Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 11:47 AM EDT

PDB ID	:	3KVE
Title	:	Structure of native L-amino acid oxidase from Vipera ammodytes ammodytes: stabilization of the quaternary structure by divalent ions and structural changes in the dynamic active site
Authors	:	Gergiova, D.; Murakami, M.T.; Perbandt, M.; Arni, R.K.; Betzel, C.
Deposited on	:	2009-11-30
Resolution	:	2.57 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:

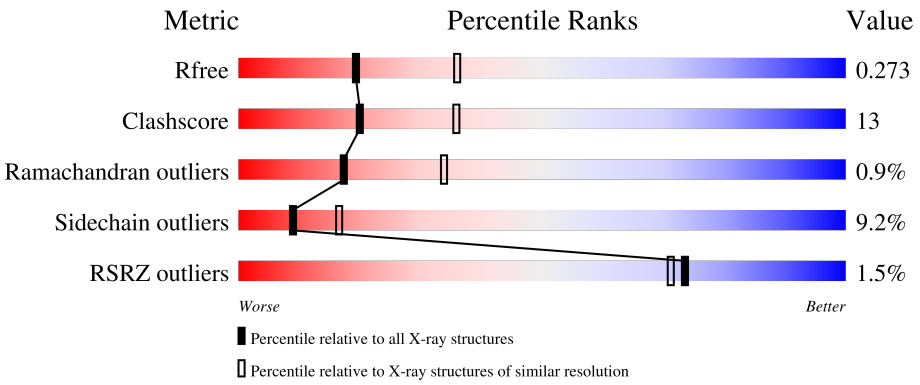
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	486	2% 69% 25% 5%
1	B	486	2% 69% 26% 5% •
1	C	486	2% 72% 24% •
1	D	486	% 72% 23% •

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
3	NAG	A	488	X	-	-	-
3	NAG	B	488	X	-	-	-
3	NAG	C	488	X	-	-	-

2 Entry composition (i)

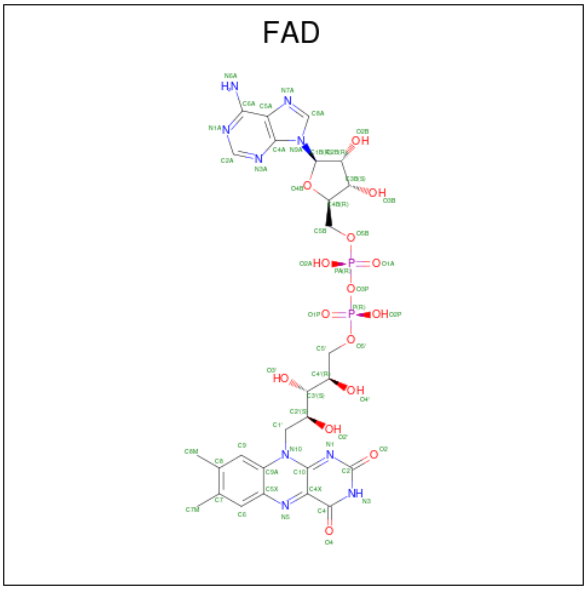
There are 5 unique types of molecules in this entry. The entry contains 16288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-amino acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	484	3870	2452	669	736	13	0	1	0
1	B	484	3864	2448	668	735	13	0	0	0
1	C	484	3864	2448	668	735	13	0	0	0
1	D	484	3864	2448	668	735	13	0	0	0

- Molecule 2 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		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0

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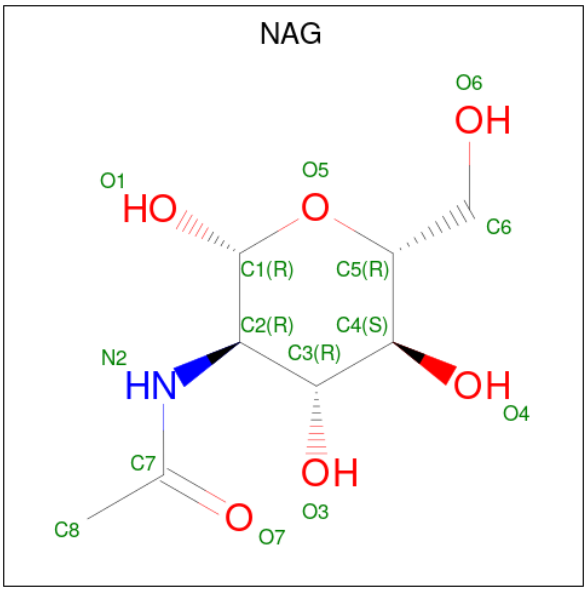
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
2	D	1	53	27	9	15	2	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
			Total	C	N	O		
3	B	1	14	8	1	5	0	0
			Total	C	N	O		
3	C	1	14	8	1	5	0	0
			Total	C	N	O		
3	D	1	14	8	1	5	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
			Total	Zn		
4	B	1	1	1	0	0
			Total	Zn		
4	C	1	1	1	0	0

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

- Molecule 5 is water.

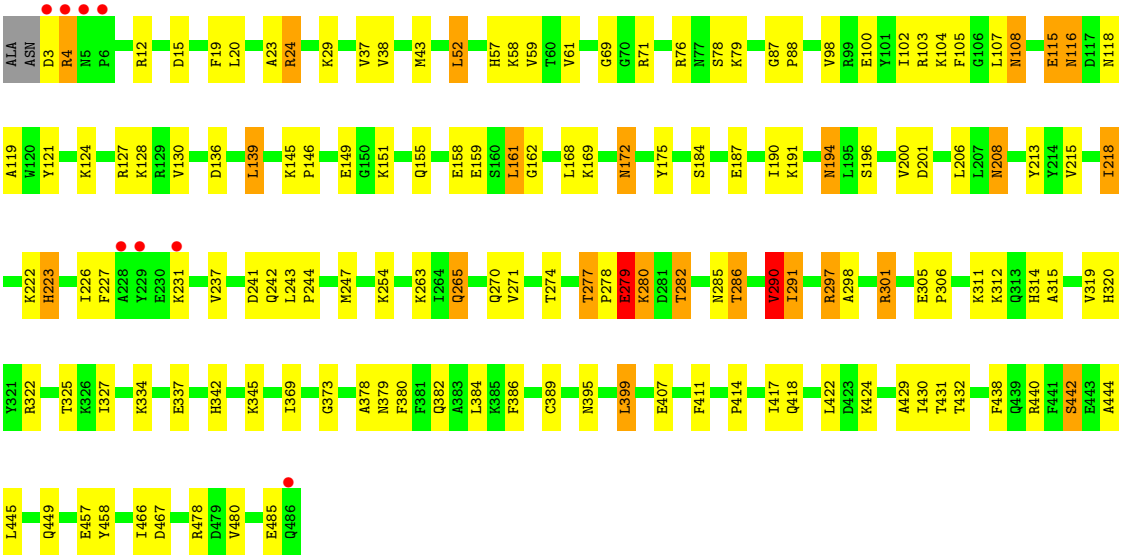
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	164	164	164	0	0
			Total	O		
5	B	129	129	129	0	0
			Total	O		
5	C	125	125	125	0	0
			Total	O		
5	D	136	136	136	0	0

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.

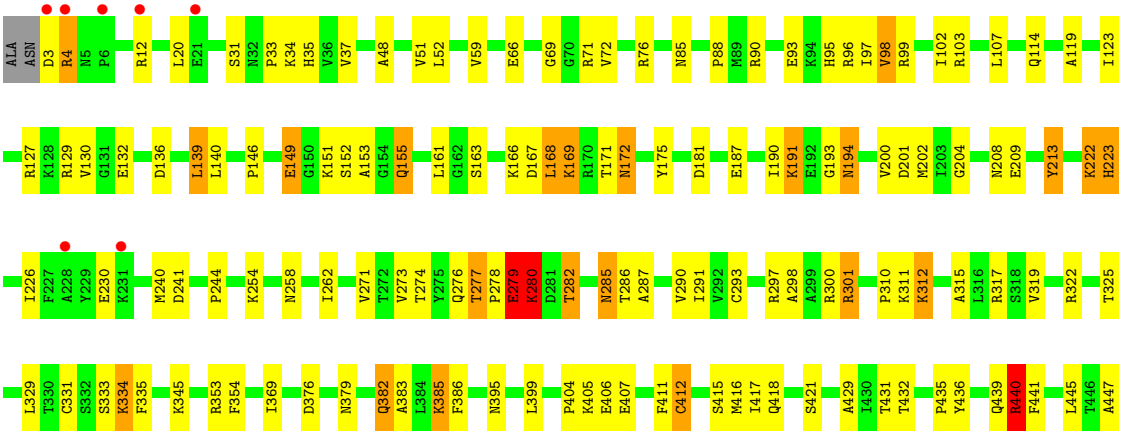
• Molecule 1: L-amino acid oxidase

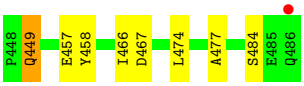
Chain A: 2% 69% 25% 5%



• Molecule 1: L-amino acid oxidase

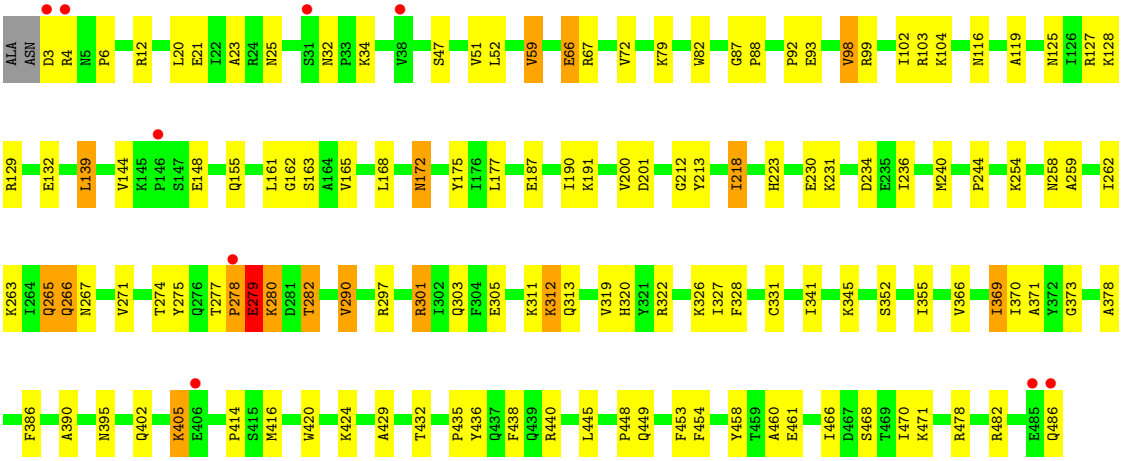
Chain B: 2% 69% 26% 5%





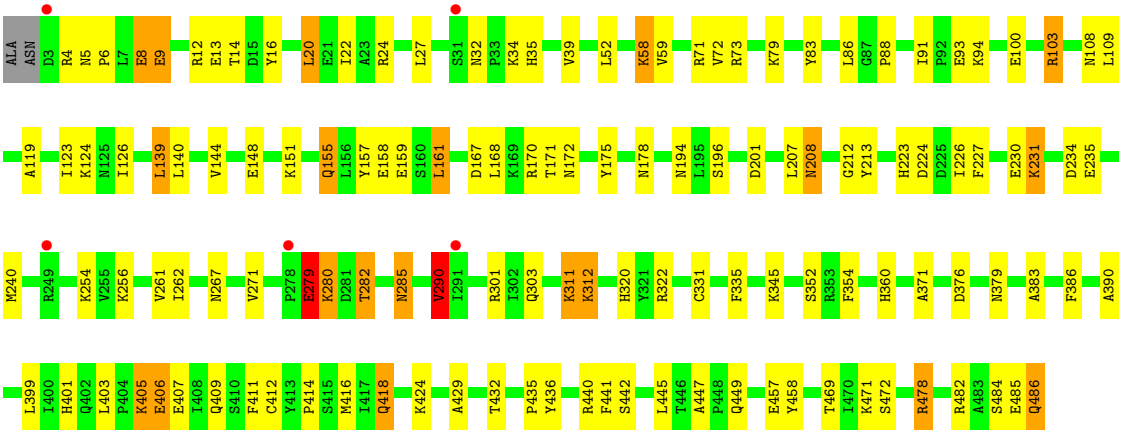
• Molecule 1: L-amino acid oxidase

Chain C:



• Molecule 1: L-amino acid oxidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.98Å 95.84Å 108.44Å 90.00° 92.53° 90.00°	Depositor
Resolution (Å)	27.40 – 2.57 27.42 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.0 (27.40-2.57) 98.2 (27.42-2.56)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.276 0.192 , 0.273	Depositor DCC
R_{free} test set	3212 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16288	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: ZN, NAG, 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	0.64	0/3962	0.75	2/5351 (0.0%)
1	B	0.62	0/3953	0.75	3/5339 (0.1%)
1	C	0.59	0/3953	0.68	0/5339
1	D	0.61	0/3953	0.71	3/5339 (0.1%)
All	All	0.62	0/15821	0.72	8/21368 (0.0%)

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
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	9

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	440	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	D	280	LYS	N-CA-C	7.30	130.71	111.00
1	B	440	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	290	VAL	CB-CA-C	-5.56	100.84	111.40
1	A	290	VAL	CB-CA-C	-5.27	101.39	111.40
1	B	279	GLU	N-CA-C	5.13	124.84	111.00
1	D	279	GLU	C-N-CA	5.10	134.45	121.70
1	A	279	GLU	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	GLU	Peptide
1	A	449	GLN	Peptide
1	B	279	GLU	Peptide
1	B	449	GLN	Peptide
1	C	278	PRO	Peptide
1	C	279	GLU	Peptide
1	C	449	GLN	Peptide
1	D	279	GLU	Peptide
1	D	449	GLN	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	3870	0	3783	106	0
1	B	3864	0	3775	116	0
1	C	3864	0	3775	88	0
1	D	3864	0	3775	97	0
2	A	53	0	31	3	0
2	B	53	0	31	5	0
2	C	53	0	31	3	0
2	D	53	0	31	5	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	164	0	0	10	0
5	B	129	0	0	5	0
5	C	125	0	0	3	0
5	D	136	0	0	1	0
All	All	16288	0	15284	391	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 13.

All (391) 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:271:VAL:HG11	1:D:290:VAL:HG22	1.21	1.12
1:A:271:VAL:HG11	1:A:290:VAL:CG2	1.85	1.07
1:C:440:ARG:CZ	1:D:201:ASP:OD1	2.08	1.01
1:C:271:VAL:HG11	1:C:290:VAL:HG22	1.43	0.98
1:A:201:ASP:OD1	1:B:440:ARG:CZ	2.12	0.98
1:A:271:VAL:HG11	1:A:290:VAL:HG22	1.49	0.93
1:B:322:ARG:HD3	1:B:432:THR:HG21	1.52	0.92
1:C:440:ARG:NH1	1:D:201:ASP:OD1	2.04	0.90
1:C:271:VAL:HG11	1:C:290:VAL:CG2	2.05	0.87
1:C:201:ASP:OD2	1:D:440:ARG:CZ	2.26	0.84
1:D:322:ARG:HD2	1:D:432:THR:OG1	1.78	0.84
1:A:201:ASP:OD1	1:B:440:ARG:NH2	2.10	0.83
1:B:37:VAL:HB	1:B:290:VAL:HG12	1.61	0.81
1:B:208:ASN:HB2	1:B:354:PHE:CZ	2.16	0.80
1:D:262:ILE:HD11	1:D:282:THR:HG21	1.64	0.79
1:A:119:ALA:HB1	1:A:345:LYS:O	1.82	0.79
1:D:86:LEU:HB3	1:D:418:GLN:HG2	1.65	0.78
1:D:124:LYS:NZ	1:D:140:LEU:O	2.15	0.78
1:A:440:ARG:CZ	1:B:201:ASP:OD2	2.31	0.78
1:B:153:ALA:N	1:B:202:MET:HE2	1.99	0.78
1:C:92:PRO:HB3	1:C:230:GLU:HG3	1.65	0.78
1:A:128:LYS:HD2	1:A:139:LEU:HG	1.65	0.77
1:B:276:GLN:HG3	1:B:282:THR:HG23	1.66	0.77
1:D:271:VAL:CG1	1:D:290:VAL:HG22	2.10	0.75
1:A:201:ASP:OD1	1:B:440:ARG:NH1	2.19	0.74
1:C:322:ARG:O	1:C:429:ALA:HB3	1.86	0.74
1:C:322:ARG:HD2	1:C:432:THR:OG1	1.87	0.73
1:D:223:HIS:CD2	1:D:227:PHE:HD1	2.05	0.73
1:C:277:THR:HG23	1:C:278:PRO:HD2	1.70	0.73
1:B:181:ASP:OD2	1:B:439:GLN:HG3	1.90	0.72
1:D:223:HIS:CD2	1:D:227:PHE:CD1	2.77	0.72
1:C:129:ARG:HB2	1:C:132:GLU:HG3	1.72	0.72
1:C:201:ASP:OD2	1:D:440:ARG:NH2	2.22	0.71
1:C:98:VAL:HG11	1:C:466:ILE:CG2	2.20	0.71
1:A:274:THR:HG23	1:A:282:THR:HG22	1.70	0.71
1:B:34:LYS:HG3	1:B:484:SER:HB2	1.71	0.70
1:B:274:THR:HG22	1:B:282:THR:CG2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLN:HG2	5:C:592:HOH:O	1.90	0.70
1:B:153:ALA:CA	1:B:202:MET:HE2	2.23	0.69
1:B:274:THR:HG22	1:B:282:THR:HG22	1.75	0.68
1:D:8:GLU:HG3	1:D:9:GLU:N	2.07	0.68
1:A:218:ILE:HG12	1:A:438:PHE:CE2	2.28	0.68
1:A:172:ASN:HD22	1:A:175:TYR:HB2	1.59	0.68
1:C:98:VAL:HG13	1:C:470:ILE:HD12	1.75	0.67
1:B:169:LYS:O	1:B:171:THR:N	2.27	0.67
1:B:271:VAL:HG11	1:B:290:VAL:HG13	1.76	0.67
1:B:329:LEU:HB3	1:B:412:CYS:SG	2.35	0.67
1:A:440:ARG:NH2	1:B:201:ASP:OD2	2.29	0.66
1:A:187:GLU:HG3	1:A:191:LYS:HE3	1.78	0.66
1:A:274:THR:CG2	1:A:282:THR:CG2	2.73	0.66
1:A:274:THR:CG2	1:A:282:THR:HG21	2.26	0.66
1:D:212:GLY:HA3	1:D:322:ARG:NH2	2.11	0.66
1:C:312:LYS:HE2	1:C:454:PHE:CE1	2.32	0.65
1:D:119:ALA:HB1	1:D:345:LYS:O	1.96	0.65
1:A:274:THR:HG23	1:A:282:THR:CG2	2.27	0.65
1:C:274:THR:HG22	1:C:282:THR:HG21	1.78	0.65
1:D:231:LYS:NZ	1:D:231:LYS:HB3	2.11	0.65
1:A:312:LYS:NZ	1:A:444:ALA:O	2.27	0.64
1:A:38:VAL:HB	1:A:61:VAL:HG22	1.79	0.64
1:A:128:LYS:CD	1:A:139:LEU:HG	2.27	0.64
1:C:277:THR:HG23	1:C:278:PRO:CD	2.28	0.64
1:D:71:ARG:HD3	2:D:487:FAD:O1A	1.98	0.64
1:A:322:ARG:HD3	1:A:432:THR:HG21	1.80	0.63
1:D:88:PRO:HA	2:D:487:FAD:C4X	2.28	0.63
1:C:128:LYS:HD2	1:C:139:LEU:HG	1.79	0.63
1:D:486:GLN:C	1:D:486:GLN:HE21	2.02	0.63
1:D:59:VAL:HG22	1:D:254:LYS:HD3	1.81	0.63
1:B:181:ASP:HB3	1:B:439:GLN:HE21	1.64	0.63
1:D:8:GLU:HG3	1:D:9:GLU:H	1.64	0.62
1:D:86:LEU:HB3	1:D:418:GLN:CG	2.29	0.62
1:C:201:ASP:OD2	1:D:440:ARG:NH1	2.32	0.62
1:C:440:ARG:NH2	1:D:201:ASP:OD1	2.31	0.62
1:D:271:VAL:HG11	1:D:290:VAL:CG2	2.13	0.62
1:C:98:VAL:HG11	1:C:466:ILE:HG21	1.80	0.61
1:C:98:VAL:CG1	1:C:466:ILE:HG22	2.31	0.61
1:D:13:GLU:HB2	1:D:16:TYR:HB2	1.81	0.61
1:B:153:ALA:N	1:B:202:MET:CE	2.63	0.61
1:D:386:PHE:CZ	1:D:414:PRO:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LYS:HZ3	1:D:79:LYS:HD3	1.67	0.60
1:A:71:ARG:NH2	1:A:457:GLU:OE1	2.35	0.60
1:A:297:ARG:HG3	5:A:545:HOH:O	2.02	0.60
1:C:301:ARG:NH2	5:C:509:HOH:O	2.35	0.60
1:B:312:LYS:NZ	1:B:447:ALA:O	2.35	0.60
1:D:312:LYS:NZ	1:D:447:ALA:O	2.35	0.60
1:A:119:ALA:CB	1:A:345:LYS:O	2.50	0.59
1:C:88:PRO:HA	2:C:487:FAD:C4X	2.32	0.59
1:A:424:LYS:HG2	5:A:587:HOH:O	2.02	0.59
1:A:105:PHE:HE2	1:A:247:MET:HE2	1.66	0.59
1:B:88:PRO:HA	2:B:487:FAD:C4X	2.33	0.59
1:A:386:PHE:CZ	1:A:414:PRO:HB2	2.37	0.59
1:C:386:PHE:CZ	1:C:414:PRO:HB2	2.38	0.59
1:A:277:THR:HG21	5:A:643:HOH:O	2.02	0.59
1:C:331:CYS:SG	1:C:369:ILE:HD11	2.42	0.59
1:A:440:ARG:NH1	1:B:201:ASP:OD2	2.36	0.59
1:D:486:GLN:HE21	1:D:486:GLN:CA	2.15	0.59
1:B:85:ASN:HD21	1:B:240:MET:H	1.50	0.58
1:A:102:ILE:HG23	1:A:107:LEU:HB2	1.84	0.58
1:A:98:VAL:HG13	1:A:467:ASP:HA	1.85	0.58
1:A:172:ASN:ND2	1:A:175:TYR:HB2	2.18	0.58
1:C:98:VAL:CG1	1:C:466:ILE:CG2	2.81	0.58
1:B:241:ASP:O	1:B:244:PRO:HG2	2.04	0.58
1:A:145:LYS:HG3	1:A:196:SER:HB3	1.85	0.58
1:D:59:VAL:CG2	1:D:254:LYS:HD3	2.34	0.58
1:C:319:VAL:HG21	1:C:445:LEU:HD11	1.86	0.58
1:D:406:GLU:H	1:D:406:GLU:CD	2.08	0.58
1:B:262:ILE:HD11	1:B:282:THR:HG21	1.86	0.57
1:D:235:GLU:OE2	1:D:360:HIS:ND1	2.30	0.57
1:A:315:ALA:HB1	1:A:445:LEU:HD21	1.85	0.57
1:D:322:ARG:O	1:D:429:ALA:HB3	2.05	0.57
1:A:88:PRO:HA	2:A:487:FAD:C4X	2.34	0.57
1:C:212:GLY:HA3	1:C:322:ARG:NH2	2.20	0.57
1:B:168:LEU:C	1:B:169:LYS:O	2.38	0.57
1:B:127:ARG:NH1	5:B:618:HOH:O	2.38	0.57
1:D:73:ARG:HD2	1:D:86:LEU:HD12	1.87	0.57
1:A:88:PRO:HA	2:A:487:FAD:N5	2.20	0.57
1:B:209:GLU:OE2	1:B:223:HIS:CE1	2.58	0.57
1:B:34:LYS:HG3	1:B:484:SER:CB	2.35	0.56
1:B:71:ARG:NH2	1:B:457:GLU:OE1	2.38	0.56
1:B:300:ARG:NH2	1:B:317:ARG:HD3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:O	1:B:429:ALA:HB3	2.06	0.56
1:D:59:VAL:H	1:D:254:LYS:HZ3	1.52	0.56
2:A:487:FAD:H8A	5:A:522:HOH:O	2.05	0.56
1:D:144:VAL:HB	1:D:148:GLU:HB2	1.86	0.56
1:D:390:ALA:CB	1:D:414:PRO:HB3	2.36	0.56
1:A:115:GLU:HA	5:A:620:HOH:O	2.06	0.55
1:B:222:LYS:O	1:B:226:ILE:HD12	2.06	0.55
1:A:108:ASN:N	1:A:108:ASN:HD22	2.04	0.55
1:B:3:ASP:O	1:B:4:ARG:HG3	2.07	0.55
1:A:270:GLN:NE2	1:A:286:THR:CG2	2.70	0.55
1:B:146:PRO:O	1:B:149:GLU:HG2	2.07	0.54
1:A:116:ASN:HD21	1:A:118:ASN:HB2	1.72	0.54
1:C:21:GLU:OE1	1:C:25:ASN:ND2	2.39	0.54
1:C:32:ASN:ND2	1:C:34:LYS:HE2	2.23	0.54
1:B:153:ALA:HA	1:B:202:MET:HE2	1.90	0.54
1:A:270:GLN:NE2	1:A:286:THR:HG21	2.22	0.54
1:B:129:ARG:HB2	1:B:132:GLU:HG3	1.90	0.54
1:A:23:ALA:O	1:A:104:LYS:NZ	2.41	0.54
1:D:407:GLU:HG2	1:D:411:PHE:CZ	2.43	0.54
1:B:435:PRO:O	1:B:436:TYR:HB2	2.08	0.53
1:A:263:LYS:NZ	1:A:305:GLU:OE2	2.40	0.53
1:C:320:HIS:HB3	1:C:432:THR:O	2.08	0.53
1:D:58:LYS:HA	1:D:254:LYS:HZ3	1.74	0.53
1:B:382:GLN:HE22	1:B:421:SER:HB3	1.74	0.53
1:C:88:PRO:HA	2:C:487:FAD:N5	2.24	0.53
1:D:331:CYS:HA	1:D:412:CYS:HA	1.89	0.53
1:A:59:VAL:O	1:A:254:LYS:HD3	2.09	0.53
1:A:254:LYS:HG3	5:A:619:HOH:O	2.08	0.52
1:B:71:ARG:HD3	2:B:487:FAD:O1A	2.08	0.52
1:A:237:VAL:O	1:A:242:GLN:NE2	2.43	0.52
1:A:270:GLN:HE21	1:A:286:THR:CG2	2.22	0.52
1:D:22:ILE:HD13	1:D:27:LEU:HD23	1.91	0.52
1:D:445:LEU:HD22	1:D:458:TYR:CD2	2.44	0.52
1:A:184:SER:HA	1:A:215:VAL:O	2.09	0.52
1:B:404:PRO:HG2	1:B:407:GLU:HB2	1.92	0.52
1:A:121:TYR:CE1	1:A:206:LEU:HD22	2.45	0.52
1:A:172:ASN:HB2	1:A:175:TYR:H	1.73	0.52
1:B:395:ASN:O	1:B:399:LEU:HD13	2.09	0.52
1:D:158:GLU:O	1:D:161:LEU:HB2	2.09	0.52
1:C:277:THR:CG2	1:C:280:LYS:HD3	2.40	0.51
1:A:52:LEU:HD12	1:A:57:HIS:CD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ALA:O	1:C:104:LYS:NZ	2.43	0.51
1:C:390:ALA:HB1	1:C:414:PRO:HB3	1.92	0.51
1:D:39:VAL:HG22	1:D:261:VAL:HG21	1.92	0.51
1:B:301:ARG:HD3	5:B:604:HOH:O	2.11	0.51
1:C:274:THR:HG22	1:C:282:THR:CG2	2.40	0.51
1:D:123:ILE:HG22	1:D:124:LYS:HG2	1.93	0.51
1:C:424:LYS:HA	1:D:383:ALA:HB1	1.92	0.51
1:A:43:MET:HG3	1:A:466:ILE:HG23	1.91	0.51
1:B:168:LEU:HD22	1:B:168:LEU:O	2.11	0.51
1:A:223:HIS:CD2	1:A:227:PHE:CD1	2.99	0.51
1:A:291:ILE:HD11	1:A:480:VAL:HG21	1.93	0.51
1:D:5:ASN:HB3	1:D:8:GLU:HB3	1.93	0.51
1:D:72:VAL:HG22	1:D:88:PRO:HG2	1.92	0.51
1:B:52:LEU:CD2	1:B:477:ALA:HB1	2.41	0.50
1:B:274:THR:HG22	1:B:282:THR:HG21	1.92	0.50
1:B:382:GLN:HE22	1:B:421:SER:CB	2.24	0.50
1:D:20:LEU:O	1:D:24:ARG:HG3	2.11	0.50
1:B:35:HIS:O	1:B:287:ALA:HB1	2.11	0.50
1:B:98:VAL:HG13	1:B:467:ASP:HA	1.93	0.50
1:A:79:LYS:HE2	1:C:405:LYS:HE3	1.92	0.50
1:A:124:LYS:HG2	1:B:310:PRO:HB3	1.93	0.50
1:D:93:GLU:HB3	1:D:230:GLU:OE2	2.11	0.50
1:D:401:HIS:O	1:D:403:LEU:HG	2.12	0.50
1:B:98:VAL:O	1:B:102:ILE:HG13	2.12	0.50
1:A:190:ILE:O	1:A:194:ASN:HA	2.12	0.50
1:D:445:LEU:HD22	1:D:458:TYR:HD2	1.77	0.50
1:B:136:ASP:HB3	1:B:139:LEU:HD22	1.94	0.50
1:C:98:VAL:HG13	1:C:466:ILE:HG22	1.93	0.50
1:A:373:GLY:O	1:A:378:ALA:HB2	2.11	0.50
1:B:385:LYS:HG3	5:B:547:HOH:O	2.10	0.50
1:A:116:ASN:ND2	1:A:118:ASN:HB2	2.27	0.49
1:A:265:GLN:HB3	1:A:305:GLU:HB3	1.93	0.49
1:B:52:LEU:HD21	1:B:477:ALA:HB1	1.94	0.49
1:A:337:GLU:HG2	1:A:342:HIS:CE1	2.47	0.49
1:B:37:VAL:O	1:B:290:VAL:HA	2.12	0.49
1:C:99:ARG:NH2	1:C:234:ASP:OD2	2.35	0.49
5:C:496:HOH:O	1:D:440:ARG:HB2	2.11	0.49
1:D:226:ILE:O	1:D:230:GLU:HB3	2.12	0.49
1:A:121:TYR:CE2	1:A:130:VAL:HG22	2.48	0.49
1:B:90:ARG:NH1	1:B:114:GLN:OE1	2.46	0.49
1:B:258:ASN:O	1:B:277:THR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:TYR:CD1	1:D:83:TYR:C	2.85	0.49
1:B:226:ILE:O	1:B:230:GLU:HB2	2.13	0.49
1:B:85:ASN:ND2	1:B:240:MET:H	2.11	0.48
1:B:187:GLU:OE2	1:B:191:LYS:NZ	2.45	0.48
1:C:395:ASN:OD1	1:C:405:LYS:HD2	2.13	0.48
1:A:438:PHE:O	1:A:442:SER:HB2	2.12	0.48
1:D:208:ASN:HB2	1:D:354:PHE:CZ	2.49	0.48
1:B:97:ILE:HB	1:B:467:ASP:OD1	2.13	0.48
1:C:262:ILE:HD11	1:C:282:THR:HG21	1.94	0.48
1:C:445:LEU:HD22	1:C:458:TYR:CD2	2.48	0.48
1:B:315:ALA:HB1	1:B:445:LEU:HD21	1.94	0.48
1:A:158:GLU:O	1:A:161:LEU:HB2	2.12	0.48
1:A:422:LEU:HA	1:B:383:ALA:HB2	1.96	0.48
1:D:91:ILE:HD11	1:D:240:MET:HE1	1.94	0.48
1:B:449:GLN:NE2	5:B:570:HOH:O	2.47	0.48
1:D:267:ASN:HB2	5:D:519:HOH:O	2.13	0.48
1:C:82:TRP:HB3	1:C:366:VAL:HG21	1.96	0.48
1:D:435:PRO:O	1:D:436:TYR:HB2	2.14	0.48
1:D:100:GLU:O	1:D:103:ARG:HG3	2.14	0.48
1:B:278:PRO:C	1:B:280:LYS:HB2	2.34	0.47
1:B:123:ILE:HB	1:B:140:LEU:HD22	1.95	0.47
1:C:277:THR:CG2	1:C:278:PRO:HD2	2.41	0.47
1:B:333:SER:O	1:B:335:PHE:N	2.43	0.47
1:D:148:GLU:OE1	1:D:196:SER:OG	2.23	0.47
1:A:76:ARG:HB2	1:D:279:GLU:O	2.14	0.47
1:A:263:LYS:HB3	1:A:274:THR:HB	1.96	0.47
1:B:273:VAL:HG21	1:B:290:VAL:HG11	1.95	0.47
1:B:322:ARG:HD3	1:B:432:THR:CG2	2.35	0.47
1:C:116:ASN:HD21	1:C:341:ILE:HA	1.80	0.47
1:D:59:VAL:H	1:D:254:LYS:NZ	2.13	0.47
1:A:215:VAL:HG11	1:A:432:THR:CG2	2.45	0.47
1:A:325:THR:HA	1:A:418:GLN:O	2.14	0.47
1:C:187:GLU:OE2	1:C:191:LYS:NZ	2.43	0.47
1:D:5:ASN:HA	1:D:6:PRO:HD2	1.76	0.47
1:B:119:ALA:HB1	1:B:345:LYS:O	2.15	0.47
1:B:273:VAL:CG2	1:B:290:VAL:HG11	2.44	0.47
1:C:266:GLN:HG2	1:C:267:ASN:N	2.29	0.46
1:C:279:GLU:N	1:C:280:LYS:HB2	2.30	0.46
1:B:48:ALA:HA	1:B:477:ALA:HB2	1.98	0.46
1:B:431:THR:HG21	1:B:458:TYR:HA	1.97	0.46
1:C:98:VAL:HG11	1:C:466:ILE:HG22	1.91	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:THR:CG2	1:C:282:THR:HG21	2.44	0.46
1:D:126:ILE:HG21	1:D:139:LEU:O	2.15	0.46
1:D:285:ASN:HD22	1:D:285:ASN:HA	1.61	0.46
1:A:222:LYS:O	1:A:226:ILE:HD12	2.15	0.46
1:A:4:ARG:NH2	5:A:633:HOH:O	2.47	0.46
1:C:277:THR:CG2	1:C:278:PRO:CD	2.93	0.46
1:D:88:PRO:HA	2:D:487:FAD:N5	2.30	0.46
1:C:478:ARG:HD3	1:C:482:ARG:CZ	2.46	0.46
1:D:320:HIS:HB3	1:D:432:THR:O	2.16	0.46
1:A:277:THR:O	1:A:280:LYS:HB2	2.15	0.46
1:B:59:VAL:O	1:B:254:LYS:HD2	2.16	0.46
1:B:102:ILE:HG23	1:B:107:LEU:HB2	1.97	0.46
1:B:319:VAL:HG21	1:B:445:LEU:HD11	1.98	0.46
1:C:66:GLU:HG3	1:C:258:ASN:OD1	2.16	0.46
1:C:87:GLY:O	1:C:326:LYS:NZ	2.42	0.46
1:A:265:GLN:HA	1:A:305:GLU:O	2.15	0.46
1:D:352:SER:O	1:D:354:PHE:N	2.47	0.46
1:B:69:GLY:HA2	1:B:244:PRO:HB3	1.97	0.46
1:C:119:ALA:HB1	1:C:345:LYS:O	2.16	0.46
1:C:312:LYS:HE2	1:C:454:PHE:CD1	2.51	0.46
1:B:76:ARG:HG3	1:B:76:ARG:HH11	1.80	0.45
1:B:376:ASP:HA	1:B:379:ASN:HB2	1.96	0.45
1:A:69:GLY:HA2	1:A:244:PRO:HB3	1.98	0.45
1:B:291:ILE:HG22	1:B:293:CYS:SG	2.56	0.45
1:C:263:LYS:HB3	1:C:274:THR:HB	1.98	0.45
1:A:270:GLN:HE21	1:A:286:THR:HG21	1.81	0.45
1:C:266:GLN:HE21	1:C:266:GLN:HB3	1.66	0.45
1:B:445:LEU:HD22	1:B:458:TYR:CD2	2.51	0.45
1:D:35:HIS:HD2	1:D:58:LYS:O	2.00	0.45
1:D:354:PHE:O	1:D:371:ALA:HA	2.15	0.45
1:A:37:VAL:HB	1:A:290:VAL:HG13	1.98	0.45
1:B:153:ALA:HB2	1:B:202:MET:HE3	1.99	0.45
1:A:196:SER:O	1:A:200:VAL:HG23	2.17	0.45
1:B:35:HIS:HE1	1:B:285:ASN:ND2	2.15	0.45
1:B:213:TYR:HD1	1:B:213:TYR:HA	1.66	0.45
1:C:218:ILE:HG12	1:C:438:PHE:CE2	2.50	0.45
1:A:146:PRO:HA	1:A:149:GLU:HG3	1.99	0.45
1:A:312:LYS:HE3	5:A:628:HOH:O	2.16	0.45
1:C:93:GLU:HA	1:C:99:ARG:CZ	2.46	0.45
1:B:31:SER:O	1:B:33:PRO:HD3	2.17	0.45
1:A:322:ARG:O	1:A:429:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:VAL:HG11	1:B:474:LEU:HD22	1.99	0.44
1:C:448:PRO:HB3	1:C:453:PHE:CD1	2.53	0.44
1:D:457:GLU:HB2	2:D:487:FAD:H5'2	1.98	0.44
1:B:298:ALA:O	1:B:301:ARG:HB2	2.17	0.44
1:B:440:ARG:HD3	1:B:441:PHE:CE1	2.52	0.44
1:A:431:THR:HG21	1:A:458:TYR:HA	1.99	0.44
1:D:335:PHE:HE2	1:D:412:CYS:SG	2.39	0.44
1:C:98:VAL:CG1	1:C:466:ILE:HG21	2.47	0.44
1:C:327:ILE:HB	1:C:371:ALA:HB3	2.00	0.44
1:B:95:HIS:HB3	1:B:467:ASP:HB2	1.99	0.44
1:C:259:ALA:HB1	1:C:275:TYR:CD1	2.53	0.44
1:A:87:GLY:HA3	1:A:88:PRO:HD2	1.87	0.44
1:A:379:ASN:O	1:A:380:PHE:C	2.56	0.44
1:A:384:LEU:HB2	1:A:389:CYS:SG	2.58	0.44
1:B:385:LYS:HE3	1:B:385:LYS:HB3	1.66	0.44
1:C:72:VAL:HG22	1:C:88:PRO:HG2	1.99	0.44
1:C:127:ARG:O	1:C:128:LYS:HG2	2.18	0.44
1:C:144:VAL:HB	1:C:148:GLU:HB2	2.00	0.43
1:C:435:PRO:O	1:C:436:TYR:HB2	2.18	0.43
1:A:407:GLU:HG2	1:A:411:PHE:CZ	2.53	0.43
1:A:325:THR:HB	5:A:590:HOH:O	2.18	0.43
1:B:331:CYS:HA	1:B:411:PHE:O	2.19	0.43
1:A:279:GLU:N	1:A:280:LYS:HB2	2.33	0.43
1:B:331:CYS:HA	1:B:412:CYS:HA	1.99	0.43
1:D:32:ASN:ND2	1:D:34:LYS:HE2	2.33	0.43
1:D:231:LYS:HB3	1:D:231:LYS:HZ1	1.80	0.43
1:A:208:ASN:ND2	5:A:570:HOH:O	2.52	0.43
1:D:172:ASN:HD22	1:D:175:TYR:HB2	1.82	0.43
1:A:278:PRO:O	1:A:279:GLU:HB2	2.19	0.43
1:A:298:ALA:O	1:A:301:ARG:HB2	2.19	0.43
1:A:320:HIS:HB3	1:A:432:THR:O	2.19	0.43
1:A:215:VAL:HG11	1:A:432:THR:HG21	2.00	0.43
1:B:415:SER:O	1:B:416:MET:HB2	2.18	0.43
1:C:265:GLN:HA	1:C:305:GLU:O	2.18	0.43
1:C:373:GLY:O	1:C:378:ALA:HB2	2.18	0.43
1:B:279:GLU:N	1:B:280:LYS:HB2	2.34	0.43
1:C:6:PRO:HB2	1:C:165:VAL:HG21	2.01	0.43
1:C:265:GLN:HB3	1:C:305:GLU:HB2	2.01	0.43
1:D:109:LEU:HD22	1:D:234:ASP:HB3	2.00	0.43
1:C:47:SER:O	1:C:51:VAL:HG22	2.19	0.43
1:C:102:ILE:HG12	1:C:236:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ASN:HD22	1:B:175:TYR:HB2	1.84	0.43
1:A:241:ASP:HA	1:A:244:PRO:HG2	2.01	0.42
1:A:243:LEU:HB3	1:A:244:PRO:HD2	2.00	0.42
1:C:172:ASN:HD22	1:C:175:TYR:HB2	1.83	0.42
1:C:277:THR:HG22	1:C:280:LYS:HD3	2.00	0.42
1:C:328:PHE:HB2	1:C:416:MET:HB3	2.01	0.42
1:D:8:GLU:O	1:D:9:GLU:C	2.58	0.42
1:D:170:ARG:HE	1:D:171:THR:HG23	1.84	0.42
1:B:37:VAL:HB	1:B:290:VAL:CG1	2.40	0.42
1:B:93:GLU:HA	1:B:99:ARG:CZ	2.48	0.42
2:B:487:FAD:H8A	5:B:501:HOH:O	2.18	0.42
1:D:94:LYS:HE2	1:D:94:LYS:HB3	1.77	0.42
1:B:405:LYS:HZ3	1:D:79:LYS:CD	2.31	0.42
1:C:328:PHE:CD2	1:C:370:ILE:HG12	2.55	0.42
1:D:71:ARG:CD	2:D:487:FAD:O1A	2.66	0.42
1:A:280:LYS:HD2	1:A:280:LYS:HA	1.78	0.42
1:A:327:ILE:HG12	1:A:417:ILE:HD12	2.02	0.42
1:B:72:VAL:HG22	1:B:88:PRO:HG2	2.01	0.42
1:C:59:VAL:O	1:C:254:LYS:HD2	2.19	0.42
1:C:420:TRP:CD1	2:C:487:FAD:HM71	2.53	0.42
1:A:305:GLU:HA	1:A:306:PRO:C	2.38	0.42
1:B:151:LYS:HG2	1:B:155:GLN:NE2	2.34	0.42
1:B:193:GLY:O	1:B:194:ASN:CB	2.68	0.42
1:D:157:TYR:HE2	1:D:224:ASP:CG	2.22	0.42
1:A:136:ASP:HB3	1:A:139:LEU:HD22	2.02	0.42
1:B:190:ILE:HG13	1:B:200:VAL:HG21	2.02	0.42
1:B:386:PHE:CE1	1:B:417:ILE:HB	2.55	0.41
1:B:48:ALA:O	1:B:52:LEU:HG	2.19	0.41
1:C:190:ILE:HG13	1:C:200:VAL:HG21	2.03	0.41
1:C:460:ALA:HB1	1:C:468:SER:OG	2.21	0.41
1:D:34:LYS:HG2	1:D:484:SER:HB2	2.03	0.41
1:A:15:ASP:OD2	1:A:19:PHE:HE2	2.04	0.41
1:A:127:ARG:O	1:A:128:LYS:HG2	2.20	0.41
1:D:390:ALA:HB2	1:D:414:PRO:HB3	2.02	0.41
1:B:88:PRO:HA	2:B:487:FAD:N5	2.35	0.41
1:A:270:GLN:NE2	1:A:286:THR:HG23	2.35	0.41
1:B:152:SER:C	1:B:202:MET:HE2	2.41	0.41
1:D:405:LYS:O	1:D:409:GLN:HG3	2.21	0.41
1:B:3:ASP:O	1:B:4:ARG:CG	2.68	0.41
1:B:98:VAL:CG1	1:B:466:ILE:HG22	2.51	0.41
1:D:390:ALA:HB1	1:D:414:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:HIS:ND1	1:A:440:ARG:NH2	2.57	0.41
1:A:322:ARG:CD	1:A:432:THR:HG21	2.49	0.41
1:B:76:ARG:HG3	1:B:76:ARG:NH1	2.36	0.41
1:C:240:MET:O	1:C:244:PRO:HD2	2.21	0.41
1:D:170:ARG:HG2	1:D:170:ARG:O	2.20	0.41
1:D:440:ARG:HG2	1:D:441:PHE:CE1	2.55	0.41
1:A:243:LEU:HB3	1:A:244:PRO:CD	2.51	0.41
1:B:204:GLY:HA2	1:B:209:GLU:HB2	2.03	0.41
1:D:478:ARG:HD3	1:D:482:ARG:HD2	2.02	0.40
1:B:119:ALA:C	1:B:130:VAL:HG23	2.41	0.40
1:B:325:THR:HA	1:B:418:GLN:O	2.21	0.40
1:B:329:LEU:HB2	1:B:369:ILE:HG13	2.03	0.40
1:C:352:SER:HB3	1:C:355:ILE:HD11	2.03	0.40
1:D:311:LYS:H	1:D:311:LYS:HG2	1.70	0.40
1:A:24:ARG:HB2	1:A:100:GLU:HG2	2.02	0.40
1:A:395:ASN:O	1:A:399:LEU:HD13	2.20	0.40
1:D:155:GLN:NE2	1:D:159:GLU:OE2	2.54	0.40
1:D:469:THR:O	1:D:472:SER:OG	2.28	0.40
1:A:151:LYS:HG2	1:A:155:GLN:OE1	2.21	0.40
2:B:487:FAD:HM83	2:B:487:FAD:HM71	1.96	0.40
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.91	0.40
1:C:445:LEU:HD22	1:C:458:TYR:HD2	1.86	0.40
1:D:139:LEU:HD13	1:D:139:LEU:HA	1.97	0.40
1:D:151:LYS:HE2	1:D:159:GLU:OE2	2.21	0.40
1:D:376:ASP:HA	1:D:379:ASN:HB2	2.03	0.40
1:B:85:ASN:HD22	1:B:85:ASN:HA	1.77	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	483/486 (99%)	456 (94%)	22 (5%)	5 (1%)	15	31
1	B	482/486 (99%)	453 (94%)	23 (5%)	6 (1%)	13	26
1	C	482/486 (99%)	458 (95%)	20 (4%)	4 (1%)	19	37
1	D	482/486 (99%)	453 (94%)	26 (5%)	3 (1%)	25	45
All	All	1929/1944 (99%)	1820 (94%)	91 (5%)	18 (1%)	17	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	LYS
1	B	280	LYS
1	C	280	LYS
1	D	280	LYS
1	A	4	ARG
1	A	162	GLY
1	A	279	GLU
1	C	279	GLU
1	D	4	ARG
1	B	169	LYS
1	B	334	LYS
1	B	353	ARG
1	D	9	GLU
1	B	4	ARG
1	B	279	GLU
1	C	4	ARG
1	C	162	GLY
1	A	319	VAL

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	415/415 (100%)	372 (90%)	43 (10%)	7	12
1	B	414/415 (100%)	378 (91%)	36 (9%)	10	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	414/415 (100%)	377 (91%)	37 (9%)	9	18
1	D	414/415 (100%)	376 (91%)	38 (9%)	9	16
All	All	1657/1660 (100%)	1503 (91%)	154 (9%)	9	16

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	12	ARG
1	A	20	LEU
1	A	24	ARG
1	A	29	LYS
1	A	52	LEU
1	A	58	LYS
1	A	78	SER
1	A	103	ARG
1	A	108	ASN
1	A	115	GLU
1	A	116	ASN
1	A	139	LEU
1	A	159	GLU
1	A	161	LEU
1	A	168	LEU
1	A	169	LYS
1	A	172	ASN
1	A	194	ASN
1	A	208	ASN
1	A	213	TYR
1	A	218	ILE
1	A	223	HIS
1	A	231	LYS
1	A	265	GLN
1	A	277	THR
1	A	282	THR
1	A	285	ASN
1	A	286	THR
1	A	290	VAL
1	A	291	ILE
1	A	297	ARG
1	A	301	ARG
1	A	311	LYS

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Mol	Chain	Res	Type
1	A	334	LYS
1	A	369	ILE
1	A	382[A]	GLN
1	A	382[B]	GLN
1	A	399	LEU
1	A	430	ILE
1	A	442	SER
1	A	478	ARG
1	A	485	GLU
1	B	12	ARG
1	B	20	LEU
1	B	66	GLU
1	B	96	ARG
1	B	98	VAL
1	B	103	ARG
1	B	139	LEU
1	B	149	GLU
1	B	155	GLN
1	B	161	LEU
1	B	163	SER
1	B	166	LYS
1	B	167	ASP
1	B	168	LEU
1	B	172	ASN
1	B	191	LYS
1	B	194	ASN
1	B	213	TYR
1	B	222	LYS
1	B	223	HIS
1	B	277	THR
1	B	279	GLU
1	B	280	LYS
1	B	282	THR
1	B	285	ASN
1	B	286	THR
1	B	297	ARG
1	B	301	ARG
1	B	311	LYS
1	B	312	LYS
1	B	334	LYS
1	B	382	GLN
1	B	385	LYS

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Mol	Chain	Res	Type
1	B	406	GLU
1	B	412	CYS
1	B	440	ARG
1	C	3	ASP
1	C	12	ARG
1	C	20	LEU
1	C	52	LEU
1	C	59	VAL
1	C	66	GLU
1	C	67	ARG
1	C	79	LYS
1	C	98	VAL
1	C	103	ARG
1	C	125	ASN
1	C	139	LEU
1	C	155	GLN
1	C	161	LEU
1	C	163	SER
1	C	168	LEU
1	C	172	ASN
1	C	213	TYR
1	C	218	ILE
1	C	223	HIS
1	C	231	LYS
1	C	265	GLN
1	C	266	GLN
1	C	282	THR
1	C	290	VAL
1	C	297	ARG
1	C	301	ARG
1	C	303	GLN
1	C	311	LYS
1	C	312	LYS
1	C	313	GLN
1	C	369	ILE
1	C	402	GLN
1	C	405	LYS
1	C	461	GLU
1	C	471	LYS
1	C	486	GLN
1	D	8	GLU
1	D	12	ARG

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Mol	Chain	Res	Type
1	D	14	THR
1	D	20	LEU
1	D	52	LEU
1	D	58	LYS
1	D	103	ARG
1	D	108	ASN
1	D	139	LEU
1	D	155	GLN
1	D	161	LEU
1	D	167	ASP
1	D	168	LEU
1	D	178	ASN
1	D	194	ASN
1	D	207	LEU
1	D	208	ASN
1	D	213	TYR
1	D	231	LYS
1	D	256	LYS
1	D	282	THR
1	D	285	ASN
1	D	290	VAL
1	D	301	ARG
1	D	303	GLN
1	D	311	LYS
1	D	312	LYS
1	D	399	LEU
1	D	405	LYS
1	D	406	GLU
1	D	416	MET
1	D	418	GLN
1	D	424	LYS
1	D	442	SER
1	D	471	LYS
1	D	478	ARG
1	D	485	GLU
1	D	486	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	134	ASN
1	A	208	ASN
1	A	223	HIS
1	A	265	GLN
1	A	270	GLN
1	A	276	GLN
1	A	285	ASN
1	A	409	GLN
1	B	85	ASN
1	B	116	ASN
1	B	134	ASN
1	B	155	GLN
1	B	178	ASN
1	B	208	ASN
1	B	223	HIS
1	B	242	GLN
1	B	285	ASN
1	B	313	GLN
1	B	382	GLN
1	B	402	GLN
1	B	439	GLN
1	C	118	ASN
1	C	155	GLN
1	C	303	GLN
1	C	382	GLN
1	C	402	GLN
1	C	486	GLN
1	D	32	ASN
1	D	134	ASN
1	D	208	ASN
1	D	223	HIS
1	D	242	GLN
1	D	285	ASN
1	D	313	GLN
1	D	342	HIS
1	D	382	GLN
1	D	402	GLN
1	D	486	GLN

5.3.3 RNA (i)

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)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	NAG	B	488	1	14,14,15	0.45	0	17,19,21	1.52	1 (5%)
2	FAD	D	487	-	53,58,58	1.29	5 (9%)	68,89,89	1.56	11 (16%)
3	NAG	D	488	1	14,14,15	0.91	1 (7%)	17,19,21	1.92	4 (23%)
3	NAG	C	488	1	14,14,15	0.54	0	17,19,21	2.26	3 (17%)
2	FAD	B	487	-	53,58,58	1.16	5 (9%)	68,89,89	1.64	16 (23%)
2	FAD	A	487	-	53,58,58	1.23	5 (9%)	68,89,89	1.32	9 (13%)
2	FAD	C	487	-	53,58,58	1.19	4 (7%)	68,89,89	1.58	16 (23%)
3	NAG	A	488	1	14,14,15	0.42	0	17,19,21	1.89	2 (11%)

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
3	NAG	B	488	1	1/1/5/7	4/6/23/26	0/1/1/1
2	FAD	D	487	-	-	5/30/50/50	0/6/6/6
3	NAG	D	488	1	-	4/6/23/26	0/1/1/1
3	NAG	C	488	1	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	487	-	-	8/30/50/50	0/6/6/6
2	FAD	A	487	-	-	9/30/50/50	0/6/6/6
2	FAD	C	487	-	-	2/30/50/50	0/6/6/6
3	NAG	A	488	1	1/1/5/7	4/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	487	FAD	C2A-N3A	4.74	1.39	1.32
2	D	487	FAD	C4X-N5	4.73	1.39	1.30
2	A	487	FAD	C2A-N3A	4.70	1.39	1.32
2	A	487	FAD	C4X-N5	4.06	1.38	1.30
2	B	487	FAD	C2A-N3A	3.93	1.38	1.32
2	C	487	FAD	C2A-N3A	3.90	1.38	1.32
2	C	487	FAD	C4X-N5	3.68	1.37	1.30
2	B	487	FAD	C4X-N5	3.51	1.37	1.30
2	C	487	FAD	C2A-N1A	2.79	1.39	1.33
3	D	488	NAG	C1-C2	2.68	1.56	1.52
2	A	487	FAD	C10-N1	2.62	1.38	1.33
2	D	487	FAD	O4B-C4B	-2.49	1.39	1.45
2	B	487	FAD	C2A-N1A	2.42	1.38	1.33
2	A	487	FAD	C2A-N1A	2.38	1.38	1.33
2	B	487	FAD	C10-N1	2.38	1.38	1.33
2	C	487	FAD	C10-N1	2.33	1.38	1.33
2	A	487	FAD	O4B-C4B	-2.28	1.39	1.45
2	D	487	FAD	C2A-N1A	2.24	1.38	1.33
2	B	487	FAD	O4B-C4B	-2.18	1.40	1.45
2	D	487	FAD	C10-N1	2.05	1.37	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	488	NAG	C1-O5-C5	7.41	122.23	112.19
2	B	487	FAD	N3A-C2A-N1A	-6.81	118.04	128.68
2	D	487	FAD	N3A-C2A-N1A	-6.56	118.42	128.68
3	A	488	NAG	C1-O5-C5	6.46	120.95	112.19
2	C	487	FAD	N3A-C2A-N1A	-5.86	119.53	128.68
3	D	488	NAG	C1-O5-C5	5.71	119.92	112.19
2	A	487	FAD	N3A-C2A-N1A	-5.15	120.62	128.68
3	B	488	NAG	C1-O5-C5	4.73	118.60	112.19
3	D	488	NAG	C2-N2-C7	3.42	127.78	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	487	FAD	C4X-C10-N10	3.41	121.47	116.48
2	D	487	FAD	O4-C4-C4X	-3.22	118.05	126.60
2	C	487	FAD	C1B-N9A-C4A	-3.20	121.02	126.64
3	C	488	NAG	C3-C4-C5	3.20	115.94	110.24
2	B	487	FAD	C9A-C5X-N5	-3.04	119.13	122.43
2	B	487	FAD	O4B-C1B-C2B	-3.01	102.53	106.93
2	C	487	FAD	C4-N3-C2	-3.00	120.10	125.64
2	B	487	FAD	C10-C4X-N5	-2.95	118.59	124.86
2	C	487	FAD	C10-C4X-N5	-2.93	118.63	124.86
2	B	487	FAD	C4X-C10-N10	2.89	120.71	116.48
2	D	487	FAD	C4X-C4-N3	2.88	120.52	113.19
2	A	487	FAD	C9A-C5X-N5	-2.84	119.34	122.43
2	D	487	FAD	C4-N3-C2	-2.84	120.40	125.64
2	B	487	FAD	C4-N3-C2	-2.81	120.45	125.64
2	A	487	FAD	O4-C4-C4X	-2.73	119.36	126.60
3	C	488	NAG	O5-C5-C4	2.67	117.32	110.83
2	D	487	FAD	C4X-C10-N10	2.66	120.36	116.48
2	B	487	FAD	C5X-N5-C4X	2.61	122.41	118.07
2	A	487	FAD	C4X-C4-N3	2.59	119.77	113.19
2	C	487	FAD	C5'-C4'-C3'	-2.57	107.23	112.20
2	B	487	FAD	C5'-C4'-C3'	-2.55	107.28	112.20
2	C	487	FAD	C7M-C7-C6	-2.54	114.79	119.49
2	A	487	FAD	C4-N3-C2	-2.49	121.03	125.64
2	C	487	FAD	O3B-C3B-C4B	-2.48	103.89	111.05
2	B	487	FAD	C4X-C4-N3	2.48	119.48	113.19
2	C	487	FAD	O2-C2-N1	-2.47	117.73	121.83
2	D	487	FAD	C1B-N9A-C4A	-2.45	122.34	126.64
2	B	487	FAD	C4X-C10-N1	-2.44	119.06	124.73
2	D	487	FAD	C10-N1-C2	2.44	121.78	116.90
2	D	487	FAD	P-O3P-PA	-2.41	124.55	132.83
2	D	487	FAD	C9A-C5X-N5	-2.41	119.81	122.43
2	C	487	FAD	C4X-C10-N1	-2.38	119.20	124.73
2	A	487	FAD	C5X-C9A-N10	2.36	120.39	117.95
2	A	487	FAD	O4B-C1B-C2B	-2.35	103.48	106.93
3	D	488	NAG	O7-C7-C8	-2.34	117.71	122.06
2	C	487	FAD	C4-C4X-C10	2.28	120.63	116.79
2	B	487	FAD	C8M-C8-C9	-2.27	115.29	119.49
2	C	487	FAD	C8M-C8-C9	-2.22	115.38	119.49
3	A	488	NAG	O7-C7-C8	-2.16	118.05	122.06
2	D	487	FAD	C10-C4X-N5	-2.15	120.29	124.86
2	B	487	FAD	P-O3P-PA	-2.15	125.45	132.83
2	C	487	FAD	O4-C4-C4X	-2.13	120.95	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	487	FAD	C5X-C9A-N10	2.12	120.14	117.95
2	C	487	FAD	C5X-C9A-N10	2.11	120.13	117.95
2	B	487	FAD	C4-C4X-C10	2.10	120.33	116.79
2	B	487	FAD	C8M-C8-C7	-2.10	116.44	120.74
2	C	487	FAD	C4X-C4-N3	2.10	118.51	113.19
2	C	487	FAD	P-O3P-PA	-2.08	125.68	132.83
2	A	487	FAD	C4X-C10-N1	-2.08	119.91	124.73
2	A	487	FAD	P-O3P-PA	-2.06	125.77	132.83
3	D	488	NAG	C8-C7-N2	2.04	119.55	116.10
2	B	487	FAD	O5B-C5B-C4B	-2.02	102.03	108.99
2	B	487	FAD	C4-C4X-N5	2.00	121.08	118.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	488	NAG	C1
3	B	488	NAG	C1
3	C	488	NAG	C1

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	487	FAD	C5B-O5B-PA-O1A
2	B	487	FAD	C2'-C3'-C4'-C5'
2	B	487	FAD	O3'-C3'-C4'-C5'
2	C	487	FAD	PA-O3P-P-O5'
2	D	487	FAD	PA-O3P-P-O5'
3	B	488	NAG	C8-C7-N2-C2
3	B	488	NAG	O7-C7-N2-C2
3	D	488	NAG	C8-C7-N2-C2
3	D	488	NAG	O7-C7-N2-C2
3	A	488	NAG	C8-C7-N2-C2
3	A	488	NAG	O7-C7-N2-C2
3	A	488	NAG	O5-C5-C6-O6
3	C	488	NAG	O5-C5-C6-O6
2	B	487	FAD	O3'-C3'-C4'-O4'
2	B	487	FAD	C2'-C3'-C4'-O4'
3	B	488	NAG	O5-C5-C6-O6
3	A	488	NAG	C4-C5-C6-O6
3	C	488	NAG	C4-C5-C6-O6
3	D	488	NAG	C1-C2-N2-C7
3	B	488	NAG	C4-C5-C6-O6

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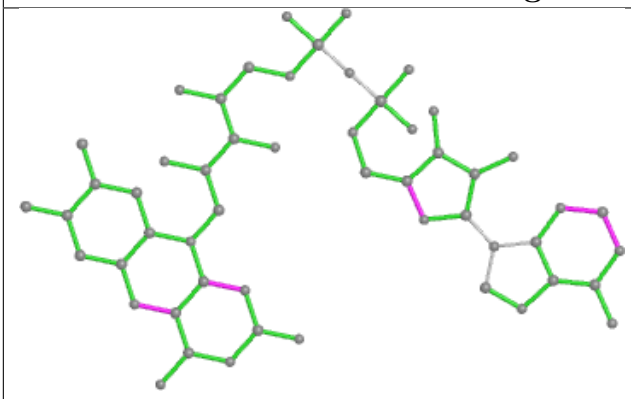
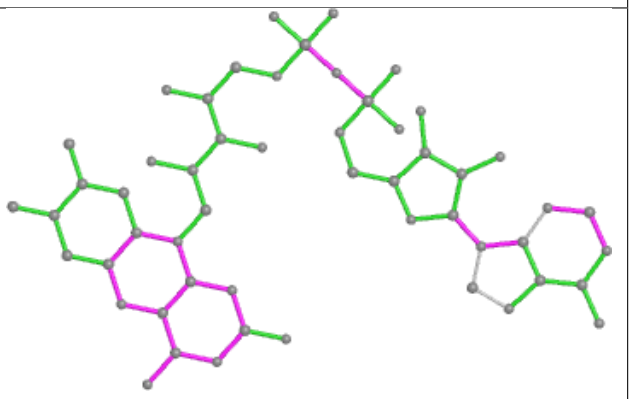
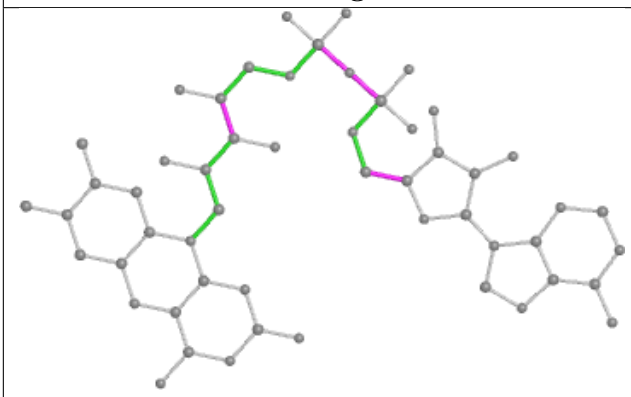
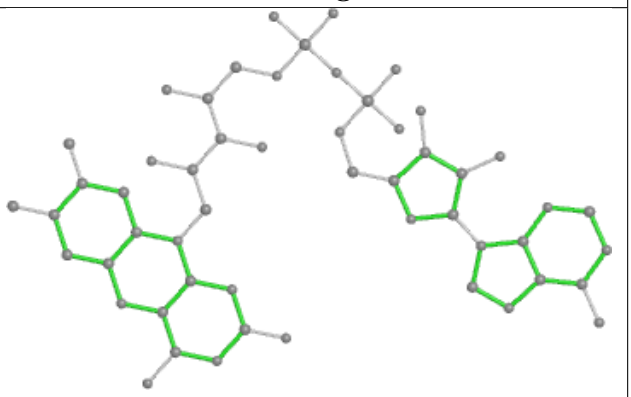
Mol	Chain	Res	Type	Atoms
3	C	488	NAG	C8-C7-N2-C2
3	C	488	NAG	O7-C7-N2-C2
2	A	487	FAD	O3'-C3'-C4'-C5'
2	A	487	FAD	C2'-C3'-C4'-O4'
2	B	487	FAD	P-O3P-PA-O1A
2	A	487	FAD	O3'-C3'-C4'-O4'
2	B	487	FAD	PA-O3P-P-O5'
2	A	487	FAD	O4B-C4B-C5B-O5B
2	D	487	FAD	C2'-C3'-C4'-C5'
2	A	487	FAD	C5B-O5B-PA-O2A
2	A	487	FAD	C2'-C3'-C4'-C5'
3	D	488	NAG	C3-C2-N2-C7
2	D	487	FAD	O4B-C4B-C5B-O5B
2	A	487	FAD	C3B-C4B-C5B-O5B
2	A	487	FAD	C5B-O5B-PA-O3P
2	B	487	FAD	O4B-C4B-C5B-O5B
2	B	487	FAD	P-O3P-PA-O2A
2	D	487	FAD	P-O3P-PA-O2A
2	C	487	FAD	O4B-C4B-C5B-O5B
2	D	487	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

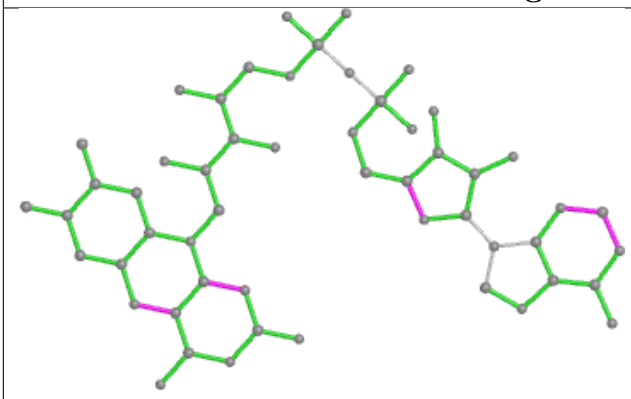
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	487	FAD	5	0
2	B	487	FAD	5	0
2	A	487	FAD	3	0
2	C	487	FAD	3	0

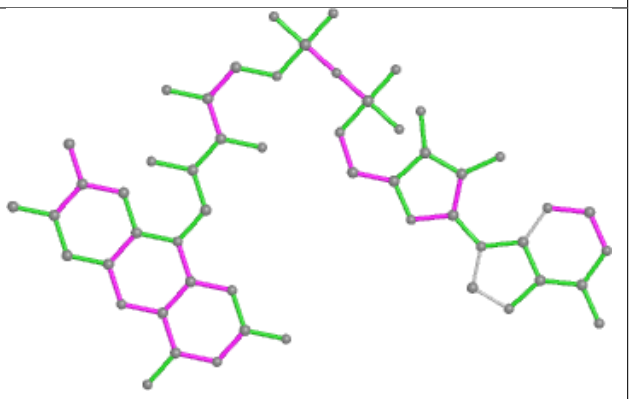
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FAD D 487	
 Bond lengths	 Bond angles
 Torsions	 Rings

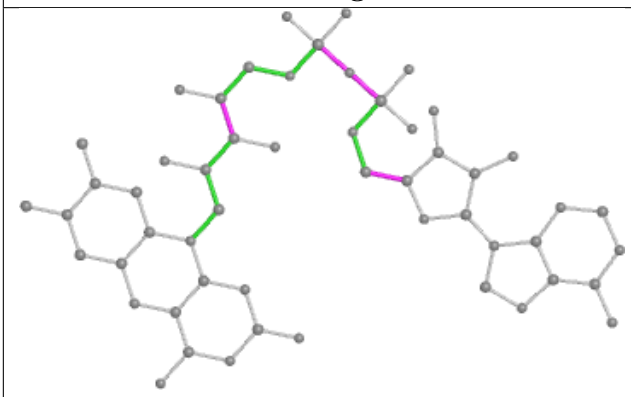
Ligand FAD B 487



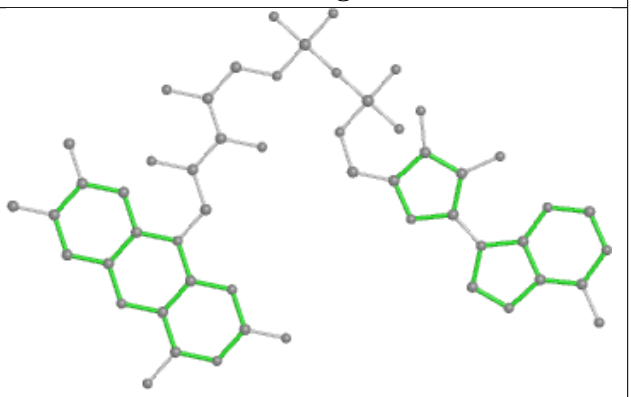
Bond lengths



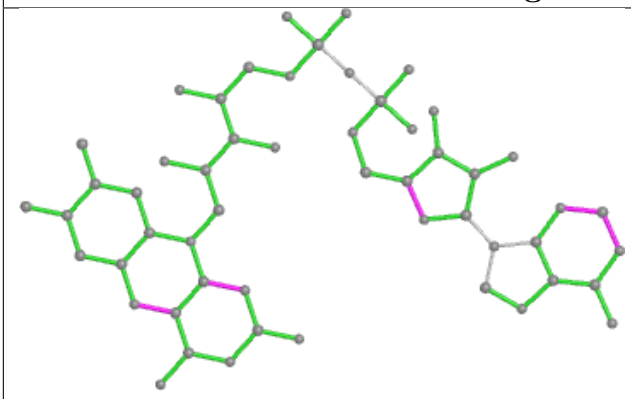
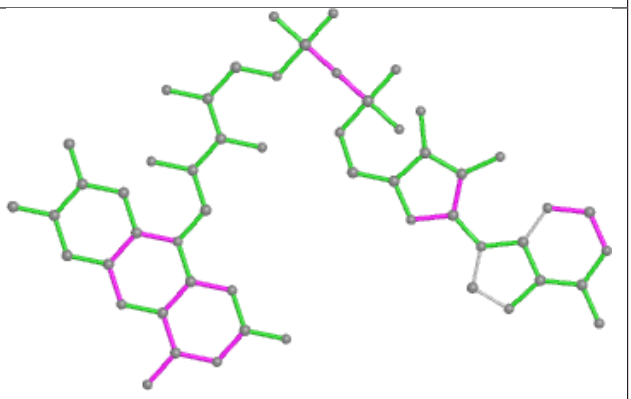
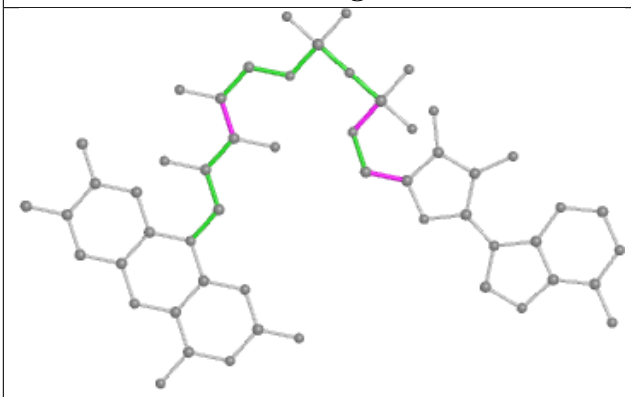
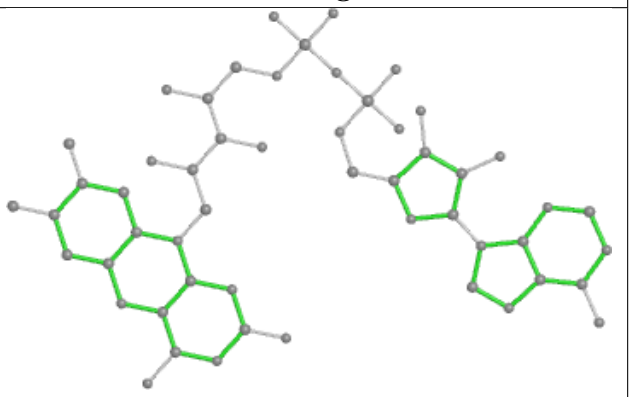
Bond angles



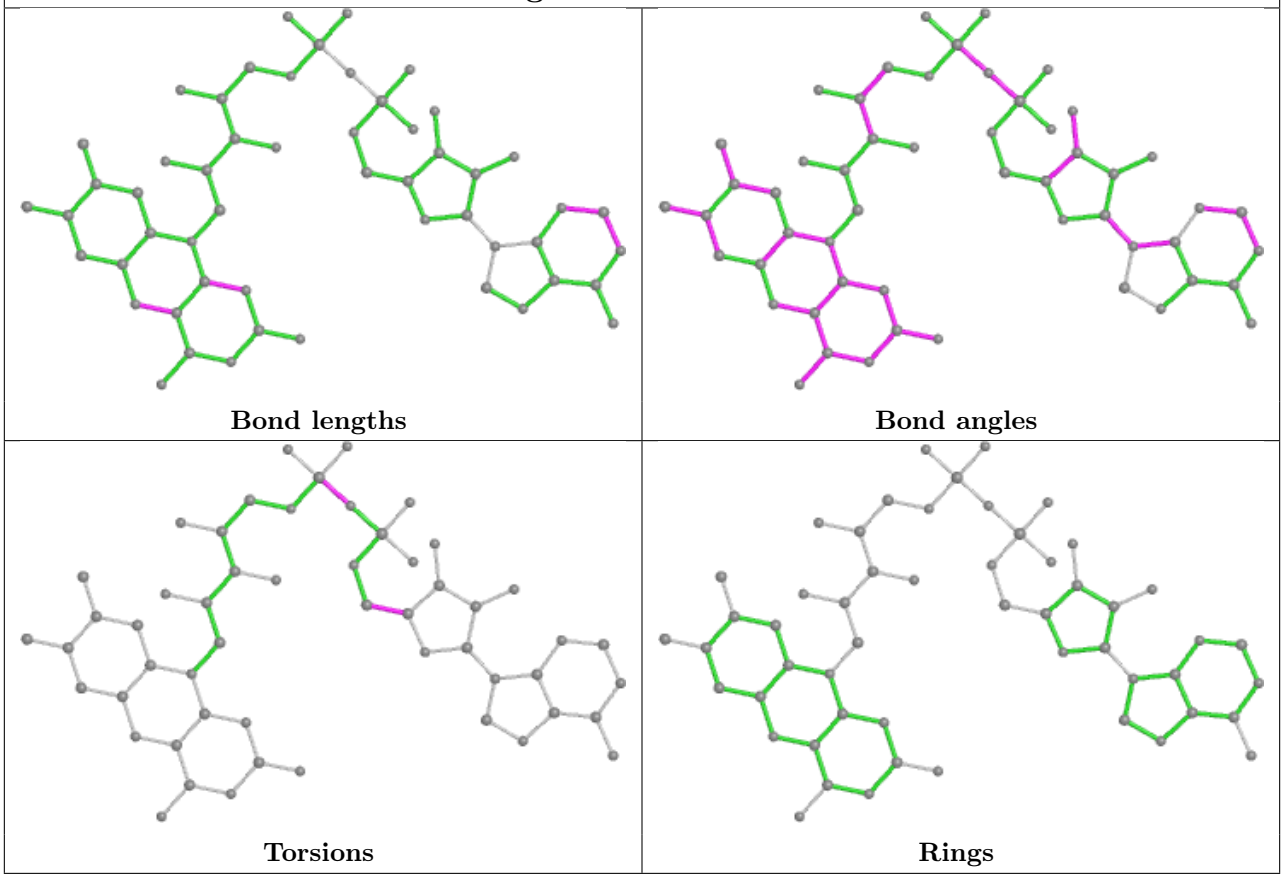
Torsions



Rings

Ligand FAD A 487	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD C 487



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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å^2)	Q<0.9
1	A	484/486 (99%)	-0.20	8 (1%)	70	67	5, 15, 33, 52	1 (0%)
1	B	484/486 (99%)	-0.17	8 (1%)	70	67	5, 17, 34, 46	3 (0%)
1	C	484/486 (99%)	-0.00	9 (1%)	66	64	8, 22, 38, 54	3 (0%)
1	D	484/486 (99%)	-0.08	5 (1%)	82	81	8, 18, 40, 52	1 (0%)
All	All	1936/1944 (99%)	-0.11	30 (1%)	73	71	5, 18, 38, 54	8 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	486	GLN	5.6
1	A	4	ARG	5.5
1	A	3	ASP	4.9
1	B	3	ASP	4.0
1	A	486	GLN	3.8
1	B	486	GLN	3.8
1	C	4	ARG	3.5
1	A	229	TYR	3.3
1	B	4	ARG	3.0
1	B	6	PRO	3.0
1	D	31	SER	2.9
1	D	3	ASP	2.9
1	C	485	GLU	2.9
1	D	278	PRO	2.7
1	C	278	PRO	2.6
1	C	31	SER	2.6
1	A	228	ALA	2.6
1	B	12	ARG	2.4
1	B	231	LYS	2.4
1	A	231	LYS	2.3
1	C	3	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	146	PRO	2.2
1	B	21	GLU	2.2
1	D	291	ILE	2.1
1	D	249	ARG	2.1
1	B	228	ALA	2.1
1	A	5	ASN	2.1
1	A	6	PRO	2.1
1	C	38	VAL	2.1
1	C	406	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.

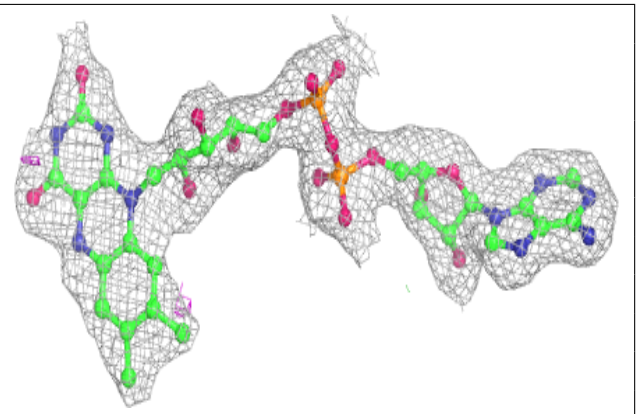
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	488	14/15	0.72	0.23	51,53,54,55	0
3	NAG	C	488	14/15	0.75	0.24	49,51,53,53	0
3	NAG	B	488	14/15	0.82	0.19	41,45,51,51	0
3	NAG	A	488	14/15	0.83	0.16	40,42,43,43	0
2	FAD	A	487	53/53	0.97	0.15	6,9,11,12	0
2	FAD	C	487	53/53	0.97	0.14	2,12,17,17	0
2	FAD	B	487	53/53	0.98	0.13	2,5,8,9	0
2	FAD	D	487	53/53	0.98	0.14	2,8,11,12	0
4	ZN	B	489	1/1	0.98	0.05	19,19,19,19	0
4	ZN	D	489	1/1	0.98	0.06	22,22,22,22	0
4	ZN	C	489	1/1	0.99	0.06	29,29,29,29	0
4	ZN	A	489	1/1	0.99	0.09	19,19,19,19	0

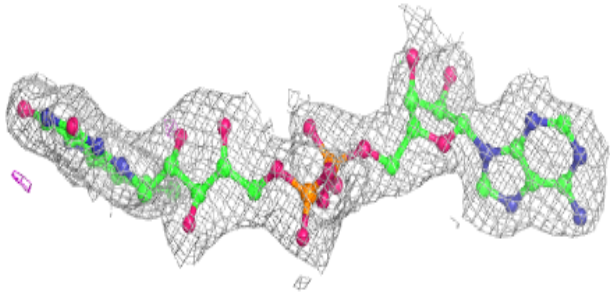
The following is a graphical depiction of the model fit to experimental electron density of all

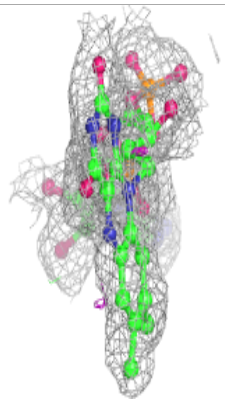
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 487:

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

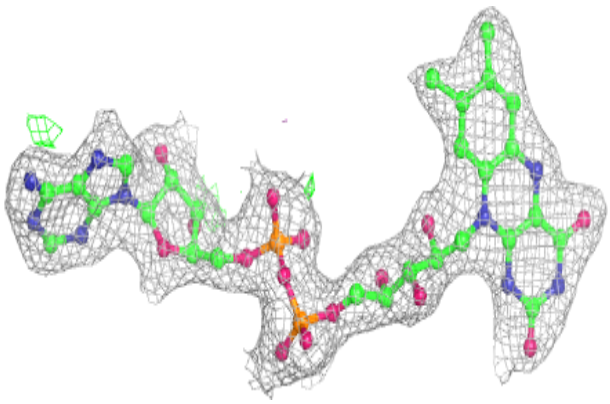


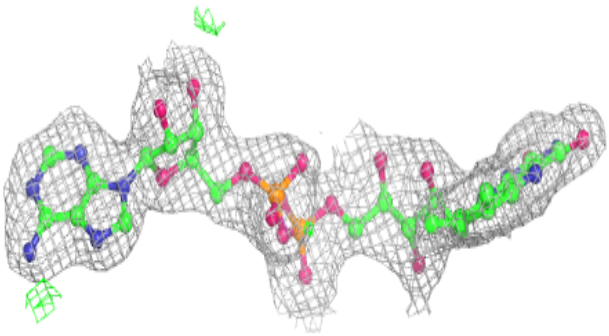


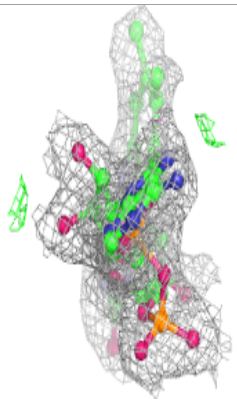


Electron density around FAD C 487:

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

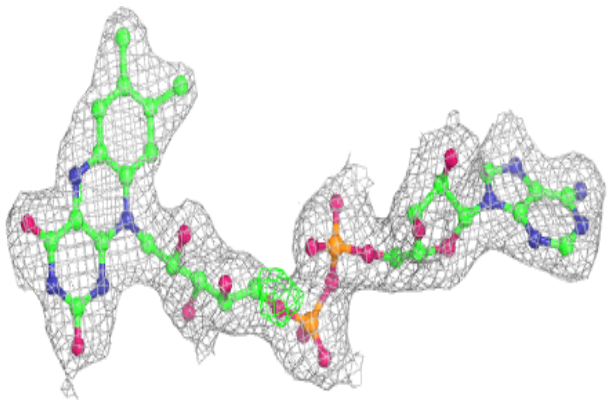


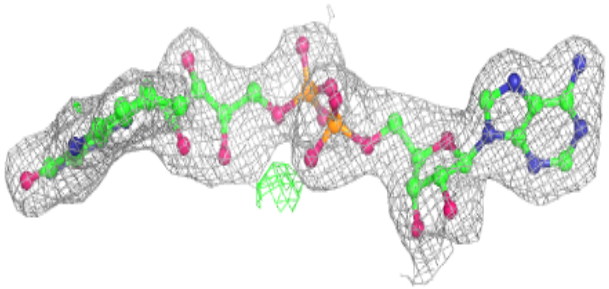


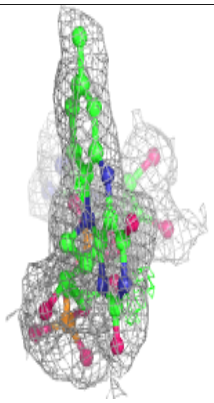


Electron density around FAD B 487:

$2mF_o$-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 D 487:

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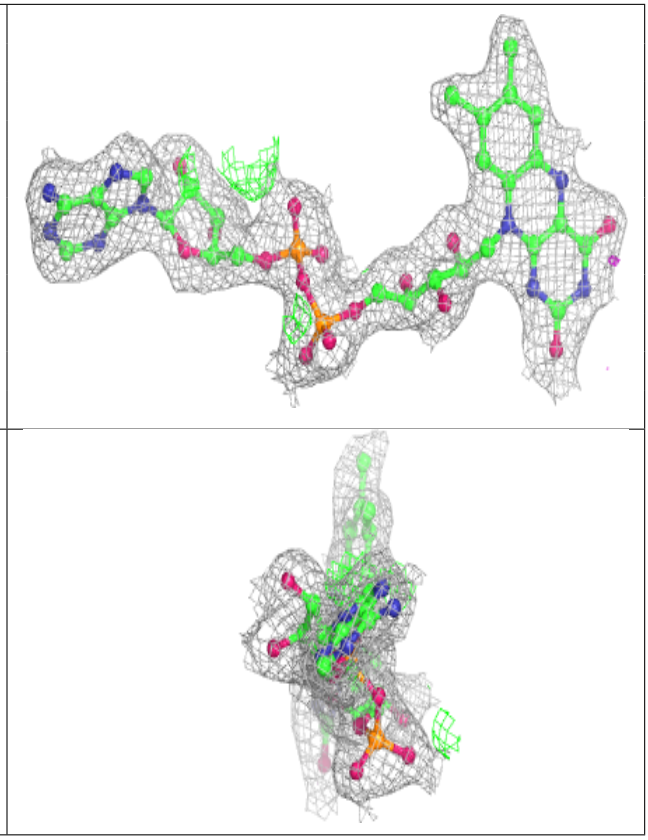
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.