-C	-5.88	95.12	111.00
1	B	283	LEU	N-CA-C	5.53	125.94	111.00
1	A	71	ILE	N-CA-C	-5.45	96.30	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2846	0	2841	129	0
1	B	2829	0	2824	128	0
2	A	64	0	0	14	0
2	B	58	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5797	0	5665	251	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 22.

All (251) 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:139:LYS:HB3	1:B:140:PRO:HD3	1.28	1.12
1:A:284:GLY:HA3	1:B:243:ASN:OD1	1.63	0.98
1:B:119:LEU:HA	1:B:122:THR:HG22	1.46	0.97
1:B:362:LEU:H	1:B:362:LEU:HD12	1.31	0.96
1:B:139:LYS:HB3	1:B:140:PRO:CD	1.95	0.95
1:A:127:ALA:HB3	1:A:128:PRO:HD3	1.49	0.93
1:A:69:ILE:HG22	1:A:70:PRO:HD3	1.47	0.93
1:A:68:LEU:HG	1:A:69:ILE:H	1.31	0.92
1:A:221:PRO:O	1:A:222:GLN:HB3	1.68	0.92
1:A:122:THR:HG23	1:A:354:LYS:HD2	1.55	0.89
1:A:274:GLN:HA	1:A:276:GLN:HE22	1.38	0.88
1:A:76:GLN:HA	1:A:79:ILE:HG12	1.56	0.88
1:B:127:ALA:HB1	1:B:128:PRO:CD	2.04	0.87
1:B:283:LEU:HD12	1:B:284:GLY:H	1.39	0.87
1:B:68:LEU:CD1	1:B:69:ILE:HG13	2.07	0.84
1:A:69:ILE:CG2	1:A:70:PRO:HD3	2.08	0.83
1:A:210:SER:O	1:A:211:GLU:HB2	1.80	0.81
1:A:298:VAL:HG21	1:A:301:LEU:HD13	1.63	0.80
1:B:94:GLN:NE2	1:B:313:ILE:HD11	1.97	0.78
1:A:70:PRO:HD2	1:A:76:GLN:HE22	1.48	0.78
1:A:122:THR:CG2	1:A:354:LYS:HD2	2.15	0.77
1:A:165:HIS:HE1	1:A:255:THR:OG1	1.68	0.77
1:B:165:HIS:HE1	1:B:255:THR:OG1	1.69	0.76
1:A:127:ALA:CB	1:A:128:PRO:HD3	2.16	0.75
1:B:358:GLN:HG3	2:B:436:HOH:O	1.87	0.73
1:A:248:TYR:HB3	1:A:249:PRO:HD3	1.70	0.72
1:B:94:GLN:HE21	1:B:313:ILE:HD11	1.54	0.71
1:B:68:LEU:HD12	1:B:69:ILE:HG13	1.74	0.70
1:A:217:LEU:O	1:A:220:PHE:HB2	1.91	0.69
1:B:52:VAL:HG11	1:B:96:ARG:HD2	1.74	0.69
1:B:127:ALA:HB1	1:B:128:PRO:HD3	1.75	0.69
1:B:68:LEU:HD13	1:B:69:ILE:HG13	1.73	0.69
1:A:324:ILE:O	1:A:330:LYS:HG3	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:HB3	1:B:154:VAL:HG21	1.75	0.68
1:A:298:VAL:HG21	1:A:301:LEU:CD1	2.25	0.67
1:A:221:PRO:O	1:A:222:GLN:CB	2.42	0.67
1:A:73:ALA:O	1:A:74:LYS:HB2	1.95	0.67
1:A:229:VAL:CG1	1:A:301:LEU:HD12	2.25	0.67
1:A:95:TYR:HB3	1:A:101:GLY:H	1.59	0.66
1:B:362:LEU:N	1:B:362:LEU:HD12	2.09	0.65
1:B:360:ASN:H	1:B:360:ASN:HD22	1.45	0.65
1:B:274:GLN:O	1:B:275:SER:HB3	1.96	0.65
1:B:342:ASN:HD22	1:B:345:PHE:H	1.46	0.64
1:A:301:LEU:HD22	1:A:333:PHE:CE2	2.32	0.64
1:A:241:VAL:O	1:A:244:THR:HB	1.98	0.64
1:A:68:LEU:HG	1:A:69:ILE:N	2.09	0.64
1:A:244:THR:HG21	2:A:402:HOH:O	1.98	0.64
1:A:76:GLN:C	1:A:78:THR:N	2.51	0.64
1:A:122:THR:HG21	2:A:424:HOH:O	1.96	0.63
1:A:72:SER:CB	1:A:76:GLN:HB2	2.29	0.63
1:B:139:LYS:CB	1:B:140:PRO:HD3	2.18	0.63
1:B:72:SER:H	1:B:76:GLN:NE2	1.97	0.63
1:B:360:ASN:H	1:B:360:ASN:ND2	1.97	0.63
1:B:45:ASN:ND2	1:B:47:GLY:H	1.97	0.63
1:B:48:GLY:N	1:B:138:ALA:HB2	2.14	0.63
1:A:68:LEU:CG	1:A:69:ILE:H	2.09	0.62
1:B:302:MET:CE	1:B:336:CYS:HB2	2.29	0.62
1:A:276:GLN:NE2	1:A:276:GLN:H	1.96	0.62
1:B:367:LEU:HG	1:B:383:LEU:HD21	1.80	0.62
1:B:302:MET:HE3	1:B:336:CYS:HB2	1.81	0.62
1:A:69:ILE:HB	1:A:70:PRO:CD	2.30	0.62
1:B:248:TYR:HB3	1:B:249:PRO:HD3	1.79	0.62
1:A:69:ILE:CB	1:A:70:PRO:HD3	2.30	0.62
1:A:211:GLU:N	2:A:438:HOH:O	2.33	0.62
1:B:109:GLU:O	1:B:113:THR:HG23	1.98	0.62
1:B:283:LEU:CD1	1:B:284:GLY:H	2.10	0.62
1:B:216:LYS:HE2	1:B:335:ARG:O	2.00	0.62
1:B:277:VAL:O	1:B:280:LYS:HE2	2.00	0.61
1:B:43:LEU:HD22	1:B:160:PHE:HD2	1.65	0.61
1:B:276:GLN:HE22	1:B:286:GLN:HG2	1.65	0.61
1:A:221:PRO:HB2	1:A:224:VAL:HG12	1.81	0.61
1:A:198:ARG:HD3	1:A:251:GLU:OE2	2.00	0.61
1:A:179:TRP:CE2	1:A:183:LYS:HD2	2.35	0.61
1:B:139:LYS:O	1:B:141:LEU:N	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ARG:HB3	2:B:446:HOH:O	2.01	0.61
1:A:88:THR:O	1:A:92:GLU:HG3	2.01	0.60
1:A:77:LYS:O	1:A:81:LYS:HE2	2.02	0.60
1:A:127:ALA:HB3	1:A:128:PRO:CD	2.29	0.60
1:A:71:ILE:N	1:A:71:ILE:HD13	2.17	0.59
1:B:127:ALA:CB	1:B:128:PRO:CD	2.80	0.58
1:A:194:SER:OG	1:A:356:HIS:HE1	1.86	0.58
1:B:361:GLN:HA	1:B:361:GLN:OE1	2.03	0.58
1:A:213:ILE:HB	2:A:438:HOH:O	2.01	0.58
1:B:209:PHE:O	1:B:213:ILE:HG13	2.03	0.58
1:A:95:TYR:CD2	1:A:98:ILE:HD11	2.39	0.58
1:B:38:PRO:HB2	1:B:155:LYS:HD3	1.85	0.58
1:A:385:LEU:HD23	1:A:385:LEU:O	2.03	0.58
1:A:274:GLN:CA	1:A:276:GLN:HE22	2.13	0.58
1:B:139:LYS:CB	1:B:140:PRO:CD	2.75	0.58
1:B:43:LEU:HD22	1:B:160:PHE:CD2	2.38	0.58
1:B:206:ILE:HG21	1:B:258:ASN:ND2	2.19	0.58
1:A:71:ILE:O	1:A:72:SER:HB3	2.04	0.58
1:A:268:PRO:HA	1:B:366:GLN:HE22	1.68	0.58
1:B:206:ILE:HG21	1:B:258:ASN:HD22	1.68	0.58
1:B:71:ILE:H	1:B:76:GLN:HE22	1.52	0.57
1:A:76:GLN:C	1:A:78:THR:H	2.08	0.57
1:B:136:ARG:HG3	1:B:137:TYR:CE2	2.40	0.57
1:A:127:ALA:CB	1:A:128:PRO:CD	2.83	0.57
1:A:224:VAL:HG21	1:A:299:ASP:CG	2.25	0.57
1:A:81:LYS:O	1:A:85:LYS:HG3	2.03	0.57
1:B:146:TYR:CE2	1:B:191:ILE:HD12	2.41	0.56
1:B:43:LEU:HG	1:B:112:ALA:HB2	1.87	0.56
1:B:88:THR:O	1:B:92:GLU:HB2	2.05	0.56
1:A:366:GLN:OE1	1:B:268:PRO:HA	2.05	0.56
1:A:69:ILE:CB	1:A:70:PRO:CD	2.85	0.55
1:B:139:LYS:O	1:B:140:PRO:C	2.45	0.55
1:A:95:TYR:HD2	1:A:98:ILE:HD11	1.70	0.55
1:A:189:ARG:HB3	2:A:405:HOH:O	2.06	0.54
1:A:122:THR:HG22	1:A:123:CYS:SG	2.47	0.54
1:A:73:ALA:O	1:A:74:LYS:CB	2.54	0.54
1:B:122:THR:HG21	2:B:425:HOH:O	2.07	0.54
1:A:373:LEU:CD1	1:B:294:LEU:HD21	2.38	0.54
1:A:88:THR:HB	1:A:89:PRO:HD3	1.90	0.54
1:B:198:ARG:HD3	1:B:251:GLU:OE1	2.07	0.54
1:B:167:SER:HB2	1:B:248:TYR:HB2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HD11	1:B:353:VAL:HG11	1.90	0.53
1:B:127:ALA:HB1	1:B:128:PRO:HD2	1.88	0.53
1:A:296:PRO:HG3	1:A:329:TYR:OH	2.09	0.53
1:A:301:LEU:HD22	1:A:333:PHE:CZ	2.45	0.52
1:B:213:ILE:HA	1:B:302:MET:HE1	1.92	0.52
1:B:312:HIS:CE1	1:B:314:GLU:HB2	2.45	0.52
1:A:327:SER:O	1:A:330:LYS:HE2	2.09	0.52
1:A:63:PHE:HA	1:A:69:ILE:HG21	1.91	0.52
1:A:373:LEU:HD11	1:B:294:LEU:HD21	1.92	0.52
1:A:95:TYR:HA	1:A:98:ILE:HG12	1.92	0.52
1:B:46:MET:HG3	1:B:163:TYR:OH	2.10	0.52
1:B:314:GLU:O	1:B:318:GLU:HB2	2.09	0.52
1:B:179:TRP:CE2	1:B:183:LYS:HE3	2.45	0.51
1:B:317:HIS:CD2	1:B:321:LEU:HD12	2.45	0.51
1:B:179:TRP:CE3	1:B:386:VAL:HG22	2.45	0.51
1:A:66:ASN:HA	1:A:68:LEU:O	2.10	0.51
1:A:76:GLN:HG3	1:A:76:GLN:O	2.10	0.51
1:A:220:PHE:CE1	1:A:334:LYS:HD2	2.46	0.51
1:B:149:MET:O	1:B:154:VAL:HG22	2.11	0.51
1:A:216:LYS:HB2	2:A:433:HOH:O	2.11	0.50
1:A:287:THR:O	1:A:290:ILE:HG22	2.11	0.50
1:A:70:PRO:C	1:A:71:ILE:HD13	2.32	0.50
1:B:322:GLY:O	1:B:326:GLU:HB2	2.11	0.50
1:B:302:MET:HA	1:B:334:LYS:O	2.11	0.50
1:A:43:LEU:HG	1:A:112:ALA:HB2	1.94	0.50
1:A:62:LEU:HD23	1:A:137:TYR:CE1	2.46	0.50
1:B:206:ILE:HG13	1:B:258:ASN:ND2	2.27	0.50
1:B:143:ALA:O	1:B:147:LYS:HG3	2.11	0.50
1:B:215:LYS:HA	1:B:218:GLN:HG3	1.94	0.49
1:A:65:ASP:HA	2:A:451:HOH:O	2.13	0.49
1:B:181:GLN:HA	1:B:181:GLN:OE1	2.12	0.49
1:A:181:GLN:NE2	1:A:181:GLN:HA	2.27	0.49
1:A:349:MET:O	1:A:353:VAL:HG23	2.13	0.49
1:B:149:MET:HB3	1:B:154:VAL:CG2	2.43	0.49
1:B:146:TYR:HB3	1:B:185:LEU:HD23	1.96	0.48
1:B:98:ILE:O	1:B:98:ILE:HG13	2.13	0.48
1:A:284:GLY:O	1:A:285:ALA:CB	2.61	0.48
1:B:53:GLU:OE1	1:B:53:GLU:C	2.52	0.48
1:B:222:GLN:HB3	1:B:223:PRO:HD3	1.96	0.48
1:A:335:ARG:HG2	1:A:336:CYS:O	2.13	0.48
1:B:240:ASP:O	1:B:244:THR:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:O	1:A:210:SER:O	2.32	0.47
1:B:122:THR:C	1:B:124:PRO:HD3	2.35	0.47
1:B:165:HIS:CE1	1:B:255:THR:OG1	2.58	0.47
1:A:342:ASN:O	1:A:346:ILE:HG12	2.14	0.47
1:A:53:GLU:OE1	1:A:53:GLU:N	2.48	0.47
1:B:136:ARG:CZ	1:B:177:GLU:HG2	2.44	0.47
1:A:210:SER:C	2:A:438:HOH:O	2.53	0.47
1:B:276:GLN:NE2	1:B:286:GLN:HG2	2.30	0.47
1:B:168:TYR:CE1	1:B:374:GLY:HA3	2.50	0.47
1:B:213:ILE:HG23	1:B:302:MET:HE2	1.96	0.47
1:A:189:ARG:NH1	1:A:385:LEU:O	2.40	0.47
1:B:138:ALA:O	1:B:139:LYS:O	2.32	0.47
1:A:268:PRO:HA	1:B:366:GLN:NE2	2.30	0.47
1:B:300:GLY:HA2	1:B:332:LYS:HB2	1.97	0.47
1:A:68:LEU:HD23	1:A:69:ILE:HD13	1.98	0.46
1:B:283:LEU:CG	1:B:284:GLY:N	2.78	0.46
1:B:179:TRP:NE1	1:B:183:LYS:HE3	2.31	0.46
1:A:179:TRP:CZ2	1:A:183:LYS:HD2	2.51	0.46
1:A:189:ARG:HB3	1:A:189:ARG:HE	1.42	0.46
1:B:95:TYR:O	1:B:100:GLY:N	2.48	0.46
1:B:329:TYR:HB3	1:B:332:LYS:HG3	1.98	0.46
1:A:62:LEU:HD23	1:A:137:TYR:CD1	2.51	0.46
1:A:51:LYS:HA	2:A:457:HOH:O	2.16	0.45
1:A:68:LEU:C	1:A:69:ILE:HG12	2.36	0.45
1:A:71:ILE:N	1:A:71:ILE:CD1	2.79	0.45
1:A:37:SER:HA	1:A:38:PRO:HD3	1.86	0.45
1:B:123:CYS:N	1:B:124:PRO:HD3	2.32	0.45
1:B:119:LEU:CD1	1:B:353:VAL:HG11	2.46	0.45
1:B:195:VAL:HG12	1:B:362:LEU:O	2.17	0.45
1:B:284:GLY:O	1:B:285:ALA:HB3	2.15	0.45
1:B:283:LEU:HG	1:B:284:GLY:N	2.32	0.45
1:A:359:SER:O	1:A:360:ASN:HB2	2.17	0.45
1:A:114:GLU:OE1	1:A:114:GLU:HA	2.17	0.45
1:B:304:ILE:HA	1:B:305:PRO:HD3	1.81	0.45
1:A:339:LEU:HD13	1:A:345:PHE:CD2	2.51	0.45
1:B:133:VAL:HG11	1:B:135:PHE:CZ	2.51	0.44
1:B:199:TRP:N	1:B:200:PRO:HD3	2.32	0.44
1:B:360:ASN:O	1:B:361:GLN:O	2.35	0.44
1:B:363:TYR:HB2	1:B:367:LEU:HD22	1.98	0.44
1:A:71:ILE:O	1:A:72:SER:CB	2.65	0.44
1:B:375:LYS:NZ	2:B:416:HOH:O	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:SER:O	1:B:276:GLN:HB2	2.18	0.44
1:B:206:ILE:HG13	1:B:258:ASN:HD22	1.82	0.43
1:B:133:VAL:CG1	1:B:135:PHE:CZ	3.01	0.43
1:A:52:VAL:HG23	2:A:457:HOH:O	2.18	0.43
1:B:275:SER:O	1:B:276:GLN:CB	2.65	0.43
1:B:168:TYR:CD1	1:B:374:GLY:HA3	2.53	0.43
1:A:107:TRP:O	1:A:111:GLN:HG3	2.18	0.43
1:A:210:SER:O	1:A:211:GLU:CB	2.54	0.43
1:A:276:GLN:CD	1:A:276:GLN:H	2.21	0.43
1:A:102:SER:HA	1:A:103:PRO:HD3	1.77	0.42
1:B:47:GLY:HA3	1:B:138:ALA:HB3	2.01	0.42
1:B:56:TYR:O	1:B:57:ASP:CG	2.58	0.42
1:B:111:GLN:O	1:B:115:VAL:HG23	2.19	0.42
1:B:41:ILE:HD12	1:B:41:ILE:N	2.33	0.42
1:A:72:SER:HB2	1:A:76:GLN:HB2	2.00	0.42
1:A:100:GLY:C	2:A:457:HOH:O	2.58	0.42
1:A:312:HIS:NE2	1:A:314:GLU:HB2	2.35	0.42
1:A:330:LYS:HE3	1:A:330:LYS:HB2	1.85	0.42
1:B:274:GLN:O	1:B:275:SER:CB	2.67	0.42
1:B:298:VAL:HG21	1:B:301:LEU:HG	2.01	0.42
1:A:151:LYS:HD2	1:A:151:LYS:HA	1.90	0.42
1:B:49:PRO:HD2	1:B:95:TYR:CZ	2.55	0.42
1:A:46:MET:HE2	1:A:46:MET:HA	2.01	0.42
1:A:130:LYS:HA	1:A:131:PRO:HD3	1.81	0.41
1:A:136:ARG:NH1	2:A:409:HOH:O	2.39	0.41
1:A:312:HIS:N	1:A:312:HIS:CD2	2.87	0.41
1:A:140:PRO:HB3	1:A:144:GLU:CD	2.41	0.41
1:A:209:PHE:O	1:A:213:ILE:HG13	2.20	0.41
1:A:210:SER:CA	2:A:438:HOH:O	2.68	0.41
1:B:194:SER:HA	1:B:362:LEU:HB3	2.01	0.41
1:B:362:LEU:H	1:B:362:LEU:CD1	2.09	0.41
1:A:119:LEU:HD11	1:A:353:VAL:HG11	2.02	0.41
1:A:224:VAL:HG22	1:A:224:VAL:O	2.19	0.41
1:B:327:SER:O	1:B:330:LYS:CG	2.68	0.41
1:B:38:PRO:HB2	1:B:155:LYS:CD	2.49	0.41
1:A:218:GLN:C	1:A:220:PHE:H	2.23	0.41
1:A:229:VAL:HG12	1:A:301:LEU:HD12	1.99	0.41
1:A:297:LYS:HE2	1:A:297:LYS:HB3	1.94	0.41
1:A:53:GLU:CD	1:A:53:GLU:H	2.23	0.41
1:B:329:TYR:HB3	1:B:332:LYS:CG	2.50	0.41
1:A:360:ASN:HD22	1:A:360:ASN:HA	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:VAL:HB	1:B:387:PHE:CE2	2.55	0.41
1:B:69:ILE:HA	1:B:70:PRO:HD3	1.91	0.41
1:A:280:LYS:HA	1:A:281:PRO:HD3	1.86	0.40
1:A:72:SER:OG	1:A:76:GLN:HB2	2.21	0.40
1:B:280:LYS:HA	1:B:281:PRO:HD3	1.89	0.40
1:A:136:ARG:CZ	1:A:177:GLU:HG2	2.51	0.40
1:A:68:LEU:CG	1:A:69:ILE:N	2.78	0.40
1:A:210:SER:HA	2:A:438:HOH:O	2.21	0.40
1:B:179:TRP:CZ2	1:B:183:LYS:HD2	2.56	0.40
1:B:329:TYR:O	1:B:331:ASP:N	2.53	0.40
1:B:220:PHE:CE1	1:B:334:LYS:HD2	2.56	0.40
1:A:316:LEU:O	1:A:320:ASP:HB2	2.21	0.40
1:A:46:MET:HA	1:A:136:ARG:HB3	2.04	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	354/362 (98%)	312 (88%)	34 (10%)	8 (2%)	6	7
1	B	352/362 (97%)	315 (90%)	24 (7%)	13 (4%)	3	2
All	All	706/724 (98%)	627 (89%)	58 (8%)	21 (3%)	4	3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ILE
1	A	72	SER
1	A	127	ALA
1	A	221	PRO
1	A	222	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	285	ALA
1	B	127	ALA
1	B	139	LYS
1	B	284	GLY
1	B	361	GLN
1	A	74	LYS
1	B	57	ASP
1	B	140	PRO
1	B	275	SER
1	B	358	GLN
1	B	360	ASN
1	B	326	GLU
1	B	330	LYS
1	A	189	ARG
1	B	276	GLN
1	B	52	VAL

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	312/317 (98%)	281 (90%)	31 (10%)	8	11
1	B	310/317 (98%)	287 (93%)	23 (7%)	13	22
All	All	622/634 (98%)	568 (91%)	54 (9%)	10	15

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	62	LEU
1	A	66	ASN
1	A	69	ILE
1	A	71	ILE
1	A	75	TYR
1	A	76	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	ARG
1	A	90	LYS
1	A	96	ARG
1	A	122	THR
1	A	136	ARG
1	A	160	PHE
1	A	177	GLU
1	A	178	LEU
1	A	189	ARG
1	A	218	GLN
1	A	221	PRO
1	A	222	GLN
1	A	244	THR
1	A	258	ASN
1	A	262	LYS
1	A	276	GLN
1	A	286	GLN
1	A	299	ASP
1	A	301	LEU
1	A	312	HIS
1	A	331	ASP
1	A	352	LEU
1	A	369	LEU
1	A	389	ASN
1	B	53	GLU
1	B	61	GLN
1	B	62	LEU
1	B	87	ARG
1	B	96	ARG
1	B	122	THR
1	B	125	GLU
1	B	146	TYR
1	B	174	SER
1	B	177	GLU
1	B	183	LYS
1	B	185	LEU
1	B	199	TRP
1	B	280	LYS
1	B	312	HIS
1	B	331	ASP
1	B	337	GLU
1	B	352	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	360	ASN
1	B	362	LEU
1	B	365	ASN
1	B	383	LEU
1	B	385	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	94	GLN
1	A	165	HIS
1	A	181	GLN
1	A	222	GLN
1	A	261	GLN
1	A	274	GLN
1	A	276	GLN
1	A	356	HIS
1	A	360	ASN
1	A	377	ASN
1	A	389	ASN
1	B	45	ASN
1	B	61	GLN
1	B	76	GLN
1	B	94	GLN
1	B	148	GLN
1	B	165	HIS
1	B	176	ASN
1	B	258	ASN
1	B	274	GLN
1	B	312	HIS
1	B	342	ASN
1	B	358	GLN
1	B	360	ASN
1	B	365	ASN
1	B	377	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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	356/362 (98%)	-0.05	16 (4%) 33 31	21, 42, 80, 99	0
1	B	354/362 (97%)	-0.16	7 (1%) 65 63	21, 41, 74, 95	0
All	All	710/724 (98%)	-0.11	23 (3%) 47 46	21, 41, 76, 99	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	TYR	6.9
1	A	69	ILE	5.7
1	B	360	ASN	4.9
1	A	74	LYS	4.9
1	A	67	ASP	4.4
1	A	73	ALA	4.4
1	A	127	ALA	3.8
1	A	68	LEU	3.4
1	B	361	GLN	3.4
1	B	139	LYS	3.3
1	A	391	GLU	3.2
1	A	155	LYS	2.9
1	A	36	ARG	2.7
1	B	279	PRO	2.6
1	A	77	LYS	2.6
1	A	82	TYR	2.5
1	B	188	GLU	2.4
1	A	72	SER	2.2
1	B	53	GLU	2.2
1	B	280	LYS	2.1
1	A	360	ASN	2.1
1	A	70	PRO	2.0
1	A	86	PHE	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 carbohydrates 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.