Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 06:27 PM GMT

PDB ID	:	3ADA
Title	:	Heterotetrameric Sarcosine Oxidase from Corynebacterium sp. U-96 in complex with sulfite
Authors	:	Suzuki, H.; Moriguchi, T.; Ida, K.
Deposited on	:	2010-01-15
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

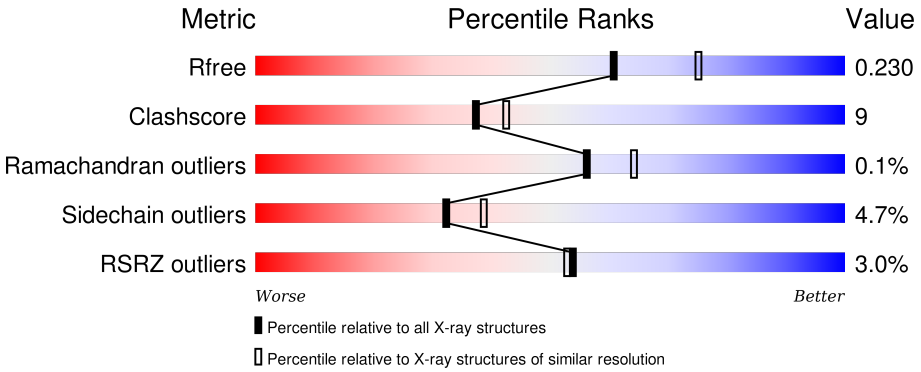
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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 <=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	5%, 81%, 17%
2	B	399	%, 82%, 15%
3	C	203	78%, 15%
4	D	99	80%, 10%, 8%

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
10	ZN	D	100	-	-	X	-
6	SO4	A	2562	-	-	X	-
6	SO4	C	2564	-	-	-	X
8	FMN	B	4	-	-	X	-
9	SO3	B	6244	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 13493 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	397	Total	C	N	O	S	0	0	0
			3057	1948	532	567	10			

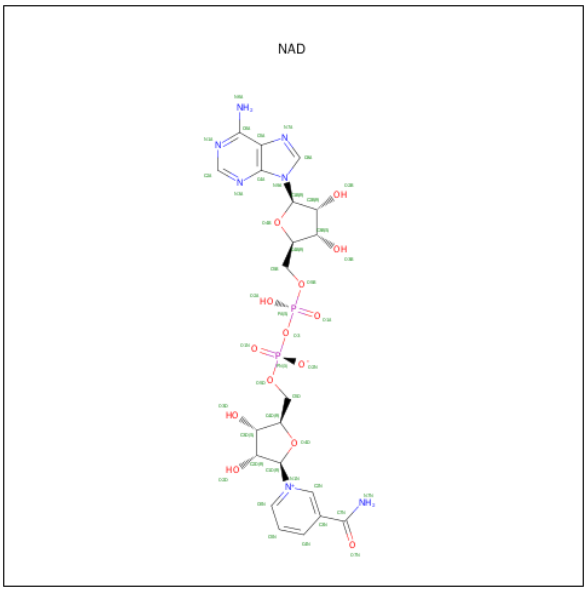
- Molecule 3 is a protein called SARCOSINE OXIDASE GAMMA SUBUNIT.

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.

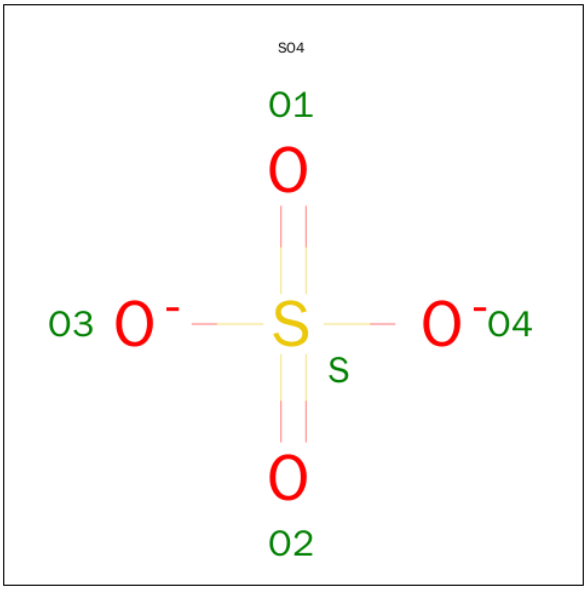
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	91	Total	C	N	O	S	0	0	0
			749	476	135	133	5			

- 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: SO4) (formula: O_4S).



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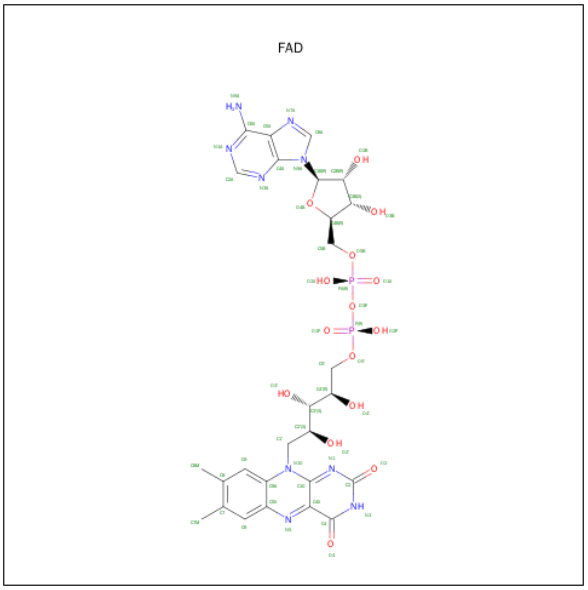
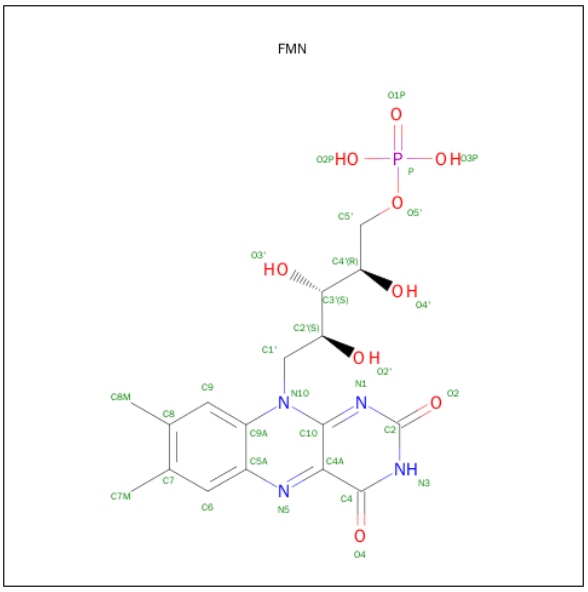
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

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



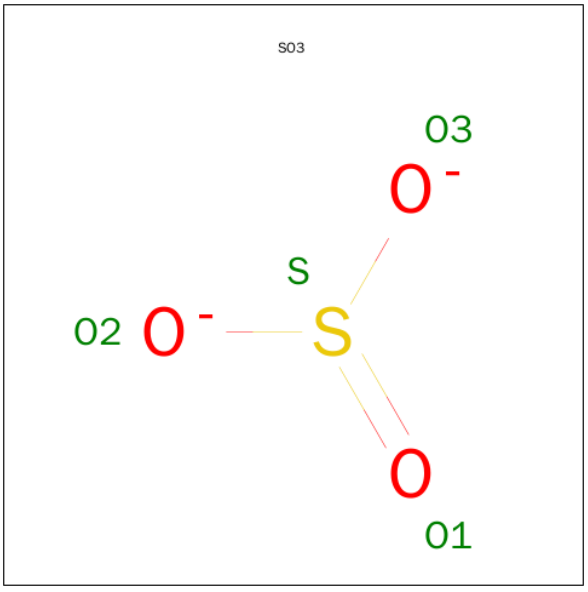
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 53 27 9 15 2	0	0

- 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 SULFITE ION (three-letter code: SO3) (formula: O_3S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	O	S		0	0
			4	3	1			

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

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

- Molecule 11 is water.

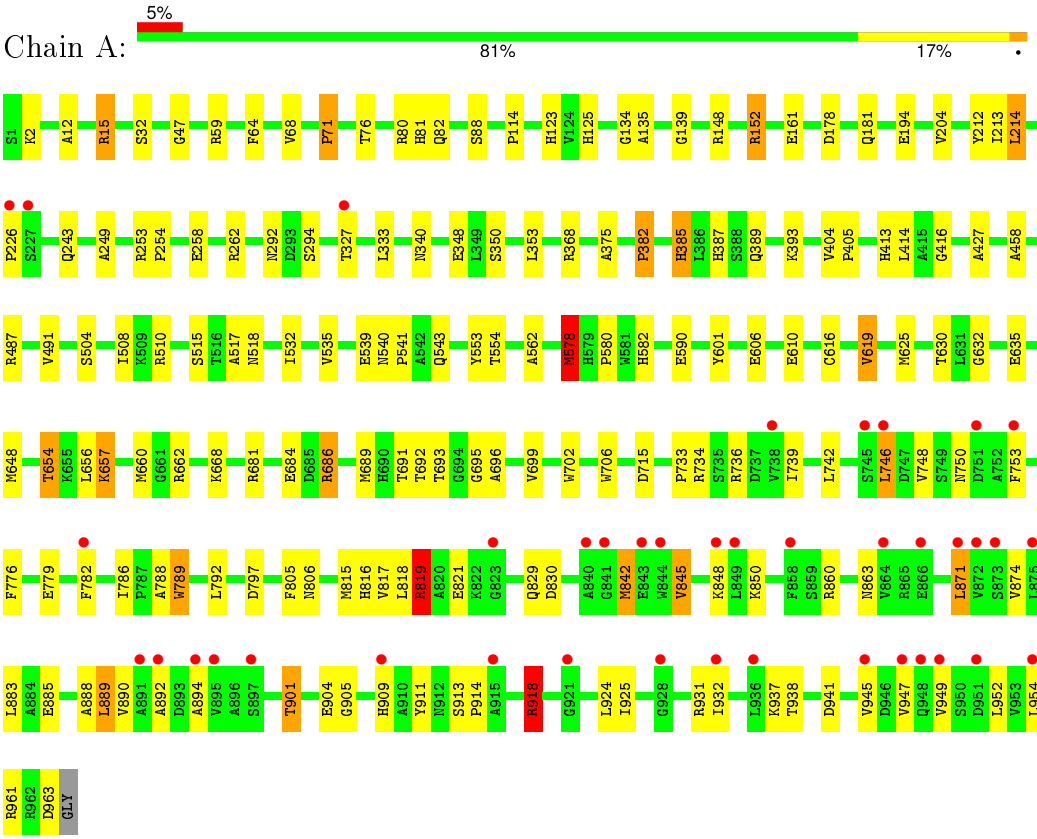
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	552	Total O 552 552	0	0
11	B	139	Total O 139 139	0	0
11	C	114	Total O 114 114	0	0
11	D	47	Total O 47 47	0	0

3 Residue-property plots (i)

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.

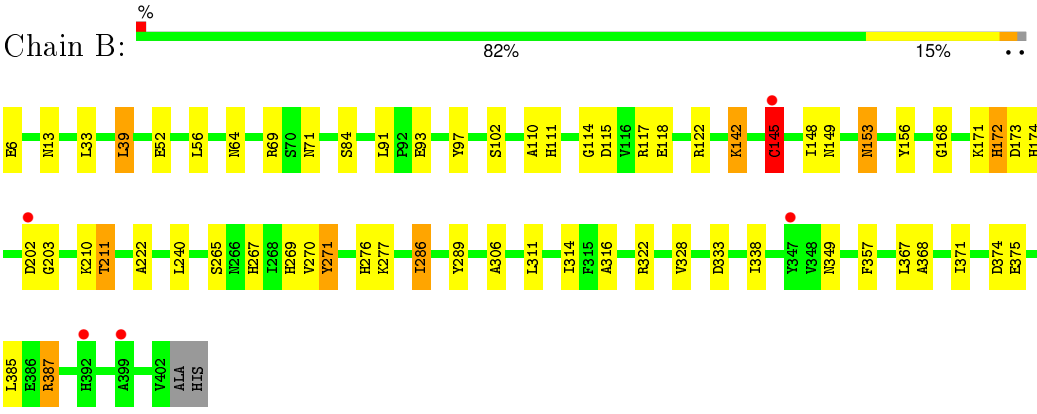
- Molecule 1: SARCOSINE OXIDASE ALPHA SUBUNIT

Chain A:



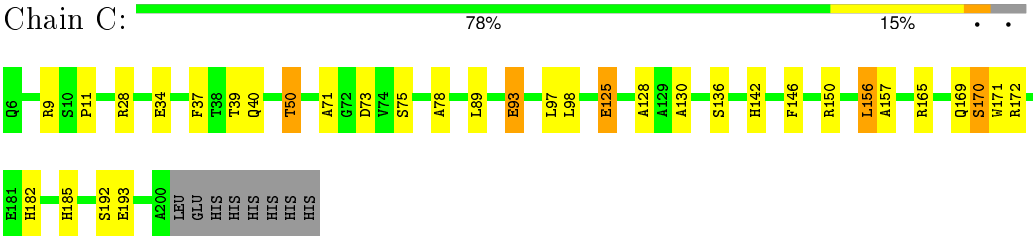
- Molecule 2: SARCOSINE OXIDASE BETA SUBUNIT

Chain B:



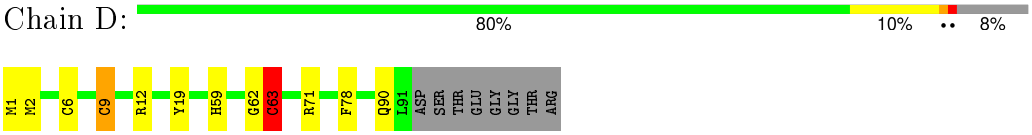
• Molecule 3: SARCOSINE OXIDASE GAMMA SUBUNIT

Chain C:



• Molecule 4: SARCOSINE OXIDASE DELTA SUBUNIT

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	198.80Å 198.80Å 197.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.98 – 2.20 69.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (69.98-2.20) 99.7 (69.98-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	6.82 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.189 , 0.232 0.186 , 0.230	Depositor DCC
R_{free} test set	5786 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 115422 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13493	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAD, FMN, SO3, SO4, 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	1.12	9/7361 (0.1%)	0.95	14/10017 (0.1%)
2	B	1.19	6/3136 (0.2%)	0.92	8/4266 (0.2%)
3	C	1.29	3/1461 (0.2%)	1.11	5/1998 (0.3%)
4	D	1.07	3/772 (0.4%)	0.95	4/1040 (0.4%)
All	All	1.16	21/12730 (0.2%)	0.97	31/17321 (0.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	145	CYS	CB-SG	29.42	2.32	1.82
2	B	145	CYS	CA-CB	7.83	1.71	1.53
4	D	63	CYS	CB-SG	6.72	1.93	1.82
1	A	212	TYR	CD2-CE2	6.52	1.49	1.39
4	D	6	CYS	CB-SG	6.07	1.92	1.82
1	A	348	GLU	CB-CG	5.91	1.63	1.52
1	A	458	ALA	CA-CB	5.82	1.64	1.52
2	B	316	ALA	CA-CB	5.71	1.64	1.52
1	A	553	TYR	CG-CD1	5.69	1.46	1.39
3	C	130	ALA	CA-CB	5.68	1.64	1.52
4	D	6	CYS	CA-CB	5.43	1.65	1.53
1	A	375	ALA	CA-CB	5.29	1.63	1.52
1	A	135	ALA	CA-CB	5.26	1.63	1.52
3	C	128	ALA	CA-CB	5.25	1.63	1.52
3	C	125	GLU	CB-CG	-5.22	1.42	1.52
2	B	271	TYR	CE1-CZ	5.19	1.45	1.38
1	A	258	GLU	CG-CD	5.18	1.59	1.51
2	B	145	CYS	N-CA	5.17	1.56	1.46
2	B	277	LYS	CE-NZ	5.09	1.61	1.49
1	A	350	SER	CB-OG	5.07	1.48	1.42
1	A	788	ALA	CA-CB	5.00	1.62	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	145	CYS	CA-CB-SG	14.70	140.47	114.00
1	A	15	ARG	NE-CZ-NH2	-10.18	115.21	120.30
3	C	176	ARG	NE-CZ-NH2	-9.58	115.51	120.30
2	B	387	ARG	NE-CZ-NH1	-9.28	115.66	120.30
2	B	145	CYS	N-CA-CB	8.15	125.26	110.60
1	A	214	LEU	CA-CB-CG	-7.85	97.25	115.30
1	A	487	ARG	NE-CZ-NH2	-7.67	116.46	120.30
2	B	145	CYS	N-CA-C	-7.25	91.41	111.00
1	A	59	ARG	NE-CZ-NH2	-7.07	116.76	120.30
2	B	322	ARG	NE-CZ-NH1	-6.95	116.83	120.30
1	A	15	ARG	NE-CZ-NH1	6.79	123.69	120.30
3	C	176	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	152	ARG	NE-CZ-NH1	6.74	123.67	120.30
4	D	12	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	819	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	12	ALA	C-N-CA	-6.37	108.92	122.30
2	B	387	ARG	NE-CZ-NH2	6.28	123.44	120.30
3	C	28	ARG	NE-CZ-NH2	-5.94	117.33	120.30
3	C	172	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	148	ARG	NE-CZ-NH1	-5.85	117.37	120.30
2	B	142	LYS	CD-CE-NZ	-5.83	98.29	111.70
3	C	165	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	262	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	918	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	214	LEU	CB-CG-CD1	5.37	120.12	111.00
2	B	117	ARG	NE-CZ-NH2	-5.32	117.64	120.30
4	D	1	MET	CG-SD-CE	-5.17	91.92	100.20
1	A	578	MET	CG-SD-CE	-5.08	92.07	100.20
4	D	9	CYS	CA-CB-SG	5.08	123.14	114.00
1	A	625	MET	CG-SD-CE	5.06	108.29	100.20
4	D	6	CYS	N-CA-CB	5.00	119.61	110.60

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	7229	0	7104	134	0
2	B	3057	0	2982	62	0
3	C	1433	0	1434	26	0
4	D	749	0	708	13	0
5	A	44	0	26	4	0
6	A	30	0	0	5	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	11	0
9	B	4	0	0	2	0
10	D	1	0	0	4	0
11	A	552	0	0	22	0
11	B	139	0	0	6	0
11	C	114	0	0	5	0
11	D	47	0	0	1	0
All	All	13493	0	12304	231	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 9.

All (231) 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:4:FMN:C8M	1.73	1.48
1:A:819:ARG:HH12	1:A:909:HIS:CE1	1.44	1.35
1:A:696:ALA:HB3	6:A:2562:SO4:O3	1.22	1.27
9:B:6244:SO3:S	9:B:6244:SO3:O2	1.99	1.21
2:B:145:CYS:SG	2:B:145:CYS:CB	2.32	1.18
1:A:696:ALA:CB	6:A:2562:SO4:O3	1.92	1.16
1:A:736:ARG:NH2	1:A:963:ASP:O	1.79	1.15
4:D:2:MET:HE1	4:D:78:PHE:CE1	1.84	1.13
2:B:172:HIS:CE1	8:B:4:FMN:HM83	1.83	1.12
2:B:276:HIS:HE1	11:B:452:HOH:O	1.31	1.11
2:B:172:HIS:NE2	8:B:4:FMN:HM83	0.77	1.10
1:A:819:ARG:NH1	1:A:909:HIS:CE1	2.18	1.10
1:A:889:LEU:HD23	1:A:925:ILE:HD11	1.29	1.10
2:B:267:HIS:HD2	11:B:434:HOH:O	1.35	1.08
1:A:15:ARG:HD2	1:A:161:GLU:OE2	1.55	1.07
4:D:2:MET:HE1	4:D:78:PHE:HE1	1.22	1.04
4:D:63:CYS:SG	10:D:100:ZN:ZN	1.49	1.00
2:B:172:HIS:CD2	8:B:4:FMN:HM83	1.97	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:GLN:NE2	3:C:171:TRP:HE1	1.61	0.97
1:A:15:ARG:CD	1:A:161:GLU:OE2	2.13	0.96
3:C:169:GLN:HE21	3:C:171:TRP:HE1	1.04	0.96
4:D:2:MET:CE	4:D:78:PHE:CE1	2.50	0.93
4:D:9:CYS:HG	10:D:100:ZN:ZN	0.81	0.87
1:A:696:ALA:HB1	11:A:1259:HOH:O	1.75	0.85
4:D:2:MET:CE	4:D:78:PHE:HE1	1.88	0.85
2:B:93:GLU:HG2	11:B:617:HOH:O	1.76	0.85
1:A:918:ARG:HH11	1:A:918:ARG:HG3	1.41	0.84
1:A:249:ALA:HB1	11:A:966:HOH:O	1.80	0.81
1:A:292:ASN:HD22	1:A:294:SER:H	1.26	0.81
3:C:93:GLU:HG3	11:C:537:HOH:O	1.81	0.80
1:A:830:ASP:OD1	1:A:909:HIS:CD2	2.35	0.79
2:B:286:ILE:HD11	2:B:328:VAL:CG2	2.13	0.79
3:C:37:PHE:O	3:C:93:GLU:HG2	1.84	0.78
1:A:504:SER:O	1:A:508:ILE:HG12	1.84	0.77
3:C:50:THR:HG22	11:C:227:HOH:O	1.83	0.77
1:A:696:ALA:HB3	6:A:2562:SO4:S	2.25	0.76
3:C:37:PHE:O	3:C:93:GLU:CG	2.34	0.75
1:A:80:ARG:NH2	11:A:1487:HOH:O	2.20	0.74
1:A:821:GLU:OE2	1:A:913:SER:HB2	1.88	0.74
1:A:68:VAL:HG21	1:A:554:THR:HG21	1.70	0.74
1:A:292:ASN:ND2	1:A:294:SER:H	1.85	0.73
1:A:249:ALA:HB2	5:A:965:NAD:PA	2.29	0.73
1:A:2:LYS:HE2	1:A:47:GLY:HA3	1.71	0.72
1:A:249:ALA:HB2	5:A:965:NAD:O3	1.89	0.72
1:A:945:VAL:HG13	11:A:1089:HOH:O	1.88	0.72
2:B:286:ILE:HD11	2:B:328:VAL:HG21	1.69	0.72
2:B:333:ASP:OD2	2:B:387:ARG:NH1	2.21	0.72
1:A:889:LEU:HD23	1:A:925:ILE:CD1	2.16	0.71
1:A:657:LYS:HE3	1:A:660:MET:HG3	1.73	0.71
11:A:1436:HOH:O	3:C:185:HIS:HD2	1.74	0.70
1:A:510:ARG:HH21	8:B:4:FMN:C5'	2.06	0.69
1:A:226:PRO:HB2	11:A:1205:HOH:O	1.91	0.69
1:A:819:ARG:NH1	1:A:909:HIS:ND1	2.33	0.68
1:A:931:ARG:O	1:A:949:VAL:CG2	2.41	0.68
1:A:860:ARG:HH21	1:A:863:ASN:HD21	1.41	0.68
1:A:510:ARG:HH21	8:B:4:FMN:H5'1	1.58	0.68
4:D:9:CYS:SG	10:D:100:ZN:ZN	1.83	0.68
1:A:639:LYS:HG3	1:A:715:ASP:OD2	1.95	0.67
1:A:249:ALA:CB	5:A:965:NAD:O2A	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:HD3	1:A:161:GLU:OE2	1.94	0.66
1:A:82:GLN:CG	11:A:1155:HOH:O	2.43	0.66
1:A:931:ARG:O	1:A:949:VAL:HG21	1.96	0.65
2:B:149:ASN:HD21	2:B:153:ASN:HD21	1.42	0.65
3:C:11:PRO:HD2	3:C:34:GLU:OE2	1.96	0.65
4:D:63:CYS:HG	10:D:100:ZN:ZN	1.09	0.64
1:A:82:GLN:HG3	11:A:1155:HOH:O	1.97	0.64
1:A:888:ALA:O	1:A:938:THR:HG23	2.00	0.62
2:B:111:HIS:HD2	2:B:156:TYR:O	1.82	0.61
1:A:243:GLN:OE1	1:A:413:HIS:HE1	1.84	0.60
11:A:1249:HOH:O	3:C:182:HIS:HD2	1.84	0.60
2:B:387:ARG:HG3	2:B:387:ARG:HH11	1.67	0.60
1:A:382:PRO:HG2	1:A:404:VAL:HG12	1.84	0.59
2:B:114:GLY:O	2:B:118:GLU:HG2	2.02	0.59
2:B:6:GLU:HB2	11:B:504:HOH:O	2.01	0.59
1:A:742:LEU:HD21	1:A:797:ASP:HB3	1.83	0.59
3:C:125:GLU:HG3	3:C:170:SER:HB3	1.85	0.59
2:B:172:HIS:HD1	2:B:173:ASP:H	1.50	0.59
1:A:819:ARG:CZ	1:A:909:HIS:CE1	2.86	0.58
1:A:635:GLU:OE2	1:A:686:ARG:NH1	2.36	0.58
1:A:689:MET:HE2	1:A:699:VAL:HG11	1.85	0.58
1:A:689:MET:CE	1:A:699:VAL:HG11	2.33	0.58
1:A:830:ASP:OD1	1:A:909:HIS:HD2	1.82	0.58
1:A:892:ALA:HA	1:A:937:LYS:HD2	1.84	0.57
1:A:125:HIS:HD2	11:A:1065:HOH:O	1.87	0.57
1:A:746:LEU:HD23	11:A:1347:HOH:O	2.05	0.57
3:C:37:PHE:O	3:C:93:GLU:HG3	2.05	0.57
2:B:64:ASN:HA	7:B:1:FAD:C6	2.35	0.56
1:A:883:LEU:HD11	1:A:947:VAL:HG11	1.87	0.56
2:B:384:ALA:O	2:B:387:ARG:HD3	2.05	0.56
1:A:578:MET:HB2	1:A:582:HIS:CE1	2.41	0.56
1:A:387:HIS:HE1	1:A:393:LYS:O	1.89	0.55
3:C:71:ALA:O	3:C:78:ALA:HA	2.06	0.55
1:A:582:HIS:CD2	1:A:601:TYR:OH	2.60	0.55
2:B:172:HIS:HD1	2:B:173:ASP:N	2.06	0.55
1:A:368:ARG:HD2	11:A:1365:HOH:O	2.07	0.55
2:B:39:LEU:HD13	2:B:368:ALA:CB	2.37	0.54
2:B:102:SER:O	2:B:168:GLY:HA3	2.08	0.54
1:A:830:ASP:OD2	1:A:909:HIS:NE2	2.39	0.54
1:A:842:MET:O	1:A:845:VAL:HG12	2.07	0.54
2:B:153:ASN:H	2:B:153:ASN:HD22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:PRO:HG3	11:C:245:HOH:O	2.07	0.54
1:A:616:CYS:SG	1:A:817:VAL:HG11	2.48	0.54
1:A:68:VAL:CG2	1:A:554:THR:HG21	2.38	0.53
1:A:736:ARG:HD3	1:A:748:VAL:O	2.09	0.53
2:B:13:ASN:HD22	2:B:184:ASN:HD21	1.56	0.53
1:A:909:HIS:HB3	1:A:911:TYR:CE1	2.44	0.52
1:A:632:GLY:HA3	1:A:696:ALA:HB2	1.92	0.51
1:A:194:GLU:O	1:A:194:GLU:HG3	2.10	0.51
1:A:539:GLU:HG3	11:A:1273:HOH:O	2.10	0.51
1:A:830:ASP:CG	1:A:909:HIS:HE2	2.13	0.51
1:A:654:THR:OG1	11:A:1390:HOH:O	2.19	0.50
1:A:580:PRO:HG2	3:C:9:ARG:HH12	1.76	0.50
1:A:770:ARG:NH2	11:A:1383:HOH:O	2.44	0.50
3:C:73:ASP:OD2	3:C:75:SER:HB2	2.10	0.50
1:A:616:CYS:HB2	1:A:914:PRO:HG2	1.93	0.50
2:B:202:ASP:OD1	2:B:203:GLY:N	2.45	0.50
1:A:178:ASP:HB2	1:A:181:GLN:HE21	1.76	0.50
2:B:270:VAL:HG22	2:B:271:TYR:N	2.27	0.50
2:B:39:LEU:HD13	2:B:368:ALA:HA	1.94	0.50
3:C:40:GLN:HA	3:C:89:LEU:O	2.11	0.49
2:B:381:ALA:N	2:B:382:PRO:CD	2.75	0.49
2:B:267:HIS:CD2	11:B:434:HOH:O	2.25	0.49
1:A:387:HIS:HD2	11:A:968:HOH:O	1.94	0.49
2:B:13:ASN:ND2	2:B:184:ASN:HD21	2.09	0.49
3:C:169:GLN:NE2	3:C:171:TRP:NE1	2.44	0.48
3:C:157:ALA:O	3:C:182:HIS:HE1	1.96	0.48
2:B:240:LEU:HD23	2:B:385:LEU:HD21	1.94	0.48
2:B:222:ALA:HB2	2:B:371:ILE:HD11	1.95	0.48
1:A:829:GLN:CD	1:A:909:HIS:CE1	2.87	0.48
3:C:176:ARG:HD3	11:C:545:HOH:O	2.13	0.48
1:A:510:ARG:NH2	8:B:4:FMN:C5'	2.77	0.48
1:A:696:ALA:CB	6:A:2562:SO4:S	2.96	0.47
1:A:829:GLN:HG2	1:A:909:HIS:NE2	2.29	0.47
1:A:648:MET:HE2	1:A:648:MET:HA	1.96	0.47
1:A:656:LEU:HD13	1:A:662:ARG:HB2	1.96	0.47
6:A:2562:SO4:O1	3:C:176:ARG:NH2	2.48	0.47
2:B:387:ARG:CG	2:B:387:ARG:HH11	2.26	0.47
1:A:776:PHE:O	1:A:819:ARG:HB2	2.14	0.47
2:B:64:ASN:HA	7:B:1:FAD:C5X	2.45	0.47
2:B:210:LYS:HE3	2:B:211:THR:O	2.14	0.47
2:B:71:ASN:O	2:B:122:ARG:HD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HB3	1:A:353:LEU:HD22	1.97	0.47
8:B:4:FMN:N5	9:B:6244:SO3:S	2.88	0.47
1:A:82:GLN:HG2	11:A:1155:HOH:O	2.13	0.46
2:B:52:GLU:HG2	2:B:56:LEU:HA	1.97	0.46
1:A:739:ILE:HG13	1:A:782:PHE:CG	2.49	0.46
2:B:145:CYS:HB3	2:B:148:ILE:HG13	1.97	0.46
1:A:249:ALA:HB2	5:A:965:NAD:O2A	2.09	0.46
1:A:606:GLU:HA	1:A:610:GLU:OE1	2.16	0.46
1:A:385:HIS:O	1:A:389:GLN:HG3	2.14	0.46
1:A:81:HIS:NE2	1:A:226:PRO:HD2	2.31	0.46
1:A:789:TRP:CZ3	3:C:37:PHE:HA	2.51	0.46
1:A:860:ARG:NH2	1:A:863:ASN:HD21	2.11	0.46
1:A:510:ARG:NH2	8:B:4:FMN:H5'2	2.31	0.45
2:B:33:LEU:HD21	2:B:56:LEU:HD11	1.98	0.45
2:B:265:SER:O	2:B:269:HIS:HD2	1.98	0.45
1:A:152:ARG:HD3	3:C:142:HIS:CD2	2.52	0.45
1:A:733:PRO:HD3	1:A:779:GLU:OE1	2.17	0.45
1:A:889:LEU:CD2	1:A:925:ILE:HD11	2.22	0.45
2:B:286:ILE:HD11	2:B:328:VAL:HG23	1.97	0.45
2:B:265:SER:O	2:B:269:HIS:HA	2.17	0.45
1:A:510:ARG:HH21	8:B:4:FMN:H5'2	1.80	0.45
1:A:668:LYS:HD3	1:A:702:TRP:CH2	2.52	0.45
2:B:172:HIS:CE1	8:B:4:FMN:C8M	2.65	0.44
2:B:69:ARG:HD2	2:B:71:ASN:OD1	2.17	0.44
1:A:776:PHE:CZ	1:A:819:ARG:HG3	2.52	0.44
1:A:562:ALA:HB1	2:B:306:ALA:HA	2.00	0.44
2:B:357:PHE:HB3	7:B:1:FAD:C2	2.48	0.44
3:C:192:SER:O	3:C:193:GLU:C	2.55	0.44
1:A:630:THR:HB	1:A:693:THR:HG23	1.98	0.44
1:A:416:GLY:HA2	1:A:427:ALA:HA	1.99	0.44
1:A:253:ARG:HB2	1:A:254:PRO:HD2	1.98	0.44
1:A:805:PHE:O	1:A:806:ASN:HB3	2.17	0.44
1:A:871:LEU:HD13	1:A:952:LEU:HD11	1.99	0.44
2:B:171:LYS:HA	2:B:171:LYS:HD2	1.67	0.44
1:A:405:PRO:HB2	1:A:414:LEU:HD13	2.00	0.43
3:C:93:GLU:CG	11:C:537:HOH:O	2.54	0.43
1:A:689:MET:HE2	1:A:691:THR:HG22	2.00	0.43
1:A:656:LEU:HD23	1:A:681:ARG:HB2	2.00	0.43
3:C:136:SER:OG	3:C:156:LEU:HD22	2.18	0.43
4:D:90:GLN:HG3	11:D:678:HOH:O	2.17	0.43
1:A:114:PRO:HA	2:B:314:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD12	1:A:226:PRO:HB3	2.00	0.43
4:D:2:MET:HE3	4:D:71:ARG:HD2	2.00	0.43
1:A:918:ARG:HG3	1:A:918:ARG:NH1	2.18	0.43
2:B:276:HIS:CE1	11:B:452:HOH:O	2.24	0.43
1:A:702:TRP:O	1:A:706:TRP:HD1	2.02	0.43
2:B:289:TYR:HA	4:D:19:TYR:CD2	2.54	0.43
1:A:890:VAL:HG22	1:A:894:ALA:HB3	2.01	0.42
2:B:142:LYS:HG2	2:B:142:LYS:HZ3	1.67	0.42
1:A:901:THR:HG23	11:A:1510:HOH:O	2.18	0.42
4:D:59:HIS:CE1	4:D:62:GLY:HA3	2.53	0.42
1:A:76:THR:HA	1:A:88:SER:HA	2.01	0.42
1:A:904:GLU:HG3	1:A:931:ARG:HH22	1.84	0.42
2:B:153:ASN:HD22	2:B:153:ASN:N	2.15	0.42
1:A:134:GLY:O	1:A:139:GLY:HA3	2.20	0.42
1:A:204:VAL:HG13	1:A:213:ILE:HG23	2.01	0.42
1:A:961:ARG:HE	1:A:961:ARG:HB3	1.68	0.42
1:A:64:PHE:HB3	1:A:71:PRO:HD2	2.01	0.42
3:C:177:ALA:O	3:C:180:THR:OG1	2.29	0.42
1:A:479:LYS:HE3	1:A:479:LYS:HB3	1.89	0.42
2:B:286:ILE:CD1	2:B:328:VAL:HG21	2.44	0.41
1:A:692:THR:OG1	1:A:695:GLY:N	2.53	0.41
2:B:374:ASP:O	2:B:375:GLU:HG2	2.19	0.41
1:A:945:VAL:CG1	11:A:1089:HOH:O	2.56	0.41
2:B:182:LYS:HA	2:B:182:LYS:HD3	1.49	0.41
2:B:349:ASN:HB2	2:B:367:LEU:HD22	2.01	0.41
4:D:2:MET:HE1	4:D:78:PHE:CZ	2.48	0.41
1:A:478:TYR:HB3	1:A:491:VAL:HB	2.03	0.41
1:A:819:ARG:NH2	1:A:909:HIS:CE1	2.89	0.41
11:A:1124:HOH:O	2:B:267:HIS:CE1	2.74	0.41
2:B:111:HIS:CE1	2:B:265:SER:OG	2.73	0.41
2:B:110:ALA:HB1	2:B:115:ASP:HB3	2.01	0.41
1:A:885:GLU:HG2	1:A:909:HIS:HA	2.01	0.41
1:A:938:THR:HG22	11:A:1385:HOH:O	2.20	0.41
2:B:111:HIS:HB3	2:B:156:TYR:HB3	2.03	0.41
1:A:539:GLU:O	1:A:541:PRO:HD3	2.21	0.41
1:A:540:ASN:HB3	1:A:543:GLN:HE21	1.85	0.41
1:A:830:ASP:CG	1:A:909:HIS:NE2	2.74	0.41
1:A:816:HIS:O	1:A:819:ARG:HD3	2.21	0.40
1:A:932:ILE:H	1:A:932:ILE:HG12	1.77	0.40
2:B:39:LEU:CD1	2:B:368:ALA:HA	2.52	0.40
1:A:532:ILE:HD13	1:A:532:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:GLY:HA3	1:A:924:LEU:O	2.21	0.40
2:B:387:ARG:HG3	2:B:387:ARG:NH1	2.33	0.40
1:A:486:GLN:OE1	1:A:517:ALA:HB1	2.22	0.40
1:A:776:PHE:CE2	1:A:819:ARG:HG3	2.56	0.40
1:A:750:ASN:ND2	1:A:963:ASP:OD1	2.54	0.40
1:A:515:SER:HA	11:A:974:HOH:O	2.21	0.40
1:A:619:VAL:HG21	1:A:818:LEU:CD1	2.51	0.40
1:A:819:ARG:HH22	1:A:909:HIS:CE1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	961/964 (100%)	930 (97%)	29 (3%)	2 (0%)	52 59
2	B	395/399 (99%)	381 (96%)	14 (4%)	0	100 100
3	C	193/203 (95%)	181 (94%)	12 (6%)	0	100 100
4	D	89/99 (90%)	86 (97%)	3 (3%)	0	100 100
All	All	1638/1665 (98%)	1578 (96%)	58 (4%)	2 (0%)	56 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	941	ASP
1	A	71	PRO

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%)	29	34
2	B	314/315 (100%)	302 (96%)	12 (4%)	40	49
3	C	143/151 (95%)	134 (94%)	9 (6%)	22	24
4	D	75/81 (93%)	74 (99%)	1 (1%)	76	87
All	All	1279/1294 (99%)	1219 (95%)	60 (5%)	32	39

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	123	HIS
1	A	214	LEU
1	A	218	ARG
1	A	327	THR
1	A	333	LEU
1	A	382	PRO
1	A	385	HIS
1	A	518	ASN
1	A	535	VAL
1	A	578	MET
1	A	590	GLU
1	A	619	VAL
1	A	639	LYS
1	A	645	LEU
1	A	654	THR
1	A	657	LYS
1	A	684	GLU
1	A	686	ARG
1	A	734	ARG
1	A	746	LEU
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

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Mol	Chain	Res	Type
1	A	842	MET
1	A	845	VAL
1	A	848	LYS
1	A	850	LYS
1	A	871	LEU
1	A	874	VAL
1	A	889	LEU
1	A	901	THR
1	A	918	ARG
1	A	954	LEU
2	B	39	LEU
2	B	84	SER
2	B	91	LEU
2	B	97	TYR
2	B	145	CYS
2	B	153	ASN
2	B	172	HIS
2	B	174	HIS
2	B	211	THR
2	B	286	ILE
2	B	311	LEU
2	B	338	ILE
3	C	39	THR
3	C	50	THR
3	C	93	GLU
3	C	97	LEU
3	C	98	LEU
3	C	146	PHE
3	C	150	ARG
3	C	156	LEU
3	C	170	SER
4	D	63	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	82	GLN
1	A	102	ASN
1	A	123	HIS
1	A	125	HIS
1	A	181	GLN

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Mol	Chain	Res	Type
1	A	238	HIS
1	A	292	ASN
1	A	362	ASN
1	A	387	HIS
1	A	413	HIS
1	A	452	GLN
1	A	503	GLN
1	A	540	ASN
1	A	543	GLN
1	A	582	HIS
1	A	750	ASN
1	A	816	HIS
1	A	863	ASN
1	A	912	ASN
2	B	13	ASN
2	B	14	ASN
2	B	111	HIS
2	B	153	ASN
2	B	269	HIS
2	B	299	HIS
2	B	344	GLN
2	B	373	HIS
3	C	6	GLN
3	C	158	ASN
3	C	169	GLN
3	C	182	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 (i)

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	0.13	0
6	SO4	A	2560	-	4,4,4	0.21	0	6,6,6	0.29	0
6	SO4	A	2561	-	4,4,4	0.36	0	6,6,6	0.20	0
6	SO4	A	2562	-	4,4,4	0.62	0	6,6,6	0.52	0
6	SO4	A	2563	-	4,4,4	0.22	0	6,6,6	0.19	0
6	SO4	A	2567	-	4,4,4	0.38	0	6,6,6	0.38	0
5	NAD	A	965	-	42,48,48	1.73	7 (16%)	46,73,73	2.44	14 (30%)
7	FAD	B	1	-	52,58,58	1.54	7 (13%)	52,89,89	2.06	8 (15%)
8	FMN	B	4	-	32,33,33	2.11	9 (28%)	34,50,50	2.44	10 (29%)
9	SO3	B	6244	-	1,3,3	11.56	1 (100%)	0,3,3	0.00	-
6	SO4	C	2564	-	4,4,4	0.93	0	6,6,6	0.39	0
6	SO4	D	2566	-	4,4,4	0.18	0	6,6,6	0.10	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	2561	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2562	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2563	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2567	-	-	0/0/0/0	0/0/0/0
5	NAD	A	965	-	-	0/22/62/62	0/5/5/5
7	FAD	B	1	-	-	0/30/50/50	0/6/6/6
8	FMN	B	4	-	-	0/18/18/18	0/3/3/3
9	SO3	B	6244	-	-	0/0/0/0	0/0/0/0
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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	4	FMN	O5'-C5'	-5.68	1.22	1.44
5	A	965	NAD	C2B-C1B	-4.62	1.46	1.53
5	A	965	NAD	PN-O5D	-3.13	1.45	1.59
5	A	965	NAD	PA-O1A	-2.96	1.40	1.51
8	B	4	FMN	C4A-C10	-2.81	1.35	1.40
8	B	4	FMN	P-O2P	-2.81	1.45	1.54
5	A	965	NAD	C5A-N7A	-2.75	1.29	1.39
8	B	4	FMN	C4-C4A	-2.46	1.36	1.41
8	B	4	FMN	C10-N10	-2.46	1.36	1.39
8	B	4	FMN	C9A-C5A	-2.29	1.37	1.42
7	B	1	FAD	C2-N3	2.02	1.42	1.38
7	B	1	FAD	O4B-C4B	2.05	1.49	1.45
5	A	965	NAD	C2N-N1N	2.20	1.38	1.35
7	B	1	FAD	C10-N1	2.22	1.39	1.35
7	B	1	FAD	O3B-C3B	2.29	1.48	1.43
5	A	965	NAD	O4D-C4D	2.92	1.51	1.45
8	B	4	FMN	P-O3P	3.22	1.65	1.54
7	B	1	FAD	C5X-N5	3.35	1.40	1.35
8	B	4	FMN	C4-N3	4.45	1.41	1.33
7	B	1	FAD	C4-N3	4.85	1.41	1.33
8	B	4	FMN	C4A-N5	5.07	1.41	1.33
5	A	965	NAD	O7N-C7N	5.49	1.35	1.24
7	B	1	FAD	C4X-N5	5.57	1.41	1.33
9	B	6244	SO3	O1-S	11.56	1.90	1.44

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	965	NAD	N3A-C2A-N1A	-10.02	121.00	128.87
7	B	1	FAD	N3A-C2A-N1A	-9.06	121.76	128.87
8	B	4	FMN	O4'-C4'-C5'	-6.99	94.85	110.09
7	B	1	FAD	C4B-O4B-C1B	-5.81	103.49	109.64
5	A	965	NAD	O4B-C1B-N9A	-5.24	98.22	108.11
5	A	965	NAD	C2D-C1D-N1N	-4.96	103.81	113.53
8	B	4	FMN	N3-C2-N1	-4.10	120.79	127.69
8	B	4	FMN	C4A-C4-N3	-4.02	118.27	123.52
5	A	965	NAD	C1B-N9A-C4A	-4.01	122.33	126.81
7	B	1	FAD	C4X-C4-N3	-3.93	118.38	123.52
5	A	965	NAD	C5B-C4B-C3B	-3.80	100.51	115.20
7	B	1	FAD	N3-C2-N1	-3.55	121.71	127.69
5	A	965	NAD	C6N-C5N-C4N	-2.87	115.07	119.43
5	A	965	NAD	O4D-C1D-N1N	-2.83	105.04	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	965	NAD	C2D-C3D-C4D	-2.67	97.18	102.64
8	B	4	FMN	C9A-C5A-N5	-2.51	118.10	122.18
7	B	1	FAD	O4B-C1B-N9A	-2.41	103.55	108.11
7	B	1	FAD	C1B-N9A-C4A	-2.33	124.20	126.81
8	B	4	FMN	C7-C6-C5A	-2.19	117.32	120.90
5	A	965	NAD	O7N-C7N-N7N	-2.15	119.52	122.58
5	A	965	NAD	C3N-C2N-N1N	-2.00	118.05	120.34
8	B	4	FMN	O3'-C3'-C2'	2.07	114.09	108.73
5	A	965	NAD	C5N-C6N-N1N	2.49	124.76	120.46
5	A	965	NAD	O7N-C7N-C3N	2.84	122.75	119.60
5	A	965	NAD	C2N-C3N-C4N	3.11	121.79	118.27
7	B	1	FAD	C4X-N5-C5X	3.18	120.47	116.72
5	A	965	NAD	C2A-N1A-C6A	3.32	124.70	118.77
8	B	4	FMN	C5A-C9A-N10	3.44	120.16	117.58
8	B	4	FMN	C4A-N5-C5A	3.73	121.12	116.72
8	B	4	FMN	C4-N3-C2	4.51	118.92	115.16
7	B	1	FAD	C4-N3-C2	5.34	119.62	115.16
8	B	4	FMN	O5'-P-O1P	5.59	121.14	107.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2562	SO4	5	0
5	A	965	NAD	4	0
7	B	1	FAD	3	0
8	B	4	FMN	11	0
9	B	6244	SO3	2	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, 95^{th} 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	963/964 (99%)	-0.06	44 (4%) 36 35	19, 35, 68, 86	0
2	B	397/399 (99%)	-0.12	5 (1%) 79 78	24, 43, 59, 76	0
3	C	195/203 (96%)	-0.26	0 100 100	24, 34, 56, 68	0
4	D	91/99 (91%)	-0.22	0 100 100	26, 37, 72, 108	0
All	All	1646/1665 (98%)	-0.11	49 (2%) 54 53	19, 38, 66, 108	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	954	LEU	4.6
1	A	849	LEU	4.2
1	A	848	LYS	4.1
1	A	897	SER	3.6
1	A	866	GLU	3.5
1	A	875	LEU	3.5
1	A	782	PHE	3.4
1	A	928	GLY	3.4
1	A	915	ALA	3.4
2	B	399	ALA	3.4
1	A	909	HIS	3.2
2	B	202	ASP	3.2
1	A	226	PRO	3.1
2	B	392	HIS	3.0
1	A	932	ILE	2.8
1	A	960	SER	2.8
1	A	947	VAL	2.7
1	A	823	GLY	2.7
1	A	948	GLN	2.7
1	A	873	SER	2.7
1	A	894	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	753	PHE	2.6
1	A	881	LEU	2.6
1	A	958	GLU	2.6
1	A	227	SER	2.5
1	A	746	LEU	2.5
1	A	891	ALA	2.4
1	A	738	VAL	2.4
1	A	327	THR	2.3
1	A	892	ALA	2.3
1	A	844	TRP	2.3
1	A	872	VAL	2.3
1	A	949	VAL	2.3
1	A	840	ALA	2.3
1	A	921	GLY	2.2
1	A	864	VAL	2.2
2	B	145	CYS	2.2
1	A	951	ASP	2.2
1	A	895	VAL	2.2
1	A	936	LEU	2.2
1	A	945	VAL	2.2
2	B	347	TYR	2.1
1	A	843	GLU	2.1
1	A	745	SER	2.1
1	A	876	PRO	2.1
1	A	858	PHE	2.1
1	A	751	ASP	2.0
1	A	871	LEU	2.0
1	A	841	GLY	2.0

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^{th} 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
6	SO4	C	2564	5/5	0.98	0.20	4.67	41,45,59,64	0
9	SO3	B	6244	4/4	0.95	0.13	1.96	56,59,62,73	0
6	SO4	A	2562	5/5	0.92	0.13	1.18	44,44,73,102	0
7	FAD	B	1	53/53	0.97	0.12	0.47	26,39,53,56	0
8	FMN	B	4	31/31	0.98	0.10	-0.19	21,27,32,42	0
5	NAD	A	965	44/44	0.99	0.11	-0.25	12,21,27,31	0
6	SO4	A	2560	5/5	0.95	0.22	-0.42	61,66,79,103	0
6	SO4	A	2559	5/5	0.97	0.10	-0.55	70,75,108,121	0
10	ZN	D	100	1/1	0.99	0.05	-3.58	32,32,32,32	0
6	SO4	A	2563	5/5	0.97	0.29	-	78,80,92,294	0
6	SO4	A	2561	5/5	0.97	0.14	-	44,55,84,100	0
6	SO4	A	2567	5/5	0.99	0.07	-	44,46,61,72	0
6	SO4	D	2566	5/5	0.97	0.09	-	74,78,102,105	0

6.5 Other polymers

There are no such residues in this entry.