



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 30, 2026 – 01:22 pm BST

PDB ID : 9SYQ / pdb_00009syq
Title : Structure of *S. pombe* Pta1 - Ssu72 - PNUTS - Swd2.2 complex - crystal form 1
Authors : Au, H.C.A.; Balikci, E.; Kus, K.; Grimes, J.M.; Vasiljeva, L.
Deposited on : 2025-10-13
Resolution : 3.79 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 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

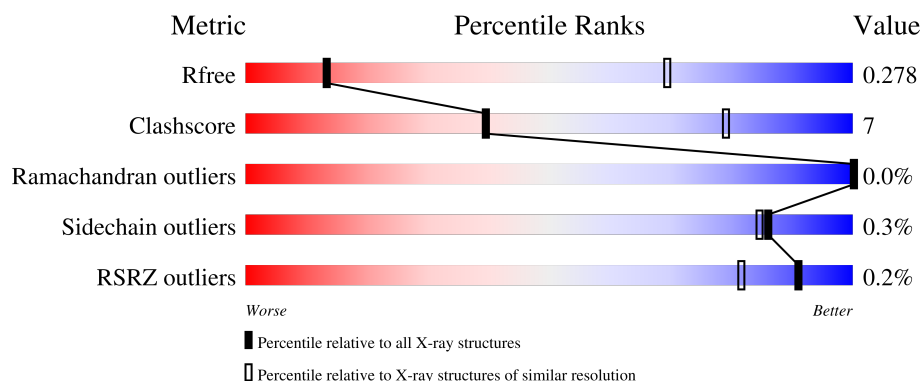
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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.



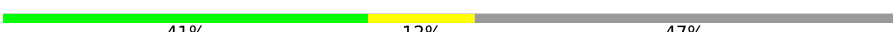
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	341	 84% 16% .
1	B	341	 84% 15% .
1	C	341	 84% 15% .
1	D	341	 84% 14% .
2	E	313	 73% 17% 10% .

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Mol	Chain	Length	Quality of chain
2	F	313	 69%22%9%
2	G	313	 79%12%9%
2	H	313	 73%17%10%
3	I	197	 41%12%47%
3	J	197	 41%8%52%
3	K	197	 40%11%49%
3	L	197	 45%7%48%
4	M	87	 84%6%10%
4	N	87	 84%6%10%
4	O	87	 85%6%9%
4	P	87	 89%1%9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51122 atoms, of which 25507 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 Uncharacterized WD repeat-containing protein C824.04.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	339	Total	C	H	N	O	S	0	0	0
			5307	1718	2605	457	517	10			
1	B	338	Total	C	H	N	O	S	0	0	0
			5287	1712	2593	456	516	10			
1	C	339	Total	C	H	N	O	S	0	0	0
			5307	1718	2605	457	517	10			
1	D	334	Total	C	H	N	O	S	0	0	0
			5223	1689	2565	447	512	10			

- Molecule 2 is a protein called mRNA cleavage and polyadenylation specificity factor complex subunit pta1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	282	Total	C	H	N	O	S	0	0	0
			4561	1439	2322	375	416	9			
2	F	284	Total	C	H	N	O	S	0	0	0
			4598	1451	2343	377	418	9			
2	G	285	Total	C	H	N	O	S	0	0	0
			4612	1455	2349	379	420	9			
2	H	283	Total	C	H	N	O	S	0	0	0
			4592	1449	2340	377	417	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	308	GLU	-	expression tag	UNP Q10222
E	309	ASP	-	expression tag	UNP Q10222
E	310	LEU	-	expression tag	UNP Q10222
E	311	TYR	-	expression tag	UNP Q10222
E	312	PHE	-	expression tag	UNP Q10222
E	313	GLN	-	expression tag	UNP Q10222
F	308	GLU	-	expression tag	UNP Q10222
F	309	ASP	-	expression tag	UNP Q10222

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Chain	Residue	Modelled	Actual	Comment	Reference
F	310	LEU	-	expression tag	UNP Q10222
F	311	TYR	-	expression tag	UNP Q10222
F	312	PHE	-	expression tag	UNP Q10222
F	313	GLN	-	expression tag	UNP Q10222
G	308	GLU	-	expression tag	UNP Q10222
G	309	ASP	-	expression tag	UNP Q10222
G	310	LEU	-	expression tag	UNP Q10222
G	311	TYR	-	expression tag	UNP Q10222
G	312	PHE	-	expression tag	UNP Q10222
G	313	GLN	-	expression tag	UNP Q10222
H	308	GLU	-	expression tag	UNP Q10222
H	309	ASP	-	expression tag	UNP Q10222
H	310	LEU	-	expression tag	UNP Q10222
H	311	TYR	-	expression tag	UNP Q10222
H	312	PHE	-	expression tag	UNP Q10222
H	313	GLN	-	expression tag	UNP Q10222

- Molecule 3 is a protein called RNA polymerase II subunit A C-terminal domain phosphatase ssu72.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	104	Total	C	H	N	O	S	0	0	0
			1678	541	826	140	167	4			
3	J	95	Total	C	H	N	O	S	0	0	0
			1530	490	760	127	149	4			
3	K	101	Total	C	H	N	O	S	0	0	0
			1619	522	801	133	158	5			
3	L	103	Total	C	H	N	O	S	0	0	0
			1651	529	817	137	164	4			

- Molecule 4 is a protein called Cleavage and polyadenylation factor complex subunit C74.02c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	M	78	Total	C	H	N	O	S	0	0	0
			1280	408	640	109	122	1			
4	N	78	Total	C	H	N	O	S	0	0	0
			1279	408	639	109	122	1			
4	O	79	Total	C	H	N	O	S	0	0	0
			1299	413	651	110	123	2			
4	P	79	Total	C	H	N	O	S	0	0	0
			1299	413	651	110	123	2			

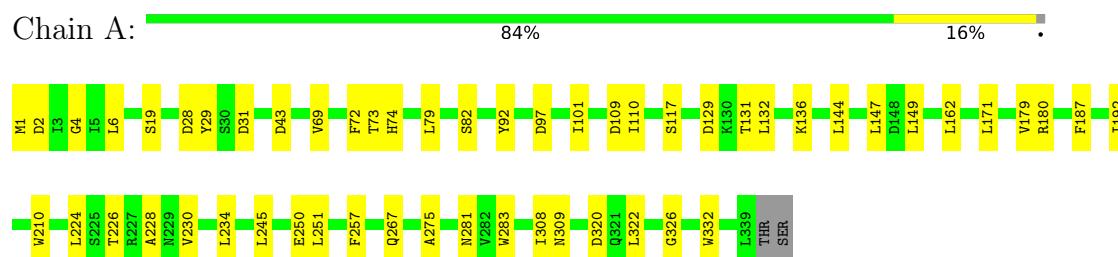
There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	MET	-	initiating methionine	UNP O74535
M	82	GLU	-	expression tag	UNP O74535
M	83	ASP	-	expression tag	UNP O74535
M	84	LEU	-	expression tag	UNP O74535
M	85	TYR	-	expression tag	UNP O74535
M	86	PHE	-	expression tag	UNP O74535
M	87	GLN	-	expression tag	UNP O74535
N	1	MET	-	initiating methionine	UNP O74535
N	82	GLU	-	expression tag	UNP O74535
N	83	ASP	-	expression tag	UNP O74535
N	84	LEU	-	expression tag	UNP O74535
N	85	TYR	-	expression tag	UNP O74535
N	86	PHE	-	expression tag	UNP O74535
N	87	GLN	-	expression tag	UNP O74535
O	1	MET	-	initiating methionine	UNP O74535
O	82	GLU	-	expression tag	UNP O74535
O	83	ASP	-	expression tag	UNP O74535
O	84	LEU	-	expression tag	UNP O74535
O	85	TYR	-	expression tag	UNP O74535
O	86	PHE	-	expression tag	UNP O74535
O	87	GLN	-	expression tag	UNP O74535
P	1	MET	-	initiating methionine	UNP O74535
P	82	GLU	-	expression tag	UNP O74535
P	83	ASP	-	expression tag	UNP O74535
P	84	LEU	-	expression tag	UNP O74535
P	85	TYR	-	expression tag	UNP O74535
P	86	PHE	-	expression tag	UNP O74535
P	87	GLN	-	expression tag	UNP O74535

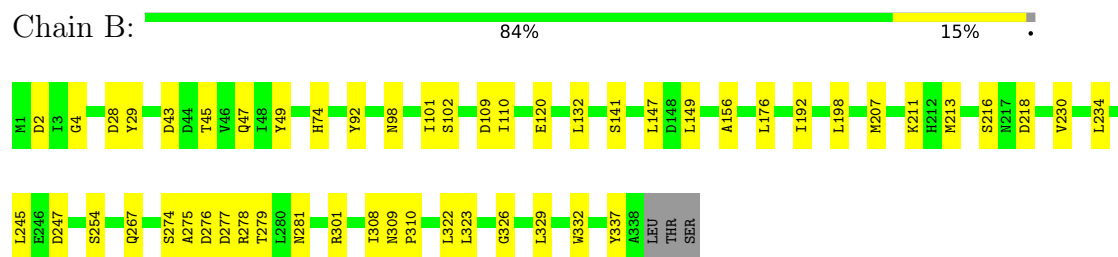
3 Residue-property plots [i](#)

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.

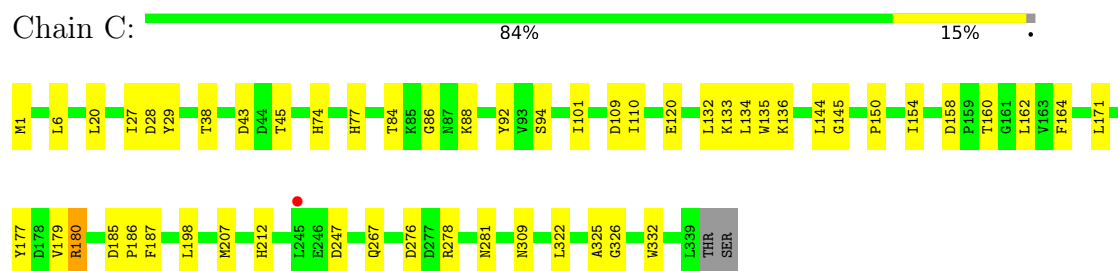
• Molecule 1: Uncharacterized WD repeat-containing protein C824.04



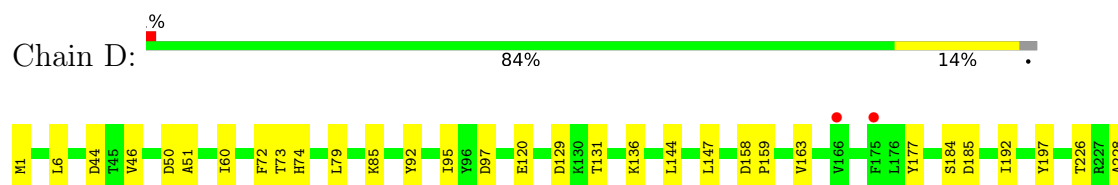
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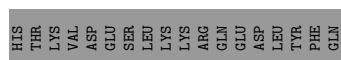
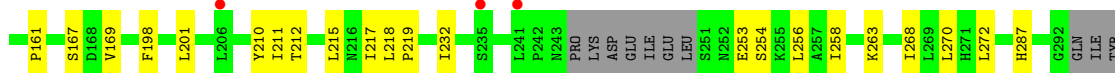
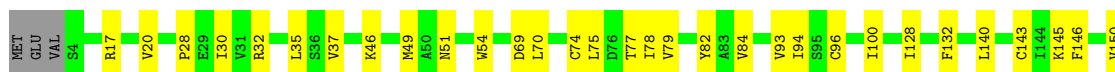
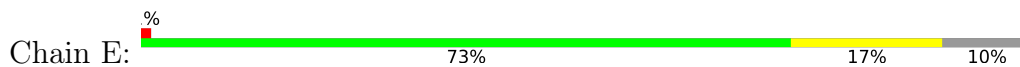


• Molecule 1: Uncharacterized WD repeat-containing protein C824.04

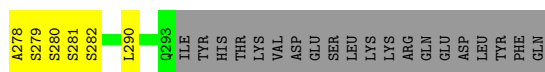




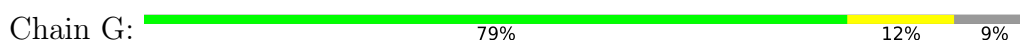
- Molecule 2: mRNA cleavage and polyadenylation specificity factor complex subunit pta1



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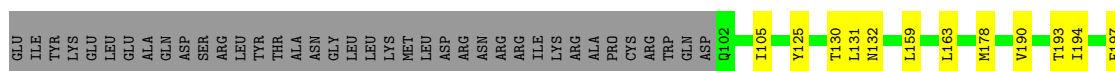
- Molecule 2: mRNA cleavage and polyadenylation specificity factor complex subunit pta1



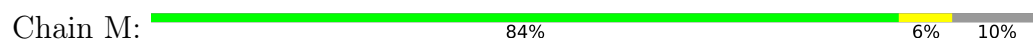
- Molecule 2: mRNA cleavage and polyadenylation specificity factor complex subunit pta1



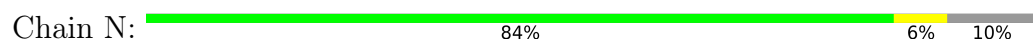
MET	ALA	PRO	LYS	T5	N6	VII	ILE	CYS	ALA	ASN	GLN	ASN	ARG	SER	LYS	ASN	ALA	GLY	TYR	GLN	VAL	VAL	ASP	SER	PHE	GLY	THR	GLY	SER	ALA	VAL	ARG	LEU	PRO	PRO	PRO	TYR	ASP
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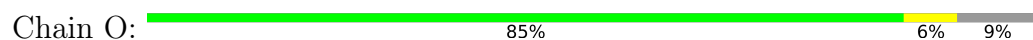
- Molecule 4: Cleavage and polyadenylation factor complex subunit C74.02c



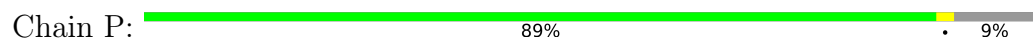
- Molecule 4: Cleavage and polyadenylation factor complex subunit C74.02c



- Molecule 4: Cleavage and polyadenylation factor complex subunit C74.02c



- Molecule 4: Cleavage and polyadenylation factor complex subunit C74.02c



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	217.04Å 217.04Å 189.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.46 – 3.79 71.46 – 3.79	Depositor EDS
% Data completeness (in resolution range)	83.4 (71.46-3.79) 83.3 (71.46-3.79)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.224 , 0.280 0.226 , 0.278	Depositor DCC
R_{free} test set	1976 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	150.5	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 98.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	51122	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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

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	0.14	0/2774	0.33	0/3771
1	B	0.13	0/2766	0.34	0/3760
1	C	0.13	0/2774	0.33	0/3771
1	D	0.11	0/2726	0.30	0/3706
2	E	0.15	0/2279	0.30	0/3088
2	F	0.15	0/2295	0.30	0/3110
2	G	0.13	0/2303	0.28	0/3121
2	H	0.12	0/2291	0.26	0/3103
3	I	0.14	0/868	0.30	0/1176
3	J	0.12	0/782	0.27	0/1056
3	K	0.17	0/832	0.32	0/1127
3	L	0.12	0/848	0.28	0/1148
4	M	0.15	0/655	0.29	0/886
4	N	0.13	0/655	0.27	0/886
4	O	0.11	0/663	0.24	0/896
4	P	0.10	0/663	0.24	0/896
All	All	0.14	0/26174	0.30	0/35501

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	180	ARG	Sidechain

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	2702	2605	2604	44	0
1	B	2694	2593	2593	37	0
1	C	2702	2605	2604	37	0
1	D	2658	2565	2564	29	0
2	E	2239	2322	2321	47	0
2	F	2255	2343	2343	45	0
2	G	2263	2349	2349	28	0
2	H	2252	2340	2340	40	0
3	I	852	826	825	21	0
3	J	770	760	759	13	0
3	K	818	801	799	18	0
3	L	834	817	817	14	0
4	M	640	640	639	6	0
4	N	640	639	639	9	0
4	O	648	651	651	4	0
4	P	648	651	651	2	0
All	All	25615	25507	25498	344	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 7.

The worst 5 of 344 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)
3:L:159:LEU:HD11	3:L:178:MET:HE1	1.60	0.83
4:O:68:ASP:OD1	4:O:70:SER:OG	1.95	0.83
2:F:256:LEU:HD21	3:K:190:VAL:HG13	1.59	0.82
2:F:147:ILE:HG23	2:F:193:LEU:HD22	1.62	0.81
2:E:28:PRO:HA	2:E:70:LEU:HD11	1.63	0.79

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	337/341 (99%)	310 (92%)	27 (8%)	0	100	100
1	B	336/341 (98%)	314 (94%)	22 (6%)	0	100	100
1	C	337/341 (99%)	307 (91%)	30 (9%)	0	100	100
1	D	330/341 (97%)	311 (94%)	19 (6%)	0	100	100
2	E	278/313 (89%)	270 (97%)	8 (3%)	0	100	100
2	F	280/313 (90%)	264 (94%)	15 (5%)	1 (0%)	30	62
2	G	281/313 (90%)	275 (98%)	6 (2%)	0	100	100
2	H	277/313 (88%)	273 (99%)	4 (1%)	0	100	100
3	I	100/197 (51%)	97 (97%)	3 (3%)	0	100	100
3	J	89/197 (45%)	82 (92%)	7 (8%)	0	100	100
3	K	95/197 (48%)	92 (97%)	3 (3%)	0	100	100
3	L	99/197 (50%)	97 (98%)	2 (2%)	0	100	100
4	M	76/87 (87%)	73 (96%)	3 (4%)	0	100	100
4	N	76/87 (87%)	73 (96%)	3 (4%)	0	100	100
4	O	77/87 (88%)	76 (99%)	1 (1%)	0	100	100
4	P	77/87 (88%)	72 (94%)	5 (6%)	0	100	100
All	All	3145/3752 (84%)	2986 (95%)	158 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	280	SER

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	306/308 (99%)	305 (100%)	1 (0%)	86	84
1	B	305/308 (99%)	305 (100%)	0	100	100
1	C	306/308 (99%)	305 (100%)	1 (0%)	86	84
1	D	302/308 (98%)	301 (100%)	1 (0%)	86	84
2	E	265/296 (90%)	264 (100%)	1 (0%)	84	83
2	F	267/296 (90%)	266 (100%)	1 (0%)	84	83
2	G	268/296 (90%)	267 (100%)	1 (0%)	84	83
2	H	267/296 (90%)	267 (100%)	0	100	100
3	I	96/175 (55%)	96 (100%)	0	100	100
3	J	88/175 (50%)	88 (100%)	0	100	100
3	K	93/175 (53%)	91 (98%)	2 (2%)	45	63
3	L	95/175 (54%)	95 (100%)	0	100	100
4	M	73/82 (89%)	73 (100%)	0	100	100
4	N	73/82 (89%)	73 (100%)	0	100	100
4	O	74/82 (90%)	74 (100%)	0	100	100
4	P	74/82 (90%)	74 (100%)	0	100	100
All	All	2952/3444 (86%)	2944 (100%)	8 (0%)	86	84

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	112	CYS
3	K	13	CYS
2	F	98	CYS
2	E	258	ILE
2	G	98	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	264	ASN
3	K	107	ASN

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Mol	Chain	Res	Type
3	I	161	ASN
3	K	184	ASN
1	C	300	HIS

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](#)

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	339/341 (99%)	-0.70	0	100	100	128, 143, 173, 194	0
1	B	338/341 (99%)	-0.69	0	100	100	128, 153, 182, 204	0
1	C	339/341 (99%)	-0.66	1 (0%)	90	78	145, 163, 192, 213	0
1	D	334/341 (97%)	-0.64	2 (0%)	85	68	156, 201, 227, 262	0
2	E	282/313 (90%)	-0.47	3 (1%)	78	56	128, 158, 201, 257	0
2	F	284/313 (90%)	-0.62	0	100	100	132, 156, 213, 256	0
2	G	285/313 (91%)	-0.50	0	100	100	145, 178, 230, 272	0
2	H	283/313 (90%)	-0.72	0	100	100	157, 191, 237, 261	0
3	I	104/197 (52%)	-0.42	0	100	100	137, 187, 236, 248	0
3	J	95/197 (48%)	-0.57	0	100	100	194, 219, 266, 286	0
3	K	101/197 (51%)	-0.61	0	100	100	141, 177, 198, 218	0
3	L	103/197 (52%)	-0.60	0	100	100	162, 200, 263, 301	0
4	M	78/87 (89%)	-0.73	0	100	100	133, 149, 170, 178	0
4	N	78/87 (89%)	-0.80	0	100	100	135, 154, 172, 184	0
4	O	79/87 (90%)	-0.87	0	100	100	151, 171, 189, 205	0
4	P	79/87 (90%)	-0.61	0	100	100	168, 208, 228, 239	0
All	All	3201/3752 (85%)	-0.63	6 (0%)	91	81	128, 169, 226, 301	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	206	LEU	3.0
1	D	175	PHE	2.9
1	D	166	VAL	2.4
2	E	241	LEU	2.3
2	E	235	SER	2.3

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.