



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:51 pm GMT

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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

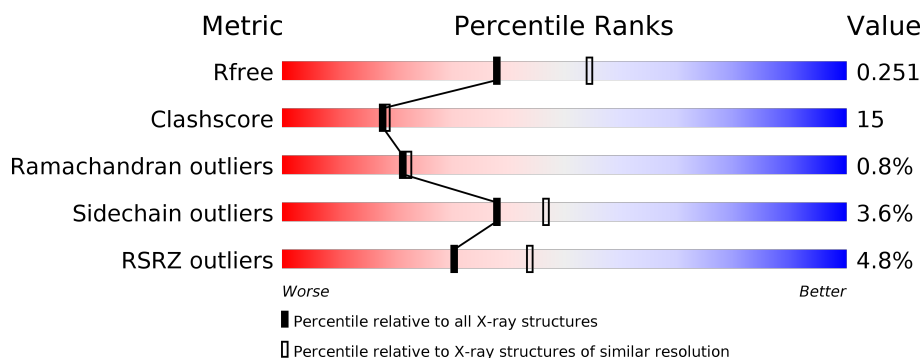
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	111664	1015 (2.36-2.36)
Clashscore	122126	1081 (2.36-2.36)
Ramachandran outliers	120053	1066 (2.36-2.36)
Sidechain outliers	120020	1067 (2.36-2.36)
RSRZ outliers	108989	1002 (2.36-2.36)

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	170	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	170	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	170	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	170	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>24%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	170	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	F	170	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>25%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7183 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 2-C-methyl-D-erythritol 2,4-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

*Continued on next page...*

*Continued from previous page...*

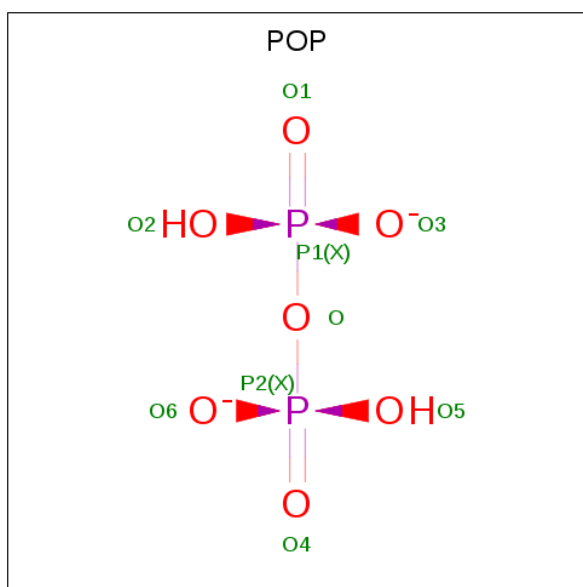
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	cloning artifact	UNP P44815
B	1	LEU	-	cloning artifact	UNP P44815
B	67	MSE	MET	modified residue	UNP P44815
B	106	MSE	MET	modified residue	UNP P44815
B	113	MSE	MET	modified residue	UNP P44815
B	159	GLU	-	cloning artifact	UNP P44815
B	160	GLY	-	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

*Continued on next page...*

*Continued from previous page...*

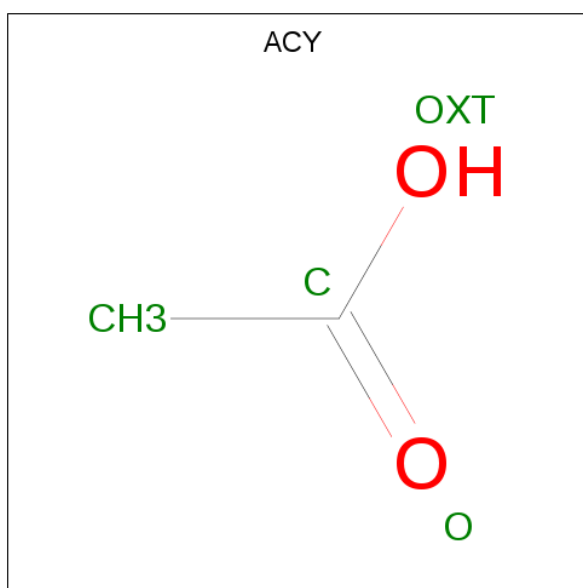
Chain	Residue	Modelled	Actual	Comment	Reference
D	164	HIS	-	cloning artifact	UNP P44815
D	165	HIS	-	cloning artifact	UNP P44815
D	166	HIS	-	cloning artifact	UNP P44815
D	167	HIS	-	cloning artifact	UNP P44815
D	168	HIS	-	cloning artifact	UNP P44815
E	-1	MSE	-	cloning artifact	UNP P44815
E	0	SER	-	cloning 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		

*Continued on next page...*

*Continued from previous page...*

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

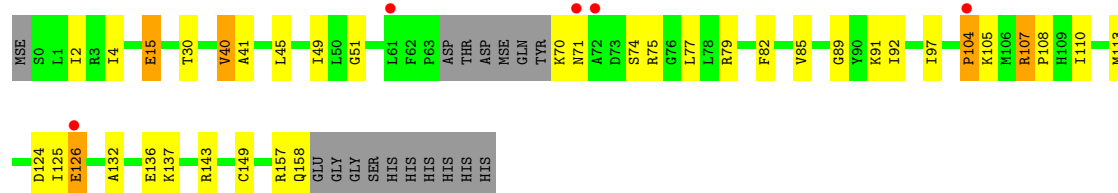
- Molecule 4 is water.

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

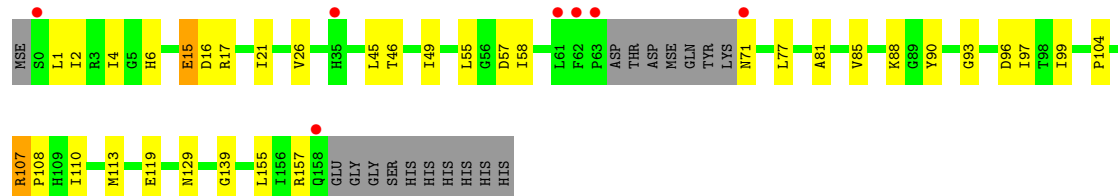
### 3 Residue-property plots [i](#)

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.

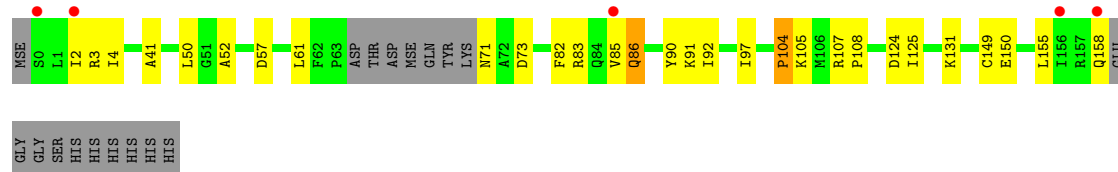
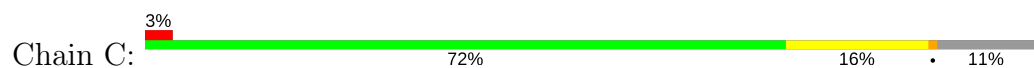
#### • Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



#### • Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



#### • Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



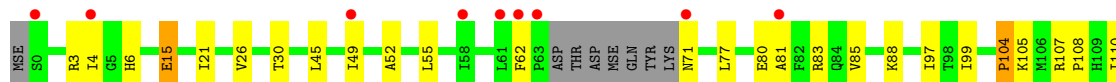
#### • Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



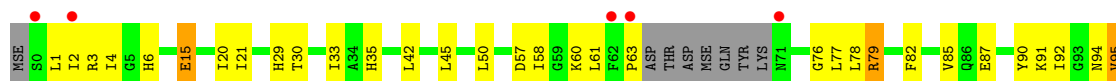




- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



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



## 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) 99.2 (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 4.0	Depositor
R, $R_{free}$	0.240 , 0.280 0.207 , 0.251	Depositor DCC
$R_{free}$ test set	2208 reflections (5.08%)	wwPDB-VP
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> )	0.33 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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 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	1155	0	1160	42	0
1	B	1146	0	1147	34	0
1	C	1146	0	1147	30	0
1	D	1145	0	1145	35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 15.

All (196) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:A:104:PRO:HG2	1:A:105:LYS:H	1.66	0.61
1:E:55:LEU:HD21	1:E:88:LYS:HD2	1.80	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:D:150:GLU:HG2	1:F:6:HIS:CE1	2.38	0.58
1:E:107:ARG:HA	1:E:110:ILE:HG12	1.85	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:HD11	1:B:77:LEU:HD13	1.85	0.58
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:C:3:ARG:HD2	1:C:52:ALA:O	2.08	0.54
1:F:76:GLY:HA2	1:F:79:ARG:HH12	1.72	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:A:4:ILE:HG13	1:C:4:ILE:HD12	1.89	0.53
1:D:45:LEU:HD22	1:D:97:ILE:HD11	1.91	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:B:55:LEU:HD21	1:B:88:LYS:HD2	1.92	0.52
1:E:136:GLU:O	1:E:137:LYS:HB2	2.09	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:B:46:THR:HG21	1:B:58:ILE:HD13	1.93	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:97:ILE:N	1:B:97:ILE:HD12	2.26	0.50
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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:PRO:HG2	1:F:105:LYS:H	1.76	0.49
1:A:2:ILE:HD11	1:C:2:ILE:HD13	1.93	0.49
1:B:107:ARG:HA	1:B:110:ILE:CG1	2.43	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:D:15:GLU:HG2	1:D:30:THR:HB	1.95	0.48
1:E:3:ARG:HB2	1:E:155:LEU:HB2	1.95	0.48
1:F:107:ARG:N	1:F:108:PRO:CD	2.76	0.48
1:C:73:ASP:OD1	1:F:87:GLU:OE2	2.30	0.48
1:E:83:ARG:HG2	1:E:83:ARG:HH11	1.78	0.48
1:F:60:LYS:O	1:F:63:PRO:HD3	2.13	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:131:LYS:HZ3	1:F:131:LYS:HB3	1.79	0.47
1:F:82:PHE:CE2	1:F:92:ILE:HD13	2.49	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:A:75:ARG:O	1:A:79:ARG:HG3	2.15	0.46
1:E:107:ARG:HB3	1:E:108:PRO:HD3	1.98	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
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
2:D:169[B]:POP:O2	3:F:169:ACY:OXT	2.34	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:CYS:HB2	1:D:127:GLN:OE1	2.16	0.45
1:C:107:ARG:N	1:C:108:PRO:CD	2.80	0.45
1:E:21:ILE:HD12	1:E:26:VAL:HG21	1.99	0.45
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:C:97:ILE:N	1:C:97:ILE:HD12	2.32	0.44
1:F:1:LEU:O	1:F:2:ILE:HD12	2.18	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:A:51:GLY:HA2	1:B:129:ASN:ND2	2.33	0.43
1:F:29:HIS:CD2	1:F:33:ILE:HD13	2.52	0.43
1:A:107:ARG:HD2	1:A:107:ARG:N	2.32	0.43
1:D:71:ASN:O	1:D:71:ASN:ND2	2.52	0.43
1:F:97:ILE:HG23	1:F:149:CYS:SG	2.59	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:E:157:ARG:HD3	1:E:157:ARG:HA	1.83	0.42
1:D:4:ILE:HG13	1:F:4:ILE:HD12	2.00	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
1:A:104:PRO:HG2	1:A:105:LYS:N	2.32	0.42
1:B:85:VAL:HG11	1:B:155:LEU:HD13	2.01	0.42
2:D:169[B]:POP:O5	1:E:143:ARG:NH2	2.41	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:A:104:PRO:CG	1:A:105:LYS:H	2.29	0.41
1:D:85:VAL:CG1	1:D:90:TYR:HB2	2.50	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

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2:ILE:O	1:D:2:ILE:HG23	2.21	0.41
1:D:5:GLY:HA3	1:D:52:ALA:HB2	2.02	0.41
1:F:42:LEU:HD22	1:F:78:LEU:HD22	2.03	0.41
1:D:104:PRO:HG2	1:D:105:LYS:N	2.35	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:D:17:ARG:HD3	1:D:19:LEU:HD21	2.04	0.40
1:F:107:ARG:HB2	1:F:107:ARG:CZ	2.51	0.40
1:A:82:PHE:CE2	1:A:92:ILE:HD13	2.56	0.40
1:E:107:ARG:N	1:E:108:PRO:CD	2.83	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%)	24	25
1	B	148/170 (87%)	142 (96%)	5 (3%)	1 (1%)	24	25
1	C	148/170 (87%)	144 (97%)	3 (2%)	1 (1%)	24	25
1	D	148/170 (87%)	141 (95%)	5 (3%)	2 (1%)	12	10
1	E	148/170 (87%)	141 (95%)	6 (4%)	1 (1%)	24	25
1	F	148/170 (87%)	142 (96%)	5 (3%)	1 (1%)	24	25
All	All	889/1020 (87%)	852 (96%)	30 (3%)	7 (1%)	21	22

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
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%)	40	49
1	B	115/129 (89%)	109 (95%)	6 (5%)	25	29
1	C	115/129 (89%)	113 (98%)	2 (2%)	63	75
1	D	115/129 (89%)	110 (96%)	5 (4%)	32	38
1	E	115/129 (89%)	112 (97%)	3 (3%)	49	59
1	F	115/129 (89%)	110 (96%)	5 (4%)	32	38
All	All	691/774 (89%)	666 (96%)	25 (4%)	38	47

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	17	ARG
1	D	35	HIS
1	D	71	ASN
1	D	107	ARG
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 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	1.51	2 (25%)	9,13,13	0.79	0
2	POP	A	169[B]	3	8,8,8	1.50	2 (25%)	9,13,13	0.81	0
2	POP	A	169[C]	3	8,8,8	1.42	1 (12%)	9,13,13	0.77	0
3	ACY	A	170	2	1,3,3	1.11	0	0,3,3	0.00	-
3	ACY	B	169	2	1,3,3	1.32	0	0,3,3	0.00	-
3	ACY	C	169	2	1,3,3	1.24	0	0,3,3	0.00	-
2	POP	D	169[A]	1,3	8,8,8	1.46	2 (25%)	9,13,13	0.77	0
2	POP	D	169[B]	3	8,8,8	1.46	1 (12%)	9,13,13	0.80	0
2	POP	D	169[C]	3	8,8,8	1.44	1 (12%)	9,13,13	0.79	0
3	ACY	D	170	2	1,3,3	1.23	0	0,3,3	0.00	-
3	ACY	E	169	2	1,3,3	1.31	0	0,3,3	0.00	-
3	ACY	F	169	2	1,3,3	1.43	0	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	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

*Continued on next page...*

*Continued from previous page...*

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	169[B]	POP	P2-O	-2.55	1.56	1.60
2	A	169[A]	POP	P2-O	-2.53	1.56	1.60
2	A	169[C]	POP	P2-O	-2.29	1.56	1.60
2	D	169[A]	POP	P2-O	-2.02	1.57	1.60
2	A	169[B]	POP	P1-O	2.06	1.63	1.60
2	A	169[A]	POP	P1-O	2.18	1.63	1.60
2	D	169[C]	POP	P1-O	2.45	1.63	1.60
2	D	169[A]	POP	P1-O	2.46	1.63	1.60
2	D	169[B]	POP	P1-O	2.54	1.63	1.60

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	169[A]	POP	1	0
2	A	169[C]	POP	3	0
3	A	170	ACY	1	0
3	B	169	ACY	1	0
2	D	169[B]	POP	2	0
3	F	169	ACY	1	0

## 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	151/170 (88%)	0.09	5 (3%)	46	60	17, 33, 58, 68	0
1	B	150/170 (88%)	0.27	7 (4%)	31	44	18, 29, 63, 93	0
1	C	150/170 (88%)	0.11	5 (3%)	46	60	16, 31, 55, 64	0
1	D	150/170 (88%)	0.22	9 (6%)	22	33	20, 38, 65, 87	0
1	E	150/170 (88%)	0.39	11 (7%)	15	23	21, 40, 68, 87	0
1	F	150/170 (88%)	0.13	6 (4%)	38	52	20, 32, 64, 94	0
All	All	901/1020 (88%)	0.20	43 (4%)	30	44	16, 34, 62, 94	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	PHE	8.4
1	F	63	PRO	7.6
1	B	71	ASN	7.2
1	B	63	PRO	6.6
1	E	62	PHE	6.0
1	F	71	ASN	5.9
1	F	62	PHE	5.3
1	B	61	LEU	5.3
1	E	63	PRO	4.6
1	C	85	VAL	4.4
1	C	158	GLN	4.1
1	D	71	ASN	4.1
1	E	58	ILE	4.0
1	D	62	PHE	4.0
1	E	71	ASN	3.7
1	F	0	SER	3.6
1	D	63	PRO	3.5
1	D	158	GLN	3.5
1	A	72	ALA	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	0	SER	3.2
1	E	49	ILE	3.2
1	D	0	SER	3.1
1	D	61	LEU	3.1
1	C	156	ILE	3.0
1	C	0	SER	3.0
1	C	2	ILE	3.0
1	A	61	LEU	2.8
1	F	104	PRO	2.8
1	E	61	LEU	2.7
1	E	81	ALA	2.7
1	F	2	ILE	2.5
1	D	72	ALA	2.4
1	D	2	ILE	2.4
1	E	0	SER	2.4
1	E	125	ILE	2.4
1	A	71	ASN	2.4
1	B	35	HIS	2.4
1	D	107	ARG	2.3
1	A	104	PRO	2.3
1	E	158	GLN	2.2
1	A	126	GLU	2.1
1	E	4	ILE	2.0
1	B	158	GLN	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACY	E	169	4/4	0.72	0.34	31,32,34,35	4
3	ACY	F	169	4/4	0.77	0.25	23,25,25,26	4
3	ACY	B	169	4/4	0.77	0.31	25,27,28,28	4
3	ACY	D	170	4/4	0.78	0.24	24,25,26,26	4
3	ACY	A	170	4/4	0.86	0.28	28,31,32,33	4
3	ACY	C	169	4/4	0.92	0.19	22,23,23,24	4
2	POP	D	169[B]	9/9	0.98	0.14	21,22,24,25	9
2	POP	D	169[A]	9/9	0.98	0.14	19,20,22,23	9
2	POP	D	169[C]	9/9	0.98	0.14	26,27,29,30	9
2	POP	A	169[C]	9/9	0.99	0.13	21,22,23,24	9
2	POP	A	169[B]	9/9	0.99	0.13	11,13,15,15	9
2	POP	A	169[A]	9/9	0.99	0.13	16,19,21,21	9

## 6.5 Other polymers [i](#)

There are no such residues in this entry.