



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 04:28 am BST

PDB ID : 4XR7
Title : Structure of the *Saccharomyces cerevisiae* PAN2-PAN3 core complex
Authors : Schafer, I.B.; Rode, M.; Bonneau, F.; Schussler, S.; Conti, E.
Deposited on : 2015-01-20
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

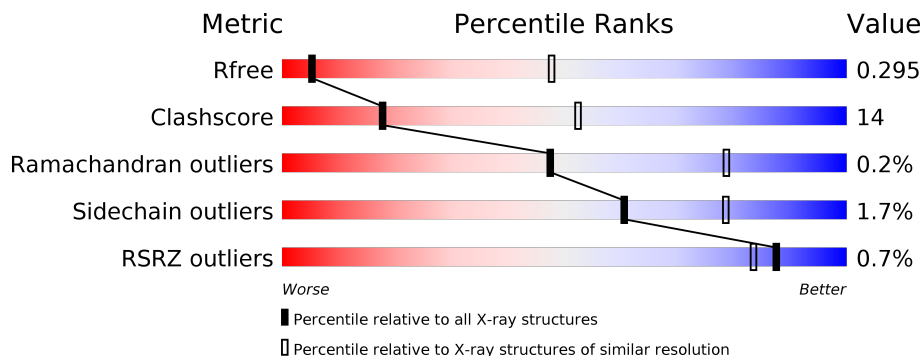
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	776	
1	D	776	
1	G	776	
1	J	776	
2	B	465	
2	C	465	

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Mol	Chain	Length	Quality of chain
2	E	465	
2	F	465	
2	H	465	
2	I	465	
2	K	465	
2	L	465	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 46467 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 PAB-dependent poly(A)-specific ribonuclease subunit PAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	683	Total 4981	C 3160	N 829	O 972	S 20	0	0	0
1	D	683	Total 4973	C 3153	N 834	O 966	S 20	0	0	0
1	J	681	Total 4958	C 3162	N 810	O 967	S 19	0	0	0
1	A	701	Total 5217	C 3323	N 860	O 1012	S 22	0	0	0

- Molecule 2 is a protein called PAB-dependent poly(A)-specific ribonuclease subunit PAN3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	441	Total 3479	C 2243	N 576	O 646	S 14	0	0	0
2	K	431	Total 3272	C 2087	N 547	O 624	S 14	0	0	0
2	E	414	Total 3084	C 1985	N 509	O 576	S 14	0	0	0
2	F	442	Total 3381	C 2186	N 553	O 628	S 14	0	0	0
2	H	420	Total 3153	C 2020	N 523	O 596	S 14	0	0	0
2	I	437	Total 3292	C 2109	N 541	O 628	S 14	0	0	0
2	C	444	Total 3405	C 2188	N 561	O 642	S 14	0	0	0
2	B	429	Total 3272	C 2093	N 545	O 620	S 14	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	225	MET	-	initiating methionine	UNP P36102

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Chain	Residue	Modelled	Actual	Comment	Reference
L	680	HIS	-	expression tag	UNP P36102
L	681	HIS	-	expression tag	UNP P36102
L	682	HIS	-	expression tag	UNP P36102
L	683	HIS	-	expression tag	UNP P36102
L	684	HIS	-	expression tag	UNP P36102
L	685	HIS	-	expression tag	UNP P36102
L	686	HIS	-	expression tag	UNP P36102
L	687	HIS	-	expression tag	UNP P36102
L	688	HIS	-	expression tag	UNP P36102
L	689	HIS	-	expression tag	UNP P36102
K	219	MET	-	initiating methionine	UNP P36102
K	680	HIS	-	expression tag	UNP P36102
K	681	HIS	-	expression tag	UNP P36102
K	682	HIS	-	expression tag	UNP P36102
K	683	HIS	-	expression tag	UNP P36102
K	684	HIS	-	expression tag	UNP P36102
K	685	HIS	-	expression tag	UNP P36102
K	686	HIS	-	expression tag	UNP P36102
K	687	HIS	-	expression tag	UNP P36102
K	688	HIS	-	expression tag	UNP P36102
K	689	HIS	-	expression tag	UNP P36102
E	225	MET	-	initiating methionine	UNP P36102
E	680	HIS	-	expression tag	UNP P36102
E	681	HIS	-	expression tag	UNP P36102
E	682	HIS	-	expression tag	UNP P36102
E	683	HIS	-	expression tag	UNP P36102
E	684	HIS	-	expression tag	UNP P36102
E	685	HIS	-	expression tag	UNP P36102
E	686	HIS	-	expression tag	UNP P36102
E	687	HIS	-	expression tag	UNP P36102
E	688	HIS	-	expression tag	UNP P36102
E	689	HIS	-	expression tag	UNP P36102
F	225	MET	-	initiating methionine	UNP P36102
F	680	HIS	-	expression tag	UNP P36102
F	681	HIS	-	expression tag	UNP P36102
F	682	HIS	-	expression tag	UNP P36102
F	683	HIS	-	expression tag	UNP P36102
F	684	HIS	-	expression tag	UNP P36102
F	685	HIS	-	expression tag	UNP P36102
F	686	HIS	-	expression tag	UNP P36102
F	687	HIS	-	expression tag	UNP P36102
F	688	HIS	-	expression tag	UNP P36102

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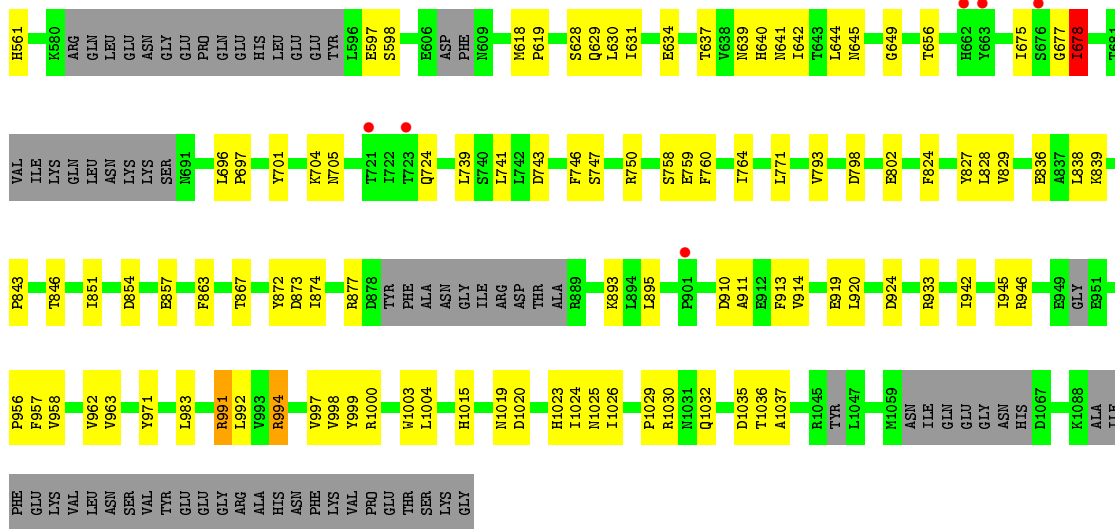
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Chain	Residue	Modelled	Actual	Comment	Reference
F	689	HIS	-	expression tag	UNP P36102
H	225	MET	-	initiating methionine	UNP P36102
H	680	HIS	-	expression tag	UNP P36102
H	681	HIS	-	expression tag	UNP P36102
H	682	HIS	-	expression tag	UNP P36102
H	683	HIS	-	expression tag	UNP P36102
H	684	HIS	-	expression tag	UNP P36102
H	685	HIS	-	expression tag	UNP P36102
H	686	HIS	-	expression tag	UNP P36102
H	687	HIS	-	expression tag	UNP P36102
H	688	HIS	-	expression tag	UNP P36102
H	689	HIS	-	expression tag	UNP P36102
I	225	MET	-	initiating methionine	UNP P36102
I	680	HIS	-	expression tag	UNP P36102
I	681	HIS	-	expression tag	UNP P36102
I	682	HIS	-	expression tag	UNP P36102
I	683	HIS	-	expression tag	UNP P36102
I	684	HIS	-	expression tag	UNP P36102
I	685	HIS	-	expression tag	UNP P36102
I	686	HIS	-	expression tag	UNP P36102
I	687	HIS	-	expression tag	UNP P36102
I	688	HIS	-	expression tag	UNP P36102
I	689	HIS	-	expression tag	UNP P36102
C	225	MET	-	initiating methionine	UNP P36102
C	680	HIS	-	expression tag	UNP P36102
C	681	HIS	-	expression tag	UNP P36102
C	682	HIS	-	expression tag	UNP P36102
C	683	HIS	-	expression tag	UNP P36102
C	684	HIS	-	expression tag	UNP P36102
C	685	HIS	-	expression tag	UNP P36102
C	686	HIS	-	expression tag	UNP P36102
C	687	HIS	-	expression tag	UNP P36102
C	688	HIS	-	expression tag	UNP P36102
C	689	HIS	-	expression tag	UNP P36102
B	225	MET	-	initiating methionine	UNP P36102
B	680	HIS	-	expression tag	UNP P36102
B	681	HIS	-	expression tag	UNP P36102
B	682	HIS	-	expression tag	UNP P36102
B	683	HIS	-	expression tag	UNP P36102
B	684	HIS	-	expression tag	UNP P36102
B	685	HIS	-	expression tag	UNP P36102
B	686	HIS	-	expression tag	UNP P36102

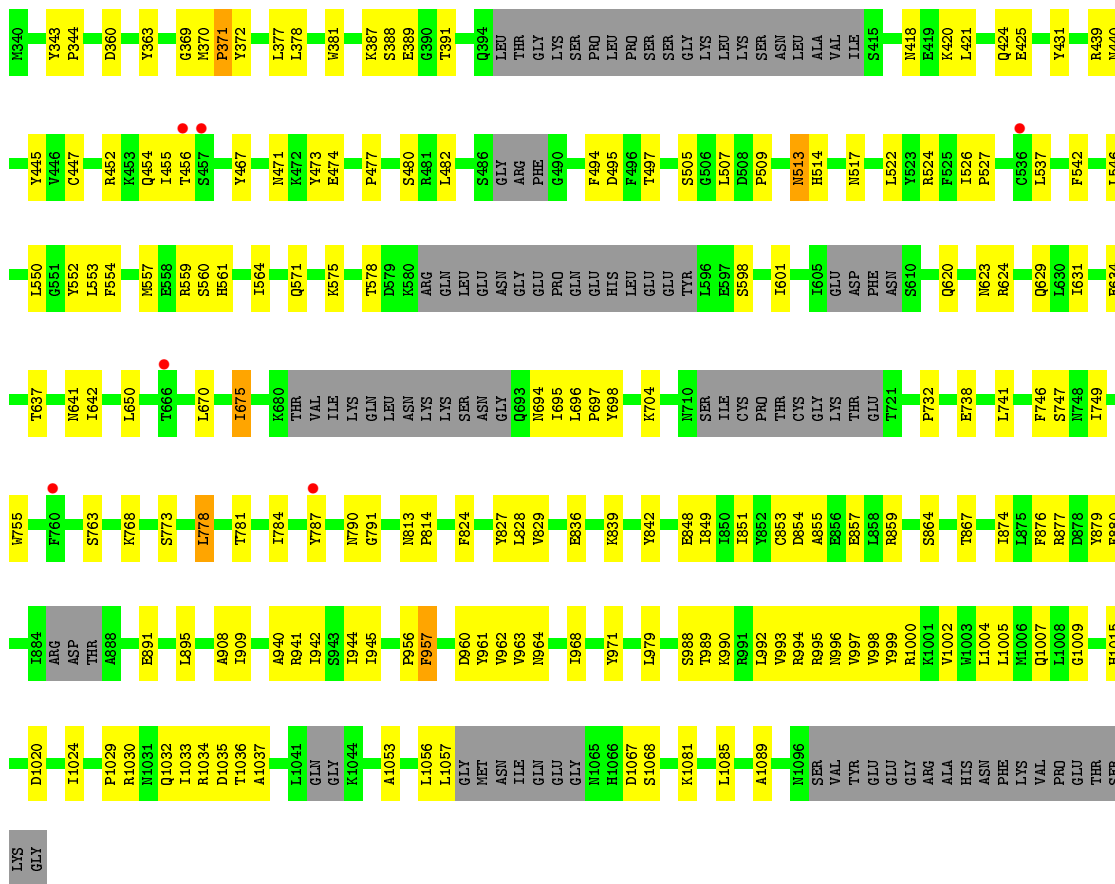
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Chain	Residue	Modelled	Actual	Comment	Reference
B	687	HIS	-	expression tag	UNP P36102
B	688	HIS	-	expression tag	UNP P36102
B	689	HIS	-	expression tag	UNP P36102

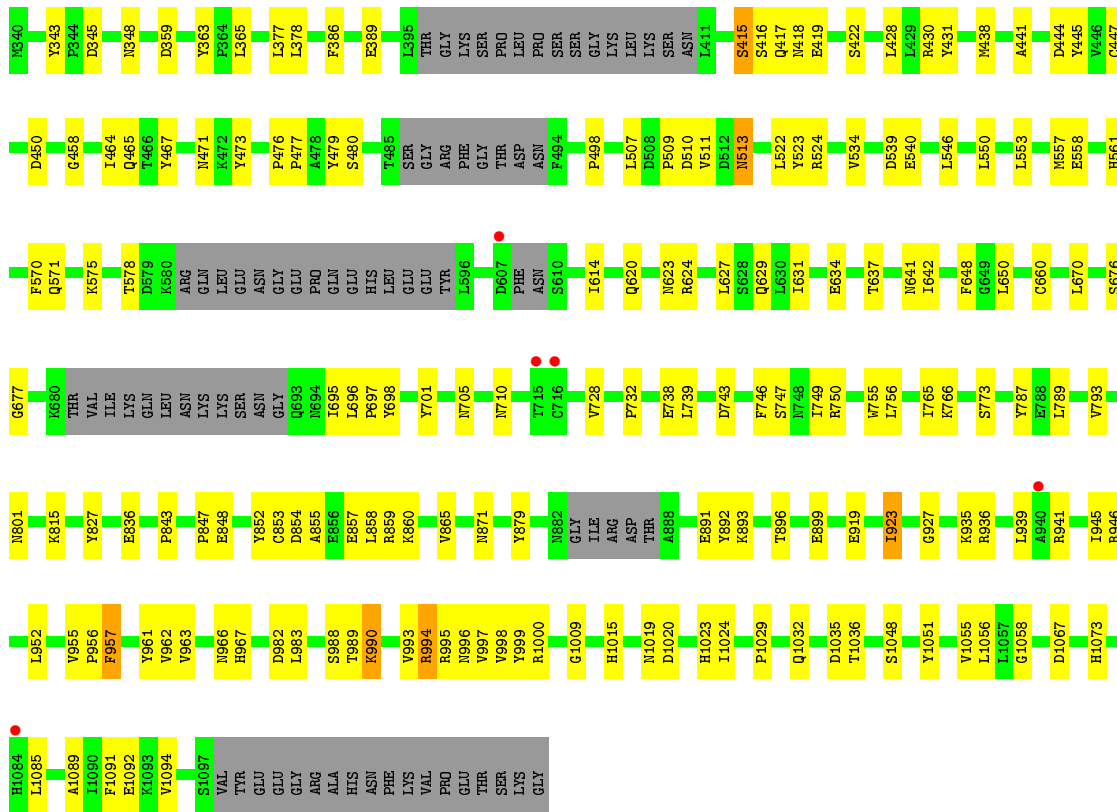


• Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2

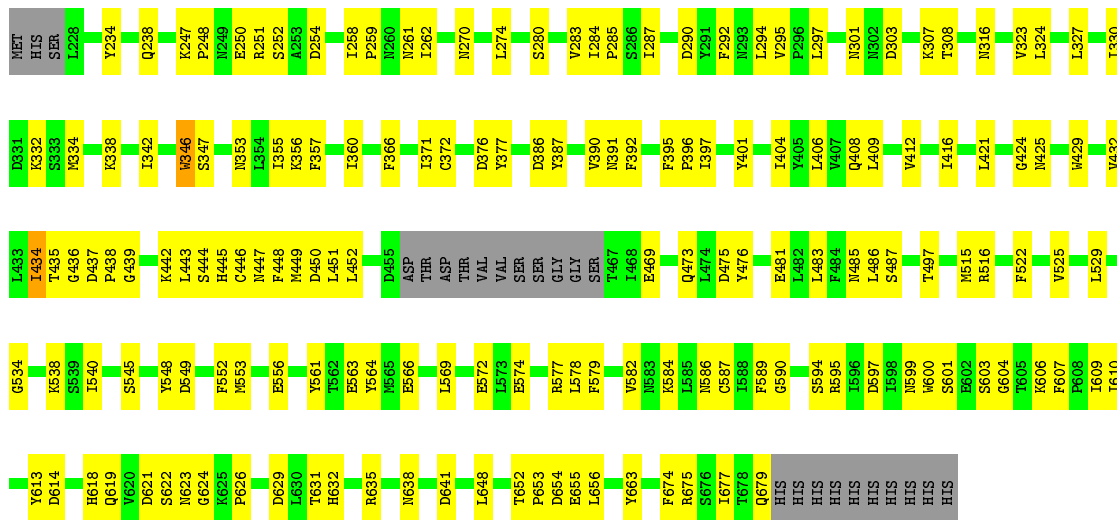


• Molecule 1: PAB-dependent poly(A)-specific ribonuclease subunit PAN2





• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3



• Molecule 2: PAB-dependent poly(A)-specific ribonuclease subunit PAN3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.44Å 205.30Å 234.41Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	48.83 – 3.80 48.83 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.83-3.80) 99.3 (48.83-3.79)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.77Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.285 , 0.299 0.281 , 0.295	Depositor DCC
R_{free} test set	6098 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	133.3	Xtrriage
Anisotropy	0.288	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	46467	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.28	0/5327	0.56	0/7277
1	D	0.28	0/5074	0.55	1/6935 (0.0%)
1	G	0.29	0/5080	0.57	1/6945 (0.0%)
1	J	0.28	0/5062	0.56	0/6924
2	B	0.32	0/3341	0.65	3/4547 (0.1%)
2	C	0.28	0/3483	0.58	0/4752
2	E	0.31	0/3150	0.61	1/4298 (0.0%)
2	F	0.29	0/3459	0.59	0/4723
2	H	0.30	0/3221	0.63	3/4392 (0.1%)
2	I	0.29	0/3365	0.58	1/4595 (0.0%)
2	K	0.30	0/3341	0.63	3/4550 (0.1%)
2	L	0.29	0/3558	0.60	1/4837 (0.0%)
All	All	0.29	0/47461	0.59	14/64775 (0.0%)

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	4
1	D	0	2
1	G	0	1
1	J	0	2
2	C	0	1
2	F	0	1
2	H	0	1
2	L	0	1
All	All	0	13

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	LEU	CA-CB-CG	7.63	132.86	115.30
2	B	652	THR	C-N-CD	-7.10	104.98	120.60
2	K	652	THR	C-N-CD	-6.95	105.30	120.60
1	G	561	HIS	N-CA-C	-6.43	93.63	111.00
2	L	534	GLY	N-CA-C	-6.28	97.40	113.10

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	431	TYR	Peptide
1	D	994	ARG	Peptide
2	F	438	PRO	Peptide
1	G	453	LYS	Peptide
2	L	366	PHE	Peptide

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	5217	0	4654	115	0
1	D	4973	0	4313	105	0
1	G	4981	0	4348	115	0
1	J	4958	0	4283	124	0
2	B	3272	0	2970	107	0
2	C	3405	0	3129	119	0
2	E	3084	0	2749	96	0
2	F	3381	0	3120	124	0
2	H	3153	0	2811	97	0
2	I	3292	0	2945	127	0
2	K	3272	0	2943	97	0
2	L	3479	0	3315	127	0
All	All	46467	0	41580	1198	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 14.

The worst 5 of 1198 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)
2:I:353:ASN:HA	2:I:442:LYS:HG2	1.55	0.89
2:K:256:LEU:HD13	2:K:404:ILE:HD11	1.56	0.87
2:H:586:ASN:OD1	2:I:586:ASN:ND2	2.08	0.85
2:K:577:ARG:NH1	1:J:370:MET:SD	2.49	0.85
2:B:256:LEU:HD13	2:B:404:ILE:HD11	1.60	0.83

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	687/776 (88%)	652 (95%)	34 (5%)	1 (0%)	51	83
1	D	663/776 (85%)	622 (94%)	39 (6%)	2 (0%)	41	74
1	G	665/776 (86%)	631 (95%)	32 (5%)	2 (0%)	41	74
1	J	661/776 (85%)	624 (94%)	35 (5%)	2 (0%)	41	74
2	B	421/465 (90%)	397 (94%)	24 (6%)	0	100	100
2	C	440/465 (95%)	417 (95%)	23 (5%)	0	100	100
2	E	408/465 (88%)	384 (94%)	24 (6%)	0	100	100
2	F	438/465 (94%)	415 (95%)	22 (5%)	1 (0%)	47	79
2	H	416/465 (90%)	394 (95%)	21 (5%)	1 (0%)	47	79
2	I	429/465 (92%)	404 (94%)	24 (6%)	1 (0%)	47	79
2	K	423/465 (91%)	408 (96%)	15 (4%)	0	100	100
2	L	437/465 (94%)	416 (95%)	21 (5%)	0	100	100
All	All	6088/6824 (89%)	5764 (95%)	314 (5%)	10 (0%)	47	79

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	455	ILE

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Mol	Chain	Res	Type
1	G	616	ARG
2	F	397	ILE
1	A	660	CYS
1	G	715	THR

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	509/712 (72%)	496 (97%)	13 (3%)	46	69
1	D	465/712 (65%)	458 (98%)	7 (2%)	65	81
1	G	469/712 (66%)	459 (98%)	10 (2%)	53	74
1	J	462/712 (65%)	454 (98%)	8 (2%)	60	78
2	B	332/444 (75%)	325 (98%)	7 (2%)	53	74
2	C	352/444 (79%)	348 (99%)	4 (1%)	73	85
2	E	297/444 (67%)	294 (99%)	3 (1%)	76	86
2	F	348/444 (78%)	343 (99%)	5 (1%)	67	81
2	H	307/444 (69%)	300 (98%)	7 (2%)	50	72
2	I	331/444 (74%)	329 (99%)	2 (1%)	86	92
2	K	328/444 (74%)	321 (98%)	7 (2%)	53	74
2	L	375/444 (84%)	370 (99%)	5 (1%)	69	82
All	All	4575/6400 (72%)	4497 (98%)	78 (2%)	60	78

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	704	LYS
2	H	658	CYS
1	A	923	ILE
1	D	991	ARG
2	H	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	641	ASN
2	H	485	ASN
2	B	632	HIS
2	H	353	ASN
2	H	408	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	701/776 (90%)	-0.14	5 (0%) 87 83	86, 110, 163, 211	0
1	D	683/776 (88%)	-0.13	8 (1%) 79 72	89, 128, 188, 213	0
1	G	683/776 (88%)	-0.14	5 (0%) 87 83	81, 108, 195, 233	0
1	J	681/776 (87%)	-0.16	6 (0%) 84 79	91, 118, 146, 174	0
2	B	429/465 (92%)	-0.22	2 (0%) 91 87	66, 111, 155, 177	0
2	C	444/465 (95%)	-0.12	3 (0%) 87 83	72, 114, 151, 172	0
2	E	414/465 (89%)	-0.26	2 (0%) 91 87	67, 109, 139, 161	0
2	F	442/465 (95%)	-0.20	1 (0%) 95 94	86, 104, 125, 136	0
2	H	420/465 (90%)	-0.31	1 (0%) 95 94	73, 103, 141, 160	0
2	I	437/465 (93%)	-0.19	3 (0%) 87 83	80, 112, 146, 161	0
2	K	431/465 (92%)	-0.13	7 (1%) 72 64	80, 116, 151, 168	0
2	L	441/465 (94%)	-0.27	0 100 100	80, 99, 127, 156	0
All	All	6206/6824 (90%)	-0.18	43 (0%) 87 83	66, 112, 160, 233	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1036	THR	4.8
2	K	246	LEU	4.3
2	B	226	HIS	4.2
2	K	277	PHE	3.9
1	A	716	CYS	3.5

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.