



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:57 AM GMT

PDB ID : 3AD9  
Title : Heterotetrameric Sarcosine Oxidase from Corynebacterium sp. U-96 sarcosine-reduced form  
Authors : Suzuki, H.; Moriguchi, T.; Ida, K.  
Deposited on : 2010-01-15  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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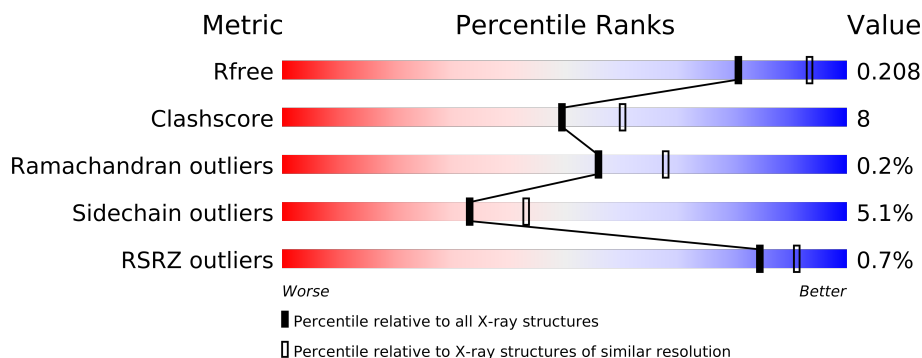
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	964	
2	B	404	
3	C	203	
4	D	99	

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

Mol	Type	Chain	Res	Geometry	Electron density
6	SO4	A	2563	-	X
6	SO4	A	2565	-	X
6	SO4	B	2561	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13569 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 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	397	Total	C	N	O	S	0	1	0
			3079	1965	533	571	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:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



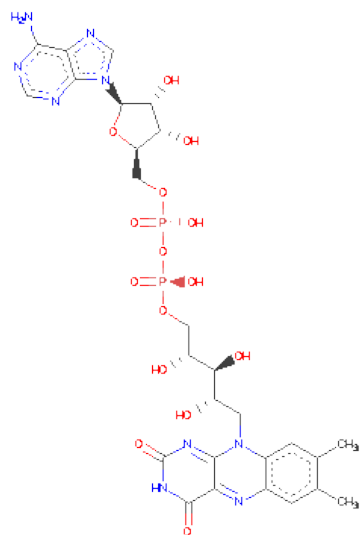
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

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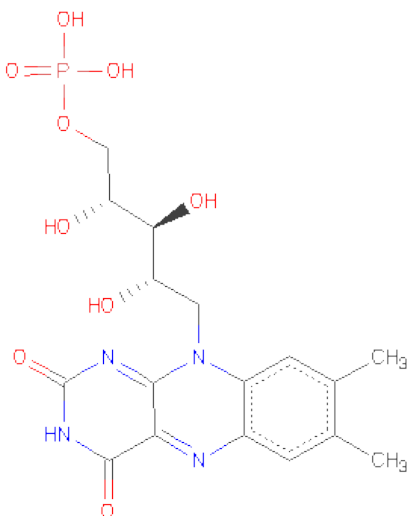
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	557	Total	O	0	0
			557	557		
10	B	163	Total	O	0	0
			163	163		
10	C	119	Total	O	0	0
			119	119		
10	D	66	Total	O	0	0
			66	66		



- Molecule 4: SARCOSINE OXIDASE DELTA SUBUNIT

Chain D: 

M1	K18	Y19	K49	F63	S60	L91	ASP	SER	THR	GLU	GLY	GLY	THR	ARG
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.56Å 198.56Å 196.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.25 – 2.30 61.25 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.25-2.30) 99.9 (61.25-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.18 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.169 , 0.211 0.169 , 0.208	Depositor DCC
$R_{free}$ test set	5043 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 20.8	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 101064 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: FMN, ZN, SO4, NAD, 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	0.98	3/7361 (0.0%)	0.91	12/10017 (0.1%)
2	B	0.99	4/3160 (0.1%)	0.88	3/4300 (0.1%)
3	C	1.06	0/1461	0.96	4/1998 (0.2%)
4	D	1.01	1/772 (0.1%)	0.92	0/1040
All	All	0.99	8/12754 (0.1%)	0.91	19/17355 (0.1%)

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
2	B	0	1
3	C	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GLU	CG-CD	6.19	1.61	1.51
2	B	118	GLU	CG-CD	5.92	1.60	1.51
1	A	616	CYS	CB-SG	-5.88	1.72	1.81
1	A	249	ALA	CA-CB	-5.52	1.40	1.52
2	B	271[A]	TYR	C-N	5.43	1.46	1.34
2	B	271[B]	TYR	C-N	5.43	1.46	1.34
4	D	53	PHE	CE1-CZ	5.39	1.47	1.37
2	B	139	GLU	CG-CD	5.29	1.59	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	387	ARG	NE-CZ-NH1	-9.56	115.52	120.30
1	A	214	LEU	CA-CB-CG	-8.58	95.57	115.30
3	C	176	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	18	ARG	NE-CZ-NH2	-7.26	116.67	120.30
3	C	176	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	5	ARG	NE-CZ-NH2	-6.50	117.05	120.30
3	C	75	SER	CB-CA-C	-6.17	98.37	110.10
1	A	12	ALA	C-N-CA	-6.15	109.39	122.30
1	A	819	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	152	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	228	GLY	N-CA-C	5.72	127.39	113.10
1	A	15	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	487	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	819	ARG	CG-CD-NE	-5.42	100.42	111.80
2	B	387	ARG	NE-CZ-NH2	5.32	122.96	120.30
3	C	98	LEU	CB-CG-CD2	5.30	120.02	111.00
2	B	122	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	909	HIS	CB-CA-C	-5.21	99.97	110.40
1	A	676	ASP	CB-CG-OD1	5.14	122.92	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	268	ILE	Peptide
3	C	199	VAL	Peptide

## 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	7229	0	7104	120	0
2	B	3079	0	3004	56	0
3	C	1433	0	1434	15	0
4	D	749	0	706	2	0
5	A	44	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	25	0	0	3	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	B	53	0	31	3	0
8	B	31	0	19	5	0
9	D	1	0	0	0	0
10	A	557	0	0	17	2
10	B	163	0	0	4	0
10	C	119	0	0	4	0
10	D	66	0	0	1	0
All	All	13569	0	12324	189	2

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 8.

All (189) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:819:ARG:HH12	1:A:909:HIS:CE1	1.38	1.41
2:B:172:HIS:NE2	8:B:406:FMN:C8M	1.79	1.41
1:A:819:ARG:NH1	1:A:909:HIS:CE1	2.11	1.16
2:B:172:HIS:NE2	8:B:406:FMN:HM83	0.83	1.15
2:B:172:HIS:CD2	8:B:406:FMN:HM83	1.84	1.13
1:A:693:THR:HG22	6:A:2559:SO4:O2	1.43	1.12
1:A:102:ASN:HB2	10:A:1443:HOH:O	1.52	1.07
1:A:768:GLU:HB2	10:A:1451:HOH:O	1.64	0.97
1:A:368:ARG:HD2	10:A:1327:HOH:O	1.66	0.95
1:A:918:ARG:HG3	1:A:918:ARG:HH11	1.31	0.95
2:B:172:HIS:CE1	8:B:406:FMN:HM83	2.01	0.95
1:A:888:ALA:O	1:A:938:THR:HG23	1.67	0.94
1:A:889:LEU:HD23	1:A:925:ILE:HD11	1.48	0.94
3:C:99:ASP:HB2	10:C:714:HOH:O	1.71	0.88
1:A:693:THR:CG2	6:A:2559:SO4:O2	2.23	0.87
3:C:37:PHE:O	3:C:93:GLU:HG2	1.76	0.85
2:B:172:HIS:HD1	2:B:173:ASP:H	1.24	0.85
1:A:102:ASN:CB	10:A:1443:HOH:O	2.18	0.82
2:B:387:ARG:HG3	2:B:387:ARG:HH11	1.44	0.81
1:A:292:ASN:HD22	1:A:294:SER:H	1.26	0.81
2:B:384:ALA:O	2:B:387:ARG:HD3	1.82	0.80
1:A:830:ASP:OD1	1:A:909:HIS:CD2	2.35	0.80
1:A:15:ARG:HD3	1:A:161:GLU:OE2	1.81	0.79
1:A:15:ARG:CD	1:A:161:GLU:OE2	2.32	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:287:ASP:OD1	10:B:656:HOH:O	2.04	0.75
1:A:226:PRO:HB2	10:A:1287:HOH:O	1.88	0.72
1:A:819:ARG:NH1	1:A:909:HIS:ND1	2.28	0.71
1:A:736:ARG:NH2	1:A:963:ASP:O	2.17	0.71
1:A:696:ALA:HB3	10:C:217:HOH:O	1.91	0.70
2:B:172:HIS:HD1	2:B:173:ASP:N	1.89	0.70
1:A:249:ALA:HB1	10:A:966:HOH:O	1.91	0.70
1:A:685:ASP:HB2	10:A:1424:HOH:O	1.92	0.69
1:A:292:ASN:ND2	1:A:294:SER:H	1.90	0.69
2:B:369:HIS:HD2	10:B:625:HOH:O	1.77	0.68
1:A:938:THR:HG22	1:A:939:PRO:HD2	1.76	0.68
1:A:243:GLN:OE1	1:A:413:HIS:HE1	1.77	0.68
1:A:248:THR:O	1:A:249:ALA:HB3	1.94	0.67
1:A:819:ARG:NH1	1:A:909:HIS:HE1	1.87	0.66
2:B:210:LYS:HD2	2:B:211:THR:H	1.61	0.66
1:A:750:ASN:ND2	1:A:773:ARG:HH12	1.93	0.66
1:A:819:ARG:CZ	1:A:909:HIS:CE1	2.80	0.65
1:A:889:LEU:HD23	1:A:925:ILE:CD1	2.27	0.64
1:A:382:PRO:HG2	1:A:404:VAL:HG12	1.81	0.63
1:A:842:MET:O	1:A:845:VAL:HG12	1.98	0.63
1:A:918:ARG:CG	1:A:918:ARG:HH11	2.08	0.62
3:C:37:PHE:O	3:C:93:GLU:CG	2.45	0.62
2:B:126:ASN:HB3	2:B:131:VAL:HG22	1.82	0.61
1:A:901:THR:CG2	10:A:1404:HOH:O	2.48	0.61
1:A:125:HIS:HD2	10:A:1346:HOH:O	1.83	0.60
2:B:387:ARG:HH11	2:B:387:ARG:CG	2.08	0.60
1:A:15:ARG:HD2	1:A:161:GLU:OE2	2.01	0.60
1:A:860:ARG:HH21	1:A:863:ASN:HD21	1.49	0.59
1:A:630:THR:O	1:A:693:THR:HB	2.03	0.59
2:B:387:ARG:HG3	2:B:387:ARG:NH1	2.16	0.59
1:A:123:HIS:CD2	1:A:238:HIS:HE1	2.19	0.59
1:A:776:PHE:CE2	1:A:819:ARG:HG3	2.39	0.58
1:A:931:ARG:O	1:A:949:VAL:CG2	2.51	0.58
1:A:114:PRO:HA	2:B:314:ILE:HG13	1.85	0.57
1:A:648:MET:HE2	1:A:648:MET:HA	1.85	0.57
10:A:1091:HOH:O	3:C:182:HIS:HD2	1.89	0.56
1:A:932:ILE:HA	1:A:949:VAL:HG23	1.88	0.55
2:B:111:HIS:HD2	2:B:156:TYR:O	1.89	0.55
1:A:815:MET:HE2	1:A:816:HIS:HD2	1.72	0.55
10:A:1191:HOH:O	2:B:277:LYS:HE2	2.07	0.55
3:C:137:CYS:HB2	3:C:156:LEU:HD23	1.89	0.54
1:A:830:ASP:OD2	1:A:909:HIS:NE2	2.41	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:887:ALA:HB1	1:A:938:THR:HG21	1.88	0.54
1:A:821:GLU:OE2	1:A:913:SER:HB2	2.08	0.54
1:A:750:ASN:HD22	1:A:773:ARG:HH12	1.56	0.53
1:A:868:ARG:O	1:A:926:LYS:O	2.26	0.53
2:B:69:ARG:HD2	2:B:71:ASN:OD1	2.09	0.53
1:A:742:LEU:HD21	1:A:798:VAL:HG22	1.89	0.53
2:B:7:HIS:CE1	2:B:174:HIS:CE1	2.96	0.53
1:A:7:SER:OG	1:A:10:GLN:HG3	2.08	0.53
1:A:511:TYR:CZ	2:B:7:HIS:HB2	2.43	0.53
1:A:582:HIS:CD2	1:A:601:TYR:OH	2.62	0.53
1:A:829:GLN:HG2	1:A:909:HIS:NE2	2.24	0.52
1:A:64:PHE:HB3	1:A:71:PRO:HD2	1.91	0.52
1:A:918:ARG:HG3	1:A:918:ARG:NH1	2.08	0.52
2:B:93:GLU:HG2	10:B:459:HOH:O	2.08	0.52
1:A:816:HIS:O	1:A:819:ARG:HD3	2.09	0.52
1:A:648:MET:CE	1:A:648:MET:HA	2.40	0.52
1:A:173:GLN:C	1:A:174:ILE:HD13	2.30	0.52
2:B:172:HIS:NE2	8:B:406:FMN:C8	2.67	0.51
2:B:333:ASP:HB2	2:B:395:ASP:HA	1.92	0.51
1:A:916:LEU:HD22	1:A:954:LEU:HD12	1.93	0.51
1:A:815:MET:HE2	1:A:816:HIS:CD2	2.45	0.51
1:A:871:LEU:HD13	1:A:952:LEU:HD11	1.93	0.51
3:C:94:ASN:HB3	3:C:97:LEU:HD22	1.91	0.51
1:A:616:CYS:HB2	1:A:914:PRO:HG2	1.94	0.50
2:B:110:ALA:HB1	2:B:115:ASP:HB3	1.93	0.50
3:C:11:PRO:HD2	3:C:34:GLU:OE2	2.11	0.50
1:A:901:THR:HG22	10:A:1404:HOH:O	2.10	0.50
1:A:578:MET:HG2	1:A:627:ASP:OD2	2.12	0.50
2:B:360:THR:HB	2:B:361:PRO:HD3	1.94	0.50
2:B:39:LEU:HD13	2:B:368:ALA:HA	1.93	0.49
1:A:387:HIS:HE1	1:A:393:LYS:O	1.95	0.49
2:B:64:ASN:HA	7:B:405:FAD:C6	2.42	0.49
1:A:635:GLU:OE2	1:A:686:ARG:NH1	2.45	0.49
2:B:7:HIS:HE1	2:B:174:HIS:CE1	2.29	0.49
1:A:656:LEU:HD23	1:A:681:ARG:HB2	1.94	0.49
2:B:388:PHE:HB2	10:D:1110:HOH:O	2.12	0.49
2:B:111:HIS:CE1	2:B:265:SER:OG	2.66	0.49
1:A:173:GLN:O	1:A:174:ILE:HD13	2.12	0.49
2:B:91:LEU:HD21	2:B:179:PHE:CZ	2.48	0.49
3:C:40:GLN:HA	3:C:89:LEU:O	2.12	0.48
1:A:696:ALA:CB	10:C:217:HOH:O	2.55	0.48
2:B:202:ASP:OD1	2:B:202:ASP:C	2.52	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:18:LYS:HG3	4:D:60:SER:OG	2.14	0.48
2:B:387:ARG:CG	2:B:387:ARG:NH1	2.71	0.48
1:A:123:HIS:HE1	1:A:560:ALA:O	1.96	0.48
1:A:909:HIS:O	1:A:921:GLY:CA	2.61	0.48
1:A:637:ARG:HG3	1:A:686:ARG:HG2	1.96	0.48
1:A:901:THR:HG23	10:A:1404:HOH:O	2.14	0.47
6:A:2559:SO4:O1	10:A:1504:HOH:O	2.20	0.47
1:A:819:ARG:NH2	1:A:909:HIS:CE1	2.83	0.47
1:A:249:ALA:HB2	5:A:965:NAD:PA	2.55	0.46
2:B:349:ASN:HB2	2:B:367:LEU:HD22	1.98	0.46
1:A:819:ARG:HH22	1:A:909:HIS:CE1	2.34	0.46
3:C:157:ALA:O	3:C:182:HIS:HE1	1.98	0.46
3:C:136:SER:OG	3:C:156:LEU:HD22	2.15	0.46
1:A:904:GLU:HG3	1:A:931:ARG:HH22	1.79	0.46
1:A:931:ARG:O	1:A:949:VAL:HG21	2.16	0.46
1:A:152:ARG:HD3	3:C:142:HIS:CD2	2.51	0.46
3:C:99:ASP:CB	10:C:714:HOH:O	2.45	0.46
1:A:590:GLU:OE1	2:B:113:LEU:HD12	2.16	0.45
3:C:44:ARG:HD2	3:C:86:GLU:HG3	1.98	0.45
2:B:381:ALA:N	2:B:382:PRO:CD	2.79	0.45
1:A:385:HIS:O	1:A:389:GLN:HG3	2.16	0.45
1:A:881:LEU:HD12	10:A:1295:HOH:O	2.16	0.45
3:C:11:PRO:HG2	3:C:120:SER:HB3	1.99	0.45
2:B:174:HIS:CD2	10:B:673:HOH:O	2.70	0.45
1:A:421:LEU:HD13	1:A:426:SER:HB3	1.99	0.45
2:B:13:ASN:ND2	2:B:184:ASN:HD21	2.15	0.45
1:A:734:ARG:HA	1:A:734:ARG:HD3	1.68	0.45
2:B:64:ASN:HA	7:B:405:FAD:C5X	2.48	0.44
2:B:357:PHE:HB3	7:B:405:FAD:C2	2.47	0.44
1:A:830:ASP:OD1	1:A:909:HIS:HD2	1.93	0.44
2:B:123:VAL:HG23	2:B:162:THR:HG22	2.00	0.44
1:A:528:ALA:O	1:A:532:ILE:HG13	2.18	0.44
2:B:367:LEU:O	2:B:371:ILE:HG13	2.18	0.44
1:A:249:ALA:HB1	1:A:250:ALA:H	1.63	0.44
2:B:289:TYR:HA	4:D:19:TYR:CD2	2.52	0.44
1:A:931:ARG:O	1:A:949:VAL:HG22	2.18	0.43
1:A:477:HIS:NE2	10:A:1498:HOH:O	1.70	0.43
1:A:249:ALA:HB2	5:A:965:NAD:O3	2.18	0.43
1:A:134:GLY:O	1:A:139:GLY:HA3	2.17	0.43
1:A:486:GLN:NE2	1:A:517:ALA:HB1	2.33	0.43
1:A:918:ARG:CG	1:A:918:ARG:NH1	2.74	0.43
3:C:44:ARG:CD	3:C:86:GLU:HG3	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:ALA:HB2	5:A:965:NAD:C5B	2.49	0.43
1:A:901:THR:HA	1:A:902:PRO:HD3	1.86	0.43
2:B:202:ASP:HB3	2:B:207:THR:HG21	2.00	0.43
2:B:270:VAL:HG22	2:B:271[B]:TYR:N	2.33	0.43
1:A:629:SER:HB3	1:A:726:ALA:HA	1.99	0.43
1:A:735:SER:O	1:A:739:ILE:HG12	2.18	0.43
2:B:265:SER:O	2:B:269:HIS:HA	2.18	0.43
2:B:106:VAL:HG13	2:B:106:VAL:O	2.17	0.42
2:B:333:ASP:OD2	2:B:387:ARG:NH1	2.33	0.42
1:A:387:HIS:HD2	10:A:975:HOH:O	2.01	0.42
2:B:13:ASN:HD22	2:B:184:ASN:HD21	1.67	0.42
1:A:830:ASP:CG	1:A:909:HIS:HE2	2.23	0.42
2:B:52:GLU:HG2	2:B:56:LEU:HA	2.02	0.42
2:B:182:LYS:HD2	2:B:182:LYS:HA	1.86	0.42
1:A:885:GLU:HG2	1:A:909:HIS:HA	2.01	0.42
1:A:819:ARG:NH1	1:A:826:ILE:HD12	2.35	0.42
1:A:227:SER:HB2	1:A:228:GLY:H	1.63	0.42
1:A:137:PRO:HD3	1:A:166:LEU:HG	2.02	0.42
2:B:91:LEU:HD21	2:B:179:PHE:HZ	1.84	0.41
1:A:909:HIS:HB3	1:A:911:TYR:CE1	2.55	0.41
1:A:248:THR:O	1:A:249:ALA:CB	2.64	0.41
2:B:111:HIS:HE1	2:B:265:SER:OG	2.03	0.41
1:A:776:PHE:CZ	1:A:819:ARG:HG3	2.55	0.41
1:A:865:ARG:HB3	1:A:867:ASP:OD1	2.21	0.41
1:A:830:ASP:CG	1:A:909:HIS:NE2	2.74	0.41
1:A:867:ASP:N	1:A:867:ASP:OD1	2.47	0.41
2:B:122:ARG:HD3	2:B:122:ARG:HH11	1.59	0.41
1:A:840:ALA:HA	1:A:871:LEU:HB2	2.02	0.41
1:A:704:GLU:HG3	1:A:708:GLN:NE2	2.36	0.41
1:A:869:LYS:HA	1:A:925:ILE:O	2.20	0.41
1:A:249:ALA:HB2	5:A:965:NAD:O2A	2.21	0.41
1:A:582:HIS:HE1	1:A:627:ASP:OD2	2.04	0.41
1:A:913:SER:HA	1:A:914:PRO:HD2	1.89	0.41
2:B:110:ALA:CB	2:B:115:ASP:HB3	2.51	0.41
1:A:883:LEU:HD11	1:A:947:VAL:HG11	2.02	0.40
1:A:776:PHE:O	1:A:819:ARG:HB2	2.20	0.40
1:A:794:VAL:O	1:A:798:VAL:HG23	2.19	0.40
1:A:223:LEU:HD12	1:A:226:PRO:HB3	2.04	0.40
2:B:102:SER:O	2:B:168:GLY:HA3	2.21	0.40

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	Distance(Å)	Clash(Å)
10:A:1013:HOH:O	10:A:1013:HOH:O[9_555]	1.63	0.57
10:A:1390:HOH:O	10:A:1390:HOH:O[10_665]	1.81	0.39

## 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%)	932 (97%)	25 (3%)	4 (0%)	43	52
2	B	396/404 (98%)	382 (96%)	14 (4%)	0	100	100
3	C	193/203 (95%)	186 (96%)	7 (4%)	0	100	100
4	D	89/99 (90%)	86 (97%)	3 (3%)	0	100	100
All	All	1639/1670 (98%)	1586 (97%)	49 (3%)	4 (0%)	56	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	228	GLY
1	A	406	ALA
1	A	71	PRO

### 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	747/747 (100%)	704 (94%)	43 (6%)	28	36
2	B	318/319 (100%)	306 (96%)	12 (4%)	44	59
3	C	143/151 (95%)	133 (93%)	10 (7%)	21	26
4	D	75/81 (93%)	74 (99%)	1 (1%)	80	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1283/1298 (99%)	1217 (95%)	66 (5%)	33	43

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	68	VAL
1	A	80	ARG
1	A	123	HIS
1	A	124	VAL
1	A	170	SER
1	A	214	LEU
1	A	218	ARG
1	A	327	THR
1	A	333	LEU
1	A	382	PRO
1	A	399	SER
1	A	466	LEU
1	A	474	ASP
1	A	515	SER
1	A	518	ASN
1	A	535	VAL
1	A	541	PRO
1	A	578	MET
1	A	616	CYS
1	A	645	LEU
1	A	684	GLU
1	A	693	THR
1	A	751	ASP
1	A	753	PHE
1	A	761	VAL
1	A	786	ILE
1	A	789	TRP
1	A	792	LEU
1	A	815	MET
1	A	819	ARG
1	A	848	LYS
1	A	850	LYS
1	A	871	LEU
1	A	874	VAL
1	A	889	LEU
1	A	890	VAL

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Mol	Chain	Res	Type
1	A	901	THR
1	A	918	ARG
1	A	932	ILE
1	A	938	THR
1	A	949	VAL
1	A	954	LEU
2	B	39	LEU
2	B	91	LEU
2	B	97	TYR
2	B	131	VAL
2	B	172	HIS
2	B	202	ASP
2	B	232	LEU
2	B	277	LYS
2	B	286	ILE
2	B	311	LEU
2	B	332	MET
2	B	387	ARG
3	C	6	GLN
3	C	33	ARG
3	C	50	THR
3	C	73	ASP
3	C	93	GLU
3	C	97	LEU
3	C	98	LEU
3	C	146	PHE
3	C	156	LEU
3	C	199	VAL
4	D	49	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	123	HIS
1	A	125	HIS
1	A	238	HIS
1	A	292	ASN
1	A	387	HIS
1	A	413	HIS
1	A	486	GLN
1	A	518	ASN

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Mol	Chain	Res	Type
1	A	582	HIS
1	A	750	ASN
1	A	816	HIS
1	A	829	GLN
1	A	863	ASN
1	A	912	ASN
2	B	13	ASN
2	B	111	HIS
2	B	174	HIS
2	B	267	HIS
2	B	344	GLN
2	B	369	HIS
3	C	6	GLN
3	C	111	GLN
3	C	118	ASN
3	C	158	ASN
3	C	182	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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	2559	-	4,4,4	0.27	0	6,6,6	0.20	0
6	SO4	A	2560	-	4,4,4	0.56	0	6,6,6	0.33	0
6	SO4	A	2563	-	4,4,4	0.13	0	6,6,6	0.30	0
6	SO4	A	2565	-	4,4,4	0.17	0	6,6,6	0.14	0
6	SO4	A	2567	-	4,4,4	0.46	0	6,6,6	0.36	0
5	NAD	A	965	-	48,48,48	2.04	11 (22%)	73,73,73	1.98	11 (15%)
6	SO4	B	2561	-	4,4,4	0.30	0	6,6,6	0.44	0
6	SO4	B	2562	-	4,4,4	0.10	0	6,6,6	0.10	0
7	FAD	B	405	-	58,58,58	1.55	10 (17%)	85,89,89	1.65	13 (15%)
8	FMN	B	406	-	33,33,33	1.73	11 (33%)	46,50,50	2.14	12 (26%)
6	SO4	C	2564	-	4,4,4	0.79	0	6,6,6	0.23	0
6	SO4	D	2566	-	4,4,4	0.18	0	6,6,6	0.17	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	2559	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2560	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2563	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2565	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2567	-	-	0/0/0/0	0/0/0/0
5	NAD	A	965	-	-	0/30/62/62	0/3/5/5
6	SO4	B	2561	-	-	0/0/0/0	0/0/0/0
6	SO4	B	2562	-	-	0/0/0/0	0/0/0/0
7	FAD	B	405	-	-	0/34/50/50	0/1/6/6
8	FMN	B	406	-	-	0/18/18/18	0/0/3/3
6	SO4	C	2564	-	-	0/0/0/0	0/0/0/0
6	SO4	D	2566	-	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	965	NAD	C2B-C1B	-6.26	1.44	1.53
5	A	965	NAD	C2N-N1N	5.62	1.42	1.35
5	A	965	NAD	O7N-C7N	5.40	1.36	1.24
7	B	405	FAD	C5X-N5	4.96	1.43	1.35
5	A	965	NAD	O4B-C1B	4.92	1.48	1.41
5	A	965	NAD	C4A-N9A	-3.97	1.32	1.37
8	B	406	FMN	C5A-N5	3.80	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	405	FAD	C10-N1	3.47	1.41	1.35
7	B	405	FAD	C9A-N10	3.31	1.43	1.38
7	B	405	FAD	C4X-N5	3.30	1.43	1.36
7	B	405	FAD	C2-N3	3.29	1.43	1.37
8	B	406	FMN	P-O1P	3.25	1.62	1.51
5	A	965	NAD	C8A-N9A	-3.22	1.31	1.36
8	B	406	FMN	C1'-C2'	3.19	1.54	1.51
7	B	405	FAD	PA-O3P	-3.10	1.54	1.59
5	A	965	NAD	C5A-N7A	-2.88	1.29	1.40
7	B	405	FAD	C4A-N9A	-2.72	1.33	1.37
8	B	406	FMN	O5'-C5'	-2.71	1.33	1.44
8	B	406	FMN	C9A-C5A	-2.44	1.37	1.42
8	B	406	FMN	C5'-C4'	2.41	1.55	1.51
7	B	405	FAD	O4'-C4'	2.34	1.48	1.43
8	B	406	FMN	C4-N3	2.32	1.41	1.37
5	A	965	NAD	O4B-C4B	-2.26	1.39	1.45
8	B	406	FMN	P-O5'	-2.26	1.52	1.60
7	B	405	FAD	C2-N1	2.24	1.41	1.35
8	B	406	FMN	C1'-N10	2.23	1.50	1.48
7	B	405	FAD	C4-N3	2.21	1.40	1.37
5	A	965	NAD	O4D-C1D	2.18	1.44	1.41
5	A	965	NAD	PN-O5D	-2.18	1.52	1.60
5	A	965	NAD	PN-O3	2.15	1.64	1.60
8	B	406	FMN	C4A-C10	-2.14	1.37	1.40
8	B	406	FMN	C4-C4A	-2.02	1.37	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	965	NAD	N3A-C2A-N1A	-7.95	122.06	128.71
8	B	406	FMN	C2-N1-C10	6.04	121.06	114.98
7	B	405	FAD	N3A-C2A-N1A	-5.99	123.70	128.71
5	A	965	NAD	C2D-C1D-N1N	-5.73	104.16	113.86
8	B	406	FMN	P-O5'-C5'	5.42	133.85	118.19
7	B	405	FAD	C4B-O4B-C1B	-5.11	104.20	109.75
5	A	965	NAD	C4A-C5A-N7A	-5.01	105.23	109.52
5	A	965	NAD	O4B-C1B-N9A	-4.93	103.86	108.44
8	B	406	FMN	C4A-N5-C5A	4.59	121.84	116.69
5	A	965	NAD	O4D-C1D-N1N	-4.49	103.36	107.95
7	B	405	FAD	C4X-N5-C5X	4.40	121.64	116.69
8	B	406	FMN	O2P-P-O5'	4.40	118.80	106.65
7	B	405	FAD	C4A-C5A-N7A	-4.34	105.80	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	965	NAD	O4B-C1B-C2B	-4.25	100.26	106.77
8	B	406	FMN	O3P-P-O5'	-4.05	95.46	106.65
8	B	406	FMN	O3P-P-O1P	-3.94	97.55	110.44
8	B	406	FMN	O2P-P-O1P	3.69	122.52	110.44
7	B	405	FAD	C4X-C10-N10	-3.61	118.71	120.51
7	B	405	FAD	N3A-C4A-N9A	3.60	131.92	125.43
5	A	965	NAD	O4D-C1D-C2D	-3.50	101.41	106.77
7	B	405	FAD	O4B-C1B-C2B	-2.94	102.27	106.77
5	A	965	NAD	N3A-C4A-N9A	2.89	130.64	125.43
7	B	405	FAD	C5A-C4A-N3A	-2.84	119.53	125.70
5	A	965	NAD	C5A-C4A-N3A	-2.66	119.91	125.70
7	B	405	FAD	C9A-C5X-N5	-2.62	118.35	122.37
7	B	405	FAD	C4-N3-C2	-2.61	120.03	125.39
8	B	406	FMN	C4-N3-C2	-2.57	120.12	125.39
5	A	965	NAD	C2A-N1A-C6A	2.43	123.17	118.77
8	B	406	FMN	C4A-C10-N1	-2.42	120.31	122.73
8	B	406	FMN	C9A-C5A-N5	-2.29	118.86	122.37
5	A	965	NAD	C5B-C4B-C3B	-2.26	106.16	115.21
7	B	405	FAD	C4-C4X-C10	2.16	120.44	116.95
7	B	405	FAD	C1'-N10-C9A	2.13	120.95	118.87
7	B	405	FAD	C5X-C9A-N10	2.10	118.87	116.80
8	B	406	FMN	C5'-C4'-C3'	2.04	115.91	112.06
8	B	406	FMN	C4-C4A-C10	2.02	120.22	116.95

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	963/964 (99%)	-0.34	8 (0%) 83 90	11, 25, 47, 67	0
2	B	397/404 (98%)	-0.36	2 (0%) 88 94	15, 28, 42, 62	0
3	C	195/203 (96%)	-0.50	0 100 100	14, 24, 44, 56	0
4	D	91/99 (91%)	-0.62	0 100 100	14, 23, 43, 55	0
All	All	1646/1670 (98%)	-0.38	10 (0%) 84 92	11, 26, 46, 67	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	909	HIS	3.1
1	A	694	GLY	3.1
1	A	848	LYS	2.5
1	A	327	THR	2.4
1	A	880	SER	2.3
2	B	202	ASP	2.3
1	A	751	ASP	2.2
1	A	226	PRO	2.1
1	A	866	GLU	2.1
2	B	392	HIS	2.1

### 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
6	SO4	A	2563	5/5	0.31	21.81	76,76,77,77	0
6	SO4	A	2565	5/5	0.65	17.82	161,161,161,162	0
6	SO4	B	2561	5/5	0.20	4.73	59,59,62,63	0
6	SO4	C	2564	5/5	0.15	1.06	33,33,37,40	0
9	ZN	D	100	1/1	0.09	0.72	21,21,21,21	0
7	FAD	B	405	53/53	0.10	0.35	15,25,31,33	0
8	FMN	B	406	31/31	0.09	-0.12	9,15,20,22	0
6	SO4	A	2559	5/5	0.12	-0.15	80,80,80,82	0
5	NAD	A	965	44/44	0.09	-0.49	5,14,18,23	0
6	SO4	A	2560	5/5	0.14	-0.78	50,51,55,55	0
6	SO4	D	2566	5/5	0.06	-1.96	73,73,75,75	0
6	SO4	A	2567	5/5	0.06	-2.62	34,35,36,39	0
6	SO4	B	2562	5/5	0.48	-	156,156,156,156	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.