



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:45 AM UTC

PDB ID : 5OQQ / pdb_00005oqq
Title : Crystal structure of the S. cerevisiae condensin Ycg1-Brn1 subcomplex
Authors : Kschonsak, M.; Hassler, M.; Haering, C.H.
Deposited on : 2017-08-14
Resolution : 2.79 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

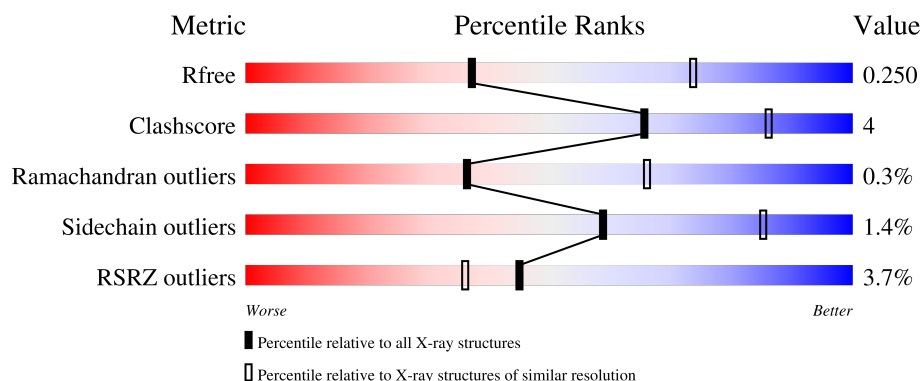
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	871	
1	B	871	
2	C	152	
2	D	152	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 28987 atoms, of which 14578 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 Condensin complex subunit 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	792	Total	C	H	N	O	S	0	0	0
			12884	4080	6506	1079	1190	29			
1	B	824	Total	C	H	N	O	S	0	0	0
			13380	4230	6742	1123	1256	29			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	initiating methionine	UNP Q06680
A	?	-	GLN	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	LYS	deletion	UNP Q06680
A	?	-	ILE	deletion	UNP Q06680
A	?	-	LYS	deletion	UNP Q06680
A	?	-	SER	deletion	UNP Q06680
A	?	-	LYS	deletion	UNP Q06680
A	?	-	LYS	deletion	UNP Q06680
A	?	-	ILE	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680
A	?	-	ARG	deletion	UNP Q06680
A	?	-	ARG	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	THR	deletion	UNP Q06680
A	?	-	SER	deletion	UNP Q06680
A	?	-	VAL	deletion	UNP Q06680
A	?	-	ASP	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	ASP	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q06680
A	?	-	THR	deletion	UNP Q06680
A	?	-	HIS	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680
A	?	-	ASP	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	VAL	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	ASP	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	ASP	deletion	UNP Q06680
A	?	-	ASP	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680
A	?	-	ILE	deletion	UNP Q06680
A	?	-	SER	deletion	UNP Q06680
A	?	-	SER	deletion	UNP Q06680
A	?	-	PHE	deletion	UNP Q06680
A	?	-	HIS	deletion	UNP Q06680
A	?	-	SER	deletion	UNP Q06680
A	?	-	ALA	deletion	UNP Q06680
A	?	-	VAL	deletion	UNP Q06680
A	?	-	GLU	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680
A	?	-	LEU	deletion	UNP Q06680
A	?	-	VAL	deletion	UNP Q06680
A	?	-	GLN	deletion	UNP Q06680
A	?	-	GLY	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680
A	?	-	GLY	deletion	UNP Q06680
A	?	-	ASN	deletion	UNP Q06680
A	?	-	VAL	deletion	UNP Q06680
B	5	MET	-	initiating methionine	UNP Q06680
B	?	-	GLN	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	LYS	deletion	UNP Q06680
B	?	-	ILE	deletion	UNP Q06680
B	?	-	LYS	deletion	UNP Q06680
B	?	-	SER	deletion	UNP Q06680
B	?	-	LYS	deletion	UNP Q06680

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP Q06680
B	?	-	ILE	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	ARG	deletion	UNP Q06680
B	?	-	ARG	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	THR	deletion	UNP Q06680
B	?	-	SER	deletion	UNP Q06680
B	?	-	VAL	deletion	UNP Q06680
B	?	-	ASP	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	ASP	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	GLY	deletion	UNP Q06680
B	?	-	THR	deletion	UNP Q06680
B	?	-	HIS	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	ASP	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	VAL	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	ASP	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	ASP	deletion	UNP Q06680
B	?	-	ASP	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	ILE	deletion	UNP Q06680
B	?	-	SER	deletion	UNP Q06680
B	?	-	SER	deletion	UNP Q06680
B	?	-	PHE	deletion	UNP Q06680
B	?	-	HIS	deletion	UNP Q06680
B	?	-	SER	deletion	UNP Q06680
B	?	-	ALA	deletion	UNP Q06680
B	?	-	VAL	deletion	UNP Q06680
B	?	-	GLU	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	LEU	deletion	UNP Q06680

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP Q06680
B	?	-	GLN	deletion	UNP Q06680
B	?	-	GLY	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	GLY	deletion	UNP Q06680
B	?	-	ASN	deletion	UNP Q06680
B	?	-	VAL	deletion	UNP Q06680

- Molecule 2 is a protein called Condensin complex subunit 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	96	Total	C	H	N	O	S	0	0	0
			1625	528	799	147	148	3			
2	C	64	Total	C	H	N	O	S	0	0	0
			1066	343	531	91	99	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	378	GLY	-	expression tag	UNP P38170
D	379	PRO	-	expression tag	UNP P38170
D	380	LEU	-	expression tag	UNP P38170
D	381	GLY	-	expression tag	UNP P38170
D	382	HIS	-	expression tag	UNP P38170
D	383	MET	-	expression tag	UNP P38170
C	378	GLY	-	expression tag	UNP P38170
C	379	PRO	-	expression tag	UNP P38170
C	380	LEU	-	expression tag	UNP P38170
C	381	GLY	-	expression tag	UNP P38170
C	382	HIS	-	expression tag	UNP P38170
C	383	MET	-	expression tag	UNP P38170

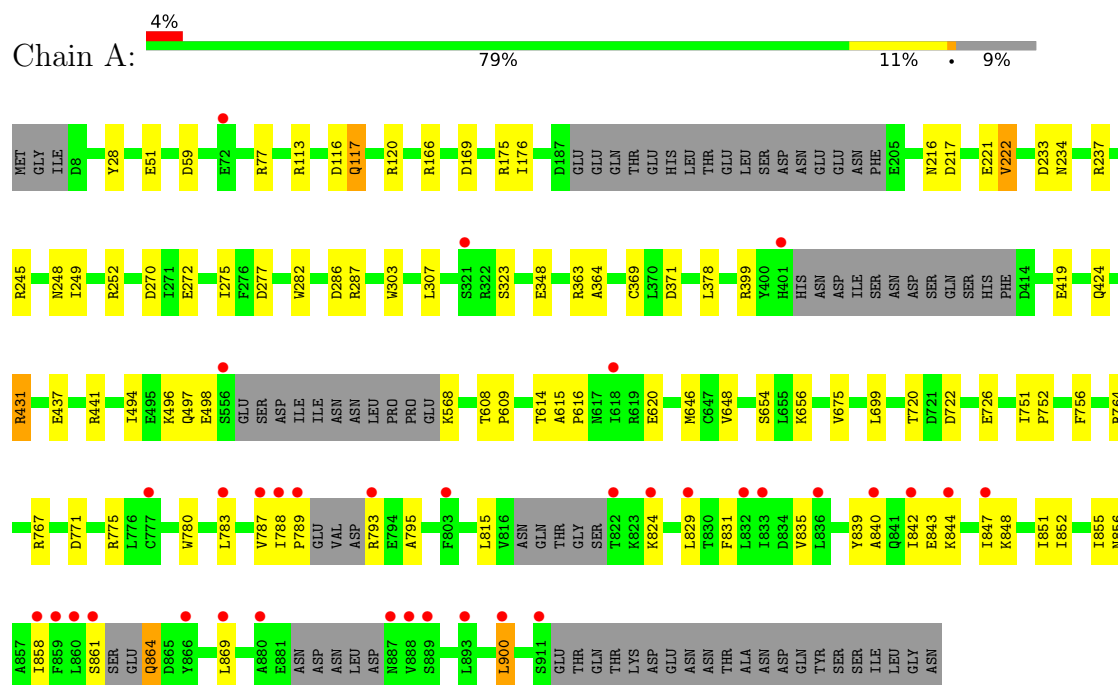
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	9	Total	O	0	0
			9	9		
3	D	4	Total	O	0	0
			4	4		

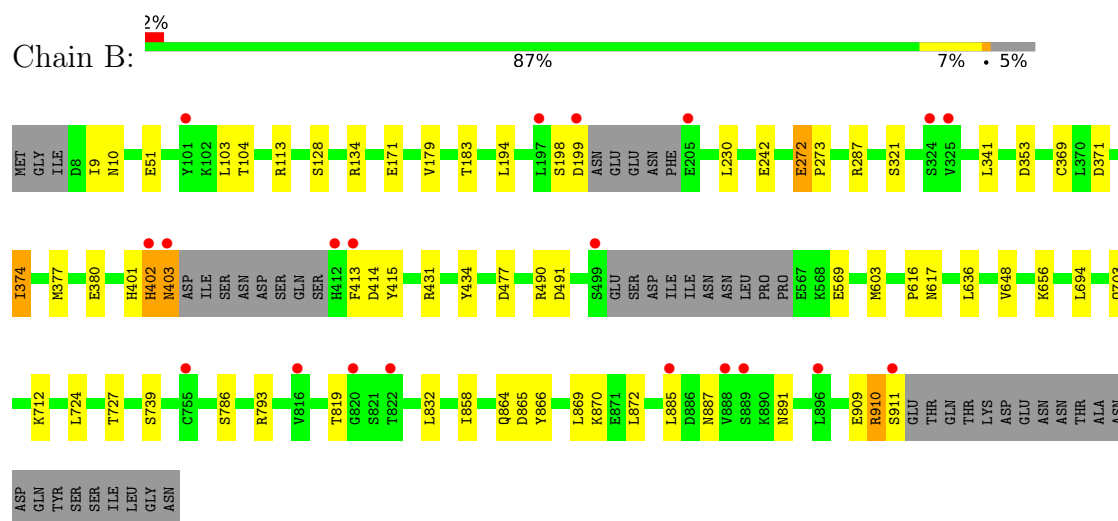
3 Residue-property plots [i](#)

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.

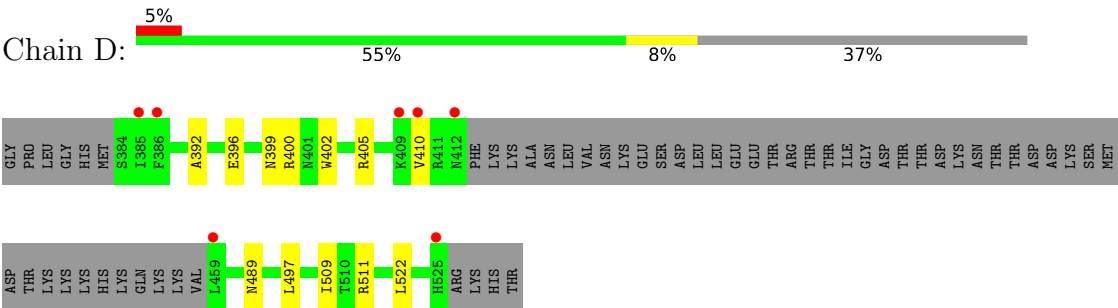
• Molecule 1: Condensin complex subunit 3



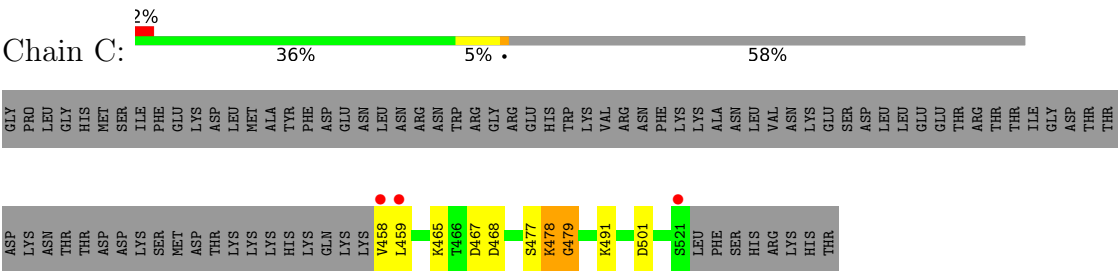
• Molecule 1: Condensin complex subunit 3



● Molecule 2: Condensin complex subunit 2



● Molecule 2: Condensin complex subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.53Å 185.53Å 148.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.25 – 2.79 47.25 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.25-2.79) 100.0 (47.25-2.79)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.249 0.206 , 0.250	Depositor DCC
R_{free} test set	1988 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28987	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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	0.13	0/6472	0.31	0/8742
1	B	0.12	0/6740	0.28	0/9113
2	C	0.14	0/547	0.41	0/732
2	D	0.12	0/847	0.30	0/1133
All	All	0.12	0/14606	0.30	0/19720

There are no bond length outliers.

There are no bond angle outliers.

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	6378	6506	6531	61	0
1	B	6638	6742	6744	41	0
2	C	535	531	531	7	0
2	D	826	799	799	9	0
3	A	19	0	0	1	0
3	B	9	0	0	2	0
3	D	4	0	0	2	0
All	All	14409	14578	14605	110	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 4.

All (110) 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:403:ASN:OD1	1:B:403:ASN:N	2.17	0.75
1:A:861:SER:O	1:A:864:GLN:NE2	2.21	0.73
1:A:793:ARG:HG2	1:A:795:ALA:H	1.54	0.72
1:A:287:ARG:NH1	2:C:501:ASP:OD1	2.24	0.70
1:A:722:ASP:OD1	1:A:764:ARG:NH1	2.25	0.70
1:A:771:ASP:OD2	1:A:775:ARG:NH1	2.27	0.68
1:A:277:ASP:OD2	1:A:323:SER:OG	2.09	0.68
2:D:405:ARG:O	3:D:601:HOH:O	2.12	0.67
1:A:237:ARG:NH1	1:A:270:ASP:O	2.29	0.66
1:B:477:ASP:OD2	3:B:1001:HOH:O	2.13	0.65
1:A:783:LEU:HD23	1:A:793:ARG:HB3	1.79	0.65
1:A:720:THR:OG1	1:A:764:ARG:NH2	2.30	0.64
1:A:399:ARG:NH2	1:A:419:GLU:OE2	2.31	0.64
2:D:489:ASN:O	3:D:602:HOH:O	2.16	0.62
1:B:786:SER:O	1:B:793:ARG:NH1	2.35	0.60
1:A:726:GLU:OE2	1:A:775:ARG:NH1	2.33	0.60
1:B:739:SER:OG	3:B:1002:HOH:O	2.16	0.59
1:A:348:GLU:OE1	3:A:1001:HOH:O	2.17	0.59
1:A:648:VAL:O	1:A:656:LYS:NZ	2.24	0.59
1:B:490:ARG:NH2	1:B:491:ASP:OD1	2.34	0.57
1:A:620:GLU:OE1	1:A:654:SER:OG	2.21	0.57
1:A:824:LYS:HZ2	1:A:864:GLN:N	2.02	0.56
1:A:116:ASP:OD2	1:A:120:ARG:NH1	2.39	0.56
1:B:909:GLU:O	1:B:911:SER:N	2.40	0.55
1:A:221:GLU:N	1:A:221:GLU:OE1	2.39	0.54
1:A:614:THR:HB	1:A:615:ALA:HA	1.89	0.54
1:B:401:HIS:O	1:B:403:ASN:N	2.42	0.53
1:A:166:ARG:NH1	1:A:169:ASP:OD1	2.42	0.52
1:A:51:GLU:OE2	1:A:113:ARG:NH1	2.42	0.52
1:B:694:LEU:O	1:B:703:GLN:NE2	2.43	0.51
1:B:832:LEU:HD22	1:B:858:ILE:CD1	2.41	0.51
1:B:832:LEU:HD23	1:B:872:LEU:HD11	1.91	0.51
1:B:51:GLU:OE2	1:B:113:ARG:NH1	2.45	0.50
1:B:866:TYR:OH	1:B:870:LYS:NZ	2.36	0.50
1:A:852:ILE:HA	1:A:855:ILE:CD1	2.42	0.50
1:A:217:ASP:CG	1:A:222:VAL:HG21	2.38	0.49
1:A:615:ALA:HB1	1:A:616:PRO:HD2	1.94	0.49
1:A:788:ILE:HG23	1:A:789:PRO:HA	1.95	0.48
1:A:175:ARG:NH1	1:A:217:ASP:OD2	2.45	0.48
1:A:843:GLU:OE1	1:B:819:THR:OG1	2.30	0.48
1:A:751:ILE:N	1:A:752:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:LYS:NZ	2:D:511:ARG:O	2.47	0.47
2:D:399:ASN:O	2:D:400:ARG:HB2	2.14	0.47
1:A:252:ARG:NH1	1:A:286:ASP:OD1	2.48	0.47
1:A:59:ASP:OD2	1:A:117:GLN:NE2	2.47	0.47
1:B:9:ILE:HD12	1:B:10:ASN:N	2.30	0.47
2:C:477:SER:O	2:C:478:LYS:CB	2.62	0.46
2:C:478:LYS:O	2:C:479:GLY:C	2.58	0.46
1:A:363:ARG:HD3	1:A:424:GLN:OE1	2.16	0.46
2:C:477:SER:O	2:C:478:LYS:HB3	2.16	0.46
1:B:603:MET:HE1	1:B:636:LEU:HD21	1.96	0.45
1:A:245:ARG:HD3	1:A:282:TRP:CD2	2.50	0.45
1:A:216:ASN:HB3	2:C:491:LYS:HA	1.99	0.45
1:A:722:ASP:OD2	1:A:767:ARG:NH1	2.48	0.45
1:B:648:VAL:O	1:B:656:LYS:HD3	2.17	0.45
1:A:176:ILE:HG13	1:A:222:VAL:HG12	1.99	0.45
1:A:497:GLN:O	1:A:568:LYS:NZ	2.42	0.45
1:B:374:ILE:O	1:B:374:ILE:CG1	2.64	0.45
1:A:303:TRP:O	1:A:307:LEU:HD12	2.17	0.45
1:B:865:ASP:O	1:B:869:LEU:HD12	2.17	0.45
1:A:842:ILE:HG23	1:A:847:ILE:HD11	1.98	0.45
1:B:380:GLU:OE2	1:B:380:GLU:N	2.42	0.45
1:B:402:HIS:O	1:B:403:ASN:C	2.60	0.45
1:B:128:SER:O	1:B:134:ARG:HD2	2.17	0.45
1:B:832:LEU:HD22	1:B:858:ILE:HD13	1.99	0.44
1:A:28:TYR:CZ	1:A:77:ARG:HG2	2.53	0.44
1:A:272:GLU:HB2	1:A:275:ILE:HG22	1.98	0.44
1:A:780:TRP:HZ3	1:A:847:ILE:HG22	1.82	0.44
1:A:788:ILE:CG2	1:A:789:PRO:HA	2.48	0.44
1:B:414:ASP:OD1	1:B:415:TYR:N	2.50	0.44
2:D:509:ILE:HG22	2:D:522:LEU:HD21	2.00	0.44
1:B:179:VAL:O	1:B:183:THR:HG23	2.18	0.44
1:B:887:ASN:O	1:B:891:ASN:N	2.38	0.44
1:A:608:THR:OG1	1:A:609:PRO:HD3	2.17	0.44
1:A:856:ASN:H	1:A:858:ILE:CD1	2.31	0.44
1:A:756:PHE:HA	1:A:815:LEU:HD23	2.00	0.44
1:A:369:CYS:HB3	1:A:378:LEU:HD11	2.00	0.43
1:A:646:MET:HE2	1:B:434:TYR:H	1.83	0.43
1:B:371:ASP:OD2	1:B:431:ARG:NH2	2.49	0.43
2:D:399:ASN:O	2:D:400:ARG:CB	2.66	0.43
1:B:374:ILE:O	1:B:374:ILE:HG12	2.18	0.43
1:B:353:ASP:N	1:B:353:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:458:VAL:O	2:C:459:LEU:C	2.61	0.43
1:A:371:ASP:OD1	1:A:431:ARG:NH2	2.45	0.43
2:D:392:ALA:O	2:D:396:GLU:HG3	2.19	0.43
1:A:494:ILE:HG22	1:A:494:ILE:O	2.19	0.43
1:A:851:ILE:O	1:A:855:ILE:HD12	2.19	0.43
1:A:369:CYS:CB	1:A:378:LEU:HD11	2.49	0.43
1:B:724:LEU:O	1:B:727:THR:OG1	2.34	0.43
1:A:233:ASP:OD1	1:A:234:ASN:N	2.51	0.43
1:A:363:ARG:HG3	1:A:364:ALA:N	2.34	0.43
1:B:369:CYS:HA	1:B:374:ILE:HG23	2.00	0.42
1:A:855:ILE:HG22	1:A:856:ASN:N	2.35	0.42
1:A:839:TYR:CD2	1:A:840:ALA:N	2.88	0.42
1:A:844:LYS:HE3	1:B:819:THR:HB	2.01	0.42
1:B:864:GLN:HB2	1:B:869:LEU:HD11	2.02	0.42
1:A:829:LEU:C	1:A:829:LEU:HD13	2.44	0.41
1:A:248:ASN:OD1	1:A:249:ILE:N	2.53	0.41
1:B:103:LEU:O	1:B:104:THR:HG22	2.20	0.41
1:B:242:GLU:HG2	2:D:497:LEU:HD21	2.02	0.41
1:B:272:GLU:HG2	1:B:273:PRO:HD2	2.01	0.41
1:B:194:LEU:HD12	1:B:194:LEU:H	1.85	0.41
1:A:848:LYS:O	1:A:851:ILE:HG22	2.21	0.41
1:B:616:PRO:O	1:B:617:ASN:HB2	2.19	0.41
1:B:198:SER:O	1:B:199:ASP:C	2.63	0.41
1:A:437:GLU:HG3	1:A:441:ARG:HE	1.86	0.40
2:C:467:ASP:O	2:C:468:ASP:C	2.64	0.40
1:A:831:PHE:CE2	1:A:835:VAL:CG2	3.05	0.40
1:B:287:ARG:HD3	2:D:402:TRP:CD1	2.57	0.40
1:A:869:LEU:HD11	1:A:900:LEU:HD13	2.03	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	776/871 (89%)	744 (96%)	32 (4%)	0	100	100
1	B	816/871 (94%)	788 (97%)	25 (3%)	3 (0%)	30	60
2	C	62/152 (41%)	56 (90%)	4 (6%)	2 (3%)	3	11
2	D	92/152 (60%)	85 (92%)	7 (8%)	0	100	100
All	All	1746/2046 (85%)	1673 (96%)	68 (4%)	5 (0%)	36	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	402	HIS
1	B	910	ARG
2	C	478	LYS
2	C	479	GLY
1	B	413	PHE

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	719/794 (91%)	709 (99%)	10 (1%)	59	85
1	B	750/794 (94%)	739 (98%)	11 (2%)	57	84
2	C	61/143 (43%)	60 (98%)	1 (2%)	55	83
2	D	91/143 (64%)	90 (99%)	1 (1%)	65	87
All	All	1621/1874 (86%)	1598 (99%)	23 (1%)	59	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	222	VAL
1	A	431	ARG
1	A	496	LYS
1	A	498	GLU
1	A	675	VAL

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Mol	Chain	Res	Type
1	A	699	LEU
1	A	787	VAL
1	A	864	GLN
1	A	900	LEU
1	B	171	GLU
1	B	230	LEU
1	B	272	GLU
1	B	321	SER
1	B	341	LEU
1	B	374	ILE
1	B	377	MET
1	B	403	ASN
1	B	569	GLU
1	B	885	LEU
1	B	910	ARG
2	D	410	VAL
2	C	465	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	A	449	ASN
1	A	596	ASN
1	A	864	GLN
1	A	908	ASN
1	B	42	GLN
1	B	235	ASN
1	B	596	ASN
1	B	804	GLN
1	B	818	GLN
1	B	884	ASN
2	D	503	HIS

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 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	792/871 (90%)	0.20	35 (4%) 39 31	55, 87, 148, 256	0
1	B	824/871 (94%)	-0.09	20 (2%) 59 49	50, 75, 125, 160	0
2	C	64/152 (42%)	0.29	3 (4%) 36 29	71, 97, 122, 141	0
2	D	96/152 (63%)	0.25	7 (7%) 21 15	55, 88, 133, 144	0
All	All	1776/2046 (86%)	0.07	65 (3%) 45 36	50, 82, 137, 256	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	SER	5.8
1	B	911	SER	4.6
2	C	459	LEU	4.3
1	A	859	PHE	4.3
2	C	458	VAL	3.8
2	D	410	VAL	3.8
1	B	499	SER	3.7
1	A	787	VAL	3.6
2	D	459	LEU	3.6
1	A	900	LEU	3.6
1	B	199	ASP	3.6
1	A	793	ARG	3.5
1	A	888	VAL	3.4
1	A	829	LEU	3.4
1	A	789	PRO	3.4
1	B	197	LEU	3.3
2	D	385	ILE	3.2
1	B	755	CYS	3.2
1	A	889	SER	3.1
1	A	836	LEU	3.0
2	D	525	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	833	ILE	3.0
1	B	403	ASN	3.0
1	A	869	LEU	3.0
1	B	324	SER	3.0
1	A	840	ALA	2.9
1	A	866	TYR	2.8
1	A	777	CYS	2.7
1	A	860	LEU	2.6
1	A	72	GLU	2.6
1	A	401	HIS	2.6
1	A	822	THR	2.6
1	B	412	HIS	2.6
1	A	880	ALA	2.6
1	A	911	SER	2.5
1	B	205	GLU	2.5
1	A	783	LEU	2.5
2	D	386	PHE	2.5
1	B	101	TYR	2.4
1	B	816	VAL	2.4
1	B	413	PHE	2.4
1	B	325	VAL	2.4
1	A	788	ILE	2.3
1	A	844	LYS	2.3
1	A	858	ILE	2.3
1	A	321	SER	2.3
1	A	832	LEU	2.3
1	A	618	ILE	2.3
1	B	889	SER	2.3
1	B	820	GLY	2.3
1	A	893	LEU	2.3
2	D	412	ASN	2.2
2	C	521	SER	2.2
1	A	842	ILE	2.2
1	B	885	LEU	2.2
1	B	896	LEU	2.2
1	B	402	HIS	2.2
1	B	888	VAL	2.2
1	A	861	SER	2.1
1	A	803	PHE	2.1
1	A	887	ASN	2.1
1	A	847	ILE	2.1
1	A	824	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	822	THR	2.1
2	D	409	LYS	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.