



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:09 PM GMT

PDB ID : 1S80  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

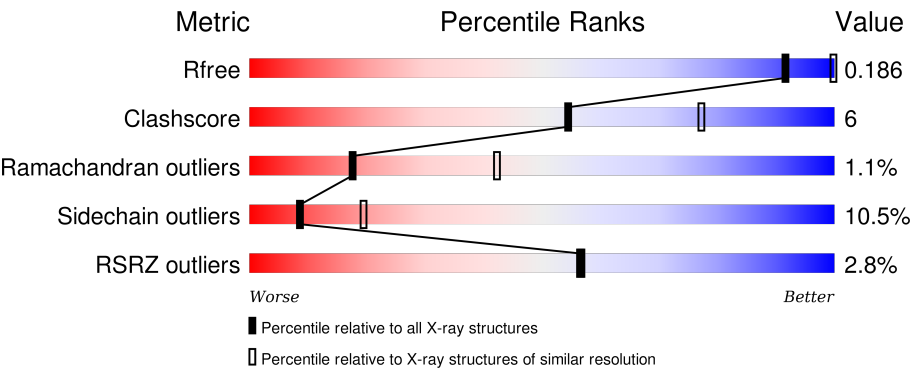
# 1 Overall quality at a glance i

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.



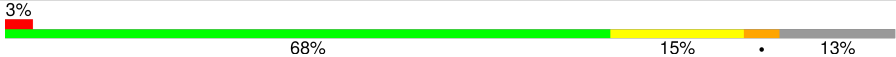
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	278	<div><div>3%</div><div>72%13%••13%</div></div>
1	B	278	<div><div>2%</div><div>71%14%•13%</div></div>
1	C	278	<div><div>3%</div><div>72%13%••13%</div></div>
1	D	278	<div><div>2%</div><div>72%11%•13%</div></div>
1	E	278	<div><div>2%</div><div>65%15%5%•13%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	278	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (3%), green (68%), yellow (15%), and grey (13%). A small black dot is located on the yellow segment. The segments are labeled with their respective percentages: 3%, 68%, 15%, and 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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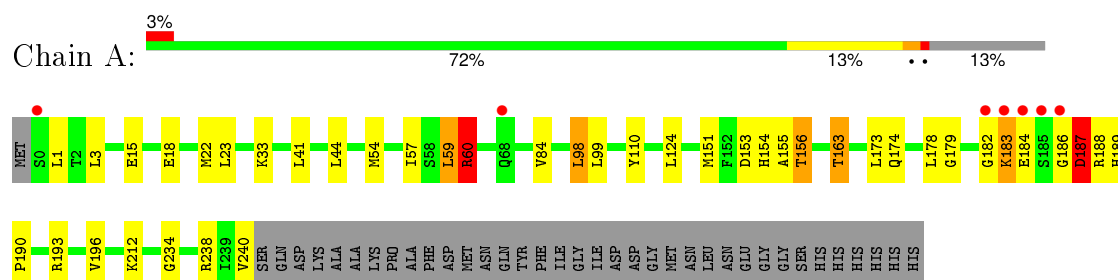
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	73	Total 73	O 73	0	0
2	C	71	Total 71	O 71	0	0
2	D	72	Total 72	O 72	0	0
2	E	74	Total 74	O 74	0	0
2	F	57	Total 57	O 57	0	0

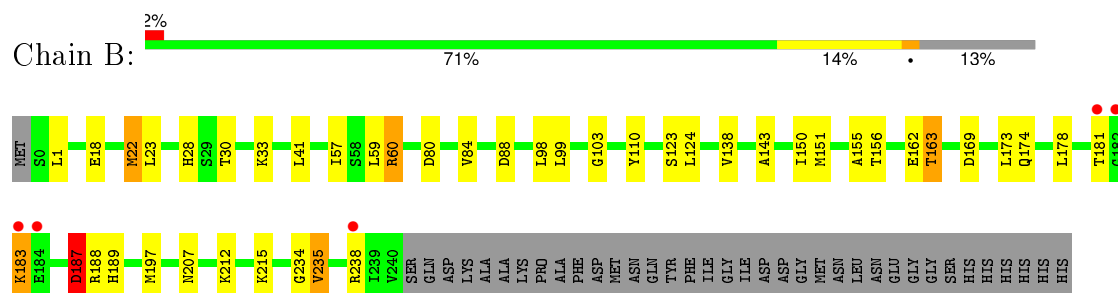
### 3 Residue-property plots [i](#)

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

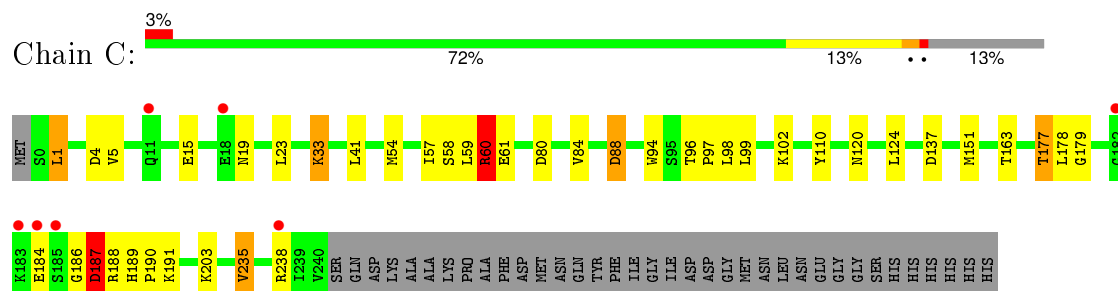
- Molecule 1: Serine acetyltransferase



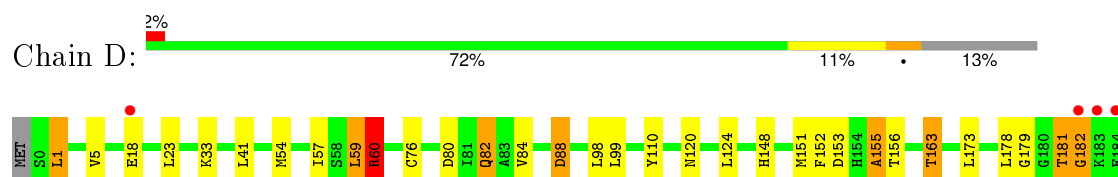
- Molecule 1: Serine acetyltransferase



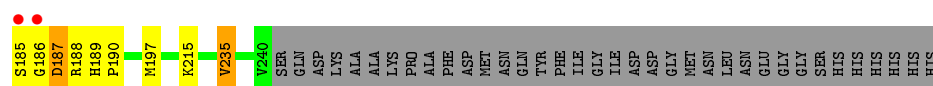
- Molecule 1: Serine acetyltransferase



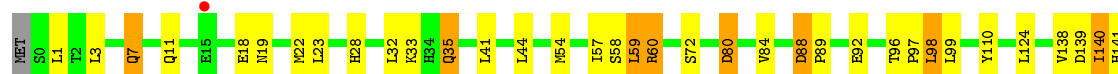
- Molecule 1: Serine acetyltransferase



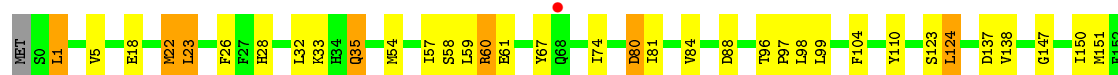




• Molecule 1: Serine acetyltransferase



• Molecule 1: Serine acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.96Å 209.67Å 136.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.70) 94.7 (19.95-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.93 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.172 , 0.219 0.181 , 0.186	Depositor DCC
$R_{free}$ test set	2479 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 48586 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 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	0.53	0/1884	0.74	2/2555 (0.1%)
1	B	0.57	0/1884	0.76	3/2555 (0.1%)
1	C	0.56	0/1884	0.77	4/2555 (0.2%)
1	D	0.57	0/1884	0.76	3/2555 (0.1%)
1	E	0.55	0/1884	0.77	5/2555 (0.2%)
1	F	0.55	0/1884	0.74	5/2555 (0.2%)
All	All	0.56	0/11304	0.76	22/15330 (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	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

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	60	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	D	187	ASP	CB-CG-OD2	6.52	124.17	118.30
1	F	187	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	187	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	187	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	187	ASP	CB-CG-OD2	6.08	123.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	137	ASP	CB-CG-OD2	6.03	123.73	118.30
1	D	88	ASP	CB-CG-OD2	5.85	123.56	118.30
1	E	88	ASP	CB-CG-OD2	5.83	123.54	118.30
1	E	139	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	4	ASP	CB-CG-OD2	5.67	123.40	118.30
1	E	80	ASP	CB-CG-OD2	5.64	123.37	118.30
1	F	169	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	60	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	E	187	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	169	ASP	CB-CG-OD2	5.39	123.15	118.30
1	F	153	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	153	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	80	ASP	CB-CG-OD2	5.18	122.97	118.30
1	F	80	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	60	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	88	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

All (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
1	D	178	LEU	Peptide
1	E	178	LEU	Peptide
1	F	178	LEU	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	23	0
1	B	1849	0	1867	28	0
1	C	1849	0	1867	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1849	0	1867	23	0
1	E	1849	0	1867	31	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	1	0
All	All	11512	0	11202	142	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 6.

All (142) 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:SE	1:D:197:MSE:CE	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
1:F:54:MSE:HE1	1:F:124:LEU:HD21	1.59	0.83
1:E:19:ASN:HB3	2:E:346:HOH:O	1.82	0.79
1:E:184:GLU:HB3	2:E:349:HOH:O	1.84	0.78
1:A:84:VAL:HA	1:A:151:MSE:HE3	1.65	0.77
1:E:163:THR:HG21	1:E:187:ASP:HA	1.67	0.76
1:B:163:THR:HB	1:B:189:HIS:ND1	1.99	0.75
1:B:88:ASP:HB2	1:B:151:MSE:CE	2.18	0.74
1:C:84:VAL:HA	1:C:151:MSE:HE3	1.71	0.73
1:B:88:ASP:HB2	1:B:151:MSE:HE1	1.71	0.71
1:D:151:MSE:HE2	1:D:153:ASP:CG	2.12	0.70
1:C:60:ARG:HG3	1:F:57:ILE:HD11	1.72	0.70
1:A:84:VAL:HA	1:A:151:MSE:CE	2.22	0.69
1:B:57:ILE:HD11	1:D:60:ARG:HG3	1.75	0.68
1:E:163:THR:HB	1:E:189:HIS:ND1	2.09	0.68
1:A:57:ILE:HD11	1:E:60:ARG:HG3	1.75	0.68
1:B:156:THR:HG21	2:C:344:HOH:O	1.92	0.67
1:D:163:THR:HG21	1:D:187:ASP:HA	1.76	0.67
1:D:155:ALA:C	2:D:348:HOH:O	2.34	0.66
1:C:163:THR:HG21	1:C:187:ASP:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ILE:CD1	1:E:146:ILE:HD11	2.27	0.65
1:F:88:ASP:HB2	1:F:151:MSE:CE	2.26	0.65
1:A:182:GLY:O	1:A:184:GLU:N	2.27	0.64
1:E:88:ASP:HB2	1:E:151:MSE:HE1	1.79	0.64
1:A:163:THR:HB	1:A:189:HIS:ND1	2.13	0.64
1:B:84:VAL:HG22	1:B:151:MSE:HG3	1.79	0.63
1:B:174:GLN:HE21	1:C:177:THR:CG2	2.13	0.61
1:A:156:THR:HG21	2:B:288:HOH:O	2.01	0.61
1:B:22:MSE:HE1	1:F:28:HIS:HB3	1.82	0.61
1:C:80:ASP:O	1:C:84:VAL:HG23	2.01	0.60
1:A:163:THR:HG21	1:A:187:ASP:HA	1.82	0.60
1:D:156:THR:N	2:D:348:HOH:O	2.35	0.60
1:B:103:GLY:HA2	1:B:155:ALA:HB2	1.84	0.60
1:F:163:THR:HG21	1:F:187:ASP:HA	1.85	0.59
1:C:61:GLU:OE2	1:F:60:ARG:NH2	2.36	0.58
1:E:7:GLN:HE21	1:E:7:GLN:CA	2.16	0.57
1:E:88:ASP:HB2	1:E:151:MSE:CE	2.35	0.57
1:A:54:MSE:HE3	1:A:59:LEU:HG	1.86	0.56
1:C:57:ILE:HD11	1:F:60:ARG:HG3	1.87	0.56
1:A:179:GLY:HA3	1:A:190:PRO:HD3	1.87	0.56
1:F:35:GLN:HE21	1:F:35:GLN:HA	1.71	0.56
1:B:103:GLY:CA	1:B:155:ALA:HB2	2.36	0.56
1:F:80:ASP:O	1:F:84:VAL:HG23	2.06	0.56
1:D:163:THR:O	1:D:163:THR:CG2	2.54	0.55
1:D:80:ASP:O	1:D:84:VAL:HG23	2.07	0.55
1:E:28:HIS:HA	1:E:32:LEU:HB2	1.88	0.54
1:C:163:THR:HG22	1:C:163:THR:O	2.08	0.54
1:C:15:GLU:O	1:C:19:ASN:ND2	2.40	0.54
1:C:102:LYS:NZ	1:C:137:ASP:OD1	2.38	0.53
1:E:35:GLN:HE21	1:E:35:GLN:CA	2.22	0.53
1:A:60:ARG:HG3	1:E:57:ILE:HD11	1.90	0.53
1:A:22:MSE:CE	2:D:344:HOH:O	2.56	0.53
1:A:44:LEU:CD1	1:A:98:LEU:HD22	2.39	0.53
1:A:163:THR:O	1:A:163:THR:CG2	2.57	0.53
1:A:153:ASP:HB3	1:A:173:LEU:HD22	1.91	0.53
1:E:35:GLN:HE21	1:E:35:GLN:HA	1.74	0.52
1:D:1:LEU:HD22	1:D:5:VAL:HG23	1.92	0.52
1:F:163:THR:HG22	1:F:163:THR:O	2.11	0.51
1:C:96:THR:HB	1:C:97:PRO:HD3	1.92	0.51
1:C:88:ASP:HB2	1:C:151:MSE:CE	2.41	0.50
1:C:163:THR:HB	1:C:189:HIS:ND1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:NH2	1:F:61:GLU:OE2	2.44	0.50
1:C:177:THR:HG22	2:C:347:HOH:O	2.10	0.50
1:C:84:VAL:HA	1:C:151:MSE:CE	2.41	0.50
1:A:153:ASP:HB3	1:A:173:LEU:CD2	2.42	0.49
1:E:173:LEU:HD23	1:E:197:MSE:HE1	1.94	0.49
1:B:163:THR:HG21	1:B:187:ASP:HA	1.93	0.49
1:F:96:THR:HB	1:F:97:PRO:HD3	1.94	0.49
1:E:138:VAL:HG12	1:E:140:ILE:HG22	1.95	0.49
1:A:154:HIS:C	2:A:347:HOH:O	2.51	0.48
1:E:153:ASP:O	1:E:154:HIS:O	2.31	0.48
1:F:28:HIS:HA	1:F:32:LEU:HB2	1.95	0.48
1:A:186:GLY:O	1:A:187:ASP:CB	2.61	0.48
1:D:181:THR:O	1:D:182:GLY:C	2.50	0.48
1:E:80:ASP:O	1:E:84:VAL:HG23	2.14	0.48
1:C:88:ASP:HB2	1:C:151:MSE:HE1	1.95	0.48
1:F:88:ASP:HB2	1:F:151:MSE:HE2	1.95	0.47
1:D:163:THR:O	1:D:163:THR:HG22	2.14	0.47
1:F:81:ILE:HG13	1:F:104:PHE:CE1	2.50	0.47
1:B:163:THR:O	1:B:163:THR:CG2	2.62	0.47
1:F:67:TYR:HB3	1:F:74:ILE:HD11	1.96	0.47
1:E:96:THR:HB	1:E:97:PRO:HD3	1.96	0.47
1:C:163:THR:O	1:C:163:THR:CG2	2.62	0.47
1:B:22:MSE:HB3	1:C:54:MSE:HE1	1.97	0.47
1:B:181:THR:C	1:B:183:LYS:H	2.18	0.47
1:A:155:ALA:N	2:A:347:HOH:O	2.48	0.47
1:B:234:GLY:HA2	1:C:235:VAL:HG22	1.97	0.47
1:B:181:THR:CG2	1:B:183:LYS:HD2	2.45	0.47
1:A:234:GLY:HA2	1:B:235:VAL:HG22	1.96	0.47
1:F:54:MSE:CE	1:F:124:LEU:HD21	2.40	0.46
1:B:181:THR:O	1:B:183:LYS:N	2.48	0.46
1:E:155:ALA:N	2:E:350:HOH:O	2.49	0.46
1:E:163:THR:CG2	1:E:187:ASP:HA	2.41	0.46
1:C:1:LEU:HD22	1:C:5:VAL:HG23	1.98	0.46
1:B:60:ARG:HG3	1:D:57:ILE:HD11	1.98	0.46
1:A:179:GLY:CA	1:A:190:PRO:HD3	2.46	0.45
1:D:88:ASP:HB2	1:D:151:MSE:HE1	1.99	0.45
1:B:28:HIS:HB3	1:F:22:MSE:HE1	1.97	0.45
1:D:54:MSE:HE3	1:D:59:LEU:HG	1.99	0.45
1:E:163:THR:HG21	1:E:188:ARG:H	1.82	0.45
1:F:181:THR:O	1:F:183:LYS:N	2.50	0.45
1:F:1:LEU:HD22	1:F:5:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:HIS:HB3	1:E:162:GLU:HA	1.98	0.44
1:C:189:HIS:O	1:C:191:LYS:NZ	2.49	0.44
1:A:193:ARG:O	1:A:196:VAL:HG23	2.18	0.44
1:D:76:CYS:SG	1:D:148:HIS:HB3	2.58	0.44
1:B:138:VAL:CG2	1:B:155:ALA:HB1	2.48	0.44
1:C:179:GLY:HA3	1:C:190:PRO:HD3	2.00	0.44
1:D:84:VAL:HG13	1:D:151:MSE:HE3	1.99	0.43
1:E:179:GLY:HA3	1:E:190:PRO:HD3	1.99	0.43
1:F:215:LYS:NZ	2:F:328:HOH:O	2.51	0.43
1:C:94:TRP:O	1:C:97:PRO:HD2	2.19	0.43
1:E:195:GLY:HA3	1:E:213:TYR:CE2	2.53	0.43
1:E:44:LEU:HD13	1:E:98:LEU:HD22	1.99	0.43
1:E:89:PRO:HG2	1:F:188:ARG:NH2	2.33	0.43
1:D:153:ASP:C	1:D:155:ALA:H	2.22	0.43
1:A:154:HIS:O	1:A:174:GLN:HB3	2.19	0.43
1:B:103:GLY:HA2	1:B:155:ALA:CB	2.48	0.43
1:F:193:ARG:O	1:F:196:VAL:HG23	2.18	0.43
1:B:138:VAL:HG21	1:B:155:ALA:HB1	2.00	0.43
1:D:179:GLY:CA	1:D:190:PRO:HD3	2.49	0.43
1:D:152:PHE:HB3	1:D:155:ALA:HB2	2.01	0.42
1:D:235:VAL:O	1:D:235:VAL:HG22	2.20	0.42
1:B:150:ILE:N	1:B:150:ILE:HD12	2.34	0.42
1:E:3:LEU:O	1:E:7:GLN:HG2	2.20	0.42
1:F:147:GLY:O	1:F:150:ILE:HD13	2.19	0.42
1:E:197:MSE:HE2	1:E:198:ILE:O	2.19	0.42
1:D:82:GLN:HE21	1:D:82:GLN:HB3	1.63	0.42
1:B:59:LEU:HD23	1:B:59:LEU:O	2.21	0.41
1:E:193:ARG:O	1:E:196:VAL:HG23	2.19	0.41
1:F:84:VAL:HG22	1:F:151:MSE:HG3	2.03	0.41
1:B:143:ALA:HB3	1:B:162:GLU:HG3	2.02	0.41
1:C:33:LYS:HD2	1:F:61:GLU:OE1	2.21	0.40
1:A:163:THR:O	1:A:163:THR:HG22	2.21	0.40
1:F:23:LEU:O	1:F:26:PHE:HB3	2.22	0.40
1:E:54:MSE:HE3	1:E:59:LEU:HG	2.03	0.40
1:F:138:VAL:HG13	1:F:158:ILE:HB	2.03	0.40
1:D:120:ASN:HD22	1:D:120:ASN:HA	1.80	0.40

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	239/278 (86%)	230 (96%)	7 (3%)	2 (1%)	24	51
1	B	239/278 (86%)	228 (95%)	9 (4%)	2 (1%)	24	51
1	C	239/278 (86%)	232 (97%)	5 (2%)	2 (1%)	24	51
1	D	239/278 (86%)	228 (95%)	8 (3%)	3 (1%)	15	37
1	E	239/278 (86%)	229 (96%)	7 (3%)	3 (1%)	15	37
1	F	239/278 (86%)	228 (95%)	7 (3%)	4 (2%)	11	29
All	All	1434/1668 (86%)	1375 (96%)	43 (3%)	16 (1%)	17	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	LYS
1	A	187	ASP
1	E	154	HIS
1	E	184	GLU
1	F	183	LYS
1	B	187	ASP
1	C	186	GLY
1	C	187	ASP
1	D	155	ALA
1	D	182	GLY
1	D	186	GLY
1	E	186	GLY
1	F	182	GLY
1	B	207	ASN
1	F	154	HIS
1	F	186	GLY

### 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	196/222 (88%)	176 (90%)	20 (10%)	9	21
1	B	196/222 (88%)	176 (90%)	20 (10%)	9	21
1	C	196/222 (88%)	179 (91%)	17 (9%)	13	29
1	D	196/222 (88%)	177 (90%)	19 (10%)	10	23
1	E	196/222 (88%)	169 (86%)	27 (14%)	4	10
1	F	196/222 (88%)	176 (90%)	20 (10%)	9	21
All	All	1176/1332 (88%)	1053 (90%)	123 (10%)	8	19

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	3	LEU
1	A	15	GLU
1	A	18	GLU
1	A	23	LEU
1	A	33	LYS
1	A	41	LEU
1	A	59	LEU
1	A	60	ARG
1	A	98	LEU
1	A	99	LEU
1	A	110	TYR
1	A	124	LEU
1	A	156	THR
1	A	163	THR
1	A	183	LYS
1	A	188	ARG
1	A	212	LYS
1	A	238	ARG
1	A	240	VAL
1	B	1	LEU
1	B	18	GLU

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Mol	Chain	Res	Type
1	B	22	MSE
1	B	23	LEU
1	B	30	THR
1	B	33	LYS
1	B	41	LEU
1	B	60	ARG
1	B	98	LEU
1	B	99	LEU
1	B	110	TYR
1	B	123	SER
1	B	124	LEU
1	B	163	THR
1	B	173	LEU
1	B	188	ARG
1	B	212	LYS
1	B	215	LYS
1	B	235	VAL
1	B	238	ARG
1	C	1	LEU
1	C	23	LEU
1	C	33	LYS
1	C	41	LEU
1	C	58	SER
1	C	59	LEU
1	C	60	ARG
1	C	98	LEU
1	C	99	LEU
1	C	110	TYR
1	C	120	ASN
1	C	124	LEU
1	C	177	THR
1	C	188	ARG
1	C	203	LYS
1	C	235	VAL
1	C	238	ARG
1	D	1	LEU
1	D	18	GLU
1	D	23	LEU
1	D	33	LYS
1	D	41	LEU
1	D	59	LEU
1	D	60	ARG

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Mol	Chain	Res	Type
1	D	82	GLN
1	D	98	LEU
1	D	99	LEU
1	D	110	TYR
1	D	124	LEU
1	D	163	THR
1	D	173	LEU
1	D	181	THR
1	D	185	SER
1	D	188	ARG
1	D	215	LYS
1	D	235	VAL
1	E	1	LEU
1	E	7	GLN
1	E	11	GLN
1	E	18	GLU
1	E	22	MSE
1	E	23	LEU
1	E	33	LYS
1	E	35	GLN
1	E	41	LEU
1	E	58	SER
1	E	59	LEU
1	E	60	ARG
1	E	72	SER
1	E	92	GLU
1	E	98	LEU
1	E	99	LEU
1	E	110	TYR
1	E	124	LEU
1	E	140	ILE
1	E	154	HIS
1	E	163	THR
1	E	173	LEU
1	E	187	ASP
1	E	188	ARG
1	E	197	MSE
1	E	215	LYS
1	E	238	ARG
1	F	1	LEU
1	F	18	GLU
1	F	22	MSE

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Mol	Chain	Res	Type
1	F	23	LEU
1	F	33	LYS
1	F	35	GLN
1	F	58	SER
1	F	59	LEU
1	F	60	ARG
1	F	98	LEU
1	F	99	LEU
1	F	110	TYR
1	F	123	SER
1	F	124	LEU
1	F	181	THR
1	F	188	ARG
1	F	197	MSE
1	F	212	LYS
1	F	215	LYS
1	F	235	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	B	82	GLN
1	C	35	GLN
1	C	129	GLN
1	D	7	GLN
1	D	82	GLN
1	D	120	ASN
1	D	129	GLN
1	D	154	HIS
1	E	7	GLN
1	E	35	GLN
1	E	154	HIS
1	F	35	GLN
1	F	129	GLN
1	F	130	ASN

### 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/278 (85%)	-0.32	7 (2%) 54 54	22, 31, 44, 62	0
1	B	237/278 (85%)	-0.38	5 (2%) 67 68	20, 29, 44, 59	0
1	C	237/278 (85%)	-0.30	7 (2%) 54 54	21, 33, 49, 59	0
1	D	237/278 (85%)	-0.34	6 (2%) 61 61	18, 28, 46, 63	0
1	E	237/278 (85%)	-0.32	6 (2%) 61 61	21, 34, 49, 60	0
1	F	237/278 (85%)	-0.20	9 (3%) 44 44	23, 38, 50, 67	0
All	All	1422/1668 (85%)	-0.31	40 (2%) 56 57	18, 32, 48, 67	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	LYS	7.5
1	D	183	LYS	6.0
1	F	182	GLY	5.4
1	E	183	LYS	4.9
1	E	184	GLU	4.6
1	A	184	GLU	4.4
1	D	182	GLY	4.4
1	C	183	LYS	4.1
1	F	183	LYS	4.0
1	B	183	LYS	4.0
1	B	182	GLY	3.9
1	C	182	GLY	3.7
1	D	184	GLU	3.4
1	C	185	SER	3.3
1	D	186	GLY	3.2
1	A	68	GLN	3.2
1	C	184	GLU	3.0
1	F	186	GLY	2.9
1	D	185	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	182	GLY	2.8
1	F	240	VAL	2.8
1	B	238	ARG	2.7
1	A	182	GLY	2.6
1	B	181	THR	2.5
1	F	187	ASP	2.5
1	B	184	GLU	2.4
1	F	68	GLN	2.4
1	F	238	ARG	2.3
1	E	238	ARG	2.3
1	D	18	GLU	2.3
1	A	186	GLY	2.3
1	F	229	TYR	2.2
1	C	238	ARG	2.2
1	C	18	GLU	2.2
1	A	185	SER	2.2
1	F	184	GLU	2.1
1	E	15	GLU	2.1
1	C	11	GLN	2.0
1	E	181	THR	2.0
1	A	0	SER	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.