



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:15 PM GMT

PDB ID : 1SSM
Title : Serine Acetyltransferase- Apoenzyme (truncated)
Authors : Olsen, L.R.; Huang, B.; Vetting, M.W.; Roderick, S.L.
Deposited on : 2004-03-24
Resolution : 2.15 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

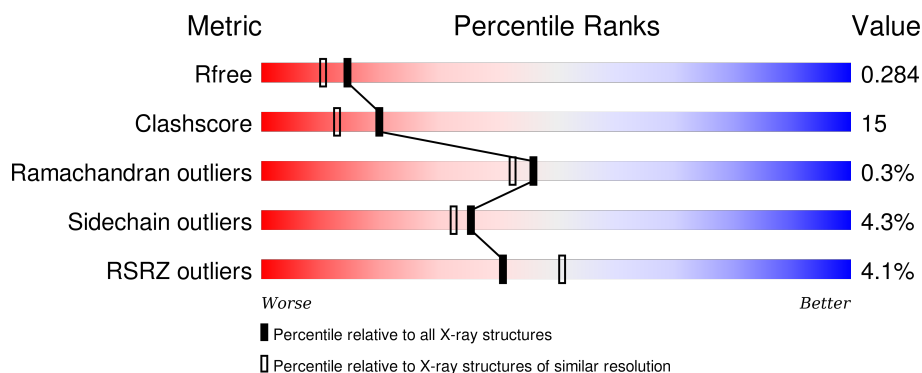
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 $\leq 5\%$. 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	242	<div> <div>5%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	B	242	<div> <div>3%</div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	C	242	<div> <div>4%</div> <div>71%</div> <div>27%</div> <div>..</div> </div>
1	D	242	<div> <div>4%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>
1	E	242	<div> <div>5%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	242	<div><div></div><div>4%</div><div>65%</div><div>31%</div><div></div><div>• •</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11514 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 acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	Se	0	0	0
			1824	1162	320	336	2	4			
1	B	240	Total	C	N	O	S	Se	0	0	0
			1826	1163	319	337	2	5			
1	C	240	Total	C	N	O	S	Se	0	0	0
			1819	1159	318	336	2	4			
1	D	240	Total	C	N	O	S	Se	0	0	0
			1823	1162	319	336	2	4			
1	E	240	Total	C	N	O	S	Se	0	0	0
			1831	1166	321	337	2	5			
1	F	240	Total	C	N	O	S	Se	0	0	0
			1822	1162	319	335	2	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P43886
A	22	MSE	MET	MODIFIED RESIDUE	UNP P43886
A	54	MSE	MET	MODIFIED RESIDUE	UNP P43886
A	151	MSE	MET	MODIFIED RESIDUE	UNP P43886
A	197	MSE	MET	MODIFIED RESIDUE	UNP P43886
B	1	MSE	MET	MODIFIED RESIDUE	UNP P43886
B	22	MSE	MET	MODIFIED RESIDUE	UNP P43886
B	54	MSE	MET	MODIFIED RESIDUE	UNP P43886
B	151	MSE	MET	MODIFIED RESIDUE	UNP P43886
B	197	MSE	MET	MODIFIED RESIDUE	UNP P43886
C	1	MSE	MET	MODIFIED RESIDUE	UNP P43886
C	22	MSE	MET	MODIFIED RESIDUE	UNP P43886
C	54	MSE	MET	MODIFIED RESIDUE	UNP P43886
C	151	MSE	MET	MODIFIED RESIDUE	UNP P43886
C	197	MSE	MET	MODIFIED RESIDUE	UNP P43886
D	1	MSE	MET	MODIFIED RESIDUE	UNP P43886
D	22	MSE	MET	MODIFIED RESIDUE	UNP P43886

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Chain	Residue	Modelled	Actual	Comment	Reference
D	54	MSE	MET	MODIFIED RESIDUE	UNP P43886
D	151	MSE	MET	MODIFIED RESIDUE	UNP P43886
D	197	MSE	MET	MODIFIED RESIDUE	UNP P43886
E	1	MSE	MET	MODIFIED RESIDUE	UNP P43886
E	22	MSE	MET	MODIFIED RESIDUE	UNP P43886
E	54	MSE	MET	MODIFIED RESIDUE	UNP P43886
E	151	MSE	MET	MODIFIED RESIDUE	UNP P43886
E	197	MSE	MET	MODIFIED RESIDUE	UNP P43886
F	1	MSE	MET	MODIFIED RESIDUE	UNP P43886
F	22	MSE	MET	MODIFIED RESIDUE	UNP P43886
F	54	MSE	MET	MODIFIED RESIDUE	UNP P43886
F	151	MSE	MET	MODIFIED RESIDUE	UNP P43886
F	197	MSE	MET	MODIFIED RESIDUE	UNP P43886

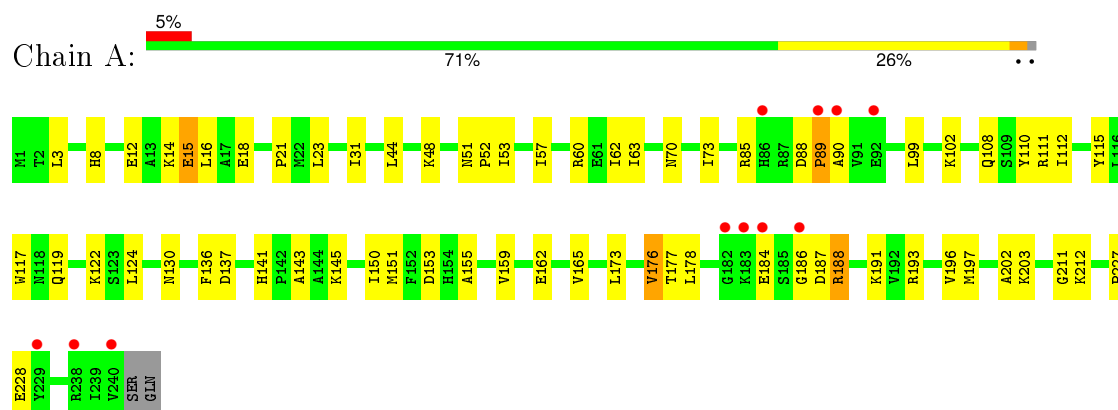
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	101	Total O 101 101	0	0
2	B	96	Total O 96 96	0	0
2	C	89	Total O 89 89	0	0
2	D	91	Total O 91 91	0	0
2	E	86	Total O 86 86	0	0
2	F	106	Total O 106 106	0	0

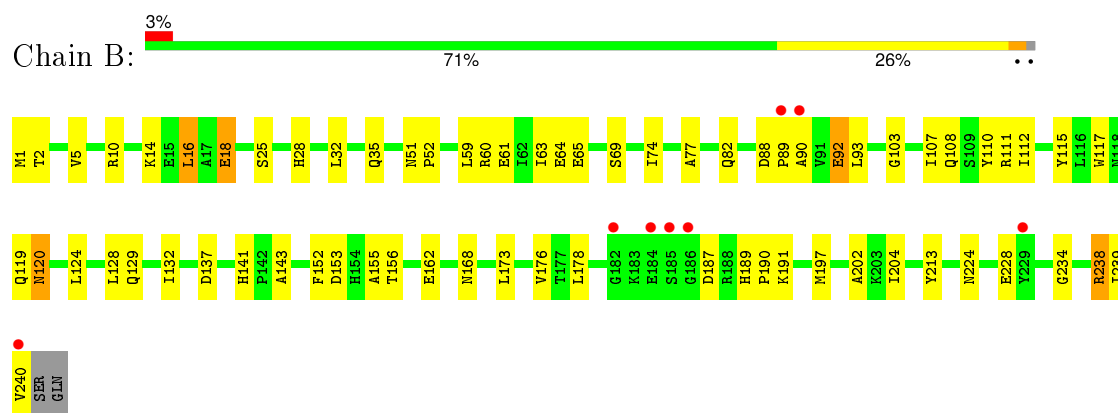
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

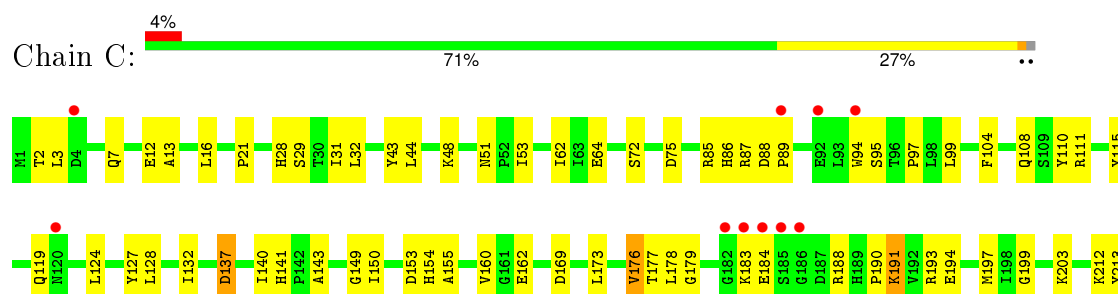
• Molecule 1: Serine acetyltransferase



• Molecule 1: Serine acetyltransferase

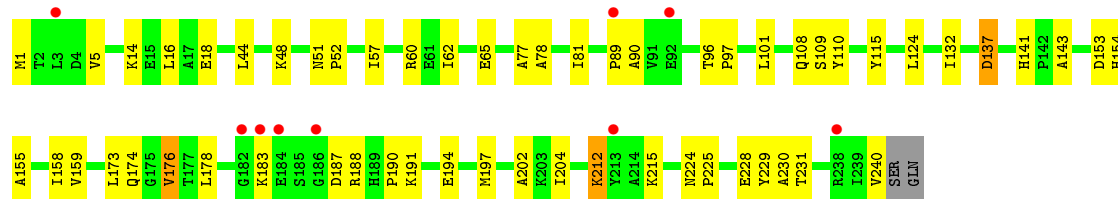
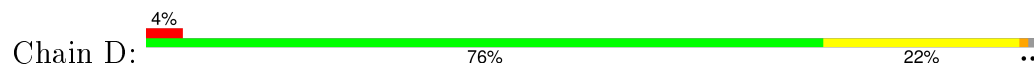


• Molecule 1: Serine acetyltransferase

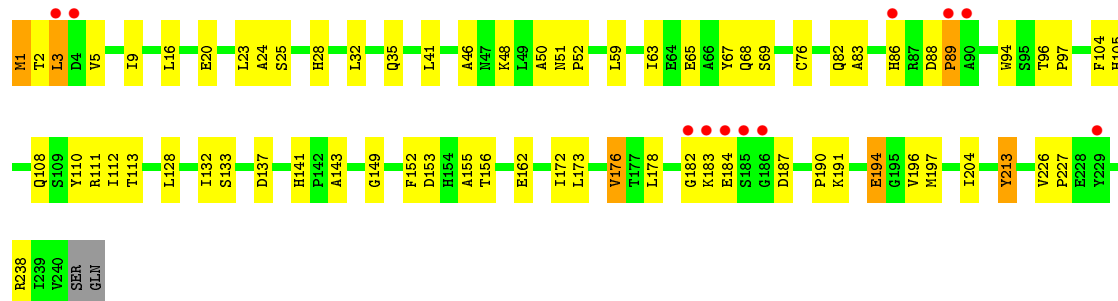




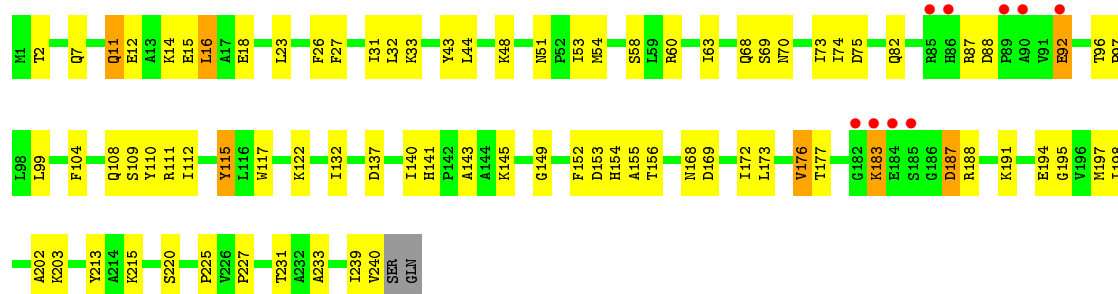
• Molecule 1: Serine acetyltransferase



• Molecule 1: Serine acetyltransferase



• Molecule 1: Serine acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.10Å 126.60Å 107.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.15 29.74 – 2.13	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.74-2.15) 90.5 (29.74-2.13)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.14Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.278 0.231 , 0.284	Depositor DCC
R_{free} test set	3575 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	8 of 147686 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11514	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.91 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.2745e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.83	2/1859 (0.1%)	0.93	3/2525 (0.1%)
1	B	0.84	1/1860 (0.1%)	0.95	2/2525 (0.1%)
1	C	0.84	0/1853	0.93	2/2517 (0.1%)
1	D	0.82	0/1857	0.93	2/2521 (0.1%)
1	E	0.85	1/1866 (0.1%)	0.93	2/2533 (0.1%)
1	F	0.81	1/1857 (0.1%)	0.92	3/2522 (0.1%)
All	All	0.83	5/11152 (0.0%)	0.93	14/15143 (0.1%)

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	B	0	1
1	C	0	1
1	E	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	76	CYS	CB-SG	7.41	1.94	1.82
1	A	15	GLU	CB-CG	5.52	1.62	1.52
1	A	15	GLU	CG-CD	5.36	1.59	1.51
1	F	43	TYR	CD2-CE2	5.22	1.47	1.39
1	B	92	GLU	CD-OE2	5.06	1.31	1.25

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	LYS	N-CA-C	-7.08	91.89	111.00
1	B	178	LEU	N-CA-C	-6.80	92.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	E	3	LEU	CB-CG-CD1	-6.50	99.96	111.00
1	A	178	LEU	N-CA-C	-6.35	93.85	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	TYR	Sidechain
1	C	127	TYR	Sidechain
1	E	213	TYR	Sidechain

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	1824	0	1821	50	0
1	B	1826	0	1829	69	0
1	C	1819	0	1816	54	0
1	D	1823	0	1827	53	0
1	E	1831	0	1834	52	0
1	F	1822	0	1823	66	0
2	A	101	0	0	14	0
2	B	96	0	0	14	0
2	C	89	0	0	11	0
2	D	91	0	0	9	0
2	E	86	0	0	4	0
2	F	106	0	0	9	0
All	All	11514	0	10950	324	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 15.

The worst 5 of 324 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:53:ILE:HB	2:A:7567:HOH:O	1.47	1.12
1:E:141:HIS:HD2	1:E:143:ALA:H	1.00	0.98
1:E:3:LEU:HG	2:E:7410:HOH:O	1.65	0.95
1:E:141:HIS:CD2	1:E:143:ALA:H	1.85	0.94
1:C:141:HIS:HD2	1:C:143:ALA:H	1.04	0.94

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	238/242 (98%)	229 (96%)	8 (3%)	1 (0%)	39	34
1	B	238/242 (98%)	225 (94%)	13 (6%)	0	100	100
1	C	238/242 (98%)	229 (96%)	9 (4%)	0	100	100
1	D	238/242 (98%)	224 (94%)	13 (6%)	1 (0%)	39	34
1	E	238/242 (98%)	225 (94%)	11 (5%)	2 (1%)	24	15
1	F	238/242 (98%)	227 (95%)	11 (5%)	0	100	100
All	All	1428/1452 (98%)	1359 (95%)	65 (5%)	4 (0%)	46	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	229	TYR
1	E	183	LYS
1	E	89	PRO
1	A	89	PRO

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	190/192 (99%)	183 (96%)	7 (4%)	41	38
1	B	191/192 (100%)	184 (96%)	7 (4%)	41	38
1	C	189/192 (98%)	181 (96%)	8 (4%)	36	34
1	D	190/192 (99%)	183 (96%)	7 (4%)	41	38
1	E	192/192 (100%)	183 (95%)	9 (5%)	32	28
1	F	190/192 (99%)	179 (94%)	11 (6%)	25	19
All	All	1142/1152 (99%)	1093 (96%)	49 (4%)	35	32

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	16	LEU
1	D	188	ARG
1	F	115	TYR
1	D	115	TYR
1	D	212	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	141	HIS
1	D	7	GLN
1	F	141	HIS
1	C	148	HIS
1	C	154	HIS

5.3.3 RNA ⓘ

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 carbohydrates 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	235/242 (97%)	0.09	11 (4%) 35 46	16, 25, 41, 56	0
1	B	235/242 (97%)	0.11	8 (3%) 49 59	16, 25, 41, 55	0
1	C	235/242 (97%)	0.14	10 (4%) 39 49	17, 25, 42, 52	0
1	D	235/242 (97%)	0.11	9 (3%) 44 54	15, 24, 40, 50	0
1	E	235/242 (97%)	0.18	11 (4%) 35 46	16, 25, 42, 52	0
1	F	235/242 (97%)	0.03	9 (3%) 44 54	16, 23, 41, 53	0
All	All	1410/1452 (97%)	0.11	58 (4%) 41 51	15, 25, 42, 56	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	GLU	6.0
1	B	185	SER	5.9
1	C	185	SER	5.8
1	E	184	GLU	5.7
1	A	184	GLU	5.7

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.