Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 10:57 PM EDT

PDB ID	:	2GAH
Title	:	Heterotetrameric sarcosine: structure of a diflavin metaloenzyme at 1.85 a resolution
Authors	:	Chen, Z.W.; Hassan-Abdulah, A.; Zhao, G.; Jorns, M.S.; Mathews, F.S.
Deposited on	:	2006-03-08
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

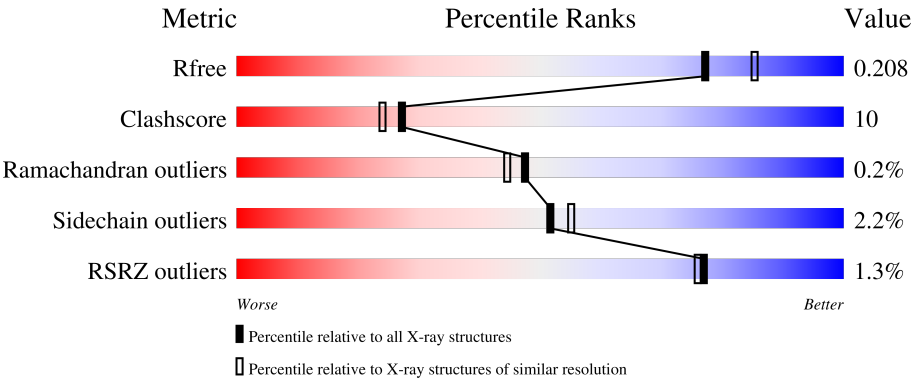
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	965	82% 18%
2	B	405	78% 20%
3	C	210	2% 70% 19% 10%
4	D	99	3% 78% 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
7	FMN	B	502	X	X	-	-
8	FOA	B	503	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14343 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 heterotetrameric sarcosine oxidase alpha-subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	965	7261	4520	1294	1428	2	17	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	90	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	155	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	267	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	419	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	503	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	579	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	609	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	626	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	661	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	667	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	673	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	757	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	816	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	843	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8
A	904	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ8

- Molecule 2 is a protein called heterotetrameric sarcosine oxidase beta-subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	403	3098	1969	542	576	3	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	62	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	160	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	187	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	236	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	265	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	283	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	306	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0
B	333	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDR0

- Molecule 3 is a protein called heterotetrameric sarcosine oxidase gamma-subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	190	Total	C	N	O	S	Se	0	0	0
			1396	877	248	266	2	3			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	23	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ7
C	176	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ7
C	193	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ7
C	203	LEU	-	CLONING ARTIFACT	UNP Q3ZDQ7
C	204	GLU	-	CLONING ARTIFACT	UNP Q3ZDQ7
C	205	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	206	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	207	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	208	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	209	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7
C	210	HIS	-	EXPRESSION TAG	UNP Q3ZDQ7

- Molecule 4 is a protein called heterotetrameric sarcosine oxidase delta-subunit.

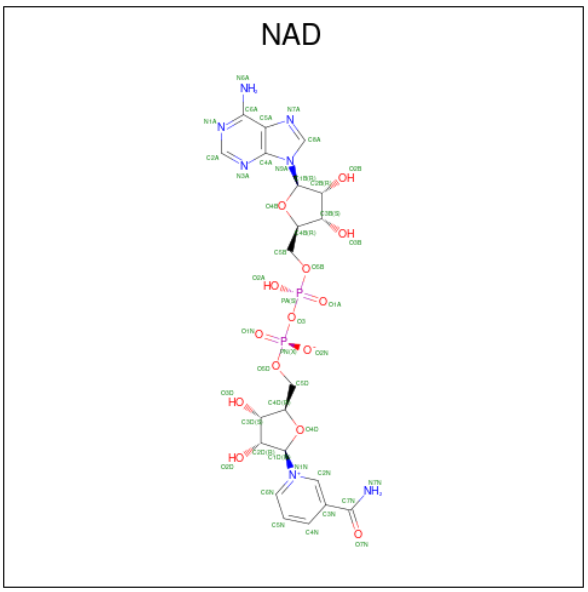
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	91	Total	C	N	O	S	Se	0	0	0
			747	480	134	128	3	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ9
D	2	MSE	MET	MODIFIED RESIDUE	UNP Q3ZDQ9

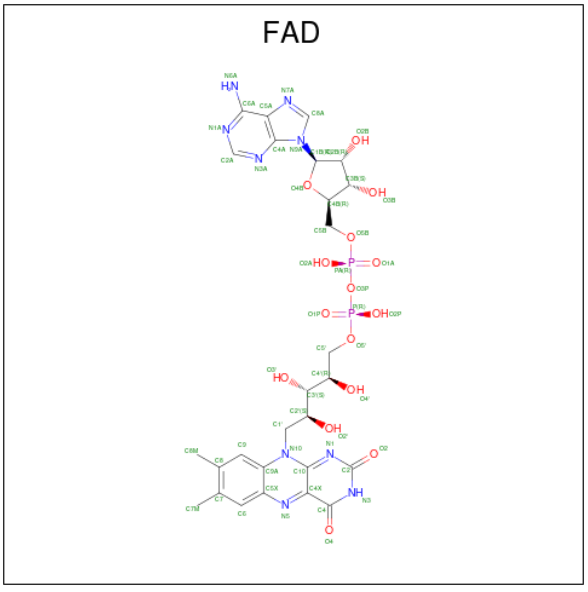
- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD)

(formula: $C_{21}H_{27}N_7O_{14}P_2$).



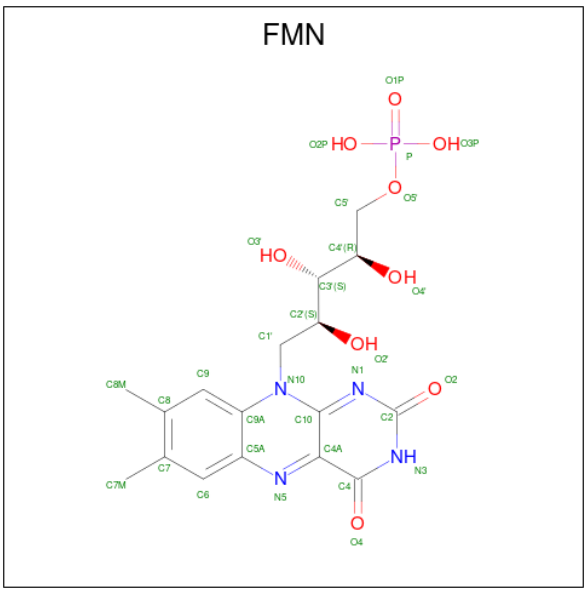
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



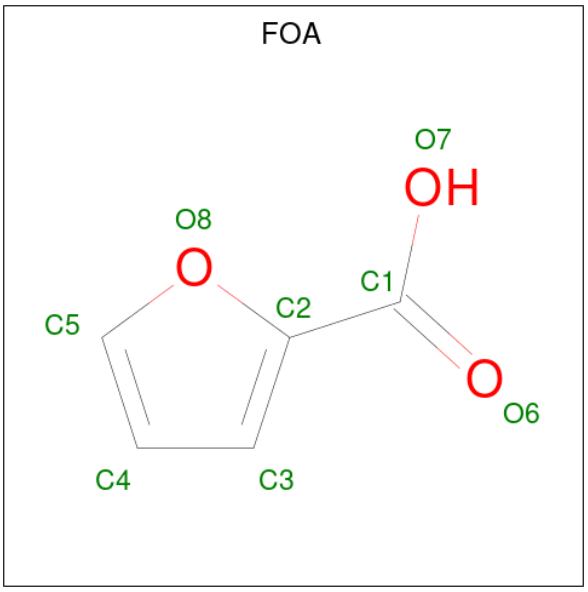
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 8 is 2-FUROIC ACID (three-letter code: FOA) (formula: $C_5H_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O		0	0
			8	5	3			

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

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

- Molecule 10 is water.

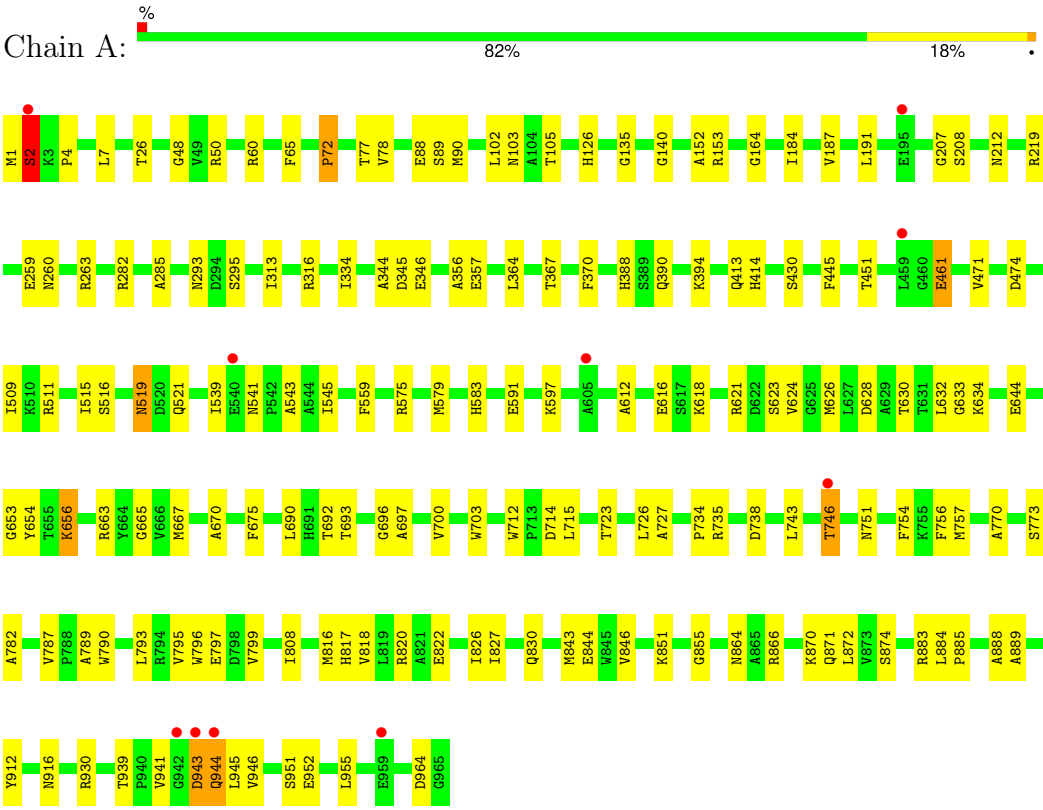
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	986	Total O 986 986	0	0
10	B	421	Total O 421 421	0	0
10	C	189	Total O 189 189	0	0
10	D	108	Total O 108 108	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

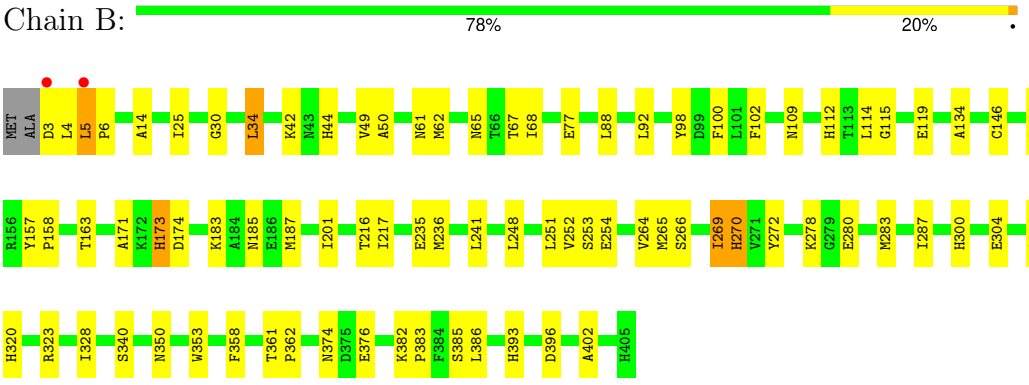
• Molecule 1: heterotetrameric sarcosine oxidase alpha-subunit

Chain A:



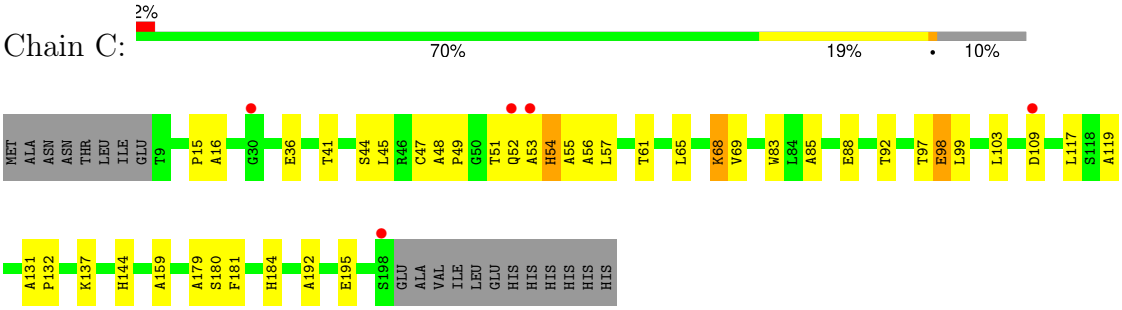
• Molecule 2: heterotetrameric sarcosine oxidase beta-subunit

Chain B:



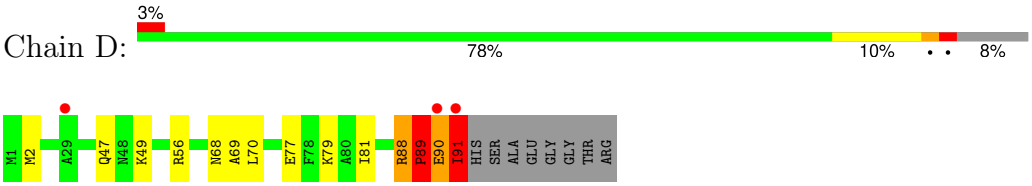
• Molecule 3: heterotetrameric sarcosine oxidase gamma-subunit

Chain C:



• Molecule 4: heterotetrameric sarcosine oxidase delta-subunit

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.26Å 132.77Å 198.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.57 – 2.00 20.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.4 (20.57-2.00) 86.5 (20.57-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.211 0.169 , 0.208	Depositor DCC
R_{free} test set	5028 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14343	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ZN, FOA, 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	0.37	0/7373	0.60	0/10004
2	B	0.38	0/3171	0.64	3/4299 (0.1%)
3	C	0.35	0/1423	0.64	1/1945 (0.1%)
4	D	0.66	3/772 (0.4%)	0.95	7/1044 (0.7%)
All	All	0.39	3/12739 (0.0%)	0.64	11/17292 (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
4	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	90	GLU	CG-CD	8.63	1.64	1.51
4	D	90	GLU	CB-CG	6.37	1.64	1.52
4	D	90	GLU	N-CA	-5.80	1.34	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	90	GLU	N-CA-CB	-11.43	90.03	110.60
4	D	91	ILE	N-CA-C	8.73	134.58	111.00
4	D	88	ARG	C-N-CD	8.65	146.56	128.40
4	D	90	GLU	CB-CG-CD	7.40	134.17	114.20
2	B	319	ALA	N-CA-C	-5.94	94.95	111.00
4	D	90	GLU	OE1-CD-OE2	-5.75	116.40	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	91	ILE	N-CA-CB	-5.46	98.25	110.80
4	D	90	GLU	CA-CB-CG	-5.32	101.69	113.40
2	B	270	HIS	N-CA-C	5.11	124.80	111.00
3	C	54	HIS	N-CA-C	-5.11	97.22	111.00
2	B	269	ILE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	89	PRO	Peptide

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	7261	0	7143	151	0
2	B	3098	0	3013	63	0
3	C	1396	0	1385	38	0
4	D	747	0	710	13	0
5	A	44	0	26	0	0
6	B	53	0	31	4	0
7	B	31	0	17	2	0
8	B	8	0	3	4	0
9	D	1	0	0	0	0
10	A	986	0	0	20	0
10	B	421	0	0	5	0
10	C	189	0	0	6	0
10	D	108	0	0	1	0
All	All	14343	0	12328	253	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 10.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:LYS:H	1:A:656:LYS:HD2	1.26	0.98
1:A:647:ASN:HD21	1:A:654:TYR:H	1.21	0.86
2:B:173:HIS:HD1	2:B:174:ASP:H	1.28	0.82
4:D:70:LEU:HD13	4:D:91:ILE:HD13	1.61	0.82
1:A:541:ASN:HD21	1:A:543:ALA:HB3	1.43	0.81
4:D:70:LEU:CD1	4:D:91:ILE:HD13	2.11	0.81
2:B:68:ILE:HD12	8:B:503:FOA:H3	1.63	0.81
1:A:541:ASN:ND2	1:A:543:ALA:HB3	1.99	0.77
1:A:656:LYS:H	1:A:656:LYS:CD	1.99	0.76
1:A:692:THR:HG21	1:A:697:ALA:HA	1.72	0.71
1:A:633:GLY:HA3	1:A:692:THR:HG22	1.70	0.71
1:A:735:ARG:HH21	1:A:735:ARG:HA	1.56	0.71
1:A:649:ILE:CG2	1:A:667:MSE:HE3	2.20	0.71
1:A:816:MSE:HE2	1:A:817:HIS:HD2	1.55	0.70
2:B:61:ASN:HD21	2:B:328:ILE:H	1.40	0.70
2:B:350:ASN:HD21	2:B:353:TRP:HE1	1.38	0.69
2:B:340:SER:HB3	2:B:385:SER:HA	1.75	0.69
1:A:539:ILE:HD12	1:A:545:ILE:HD11	1.73	0.69
3:C:53:ALA:HA	3:C:56:ALA:CB	2.22	0.69
1:A:78:VAL:HG13	1:A:102:LEU:HD11	1.75	0.68
1:A:692:THR:OG1	1:A:700:VAL:HG21	1.95	0.67
2:B:254:GLU:OE2	2:B:320:HIS:HD2	1.77	0.67
3:C:53:ALA:HA	3:C:56:ALA:HB3	1.77	0.66
1:A:770:ALA:HB2	1:A:787:VAL:HG12	1.77	0.65
3:C:48:ALA:HB3	3:C:51:THR:HG21	1.79	0.65
4:D:70:LEU:HD13	4:D:91:ILE:CD1	2.29	0.63
1:A:1:MSE:HB2	1:A:285:ALA:CB	2.28	0.63
4:D:49:LYS:HE2	10:D:1564:HOH:O	1.98	0.63
1:A:1:MSE:HB2	1:A:285:ALA:HB3	1.81	0.62
2:B:374:ASN:HB3	2:B:376:GLU:HG2	1.81	0.62
1:A:575:ARG:HD3	3:C:181:PHE:CE2	2.35	0.62
1:A:843:MSE:O	1:A:846:VAL:HG12	1.99	0.62
1:A:871:GLN:NE2	1:A:930:ARG:H	1.98	0.62
2:B:173:HIS:HD1	2:B:174:ASP:N	1.98	0.61
4:D:89:PRO:HB2	4:D:90:GLU:HG2	1.83	0.61
2:B:42:LYS:HD3	2:B:42:LYS:O	2.01	0.61
1:A:207:GLY:HA2	1:A:390:GLN:HE22	1.66	0.60
1:A:153:ARG:HD3	3:C:144:HIS:CD2	2.37	0.60
1:A:208:SER:H	1:A:390:GLN:NE2	2.00	0.60
2:B:201:ILE:HD11	2:B:216:THR:HG23	1.83	0.60
1:A:60:ARG:HH22	1:A:260:ASN:HD22	1.50	0.60
1:A:414:HIS:HD2	10:A:1528:HOH:O	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:ARG:HG2	4:D:89:PRO:O	2.01	0.60
2:B:236:MSE:HE1	10:B:1578:HOH:O	2.00	0.59
1:A:575:ARG:HD3	3:C:181:PHE:CZ	2.37	0.59
1:A:743:LEU:HD11	1:A:799:VAL:HG22	1.83	0.59
1:A:939:THR:HG23	1:A:941:VAL:CG1	2.32	0.59
3:C:57:LEU:O	3:C:61:THR:HG23	2.03	0.58
1:A:212:ASN:ND2	1:A:413:GLN:HE21	2.01	0.58
2:B:42:LYS:HD3	2:B:42:LYS:C	2.24	0.58
1:A:521:GLN:HE22	2:B:323:ARG:HD2	1.68	0.58
1:A:77:THR:HB	1:A:105:THR:CG2	2.33	0.58
2:B:300:HIS:O	2:B:304:GLU:HG3	2.04	0.58
2:B:155:ILE:HD11	2:B:158:PRO:HA	1.87	0.57
1:A:770:ALA:HB2	1:A:787:VAL:CG1	2.35	0.57
2:B:112:HIS:HD2	2:B:157:TYR:O	1.89	0.56
3:C:131:ALA:HB3	3:C:132:PRO:HD3	1.86	0.56
1:A:575:ARG:HD2	3:C:180:SER:OG	2.05	0.56
1:A:944:GLN:HE21	1:A:945:LEU:H	1.54	0.56
1:A:871:GLN:HE21	1:A:930:ARG:H	1.52	0.56
2:B:350:ASN:ND2	2:B:353:TRP:HE1	2.03	0.55
1:A:944:GLN:HE21	1:A:945:LEU:N	2.03	0.55
1:A:647:ASN:ND2	1:A:654:TYR:H	1.99	0.55
1:A:583:HIS:HE1	1:A:628:ASP:OD2	1.89	0.55
2:B:146:CYS:SG	2:B:149:ILE:HG13	2.47	0.55
1:A:102:LEU:HD12	10:A:1231:HOH:O	2.07	0.55
3:C:85:ALA:HB3	3:C:88:GLU:HB3	1.88	0.55
1:A:667:MSE:HE1	1:A:703:TRP:HD1	1.72	0.54
1:A:870:LYS:NZ	10:A:1451:HOH:O	2.40	0.54
1:A:746:THR:O	1:A:746:THR:OG1	2.22	0.54
1:A:244:GLN:OE1	1:A:414:HIS:HE1	1.90	0.54
1:A:313:ILE:CD1	1:A:334:ILE:HD12	2.37	0.54
1:A:2:SER:O	1:A:50:ARG:NH2	2.33	0.54
3:C:159:ALA:O	3:C:184:HIS:HE1	1.91	0.54
1:A:667:MSE:CE	1:A:703:TRP:CD1	2.91	0.53
3:C:52:GLN:O	3:C:53:ALA:HB3	2.08	0.53
1:A:644:GLU:HG2	10:A:2288:HOH:O	2.08	0.53
1:A:820:ARG:HD2	1:A:820:ARG:C	2.29	0.53
1:A:26:THR:HB	1:A:103:ASN:HD22	1.73	0.53
1:A:334:ILE:HD11	1:A:370:PHE:CZ	2.44	0.53
1:A:77:THR:HB	1:A:105:THR:HG23	1.91	0.53
1:A:939:THR:HG23	1:A:941:VAL:HG12	1.90	0.53
3:C:52:GLN:HG3	10:C:2358:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLU:OE2	2:B:114:LEU:HD12	2.09	0.52
2:B:361:THR:HB	2:B:362:PRO:HD3	1.91	0.52
1:A:356:ALA:HB2	1:A:367:THR:HG22	1.89	0.52
1:A:626:MSE:HE2	1:A:796:TRP:CE2	2.45	0.52
1:A:941:VAL:O	1:A:941:VAL:HG22	2.09	0.52
2:B:68:ILE:HD12	8:B:503:FOA:C3	2.37	0.52
1:A:714:ASP:HA	10:A:1508:HOH:O	2.09	0.52
3:C:98:GLU:HG2	10:C:2636:HOH:O	2.10	0.52
3:C:53:ALA:CA	3:C:56:ALA:HB3	2.40	0.51
1:A:559:PHE:HE2	2:B:283:MSE:HE1	1.75	0.51
1:A:60:ARG:HH22	1:A:260:ASN:ND2	2.09	0.51
1:A:667:MSE:HE1	1:A:703:TRP:CD1	2.45	0.51
2:B:254:GLU:OE2	2:B:320:HIS:CD2	2.60	0.51
1:A:649:ILE:HG23	1:A:667:MSE:HE3	1.91	0.51
2:B:149:ILE:HD11	2:B:264:VAL:HG21	1.92	0.51
1:A:293:ASN:HD22	1:A:295:SER:H	1.58	0.50
3:C:68:LYS:HG2	10:C:2202:HOH:O	2.11	0.50
1:A:696:GLY:O	1:A:700:VAL:HG23	2.11	0.50
2:B:358:PHE:HB3	6:B:501:FAD:C2	2.41	0.50
1:A:770:ALA:CB	1:A:787:VAL:HG12	2.41	0.50
1:A:515:ILE:O	1:A:516:SER:HB3	2.12	0.50
2:B:62:MSE:O	2:B:173:HIS:HB2	2.12	0.50
1:A:388:HIS:HD2	10:A:1557:HOH:O	1.93	0.50
1:A:487:GLN:NE2	1:A:519:ASN:H	2.10	0.49
1:A:88:GLU:OE2	2:B:320:HIS:HE1	1.95	0.49
1:A:817:HIS:HB3	1:A:912:TYR:OH	2.12	0.49
3:C:55:ALA:HB1	10:C:1561:HOH:O	2.11	0.49
2:B:67:THR:HB	2:B:171:ALA:O	2.13	0.49
2:B:266:SER:O	2:B:270:HIS:HA	2.13	0.49
2:B:248:LEU:HB3	6:B:501:FAD:HM83	1.93	0.49
1:A:126:HIS:HD2	10:A:2534:HOH:O	1.96	0.49
1:A:559:PHE:CE2	2:B:283:MSE:HE1	2.48	0.49
2:B:115:GLY:O	2:B:119:GLU:HG3	2.13	0.49
1:A:866:ARG:HD3	2:B:393:HIS:HE1	1.77	0.48
1:A:632:LEU:HD22	10:A:2147:HOH:O	2.13	0.48
1:A:773:SER:HB3	1:A:775:ILE:HD12	1.96	0.48
10:A:1309:HOH:O	3:C:184:HIS:HD2	1.95	0.48
2:B:149:ILE:HG12	2:B:313:PHE:CE1	2.49	0.48
3:C:54:HIS:CE1	3:C:65:LEU:HD12	2.48	0.48
3:C:98:GLU:HG3	3:C:99:LEU:N	2.29	0.48
4:D:89:PRO:HB2	4:D:90:GLU:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MSE:HG3	2:B:254:GLU:HG3	1.95	0.48
2:B:65:ASN:HA	6:B:501:FAD:C5X	2.44	0.48
1:A:623:SER:HB3	10:A:1500:HOH:O	2.12	0.48
2:B:251:LEU:C	2:B:251:LEU:HD12	2.34	0.48
1:A:263:ARG:HD3	1:A:344:ALA:HB2	1.95	0.48
1:A:471:VAL:HG22	10:A:1774:HOH:O	2.14	0.47
1:A:734:PRO:O	1:A:735:ARG:NH2	2.47	0.47
1:A:820:ARG:HD3	1:A:827:ILE:HD13	1.96	0.47
1:A:883:ARG:NH2	10:A:1628:HOH:O	2.43	0.47
1:A:50:ARG:HG3	10:A:1713:HOH:O	2.14	0.47
1:A:187:VAL:O	1:A:191:LEU:HG	2.14	0.47
1:A:656:LYS:HG2	1:A:663:ARG:HH12	1.80	0.47
10:A:1719:HOH:O	3:C:179:ALA:HB3	2.14	0.47
1:A:827:ILE:O	1:A:827:ILE:HG22	2.14	0.47
3:C:68:LYS:NZ	3:C:69:VAL:O	2.42	0.47
1:A:844:GLU:HB2	10:A:2704:HOH:O	2.15	0.46
1:A:692:THR:CG2	1:A:697:ALA:HA	2.43	0.46
1:A:820:ARG:HD3	1:A:827:ILE:CD1	2.45	0.46
3:C:97:THR:HG22	3:C:97:THR:O	2.15	0.46
1:A:231:GLY:O	3:C:195:GLU:HB2	2.14	0.46
1:A:519:ASN:C	1:A:519:ASN:ND2	2.68	0.46
1:A:164:GLY:HA3	1:A:184:ILE:HD13	1.97	0.46
1:A:634:LYS:HE3	1:A:726:LEU:HB2	1.97	0.46
3:C:45:LEU:HD21	3:C:103:LEU:HD13	1.98	0.46
1:A:647:ASN:HD21	1:A:654:TYR:N	2.02	0.46
2:B:25:ILE:HD11	2:B:217:ILE:HG22	1.97	0.46
1:A:656:LYS:CD	1:A:656:LYS:N	2.75	0.45
1:A:820:ARG:CD	1:A:827:ILE:HD13	2.46	0.45
2:B:65:ASN:HA	6:B:501:FAD:C6	2.47	0.45
2:B:272:TYR:CE1	8:B:503:FOA:H4	2.51	0.45
3:C:15:PRO:HG3	10:C:1338:HOH:O	2.16	0.45
3:C:44:SER:HB2	3:C:117:LEU:HD12	1.98	0.45
3:C:49:PRO:HA	3:C:54:HIS:CD2	2.52	0.45
1:A:624:VAL:HG13	1:A:808:ILE:HA	1.98	0.45
1:A:626:MSE:HE2	1:A:796:TRP:CD2	2.52	0.45
1:A:751:ASN:ND2	1:A:774:ARG:HH12	2.15	0.45
1:A:827:ILE:HG22	1:A:830:GLN:HB3	1.99	0.45
1:A:511:ARG:HH11	1:A:511:ARG:HG3	1.80	0.45
1:A:885:PRO:HG2	1:A:888:ALA:HB2	1.97	0.45
1:A:152:ALA:HB2	1:A:445:PHE:CG	2.51	0.45
1:A:388:HIS:HE1	1:A:394:LYS:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:SER:HB2	1:A:782:ALA:HB3	1.99	0.45
2:B:134:ALA:HB2	10:B:1130:HOH:O	2.16	0.45
1:A:505:SER:O	1:A:509:ILE:HG12	2.17	0.44
1:A:692:THR:HG23	1:A:693:THR:O	2.16	0.44
1:A:818:VAL:O	1:A:822:GLU:HG3	2.18	0.44
3:C:69:VAL:HA	3:C:83:TRP:CE3	2.52	0.44
1:A:259:GLU:HG3	10:A:1019:HOH:O	2.17	0.44
1:A:690:LEU:HD12	1:A:690:LEU:N	2.32	0.44
2:B:30:GLY:O	2:B:34:LEU:CD2	2.65	0.44
1:A:889:ALA:HB1	1:A:904:MSE:HE3	1.98	0.44
1:A:951:SER:HB3	10:A:2251:HOH:O	2.18	0.44
1:A:864:ASN:HB2	10:A:1835:HOH:O	2.18	0.44
2:B:5:LEU:HB2	2:B:6:PRO:HD2	1.99	0.44
3:C:137:LYS:HD2	3:C:192:ALA:HB1	1.99	0.44
1:A:219:ARG:HD2	1:A:219:ARG:N	2.33	0.44
1:A:634:LYS:HE2	1:A:723:THR:HA	2.00	0.44
2:B:14:ALA:H	2:B:185:ASN:ND2	2.16	0.44
2:B:382:LYS:N	2:B:383:PRO:CD	2.80	0.44
1:A:735:ARG:HD3	1:A:738:ASP:OD2	2.17	0.43
1:A:789:ALA:HB3	3:C:119:ALA:HB1	1.99	0.43
1:A:874:SER:HB2	1:A:952:GLU:O	2.18	0.43
2:B:100:PHE:CE1	2:B:102:PHE:HB2	2.53	0.43
2:B:248:LEU:HD13	2:B:287:ILE:HG22	2.00	0.43
1:A:647:ASN:ND2	1:A:653:GLY:HA2	2.33	0.43
1:A:316:ARG:HD2	1:A:461:GLU:HG2	1.99	0.43
2:B:183:LYS:O	2:B:187:MSE:HG3	2.18	0.43
1:A:826:ILE:HG22	1:A:872:LEU:HD22	2.00	0.43
1:A:884:LEU:HD22	1:A:939:THR:HG21	2.01	0.43
1:A:135:GLY:O	1:A:140:GLY:HA3	2.18	0.43
1:A:941:VAL:O	1:A:941:VAL:CG2	2.65	0.43
1:A:756:PHE:CE2	1:A:757:MSE:HE2	2.53	0.43
1:A:65:PHE:HB3	1:A:72:PRO:HD2	2.00	0.43
1:A:487:GLN:HE22	1:A:519:ASN:H	1.66	0.43
3:C:53:ALA:HA	3:C:56:ALA:H	1.83	0.43
1:A:656:LYS:HD2	1:A:656:LYS:N	2.09	0.43
1:A:4:PRO:O	1:A:48:GLY:HA2	2.19	0.43
1:A:612:ALA:O	1:A:616:GLU:HG3	2.18	0.43
2:B:278:LYS:HB3	2:B:280:GLU:OE1	2.19	0.43
7:B:502:FMN:H1'2	7:B:502:FMN:H4'	1.88	0.43
3:C:16:ALA:HB3	3:C:36:GLU:CD	2.38	0.42
1:A:670:ALA:O	1:A:855:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ASN:O	7:B:502:FMN:HM82	2.19	0.42
2:B:185:ASN:ND2	10:B:1330:HOH:O	2.53	0.42
1:A:1:MSE:O	1:A:2:SER:C	2.58	0.42
2:B:30:GLY:O	2:B:34:LEU:HD23	2.19	0.42
3:C:52:GLN:OE1	3:C:53:ALA:HB2	2.20	0.42
3:C:47:CYS:SG	3:C:57:LEU:HD12	2.60	0.42
3:C:52:GLN:NE2	10:C:2358:HOH:O	2.52	0.42
1:A:618:LYS:HE2	10:A:1997:HOH:O	2.19	0.42
2:B:109:ASN:HB2	2:B:163:THR:OG1	2.20	0.42
2:B:269:ILE:HG22	2:B:308:ALA:HB1	2.02	0.42
1:A:751:ASN:HD21	1:A:964:ASP:CG	2.22	0.42
1:A:539:ILE:CD1	1:A:545:ILE:HD11	2.46	0.42
2:B:44:HIS:HD2	10:B:1241:HOH:O	2.01	0.42
4:D:69:ALA:CB	4:D:81:ILE:HD13	2.50	0.42
1:A:795:VAL:O	1:A:799:VAL:HG23	2.19	0.42
1:A:7:LEU:HD21	1:A:282:ARG:HB2	2.01	0.41
1:A:621:ARG:HD2	1:A:916:ASN:CG	2.40	0.41
1:A:630:THR:HG23	1:A:727:ALA:HA	2.02	0.41
2:B:88:LEU:O	2:B:92:LEU:HG	2.20	0.41
3:C:41:THR:O	3:C:92:THR:HA	2.20	0.41
4:D:69:ALA:HB2	4:D:81:ILE:HD13	2.02	0.41
1:A:793:LEU:O	1:A:797:GLU:HG3	2.20	0.41
1:A:153:ARG:HD2	10:A:2434:HOH:O	2.19	0.41
1:A:430:SER:HA	1:A:451:THR:HG23	2.03	0.41
2:B:241:LEU:HD23	2:B:386:LEU:HD21	2.01	0.41
2:B:253:SER:HA	2:B:320:HIS:O	2.21	0.41
4:D:47:GLN:OE1	4:D:49:LYS:HD2	2.20	0.41
1:A:77:THR:HA	1:A:89:SER:HA	2.02	0.41
1:A:712:TRP:HB3	1:A:715:LEU:HG	2.01	0.41
2:B:3:ASP:N	10:B:2649:HOH:O	2.53	0.41
2:B:49:VAL:HG12	2:B:50:ALA:N	2.34	0.41
1:A:357:GLU:O	1:A:364:LEU:HA	2.20	0.41
1:A:874:SER:HB3	1:A:955:LEU:HD11	2.02	0.41
3:C:48:ALA:O	3:C:51:THR:HG23	2.21	0.41
1:A:345:ASP:HB2	1:A:346:GLU:OE1	2.20	0.41
1:A:654:TYR:OH	1:A:665:GLY:HA3	2.20	0.41
2:B:77:GLU:OE1	2:B:77:GLU:N	2.51	0.41
1:A:634:LYS:HB2	1:A:723:THR:HA	2.03	0.41
4:D:56:ARG:HG2	4:D:68:ASN:HD22	1.85	0.41
1:A:633:GLY:CA	1:A:692:THR:HG22	2.46	0.40
2:B:265:MSE:HE2	2:B:402:ALA:HB1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:77:GLU:OE2	4:D:79:LYS:HE2	2.21	0.40
1:A:597:LYS:HD3	1:A:597:LYS:HA	1.99	0.40
1:A:939:THR:HG23	1:A:946:VAL:HG22	2.03	0.40
1:A:820:ARG:NE	1:A:827:ILE:HD13	2.36	0.40
2:B:272:TYR:CD1	8:B:503:FOA:H4	2.57	0.40
4:D:89:PRO:HB2	4:D:90:GLU:CD	2.42	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	963/965 (100%)	931 (97%)	29 (3%)	3 (0%)	41 37
2	B	401/405 (99%)	388 (97%)	13 (3%)	0	100 100
3	C	188/210 (90%)	179 (95%)	9 (5%)	0	100 100
4	D	89/99 (90%)	85 (96%)	3 (3%)	1 (1%)	14 8
All	All	1641/1679 (98%)	1583 (96%)	54 (3%)	4 (0%)	47 44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	72	PRO
1	A	943	ASP
4	D	89	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	749/732 (102%)	735 (98%)	14 (2%)	57	61
2	B	319/312 (102%)	310 (97%)	9 (3%)	43	44
3	C	143/158 (90%)	140 (98%)	3 (2%)	53	57
4	D	74/77 (96%)	72 (97%)	2 (3%)	44	46
All	All	1285/1279 (100%)	1257 (98%)	28 (2%)	52	55

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	461	GLU
1	A	474	ASP
1	A	519	ASN
1	A	579	MSE
1	A	656	LYS
1	A	675	PHE
1	A	746	THR
1	A	754	PHE
1	A	775	ILE
1	A	790	TRP
1	A	851	LYS
1	A	943	ASP
1	A	944	GLN
2	B	4	LEU
2	B	5	LEU
2	B	34	LEU
2	B	98	TYR
2	B	153	ASP
2	B	173	HIS
2	B	235	GLU
2	B	252	VAL
2	B	396	ASP
3	C	68	LYS
3	C	98	GLU
3	C	109	ASP
4	D	2	MSE
4	D	91	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	126	HIS
1	A	201	GLN
1	A	212	ASN
1	A	260	ASN
1	A	277	ASN
1	A	293	ASN
1	A	368	GLN
1	A	382	ASN
1	A	388	HIS
1	A	390	GLN
1	A	412	ASN
1	A	414	HIS
1	A	487	GLN
1	A	519	ASN
1	A	521	GLN
1	A	583	HIS
1	A	586	HIS
1	A	647	ASN
1	A	751	ASN
1	A	817	HIS
1	A	830	GLN
1	A	871	GLN
1	A	916	ASN
1	A	944	GLN
2	B	15	ASN
2	B	44	HIS
2	B	61	ASN
2	B	109	ASN
2	B	112	HIS
2	B	185	ASN
2	B	218	HIS
2	B	244	GLN
2	B	249	GLN
2	B	320	HIS
2	B	350	ASN
2	B	370	HIS
2	B	393	HIS
3	C	77	GLN
3	C	184	HIS
3	C	187	HIS

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Mol	Chain	Res	Type
4	D	68	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	NAD	A	999	-	42,48,48	3.25	17 (40%)	50,73,73	2.12	14 (28%)
7	FMN	B	502	2	33,33,33	3.84	19 (57%)	48,50,50	3.04	22 (45%)
6	FAD	B	501	-	54,58,58	3.00	23 (42%)	71,89,89	1.81	17 (23%)
8	FOA	B	503	-	5,8,8	2.05	1 (20%)	4,10,10	1.22	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
7	FMN	B	502	2	1/1/4/4	8/18/18/18	0/3/3/3
6	FAD	B	501	-	-	4/30/50/50	0/6/6/6
8	FOA	B	503	-	-	0/0/4/4	0/1/1/1
5	NAD	A	999	-	-	3/26/62/62	0/5/5/5

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	NAD	C2N-N1N	11.27	1.47	1.35
7	B	502	FMN	C1'-C2'	-10.29	1.38	1.52
7	B	502	FMN	C9A-C5A	10.24	1.57	1.41
7	B	502	FMN	C8-C7	7.89	1.60	1.40
5	A	999	NAD	C2A-N3A	7.30	1.43	1.32
6	B	501	FAD	C4A-N3A	7.20	1.45	1.35
6	B	501	FAD	P-O5'	-6.73	1.33	1.59
6	B	501	FAD	C4X-N5	6.32	1.44	1.30
6	B	501	FAD	C2A-N3A	6.20	1.41	1.32
6	B	501	FAD	C10-N1	6.18	1.45	1.33
7	B	502	FMN	C6-C5A	6.18	1.49	1.40
5	A	999	NAD	C4N-C3N	6.12	1.48	1.39
7	B	502	FMN	C10-N10	6.11	1.50	1.37
5	A	999	NAD	C6N-N1N	6.01	1.49	1.35
5	A	999	NAD	C5N-C4N	5.55	1.48	1.38
5	A	999	NAD	C4A-N3A	5.52	1.43	1.35
6	B	501	FAD	C9A-C5X	5.51	1.50	1.41
6	B	501	FAD	C9-C9A	4.84	1.47	1.39
6	B	501	FAD	C6-C5X	4.81	1.47	1.40
6	B	501	FAD	C9-C8	4.75	1.46	1.39
6	B	501	FAD	O5B-C5B	-4.56	1.27	1.44
6	B	501	FAD	C2A-N1A	4.37	1.41	1.33
6	B	501	FAD	C8-C7	4.30	1.51	1.40
7	B	502	FMN	C2-N3	4.27	1.48	1.39
5	A	999	NAD	O4D-C1D	4.13	1.46	1.40
6	B	501	FAD	O4'-C4'	4.05	1.51	1.43
6	B	501	FAD	C10-N10	3.96	1.45	1.37
8	B	503	FOA	C3-C2	-3.84	1.34	1.38
5	A	999	NAD	C2A-N1A	3.78	1.40	1.33
6	B	501	FAD	P-O3P	3.65	1.63	1.59
5	A	999	NAD	PN-O3	3.59	1.63	1.59
5	A	999	NAD	C6N-C5N	3.27	1.45	1.38
7	B	502	FMN	C9A-N10	3.15	1.46	1.41
7	B	502	FMN	C9-C8	3.09	1.43	1.39
6	B	501	FAD	C6-C7	3.09	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	FMN	C4A-N5	3.06	1.37	1.30
7	B	502	FMN	O5'-C5'	-3.04	1.33	1.44
7	B	502	FMN	C2'-C3'	-3.04	1.48	1.53
5	A	999	NAD	PA-O3	3.01	1.62	1.59
7	B	502	FMN	O3'-C3'	2.83	1.50	1.43
7	B	502	FMN	C4A-C10	2.81	1.52	1.44
6	B	501	FAD	C9A-N10	2.80	1.46	1.41
7	B	502	FMN	C4-N3	2.75	1.44	1.38
7	B	502	FMN	P-O1P	-2.67	1.42	1.50
7	B	502	FMN	C9-C9A	2.66	1.43	1.39
6	B	501	FAD	C4-N3	2.65	1.43	1.38
5	A	999	NAD	O4B-C1B	2.62	1.44	1.40
7	B	502	FMN	C10-N1	2.56	1.38	1.33
7	B	502	FMN	C7M-C7	2.46	1.55	1.51
6	B	501	FAD	C2-N3	2.45	1.44	1.39
5	A	999	NAD	C5D-C4D	-2.37	1.44	1.51
6	B	501	FAD	C4'-C3'	2.29	1.57	1.53
5	A	999	NAD	C5A-N7A	-2.26	1.31	1.39
5	A	999	NAD	C6A-N1A	2.26	1.45	1.36
6	B	501	FAD	C6A-N1A	2.12	1.44	1.36
6	B	501	FAD	O3'-C3'	2.11	1.48	1.43
5	A	999	NAD	O4D-C4D	2.09	1.49	1.45
7	B	502	FMN	O4-C4	-2.03	1.19	1.23
5	A	999	NAD	C3N-C7N	2.01	1.53	1.50
6	B	501	FAD	C2-N1	2.00	1.41	1.36

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	999	NAD	N3A-C2A-N1A	-8.60	116.99	128.67
7	B	502	FMN	O4'-C4'-C3'	8.39	128.88	109.25
6	B	501	FAD	N3A-C2A-N1A	-6.71	119.56	128.67
7	B	502	FMN	C8M-C8-C9	-6.59	107.97	119.57
7	B	502	FMN	C8M-C8-C7	6.06	133.13	120.76
7	B	502	FMN	O3'-C3'-C4'	5.59	121.64	108.93
5	A	999	NAD	C5N-C4N-C3N	5.08	125.36	120.36
7	B	502	FMN	C2'-C1'-N10	5.04	134.03	110.20
7	B	502	FMN	C1'-C2'-C3'	4.63	122.21	109.66
7	B	502	FMN	O5'-C5'-C4'	4.27	120.76	109.36
7	B	502	FMN	C9-C9A-N10	4.23	127.54	121.85
6	B	501	FAD	P-O5'-C5'	4.21	145.46	121.35
5	A	999	NAD	C1B-N9A-C4A	-4.16	119.33	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	502	FMN	C5A-N5-C4A	3.94	124.45	118.09
7	B	502	FMN	O3'-C3'-C2'	-3.91	100.04	108.93
7	B	502	FMN	C10-N1-C2	3.82	125.12	116.85
7	B	502	FMN	C5'-C4'-C3'	-3.81	105.04	112.22
5	A	999	NAD	O2N-PN-O3	-3.61	97.51	107.27
7	B	502	FMN	C5A-C9A-N10	-3.54	114.77	117.97
6	B	501	FAD	C5X-N5-C4X	3.33	123.48	118.09
6	B	501	FAD	C9A-C5X-N5	-3.22	119.04	122.45
7	B	502	FMN	C4-C4A-N5	3.21	122.64	118.21
6	B	501	FAD	O2P-P-O5'	3.21	122.09	107.57
5	A	999	NAD	C4A-C5A-N7A	3.09	112.61	109.34
6	B	501	FAD	C4-C4X-N5	3.04	122.41	118.21
6	B	501	FAD	C4B-O4B-C1B	-3.03	107.15	109.92
7	B	502	FMN	C9A-C5A-N5	-3.03	119.24	122.45
6	B	501	FAD	O4B-C1B-N9A	3.00	112.73	108.75
5	A	999	NAD	O5B-C5B-C4B	-2.99	98.83	108.99
7	B	502	FMN	O5'-P-O1P	2.98	114.49	106.44
7	B	502	FMN	O2'-C2'-C3'	2.96	116.18	109.25
6	B	501	FAD	C5'-C4'-C3'	-2.94	106.68	112.22
5	A	999	NAD	O4B-C1B-N9A	-2.93	104.87	108.75
7	B	502	FMN	N3-C2-N1	-2.89	113.37	119.50
7	B	502	FMN	C9A-N10-C10	2.83	125.07	120.75
6	B	501	FAD	C4X-C4-N3	2.78	120.34	113.25
6	B	501	FAD	C4'-C3'-C2'	-2.78	108.94	113.57
5	A	999	NAD	O5D-PN-O1N	2.77	119.91	108.94
6	B	501	FAD	C10-C4X-N5	-2.74	119.22	124.81
7	B	502	FMN	O2'-C2'-C1'	2.69	121.25	110.20
5	A	999	NAD	O2D-C2D-C3D	2.62	120.23	111.82
7	B	502	FMN	O2-C2-N1	2.54	126.01	121.80
7	B	502	FMN	C7M-C7-C6	-2.45	115.26	119.57
6	B	501	FAD	PA-O5B-C5B	2.38	134.98	121.35
6	B	501	FAD	C9-C9A-N10	2.36	125.03	121.85
6	B	501	FAD	O3P-P-O1P	-2.29	103.82	110.70
5	A	999	NAD	C5B-C4B-C3B	2.24	123.27	115.21
6	B	501	FAD	C8M-C8-C9	-2.21	115.69	119.57
5	A	999	NAD	C6N-C5N-C4N	-2.13	116.39	119.45
5	A	999	NAD	PN-O5D-C5D	2.10	133.38	121.35
5	A	999	NAD	O3D-C3D-C4D	-2.07	105.13	111.08
5	A	999	NAD	N6A-C6A-N1A	2.06	122.74	118.33
6	B	501	FAD	C4-N3-C2	-2.06	121.99	125.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	502	FMN	C2'

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	502	FMN	N10-C1'-C2'-O2'
7	B	502	FMN	O2'-C2'-C3'-C4'
7	B	502	FMN	C5'-O5'-P-O2P
7	B	502	FMN	O2'-C2'-C3'-O3'
7	B	502	FMN	O4'-C4'-C5'-O5'
5	A	999	NAD	O4D-C4D-C5D-O5D
5	A	999	NAD	C3D-C4D-C5D-O5D
7	B	502	FMN	C5'-O5'-P-O1P
6	B	501	FAD	C4'-C5'-O5'-P
6	B	501	FAD	C5'-O5'-P-O1P
6	B	501	FAD	C5'-O5'-P-O3P
7	B	502	FMN	C2'-C1'-N10-C10
7	B	502	FMN	C4'-C5'-O5'-P
5	A	999	NAD	O4B-C4B-C5B-O5B
6	B	501	FAD	O4B-C4B-C5B-O5B

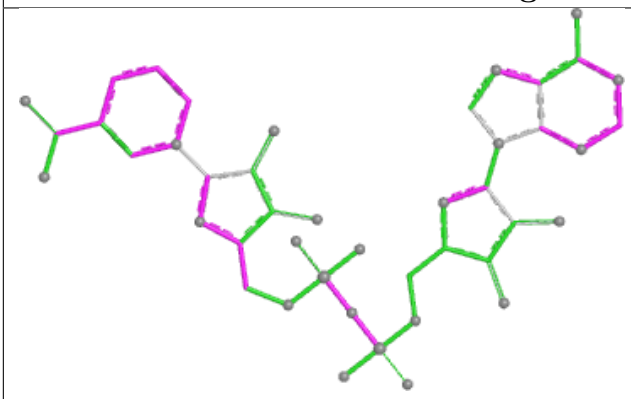
There are no ring outliers.

3 monomers are involved in 10 short contacts:

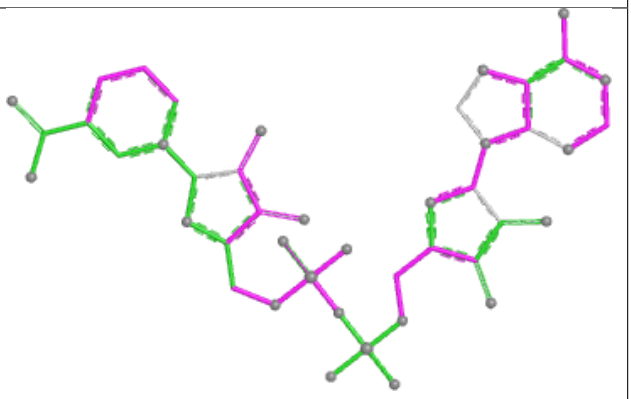
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	502	FMN	2	0
6	B	501	FAD	4	0
8	B	503	FOA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

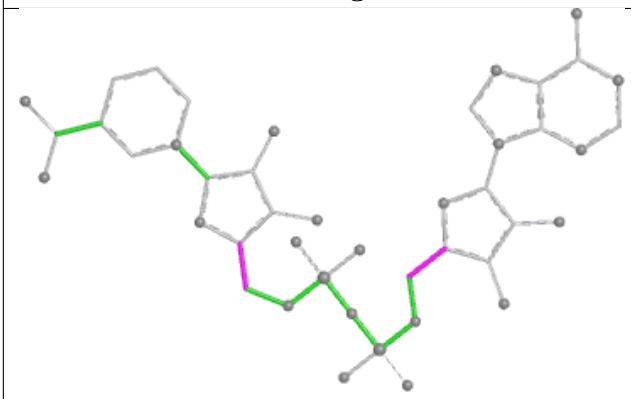
Ligand NAD A 999



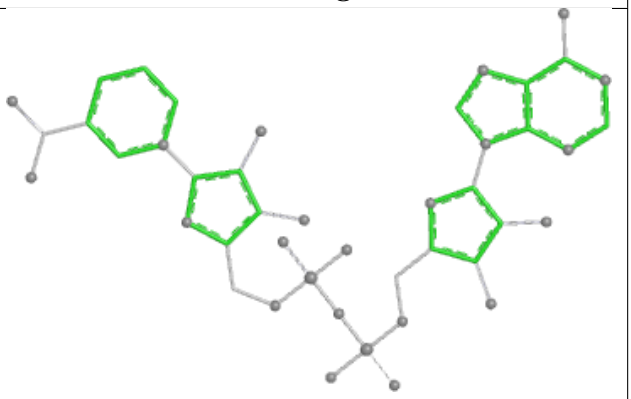
Bond lengths



Bond angles

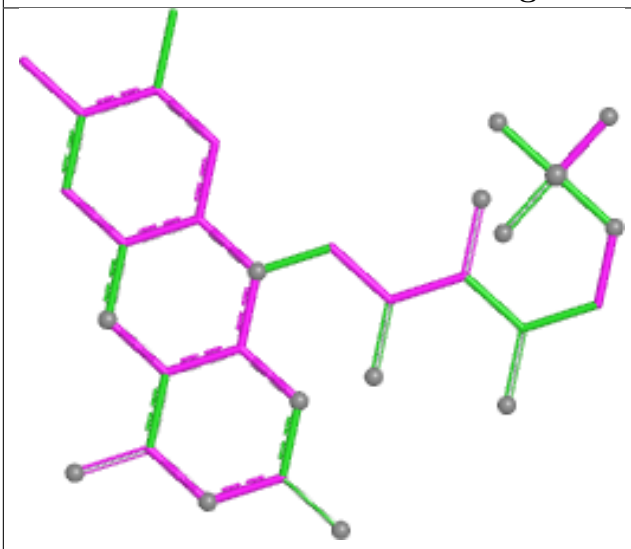


Torsions

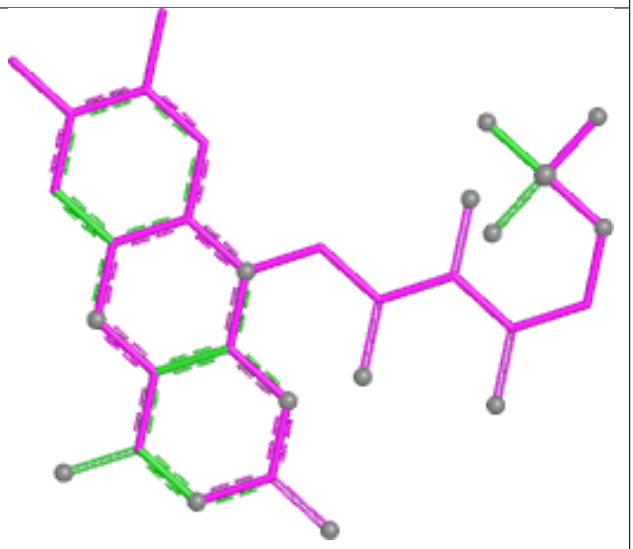


Rings

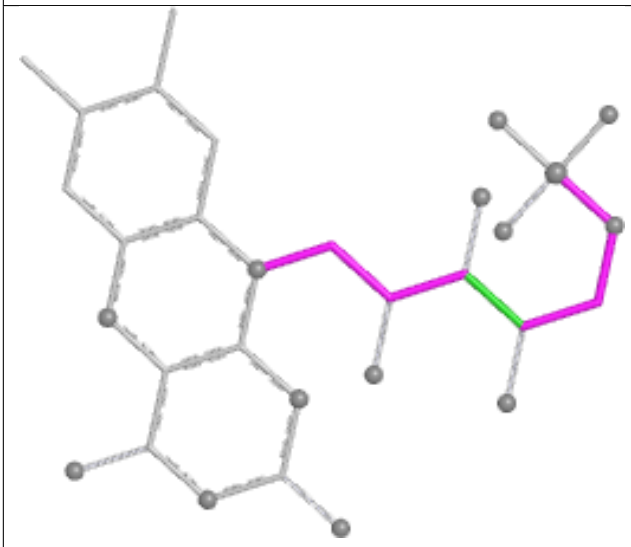
Ligand FMN B 502



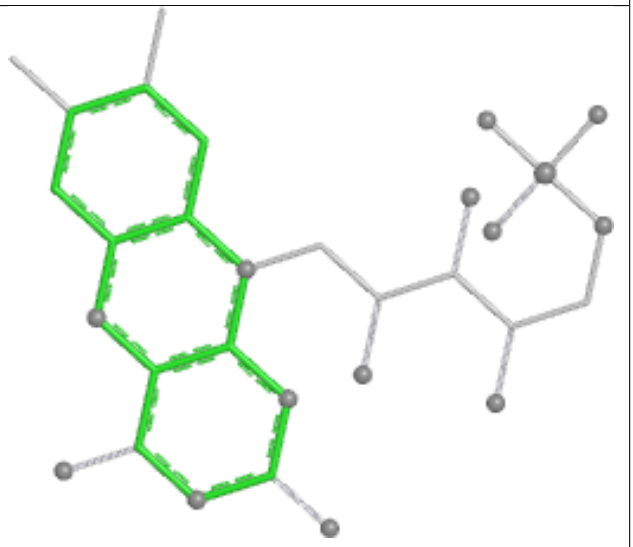
Bond lengths



Bond angles

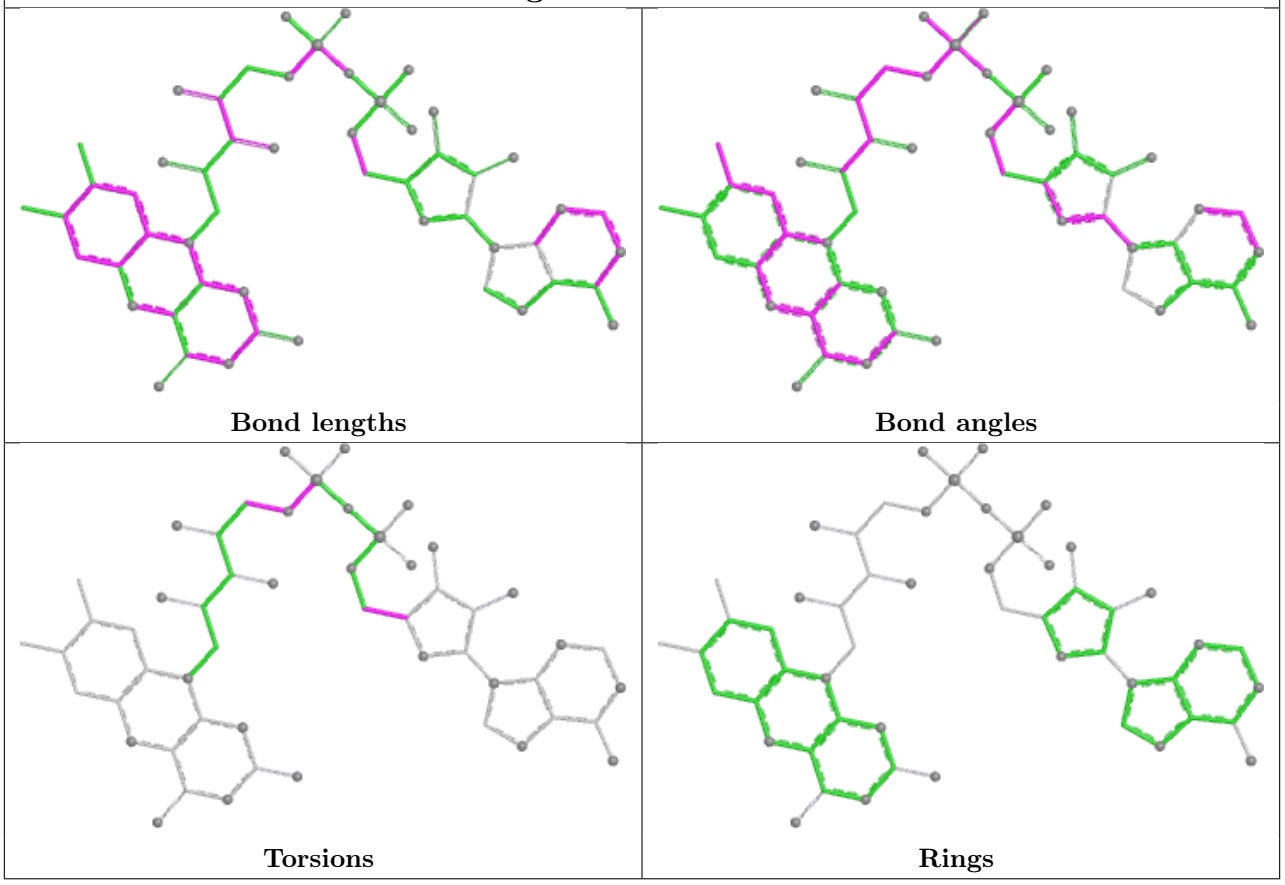


Torsions



Rings

Ligand FAD B 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	948/965 (98%)	-0.38	11 (1%)	79	78	13, 21, 36, 65	0
2	B	395/405 (97%)	-0.49	2 (0%)	91	90	12, 18, 32, 70	0
3	C	187/210 (89%)	-0.13	5 (2%)	54	53	16, 24, 41, 59	0
4	D	89/99 (89%)	-0.24	3 (3%)	45	44	16, 21, 34, 73	0
All	All	1619/1679 (96%)	-0.37	21 (1%)	77	76	12, 21, 36, 73	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	91	ILE	4.6
4	D	90	GLU	4.4
1	A	459	LEU	4.0
1	A	943	ASP	3.9
1	A	746	THR	3.7
3	C	198	SER	3.7
2	B	3	ASP	3.0
3	C	52	GLN	3.0
1	A	2	SER	2.9
3	C	53	ALA	2.8
3	C	109	ASP	2.8
1	A	942	GLY	2.7
3	C	30	GLY	2.7
4	D	29	ALA	2.7
1	A	605	ALA	2.7
1	A	959	GLU	2.6
1	A	540	GLU	2.5
2	B	5	LEU	2.2
1	A	944	GLN	2.1
1	A	195	GLU	2.1
1	A	899	GLU	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

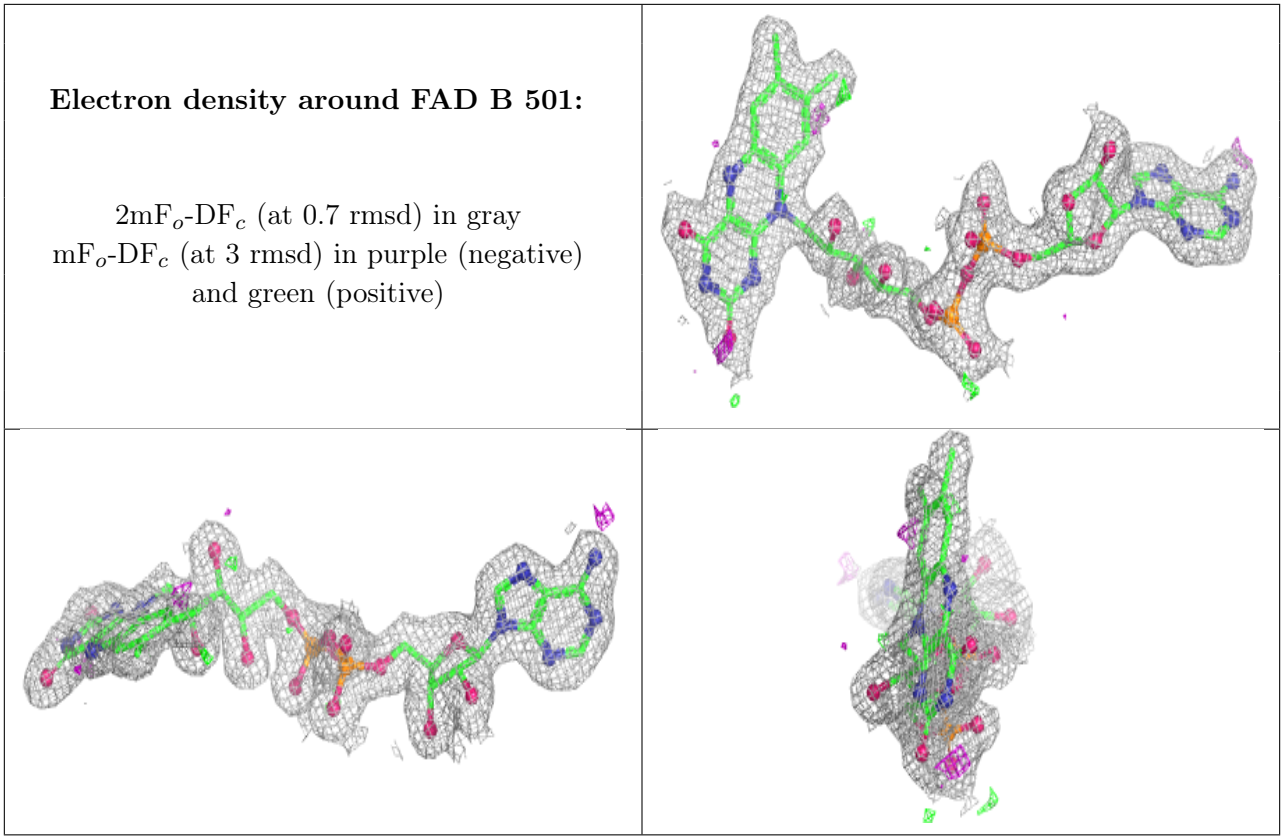
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FOA	B	503	8/8	0.95	0.12	17,22,24,26	0
6	FAD	B	501	53/53	0.97	0.09	13,17,20,22	0
7	FMN	B	502	31/31	0.98	0.07	10,15,18,20	0
5	NAD	A	999	44/44	0.98	0.08	11,17,22,25	0
9	ZN	D	101	1/1	1.00	0.03	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

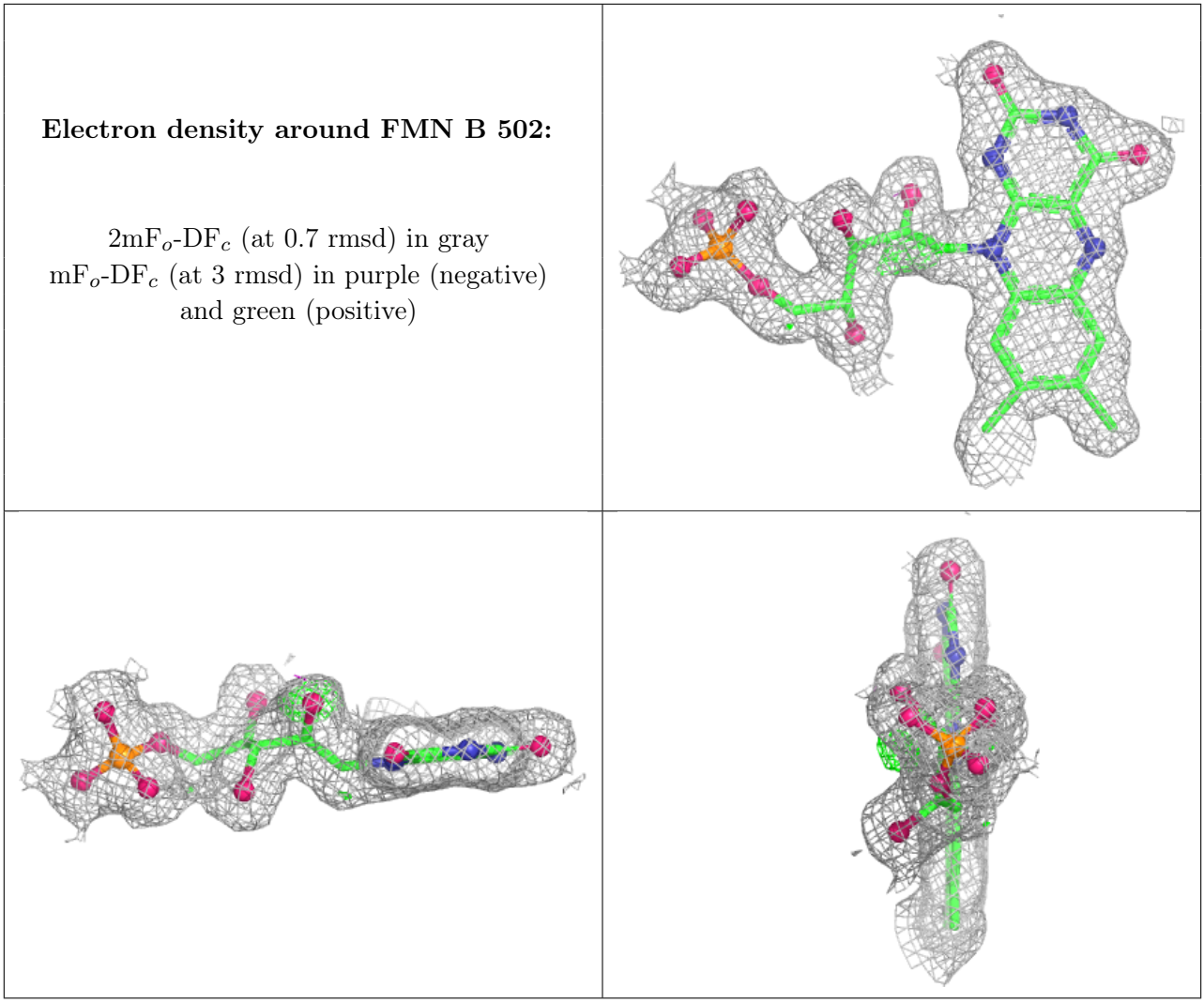
Electron density around FAD B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



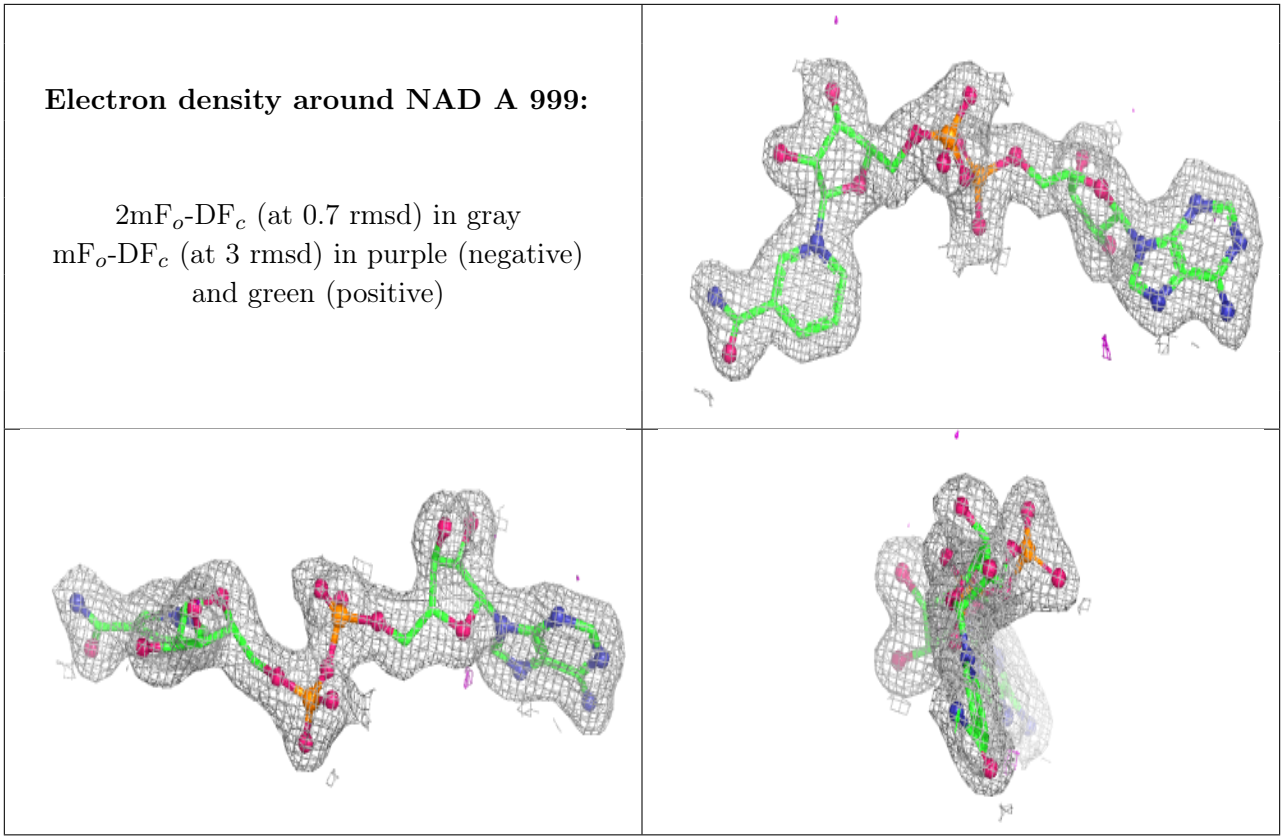
Electron density around FMN B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NAD A 999:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.