Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 06:10 PM JST

PDB ID	:	5GSN
Title	:	Tmm in complex with methimazole
Authors	:	Zhang, Y.Z.; Li, C.Y.
Deposited on	:	2016-08-16
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.270
Clashscore		14
Ramachandran outliers		0.6%
Sidechain outliers		3.6%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
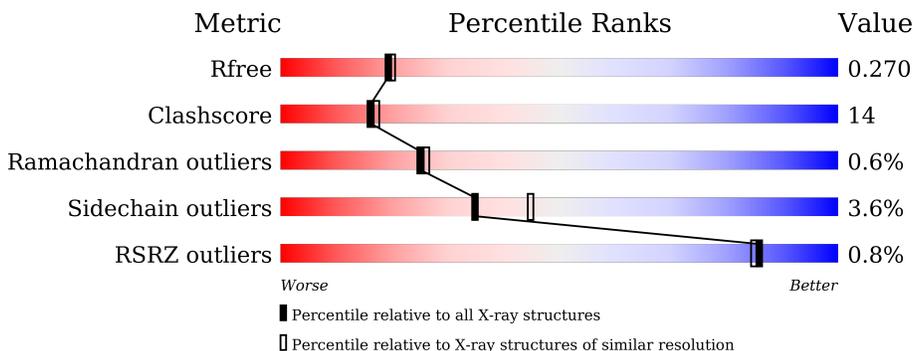
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	453	77% 20% ••
1	B	453	% 75% 22% ••
1	C	453	% 66% 29% ••
1	D	453	% 72% 24% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MMZ	C	503	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15548 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 Flavin-containing monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	1	0
			3582	2287	607	671	17			
1	B	445	Total	C	N	O	S	0	4	0
			3607	2303	613	674	17			
1	C	445	Total	C	N	O	S	0	0	0
			3573	2282	605	669	17			
1	D	445	Total	C	N	O	S	0	1	0
			3582	2287	606	672	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ALA	GLU	engineered mutation	UNP A3SLM3
A	154	ALA	ASP	engineered mutation	UNP A3SLM3
A	207	SER	TYR	engineered mutation	UNP A3SLM3
A	448	HIS	-	expression tag	UNP A3SLM3
A	449	HIS	-	expression tag	UNP A3SLM3
A	450	HIS	-	expression tag	UNP A3SLM3
A	451	HIS	-	expression tag	UNP A3SLM3
A	452	HIS	-	expression tag	UNP A3SLM3
A	453	HIS	-	expression tag	UNP A3SLM3
B	153	ALA	GLU	engineered mutation	UNP A3SLM3
B	154	ALA	ASP	engineered mutation	UNP A3SLM3
B	207	SER	TYR	engineered mutation	UNP A3SLM3
B	448	HIS	-	expression tag	UNP A3SLM3
B	449	HIS	-	expression tag	UNP A3SLM3
B	450	HIS	-	expression tag	UNP A3SLM3
B	451	HIS	-	expression tag	UNP A3SLM3
B	452	HIS	-	expression tag	UNP A3SLM3
B	453	HIS	-	expression tag	UNP A3SLM3
C	153	ALA	GLU	engineered mutation	UNP A3SLM3
C	154	ALA	ASP	engineered mutation	UNP A3SLM3
C	207	SER	TYR	engineered mutation	UNP A3SLM3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	448	HIS	-	expression tag	UNP A3SLM3
C	449	HIS	-	expression tag	UNP A3SLM3
C	450	HIS	-	expression tag	UNP A3SLM3
C	451	HIS	-	expression tag	UNP A3SLM3
C	452	HIS	-	expression tag	UNP A3SLM3
C	453	HIS	-	expression tag	UNP A3SLM3
D	153	ALA	GLU	engineered mutation	UNP A3SLM3
D	154	ALA	ASP	engineered mutation	UNP A3SLM3
D	207	SER	TYR	engineered mutation	UNP A3SLM3
D	448	HIS	-	expression tag	UNP A3SLM3
D	449	HIS	-	expression tag	UNP A3SLM3
D	450	HIS	-	expression tag	UNP A3SLM3
D	451	HIS	-	expression tag	UNP A3SLM3
D	452	HIS	-	expression tag	UNP A3SLM3
D	453	HIS	-	expression tag	UNP A3SLM3

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
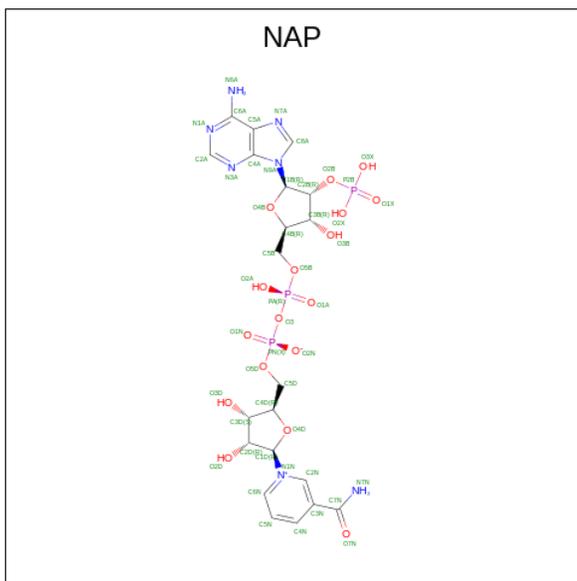

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	D	1	48	21	7	17	3	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
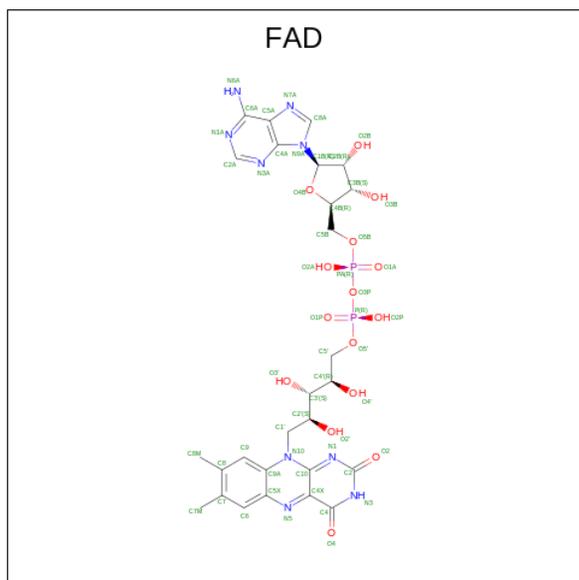
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0
3	C	1	53	27	9	15	2	0	0
3	D	1	53	27	9	15	2	0	0

- Molecule 4 is 1-METHYL-1,3-DIHYDRO-2H-IMIDAZOLE-2-THIONE (three-letter code: MMZ) (formula: $C_4H_6N_2S$).

MMZ

C4

N3

S2

C3A

C2

C1A

N1
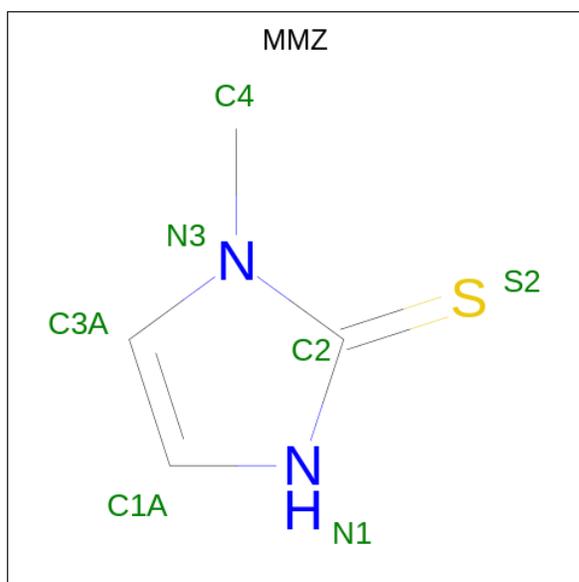
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 7	C 4	N 2	S 1	0	0
4	C	1	Total 7	C 4	N 2	S 1	0	0

• Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	186	Total 186	O 186	0	0
5	B	202	Total 202	O 202	0	0
5	C	206	Total 206	O 206	0	0
5	D	192	Total 192	O 192	0	0

3 Residue-property plots ⓘ

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: Flavin-containing monooxygenase
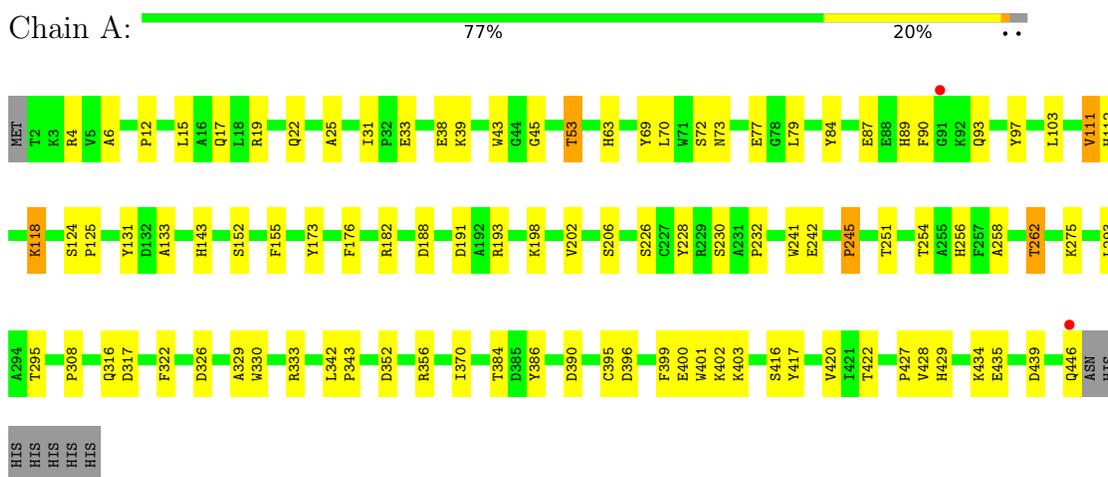
Chain A:

• Molecule 1: Flavin-containing monooxygenase

Chain B:

• Molecule 1: Flavin-containing monooxygenase

Chain C:

• Molecule 1: Flavin-containing monooxygenase

Chain D:
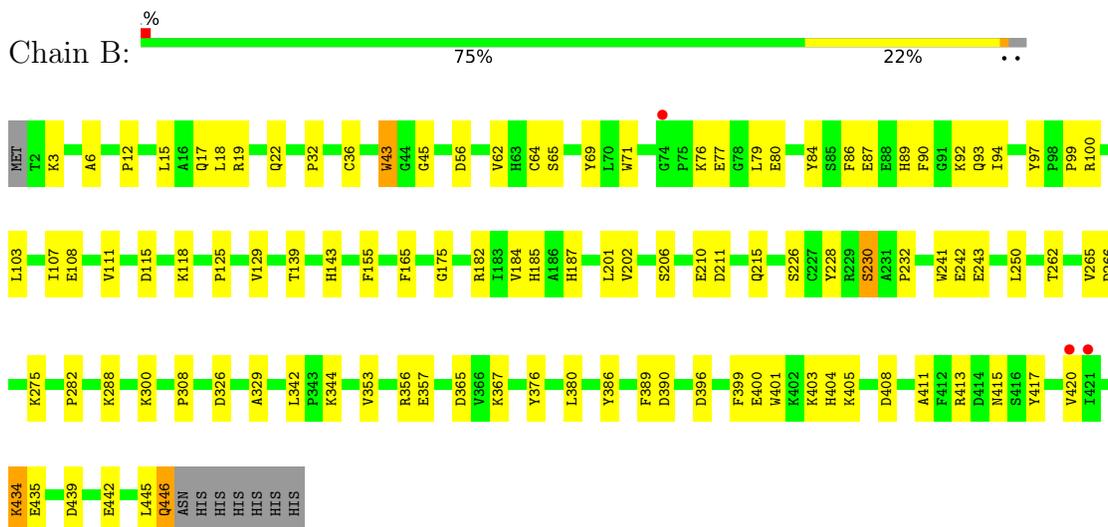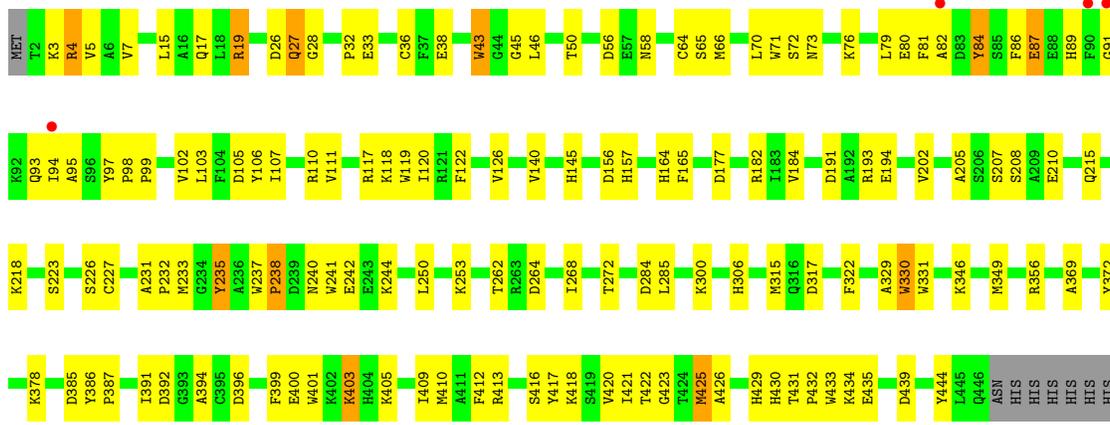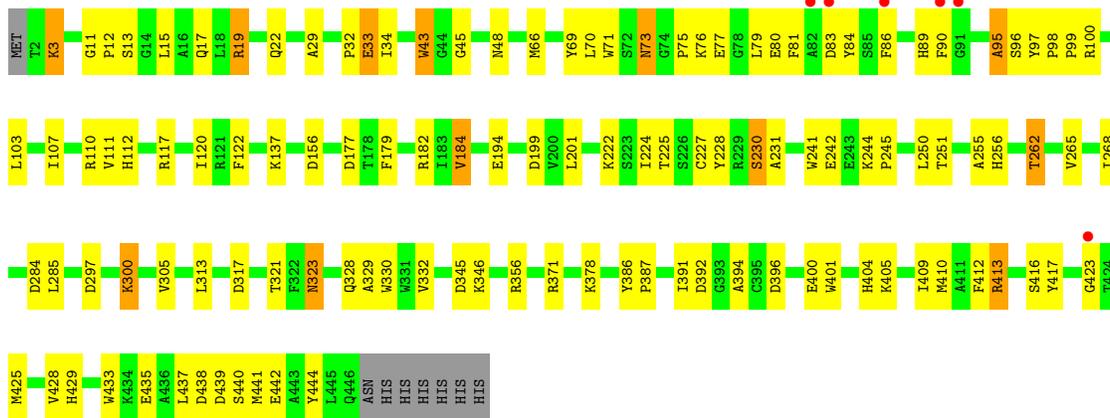
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.85Å 207.58Å 72.52Å 90.00° 90.31° 90.00°	Depositor
Resolution (Å)	46.74 – 2.20 46.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.1 (46.74-2.20) 91.4 (46.74-2.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.203 , 0.274 0.202 , 0.270	Depositor DCC
R_{free} test set	4242 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 14.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.338 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15548	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2477e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, NAP, MMZ

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	0.42	0/3691	0.55	0/5010
1	B	0.44	0/3716	0.56	0/5044
1	C	0.44	1/3682 (0.0%)	0.57	1/4998 (0.0%)
1	D	0.42	0/3691	0.55	0/5010
All	All	0.43	1/14780 (0.0%)	0.56	1/20062 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	232	PRO	N-CD	5.04	1.54	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	231	ALA	C-N-CD	5.74	140.46	128.40

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	3582	0	3363	71	0
1	B	3607	0	3391	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3573	0	3356	130	0
1	D	3582	0	3361	115	0
2	A	48	0	24	10	0
2	B	48	0	25	6	0
2	C	48	0	24	12	0
2	D	48	0	24	4	0
3	A	53	0	31	5	0
3	B	53	0	31	2	0
3	C	53	0	31	8	0
3	D	53	0	31	4	0
4	A	7	0	6	3	0
4	C	7	0	6	11	0
5	A	186	0	0	5	1
5	B	202	0	0	13	1
5	C	206	0	0	11	2
5	D	192	0	0	4	0
All	All	15548	0	13704	412	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (412) 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:D:323:ASN:HD22	1:D:323:ASN:H	1.01	1.01
1:A:87:GLU:OE2	1:A:93:GLN:NE2	1.98	0.97
1:D:323:ASN:HD22	1:D:323:ASN:N	1.64	0.95
1:C:421:ILE:HG13	1:C:422:THR:HG23	1.52	0.92
1:C:45:GLY:HA2	3:C:502:FAD:O3B	1.70	0.91
1:C:418:LYS:HG2	1:C:425:MET:HG3	1.54	0.89
1:A:390:ASP:HB3	1:A:420:VAL:HG13	1.54	0.87
1:D:323:ASN:H	1:D:323:ASN:ND2	1.67	0.86
1:C:72:SER:HB2	1:C:103:LEU:HD11	1.57	0.84
1:B:446:GLN:HE21	1:B:446:GLN:HA	1.43	0.82
1:C:208:SER:OG	4:C:503:MMZ:H3A	1.80	0.82
1:C:15:LEU:HD13	1:C:111:VAL:HG11	1.62	0.82
1:B:165:PHE:CZ	2:B:501:NAP:H1D	2.15	0.81
1:C:81:PHE:HB2	1:C:84:TYR:O	1.81	0.80
1:C:439:ASP:HB3	5:C:732:HOH:O	1.82	0.80
3:C:502:FAD:C6	4:C:503:MMZ:C2	2.59	0.80
1:C:250:LEU:HD11	1:C:268:ILE:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:HIS:CE1	1:D:417:TYR:HE1	2.01	0.78
1:A:124:SER:O	5:A:601:HOH:O	2.03	0.77
1:B:390:ASP:HB3	1:B:420:VAL:HG13	1.65	0.77
1:C:87:GLU:OE2	1:C:93:GLN:NE2	2.18	0.76
1:D:81:PHE:CD1	1:D:110:ARG:NH1	2.55	0.74
1:A:295:THR:OG1	1:A:316:GLN:HG3	1.88	0.73
1:D:378:LYS:HG3	1:D:391:ILE:HD13	1.71	0.72
1:D:242:GLU:OE2	1:D:244:LYS:HE2	1.88	0.72
1:A:401:TRP:HH2	2:A:501:NAP:H4N	1.55	0.71
1:D:19:ARG:HG2	1:D:110:ARG:NH2	2.04	0.71
1:C:317:ASP:OD1	2:C:501:NAP:O3D	2.05	0.70
1:C:76:LYS:HE3	1:C:94:ILE:HG13	1.73	0.70
1:D:66:MET:HG2	1:D:70:LEU:HD13	1.73	0.70
1:B:446:GLN:HA	1:B:446:GLN:NE2	2.06	0.70
1:D:401:TRP:NE1	1:D:405:LYS:HD2	2.08	0.69
1:B:19:ARG:HD2	1:B:22[B]:GLN:HE22	1.58	0.69
2:C:501:NAP:C6N	4:C:503:MMZ:N1	2.56	0.69
1:D:81:PHE:HD1	1:D:110:ARG:HH11	1.38	0.68
1:C:81:PHE:CD1	1:C:110:ARG:NH1	2.62	0.68
1:A:241:TRP:HD1	1:A:242:GLU:N	1.91	0.68
1:C:210:GLU:HG3	1:C:233:MET:SD	2.34	0.68
1:D:45:GLY:HA2	3:D:502:FAD:O3B	1.94	0.67
1:C:306:HIS:HA	5:C:706:HOH:O	1.93	0.66
1:C:98:PRO:HB2	1:C:103:LEU:HG	1.77	0.66
1:D:84:TYR:OH	1:D:89:HIS:HB2	1.95	0.66
1:B:15:LEU:HD22	1:B:111:VAL:HG11	1.77	0.66
1:C:4:ARG:HB3	1:C:33:GLU:HG3	1.76	0.66
1:D:300:LYS:HD3	1:D:356:ARG:NH2	2.09	0.66
1:D:313:LEU:HD21	1:D:332:VAL:HG21	1.77	0.66
1:A:45:GLY:HA2	3:A:502:FAD:O3B	1.95	0.66
1:B:19:ARG:HD2	1:B:22[B]:GLN:NE2	2.11	0.66
1:A:38:GLU:C	5:A:601:HOH:O	2.33	0.66
1:B:12:PRO:HG2	3:B:502:FAD:H4'	1.76	0.66
1:C:349:MET:SD	5:C:726:HOH:O	2.53	0.65
1:D:404:HIS:CE1	1:D:417:TYR:CE1	2.85	0.65
1:A:72:SER:HB2	1:A:103:LEU:HD11	1.79	0.65
1:D:12:PRO:HG2	3:D:502:FAD:H4'	1.79	0.65
1:B:64:CYS:O	5:B:601:HOH:O	2.15	0.65
1:A:19:ARG:HD2	1:A:22[B]:GLN:HE22	1.62	0.64
1:A:434:LYS:HE3	1:A:435:GLU:OE2	1.98	0.64
1:D:75:PRO:HB3	1:D:417:TYR:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:HIS:HD2	1:C:431:THR:OG1	1.81	0.64
1:C:5:VAL:HG22	1:C:157:HIS:HB2	1.80	0.64
1:C:3:LYS:HB2	1:C:32:PRO:HB3	1.81	0.63
3:C:502:FAD:C5X	4:C:503:MMZ:S2	2.87	0.63
1:A:19:ARG:HD2	1:A:22[B]:GLN:NE2	2.14	0.62
1:B:87:GLU:HA	5:B:602:HOH:O	1.99	0.62
1:A:228:TYR:CZ	1:A:232:PRO:HG3	2.34	0.62
1:D:323:ASN:N	1:D:323:ASN:ND2	2.36	0.62
1:B:344:LYS:HD3	1:C:118:LYS:O	1.99	0.62
1:C:378:LYS:HE2	1:C:391:ILE:HD12	1.81	0.62
1:C:84:TYR:CE1	1:C:89:HIS:HB2	2.34	0.62
1:C:120:ILE:HG21	1:C:122:PHE:CE1	2.36	0.61
1:B:17:GLN:HA	1:B:329:ALA:HB1	1.81	0.61
1:D:75:PRO:HG3	1:D:401:TRP:HB2	1.81	0.61
1:D:404:HIS:HE1	1:D:417:TYR:HE1	1.48	0.61
1:C:300:LYS:HD3	1:C:356:ARG:NH2	2.16	0.61
1:B:434:LYS:HB3	5:B:757:HOH:O	2.00	0.60
1:B:69:TYR:HD1	1:B:439:ASP:OD1	1.84	0.60
1:D:201:LEU:HB2	1:D:265:VAL:HG11	1.82	0.60
1:A:308:PRO:HB2	1:A:342:LEU:HD13	1.83	0.60
1:A:399:PHE:O	1:A:403:LYS:HG3	2.01	0.60
2:C:501:NAP:N1N	4:C:503:MMZ:N1	2.49	0.60
1:D:201:LEU:HD12	1:D:225:THR:O	2.01	0.60
3:C:502:FAD:C7	4:C:503:MMZ:C2	2.79	0.60
1:D:19:ARG:HH21	1:D:22:GLN:HB3	1.67	0.60
1:D:346:LYS:HE2	5:D:614:HOH:O	2.01	0.60
1:D:378:LYS:CG	1:D:391:ILE:HD13	2.31	0.59
1:D:428:VAL:HG12	1:D:429:HIS:O	2.02	0.59
2:D:501:NAP:H51N	2:D:501:NAP:O1A	2.02	0.59
1:C:399:PHE:O	1:C:403:LYS:HD2	2.03	0.58
1:C:409:ILE:HG23	1:C:410:MET:HG2	1.84	0.58
1:D:71:TRP:CZ3	1:D:433:TRP:HD1	2.21	0.58
1:A:39:LYS:HG3	1:A:125:PRO:HB3	1.86	0.58
1:C:432:PRO:HB2	1:C:435:GLU:OE1	2.03	0.58
3:C:502:FAD:C5X	4:C:503:MMZ:C2	2.81	0.58
1:C:84:TYR:OH	1:C:89:HIS:HB2	2.04	0.57
1:A:326:ASP:HB3	1:A:386:TYR:CE1	2.39	0.57
1:C:17:GLN:HA	1:C:329:ALA:HB1	1.86	0.57
1:A:118:LYS:HD3	1:D:345:ASP:HB2	1.86	0.57
1:D:80:GLU:HG2	1:D:86:PHE:HD1	1.69	0.57
1:D:81:PHE:HD1	1:D:110:ARG:NH1	1.99	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:TRP:CD1	1:A:242:GLU:N	2.71	0.57
1:A:317:ASP:OD1	2:A:501:NAP:O3D	2.21	0.57
1:C:19:ARG:HD3	1:C:110:ARG:NH2	2.20	0.57
1:C:46:LEU:O	1:C:66:MET:HG3	2.06	0.56
1:D:120:ILE:HG21	1:D:122:PHE:CE1	2.39	0.56
1:A:15:LEU:HD22	1:A:111:VAL:HG11	1.85	0.56
1:B:228:TYR:CZ	1:B:232:PRO:HG3	2.40	0.56
1:C:81:PHE:CE1	1:C:110:ARG:HD3	2.41	0.56
1:C:378:LYS:NZ	1:C:392:ASP:OD1	2.39	0.56
1:A:330:TRP:CD1	1:A:333:ARG:NH2	2.73	0.56
1:D:80:GLU:HG2	1:D:86:PHE:CD1	2.41	0.55
1:D:409:ILE:O	1:D:412:PHE:HD1	1.87	0.55
1:D:17:GLN:HA	1:D:329:ALA:HB1	1.88	0.55
1:D:416:SER:HB2	1:D:425:MET:HE3	1.89	0.55
1:A:124:SER:C	5:A:601:HOH:O	2.44	0.55
1:B:76:LYS:HE3	1:B:94:ILE:CG1	2.37	0.55
1:B:115:ASP:O	1:B:118:LYS:HE3	2.07	0.55
1:B:308:PRO:HB2	1:B:342:LEU:HD13	1.89	0.55
2:C:501:NAP:C6N	4:C:503:MMZ:S2	2.95	0.55
1:C:182:ARG:NH1	1:C:194:GLU:OE1	2.34	0.55
1:C:182:ARG:CZ	1:C:184:VAL:HG11	2.36	0.55
1:A:125:PRO:HD2	1:A:143:HIS:O	2.07	0.54
1:D:84:TYR:CZ	1:D:89:HIS:HB2	2.42	0.54
1:C:238:PRO:HG3	1:C:410:MET:HG3	1.89	0.54
1:D:43:TRP:CZ3	1:D:117:ARG:HB2	2.42	0.54
1:C:396:ASP:O	1:C:400:GLU:HG2	2.08	0.54
1:A:293:LEU:HD23	1:A:317:ASP:HB3	1.89	0.54
1:B:65:SER:OG	1:B:187:HIS:ND1	2.33	0.54
1:C:76:LYS:HD2	1:C:86:PHE:CE2	2.43	0.54
1:A:22[A]:GLN:HE22	1:A:118:LYS:NZ	2.06	0.54
1:B:19:ARG:HH11	1:B:22[B]:GLN:HE22	1.57	0.53
1:D:3:LYS:O	1:D:32:PRO:HB2	2.08	0.53
1:D:330:TRP:CD2	1:D:386:TYR:HD1	2.26	0.53
1:C:3:LYS:HD3	1:C:156:ASP:CG	2.29	0.53
1:C:418:LYS:HA	1:C:425:MET:HA	1.90	0.53
1:D:76:LYS:HD3	1:D:95:ALA:O	2.07	0.53
1:D:317:ASP:OD1	2:D:501:NAP:O3D	2.21	0.53
1:C:401:TRP:NE1	1:C:405:LYS:HD2	2.23	0.53
1:C:409:ILE:O	1:C:412:PHE:HD2	1.91	0.53
1:C:84:TYR:HE1	1:C:89:HIS:HB2	1.74	0.53
1:C:300:LYS:HD3	1:C:356:ARG:HH21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:LYS:NZ	1:D:392:ASP:OD1	2.38	0.53
1:C:82:ALA:HB3	1:C:386:TYR:OH	2.09	0.53
1:D:3:LYS:HD3	1:D:156:ASP:CG	2.29	0.52
1:D:75:PRO:HB3	1:D:417:TYR:CD2	2.44	0.52
1:D:120:ILE:HG21	1:D:122:PHE:CZ	2.44	0.52
1:B:76:LYS:HE3	1:B:94:ILE:HG12	1.92	0.52
1:C:97:TYR:CG	1:C:413:ARG:HG2	2.44	0.52
1:C:429:HIS:CE1	1:C:444:TYR:CD1	2.97	0.52
1:C:207:SER:HB3	2:C:501:NAP:H5N	1.92	0.52
1:D:97:TYR:CD2	1:D:413:ARG:HA	2.44	0.52
1:C:107:ILE:O	1:C:111:VAL:HG22	2.09	0.52
1:D:300:LYS:HD3	1:D:356:ARG:HH22	1.74	0.52
2:A:501:NAP:H2N	4:A:503:MMZ:S2	2.48	0.52
1:C:120:ILE:HG21	1:C:122:PHE:CZ	2.44	0.52
1:C:253:LYS:O	1:C:264:ASP:HA	2.10	0.52
1:C:81:PHE:CD1	1:C:110:ARG:HD3	2.44	0.52
1:D:391:ILE:O	1:D:394:ALA:N	2.42	0.52
1:B:182:ARG:HG3	1:B:184[A]:VAL:HG23	1.91	0.52
1:D:250:LEU:HD11	1:D:268:ILE:CD1	2.40	0.52
1:A:118:LYS:CD	1:D:345:ASP:HB2	2.40	0.52
1:C:242:GLU:CD	1:C:244:LYS:HE3	2.29	0.51
1:B:71:TRP:HA	1:B:99:PRO:HA	1.92	0.51
1:D:81:PHE:HB2	1:D:84:TYR:HB3	1.91	0.51
1:D:251:THR:OG1	1:D:256:HIS:HE1	1.94	0.51
1:A:251:THR:OG1	1:A:256:HIS:HE1	1.93	0.51
1:B:76:LYS:HA	1:B:79:LEU:HG	1.92	0.51
1:C:330:TRP:CD2	1:C:386:TYR:HD1	2.27	0.51
1:B:408:ASP:CG	1:B:411:ALA:HB3	2.30	0.51
1:A:4:ARG:HG2	1:A:33:GLU:HB2	1.93	0.51
1:A:73:ASN:ND2	2:A:501:NAP:O7N	2.44	0.51
1:A:124:SER:HA	1:A:143:HIS:O	2.11	0.51
1:A:38:GLU:N	5:A:601:HOH:O	2.44	0.51
2:B:501:NAP:H51N	2:B:501:NAP:O1A	2.10	0.51
1:A:77:GLU:OE1	1:A:417:TYR:HB2	2.11	0.51
1:D:224:ILE:O	1:D:241:TRP:HA	2.10	0.51
1:D:250:LEU:HD11	1:D:268:ILE:HD11	1.92	0.51
1:B:405:LYS:HE3	5:B:607:HOH:O	2.10	0.51
1:C:215:GLN:OE1	1:C:215:GLN:HA	2.11	0.51
1:B:211:ASP:O	1:B:215:GLN:HG2	2.12	0.50
1:C:218:LYS:HE3	1:C:433:TRP:O	2.11	0.50
1:D:297:ASP:O	1:D:305:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:GLN:O	1:D:332:VAL:HG23	2.10	0.50
1:D:371:ARG:HH22	1:D:378:LYS:HE2	1.75	0.50
1:C:346:LYS:NZ	5:C:606:HOH:O	2.40	0.50
1:A:93:GLN:O	1:A:427:PRO:HG2	2.12	0.50
1:B:230:SER:O	1:D:231:ALA:HB2	2.11	0.50
1:D:96:SER:OG	1:D:416:SER:HA	2.11	0.50
1:C:38:GLU:OE2	3:C:502:FAD:O2B	2.29	0.50
1:C:79:LEU:HA	5:C:688:HOH:O	2.10	0.50
1:D:391:ILE:O	1:D:394:ALA:HB3	2.12	0.50
1:A:6:ALA:HB2	1:A:155:PHE:CD2	2.47	0.50
1:B:80:GLU:HG3	1:B:86:PHE:CD2	2.47	0.50
1:B:103:LEU:O	1:B:107:ILE:HG13	2.12	0.50
1:C:3:LYS:CB	1:C:32:PRO:HB3	2.40	0.50
2:C:501:NAP:C5N	4:C:503:MMZ:S2	3.00	0.50
1:D:66:MET:HG2	1:D:70:LEU:CD1	2.42	0.49
1:A:396:ASP:O	1:A:400:GLU:HG2	2.12	0.49
1:C:80:GLU:HG3	1:C:86:PHE:HD1	1.75	0.49
1:C:418:LYS:N	1:C:425:MET:HG2	2.27	0.49
1:B:182:ARG:CZ	1:B:184[A]:VAL:HG21	2.42	0.49
1:D:107:ILE:O	1:D:111:VAL:HG22	2.12	0.49
1:A:254:THR:CG2	1:A:262:THR:HG23	2.43	0.49
1:C:71:TRP:CZ3	1:C:433:TRP:HD1	2.31	0.49
1:C:177:ASP:OD1	1:C:177:ASP:N	2.44	0.49
1:C:223:SER:HA	1:C:240:ASN:HB2	1.94	0.49
1:C:385:ASP:C	1:C:385:ASP:OD1	2.50	0.49
1:A:202:VAL:O	1:A:226:SER:HA	2.13	0.49
1:A:446:GLN:HE21	1:A:446:GLN:HA	1.76	0.49
1:A:317:ASP:OD1	2:A:501:NAP:C2D	2.60	0.49
1:A:63:HIS:ND1	3:A:502:FAD:H2B	2.27	0.49
1:C:107:ILE:HD11	1:C:322:PHE:CZ	2.48	0.49
2:A:501:NAP:H51N	2:A:501:NAP:O1A	2.13	0.48
1:C:202:VAL:O	1:C:226:SER:HA	2.12	0.48
1:C:227:CYS:HA	1:C:244:LYS:O	2.13	0.48
1:C:81:PHE:HD2	1:C:106:TYR:CZ	2.31	0.48
1:D:83:ASP:N	1:D:83:ASP:OD1	2.44	0.48
1:D:89:HIS:HD2	1:D:90:PHE:CD1	2.31	0.48
1:C:207:SER:HB2	2:C:501:NAP:H6N	1.94	0.48
1:D:19:ARG:HH21	1:D:22:GLN:CG	2.26	0.48
1:A:17:GLN:HA	1:A:329:ALA:HB1	1.95	0.48
1:D:11:GLY:O	1:D:15:LEU:HG	2.14	0.48
1:D:177:ASP:N	1:D:177:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22[A]:GLN:HE22	1:A:118:LYS:HZ1	1.61	0.48
1:D:19:ARG:HH21	1:D:22:GLN:CB	2.26	0.48
1:D:437:LEU:HD11	5:D:761:HOH:O	2.14	0.48
1:C:71:TRP:HA	1:C:99:PRO:HA	1.94	0.47
1:C:401:TRP:HE1	1:C:405:LYS:HD2	1.78	0.47
1:C:434:LYS:HG3	1:C:435:GLU:OE2	2.14	0.47
2:C:501:NAP:H51N	2:C:501:NAP:O1A	2.14	0.47
1:D:70:LEU:C	1:D:70:LEU:HD23	2.34	0.47
1:B:211:ASP:HA	5:B:753:HOH:O	2.13	0.47
1:C:210:GLU:OE2	1:C:235:TYR:HE2	1.97	0.47
1:B:45:GLY:HA2	3:B:502:FAD:O3B	2.14	0.47
1:B:241:TRP:CD1	1:B:241:TRP:C	2.87	0.47
1:A:245:PRO:HB2	1:A:258:ALA:HB3	1.96	0.47
1:C:99:PRO:HG2	1:C:102:VAL:HG23	1.97	0.47
1:D:409:ILE:HG23	1:D:410:MET:N	2.29	0.47
1:B:202:VAL:O	1:B:226:SER:HA	2.15	0.47
1:B:326:ASP:HB3	1:B:386:TYR:CE1	2.49	0.47
1:B:353:VAL:O	1:B:357:GLU:HG3	2.15	0.47
1:B:365:ASP:OD2	1:B:367:LYS:HB2	2.15	0.47
1:A:6:ALA:HB2	1:A:155:PHE:CE2	2.50	0.47
1:C:317:ASP:OD1	2:C:501:NAP:O2D	2.33	0.47
1:D:89:HIS:CD2	1:D:90:PHE:CD1	3.02	0.47
1:D:227:CYS:HA	1:D:244:LYS:O	2.15	0.47
1:A:79:LEU:O	1:A:322:PHE:HB2	2.14	0.47
1:B:230:SER:O	1:D:231:ALA:CB	2.63	0.47
1:C:205:ALA:HB3	5:C:729:HOH:O	2.15	0.47
1:A:173:TYR:HB2	1:A:176:PHE:CZ	2.50	0.46
1:B:401:TRP:NE1	1:B:405:LYS:HD2	2.30	0.46
1:C:76:LYS:HE3	1:C:94:ILE:CG1	2.43	0.46
1:D:77:GLU:OE1	1:D:417:TYR:HB2	2.14	0.46
1:D:79:LEU:HA	1:D:323:ASN:HD21	1.79	0.46
1:D:244:LYS:HB3	1:D:245:PRO:HD2	1.97	0.46
1:A:206:SER:HB3	2:A:501:NAP:O1N	2.14	0.46
1:B:165:PHE:CE2	2:B:501:NAP:H1D	2.49	0.46
1:B:445:LEU:O	1:B:446:GLN:HB2	2.15	0.46
1:C:119:TRP:HA	5:C:646:HOH:O	2.15	0.46
1:C:416:SER:HB3	1:C:426:ALA:HB3	1.97	0.46
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.80	0.46
1:B:401:TRP:CE2	1:B:405:LYS:HD2	2.50	0.46
1:B:165:PHE:CZ	2:B:501:NAP:C1D	2.96	0.46
1:D:346:LYS:HB2	1:D:346:LYS:HE3	1.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:NAP:C2N	4:C:503:MMZ:HN1	2.29	0.46
1:D:182:ARG:NH2	1:D:184:VAL:HG11	2.31	0.46
2:A:501:NAP:O4D	4:A:503:MMZ:N1	2.49	0.46
1:B:139:THR:HG22	5:B:682:HOH:O	2.14	0.46
1:D:73:ASN:HA	1:D:413:ARG:NH2	2.30	0.46
1:D:284:ASP:O	1:D:285:LEU:HD23	2.16	0.46
1:B:69:TYR:CD1	1:B:439:ASP:OD1	2.67	0.46
1:B:97:TYR:CE2	1:B:413:ARG:HA	2.51	0.46
1:C:300:LYS:HG3	1:C:331:TRP:CZ2	2.51	0.46
1:D:33[B]:GLU:O	1:D:34:ILE:HD13	2.15	0.46
1:C:250:LEU:HD11	1:C:268:ILE:CD1	2.41	0.46
1:A:428:VAL:HG12	1:A:429:HIS:O	2.16	0.46
1:B:389:PHE:HB3	5:B:623:HOH:O	2.14	0.46
1:D:300:LYS:HA	1:D:356:ARG:NH2	2.31	0.46
1:A:22[B]:GLN:HE21	1:A:22[B]:GLN:HB3	1.56	0.45
1:A:191:ASP:OD1	1:A:193:ARG:N	2.46	0.45
2:B:501:NAP:O1A	2:B:501:NAP:H4D	2.16	0.45
1:C:431:THR:HG22	1:C:432:PRO:O	2.16	0.45
1:A:228:TYR:CE2	1:A:232:PRO:HG3	2.52	0.45
1:A:446:GLN:HA	1:A:446:GLN:NE2	2.31	0.45
1:C:98:PRO:HG2	1:C:103:LEU:HD21	1.98	0.45
1:B:93:GLN:HA	5:B:625:HOH:O	2.15	0.45
1:D:45:GLY:N	5:D:611:HOH:O	2.44	0.45
2:D:501:NAP:H2N	2:D:501:NAP:H2D	1.60	0.45
1:B:175:GLY:HA3	1:B:250:LEU:HB2	1.99	0.45
1:C:439:ASP:OD1	1:C:439:ASP:C	2.55	0.45
1:D:404:HIS:HE1	1:D:417:TYR:CE1	2.27	0.45
1:B:182:ARG:NH2	1:B:184[B]:VAL:HG11	2.31	0.45
1:C:97:TYR:CE2	1:C:413:ARG:HA	2.52	0.45
1:B:18:LEU:HD21	1:B:36:CYS:HB2	1.99	0.45
1:B:84:TYR:CE2	1:B:89:HIS:HB2	2.51	0.45
1:B:242:GLU:HG2	1:B:243:GLU:N	2.31	0.45
1:C:89:HIS:NE2	1:C:105:ASP:OD1	2.42	0.45
3:C:502:FAD:N5	4:C:503:MMZ:S2	2.90	0.45
1:D:98:PRO:HB2	1:D:103:LEU:HG	1.97	0.45
1:B:201:LEU:HB2	1:B:265:VAL:HG11	1.99	0.45
1:D:442:GLU:OE2	1:D:442:GLU:HA	2.17	0.44
1:B:100:ARG:HD3	5:B:648:HOH:O	2.17	0.44
2:B:501:NAP:H2D	2:B:501:NAP:H2N	1.58	0.44
1:C:417:TYR:C	1:C:425:MET:HG2	2.38	0.44
1:C:369:ALA:O	1:C:372:TYR:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TYR:CE2	1:A:133:ALA:HA	2.52	0.44
1:D:69:TYR:N	1:D:439:ASP:OD2	2.40	0.44
1:A:70:LEU:C	1:A:70:LEU:HD23	2.38	0.44
1:D:19:ARG:HG2	1:D:110:ARG:HH21	1.81	0.44
1:D:228:TYR:CD2	1:D:230:SER:O	2.71	0.44
1:B:399:PHE:O	1:B:403:LYS:HG3	2.18	0.44
1:D:71:TRP:HA	1:D:99:PRO:HA	1.98	0.44
1:C:84:TYR:CZ	1:C:89:HIS:HB2	2.52	0.44
1:C:241:TRP:CD1	1:C:241:TRP:C	2.91	0.44
1:A:89:HIS:HD2	1:A:90:PHE:CD2	2.36	0.43
3:A:502:FAD:H2A	5:A:601:HOH:O	2.17	0.43
1:D:71:TRP:CE3	1:D:433:TRP:HD1	2.34	0.43
1:D:84:TYR:CE2	1:D:89:HIS:HB2	2.53	0.43
1:B:15:LEU:HB3	1:B:111:VAL:HG11	1.99	0.43
1:C:70:LEU:C	1:C:70:LEU:HD23	2.38	0.43
1:C:378:LYS:HE3	1:C:378:LYS:HB2	1.79	0.43
1:C:420:VAL:HG12	1:C:420:VAL:O	2.18	0.43
1:B:125:PRO:HD2	1:B:143:HIS:O	2.18	0.43
1:C:27:GLN:HB2	5:C:624:HOH:O	2.18	0.43
2:D:501:NAP:C6N	3:D:502:FAD:HM83	2.48	0.43
1:A:12:PRO:HG2	3:A:502:FAD:H4'	2.01	0.43
1:C:346:LYS:HD3	5:C:706:HOH:O	2.19	0.43
1:D:438:ASP:OD1	1:D:440:SER:N	2.49	0.43
1:B:3:LYS:HB2	1:B:32:PRO:HB3	2.00	0.43
1:B:396:ASP:O	1:B:400:GLU:HG2	2.18	0.43
1:D:89:HIS:CD2	1:D:90:PHE:CE1	3.06	0.43
1:C:87:GLU:O	1:C:91:GLY:N	2.50	0.43
1:D:371:ARG:HH22	1:D:378:LYS:CD	2.32	0.43
1:B:79:LEU:HD12	1:B:79:LEU:C	2.39	0.43
1:B:376:TYR:CZ	1:B:380:LEU:HD11	2.53	0.43
1:C:103:LEU:O	1:C:107:ILE:HG13	2.18	0.43
1:D:241:TRP:CZ3	1:D:410:MET:HE1	2.53	0.43
1:C:64:CYS:HB2	5:C:691:HOH:O	2.18	0.43
1:C:191:ASP:OD1	1:C:193:ARG:HG3	2.18	0.43
1:A:401:TRP:CH2	2:A:501:NAP:H4N	2.43	0.43
1:B:43:TRP:NE1	1:B:108:GLU:HG3	2.34	0.43
1:B:43:TRP:HE1	1:B:108:GLU:HG3	1.83	0.43
1:C:284:ASP:O	1:C:285:LEU:HD23	2.19	0.43
1:D:179:PHE:CD1	1:D:250:LEU:HD13	2.54	0.43
1:C:272:THR:HA	2:C:501:NAP:O4B	2.19	0.42
1:C:405:LYS:HG2	1:C:412:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:TRP:CZ3	1:C:117:ARG:HB2	2.54	0.42
1:C:71:TRP:CE3	1:C:433:TRP:HD1	2.36	0.42
1:A:370:ILE:HG22	1:A:395:CYS:SG	2.59	0.42
1:C:102:VAL:HG21	1:C:444:TYR:CD2	2.54	0.42
1:A:191:ASP:OD1	1:A:193:ARG:HB2	2.19	0.42
1:C:207:SER:CB	2:C:501:NAP:H6N	2.49	0.42
1:A:241:TRP:CD1	1:A:241:TRP:C	2.92	0.42
1:C:95:ALA:HB3	1:C:444:TYR:OH	2.20	0.42
1:D:97:TYR:CE2	1:D:413:ARG:HA	2.54	0.42
1:B:90:PHE:CE1	1:B:445:LEU:HD11	2.55	0.42
1:D:255:ALA:O	1:D:262:THR:HA	2.19	0.42
1:C:391:ILE:O	1:C:394:ALA:HB3	2.20	0.42
1:D:199:ASP:OD1	1:D:222:LYS:HD2	2.20	0.42
1:D:330:TRP:CE2	1:D:386:TYR:HD1	2.38	0.42
1:B:77:GLU:OE1	1:B:417:TYR:HB2	2.20	0.42
1:A:25:ALA:HB2	1:A:31:ILE:HD13	2.01	0.42
1:A:97:TYR:HH	1:A:401:TRP:HD1	1.68	0.42
1:D:29:ALA:HB2	5:D:603:HOH:O	2.19	0.42
1:A:53:THR:HG21	1:A:188:ASP:O	2.20	0.41
1:A:352:ASP:O	1:A:356:ARG:HG3	2.19	0.41
1:C:164:HIS:CD2	1:C:315:MET:HA	2.55	0.41
1:B:100:ARG:NH1	5:B:619:HOH:O	2.49	0.41
1:C:237:TRP:HB3	1:C:241:TRP:HB3	2.02	0.41
1:D:182:ARG:CZ	1:D:184:VAL:HG11	2.50	0.41
1:A:416:SER:C	1:A:417:TYR:CD1	2.94	0.41
1:B:404:HIS:CE1	1:B:415:ASN:ND2	2.88	0.41
1:C:26:ASP:O	1:C:28:GLY:N	2.54	0.41
1:C:56:ASP:HB2	5:C:778:HOH:O	2.20	0.41
1:C:81:PHE:CD2	1:C:106:TYR:CZ	3.08	0.41
1:D:194:GLU:O	1:D:194:GLU:HG2	2.20	0.41
1:B:184[A]:VAL:HG12	1:B:185:HIS:O	2.21	0.41
1:D:33[B]:GLU:C	1:D:34:ILE:HD13	2.41	0.41
1:C:416:SER:HB2	1:C:425:MET:HE1	2.02	0.41
1:D:95:ALA:CB	1:D:429:HIS:HB2	2.51	0.41
1:A:330:TRP:HB3	1:A:384:THR:HG21	2.02	0.41
3:A:502:FAD:HM73	4:A:503:MMZ:H3A	2.02	0.41
1:B:62:VAL:CG1	5:B:601:HOH:O	2.67	0.41
1:B:129:VAL:O	1:B:282:PRO:HD3	2.21	0.41
1:C:99:PRO:HG2	1:C:102:VAL:CG2	2.51	0.41
1:B:92:LYS:O	5:B:602:HOH:O	2.21	0.41
1:C:165:PHE:CB	3:C:502:FAD:HM81	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:SER:HB2	1:C:425:MET:CE	2.51	0.41
1:D:396:ASP:O	1:D:400:GLU:HG2	2.21	0.41
1:A:342:LEU:HA	1:A:343:PRO:HD3	1.87	0.41
1:B:56:ASP:HB2	5:B:749:HOH:O	2.21	0.41
1:C:330:TRP:CE2	1:C:386:TYR:HD1	2.39	0.41
1:D:242:GLU:CD	1:D:244:LYS:HE2	2.41	0.41
1:C:391:ILE:O	1:C:394:ALA:N	2.54	0.41
1:A:317:ASP:OD1	2:A:501:NAP:C3D	2.69	0.41
1:B:76:LYS:O	1:B:79:LEU:HG	2.21	0.41
1:C:58:ASN:HB3	1:C:145:HIS:CD2	2.56	0.41
1:B:6:ALA:HB2	1:B:155:PHE:CD2	2.56	0.40
1:C:7:VAL:O	1:C:36:CYS:HA	2.21	0.40
1:C:87:GLU:O	1:C:91:GLY:CA	2.69	0.40
1:C:429:HIS:CE1	1:C:444:TYR:CE1	3.09	0.40
1:D:12:PRO:HD2	3:D:502:FAD:O5'	2.20	0.40
1:A:251:THR:OG1	1:A:256:HIS:CE1	2.73	0.40
1:C:430:HIS:CD2	1:C:431:THR:OG1	2.67	0.40
1:D:241:TRP:CD1	1:D:241:TRP:C	2.95	0.40
1:D:378:LYS:HZ2	1:D:391:ILE:HB	1.84	0.40
1:B:206:SER:O	1:B:210:GLU:HG2	2.22	0.40
1:C:126:VAL:HG13	1:C:140:VAL:HG13	2.03	0.40
1:C:418:LYS:HG2	1:C:425:MET:CG	2.39	0.40
1:B:19:ARG:HH11	1:B:22[B]:GLN:NE2	2.20	0.40
1:B:300:LYS:HD3	1:B:356:ARG:NH2	2.37	0.40
1:D:79:LEU:HD12	1:D:79:LEU:O	2.22	0.40
1:D:441:MET:O	1:D:444:TYR:HB3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:772:HOH:O	5:C:779:HOH:O[1_556]	1.94	0.26
5:B:794:HOH:O	5:C:803:HOH:O[1_455]	2.19	0.01

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/453 (98%)	417 (94%)	25 (6%)	2 (0%)	29	31
1	B	447/453 (99%)	423 (95%)	24 (5%)	0	100	100
1	C	443/453 (98%)	411 (93%)	27 (6%)	5 (1%)	14	12
1	D	444/453 (98%)	405 (91%)	35 (8%)	4 (1%)	17	16
All	All	1778/1812 (98%)	1656 (93%)	111 (6%)	11 (1%)	25	26

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	300	LYS
1	C	27	GLN
1	D	95	ALA
1	A	84	TYR
1	C	235	TYR
1	C	238	PRO
1	D	423	GLY
1	A	245	PRO
1	C	387	PRO
1	D	387	PRO
1	C	423	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/373 (98%)	352 (96%)	14 (4%)	33	42
1	B	369/373 (99%)	359 (97%)	10 (3%)	44	57
1	C	365/373 (98%)	353 (97%)	12 (3%)	38	49
1	D	366/373 (98%)	348 (95%)	18 (5%)	25	31
All	All	1466/1492 (98%)	1412 (96%)	54 (4%)	35	43

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	TRP
1	A	53	THR
1	A	69	TYR
1	A	111	VAL
1	A	112	HIS
1	A	118	LYS
1	A	152	SER
1	A	198	LYS
1	A	230	SER
1	A	262	THR
1	A	275	LYS
1	A	402	LYS
1	A	422	THR
1	A	439	ASP
1	B	43	TRP
1	B	230	SER
1	B	262	THR
1	B	266	ASP
1	B	275	LYS
1	B	288	LYS
1	B	434	LYS
1	B	435	GLU
1	B	442	GLU
1	B	446	GLN
1	C	4	ARG
1	C	19	ARG
1	C	43	TRP
1	C	50	THR
1	C	65	SER
1	C	73	ASN
1	C	84	TYR
1	C	87	GLU
1	C	262	THR
1	C	330	TRP
1	C	403	LYS
1	C	425	MET
1	D	3	LYS
1	D	13	SER
1	D	19	ARG
1	D	33[A]	GLU
1	D	33[B]	GLU
1	D	43	TRP

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Mol	Chain	Res	Type
1	D	48	ASN
1	D	73	ASN
1	D	100	ARG
1	D	112	HIS
1	D	137	LYS
1	D	184	VAL
1	D	230	SER
1	D	262	THR
1	D	321	THR
1	D	323	ASN
1	D	413	ARG
1	D	435	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	256	HIS
1	A	446	GLN
1	B	415	ASN
1	B	446	GLN
1	C	48	ASN
1	C	256	HIS
1	C	323	ASN
1	C	415	ASN
1	C	429	HIS
1	C	430	HIS
1	D	48	ASN
1	D	89	HIS
1	D	256	HIS
1	D	323	ASN
1	D	415	ASN
1	D	446	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates (i)

There are no monosaccharides in this entry.

5.6   Ligand geometry (i)

10 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	NAP	C	501	-	45,52,52	2.94	17 (37%)	56,80,80	2.11	13 (23%)
3	FAD	D	502	-	53,58,58	1.27	5 (9%)	68,89,89	1.25	10 (14%)
4	MMZ	A	503	-	5,7,7	2.05	2 (40%)	4,9,9	1.80	1 (25%)
3	FAD	C	502	-	53,58,58	1.26	6 (11%)	68,89,89	1.25	9 (13%)
2	NAP	A	501	-	45,52,52	3.03	16 (35%)	56,80,80	1.74	10 (17%)
2	NAP	B	501	-	45,52,52	2.93	17 (37%)	56,80,80	1.87	10 (17%)
2	NAP	D	501	-	45,52,52	2.96	16 (35%)	56,80,80	1.80	11 (19%)
3	FAD	A	502	-	53,58,58	1.28	6 (11%)	68,89,89	1.26	9 (13%)
4	MMZ	C	503	-	5,7,7	2.06	3 (60%)	4,9,9	1.59	1 (25%)
3	FAD	B	502	-	53,58,58	1.27	6 (11%)	68,89,89	1.26	10 (14%)

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
2	NAP	C	501	-	-	13/31/67/67	0/5/5/5
3	FAD	D	502	-	-	4/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MMZ	A	503	-	-	-	0/1/1/1
3	FAD	C	502	-	-	11/30/50/50	0/6/6/6
2	NAP	A	501	-	-	15/31/67/67	0/5/5/5
2	NAP	B	501	-	-	8/31/67/67	0/5/5/5
2	NAP	D	501	-	-	10/31/67/67	0/5/5/5
3	FAD	A	502	-	-	4/30/50/50	0/6/6/6
4	MMZ	C	503	-	-	-	0/1/1/1
3	FAD	B	502	-	-	6/30/50/50	0/6/6/6

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAP	C2N-N1N	8.55	1.45	1.35
2	A	501	NAP	C2N-N1N	8.42	1.45	1.35
2	B	501	NAP	C2N-N1N	8.08	1.44	1.35
2	C	501	NAP	C2N-N1N	7.84	1.44	1.35
2	D	501	NAP	C2N-C3N	7.62	1.50	1.39
2	C	501	NAP	C2N-C3N	7.01	1.49	1.39
2	A	501	NAP	C3B-C2B	-6.98	1.37	1.52
2	A	501	NAP	C2N-C3N	6.95	1.49	1.39
2	C	501	NAP	C4N-C3N	6.95	1.51	1.39
2	B	501	NAP	C3B-C2B	-6.91	1.37	1.52
2	A	501	NAP	C4N-C3N	6.84	1.51	1.39
2	B	501	NAP	C2N-C3N	6.82	1.49	1.39
2	D	501	NAP	C3B-C2B	-6.68	1.38	1.52
2	B	501	NAP	C7N-N7N	6.58	1.45	1.33
2	C	501	NAP	C3B-C2B	-6.50	1.38	1.52
2	D	501	NAP	C7N-N7N	6.50	1.45	1.33
2	A	501	NAP	C7N-N7N	6.48	1.45	1.33
2	B	501	NAP	C4N-C3N	6.43	1.50	1.39
2	C	501	NAP	C7N-N7N	6.05	1.44	1.33
2	D	501	NAP	C4N-C3N	6.00	1.49	1.39
2	C	501	NAP	C5N-C4N	5.63	1.50	1.38
2	A	501	NAP	C5N-C4N	5.46	1.50	1.38
2	B	501	NAP	C5N-C4N	5.35	1.50	1.38
2	D	501	NAP	C5N-C4N	5.16	1.49	1.38
2	A	501	NAP	C6N-C5N	5.08	1.49	1.38
3	A	502	FAD	C9A-C5X	5.05	1.49	1.41
3	D	502	FAD	C9A-C5X	5.03	1.49	1.41
3	C	502	FAD	C9A-C5X	5.03	1.49	1.41
2	D	501	NAP	C6N-C5N	5.01	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	FAD	C9A-C5X	4.99	1.49	1.41
2	B	501	NAP	C6N-C5N	4.94	1.49	1.38
2	C	501	NAP	C6N-C5N	4.89	1.49	1.38
2	A	501	NAP	C6N-N1N	4.29	1.45	1.35
2	B	501	NAP	C6N-N1N	3.94	1.45	1.35
2	C	501	NAP	C6N-N1N	3.64	1.44	1.35
2	D	501	NAP	C6N-N1N	3.55	1.44	1.35
2	C	501	NAP	C6A-N6A	3.47	1.46	1.34
2	A	501	NAP	C6A-N6A	3.37	1.46	1.34
3	B	502	FAD	C8-C7	3.30	1.49	1.40
3	D	502	FAD	C8-C7	3.28	1.49	1.40
3	C	502	FAD	C8-C7	3.24	1.49	1.40
3	A	502	FAD	C8-C7	3.24	1.49	1.40
2	D	501	NAP	C6A-N6A	3.22	1.45	1.34
2	A	501	NAP	C2D-C1D	-3.21	1.48	1.53
2	B	501	NAP	C6A-N6A	3.01	1.45	1.34
2	C	501	NAP	C5D-C4D	-2.95	1.42	1.51
4	C	503	MMZ	C3A-N3	2.89	1.43	1.37
4	A	503	MMZ	C3A-N3	2.85	1.43	1.37
4	A	503	MMZ	C3A-C1A	2.83	1.47	1.36
2	A	501	NAP	O2D-C2D	-2.80	1.36	1.43
2	D	501	NAP	O4B-C4B	-2.79	1.38	1.45
2	B	501	NAP	C3N-C7N	-2.76	1.46	1.50
4	C	503	MMZ	C3A-C1A	2.75	1.47	1.36
2	C	501	NAP	O4B-C4B	-2.68	1.39	1.45
2	D	501	NAP	C2D-C1D	-2.68	1.49	1.53
2	C	501	NAP	O2D-C2D	-2.65	1.36	1.43
3	A	502	FAD	C4-N3	-2.63	1.34	1.38
2	D	501	NAP	O2D-C2D	-2.62	1.36	1.43
3	B	502	FAD	C4-N3	-2.59	1.34	1.38
3	C	502	FAD	C4-N3	-2.57	1.34	1.38
3	D	502	FAD	C4-N3	-2.56	1.34	1.38
2	C	501	NAP	C3D-C4D	-2.52	1.46	1.53
2	A	501	NAP	O4B-C4B	-2.50	1.39	1.45
3	D	502	FAD	C4X-N5	2.40	1.35	1.30
3	A	502	FAD	C5A-C4A	2.38	1.47	1.40
3	B	502	FAD	C5A-C4A	2.38	1.47	1.40
2	B	501	NAP	O4B-C4B	-2.38	1.39	1.45
3	C	502	FAD	C4X-N5	2.36	1.35	1.30
2	A	501	NAP	C5D-C4D	-2.36	1.44	1.51
3	D	502	FAD	C5A-C4A	2.34	1.47	1.40
2	B	501	NAP	O2D-C2D	-2.34	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	FAD	C5A-C4A	2.32	1.47	1.40
3	A	502	FAD	C4X-N5	2.31	1.35	1.30
3	B	502	FAD	C4X-N5	2.29	1.35	1.30
2	D	501	NAP	C5D-C4D	-2.25	1.44	1.51
2	B	501	NAP	C2D-C1D	-2.25	1.50	1.53
2	A	501	NAP	C3D-C4D	-2.20	1.47	1.53
2	D	501	NAP	C3D-C4D	-2.18	1.47	1.53
2	C	501	NAP	C2D-C1D	-2.17	1.50	1.53
2	B	501	NAP	C2A-N3A	2.17	1.35	1.32
3	A	502	FAD	C5X-N5	-2.12	1.35	1.39
2	A	501	NAP	C2A-N3A	2.11	1.35	1.32
2	B	501	NAP	C5D-C4D	-2.10	1.45	1.51
2	C	501	NAP	P2B-O3X	-2.10	1.46	1.54
2	D	501	NAP	P2B-O3X	-2.06	1.46	1.54
4	C	503	MMZ	C2-S2	2.05	1.71	1.66
3	C	502	FAD	C5X-N5	-2.05	1.35	1.39
2	B	501	NAP	O4B-C1B	-2.03	1.38	1.41
2	A	501	NAP	O4B-C1B	-2.03	1.38	1.41
2	B	501	NAP	C3D-C4D	-2.03	1.47	1.53
2	C	501	NAP	C3N-C7N	-2.03	1.47	1.50
3	B	502	FAD	C5X-N5	-2.02	1.35	1.39
2	D	501	NAP	C2D-C3D	-2.01	1.47	1.53
2	C	501	NAP	O4B-C1B	-2.01	1.38	1.41

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAP	C2N-N1N-C1D	-7.70	101.98	119.14
2	C	501	NAP	C2N-N1N-C1D	-7.17	103.16	119.14
2	B	501	NAP	C2N-N1N-C1D	-7.12	103.27	119.14
2	C	501	NAP	C3N-C2N-N1N	-6.61	113.96	120.43
2	D	501	NAP	C5N-C4N-C3N	-6.46	112.69	120.34
2	C	501	NAP	C5N-C4N-C3N	-5.59	113.73	120.34
2	D	501	NAP	C2N-N1N-C1D	-5.41	107.08	119.14
2	B	501	NAP	N3A-C2A-N1A	-5.09	120.72	128.68
2	B	501	NAP	C5N-C4N-C3N	-5.02	114.40	120.34
2	D	501	NAP	N3A-C2A-N1A	-4.37	121.84	128.68
2	C	501	NAP	N3A-C2A-N1A	-4.17	122.16	128.68
2	A	501	NAP	C5N-C4N-C3N	-4.08	115.51	120.34
2	A	501	NAP	N3A-C2A-N1A	-4.05	122.35	128.68
2	C	501	NAP	C5N-C6N-N1N	-4.00	114.67	120.40
2	D	501	NAP	C3D-C2D-C1D	3.86	106.78	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	NAP	C6N-N1N-C2N	-3.44	118.83	121.97
2	A	501	NAP	C3D-C2D-C1D	3.41	106.11	100.98
2	B	501	NAP	O5D-C5D-C4D	3.39	120.67	108.99
2	B	501	NAP	C3D-C2D-C1D	3.29	105.93	100.98
3	C	502	FAD	N3A-C2A-N1A	-3.24	123.61	128.68
3	A	502	FAD	N3A-C2A-N1A	-3.19	123.70	128.68
3	B	502	FAD	N3A-C2A-N1A	-3.17	123.73	128.68
2	C	501	NAP	C3D-C2D-C1D	3.09	105.64	100.98
3	D	502	FAD	N3A-C2A-N1A	-3.09	123.84	128.68
2	C	501	NAP	C5D-C4D-C3D	-3.08	103.63	115.18
2	D	501	NAP	C6N-N1N-C2N	-3.04	119.21	121.97
3	A	502	FAD	C4X-C10-N1	-2.88	118.06	124.73
3	D	502	FAD	C4-C4X-N5	2.87	122.32	118.23
3	D	502	FAD	C4A-C5A-N7A	-2.84	106.44	109.40
3	A	502	FAD	C4A-C5A-N7A	-2.84	106.44	109.40
4	A	503	MMZ	C3A-N3-C2	-2.83	105.63	108.51
3	B	502	FAD	C4A-C5A-N7A	-2.82	106.46	109.40
3	C	502	FAD	C4A-C5A-N7A	-2.76	106.52	109.40
2	D	501	NAP	O5B-C5B-C4B	2.76	118.50	108.99
3	B	502	FAD	C4-C4X-N5	2.74	122.13	118.23
3	C	502	FAD	C4-C4X-N5	2.74	122.13	118.23
3	B	502	FAD	C4X-C10-N1	-2.73	118.38	124.73
2	D	501	NAP	O5D-C5D-C4D	2.71	118.31	108.99
3	C	502	FAD	C4X-C10-N1	-2.69	118.48	124.73
2	A	501	NAP	C3N-C7N-N7N	2.68	120.97	117.75
3	B	502	FAD	P-O3P-PA	-2.67	123.65	132.83
2	B	501	NAP	C3N-C2N-N1N	-2.62	117.87	120.43
3	D	502	FAD	C4X-C10-N1	-2.62	118.66	124.73
2	A	501	NAP	O5D-C5D-C4D	2.61	117.97	108.99
3	D	502	FAD	P-O3P-PA	-2.60	123.92	132.83
2	B	501	NAP	C2N-C3N-C4N	2.58	121.18	118.26
2	D	501	NAP	C3N-C2N-N1N	-2.58	117.91	120.43
2	C	501	NAP	C6N-N1N-C2N	-2.53	119.67	121.97
3	C	502	FAD	P-O3P-PA	-2.47	124.36	132.83
3	A	502	FAD	C4-C4X-N5	2.46	121.74	118.23
2	D	501	NAP	C3N-C7N-N7N	2.44	120.68	117.75
2	B	501	NAP	C1B-N9A-C4A	-2.40	122.43	126.64
2	D	501	NAP	C2D-C3D-C4D	2.36	107.22	102.64
3	A	502	FAD	C10-N1-C2	2.35	121.61	116.90
3	B	502	FAD	C4X-C10-N10	2.32	119.88	116.48
3	C	502	FAD	C10-N1-C2	2.32	121.54	116.90
3	A	502	FAD	P-O3P-PA	-2.29	124.98	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	FAD	C10-N1-C2	2.29	121.47	116.90
3	D	502	FAD	C10-N1-C2	2.27	121.44	116.90
3	A	502	FAD	C4X-C10-N10	2.24	119.76	116.48
3	D	502	FAD	C4X-C10-N10	2.22	119.73	116.48
3	C	502	FAD	O4-C4-C4X	-2.21	120.74	126.60
4	C	503	MMZ	C3A-N3-C2	-2.20	106.28	108.51
2	A	501	NAP	C6N-N1N-C2N	-2.16	120.01	121.97
2	C	501	NAP	O5B-C5B-C4B	2.15	116.39	108.99
2	B	501	NAP	O5B-C5B-C4B	2.14	116.35	108.99
3	A	502	FAD	O4-C4-C4X	-2.12	120.96	126.60
3	C	502	FAD	C4X-C4-N3	2.12	118.56	113.19
2	D	501	NAP	C2N-C3N-C4N	2.10	120.64	118.26
3	B	502	FAD	O2-C2-N1	-2.10	118.35	121.83
2	C	501	NAP	O3D-C3D-C2D	2.09	118.59	111.82
3	C	502	FAD	C4X-C10-N10	2.09	119.54	116.48
3	D	502	FAD	O4-C4-C4X	-2.08	121.07	126.60
2	C	501	NAP	C3N-C7N-N7N	2.07	120.24	117.75
3	B	502	FAD	O4-C4-C4X	-2.07	121.11	126.60
3	D	502	FAD	C4X-C4-N3	2.06	118.43	113.19
2	A	501	NAP	C2N-C3N-C4N	2.04	120.57	118.26
3	A	502	FAD	C4X-C4-N3	2.04	118.36	113.19
2	C	501	NAP	O5D-C5D-C4D	2.04	116.00	108.99
3	B	502	FAD	C4X-C4-N3	2.02	118.33	113.19
2	A	501	NAP	C5D-C4D-C3D	-2.02	107.61	115.18
2	C	501	NAP	C2D-C3D-C4D	2.01	106.55	102.64
3	D	502	FAD	O2-C2-N1	-2.00	118.51	121.83
2	A	501	NAP	O7N-C7N-N7N	-2.00	119.73	122.58

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAP	C2B-O2B-P2B-O2X
2	A	501	NAP	O4D-C1D-N1N-C2N
2	A	501	NAP	O4D-C1D-N1N-C6N
2	A	501	NAP	C2D-C1D-N1N-C2N
2	A	501	NAP	C2D-C1D-N1N-C6N
2	A	501	NAP	C2N-C3N-C7N-N7N
2	B	501	NAP	C2B-O2B-P2B-O2X
2	B	501	NAP	O4D-C4D-C5D-O5D
2	B	501	NAP	C3D-C4D-C5D-O5D
2	B	501	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	B	501	NAP	C2D-C1D-N1N-C6N
2	C	501	NAP	PN-O3-PA-O5B
2	C	501	NAP	C2B-O2B-P2B-O2X
2	C	501	NAP	C5D-O5D-PN-O1N
2	D	501	NAP	PN-O3-PA-O5B
2	D	501	NAP	C5D-O5D-PN-O1N
2	D	501	NAP	O4D-C4D-C5D-O5D
2	D	501	NAP	C3D-C4D-C5D-O5D
2	D	501	NAP	C2D-C1D-N1N-C2N
2	D	501	NAP	C2D-C1D-N1N-C6N
3	A	502	FAD	N10-C1'-C2'-O2'
3	A	502	FAD	N10-C1'-C2'-C3'
3	B	502	FAD	N10-C1'-C2'-O2'
3	B	502	FAD	N10-C1'-C2'-C3'
3	C	502	FAD	N10-C1'-C2'-O2'
3	C	502	FAD	N10-C1'-C2'-C3'
3	C	502	FAD	C3'-C4'-C5'-O5'
3	C	502	FAD	C5'-O5'-P-O3P
3	D	502	FAD	N10-C1'-C2'-O2'
3	D	502	FAD	N10-C1'-C2'-C3'
2	A	501	NAP	C4N-C3N-C7N-O7N
2	A	501	NAP	C4N-C3N-C7N-N7N
2	C	501	NAP	C4N-C3N-C7N-O7N
2	C	501	NAP	C4N-C3N-C7N-N7N
2	A	501	NAP	C2N-C3N-C7N-O7N
2	A	501	NAP	C3D-C4D-C5D-O5D
3	C	502	FAD	O4B-C4B-C5B-O5B
3	C	502	FAD	O4'-C4'-C5'-O5'
2	A	501	NAP	O4D-C4D-C5D-O5D
3	A	502	FAD	O4B-C4B-C5B-O5B
2	A	501	NAP	C2B-O2B-P2B-O3X
2	C	501	NAP	C5B-O5B-PA-O3
2	D	501	NAP	C5B-O5B-PA-O3
2	C	501	NAP	O4B-C4B-C5B-O5B
3	C	502	FAD	C5B-O5B-PA-O1A
3	C	502	FAD	C5'-O5'-P-O1P
3	C	502	FAD	C5'-O5'-P-O2P
3	C	502	FAD	C3B-C4B-C5B-O5B
3	B	502	FAD	C2'-C3'-C4'-C5'
2	C	501	NAP	C2N-C3N-C7N-O7N
2	B	501	NAP	C4D-C5D-O5D-PN
2	C	501	NAP	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
3	A	502	FAD	C3B-C4B-C5B-O5B
3	B	502	FAD	O3'-C3'-C4'-C5'
3	B	502	FAD	O3'-C3'-C4'-O4'
3	D	502	FAD	O3'-C3'-C4'-O4'
2	B	501	NAP	O4B-C4B-C5B-O5B
2	D	501	NAP	O4B-C4B-C5B-O5B
2	B	501	NAP	C2B-O2B-P2B-O3X
2	C	501	NAP	C2B-O2B-P2B-O3X
2	D	501	NAP	C5D-O5D-PN-O3
3	C	502	FAD	C5B-O5B-PA-O3P
2	A	501	NAP	O4B-C4B-C5B-O5B
2	C	501	NAP	C3B-C4B-C5B-O5B
3	D	502	FAD	O4B-C4B-C5B-O5B
2	C	501	NAP	C4D-C5D-O5D-PN
2	A	501	NAP	C5B-O5B-PA-O1A
2	A	501	NAP	C5D-O5D-PN-O1N
2	C	501	NAP	C5B-O5B-PA-O1A
2	D	501	NAP	C5B-O5B-PA-O1A
3	B	502	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

10 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAP	12	0
3	D	502	FAD	4	0
4	A	503	MMZ	3	0
3	C	502	FAD	8	0
2	A	501	NAP	10	0
2	B	501	NAP	6	0
2	D	501	NAP	4	0
3	A	502	FAD	5	0
4	C	503	MMZ	11	0
3	B	502	FAD	2	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 NAP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 502

Bond lengths

Bond angles

Torsions

Rings

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, 95th 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(Å²)	Q<0.9
1	A	445/453 (98%)	-0.51	2 (0%)	92	91	17, 30, 49, 66	0
1	B	445/453 (98%)	-0.51	3 (0%)	87	86	14, 30, 50, 65	0
1	C	445/453 (98%)	-0.36	4 (0%)	84	83	16, 32, 63, 86	0
1	D	445/453 (98%)	-0.34	6 (1%)	77	75	17, 31, 65, 86	0
All	All	1780/1812 (98%)	-0.43	15 (0%)	86	85	14, 30, 57, 86	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	82	ALA	6.0
1	C	91	GLY	5.4
1	D	86	PHE	3.4
1	D	423	GLY	3.4
1	C	82	ALA	3.1
1	D	91	GLY	3.0
1	D	90	PHE	2.7
1	C	94	ILE	2.7
1	C	90	PHE	2.4
1	B	74	GLY	2.2
1	A	91	GLY	2.2
1	B	421	ILE	2.1
1	B	420	VAL	2.1
1	A	446	GLN	2.0
1	D	83	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (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, 95th 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
4	MMZ	A	503	7/7	0.84	0.17	35,41,46,59	0
4	MMZ	C	503	7/7	0.84	0.19	37,41,48,64	0
2	NAP	A	501	48/48	0.93	0.14	25,34,53,61	0
2	NAP	C	501	48/48	0.94	0.13	25,35,53,56	0
3	FAD	A	502	53/53	0.95	0.12	13,22,36,37	0
3	FAD	D	502	53/53	0.95	0.11	15,26,33,35	0
2	NAP	B	501	48/48	0.95	0.11	21,32,44,49	0
2	NAP	D	501	48/48	0.95	0.12	23,33,46,52	0
3	FAD	C	502	53/53	0.96	0.11	14,24,40,41	0
3	FAD	B	502	53/53	0.96	0.11	14,22,30,37	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 NAP A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
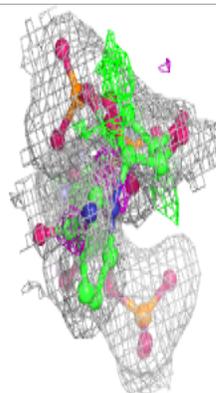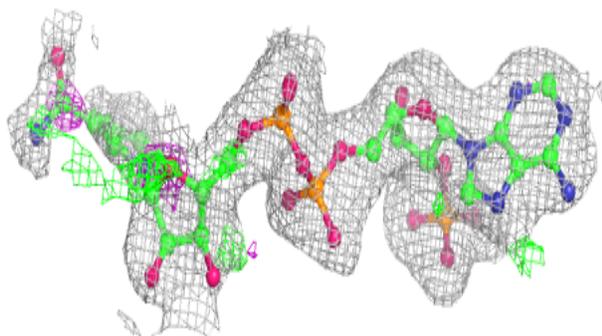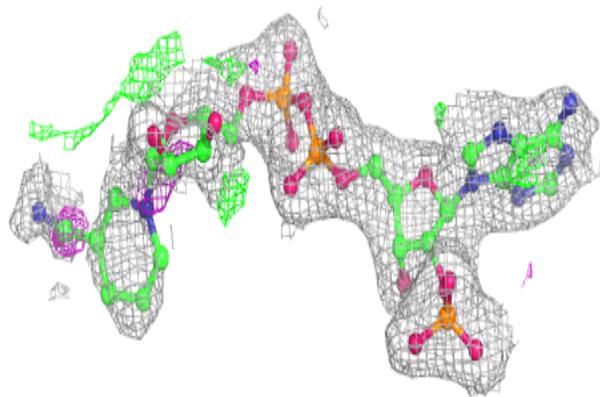
Electron density around NAP C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
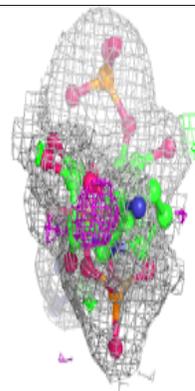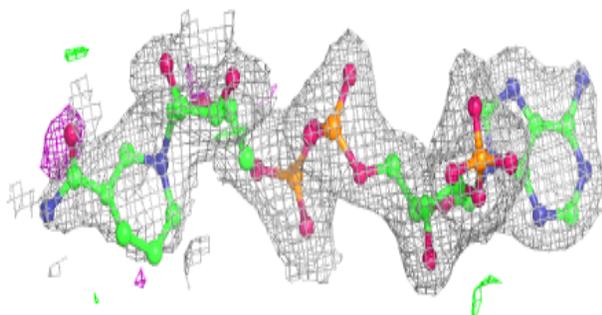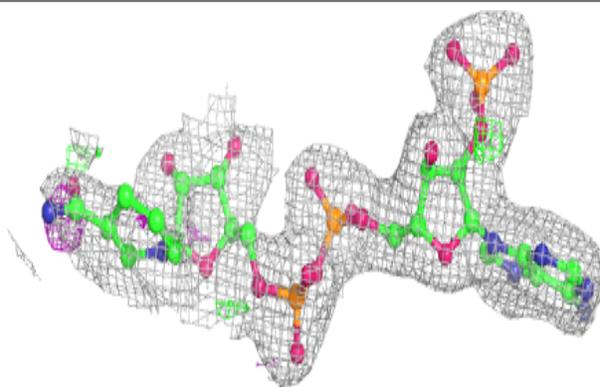
Electron density around FAD A 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
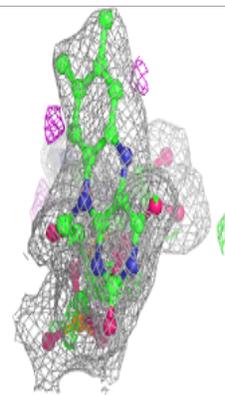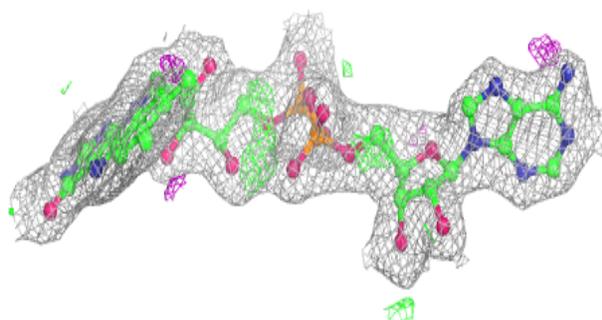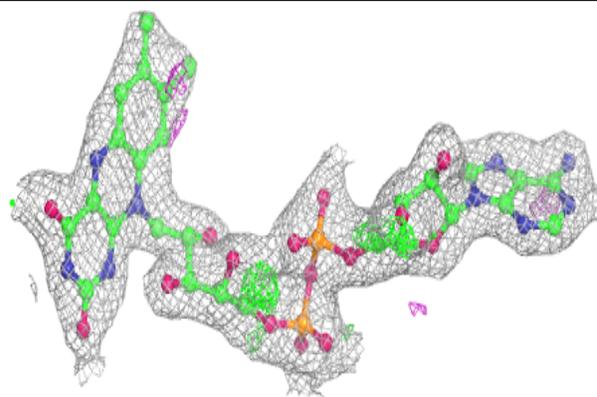
Electron density around FAD D 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
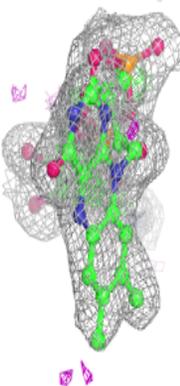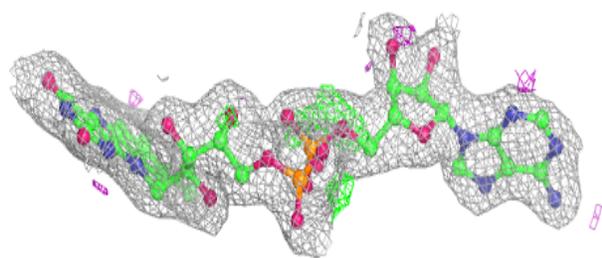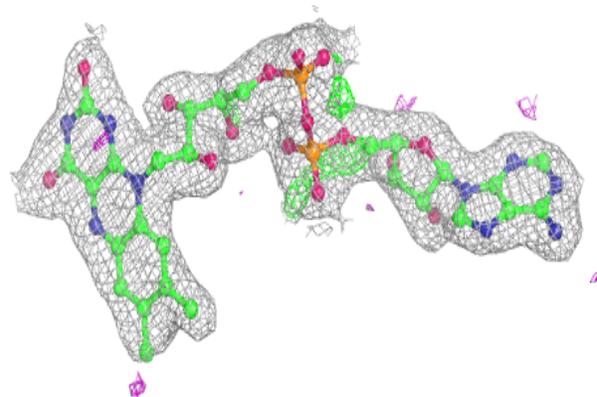
Electron density around NAP B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
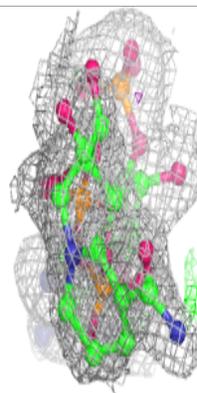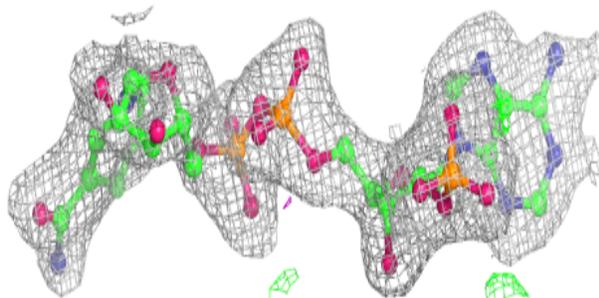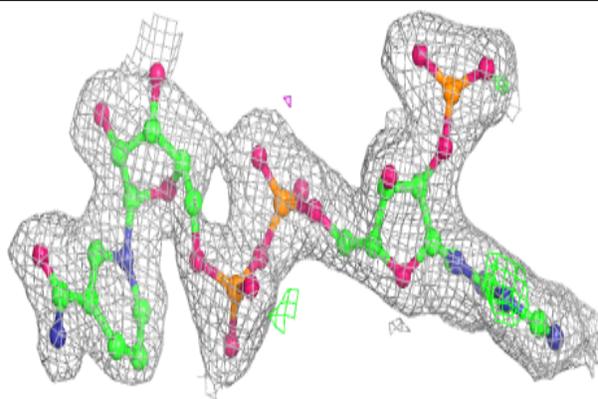
Electron density around NAP D 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
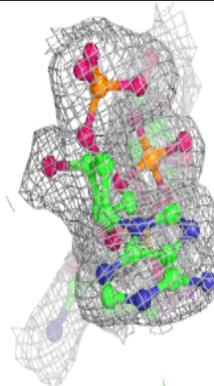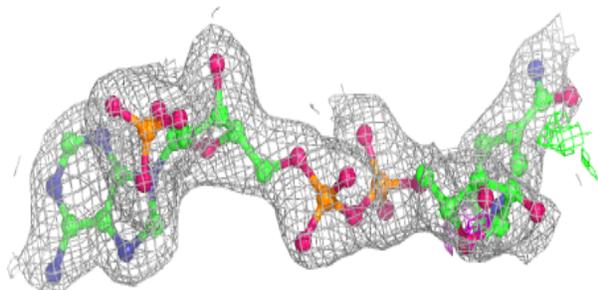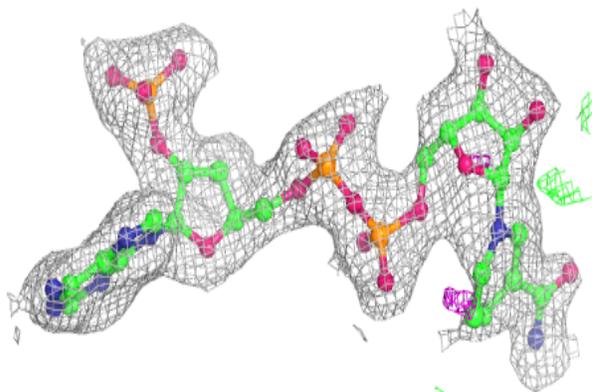
Electron density around FAD C 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
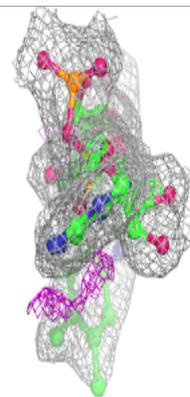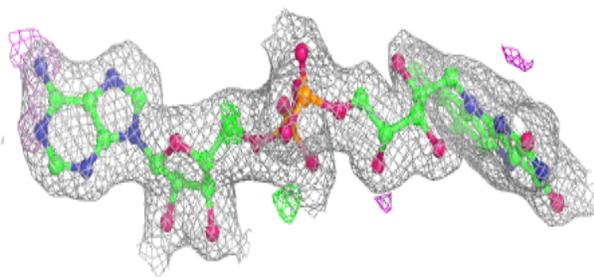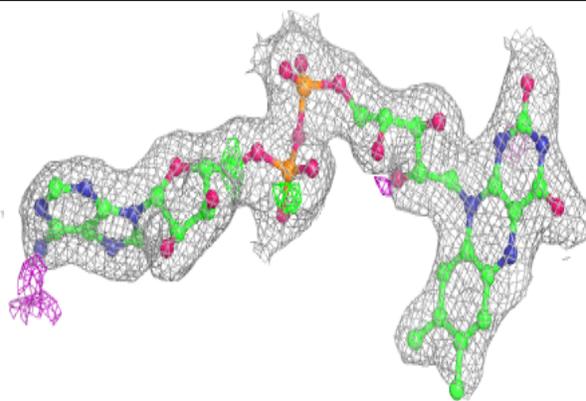
Electron density around FAD B 502:

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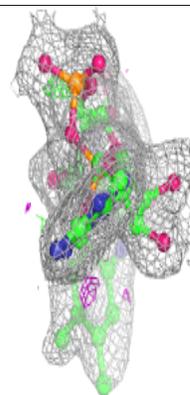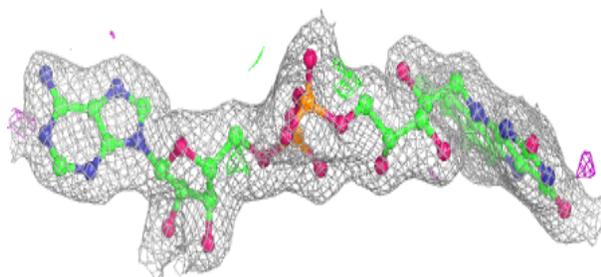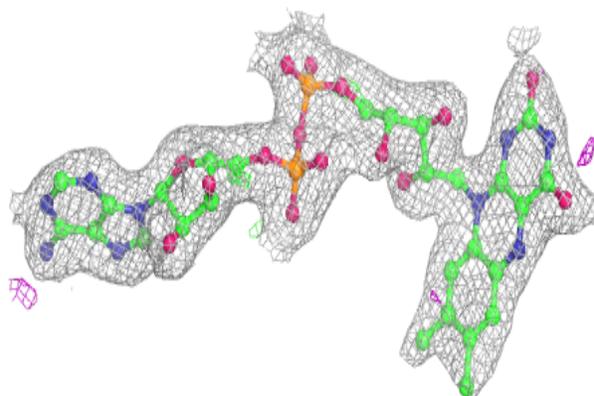
6.5 Other polymers (i)

There are no such residues in this entry.