



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:15 PM UTC

PDB ID : 3BTv / pdb_00003btv
Title : Crystal structure of the super-repressor mutant of Gal80p from *Saccharomyces cerevisiae*; Gal80(S0)-[G301R]
Authors : Kumar, P.R.; Joshua-Tor, L.
Deposited on : 2007-12-31
Resolution : 2.10 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

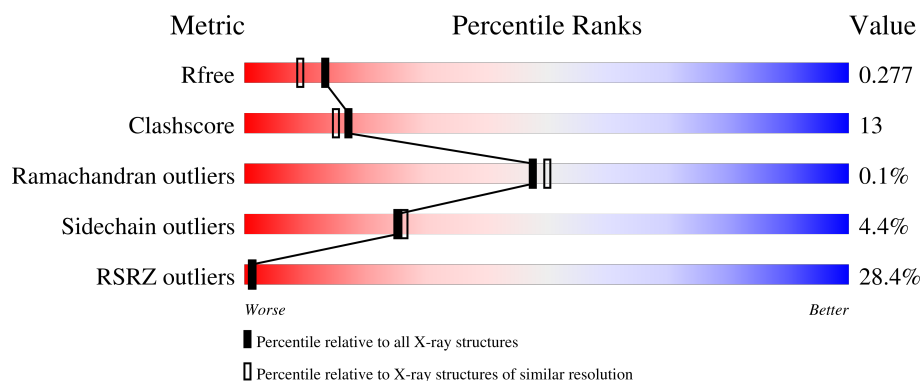
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	438	22% 63% 24% 11%
1	B	438	29% 63% 26% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6380 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	4	0
			3107	1995	524	576	12			
1	B	392	Total	C	N	O	S	0	1	0
			3106	1999	519	576	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P04387
A	-1	SER	-	expression tag	UNP P04387
A	0	HIS	-	expression tag	UNP P04387
A	301	ARG	GLY	engineered mutation	UNP P04387
B	-2	GLY	-	expression tag	UNP P04387
B	-1	SER	-	expression tag	UNP P04387
B	0	HIS	-	expression tag	UNP P04387
B	301	ARG	GLY	engineered mutation	UNP P04387

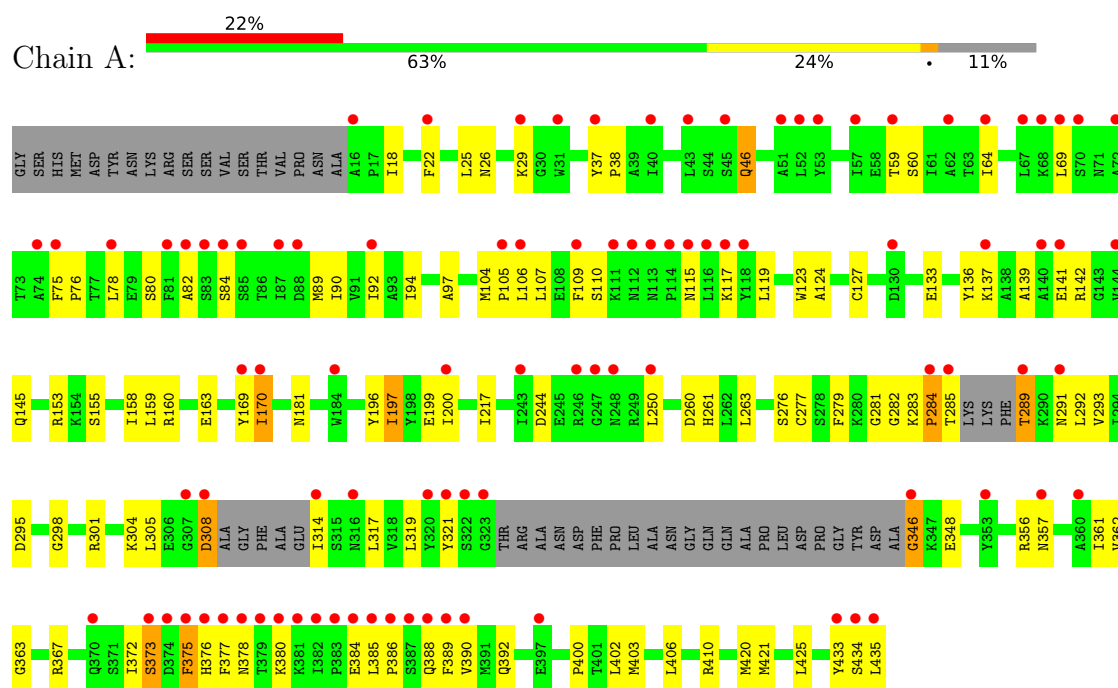
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	113	Total	O	0	0
			113	113		
2	B	54	Total	O	0	0
			54	54		

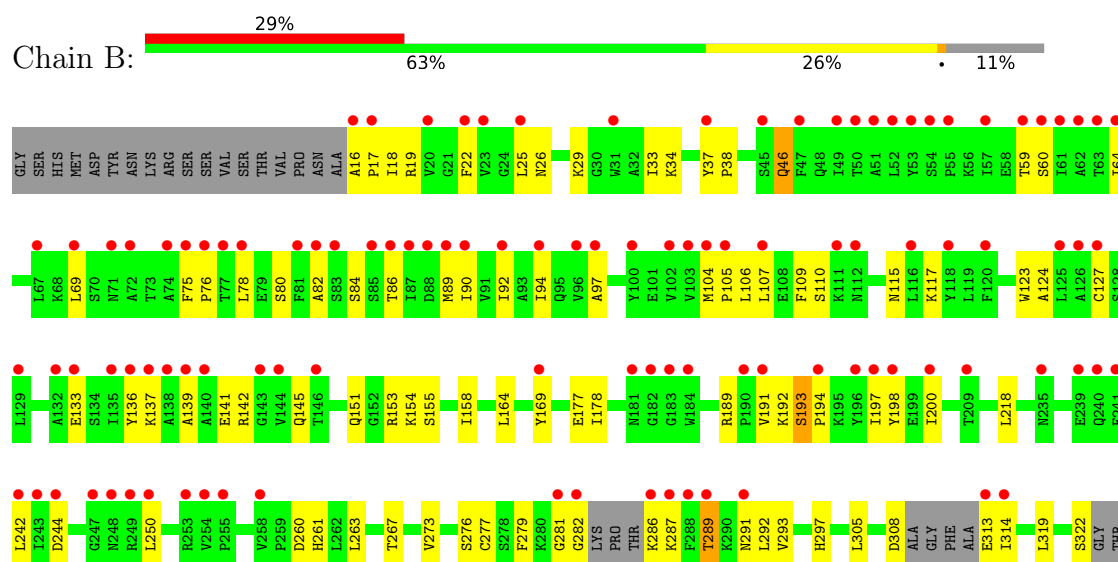
3 Residue-property plots

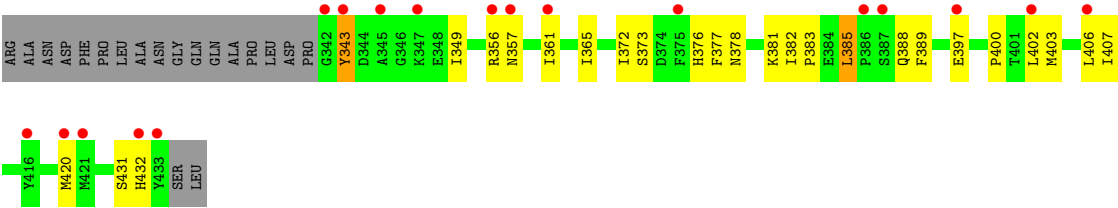
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Galactose/lactose metabolism regulatory protein GAL80



- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.09Å 103.95Å 106.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.61 – 2.10 46.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.61-2.10) 99.8 (46.61-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.215 , 0.257 0.240 , 0.277	Depositor DCC
R_{free} test set	2867 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6380	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	0.53	0/3173	0.85	3/4297 (0.1%)
1	B	0.43	0/3173	0.83	7/4295 (0.2%)
All	All	0.48	0/6346	0.84	10/8592 (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	A	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	GLY	CA-C-N	9.22	138.29	121.70
1	B	281	GLY	C-N-CA	9.22	138.29	121.70
1	A	346	GLY	N-CA-C	-6.78	93.62	113.30
1	A	308	ASP	N-CA-C	-6.56	92.64	111.00
1	B	193	SER	CA-C-N	6.48	126.87	119.93
1	B	193	SER	C-N-CA	6.48	126.87	119.93
1	B	282	GLY	N-CA-C	-5.58	97.12	113.30
1	B	432	HIS	N-CA-C	5.30	119.50	112.72
1	A	361	ILE	N-CA-C	5.27	115.48	110.42
1	B	313	GLU	N-CA-C	-5.26	96.28	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	346	GLY	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	3107	0	3117	76	0
1	B	3106	0	3111	85	0
2	A	113	0	0	4	0
2	B	54	0	0	1	0
All	All	6380	0	6228	157	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 13.

All (157) 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:164:LEU:HD13	1:B:319:LEU:HD11	1.36	1.02
1:A:89:MET:HE1	1:A:372:ILE:HG21	1.42	1.01
1:A:46:GLN:HE21	1:A:46:GLN:H	1.14	0.96
1:B:46:GLN:HE21	1:B:46:GLN:H	1.14	0.96
1:B:286:LYS:HD3	1:B:289:THR:HG23	1.50	0.92
1:B:145:GLN:HE22	1:B:389:PHE:H	1.20	0.90
1:A:301[B]:ARG:NH1	1:A:319:LEU:HD21	1.97	0.80
1:A:301[B]:ARG:HG2	1:A:321:TYR:HB3	1.66	0.77
1:A:434:SER:HA	1:A:435:LEU:C	2.08	0.76
1:B:286:LYS:HD3	1:B:289:THR:CG2	2.17	0.75
1:B:151:GLN:HG3	1:B:365:ILE:HD12	1.68	0.74
1:A:301[A]:ARG:HG2	1:A:321:TYR:HB3	1.71	0.73
1:A:385:LEU:HD12	1:A:386:PRO:HD2	1.70	0.72
1:A:285:THR:HG23	1:B:322:SER:OG	1.90	0.72
1:A:295:ASP:OD2	1:A:304:LYS:HE2	1.89	0.71
1:A:375:PHE:O	1:A:378[B]:ASN:ND2	2.23	0.71
1:B:191:VAL:HA	1:B:242:LEU:HD22	1.73	0.71
1:B:189:ARG:O	1:B:242:LEU:HA	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:HE21	1:A:46:GLN:N	1.88	0.70
1:B:46:GLN:HE21	1:B:46:GLN:N	1.89	0.70
1:B:291:ASN:CB	1:B:308:ASP:HA	2.24	0.68
1:A:104:MET:HB2	1:A:105:PRO:HD3	1.76	0.67
1:B:382:ILE:O	1:B:382:ILE:HG13	1.95	0.67
1:A:378[B]:ASN:ND2	1:A:385:LEU:HD23	2.09	0.67
1:B:145:GLN:NE2	1:B:389:PHE:H	1.93	0.66
1:A:301[B]:ARG:HD3	1:A:319:LEU:HD11	1.77	0.66
1:B:104:MET:HB2	1:B:105:PRO:HD3	1.77	0.66
1:B:378:ASN:ND2	1:B:385:LEU:HD11	2.10	0.66
1:B:291:ASN:HB2	1:B:308:ASP:HA	1.78	0.65
1:A:363:GLY:O	1:A:367:ARG:HG3	1.95	0.65
1:B:136:TYR:CZ	1:B:403:MET:HE2	2.33	0.64
1:A:137:LYS:O	1:A:141:GLU:HG2	1.98	0.63
1:B:381:LYS:O	1:B:383:PRO:HD3	1.97	0.63
1:A:433:TYR:HB2	2:A:542:HOH:O	1.99	0.62
1:A:145:GLN:HE22	1:A:389:PHE:H	1.49	0.61
1:B:343:TYR:N	1:B:343:TYR:CD2	2.67	0.61
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.36	0.61
1:A:60:SER:O	1:A:64:ILE:HG13	2.01	0.60
1:A:136:TYR:CZ	1:A:403:MET:HE2	2.36	0.60
1:A:153:ARG:HD2	1:A:400:PRO:HG3	1.83	0.60
1:B:60:SER:O	1:B:64:ILE:HG13	2.02	0.59
1:B:133:GLU:HG3	1:B:406:LEU:HD11	1.83	0.59
1:B:137:LYS:O	1:B:141:GLU:HG2	2.01	0.59
1:B:153:ARG:HD2	1:B:400:PRO:HG3	1.83	0.59
1:B:189:ARG:HD3	1:B:198:TYR:CE1	2.37	0.59
1:A:181[B]:ASN:HD21	1:A:282:GLY:C	2.11	0.59
1:B:123:TRP:CD2	1:B:124:ALA:HA	2.38	0.59
1:A:263:LEU:HD22	1:B:276:SER:HB2	1.84	0.59
1:B:155:SER:HB3	1:B:158:ILE:HG12	1.85	0.58
1:A:90:ILE:HD13	1:A:106:LEU:HD21	1.84	0.58
1:B:107:LEU:O	1:B:110:SER:HB3	2.04	0.57
1:B:292:LEU:HD12	1:B:314:ILE:CD1	2.34	0.57
1:A:291:ASN:HB2	1:A:308:ASP:OD2	2.04	0.57
1:A:261:HIS:HD2	2:B:470:HOH:O	1.87	0.57
1:A:155:SER:HB3	1:A:158:ILE:HG12	1.85	0.57
1:A:196:TYR:CE1	1:A:197:ILE:HG22	2.40	0.56
1:B:145:GLN:NE2	1:B:388:GLN:HG3	2.21	0.56
1:B:37:TYR:HB3	1:B:38:PRO:HD3	1.88	0.56
2:A:505:HOH:O	1:B:261:HIS:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD12	1:A:386:PRO:CD	2.35	0.55
1:B:145:GLN:HE21	1:B:388:GLN:HA	1.72	0.55
1:B:89:MET:HE1	1:B:372:ILE:HG21	1.88	0.55
1:A:107:LEU:O	1:A:110:SER:HB3	2.08	0.54
1:A:410:ARG:NH1	2:A:542:HOH:O	2.40	0.54
1:B:90:ILE:HD13	1:B:106:LEU:HD21	1.89	0.54
1:A:37:TYR:HB3	1:A:38:PRO:HD3	1.91	0.53
1:A:284:PRO:HB2	1:A:289:THR:OG1	2.09	0.53
1:A:348:GLU:OE1	1:B:287:LYS:HB3	2.08	0.53
1:B:169:TYR:CE2	1:B:319:LEU:HD13	2.44	0.52
1:B:291:ASN:HB3	1:B:308:ASP:HA	1.89	0.52
1:A:181[B]:ASN:OD1	1:A:282:GLY:O	2.28	0.52
1:A:133:GLU:HG3	1:A:406:LEU:HD11	1.91	0.52
1:B:164:LEU:CD1	1:B:319:LEU:HD11	2.26	0.51
1:B:277[A]:CYS:SG	1:B:279:PHE:CE2	3.04	0.51
1:A:305:LEU:HB3	1:A:314:ILE:CD1	2.41	0.51
1:B:19:ARG:NH1	1:B:86:THR:HA	2.26	0.51
1:B:177:GLU:OE1	1:B:297:HIS:NE2	2.37	0.51
1:B:22:PHE:CD1	1:B:25:LEU:HB2	2.46	0.50
1:A:277[A]:CYS:SG	1:A:279:PHE:CE2	3.04	0.50
1:A:378[B]:ASN:ND2	1:A:385:LEU:CD2	2.74	0.50
1:A:420:MET:HE2	1:A:421:MET:HG3	1.93	0.49
1:A:76:PRO:HD2	1:A:80:SER:OG	2.12	0.49
1:B:292:LEU:HD12	1:B:314:ILE:HD11	1.94	0.49
1:B:76:PRO:HD2	1:B:80:SER:OG	2.12	0.49
1:B:244:ASP:HB3	1:B:250:LEU:HD21	1.95	0.49
1:A:22:PHE:CD1	1:A:25:LEU:HB2	2.47	0.49
1:A:292:LEU:C	1:A:292:LEU:HD13	2.39	0.47
1:A:46:GLN:HG2	1:A:373:SER:OG	2.14	0.47
1:A:115:ASN:O	1:A:117:LYS:HG2	2.14	0.47
1:A:356:ARG:HA	1:A:357:ASN:HA	1.44	0.47
1:B:115:ASN:O	1:B:117:LYS:HG2	2.13	0.47
1:B:192:LYS:HG2	1:B:192:LYS:O	2.15	0.47
1:B:292:LEU:C	1:B:292:LEU:HD13	2.39	0.47
1:B:151:GLN:HG3	1:B:365:ILE:CD1	2.43	0.47
1:A:244:ASP:HB3	1:A:250:LEU:HD21	1.97	0.46
1:B:26:ASN:HB3	1:B:29:LYS:O	2.15	0.46
1:B:193:SER:HA	1:B:194:PRO:HD3	1.82	0.46
1:A:18:ILE:HD11	1:A:376:HIS:CD2	2.50	0.46
1:B:178:ILE:HD11	1:B:218:LEU:HD22	1.97	0.46
1:A:92:ILE:HG23	1:A:94:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:HA	1:A:69:LEU:HD12	1.98	0.46
1:A:26:ASN:HB3	1:A:29:LYS:O	2.16	0.46
1:A:145:GLN:NE2	1:A:388:GLN:HB2	2.31	0.46
1:B:373:SER:O	1:B:377:PHE:N	2.46	0.45
1:B:75:PHE:HA	1:B:76:PRO:HD3	1.79	0.45
1:B:92:ILE:HG23	1:B:94:ILE:HG12	1.99	0.45
1:B:356:ARG:O	1:B:357:ASN:HB2	2.16	0.45
1:B:194:PRO:HB2	1:B:197:ILE:HG13	1.97	0.45
1:A:377:PHE:O	1:A:378[A]:ASN:C	2.59	0.45
1:A:435:LEU:HD23	2:A:542:HOH:O	2.16	0.45
1:A:384:GLU:O	1:A:385:LEU:C	2.58	0.45
1:B:64:ILE:HA	1:B:69:LEU:HD12	1.99	0.45
1:A:75:PHE:CE2	1:A:84:SER:HB2	2.52	0.44
1:A:153:ARG:HD3	1:A:392:GLN:OE1	2.17	0.44
1:A:169:TYR:O	1:A:301[B]:ARG:HD2	2.16	0.44
1:B:191:VAL:HB	1:B:250:LEU:CD1	2.47	0.44
1:A:75:PHE:HA	1:A:76:PRO:HD3	1.78	0.44
1:A:90:ILE:HG22	1:A:92:ILE:HD12	2.00	0.44
1:A:159:LEU:O	1:A:163:GLU:HG3	2.17	0.44
1:B:145:GLN:NE2	1:B:388:GLN:HA	2.32	0.43
1:A:420:MET:HE2	1:A:421:MET:CG	2.48	0.43
1:A:276:SER:HB2	1:B:263:LEU:HD22	2.00	0.43
1:B:18:ILE:HD11	1:B:376:HIS:CD2	2.54	0.43
1:B:407:ILE:HG12	1:B:431:SER:HA	2.01	0.43
1:A:64:ILE:HG23	1:A:69:LEU:HB2	2.01	0.42
1:A:305:LEU:CD2	1:A:317:LEU:HD13	2.49	0.42
1:B:16:ALA:HB3	1:B:17:PRO:HD3	2.01	0.42
1:B:33:ILE:HG23	1:B:34:LYS:HG3	2.01	0.42
1:B:277[A]:CYS:SG	1:B:279:PHE:HE2	2.43	0.42
1:A:375:PHE:CD2	1:A:375:PHE:C	2.98	0.42
1:A:92:ILE:HD13	1:A:119:LEU:HD11	2.01	0.42
1:B:90:ILE:HG22	1:B:92:ILE:HD12	2.01	0.42
1:B:75:PHE:CE2	1:B:84:SER:HB2	2.55	0.42
1:B:292:LEU:CD1	1:B:314:ILE:HD11	2.50	0.42
1:B:378:ASN:HD21	1:B:385:LEU:HD11	1.83	0.42
1:A:170:ILE:CG2	1:A:298:GLY:HA3	2.50	0.42
1:B:82:ALA:HB3	1:B:109:PHE:HB2	2.01	0.42
1:A:277[A]:CYS:SG	1:A:279:PHE:HE2	2.43	0.42
1:A:82:ALA:HB3	1:A:109:PHE:HB2	2.02	0.42
1:A:377:PHE:O	1:A:378[B]:ASN:C	2.60	0.42
1:B:97:ALA:HA	1:B:127:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:THR:HA	1:B:273:VAL:O	2.21	0.41
1:B:277[A]:CYS:SG	1:B:279:PHE:CD2	3.14	0.41
1:B:139:ALA:O	1:B:142:ARG:HB3	2.20	0.41
1:A:78:LEU:HD11	1:A:106:LEU:HD12	2.03	0.41
1:B:64:ILE:HG23	1:B:69:LEU:HB2	2.02	0.41
1:B:305:LEU:HD22	1:B:314:ILE:HG21	2.02	0.41
1:B:78:LEU:HD11	1:B:106:LEU:HD12	2.02	0.41
1:B:361:ILE:O	1:B:365:ILE:HD13	2.20	0.41
1:A:139:ALA:O	1:A:142:ARG:HB3	2.21	0.41
1:B:123:TRP:CG	1:B:124:ALA:HA	2.55	0.41
1:B:169:TYR:HE2	1:B:319:LEU:HD13	1.83	0.41
1:B:145:GLN:HE22	1:B:389:PHE:N	2.00	0.40
1:A:97:ALA:HA	1:A:127:CYS:SG	2.60	0.40
1:A:158:ILE:CD1	1:A:217:ILE:HD12	2.51	0.40
1:B:154:LYS:HA	1:B:154:LYS:HD3	1.94	0.40
1:B:373:SER:HA	1:B:376:HIS:HB3	2.03	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	386/438 (88%)	366 (95%)	19 (5%)	1 (0%)	36	36
1	B	385/438 (88%)	367 (95%)	18 (5%)	0	100	100
All	All	771/876 (88%)	733 (95%)	37 (5%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	PRO

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	343/376 (91%)	325 (95%)	18 (5%)	21	20
1	B	341/376 (91%)	329 (96%)	12 (4%)	32	35
All	All	684/752 (91%)	654 (96%)	30 (4%)	25	26

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	59	THR
1	A	160	ARG
1	A	170	ILE
1	A	197	ILE
1	A	199	GLU
1	A	200	ILE
1	A	260	ASP
1	A	283	LYS
1	A	289	THR
1	A	293	VAL
1	A	362	VAL
1	A	373	SER
1	A	375	PHE
1	A	380	LYS
1	A	390	VAL
1	A	402	LEU
1	A	425	LEU
1	B	46	GLN
1	B	59	THR
1	B	200	ILE
1	B	260	ASP
1	B	289	THR
1	B	293	VAL
1	B	343	TYR
1	B	349	ILE
1	B	385	LEU

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Mol	Chain	Res	Type
1	B	397	GLU
1	B	402	LEU
1	B	420	MET

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

Mol	Chain	Res	Type
1	A	46	GLN
1	A	71	ASN
1	A	95	GLN
1	A	112	ASN
1	A	145	GLN
1	A	202	ASN
1	A	230	ASN
1	A	261	HIS
1	A	265	GLN
1	A	291	ASN
1	A	388	GLN
1	B	46	GLN
1	B	71	ASN
1	B	95	GLN
1	B	112	ASN
1	B	145	GLN
1	B	174	ASN
1	B	181	ASN
1	B	202	ASN
1	B	230	ASN
1	B	261	HIS
1	B	265	GLN
1	B	366	HIS
1	B	370	GLN
1	B	378	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	390/438 (89%)	1.22	95 (24%) 2 2	16, 53, 107, 136	4 (1%)
1	B	392/438 (89%)	1.53	127 (32%) 1 1	18, 67, 117, 157	1 (0%)
All	All	782/876 (89%)	1.38	222 (28%) 1 1	16, 59, 112, 157	5 (0%)

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	GLY	6.5
1	A	380	LYS	6.3
1	B	75	PHE	6.2
1	B	52	LEU	6.1
1	A	250	LEU	5.8
1	A	31	TRP	5.7
1	A	435	LEU	5.5
1	B	57	ILE	5.4
1	B	74	ALA	5.2
1	A	289	THR	5.2
1	A	386	PRO	5.1
1	B	250	LEU	4.9
1	A	248	ASN	4.8
1	B	184	TRP	4.8
1	A	40	ILE	4.7
1	B	243	ILE	4.7
1	A	200	ILE	4.6
1	B	433	TYR	4.4
1	A	323	GLY	4.4
1	A	109	PHE	4.3
1	A	75	PHE	4.2
1	B	51	ALA	4.2
1	A	375	PHE	4.2
1	B	247	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	53	TYR	4.2
1	A	385	LEU	4.1
1	B	60	SER	4.1
1	B	386	PRO	4.0
1	A	389	PHE	4.0
1	B	102	VAL	4.0
1	B	288	PHE	4.0
1	B	22	PHE	3.9
1	B	196	TYR	3.9
1	B	53	TYR	3.9
1	A	52	LEU	3.9
1	B	254	VAL	3.9
1	B	76	PRO	3.9
1	A	83	SER	3.8
1	B	191	VAL	3.8
1	B	197	ILE	3.8
1	A	383	PRO	3.7
1	B	16	ALA	3.7
1	A	57	ILE	3.7
1	B	81	PHE	3.6
1	B	82	ALA	3.6
1	B	282	GLY	3.6
1	B	59	THR	3.5
1	B	23	VAL	3.5
1	B	126	ALA	3.5
1	A	379	THR	3.5
1	A	314	ILE	3.4
1	A	84	SER	3.4
1	A	285	THR	3.4
1	B	144	VAL	3.4
1	B	64	ILE	3.4
1	B	87	ILE	3.4
1	B	69	LEU	3.4
1	A	169	TYR	3.4
1	B	343	TYR	3.4
1	A	384	GLU	3.4
1	B	387	SER	3.3
1	B	61	ILE	3.3
1	A	16	ALA	3.3
1	A	85	SER	3.3
1	B	116	LEU	3.2
1	B	313	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	377	PHE	3.2
1	B	31	TRP	3.1
1	A	381	LYS	3.1
1	A	114	PRO	3.1
1	B	78	LEU	3.1
1	B	54	SER	3.1
1	B	342	GLY	3.1
1	B	72	ALA	3.1
1	A	69	LEU	3.1
1	A	64	ILE	3.1
1	A	45	SER	3.1
1	A	307	GLY	3.1
1	A	112	ASN	3.1
1	B	20	VAL	3.1
1	B	100	TYR	3.0
1	B	375	PHE	3.0
1	B	133	GLU	3.0
1	A	118	TYR	3.0
1	B	281	GLY	3.0
1	B	182	GLY	3.0
1	A	111	LYS	3.0
1	A	243	ILE	2.9
1	A	388	GLN	2.9
1	B	356	ARG	2.9
1	A	141	GLU	2.9
1	A	51	ALA	2.9
1	B	291	ASN	2.9
1	B	55	PRO	2.9
1	A	87	ILE	2.9
1	A	378[A]	ASN	2.9
1	B	103	VAL	2.8
1	B	94	ILE	2.8
1	B	287	LYS	2.8
1	A	74	ALA	2.8
1	A	82	ALA	2.8
1	B	132	ALA	2.8
1	B	345	ALA	2.8
1	A	170	ILE	2.8
1	A	387	SER	2.8
1	A	374	ASP	2.8
1	A	59	THR	2.8
1	B	90	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	320	TYR	2.7
1	B	67	LEU	2.7
1	B	105	PRO	2.7
1	B	137	LYS	2.7
1	A	140	ALA	2.7
1	A	397	GLU	2.7
1	B	49	ILE	2.7
1	A	247	GLY	2.7
1	A	78	LEU	2.6
1	B	255	PRO	2.6
1	B	397	GLU	2.6
1	B	181	ASN	2.6
1	A	105	PRO	2.6
1	B	111	LYS	2.6
1	A	321	TYR	2.6
1	B	420	MET	2.6
1	A	291	ASN	2.6
1	A	62	ALA	2.6
1	B	209	THR	2.6
1	A	137	LYS	2.6
1	B	129	LEU	2.6
1	B	85	SER	2.6
1	B	146	THR	2.6
1	B	88	ASP	2.6
1	B	244	ASP	2.6
1	A	68	LYS	2.5
1	B	347	LYS	2.5
1	A	88	ASP	2.5
1	A	284	PRO	2.5
1	B	118	TYR	2.5
1	B	77	THR	2.5
1	A	360	ALA	2.5
1	B	421	MET	2.5
1	A	316	ASN	2.5
1	A	308	ASP	2.5
1	B	406	LEU	2.5
1	B	104	MET	2.5
1	B	120	PHE	2.5
1	B	357	ASN	2.5
1	B	136	TYR	2.4
1	B	83	SER	2.4
1	B	190	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	25	LEU	2.4
1	B	249	ARG	2.4
1	B	432	HIS	2.4
1	A	382	ILE	2.4
1	B	258	VAL	2.4
1	A	70	SER	2.4
1	B	169	TYR	2.4
1	B	289	THR	2.4
1	B	416	TYR	2.4
1	B	62	ALA	2.4
1	B	143	GLY	2.4
1	A	130	ASP	2.4
1	B	239	GLU	2.3
1	B	253	ARG	2.3
1	A	322	SER	2.3
1	B	45	SER	2.3
1	B	92	ILE	2.3
1	B	314	ILE	2.3
1	B	127	CYS	2.3
1	A	353	TYR	2.3
1	A	43	LEU	2.3
1	B	107	LEU	2.3
1	B	242	LEU	2.3
1	B	47	PHE	2.3
1	A	390	VAL	2.3
1	B	194	PRO	2.3
1	B	97	ALA	2.3
1	A	117	LYS	2.3
1	A	434	SER	2.3
1	A	116	LEU	2.3
1	A	433	TYR	2.3
1	B	17	PRO	2.2
1	B	63	THR	2.2
1	B	138	ALA	2.2
1	B	139	ALA	2.2
1	A	113	ASN	2.2
1	A	115	ASN	2.2
1	B	200	ILE	2.2
1	B	96	VAL	2.2
1	A	72	ALA	2.2
1	A	373	SER	2.2
1	B	50	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	286	LYS	2.2
1	B	71	ASN	2.2
1	B	361	ILE	2.1
1	A	370	GLN	2.1
1	B	240	GLN	2.1
1	B	140	ALA	2.1
1	A	37	TYR	2.1
1	A	376	HIS	2.1
1	B	235	ASN	2.1
1	B	241	GLU	2.1
1	B	86	THR	2.1
1	B	135	ILE	2.1
1	A	246	ARG	2.1
1	B	198	TYR	2.1
1	A	92	ILE	2.1
1	A	81	PHE	2.1
1	A	144	VAL	2.1
1	A	106	LEU	2.0
1	B	125	LEU	2.0
1	B	402	LEU	2.0
1	B	112	ASN	2.0
1	B	248	ASN	2.0
1	A	29	LYS	2.0
1	B	37	TYR	2.0
1	A	22	PHE	2.0
1	B	89	MET	2.0
1	A	184	TRP	2.0
1	A	357	ASN	2.0
1	A	67	LEU	2.0
1	B	183	GLY	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 ⓘ

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.