



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:09 AM UTC

PDB ID : 4B8B / pdb_00004b8b
Title : N-Terminal domain of the yeast Not1
Authors : Basquin, J.; Conti, E.
Deposited on : 2012-08-26
Resolution : 2.80 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

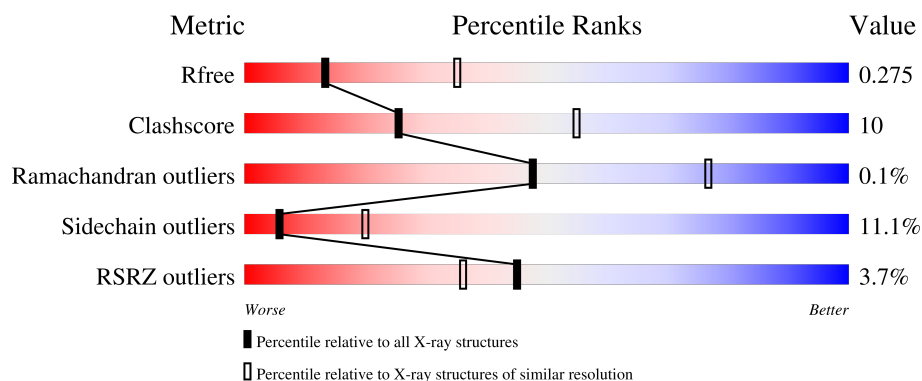
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	603	 3% 62% 23% 12%
1	B	603	 3% 61% 23% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8410 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 GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	0	0
			4179	2705	680	776	18			
1	B	529	Total	C	N	O	S	0	0	0
			4202	2716	687	781	18			

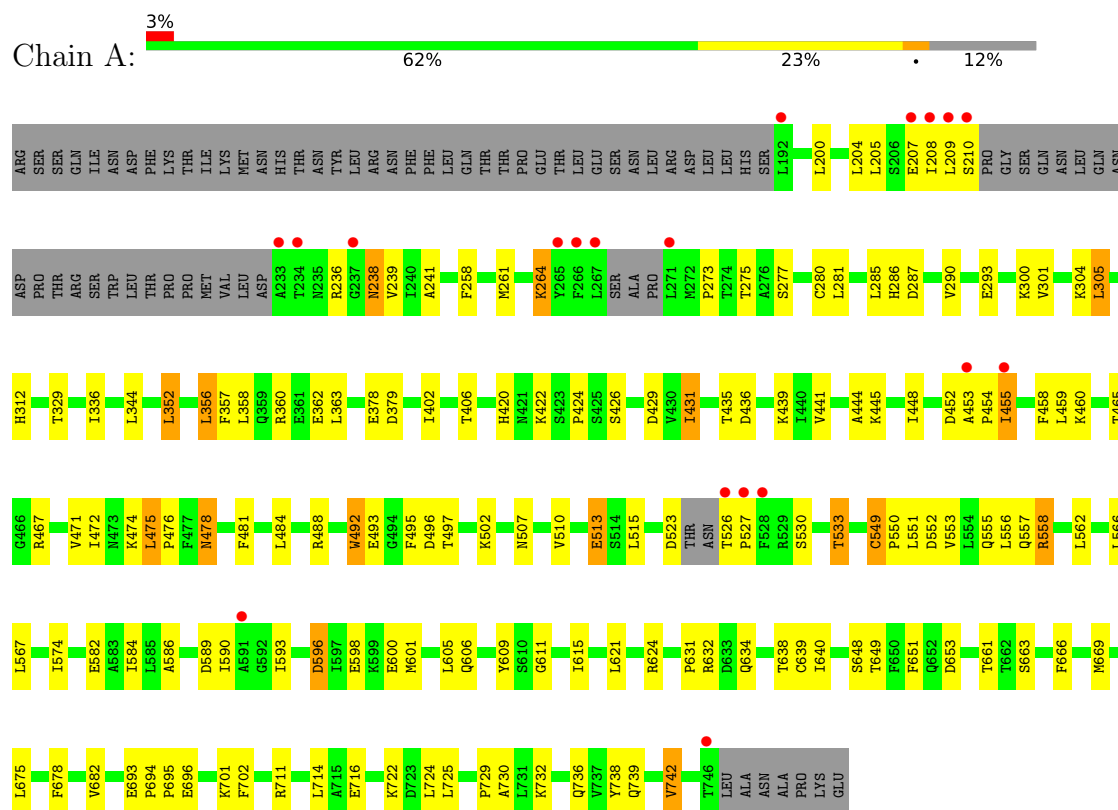
- Molecule 2 is GOLD ION (CCD ID: AU) (formula: Au).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	Au	0	0
			15	15		
2	B	14	Total	Au	0	0
			14	14		

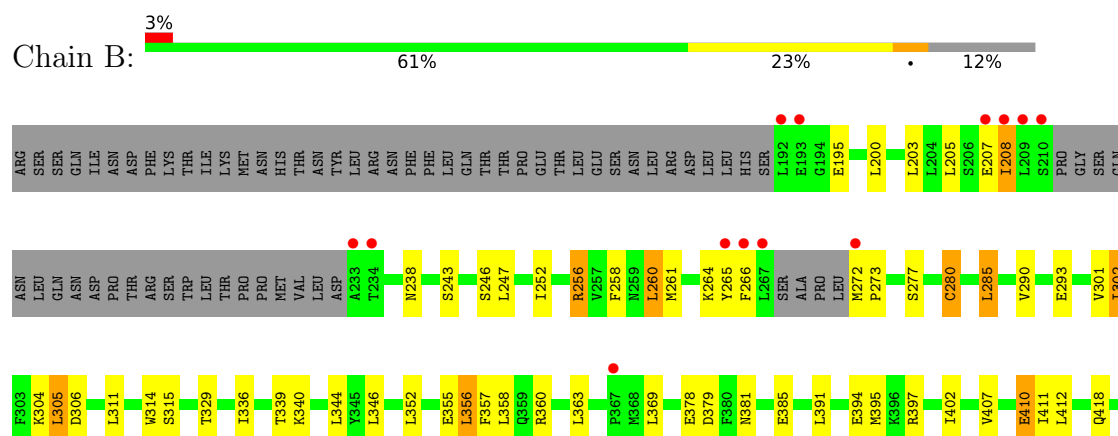
3 Residue-property plots

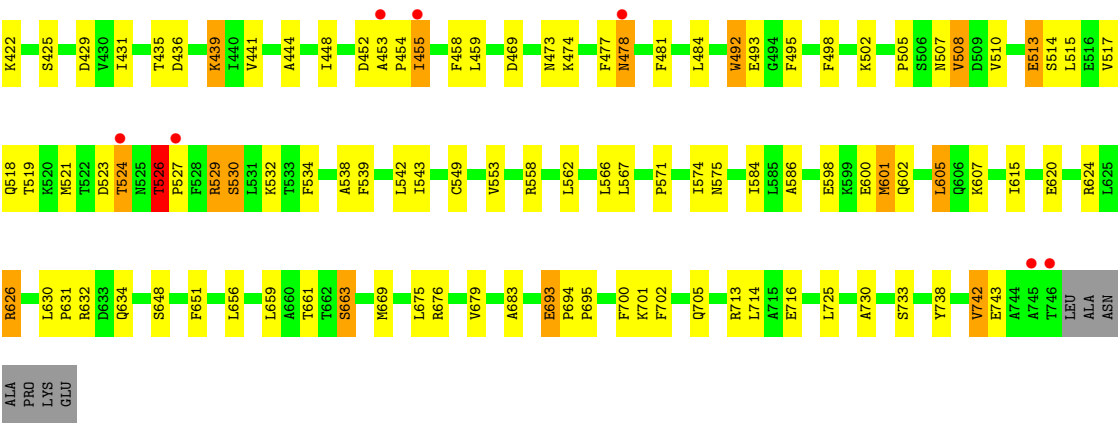
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1



• Molecule 1: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.10Å 164.51Å 86.14Å 90.00° 100.05° 90.00°	Depositor
Resolution (Å)	46.05 – 2.80 46.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.05-2.80) 99.8 (46.05-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.238 , 0.276 0.237 , 0.275	Depositor DCC
R_{free} test set	1855 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8410	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
AU

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	0.59	0/4257	1.00	7/5768 (0.1%)
1	B	0.56	0/4281	0.98	10/5800 (0.2%)
All	All	0.58	0/8538	0.99	17/11568 (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	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	526	THR	CA-C-N	11.73	134.50	119.84
1	A	526	THR	C-N-CA	11.73	134.50	119.84
1	B	530	SER	N-CA-C	-7.55	102.41	111.69
1	B	395	MET	N-CA-C	7.20	120.05	111.33
1	B	495	PHE	N-CA-C	6.33	117.84	111.07
1	B	492	TRP	N-CA-C	6.29	118.66	111.11
1	B	526	THR	CA-C-N	6.20	126.39	119.32
1	B	526	THR	C-N-CA	6.20	126.39	119.32
1	B	493	GLU	N-CA-C	6.05	119.89	111.90
1	B	507	ASN	N-CA-C	6.03	120.77	113.17
1	A	452	ASP	N-CA-C	-5.91	102.72	110.53
1	B	452	ASP	N-CA-C	-5.90	102.74	110.53
1	A	492	TRP	N-CA-C	5.63	117.86	111.11
1	A	574	ILE	N-CA-C	5.62	115.75	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	TYR	CA-C-N	-5.49	114.61	123.23
1	A	609	TYR	C-N-CA	-5.49	114.61	123.23
1	B	381	ASN	N-CA-C	5.07	117.92	111.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	LYS	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	4179	0	4197	76	0
1	B	4202	0	4235	89	0
2	A	15	0	0	0	0
2	B	14	0	0	0	0
All	All	8410	0	8432	162	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 10.

All (162) 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:575:ASN:ND2	1:B:634:GLN:OE1	2.10	0.83
1:A:533:THR:HG21	1:A:590:ILE:HD13	1.60	0.83
1:A:455:ILE:HG23	1:A:458:PHE:HB3	1.66	0.76
1:B:478:ASN:HB2	1:B:510:VAL:HG11	1.71	0.71
1:B:336:ILE:HD11	1:B:429:ASP:HB3	1.73	0.70
1:A:357:PHE:O	1:A:360:ARG:HG3	1.93	0.69
1:A:208:ILE:HG23	1:A:273:PRO:HG3	1.77	0.65
1:A:600:GLU:OE1	1:A:632:ARG:NH2	2.29	0.65
1:B:205:LEU:HD11	1:B:266:PHE:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:ARG:HG3	1:B:676:ARG:HH21	1.62	0.65
1:A:286:HIS:ND1	1:A:287:ASP:OD1	2.29	0.65
1:B:357:PHE:O	1:B:360:ARG:HG3	1.96	0.64
1:A:693:GLU:HG3	1:A:694:PRO:HD2	1.80	0.63
1:A:562:LEU:O	1:A:566:LEU:HB2	1.98	0.62
1:B:513:GLU:HG2	1:B:558:ARG:HH22	1.63	0.62
1:B:455:ILE:HG23	1:B:458:PHE:HB3	1.82	0.62
1:B:304:LYS:NZ	1:B:355:GLU:OE2	2.33	0.61
1:B:701:LYS:O	1:B:705:GLN:HG3	2.00	0.61
1:B:340:LYS:NZ	1:B:385:GLU:OE2	2.32	0.61
1:B:669:MET:HB3	1:B:675:LEU:HD13	1.82	0.60
1:B:410:GLU:HG3	1:B:411:ILE:HD13	1.83	0.60
1:B:258:PHE:HA	1:B:261:MET:HE3	1.84	0.60
1:A:357:PHE:CE1	1:A:360:ARG:HD3	2.37	0.59
1:A:527:PRO:HB2	1:B:524:THR:HA	1.83	0.59
1:B:444:ALA:O	1:B:448:ILE:HG12	2.02	0.59
1:A:653:ASP:HA	1:B:378:GLU:HG2	1.85	0.58
1:A:513:GLU:HG2	1:A:558:ARG:HH22	1.69	0.58
1:B:693:GLU:HG3	1:B:694:PRO:HD2	1.85	0.58
1:A:441:VAL:HG22	1:A:471:VAL:HG22	1.85	0.57
1:A:472:ILE:HD13	1:A:492:TRP:CE2	2.39	0.57
1:A:475:LEU:HD23	1:A:476:PRO:HD2	1.87	0.57
1:B:344:LEU:HD11	1:B:379:ASP:HB3	1.87	0.56
1:B:272:MET:HE3	1:B:306:ASP:HB2	1.87	0.56
1:B:586:ALA:HB3	1:B:631:PRO:HB3	1.88	0.56
1:A:621:LEU:HA	1:A:624:ARG:HH21	1.70	0.55
1:B:601:MET:HE3	1:B:605:LEU:HD22	1.88	0.55
1:A:336:ILE:HD11	1:A:429:ASP:HB3	1.89	0.55
1:B:659:LEU:HD23	1:B:701:LYS:HZ2	1.72	0.55
1:B:394:GLU:OE1	1:B:397:ARG:HD3	2.06	0.54
1:B:562:LEU:O	1:B:566:LEU:HB2	2.08	0.54
1:A:305:LEU:HD13	1:A:356:LEU:HG	1.89	0.54
1:B:247:LEU:HD13	1:B:252:ILE:HD11	1.90	0.54
1:B:441:VAL:HG21	1:B:474:LYS:HE3	1.91	0.52
1:B:675:LEU:HD23	1:B:683:ALA:HB2	1.91	0.52
1:B:256:ARG:HD2	1:B:260:LEU:HD22	1.92	0.52
1:B:243:SER:O	1:B:246:SER:HB3	2.10	0.52
1:B:626:ARG:HG3	1:B:676:ARG:NH2	2.23	0.52
1:B:527:PRO:HG2	1:B:532:LYS:NZ	2.25	0.52
1:A:601:MET:HE2	1:A:639:CYS:SG	2.50	0.51
1:B:481:PHE:HA	1:B:484:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:GLU:OE1	1:B:397:ARG:NH1	2.44	0.51
1:A:358:LEU:HB3	1:A:402:ILE:HD11	1.94	0.50
1:A:584:ILE:HG12	1:A:634:GLN:HG2	1.93	0.50
1:A:553:VAL:O	1:A:557:GLN:HG2	2.11	0.50
1:B:663:SER:HA	1:B:702:PHE:CE1	2.45	0.50
1:A:453:ALA:HB1	1:A:454:PRO:HA	1.93	0.50
1:A:472:ILE:HG21	1:A:492:TRP:CZ2	2.47	0.50
1:B:407:VAL:O	1:B:411:ILE:HG12	2.11	0.50
1:A:484:LEU:HD22	1:A:492:TRP:CZ3	2.47	0.49
1:A:444:ALA:O	1:A:448:ILE:HG12	2.12	0.49
1:A:481:PHE:HA	1:A:484:LEU:HG	1.93	0.49
1:B:208:ILE:HG23	1:B:273:PRO:HG3	1.93	0.49
1:B:521:MET:HG2	1:B:526:THR:HG21	1.94	0.49
1:A:533:THR:CG2	1:A:590:ILE:HD13	2.38	0.49
1:A:584:ILE:HG12	1:A:634:GLN:CG	2.42	0.49
1:A:601:MET:HG3	1:A:639:CYS:SG	2.53	0.48
1:B:484:LEU:HD22	1:B:492:TRP:CZ3	2.49	0.48
1:B:469:ASP:O	1:B:473:ASN:ND2	2.45	0.48
1:B:534:PHE:HB3	1:B:538:ALA:HB3	1.96	0.48
1:A:460:LYS:HE3	1:A:460:LYS:HB2	1.69	0.47
1:B:738:TYR:O	1:B:742:VAL:HG13	2.14	0.47
1:B:305:LEU:HD13	1:B:356:LEU:HG	1.97	0.47
1:B:567:LEU:CD1	1:B:574:ILE:HG12	2.45	0.47
1:A:238:ASN:HA	1:A:241:ALA:HB3	1.96	0.47
1:A:615:ILE:HD11	1:A:661:THR:HG23	1.96	0.47
1:B:517:VAL:HG12	1:B:521:MET:HE3	1.95	0.47
1:B:453:ALA:HB1	1:B:454:PRO:HA	1.96	0.47
1:A:488:ARG:HH11	1:A:495:PHE:HB3	1.79	0.47
1:B:527:PRO:HG2	1:B:532:LYS:HZ1	1.79	0.47
1:A:441:VAL:HG21	1:A:474:LYS:HE3	1.97	0.46
1:A:358:LEU:HD13	1:A:402:ILE:HD11	1.96	0.46
1:B:515:LEU:O	1:B:519:THR:HG23	2.16	0.46
1:A:301:VAL:HG11	1:A:363:LEU:HD22	1.98	0.46
1:B:513:GLU:HG2	1:B:558:ARG:NH2	2.30	0.46
1:A:663:SER:HA	1:A:702:PHE:CE1	2.51	0.46
1:A:711:ARG:HA	1:A:714:LEU:HG	1.98	0.46
1:B:412:LEU:HD23	1:B:439:LYS:HG2	1.97	0.46
1:B:529:ARG:HA	1:B:532:LYS:HB2	1.98	0.46
1:A:502:LYS:O	1:A:507:ASN:ND2	2.41	0.46
1:B:648:SER:HA	1:B:651:PHE:CZ	2.51	0.45
1:B:391:LEU:HD23	1:B:412:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:LYS:HB2	1:B:607:LYS:HE2	1.61	0.45
1:A:598:GLU:O	1:A:601:MET:HE3	2.17	0.45
1:B:571:PRO:O	1:B:574:ILE:HG13	2.17	0.45
1:B:620:GLU:O	1:B:624:ARG:HD3	2.16	0.45
1:B:418:GLN:HE22	1:B:422:LYS:HE3	1.81	0.44
1:A:431:ILE:HG22	1:A:465:THR:HG21	1.99	0.44
1:A:344:LEU:HD11	1:A:379:ASP:HB3	2.00	0.44
1:A:527:PRO:CB	1:B:524:THR:HA	2.48	0.44
1:A:208:ILE:HD11	1:A:281:LEU:HD13	1.99	0.44
1:B:600:GLU:OE1	1:B:632:ARG:NH2	2.45	0.44
1:A:436:ASP:HB3	1:A:439:LYS:HD2	2.00	0.44
1:A:478:ASN:HB2	1:A:510:VAL:HG21	2.00	0.44
1:B:477:PHE:O	1:B:478:ASN:HB3	2.18	0.44
1:B:615:ILE:HD11	1:B:661:THR:HG23	2.00	0.44
1:B:505:PRO:HA	1:B:508:VAL:HG22	2.00	0.43
1:A:207:GLU:O	1:A:277:SER:HB2	2.18	0.43
1:A:551:LEU:HD22	1:A:555:GLN:HB3	2.01	0.43
1:A:552:ASP:HB3	1:A:555:GLN:HG3	2.00	0.43
1:B:203:LEU:O	1:B:207:GLU:HB2	2.19	0.43
1:B:695:PRO:HA	1:B:700:PHE:CG	2.52	0.43
1:A:695:PRO:HG3	1:A:730:ALA:HB1	2.00	0.43
1:A:695:PRO:O	1:A:696:GLU:HB3	2.18	0.43
1:B:301:VAL:HG11	1:B:363:LEU:HD22	1.99	0.43
1:B:584:ILE:HG12	1:B:634:GLN:CG	2.49	0.43
1:A:666:PHE:O	1:A:669:MET:HB2	2.19	0.43
1:B:256:ARG:O	1:B:260:LEU:HB2	2.18	0.43
1:B:656:LEU:HD22	1:B:701:LYS:HE3	2.01	0.43
1:A:596:ASP:OD1	1:A:596:ASP:N	2.41	0.43
1:B:502:LYS:HD3	1:B:502:LYS:HA	1.89	0.43
1:B:207:GLU:OE1	1:B:280:CYS:HB3	2.19	0.43
1:A:420:HIS:O	1:A:424:PRO:HG3	2.19	0.42
1:A:738:TYR:O	1:A:742:VAL:HG13	2.19	0.42
1:B:436:ASP:OD2	1:B:439:LYS:HD3	2.19	0.42
1:B:311:LEU:O	1:B:314:TRP:HB2	2.19	0.42
1:A:549:CYS:HA	1:A:550:PRO:HD3	1.90	0.42
1:A:258:PHE:CE2	1:A:293:GLU:HG3	2.54	0.42
1:B:567:LEU:HD11	1:B:574:ILE:HG12	2.01	0.42
1:A:648:SER:HA	1:A:651:PHE:CE2	2.54	0.42
1:A:290:VAL:O	1:A:293:GLU:HB3	2.19	0.42
1:A:678:PHE:O	1:A:682:VAL:HG23	2.19	0.42
1:B:205:LEU:HD21	1:B:265:TYR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:HIS:NE2	1:A:378:GLU:OE1	2.37	0.42
1:A:648:SER:HA	1:A:651:PHE:CZ	2.55	0.42
1:B:584:ILE:HG12	1:B:634:GLN:HG2	2.00	0.42
1:B:714:LEU:HD23	1:B:714:LEU:HA	1.93	0.42
1:A:204:LEU:HD12	1:A:261:MET:HE1	2.03	0.41
1:B:272:MET:HE1	1:B:302:ILE:HG23	2.02	0.41
1:B:515:LEU:HD21	1:B:542:LEU:HD13	2.02	0.41
1:B:620:GLU:OE2	1:B:624:ARG:NH2	2.44	0.41
1:A:515:LEU:HA	1:A:515:LEU:HD23	1.81	0.41
1:B:285:LEU:HG	1:B:290:VAL:HG12	2.03	0.41
1:B:195:GLU:OE2	1:B:256:ARG:NE	2.50	0.41
1:B:514:SER:O	1:B:518:GLN:HG3	2.20	0.41
1:A:601:MET:HG2	1:A:640:ILE:HG13	2.01	0.41
1:A:724:LEU:HD23	1:A:724:LEU:HA	1.91	0.41
1:A:352:LEU:HD22	1:A:356:LEU:HD22	2.01	0.41
1:B:539:PHE:O	1:B:543:ILE:HG13	2.21	0.41
1:B:695:PRO:HG3	1:B:730:ALA:CB	2.51	0.41
1:B:358:LEU:HB3	1:B:402:ILE:HD11	2.03	0.41
1:A:621:LEU:HA	1:A:624:ARG:NH2	2.36	0.41
1:B:498:PHE:O	1:B:502:LYS:HB2	2.20	0.41
1:A:729:PRO:HA	1:A:732:LYS:HE3	2.03	0.41
1:A:732:LYS:HG2	1:A:738:TYR:CE1	2.56	0.40
1:B:713:ARG:HD2	1:B:716:GLU:OE1	2.22	0.40
1:A:696:GLU:HA	1:A:701:LYS:HE3	2.02	0.40
1:B:574:ILE:HA	1:B:679:VAL:HG21	2.04	0.40
1:B:648:SER:HA	1:B:651:PHE:CE2	2.56	0.40
1:A:478:ASN:HB2	1:A:510:VAL:HG11	2.04	0.40
1:A:586:ALA:HB3	1:A:631:PRO:HB3	2.03	0.40
1:A:694:PRO:HA	1:A:695:PRO:HD3	1.99	0.40
1:A:488:ARG:HH11	1:A:495:PHE:CB	2.35	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	520/603 (86%)	500 (96%)	19 (4%)	1 (0%)	43	72
1	B	523/603 (87%)	501 (96%)	22 (4%)	0	100	100
All	All	1043/1206 (86%)	1001 (96%)	41 (4%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	611	GLY

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	461/544 (85%)	406 (88%)	55 (12%)	5	17
1	B	466/544 (86%)	418 (90%)	48 (10%)	7	23
All	All	927/1088 (85%)	824 (89%)	103 (11%)	6	20

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	LEU
1	A	205	LEU
1	A	209	LEU
1	A	210	SER
1	A	236	ARG
1	A	238	ASN
1	A	239	VAL
1	A	264	LYS
1	A	275	THR
1	A	280	CYS
1	A	285	LEU
1	A	300	LYS

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Mol	Chain	Res	Type
1	A	304	LYS
1	A	305	LEU
1	A	329	THR
1	A	352	LEU
1	A	356	LEU
1	A	362	GLU
1	A	406	THR
1	A	422	LYS
1	A	426	SER
1	A	431	ILE
1	A	435	THR
1	A	445	LYS
1	A	455	ILE
1	A	459	LEU
1	A	467	ARG
1	A	475	LEU
1	A	478	ASN
1	A	493	GLU
1	A	496	ASP
1	A	497	THR
1	A	513	GLU
1	A	523	ASP
1	A	530	SER
1	A	533	THR
1	A	549	CYS
1	A	556	LEU
1	A	558	ARG
1	A	567	LEU
1	A	582	GLU
1	A	589	ASP
1	A	593	ILE
1	A	596	ASP
1	A	605	LEU
1	A	606	GLN
1	A	638	THR
1	A	649	THR
1	A	675	LEU
1	A	716	GLU
1	A	722	LYS
1	A	725	LEU
1	A	736	GLN
1	A	739	GLN

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Mol	Chain	Res	Type
1	A	742	VAL
1	B	200	LEU
1	B	208	ILE
1	B	238	ASN
1	B	256	ARG
1	B	260	LEU
1	B	264	LYS
1	B	277	SER
1	B	280	CYS
1	B	285	LEU
1	B	293	GLU
1	B	302	ILE
1	B	305	LEU
1	B	315	SER
1	B	329	THR
1	B	339	THR
1	B	346	LEU
1	B	352	LEU
1	B	356	LEU
1	B	369	LEU
1	B	410	GLU
1	B	425	SER
1	B	431	ILE
1	B	435	THR
1	B	439	LYS
1	B	455	ILE
1	B	459	LEU
1	B	478	ASN
1	B	508	VAL
1	B	513	GLU
1	B	523	ASP
1	B	524	THR
1	B	526	THR
1	B	529	ARG
1	B	530	SER
1	B	549	CYS
1	B	553	VAL
1	B	598	GLU
1	B	601	MET
1	B	602	GLN
1	B	605	LEU
1	B	626	ARG

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Mol	Chain	Res	Type
1	B	630	LEU
1	B	663	SER
1	B	693	GLU
1	B	725	LEU
1	B	733	SER
1	B	742	VAL
1	B	743	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
1	A	310	GLN
1	A	317	GLN
1	A	736	GLN
1	B	317	GLN
1	B	341	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 29 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	528/603 (87%)	0.19	19 (3%) 46 37	28, 54, 98, 145	0
1	B	529/603 (87%)	0.09	20 (3%) 44 35	35, 54, 102, 169	0
All	All	1057/1206 (87%)	0.14	39 (3%) 45 36	28, 54, 101, 169	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	TYR	6.1
1	B	453	ALA	4.8
1	A	207	GLU	4.7
1	B	209	LEU	4.7
1	A	266	PHE	4.7
1	A	526	THR	4.4
1	A	528	PHE	4.3
1	A	746	THR	4.1
1	B	208	ILE	3.9
1	A	271	LEU	3.9
1	B	746	THR	3.9
1	B	527	PRO	3.8
1	B	210	SER	3.8
1	A	210	SER	3.7
1	B	267	LEU	3.7
1	B	745	ALA	3.7
1	A	233	ALA	3.5
1	A	265	TYR	3.5
1	A	237	GLY	3.4
1	A	453	ALA	3.3
1	A	267	LEU	3.2
1	A	192	LEU	3.2
1	B	266	PHE	3.2
1	B	192	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	209	LEU	3.0
1	B	233	ALA	2.9
1	B	234	THR	2.9
1	B	367	PRO	2.9
1	A	591	ALA	2.8
1	B	524	THR	2.6
1	B	207	GLU	2.6
1	A	208	ILE	2.5
1	A	455	ILE	2.5
1	A	234	THR	2.4
1	A	527	PRO	2.3
1	B	455	ILE	2.2
1	B	478	ASN	2.1
1	B	272	MET	2.1
1	B	193	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AU	B	1801	1/1	0.23	0.12	180,180,180,180	1
2	AU	B	1754	1/1	0.34	0.22	120,120,120,120	1
2	AU	B	1800	1/1	0.42	0.26	543,543,543,543	0
2	AU	B	1751	1/1	0.55	0.35	156,156,156,156	1
2	AU	A	1801	1/1	0.67	0.18	127,127,127,127	1
2	AU	A	1750	1/1	0.68	0.14	100,100,100,100	1
2	AU	B	1756	1/1	0.68	0.26	154,154,154,154	1
2	AU	A	1802	1/1	0.68	0.26	147,147,147,147	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AU	A	1754	1/1	0.68	0.21	101,101,101,101	1
2	AU	A	1751	1/1	0.70	0.39	217,217,217,217	1
2	AU	A	1803	1/1	0.71	0.21	138,138,138,138	1
2	AU	B	1750	1/1	0.76	0.35	127,127,127,127	1
2	AU	A	1757	1/1	0.82	0.29	120,120,120,120	1
2	AU	A	1756	1/1	0.83	0.19	115,115,115,115	1
2	AU	B	1803	1/1	0.85	0.21	118,118,118,118	1
2	AU	A	1748	1/1	0.90	0.13	77,77,77,77	1
2	AU	B	1747	1/1	0.90	0.12	63,63,63,63	1
2	AU	A	1755	1/1	0.90	0.29	103,103,103,103	1
2	AU	B	1755	1/1	0.91	0.25	139,139,139,139	1
2	AU	B	1753	1/1	0.92	0.23	93,93,93,93	1
2	AU	A	1753	1/1	0.93	0.24	71,71,71,71	1
2	AU	A	1747	1/1	0.93	0.12	66,66,66,66	1
2	AU	A	1749	1/1	0.93	0.22	5,5,5,5	1
2	AU	B	1802	1/1	0.94	0.14	82,82,82,82	1
2	AU	B	1748	1/1	0.95	0.15	67,67,67,67	1
2	AU	A	1752	1/1	0.95	0.13	71,71,71,71	1
2	AU	A	1800	1/1	0.95	0.05	76,76,76,76	0
2	AU	B	1752	1/1	0.95	0.21	38,38,38,38	1
2	AU	B	1749	1/1	0.97	0.16	1,1,1,1	1

6.5 Other polymers

There are no such residues in this entry.