Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 06:32 PM GMT

PDB ID	:	1X31
Title	:	Crystal Structure of Heterotetrameric Sarcosine Oxidase from Corynebacterium sp. U-96
Authors	:	Ida, K.; Moriguchi, T.; Suzuki, H.
Deposited on	:	2005-04-27
Resolution	:	2.15 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:

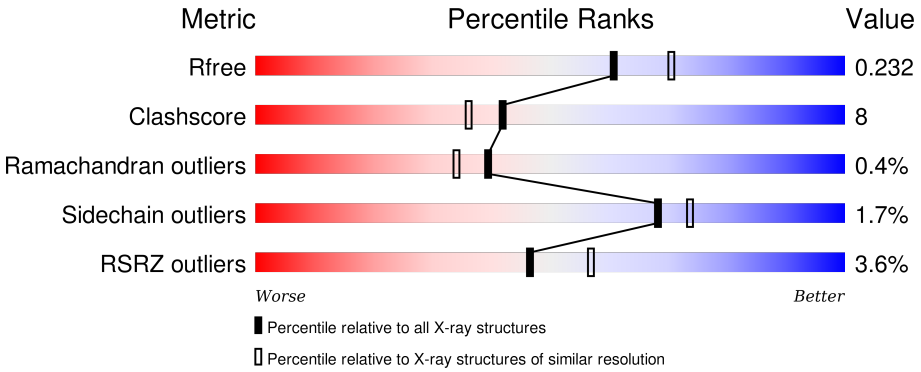
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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% 82% 17%
2	B	404	% 83% 16%
3	C	206	2% 73% 22% 5%
4	D	99	% 81% 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	DMG	B	1005	-	-	X	X
6	SO4	A	2002	-	-	X	-
6	SO4	B	2007	-	-	-	X
9	FMN	B	1004	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13814 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	402	Total	C	N	O	S	0	0	0
			3093	1972	537	574	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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	201	HIS	-	EXPRESSION TAG	UNP Q50LE9
C	202	HIS	-	EXPRESSION TAG	UNP Q50LE9
C	203	HIS	-	EXPRESSION TAG	UNP Q50LE9
C	204	HIS	-	EXPRESSION TAG	UNP Q50LE9
C	205	HIS	-	EXPRESSION TAG	UNP Q50LE9
C	206	HIS	-	EXPRESSION TAG	UNP Q50LE9

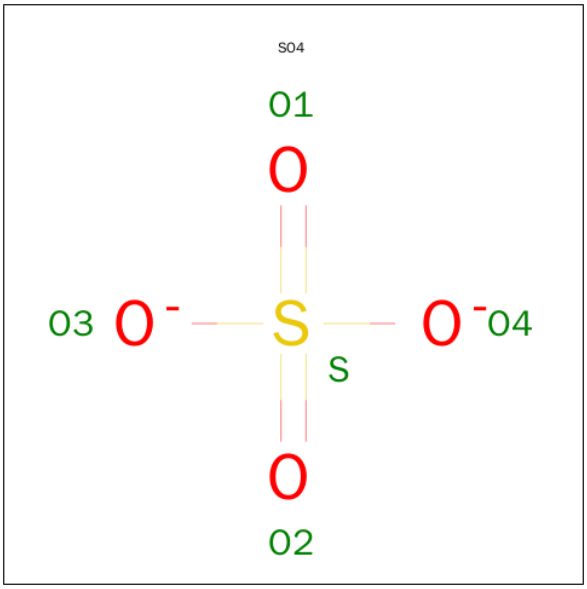
- Molecule 4 is a protein called Sarcosine oxidase delta subunit.

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

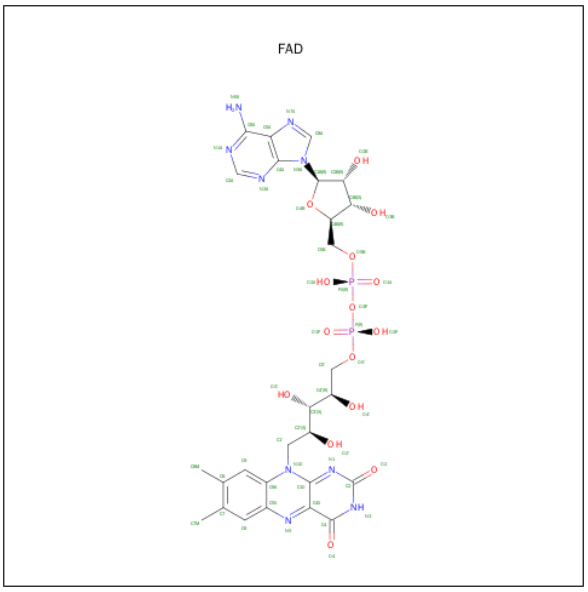
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Zn 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



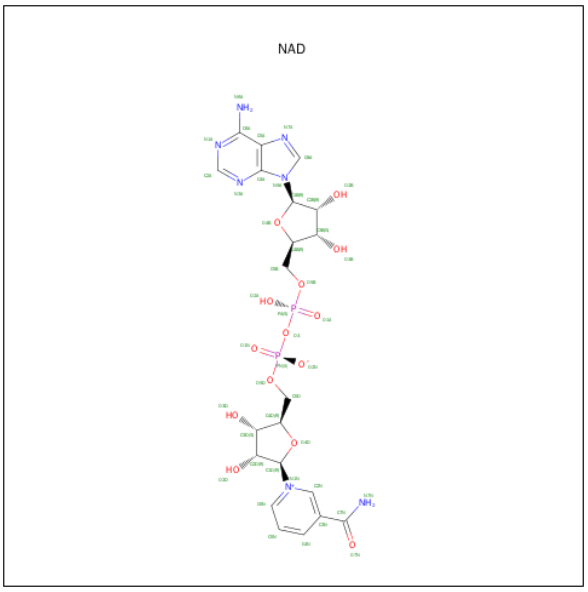
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

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



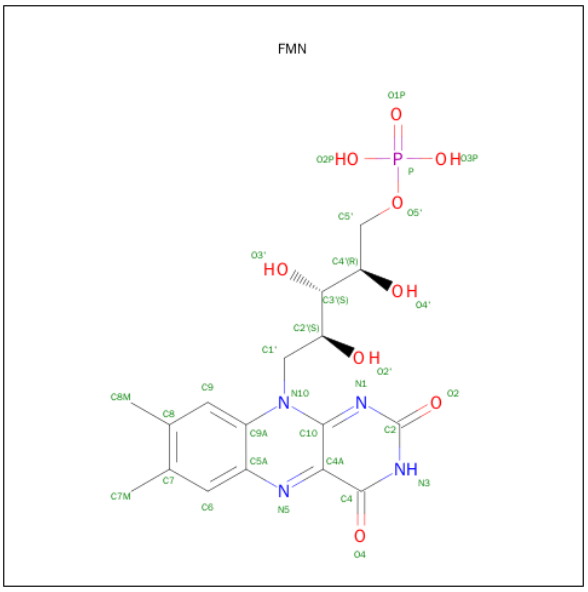
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



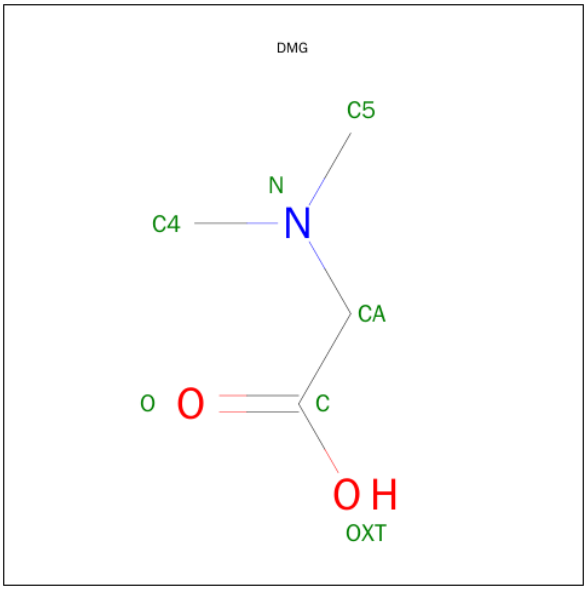
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 9 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 10 is N,N-DIMETHYLGLYCINE (three-letter code: DMG) (formula: $C_4H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 11 is water.

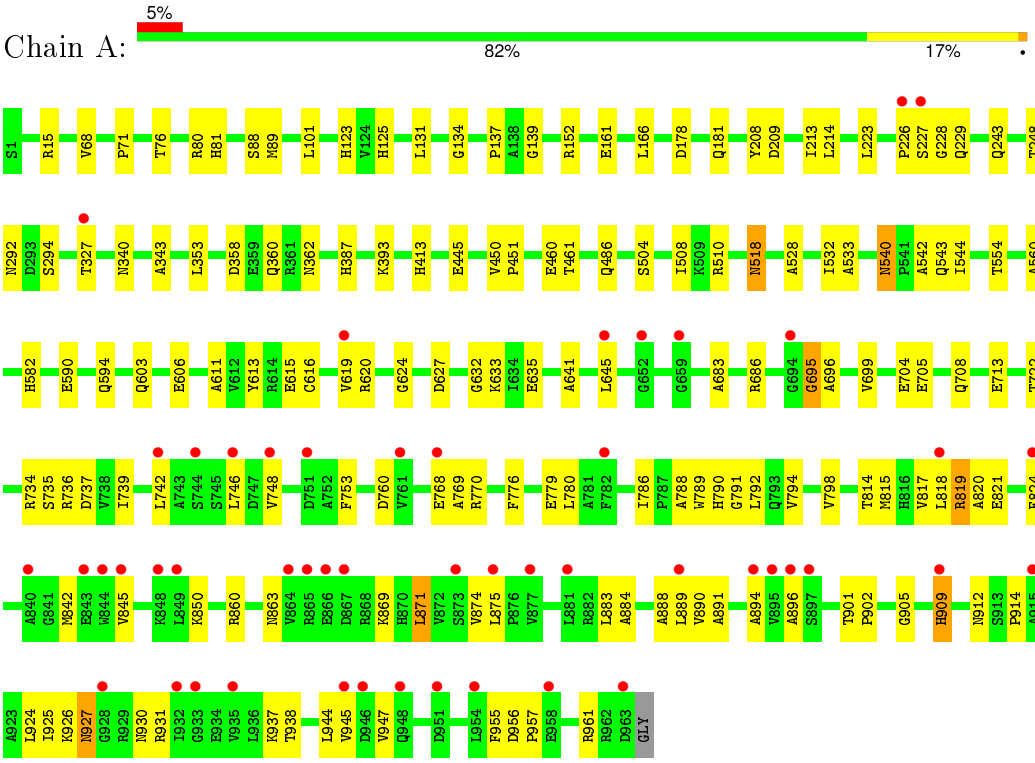
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	696	Total O 696 696	0	0
11	B	199	Total O 199 199	0	0
11	C	151	Total O 151 151	0	0
11	D	88	Total O 88 88	0	0

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.

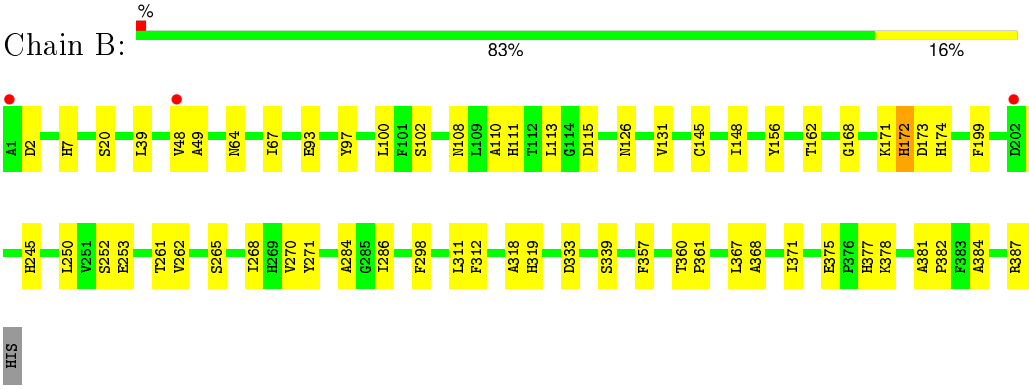
- Molecule 1: Sarcosine oxidase alpha subunit

Chain A:



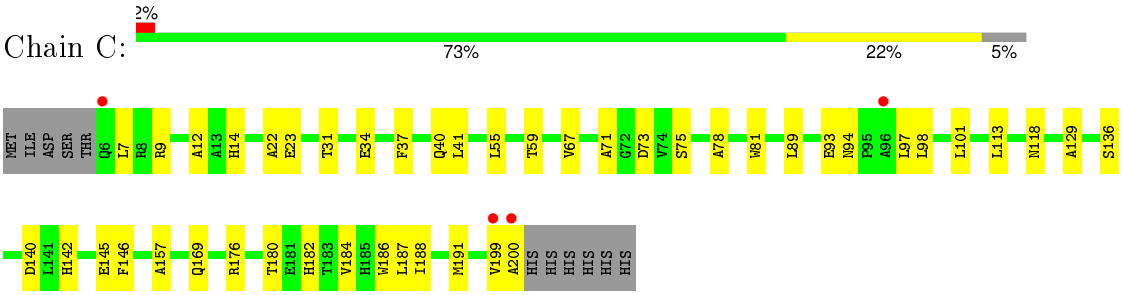
- Molecule 2: Sarcosine oxidase beta subunit

Chain B:



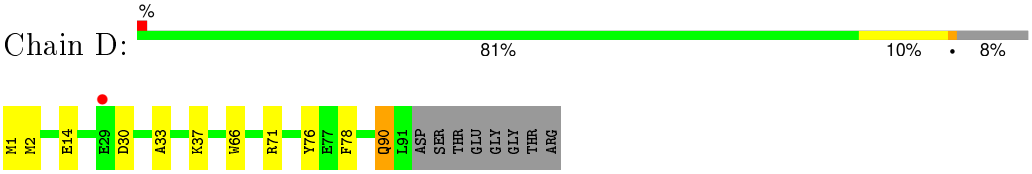
- Molecule 3: Sarcosine oxidase gamma subunit

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	199.11Å 199.11Å 197.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.06 – 2.15 70.06 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.06-2.15) 99.7 (70.06-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 2.14Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.232 0.188 , 0.232	Depositor DCC
R_{free} test set	12401 reflections (9.99%)	DCC
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 124152 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13814	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 2.13% 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, DMG, FMN, 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	0.31	0/7361	0.60	0/10017
2	B	0.30	0/3173	0.59	1/4318 (0.0%)
3	C	0.36	0/1461	0.62	0/1998
4	D	0.35	0/772	0.60	0/1040
All	All	0.32	0/12767	0.60	1/17373 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	318	ALA	N-CA-C	-5.85	95.20	111.00

There are no chirality outliers.

There are no planarity outliers.

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	127	0
2	B	3093	0	3023	50	0
3	C	1433	0	1434	29	0
4	D	749	0	706	9	0
5	D	1	0	0	0	0
6	A	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	B	53	0	31	5	0
8	A	44	0	26	4	0
9	B	31	0	19	10	0
10	B	7	0	8	6	0
11	A	696	0	0	8	1
11	B	199	0	0	3	0
11	C	151	0	0	2	0
11	D	88	0	0	1	0
All	All	13814	0	12351	210	1

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 8.

All (210) 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	9:B:1004:FMN:HM83	1.46	1.27
2:B:172:HIS:HE2	9:B:1004:FMN:C8M	1.58	1.16
10:B:1005:DMG:H43	10:B:1005:DMG:O	1.46	1.11
2:B:172:HIS:HE2	9:B:1004:FMN:HM83	0.89	1.04
2:B:172:HIS:CD2	9:B:1004:FMN:HM83	2.06	0.90
2:B:100:LEU:HD12	2:B:171:LYS:HD2	1.52	0.89
1:A:510:ARG:HH21	9:B:1004:FMN:H5'2	1.41	0.86
10:B:1005:DMG:O	10:B:1005:DMG:C4	2.24	0.85
2:B:67:ILE:HD12	10:B:1005:DMG:C4	2.09	0.83
1:A:510:ARG:NH2	9:B:1004:FMN:H5'2	1.95	0.80
3:C:23:GLU:HG3	3:C:31:THR:HG22	1.61	0.80
1:A:632:GLY:HA3	1:A:696:ALA:HB2	1.65	0.79
1:A:249:ALA:HB1	11:A:3001:HOH:O	1.83	0.78
1:A:896:ALA:HA	1:A:901:THR:HG22	1.66	0.77
1:A:292:ASN:HD22	1:A:294:SER:H	1.29	0.77
1:A:633:LYS:HE3	1:A:725:LEU:HB2	1.66	0.76
2:B:245:HIS:HB2	2:B:286:ILE:HD11	1.68	0.74
1:A:249:ALA:HB2	8:A:1002:NAD:O3	1.89	0.72
1:A:842:MET:O	1:A:845:VAL:HG12	1.92	0.70
1:A:742:LEU:HD21	1:A:798:VAL:HG22	1.74	0.70
1:A:704:GLU:HG3	1:A:708:GLN:HE21	1.57	0.69
1:A:292:ASN:ND2	1:A:294:SER:H	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:ILE:HD11	2:B:311:LEU:HD22	1.76	0.68
3:C:37:PHE:O	3:C:93:GLU:HG2	1.93	0.67
1:A:540:ASN:HB3	1:A:543:GLN:HG3	1.78	0.66
3:C:41:LEU:HD22	3:C:98:LEU:HD23	1.78	0.64
1:A:704:GLU:HG3	1:A:708:GLN:NE2	2.12	0.64
1:A:510:ARG:HH21	9:B:1004:FMN:C5'	2.10	0.64
1:A:891:ALA:HB3	1:A:894:ALA:HB2	1.80	0.64
1:A:504:SER:O	1:A:508:ILE:HG12	1.98	0.63
1:A:68:VAL:HG21	1:A:554:THR:HG21	1.81	0.62
1:A:884:ALA:HB3	11:A:3652:HOH:O	2.00	0.62
2:B:172:HIS:ND1	2:B:173:ASP:N	2.49	0.61
1:A:249:ALA:HB2	8:A:1002:NAD:PA	2.40	0.61
3:C:94:ASN:HD22	3:C:97:LEU:HB2	1.66	0.61
1:A:360:GLN:HG2	11:A:3591:HOH:O	2.01	0.60
2:B:339:SER:HB3	2:B:384:ALA:HA	1.84	0.60
2:B:265:SER:OG	2:B:268:ILE:HG12	2.02	0.60
1:A:619:VAL:HG21	1:A:818:LEU:HD11	1.84	0.59
2:B:93:GLU:HG2	11:B:3617:HOH:O	2.02	0.59
1:A:860:ARG:HH21	1:A:863:ASN:HD21	1.51	0.58
2:B:360:THR:HB	2:B:361:PRO:HD3	1.86	0.58
1:A:927:ASN:HB3	1:A:931:ARG:HD2	1.85	0.57
1:A:152:ARG:HD3	3:C:142:HIS:CD2	2.38	0.57
3:C:184:VAL:O	3:C:188:ILE:HG12	2.04	0.57
1:A:829:GLN:HG2	1:A:909:HIS:CE1	2.40	0.57
2:B:67:ILE:HD12	10:B:1005:DMG:H43	1.87	0.56
2:B:64:ASN:HA	7:B:1001:FAD:C6	2.34	0.56
3:C:187:LEU:O	3:C:191:MET:HG2	2.04	0.56
1:A:734:ARG:HD3	1:A:737:ASP:OD2	2.05	0.56
1:A:819:ARG:HH22	1:A:909:HIS:CD2	2.23	0.56
1:A:695:GLY:O	1:A:699:VAL:HG23	2.06	0.56
1:A:611:ALA:O	1:A:615:GLU:HG3	2.06	0.56
1:A:603:GLN:O	1:A:606:GLU:HB2	2.05	0.56
2:B:111:HIS:HD2	2:B:156:TYR:O	1.90	0.54
1:A:736:ARG:HB2	1:A:780:LEU:HD21	1.90	0.54
1:A:619:VAL:HG12	1:A:624:GLY:HA3	1.89	0.53
1:A:208:TYR:CE2	1:A:214:LEU:HD12	2.44	0.53
1:A:340:ASN:HB3	1:A:353:LEU:HD22	1.90	0.53
1:A:683:ALA:HB3	1:A:686:ARG:HB2	1.91	0.53
2:B:171:LYS:HE2	2:B:174:HIS:CD2	2.44	0.53
1:A:819:ARG:HG2	1:A:824:PHE:HB2	1.90	0.53
1:A:819:ARG:HD3	1:A:820:ALA:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1001:FAD:C4	10:B:1005:DMG:HA2	2.39	0.52
1:A:243:GLN:OE1	1:A:413:HIS:HE1	1.93	0.52
4:D:90:GLN:NE2	4:D:90:GLN:H	2.07	0.52
3:C:55:LEU:O	3:C:59:THR:HG23	2.09	0.52
1:A:723:GLU:HB2	3:C:118:ASN:ND2	2.25	0.52
1:A:937:LYS:HB3	1:A:944:LEU:HB3	1.92	0.51
1:A:955:PHE:HZ	1:A:961:ARG:HH11	1.57	0.51
1:A:830:ASP:CG	1:A:909:HIS:HE2	2.13	0.51
1:A:131:LEU:HD23	1:A:213:ILE:HG13	1.91	0.51
2:B:126:ASN:HB3	2:B:131:VAL:HG23	1.93	0.51
1:A:776:PHE:CE2	1:A:819:ARG:HG3	2.46	0.51
1:A:613:TYR:CD1	1:A:914:PRO:HG3	2.46	0.51
2:B:172:HIS:HE2	9:B:1004:FMN:C8	2.20	0.51
1:A:830:ASP:OD1	1:A:909:HIS:NE2	2.42	0.51
1:A:635:GLU:HG2	3:C:113:LEU:HD11	1.93	0.51
1:A:901:THR:HG23	11:A:3550:HOH:O	2.10	0.51
1:A:760:ASP:OD1	1:A:770:ARG:HD3	2.10	0.51
2:B:375:GLU:HG3	11:B:3585:HOH:O	2.11	0.50
1:A:590:GLU:OE1	2:B:113:LEU:HD12	2.12	0.50
4:D:2:MET:HE1	4:D:78:PHE:CE1	2.45	0.50
1:A:696:ALA:HB3	6:A:2002:SO4:O4	2.11	0.50
1:A:123:HIS:HE1	1:A:560:ALA:O	1.94	0.50
4:D:2:MET:HE3	4:D:76:TYR:O	2.11	0.50
3:C:94:ASN:ND2	3:C:97:LEU:HB2	2.26	0.49
2:B:252:SER:HA	2:B:319:HIS:O	2.12	0.49
2:B:333:ASP:OD2	2:B:387:ARG:NH1	2.42	0.49
3:C:9:ARG:NH2	3:C:14:HIS:HB3	2.28	0.49
3:C:41:LEU:HD13	3:C:101:LEU:HD12	1.95	0.48
1:A:860:ARG:HB2	1:A:863:ASN:HD22	1.78	0.48
1:A:125:HIS:HD2	11:A:3193:HOH:O	1.96	0.48
2:B:108:ASN:HB2	2:B:162:THR:OG1	2.13	0.48
1:A:786:ILE:HD13	1:A:790:HIS:HB2	1.95	0.48
1:A:726:ALA:HB2	1:A:788:ALA:HA	1.94	0.48
1:A:387:HIS:HE1	1:A:393:LYS:O	1.97	0.48
1:A:888:ALA:O	1:A:938:THR:HG23	2.13	0.48
1:A:249:ALA:CB	8:A:1002:NAD:O2A	2.62	0.48
1:A:786:ILE:HG12	1:A:794:VAL:HG21	1.96	0.47
1:A:869:LYS:HA	1:A:925:ILE:O	2.13	0.47
1:A:769:ALA:HB2	1:A:786:ILE:CG2	2.44	0.47
2:B:250:LEU:HD12	2:B:250:LEU:C	2.35	0.47
1:A:486:GLN:HE22	1:A:518:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:VAL:HA	11:B:4107:HOH:O	2.13	0.47
1:A:633:LYS:HE2	1:A:722:THR:HA	1.97	0.47
1:A:829:GLN:HG2	1:A:909:HIS:ND1	2.30	0.47
1:A:582:HIS:HE1	1:A:627:ASP:OD2	1.98	0.47
1:A:896:ALA:CA	1:A:901:THR:HG22	2.42	0.47
1:A:696:ALA:HB3	6:A:2002:SO4:S	2.56	0.46
1:A:776:PHE:HE2	1:A:815:MET:HE3	1.80	0.46
1:A:101:LEU:C	1:A:101:LEU:HD23	2.36	0.46
1:A:540:ASN:ND2	1:A:542:ALA:H	2.14	0.46
3:C:22:ALA:HB2	3:C:188:ILE:HD12	1.98	0.46
2:B:389:GLU:HG3	4:D:37:LYS:HA	1.97	0.46
1:A:883:LEU:HD11	1:A:947:VAL:HG11	1.98	0.46
1:A:937:LYS:HA	1:A:945:VAL:O	2.16	0.46
1:A:860:ARG:NH2	1:A:863:ASN:HD21	2.13	0.46
3:C:180:THR:O	3:C:184:VAL:HG23	2.16	0.46
2:B:64:ASN:HA	7:B:1001:FAD:C5X	2.46	0.46
2:B:64:ASN:O	9:B:1004:FMN:HM82	2.16	0.45
1:A:641:ALA:O	1:A:645:LEU:HD13	2.16	0.45
3:C:12:ALA:HB3	3:C:34:GLU:CD	2.36	0.45
1:A:871:LEU:HD21	1:A:922:LEU:HB3	1.97	0.45
11:A:3110:HOH:O	2:B:7:HIS:HE1	2.00	0.45
1:A:226:PRO:HB2	11:A:3568:HOH:O	2.17	0.45
3:C:40:GLN:HA	3:C:89:LEU:O	2.16	0.45
9:B:1004:FMN:H1'2	9:B:1004:FMN:H9	1.75	0.45
1:A:723:GLU:HG3	3:C:176:ARG:HB3	1.99	0.45
3:C:176:ARG:HD3	11:C:3630:HOH:O	2.17	0.45
1:A:918:ARG:HH11	1:A:918:ARG:HG3	1.81	0.44
2:B:171:LYS:HE2	2:B:174:HIS:HD2	1.82	0.44
1:A:713:GLU:H	1:A:713:GLU:CD	2.21	0.44
1:A:292:ASN:HD21	1:A:294:SER:CB	2.30	0.44
4:D:1:MET:SD	4:D:14:GLU:HG2	2.58	0.44
2:B:102:SER:O	2:B:168:GLY:HA3	2.18	0.44
4:D:90:GLN:H	4:D:90:GLN:HE21	1.63	0.44
1:A:635:GLU:HG2	3:C:113:LEU:HD21	1.99	0.44
1:A:889:LEU:HD12	1:A:925:ILE:HD11	2.00	0.44
1:A:635:GLU:HG3	11:C:3560:HOH:O	2.18	0.44
2:B:145:CYS:SG	2:B:148:ILE:HG13	2.58	0.44
1:A:620:ARG:NH1	1:A:779:GLU:HG2	2.33	0.44
1:A:178:ASP:HB2	1:A:181:GLN:HE21	1.83	0.44
1:A:613:TYR:CE1	1:A:914:PRO:HG3	2.53	0.43
1:A:817:VAL:O	1:A:821:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:HIS:NE2	1:A:226:PRO:HD2	2.33	0.43
1:A:76:THR:HA	1:A:88:SER:HA	2.00	0.43
1:A:89:MET:HG3	2:B:253:GLU:HG3	2.00	0.43
1:A:632:GLY:CA	1:A:696:ALA:HB2	2.41	0.43
1:A:616:CYS:HB3	1:A:814:THR:HG23	2.00	0.43
3:C:73:ASP:OD2	3:C:75:SER:HB2	2.19	0.43
1:A:358:ASP:OD2	1:A:362:ASN:HB2	2.19	0.43
2:B:357:PHE:HB3	7:B:1001:FAD:C2	2.49	0.43
2:B:148:ILE:HG12	2:B:312:PHE:CE1	2.53	0.43
1:A:768:GLU:O	1:A:786:ILE:HG22	2.19	0.43
2:B:39:LEU:HD13	2:B:368:ALA:HA	2.01	0.43
1:A:746:LEU:HD12	1:A:748:VAL:CG1	2.49	0.43
1:A:890:VAL:HG13	1:A:902:PRO:O	2.19	0.42
1:A:927:ASN:ND2	1:A:930:ASN:HB2	2.34	0.42
1:A:387:HIS:HD2	11:A:3003:HOH:O	2.00	0.42
1:A:137:PRO:HD3	1:A:166:LEU:HG	2.01	0.42
1:A:905:GLY:HA3	1:A:924:LEU:O	2.19	0.42
1:A:769:ALA:HB2	1:A:786:ILE:HG22	2.00	0.42
1:A:528:ALA:O	1:A:532:ILE:HG13	2.20	0.42
1:A:248:THR:O	1:A:249:ALA:HB3	2.18	0.42
1:A:909:HIS:CD2	1:A:922:LEU:HD12	2.54	0.42
1:A:214:LEU:HD13	2:B:298:PHE:CD2	2.55	0.42
3:C:129:ALA:HB3	3:C:169:GLN:NE2	2.33	0.42
1:A:825:ILE:HG22	1:A:871:LEU:CD1	2.49	0.42
1:A:249:ALA:HB2	8:A:1002:NAD:O2A	2.20	0.42
4:D:30:ASP:OD2	4:D:33:ALA:HB2	2.20	0.42
3:C:67:VAL:HA	3:C:81:TRP:CE3	2.54	0.42
1:A:890:VAL:HG12	1:A:894:ALA:HB3	2.00	0.42
1:A:776:PHE:O	1:A:819:ARG:HB2	2.19	0.42
3:C:157:ALA:O	3:C:182:HIS:HE1	2.03	0.42
3:C:136:SER:HB3	3:C:186:TRP:CZ2	2.55	0.42
2:B:367:LEU:O	2:B:371:ILE:HG13	2.20	0.42
2:B:377:HIS:ND1	2:B:378:LYS:N	2.68	0.42
2:B:110:ALA:HB1	2:B:115:ASP:HB3	2.01	0.42
2:B:381:ALA:HB3	2:B:382:PRO:HD3	2.01	0.42
1:A:875:LEU:HD22	1:A:918:ARG:NH1	2.34	0.42
7:B:1001:FAD:O4	10:B:1005:DMG:H42	2.20	0.42
2:B:39:LEU:HA	2:B:39:LEU:HD12	1.96	0.42
2:B:199:PHE:CD1	2:B:209:VAL:HG12	2.55	0.42
1:A:956:ASP:N	1:A:957:PRO:HD3	2.35	0.42
2:B:381:ALA:N	2:B:382:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:GLU:HG3	4:D:66:TRP:CZ2	2.55	0.41
1:A:262:ARG:HD3	1:A:343:ALA:HB2	2.02	0.41
1:A:735:SER:O	1:A:739:ILE:HG12	2.20	0.41
1:A:776:PHE:CE2	1:A:815:MET:HE3	2.56	0.41
2:B:20:SER:HB3	2:B:217:LEU:HB2	2.01	0.41
1:A:450:VAL:HA	1:A:451:PRO:HD3	1.99	0.41
2:B:271:TYR:CD2	2:B:284:ALA:HA	2.56	0.41
1:A:572:PRO:HD2	1:A:594:GLN:NE2	2.35	0.41
1:A:15:ARG:HD3	1:A:161:GLU:OE2	2.20	0.41
3:C:140:ASP:OD2	3:C:145:GLU:HG3	2.20	0.41
1:A:786:ILE:HD11	1:A:791:GLY:HA2	2.03	0.41
2:B:388:PHE:HB2	11:D:3393:HOH:O	2.20	0.41
3:C:71:ALA:O	3:C:78:ALA:HA	2.21	0.41
1:A:616:CYS:SG	1:A:914:PRO:HG2	2.60	0.41
3:C:129:ALA:HB3	3:C:169:GLN:HE21	1.84	0.41
1:A:134:GLY:O	1:A:139:GLY:HA3	2.20	0.41
4:D:2:MET:HE3	4:D:71:ARG:HD2	2.03	0.40
1:A:874:VAL:CG1	1:A:947:VAL:HB	2.51	0.40
1:A:533:ALA:HB2	1:A:544:ILE:HD12	2.04	0.40
3:C:199:VAL:O	3:C:200:ALA:HB3	2.21	0.40
1:A:460:GLU:HG2	1:A:461:THR:N	2.36	0.40
1:A:223:LEU:HD12	1:A:226:PRO:HB3	2.04	0.40
2:B:48:VAL:HG12	2:B:49:ALA:N	2.35	0.40
2:B:261:THR:OG1	2:B:262:VAL:N	2.55	0.40

All (1) 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)
11:A:3832:HOH:O	11:A:3832:HOH:O[10_665]	1.82	0.38

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%)	25 (3%)	6 (1%)	30 21
2	B	400/404 (99%)	387 (97%)	12 (3%)	1 (0%)	46 42
3	C	193/206 (94%)	179 (93%)	14 (7%)	0	100 100
4	D	89/99 (90%)	86 (97%)	3 (3%)	0	100 100
All	All	1643/1673 (98%)	1582 (96%)	54 (3%)	7 (0%)	39 34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	GLY
1	A	227	SER
1	A	926	LYS
1	A	927	ASN
2	B	203	GLY
1	A	695	GLY
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%)	731 (98%)	16 (2%)	61 65
2	B	318/319 (100%)	315 (99%)	3 (1%)	84 89
3	C	143/154 (93%)	141 (99%)	2 (1%)	74 80
4	D	75/81 (93%)	74 (99%)	1 (1%)	76 82
All	All	1283/1301 (99%)	1261 (98%)	22 (2%)	68 74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	209	ASP

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Mol	Chain	Res	Type
1	A	229	GLN
1	A	327	THR
1	A	445	GLU
1	A	518	ASN
1	A	540	ASN
1	A	578	MET
1	A	753	PHE
1	A	789	TRP
1	A	792	LEU
1	A	819	ARG
1	A	850	LYS
1	A	871	LEU
1	A	909	HIS
1	A	912	ASN
2	B	2	ASP
2	B	97	TYR
2	B	172	HIS
3	C	7	LEU
3	C	146	PHE
4	D	90	GLN

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	30	GLN
1	A	82	GLN
1	A	125	HIS
1	A	181	GLN
1	A	292	ASN
1	A	387	HIS
1	A	413	HIS
1	A	452	GLN
1	A	518	ASN
1	A	540	ASN
1	A	543	GLN
1	A	582	HIS
1	A	594	GLN
1	A	750	ASN
1	A	816	HIS
1	A	829	GLN
1	A	863	ASN
1	A	912	ASN

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Mol	Chain	Res	Type
1	A	927	ASN
1	A	930	ASN
2	B	7	HIS
2	B	13	ASN
2	B	111	HIS
2	B	126	ASN
2	B	129	ASN
2	B	299	HIS
2	B	344	GLN
3	C	94	ASN
3	C	118	ASN
3	C	169	GLN
3	C	182	HIS
4	D	90	GLN

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

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	$\#\|Z\|>2$
8	NAD	A	1002	-	42,48,48	1.36	4 (9%)	46,73,73	1.71	3 (6%)
6	SO4	A	2001	-	4,4,4	0.28	0	6,6,6	0.07	0
6	SO4	A	2002	-	4,4,4	0.23	0	6,6,6	0.05	0
6	SO4	A	2003	-	4,4,4	0.22	0	6,6,6	0.08	0
6	SO4	A	2006	-	4,4,4	0.28	0	6,6,6	0.07	0
6	SO4	A	2008	-	4,4,4	0.28	0	6,6,6	0.08	0
7	FAD	B	1001	-	52,58,58	1.35	4 (7%)	52,89,89	2.11	7 (13%)
9	FMN	B	1004	-	32,33,33	1.66	4 (12%)	34,50,50	1.82	6 (17%)
10	DMG	B	1005	-	3,6,6	0.60	0	3,7,7	1.11	0
6	SO4	B	2007	-	4,4,4	0.30	0	6,6,6	0.10	0
6	SO4	C	2005	-	4,4,4	0.20	0	6,6,6	0.09	0
6	SO4	D	2004	-	4,4,4	0.27	0	6,6,6	0.06	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
8	NAD	A	1002	-	-	0/22/62/62	0/5/5/5
6	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2003	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2006	-	-	0/0/0/0	0/0/0/0
6	SO4	A	2008	-	-	0/0/0/0	0/0/0/0
7	FAD	B	1001	-	-	0/30/50/50	0/6/6/6
9	FMN	B	1004	-	-	0/18/18/18	0/3/3/3
10	DMG	B	1005	-	-	0/2/4/4	0/0/0/0
6	SO4	B	2007	-	-	0/0/0/0	0/0/0/0
6	SO4	C	2005	-	-	0/0/0/0	0/0/0/0
6	SO4	D	2004	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1002	NAD	C3N-C7N	2.01	1.53	1.50
8	A	1002	NAD	O4D-C1D	2.08	1.44	1.41
7	B	1001	FAD	C10-N1	2.94	1.40	1.35
9	B	1004	FMN	C10-N1	3.06	1.40	1.35
9	B	1004	FMN	C5A-N5	3.35	1.40	1.35
7	B	1001	FAD	C5X-N5	3.46	1.40	1.35
8	A	1002	NAD	C2N-N1N	3.96	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1004	FMN	C4-N3	4.19	1.40	1.33
7	B	1001	FAD	C4-N3	4.21	1.40	1.33
7	B	1001	FAD	C4X-N5	4.71	1.40	1.33
9	B	1004	FMN	C4A-N5	4.72	1.40	1.33
8	A	1002	NAD	O7N-C7N	5.82	1.36	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1002	NAD	N3A-C2A-N1A	-9.76	121.21	128.87
7	B	1001	FAD	N3A-C2A-N1A	-9.60	121.33	128.87
7	B	1001	FAD	C4B-O4B-C1B	-5.90	103.39	109.64
7	B	1001	FAD	N3-C2-N1	-4.97	119.33	127.69
9	B	1004	FMN	N3-C2-N1	-4.97	119.33	127.69
8	A	1002	NAD	C4B-O4B-C1B	-3.04	106.42	109.64
9	B	1004	FMN	C4A-C4-N3	-2.55	120.19	123.52
7	B	1001	FAD	C4X-C4-N3	-2.43	120.35	123.52
8	A	1002	NAD	O4D-C1D-N1N	2.67	110.99	108.10
7	B	1001	FAD	C5X-C9A-N10	2.70	119.60	117.58
9	B	1004	FMN	C4A-N5-C5A	3.19	120.49	116.72
7	B	1001	FAD	C4X-N5-C5X	3.33	120.64	116.72
9	B	1004	FMN	C5A-C9A-N10	3.37	120.10	117.58
9	B	1004	FMN	O5'-P-O1P	3.60	116.12	107.08
9	B	1004	FMN	C4-N3-C2	5.89	120.07	115.16
7	B	1001	FAD	C4-N3-C2	5.91	120.09	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1002	NAD	4	0
6	A	2002	SO4	2	0
7	B	1001	FAD	5	0
9	B	1004	FMN	10	0
10	B	1005	DMG	6	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%)	0.14	51 (5%) 30 40	18, 36, 64, 83	0
2	B	402/404 (99%)	0.05	4 (0%) 84 88	21, 39, 57, 80	0
3	C	195/206 (94%)	0.05	4 (2%) 67 74	24, 35, 60, 81	0
4	D	91/99 (91%)	0.14	1 (1%) 82 86	25, 33, 56, 76	0
All	All	1651/1673 (98%)	0.11	60 (3%) 46 57	18, 37, 63, 83	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	200	ALA	4.7
2	B	202	ASP	4.4
1	A	866	GLU	4.2
1	A	226	PRO	4.0
1	A	935	VAL	3.8
1	A	954	LEU	3.7
1	A	864	VAL	3.6
1	A	751	ASP	3.4
3	C	96	ALA	3.3
1	A	761	VAL	3.2
1	A	875	LEU	3.2
1	A	932	ILE	3.0
1	A	909	HIS	2.9
1	A	881	LEU	2.8
1	A	327	THR	2.8
1	A	849	LEU	2.8
1	A	897	SER	2.8
1	A	867	ASP	2.7
1	A	873	SER	2.7
1	A	742	LEU	2.7
1	A	933	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	748	VAL	2.6
1	A	694	GLY	2.6
1	A	782	PHE	2.6
2	B	1	ALA	2.5
1	A	894	ALA	2.5
1	A	227	SER	2.5
1	A	865	ARG	2.5
1	A	830	ASP	2.5
1	A	895	VAL	2.5
1	A	845	VAL	2.4
1	A	652	GLY	2.4
1	A	844	TRP	2.4
1	A	915	ALA	2.4
1	A	843	GLU	2.3
1	A	958	GLU	2.3
1	A	877	VAL	2.3
1	A	946	ASP	2.3
1	A	889	LEU	2.3
1	A	818	LEU	2.3
2	B	48	VAL	2.3
2	B	402	VAL	2.3
1	A	840	ALA	2.2
1	A	896	ALA	2.2
3	C	199	VAL	2.2
1	A	824	PHE	2.2
1	A	848	LYS	2.2
1	A	659	GLY	2.2
1	A	928	GLY	2.2
1	A	951	ASP	2.2
1	A	945	VAL	2.1
3	C	6	GLN	2.1
1	A	746	LEU	2.1
1	A	744	SER	2.0
1	A	645	LEU	2.0
1	A	768	GLU	2.0
1	A	619	VAL	2.0
4	D	29	GLU	2.0
1	A	963	ASP	2.0
1	A	948	GLN	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
10	DMG	B	1005	7/7	0.78	0.25	6.92	55,60,62,66	0
6	SO4	B	2007	5/5	0.95	0.18	2.07	71,74,76,76	0
9	FMN	B	1004	31/31	0.95	0.15	1.96	14,24,33,37	0
6	SO4	A	2002	5/5	0.94	0.14	1.08	62,63,68,69	0
6	SO4	A	2001	5/5	0.98	0.13	0.50	49,52,54,55	0
5	ZN	D	1006	1/1	0.99	0.14	0.39	30,30,30,30	0
8	NAD	A	1002	44/44	0.98	0.12	0.38	17,24,38,41	0
6	SO4	A	2003	5/5	0.96	0.09	-0.38	71,72,76,76	0
7	FAD	B	1001	53/53	0.96	0.10	-0.49	22,31,37,41	0
6	SO4	A	2006	5/5	0.97	0.18	-0.77	60,62,65,66	0
6	SO4	D	2004	5/5	0.97	0.07	-	86,87,88,89	0
6	SO4	A	2008	5/5	0.97	0.12	-	64,65,68,71	0
6	SO4	C	2005	5/5	0.98	0.08	-	49,52,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.