wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 09:43 PM EDT

PDB ID	:	3FMV
Title	:	Crystal structure of the serine phosphatase of RNA polymerase II CTD (SSU72 superfamily) from Drosophila melanogaster. Monoclinic crystal form. Northeast Structural Genomics Consortium target FR253.
Authors	:	Kuzin, A.P.; Chen, Y.; Seetharaman, J.; Forouhar, F.; Chinag, Y.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2008-12-22
Resolution	:	3.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

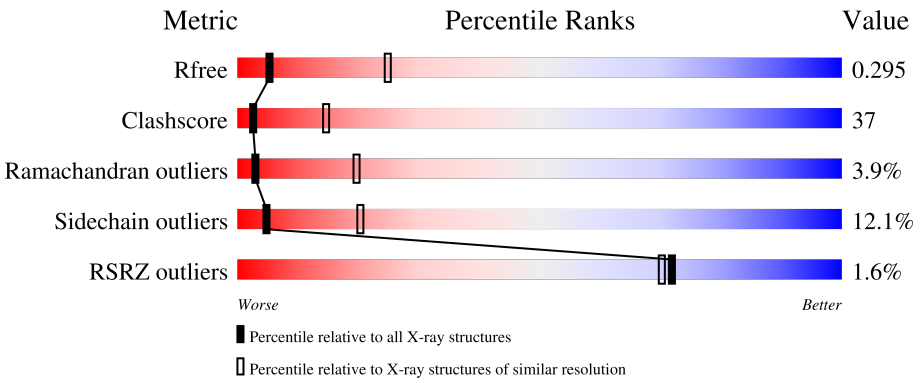
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	A	195	% 36% 53% 8% •
1	B	195	% 38% 47% 11% • •
1	C	195	% 39% 48% 9% • •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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Mol	Chain	Length	Quality of chain
1	D	195	2% 42% 49% 6%
1	E	195	% 36% 47% 14%
1	F	195	4% 39% 51% 7%
1	G	195	3% 46% 45% 6%
1	H	195	43% 48% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 12432 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 Serine phosphatase of RNA polymerase II CTD.

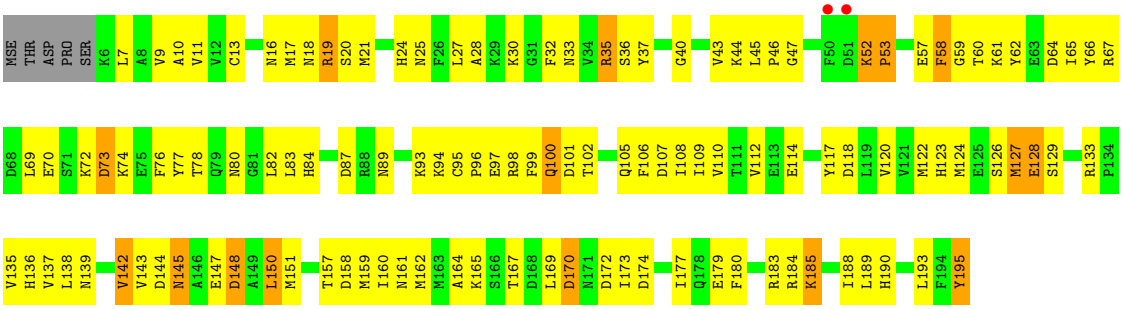
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	190	1554	975	268	298	2	11	0	0	0
1	B	190	1554	975	268	298	2	11	0	0	0
1	C	190	1554	975	268	298	2	11	0	0	0
1	D	190	1554	975	268	298	2	11	0	0	0
1	E	190	1554	975	268	298	2	11	0	0	0
1	F	190	1554	975	268	298	2	11	0	0	0
1	G	190	1554	975	268	298	2	11	0	0	0
1	H	190	1554	975	268	298	2	11	0	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.

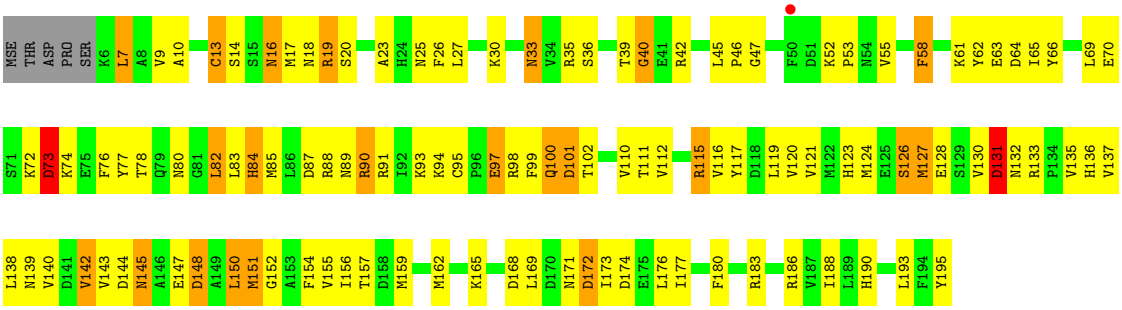
• Molecule 1: Serine phosphatase of RNA polymerase II CTD

Chain A:



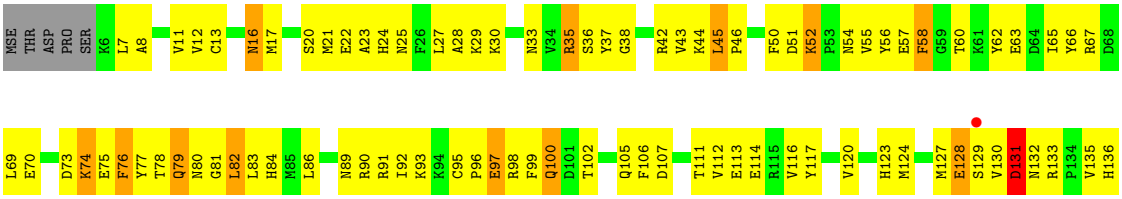
• Molecule 1: Serine phosphatase of RNA polymerase II CTD

Chain B:



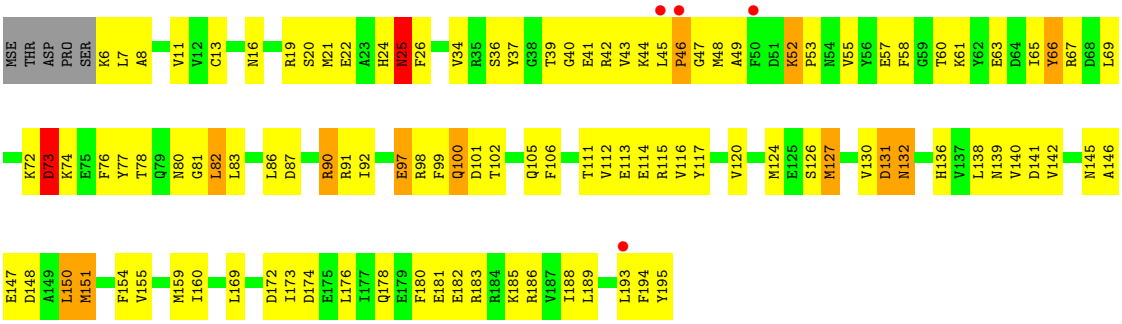
• Molecule 1: Serine phosphatase of RNA polymerase II CTD

Chain C:



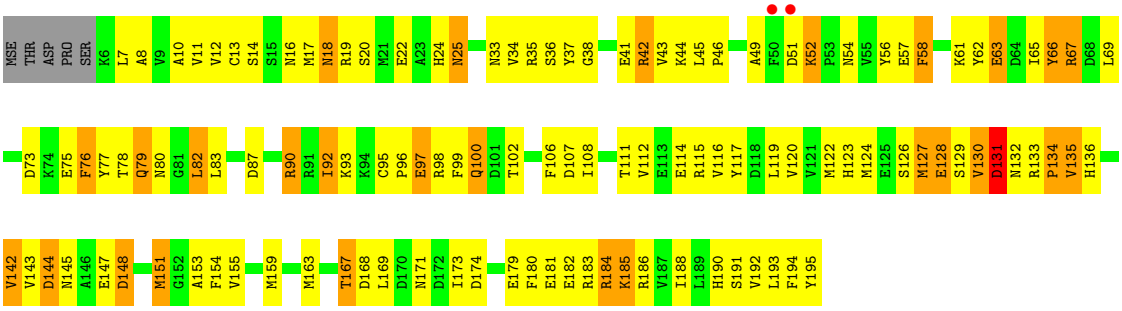
• Molecule 1: Serine phosphatase of RNA polymerase II CTD

Chain D:



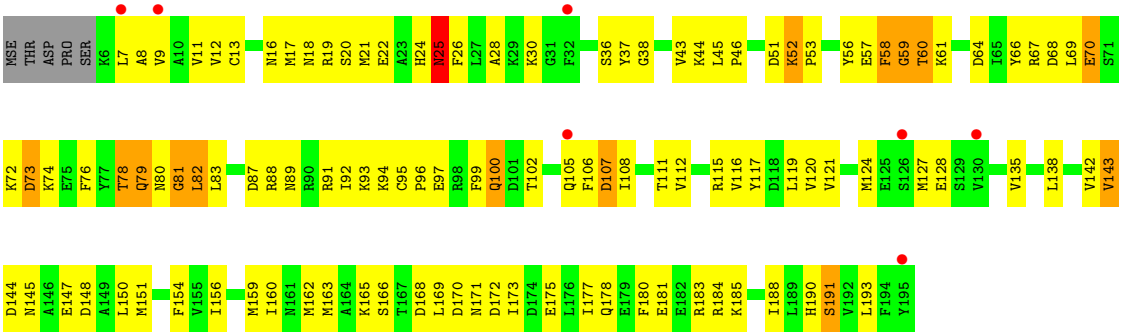
• Molecule 1: Serine phosphatase of RNA polymerase II CTD

Chain E:



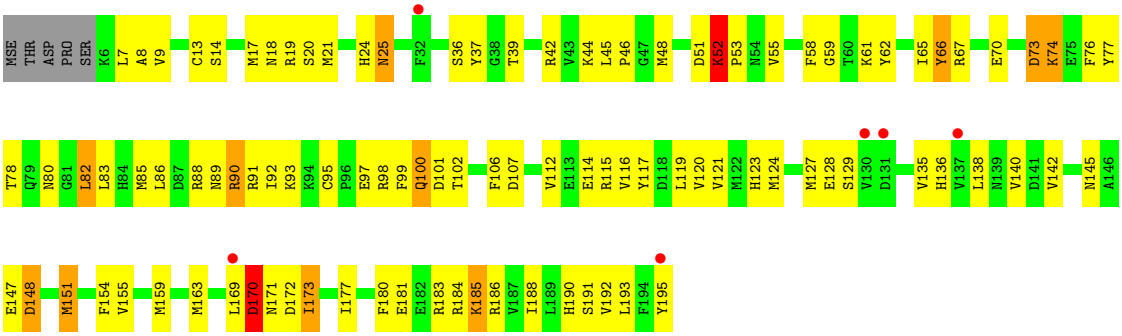
• Molecule 1: Serine phosphatase of RNA polymerase II CTD

Chain F:



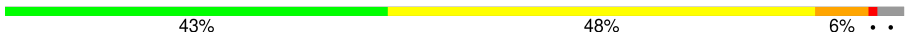
• Molecule 1: Serine phosphatase of RNA polymerase II CTD

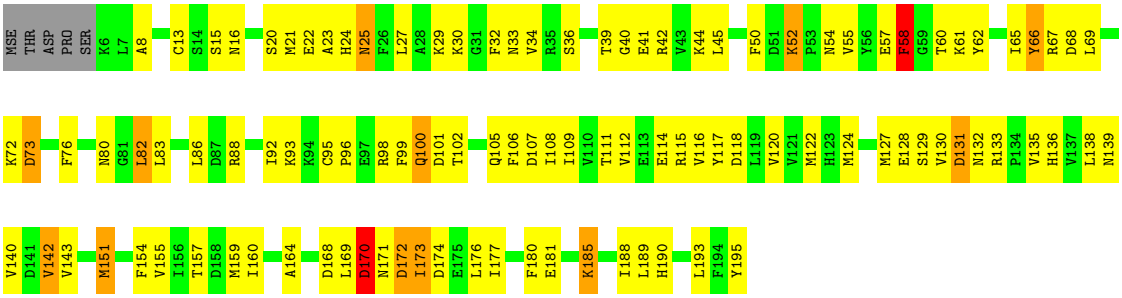
Chain G:



- Molecule 1: Serine phosphatase of RNA polymerase II CTD

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.98Å 99.00Å 158.12Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	19.93 – 3.31 30.12 – 3.31	Depositor EDS
% Data completeness (in resolution range)	87.5 (19.93-3.31) 93.2 (30.12-3.31)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 3.31Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.280 0.245 , 0.295	Depositor DCC
R_{free} test set	2701 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 14.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12432	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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 (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	0.59	0/1568	0.85	0/2088
1	B	0.58	0/1568	0.82	1/2088 (0.0%)
1	C	0.60	0/1568	0.80	0/2088
1	D	0.51	0/1568	0.73	0/2088
1	E	0.60	0/1568	0.83	0/2088
1	F	0.48	0/1568	0.70	0/2088
1	G	0.54	0/1568	0.72	0/2088
1	H	0.54	0/1568	0.78	0/2088
All	All	0.56	0/12544	0.78	1/16704 (0.0%)

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
1	C	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13	CYS	CA-CB-SG	6.02	124.84	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	37	TYR	Sidechain
1	E	66	TYR	Sidechain

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	1554	0	1529	131	0
1	B	1554	0	1529	125	0
1	C	1554	0	1529	132	0
1	D	1554	0	1529	106	0
1	E	1554	0	1529	131	0
1	F	1554	0	1529	98	0
1	G	1554	0	1529	99	0
1	H	1554	0	1529	113	0
All	All	12432	0	12232	903	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 37.

The worst 5 of 903 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:G:100:GLN:H	1:G:100:GLN:NE2	1.53	1.04
1:E:51:ASP:O	1:E:52:LYS:HE3	1.56	1.04
1:C:100:GLN:HE21	1:C:100:GLN:N	1.59	0.99
1:C:13:CYS:SG	1:C:20:SER:HB2	2.01	0.99
1:D:100:GLN:H	1:D:100:GLN:NE2	1.61	0.99

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	188/195 (96%)	160 (85%)	23 (12%)	5 (3%)	5	27
1	B	188/195 (96%)	157 (84%)	24 (13%)	7 (4%)	3	21
1	C	188/195 (96%)	146 (78%)	35 (19%)	7 (4%)	3	21
1	D	188/195 (96%)	155 (82%)	22 (12%)	11 (6%)	1	11
1	E	188/195 (96%)	147 (78%)	32 (17%)	9 (5%)	2	15
1	F	188/195 (96%)	150 (80%)	31 (16%)	7 (4%)	3	21
1	G	188/195 (96%)	147 (78%)	33 (18%)	8 (4%)	2	18
1	H	188/195 (96%)	153 (81%)	31 (16%)	4 (2%)	7	32
All	All	1504/1560 (96%)	1215 (81%)	231 (15%)	58 (4%)	3	20

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	131	ASP
1	C	74	LYS
1	C	90	ARG
1	C	191	SER
1	D	73	ASP

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	A	174/167 (104%)	152 (87%)	22 (13%)	4	19
1	B	174/167 (104%)	147 (84%)	27 (16%)	2	12
1	C	174/167 (104%)	155 (89%)	19 (11%)	6	25
1	D	174/167 (104%)	155 (89%)	19 (11%)	6	25
1	E	174/167 (104%)	150 (86%)	24 (14%)	3	16
1	F	174/167 (104%)	154 (88%)	20 (12%)	5	22
1	G	174/167 (104%)	155 (89%)	19 (11%)	6	25
1	H	174/167 (104%)	156 (90%)	18 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1392/1336 (104%)	1224 (88%)	168 (12%)	5 20

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	58	PHE
1	G	128	GLU
1	F	73	ASP
1	F	151	MSE
1	H	25	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	16	ASN
1	H	24	HIS
1	H	136	HIS
1	D	54	ASN
1	D	33	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	179/195 (91%)	-0.07	2 (1%)	80	81	39, 67, 100, 109	0
1	B	179/195 (91%)	-0.02	1 (0%)	89	90	37, 67, 108, 123	0
1	C	179/195 (91%)	-0.08	1 (0%)	89	90	42, 71, 96, 111	0
1	D	179/195 (91%)	0.09	4 (2%)	62	60	53, 84, 112, 127	0
1	E	179/195 (91%)	-0.01	2 (1%)	80	81	30, 67, 99, 114	0
1	F	179/195 (91%)	0.26	7 (3%)	39	38	63, 96, 136, 140	0
1	G	179/195 (91%)	0.30	6 (3%)	45	43	60, 103, 143, 147	0
1	H	179/195 (91%)	-0.04	0	100	100	44, 74, 99, 104	0
All	All	1432/1560 (91%)	0.05	23 (1%)	72	70	30, 77, 130, 147	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	126	SER	4.5
1	G	131	ASP	4.5
1	G	130	VAL	3.9
1	F	195	TYR	3.8
1	F	32	PHE	3.2

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.