



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:26 pm GMT

PDB ID : 4ZRB
Title : Crystal Structure of Hypothetical Thioesterase Protein SP_1851 with Coenzyme A from *Streptococcus pneumoniae* TIGR4
Authors : Khandokar, Y.B.; Srivastava, P.; Forwood, J.K.
Deposited on : 2015-05-12
Resolution : 2.20 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

<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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

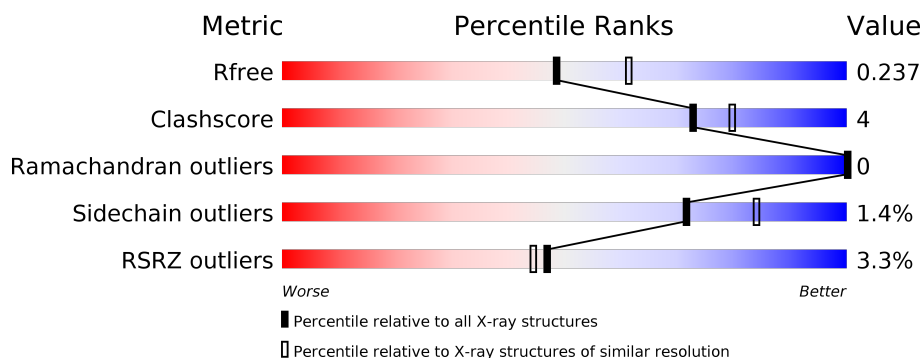
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	137	<div> <div>4%</div> <div>86%</div> <div>10%</div> </div>
1	B	137	<div> <div>4%</div> <div>81%</div> <div>9%</div> <div>10%</div> </div>
1	C	137	<div> <div>2%</div> <div>86%</div> <div>10%</div> </div>
1	D	137	<div> <div>2%</div> <div>83%</div> <div>7%</div> <div>9%</div> </div>
1	E	137	<div> <div>4%</div> <div>85%</div> <div>9%</div> <div>7%</div> </div>
1	F	137	<div> <div>4%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	137	<div><div>%</div><div><div></div><div>83%</div><div>9%</div><div>7%</div></div></div>
1	H	137	<div><div>4%</div><div><div></div><div>77%</div><div>15%</div><div>8%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8324 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 Hypothetical Thioesterase Protein SP_1851.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			948	596	161	184	7			
1	B	123	Total	C	N	O	S	0	0	0
			948	596	161	184	7			
1	C	123	Total	C	N	O	S	0	0	0
			948	596	161	184	7			
1	D	124	Total	C	N	O	S	0	0	0
			954	599	162	186	7			
1	E	128	Total	C	N	O	S	0	0	0
			981	615	165	193	8			
1	G	128	Total	C	N	O	S	0	0	0
			984	617	167	192	8			
1	H	126	Total	C	N	O	S	0	0	0
			973	611	165	189	8			
1	F	126	Total	C	N	O	S	0	0	0
			967	608	162	189	8			

There are 24 discrepancies between the modelled and reference sequences:

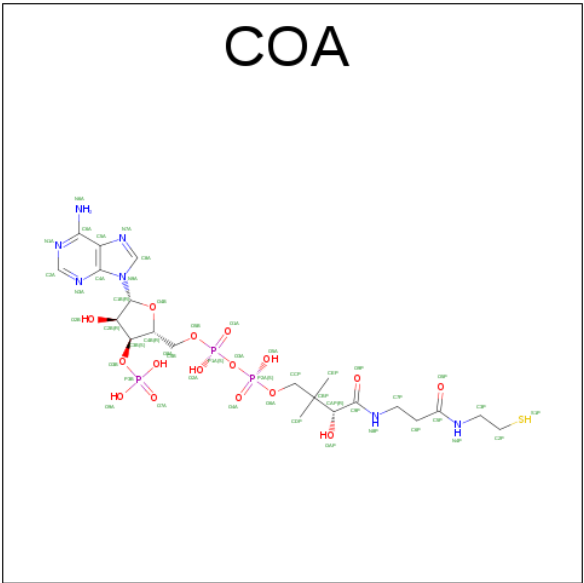
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q97NZ8
A	-1	ASN	-	expression tag	UNP Q97NZ8
A	0	ALA	-	expression tag	UNP Q97NZ8
B	-2	SER	-	expression tag	UNP Q97NZ8
B	-1	ASN	-	expression tag	UNP Q97NZ8
B	0	ALA	-	expression tag	UNP Q97NZ8
C	-2	SER	-	expression tag	UNP Q97NZ8
C	-1	ASN	-	expression tag	UNP Q97NZ8
C	0	ALA	-	expression tag	UNP Q97NZ8
D	-2	SER	-	expression tag	UNP Q97NZ8
D	-1	ASN	-	expression tag	UNP Q97NZ8
D	0	ALA	-	expression tag	UNP Q97NZ8
E	-2	SER	-	expression tag	UNP Q97NZ8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q97NZ8
E	0	ALA	-	expression tag	UNP Q97NZ8
G	-2	SER	-	expression tag	UNP Q97NZ8
G	-1	ASN	-	expression tag	UNP Q97NZ8
G	0	ALA	-	expression tag	UNP Q97NZ8
H	-2	SER	-	expression tag	UNP Q97NZ8
H	-1	ASN	-	expression tag	UNP Q97NZ8
H	0	ALA	-	expression tag	UNP Q97NZ8
F	-2	SER	-	expression tag	UNP Q97NZ8
F	-1	ASN	-	expression tag	UNP Q97NZ8
F	0	ALA	-	expression tag	UNP Q97NZ8

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

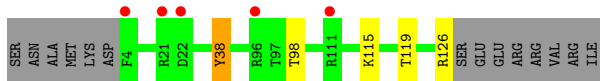
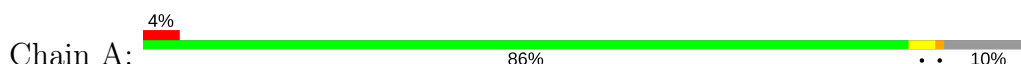
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	45	Total 45	O 45	0	0
3	C	48	Total 48	O 48	0	0
3	D	65	Total 65	O 65	0	0
3	E	53	Total 53	O 53	0	0
3	G	57	Total 57	O 57	0	0
3	H	49	Total 49	O 49	0	0
3	F	55	Total 55	O 55	0	0

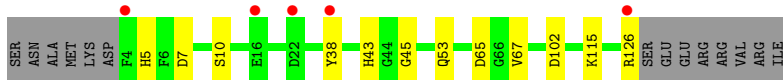
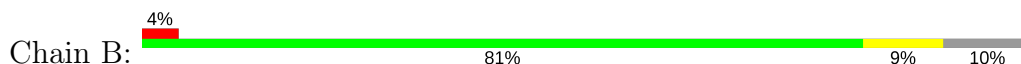
3 Residue-property plots [i](#)

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.

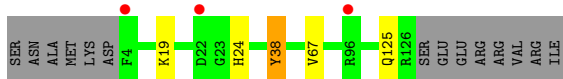
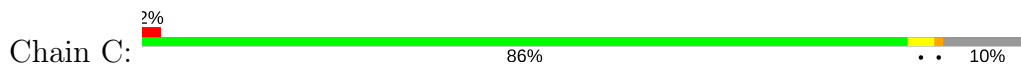
- Molecule 1: Hypothetical Thioesterase Protein SP_1851



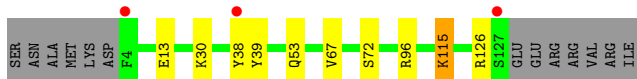
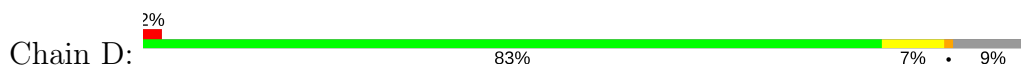
- Molecule 1: Hypothetical Thioesterase Protein SP_1851



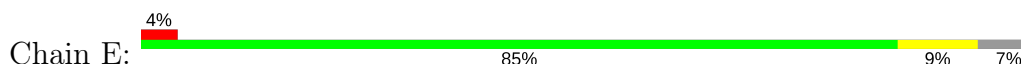
- Molecule 1: Hypothetical Thioesterase Protein SP_1851



- Molecule 1: Hypothetical Thioesterase Protein SP_1851

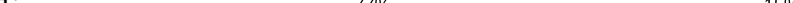


- Molecule 1: Hypothetical Thioesterase Protein SP_1851




- Molecule 1: Hypothetical Thioesterase Protein SP_1851

SER	ASN	ASP	GLY	GLU	GLN	ARG	ARG	ARG	VAL	ARG	ILE
A0	M1	K2	D3	F4	K19	H24	N41	L57	K80	K88	R96
D102	C114	K115	R126	S127	GLU	GLU	ARG	ARG	VAL	ARG	ILE

- Chain H: 

SER
ASN
ALA
M1
F4
H5
I9
F12
Y15
E16
I17
E18
K18
X19
M20
R21
D22
V26
L36
L50
L57
G63
L64
D65
L69
Q70
L81
R96
E109
Q125
R126
SER
GLU
GLU
ARG
ARG
VAL
TRP

- Chain F:  4% 83% 9% 8%

SER	ASN	ASP	GLN	GLU	ARG	VAL	ILE
A0							
H5							
I9							
F12							
Y15							
E16							
I17							
E18							
K19							
M20							
R21							
D22							
G23							
H24							
N37							
H43							
Q53							
V59							
T97							
M120							
Q125							
ARG							
SER							
GLU							
GLU							
ARG							
ARG							
VAL							
ARG							
ILE							

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.16Å 71.86Å 82.43Å 82.65° 81.38° 79.65°	Depositor
Resolution (Å)	81.06 – 2.20 44.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (81.06-2.20) 92.4 (44.53-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.203 , 0.237 0.203 , 0.237	Depositor DCC
R_{free} test set	2715 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8324	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA

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	0.27	0/962	0.47	0/1300
1	B	0.44	0/962	0.55	0/1300
1	C	0.34	0/962	0.55	0/1300
1	D	0.33	0/968	0.54	1/1308 (0.1%)
1	E	0.36	0/995	0.56	0/1344
1	F	0.31	0/981	0.55	0/1325
1	G	0.33	0/998	0.53	0/1347
1	H	0.32	0/987	0.54	0/1332
All	All	0.34	0/7815	0.54	1/10556 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	ARG	NE-CZ-NH2	-5.46	117.57	120.30

There are no chirality outliers.

There are no planarity outliers.

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	948	0	933	5	0
1	B	948	0	933	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	948	0	933	2	0
1	D	954	0	938	6	0
1	E	981	0	965	9	0
1	F	967	0	954	7	0
1	G	984	0	972	11	0
1	H	973	0	962	16	0
2	E	48	0	32	1	0
2	F	48	0	32	2	0
2	G	48	0	32	2	0
2	H	48	0	32	2	0
3	A	57	0	0	1	0
3	B	45	0	0	1	0
3	C	48	0	0	0	0
3	D	65	0	0	4	0
3	E	53	0	0	1	0
3	F	55	0	0	0	0
3	G	57	0	0	0	0
3	H	49	0	0	2	0
All	All	8324	0	7718	61	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 4.

All (61) 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)
2:F:201:COA:O4B	2:F:201:COA:C1B	1.65	1.26
2:E:201:COA:O4B	2:E:201:COA:C1B	1.65	1.22
2:H:201:COA:C1B	2:H:201:COA:O4B	1.65	1.17
2:G:201:COA:C1B	2:G:201:COA:O4B	1.65	1.16
1:B:43:HIS:HD1	1:B:45:GLY:H	1.30	0.80
1:F:12:PHE:HE1	1:F:53:GLN:HG2	1.53	0.74
1:G:24:HIS:HE1	1:G:88:LYS:HE2	1.53	0.73
1:A:119:THR:HG21	1:H:69:LEU:HD21	1.75	0.69
1:G:3:ASP:OD2	1:G:126:ARG:NH2	2.21	0.68
1:A:98:THR:HG21	1:H:69:LEU:HD11	1.76	0.67
1:H:125:GLN:O	1:H:126:ARG:HB3	1.94	0.66
1:H:65:ASP:OD2	1:H:126:ARG:HB2	1.96	0.64
1:H:1:MET:N	3:H:301:HOH:O	2.31	0.62
1:G:24:HIS:CE1	1:G:88:LYS:HE2	2.36	0.57
1:A:38:TYR:HE2	1:D:53:GLN:HE22	1.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:ARG:NH1	3:H:303:HOH:O	2.34	0.56
1:B:102:ASP:CG	1:G:115:LYS:HZ2	2.10	0.55
1:B:53:GLN:HE22	1:C:38:TYR:HE2	1.55	0.55
1:H:96:ARG:NH1	2:H:201:COA:O2B	2.39	0.55
1:G:41:ASN:OD1	1:G:80:LYS:NZ	2.30	0.54
1:E:12:PHE:HE2	1:E:53:GLN:HG2	1.73	0.53
1:E:6:PHE:O	1:E:9:ILE:HG12	2.09	0.52
1:F:19:LYS:HE3	1:F:21:ARG:HH21	1.74	0.51
1:H:5:HIS:O	1:H:9:ILE:HD12	2.11	0.50
1:E:37:ASN:HB3	1:E:43:HIS:HB3	1.94	0.50
1:E:4:PHE:HE1	1:E:53:GLN:HG3	1.77	0.49
1:F:37:ASN:HB3	1:F:43:HIS:HB3	1.95	0.49
1:C:19:LYS:HD2	1:C:24:HIS:CD2	2.47	0.49
1:A:126:ARG:HA	3:A:210:HOH:O	2.12	0.49
1:H:69:LEU:HD23	1:H:70:GLN:HB2	1.95	0.48
1:H:9:ILE:HG13	1:H:15:TYR:HE2	1.79	0.48
1:D:38:TYR:HE1	1:D:39:TYR:CZ	2.31	0.48
1:B:43:HIS:HD1	1:B:45:GLY:N	2.07	0.48
1:B:10:SER:O	3:B:201:HOH:O	2.20	0.47
1:B:65:ASP:OD1	1:B:126:ARG:NH1	2.44	0.46
1:B:5:HIS:HE1	1:B:7:ASP:OD1	1.98	0.46
1:H:12:PHE:CZ	1:H:50:LEU:HD23	2.51	0.46
1:E:4:PHE:CE1	1:E:53:GLN:HG3	2.50	0.46
1:H:19:LYS:HB3	1:H:26:VAL:HB	1.98	0.45
1:H:4:PHE:CE2	1:H:57:LEU:HG	2.51	0.45
1:D:30:LYS:HE2	3:D:204:HOH:O	2.16	0.45
1:G:4:PHE:CE2	1:G:57:LEU:HG	2.52	0.45
1:D:115:LYS:HE2	3:D:222:HOH:O	2.17	0.44
1:E:90:GLU:OE2	3:E:301:HOH:O	2.21	0.44
1:A:115:LYS:HE2	1:E:102:ASP:OD1	2.18	0.44
1:G:1:MET:HG2	1:G:4:PHE:HB3	1.99	0.44
1:D:13:GLU:OE1	3:D:201:HOH:O	2.21	0.44
1:B:115:LYS:HE3	1:G:102:ASP:OD2	2.18	0.43
1:H:65:ASP:CG	1:H:126:ARG:HB2	2.38	0.43
1:F:5:HIS:O	1:F:9:ILE:HG23	2.18	0.43
1:F:59:VAL:HG21	1:F:120:MET:SD	2.59	0.43
1:F:12:PHE:CD2	1:F:15:TYR:HB3	2.54	0.42
1:H:63:GLY:O	1:H:125:GLN:O	2.36	0.42
1:G:96:ARG:HH21	2:G:201:COA:C2B	2.31	0.42
1:H:36:LEU:HD11	1:H:81:LEU:HB2	2.01	0.42
1:F:97:THR:HG22	2:F:201:COA:O4A	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:GLY:O	1:E:90:GLU:HA	2.19	0.41
1:G:19:LYS:CE	1:G:24:HIS:HD2	2.33	0.41
1:E:12:PHE:CD1	1:E:15:TYR:HB3	2.55	0.41
1:D:72:SER:HB3	3:D:217:HOH:O	2.21	0.41
1:G:3:ASP:OD1	1:G:3:ASP:N	2.54	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	121/137 (88%)	119 (98%)	2 (2%)	0	100	100
1	B	121/137 (88%)	119 (98%)	2 (2%)	0	100	100
1	C	121/137 (88%)	119 (98%)	2 (2%)	0	100	100
1	D	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
1	E	126/137 (92%)	123 (98%)	3 (2%)	0	100	100
1	F	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
1	G	126/137 (92%)	124 (98%)	2 (2%)	0	100	100
1	H	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
All	All	985/1096 (90%)	968 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	106/119 (89%)	105 (99%)	1 (1%)	82	91
1	B	106/119 (89%)	104 (98%)	2 (2%)	62	76
1	C	106/119 (89%)	103 (97%)	3 (3%)	49	61
1	D	107/119 (90%)	104 (97%)	3 (3%)	49	61
1	E	110/119 (92%)	109 (99%)	1 (1%)	82	91
1	F	108/119 (91%)	108 (100%)	0	100	100
1	G	110/119 (92%)	108 (98%)	2 (2%)	64	77
1	H	109/119 (92%)	109 (100%)	0	100	100
All	All	862/952 (90%)	850 (99%)	12 (1%)	71	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	TYR
1	B	38	TYR
1	B	67	VAL
1	C	38	TYR
1	C	67	VAL
1	C	125	GLN
1	D	67	VAL
1	D	96	ARG
1	D	115	LYS
1	E	-2	SER
1	G	114	CYS
1	G	126	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	HIS
1	C	24	HIS
1	C	53	GLN
1	G	24	HIS

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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	COA	E	201	-	43,50,50	4.07	14 (32%)	48,75,75	2.01	5 (10%)
2	COA	F	201	-	43,50,50	4.02	13 (30%)	48,75,75	2.02	5 (10%)
2	COA	G	201	-	43,50,50	4.02	13 (30%)	48,75,75	2.03	5 (10%)
2	COA	H	201	-	43,50,50	4.01	13 (30%)	48,75,75	2.13	9 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	E	201	-	-	0/44/64/64	0/3/3/3
2	COA	F	201	-	-	0/44/64/64	0/3/3/3
2	COA	G	201	-	-	0/44/64/64	0/3/3/3
2	COA	H	201	-	-	0/44/64/64	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	COA	C2B-C1B	-12.79	1.33	1.53
2	H	201	COA	C2B-C1B	-12.77	1.33	1.53
2	G	201	COA	C2B-C1B	-12.68	1.33	1.53
2	F	201	COA	C2B-C1B	-12.63	1.33	1.53
2	E	201	COA	O4B-C4B	-5.60	1.32	1.45
2	F	201	COA	O4B-C4B	-5.59	1.32	1.45
2	H	201	COA	O4B-C4B	-5.52	1.32	1.45
2	G	201	COA	O4B-C4B	-5.49	1.32	1.45
2	H	201	COA	O3B-C3B	-2.82	1.33	1.44
2	E	201	COA	O3B-C3B	-2.80	1.33	1.44
2	F	201	COA	O3B-C3B	-2.79	1.33	1.44
2	G	201	COA	O3B-C3B	-2.78	1.33	1.44
2	F	201	COA	C5A-C4A	-2.54	1.34	1.40
2	H	201	COA	C5A-C4A	-2.53	1.34	1.40
2	H	201	COA	OAP-CAP	-2.52	1.37	1.42
2	E	201	COA	C5A-C4A	-2.48	1.34	1.40
2	G	201	COA	OAP-CAP	-2.45	1.37	1.42
2	G	201	COA	C5A-C4A	-2.45	1.35	1.40
2	E	201	COA	OAP-CAP	-2.43	1.37	1.42
2	F	201	COA	OAP-CAP	-2.38	1.37	1.42
2	F	201	COA	O9P-C9P	-2.30	1.18	1.23
2	E	201	COA	O9P-C9P	-2.26	1.19	1.23
2	G	201	COA	O9P-C9P	-2.18	1.19	1.23
2	H	201	COA	O9P-C9P	-2.17	1.19	1.23
2	E	201	COA	O5P-C5P	-2.15	1.18	1.23
2	F	201	COA	O5P-C5P	-2.11	1.18	1.23
2	H	201	COA	O5P-C5P	-2.10	1.18	1.23
2	G	201	COA	O5P-C5P	-2.06	1.18	1.23
2	E	201	COA	C3B-C4B	2.03	1.58	1.52
2	H	201	COA	C2A-N3A	2.60	1.36	1.32
2	F	201	COA	C2A-N3A	2.61	1.36	1.32
2	G	201	COA	C2A-N3A	2.67	1.36	1.32
2	E	201	COA	C2A-N3A	2.69	1.36	1.32
2	E	201	COA	C6A-N6A	3.07	1.46	1.34
2	G	201	COA	C6A-N6A	3.09	1.46	1.34
2	H	201	COA	C6A-N6A	3.10	1.46	1.34
2	F	201	COA	C6A-N6A	3.11	1.46	1.34
2	E	201	COA	P3B-O3B	3.23	1.65	1.59
2	H	201	COA	P3B-O3B	3.24	1.65	1.59
2	F	201	COA	P3B-O3B	3.26	1.65	1.59
2	G	201	COA	P3B-O3B	3.41	1.65	1.59
2	H	201	COA	C5P-N4P	6.31	1.48	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	201	COA	C5P-N4P	6.49	1.48	1.33
2	E	201	COA	C5P-N4P	6.53	1.48	1.33
2	F	201	COA	C5P-N4P	6.54	1.48	1.33
2	H	201	COA	C9P-N8P	8.07	1.50	1.33
2	G	201	COA	C9P-N8P	8.27	1.50	1.33
2	F	201	COA	C9P-N8P	8.27	1.50	1.33
2	E	201	COA	C9P-N8P	8.40	1.50	1.33
2	F	201	COA	O4B-C1B	17.39	1.65	1.41
2	G	201	COA	O4B-C1B	17.43	1.65	1.41
2	H	201	COA	O4B-C1B	17.47	1.65	1.41
2	E	201	COA	O4B-C1B	17.66	1.65	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	COA	N3A-C2A-N1A	-10.13	120.04	128.86
2	H	201	COA	N3A-C2A-N1A	-10.13	120.04	128.86
2	E	201	COA	N3A-C2A-N1A	-10.04	120.12	128.86
2	G	201	COA	N3A-C2A-N1A	-9.80	120.33	128.86
2	G	201	COA	N6A-C6A-N1A	-5.09	108.68	118.77
2	H	201	COA	N6A-C6A-N1A	-5.00	108.86	118.77
2	F	201	COA	N6A-C6A-N1A	-4.79	109.27	118.77
2	E	201	COA	N6A-C6A-N1A	-4.77	109.31	118.77
2	H	201	COA	C7P-C6P-C5P	-3.21	107.06	112.22
2	H	201	COA	C3P-N4P-C5P	-2.35	118.33	122.84
2	H	201	COA	C7P-N8P-C9P	-2.22	118.45	122.59
2	H	201	COA	C2P-C3P-N4P	-2.21	107.69	112.50
2	G	201	COA	C6P-C7P-N8P	-2.19	107.34	111.87
2	F	201	COA	C7P-C6P-C5P	-2.17	108.74	112.22
2	H	201	COA	C6P-C7P-N8P	-2.11	107.50	111.87
2	E	201	COA	O6A-CCP-CBP	-2.09	107.19	110.55
2	G	201	COA	C4B-O4B-C1B	-2.03	107.60	109.77
2	H	201	COA	C4B-O4B-C1B	-2.01	107.63	109.77
2	E	201	COA	C6P-C5P-N4P	2.18	120.25	116.49
2	F	201	COA	C6P-C5P-N4P	2.23	120.34	116.49
2	E	201	COA	C5A-C6A-N6A	4.99	130.64	120.47
2	F	201	COA	C5A-C6A-N6A	5.04	130.74	120.47
2	H	201	COA	C5A-C6A-N6A	5.27	131.22	120.47
2	G	201	COA	C5A-C6A-N6A	5.37	131.42	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	COA	1	0
2	F	201	COA	2	0
2	G	201	COA	2	0
2	H	201	COA	2	0

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, 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	123/137 (89%)	0.35	5 (4%) 38 36	17, 30, 48, 66	0
1	B	123/137 (89%)	0.23	5 (4%) 38 36	16, 29, 50, 67	0
1	C	123/137 (89%)	0.19	3 (2%) 59 57	16, 29, 47, 64	0
1	D	124/137 (90%)	0.12	3 (2%) 59 57	17, 25, 45, 65	0
1	E	128/137 (93%)	0.41	5 (3%) 40 38	17, 31, 49, 56	0
1	F	126/137 (91%)	0.26	5 (3%) 39 37	18, 32, 47, 62	0
1	G	128/137 (93%)	0.23	1 (0%) 86 85	18, 27, 43, 53	0
1	H	126/137 (91%)	0.34	6 (4%) 31 30	19, 32, 47, 64	0
All	All	1001/1096 (91%)	0.27	33 (3%) 47 44	16, 30, 48, 67	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	21	ARG	3.9
1	D	127	SER	3.7
1	D	38	TYR	3.5
1	D	4	PHE	3.5
1	F	21	ARG	3.4
1	C	4	PHE	3.3
1	A	22	ASP	3.2
1	A	21	ARG	3.0
1	H	17	ILE	3.0
1	H	9	ILE	2.9
1	F	22	ASP	2.7
1	C	96	ARG	2.6
1	A	96	ARG	2.6
1	G	0	ALA	2.6
1	B	38	TYR	2.6
1	C	22	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	4	PHE	2.5
1	F	17	ILE	2.5
1	E	110	GLY	2.4
1	E	84	VAL	2.4
1	E	68	THR	2.3
1	E	65	ASP	2.2
1	H	16	GLU	2.2
1	F	24	HIS	2.2
1	E	21	ARG	2.2
1	B	16	GLU	2.2
1	A	4	PHE	2.1
1	B	22	ASP	2.1
1	A	111	ARG	2.1
1	B	126	ARG	2.1
1	H	109	GLU	2.0
1	H	22	ASP	2.0
1	F	18	GLU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	COA	F	201	48/48	0.93	0.15	0.03	22,37,64,75	0
2	COA	E	201	48/48	0.94	0.14	-0.56	23,37,60,66	0
2	COA	H	201	48/48	0.95	0.12	-0.66	18,34,47,65	0
2	COA	G	201	48/48	0.94	0.14	-0.75	17,33,56,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.