



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:56 PM GMT

PDB ID : 1VH8  
Title : Crystal structure of a 2C-methyl-D-erythritol2,4-cyclodiphosphate synthase  
Authors : Structural GenomiX  
Deposited on : 2003-12-01  
Resolution : 2.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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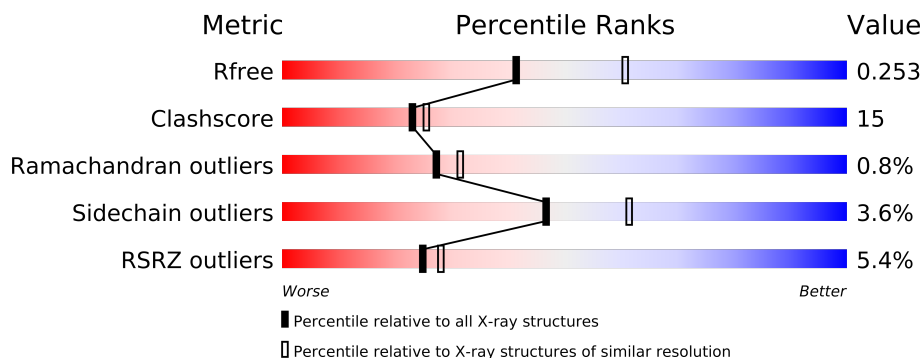
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.35 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))
$R_{free}$	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	170	
1	B	170	
1	C	170	
1	D	170	
1	E	170	
1	F	170	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACY	A	170	-	X
3	ACY	B	169	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	ACY	C	169	-	X
3	ACY	D	170	-	X
3	ACY	E	169	-	X
3	ACY	F	169	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7183 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2-C-methyl-D-erythritol2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	Se	0	0	0
			1155	728	208	215	2	2			
1	B	152	Total	C	N	O	S	Se	0	0	0
			1146	722	206	214	2	2			
1	C	152	Total	C	N	O	S	Se	0	0	0
			1146	722	206	214	2	2			
1	D	152	Total	C	N	O	S	Se	0	0	0
			1145	721	206	214	2	2			
1	E	152	Total	C	N	O	S	Se	0	0	0
			1145	721	206	214	2	2			
1	F	152	Total	C	N	O	S	Se	0	0	0
			1145	721	206	214	2	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP P44815
A	0	SER	-	cloning artifact	UNP P44815
A	1	LEU	-	cloning artifact	UNP P44815
A	67	MSE	MET	modified residue	UNP P44815
A	106	MSE	MET	modified residue	UNP P44815
A	113	MSE	MET	modified residue	UNP P44815
A	159	GLU	-	cloning artifact	UNP P44815
A	160	GLY	-	cloning artifact	UNP P44815
A	161	GLY	-	cloning artifact	UNP P44815
A	162	SER	-	cloning artifact	UNP P44815
A	163	HIS	-	cloning artifact	UNP P44815
A	164	HIS	-	cloning artifact	UNP P44815
A	165	HIS	-	cloning artifact	UNP P44815
A	166	HIS	-	cloning artifact	UNP P44815
A	167	HIS	-	cloning artifact	UNP P44815
A	168	HIS	-	cloning artifact	UNP P44815
B	-1	MSE	-	cloning artifact	UNP P44815

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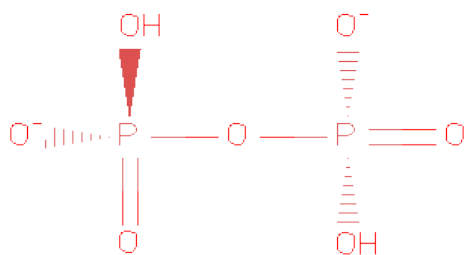
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	cloning artifact	UNP P44815
B	1	LEU	-	cloning artifact	UNP P44815
B	67	MSE	MET	modified residue	UNP P44815
B	106	MSE	MET	modified residue	UNP P44815
B	113	MSE	MET	modified residue	UNP P44815
B	159	GLU	-	cloning artifact	UNP P44815
B	160	GLY	-	cloning artifact	UNP P44815
B	161	GLY	-	cloning artifact	UNP P44815
B	162	SER	-	cloning artifact	UNP P44815
B	163	HIS	-	cloning artifact	UNP P44815
B	164	HIS	-	cloning artifact	UNP P44815
B	165	HIS	-	cloning artifact	UNP P44815
B	166	HIS	-	cloning artifact	UNP P44815
B	167	HIS	-	cloning artifact	UNP P44815
B	168	HIS	-	cloning artifact	UNP P44815
C	-1	MSE	-	cloning artifact	UNP P44815
C	0	SER	-	cloning artifact	UNP P44815
C	1	LEU	-	cloning artifact	UNP P44815
C	67	MSE	MET	modified residue	UNP P44815
C	106	MSE	MET	modified residue	UNP P44815
C	113	MSE	MET	modified residue	UNP P44815
C	159	GLU	-	cloning artifact	UNP P44815
C	160	GLY	-	cloning artifact	UNP P44815
C	161	GLY	-	cloning artifact	UNP P44815
C	162	SER	-	cloning artifact	UNP P44815
C	163	HIS	-	cloning artifact	UNP P44815
C	164	HIS	-	cloning artifact	UNP P44815
C	165	HIS	-	cloning artifact	UNP P44815
C	166	HIS	-	cloning artifact	UNP P44815
C	167	HIS	-	cloning artifact	UNP P44815
C	168	HIS	-	cloning artifact	UNP P44815
D	-1	MSE	-	cloning artifact	UNP P44815
D	0	SER	-	cloning artifact	UNP P44815
D	1	LEU	-	cloning artifact	UNP P44815
D	67	MSE	MET	modified residue	UNP P44815
D	106	MSE	MET	modified residue	UNP P44815
D	113	MSE	MET	modified residue	UNP P44815
D	159	GLU	-	cloning artifact	UNP P44815
D	160	GLY	-	cloning artifact	UNP P44815
D	161	GLY	-	cloning artifact	UNP P44815
D	162	SER	-	cloning artifact	UNP P44815
D	163	HIS	-	cloning artifact	UNP P44815

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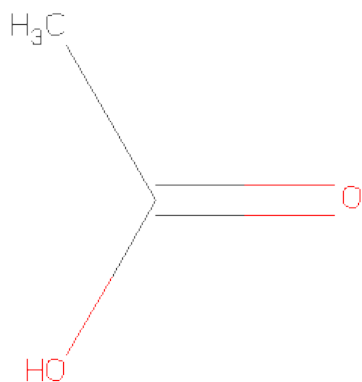
Chain	Residue	Modelled	Actual	Comment	Reference
D	164	HIS	-	cloning artifact	UNP P44815
D	165	HIS	-	cloning artifact	UNP P44815
D	166	HIS	-	cloning artifact	UNP P44815
D	167	HIS	-	cloning artifact	UNP P44815
D	168	HIS	-	cloning artifact	UNP P44815
E	-1	MSE	-	cloning artifact	UNP P44815
E	0	SER	-	cloning artifact	UNP P44815
E	1	LEU	-	cloning artifact	UNP P44815
E	67	MSE	MET	modified residue	UNP P44815
E	106	MSE	MET	modified residue	UNP P44815
E	113	MSE	MET	modified residue	UNP P44815
E	159	GLU	-	cloning artifact	UNP P44815
E	160	GLY	-	cloning artifact	UNP P44815
E	161	GLY	-	cloning artifact	UNP P44815
E	162	SER	-	cloning artifact	UNP P44815
E	163	HIS	-	cloning artifact	UNP P44815
E	164	HIS	-	cloning artifact	UNP P44815
E	165	HIS	-	cloning artifact	UNP P44815
E	166	HIS	-	cloning artifact	UNP P44815
E	167	HIS	-	cloning artifact	UNP P44815
E	168	HIS	-	cloning artifact	UNP P44815
F	-1	MSE	-	cloning artifact	UNP P44815
F	0	SER	-	cloning artifact	UNP P44815
F	1	LEU	-	cloning artifact	UNP P44815
F	67	MSE	MET	modified residue	UNP P44815
F	106	MSE	MET	modified residue	UNP P44815
F	113	MSE	MET	modified residue	UNP P44815
F	159	GLU	-	cloning artifact	UNP P44815
F	160	GLY	-	cloning artifact	UNP P44815
F	161	GLY	-	cloning artifact	UNP P44815
F	162	SER	-	cloning artifact	UNP P44815
F	163	HIS	-	cloning artifact	UNP P44815
F	164	HIS	-	cloning artifact	UNP P44815
F	165	HIS	-	cloning artifact	UNP P44815
F	166	HIS	-	cloning artifact	UNP P44815
F	167	HIS	-	cloning artifact	UNP P44815
F	168	HIS	-	cloning artifact	UNP P44815

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	1
			27	21	6		
2	D	1	Total	O	P	0	1
			27	21	6		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total 40	O 40	0	0
4	B	40	Total 40	O 40	0	0
4	C	50	Total 50	O 50	0	0
4	D	32	Total 32	O 32	0	0
4	E	27	Total 27	O 27	0	0
4	F	34	Total 34	O 34	0	0

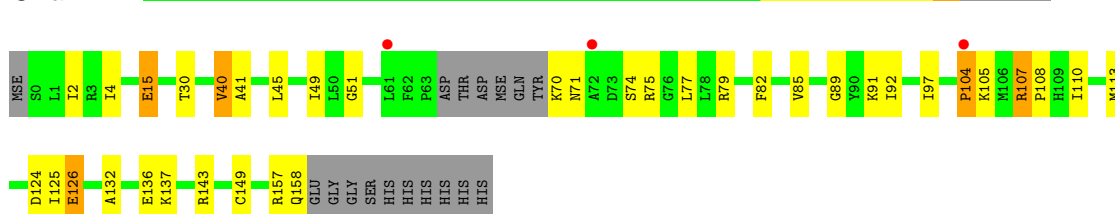


### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

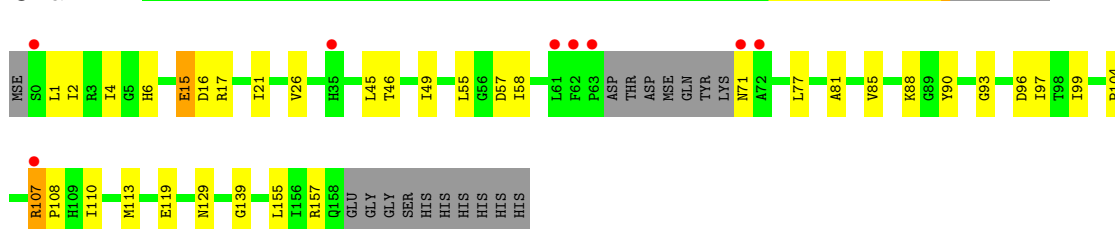
- Molecule 1: 2-C-methyl-D-erythritol2,4-cyclodiphosphate synthase

Chain A:



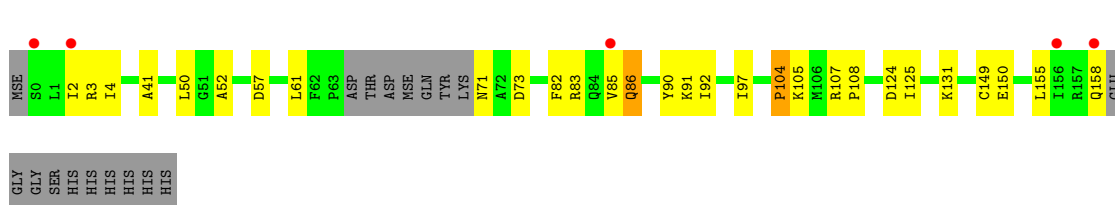
- Molecule 1: 2-C-methyl-D-erythritol2,4-cyclodiphosphate synthase

Chain B:



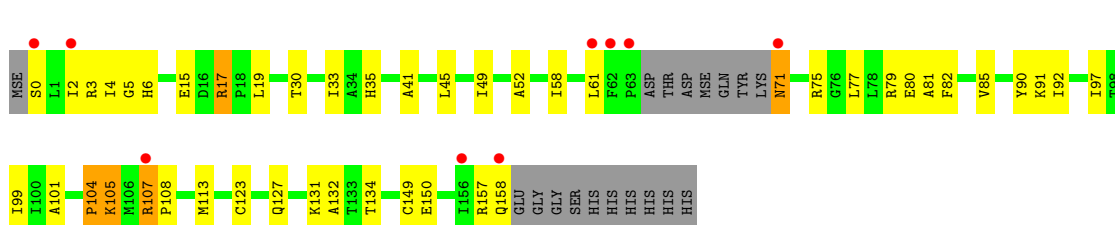
- Molecule 1: 2-C-methyl-D-erythritol2,4-cyclodiphosphate synthase

Chain C:



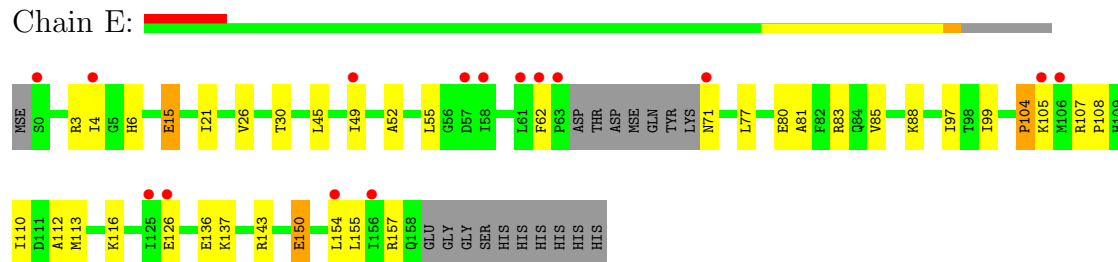
- Molecule 1: 2-C-methyl-D-erythritol2,4-cyclodiphosphate synthase

Chain D:



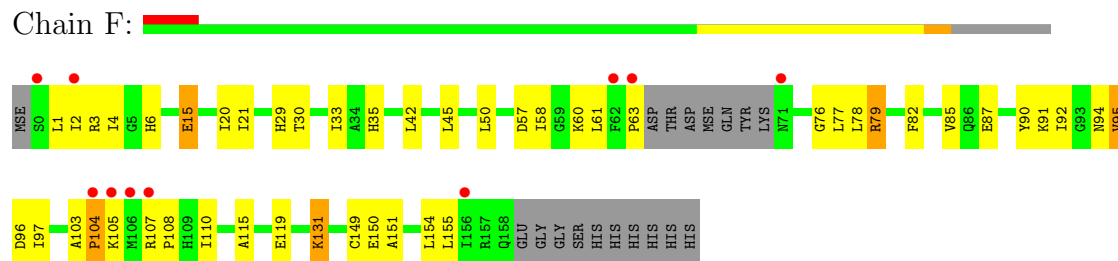
- Molecule 1: 2-C-methyl-D-erythritol2,4-cyclodiphosphate synthase

Chain E:



- Molecule 1: 2-C-methyl-D-erythritol2,4-cyclodiphosphate synthase

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.85Å 104.85Å 195.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.35 48.94 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.94-2.35) 99.3 (48.94-2.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.34Å)	Xtriage
Refinement program	REFMAC 4	Depositor
R, $R_{free}$	0.240 , 0.280 0.207 , 0.253	Depositor DCC
$R_{free}$ test set	2208 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.7	EDS
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 43488 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.36	0/1170	0.57	0/1576
1	B	0.36	0/1161	0.58	1/1565 (0.1%)
1	C	0.39	0/1161	0.58	0/1565
1	D	0.33	0/1160	0.55	0/1564
1	E	0.32	0/1160	0.55	0/1564
1	F	0.37	0/1160	0.58	0/1564
All	All	0.35	0/6972	0.57	1/9398 (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	93	GLY	N-CA-C	-5.22	100.04	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1155	0	1160	42	0
1	B	1146	0	1147	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1146	0	1147	30	0
1	D	1145	0	1145	35	0
1	E	1145	0	1145	31	0
1	F	1145	0	1145	46	0
2	A	27	0	0	4	0
2	D	27	0	0	2	0
3	A	4	0	3	1	0
3	B	4	0	3	1	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	1	0
4	A	40	0	0	1	0
4	B	40	0	0	0	0
4	C	50	0	0	0	0
4	D	32	0	0	1	0
4	E	27	0	0	0	0
4	F	34	0	0	1	0
All	All	7183	0	6907	196	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (196) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:ARG:HH12	1:A:132:ALA:H	1.08	1.01
1:B:107:ARG:HB2	1:B:107:ARG:HH21	1.27	0.95
1:A:107:ARG:HH22	1:A:132:ALA:HB3	1.32	0.94
1:A:70:LYS:HG2	1:A:71:ASN:H	1.30	0.93
1:A:15:GLU:HG2	1:A:30:THR:HB	1.49	0.92
1:F:2:ILE:HG23	1:F:154:LEU:HD11	1.54	0.89
1:B:107:ARG:HB2	1:B:107:ARG:NH2	1.88	0.88
1:A:40:VAL:HG13	1:A:149:CYS:HB2	1.55	0.87
1:D:58:ILE:HD11	1:D:77:LEU:HD13	1.55	0.86
1:D:99:ILE:HD11	1:D:113:MSE:HE1	1.56	0.86
1:C:85:VAL:HG22	1:C:90:TYR:HB2	1.63	0.80
1:B:99:ILE:HD11	1:B:113:MSE:HE1	1.64	0.80
1:D:81:ALA:O	1:D:85:VAL:HG23	1.82	0.79
1:F:107:ARG:HB2	1:F:107:ARG:NH2	1.97	0.79
1:C:91:LYS:HD2	1:C:158:GLN:HG3	1.66	0.77
1:D:91:LYS:HB2	1:D:158:GLN:HB2	1.67	0.76
1:B:6:HIS:CE1	1:C:150:GLU:HG2	2.21	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:6:HIS:NE2	1:C:150:GLU:HG2	2.02	0.74
1:A:107:ARG:NH2	1:A:132:ALA:HB3	2.02	0.74
1:B:85:VAL:HG12	1:B:90:TYR:HB2	1.68	0.74
1:A:91:LYS:HD3	1:A:158:GLN:HB3	1.72	0.72
1:A:107:ARG:NH1	1:A:132:ALA:H	1.85	0.72
1:F:45:LEU:HD13	1:F:97:ILE:HD11	1.72	0.71
1:A:40:VAL:HG13	1:A:149:CYS:CB	2.20	0.70
1:B:1:LEU:HA	1:B:157:ARG:HB2	1.74	0.70
1:B:45:LEU:HD13	1:B:97:ILE:HD11	1.75	0.69
1:C:86:GLN:HE21	1:C:86:GLN:HA	1.58	0.67
1:D:49:ILE:CG2	1:D:85:VAL:HG21	2.24	0.67
1:D:49:ILE:HG22	1:D:85:VAL:HG21	1.76	0.67
1:A:143:ARG:NH2	2:A:169[A]:POP:O5	2.19	0.67
1:F:107:ARG:HB2	1:F:107:ARG:HH21	1.60	0.67
1:D:61:LEU:HD22	1:D:80:GLU:HG3	1.76	0.66
1:C:104:PRO:HG2	1:C:105:LYS:H	1.61	0.66
1:E:49:ILE:HG22	1:E:85:VAL:HG21	1.75	0.66
1:A:49:ILE:CG2	1:A:85:VAL:HG21	2.26	0.65
1:B:107:ARG:HA	1:B:110:ILE:HG12	1.80	0.64
1:C:85:VAL:HG21	1:C:155:LEU:HD13	1.78	0.64
1:E:3:ARG:O	1:E:154:LEU:HD12	1.97	0.64
1:F:85:VAL:HG13	1:F:90:TYR:HB2	1.80	0.64
1:E:112:ALA:O	1:E:116:LYS:HG3	1.99	0.62
1:F:15:GLU:HG2	1:F:30:THR:HB	1.81	0.62
1:E:55:LEU:HD21	1:E:88:LYS:HD2	1.80	0.61
1:A:104:PRO:HG2	1:A:105:LYS:H	1.66	0.61
1:F:76:GLY:HA2	1:F:79:ARG:NH1	2.16	0.61
1:D:107:ARG:HB3	1:D:108:PRO:HD3	1.82	0.60
1:D:85:VAL:HG12	1:D:90:TYR:HB2	1.82	0.60
1:A:2:ILE:CD1	1:C:2:ILE:HD13	2.31	0.60
1:D:107:ARG:HH12	1:D:132:ALA:H	1.49	0.59
1:E:45:LEU:HD22	1:E:97:ILE:HD11	1.84	0.59
1:A:91:LYS:HD3	1:A:158:GLN:CB	2.32	0.59
1:F:29:HIS:HD2	1:F:33:ILE:HD13	1.68	0.59
1:E:104:PRO:HG2	1:E:105:LYS:H	1.68	0.59
1:E:15:GLU:HG2	1:E:30:THR:HB	1.84	0.58
1:E:107:ARG:HA	1:E:110:ILE:HG12	1.85	0.58
1:D:150:GLU:HG2	1:F:6:HIS:CE1	2.38	0.58
1:F:1:LEU:C	1:F:2:ILE:HD12	2.24	0.58
1:D:150:GLU:HG2	1:F:6:HIS:NE2	2.18	0.58
1:A:89:GLY:O	1:A:157:ARG:HD3	2.04	0.58
1:B:58:ILE:HD11	1:B:77:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:ASN:HD22	1:A:77:LEU:HD21	1.68	0.57
1:A:124:ASP:OD2	1:A:125:ILE:N	2.37	0.57
1:F:20:ILE:O	1:F:21:ILE:HD13	2.04	0.57
1:B:107:ARG:N	1:B:108:PRO:CD	2.68	0.56
1:E:49:ILE:CG2	1:E:85:VAL:HG21	2.35	0.56
1:D:6:HIS:NE2	1:E:150:GLU:HG2	2.22	0.55
1:C:82:PHE:O	1:C:85:VAL:HG12	2.06	0.55
1:C:85:VAL:CG2	1:C:155:LEU:HD13	2.37	0.54
1:C:85:VAL:HG21	1:C:155:LEU:CD1	2.37	0.54
1:E:99:ILE:HD11	1:E:113:MSE:HE1	1.89	0.54
1:F:76:GLY:HA2	1:F:79:ARG:HH12	1.72	0.54
1:C:3:ARG:HD2	1:C:52:ALA:O	2.08	0.54
1:A:70:LYS:HG2	1:A:71:ASN:N	2.11	0.54
1:B:49:ILE:HG22	1:B:85:VAL:HG21	1.90	0.54
1:B:96:ASP:C	1:B:97:ILE:HD12	2.28	0.53
1:B:81:ALA:O	1:B:85:VAL:HG23	2.09	0.53
1:C:83:ARG:HG2	1:C:83:ARG:HH11	1.74	0.53
1:D:45:LEU:HD22	1:D:97:ILE:HD11	1.91	0.53
1:A:4:ILE:HG13	1:C:4:ILE:HD12	1.89	0.53
1:A:71:ASN:ND2	1:A:77:LEU:HD21	2.24	0.53
1:B:21:ILE:HD12	1:B:26:VAL:HG21	1.91	0.52
1:E:81:ALA:O	1:E:85:VAL:HG23	2.09	0.52
1:A:40:VAL:CG1	1:A:149:CYS:HB2	2.34	0.52
1:C:82:PHE:CE2	1:C:92:ILE:HD13	2.45	0.52
1:E:136:GLU:O	1:E:137:LYS:HB2	2.09	0.52
1:B:55:LEU:HD21	1:B:88:LYS:HD2	1.92	0.52
1:D:75:ARG:O	1:D:79:ARG:HG3	2.09	0.51
1:E:6:HIS:CE1	1:F:150:GLU:HG2	2.45	0.51
1:A:45:LEU:HD22	1:A:97:ILE:HD11	1.91	0.51
1:F:2:ILE:CG2	1:F:154:LEU:HD11	2.35	0.51
1:B:2:ILE:HD13	1:C:2:ILE:CD1	2.41	0.51
1:F:45:LEU:HD11	1:F:95:VAL:HG21	1.93	0.51
1:F:96:ASP:C	1:F:97:ILE:HD12	2.31	0.51
1:B:46:THR:HG21	1:B:58:ILE:HD13	1.93	0.51
1:D:58:ILE:HG13	1:D:61:LEU:HD12	1.94	0.50
1:F:107:ARG:HA	1:F:110:ILE:HG12	1.92	0.50
1:B:97:ILE:HD12	1:B:97:ILE:N	2.26	0.50
1:F:3:ARG:O	1:F:154:LEU:HD12	2.11	0.50
1:E:4:ILE:HD12	1:F:4:ILE:HG13	1.92	0.50
1:B:15:GLU:N	1:B:15:GLU:CD	2.65	0.50
1:F:104:PRO:HG2	1:F:105:LYS:H	1.76	0.49
1:B:107:ARG:HA	1:B:110:ILE:CG1	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:ILE:HD11	1:C:2:ILE:HD13	1.93	0.49
1:D:4:ILE:HD12	1:E:4:ILE:HG13	1.94	0.49
1:E:4:ILE:HG22	1:F:94:ASN:OD1	2.13	0.49
1:E:62:PHE:CZ	1:E:80:GLU:HG2	2.48	0.49
1:D:104:PRO:HG2	1:D:105:LYS:H	1.78	0.49
1:F:97:ILE:HG13	1:F:151:ALA:HB2	1.95	0.49
1:A:136:GLU:O	1:A:137:LYS:HB2	2.12	0.48
2:A:169[C]:POP:O2	3:A:170:ACY:OXT	2.31	0.48
1:F:107:ARG:N	1:F:108:PRO:CD	2.76	0.48
1:E:3:ARG:HB2	1:E:155:LEU:HB2	1.95	0.48
1:C:73:ASP:OD1	1:F:87:GLU:OE2	2.30	0.48
1:D:15:GLU:HG2	1:D:30:THR:HB	1.95	0.48
1:F:60:LYS:O	1:F:63:PRO:HD3	2.13	0.48
1:E:83:ARG:HG2	1:E:83:ARG:HH11	1.78	0.48
1:B:57:ASP:HB3	1:C:131:LYS:HB2	1.94	0.48
1:E:71:ASN:HA	1:E:77:LEU:HD21	1.94	0.48
1:D:82:PHE:CE2	1:D:92:ILE:HD13	2.49	0.48
1:A:107:ARG:HA	1:A:110:ILE:HG12	1.94	0.48
1:C:83:ARG:NH1	1:C:83:ARG:HG2	2.28	0.48
1:F:115:ALA:O	1:F:119:GLU:HG3	2.14	0.47
1:B:85:VAL:CG1	1:B:90:TYR:HB2	2.42	0.47
1:A:107:ARG:N	1:A:108:PRO:CD	2.78	0.47
1:F:82:PHE:CE2	1:F:92:ILE:HD13	2.49	0.47
1:F:131:LYS:HZ3	1:F:131:LYS:HB3	1.79	0.47
1:F:58:ILE:HD11	1:F:77:LEU:HD13	1.96	0.47
1:A:49:ILE:HG22	1:A:85:VAL:HG21	1.97	0.47
1:D:101:ALA:O	1:D:134:THR:HG22	2.15	0.47
1:D:107:ARG:CB	1:D:108:PRO:HD3	2.45	0.47
1:A:157:ARG:HA	1:A:157:ARG:HD3	1.76	0.47
1:F:3:ARG:HB2	1:F:155:LEU:HB2	1.97	0.46
1:D:0:SER:CB	1:D:3:ARG:HD3	2.44	0.46
1:F:95:VAL:HG13	1:F:97:ILE:HD13	1.96	0.46
1:E:107:ARG:HB3	1:E:108:PRO:HD3	1.98	0.46
1:A:75:ARG:O	1:A:79:ARG:HG3	2.15	0.46
1:A:126:GLU:O	1:A:126:GLU:OE1	2.34	0.46
1:E:15:GLU:N	1:E:15:GLU:CD	2.69	0.45
2:D:169[B]:POP:O2	3:F:169:ACY:OXT	2.34	0.45
1:A:74:SER:HB2	4:A:180:HOH:O	2.15	0.45
1:F:103:ALA:HA	4:F:195:HOH:O	2.16	0.45
1:D:123:CYS:HB2	1:D:127:GLN:OE1	2.16	0.45
1:E:21:ILE:HD12	1:E:26:VAL:HG21	1.99	0.45
1:C:107:ARG:N	1:C:108:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:85:VAL:CG1	1:F:90:TYR:HB2	2.47	0.45
1:B:2:ILE:HD13	1:C:2:ILE:HD12	1.99	0.44
1:A:2:ILE:HD13	1:B:2:ILE:CD1	2.47	0.44
1:C:124:ASP:OD2	1:C:125:ILE:N	2.50	0.44
1:F:1:LEU:O	1:F:2:ILE:HD12	2.18	0.44
1:C:97:ILE:N	1:C:97:ILE:HD12	2.32	0.44
1:F:91:LYS:HE2	1:F:91:LYS:HB3	1.84	0.44
1:B:85:VAL:CG1	1:B:155:LEU:HD13	2.48	0.44
1:B:46:THR:HG21	1:B:58:ILE:CD1	2.48	0.44
1:E:4:ILE:CD1	1:F:4:ILE:HG13	2.48	0.43
1:F:29:HIS:CD2	1:F:33:ILE:HD13	2.52	0.43
1:A:51:GLY:HA2	1:B:129:ASN:ND2	2.33	0.43
1:A:107:ARG:HD2	1:A:107:ARG:N	2.32	0.43
1:F:97:ILE:HG23	1:F:149:CYS:SG	2.59	0.43
1:D:71:ASN:O	1:D:71:ASN:ND2	2.52	0.43
1:C:97:ILE:HG23	1:C:149:CYS:SG	2.59	0.43
1:C:86:GLN:NE2	1:C:90:TYR:O	2.52	0.43
1:E:3:ARG:NH1	1:E:52:ALA:O	2.51	0.43
1:A:4:ILE:HD12	1:B:4:ILE:HG13	2.01	0.42
1:D:131:LYS:HB2	1:F:57:ASP:HB3	2.00	0.42
1:D:4:ILE:HG13	1:F:4:ILE:HD12	2.00	0.42
1:E:157:ARG:HD3	1:E:157:ARG:HA	1.83	0.42
2:A:169[C]:POP:O3	3:B:169:ACY:OXT	2.37	0.42
1:F:96:ASP:O	1:F:97:ILE:HD12	2.20	0.42
2:D:169[B]:POP:O5	1:E:143:ARG:NH2	2.41	0.42
1:B:85:VAL:HG11	1:B:155:LEU:HD13	2.01	0.42
1:A:104:PRO:HG2	1:A:105:LYS:N	2.32	0.42
1:F:50:LEU:HD11	1:F:61:LEU:HD21	2.01	0.42
1:D:33:ILE:HB	4:D:184:HOH:O	2.20	0.42
1:B:2:ILE:O	1:B:2:ILE:HG23	2.20	0.42
1:D:0:SER:HB2	1:D:3:ARG:HD3	2.01	0.42
1:C:50:LEU:HD11	1:C:61:LEU:HD21	2.02	0.41
1:D:85:VAL:CG1	1:D:90:TYR:HB2	2.50	0.41
1:A:104:PRO:CG	1:A:105:LYS:H	2.29	0.41
1:A:107:ARG:NH1	1:C:57:ASP:OD2	2.53	0.41
1:D:41:ALA:HA	1:D:149:CYS:SG	2.60	0.41
2:A:169[C]:POP:O4	1:B:139:GLY:HA2	2.20	0.41
1:C:41:ALA:HA	1:C:149:CYS:SG	2.61	0.41
1:E:6:HIS:NE2	1:F:150:GLU:HG2	2.35	0.41
1:E:83:ARG:HG2	1:E:83:ARG:NH1	2.34	0.41
1:D:104:PRO:HG2	1:D:105:LYS:N	2.35	0.41
1:D:5:GLY:HA3	1:D:52:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:42:LEU:HD22	1:F:78:LEU:HD22	2.03	0.41
1:D:2:ILE:O	1:D:2:ILE:HG23	2.21	0.41
1:A:41:ALA:HA	1:A:149:CYS:SG	2.61	0.40
1:A:110:ILE:O	1:A:113:MSE:HB2	2.21	0.40
1:B:4:ILE:HD12	1:C:4:ILE:HG13	2.03	0.40
1:F:107:ARG:HB2	1:F:107:ARG:CZ	2.51	0.40
1:D:17:ARG:HD3	1:D:19:LEU:HD21	2.04	0.40
1:E:107:ARG:N	1:E:108:PRO:CD	2.83	0.40
1:A:82:PHE:CE2	1:A:92:ILE:HD13	2.56	0.40
1:A:91:LYS:HB3	1:A:158:GLN:HB3	2.03	0.40
1:B:1:LEU:CA	1:B:157:ARG:HB2	2.49	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	149/170 (88%)	142 (95%)	6 (4%)	1 (1%)	30	34
1	B	148/170 (87%)	142 (96%)	5 (3%)	1 (1%)	30	34
1	C	148/170 (87%)	144 (97%)	3 (2%)	1 (1%)	30	34
1	D	148/170 (87%)	141 (95%)	5 (3%)	2 (1%)	16	15
1	E	148/170 (87%)	141 (95%)	6 (4%)	1 (1%)	30	34
1	F	148/170 (87%)	142 (96%)	5 (3%)	1 (1%)	30	34
All	All	889/1020 (87%)	852 (96%)	30 (3%)	7 (1%)	27	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	PRO
1	C	104	PRO
1	D	104	PRO
1	E	104	PRO

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Mol	Chain	Res	Type
1	F	104	PRO
1	B	104	PRO
1	D	105	LYS

### 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	116/129 (90%)	112 (97%)	4 (3%)	49	64
1	B	115/129 (89%)	109 (95%)	6 (5%)	32	40
1	C	115/129 (89%)	113 (98%)	2 (2%)	73	86
1	D	115/129 (89%)	110 (96%)	5 (4%)	40	51
1	E	115/129 (89%)	112 (97%)	3 (3%)	59	75
1	F	115/129 (89%)	110 (96%)	5 (4%)	40	51
All	All	691/774 (89%)	666 (96%)	25 (4%)	47	61

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	40	VAL
1	A	107	ARG
1	A	126	GLU
1	B	15	GLU
1	B	16	ASP
1	B	17	ARG
1	B	71	ASN
1	B	107	ARG
1	B	119	GLU
1	C	71	ASN
1	C	86	GLN
1	D	17	ARG
1	D	35	HIS
1	D	71	ASN
1	D	107	ARG

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Mol	Chain	Res	Type
1	D	157	ARG
1	E	15	GLU
1	E	126	GLU
1	E	150	GLU
1	F	15	GLU
1	F	35	HIS
1	F	79	ARG
1	F	95	VAL
1	F	131	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	122	GLN
1	B	71	ASN
1	B	122	GLN
1	C	86	GLN
1	C	122	GLN
1	C	158	GLN
1	D	35	HIS
1	D	71	ASN
1	D	84	GLN
1	D	122	GLN
1	E	43	HIS
1	E	122	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

12 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	POP	A	169[A]	3	8,8,8	1.34	1 (12%)	13,13,13	0.69	0
2	POP	A	169[B]	3	8,8,8	1.34	1 (12%)	13,13,13	0.69	0
2	POP	A	169[C]	3	8,8,8	1.29	0	13,13,13	0.68	0
3	ACY	A	170	2	3,3,3	0.78	0	3,3,3	1.54	1 (33%)
3	ACY	B	169	2	3,3,3	0.75	0	3,3,3	1.54	1 (33%)
3	ACY	C	169	2	3,3,3	0.75	0	3,3,3	1.52	1 (33%)
2	POP	D	169[A]	1,3	8,8,8	1.27	0	13,13,13	0.69	0
2	POP	D	169[B]	3	8,8,8	1.27	0	13,13,13	0.70	0
2	POP	D	169[C]	3	8,8,8	1.27	0	13,13,13	0.68	0
3	ACY	D	170	2	3,3,3	0.72	0	3,3,3	1.50	1 (33%)
3	ACY	E	169	2	3,3,3	0.77	0	3,3,3	1.56	1 (33%)
3	ACY	F	169	2	3,3,3	0.82	0	3,3,3	1.51	1 (33%)

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	POP	A	169[A]	3	-	0/6/6/6	0/0/0/0
2	POP	A	169[B]	3	-	0/6/6/6	0/0/0/0
2	POP	A	169[C]	3	-	0/6/6/6	0/0/0/0
3	ACY	A	170	2	-	0/0/0/0	0/0/0/0
3	ACY	B	169	2	-	0/0/0/0	0/0/0/0
3	ACY	C	169	2	-	0/0/0/0	0/0/0/0
2	POP	D	169[A]	1,3	-	0/6/6/6	0/0/0/0
2	POP	D	169[B]	3	-	0/6/6/6	0/0/0/0
2	POP	D	169[C]	3	-	0/6/6/6	0/0/0/0
3	ACY	D	170	2	-	0/0/0/0	0/0/0/0
3	ACY	E	169	2	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACY	F	169	2	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	169[B]	POP	P2-O	-2.17	1.56	1.60
2	A	169[A]	POP	P2-O	-2.16	1.56	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	169	ACY	O-C-CH3	-2.16	112.66	122.06
3	B	169	ACY	O-C-CH3	-2.14	112.74	122.06
3	A	170	ACY	O-C-CH3	-2.13	112.78	122.06
3	C	169	ACY	O-C-CH3	-2.11	112.85	122.06
3	F	169	ACY	O-C-CH3	-2.08	112.96	122.06
3	D	170	ACY	O-C-CH3	-2.07	113.01	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	153/170 (90%)	0.08	3 (1%) 62 65	17, 33, 61, 68	0
1	B	152/170 (89%)	0.30	8 (5%) 25 29	18, 29, 64, 93	0
1	C	152/170 (89%)	0.21	5 (3%) 44 48	16, 31, 55, 68	0
1	D	152/170 (89%)	0.24	9 (5%) 22 25	20, 38, 65, 87	0
1	E	152/170 (89%)	0.43	15 (9%) 8 9	21, 40, 71, 87	0
1	F	152/170 (89%)	0.19	10 (6%) 18 20	20, 32, 64, 94	0
All	All	913/1020 (89%)	0.24	50 (5%) 25 27	16, 34, 64, 94	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	PHE	8.3
1	B	71	ASN	8.1
1	F	63	PRO	8.0
1	B	63	PRO	6.3
1	B	61	LEU	5.4
1	F	71	ASN	5.0
1	E	63	PRO	4.8
1	E	62	PHE	4.7
1	F	62	PHE	4.5
1	C	85	VAL	4.4
1	C	156	ILE	4.0
1	B	0	SER	4.0
1	C	2	ILE	3.9
1	F	0	SER	3.8
1	C	158	GLN	3.7
1	F	2	ILE	3.6
1	C	0	SER	3.5
1	D	2	ILE	3.4
1	E	49	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	0	SER	3.3
1	E	58	ILE	3.3
1	F	104	PRO	3.2
1	D	71	ASN	3.2
1	E	106	MSE	3.1
1	E	125	ILE	3.0
1	D	62	PHE	3.0
1	D	63	PRO	3.0
1	E	71	ASN	3.0
1	D	61	LEU	2.9
1	D	158	GLN	2.9
1	E	126	GLU	2.8
1	A	61	LEU	2.7
1	D	107	ARG	2.7
1	F	106	MSE	2.6
1	E	4	ILE	2.5
1	A	72	ALA	2.5
1	B	72	ALA	2.4
1	F	107	ARG	2.4
1	A	104	PRO	2.3
1	E	0	SER	2.3
1	D	156	ILE	2.3
1	E	156	ILE	2.3
1	E	57	ASP	2.2
1	B	35	HIS	2.2
1	E	61	LEU	2.1
1	F	156	ILE	2.1
1	F	105	LYS	2.0
1	E	154	LEU	2.0
1	B	107	ARG	2.0
1	E	105	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACY	A	170	4/4	0.28	16.69	28,31,32,33	4
3	ACY	E	169	4/4	0.30	10.86	31,32,34,35	4
3	ACY	B	169	4/4	0.28	8.65	25,27,28,28	4
3	ACY	D	170	4/4	0.22	7.29	24,25,26,26	4
3	ACY	F	169	4/4	0.25	5.16	23,25,25,26	4
3	ACY	C	169	4/4	0.18	4.81	22,23,23,24	4
2	POP	D	169[B]	9/9	0.13	0.20	21,22,24,25	9
2	POP	D	169[A]	9/9	0.13	0.06	19,20,22,23	9
2	POP	D	169[C]	9/9	0.13	0.06	26,27,29,30	9
2	POP	A	169[B]	9/9	0.12	-0.97	11,13,15,15	9
2	POP	A	169[C]	9/9	0.12	-0.98	21,22,23,24	9
2	POP	A	169[A]	9/9	0.12	-1.04	16,19,21,21	9

## 6.5 Other polymers ⓘ

There are no such residues in this entry.