Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:04 am BST

PDB ID	:	4C8H
Title	:	Crystal structure of the C-terminal region of yeast Ctf4, selenomethionine protein.
Authors	:	Simon, A.C.; Pellegrini, L.
Deposited on	:	2013-10-01
Resolution	:	2.69 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 following versions of software and data (see references ①) were used in the production of this report:

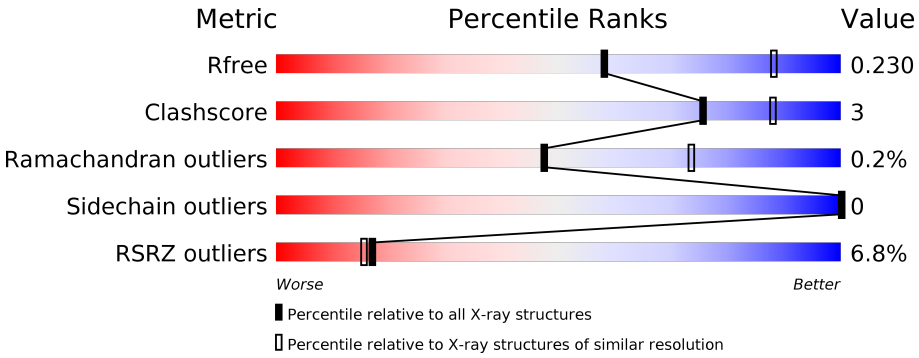
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	A	478	2% 82% 8% 10%
1	B	478	9% 81% 7% 12%
1	C	478	6% 81% 8% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10421 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 CTF4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	Se	0	1	0
			3475	2233	577	649	5	11			
1	B	419	Total	C	N	O	S	Se	0	0	0
			3371	2170	557	629	5	10			
1	C	425	Total	C	N	O	S	Se	0	0	0
			3412	2192	565	640	5	10			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	MSE	-	expression tag	UNP Q01454
A	451	GLY	-	expression tag	UNP Q01454
A	452	SER	-	expression tag	UNP Q01454
A	453	SER	-	expression tag	UNP Q01454
A	454	HIS	-	expression tag	UNP Q01454
A	455	HIS	-	expression tag	UNP Q01454
A	456	HIS	-	expression tag	UNP Q01454
A	457	HIS	-	expression tag	UNP Q01454
A	458	HIS	-	expression tag	UNP Q01454
A	459	HIS	-	expression tag	UNP Q01454
A	460	SER	-	expression tag	UNP Q01454
A	461	GLN	-	expression tag	UNP Q01454
A	462	ASP	-	expression tag	UNP Q01454
A	463	PRO	-	expression tag	UNP Q01454
A	464	GLU	-	expression tag	UNP Q01454
A	465	ASN	-	expression tag	UNP Q01454
A	466	LEU	-	expression tag	UNP Q01454
A	467	TYR	-	expression tag	UNP Q01454
A	468	PHE	-	expression tag	UNP Q01454
A	469	GLN	-	expression tag	UNP Q01454
A	470	GLY	-	expression tag	UNP Q01454
B	450	MSE	-	expression tag	UNP Q01454
B	451	GLY	-	expression tag	UNP Q01454

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	SER	-	expression tag	UNP Q01454
B	453	SER	-	expression tag	UNP Q01454
B	454	HIS	-	expression tag	UNP Q01454
B	455	HIS	-	expression tag	UNP Q01454
B	456	HIS	-	expression tag	UNP Q01454
B	457	HIS	-	expression tag	UNP Q01454
B	458	HIS	-	expression tag	UNP Q01454
B	459	HIS	-	expression tag	UNP Q01454
B	460	SER	-	expression tag	UNP Q01454
B	461	GLN	-	expression tag	UNP Q01454
B	462	ASP	-	expression tag	UNP Q01454
B	463	PRO	-	expression tag	UNP Q01454
B	464	GLU	-	expression tag	UNP Q01454
B	465	ASN	-	expression tag	UNP Q01454
B	466	LEU	-	expression tag	UNP Q01454
B	467	TYR	-	expression tag	UNP Q01454
B	468	PHE	-	expression tag	UNP Q01454
B	469	GLN	-	expression tag	UNP Q01454
B	470	GLY	-	expression tag	UNP Q01454
C	450	MSE	-	expression tag	UNP Q01454
C	451	GLY	-	expression tag	UNP Q01454
C	452	SER	-	expression tag	UNP Q01454
C	453	SER	-	expression tag	UNP Q01454
C	454	HIS	-	expression tag	UNP Q01454
C	455	HIS	-	expression tag	UNP Q01454
C	456	HIS	-	expression tag	UNP Q01454
C	457	HIS	-	expression tag	UNP Q01454
C	458	HIS	-	expression tag	UNP Q01454
C	459	HIS	-	expression tag	UNP Q01454
C	460	SER	-	expression tag	UNP Q01454
C	461	GLN	-	expression tag	UNP Q01454
C	462	ASP	-	expression tag	UNP Q01454
C	463	PRO	-	expression tag	UNP Q01454
C	464	GLU	-	expression tag	UNP Q01454
C	465	ASN	-	expression tag	UNP Q01454
C	466	LEU	-	expression tag	UNP Q01454
C	467	TYR	-	expression tag	UNP Q01454
C	468	PHE	-	expression tag	UNP Q01454
C	469	GLN	-	expression tag	UNP Q01454
C	470	GLY	-	expression tag	UNP Q01454

- Molecule 2 is water.

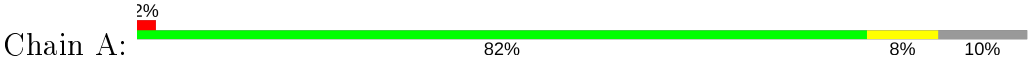
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	113	Total O 113 113	0	0
2	B	15	Total O 15 15	0	0
2	C	35	Total O 35 35	0	0

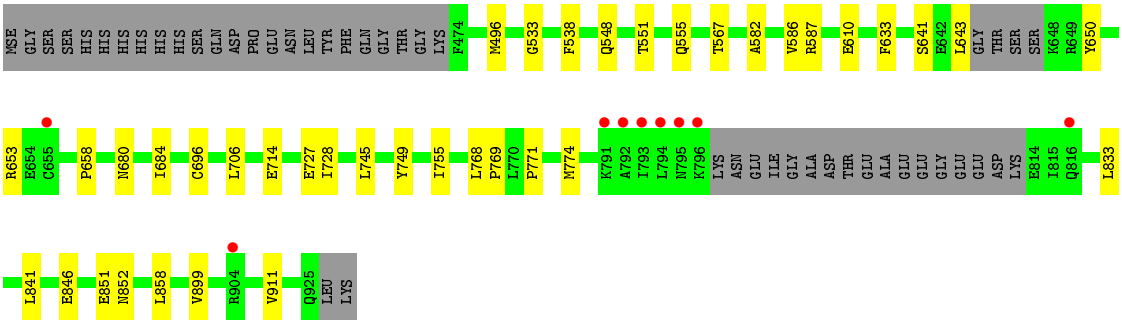
3 Residue-property plots (i)

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: CTF4

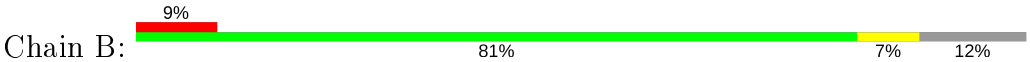
Chain A:

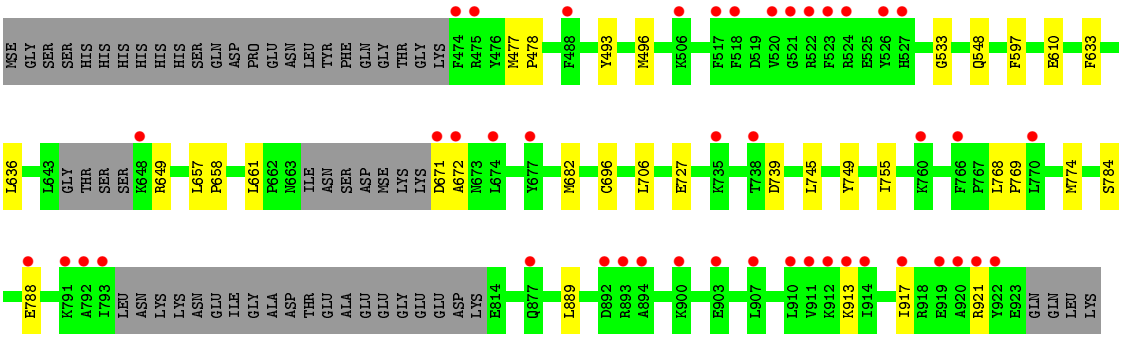




- Molecule 1: CTF4

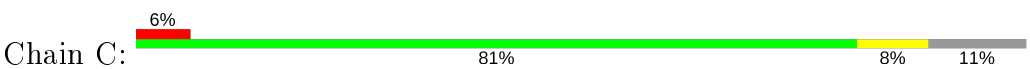
Chain B:

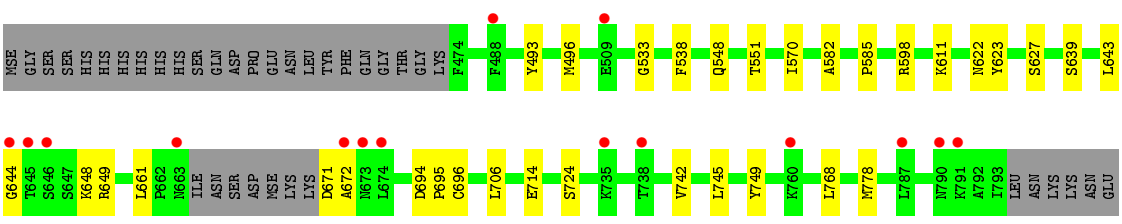


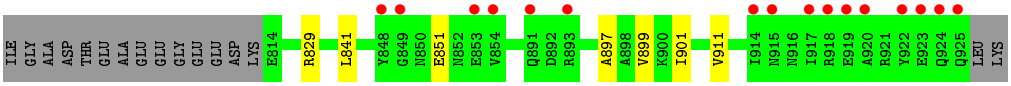


- Molecule 1: CTF4

Chain C:






ILE
GLY
ALA
ASP
THR
GLU
ALA
GLU
GLU
GLY
GLU
GLU
ASP
LYS
E814
R829
L841
Y848
G849
N850
E851
N852
E853
V854
Q891
D892
R893
A897
A898
V899
K900
I901
V911
I914
N915
N916
I917
R918
E919
A920
R921
Y922
E923
Q924
Q925
LEU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.29Å 118.43Å 155.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 2.69 49.19 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.19-2.69) 99.4 (49.19-2.69)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.225 0.197 , 0.230	Depositor DCC
R_{free} test set	2813 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10421	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	A	0.23	0/3552	0.39	0/4790
1	B	0.22	0/3445	0.39	0/4649
1	C	0.23	0/3487	0.40	0/4707
All	All	0.22	0/10484	0.39	0/14146

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

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	3475	0	3433	26	0
1	B	3371	0	3319	20	0
1	C	3412	0	3356	23	0
2	A	113	0	0	0	0
2	B	15	0	0	0	0
2	C	35	0	0	0	0
All	All	10421	0	10108	63	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 3.

All (63) 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:A:496:MSE:HE2	1:A:745:LEU:HD21	1.63	0.79
1:B:496:MSE:HE2	1:B:745:LEU:HD21	1.68	0.76
1:C:496:MSE:HE2	1:C:745:LEU:HD21	1.70	0.73
1:C:778:MSE:HE3	1:C:829:ARG:HA	1.77	0.66
1:B:533:GLY:O	1:B:548:GLN:NE2	2.28	0.66
1:A:768:LEU:HD12	1:A:769:PRO:HD2	1.81	0.63
1:A:846:GLU:OE2	1:A:852:ASN:ND2	2.30	0.61
1:B:477:MSE:HE3	1:B:478:PRO:HD2	1.81	0.61
1:A:533:GLY:O	1:A:548:GLN:NE2	2.34	0.60
1:B:768:LEU:HD12	1:B:769:PRO:HD2	1.83	0.60
1:C:533:GLY:O	1:C:548:GLN:NE2	2.35	0.59
1:C:643:LEU:HD13	1:C:648:LYS:HG2	1.84	0.59
1:B:496:MSE:HE1	1:B:755:ILE:HG13	1.84	0.58
1:A:496:MSE:HE1	1:A:755:ILE:HG13	1.86	0.57
1:B:727:GLU:HB2	1:B:774:MSE:HE2	1.88	0.56
1:A:899:VAL:HG13	1:A:911:VAL:HG13	1.88	0.55
1:A:833:LEU:HB3	1:A:858:LEU:HD21	1.91	0.53
1:C:841:LEU:HD21	1:C:851:GLU:HB3	1.91	0.52
1:B:889:LEU:O	1:B:921:ARG:NH1	2.42	0.51
1:B:671:ASP:OD1	1:B:672:ALA:N	2.45	0.50
1:A:714:GLU:OE1	1:C:649:ARG:NH1	2.45	0.50
1:A:728:ILE:HG13	1:A:774:MSE:HE1	1.95	0.49
1:B:696:CYS:SG	1:B:706:LEU:HD13	2.53	0.48
1:A:658:PRO:HB2	1:C:611:LYS:HG3	1.95	0.48
1:B:633:PHE:CG	1:C:661:LEU:HD12	2.48	0.48
1:A:841:LEU:HD21	1:A:851:GLU:HB3	1.97	0.47
1:B:739:ASP:OD1	1:B:739:ASP:N	2.48	0.47
1:A:633:PHE:CG	1:B:661:LEU:HD12	2.50	0.47
1:B:493:TYR:OH	1:B:768:LEU:HB2	2.14	0.46
1:C:671:ASP:OD1	1:C:672:ALA:N	2.48	0.46
1:C:548:GLN:HG3	1:C:551:THR:H	1.81	0.46
1:C:585:PRO:HD2	1:C:622:ASN:O	2.16	0.46
1:A:633:PHE:CD2	1:B:661:LEU:HD12	2.50	0.46
1:A:641:SER:HB3	1:A:650:TYR:CD2	2.51	0.46
1:A:555:GLN:HG3	1:A:567:THR:HG22	1.99	0.45
1:A:696:CYS:SG	1:A:706:LEU:HD13	2.57	0.45
1:C:623:TYR:CD1	1:C:644:GLY:HA2	2.52	0.44
1:B:636:LEU:HD13	1:B:682:MSE:HE1	2.00	0.44
1:A:755:ILE:HD13	1:A:771:PRO:HA	2.00	0.44
1:C:493:TYR:OH	1:C:768:LEU:HG	2.19	0.43
1:C:851:GLU:N	1:C:851:GLU:OE1	2.50	0.43
1:C:899:VAL:HG13	1:C:911:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ARG:NE	1:C:714:GLU:OE1	2.46	0.43
1:A:727:GLU:HB2	1:A:774:MSE:HE2	2.01	0.43
1:C:570:ILE:HG23	1:C:598:ARG:HD2	2.00	0.43
1:A:680:ASN:ND2	1:A:684:ILE:O	2.48	0.42
1:A:586:VAL:O	1:A:587:ARG:NH1	2.47	0.42
1:C:696:CYS:SG	1:C:706:LEU:HD13	2.59	0.42
1:B:784:SER:O	1:B:788:GLU:HG3	2.18	0.42
1:A:841:LEU:HD21	1:A:851:GLU:CB	2.49	0.42
1:A:610:GLU:OE2	1:A:653:ARG:NH2	2.50	0.42
1:A:548:GLN:HG3	1:A:551:THR:H	1.84	0.42
1:A:587:ARG:HE	1:A:643:LEU:CD2	2.33	0.41
1:C:897:ALA:O	1:C:901:ILE:HG13	2.21	0.41
1:A:610:GLU:OE1	1:A:650:TYR:OH	2.36	0.41
1:B:657:LEU:HA	1:B:658:PRO:HD3	1.78	0.41
1:A:538:PHE:CG	1:A:582:ALA:HA	2.55	0.41
1:B:913:LYS:O	1:B:917:ILE:HG13	2.21	0.41
1:C:694:ASP:HA	1:C:695:PRO:HD3	1.85	0.40
1:C:538:PHE:CG	1:C:582:ALA:HA	2.56	0.40
1:C:627:SER:OG	1:C:639:SER:HB2	2.21	0.40
1:C:724:SER:HB2	1:C:742:VAL:HG21	2.02	0.40
1:B:597:PHE:HB3	1:B:610:GLU:HB2	2.03	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	426/478 (89%)	417 (98%)	8 (2%)	1 (0%)	47	73
1	B	411/478 (86%)	401 (98%)	9 (2%)	1 (0%)	47	73
1	C	419/478 (88%)	410 (98%)	8 (2%)	1 (0%)	47	73
All	All	1256/1434 (88%)	1228 (98%)	25 (2%)	3 (0%)	47	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	749	TYR
1	B	749	TYR
1	C	749	TYR

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	384/410 (94%)	384 (100%)	0	100	100
1	B	371/410 (90%)	371 (100%)	0	100	100
1	C	376/410 (92%)	376 (100%)	0	100	100
All	All	1131/1230 (92%)	1131 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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, 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	A	420/478 (87%)	0.30	9 (2%) 63 65	35, 57, 92, 134	0
1	B	409/478 (85%)	0.64	44 (10%) 5 4	50, 84, 124, 160	0
1	C	415/478 (86%)	0.48	31 (7%) 14 12	40, 71, 109, 151	0
All	All	1244/1434 (86%)	0.47	84 (6%) 17 15	35, 70, 116, 160	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	PHE	7.4
1	B	917	ILE	7.0
1	C	922	TYR	6.7
1	C	646	SER	5.5
1	A	793	ILE	5.5
1	B	922	TYR	5.4
1	C	923	GLU	5.3
1	C	645	THR	5.1
1	B	920	ALA	5.1
1	B	910	LEU	4.9
1	C	925	GLN	4.8
1	A	796	LYS	4.7
1	B	793	ILE	4.3
1	B	900	LYS	4.3
1	B	738	THR	4.3
1	B	474	PHE	4.2
1	A	794	LEU	4.1
1	C	488	PHE	4.0
1	B	521	GLY	3.9
1	C	672	ALA	3.7
1	C	760	LYS	3.7
1	B	907	LEU	3.7
1	B	919	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	792	ALA	3.6
1	C	924	GLN	3.5
1	A	795	ASN	3.5
1	B	520	VAL	3.5
1	B	524	ARG	3.4
1	B	674	LEU	3.4
1	B	527	HIS	3.3
1	C	915	ASN	3.3
1	B	893	ARG	3.3
1	C	919	GLU	3.3
1	B	914	ILE	3.1
1	B	911	VAL	3.1
1	B	921	ARG	3.1
1	B	792	ALA	3.1
1	B	677	TYR	3.1
1	C	790	ASN	3.0
1	B	912	LYS	2.9
1	B	518	PHE	2.9
1	A	791	LYS	2.9
1	C	674	LEU	2.8
1	B	788	GLU	2.8
1	B	766	PHE	2.8
1	C	891	GLN	2.8
1	C	918	ARG	2.8
1	B	770	LEU	2.7
1	C	917	ILE	2.7
1	B	671	ASP	2.7
1	C	920	ALA	2.7
1	C	787	LEU	2.6
1	C	738	THR	2.6
1	B	892	ASP	2.6
1	B	894	ALA	2.5
1	B	877	GLN	2.5
1	B	648	LYS	2.5
1	C	735	LYS	2.5
1	B	903	GLU	2.4
1	C	673	ASN	2.4
1	C	893	ARG	2.3
1	B	475	ARG	2.3
1	B	517	PHE	2.3
1	B	523	PHE	2.3
1	C	848	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	509	GLU	2.2
1	C	914	ILE	2.2
1	B	735	LYS	2.2
1	B	791	LYS	2.2
1	C	663	ASN	2.2
1	A	904	ARG	2.2
1	B	913	LYS	2.2
1	C	791	LYS	2.2
1	B	760	LYS	2.1
1	C	644	GLY	2.1
1	C	849	GLY	2.1
1	B	526	TYR	2.1
1	C	854	VAL	2.0
1	B	522	ARG	2.0
1	A	655	CYS	2.0
1	C	853	GLU	2.0
1	B	672	ALA	2.0
1	A	816	GLN	2.0
1	B	506	LYS	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 carbohydrates 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.