



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 03:00 PM EDT

PDB ID : 6MJE
Title : Structure of Candida glabrata Csm1: S. cerevisiae Dsn1 complex
Authors : Singh, N.; Corbett, K.D.
Deposited on : 2018-09-20
Resolution : 2.50 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

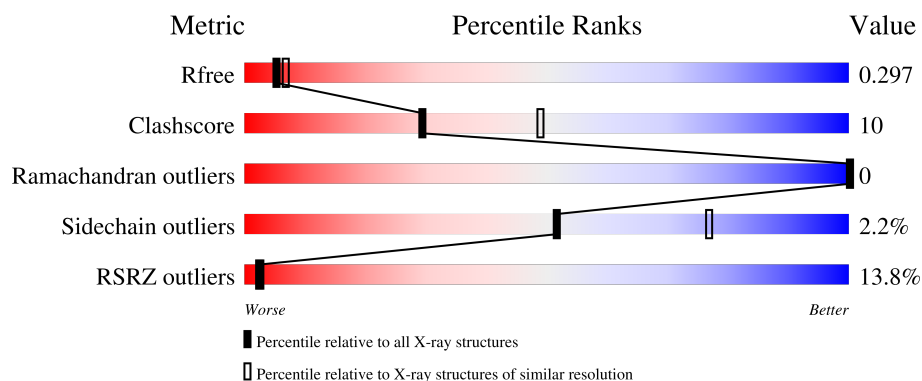
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	132	<div> <div>8%</div> <div>65%</div> <div>17%</div> <div>•</div> <div>17%</div> </div>
1	C	132	<div> <div>8%</div> <div>59%</div> <div>24%</div> <div>17%</div> </div>
1	E	132	<div> <div>10%</div> <div>60%</div> <div>21%</div> <div>•</div> <div>17%</div> </div>
1	G	132	<div> <div>14%</div> <div>61%</div> <div>22%</div> <div>17%</div> </div>
2	B	40	<div> <div>15%</div> <div>45%</div> <div>30%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	40	
2	F	40	
2	H	40	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4561 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 Monopolin complex subunit CSM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	0	0
			897	578	144	172	3			
1	C	110	Total	C	N	O	S	0	0	0
			894	577	144	170	3			
1	E	109	Total	C	N	O	S	0	0	0
			889	574	143	169	3			
1	G	109	Total	C	N	O	S	0	0	0
			889	574	143	169	3			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	expression tag	UNP A0A0W0CH22
A	51	LYS	-	expression tag	UNP A0A0W0CH22
A	52	SER	-	expression tag	UNP A0A0W0CH22
A	53	SER	-	expression tag	UNP A0A0W0CH22
A	54	HIS	-	expression tag	UNP A0A0W0CH22
A	55	HIS	-	expression tag	UNP A0A0W0CH22
A	56	HIS	-	expression tag	UNP A0A0W0CH22
A	57	HIS	-	expression tag	UNP A0A0W0CH22
A	58	HIS	-	expression tag	UNP A0A0W0CH22
A	59	HIS	-	expression tag	UNP A0A0W0CH22
A	60	GLU	-	expression tag	UNP A0A0W0CH22
A	61	ASN	-	expression tag	UNP A0A0W0CH22
A	62	LEU	-	expression tag	UNP A0A0W0CH22
A	63	TYR	-	expression tag	UNP A0A0W0CH22
A	64	PHE	-	expression tag	UNP A0A0W0CH22
A	65	GLN	-	expression tag	UNP A0A0W0CH22
A	66	SER	-	expression tag	UNP A0A0W0CH22
A	67	ASN	-	expression tag	UNP A0A0W0CH22
A	68	ALA	-	expression tag	UNP A0A0W0CH22
C	50	MET	-	expression tag	UNP A0A0W0CH22
C	51	LYS	-	expression tag	UNP A0A0W0CH22

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Chain	Residue	Modelled	Actual	Comment	Reference
C	52	SER	-	expression tag	UNP A0A0W0CH22
C	53	SER	-	expression tag	UNP A0A0W0CH22
C	54	HIS	-	expression tag	UNP A0A0W0CH22
C	55	HIS	-	expression tag	UNP A0A0W0CH22
C	56	HIS	-	expression tag	UNP A0A0W0CH22
C	57	HIS	-	expression tag	UNP A0A0W0CH22
C	58	HIS	-	expression tag	UNP A0A0W0CH22
C	59	HIS	-	expression tag	UNP A0A0W0CH22
C	60	GLU	-	expression tag	UNP A0A0W0CH22
C	61	ASN	-	expression tag	UNP A0A0W0CH22
C	62	LEU	-	expression tag	UNP A0A0W0CH22
C	63	TYR	-	expression tag	UNP A0A0W0CH22
C	64	PHE	-	expression tag	UNP A0A0W0CH22
C	65	GLN	-	expression tag	UNP A0A0W0CH22
C	66	SER	-	expression tag	UNP A0A0W0CH22
C	67	ASN	-	expression tag	UNP A0A0W0CH22
C	68	ALA	-	expression tag	UNP A0A0W0CH22
E	50	MET	-	expression tag	UNP A0A0W0CH22
E	51	LYS	-	expression tag	UNP A0A0W0CH22
E	52	SER	-	expression tag	UNP A0A0W0CH22
E	53	SER	-	expression tag	UNP A0A0W0CH22
E	54	HIS	-	expression tag	UNP A0A0W0CH22
E	55	HIS	-	expression tag	UNP A0A0W0CH22
E	56	HIS	-	expression tag	UNP A0A0W0CH22
E	57	HIS	-	expression tag	UNP A0A0W0CH22
E	58	HIS	-	expression tag	UNP A0A0W0CH22
E	59	HIS	-	expression tag	UNP A0A0W0CH22
E	60	GLU	-	expression tag	UNP A0A0W0CH22
E	61	ASN	-	expression tag	UNP A0A0W0CH22
E	62	LEU	-	expression tag	UNP A0A0W0CH22
E	63	TYR	-	expression tag	UNP A0A0W0CH22
E	64	PHE	-	expression tag	UNP A0A0W0CH22
E	65	GLN	-	expression tag	UNP A0A0W0CH22
E	66	SER	-	expression tag	UNP A0A0W0CH22
E	67	ASN	-	expression tag	UNP A0A0W0CH22
E	68	ALA	-	expression tag	UNP A0A0W0CH22
G	50	MET	-	expression tag	UNP A0A0W0CH22
G	51	LYS	-	expression tag	UNP A0A0W0CH22
G	52	SER	-	expression tag	UNP A0A0W0CH22
G	53	SER	-	expression tag	UNP A0A0W0CH22
G	54	HIS	-	expression tag	UNP A0A0W0CH22
G	55	HIS	-	expression tag	UNP A0A0W0CH22

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Chain	Residue	Modelled	Actual	Comment	Reference
G	56	HIS	-	expression tag	UNP A0A0W0CH22
G	57	HIS	-	expression tag	UNP A0A0W0CH22
G	58	HIS	-	expression tag	UNP A0A0W0CH22
G	59	HIS	-	expression tag	UNP A0A0W0CH22
G	60	GLU	-	expression tag	UNP A0A0W0CH22
G	61	ASN	-	expression tag	UNP A0A0W0CH22
G	62	LEU	-	expression tag	UNP A0A0W0CH22
G	63	TYR	-	expression tag	UNP A0A0W0CH22
G	64	PHE	-	expression tag	UNP A0A0W0CH22
G	65	GLN	-	expression tag	UNP A0A0W0CH22
G	66	SER	-	expression tag	UNP A0A0W0CH22
G	67	ASN	-	expression tag	UNP A0A0W0CH22
G	68	ALA	-	expression tag	UNP A0A0W0CH22

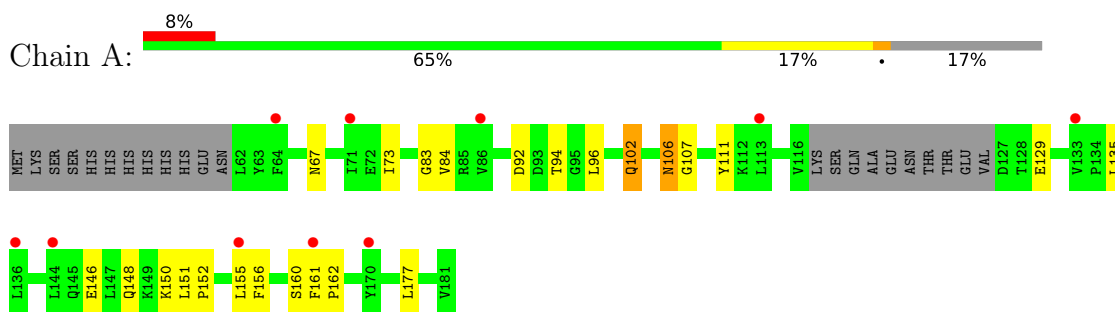
- Molecule 2 is a protein called Dsn1p.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	0	0	0
			248	156	49	43			
2	D	30	Total	C	N	O	0	0	0
			248	156	49	43			
2	F	30	Total	C	N	O	0	0	0
			248	156	49	43			
2	H	30	Total	C	N	O	0	0	0
			248	156	49	43			

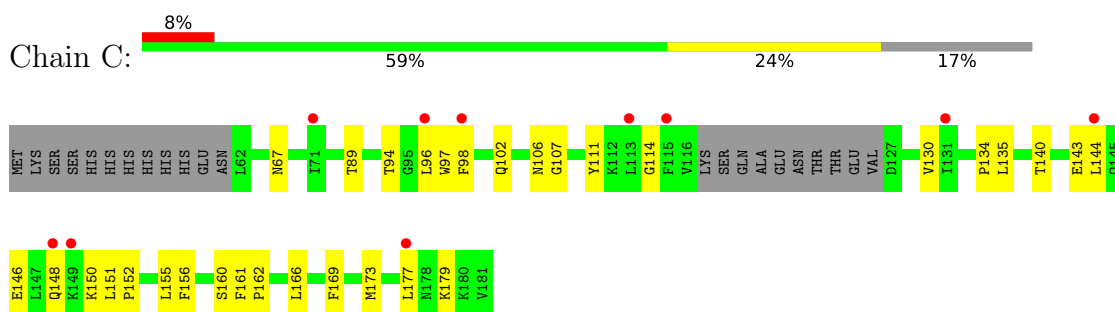
3 Residue-property plots [i](#)

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.

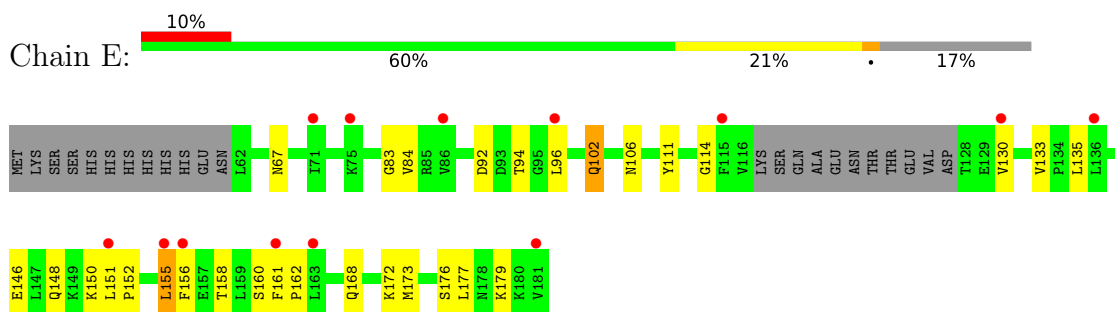
• Molecule 1: Monopolin complex subunit CSM1



• Molecule 1: Monopolin complex subunit CSM1

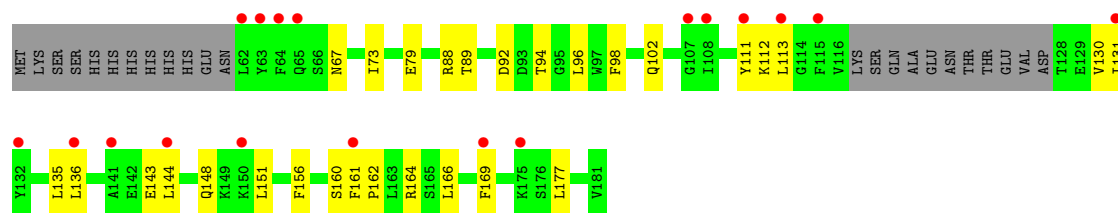


• Molecule 1: Monopolin complex subunit CSM1

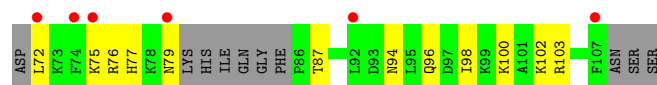


• Molecule 1: Monopolin complex subunit CSM1

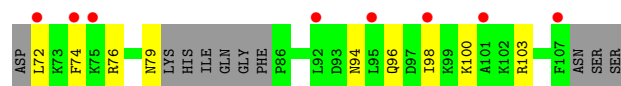




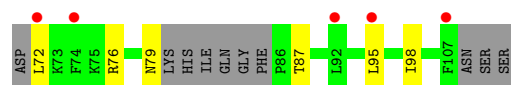
● Molecule 2: Dsn1p



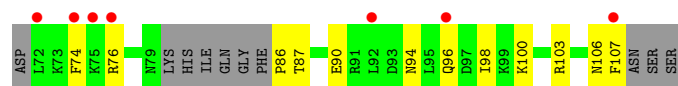
● Molecule 2: Dsn1p



● Molecule 2: Dsn1p



● Molecule 2: Dsn1p



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.37Å 203.75Å 44.26Å 90.00° 90.36° 90.00°	Depositor
Resolution (Å)	43.35 – 2.50 43.35 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.2 (43.35-2.50) 94.6 (43.35-2.49)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.240 , 0.297 0.240 , 0.297	Depositor DCC
R_{free} test set	1305 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.801	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.390 for -l,k,h 0.428 for -h,-k,l 0.427 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4561	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.14% 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 [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	0.43	0/915	0.54	0/1235
1	C	0.43	0/912	0.56	0/1231
1	E	0.43	0/907	0.53	0/1224
1	G	0.40	0/907	0.56	0/1224
2	B	0.36	0/250	0.52	0/330
2	D	0.37	0/250	0.52	0/330
2	F	0.39	0/250	0.51	0/330
2	H	0.37	0/250	0.52	0/330
All	All	0.41	0/4641	0.54	0/6234

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	897	0	864	18	0
1	C	894	0	862	20	0
1	E	889	0	860	19	0
1	G	889	0	860	21	0
2	B	248	0	251	7	0
2	D	248	0	251	7	0
2	F	248	0	251	3	0
2	H	248	0	251	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4561	0	4450	86	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 10.

All (86) 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:67:ASN:HB3	1:E:67:ASN:HB3	1.73	0.71
1:G:92:ASP:OD1	1:G:94:THR:N	2.30	0.64
1:G:79:GLU:OE1	2:H:76:ARG:NH1	2.31	0.62
2:H:106:ASN:ND2	2:H:107:PHE:O	2.33	0.61
1:A:146:GLU:HG3	2:B:72:LEU:HD23	1.81	0.61
1:A:67:ASN:HB3	1:G:67:ASN:HB3	1.83	0.61
1:A:106:ASN:O	1:A:150:LYS:NZ	2.36	0.59
1:E:146:GLU:HG3	2:F:72:LEU:HD23	1.87	0.57
1:E:152:PRO:HD2	1:E:155:LEU:HD22	1.87	0.56
2:D:76:ARG:HH22	2:D:79:ASN:HD21	1.54	0.55
2:H:87:THR:N	2:H:90:GLU:OE1	2.37	0.54
2:B:94:ASN:O	2:B:98:ILE:HG12	2.08	0.54
1:C:151:LEU:HD21	1:C:177:LEU:HD23	1.91	0.53
1:E:168:GLN:O	1:E:172:LYS:HG2	2.09	0.53
1:C:143:GLU:HB3	2:D:74:PHE:CE1	2.43	0.53
1:A:151:LEU:HD21	1:A:177:LEU:HD23	1.90	0.52
1:E:148:GLN:HA	1:E:156:PHE:CZ	2.44	0.52
1:E:161:PHE:HB2	1:E:162:PRO:HD2	1.92	0.52
1:C:161:PHE:HB2	1:C:162:PRO:HD2	1.90	0.52
1:A:111:TYR:HA	1:A:135:LEU:HG	1.92	0.52
2:F:95:LEU:O	2:F:98:ILE:HG22	2.10	0.52
1:A:96:LEU:HD21	1:G:73:ILE:HG23	1.93	0.51
1:A:148:GLN:HA	1:A:156:PHE:HZ	1.76	0.51
1:C:146:GLU:HG3	2:D:72:LEU:HD23	1.93	0.50
1:G:111:TYR:HA	1:G:135:LEU:HG	1.94	0.50
1:E:111:TYR:HA	1:E:135:LEU:HG	1.93	0.50
1:E:148:GLN:HA	1:E:156:PHE:HZ	1.76	0.50
1:E:96:LEU:O	1:E:114:GLY:HA2	2.11	0.50
2:D:94:ASN:O	2:D:98:ILE:HG12	2.11	0.50
2:F:76:ARG:HH22	2:F:79:ASN:HD21	1.59	0.49
1:E:92:ASP:OD1	1:E:94:THR:N	2.44	0.49
2:B:96:GLN:O	2:B:100:LYS:HG3	2.12	0.49
1:E:173:MET:O	1:E:177:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:96:GLN:O	2:H:100:LYS:HG3	2.14	0.48
1:C:111:TYR:HA	1:C:135:LEU:HG	1.96	0.48
1:A:106:ASN:N	1:A:106:ASN:OD1	2.47	0.48
1:E:106:ASN:O	1:E:150:LYS:NZ	2.46	0.48
1:A:148:GLN:HA	1:A:156:PHE:CZ	2.49	0.47
1:A:161:PHE:HB2	1:A:162:PRO:HD2	1.95	0.47
1:C:106:ASN:O	1:C:150:LYS:NZ	2.48	0.47
1:C:96:LEU:O	1:C:114:GLY:HA2	2.15	0.47
1:C:130:VAL:O	1:C:160:SER:HA	2.14	0.47
1:C:150:LYS:HE2	1:C:179:LYS:O	2.15	0.47
1:G:89:THR:HG22	1:G:98:PHE:CD2	2.50	0.47
1:A:160:SER:O	2:B:103:ARG:HD2	2.16	0.46
1:G:160:SER:O	2:H:103:ARG:HD2	2.16	0.46
1:G:148:GLN:HA	1:G:156:PHE:HZ	1.81	0.45
1:C:107:GLY:HA2	2:D:74:PHE:CD2	2.51	0.45
1:E:84:VAL:HG22	1:E:102:GLN:HB2	1.98	0.45
1:E:150:LYS:HE2	1:E:179:LYS:O	2.16	0.45
1:G:148:GLN:HA	1:G:156:PHE:CZ	2.51	0.45
1:E:83:GLY:O	1:E:102:GLN:HA	2.17	0.44
1:G:130:VAL:O	1:G:160:SER:HA	2.16	0.44
1:G:136:LEU:HD13	1:G:144:LEU:HD21	1.99	0.44
1:G:151:LEU:HD21	1:G:177:LEU:HD23	1.99	0.44
1:G:88:ARG:NH2	2:H:86:PRO:HA	2.33	0.44
1:A:92:ASP:OD1	1:A:94:THR:N	2.50	0.43
1:G:112:LYS:NZ	2:H:94:ASN:OD1	2.40	0.43
1:A:83:GLY:O	1:A:102:GLN:HA	2.18	0.43
1:G:164:ARG:H	1:G:164:ARG:HG2	1.55	0.43
1:A:129:GLU:HG2	2:B:103:ARG:HH12	1.83	0.43
1:C:152:PRO:HD2	1:C:155:LEU:HD12	1.99	0.43
1:E:151:LEU:HD22	1:E:176:SER:HB3	2.00	0.43
1:G:161:PHE:HB2	1:G:162:PRO:HD2	1.99	0.43
1:C:160:SER:O	2:D:103:ARG:HD2	2.18	0.43
1:C:148:GLN:HA	1:C:156:PHE:CZ	2.54	0.43
1:A:152:PRO:HD2	1:A:155:LEU:HD12	2.00	0.43
1:A:84:VAL:HG22	1:A:102:GLN:HB2	2.01	0.43
1:E:155:LEU:HA	1:E:155:LEU:HD12	1.76	0.42
1:A:107:GLY:O	1:A:177:LEU:HD13	2.20	0.42
1:C:97:TRP:CZ3	1:C:114:GLY:HA3	2.55	0.42
1:E:133:VAL:HG22	1:E:158:THR:HG23	2.02	0.42
1:E:130:VAL:O	1:E:160:SER:HA	2.20	0.42
1:C:144:LEU:HD13	2:H:96:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:MET:O	1:C:177:LEU:HG	2.19	0.42
1:G:113:LEU:HD23	1:G:113:LEU:HA	1.92	0.42
2:B:76:ARG:HH22	2:B:79:ASN:HD21	1.68	0.42
2:B:75:LYS:HE3	2:B:77:HIS:ND1	2.34	0.41
1:C:166:LEU:O	1:C:169:PHE:HB3	2.19	0.41
2:D:96:GLN:O	2:D:100:LYS:HG3	2.20	0.41
1:G:143:GLU:HB3	2:H:74:PHE:CE1	2.55	0.41
1:C:89:THR:HG22	1:C:98:PHE:CD2	2.56	0.41
1:G:166:LEU:O	1:G:169:PHE:HB3	2.21	0.41
1:G:131:ILE:HG12	2:H:98:ILE:HD13	2.03	0.41
1:A:73:ILE:HG23	1:G:96:LEU:HD21	2.04	0.40
1:C:134:PRO:O	1:C:135:LEU:HD23	2.21	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	106/132 (80%)	104 (98%)	2 (2%)	0	100	100
1	C	106/132 (80%)	104 (98%)	2 (2%)	0	100	100
1	E	105/132 (80%)	102 (97%)	3 (3%)	0	100	100
1	G	105/132 (80%)	102 (97%)	3 (3%)	0	100	100
2	B	26/40 (65%)	26 (100%)	0	0	100	100
2	D	26/40 (65%)	26 (100%)	0	0	100	100
2	F	26/40 (65%)	26 (100%)	0	0	100	100
2	H	26/40 (65%)	26 (100%)	0	0	100	100
All	All	526/688 (76%)	516 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	98/124 (79%)	96 (98%)	2 (2%)	55	79
1	C	97/124 (78%)	94 (97%)	3 (3%)	40	67
1	E	97/124 (78%)	95 (98%)	2 (2%)	53	78
1	G	97/124 (78%)	96 (99%)	1 (1%)	76	90
2	B	26/37 (70%)	24 (92%)	2 (8%)	13	25
2	D	26/37 (70%)	26 (100%)	0	100	100
2	F	26/37 (70%)	25 (96%)	1 (4%)	33	58
2	H	26/37 (70%)	26 (100%)	0	100	100
All	All	493/644 (77%)	482 (98%)	11 (2%)	52	77

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	106	ASN
2	B	87	THR
2	B	102	LYS
1	C	94	THR
1	C	102	GLN
1	C	140	THR
1	E	102	GLN
1	E	155	LEU
2	F	87	THR
1	G	102	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
2	B	79	ASN
1	C	102	GLN

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Mol	Chain	Res	Type
2	D	79	ASN
1	E	102	GLN
1	E	106	ASN
2	F	79	ASN
2	F	106	ASN
1	G	102	GLN
1	G	106	ASN
2	H	106	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 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

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	110/132 (83%)	0.70	10 (9%) 9 9	59, 81, 116, 123	0
1	C	110/132 (83%)	0.77	10 (9%) 9 9	57, 80, 114, 125	0
1	E	109/132 (82%)	0.74	13 (11%) 4 4	58, 84, 116, 123	0
1	G	109/132 (82%)	0.86	18 (16%) 1 1	58, 80, 116, 126	0
2	B	30/40 (75%)	0.92	6 (20%) 1 0	75, 89, 137, 152	0
2	D	30/40 (75%)	0.74	8 (26%) 0 0	76, 86, 130, 136	0
2	F	30/40 (75%)	1.15	5 (16%) 1 1	72, 87, 133, 139	0
2	H	30/40 (75%)	1.07	7 (23%) 0 0	72, 88, 141, 143	0
All	All	558/688 (81%)	0.81	77 (13%) 2 2	57, 84, 123, 152	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	72	LEU	8.7
1	G	63	TYR	7.6
2	B	72	LEU	6.4
2	H	72	LEU	5.8
2	H	74	PHE	5.8
1	A	155	LEU	5.4
2	F	74	PHE	4.8
1	A	161	PHE	4.4
1	G	64	PHE	4.3
1	E	86	VAL	4.2
1	A	64	PHE	3.9
1	E	136	LEU	3.8
1	G	115	PHE	3.7
1	C	177	LEU	3.7
1	E	151	LEU	3.4
1	C	144	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	115	PHE	3.3
2	D	74	PHE	3.3
1	E	71	ILE	3.3
1	E	155	LEU	3.3
2	D	72	LEU	3.2
1	G	161	PHE	3.2
1	E	96	LEU	3.2
1	G	144	LEU	3.2
2	H	107	PHE	3.1
2	B	74	PHE	3.1
1	G	65	GLN	3.0
1	G	169	PHE	3.0
1	A	144	LEU	2.9
1	G	107	GLY	2.9
1	G	175	LYS	2.9
2	H	75	LYS	2.9
1	C	113	LEU	2.8
1	G	132	TYR	2.8
1	G	136	LEU	2.8
1	A	113	LEU	2.8
1	A	136	LEU	2.7
2	F	95	LEU	2.7
1	G	111	TYR	2.7
2	F	92	LEU	2.7
1	G	131	ILE	2.6
2	B	107	PHE	2.6
2	H	92	LEU	2.6
1	G	141	ALA	2.6
1	E	161	PHE	2.6
1	E	75	LYS	2.5
2	F	107	PHE	2.5
1	E	163	LEU	2.5
2	H	76	ARG	2.5
2	D	98	ILE	2.5
1	C	148	GLN	2.4
2	D	75	LYS	2.4
1	G	113	LEU	2.4
1	E	115	PHE	2.4
1	G	62	LEU	2.4
1	C	96	LEU	2.3
1	C	98	PHE	2.3
1	C	149	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	92	LEU	2.3
1	C	131	ILE	2.3
2	H	96	GLN	2.2
1	A	133	VAL	2.2
1	E	130	VAL	2.2
1	A	71	ILE	2.2
1	C	71	ILE	2.2
2	D	95	LEU	2.2
1	G	108	ILE	2.2
2	D	107	PHE	2.2
2	B	75	LYS	2.1
1	E	156	PHE	2.1
2	D	101	ALA	2.1
2	D	92	LEU	2.1
2	B	79	ASN	2.1
1	A	86	VAL	2.1
1	G	150	LYS	2.1
1	E	181	VAL	2.0
1	A	170	TYR	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.