



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:36 am GMT

PDB ID : 3AD8  
Title : Heterotetrameric Sarcosine Oxidase from *Corynebacterium* sp. U-96 in complex with pyrrole 2-carboxylate  
Authors : Suzuki, H.; Moriguchi, T.; Ida, K.  
Deposited on : 2010-01-15  
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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

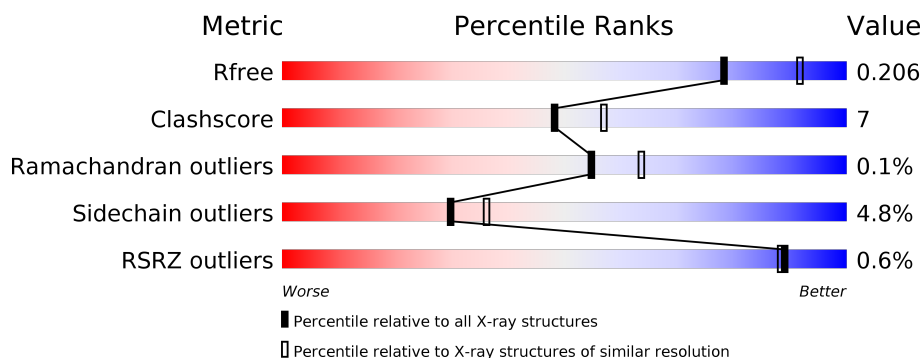
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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  $\geq 3$ , 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	964	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>87%</span> <span>11%</span> </div> </div>
2	B	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>85%</span> <span>12%</span> </div> </div>
3	C	203	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 80%, yellow 13%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>80%</span> <span>13%</span> </div> </div>
4	D	99	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 87%, yellow 5%, orange 8%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>87%</span> <span>5%</span> <span>8%</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	2506	-	-	-	X
6	SO4	A	2509	-	-	X	X
8	FMN	B	406	-	-	X	-
9	PYC	B	801	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13736 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 SARCOSINE OXIDASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	963	Total	C	N	O	S	0	0	0
			7229	4507	1287	1413	22			

- Molecule 2 is a protein called SARCOSINE OXIDASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3108	1981	541	576	10			

- Molecule 3 is a protein called SARCOSINE OXIDASE GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	0	0
			1433	902	257	271	3			

- Molecule 4 is a protein called SARCOSINE OXIDASE DELTA SUBUNIT.

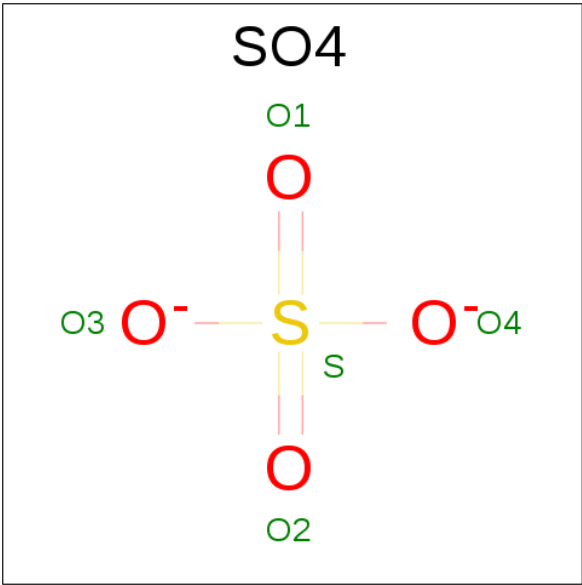
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	91	Total	C	N	O	S	0	0	0
			749	476	135	133	5			

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



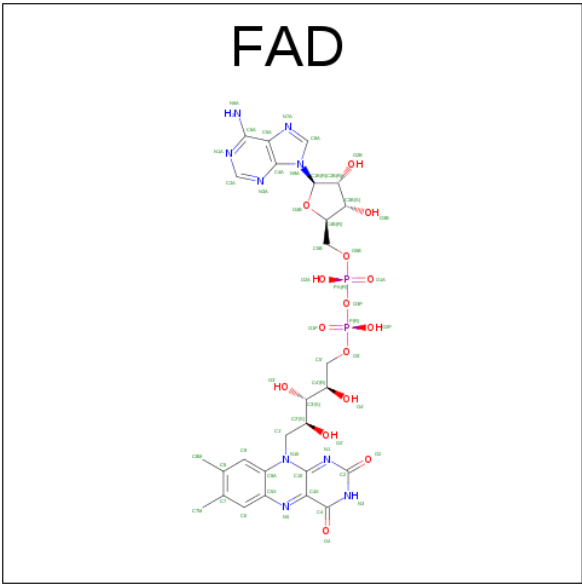
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

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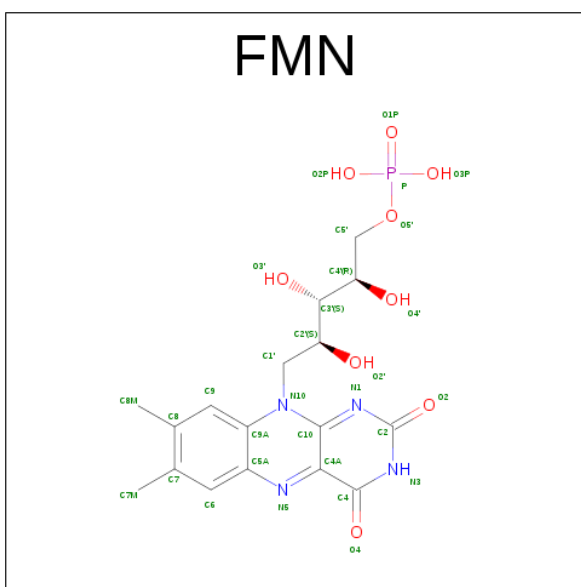
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



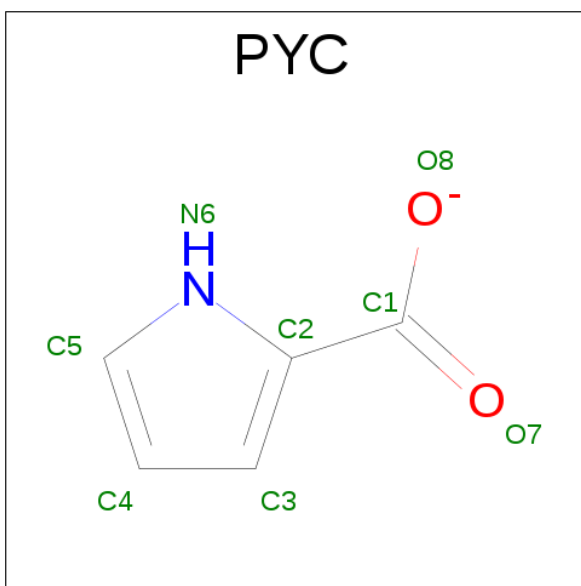
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O P	0	0
			53	27	9	15 2		

- Molecule 8 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 9 is PYRROLE-2-CARBOXYLATE (three-letter code: PYC) (formula:  $C_5H_4NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total 1	Zn 1	0	0

- Molecule 11 is water.

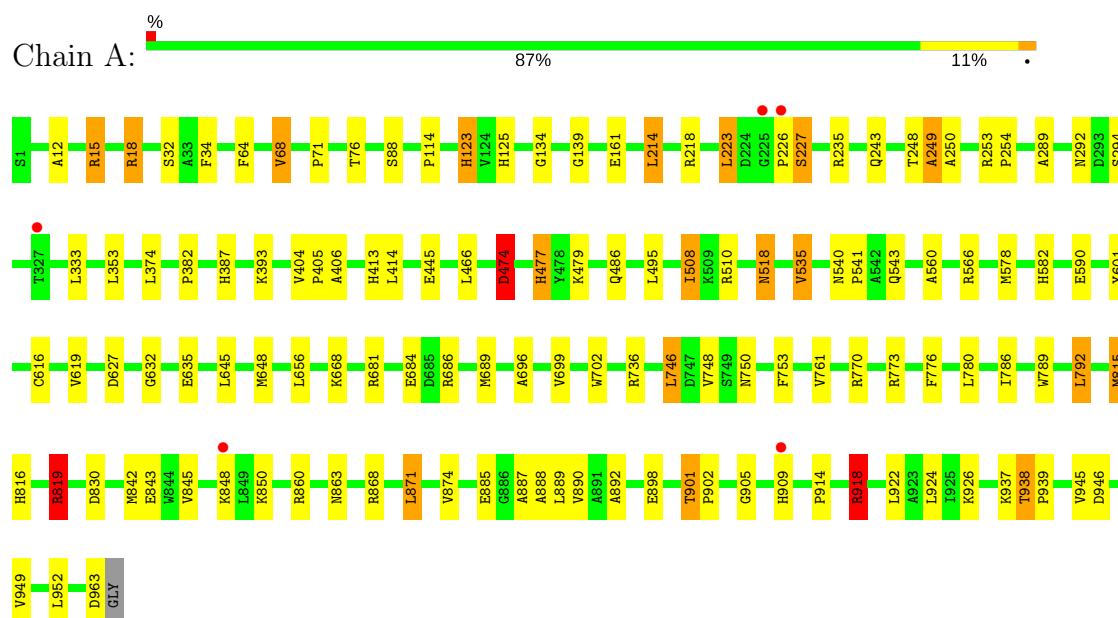
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	631	Total 631	O 631	0	0
11	B	189	Total 189	O 189	0	0
11	C	133	Total 133	O 133	0	0
11	D	67	Total 67	O 67	0	0



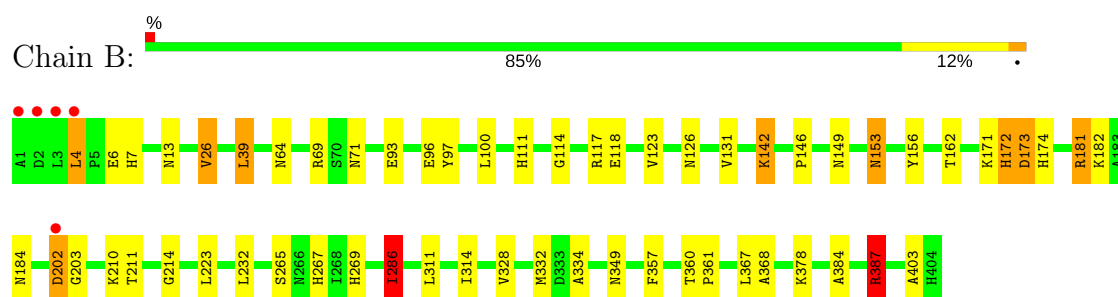
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

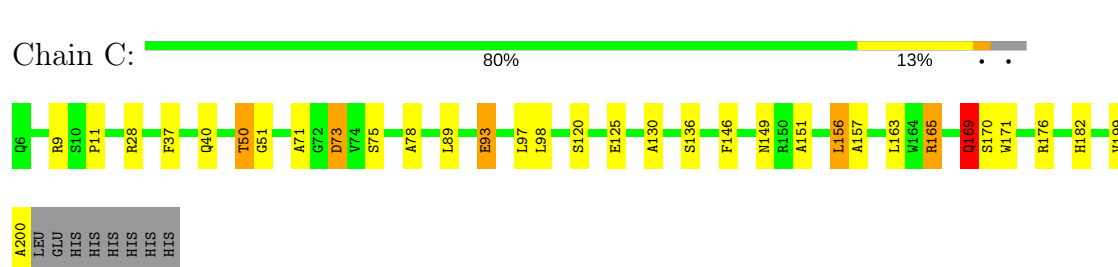
#### • Molecule 1: SARCOSINE OXIDASE ALPHA SUBUNIT




#### • Molecule 2: SARCOSINE OXIDASE BETA SUBUNIT

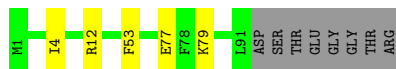


#### • Molecule 3: SARCOSINE OXIDASE GAMMA SUBUNIT



- Molecule 4: SARCOSINE OXIDASE DELTA SUBUNIT

Chain D:  87% 5% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.80Å 198.80Å 196.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.31 – 2.20 61.31 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.31-2.20) 100.0 (61.31-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.161 , 0.206 0.161 , 0.206	Depositor DCC
$R_{free}$ test set	5799 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.4	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAD, FMN, SO4, PYC, FAD

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	1.04	5/7361 (0.1%)	0.93	19/10017 (0.2%)
2	B	1.01	2/3189 (0.1%)	0.91	6/4340 (0.1%)
3	C	1.11	3/1461 (0.2%)	1.00	6/1998 (0.3%)
4	D	1.03	1/772 (0.1%)	0.88	1/1040 (0.1%)
All	All	1.04	11/12783 (0.1%)	0.93	32/17395 (0.2%)

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
3	C	0	1
All	All	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	477	HIS	CB-CG	9.30	1.66	1.50
1	A	477	HIS	CA-CB	8.05	1.71	1.53
1	A	477	HIS	CA-C	6.84	1.70	1.52
4	D	53	PHE	CE1-CZ	6.38	1.49	1.37
1	A	249	ALA	CA-CB	-5.99	1.39	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	387	ARG	NE-CZ-NH1	-14.34	113.13	120.30
1	A	15	ARG	NE-CZ-NH2	-12.63	113.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	819	ARG	NE-CZ-NH2	-12.61	113.99	120.30
1	A	819	ARG	NE-CZ-NH1	10.36	125.48	120.30
3	C	176	ARG	NE-CZ-NH2	-8.83	115.88	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	SER	Peptide
3	C	199	VAL	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	7229	0	7104	101	1
2	B	3108	0	3035	54	0
3	C	1433	0	1434	17	0
4	D	749	0	706	3	0
5	A	44	0	26	4	0
6	A	35	0	0	3	0
6	B	15	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	B	53	0	31	4	0
8	B	31	0	18	9	0
9	B	8	0	4	0	0
10	D	1	0	0	0	0
11	A	631	0	0	13	1
11	B	189	0	0	5	0
11	C	133	0	0	2	0
11	D	67	0	0	0	0
All	All	13736	0	12358	173	2

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 173 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)
2:B:172:HIS:NE2	8:B:406:FMN:C8M	1.71	1.50
1:A:830:ASP:OD1	1:A:909:HIS:CE1	1.88	1.26
1:A:696:ALA:HB3	6:A:2509:SO4:O3	1.41	1.17
2:B:384:ALA:O	2:B:387:ARG:HD3	1.44	1.12
2:B:387:ARG:HH11	2:B:387:ARG:HG3	0.98	1.11

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:HIS:NE2	1:A:477:HIS:NE2[11_555]	1.27	0.93
11:A:1080:HOH:O	11:A:1080:HOH:O[9_555]	1.63	0.57

## 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	961/964 (100%)	941 (98%)	18 (2%)	2 (0%)	51	58
2	B	402/404 (100%)	387 (96%)	15 (4%)	0	100	100
3	C	193/203 (95%)	187 (97%)	6 (3%)	0	100	100
4	D	89/99 (90%)	87 (98%)	2 (2%)	0	100	100
All	All	1645/1670 (98%)	1602 (97%)	41 (2%)	2 (0%)	55	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	406	ALA

### 5.3.2 Protein sidechains [i](#)

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	747/747 (100%)	709 (95%)	38 (5%)	28	33
2	B	319/319 (100%)	305 (96%)	14 (4%)	33	40
3	C	143/151 (95%)	134 (94%)	9 (6%)	21	23
4	D	75/81 (93%)	74 (99%)	1 (1%)	73	85
All	All	1284/1298 (99%)	1222 (95%)	62 (5%)	30	36

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	848	LYS
1	A	901	THR
3	C	146	PHE
1	A	874	VAL
1	A	938	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	750	ASN
1	A	912	ASN
3	C	158	ASN
1	A	863	ASN
2	B	7	HIS

### 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 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\# Z  > 2$
6	SO4	A	2500	-	4,4,4	0.12	0	6,6,6	0.26	0
6	SO4	A	2501	-	4,4,4	0.36	0	6,6,6	0.56	0
6	SO4	A	2502	-	4,4,4	0.28	0	6,6,6	0.27	0
6	SO4	A	2504	-	4,4,4	0.11	0	6,6,6	0.33	0
6	SO4	A	2506	-	4,4,4	0.34	0	6,6,6	0.32	0
6	SO4	A	2507	-	4,4,4	0.22	0	6,6,6	0.44	0
6	SO4	A	2509	-	4,4,4	0.42	0	6,6,6	0.43	0
5	NAD	A	965	-	41,48,48	1.41	4 (9%)	43,73,73	1.69	4 (9%)
6	SO4	B	2505	-	4,4,4	0.21	0	6,6,6	0.24	0
6	SO4	B	2510	-	4,4,4	0.50	0	6,6,6	0.62	0
6	SO4	B	2511	-	4,4,4	0.23	0	6,6,6	0.44	0
7	FAD	B	405	-	51,58,58	1.83	7 (13%)	54,89,89	1.94	12 (22%)
8	FMN	B	406	-	31,33,33	2.21	11 (35%)	38,50,50	2.49	12 (31%)
9	PYC	B	801	-	5,8,8	2.95	1 (20%)	4,10,10	1.27	0
6	SO4	C	2508	-	4,4,4	0.66	0	6,6,6	0.27	0
6	SO4	D	2503	-	4,4,4	0.22	0	6,6,6	0.19	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
6	SO4	A	2500	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2501	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2502	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	A	2504	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2506	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2507	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2509	-	-	0/0/0/0	0/0/0/0
5	NAD	A	965	-	-	0/22/62/62	0/5/5/5
6	SO4	B	2505	-	-	0/0/0/0	0/0/0/0
6	SO4	B	2510	-	-	0/0/0/0	0/0/0/0
6	SO4	B	2511	-	-	0/0/0/0	0/0/0/0
7	FAD	B	405	-	-	0/28/50/50	0/6/6/6
8	FMN	B	406	-	-	0/16/18/18	0/3/3/3
9	PYC	B	801	-	-	0/0/4/4	0/1/1/1
6	SO4	C	2508	-	-	0/0/0/0	0/0/0/0
6	SO4	D	2503	-	-	0/0/0/0	0/0/0/0

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	801	PYC	C3-C2	-6.07	1.32	1.40
8	B	406	FMN	O5'-C5'	-6.05	1.20	1.44
5	A	965	NAD	C2B-C1B	-3.06	1.48	1.53
8	B	406	FMN	C9A-C5A	-3.06	1.36	1.42
5	A	965	NAD	C5A-N7A	-2.45	1.31	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	965	NAD	N3A-C2A-N1A	-7.59	122.25	128.86
8	B	406	FMN	O4'-C4'-C5'	-6.23	96.13	110.00
7	B	405	FAD	N3A-C2A-N1A	-6.20	123.45	128.86
7	B	405	FAD	C4B-O4B-C1B	-5.56	103.85	109.77
8	B	406	FMN	C4A-C4-N3	-3.66	118.27	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2509	SO4	3	0
5	A	965	NAD	4	0
7	B	405	FAD	4	0

*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	406	FMN	9	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	963/964 (99%)	-0.62	5 (0%) 90 90	11, 24, 41, 59	0
2	B	404/404 (100%)	-0.55	5 (1%) 79 77	13, 25, 39, 84	0
3	C	195/203 (96%)	-0.74	0 100 100	14, 22, 42, 49	0
4	D	91/99 (91%)	-0.80	0 100 100	15, 22, 42, 54	0
All	All	1653/1670 (98%)	-0.63	10 (0%) 89 88	11, 24, 41, 84	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ASP	8.3
2	B	1	ALA	7.4
2	B	3	LEU	7.3
1	A	909	HIS	3.8
1	A	226	PRO	2.8

### 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( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	2506	5/5	0.93	0.27	7.66	65,65,67,68	0
9	PYC	B	801	8/8	0.96	0.14	4.42	44,44,46,48	0
6	SO4	A	2509	5/5	0.98	0.13	3.15	44,46,49,52	0
6	SO4	B	2510	5/5	0.94	0.23	1.94	52,53,57,57	0
6	SO4	C	2508	5/5	0.99	0.13	1.24	30,33,35,35	0
7	FAD	B	405	53/53	0.97	0.10	0.76	11,22,27,28	0
6	SO4	A	2500	5/5	0.99	0.13	0.59	65,66,67,68	0
10	ZN	D	100	1/1	1.00	0.08	0.24	19,19,19,19	0
6	SO4	B	2511	5/5	0.90	0.11	0.22	73,73,75,76	0
8	FMN	B	406	31/31	0.98	0.09	0.02	11,15,19,23	0
5	NAD	A	965	44/44	0.99	0.09	-0.38	8,14,19,25	0
6	SO4	A	2501	5/5	0.97	0.12	-0.47	46,47,50,51	0
6	SO4	D	2503	5/5	0.94	0.13	-	82,82,83,83	0
6	SO4	B	2505	5/5	0.97	0.20	-	56,57,58,60	0
6	SO4	A	2504	5/5	1.00	0.08	-	29,30,35,37	0
6	SO4	A	2502	5/5	0.95	0.29	-	76,76,77,78	0
6	SO4	A	2507	5/5	0.96	0.20	-	59,60,62,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.