WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 01:45 am GMT

PDB ID : 2YFW

Title : HETEROTETRAMER STRUCTURE OF KLUYVEROMYCES LACTIS CSE4,H4

Authors : Cho, U.S.; Harrison, S.C.

Deposited on : 2011-04-08

Resolution : 2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949
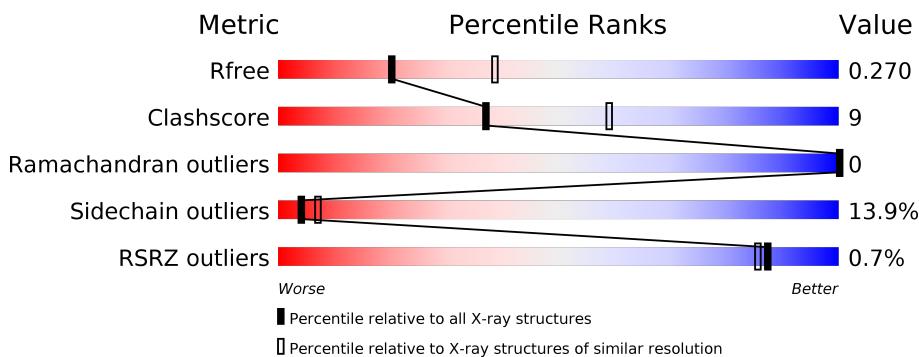
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		13.9%
RSRZ outliers		0.7%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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 <=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	92	62% 21% • 15%
1	C	92	3% / 64% 12% • 23%
1	E	92	73% 17% 5% •
1	G	92	62% 21% • 15%
2	B	103	% / 46% 15% • 36%
2	D	103	52% 14% •• 31%

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Mol	Chain	Length	Quality of chain
2	F	103	51% 14% 5% 30%
2	H	103	56% 17% 5% 22%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4822 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 HISTONE H3-LIKE CENTROMERIC PROTEIN CSE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			629	401	116	107	5			
1	C	71	Total	C	N	O	S	0	0	0
			567	360	107	95	5			
1	E	88	Total	C	N	O	S	0	0	0
			694	442	127	120	5			
1	G	78	Total	C	N	O	S	0	0	0
			628	397	115	111	5			

- Molecule 2 is a protein called HISTONE H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	66	Total	C	N	O	0	0	0
			531	336	103	92			
2	D	71	Total	C	N	O	0	0	0
			559	352	109	98			
2	F	72	Total	C	N	O	0	0	0
			570	359	111	100			
2	H	80	Total	C	N	O	0	0	0
			630	398	121	111			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	3	Total	O	0	0
			3	3		
3	C	6	Total	O	0	0
			6	6		
3	E	2	Total	O	0	0
			2	2		

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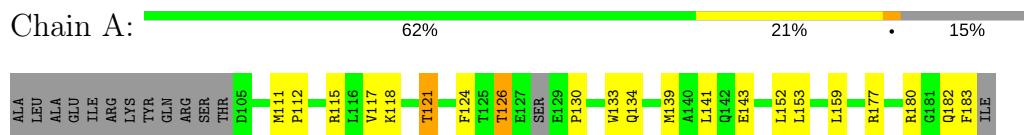
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total 2	O 2	0	0
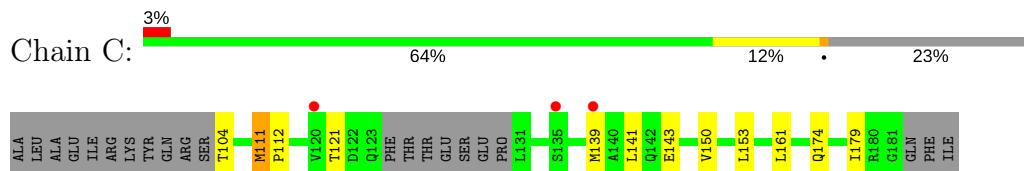
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.
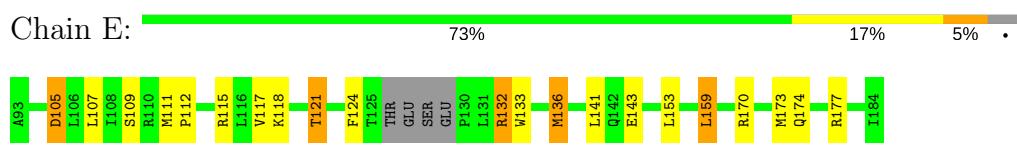
• Molecule 1: HISTONE H3-LIKE CENTROMERIC PROTEIN CSE4
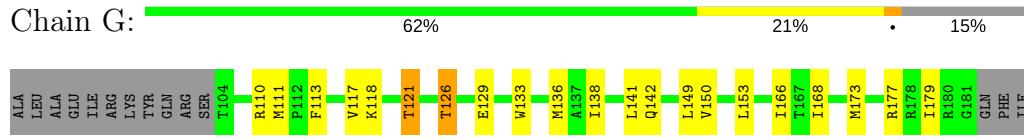
Chain A:

• Molecule 1: HISTONE H3-LIKE CENTROMERIC PROTEIN CSE4

Chain C:

• Molecule 1: HISTONE H3-LIKE CENTROMERIC PROTEIN CSE4

Chain E:

• Molecule 1: HISTONE H3-LIKE CENTROMERIC PROTEIN CSE4

Chain G:

• Molecule 2: HISTONE H4

Chain B:

• Molecule 2: HISTONE H4

Chain D:

52%   14%   · ·   31%

MET SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS ILE LEU ARG **D24 N25** I26 **T30 K31 P32** L37 **R40** R45 I46 S47 L58 K59 **L62 E63** S64 Y72 S83 L90 K91 R92 Q93 G94 ARG THR LEU TYR
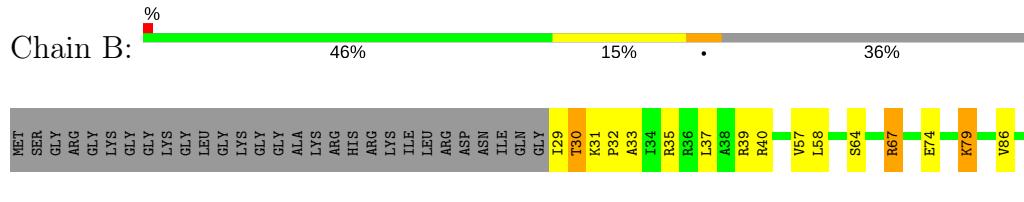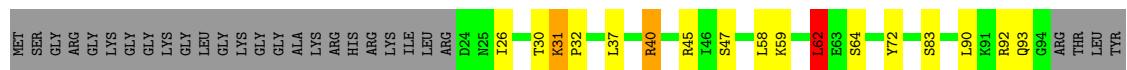
GLY PHE GLY GLY

● Molecule 2: HISTONE H4

Chain F:

51%   14%   5%   30%

MET SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS ILE LEU R23 D24 N25 T30 K31 P32 A33 R36 L37 R40 S47 L58 K59 L62 R67 D68 A69 H75 K79 T80 V81 L90 G94 ARG THR LEU

TYR GLY PHE GLY

● Molecule 2: HISTONE H4

Chain H:

56%   17%   5%   22%

MET SER GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG LYS ILE LEU R23 D24 Q27 T30 K31 P32 A33 L37 R40 R45 I46 S47 Y51 L58 L62 R67 V70 E74 K77 R78 K79 L84 L90

R95 T96 L97 G102

4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	169.48Å　　169.48Å　　81.22Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	50.00　–　2.60 45.81　–　2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.60) 99.4 (45.81-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218　,　0.276 0.213　,　0.270	Depositor DCC
R_{free} test set	1339 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	49.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4822	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.64	0/637	0.69	0/855
1	C	0.53	0/572	0.65	0/766
1	E	0.51	0/703	0.62	0/945
1	G	0.53	0/636	0.69	0/855
2	B	0.64	0/536	0.73	0/719
2	D	0.51	0/564	0.72	1/757 (0.1%)
2	F	0.54	0/575	0.67	0/772
2	H	0.56	0/637	0.79	1/855 (0.1%)
All	All	0.56	0/4860	0.70	2/6524 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	62	LEU	CA-CB-CG	7.83	133.32	115.30
2	D	62	LEU	CA-CB-CG	6.95	131.28	115.30

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	629	0	656	17	0
1	C	567	0	604	8	0
1	E	694	0	708	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	628	0	655	16	0
2	B	531	0	577	17	0
2	D	559	0	594	10	0
2	F	570	0	609	12	0
2	H	630	0	663	13	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
3	C	6	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	4822	0	5066	88	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 9.

All (88) 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:B:30:THR:HG23	2:B:32:PRO:HD2	1.22	1.07
1:A:117:VAL:O	1:A:121:THR:HG22	1.61	1.00
1:E:117:VAL:O	1:E:121:THR:HG22	1.62	0.97
2:B:30:THR:HG23	2:B:32:PRO:CD	1.94	0.97
1:G:117:VAL:O	1:G:121:THR:HG22	1.66	0.95
2:B:30:THR:HG22	2:B:33:ALA:H	1.32	0.95
2:D:64:SER:HB3	2:D:93:GLN:HE22	1.35	0.92
2:H:30:THR:HG23	2:H:32:PRO:HD2	1.58	0.86
2:D:64:SER:HB3	2:D:93:GLN:NE2	2.01	0.75
1:E:124:PHE:CE1	2:F:67:ARG:HG3	2.21	0.75
2:D:26:ILE:CB	2:D:59:LYS:HE2	2.16	0.75
1:G:117:VAL:O	1:G:121:THR:CG2	2.40	0.68
2:F:75:HIS:C	2:F:75:HIS:ND1	2.48	0.66
1:A:159:LEU:HD11	1:C:179:ILE:HD13	1.79	0.65
1:E:136:MET:HE2	1:E:136:MET:HA	1.80	0.63
1:G:166:ILE:HD12	2:H:45:ARG:HD2	1.82	0.62
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.81	0.62
1:C:111:MET:HB2	1:C:112:PRO:HD3	1.81	0.62
1:E:105:ASP:N	1:E:105:ASP:OD1	2.33	0.62
1:A:126:THR:HB	2:B:74:GLU:OE1	1.99	0.61
1:G:121:THR:HG21	1:G:133:TRP:HE1	1.64	0.61
1:A:111:MET:HB2	1:A:112:PRO:HD3	1.81	0.61
1:E:107:LEU:HD12	2:F:37:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:VAL:HG12	2:B:90:LEU:HD22	1.83	0.60
2:D:30:THR:HG22	2:D:32:PRO:HD2	1.82	0.59
1:G:149:LEU:HD11	2:H:58:LEU:HD13	1.83	0.59
2:B:29:ILE:HD13	2:B:29:ILE:N	2.17	0.59
2:D:30:THR:CG2	2:D:32:PRO:HD2	2.32	0.59
2:B:30:THR:CG2	2:B:33:ALA:H	2.12	0.58
2:D:30:THR:HG22	2:D:32:PRO:CD	2.35	0.57
1:E:111:MET:CB	1:E:112:PRO:HD3	2.35	0.56
2:B:30:THR:HG22	2:B:33:ALA:N	2.14	0.56
2:B:91:LYS:NZ	2:H:95:ARG:O	2.39	0.56
1:E:159:LEU:HD11	1:G:179:ILE:CD1	2.35	0.56
2:H:30:THR:HG23	2:H:32:PRO:CD	2.35	0.55
2:B:64:SER:HB3	2:B:93:GLN:NE2	2.22	0.54
1:A:130:PRO:O	2:B:79:LYS:NZ	2.41	0.54
1:A:159:LEU:HD11	1:C:179:ILE:CD1	2.37	0.54
1:G:126:THR:HB	2:H:74:GLU:OE1	2.07	0.53
1:E:136:MET:CE	1:E:136:MET:HA	2.39	0.53
2:F:75:HIS:O	2:F:75:HIS:ND1	2.41	0.53
1:G:150:VAL:HG21	2:H:40:ARG:HD2	1.91	0.52
1:A:143:GLU:HG3	2:H:84:LEU:HD13	1.92	0.52
1:E:159:LEU:HD11	1:G:179:ILE:HD13	1.91	0.51
1:E:173:MET:O	1:E:177:ARG:HG3	2.10	0.51
1:E:132:ARG:HG2	1:E:133:TRP:H	1.74	0.51
1:E:111:MET:HB3	1:E:112:PRO:HD3	1.93	0.51
2:H:30:THR:HG22	2:H:33:ALA:H	1.76	0.50
2:B:29:ILE:HG13	2:B:58:LEU:HD23	1.92	0.50
2:B:29:ILE:HG13	2:B:58:LEU:CD2	2.43	0.48
1:E:170:ARG:NH1	1:E:174:GLN:HE22	2.11	0.48
1:E:121:THR:HG21	1:E:133:TRP:HE1	1.79	0.48
1:G:133:TRP:HB2	1:G:138:ILE:HD11	1.95	0.48
1:C:139:MET:HA	1:C:139:MET:CE	2.44	0.48
1:A:159:LEU:CD1	1:C:179:ILE:CD1	2.91	0.47
1:A:124:PHE:CD1	2:B:67:ARG:HG3	2.49	0.47
2:D:31:LYS:HB3	2:D:32:PRO:HD3	1.97	0.47
1:C:139:MET:HE2	1:C:139:MET:HA	1.95	0.47
1:E:115:ARG:HB3	2:F:25:ASN:OD1	2.13	0.47
1:E:124:PHE:CD1	2:F:67:ARG:HG3	2.49	0.46
2:F:68:ASP:O	2:F:69:ALA:C	2.54	0.46
1:C:150:VAL:HG21	2:D:40:ARG:HG2	1.97	0.46
1:G:173:MET:O	1:G:177:ARG:HG3	2.15	0.46
1:E:107:LEU:HD13	2:F:36:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HG21	1:A:133:TRP:HE1	1.80	0.46
1:G:111:MET:CE	1:G:111:MET:HA	2.46	0.46
1:A:118:LYS:HA	1:A:121:THR:HG23	1.99	0.45
1:A:121:THR:HG21	1:A:133:TRP:NE1	2.32	0.45
2:D:58:LEU:O	2:D:62:LEU:HD22	2.17	0.44
1:E:118:LYS:HD3	1:E:118:LYS:HA	1.80	0.44
2:B:35:ARG:O	2:B:39:ARG:HG2	2.18	0.43
2:F:30:THR:HG23	2:F:33:ALA:H	1.83	0.43
1:G:118:LYS:HA	1:G:121:THR:HG23	2.00	0.43
2:F:58:LEU:O	2:F:62:LEU:HD22	2.18	0.43
1:E:109:SER:HB3	1:E:112:PRO:HD2	2.00	0.43
1:G:168:ILE:O	2:H:47:SER:HB3	2.19	0.43
1:A:124:PHE:CE1	2:B:67:ARG:HG3	2.54	0.43
2:H:70:VAL:HG13	2:H:74:GLU:OE2	2.20	0.42
1:A:152:LEU:CD2	2:B:57:VAL:HG11	2.49	0.42
1:E:132:ARG:O	2:F:81:VAL:HG23	2.19	0.42
1:E:159:LEU:CD1	1:G:179:ILE:HD11	2.49	0.42
2:H:30:THR:CG2	2:H:33:ALA:H	2.33	0.41
1:A:177:ARG:HH21	1:A:183:PHE:HB2	1.85	0.41
2:H:31:LYS:HG3	2:H:51:TYR:CD1	2.55	0.41
1:A:118:LYS:HA	1:A:121:THR:CG2	2.50	0.41
1:G:113:PHE:CD2	1:G:142:GLN:HG3	2.56	0.41
1:A:159:LEU:CD1	1:C:179:ILE:HD13	2.49	0.40
2:D:72:TYR:CE2	2:D:92:ARG:HD3	2.56	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	74/92 (80%)	74 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	67/92 (73%)	67 (100%)	0	0	100	100
1	E	84/92 (91%)	80 (95%)	4 (5%)	0	100	100
1	G	76/92 (83%)	76 (100%)	0	0	100	100
2	B	64/103 (62%)	63 (98%)	1 (2%)	0	100	100
2	D	69/103 (67%)	66 (96%)	3 (4%)	0	100	100
2	F	70/103 (68%)	70 (100%)	0	0	100	100
2	H	78/103 (76%)	74 (95%)	4 (5%)	0	100	100
All	All	582/780 (75%)	570 (98%)	12 (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	66/80 (82%)	57 (86%)	9 (14%)	4	7
1	C	59/80 (74%)	51 (86%)	8 (14%)	4	7
1	E	70/80 (88%)	62 (89%)	8 (11%)	7	12
1	G	67/80 (84%)	60 (90%)	7 (10%)	8	15
2	B	57/81 (70%)	50 (88%)	7 (12%)	5	10
2	D	58/81 (72%)	50 (86%)	8 (14%)	4	7
2	F	60/81 (74%)	50 (83%)	10 (17%)	2	4
2	H	65/81 (80%)	52 (80%)	13 (20%)	1	2
All	All	502/644 (78%)	432 (86%)	70 (14%)	4	7

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	121	THR

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Mol	Chain	Res	Type
1	A	126	THR
1	A	134	GLN
1	A	139	MET
1	A	141	LEU
1	A	153	LEU
1	A	180	ARG
1	A	182	GLN
2	B	30	THR
2	B	31	LYS
2	B	37	LEU
2	B	40	ARG
2	B	67	ARG
2	B	79	LYS
2	B	90	LEU
1	C	104	THR
1	C	111	MET
1	C	121	THR
1	C	141	LEU
1	C	143	GLU
1	C	153	LEU
1	C	161	LEU
1	C	174	GLN
2	D	31	LYS
2	D	37	LEU
2	D	40	ARG
2	D	45	ARG
2	D	47	SER
2	D	62	LEU
2	D	83	SER
2	D	90	LEU
1	E	105	ASP
1	E	121	THR
1	E	132	ARG
1	E	136	MET
1	E	141	LEU
1	E	143	GLU
1	E	153	LEU
1	E	159	LEU
2	F	25	ASN
2	F	37	LEU
2	F	40	ARG
2	F	47	SER

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Mol	Chain	Res	Type
2	F	59	LYS
2	F	62	LEU
2	F	67	ARG
2	F	75	HIS
2	F	79	LYS
2	F	90	LEU
1	G	110	ARG
1	G	121	THR
1	G	126	THR
1	G	129	GLU
1	G	136	MET
1	G	141	LEU
1	G	153	LEU
2	H	24	ASP
2	H	27	GLN
2	H	30	THR
2	H	31	LYS
2	H	37	LEU
2	H	45	ARG
2	H	47	SER
2	H	62	LEU
2	H	67	ARG
2	H	77	LYS
2	H	79	LYS
2	H	90	LEU
2	H	97	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	56	ASN
2	D	93	GLN
1	E	123	GLN
1	E	174	GLN
2	F	93	GLN
2	H	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no ligands in this entry.

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, 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	78/92 (84%)	-0.08	0	100	100	26, 38, 59, 63	0
1	C	71/92 (77%)	0.19	3 (4%)	37	29	32, 50, 87, 92	0
1	E	88/92 (95%)	0.00	0	100	100	37, 55, 78, 80	0
1	G	78/92 (84%)	-0.12	0	100	100	37, 50, 62, 66	0
2	B	66/103 (64%)	-0.10	1 (1%)	74	69	26, 37, 49, 54	0
2	D	71/103 (68%)	-0.01	0	100	100	46, 59, 82, 92	0
2	F	72/103 (69%)	-0.00	0	100	100	36, 49, 72, 79	0
2	H	80/103 (77%)	-0.02	0	100	100	33, 52, 65, 77	0
All	All	604/780 (77%)	-0.02	4 (0%)	87	85	26, 49, 77, 92	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	139	MET	2.5
1	C	135	SER	2.4
2	B	94	GLY	2.3
1	C	120	VAL	2.1

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.