Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 06:29 PM JST

PDB ID	:	7F90
Title	:	Crystal structure of SARS auxiliary protein in complex with human nuclear protein
Authors	:	Gao, X.; Cui, S.
Deposited on	:	2021-07-03
Resolution	:	2.39 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:

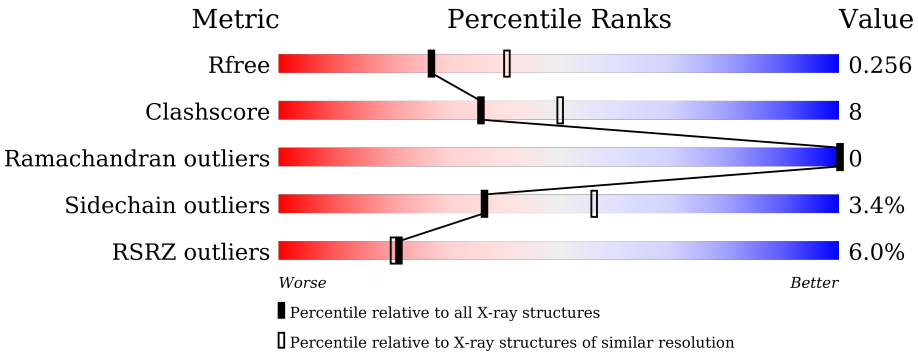
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 <=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	E	63	3% 11% 5% 84%
1	F	63	10% 11% 8% 81%
2	A	368	4% 73% 15% 11%
2	C	368	2% 73% 16% 11%
3	B	1817	% 98%
3	D	1817	97%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12124 atoms, of which 5832 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 ORF6 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	10	Total	C	H	N	O	S	0	0	0
			151	52	65	10	23	1			
1	F	12	Total	C	H	N	O	S	0	0	0
			162	63	61	12	25	1			

- Molecule 2 is a protein called mRNA export factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	328	Total	C	H	N	O	S	0	0	0
			5096	1645	2499	452	483	17			
2	C	327	Total	C	H	N	O	S	0	1	0
			5086	1643	2494	449	483	17			

- Molecule 3 is a protein called Nuclear pore complex protein Nup98-Nup96.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	B	45	Total	C	H	N	O	S	0	0	0
			713	221	353	62	75	2			
3	D	46	Total	C	H	N	O	S	0	0	0
			727	225	360	63	77	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		
4	A	83	Total	O	0	0
			83	83		
4	C	90	Total	O	0	0
			90	90		

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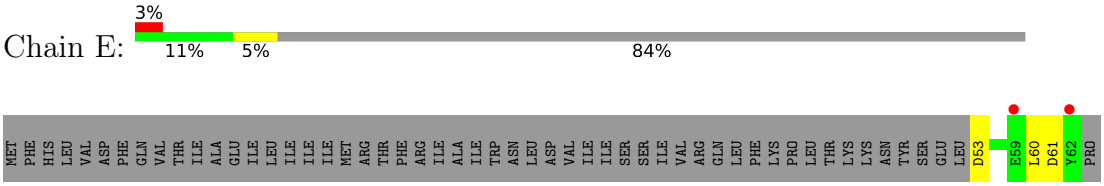
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total O 5 5	0	0
4	D	8	Total O 8 8	0	0

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.

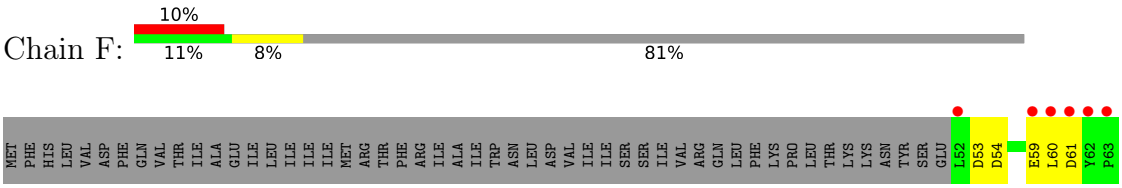
• Molecule 1: ORF6 protein

Chain E:



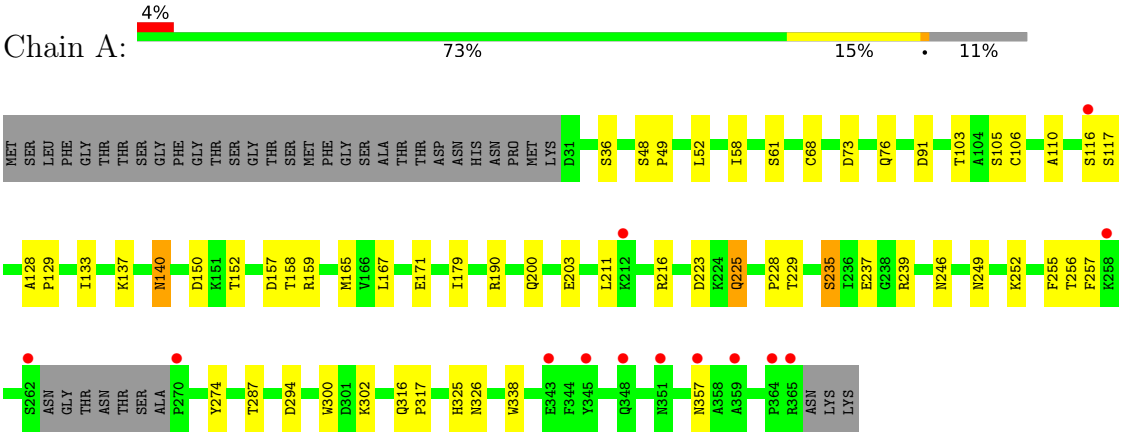
• Molecule 1: ORF6 protein

Chain F:



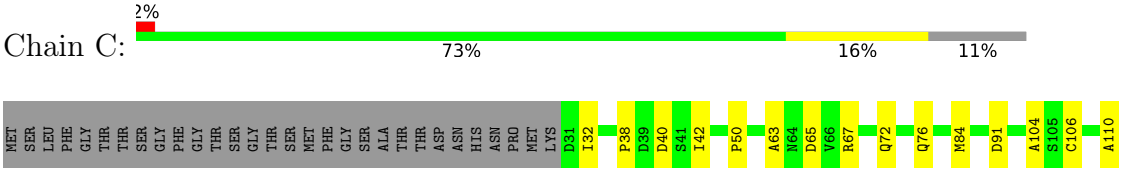
• Molecule 2: mRNA export factor

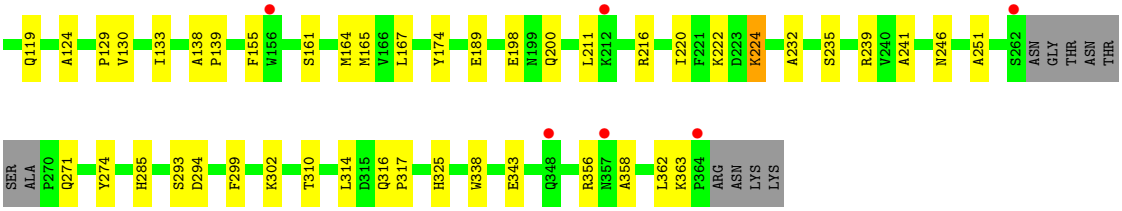
Chain A:



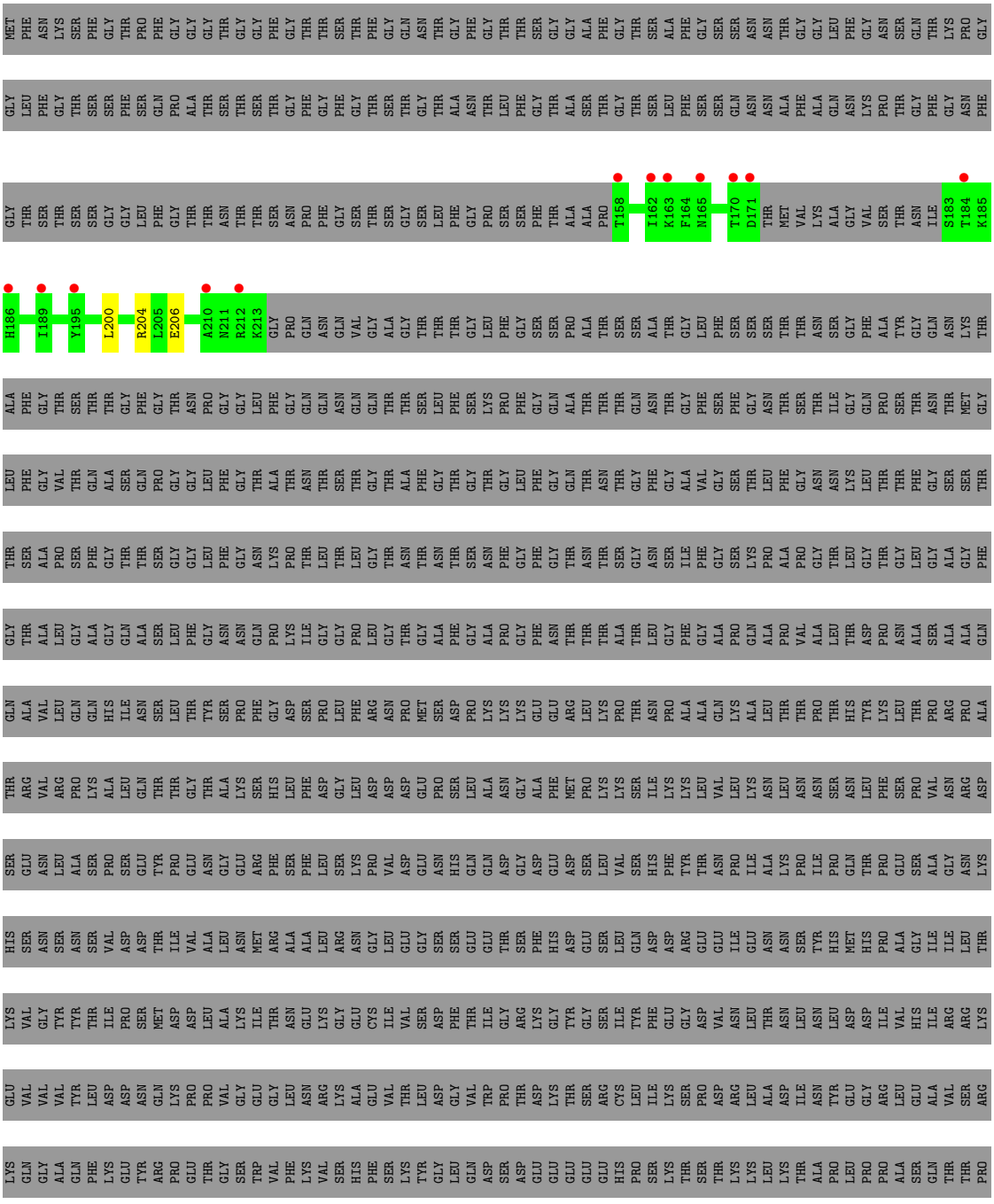
• Molecule 2: mRNA export factor

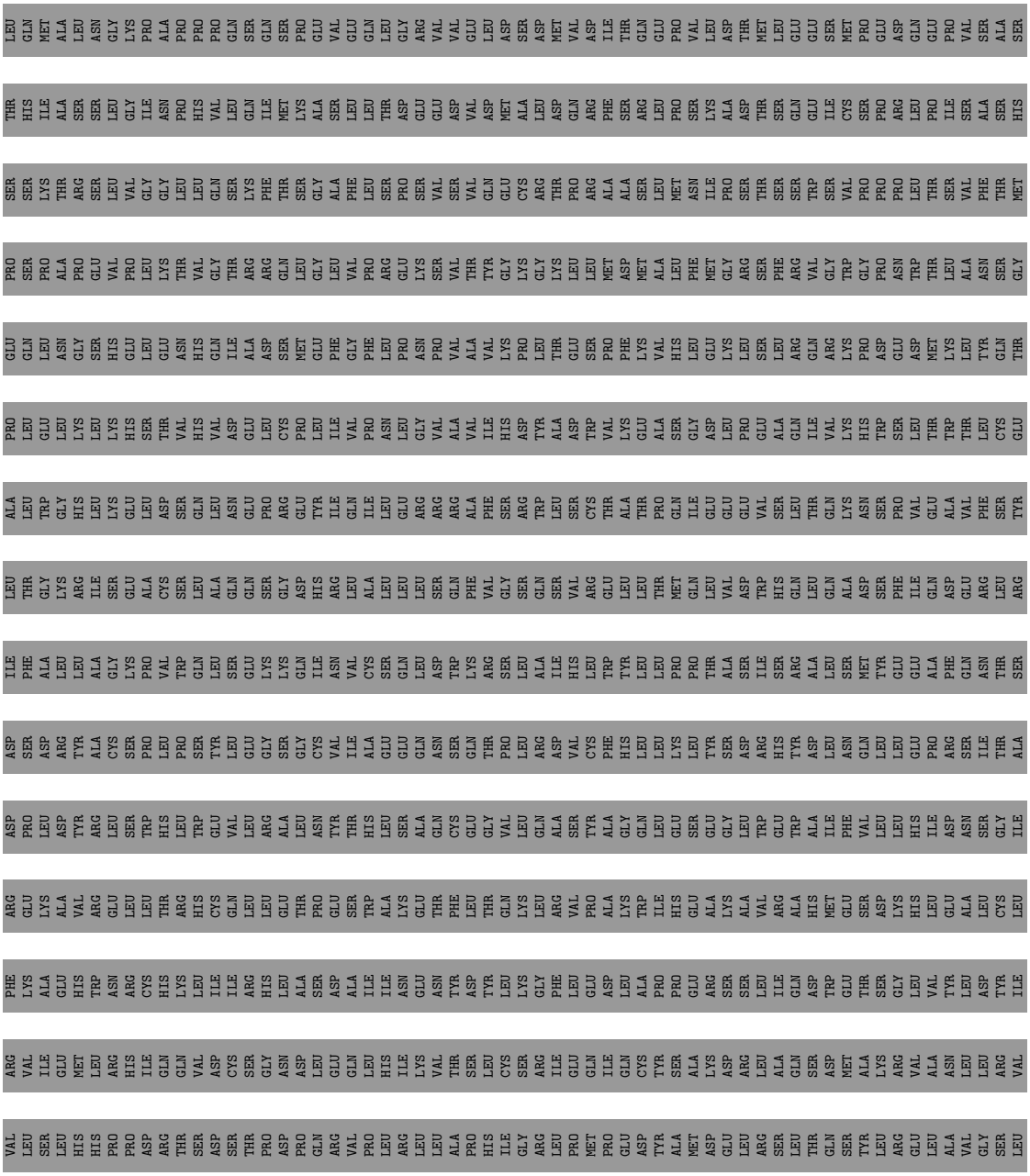
Chain C:





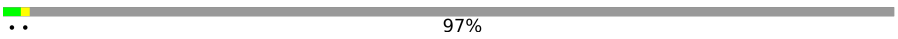
• Molecule 3: Nuclear pore complex protein Nup98-Nup96

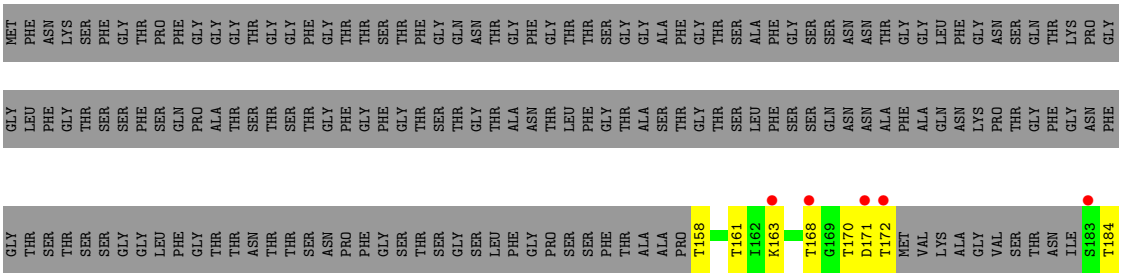


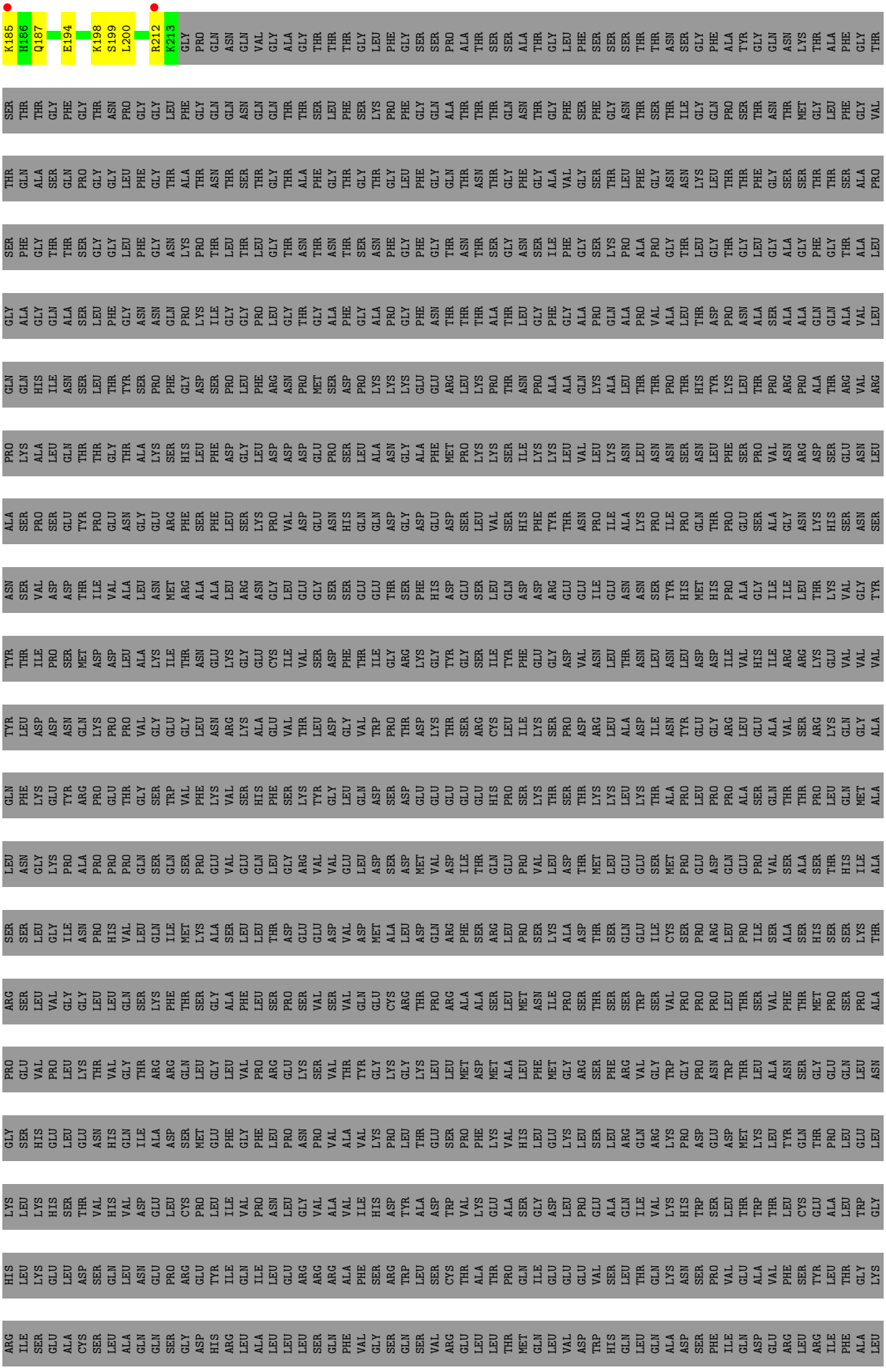


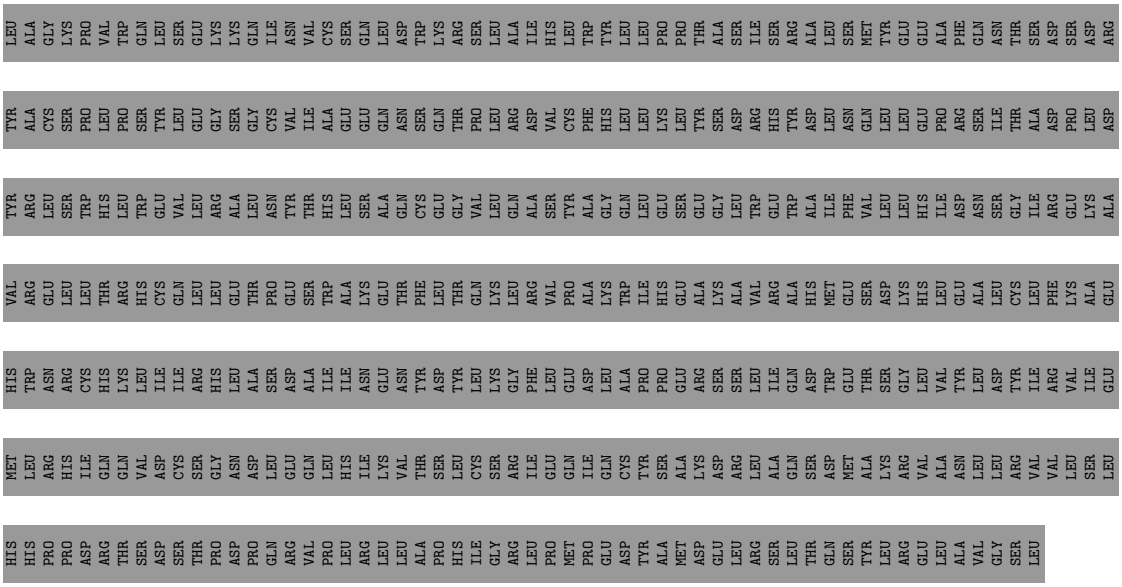
• Molecule 3: Nuclear pore complex protein Nup98-Nup96

Chain D:






K185
H186
Q187
E194
K198
S199
L200
R212
K213


LEU ALA GLY LYS PRO VAL TRP GLN LEU SER GLU LYS LYS GLN ILE ASN VAL CYS SER GLN LEU ASP TRP LYS ARG SER LEU ALA ILE HIS LEU TRP TYR LEU LEU PRO PRO THR ALA SER ILE SER ARG ALA LEU SER MET TYR GLU GLU ALA PHE GLN ASN THR SER ASP SER ASP ARG
TYR ALA CYS SER PRO LEU PRO SER TYR LEU GLU GLY SER GLY CYS VAL ILE ALA GLU GLU GLN ASN SER GLN THR PRO LEU ARG ASP VAL CYS PHE HIS LEU LEU LYS LEU TYR SER ASP ARG HIS TYR ASP LEU ASN GLN LEU LEU LEU GLU GLU PRO ARG SER ILE THR ALA ASP PRO LEU ASP
TYR ARG LEU SER TRP HIS LEU TRP GLU VAL LEU ARG ALA LEU ASN TYR THR HIS LEU SER ALA GLN CYS GLU GLY VAL LEU GLN ALA SER TYR ALA GLY GLN LEU GLU SER GLU GLY LEU TRP GLU TRP ALA ILE PHE VAL LEU LEU LEU HIS ILE ASP ASN SER GLY ILE ARG GLU LYS ALA
VAL ARG GLU LEU LEU THR ARG HIS CYS GLN LEU LEU LEU GLU THR PRO GLU SER TRP ALA LYS GLU THR PHE LEU THR GLN LYS LEU ARG VAL PRO ALA LYS TRP ILE HIS GLU ALA LYS ALA VAL ARG ALA HIS MET GLU SER ASP LYS HIS LEU GLU ALA LEU CYS LEU PHE LYS ALA GLU
HIS TRP ASN ARG CYS HIS LYS LEU ILE ILE ARG HIS LEU ALA SER ASP ALA ILE ILE ASN GLU ASN TYR ASP TYR LEU LYS GLY PHE LEU GLU ASP LEU ALA PRO PRO GLU ARG SER SER LEU ILE GLN ASP TRP GLU THR SER GLY LEU VAL TYR LEU ASP TYR ILE ARG VAL ILE GLU
MET LEU ARG HIS ILE GLN VAL ASP CYS SER GLY ASN ASP LEU GLU GLN LEU HIS ILE LYS VAL THR SER LEU CYS SER ARG ILE GLN CYS TYR SER ALA LYS ASP ARG LEU ALA GLN SER ASP MET ALA LYS ARG VAL ALA ASN LEU LEU ARG VAL ALA VAL LEU SER LEU
HIS HIS PRO PRO ASP ARG THR SER ASP SER THR PRO ASP PRO GLN ARG VAL PRO LEU ARG LEU LEU ALA PRO HIS ILE GLY ARG LEU PRO MET PRO GLU ASP TYR ALA MET ASP GLU LEU ARG SER LEU THR GLN SER TYR LEU ARG GLU LEU ALA VAL GLY SER LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	189.33Å 86.79Å 47.91Å 90.00° 92.09° 90.00°	Depositor
Resolution (Å)	47.87 – 2.39 47.87 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.87-2.39) 99.9 (47.87-2.39)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.220 , 0.258 0.222 , 0.256	Depositor DCC
R_{free} test set	1603 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12124	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	E	0.31	0/87	0.54	0/117
1	F	0.50	0/103	0.68	0/140
2	A	0.34	0/2672	0.57	1/3631 (0.0%)
2	C	0.32	0/2670	0.54	0/3629
3	B	0.26	0/364	0.47	0/487
3	D	0.27	0/371	0.51	0/497
All	All	0.32	0/6267	0.55	1/8501 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	190	ARG	NE-CZ-NH1	5.28	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

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	E	86	65	65	8	0
1	F	101	61	83	1	0
2	A	2597	2499	2499	39	0
2	C	2592	2494	2494	42	0
3	B	360	353	352	3	0
3	D	367	360	359	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	83	0	0	14	0
4	B	5	0	0	2	0
4	C	90	0	0	12	1
4	D	8	0	0	6	0
4	E	2	0	0	1	0
4	F	1	0	0	0	0
All	All	6292	5832	5852	95	1

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 8.

All (95) 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:A:246:ASN:OD1	4:A:401:HOH:O	1.83	0.95
2:C:76:GLN:OE1	4:C:401:HOH:O	1.85	0.95
2:C:220:ILE:O	4:C:402:HOH:O	1.88	0.91
1:E:61:ASP:OD1	2:A:239:ARG:NH1	2.05	0.89
2:A:150:ASP:OD1	2:A:152:THR:OG1	1.91	0.88
2:A:357:ASN:ND2	4:A:403:HOH:O	1.96	0.87
2:A:76:GLN:NE2	4:A:406:HOH:O	2.12	0.82
3:D:161:THR:OG1	4:D:1901:HOH:O	1.98	0.80
3:D:158:THR:O	4:D:1901:HOH:O	1.99	0.79
3:D:187:GLN:O	4:D:1902:HOH:O	2.02	0.78
2:A:91:ASP:HB3	2:A:133:ILE:HG22	1.68	0.74
3:D:200:LEU:H	3:D:200:LEU:HD12	1.56	0.69
2:C:84:MET:O	4:C:403:HOH:O	2.09	0.69
2:C:161:SER:OG	4:C:404:HOH:O	2.10	0.69
3:D:158:THR:HA	4:D:1903:HOH:O	1.92	0.68
2:C:222:LYS:O	4:C:406:HOH:O	2.13	0.67
2:A:326:ASN:ND2	4:A:405:HOH:O	2.05	0.66
2:C:211:LEU:HD13	2:C:235:SER:HB3	1.79	0.65
2:C:246:ASN:OD1	4:C:407:HOH:O	2.15	0.65
2:C:310:THR:HG21	4:C:412:HOH:O	1.95	0.64
2:A:179:ILE:HG22	2:A:228:PRO:HG3	1.82	0.61
1:F:61:ASP:OD1	2:C:239:ARG:NH1	2.32	0.61
2:C:310:THR:CB	4:C:412:HOH:O	2.49	0.61
2:A:223:ASP:OD2	4:A:407:HOH:O	2.16	0.61
3:B:204:ARG:NH1	4:B:1902:HOH:O	2.32	0.60
2:A:252:LYS:NZ	4:A:414:HOH:O	2.32	0.60
2:C:356:ARG:HG2	2:C:358:ALA:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:203:GLU:OE1	4:A:408:HOH:O	2.17	0.59
2:A:225:GLN:NE2	4:A:407:HOH:O	2.36	0.58
2:A:73:ASP:OD1	4:A:409:HOH:O	2.17	0.58
2:A:140:ASN:HB2	4:A:426:HOH:O	2.06	0.56
3:D:194:GLU:OE2	3:D:194:GLU:N	2.33	0.56
2:C:316:GLN:HB2	2:C:317:PRO:HD2	1.89	0.55
3:D:212:ARG:NH2	4:D:1901:HOH:O	2.41	0.52
2:C:299:PHE:CG	2:C:362:LEU:HD21	2.45	0.52
2:A:157:ASP:O	2:A:158:THR:OG1	2.22	0.51
2:C:174:TYR:CZ	3:D:199:SER:HB3	2.46	0.51
2:C:110:ALA:HB3	2:C:124:ALA:HB3	1.93	0.51
2:C:138:ALA:HB1	2:C:139:PRO:HD2	1.94	0.50
2:A:211:LEU:HD13	2:A:235:SER:HB3	1.94	0.49
1:E:61:ASP:OD2	2:A:256:THR:OG1	2.24	0.49
2:A:316:GLN:HB3	2:A:317:PRO:HD2	1.93	0.49
2:C:32:ILE:H	2:C:32:ILE:HD12	1.78	0.49
2:C:38:PRO:HD2	2:C:42:ILE:HD11	1.94	0.48
1:E:61:ASP:O	4:E:101:HOH:O	2.19	0.48
2:C:274:TYR:CD1	2:C:294:ASP:HB3	2.49	0.48
2:C:119:GLN:NE2	4:C:410:HOH:O	2.22	0.48
1:E:60:LEU:HD23	2:A:257:PHE:HB3	1.96	0.48
1:E:61:ASP:CG	2:A:239:ARG:HH11	2.18	0.47
2:C:216:ARG:NH1	3:D:200:LEU:HD13	2.29	0.47
2:C:224:LYS:N	2:C:224:LYS:HD3	2.30	0.47
2:C:274:TYR:HB3	2:C:293:SER:HB2	1.96	0.47
2:C:40:ASP:HB2	2:C:63:ALA:HB2	1.96	0.47
2:A:48:SER:HB2	2:A:52:LEU:HD12	1.97	0.46
2:A:211:LEU:HD13	2:A:235:SER:CB	2.45	0.46
2:C:50:PRO:HG3	2:C:325:HIS:HB2	1.98	0.46
2:C:310:THR:CG2	4:C:412:HOH:O	2.58	0.46
2:A:106:CYS:HA	2:A:129:PRO:HB3	1.96	0.46
2:A:274:TYR:CD2	2:A:294:ASP:HB3	2.51	0.45
2:C:271:GLN:HB3	3:D:184:THR:HG22	1.98	0.45
2:A:103:THR:O	2:A:110:ALA:HA	2.17	0.45
2:C:91:ASP:HB3	2:C:133:ILE:HG22	1.98	0.45
2:C:65:ASP:OD2	2:C:67:ARG:NE	2.48	0.44
2:C:189:GLU:OE2	4:C:409:HOH:O	2.21	0.44
2:A:165:MET:HE3	2:A:167:LEU:HG	1.98	0.44
2:A:128:ALA:HB1	2:A:129:PRO:HD2	1.99	0.44
2:C:232:ALA:HA	2:C:241:ALA:O	2.18	0.44
2:A:137:LYS:O	4:A:410:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:LEU:HD22	2:A:255:PHE:CD2	2.53	0.43
2:A:357:ASN:ND2	4:A:417:HOH:O	2.36	0.43
2:A:58:ILE:HD13	2:A:68:CYS:HB2	2.00	0.43
2:A:216:ARG:CZ	3:B:200:LEU:HD12	2.48	0.43
2:A:325:HIS:CE1	4:A:405:HOH:O	2.71	0.43
2:C:155:PHE:O	2:C:164:MET:HG2	2.18	0.43
2:C:165:MET:CE	2:C:167:LEU:HD21	2.48	0.43
2:A:116:SER:OG	2:A:117:SER:N	2.52	0.43
2:C:343:GLU:OE2	3:D:163:LYS:HG3	2.19	0.43
2:C:198:GLU:O	2:C:200:GLN:N	2.51	0.43
3:D:171:ASP:OD1	3:D:172:THR:N	2.51	0.43
2:C:299:PHE:CG	2:C:362:LEU:CD2	3.02	0.42
2:C:251:ALA:HB3	4:C:432:HOH:O	2.18	0.42
2:A:48:SER:HB2	2:A:49:PRO:HD2	2.01	0.42
2:C:293:SER:HA	2:C:317:PRO:HB3	2.02	0.42
2:A:140:ASN:ND2	4:A:426:HOH:O	2.52	0.42
3:D:168:THR:HG22	3:D:185:LYS:HE2	2.02	0.42
1:E:61:ASP:CG	2:A:239:ARG:NH1	2.73	0.42
2:C:104:ALA:HB1	2:C:130:VAL:HG12	2.01	0.41
3:D:170:THR:HG22	3:D:171:ASP:N	2.35	0.41
3:D:198:LYS:NZ	4:D:1903:HOH:O	2.53	0.41
2:C:285:HIS:CD2	2:C:363:LYS:HG3	2.55	0.41
2:C:314:LEU:HD12	2:C:314:LEU:N	2.35	0.41
3:B:206:GLU:OE2	4:B:1901:HOH:O	2.22	0.41
1:E:60:LEU:HD22	2:A:255:PHE:HD2	1.86	0.41
2:A:287:THR:HB	2:A:300:TRP:O	2.21	0.41
2:C:106:CYS:HA	2:C:129:PRO:HB3	2.03	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:411:HOH:O	4:C:437:HOH:O[2_556]	2.07	0.13

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	E	8/63 (13%)	8 (100%)	0	0	100 100
1	F	10/63 (16%)	10 (100%)	0	0	100 100
2	A	324/368 (88%)	305 (94%)	19 (6%)	0	100 100
2	C	324/368 (88%)	311 (96%)	13 (4%)	0	100 100
3	B	41/1817 (2%)	41 (100%)	0	0	100 100
3	D	42/1817 (2%)	42 (100%)	0	0	100 100
All	All	749/4496 (17%)	717 (96%)	32 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	E	10/61 (16%)	9 (90%)	1 (10%)	7 11
1	F	12/61 (20%)	8 (67%)	4 (33%)	0 0
2	A	285/317 (90%)	271 (95%)	14 (5%)	25 40
2	C	285/317 (90%)	281 (99%)	4 (1%)	67 82
3	B	41/1543 (3%)	41 (100%)	0	100 100
3	D	42/1543 (3%)	42 (100%)	0	100 100
All	All	675/3842 (18%)	652 (97%)	23 (3%)	37 56

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	53	ASP
1	F	53	ASP
1	F	54	ASP

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Mol	Chain	Res	Type
1	F	59	GLU
1	F	60	LEU
2	A	36	SER
2	A	61	SER
2	A	105	SER
2	A	140	ASN
2	A	159	ARG
2	A	171	GLU
2	A	200	GLN
2	A	225	GLN
2	A	229	THR
2	A	235	SER
2	A	237	GLU
2	A	249	ASN
2	A	302	LYS
2	A	338	TRP
2	C	72	GLN
2	C	224	LYS
2	C	302	LYS
2	C	338	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	246	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

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, 95^{th} 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	E	10/63 (15%)	1.57	2 (20%) 1 0	48, 57, 89, 92	0
1	F	12/63 (19%)	2.70	6 (50%) 0 0	44, 74, 100, 114	0
2	A	328/368 (89%)	0.69	13 (3%) 38 37	24, 36, 59, 89	0
2	C	327/368 (88%)	0.62	6 (1%) 68 66	22, 33, 53, 69	0
3	B	45/1817 (2%)	1.51	12 (26%) 0 0	35, 59, 77, 87	0
3	D	46/1817 (2%)	1.00	7 (15%) 2 1	31, 48, 67, 76	0
All	All	768/4496 (17%)	0.77	46 (5%) 21 20	22, 36, 65, 114	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	63	PRO	9.4
1	E	62	TYR	7.1
3	B	163	LYS	5.7
1	F	62	TYR	4.7
2	A	262	SER	4.7
1	F	52	LEU	4.5
2	C	348	GLN	4.2
2	A	348	GLN	3.8
2	C	212	LYS	3.8
2	A	364	PRO	3.8
2	A	365	ARG	3.7
2	C	262	SER	3.7
2	A	258	LYS	3.6
3	B	210	ALA	3.5
3	B	212	ARG	3.2
2	A	212	LYS	3.1
3	D	171	ASP	3.1
2	C	357	ASN	3.1
2	A	357	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	B	186	HIS	2.8
3	D	163	LYS	2.8
3	D	172	THR	2.7
3	D	168	THR	2.6
3	D	212	ARG	2.6
2	A	270	PRO	2.6
1	F	60	LEU	2.5
3	B	162	ILE	2.5
3	B	158	THR	2.5
3	D	185	LYS	2.5
3	B	171	ASP	2.4
2	A	351	ASN	2.4
3	B	165	ASN	2.3
3	B	184	THR	2.3
3	D	183	SER	2.3
2	A	343	GLU	2.3
2	C	364	PRO	2.2
2	A	359	ALA	2.2
3	B	189	ILE	2.2
3	B	195	TYR	2.2
2	C	156	TRP	2.2
1	F	59	GLU	2.2
1	E	59	GLU	2.2
2	A	345	TYR	2.2
2	A	116	SER	2.1
1	F	61	ASP	2.1
3	B	170	THR	2.1

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.