Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 05:54 AM EDT

PDB ID	:	5OQQ
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 (i) 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 (1)) were used in the production of this report:

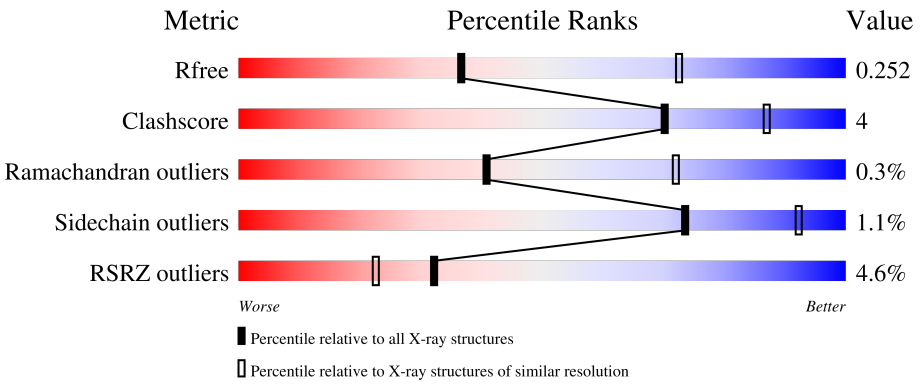
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	7%, 80%, 11%, 9%
1	B	871	2%, 88%, 6%, 5%
2	C	152	%, 39%, 58%
2	D	152	3%, 55%, 8%, 37%

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
			Total	C	H	N	O	S			
1	A	792	12884	4080	6506	1079	1190	29	0	0	0
1	B	824	13380	4230	6742	1123	1256	29	0	0	0

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
			Total	C	H	N	O	S			
2	D	96	1625	528	799	147	148	3	0	0	0
			Total	C	H	N	O	S			
2	C	64	1066	343	531	91	99	2	0	0	0

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.

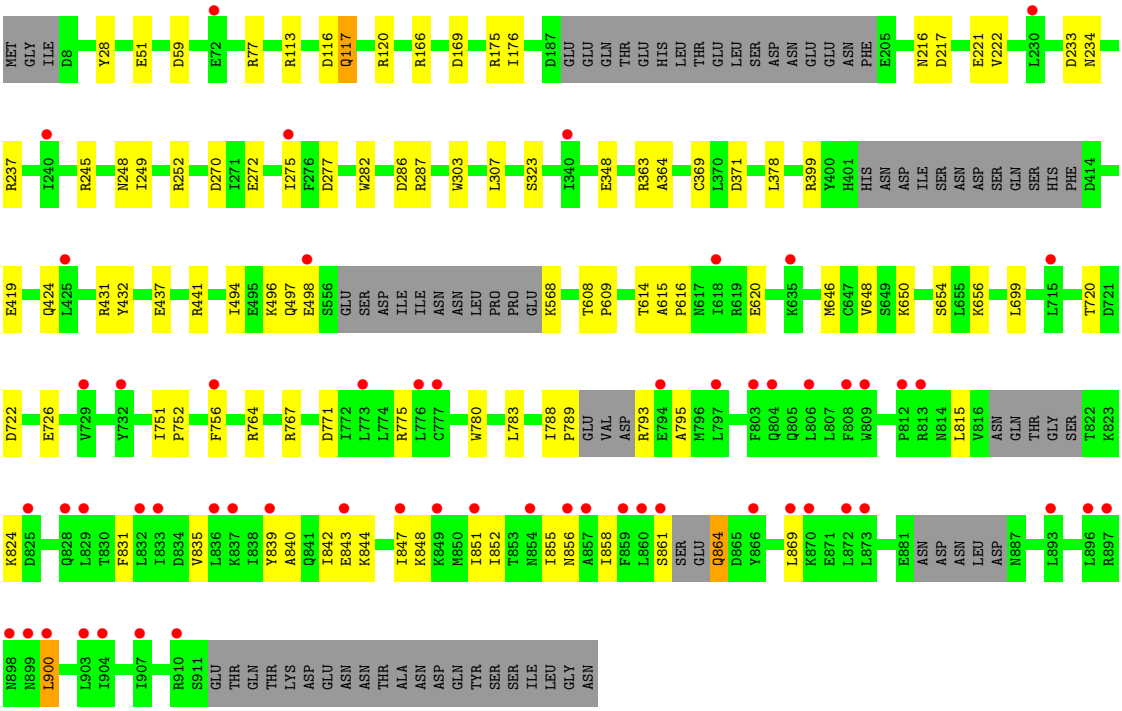
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	19	19	19	0	0
			Total	O		
3	B	9	9	9	0	0
			Total	O		
3	D	4	4	4	0	0

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.

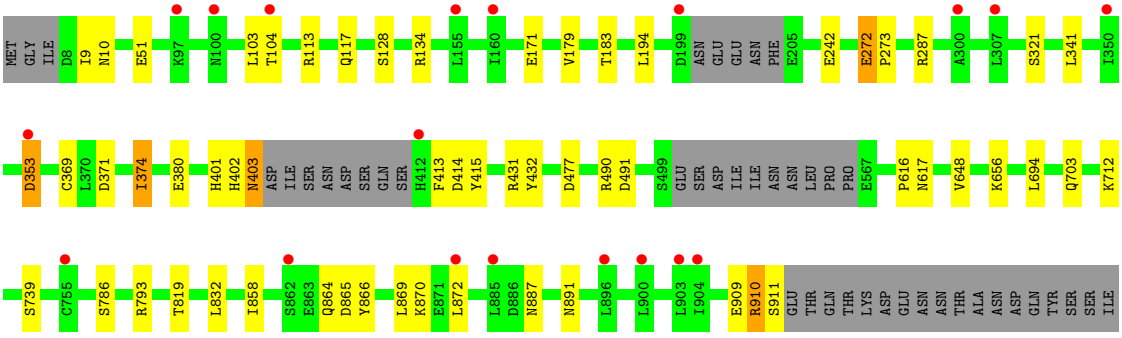
• Molecule 1: Condensin complex subunit 3

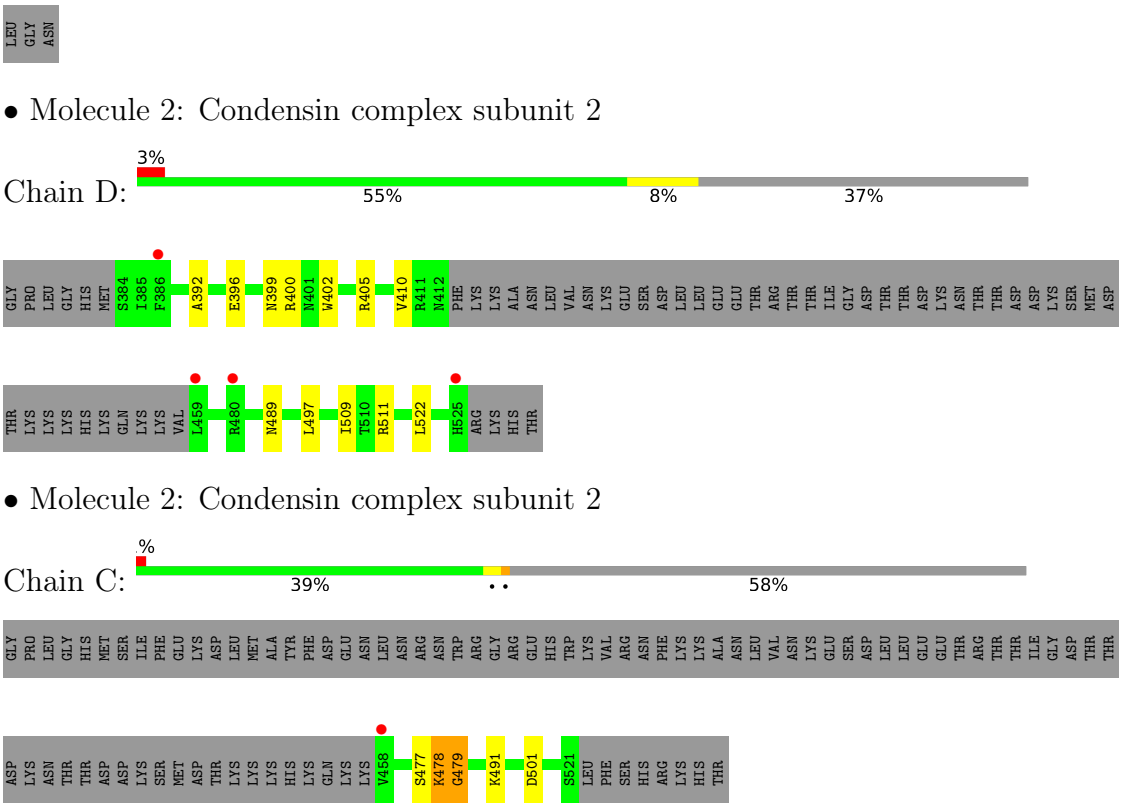
Chain A: 7% 80% 11% 9%



• Molecule 1: Condensin complex subunit 3

Chain B: 2% 88% 6% • 5%




LEU GLY ASN
• Molecule 2: Condensin complex subunit 2
Chain D:
3%
55%
8%
37%
GLY PRO LEU GLY HIS MET S384 I385 F386 A392 E396 N399 R400 N401 W402 R405 V410 R411 N412 PHE LYS LYS ALA ASN LEU VAL ASN LYS GLU SER ASP LEU LEU GLU GLU THR ARG THR THR ILE GLY ASP THR THR ASP LYS ASN THR THR ASP ASP LYS SER MET ASP
THR LYS LYS LYS HIS LYS GLN LYS LYS VAL L459 R480 N489 L497 I509 T510 R511 L522 H525 ARG LYS HIS THR
• Molecule 2: Condensin complex subunit 2
Chain C:
%
39%
58%
GLY PRO LEU GLY HIS MET SER ILE PHE GLU LYS ASP LEU MET ALA TYR PHE ASP GLU ASN LEU ASN ARG ASN TRP ARG GLY ARG GLU HIS TRP LYS VAL ARG ASN PHE LYS LYS ALA ASN LEU VAL ASN LYS GLU SER ASP LEU LEU GLU GLU THR ARG THR THR ILE GLY ASP THR THR
ASP LYS ASN THR THR ASP ASP LYS SER MET ASP THR LYS LYS LYS HIS LYS GLN LYS LYS V458 S477 K478 G479 K491 D501 S521 LEU PHE SER HIS ARG LYS HIS THR

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.44 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.249 0.206 , 0.252	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 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/6472	0.40	0/8742
1	B	0.24	0/6740	0.40	0/9113
2	C	0.25	0/547	0.48	0/732
2	D	0.25	0/847	0.43	0/1133
All	All	0.24	0/14606	0.40	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	60	0
1	B	6638	6742	6744	36	0
2	C	535	531	531	5	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	103	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 (103) 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:824:LYS:HZ2	1:A:864:GLN:N	1.95	0.64
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: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:A:646:MET:HE3	1:A:650:LYS:HG3	1.90	0.54
1:B:401:HIS:O	1:B:403:ASN:N	2.42	0.53
1:A:620:GLU:OE1	1:A:654:SER:OG	2.21	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: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
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: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:A:217:ASP:CG	1:A:222:VAL:HG21	2.38	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:353:ASP:N	1:B:353:ASP:OD1	2.50	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:C:478:LYS:O	2:C:479:GLY:C	2.58	0.41
1:B:616:PRO:O	1:B:617:ASN:HB2	2.19	0.41
1:A:437:GLU:HG3	1:A:441:ARG:HE	1.86	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%)	34 66
2	C	62/152 (41%)	56 (90%)	4 (6%)	2 (3%)	4 13
2	D	92/152 (60%)	85 (92%)	7 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1746/2046 (85%)	1673 (96%)	68 (4%)	5 (0%)	41	72

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 (i)

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%)	712 (99%)	7 (1%)	76	93
1	B	750/794 (94%)	740 (99%)	10 (1%)	69	91
2	C	61/143 (43%)	61 (100%)	0	100	100
2	D	91/143 (64%)	90 (99%)	1 (1%)	73	92
All	All	1621/1874 (86%)	1603 (99%)	18 (1%)	73	92

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	432	TYR
1	A	496	LYS
1	A	498	GLU
1	A	699	LEU
1	A	864	GLN
1	A	900	LEU
1	B	117	GLN
1	B	171	GLU
1	B	272	GLU

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Mol	Chain	Res	Type
1	B	321	SER
1	B	341	LEU
1	B	353	ASP
1	B	374	ILE
1	B	403	ASN
1	B	432	TYR
1	B	910	ARG
2	D	410	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	864	GLN
1	B	117	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.51	58 (7%)	15	8	51, 79, 136, 256	0
1	B	824/871 (94%)	0.35	19 (2%)	60	51	46, 68, 114, 145	0
2	C	64/152 (42%)	0.19	1 (1%)	72	66	64, 88, 108, 122	0
2	D	96/152 (63%)	0.42	4 (4%)	36	26	50, 81, 122, 131	0
All	All	1776/2046 (86%)	0.42	82 (4%)	32	22	46, 74, 127, 256	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	866	TYR	5.5
1	A	860	LEU	5.5
1	A	900	LEU	5.1
1	B	885	LEU	4.8
1	A	833	ILE	4.4
1	A	832	LEU	4.4
1	A	904	ILE	4.3
1	A	907	ILE	4.1
1	A	829	LEU	3.9
1	A	851	ILE	3.9
1	A	813	ARG	3.8
1	A	836	LEU	3.5
1	A	803	PHE	3.4
2	D	525	HIS	3.3
1	A	794	GLU	3.2
1	A	776	LEU	3.1
1	A	872	LEU	3.1
1	A	804	GLN	3.0
1	A	861	SER	3.0
1	A	898	ASN	2.9
1	A	897	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	618	ILE	2.9
1	B	307	LEU	2.8
2	D	386	PHE	2.8
1	A	859	PHE	2.8
1	B	350	ILE	2.7
1	A	756	PHE	2.7
1	A	896	LEU	2.6
1	A	715	LEU	2.6
1	A	797	LEU	2.5
1	B	903	LEU	2.5
1	B	104	THR	2.5
1	A	828	GLN	2.5
1	A	837	LYS	2.5
2	D	480	ARG	2.5
1	B	100	ASN	2.5
1	B	97	LYS	2.5
1	A	425	LEU	2.5
1	A	732	TYR	2.5
1	A	777	CYS	2.5
1	A	870	LYS	2.4
1	A	808	PHE	2.4
1	A	893	LEU	2.4
1	A	869	LEU	2.4
1	A	498	GLU	2.4
1	B	755	CYS	2.4
1	B	872	LEU	2.3
1	A	856	ASN	2.3
1	A	773	LEU	2.3
1	B	155	LEU	2.3
1	B	904	ILE	2.3
1	A	809	TRP	2.3
2	C	458	VAL	2.3
1	A	825	ASP	2.3
1	A	230	LEU	2.3
1	A	843	GLU	2.3
1	A	275	ILE	2.3
1	A	240	ILE	2.2
1	A	812	PRO	2.2
1	B	896	LEU	2.2
1	A	849	LYS	2.2
1	A	729	VAL	2.2
1	A	873	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	459	LEU	2.2
1	B	300	ALA	2.2
1	B	862	SER	2.2
1	A	635	LYS	2.1
1	A	903	LEU	2.1
1	A	854	ASN	2.1
1	A	340	ILE	2.1
1	B	160	ILE	2.1
1	A	72	GLU	2.1
1	A	857	ALA	2.1
1	A	899	ASN	2.1
1	A	910	ARG	2.1
1	B	353	ASP	2.1
1	A	806	LEU	2.0
1	A	847	ILE	2.0
1	B	900	LEU	2.0
1	B	412	HIS	2.0
1	A	839	TYR	2.0
1	B	199	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.