



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:51 PM UTC

PDB ID : 1S80 / pdb_00001s80
Title : Structure of Serine Acetyltransferase from Haemophilis influenzae Rd
Authors : Gorman, J.; Gogos, A.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-01-30
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

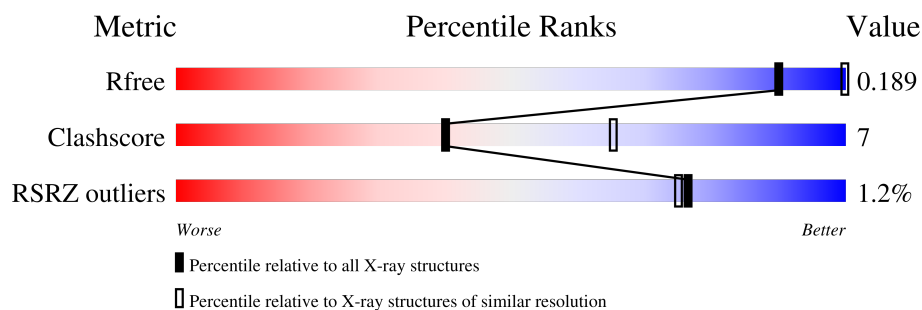
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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 $\leq 5\%$. 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	278	76% 10% 13%
1	B	278	77% 9% 13%
1	C	278	77% 9% 13%
1	D	278	76% 10% 13%
1	E	278	70% 16% 13%
1	F	278	73% 14% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11512 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	241	Total	C	N	O	S	Se	0	0	0
			1849	1178	324	341	2	4			
1	B	241	Total	C	N	O	S	Se	0	0	0
			1849	1178	324	341	2	4			
1	C	241	Total	C	N	O	S	Se	0	0	0
			1849	1178	324	341	2	4			
1	D	241	Total	C	N	O	S	Se	0	0	0
			1849	1178	324	341	2	4			
1	E	241	Total	C	N	O	S	Se	0	0	0
			1849	1178	324	341	2	4			
1	F	241	Total	C	N	O	S	Se	0	0	0
			1849	1178	324	341	2	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP P43886
A	1	LEU	-	cloning artifact	UNP P43886
A	22	MSE	-	modified residue	UNP P43886
A	54	MSE	-	modified residue	UNP P43886
A	151	MSE	-	modified residue	UNP P43886
A	197	MSE	-	modified residue	UNP P43886
A	267	GLU	-	expression tag	UNP P43886
A	268	GLY	-	expression tag	UNP P43886
A	269	GLY	-	expression tag	UNP P43886
A	270	SER	-	expression tag	UNP P43886
A	271	HIS	-	expression tag	UNP P43886
A	272	HIS	-	expression tag	UNP P43886
A	273	HIS	-	expression tag	UNP P43886
A	274	HIS	-	expression tag	UNP P43886
A	275	HIS	-	expression tag	UNP P43886
A	276	HIS	-	expression tag	UNP P43886
B	0	SER	-	cloning artifact	UNP P43886

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	cloning artifact	UNP P43886
B	22	MSE	-	modified residue	UNP P43886
B	54	MSE	-	modified residue	UNP P43886
B	151	MSE	-	modified residue	UNP P43886
B	197	MSE	-	modified residue	UNP P43886
B	267	GLU	-	expression tag	UNP P43886
B	268	GLY	-	expression tag	UNP P43886
B	269	GLY	-	expression tag	UNP P43886
B	270	SER	-	expression tag	UNP P43886
B	271	HIS	-	expression tag	UNP P43886
B	272	HIS	-	expression tag	UNP P43886
B	273	HIS	-	expression tag	UNP P43886
B	274	HIS	-	expression tag	UNP P43886
B	275	HIS	-	expression tag	UNP P43886
B	276	HIS	-	expression tag	UNP P43886
C	0	SER	-	cloning artifact	UNP P43886
C	1	LEU	-	cloning artifact	UNP P43886
C	22	MSE	-	modified residue	UNP P43886
C	54	MSE	-	modified residue	UNP P43886
C	151	MSE	-	modified residue	UNP P43886
C	197	MSE	-	modified residue	UNP P43886
C	267	GLU	-	expression tag	UNP P43886
C	268	GLY	-	expression tag	UNP P43886
C	269	GLY	-	expression tag	UNP P43886
C	270	SER	-	expression tag	UNP P43886
C	271	HIS	-	expression tag	UNP P43886
C	272	HIS	-	expression tag	UNP P43886
C	273	HIS	-	expression tag	UNP P43886
C	274	HIS	-	expression tag	UNP P43886
C	275	HIS	-	expression tag	UNP P43886
C	276	HIS	-	expression tag	UNP P43886
D	0	SER	-	cloning artifact	UNP P43886
D	1	LEU	-	cloning artifact	UNP P43886
D	22	MSE	-	modified residue	UNP P43886
D	54	MSE	-	modified residue	UNP P43886
D	151	MSE	-	modified residue	UNP P43886
D	197	MSE	-	modified residue	UNP P43886
D	267	GLU	-	expression tag	UNP P43886
D	268	GLY	-	expression tag	UNP P43886
D	269	GLY	-	expression tag	UNP P43886
D	270	SER	-	expression tag	UNP P43886
D	271	HIS	-	expression tag	UNP P43886

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Chain	Residue	Modelled	Actual	Comment	Reference
D	272	HIS	-	expression tag	UNP P43886
D	273	HIS	-	expression tag	UNP P43886
D	274	HIS	-	expression tag	UNP P43886
D	275	HIS	-	expression tag	UNP P43886
D	276	HIS	-	expression tag	UNP P43886
E	0	SER	-	cloning artifact	UNP P43886
E	1	LEU	-	cloning artifact	UNP P43886
E	22	MSE	-	modified residue	UNP P43886
E	54	MSE	-	modified residue	UNP P43886
E	151	MSE	-	modified residue	UNP P43886
E	197	MSE	-	modified residue	UNP P43886
E	267	GLU	-	expression tag	UNP P43886
E	268	GLY	-	expression tag	UNP P43886
E	269	GLY	-	expression tag	UNP P43886
E	270	SER	-	expression tag	UNP P43886
E	271	HIS	-	expression tag	UNP P43886
E	272	HIS	-	expression tag	UNP P43886
E	273	HIS	-	expression tag	UNP P43886
E	274	HIS	-	expression tag	UNP P43886
E	275	HIS	-	expression tag	UNP P43886
E	276	HIS	-	expression tag	UNP P43886
F	0	SER	-	cloning artifact	UNP P43886
F	1	LEU	-	cloning artifact	UNP P43886
F	22	MSE	-	modified residue	UNP P43886
F	54	MSE	-	modified residue	UNP P43886
F	151	MSE	-	modified residue	UNP P43886
F	197	MSE	-	modified residue	UNP P43886
F	267	GLU	-	expression tag	UNP P43886
F	268	GLY	-	expression tag	UNP P43886
F	269	GLY	-	expression tag	UNP P43886
F	270	SER	-	expression tag	UNP P43886
F	271	HIS	-	expression tag	UNP P43886
F	272	HIS	-	expression tag	UNP P43886
F	273	HIS	-	expression tag	UNP P43886
F	274	HIS	-	expression tag	UNP P43886
F	275	HIS	-	expression tag	UNP P43886
F	276	HIS	-	expression tag	UNP P43886

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	71	Total O 71 71	0	0

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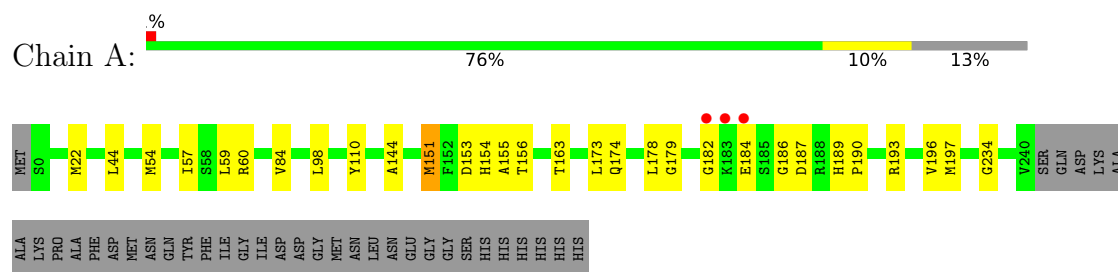
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	73	Total 73	O 73	0	0
2	C	71	Total 71	O 71	0	0
2	D	72	Total 72	O 72	0	0
2	E	74	Total 74	O 74	0	0
2	F	57	Total 57	O 57	0	0

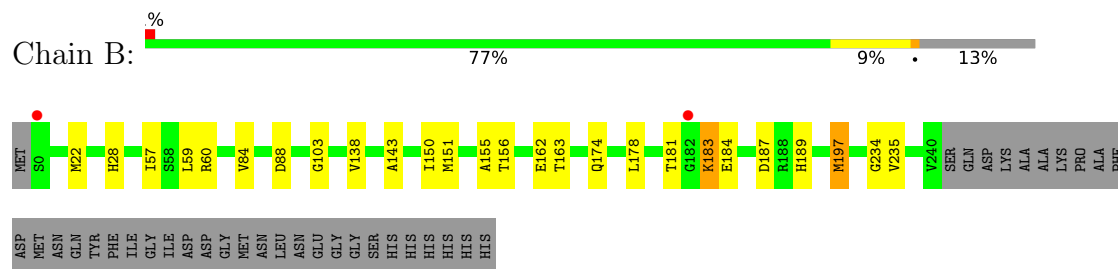
3 Residue-property plots

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.

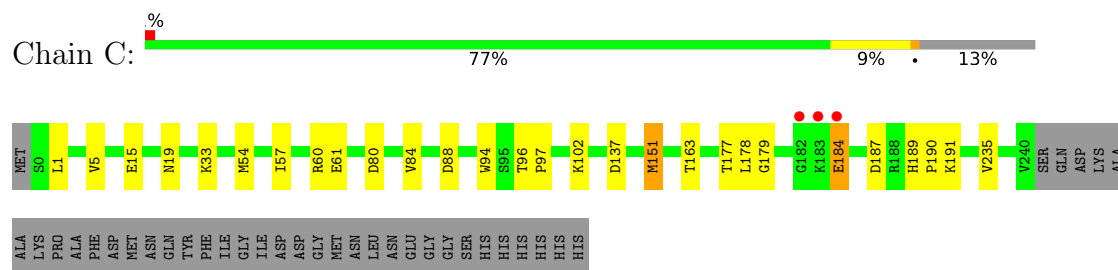
• Molecule 1: Serine acetyltransferase



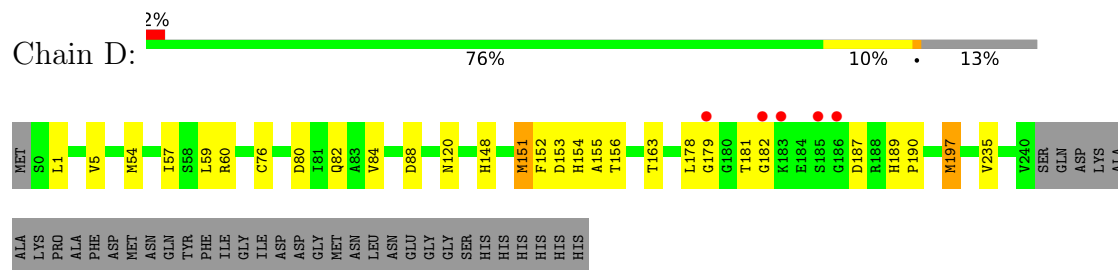
• Molecule 1: Serine acetyltransferase



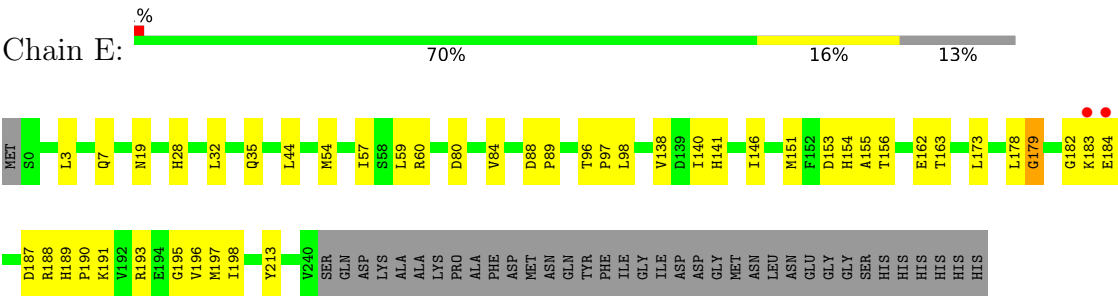
• Molecule 1: Serine acetyltransferase



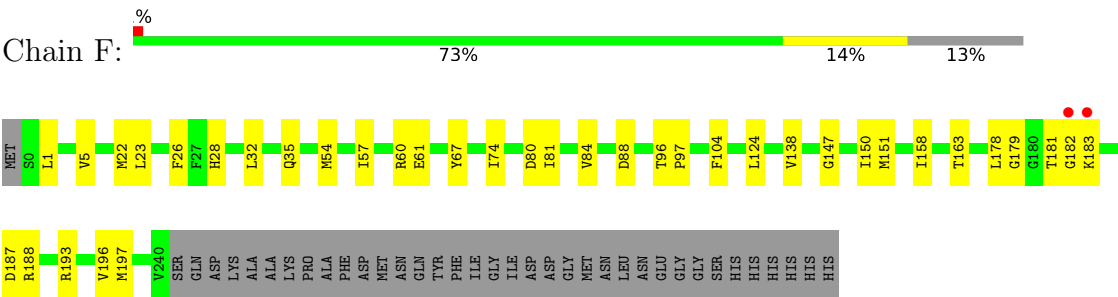
• Molecule 1: Serine acetyltransferase



● Molecule 1: Serine acetyltransferase



● Molecule 1: Serine acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.96Å 209.67Å 136.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.70) 94.4 (20.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.93 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.172 , 0.219 (Not available) , 0.189	Depositor DCC
R_{free} test set	2479 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11512	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.73	2/1884 (0.1%)	0.92	0/2555
1	B	0.78	1/1884 (0.1%)	0.94	1/2555 (0.0%)
1	C	0.75	1/1884 (0.1%)	0.97	1/2555 (0.0%)
1	D	0.76	2/1884 (0.1%)	0.93	0/2555
1	E	0.73	0/1884	0.98	1/2555 (0.0%)
1	F	0.74	1/1884 (0.1%)	0.92	1/2555 (0.0%)
All	All	0.75	7/11304 (0.1%)	0.95	4/15330 (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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	197	MSE	SE-CE	9.03	2.22	1.95
1	B	197	MSE	SE-CE	7.46	2.17	1.95
1	F	197	MSE	SE-CE	6.05	2.13	1.95
1	A	197	MSE	SE-CE	5.99	2.13	1.95
1	A	151	MSE	SE-CE	-5.17	1.79	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	GLU	N-CA-C	6.26	119.56	109.79
1	F	179	GLY	N-CA-C	5.45	118.40	112.29
1	C	184	GLU	N-CA-C	5.31	117.14	109.07
1	E	179	GLY	N-CA-C	5.21	117.36	112.04

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	LEU	Peptide
1	B	178	LEU	Peptide
1	B	183	LYS	Peptide
1	C	178	LEU	Peptide
1	C	184	GLU	Peptide

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	1849	0	1867	24	0
1	B	1849	0	1867	28	0
1	C	1849	0	1867	26	0
1	D	1849	0	1867	24	0
1	E	1849	0	1867	34	0
1	F	1849	0	1867	28	0
2	A	71	0	0	2	0
2	B	73	0	0	1	0
2	C	71	0	0	2	0
2	D	72	0	0	3	0
2	E	74	0	0	3	0
2	F	57	0	0	0	0
All	All	11512	0	11202	147	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 7.

The worst 5 of 147 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:B:197:MSE:SE	1:B:197:MSE:CE	2.17	1.43
1:D:197:MSE:CE	1:D:197:MSE:SE	2.22	1.36
1:B:174:GLN:HE21	1:C:177:THR:HG21	1.41	0.85
1:D:163:THR:HB	1:D:189:HIS:ND1	1.93	0.84
1:E:7:GLN:HE21	1:E:7:GLN:HA	1.44	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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 oligosaccharides 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 ⓘ

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	237/278 (85%)	-0.42	3 (1%) 75 73	22, 31, 44, 62	0
1	B	237/278 (85%)	-0.45	2 (0%) 82 81	20, 29, 44, 59	0
1	C	237/278 (85%)	-0.39	3 (1%) 75 73	21, 33, 49, 59	0
1	D	237/278 (85%)	-0.43	5 (2%) 63 61	18, 28, 46, 63	0
1	E	237/278 (85%)	-0.33	2 (0%) 82 81	21, 34, 49, 60	0
1	F	237/278 (85%)	-0.22	2 (0%) 82 81	23, 38, 50, 67	0
All	All	1422/1668 (85%)	-0.38	17 (1%) 76 75	18, 32, 48, 67	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	LYS	4.6
1	D	182	GLY	3.2
1	F	182	GLY	3.0
1	F	183	LYS	2.9
1	E	184	GLU	2.8

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 oligosaccharides 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.