



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:54 AM GMT

PDB ID : 4C8Q  
Title : Crystal structure of the yeast Lsm1-7-Pat1 complex  
Authors : Sharif, H.; Conti, E.  
Deposited on : 2013-10-01  
Resolution : 3.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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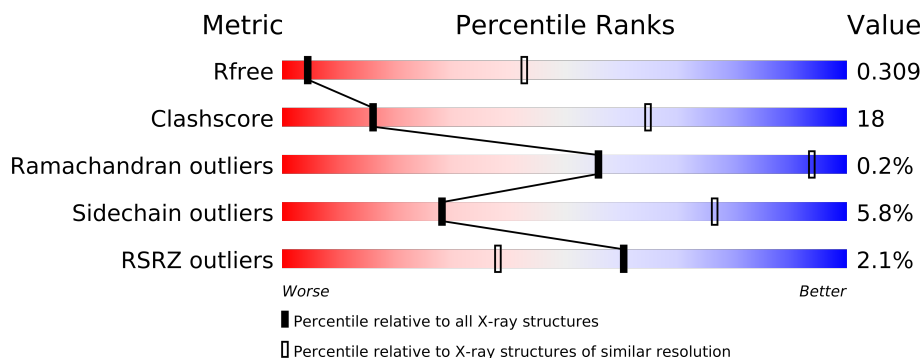
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.70 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))
$R_{free}$	66092	1098 (4.00-3.40)
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	101	
2	B	105	
3	C	89	
4	D	114	
5	E	93	
6	F	86	
7	G	115	
8	H	328	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6280 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SM-LIKE PROTEIN LSM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			673	428	115	125	5			

- Molecule 2 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			796	505	134	154	3			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	EXPRESSION TAG	UNP P38203
B	-8	GLU	-	EXPRESSION TAG	UNP P38203
B	-7	ASN	-	EXPRESSION TAG	UNP P38203
B	-6	LEU	-	EXPRESSION TAG	UNP P38203
B	-5	TYR	-	EXPRESSION TAG	UNP P38203
B	-4	PHE	-	EXPRESSION TAG	UNP P38203
B	-3	GLN	-	EXPRESSION TAG	UNP P38203
B	-2	GLY	-	EXPRESSION TAG	UNP P38203
B	-1	SER	-	EXPRESSION TAG	UNP P38203
B	0	GLY	-	EXPRESSION TAG	UNP P38203
B	1	SER	-	EXPRESSION TAG	UNP P38203

- Molecule 3 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	79	Total	C	N	O	S	0	0	0
			589	369	105	112	3			

- Molecule 4 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	81	Total	C	N	O	S	0	0	0
			504	321	85	97	1			

- Molecule 5 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	83	Total	C	N	O	S	0	0	0
			600	383	104	111	2			

- Molecule 6 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	77	Total	C	N	O	S	0	0	0
			571	361	95	113	2			

- Molecule 7 is a protein called U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	69	Total	C	N	O	S	0	0	0
			456	289	79	87	1			

- Molecule 8 is a protein called DNA TOPOISOMERASE 2-ASSOCIATED PROTEIN PAT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	279	Total	C	N	O	S	0	0	0
			2089	1366	332	384	7			

- Molecule 9 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	Co	0	0
			1	1		
9	C	1	Total	Co	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

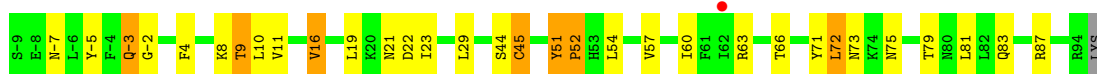
- Molecule 1: SM-LIKE PROTEIN LSM1

Chain A: 



- Molecule 2: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM2

Chain B: 



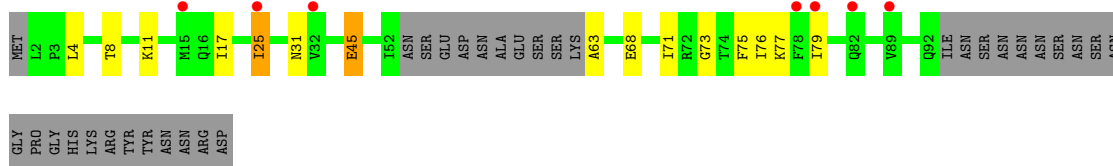
- Molecule 3: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM3

Chain C: 



- Molecule 4: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM4

Chain D: 



- Molecule 5: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM5

Chain E: 



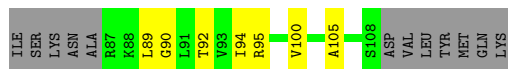
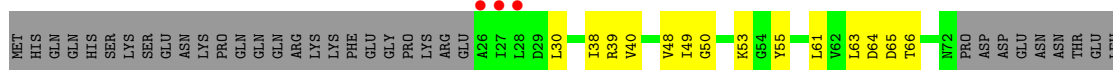
- Molecule 6: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM6

Chain F: 



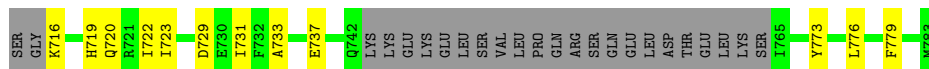
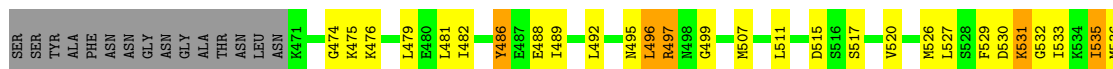
• Molecule 7: U6 SNRNA-ASSOCIATED SM-LIKE PROTEIN LSM7

Chain G:



• Molecule 8: DNA TOPOISOMERASE 2-ASSOCIATED PROTEIN PAT1

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	258.69Å 258.69Å 47.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.42 – 3.70 84.68 – 3.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (43.42-3.70) 99.3 (84.68-3.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.67Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.249 , 0.295 0.272 , 0.309	Depositor DCC
$R_{free}$ test set	988 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	135.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 95.3	EDS
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 19814 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
CO

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	0.41	1/684 (0.1%)	0.81	1/929 (0.1%)
2	B	0.35	0/806	0.73	2/1093 (0.2%)
3	C	0.43	0/594	0.85	2/807 (0.2%)
4	D	0.35	0/509	0.77	0/698
5	E	0.37	0/609	0.78	0/831
6	F	0.38	0/578	0.73	0/784
7	G	0.33	0/456	0.85	1/618 (0.2%)
8	H	0.33	0/2120	0.54	1/2881 (0.0%)
All	All	0.36	1/6356 (0.0%)	0.71	7/8641 (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
8	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	PRO	N-CD	5.08	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	75	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	122	GLN	C-N-CD	5.72	140.40	128.40
7	G	61	LEU	CA-CB-CG	5.40	127.71	115.30
8	H	499	GLY	N-CA-C	-5.40	99.61	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	43	ASP	CB-CG-OD2	5.25	123.02	118.30
2	B	51	TYR	C-N-CD	-5.13	109.30	120.60
2	B	72	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	496	LEU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	673	0	558	36	0
2	B	796	0	755	22	0
3	C	589	0	565	23	0
4	D	504	0	370	15	0
5	E	600	0	558	24	0
6	F	571	0	530	16	0
7	G	456	0	428	24	0
8	H	2089	0	1978	78	0
9	C	1	0	0	0	0
9	H	1	0	0	0	0
All	All	6280	0	5742	220	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (220) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:72:ASP:HA	1:A:75:ALA:HA	1.29	1.07
5:E:73:LEU:HD13	5:E:78:ILE:HD11	1.27	1.05
1:A:72:ASP:HA	1:A:75:ALA:CA	1.92	0.99
3:C:30:LEU:HD12	3:C:31:GLN:N	1.80	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:4:PRO:HG3	6:F:40:SER:CB	1.96	0.95
5:E:73:LEU:O	5:E:73:LEU:HD12	1.73	0.89
3:C:42:SER:O	3:C:43:ASP:OD1	1.95	0.84
5:E:43:VAL:HB	5:E:73:LEU:HD11	1.61	0.82
6:F:47:VAL:HG23	6:F:73:LEU:HB2	1.62	0.80
2:B:16:VAL:HG13	2:B:71:TYR:HB2	1.63	0.79
5:E:45:LEU:HD13	5:E:73:LEU:HD23	1.65	0.79
7:G:39:ARG:HG2	7:G:39:ARG:HH11	1.49	0.78
8:H:495:ASN:O	8:H:496:LEU:HD12	1.84	0.77
4:D:17:ILE:HG23	4:D:79:ILE:HG22	1.66	0.77
7:G:39:ARG:HG2	7:G:39:ARG:NH1	2.01	0.75
1:A:72:ASP:HA	1:A:75:ALA:N	2.02	0.74
1:A:74:TYR:O	1:A:75:ALA:HB3	1.88	0.73
8:H:539:ILE:O	8:H:543:LEU:HD23	1.88	0.73
3:C:73:VAL:O	6:F:74:ARG:HG3	1.87	0.73
6:F:25:ASN:HB3	6:F:33:LEU:HD11	1.69	0.73
1:A:121:ASP:O	1:A:124:LEU:HB2	1.88	0.73
8:H:632:ASN:HD21	8:H:703:TYR:HB2	1.55	0.71
5:E:21:LEU:HD13	5:E:86:LYS:CB	2.20	0.71
8:H:621:VAL:O	8:H:622:SER:HB3	1.92	0.70
3:C:45:VAL:HG12	3:C:62:ARG:HB3	1.72	0.70
8:H:605:PHE:HD2	8:H:644:ILE:HD12	1.55	0.69
7:G:38:ILE:O	7:G:49:ILE:HA	1.92	0.69
4:D:11:LYS:HE3	4:D:31:ASN:HA	1.74	0.69
7:G:38:ILE:HG22	7:G:40:VAL:HG23	1.75	0.69
1:A:68:LEU:HD21	1:A:71:PHE:CB	2.23	0.68
3:C:30:LEU:HD12	3:C:31:GLN:H	1.54	0.68
8:H:659:ILE:O	8:H:663:ASN:ND2	2.27	0.68
8:H:489:ILE:HG21	8:H:535:ILE:HD11	1.76	0.66
7:G:38:ILE:HB	7:G:50:GLY:O	1.95	0.66
5:E:21:LEU:HD12	5:E:31:GLU:HB3	1.78	0.65
1:A:121:ASP:HA	1:A:124:LEU:HD12	1.78	0.65
5:E:73:LEU:HD13	5:E:78:ILE:CD1	2.16	0.65
2:B:73:ASN:OD1	2:B:73:ASN:N	2.30	0.64
8:H:515:ASP:OD1	8:H:517:SER:HB3	1.97	0.63
8:H:533:ILE:HG21	8:H:587:PHE:HA	1.81	0.62
1:A:120:GLU:O	1:A:123:PRO:HG2	2.00	0.62
5:E:73:LEU:CD1	5:E:78:ILE:HD11	2.19	0.60
4:D:25:ILE:HD12	4:D:25:ILE:O	2.01	0.60
7:G:39:ARG:CG	7:G:39:ARG:HH11	2.15	0.59
1:A:72:ASP:HA	1:A:75:ALA:H	1.65	0.59
8:H:492:LEU:HB3	8:H:542:PHE:CE2	2.38	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:568:SER:HB2	8:H:627:SER:HB2	1.83	0.59
1:A:72:ASP:CA	1:A:75:ALA:HA	2.19	0.59
3:C:24:ARG:HG2	3:C:48:ILE:HG12	1.86	0.58
8:H:511:LEU:HD11	8:H:539:ILE:HD11	1.86	0.58
8:H:622:SER:HA	8:H:625:THR:HG23	1.84	0.58
8:H:731:ILE:HG23	8:H:776:LEU:HD11	1.86	0.58
7:G:39:ARG:HA	7:G:49:ILE:HG13	1.85	0.58
7:G:66:THR:H	7:G:90:GLY:HA2	1.68	0.58
4:D:17:ILE:HG12	4:D:79:ILE:HB	1.86	0.58
3:C:75:LEU:HD11	6:F:67:PHE:HE2	1.69	0.58
4:D:73:GLY:O	4:D:76:ILE:HG12	2.03	0.58
1:A:108:ASN:HD21	4:D:77:LYS:HA	1.69	0.58
8:H:520:VAL:HG12	8:H:561:HIS:ND1	2.18	0.58
3:C:63:CYS:SG	3:C:66:VAL:HG11	2.45	0.57
3:C:76:ILE:HB	6:F:72:PHE:HB3	1.86	0.57
1:A:68:LEU:HD11	1:A:71:PHE:CB	2.35	0.56
8:H:495:ASN:C	8:H:496:LEU:HD12	2.25	0.56
1:A:72:ASP:C	1:A:75:ALA:H	2.09	0.56
2:B:10:LEU:HD11	2:B:72:LEU:HD21	1.86	0.56
1:A:74:TYR:O	1:A:75:ALA:CB	2.52	0.55
1:A:103:MET:HB2	4:D:79:ILE:HG12	1.89	0.55
6:F:35:SER:O	6:F:52:ALA:HA	2.05	0.55
2:B:54:LEU:O	2:B:57:VAL:HG12	2.06	0.54
7:G:89:LEU:HD11	7:G:92:THR:HG22	1.88	0.54
3:C:30:LEU:C	3:C:30:LEU:HD12	2.28	0.54
5:E:28:ARG:NH2	6:F:57:GLU:OE2	2.40	0.54
7:G:89:LEU:HD11	7:G:92:THR:CG2	2.38	0.54
3:C:16:VAL:N	3:C:28:GLY:O	2.32	0.53
5:E:46:GLU:HG3	5:E:70:ARG:HG2	1.89	0.53
8:H:543:LEU:HD12	8:H:547:GLN:HB3	1.90	0.53
8:H:673:LEU:O	8:H:676:LYS:N	2.41	0.53
8:H:552:LEU:HD22	8:H:598:PHE:CD2	2.44	0.53
3:C:30:LEU:HA	3:C:41:LEU:HD23	1.92	0.52
8:H:536:MET:HA	8:H:539:ILE:HG22	1.89	0.52
2:B:19:LEU:HD22	2:B:66:THR:HG23	1.89	0.52
8:H:729:ASP:O	8:H:733:ALA:N	2.42	0.52
4:D:25:ILE:HG12	4:D:71:ILE:CD1	2.39	0.52
6:F:75:GLY:O	6:F:78:VAL:HG22	2.10	0.52
8:H:475:LYS:O	8:H:479:LEU:HD23	2.08	0.52
1:A:72:ASP:CA	1:A:75:ALA:H	2.22	0.52
8:H:482:ILE:HG21	8:H:531:LYS:HD3	1.91	0.52
1:A:120:GLU:O	1:A:123:PRO:CG	2.58	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:64:ASP:OD1	7:G:65:ASP:N	2.43	0.52
8:H:474:GLY:O	8:H:475:LYS:HB3	2.11	0.51
7:G:38:ILE:CB	7:G:50:GLY:O	2.58	0.51
7:G:38:ILE:HG22	7:G:40:VAL:CG2	2.39	0.51
5:E:41:VAL:HG11	7:G:95:ARG:HD2	1.93	0.51
7:G:30:LEU:HD11	7:G:55:TYR:CD1	2.45	0.51
2:B:63:ARG:O	2:B:66:THR:HG22	2.11	0.51
2:B:21:ASN:O	2:B:22:ASP:HB2	2.11	0.51
8:H:682:PRO:HG2	8:H:687:ASN:HD21	1.77	0.50
2:B:-5:TYR:HE1	2:B:9:THR:HG21	1.76	0.50
3:C:68:ILE:HG23	3:C:68:ILE:O	2.12	0.50
2:B:79:THR:HB	3:C:31:GLN:OE1	2.12	0.50
8:H:588:GLN:HG3	8:H:592:LEU:HD12	1.94	0.50
1:A:121:ASP:O	1:A:124:LEU:N	2.45	0.50
8:H:568:SER:HB3	8:H:628:LYS:H	1.77	0.50
8:H:479:LEU:HD21	8:H:529:PHE:CE2	2.46	0.50
1:A:82:CYS:SG	1:A:102:PHE:HB2	2.51	0.50
6:F:56:TYR:C	6:F:56:TYR:CD1	2.85	0.50
8:H:486:TYR:CD2	8:H:535:ILE:HD12	2.47	0.49
8:H:488:GLU:HG2	8:H:507:MET:HA	1.94	0.49
8:H:623:PHE:C	8:H:623:PHE:CD1	2.85	0.49
3:C:10:LEU:HD22	8:H:479:LEU:HB3	1.95	0.49
5:E:45:LEU:HD13	5:E:73:LEU:CD2	2.38	0.49
8:H:568:SER:HB3	8:H:628:LYS:N	2.27	0.49
1:A:82:CYS:N	1:A:99:ARG:O	2.46	0.49
4:D:75:PHE:CD1	7:G:100:VAL:HG22	2.47	0.49
1:A:113:GLY:HA3	2:B:60:ILE:HD13	1.94	0.49
3:C:39:ILE:O	3:C:68:ILE:HG22	2.13	0.49
8:H:543:LEU:HD12	8:H:547:GLN:CB	2.42	0.48
8:H:683:PRO:O	8:H:687:ASN:ND2	2.45	0.48
1:A:122:GLN:N	1:A:123:PRO:HD2	2.27	0.48
4:D:45:GLU:O	4:D:63:ALA:N	2.47	0.48
3:C:7:LEU:O	3:C:10:LEU:HB2	2.13	0.48
5:E:16:ILE:HG12	5:E:34:LEU:HD22	1.96	0.48
5:E:11:VAL:O	5:E:15:THR:HG23	2.14	0.48
1:A:108:ASN:ND2	4:D:77:LYS:HA	2.28	0.48
8:H:556:PHE:CZ	8:H:637:LEU:HD21	2.48	0.48
8:H:559:LEU:HD21	8:H:633:LEU:HD23	1.95	0.48
7:G:40:VAL:N	7:G:48:VAL:O	2.42	0.48
6:F:43:GLY:C	6:F:45:MET:H	2.15	0.48
8:H:605:PHE:CD2	8:H:644:ILE:HD12	2.43	0.47
8:H:716:LYS:O	8:H:720:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:709:ALA:HB2	8:H:779:PHE:HA	1.95	0.47
1:A:121:ASP:OD1	1:A:124:LEU:HD12	2.15	0.47
8:H:733:ALA:O	8:H:737:GLU:N	2.48	0.47
1:A:65:PHE:O	1:A:82:CYS:HA	2.14	0.47
7:G:38:ILE:O	7:G:49:ILE:HG23	2.15	0.47
8:H:495:ASN:C	8:H:497:ARG:O	2.53	0.47
5:E:73:LEU:HD12	5:E:73:LEU:C	2.33	0.47
8:H:536:MET:HG3	8:H:591:ILE:HD11	1.96	0.47
4:D:4:LEU:O	4:D:8:THR:OG1	2.31	0.47
5:E:22:ILE:CG2	5:E:78:ILE:HD12	2.46	0.46
7:G:39:ARG:HB2	7:G:105:ALA:HB2	1.97	0.46
8:H:612:LEU:O	8:H:616:ILE:HG12	2.15	0.46
8:H:474:GLY:C	8:H:476:LYS:H	2.17	0.46
5:E:40:PHE:O	5:E:41:VAL:HG12	2.15	0.46
2:B:51:TYR:HA	2:B:52:PRO:HD2	1.73	0.46
8:H:632:ASN:O	8:H:636:ILE:HG13	2.16	0.46
1:A:103:MET:SD	4:D:79:ILE:HD11	2.55	0.46
8:H:674:GLU:HG3	8:H:722:ILE:HG21	1.98	0.46
2:B:73:ASN:HB2	2:B:75:ASN:OD1	2.15	0.46
1:A:121:ASP:O	1:A:124:LEU:CB	2.63	0.46
2:B:44:SER:C	2:B:45:CYS:SG	2.94	0.46
5:E:43:VAL:HG12	5:E:45:LEU:HD12	1.98	0.46
5:E:71:MET:CB	6:F:82:SER:HB2	2.45	0.46
8:H:481:LEU:HB3	8:H:526:MET:HE2	1.98	0.45
8:H:630:GLY:O	8:H:634:ILE:HG12	2.15	0.45
1:A:120:GLU:O	1:A:124:LEU:HG	2.16	0.45
5:E:43:VAL:O	5:E:73:LEU:HG	2.17	0.45
2:B:75:ASN:N	2:B:75:ASN:OD1	2.47	0.45
8:H:546:GLN:HA	8:H:549:LEU:HB3	1.98	0.45
3:C:17:TYR:HB3	3:C:77:SER:O	2.17	0.45
8:H:719:HIS:O	8:H:723:ILE:HG12	2.17	0.45
6:F:47:VAL:CG2	6:F:73:LEU:HB2	2.42	0.45
8:H:622:SER:HA	8:H:625:THR:CG2	2.47	0.44
3:C:63:CYS:SG	3:C:66:VAL:CG1	3.05	0.44
5:E:43:VAL:HB	5:E:73:LEU:CD1	2.40	0.44
8:H:546:GLN:O	8:H:550:LYS:HB2	2.17	0.44
8:H:482:ILE:HD11	8:H:532:GLY:CA	2.48	0.44
8:H:620:ASN:O	8:H:623:PHE:HB3	2.18	0.44
8:H:545:LYS:HD2	8:H:602:ASN:OD1	2.17	0.44
1:A:73:GLN:O	1:A:74:TYR:HD1	2.00	0.44
1:A:120:GLU:C	1:A:123:PRO:HD2	2.37	0.44
7:G:66:THR:N	7:G:90:GLY:HA2	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:26:SER:OG	5:E:27:ASN:N	2.50	0.44
3:C:4:PRO:CG	6:F:40:SER:CB	2.84	0.44
1:A:82:CYS:HB2	1:A:99:ARG:CB	2.48	0.44
5:E:57:ASP:O	5:E:60:ARG:N	2.48	0.44
8:H:527:LEU:HD12	8:H:527:LEU:HA	1.84	0.44
5:E:75:GLY:HA2	5:E:78:ILE:HG12	1.99	0.43
8:H:515:ASP:OD1	8:H:517:SER:N	2.50	0.43
8:H:533:ILE:O	8:H:590:ILE:HG21	2.18	0.43
8:H:673:LEU:O	8:H:677:ILE:HG13	2.18	0.43
8:H:612:LEU:HG	8:H:637:LEU:HB3	2.01	0.43
8:H:662:TRP:HA	8:H:665:ILE:HD12	2.00	0.43
8:H:623:PHE:O	8:H:623:PHE:HD1	2.01	0.43
3:C:42:SER:O	3:C:64:GLU:O	2.37	0.43
7:G:53:LYS:HG3	7:G:64:ASP:HB2	1.98	0.43
8:H:564:ILE:HD11	8:H:584:VAL:HA	2.01	0.43
8:H:578:LEU:HA	8:H:581:LEU:HD12	2.00	0.43
8:H:564:ILE:HG21	8:H:587:PHE:CD2	2.54	0.43
8:H:620:ASN:OD1	8:H:623:PHE:HB2	2.19	0.43
2:B:11:VAL:HA	2:B:29:LEU:HD23	2.01	0.42
8:H:661:THR:HG22	8:H:665:ILE:HD11	2.01	0.42
1:A:56:VAL:HG22	1:A:112:LEU:HB3	2.00	0.42
1:A:73:GLN:C	1:A:74:TYR:HD1	2.22	0.42
6:F:42:ASP:CB	6:F:46:ASN:HB2	2.49	0.42
1:A:74:TYR:CD1	1:A:74:TYR:N	2.86	0.42
8:H:660:SER:HA	8:H:663:ASN:HD22	1.84	0.42
3:C:75:LEU:HD11	6:F:67:PHE:CE2	2.53	0.42
2:B:19:LEU:HD12	2:B:23:ILE:HB	2.01	0.42
8:H:691:MET:HE2	8:H:699:MET:HG2	2.00	0.42
1:A:68:LEU:HD12	1:A:69:ARG:H	1.85	0.42
2:B:57:VAL:HG21	2:B:60:ILE:HD11	2.02	0.42
7:G:63:LEU:HD13	7:G:94:ILE:HG12	2.00	0.42
8:H:475:LYS:HG3	8:H:529:PHE:HZ	1.84	0.42
8:H:570:TYR:OH	8:H:679:LEU:O	2.23	0.41
8:H:629:ILE:HA	8:H:629:ILE:HD13	1.78	0.41
4:D:45:GLU:OE2	7:G:39:ARG:NH2	2.52	0.41
2:B:4:PHE:O	2:B:8:LYS:HG3	2.19	0.41
8:H:495:ASN:O	8:H:497:ARG:O	2.39	0.41
8:H:632:ASN:HD22	8:H:632:ASN:HA	1.76	0.41
8:H:604:ASN:OD1	8:H:605:PHE:N	2.54	0.41
2:B:-3:GLN:HG2	2:B:-2:GLY:N	2.36	0.41
8:H:482:ILE:HD12	8:H:526:MET:HB2	2.03	0.40
4:D:17:ILE:HB	4:D:25:ILE:CD1	2.50	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:8:LYS:HE2	2:B:8:LYS:HB3	1.63	0.40
7:G:55:TYR:C	7:G:55:TYR:CD2	2.93	0.40
2:B:83:GLN:O	2:B:87:ARG:HG3	2.22	0.40
8:H:511:LEU:HD11	8:H:539:ILE:CD1	2.51	0.40
1:A:79:LEU:HB2	1:A:82:CYS:SG	2.61	0.40
2:B:-7:ASN:CB	2:B:81:LEU:HD21	2.51	0.40

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	92/101 (91%)	88 (96%)	3 (3%)	1 (1%)	21	79
2	B	102/105 (97%)	93 (91%)	8 (8%)	1 (1%)	22	81
3	C	77/89 (86%)	75 (97%)	2 (3%)	0	100	100
4	D	77/114 (68%)	73 (95%)	4 (5%)	0	100	100
5	E	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
6	F	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
7	G	65/115 (56%)	62 (95%)	3 (5%)	0	100	100
8	H	269/328 (82%)	253 (94%)	16 (6%)	0	100	100
All	All	838/1031 (81%)	792 (94%)	44 (5%)	2 (0%)	56	94

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	GLY
2	B	52	PRO

### 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	53/91 (58%)	47 (89%)	6 (11%)	9	44
2	B	84/99 (85%)	80 (95%)	4 (5%)	35	82
3	C	59/81 (73%)	56 (95%)	3 (5%)	33	81
4	D	29/104 (28%)	26 (90%)	3 (10%)	10	51
5	E	58/84 (69%)	56 (97%)	2 (3%)	49	88
6	F	58/75 (77%)	55 (95%)	3 (5%)	32	80
7	G	39/103 (38%)	39 (100%)	0	100	100
8	H	204/307 (66%)	191 (94%)	13 (6%)	25	74
All	All	584/944 (62%)	550 (94%)	34 (6%)	28	76

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	102	PHE
1	A	109	VAL
1	A	115	VAL
1	A	121	ASP
1	A	122	GLN
2	B	-3	GLN
2	B	9	THR
2	B	16	VAL
2	B	45	CYS
3	C	62	ARG
3	C	63	CYS
3	C	75	LEU
4	D	25	ILE
4	D	45	GLU
4	D	68	GLU
5	E	21	LEU
5	E	28	ARG
6	F	17	SER
6	F	47	VAL
6	F	60	ASN

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Mol	Chain	Res	Type
8	H	486	TYR
8	H	497	ARG
8	H	530	ASP
8	H	531	LYS
8	H	535	ILE
8	H	540	PHE
8	H	565	ILE
8	H	585	ASP
8	H	612	LEU
8	H	623	PHE
8	H	637	LEU
8	H	672	SER
8	H	773	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	108	ASN
8	H	588	GLN
8	H	632	ASN
8	H	663	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	94/101 (93%)	0.53	6 (6%) 19 13	102, 179, 212, 225	0
2	B	104/105 (99%)	0.11	1 (0%) 79 57	92, 125, 187, 198	0
3	C	79/89 (88%)	0.08	0 100 100	50, 100, 192, 209	0
4	D	81/114 (71%)	0.56	7 (8%) 11 9	157, 181, 208, 213	0
5	E	83/93 (89%)	0.07	1 (1%) 75 52	71, 133, 177, 183	0
6	F	77/86 (89%)	0.07	0 100 100	79, 106, 145, 153	0
7	G	69/115 (60%)	0.19	3 (4%) 34 22	84, 157, 190, 219	0
8	H	279/328 (85%)	-0.03	0 100 100	50, 95, 163, 231	0
All	All	866/1031 (83%)	0.15	18 (2%) 60 38	50, 126, 197, 231	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	LEU	3.8
4	D	79	ILE	3.7
4	D	32	VAL	3.6
7	G	28	LEU	3.5
7	G	27	ILE	3.5
1	A	64	LEU	3.4
1	A	102	PHE	3.3
1	A	103	MET	3.2
4	D	15	MET	2.9
5	E	73	LEU	2.8
4	D	78	PHE	2.8
7	G	26	ALA	2.6
1	A	104	ILE	2.4
1	A	68	LEU	2.3
4	D	25	ILE	2.3
4	D	89	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	62	ILE	2.0
4	D	82	GLN	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	CO	H	1080	1/1	0.41	1.13	189,189,189,189	0
9	CO	C	1080	1/1	0.39	1.03	144,144,144,144	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.