



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:37 PM GMT

PDB ID : 1RM6  
Title : Structure of 4-hydroxybenzoyl-CoA reductase from *Thauera aromatica*  
Authors : Unciuleac, M.; Warkentin, E.; Page, C.C.; Dutton, P.L.; Boll, M.; Ermler, U.  
Deposited on : 2003-11-27  
Resolution : 1.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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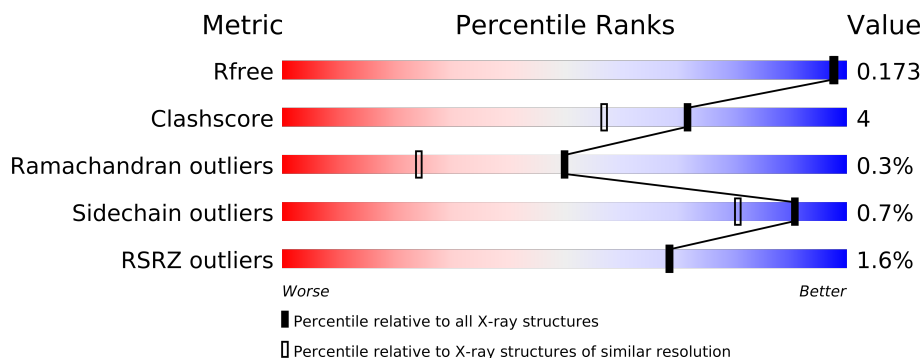
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.60 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	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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	769	
1	D	769	
2	B	324	
2	E	324	
3	C	161	
3	F	161	

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

Mol	Type	Chain	Res	Geometry	Electron density
12	EPE	A	932	-	X
12	EPE	A	933	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	CL	A	770	-	X
4	CL	D	770	-	X
7	SO4	D	773	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21258 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 4-hydroxybenzoyl-CoA reductase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	17	0
			5794	3667	993	1103	31			
1	D	760	Total	C	N	O	S	0	18	0
			5782	3660	994	1098	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ALA	GLY	SEE REMARK 999	UNP O33819
D	251	ALA	GLY	SEE REMARK 999	UNP O33819

- Molecule 2 is a protein called 4-hydroxybenzoyl-CoA reductase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	323	Total	C	N	O	S	0	9	0
			2438	1528	444	458	8			
2	E	323	Total	C	N	O	S	0	6	0
			2427	1521	446	452	8			

- Molecule 3 is a protein called 4-hydroxybenzoyl-CoA reductase gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	157	Total	C	N	O	S	0	4	0
			1186	729	219	225	13			
3	F	157	Total	C	N	O	S	0	3	0
			1177	725	215	224	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	142	LYS	ARG	SEE REMARK 999	UNP O33818
C	143	ILE	SER	SEE REMARK 999	UNP O33818

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Chain	Residue	Modelled	Actual	Comment	Reference
C	144	ILE	SER	SEE REMARK 999	UNP O33818
F	142	LYS	ARG	SEE REMARK 999	UNP O33818
F	143	ILE	SER	SEE REMARK 999	UNP O33818
F	144	ILE	SER	SEE REMARK 999	UNP O33818

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

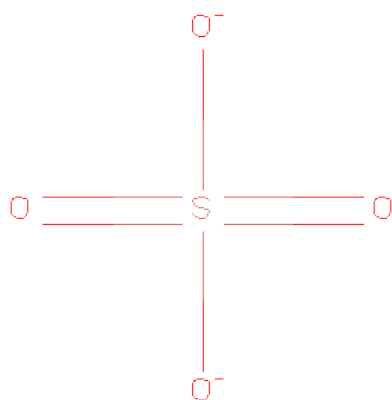
- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total K 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

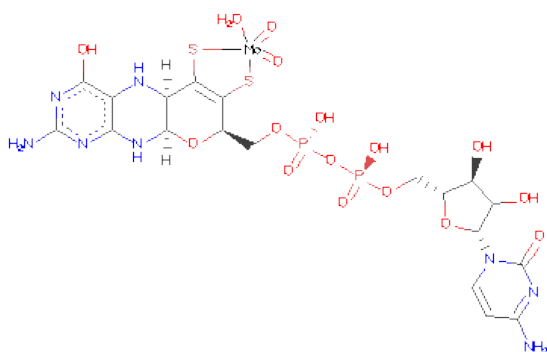
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	D	1	Total Na 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



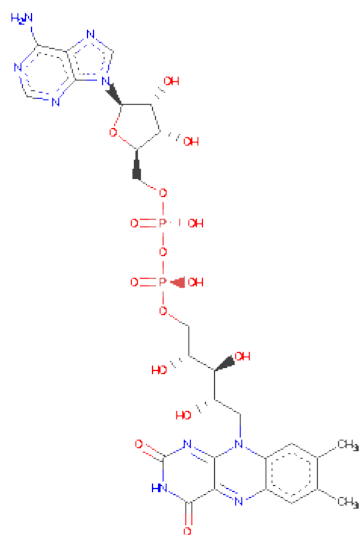
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is (MOLYBDOPTERIN-CYTOSINEDINUCLEOTIDE-S,S)-DIOXO-AQUA-MOLYBDENUM(V) (three-letter code: PCD) (formula:  $C_{19}H_{26}MoN_8O_{16}P_2S_2$ ).



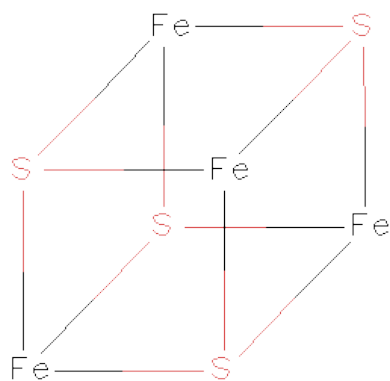
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	A	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		
8	D	1	Total	C	Mo	N	O	P	S	0	0
			48	19	1	8	16	2	2		

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



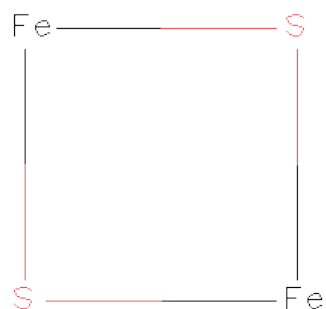
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	53	27	9	15	2	0	0
9	E	1	53	27	9	15	2	0	0

- Molecule 10 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	Fe	S	0	1
			16	8	8		
10	E	1	Total	Fe	S	0	1
			16	8	8		

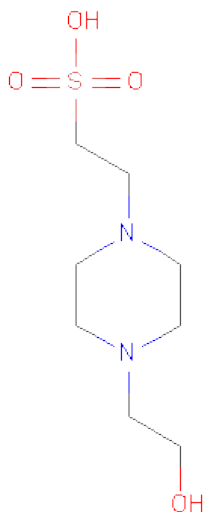
- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	Fe	S	0	0
			4	2	2		
11	C	1	Total	Fe	S	0	0
			4	2	2		
11	F	1	Total	Fe	S	0	0
			4	2	2		
11	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 12 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula:  $\text{C}_8\text{H}_{18}\text{N}_2\text{O}_4\text{S}$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
12	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
12	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
12	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

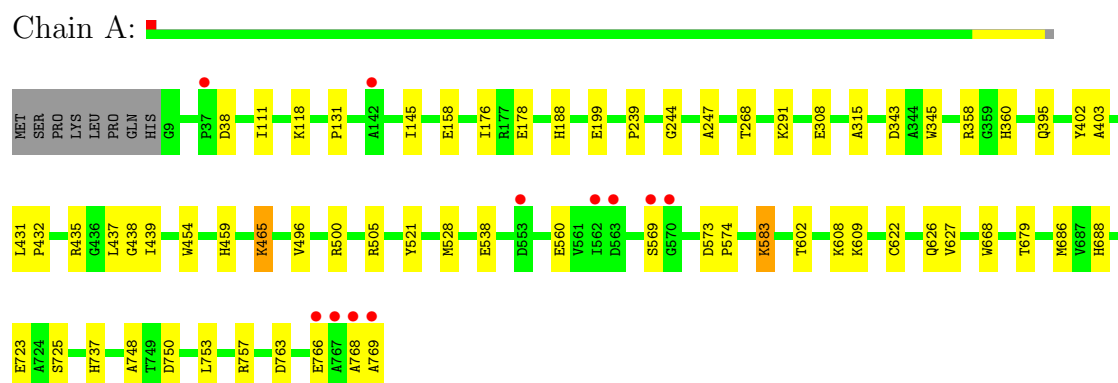
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	630	Total	O	0	0
			630	630		
13	B	290	Total	O	0	0
			290	290		
13	C	172	Total	O	0	0
			172	172		
13	D	663	Total	O	0	0
			663	663		
13	E	233	Total	O	0	0
			233	233		
13	F	146	Total	O	0	0
			146	146		

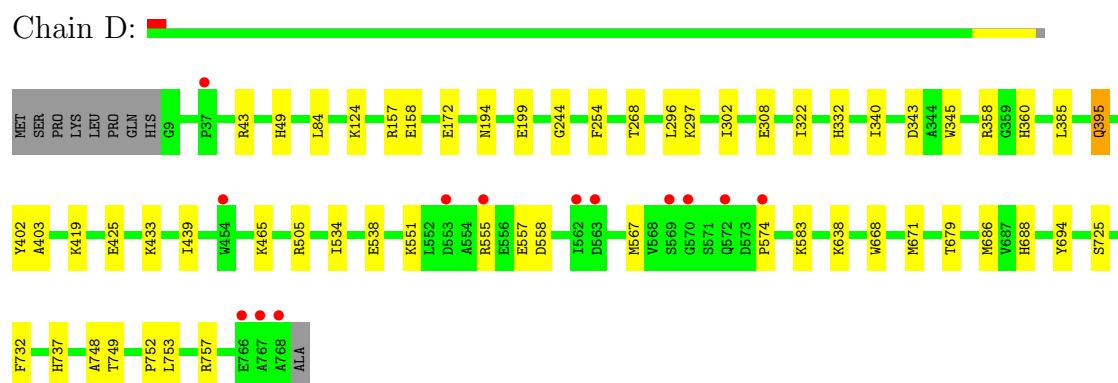
### 3 Residue-property plots

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.

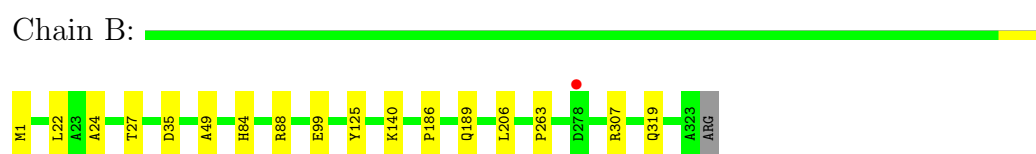
- Molecule 1: 4-hydroxybenzoyl-CoA reductase alpha subunit



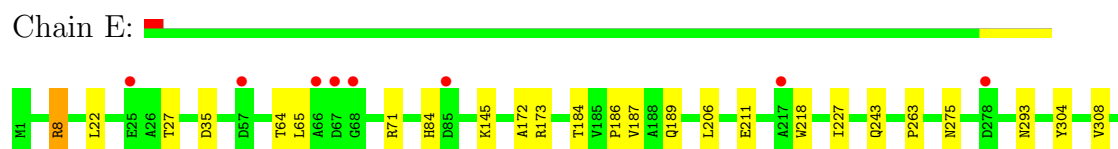
- Molecule 1: 4-hydroxybenzoyl-CoA reductase alpha subunit



- Molecule 2: 4-hydroxybenzoyl-CoA reductase beta subunit



- Molecule 2: 4-hydroxybenzoyl-CoA reductase beta subunit





- Molecule 3: 4-hydroxybenzoyl-CoA reductase gamma subunit



- Molecule 3: 4-hydroxybenzoyl-CoA reductase gamma subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.02Å 151.84Å 174.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 1.60 19.90 – 1.60	Depositor EDS
% Data completeness (in resolution range)	86.0 (19.91-1.60) 86.2 (19.90-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.152 , 0.173 0.151 , 0.173	Depositor DCC
$R_{free}$ test set	16885 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 338357 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	21258	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: CL, NA, SF4, PCD, FES, EPE, K, FAD, SO4

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	0.65	0/5959	0.79	1/8086 (0.0%)
1	D	0.65	0/5967	0.79	1/8094 (0.0%)
2	B	0.60	0/2518	0.78	1/3431 (0.0%)
2	E	0.57	0/2499	0.77	1/3405 (0.0%)
3	C	0.61	0/1210	0.80	0/1628
3	F	0.63	0/1199	0.82	0/1614
All	All	0.63	0/19352	0.79	4/26258 (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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	263	PRO	N-CA-C	-5.31	98.30	112.10
1	D	694	TYR	N-CA-C	-5.25	96.82	111.00
1	A	315	ALA	N-CA-C	5.10	124.77	111.00
2	B	263	PRO	N-CA-C	-5.08	98.89	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	TYR	Sidechain

## 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	5794	0	5838	45	0
1	D	5782	0	5834	45	0
2	B	2438	0	2459	18	0
2	E	2427	0	2463	23	0
3	C	1186	0	1230	20	0
3	F	1177	0	1221	27	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	D	5	0	0	0	0
8	A	48	0	21	3	0
8	D	48	0	21	2	0
9	B	53	0	30	1	0
9	E	53	0	31	1	0
10	B	16	0	0	0	0
10	E	16	0	0	0	0
11	C	8	0	0	0	0
11	F	8	0	0	0	0
12	A	45	0	54	5	0
12	D	15	0	18	0	0
13	A	630	0	0	7	0
13	B	290	0	0	3	0
13	C	172	0	0	4	0
13	D	663	0	0	13	0
13	E	233	0	0	6	0
13	F	146	0	0	10	0
All	All	21258	0	19220	171	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 4.

The worst 5 of 171 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:173[A]:ARG:NH1	2:E:184:THR:HG21	1.85	0.91
1:A:178[B]:GLU:OE1	1:A:291:LYS:HD2	1.76	0.86
3:F:145[A]:LYS:HG2	13:F:9545:HOH:O	1.76	0.86
3:C:145[B]:LYS:HE2	13:C:7445:HOH:O	1.78	0.83
2:E:145:LYS:HE3	13:E:7688:HOH:O	1.79	0.83

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	776/769 (101%)	755 (97%)	17 (2%)	4 (0%)	38	13
1	D	776/769 (101%)	752 (97%)	21 (3%)	3 (0%)	43	18
2	B	330/324 (102%)	325 (98%)	5 (2%)	0	100	100
2	E	327/324 (101%)	321 (98%)	6 (2%)	0	100	100
3	C	159/161 (99%)	155 (98%)	3 (2%)	1 (1%)	33	10
3	F	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
All	All	2526/2508 (101%)	2463 (98%)	55 (2%)	8 (0%)	50	24

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	HIS
3	C	156	CYS
1	D	360	HIS
1	A	358	ARG
1	D	358	ARG

### 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	605/597 (101%)	600 (99%)	5 (1%)	89	78
1	D	606/597 (102%)	603 (100%)	3 (0%)	94	87
2	B	250/243 (103%)	249 (100%)	1 (0%)	95	89
2	E	248/243 (102%)	246 (99%)	2 (1%)	89	78
3	C	130/128 (102%)	129 (99%)	1 (1%)	89	78
3	F	129/128 (101%)	128 (99%)	1 (1%)	89	78
All	All	1968/1936 (102%)	1955 (99%)	13 (1%)	91	81

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	319	GLN
3	C	7	LEU
2	E	8	ARG
1	A	766	GLU
1	D	558	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	49	HIS
1	D	395	GLN
2	E	243	GLN
3	C	133	ASN
2	E	84	HIS

### 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 ⓘ

Of 22 ligands modelled in this entry, 5 are monoatomic - leaving 17 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$
8	PCD	A	920	-	52,53,53	2.54	16 (30%)	70,86,86	4.32	29 (41%)
12	EPE	A	930	-	15,15,15	2.24	2 (13%)	20,20,20	1.70	5 (25%)
12	EPE	A	932	-	15,15,15	2.47	3 (20%)	20,20,20	1.86	6 (30%)
12	EPE	A	933	-	15,15,15	2.33	2 (13%)	20,20,20	1.82	5 (25%)
9	FAD	B	900	-	58,58,58	2.00	15 (25%)	85,89,89	2.01	17 (20%)
10	SF4	B	910[A]	2	12,12,12	12.89	12 (100%)	0,24,24	0.00	-
10	SF4	B	910[B]	2	12,12,12	11.38	12 (100%)	0,24,24	0.00	-
11	FES	C	907	3	0,4,4	0.00	-	0,4,4	0.00	-
11	FES	C	908	3	0,4,4	0.00	-	0,4,4	0.00	-
7	SO4	D	773	-	4,4,4	0.24	0	6,6,6	0.11	0
8	PCD	D	920	-	52,53,53	2.68	12 (23%)	70,86,86	4.30	28 (40%)
12	EPE	D	931	-	15,15,15	2.34	4 (26%)	20,20,20	1.37	3 (15%)
9	FAD	E	900	-	58,58,58	1.96	16 (27%)	85,89,89	2.12	17 (20%)
10	SF4	E	910[A]	2	12,12,12	10.92	12 (100%)	0,24,24	0.00	-
10	SF4	E	910[B]	2	12,12,12	17.24	12 (100%)	0,24,24	0.00	-
11	FES	F	907	3	0,4,4	0.00	-	0,4,4	0.00	-
11	FES	F	908	3	0,4,4	0.00	-	0,4,4	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
8	PCD	A	920	-	-	0/20/78/78	0/2/6/6
12	EPE	A	930	-	-	0/9/19/19	0/1/1/1
12	EPE	A	932	-	-	0/9/19/19	0/1/1/1
12	EPE	A	933	-	-	0/9/19/19	0/1/1/1
9	FAD	B	900	-	-	0/34/50/50	0/1/6/6
10	SF4	B	910[A]	2	-	0/0/48/48	0/0/5/5
10	SF4	B	910[B]	2	-	0/0/48/48	0/0/5/5
11	FES	C	907	3	-	0/0/4/4	0/0/1/1
11	FES	C	908	3	-	0/0/4/4	0/0/1/1
7	SO4	D	773	-	-	0/0/0/0	0/0/0/0
8	PCD	D	920	-	-	0/20/78/78	0/2/6/6
12	EPE	D	931	-	-	0/9/19/19	0/1/1/1
9	FAD	E	900	-	-	0/34/50/50	0/1/6/6
10	SF4	E	910[A]	2	-	0/0/48/48	0/0/5/5
10	SF4	E	910[B]	2	-	0/0/48/48	0/0/5/5
11	FES	F	907	3	-	0/0/4/4	0/0/1/1
11	FES	F	908	3	-	0/0/4/4	0/0/1/1

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	910[B]	SF4	S1-FE3	-25.12	2.16	2.33
10	E	910[B]	SF4	S3-FE1	-23.26	2.17	2.33
10	E	910[B]	SF4	S2-FE4	-21.85	2.18	2.33
10	E	910[B]	SF4	S2-FE3	-21.35	2.18	2.33
10	B	910[A]	SF4	S2-FE3	-21.31	2.18	2.33

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	920	PCD	C4A-C4B-N8'	-15.93	100.98	119.12
8	D	920	PCD	C4A-C4B-N8'	-15.92	100.99	119.12
8	D	920	PCD	C4B-C4A-N5'	14.21	137.99	118.50
8	A	920	PCD	C4B-C4A-N5'	13.61	137.16	118.50
8	A	920	PCD	N2'-C2'-N3'	11.20	136.52	117.19

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	761/769 (98%)	-0.53	11 (1%) 72 73	8, 15, 30, 67	0
1	D	760/769 (98%)	-0.52	13 (1%) 67 67	7, 14, 35, 76	0
2	B	323/324 (99%)	-0.44	1 (0%) 91 93	10, 17, 35, 47	0
2	E	323/324 (99%)	-0.16	8 (2%) 54 54	10, 20, 38, 53	0
3	C	157/161 (97%)	-0.56	3 (1%) 64 64	8, 13, 26, 79	0
3	F	157/161 (97%)	-0.62	1 (0%) 86 89	8, 13, 27, 55	0
All	All	2481/2508 (98%)	-0.48	37 (1%) 68 71	7, 15, 34, 79	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	157	GLU	7.5
1	D	572	GLN	7.3
1	A	769	ALA	7.1
3	C	156	CYS	6.8
1	A	767	ALA	6.7

### 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
12	EPE	A	933	15/15	0.79	33.21	40,55,59,60	15
7	SO4	D	773	5/5	0.44	13.29	48,51,52,53	5
12	EPE	A	932	15/15	0.38	12.90	51,53,57,58	15
4	CL	A	770	1/1	0.07	3.41	15,15,15,15	1
4	CL	D	770	1/1	0.07	3.34	14,14,14,14	1
12	EPE	D	931	15/15	0.13	1.43	15,33,44,53	15
12	EPE	A	930	15/15	0.13	0.77	25,31,39,41	15
6	NA	A	771	1/1	0.06	-0.53	18,18,18,18	0
9	FAD	E	900	53/53	0.05	-0.53	9,14,20,20	0
6	NA	D	772	1/1	0.06	-0.57	18,18,18,18	0
8	PCD	A	920	48/48	0.04	-0.85	7,9,12,13	0
8	PCD	D	920	48/48	0.04	-0.88	6,8,10,12	0
9	FAD	B	900	53/53	0.04	-1.06	9,12,15,17	0
10	SF4	B	910[A]	8/8	0.04	-1.25	8,10,13,15	8
10	SF4	B	910[B]	8/8	0.04	-1.30	6,10,11,11	8
10	SF4	E	910[B]	8/8	0.05	-1.43	9,11,13,13	8
10	SF4	E	910[A]	8/8	0.05	-1.45	8,10,11,11	8
11	FES	C	908	4/4	0.03	-1.61	9,9,10,10	0
11	FES	C	907	4/4	0.03	-1.79	8,9,9,9	0
5	K	D	771	1/1	0.03	-1.80	19,19,19,19	0
11	FES	F	907	4/4	0.03	-1.82	7,7,8,8	0
11	FES	F	908	4/4	0.03	-1.88	9,9,9,10	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.