



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2016 – 02:11 PM EDT

PDB ID : 4RUK  
Title : crystal structure of Phosphoapantetheine adenylyltransferase PPAT/CoaD with CoA and pyrophosphate from Pseudomonas aeruginosa  
Authors : Chatterjee, R.; Datta, S.  
Deposited on : 2014-11-20  
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](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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027257  
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) : rb-20027257

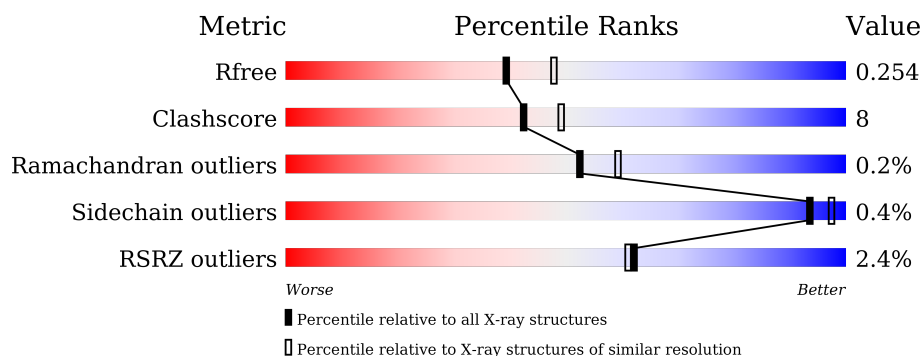
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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  $\geq 3$ , 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	159	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	159	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>18%</div> <div>.</div> </div> </div>
1	C	159	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	D	159	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>16%</div> <div>.</div> </div> </div>
1	E	159	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>.</div> </div> </div>
1	F	159	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>16%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	COA	B	201	-	-	-	X
2	COA	C	201	-	-	-	X
2	COA	E	202[A]	-	-	-	X
2	COA	E	202[B]	-	-	-	X
2	COA	F	201[A]	-	-	-	X
2	COA	F	201[B]	-	-	-	X
3	DMS	A	204	-	-	-	X
3	DMS	D	203	-	-	-	X
4	FMT	B	207	-	-	-	X
5	ACT	A	208	-	-	-	X
5	ACT	C	206	-	-	-	X

## 2 Entry composition [i](#)

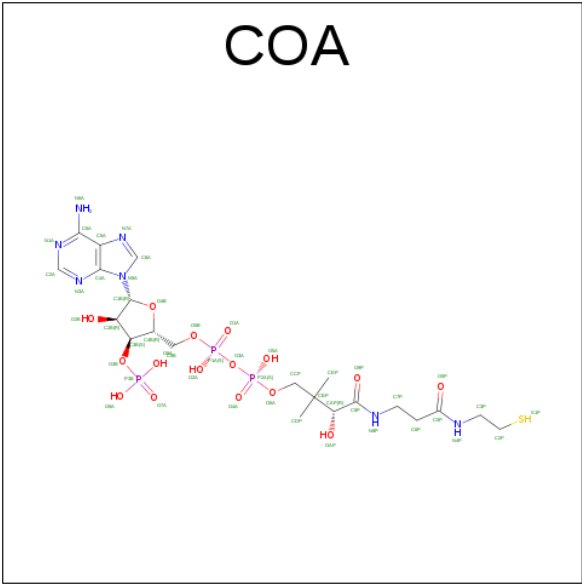
There are 9 unique types of molecules in this entry. The entry contains 8172 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphopantetheine adenylyltransferase.

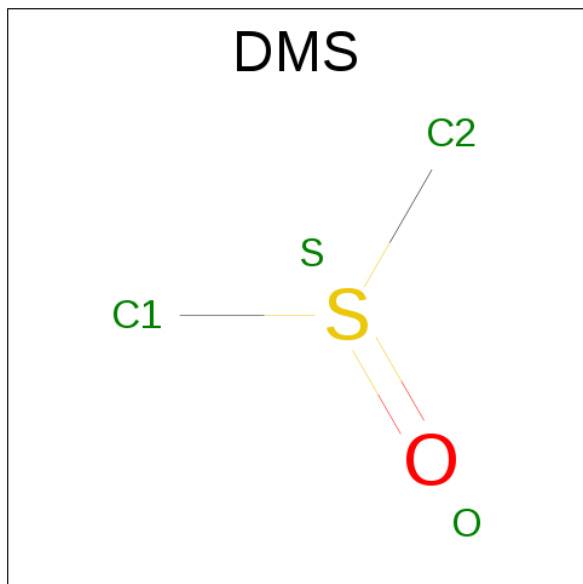
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	1	0
			1247	802	218	225	2			
1	B	158	Total	C	N	O	S	0	1	0
			1255	807	219	226	3			
1	C	158	Total	C	N	O	S	0	2	0
			1261	810	220	228	3			
1	D	158	Total	C	N	O	S	0	1	0
			1255	807	219	226	3			
1	E	158	Total	C	N	O	S	0	2	0
			1263	812	220	227	4			
1	F	158	Total	C	N	O	S	0	0	0
			1244	801	215	225	3			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		
2	F	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



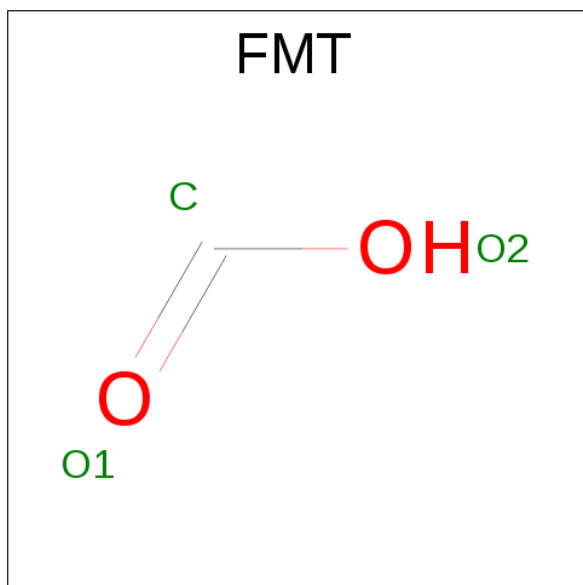
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	F	1	Total	C	O	S	0	0
			4	2	1	1		
3	F	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



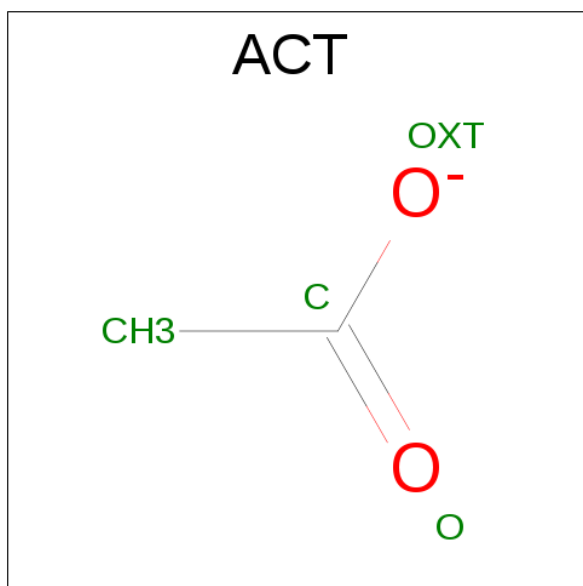
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			3	1	2			
4	A	1	Total	C	O		0	0
			3	1	2			
4	E	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			
4	B	1	Total	C	O		0	0
			3	1	2			

*Continued on next page...*

Continued from previous page...

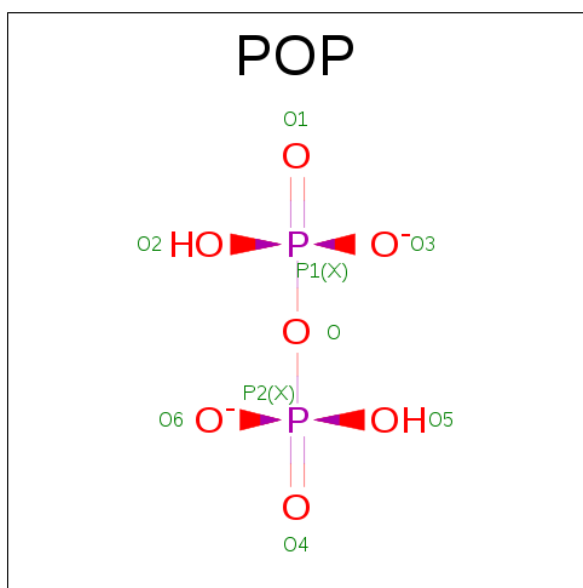
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



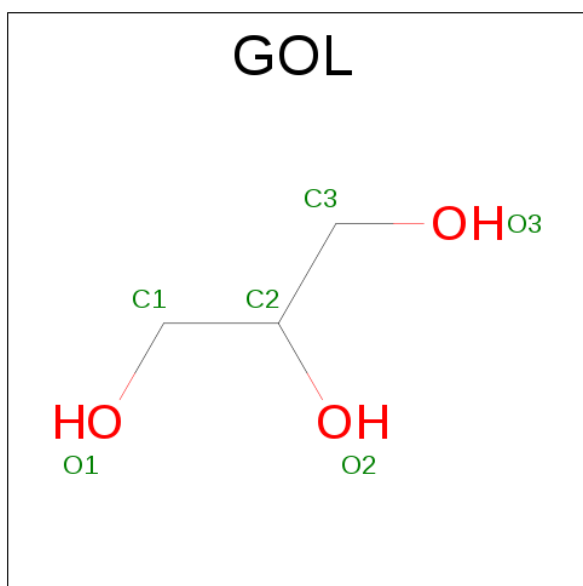
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	P	0	0
			9	7	2		
6	F	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		



- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	1	Total 1	Ca 1	0	0
8	E	1	Total 1	Ca 1	0	0

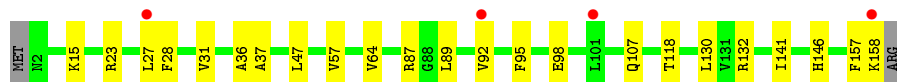
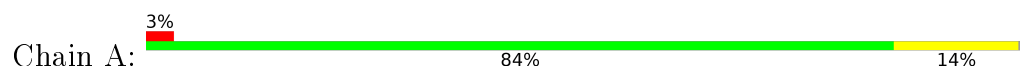
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	25	Total 25	O 25	0	0
9	B	24	Total 24	O 24	0	0
9	C	25	Total 25	O 25	0	0
9	D	24	Total 24	O 24	0	0
9	E	19	Total 19	O 19	0	0
9	F	23	Total 23	O 23	0	0

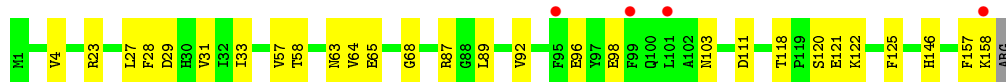
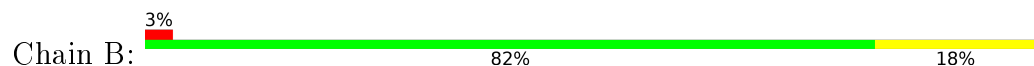
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

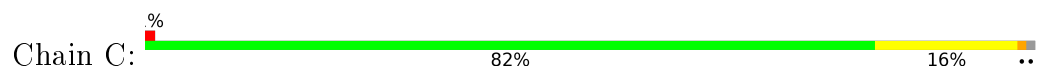
- Molecule 1: Phosphopantetheine adenylyltransferase



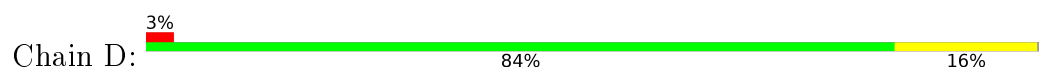
- Molecule 1: Phosphopantetheine adenylyltransferase



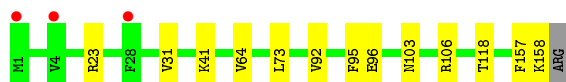
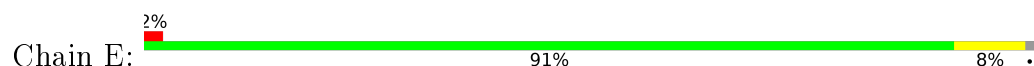
- Molecule 1: Phosphopantetheine adenylyltransferase



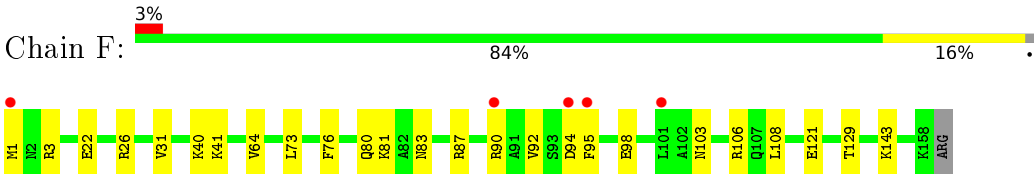
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.60Å 89.48Å 79.62Å 90.00° 97.93° 90.00°	Depositor
Resolution (Å)	45.13 – 2.20 45.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (45.13-2.20) 89.7 (45.13-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.204 , 0.254 0.207 , 0.254	Depositor DCC
$R_{free}$ test set	1840 reflections (3.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.468 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, POP, COA, DMS, ACT, CA

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	0.48	0/1274	0.62	0/1724
1	B	0.51	0/1282	0.64	1/1734 (0.1%)
1	C	0.45	0/1288	0.60	0/1742
1	D	0.44	0/1282	0.56	0/1734
1	E	0.45	0/1290	0.62	0/1744
1	F	0.43	0/1271	0.58	0/1720
All	All	0.46	0/7687	0.60	1/10398 (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	B	122	LYS	CA-CB-CG	5.03	124.47	113.40

There are no chirality outliers.

There are no planarity outliers.

### 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	1247	0	1261	20	0
1	B	1255	0	1273	26	0
1	C	1261	0	1277	24	0
1	D	1255	0	1273	24	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1263	0	1283	19	0
1	F	1244	0	1261	23	0
2	A	48	0	30	8	0
2	B	48	0	32	5	0
2	C	48	0	31	5	0
2	D	48	0	32	4	0
2	E	96	0	64	14	0
2	F	96	0	64	9	0
3	A	16	0	24	5	0
3	D	8	0	12	1	0
3	E	4	0	6	0	0
3	F	8	0	12	1	0
4	A	6	0	2	0	0
4	B	18	0	6	2	0
4	C	12	0	4	0	0
4	D	3	0	1	0	0
4	E	6	0	2	0	0
5	A	4	0	3	0	0
5	C	4	0	3	0	0
5	E	4	0	3	0	0
5	F	4	0	3	0	0
6	D	9	0	0	0	0
6	F	9	0	0	0	0
7	D	6	0	8	1	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	25	0	0	0	0
9	B	24	0	0	0	0
9	C	25	0	0	2	0
9	D	24	0	0	0	0
9	E	19	0	0	0	0
9	F	23	0	0	1	0
All	All	8172	0	7970	133	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 8.

All (133) 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:C:201:COA:O4B	2:C:201:COA:C1B	1.63	1.27

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201[A]:COA:O4B	2:F:201[A]:COA:C1B	1.64	1.24
2:B:201:COA:C1B	2:B:201:COA:O4B	1.63	1.23
2:E:202[A]:COA:C1B	2:E:202[A]:COA:O4B	1.64	1.23
2:F:201[B]:COA:C1B	2:F:201[B]:COA:O4B	1.64	1.21
2:E:202[B]:COA:C1B	2:E:202[B]:COA:O4B	1.64	1.20
2:D:201:COA:O4B	2:D:201:COA:C1B	1.63	1.16
2:A:201:COA:H8A	2:A:201:COA:H51A	1.53	0.90
1:F:73:LEU:HB2	2:F:201[A]:COA:H61	1.54	0.89
1:D:37:ALA:O	1:D:39:PRO:HD3	1.87	0.75
2:B:201:COA:H72	2:B:201:COA:H141	1.68	0.74
1:C:73:LEU:N	2:C:201:COA:O5P	2.22	0.70
1:B:96:GLU:OE2	1:E:92:VAL:HG22	1.91	0.70
1:C:55:GLN:NE2	9:C:303:HOH:O	2.25	0.68
1:B:65:GLU:HB2	4:B:205:FMT:H	1.77	0.66
1:F:41:LYS:NZ	2:F:201[A]:COA:O4A	2.28	0.66
1:C:124[B]:SER:O	1:C:126:ILE:N	2.28	0.66
1:E:41:LYS:NZ	2:E:202[A]:COA:O4A	2.30	0.65
1:C:124[A]:SER:O	1:C:126:ILE:N	2.30	0.64
1:F:41:LYS:NZ	2:F:201[B]:COA:O3A	2.32	0.63
2:A:201:COA:H8A	2:A:201:COA:C5B	2.27	0.62
1:E:103:ASN:OD1	1:E:106[B]:ARG:NH1	2.32	0.62
1:B:87:ARG:NH2	1:B:98:GLU:OE2	2.32	0.61
1:C:41:LYS:O	1:C:43:PRO:HD3	2.01	0.61
1:B:103:ASN:ND2	1:F:121:GLU:HB3	2.15	0.61
1:F:1:MET:O	1:F:1:MET:HG2	2.03	0.59
1:F:73:LEU:HB3	2:F:201[B]:COA:HN4	1.68	0.59
1:E:73:LEU:HB2	2:E:202[A]:COA:H72	1.85	0.59
1:B:103:ASN:HD21	1:F:121:GLU:HB3	1.68	0.59
1:A:157:PHE:O	1:A:158:LYS:HB3	2.03	0.58
1:E:41:LYS:NZ	2:E:202[B]:COA:O3A	2.35	0.58
1:D:37:ALA:HB2	1:D:47:LEU:HD22	1.84	0.58
1:C:15:LYS:NZ	9:C:315:HOH:O	2.37	0.57
1:A:132:ARG:NH2	2:A:201:COA:H2A	2.19	0.57
1:B:157:PHE:O	1:B:158:LYS:HB3	2.03	0.57
1:A:92:VAL:HB	1:E:92:VAL:HB	1.87	0.57
1:A:36:ALA:HB1	3:A:204:DMS:H21	1.87	0.56
1:A:31:VAL:HB	1:A:64:VAL:HG22	1.88	0.56
1:D:41:LYS:O	7:D:206:GOL:H32	2.06	0.56
1:E:157:PHE:O	1:E:158:LYS:HB3	2.06	0.56
1:D:130:LEU:HD22	2:E:202[B]:COA:S1P	2.46	0.56
1:E:31:VAL:HB	1:E:64:VAL:HG22	1.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ASN:OD1	1:C:106[B]:ARG:NH1	2.40	0.55
1:A:15:LYS:HG2	3:A:202:DMS:H22	1.89	0.55
1:F:31:VAL:HB	1:F:64:VAL:HG22	1.88	0.55
1:E:73:LEU:H	2:E:202[B]:COA:H61	1.73	0.54
1:A:92:VAL:HG22	1:C:96:GLU:OE2	2.06	0.54
1:A:57:VAL:HG22	1:A:146:HIS:CG	2.42	0.54
1:A:95:PHE:HD2	1:E:92:VAL:HG12	1.73	0.54
1:C:41:LYS:NZ	2:C:201:COA:O4B	2.39	0.54
1:C:157:PHE:O	1:C:158:LYS:HB3	2.08	0.53
1:B:31:VAL:HB	1:B:64:VAL:HG22	1.90	0.53
1:C:92:VAL:HG12	1:D:92:VAL:HB	1.91	0.53
1:A:107:GLN:HB3	1:F:143:LYS:HD2	1.91	0.53
1:A:37:ALA:HB2	1:A:47:LEU:HD22	1.91	0.53
1:D:122:LYS:O	1:D:122:LYS:HD2	2.09	0.52
1:F:41:LYS:HZ1	2:F:201[B]:COA:P2A	2.33	0.52
1:A:27:LEU:HD22	1:A:28:PHE:CE1	2.45	0.51
1:B:92:VAL:HG22	1:D:96:GLU:OE2	2.11	0.51
1:B:57:VAL:HG22	1:B:146:HIS:CG	2.46	0.50
2:A:201:COA:HN8	3:A:204:DMS:H22	1.76	0.50
1:A:37:ALA:O	3:A:204:DMS:S	2.70	0.50
1:B:23:ARG:NH2	1:B:118:THR:O	2.42	0.49
1:A:87:ARG:NH2	1:A:98:GLU:OE2	2.44	0.49
1:D:92:VAL:HG22	1:E:96:GLU:OE2	2.13	0.49
1:B:118:THR:HG22	9:F:302:HOH:O	2.12	0.48
1:B:125:PHE:O	1:D:100:GLN:HG3	2.13	0.48
1:F:83:ASN:HB2	3:F:204:DMS:H22	1.95	0.48
1:D:90:ARG:HD2	1:D:124:SER:O	2.13	0.48
1:F:87:ARG:NH1	2:F:201[B]:COA:H132	2.29	0.48
1:C:92:VAL:CG1	1:D:92:VAL:HB	2.44	0.47
1:C:130:LEU:HD23	1:C:130:LEU:HA	1.77	0.47
1:F:73:LEU:H	2:F:201[B]:COA:H61	1.80	0.47
1:D:157:PHE:O	1:D:158:LYS:HB2	2.14	0.47
1:A:92:VAL:HG12	1:E:95:PHE:HD2	1.79	0.47
1:B:92:VAL:N	1:D:96:GLU:OE2	2.47	0.47
1:D:8:GLY:HA2	2:D:201:COA:O1A	2.14	0.47
2:D:201:COA:P1A	2:D:201:COA:H121	2.56	0.46
2:A:201:COA:O4A	2:A:201:COA:OAP	2.33	0.46
1:A:130:LEU:HA	1:A:130:LEU:HD23	1.79	0.46
1:D:37:ALA:O	3:D:203:DMS:S	2.74	0.46
1:F:22:GLU:O	1:F:26:ARG:NH1	2.49	0.45
1:A:23:ARG:HH12	1:E:106[B]:ARG:HD3	1.82	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:COA:H141	2:A:201:COA:N8P	2.32	0.45
2:E:202[A]:COA:H61	2:E:202[A]:COA:H32	1.67	0.45
1:D:93:SER:N	1:E:96:GLU:OE2	2.49	0.45
1:C:31:VAL:HB	1:C:64:VAL:HG22	1.98	0.44
1:E:41:LYS:HZ1	2:E:202[B]:COA:P2A	2.40	0.44
1:B:27:LEU:HD22	1:B:28:PHE:CE1	2.52	0.44
2:B:201:COA:N9A	2:B:201:COA:O4B	2.40	0.44
1:D:130:LEU:HA	1:D:130:LEU:HD23	1.87	0.44
1:D:3:ARG:HD3	1:D:32:ILE:HD11	1.99	0.44
1:E:41:LYS:NZ	2:E:202[B]:COA:H51A	2.33	0.44
1:C:12:PRO:HG3	1:C:153:LEU:HD21	2.00	0.44
1:E:41:LYS:NZ	2:E:202[A]:COA:H142	2.33	0.44
1:C:106[B]:ARG:NH1	1:D:120:SER:HA	2.32	0.44
2:D:201:COA:H121	2:D:201:COA:O1A	2.17	0.44
1:B:120:SER:HA	1:F:106:ARG:NH1	2.33	0.43
1:B:29:ASP:O	1:B:63:ASN:HB2	2.18	0.43
1:C:45:PHE:HB2	1:C:50:ARG:HG3	2.00	0.43
1:C:73:LEU:HB2	2:C:201:COA:H71	1.99	0.43
1:B:68:GLY:H	4:B:204:FMT:C	2.30	0.43
1:B:87:ARG:HH22	2:B:201:COA:P2A	2.41	0.43
1:C:4:VAL:CG1	1:C:31:VAL:HG22	2.49	0.43
1:A:141:ILE:HG13	3:A:203:DMS:O	2.19	0.43
2:A:201:COA:H4B	2:A:201:COA:O1A	2.19	0.43
1:E:73:LEU:HB3	2:E:202[B]:COA:HN4	1.84	0.42
2:A:201:COA:H32	2:A:201:COA:H62	1.82	0.42
1:B:111:ASP:N	1:B:111:ASP:OD1	2.51	0.42
1:D:3:ARG:HD3	1:D:32:ILE:CD1	2.50	0.42
1:D:7:PRO:HA	1:D:34:ALA:O	2.20	0.42
1:A:89:LEU:O	1:A:118:THR:HG22	2.18	0.42
1:F:76:PHE:O	1:F:80:GLN:HG2	2.19	0.42
1:D:23:ARG:NH2	1:D:118:THR:O	2.43	0.42
1:B:87:ARG:HE	1:B:98:GLU:CD	2.22	0.42
1:C:7:PRO:HA	1:C:34:ALA:O	2.20	0.42
1:C:23:ARG:NH2	1:C:119:PRO:HA	2.35	0.41
1:B:33:ILE:HD11	1:B:58:THR:HG21	2.01	0.41
1:B:92:VAL:HB	1:F:92:VAL:HB	2.02	0.41
1:A:92:VAL:N	1:C:96:GLU:OE2	2.53	0.41
1:E:23:ARG:NH2	1:E:118:THR:O	2.39	0.41
1:B:89:LEU:HB3	1:F:95:PHE:CE1	2.56	0.41
2:E:202[B]:COA:H2B	2:E:202[B]:COA:H8A	1.93	0.41
1:C:72:LEU:HD12	2:C:201:COA:C5P	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:LEU:CD1	2:E:202[B]:COA:H62	2.50	0.41
1:F:40:LYS:HD3	1:F:40:LYS:HA	1.83	0.41
1:F:3:ARG:NH1	1:F:81:LYS:O	2.50	0.41
1:D:55:GLN:O	1:D:59:LYS:HG3	2.20	0.41
1:B:121:GLU:HB3	1:F:103:ASN:ND2	2.36	0.40
1:F:94:ASP:O	1:F:98:GLU:HG2	2.20	0.40
1:C:134:ILE:HD13	1:F:108:LEU:HD11	2.02	0.40
1:B:4:VAL:CG1	1:B:31:VAL:HG22	2.51	0.40
1:B:87:ARG:NH1	2:B:201:COA:O5A	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	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
1	B	157/159 (99%)	156 (99%)	1 (1%)	0	100	100
1	C	158/159 (99%)	154 (98%)	1 (1%)	3 (2%)	10	6
1	D	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	E	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
1	F	156/159 (98%)	154 (99%)	2 (1%)	0	100	100
All	All	941/954 (99%)	924 (98%)	14 (2%)	3 (0%)	52	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	125	PHE
1	C	124[A]	SER
1	C	124[B]	SER

### 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	134/135 (99%)	134 (100%)	0	100	100
1	B	135/135 (100%)	135 (100%)	0	100	100
1	C	136/135 (101%)	135 (99%)	1 (1%)	88	94
1	D	135/135 (100%)	135 (100%)	0	100	100
1	E	136/135 (101%)	136 (100%)	0	100	100
1	F	134/135 (99%)	132 (98%)	2 (2%)	72	84
All	All	810/810 (100%)	807 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	158	LYS
1	F	90	ARG
1	F	129	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	103	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 for Mogul analysis.

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	A	201	-	41,50,50	3.63	9 (21%)	49,75,75	2.44	11 (22%)
3	DMS	A	202	-	3,3,3	0.52	0	3,3,3	0.58	0
3	DMS	A	203	-	3,3,3	0.67	0	3,3,3	1.04	0
3	DMS	A	204	-	3,3,3	0.67	0	3,3,3	0.82	0
3	DMS	A	205	-	3,3,3	0.66	0	3,3,3	0.51	0
4	FMT	A	206	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	207	-	0,2,2	0.00	-	0,1,1	0.00	-
5	ACT	A	208	-	0,3,3	0.00	-	0,3,3	0.00	-
2	COA	B	201	-	41,50,50	3.81	11 (26%)	49,75,75	2.47	9 (18%)
4	FMT	B	202	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	203	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	204	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	205	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	206	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	207	-	0,2,2	0.00	-	0,1,1	0.00	-
2	COA	C	201	-	41,50,50	3.81	11 (26%)	49,75,75	2.54	8 (16%)
4	FMT	C	202	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	203	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	204	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	C	205	-	0,2,2	0.00	-	0,1,1	0.00	-
5	ACT	C	206	-	0,3,3	0.00	-	0,3,3	0.00	-
2	COA	D	201	-	41,50,50	3.84	10 (24%)	49,75,75	2.57	12 (24%)
6	POP	D	202	-	8,8,8	0.70	0	13,13,13	1.44	1 (7%)
3	DMS	D	203	-	3,3,3	0.67	0	3,3,3	0.75	0
3	DMS	D	204	-	3,3,3	0.66	0	3,3,3	0.71	0
4	FMT	D	205	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	D	206	-	5,5,5	0.32	0	5,5,5	0.36	0
4	FMT	E	201	-	0,2,2	0.00	-	0,1,1	0.00	-
2	COA	E	202[A]	8	41,50,50	3.91	12 (29%)	49,75,75	2.20	5 (10%)
2	COA	E	202[B]	8	41,50,50	3.87	11 (26%)	49,75,75	2.27	5 (10%)
3	DMS	E	204	-	3,3,3	0.66	0	3,3,3	0.30	0
4	FMT	E	205	-	0,2,2	0.00	-	0,1,1	0.00	-
5	ACT	E	206	-	0,3,3	0.00	-	0,3,3	0.00	-
2	COA	F	201[A]	8	41,50,50	3.87	11 (26%)	49,75,75	2.21	6 (12%)
2	COA	F	201[B]	8	41,50,50	3.85	11 (26%)	49,75,75	2.29	6 (12%)
6	POP	F	202	-	8,8,8	0.57	0	13,13,13	1.34	2 (15%)
3	DMS	F	204	-	3,3,3	0.68	0	3,3,3	0.54	0
3	DMS	F	205	-	3,3,3	0.64	0	3,3,3	0.40	0
5	ACT	F	206	-	0,3,3	0.00	-	0,3,3	0.00	-

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	A	201	-	-	1/44/64/64	0/3/3/3
3	DMS	A	202	-	-	0/0/0/0	0/0/0/0
3	DMS	A	203	-	-	0/0/0/0	0/0/0/0
3	DMS	A	204	-	-	0/0/0/0	0/0/0/0
3	DMS	A	205	-	-	0/0/0/0	0/0/0/0
4	FMT	A	206	-	-	0/0/0/0	0/0/0/0
4	FMT	A	207	-	-	0/0/0/0	0/0/0/0
5	ACT	A	208	-	-	0/0/0/0	0/0/0/0
2	COA	B	201	-	-	1/44/64/64	0/3/3/3
4	FMT	B	202	-	-	0/0/0/0	0/0/0/0
4	FMT	B	203	-	-	0/0/0/0	0/0/0/0
4	FMT	B	204	-	-	0/0/0/0	0/0/0/0
4	FMT	B	205	-	-	0/0/0/0	0/0/0/0
4	FMT	B	206	-	-	0/0/0/0	0/0/0/0
4	FMT	B	207	-	-	0/0/0/0	0/0/0/0
2	COA	C	201	-	-	0/44/64/64	0/3/3/3
4	FMT	C	202	-	-	0/0/0/0	0/0/0/0
4	FMT	C	203	-	-	0/0/0/0	0/0/0/0
4	FMT	C	204	-	-	0/0/0/0	0/0/0/0
4	FMT	C	205	-	-	0/0/0/0	0/0/0/0
5	ACT	C	206	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	D	201	-	-	0/44/64/64	0/3/3/3
6	POP	D	202	-	-	0/6/6/6	0/0/0/0
3	DMS	D	203	-	-	0/0/0/0	0/0/0/0
3	DMS	D	204	-	-	0/0/0/0	0/0/0/0
4	FMT	D	205	-	-	0/0/0/0	0/0/0/0
7	GOL	D	206	-	-	0/4/4/4	0/0/0/0
4	FMT	E	201	-	-	0/0/0/0	0/0/0/0
2	COA	E	202[A]	8	-	1/44/64/64	0/3/3/3
2	COA	E	202[B]	8	-	0/44/64/64	0/3/3/3
3	DMS	E	204	-	-	0/0/0/0	0/0/0/0
4	FMT	E	205	-	-	0/0/0/0	0/0/0/0
5	ACT	E	206	-	-	0/0/0/0	0/0/0/0
2	COA	F	201[A]	8	-	1/44/64/64	0/3/3/3
2	COA	F	201[B]	8	-	0/44/64/64	0/3/3/3
6	POP	F	202	-	-	0/6/6/6	0/0/0/0
3	DMS	F	204	-	-	0/0/0/0	0/0/0/0
3	DMS	F	205	-	-	0/0/0/0	0/0/0/0
5	ACT	F	206	-	-	0/0/0/0	0/0/0/0

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	201[A]	COA	C2B-C1B	-13.42	1.32	1.53
2	F	201[B]	COA	C2B-C1B	-13.34	1.32	1.53
2	E	202[A]	COA	C2B-C1B	-13.34	1.32	1.53
2	D	201	COA	C2B-C1B	-13.24	1.32	1.53
2	E	202[B]	COA	C2B-C1B	-12.99	1.33	1.53
2	C	201	COA	C2B-C1B	-12.86	1.33	1.53
2	B	201	COA	C2B-C1B	-12.29	1.34	1.53
2	A	201	COA	C2B-C1B	-12.02	1.34	1.53
2	B	201	COA	O4B-C4B	-6.57	1.30	1.45
2	C	201	COA	O4B-C4B	-6.45	1.30	1.45
2	F	201[B]	COA	O4B-C4B	-6.40	1.30	1.45
2	E	202[B]	COA	O4B-C4B	-6.34	1.30	1.45
2	D	201	COA	O4B-C4B	-6.31	1.30	1.45
2	F	201[A]	COA	O4B-C4B	-6.21	1.30	1.45
2	E	202[A]	COA	O4B-C4B	-6.17	1.30	1.45
2	A	201	COA	O4B-C4B	-5.96	1.31	1.45
2	D	201	COA	O3B-C3B	-3.52	1.33	1.44
2	C	201	COA	O3B-C3B	-3.44	1.33	1.44
2	E	202[B]	COA	O3B-C3B	-3.27	1.33	1.44
2	F	201[A]	COA	O3B-C3B	-3.27	1.33	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	202[A]	COA	O3B-C3B	-3.22	1.33	1.44
2	B	201	COA	O3B-C3B	-3.22	1.33	1.44
2	F	201[B]	COA	O3B-C3B	-3.16	1.34	1.44
2	A	201	COA	OAP-CAP	-2.93	1.36	1.42
2	C	201	COA	OAP-CAP	-2.76	1.36	1.42
2	B	201	COA	OAP-CAP	-2.66	1.36	1.42
2	D	201	COA	OAP-CAP	-2.62	1.37	1.42
2	F	201[A]	COA	OAP-CAP	-2.54	1.37	1.42
2	E	202[A]	COA	OAP-CAP	-2.41	1.37	1.42
2	B	201	COA	C5A-C4A	-2.38	1.35	1.40
2	D	201	COA	C5A-C4A	-2.34	1.35	1.40
2	E	202[B]	COA	OAP-CAP	-2.32	1.37	1.42
2	E	202[B]	COA	C5A-C4A	-2.29	1.35	1.40
2	F	201[B]	COA	C5A-C4A	-2.26	1.35	1.40
2	E	202[A]	COA	C5A-C4A	-2.22	1.35	1.40
2	F	201[B]	COA	OAP-CAP	-2.22	1.37	1.42
2	A	201	COA	O3B-C3B	-2.22	1.37	1.44
2	C	201	COA	C5A-C4A	-2.20	1.35	1.40
2	F	201[A]	COA	C5A-C4A	-2.12	1.35	1.40
2	A	201	COA	C6A-N6A	2.02	1.42	1.34
2	E	202[A]	COA	C3B-C4B	2.04	1.58	1.52
2	B	201	COA	C6A-N6A	2.06	1.42	1.34
2	E	202[A]	COA	C6A-N6A	2.07	1.42	1.34
2	F	201[B]	COA	C6A-N6A	2.07	1.42	1.34
2	E	202[B]	COA	C6A-N6A	2.07	1.42	1.34
2	C	201	COA	C6A-N6A	2.10	1.42	1.34
2	F	201[A]	COA	C6A-N6A	2.10	1.42	1.34
2	F	201[B]	COA	O2B-C2B	2.11	1.47	1.43
2	D	201	COA	O2B-C2B	2.14	1.48	1.43
2	F	201[A]	COA	O2B-C2B	2.17	1.48	1.43
2	E	202[B]	COA	O2B-C2B	2.28	1.48	1.43
2	C	201	COA	O2B-C2B	2.30	1.48	1.43
2	E	202[A]	COA	O2B-C2B	2.32	1.48	1.43
2	B	201	COA	O2B-C2B	2.42	1.48	1.43
2	D	201	COA	C2A-N3A	2.63	1.36	1.32
2	E	202[B]	COA	C2A-N3A	2.69	1.36	1.32
2	F	201[B]	COA	C2A-N3A	2.77	1.37	1.32
2	E	202[A]	COA	C2A-N3A	2.81	1.37	1.32
2	C	201	COA	C2A-N3A	2.82	1.37	1.32
2	F	201[A]	COA	C2A-N3A	2.84	1.37	1.32
2	A	201	COA	C2A-N3A	3.11	1.37	1.32
2	B	201	COA	C2A-N3A	3.13	1.37	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	COA	C5P-N4P	4.53	1.44	1.33
2	C	201	COA	C5P-N4P	4.81	1.45	1.33
2	D	201	COA	C5P-N4P	4.84	1.45	1.33
2	F	201[A]	COA	C5P-N4P	4.86	1.45	1.33
2	E	202[A]	COA	C5P-N4P	4.92	1.45	1.33
2	F	201[B]	COA	C5P-N4P	5.02	1.45	1.33
2	E	202[B]	COA	C5P-N4P	5.14	1.45	1.33
2	B	201	COA	C5P-N4P	5.17	1.45	1.33
2	F	201[B]	COA	C9P-N8P	7.17	1.48	1.33
2	F	201[A]	COA	C9P-N8P	7.43	1.49	1.33
2	D	201	COA	C9P-N8P	7.47	1.49	1.33
2	C	201	COA	C9P-N8P	7.55	1.49	1.33
2	E	202[B]	COA	C9P-N8P	7.59	1.49	1.33
2	B	201	COA	C9P-N8P	7.89	1.50	1.33
2	A	201	COA	C9P-N8P	7.92	1.50	1.33
2	E	202[A]	COA	C9P-N8P	8.15	1.50	1.33
2	A	201	COA	O4B-C1B	14.95	1.62	1.41
2	C	201	COA	O4B-C1B	15.73	1.63	1.41
2	B	201	COA	O4B-C1B	15.81	1.63	1.41
2	D	201	COA	O4B-C1B	15.85	1.63	1.41
2	F	201[B]	COA	O4B-C1B	15.92	1.64	1.41
2	F	201[A]	COA	O4B-C1B	15.97	1.64	1.41
2	E	202[A]	COA	O4B-C1B	16.05	1.64	1.41
2	E	202[B]	COA	O4B-C1B	16.20	1.64	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	COA	N3A-C2A-N1A	-11.52	119.82	128.87
2	C	201	COA	N3A-C2A-N1A	-11.36	119.95	128.87
2	F	201[B]	COA	N3A-C2A-N1A	-11.23	120.05	128.87
2	E	202[B]	COA	N3A-C2A-N1A	-11.20	120.07	128.87
2	B	201	COA	N3A-C2A-N1A	-11.09	120.16	128.87
2	F	201[A]	COA	N3A-C2A-N1A	-11.05	120.19	128.87
2	E	202[A]	COA	N3A-C2A-N1A	-11.05	120.19	128.87
2	A	201	COA	N3A-C2A-N1A	-8.67	122.06	128.87
2	B	201	COA	N6A-C6A-N1A	-8.61	104.06	118.52
2	A	201	COA	N6A-C6A-N1A	-8.55	104.17	118.52
2	C	201	COA	N6A-C6A-N1A	-8.19	104.78	118.52
2	F	201[B]	COA	N6A-C6A-N1A	-7.90	105.26	118.52
2	E	202[B]	COA	N6A-C6A-N1A	-7.82	105.40	118.52
2	E	202[A]	COA	N6A-C6A-N1A	-7.77	105.48	118.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	COA	N6A-C6A-N1A	-7.72	105.56	118.52
2	F	201[A]	COA	N6A-C6A-N1A	-7.69	105.61	118.52
2	C	201	COA	C2P-C3P-N4P	-5.46	101.62	112.44
2	D	201	COA	C7P-C6P-C5P	-5.42	102.93	112.22
2	B	201	COA	OAP-CAP-C9P	-4.78	99.16	110.52
2	D	201	COA	C2P-C3P-N4P	-4.67	103.19	112.44
2	A	201	COA	OAP-CAP-C9P	-4.45	99.94	110.52
2	E	202[B]	COA	C7P-C6P-C5P	-4.39	104.69	112.22
2	C	201	COA	C6P-C7P-N8P	-3.80	103.43	111.94
2	F	201[B]	COA	C6P-C7P-N8P	-3.37	104.39	111.94
2	B	201	COA	CEP-CBP-CCP	-3.33	104.18	108.50
2	F	201[A]	COA	C3P-N4P-C5P	-3.30	116.26	122.79
2	D	201	COA	C1B-N9A-C4A	-3.26	123.17	126.81
2	A	201	COA	C6P-C7P-N8P	-3.17	104.85	111.94
6	D	202	POP	P2-O-P1	-3.08	123.69	132.51
2	A	201	COA	C2P-C3P-N4P	-3.07	106.36	112.44
2	F	201[A]	COA	C7P-N8P-C9P	-3.05	116.50	122.62
2	C	201	COA	O5P-C5P-N4P	-3.02	116.96	122.96
2	E	202[B]	COA	C4B-O4B-C1B	-2.79	106.68	109.64
2	D	201	COA	P3B-O3B-C3B	-2.61	114.88	121.56
2	F	201[A]	COA	C4B-O4B-C1B	-2.58	106.91	109.64
2	E	202[A]	COA	C3P-N4P-C5P	-2.57	117.71	122.79
2	F	201[B]	COA	C1B-N9A-C4A	-2.47	124.05	126.81
2	B	201	COA	O4B-C1B-N9A	-2.42	103.53	108.11
2	A	201	COA	O5P-C5P-N4P	-2.40	118.19	122.96
2	B	201	COA	O2B-C2B-C3B	-2.30	104.50	111.13
2	E	202[B]	COA	C6P-C7P-N8P	-2.21	106.99	111.94
2	D	201	COA	C7P-N8P-C9P	-2.21	118.19	122.62
2	E	202[A]	COA	C4B-O4B-C1B	-2.09	107.43	109.64
2	F	201[A]	COA	C7P-C6P-C5P	-2.07	108.67	112.22
2	D	201	COA	O5P-C5P-C6P	-2.06	118.39	121.97
2	B	201	COA	C3B-C2B-C1B	2.21	104.87	100.06
6	F	202	POP	O2-P1-O	2.23	111.35	104.29
2	A	201	COA	P3B-O3B-C3B	2.26	127.35	121.56
2	F	201[B]	COA	CEP-CBP-CCP	2.30	111.48	108.50
6	F	202	POP	O5-P2-O	2.32	111.64	104.29
2	C	201	COA	CEP-CBP-CAP	2.53	113.78	109.17
2	B	201	COA	C6P-C5P-N4P	2.65	121.07	116.46
2	D	201	COA	CDP-CBP-CCP	2.66	111.95	108.50
2	D	201	COA	C6P-C5P-N4P	2.73	121.20	116.46
2	D	201	COA	CEP-CBP-CCP	2.77	112.09	108.50
2	A	201	COA	C6P-C5P-N4P	2.91	121.51	116.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	COA	CAP-C9P-N8P	2.95	123.27	116.31
2	D	201	COA	O4B-C1B-N9A	2.97	113.72	108.11
2	E	202[A]	COA	CAP-C9P-N8P	3.11	123.63	116.31
2	C	201	COA	C3B-C2B-C1B	3.11	106.84	100.06
2	F	201[B]	COA	C3B-C2B-C1B	3.27	107.19	100.06
2	C	201	COA	C6P-C5P-N4P	3.75	122.97	116.46
2	A	201	COA	C2B-C1B-N9A	3.96	124.06	113.47
2	A	201	COA	O3B-P3B-O7A	3.98	116.97	107.48
2	A	201	COA	C3B-C2B-C1B	4.01	108.79	100.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	COA	P1A-O5B-C5B-C4B
2	E	202[A]	COA	CAP-C9P-N8P-C7P
2	B	201	COA	CAP-C9P-N8P-C7P
2	F	201[A]	COA	CAP-C9P-N8P-C7P

There are no ring outliers.

16 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	COA	8	0
3	A	202	DMS	1	0
3	A	203	DMS	1	0
3	A	204	DMS	3	0
2	B	201	COA	5	0
4	B	204	FMT	1	0
4	B	205	FMT	1	0
2	C	201	COA	5	0
2	D	201	COA	4	0
3	D	203	DMS	1	0
7	D	206	GOL	1	0
2	E	202[A]	COA	5	0
2	E	202[B]	COA	9	0
2	F	201[A]	COA	3	0
2	F	201[B]	COA	6	0
3	F	204	DMS	1	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, 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	157/159 (98%)	0.11	4 (2%) 61 60	24, 36, 62, 69	0
1	B	158/159 (99%)	0.08	4 (2%) 61 60	25, 36, 62, 70	0
1	C	158/159 (99%)	0.13	2 (1%) 79 78	31, 43, 62, 75	0
1	D	158/159 (99%)	0.21	5 (3%) 51 50	31, 43, 64, 74	0
1	E	158/159 (99%)	0.20	3 (1%) 70 68	28, 42, 64, 73	0
1	F	158/159 (99%)	0.19	5 (3%) 51 50	30, 42, 63, 83	0
All	All	947/954 (99%)	0.15	23 (2%) 62 61	24, 40, 63, 83	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1[A]	MET	4.2
1	E	28	PHE	3.5
1	B	99	PHE	3.5
1	F	95	PHE	3.3
1	F	1	MET	3.2
1	A	27	LEU	3.1
1	A	92	VAL	2.7
1	D	92	VAL	2.7
1	A	101	LEU	2.6
1	C	125	PHE	2.6
1	D	27	LEU	2.6
1	D	97	TYR	2.6
1	B	158	LYS	2.6
1	A	158	LYS	2.5
1	D	157	PHE	2.5
1	C	28	PHE	2.4
1	F	90	ARG	2.4
1	D	101	LEU	2.4
1	B	101	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	101	LEU	2.1
1	E	4	VAL	2.1
1	F	94	ASP	2.1
1	B	95	PHE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	COA	E	202[A]	48/48	0.85	0.30	4.94	26,51,69,70	48
4	FMT	B	207	3/3	0.86	0.27	4.72	48,48,49,59	0
2	COA	E	202[B]	48/48	0.85	0.30	4.25	36,53,69,69	48
2	COA	C	201	48/48	0.86	0.24	3.79	42,70,84,87	48
3	DMS	A	204	4/4	0.96	0.22	3.69	32,37,39,46	4
3	DMS	D	203	4/4	0.98	0.19	3.37	42,48,53,64	0
2	COA	F	201[B]	48/48	0.86	0.29	3.26	36,54,70,73	48
2	COA	F	201[A]	48/48	0.86	0.29	2.56	30,54,69,70	48
5	ACT	C	206	4/4	0.88	0.19	2.48	49,50,50,52	0
2	COA	B	201	48/48	0.83	0.26	2.15	31,55,65,69	48
5	ACT	A	208	4/4	0.97	0.21	2.06	37,41,48,54	0
2	COA	A	201	48/48	0.87	0.24	1.74	36,57,69,73	48
6	POP	D	202	9/9	0.86	0.24	1.72	42,52,60,63	9
3	DMS	A	203	4/4	0.99	0.19	1.65	32,42,45,56	0
6	POP	F	202	9/9	0.90	0.20	1.59	44,46,62,62	9
3	DMS	D	204	4/4	0.97	0.16	1.48	46,51,55,57	0
2	COA	D	201	48/48	0.86	0.22	1.28	38,64,78,81	48

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	FMT	C	202	3/3	0.96	0.19	1.12	48,48,50,56	0
4	FMT	C	205	3/3	0.97	0.22	1.01	45,45,46,49	0
4	FMT	A	207	3/3	0.90	0.26	0.88	46,46,48,55	0
3	DMS	F	204	4/4	0.98	0.18	0.31	54,57,57,62	0
5	ACT	F	206	4/4	0.95	0.18	0.26	37,42,47,52	0
3	DMS	A	205	4/4	0.97	0.12	-0.16	51,54,61,69	0
4	FMT	E	205	3/3	0.94	0.17	-0.22	52,52,56,62	0
4	FMT	A	206	3/3	0.94	0.13	-0.60	47,47,48,50	0
3	DMS	E	204	4/4	0.97	0.12	-0.73	56,57,60,64	0
5	ACT	E	206	4/4	0.96	0.08	-3.16	34,38,43,51	0
7	GOL	D	206	6/6	0.86	0.21	-	61,69,74,77	0
4	FMT	B	202	3/3	0.86	0.17	-	55,55,57,58	0
4	FMT	C	204	3/3	0.89	0.13	-	58,58,60,64	0
3	DMS	F	205	4/4	0.95	0.17	-	65,74,75,84	0
8	CA	E	203	1/1	0.99	0.06	-	64,64,64,64	0
4	FMT	C	203	3/3	0.96	0.20	-	42,42,43,45	0
4	FMT	E	201	3/3	0.90	0.18	-	53,53,55,58	0
4	FMT	B	206	3/3	0.95	0.16	-	63,63,63,69	0
4	FMT	B	204	3/3	0.94	0.17	-	47,47,55,56	0
4	FMT	B	205	3/3	0.93	0.18	-	44,44,48,64	0
3	DMS	A	202	4/4	0.96	0.13	-	43,51,56,57	0
4	FMT	B	203	3/3	0.85	0.16	-	62,62,68,68	0
4	FMT	D	205	3/3	0.94	0.12	-	53,53,65,70	0
8	CA	F	203	1/1	0.94	0.15	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.