



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:09 PM GMT

PDB ID : 1SB3
Title : Structure of 4-hydroxybenzoyl-CoA reductase from *Thauera aromatica*
Authors : Unciuleac, M.; Warkentin, E.; Page, C.C.; Boll, M.; Ermler, U.
Deposited on : 2004-02-10
Resolution : 2.20 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

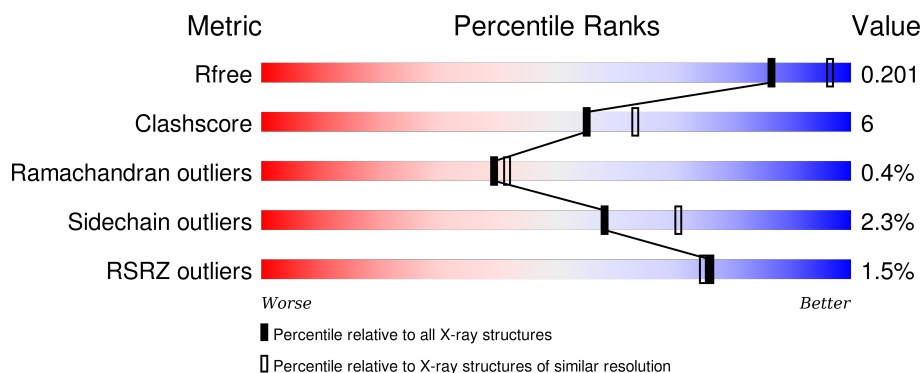
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	769	<div> <div>2%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	D	769	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
2	B	324	<div> <div>%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	E	324	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
3	C	161	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	161	

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
4	SO4	D	1112	-	-	-	X
4	SO4	E	1113	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19897 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 4-hydroxybenzoyl-CoA reductase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	0	0
			5716	3618	984	1085	29			
1	D	760	Total	C	N	O	S	0	0	0
			5710	3615	983	1083	29			

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	0	0
			2407	1508	441	450	8			
2	E	323	Total	C	N	O	S	0	0	0
			2407	1508	441	450	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	161	Total	C	N	O	S	0	0	0
			1193	732	218	230	13			
3	F	157	Total	C	N	O	S	0	0	0
			1163	716	211	223	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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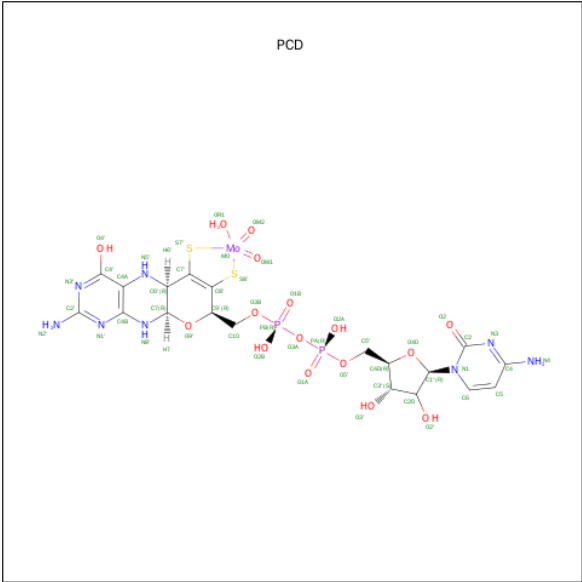
Chain	Residue	Modelled	Actual	Comment	Reference
C	144	ILE	SER	see remark 999	UNP O33818
F	142	LYS	ARG	see remark 999	UNP O33818
F	143	ILE	SER	see remark 999	UNP O33818
F	144	ILE	SER	see remark 999	UNP O33818

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



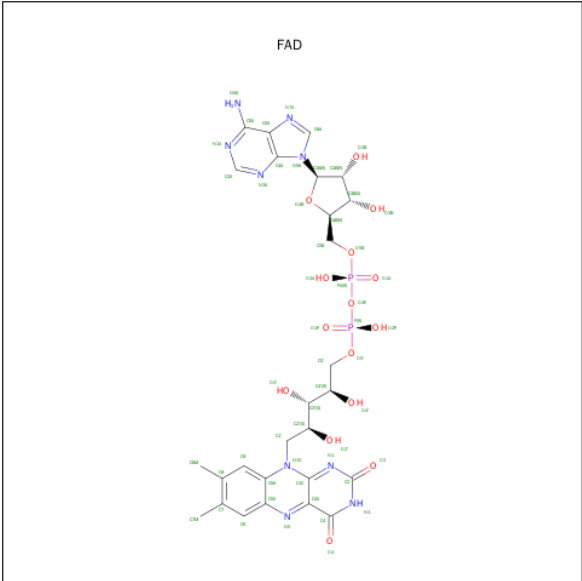
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (MOLYBDOPTERIN-CYTOSINE DINUCLEOTIDE-S,S)-DIOXO-AQUA-MOLYBDENUM(V) (three-letter code: PCD) (formula: C₁₉H₂₆MoN₈O₁₆P₂S₂).



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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



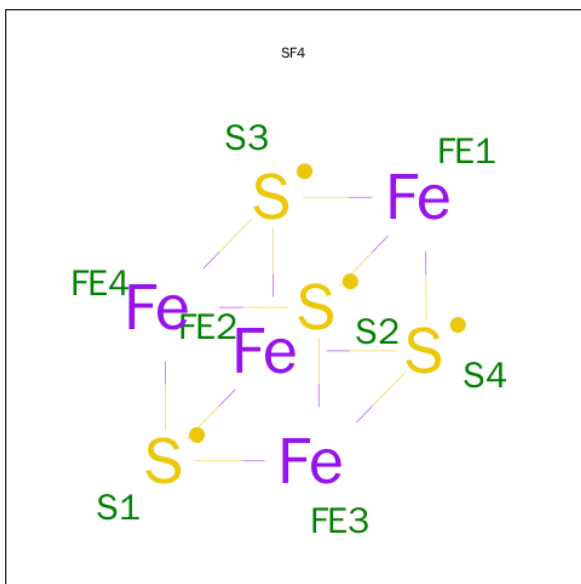
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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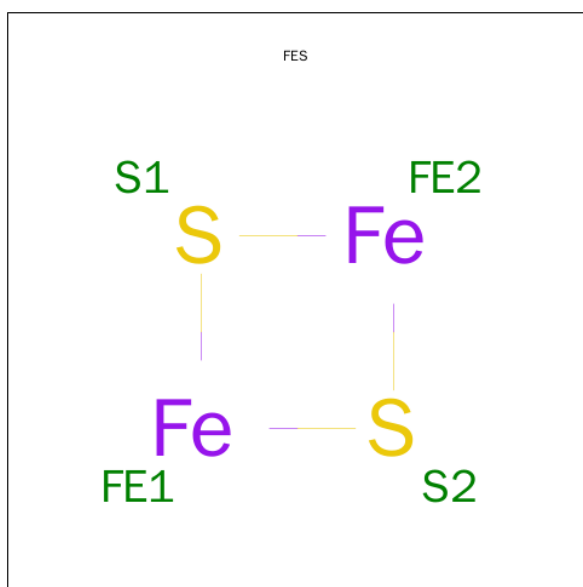
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



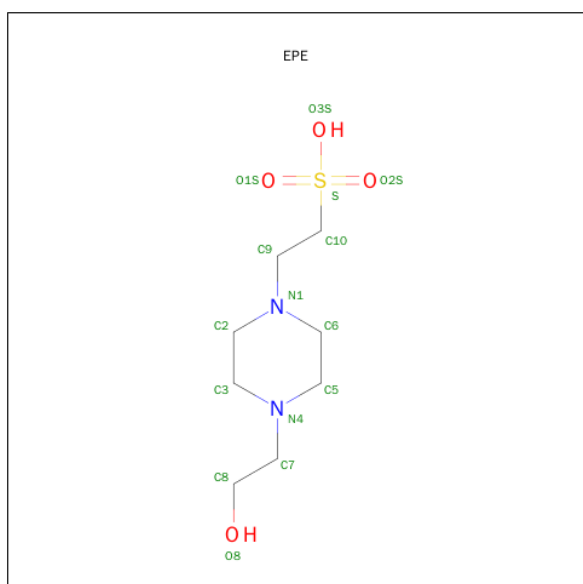
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

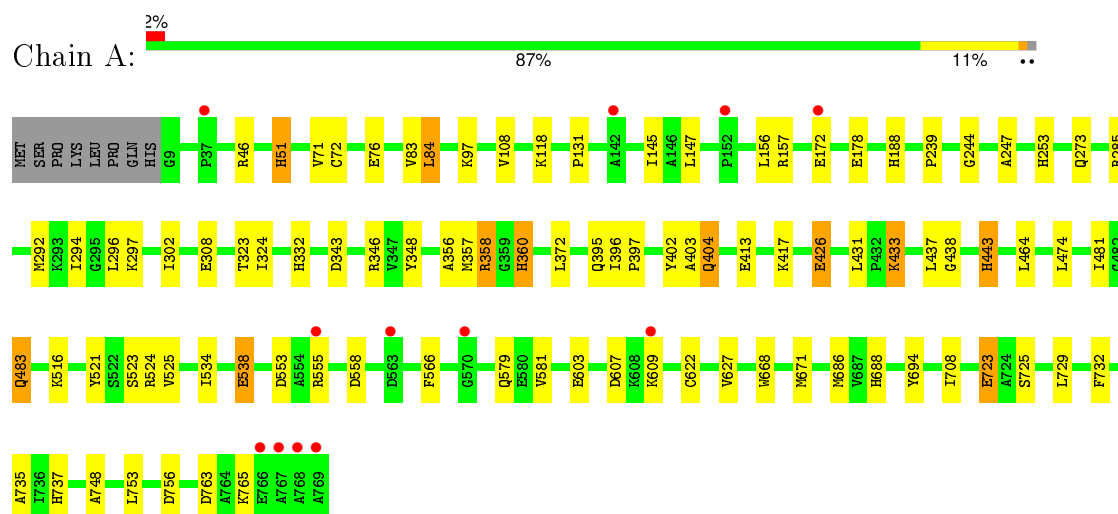
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	319	Total	O	0	0
			319	319		
10	B	115	Total	O	0	0
			115	115		
10	C	103	Total	O	0	0
			103	103		
10	D	319	Total	O	0	0
			319	319		
10	E	96	Total	O	0	0
			96	96		
10	F	90	Total	O	0	0
			90	90		

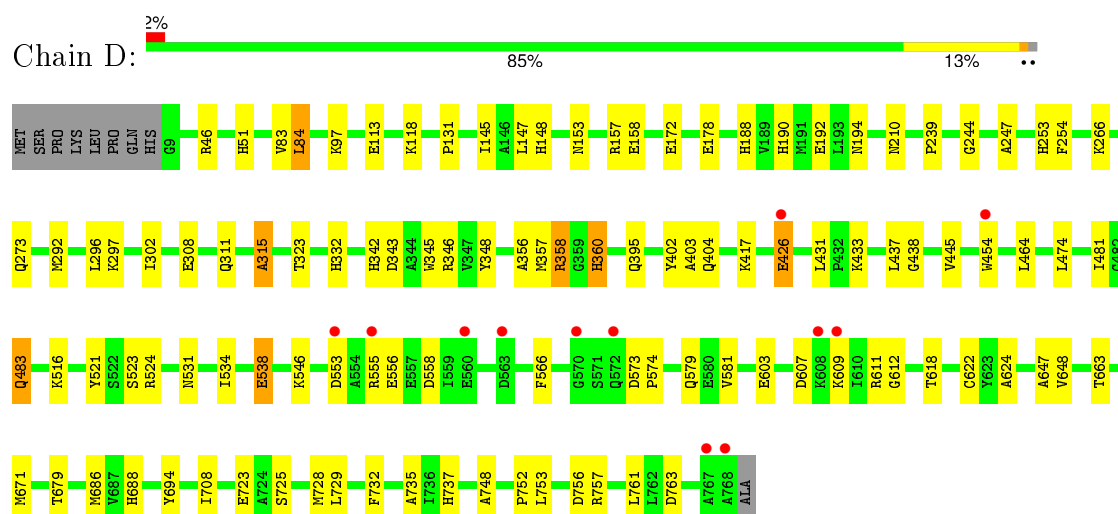
3 Residue-property plots

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.

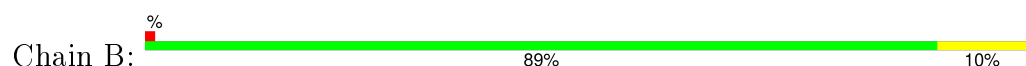
- Molecule 1: 4-hydroxybenzoyl-CoA reductase alpha subunit

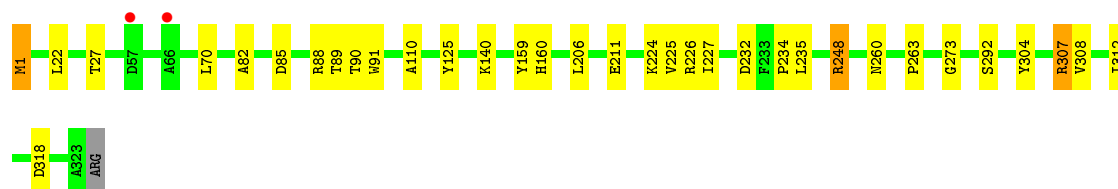


- Molecule 1: 4-hydroxybenzoyl-CoA reductase alpha subunit

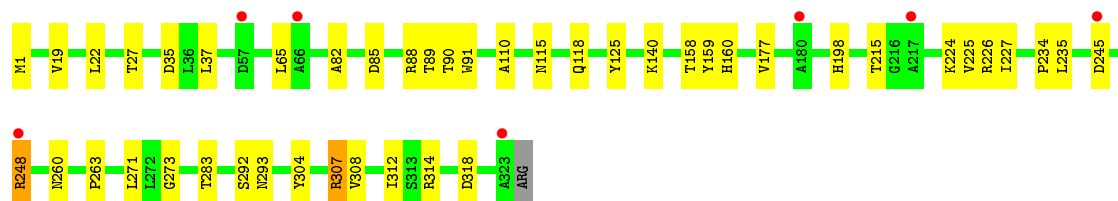
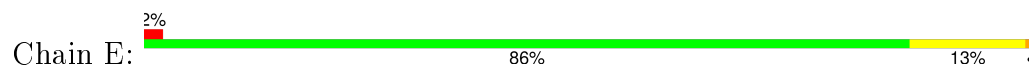


- Molecule 2: 4-hydroxybenzoyl-CoA reductase beta subunit

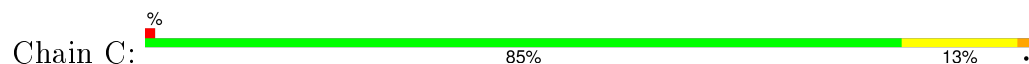




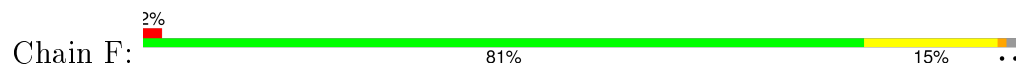
- Molecule 2: 4-hydroxybenzoyl-CoA reductase beta subunit



- 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, α , β , γ	116.62Å 150.20Å 175.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.20 19.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.90-2.20) 96.2 (19.90-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.21Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.171 , 0.205 0.168 , 0.201	Depositor DCC
R_{free} test set	7543 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 149240 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19897	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SF4, FES, FAD, EPE, PCD, 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	0.58	0/5823	0.76	1/7903 (0.0%)
1	D	0.57	0/5817	0.76	4/7896 (0.1%)
2	B	0.51	0/2450	0.73	0/3340
2	E	0.51	0/2450	0.73	0/3340
3	C	0.62	0/1203	0.81	1/1618 (0.1%)
3	F	0.55	0/1173	0.79	0/1580
All	All	0.56	0/18916	0.76	6/25677 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	694	TYR	N-CA-C	-6.03	94.72	111.00
1	A	694	TYR	N-CA-C	-5.94	94.97	111.00
1	D	113	GLU	OE1-CD-OE2	-5.32	116.92	123.30
3	C	112	GLU	OE1-CD-OE2	-5.06	117.22	123.30
1	D	315	ALA	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5716	0	5769	74	0
1	D	5710	0	5764	77	0
2	B	2407	0	2434	28	0
2	E	2407	0	2434	31	0
3	C	1193	0	1225	17	0
3	F	1163	0	1198	17	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
5	A	48	0	22	7	0
5	D	48	0	22	5	0
6	B	53	0	31	1	0
6	E	53	0	31	3	0
7	B	8	0	0	0	0
7	E	8	0	0	0	0
8	C	8	0	0	0	0
8	F	8	0	0	0	0
9	A	15	0	18	0	0
10	A	319	0	0	5	0
10	B	115	0	0	1	0
10	C	103	0	0	4	0
10	D	319	0	0	9	0
10	E	96	0	0	2	0
10	F	90	0	0	2	0
All	All	19897	0	18948	239	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 6.

The worst 5 of 239 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:172:GLU:HG2	1:A:297:LYS:NZ	1.85	0.90
1:D:483:GLN:H	1:D:483:GLN:HE21	1.19	0.90
1:D:46:ARG:HH22	1:D:253:HIS:HE1	1.20	0.88
1:D:172:GLU:HG2	1:D:297:LYS:NZ	1.91	0.85
1:A:131:PRO:HD2	1:A:145:ILE:HD12	1.57	0.84

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	759/769 (99%)	733 (97%)	22 (3%)	4 (0%)	34	35
1	D	758/769 (99%)	731 (96%)	23 (3%)	4 (0%)	34	35
2	B	321/324 (99%)	312 (97%)	9 (3%)	0	100	100
2	E	321/324 (99%)	308 (96%)	13 (4%)	0	100	100
3	C	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
3	F	155/161 (96%)	150 (97%)	4 (3%)	1 (1%)	30	29
All	All	2473/2508 (99%)	2388 (97%)	76 (3%)	9 (0%)	39	42

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	HIS
1	A	358	ARG
1	D	358	ARG
1	D	360	HIS
1	D	244	GLY

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	589/597 (99%)	574 (98%)	15 (2%)	55	67
1	D	589/597 (99%)	578 (98%)	11 (2%)	65	77
2	B	242/243 (100%)	238 (98%)	4 (2%)	68	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	242/243 (100%)	237 (98%)	5 (2%)	61	74
3	C	128/128 (100%)	124 (97%)	4 (3%)	47	59
3	F	126/128 (98%)	121 (96%)	5 (4%)	38	47
All	All	1916/1936 (99%)	1872 (98%)	44 (2%)	58	71

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	7	LEU
1	D	118	LYS
3	F	21	ASN
3	C	21	ASN
3	C	158	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	66	HIS
1	D	190	HIS
2	E	293	ASN
1	D	51	HIS
1	D	220	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

13 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$
9	EPE	A	1111	-	14,15,15	2.45	4 (28%)	18,20,20	2.18	5 (27%)
5	PCD	A	1920	-	40,53,53	2.28	14 (35%)	45,86,86	5.22	21 (46%)
6	FAD	B	1900	-	48,58,58	2.18	13 (27%)	54,89,89	2.35	15 (27%)
7	SF4	B	1910	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FES	C	1907	3	0,4,4	0.00	-	0,4,4	0.00	-
8	FES	C	1908	3	0,4,4	0.00	-	0,4,4	0.00	-
4	SO4	D	1112	-	4,4,4	0.10	0	6,6,6	0.16	0
5	PCD	D	1921	-	40,53,53	2.04	11 (27%)	45,86,86	5.27	20 (44%)
4	SO4	E	1113	-	4,4,4	0.16	0	6,6,6	0.15	0
6	FAD	E	1901	-	48,58,58	2.26	14 (29%)	54,89,89	2.45	17 (31%)
7	SF4	E	1911	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FES	F	1917	3	0,4,4	0.00	-	0,4,4	0.00	-
8	FES	F	1918	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
9	EPE	A	1111	-	-	0/9/19/19	0/1/1/1
5	PCD	A	1920	-	-	0/18/78/78	0/6/6/6
6	FAD	B	1900	-	-	0/30/50/50	0/6/6/6
7	SF4	B	1910	2	-	0/0/48/48	0/6/5/5
8	FES	C	1907	3	-	0/0/4/4	0/1/1/1
8	FES	C	1908	3	-	0/0/4/4	0/1/1/1
4	SO4	D	1112	-	-	0/0/0/0	0/0/0/0
5	PCD	D	1921	-	-	0/18/78/78	0/6/6/6
4	SO4	E	1113	-	-	0/0/0/0	0/0/0/0
6	FAD	E	1901	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	E	1911	2	-	0/0/48/48	0/6/5/5
8	FES	F	1917	3	-	0/0/4/4	0/1/1/1
8	FES	F	1918	3	-	0/0/4/4	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1900	FAD	PA-O2A	-4.17	1.37	1.54
6	E	1901	FAD	PA-O2A	-4.05	1.37	1.54
6	B	1900	FAD	P-O2P	-3.21	1.41	1.54
6	E	1901	FAD	P-O2P	-2.58	1.43	1.54
9	A	1111	EPE	C9-C10	-2.30	1.44	1.52

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1921	PCD	C4A-C4B-N8'	-18.25	99.25	118.34
5	A	1920	PCD	C4A-C4B-N8'	-17.60	99.93	118.34
5	D	1921	PCD	N2'-C2'-N1'	-10.24	100.24	117.20
5	A	1920	PCD	N2'-C2'-N1'	-10.02	100.61	117.20
5	A	1920	PCD	O4'-C4'-N3'	-6.59	98.92	116.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1920	PCD	7	0
6	B	1900	FAD	1	0
5	D	1921	PCD	5	0
6	E	1901	FAD	3	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, 95th 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 ²)	Q<0.9
1	A	761/769 (98%)	-0.56	12 (1%) 74 73	18, 30, 55, 100	0
1	D	760/769 (98%)	-0.60	12 (1%) 74 73	16, 29, 57, 92	0
2	B	323/324 (99%)	-0.51	2 (0%) 90 90	21, 34, 59, 78	0
2	E	323/324 (99%)	-0.28	7 (2%) 65 64	21, 37, 61, 80	0
3	C	161/161 (100%)	-0.74	2 (1%) 81 80	17, 24, 46, 74	0
3	F	157/161 (97%)	-0.67	3 (1%) 70 68	19, 26, 41, 103	0
All	All	2485/2508 (99%)	-0.54	38 (1%) 76 75	16, 31, 57, 103	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	769	ALA	8.5
3	F	157	GLU	4.7
3	F	156	CYS	4.3
1	A	768	ALA	4.0
1	D	563	ASP	3.8

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 [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, 95th 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 ²)	Q<0.9
4	SO4	D	1112	5/5	0.96	0.15	2.73	49,49,52,53	5
4	SO4	E	1113	5/5	0.92	0.17	2.16	41,43,46,46	5
9	EPE	A	1111	15/15	0.95	0.16	0.45	39,43,53,61	15
6	FAD	B	1900	53/53	0.98	0.07	-0.36	18,24,29,33	0
5	PCD	A	1920	48/48	0.99	0.08	-0.44	17,24,28,37	0
6	FAD	E	1901	53/53	0.98	0.07	-0.56	23,29,32,35	0
5	PCD	D	1921	48/48	0.99	0.08	-0.73	18,24,29,33	0
8	FES	C	1908	4/4	0.99	0.05	-1.51	20,20,22,23	0
8	FES	C	1907	4/4	0.99	0.06	-1.52	15,18,19,21	0
8	FES	F	1918	4/4	1.00	0.05	-1.57	23,24,24,24	0
7	SF4	B	1910	8/8	0.99	0.05	-1.89	28,29,29,30	0
8	FES	F	1917	4/4	1.00	0.05	-1.94	19,21,23,23	0
7	SF4	E	1911	8/8	0.99	0.05	-1.98	26,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.