



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:45 AM UTC

PDB ID : 5LSB / pdb_00005lsb
Title : Crystal structure of yeast Hsh49p in complex with Cus1p binding domain.
Authors : van Roon, A.M.; Obayashi, E.; Sposito, B.; Oubridge, C.; Nagai, K.
Deposited on : 2016-08-24
Resolution : 2.70 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

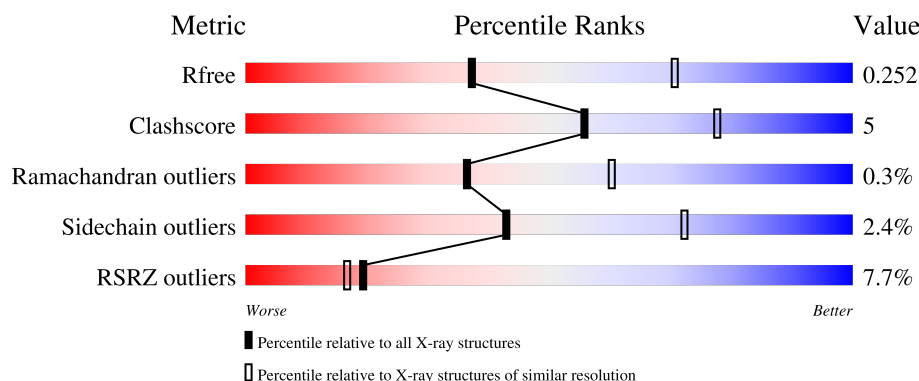
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	215	4% 71% 9% 18%
1	C	215	8% 71% 8% 18%
1	F	215	9% 69% 11% 19%
2	B	84	5% 65% 8% 26%
2	D	84	4% 68% 6% 26%

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Mol	Chain	Length	Quality of chain
2	H	84	4% 73% 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5799 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 Protein HSH49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1451	943	243	263	2			
1	C	176	Total	C	N	O	S	0	0	0
			1451	943	243	263	2			
1	F	174	Total	C	N	O	S	0	0	0
			1439	937	240	260	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q99181
A	0	GLY	-	expression tag	UNP Q99181
A	1	SER	-	expression tag	UNP Q99181
C	-1	GLY	-	expression tag	UNP Q99181
C	0	GLY	-	expression tag	UNP Q99181
C	1	SER	-	expression tag	UNP Q99181
F	-1	GLY	-	expression tag	UNP Q99181
F	0	GLY	-	expression tag	UNP Q99181
F	1	SER	-	expression tag	UNP Q99181

- Molecule 2 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	62	Total	C	N	O	S	0	0	0
			484	312	83	85	4			
2	D	62	Total	C	N	O	S	0	0	0
			484	312	83	85	4			
2	H	62	Total	C	N	O	S	0	0	0
			484	312	83	85	4			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	285	MET	-	initiating methionine	UNP Q02554
B	286	ALA	-	expression tag	UNP Q02554
B	287	VAL	-	expression tag	UNP Q02554
B	288	GLY	-	expression tag	UNP Q02554
B	289	SER	-	expression tag	UNP Q02554
D	285	MET	-	initiating methionine	UNP Q02554
D	286	ALA	-	expression tag	UNP Q02554
D	287	VAL	-	expression tag	UNP Q02554
D	288	GLY	-	expression tag	UNP Q02554
D	289	SER	-	expression tag	UNP Q02554
H	285	MET	-	initiating methionine	UNP Q02554
H	286	ALA	-	expression tag	UNP Q02554
H	287	VAL	-	expression tag	UNP Q02554
H	288	GLY	-	expression tag	UNP Q02554
H	289	SER	-	expression tag	UNP Q02554

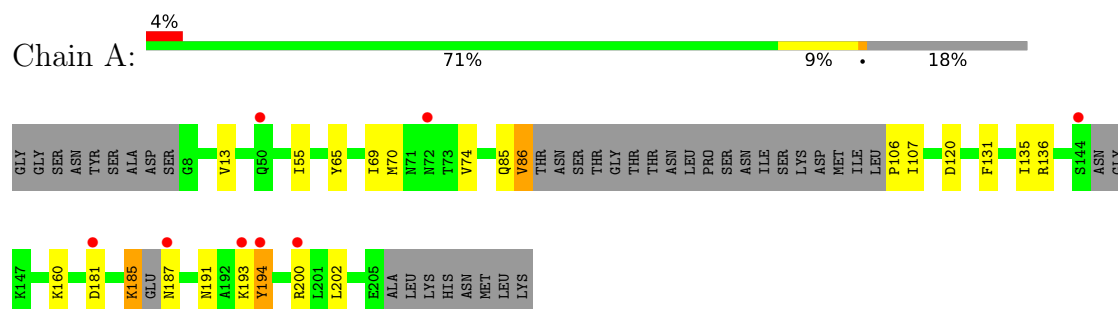
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	H	2	Total O 2 2	0	0

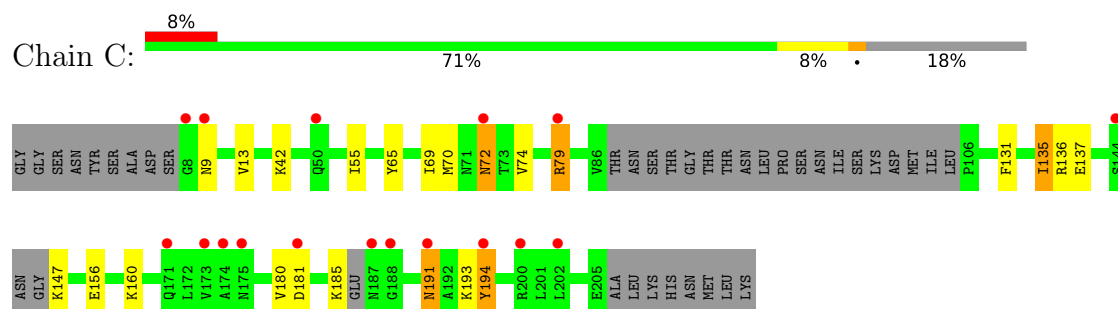
3 Residue-property plots [i](#)

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.

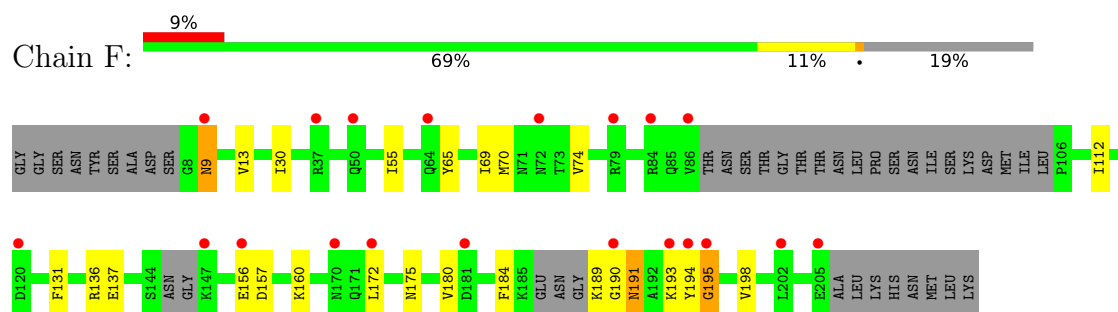
• Molecule 1: Protein HSH49



• Molecule 1: Protein HSH49



• Molecule 1: Protein HSH49

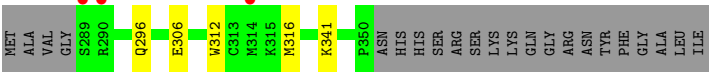


• Molecule 2: Cold sensitive U2 snRNA suppressor 1





● Molecule 2: Cold sensitive U2 snRNA suppressor 1



● Molecule 2: Cold sensitive U2 snRNA suppressor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	142.08Å 142.08Å 40.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.52 – 2.70 35.52 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.52-2.70) 100.0 (35.52-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.184 , 0.233 0.211 , 0.252	Depositor DCC
R_{free} test set	1301 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.005 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.638 for H, K, L \\ 0.362 for -K, -H, -L \	Depositor
Outliers	0 of 24999 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5799	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% 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	0.70	0/1475	0.88	1/1982 (0.1%)
1	C	0.62	0/1475	0.88	0/1982
1	F	0.63	0/1463	0.95	2/1966 (0.1%)
2	B	0.70	0/496	0.91	1/672 (0.1%)
2	D	0.68	0/496	0.85	0/672
2	H	0.68	0/496	0.84	0/672
All	All	0.66	0/5901	0.89	4/7946 (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
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	184	PHE	N-CA-C	14.15	126.21	111.07
1	F	195	GLY	N-CA-C	-10.70	99.90	112.73
2	B	335	TRP	CA-CB-CG	6.76	126.44	113.60
1	A	86	VAL	N-CA-CB	5.20	120.34	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	C	194	TYR	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	1451	0	1480	10	0
1	C	1451	0	1480	15	0
1	F	1439	0	1471	22	0
2	B	484	0	502	6	0
2	D	484	0	502	2	0
2	H	484	0	502	1	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	H	2	0	0	0	0
All	All	5799	0	5937	55	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 5.

All (55) 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:C:185:LYS:HE2	1:C:194:TYR:OH	1.50	1.11
1:F:172:LEU:HD11	1:F:175:ASN:HA	1.43	0.98
1:F:190:GLY:N	1:F:194:TYR:CE2	2.39	0.91
1:C:136:ARG:NH1	1:C:137:GLU:O	2.12	0.83
1:F:136:ARG:NH1	1:F:137:GLU:O	2.13	0.81
1:F:190:GLY:N	1:F:194:TYR:HE2	1.77	0.81
2:B:316:MET:HE3	2:B:322:PRO:HD3	1.64	0.79
1:F:112:ILE:HD12	1:F:180:VAL:HG22	1.68	0.76
1:C:185:LYS:CE	1:C:194:TYR:OH	2.32	0.76
1:A:70:MET:HE1	1:A:74:VAL:HG21	1.73	0.69
1:C:70:MET:HE1	1:C:74:VAL:HG21	1.75	0.67
1:C:180:VAL:O	1:C:181:ASP:OD1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:LEU:HD11	1:F:175:ASN:CA	2.24	0.65
2:B:316:MET:CE	2:B:321:LEU:HD23	2.28	0.63
1:F:70:MET:HE1	1:F:74:VAL:HG21	1.79	0.63
1:F:112:ILE:CD1	1:F:180:VAL:HG13	2.32	0.60
1:A:135:ILE:HG23	1:A:136:ARG:HG2	1.85	0.59
1:A:85:GLN:O	1:A:86:VAL:HG12	2.03	0.57
1:A:106:PRO:HG2	1:A:200:ARG:HD2	1.87	0.56
1:F:195:GLY:O	1:F:198:VAL:N	2.38	0.56
2:B:296:GLN:NE2	2:B:306:GLU:OE2	2.39	0.56
2:B:316:MET:CE	2:B:322:PRO:HD3	2.36	0.54
1:F:189:LYS:HA	1:F:194:TYR:CE2	2.44	0.51
2:B:316:MET:HE2	2:B:321:LEU:HD23	1.92	0.50
1:A:191:ASN:ND2	1:A:194:TYR:CE2	2.80	0.49
1:C:72:ASN:HD22	1:C:72:ASN:N	2.10	0.49
1:F:156:GLU:HG3	1:F:157:ASP:N	2.27	0.49
1:C:79:ARG:HD3	1:C:193:LYS:CE	2.43	0.49
1:F:189:LYS:HA	1:F:194:TYR:HE2	1.78	0.48
2:D:296:GLN:NE2	2:D:306:GLU:OE2	2.41	0.48
1:F:156:GLU:HG3	1:F:157:ASP:HB2	1.96	0.48
1:A:70:MET:HE1	1:A:74:VAL:CG2	2.42	0.48
1:C:13:VAL:HG21	1:C:55:ILE:HD12	1.96	0.48
1:F:30:ILE:HD11	2:H:289:SER:HB3	1.95	0.47
1:C:135:ILE:HG12	1:C:156:GLU:HG2	1.95	0.47
1:F:193:LYS:C	1:F:195:GLY:H	2.22	0.46
1:F:9:ASN:OD1	1:F:9:ASN:N	2.48	0.46
1:A:13:VAL:HG21	1:A:55:ILE:HD12	1.98	0.46
2:D:312:TRP:HD1	2:D:316:MET:HE3	1.81	0.46
1:C:70:MET:HE1	1:C:74:VAL:CG2	2.44	0.45
1:C:191:ASN:HB2	1:C:194:TYR:CE2	2.53	0.44
1:F:70:MET:HE1	1:F:74:VAL:CG2	2.47	0.44
2:B:316:MET:HE1	2:B:330:ILE:HD11	2.00	0.43
1:C:65:TYR:CZ	1:C:69:ILE:HG13	2.53	0.43
1:F:13:VAL:HG21	1:F:55:ILE:HD12	2.00	0.43
1:F:131:PHE:O	1:F:160:LYS:HD2	2.18	0.43
1:F:190:GLY:N	1:F:194:TYR:CD2	2.78	0.43
1:C:79:ARG:HH11	1:C:193:LYS:HE2	1.83	0.42
1:A:131:PHE:O	1:A:160:LYS:HD2	2.19	0.42
1:C:79:ARG:NH1	1:C:193:LYS:HE2	2.34	0.42
1:C:131:PHE:O	1:C:160:LYS:HD2	2.19	0.42
1:A:65:TYR:CZ	1:A:69:ILE:HG13	2.55	0.42
1:A:185:LYS:HD2	1:A:194:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:TYR:CZ	1:F:69:ILE:HG13	2.56	0.41
1:F:191:ASN:N	1:F:194:TYR:CD2	2.89	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	168/215 (78%)	162 (96%)	6 (4%)	0	100	100
1	C	168/215 (78%)	160 (95%)	7 (4%)	1 (1%)	21	44
1	F	166/215 (77%)	157 (95%)	8 (5%)	1 (1%)	21	44
2	B	60/84 (71%)	59 (98%)	1 (2%)	0	100	100
2	D	60/84 (71%)	59 (98%)	1 (2%)	0	100	100
2	H	60/84 (71%)	58 (97%)	2 (3%)	0	100	100
All	All	682/897 (76%)	655 (96%)	25 (4%)	2 (0%)	36	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	191	ASN
1	F	191	ASN

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	156/189 (82%)	149 (96%)	7 (4%)	24	52
1	C	156/189 (82%)	150 (96%)	6 (4%)	29	58
1	F	155/189 (82%)	154 (99%)	1 (1%)	78	91
2	B	53/70 (76%)	53 (100%)	0	100	100
2	D	53/70 (76%)	52 (98%)	1 (2%)	50	77
2	H	53/70 (76%)	53 (100%)	0	100	100
All	All	626/777 (81%)	611 (98%)	15 (2%)	43	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	120	ASP
1	A	181	ASP
1	A	185	LYS
1	A	187	ASN
1	A	193	LYS
1	A	202	LEU
1	C	9	ASN
1	C	42	LYS
1	C	72	ASN
1	C	79	ARG
1	C	135	ILE
1	C	147	LYS
2	D	341	LYS
1	F	9	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	170	ASN
2	B	303	ASN
1	C	9	ASN
1	C	47	GLN
1	C	170	ASN
1	F	64	GLN
1	F	170	ASN
1	F	176	ASN

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	176/215 (81%)	0.29	8 (4%) 38 34	11, 24, 38, 51	1 (0%)
1	C	176/215 (81%)	0.61	17 (9%) 13 11	17, 31, 52, 67	1 (0%)
1	F	174/215 (80%)	0.76	20 (11%) 9 8	19, 32, 52, 61	1 (0%)
2	B	62/84 (73%)	0.33	4 (6%) 25 22	10, 23, 41, 56	0
2	D	62/84 (73%)	0.31	3 (4%) 35 32	16, 27, 45, 59	0
2	H	62/84 (73%)	0.63	3 (4%) 35 32	23, 36, 57, 69	0
All	All	712/897 (79%)	0.52	55 (7%) 19 17	10, 29, 50, 69	3 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	194	TYR	7.3
1	C	175	ASN	5.4
1	C	50	GLN	4.2
1	F	195	GLY	4.1
1	C	194	TYR	3.8
1	F	72	ASN	3.5
1	C	187	ASN	3.4
1	A	50	GLN	3.3
1	F	156	GLU	3.2
1	A	194	TYR	3.1
1	F	50	GLN	3.1
1	F	86	VAL	3.1
2	B	318	ASP	3.1
1	C	174	ALA	3.0
1	A	187	ASN	3.0
1	F	64	GLN	3.0
1	F	202	LEU	2.9
1	A	200	ARG	2.9
1	C	181	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	314	MET	2.8
1	F	193	LYS	2.8
2	B	307	GLY	2.8
1	F	79	ARG	2.8
1	C	191	ASN	2.7
2	D	290	ARG	2.7
1	F	120	ASP	2.5
1	C	9	ASN	2.5
1	C	72	ASN	2.4
2	H	293	ARG	2.4
2	D	314	MET	2.4
2	D	289	SER	2.4
1	F	181	ASP	2.4
2	B	319	ILE	2.4
1	C	171	GLN	2.4
2	H	297	GLU	2.4
1	F	147	LYS	2.4
1	F	37	ARG	2.4
1	F	172	LEU	2.3
1	F	9	ASN	2.3
1	C	144	SER	2.3
1	C	200	ARG	2.3
1	F	84	ARG	2.3
1	A	181	ASP	2.2
2	H	314	MET	2.2
1	C	79	ARG	2.2
1	C	202	LEU	2.2
1	A	144	SER	2.2
1	C	173	VAL	2.2
1	C	8	GLY	2.1
1	C	188	GLY	2.1
1	F	170	ASN	2.1
1	F	205	GLU	2.1
1	F	190	GLY	2.1
1	A	193	LYS	2.1
1	A	72	ASN	2.0

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

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.