



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:33 AM GMT

PDB ID : 2HG4  
Title : Structure of the ketosynthase-acyltransferase didomain of module 5 from DEBS.  
Authors : Tang, Y.; Kim, C.Y.; Mathews, I.I.; Cane, D.E.; Khosla, C.  
Deposited on : 2006-06-26  
Resolution : 2.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

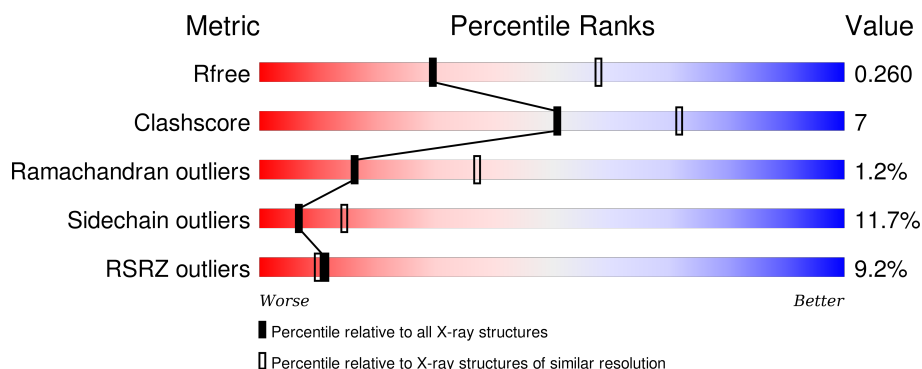
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	917	
1	B	917	
1	C	917	
1	D	917	
1	E	917	

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Mol	Chain	Length	Quality of chain
1	F	917	

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	ACT	B	950	-	-	X	-
2	ACT	C	950	-	-	X	-
3	SO4	C	975	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 39402 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 6-Deoxyerythronolide B Synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	882	Total	C	N	O	S	Se	0	0	0
			6520	4046	1204	1247	8	15			
1	B	882	Total	C	N	O	S	Se	0	0	0
			6534	4054	1208	1249	8	15			
1	C	882	Total	C	N	O	S	Se	0	0	0
			6520	4046	1204	1247	8	15			
1	D	884	Total	C	N	O	S	Se	0	0	0
			6550	4064	1210	1252	8	16			
1	E	877	Total	C	N	O	S	Se	0	0	0
			6474	4016	1196	1239	8	15			
1	F	874	Total	C	N	O	S	Se	0	0	0
			6440	3995	1189	1233	8	15			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	210	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	229	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	385	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	525	GLU	ASP	CONFLICT	UNP Q5UNP4
A	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
A	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	732	ALA	GLY	CONFLICT	UNP Q5UNP4
A	733	HIS	ILE	CONFLICT	UNP Q5UNP4
A	734	LYS	THR	CONFLICT	UNP Q5UNP4
A	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	210	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	229	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	385	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	525	GLU	ASP	CONFLICT	UNP Q5UNP4
B	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
B	732	ALA	GLY	CONFLICT	UNP Q5UNP4
B	733	HIS	ILE	CONFLICT	UNP Q5UNP4
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B	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	210	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
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C	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	525	GLU	ASP	CONFLICT	UNP Q5UNP4
C	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
C	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4

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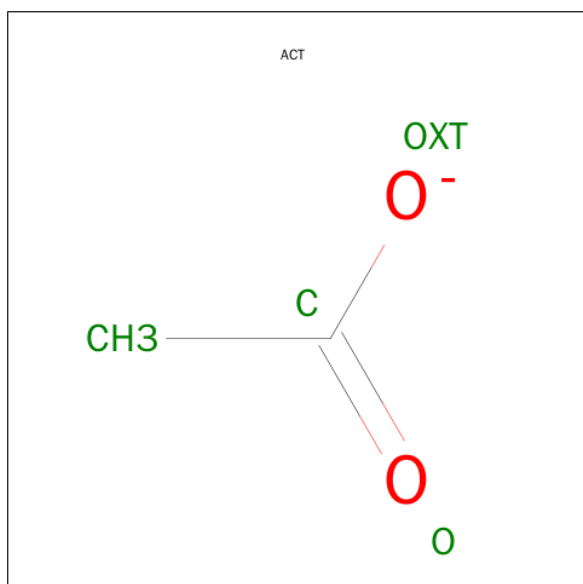
Chain	Residue	Modelled	Actual	Comment	Reference
C	732	ALA	GLY	CONFLICT	UNP Q5UNP4
C	733	HIS	ILE	CONFLICT	UNP Q5UNP4
C	734	LYS	THR	CONFLICT	UNP Q5UNP4
C	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	210	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
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D	385	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	525	GLU	ASP	CONFLICT	UNP Q5UNP4
D	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
D	732	ALA	GLY	CONFLICT	UNP Q5UNP4
D	733	HIS	ILE	CONFLICT	UNP Q5UNP4
D	734	LYS	THR	CONFLICT	UNP Q5UNP4
D	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	120	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	193	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
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E	229	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	385	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	525	GLU	ASP	CONFLICT	UNP Q5UNP4
E	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
E	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4

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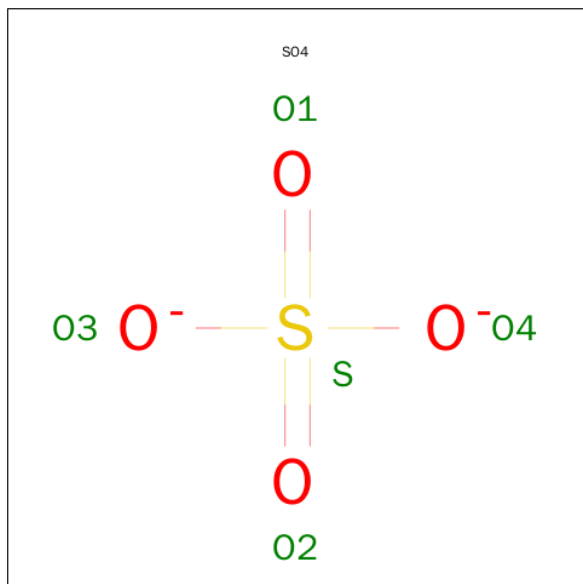
Chain	Residue	Modelled	Actual	Comment	Reference
E	732	ALA	GLY	CONFLICT	UNP Q5UNP4
E	733	HIS	ILE	CONFLICT	UNP Q5UNP4
E	734	LYS	THR	CONFLICT	UNP Q5UNP4
E	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	7	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	46	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	91	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	113	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
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F	396	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	480	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	525	GLU	ASP	CONFLICT	UNP Q5UNP4
F	555	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	567	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	621	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	680	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4
F	732	ALA	GLY	CONFLICT	UNP Q5UNP4
F	733	HIS	ILE	CONFLICT	UNP Q5UNP4
F	734	LYS	THR	CONFLICT	UNP Q5UNP4
F	786	MSE	MET	MODIFIED RESIDUE	UNP Q5UNP4

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

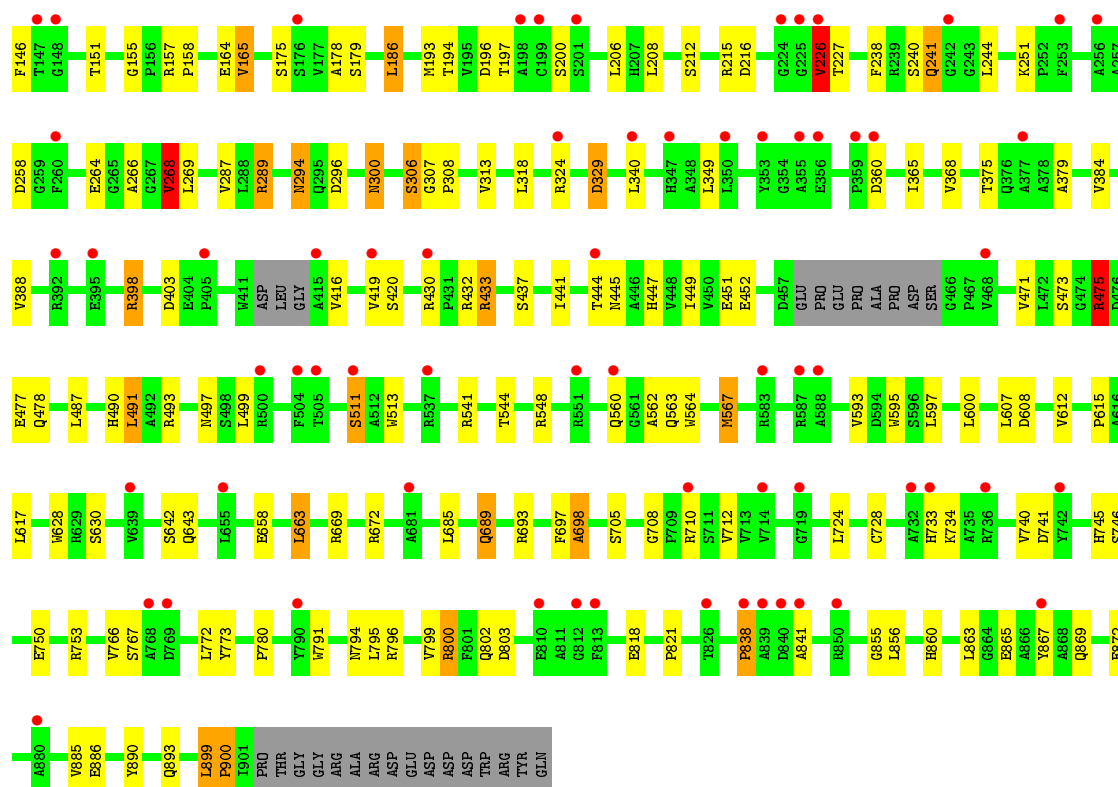


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0

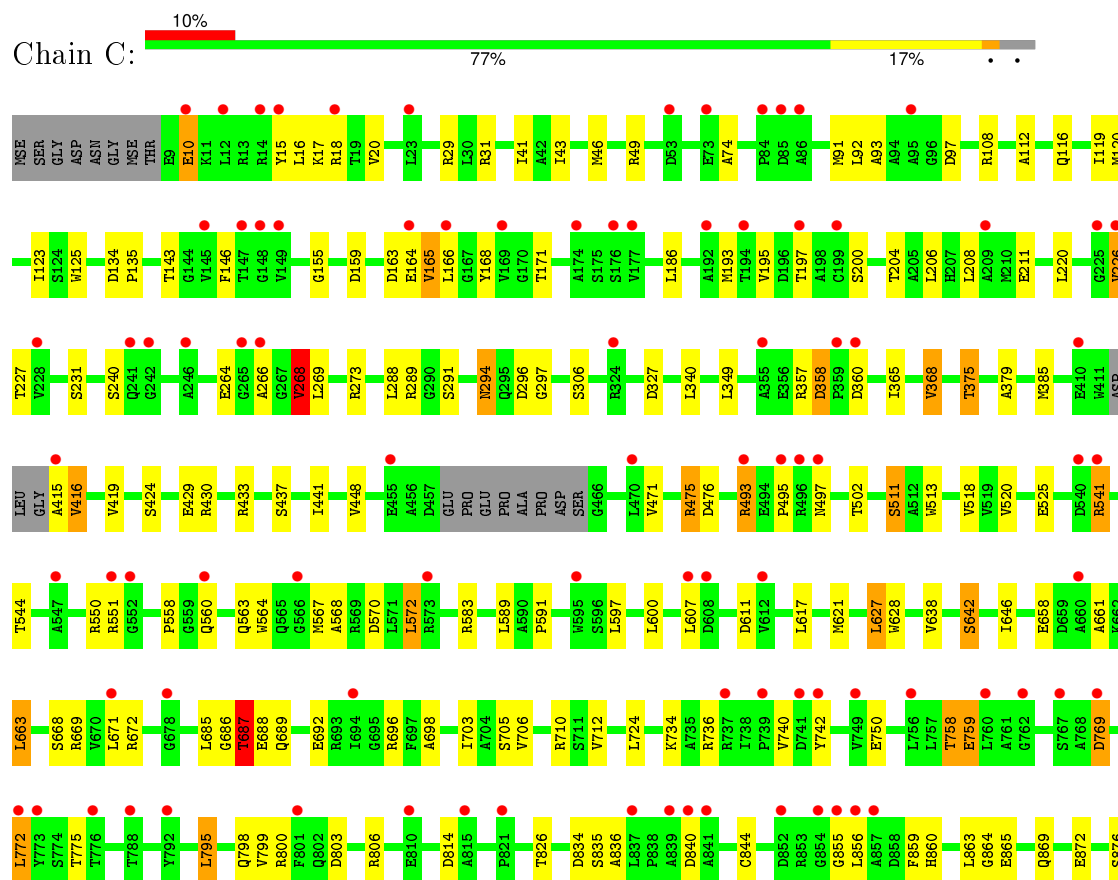
- Molecule 5 is water.

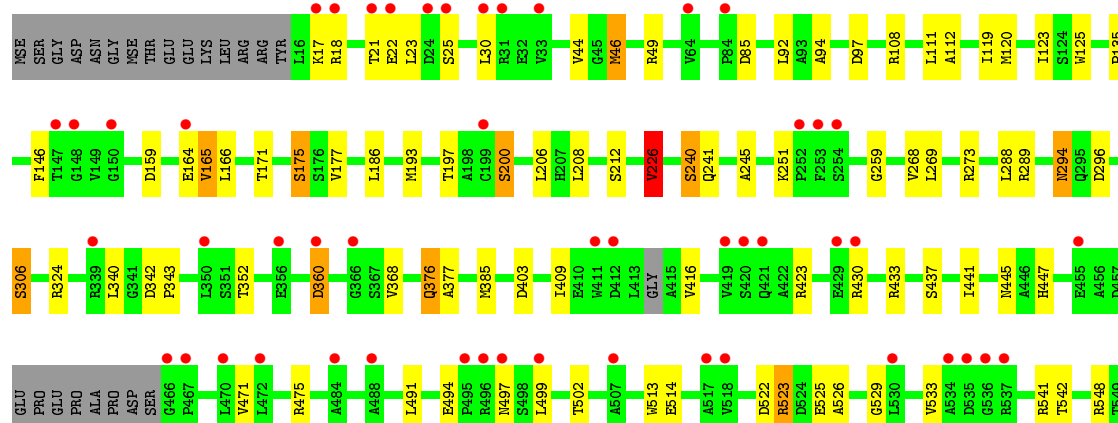
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total 74	O 74	0	0
5	B	57	Total 57	O 57	0	0
5	C	42	Total 42	O 42	0	0
5	D	50	Total 50	O 50	0	0
5	E	49	Total 49	O 49	0	0
5	F	38	Total 38	O 38	0	0

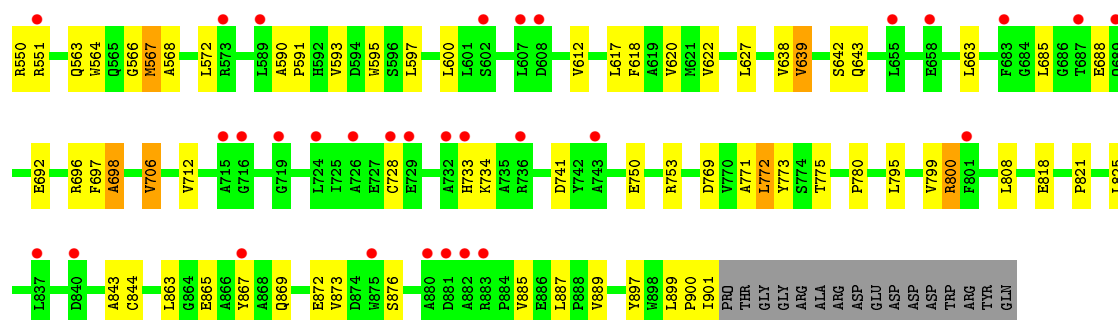




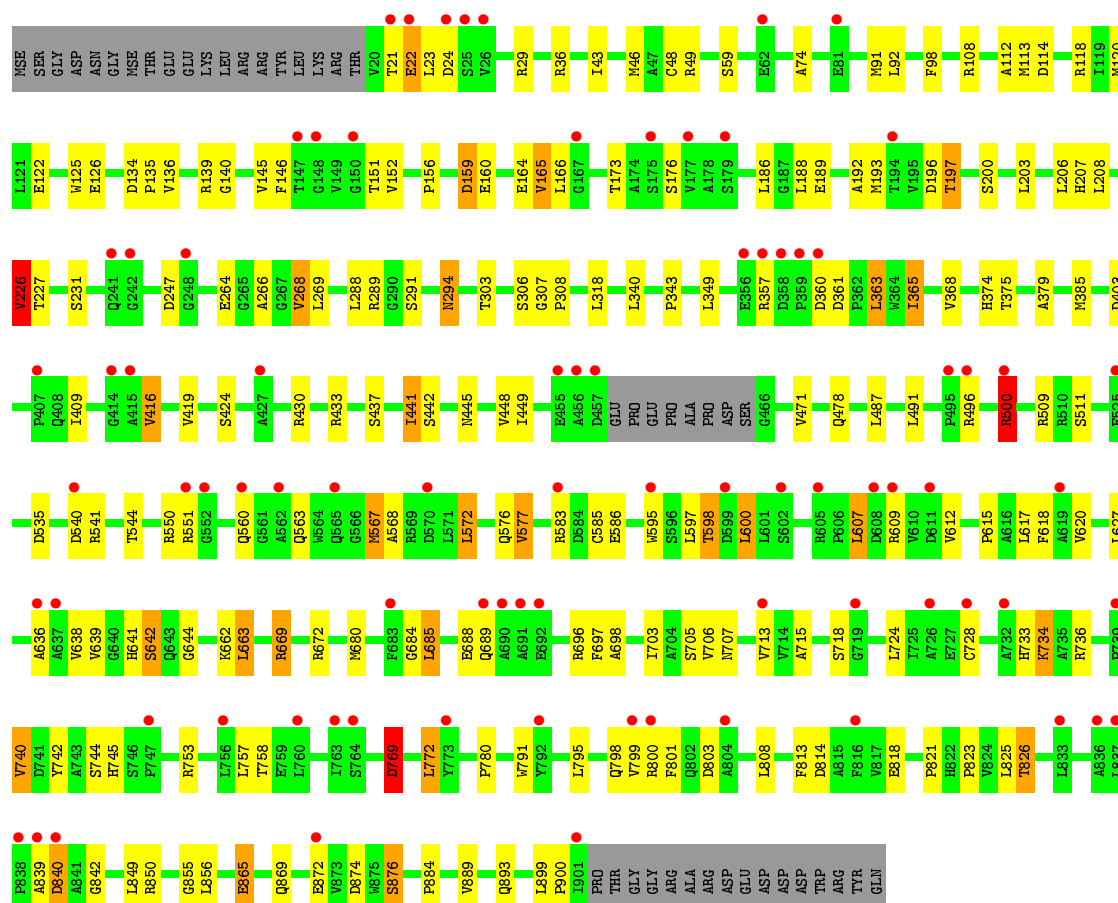
• Molecule 1: 6-Deoxyerythronolide B Synthase







• Molecule 1: 6-Deoxyerythronolide B Synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	305.26Å 150.15Å 184.38Å 90.00° 110.03° 90.00°	Depositor
Resolution (Å)	48.03 – 2.73 48.17 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.03-2.73) 99.8 (48.17-2.73)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.216 , 0.255 0.222 , 0.260	Depositor DCC
$R_{free}$ test set	10395 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 65.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 206602 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	39402	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.93% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, ACT

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	0.71	1/6634 (0.0%)	0.79	7/8999 (0.1%)
1	B	0.63	1/6648 (0.0%)	0.76	5/9015 (0.1%)
1	C	0.64	1/6634 (0.0%)	0.74	2/8999 (0.0%)
1	D	0.60	0/6663	0.73	5/9034 (0.1%)
1	E	0.58	0/6587	0.71	1/8936 (0.0%)
1	F	0.66	2/6554 (0.0%)	0.77	5/8894 (0.1%)
All	All	0.64	5/39720 (0.0%)	0.75	25/53877 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
1	C	0	3
1	F	0	2
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	872	GLU	CG-CD	7.16	1.62	1.51
1	B	48	CYS	CB-SG	-5.58	1.72	1.81
1	C	211	GLU	CG-CD	5.11	1.59	1.51
1	F	585	CYS	CB-SG	-5.11	1.73	1.81
1	A	585	CYS	CB-SG	-5.10	1.73	1.81

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	475	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	D	475	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	F	226	VAL	CB-CA-C	-7.03	98.05	111.40
1	A	226	VAL	CB-CA-C	-6.84	98.40	111.40
1	A	475	ARG	NE-CZ-NH1	6.65	123.62	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	GLY	Peptide
1	A	840	ASP	Peptide
1	A	841	ALA	Peptide
1	A	842	GLY	Peptide
1	B	155	GLY	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6520	0	6359	84	0
1	B	6534	0	6385	100	0
1	C	6520	0	6359	97	0
1	D	6550	0	6396	91	0
1	E	6474	0	6316	75	0
1	F	6440	0	6274	97	0
2	A	4	0	3	0	0
2	B	4	0	3	2	0
2	C	4	0	3	4	0
2	D	4	0	3	1	0
2	E	4	0	3	1	0
2	F	4	0	3	1	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	74	0	0	3	0
5	B	57	0	0	1	0
5	C	42	0	0	5	0
5	D	50	0	0	1	0
5	E	49	0	0	3	0
5	F	38	0	0	1	0
All	All	39402	0	38107	533	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 7.

The worst 5 of 533 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:SER:OG	2:B:950:ACT:O	1.71	1.06
1:F:207:HIS:HD1	1:F:291:SER:HG	1.16	0.94
1:D:617:LEU:HD22	1:D:621:MSE:HE3	1.53	0.91
1:C:193:MSE:HE3	1:C:208:LEU:HD13	1.56	0.86
1:E:564:TRP:O	1:E:567:MSE:HG3	1.78	0.84

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	876/917 (96%)	823 (94%)	43 (5%)	10 (1%)	17 40
1	B	876/917 (96%)	813 (93%)	55 (6%)	8 (1%)	21 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	876/917 (96%)	796 (91%)	69 (8%)	11 (1%)	15	35
1	D	876/917 (96%)	808 (92%)	58 (7%)	10 (1%)	17	40
1	E	871/917 (95%)	795 (91%)	65 (8%)	11 (1%)	15	35
1	F	870/917 (95%)	795 (91%)	61 (7%)	14 (2%)	12	28
All	All	5245/5502 (95%)	4830 (92%)	351 (7%)	64 (1%)	16	37

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	ASP
1	A	567	MSE
1	B	403	ASP
1	B	698	ALA
1	C	687	THR

### 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	647/668 (97%)	558 (86%)	89 (14%)	4	9
1	B	650/668 (97%)	581 (89%)	69 (11%)	8	18
1	C	647/668 (97%)	571 (88%)	76 (12%)	7	14
1	D	652/668 (98%)	572 (88%)	80 (12%)	6	13
1	E	643/668 (96%)	579 (90%)	64 (10%)	9	21
1	F	638/668 (96%)	561 (88%)	77 (12%)	6	13
All	All	3877/4008 (97%)	3422 (88%)	455 (12%)	7	14

5 of 455 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	607	LEU
1	D	294	ASN

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Mol	Chain	Res	Type
1	F	563	GLN
1	C	687	THR
1	C	889	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	320	ASN
1	C	560	GLN
1	F	334	HIS
1	C	334	HIS
1	C	478	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	ACT	A	950	-	1,3,3	0.91	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	975	-	4,4,4	0.22	0	6,6,6	0.21	0
2	ACT	B	950	-	1,3,3	1.11	0	0,3,3	0.00	-
3	SO4	B	975	-	4,4,4	0.21	0	6,6,6	0.35	0
2	ACT	C	950	-	1,3,3	1.15	0	0,3,3	0.00	-
3	SO4	C	975	-	4,4,4	0.17	0	6,6,6	0.21	0
2	ACT	D	950	-	1,3,3	1.65	0	0,3,3	0.00	-
2	ACT	E	950	-	1,3,3	0.46	0	0,3,3	0.00	-
3	SO4	E	975	-	4,4,4	0.21	0	6,6,6	0.14	0
2	ACT	F	950	-	1,3,3	1.52	0	0,3,3	0.00	-
3	SO4	F	975	-	4,4,4	0.16	0	6,6,6	0.34	0

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	ACT	A	950	-	-	0/0/0/0	0/0/0/0
3	SO4	A	975	-	-	0/0/0/0	0/0/0/0
2	ACT	B	950	-	-	0/0/0/0	0/0/0/0
3	SO4	B	975	-	-	0/0/0/0	0/0/0/0
2	ACT	C	950	-	-	0/0/0/0	0/0/0/0
3	SO4	C	975	-	-	0/0/0/0	0/0/0/0
2	ACT	D	950	-	-	0/0/0/0	0/0/0/0
2	ACT	E	950	-	-	0/0/0/0	0/0/0/0
3	SO4	E	975	-	-	0/0/0/0	0/0/0/0
2	ACT	F	950	-	-	0/0/0/0	0/0/0/0
3	SO4	F	975	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	950	ACT	2	0
3	B	975	SO4	1	0
2	C	950	ACT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	950	ACT	1	0
2	E	950	ACT	1	0
3	E	975	SO4	1	0
2	F	950	ACT	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	867/917 (94%)	0.58	61 (7%) 19 18	34, 67, 80, 94	0
1	B	867/917 (94%)	0.70	72 (8%) 14 12	46, 67, 80, 93	0
1	C	867/917 (94%)	0.76	92 (10%) 8 6	47, 67, 80, 93	0
1	D	868/917 (94%)	0.74	90 (10%) 8 7	48, 67, 80, 93	0
1	E	862/917 (94%)	0.71	81 (9%) 11 9	48, 67, 81, 93	0
1	F	859/917 (93%)	0.70	82 (9%) 10 9	48, 67, 80, 93	0
All	All	5190/5502 (94%)	0.70	478 (9%) 11 10	34, 67, 80, 94	0

The worst 5 of 478 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	732	ALA	8.2
1	C	496	ARG	7.1
1	B	840	ASP	6.9
1	C	551	ARG	6.8
1	D	551	ARG	6.5

### 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
3	SO4	B	975	5/5	0.85	0.36	1.80	109,109,109,109	0
3	SO4	F	975	5/5	0.94	0.34	0.77	82,82,83,83	0
3	SO4	C	975	5/5	0.75	0.41	0.20	84,84,85,86	5
3	SO4	E	975	5/5	0.76	0.30	-0.43	101,101,102,102	5
2	ACT	F	950	4/4	0.91	0.18	-0.89	44,44,45,45	0
2	ACT	C	950	4/4	0.96	0.15	-1.14	54,54,54,54	0
2	ACT	B	950	4/4	0.94	0.12	-1.14	50,50,50,50	0
2	ACT	D	950	4/4	0.92	0.17	-1.25	61,61,61,62	0
2	ACT	A	950	4/4	0.94	0.10	-1.93	51,51,51,51	0
2	ACT	E	950	4/4	0.96	0.11	-3.34	47,48,48,48	0
4	CL	C	976	1/1	0.85	0.23	-	82,82,82,82	0
4	CL	E	976	1/1	0.82	0.17	-	70,70,70,70	0
4	CL	F	976	1/1	0.76	0.25	-	76,76,76,76	0
4	CL	D	951	1/1	0.96	0.13	-	90,90,90,90	0
4	CL	B	976	1/1	0.88	0.13	-	57,57,57,57	0
3	SO4	A	975	5/5	0.91	0.30	-	87,87,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.