



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:06 am BST

PDB ID : 4I59
Title : Cyclohexylamine Oxidase from *Brevibacterium oxydans* IH-35A complexed with cyclohexanone
Authors : Mirza, I.A.; Berghuis, A.M.
Deposited on : 2012-11-28
Resolution : 2.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

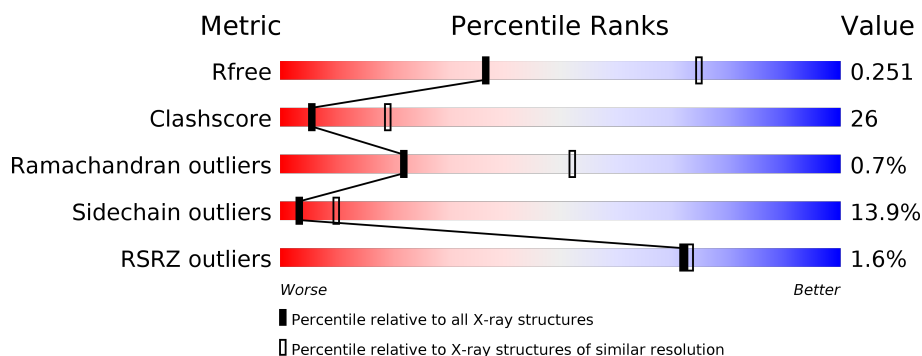
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. 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.

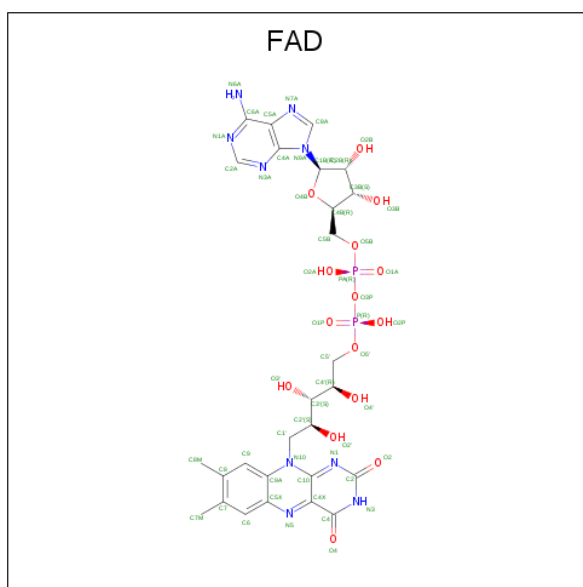
Mol	Chain	Length	Quality of chain
1	A	471	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>31%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	471	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>31%</div> <div>9%</div> <div>5%</div> </div> </div>
1	C	471	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>30%</div> <div>9%</div> <div>5%</div> </div> </div>
1	D	471	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>30%</div> <div>9%</div> <div>5%</div> </div> </div>

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 Cyclohexylamine Oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total 3432	C 2186	N 585	O 653	S 8	0	0	0
1	B	449	Total 3432	C 2186	N 585	O 653	S 8	0	0	0
1	C	449	Total 3432	C 2186	N 585	O 653	S 8	0	0	0
1	D	449	Total 3432	C 2186	N 585	O 653	S 8	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



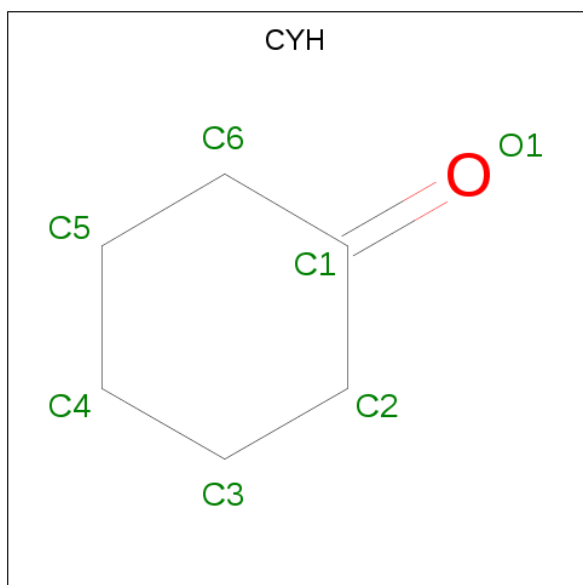
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

- Molecule 3 is CYCLOHEXANONE (three-letter code: CYH) (formula: C₆H₁₀O).

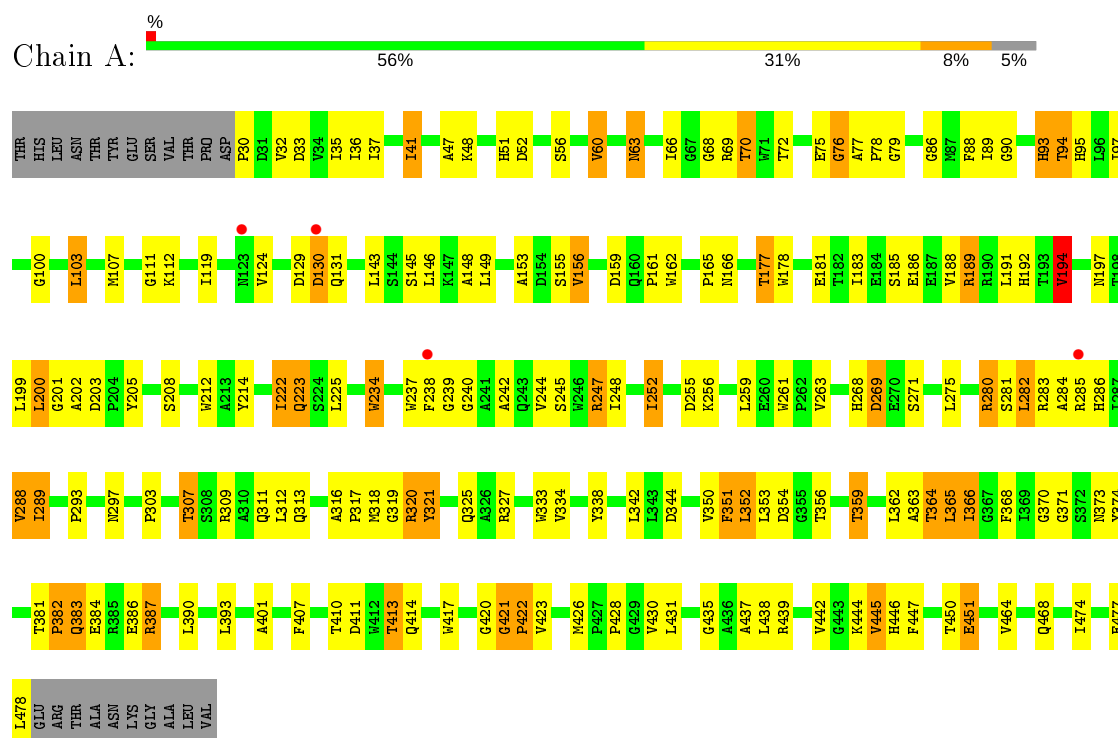


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	6	1		
3	B	1	Total	C	O	0	0
			7	6	1		
3	C	1	Total	C	O	0	0
			7	6	1		
3	D	1	Total	C	O	0	0
			7	6	1		

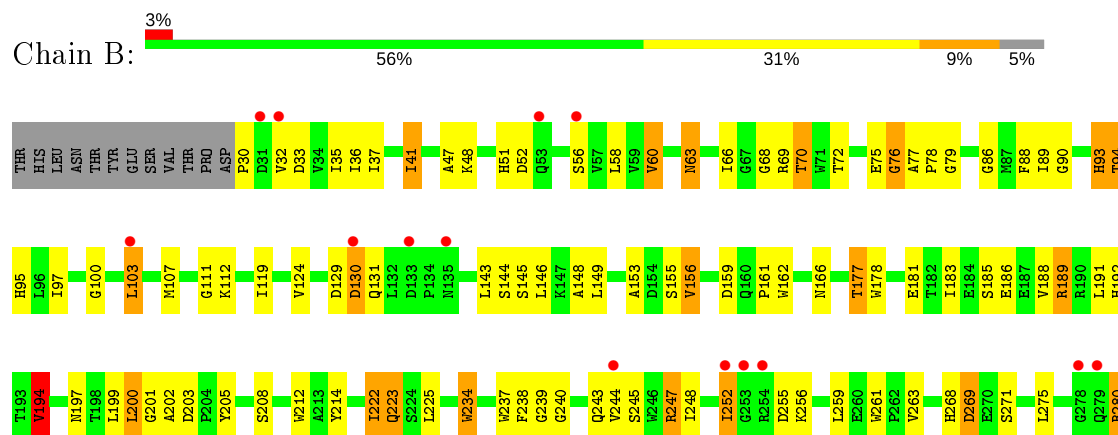
3 Residue-property plots [i](#)

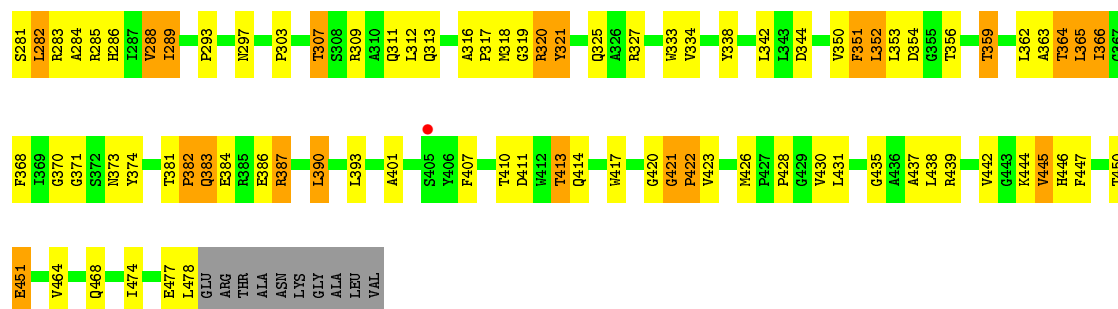
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Cyclohexylamine Oxidase



• Molecule 1: Cyclohexylamine Oxidase





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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.52Å 139.46Å 177.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.93 48.78 – 2.93	Depositor EDS
% Data completeness (in resolution range)	90.2 (48.78-2.93) 90.3 (48.78-2.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.86 (at 2.96Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.228 , 0.255 0.224 , 0.251	Depositor DCC
R_{free} test set	4488 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	1.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13968	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: CYH, 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	0.60	0/3526	0.84	4/4813 (0.1%)
1	B	0.60	0/3526	0.84	4/4813 (0.1%)
1	C	0.60	0/3526	0.84	4/4813 (0.1%)
1	D	0.60	0/3526	0.84	4/4813 (0.1%)
All	All	0.60	0/14104	0.84	16/19252 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	THR	N-CA-C	-5.83	95.25	111.00
1	A	70	THR	N-CA-C	-5.83	95.25	111.00
1	D	70	THR	N-CA-C	-5.83	95.25	111.00
1	C	70	THR	N-CA-C	-5.83	95.27	111.00
1	D	69	ARG	N-CA-C	-5.50	96.15	111.00
1	B	69	ARG	N-CA-C	-5.50	96.15	111.00
1	A	69	ARG	N-CA-C	-5.50	96.16	111.00
1	C	69	ARG	N-CA-C	-5.49	96.19	111.00
1	C	194	VAL	CB-CA-C	-5.37	101.20	111.40
1	D	194	VAL	CB-CA-C	-5.37	101.20	111.40
1	A	194	VAL	CB-CA-C	-5.37	101.21	111.40
1	B	194	VAL	CB-CA-C	-5.35	101.24	111.40
1	A	200	LEU	N-CA-C	-5.13	97.16	111.00
1	B	200	LEU	N-CA-C	-5.13	97.16	111.00
1	C	200	LEU	N-CA-C	-5.12	97.18	111.00
1	D	200	LEU	N-CA-C	-5.12	97.18	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3432	0	3293	176	0
1	B	3432	0	3293	178	0
1	C	3432	0	3293	177	0
1	D	3432	0	3293	179	0
2	A	53	0	31	6	0
2	B	53	0	31	5	0
2	C	53	0	31	5	0
2	D	53	0	31	5	0
3	A	7	0	10	0	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	D	7	0	10	0	0
All	All	13968	0	13336	698	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 26.

All (698) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:HD13	1:A:222:ILE:H	1.09	1.16
1:C:222:ILE:H	1:C:222:ILE:HD13	1.09	1.15
1:B:222:ILE:H	1:B:222:ILE:HD13	1.09	1.12
1:C:41:ILE:H	1:C:41:ILE:CD1	1.62	1.11
1:A:41:ILE:H	1:A:41:ILE:CD1	1.62	1.11
1:B:41:ILE:CD1	1:B:41:ILE:H	1.62	1.10
1:D:222:ILE:H	1:D:222:ILE:HD13	1.09	1.08
1:D:41:ILE:H	1:D:41:ILE:CD1	1.62	1.07
1:B:327:ARG:HG2	1:B:364:THR:HB	1.36	1.06
1:A:41:ILE:HD12	1:A:41:ILE:H	0.89	1.06
1:B:41:ILE:H	1:B:41:ILE:HD12	0.89	1.05
1:C:327:ARG:HG2	1:C:364:THR:HB	1.36	1.04
1:A:327:ARG:HG2	1:A:364:THR:HB	1.36	1.04
1:C:41:ILE:HD12	1:C:41:ILE:H	0.89	1.04
1:D:327:ARG:HG2	1:D:364:THR:HB	1.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ILE:H	1:D:41:ILE:HD12	0.89	1.02
1:A:41:ILE:HD12	1:A:41:ILE:N	1.74	1.02
1:B:41:ILE:HD12	1:B:41:ILE:N	1.74	1.01
1:C:41:ILE:HD12	1:C:41:ILE:N	1.74	1.00
1:D:41:ILE:N	1:D:41:ILE:HD12	1.74	1.00
1:D:321:TYR:H	1:D:413:THR:HG22	1.28	0.98
1:B:321:TYR:H	1:B:413:THR:HG22	1.28	0.97
1:C:321:TYR:H	1:C:413:THR:HG22	1.28	0.96
1:C:222:ILE:N	1:C:222:ILE:HD13	1.78	0.95
1:A:222:ILE:H	1:A:222:ILE:CD1	1.80	0.95
1:B:222:ILE:HD13	1:B:222:ILE:N	1.78	0.95
1:B:222:ILE:H	1:B:222:ILE:CD1	1.80	0.95
1:A:321:TYR:H	1:A:413:THR:HG22	1.28	0.94
1:C:222:ILE:CD1	1:C:222:ILE:H	1.80	0.94
1:D:222:ILE:CD1	1:D:222:ILE:H	1.80	0.93
1:A:222:ILE:N	1:A:222:ILE:HD13	1.78	0.93
1:D:222:ILE:HD13	1:D:222:ILE:N	1.78	0.92
1:B:289:ILE:O	1:B:289:ILE:HD13	1.70	0.92
1:D:289:ILE:O	1:D:289:ILE:HD13	1.70	0.92
1:C:293:PRO:HD3	1:C:451:GLU:HG3	1.52	0.91
1:B:293:PRO:HD3	1:B:451:GLU:HG3	1.52	0.91
1:A:289:ILE:O	1:A:289:ILE:HD13	1.70	0.91
1:C:289:ILE:O	1:C:289:ILE:HD13	1.70	0.90
1:A:366:ILE:HD11	1:A:368:PHE:CE1	2.07	0.89
1:B:366:ILE:HD11	1:B:368:PHE:CE1	2.07	0.89
1:C:366:ILE:HD11	1:C:368:PHE:CE1	2.07	0.89
1:D:366:ILE:HD11	1:D:368:PHE:CE1	2.07	0.89
1:A:311:GLN:HE22	1:D:320:ARG:CZ	1.86	0.88
1:A:293:PRO:HD3	1:A:451:GLU:HG3	1.52	0.88
1:D:293:PRO:HD3	1:D:451:GLU:HG3	1.52	0.88
1:B:327:ARG:CG	1:B:364:THR:HB	2.07	0.84
1:C:413:THR:HA	1:C:420:GLY:HA2	1.58	0.84
1:A:327:ARG:CG	1:A:364:THR:HB	2.07	0.84
1:D:327:ARG:CG	1:D:364:THR:HB	2.07	0.84
1:C:327:ARG:CG	1:C:364:THR:HB	2.07	0.84
1:A:413:THR:HA	1:A:420:GLY:HA2	1.58	0.83
1:B:177:THR:O	1:B:181:GLU:HG3	1.79	0.83
1:D:177:THR:O	1:D:181:GLU:HG3	1.79	0.83
1:A:177:THR:O	1:A:181:GLU:HG3	1.79	0.82
1:D:413:THR:HA	1:D:420:GLY:HA2	1.58	0.82
1:B:413:THR:HA	1:B:420:GLY:HA2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:O	1:A:478:LEU:HD13	1.80	0.82
1:C:177:THR:O	1:C:181:GLU:HG3	1.79	0.82
1:C:474:ILE:O	1:C:478:LEU:HD13	1.80	0.82
1:B:474:ILE:O	1:B:478:LEU:HD13	1.80	0.81
1:D:474:ILE:O	1:D:478:LEU:HD13	1.80	0.81
1:A:321:TYR:HB2	1:A:421:GLY:HA2	1.64	0.80
1:D:321:TYR:HB2	1:D:421:GLY:HA2	1.63	0.79
1:B:321:TYR:HB2	1:B:421:GLY:HA2	1.64	0.79
1:A:350:VAL:HG23	1:A:368:PHE:O	1.83	0.79
1:A:119:ILE:HD12	1:A:124:VAL:HG22	1.65	0.79
1:B:350:VAL:HG23	1:B:368:PHE:O	1.83	0.78
1:D:350:VAL:HG23	1:D:368:PHE:O	1.83	0.78
1:C:321:TYR:HB2	1:C:421:GLY:HA2	1.64	0.78
1:D:119:ILE:HD12	1:D:124:VAL:HG22	1.65	0.78
1:B:119:ILE:HD12	1:B:124:VAL:HG22	1.65	0.78
1:C:350:VAL:HG23	1:C:368:PHE:O	1.83	0.78
1:C:119:ILE:HD12	1:C:124:VAL:HG22	1.65	0.77
1:D:36:ILE:HG13	1:D:288:VAL:HG13	1.69	0.75
1:B:311:GLN:HE22	1:C:320:ARG:CZ	1.99	0.75
1:B:36:ILE:HG13	1:B:288:VAL:HG13	1.69	0.74
1:C:321:TYR:N	1:C:413:THR:HG22	2.03	0.73
1:A:36:ILE:HG13	1:A:288:VAL:HG13	1.69	0.73
1:D:95:HIS:HD2	1:D:468:GLN:OE1	1.72	0.72
1:C:36:ILE:HG13	1:C:288:VAL:HG13	1.69	0.72
1:C:383:GLN:H	1:C:383:GLN:CD	1.93	0.72
1:A:383:GLN:CD	1:A:383:GLN:H	1.93	0.72
1:C:95:HIS:HD2	1:C:468:GLN:OE1	1.72	0.72
1:B:320:ARG:CZ	1:C:311:GLN:HE22	2.03	0.72
1:B:383:GLN:CD	1:B:383:GLN:H	1.93	0.72
1:D:383:GLN:CD	1:D:383:GLN:H	1.93	0.72
1:A:95:HIS:HD2	1:A:468:GLN:OE1	1.72	0.72
1:B:95:HIS:HD2	1:B:468:GLN:OE1	1.72	0.71
1:D:321:TYR:N	1:D:413:THR:HG22	2.03	0.71
1:A:321:TYR:N	1:A:413:THR:HG22	2.03	0.70
1:B:321:TYR:N	1:B:413:THR:HG22	2.03	0.70
1:D:477:GLU:C	1:D:478:LEU:HD12	2.12	0.70
1:A:477:GLU:C	1:A:478:LEU:HD12	2.12	0.69
1:C:477:GLU:C	1:C:478:LEU:HD12	2.12	0.69
1:A:464:VAL:O	1:A:468:GLN:HG3	1.93	0.69
1:D:464:VAL:O	1:D:468:GLN:HG3	1.93	0.69
1:B:477:GLU:C	1:B:478:LEU:HD12	2.12	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:VAL:O	1:C:468:GLN:HG3	1.93	0.69
1:B:464:VAL:O	1:B:468:GLN:HG3	1.93	0.69
1:B:100:GLY:HA3	1:B:237:TRP:CH2	2.29	0.68
1:C:41:ILE:CD1	1:C:41:ILE:N	2.42	0.68
1:A:90:GLY:H	1:A:93:HIS:CD2	2.12	0.68
1:B:381:THR:HB	1:B:383:GLN:HE21	1.59	0.67
1:B:90:GLY:H	1:B:93:HIS:CD2	2.12	0.67
1:D:90:GLY:H	1:D:93:HIS:CD2	2.12	0.67
1:C:100:GLY:HA3	1:C:237:TRP:CH2	2.29	0.67
1:A:442:VAL:O	1:A:445:VAL:HG13	1.95	0.67
1:B:238:PHE:CE1	1:B:359:THR:HG21	2.30	0.67
1:D:244:VAL:O	1:D:248:ILE:HG12	1.94	0.67
1:D:381:THR:HB	1:D:383:GLN:HE21	1.59	0.67
1:A:244:VAL:O	1:A:248:ILE:HG12	1.95	0.67
1:A:381:THR:HB	1:A:383:GLN:HE21	1.59	0.67
1:A:100:GLY:HA3	1:A:237:TRP:CH2	2.29	0.67
1:A:238:PHE:CE1	1:A:359:THR:HG21	2.30	0.67
1:A:63:ASN:HB3	1:A:417:TRP:NE1	2.10	0.67
1:D:63:ASN:HB3	1:D:417:TRP:NE1	2.10	0.67
1:C:244:VAL:O	1:C:248:ILE:HG12	1.95	0.66
1:C:90:GLY:H	1:C:93:HIS:CD2	2.12	0.66
1:B:244:VAL:O	1:B:248:ILE:HG12	1.95	0.66
1:C:238:PHE:CE1	1:C:359:THR:HG21	2.30	0.66
1:C:442:VAL:O	1:C:445:VAL:HG13	1.95	0.66
1:D:100:GLY:HA3	1:D:237:TRP:CH2	2.29	0.66
1:D:366:ILE:HD11	1:D:368:PHE:CZ	2.31	0.66
1:A:366:ILE:HD11	1:A:368:PHE:CZ	2.31	0.66
1:C:381:THR:HB	1:C:383:GLN:HE21	1.59	0.66
1:C:63:ASN:HB3	1:C:417:TRP:NE1	2.10	0.66
1:D:238:PHE:CE1	1:D:359:THR:HG21	2.30	0.66
1:D:442:VAL:O	1:D:445:VAL:HG13	1.95	0.66
1:B:442:VAL:O	1:B:445:VAL:HG13	1.95	0.66
1:C:77:ALA:HB1	1:C:78:PRO:HD2	1.78	0.66
1:B:77:ALA:HB1	1:B:78:PRO:HD2	1.78	0.66
1:C:333:TRP:CE2	1:C:365:LEU:HD13	2.31	0.66
1:D:156:VAL:HG23	1:D:161:PRO:HA	1.78	0.65
1:A:333:TRP:CE2	1:A:365:LEU:HD13	2.31	0.65
1:C:156:VAL:HG23	1:C:161:PRO:HA	1.78	0.65
1:A:77:ALA:HB1	1:A:78:PRO:HD2	1.78	0.65
1:B:366:ILE:HD11	1:B:368:PHE:CZ	2.31	0.65
1:B:63:ASN:HB3	1:B:417:TRP:NE1	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:HG23	1:A:161:PRO:HA	1.78	0.65
1:B:333:TRP:CE2	1:B:365:LEU:HD13	2.31	0.65
1:C:366:ILE:HD11	1:C:368:PHE:CZ	2.31	0.65
1:D:333:TRP:CE2	1:D:365:LEU:HD13	2.31	0.64
1:B:156:VAL:HG23	1:B:161:PRO:HA	1.78	0.64
1:C:426:MET:HB3	1:C:430:VAL:CG2	2.27	0.64
1:D:426:MET:HB3	1:D:430:VAL:CG2	2.27	0.64
1:D:77:ALA:HB1	1:D:78:PRO:HD2	1.78	0.64
1:B:426:MET:HB3	1:B:430:VAL:CG2	2.27	0.64
1:A:320:ARG:CZ	1:D:311:GLN:HE22	2.11	0.63
1:A:426:MET:HB3	1:A:430:VAL:CG2	2.27	0.63
1:D:41:ILE:N	1:D:41:ILE:CD1	2.42	0.63
1:B:289:ILE:HD13	1:B:289:ILE:C	2.18	0.63
1:A:289:ILE:HD13	1:A:289:ILE:C	2.18	0.63
1:D:289:ILE:C	1:D:289:ILE:HD13	2.18	0.63
1:C:289:ILE:C	1:C:289:ILE:HD13	2.18	0.62
1:D:145:SER:OG	1:D:192:HIS:HE1	1.82	0.62
1:A:145:SER:OG	1:A:192:HIS:HE1	1.82	0.62
1:B:145:SER:OG	1:B:192:HIS:HE1	1.82	0.61
1:C:350:VAL:HG22	1:C:351:PHE:N	2.15	0.61
1:C:430:VAL:HG23	1:C:431:LEU:H	1.66	0.61
1:A:350:VAL:HG22	1:A:351:PHE:N	2.15	0.61
1:A:430:VAL:HG23	1:A:431:LEU:H	1.66	0.61
1:C:145:SER:OG	1:C:192:HIS:HE1	1.82	0.61
1:D:293:PRO:HD3	1:D:451:GLU:CG	2.30	0.61
1:A:311:GLN:HE22	1:D:320:ARG:NE	1.97	0.61
1:D:350:VAL:HG22	1:D:351:PHE:N	2.15	0.61
1:D:430:VAL:HG23	1:D:431:LEU:H	1.66	0.61
1:B:41:ILE:CD1	1:B:41:ILE:N	2.42	0.61
1:B:430:VAL:HG23	1:B:431:LEU:H	1.65	0.61
1:B:350:VAL:HG22	1:B:351:PHE:N	2.15	0.60
1:D:112:LYS:NZ	1:D:354:ASP:OD2	2.33	0.60
1:A:318:MET:O	1:A:320:ARG:NH2	2.34	0.60
1:B:155:SER:HB2	1:B:166:ASN:HD21	1.66	0.60
1:D:155:SER:HB2	1:D:166:ASN:HD21	1.66	0.60
1:B:318:MET:O	1:B:320:ARG:NH2	2.34	0.60
1:C:319:GLY:O	1:C:421:GLY:N	2.32	0.60
1:B:66:ILE:HD11	1:B:259:LEU:HD21	1.84	0.60
1:C:318:MET:O	1:C:320:ARG:NH2	2.34	0.60
1:A:89:ILE:O	1:A:234:TRP:HD1	1.85	0.60
1:A:112:LYS:NZ	1:A:354:ASP:OD2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HD11	1:A:259:LEU:HD21	1.84	0.60
1:D:89:ILE:O	1:D:234:TRP:HD1	1.85	0.60
1:A:63:ASN:HB3	1:A:417:TRP:CD1	2.37	0.59
1:D:318:MET:O	1:D:320:ARG:NH2	2.34	0.59
1:D:63:ASN:HB3	1:D:417:TRP:CD1	2.37	0.59
1:C:155:SER:HB2	1:C:166:ASN:HD21	1.66	0.59
1:B:293:PRO:HD3	1:B:451:GLU:CG	2.30	0.59
1:B:89:ILE:O	1:B:234:TRP:HD1	1.85	0.59
1:C:66:ILE:HD11	1:C:259:LEU:HD21	1.84	0.59
1:B:112:LYS:NZ	1:B:354:ASP:OD2	2.33	0.59
1:A:155:SER:HB2	1:A:166:ASN:HD21	1.66	0.59
1:C:112:LYS:NZ	1:C:354:ASP:OD2	2.33	0.59
1:C:183:ILE:HB	1:C:189:ARG:HD3	1.85	0.59
1:B:63:ASN:HB3	1:B:417:TRP:CD1	2.37	0.59
1:C:89:ILE:O	1:C:234:TRP:HD1	1.85	0.59
1:D:183:ILE:HB	1:D:189:ARG:HD3	1.85	0.59
1:D:286:HIS:HD2	1:D:446:HIS:HE1	1.51	0.59
1:A:183:ILE:HB	1:A:189:ARG:HD3	1.85	0.58
1:A:387:ARG:NH1	1:A:387:ARG:HB2	2.18	0.58
1:B:183:ILE:HB	1:B:189:ARG:HD3	1.85	0.58
1:C:63:ASN:HB3	1:C:417:TRP:CD1	2.37	0.58
1:B:420:GLY:O	1:B:421:GLY:O	2.21	0.58
1:C:286:HIS:HD2	1:C:446:HIS:HE1	1.51	0.58
1:C:420:GLY:O	1:C:421:GLY:O	2.21	0.58
1:B:197:ASN:HA	1:B:202:ALA:O	2.04	0.58
1:B:286:HIS:HD2	1:B:446:HIS:HE1	1.51	0.58
1:A:197:ASN:HA	1:A:202:ALA:O	2.04	0.58
1:B:261:TRP:CZ2	1:B:282:LEU:HD22	2.39	0.58
1:D:197:ASN:HA	1:D:202:ALA:O	2.04	0.58
1:D:261:TRP:CZ2	1:D:282:LEU:HD22	2.39	0.58
1:D:420:GLY:O	1:D:421:GLY:O	2.21	0.58
1:D:66:ILE:HD11	1:D:259:LEU:HD21	1.84	0.58
1:D:387:ARG:NH1	1:D:387:ARG:HB2	2.18	0.58
1:A:261:TRP:CZ2	1:A:282:LEU:HD22	2.39	0.58
1:A:286:HIS:HD2	1:A:446:HIS:HE1	1.51	0.58
1:C:261:TRP:CZ2	1:C:282:LEU:HD22	2.39	0.58
1:C:387:ARG:HB2	1:C:387:ARG:NH1	2.18	0.58
1:D:86:GLY:HA2	2:D:501:FAD:N5	2.19	0.58
1:B:319:GLY:O	1:B:421:GLY:N	2.32	0.58
1:B:86:GLY:HA2	2:B:501:FAD:N5	2.19	0.58
1:D:366:ILE:O	1:D:366:ILE:HD13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASN:HA	1:C:202:ALA:O	2.03	0.57
1:A:319:GLY:O	1:A:421:GLY:N	2.32	0.57
1:A:420:GLY:O	1:A:421:GLY:O	2.21	0.57
1:C:86:GLY:HA2	2:C:501:FAD:N5	2.19	0.57
1:A:478:LEU:N	1:A:478:LEU:HD12	2.20	0.57
1:C:478:LEU:N	1:C:478:LEU:HD12	2.20	0.57
1:A:366:ILE:HD13	1:A:366:ILE:O	2.04	0.57
1:A:86:GLY:HA2	2:A:501:FAD:N5	2.19	0.57
1:B:268:HIS:CD2	1:B:303:PRO:HD2	2.40	0.57
1:B:366:ILE:HD13	1:B:366:ILE:O	2.04	0.57
1:B:387:ARG:NH1	1:B:387:ARG:HB2	2.18	0.57
1:C:366:ILE:HD13	1:C:366:ILE:O	2.04	0.57
1:B:430:VAL:HG23	1:B:431:LEU:N	2.20	0.57
1:D:319:GLY:O	1:D:421:GLY:N	2.32	0.57
1:A:47:ALA:O	1:A:252:ILE:HD11	2.05	0.57
1:A:430:VAL:HG23	1:A:431:LEU:N	2.20	0.57
1:D:268:HIS:CD2	1:D:303:PRO:HD2	2.40	0.57
1:C:47:ALA:O	1:C:252:ILE:HD11	2.05	0.56
1:C:293:PRO:HD3	1:C:451:GLU:CG	2.30	0.56
1:B:478:LEU:N	1:B:478:LEU:HD12	2.20	0.56
1:B:47:ALA:O	1:B:252:ILE:HD11	2.05	0.56
1:A:381:THR:OG1	1:A:384:GLU:HG3	2.05	0.56
1:B:381:THR:OG1	1:B:384:GLU:HG3	2.05	0.56
1:C:268:HIS:CD2	1:C:303:PRO:HD2	2.40	0.56
1:A:129:ASP:O	1:A:131:GLN:HG2	2.06	0.56
1:B:129:ASP:O	1:B:131:GLN:HG2	2.06	0.56
1:C:430:VAL:HG23	1:C:431:LEU:N	2.20	0.56
1:A:268:HIS:CD2	1:A:303:PRO:HD2	2.40	0.56
1:D:129:ASP:O	1:D:131:GLN:HG2	2.06	0.56
1:D:430:VAL:HG23	1:D:431:LEU:N	2.20	0.56
1:C:129:ASP:O	1:C:131:GLN:HG2	2.06	0.56
1:C:381:THR:OG1	1:C:384:GLU:HG3	2.05	0.56
1:D:381:THR:OG1	1:D:384:GLU:HG3	2.05	0.56
1:B:411:ASP:CG	1:B:414:GLN:HG2	2.27	0.55
1:D:47:ALA:O	1:D:252:ILE:HD11	2.05	0.55
1:D:478:LEU:N	1:D:478:LEU:HD12	2.20	0.55
1:B:222:ILE:CD1	1:B:222:ILE:N	2.50	0.55
1:C:411:ASP:CG	1:C:414:GLN:HG2	2.27	0.55
1:A:293:PRO:HD3	1:A:451:GLU:CG	2.30	0.55
1:D:411:ASP:CG	1:D:414:GLN:HG2	2.27	0.55
1:A:289:ILE:HD12	1:A:447:PHE:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:HD12	1:B:447:PHE:CD2	2.42	0.55
1:C:68:GLY:C	1:C:70:THR:H	2.09	0.55
1:B:185:SER:HB3	1:B:188:VAL:HG23	1.89	0.54
1:D:185:SER:HB3	1:D:188:VAL:HG23	1.89	0.54
1:C:48:LYS:HA	1:C:252:ILE:HD11	1.90	0.54
1:D:334:VAL:HA	1:D:338:TYR:O	2.08	0.54
1:A:185:SER:HB3	1:A:188:VAL:HG23	1.89	0.54
1:C:334:VAL:HA	1:C:338:TYR:O	2.08	0.54
1:A:48:LYS:HA	1:A:252:ILE:HD11	1.90	0.54
1:A:411:ASP:CG	1:A:414:GLN:HG2	2.27	0.54
1:C:289:ILE:HD12	1:C:447:PHE:CD2	2.42	0.54
1:B:334:VAL:HA	1:B:338:TYR:O	2.08	0.54
1:D:289:ILE:HD12	1:D:447:PHE:CD2	2.42	0.54
1:A:100:GLY:HA3	1:A:237:TRP:CZ2	2.42	0.54
1:B:100:GLY:HA3	1:B:237:TRP:CZ2	2.42	0.54
1:B:103:LEU:HG	1:B:247:ARG:HB3	1.90	0.54
1:B:48:LYS:HA	1:B:252:ILE:HD11	1.90	0.54
1:D:100:GLY:HA3	1:D:237:TRP:CZ2	2.42	0.54
1:D:297:ASN:HB2	1:D:313:GLN:HB3	1.90	0.54
1:B:223:GLN:HA	1:B:223:GLN:NE2	2.23	0.54
1:C:51:HIS:CG	1:C:252:ILE:HG12	2.43	0.54
1:C:103:LEU:HG	1:C:247:ARG:HB3	1.90	0.53
1:D:223:GLN:HA	1:D:223:GLN:NE2	2.23	0.53
1:D:35:ILE:HG13	1:D:284:ALA:HB2	1.90	0.53
1:A:51:HIS:CG	1:A:252:ILE:HG12	2.44	0.53
1:C:51:HIS:CD2	1:C:252:ILE:HG12	2.44	0.53
1:D:350:VAL:CG2	1:D:351:PHE:N	2.72	0.53
1:C:100:GLY:HA3	1:C:237:TRP:CZ2	2.42	0.53
1:D:51:HIS:CD2	1:D:252:ILE:HG12	2.44	0.53
1:B:51:HIS:CD2	1:B:252:ILE:HG12	2.44	0.53
1:D:51:HIS:CG	1:D:252:ILE:HG12	2.43	0.53
1:A:297:ASN:HB2	1:A:313:GLN:HB3	1.90	0.53
1:A:223:GLN:HA	1:A:223:GLN:NE2	2.23	0.53
1:A:334:VAL:HA	1:A:338:TYR:O	2.08	0.53
1:D:103:LEU:HG	1:D:247:ARG:HB3	1.90	0.53
1:D:48:LYS:HA	1:D:252:ILE:HD11	1.90	0.53
1:A:51:HIS:CD2	1:A:252:ILE:HG12	2.44	0.53
1:B:350:VAL:CG2	1:B:351:PHE:N	2.72	0.53
1:D:197:ASN:OD1	1:D:371:GLY:HA3	2.09	0.53
1:A:197:ASN:OD1	1:A:371:GLY:HA3	2.09	0.53
1:C:185:SER:HB3	1:C:188:VAL:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:VAL:CG2	1:C:351:PHE:N	2.72	0.53
1:A:103:LEU:HG	1:A:247:ARG:HB3	1.90	0.52
1:B:197:ASN:OD1	1:B:371:GLY:HA3	2.09	0.52
1:D:189:ARG:HH11	1:D:189:ARG:HG2	1.74	0.52
1:B:297:ASN:HB2	1:B:313:GLN:HB3	1.90	0.52
1:C:35:ILE:HG13	1:C:284:ALA:HB2	1.91	0.52
1:C:297:ASN:HB2	1:C:313:GLN:HB3	1.90	0.52
1:C:383:GLN:H	1:C:383:GLN:NE2	2.07	0.52
1:C:94:THR:HG22	1:C:95:HIS:ND1	2.25	0.52
1:B:35:ILE:HG13	1:B:284:ALA:HB2	1.90	0.52
1:B:94:THR:HG22	1:B:95:HIS:ND1	2.25	0.52
1:D:162:TRP:CE3	1:D:435:GLY:HA3	2.45	0.52
1:B:189:ARG:HG2	1:B:189:ARG:HH11	1.74	0.52
1:A:35:ILE:HG13	1:A:284:ALA:HB2	1.90	0.52
1:B:51:HIS:CG	1:B:252:ILE:HG12	2.43	0.52
1:C:197:ASN:OD1	1:C:371:GLY:HA3	2.09	0.52
1:A:350:VAL:CG2	1:A:351:PHE:N	2.72	0.52
1:C:162:TRP:CE3	1:C:435:GLY:HA3	2.45	0.52
1:C:223:GLN:HA	1:C:223:GLN:NE2	2.23	0.52
1:B:162:TRP:CE3	1:B:435:GLY:HA3	2.45	0.52
1:C:189:ARG:HH11	1:C:189:ARG:HG2	1.74	0.52
1:D:383:GLN:NE2	1:D:383:GLN:H	2.07	0.52
1:A:478:LEU:N	1:A:478:LEU:CD1	2.73	0.52
1:B:383:GLN:NE2	1:B:383:GLN:H	2.07	0.52
1:C:478:LEU:CD1	1:C:478:LEU:N	2.73	0.52
1:A:162:TRP:CE3	1:A:435:GLY:HA3	2.45	0.51
1:B:382:PRO:HD2	1:B:383:GLN:HE22	1.75	0.51
1:A:382:PRO:HD2	1:A:383:GLN:HE22	1.75	0.51
1:A:68:GLY:C	1:A:70:THR:H	2.09	0.51
1:A:94:THR:HG22	1:A:95:HIS:ND1	2.25	0.51
1:B:79:GLY:CA	1:B:362:LEU:HB2	2.41	0.51
1:B:478:LEU:CD1	1:B:478:LEU:N	2.73	0.51
1:D:94:THR:HG22	1:D:95:HIS:ND1	2.25	0.51
1:A:383:GLN:NE2	1:A:383:GLN:H	2.07	0.51
1:B:68:GLY:C	1:B:70:THR:H	2.09	0.51
1:D:252:ILE:HG23	1:D:256:LYS:HD2	1.93	0.51
1:D:382:PRO:HD2	1:D:383:GLN:HE22	1.75	0.51
1:D:478:LEU:N	1:D:478:LEU:CD1	2.73	0.51
1:A:41:ILE:N	1:A:41:ILE:CD1	2.42	0.51
1:D:68:GLY:C	1:D:70:THR:H	2.09	0.51
1:B:36:ILE:HG13	1:B:288:VAL:CG1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:SER:HB2	1:D:428:PRO:HA	1.92	0.51
1:A:189:ARG:HH11	1:A:189:ARG:HG2	1.75	0.51
1:D:79:GLY:CA	1:D:362:LEU:HB2	2.41	0.51
1:A:41:ILE:HD13	2:A:501:FAD:O5'	2.11	0.51
1:B:366:ILE:HD11	1:B:368:PHE:HE1	1.73	0.51
1:C:382:PRO:HD2	1:C:383:GLN:HE22	1.75	0.51
1:D:222:ILE:CD1	1:D:222:ILE:N	2.50	0.51
1:B:252:ILE:HG23	1:B:256:LYS:HD2	1.93	0.51
1:C:79:GLY:CA	1:C:362:LEU:HB2	2.41	0.51
1:C:259:LEU:HD23	1:C:259:LEU:N	2.27	0.50
1:D:259:LEU:HD23	1:D:259:LEU:N	2.27	0.50
1:B:97:ILE:HG23	1:B:107:MET:HE2	1.94	0.50
1:C:41:ILE:HD13	2:C:501:FAD:O5'	2.11	0.50
1:A:79:GLY:CA	1:A:362:LEU:HB2	2.41	0.50
1:B:208:SER:HB2	1:B:428:PRO:HA	1.92	0.50
1:B:259:LEU:N	1:B:259:LEU:HD23	2.27	0.50
1:B:41:ILE:HD13	2:B:501:FAD:O5'	2.11	0.50
1:D:30:PRO:HA	1:D:283:ARG:CG	2.42	0.50
1:D:36:ILE:HG13	1:D:288:VAL:CG1	2.40	0.50
1:B:30:PRO:HA	1:B:283:ARG:CG	2.42	0.50
1:C:366:ILE:HD11	1:C:368:PHE:HE1	1.73	0.50
1:C:289:ILE:HD12	1:C:447:PHE:HD2	1.76	0.50
1:C:252:ILE:HG23	1:C:256:LYS:HD2	1.93	0.50
1:C:309:ARG:HA	1:C:437:ALA:HB1	1.94	0.50
1:A:30:PRO:HA	1:A:283:ARG:CG	2.42	0.50
1:A:342:LEU:HB3	1:A:352:LEU:HB2	1.94	0.50
1:A:289:ILE:HD12	1:A:447:PHE:HD2	1.76	0.50
1:C:381:THR:CB	1:C:383:GLN:HE21	2.25	0.50
1:D:268:HIS:NE2	1:D:303:PRO:HD2	2.27	0.50
1:A:268:HIS:NE2	1:A:303:PRO:HD2	2.27	0.49
1:D:41:ILE:HD13	2:D:501:FAD:O5'	2.11	0.49
1:A:208:SER:HB2	1:A:428:PRO:HA	1.92	0.49
1:B:289:ILE:HD12	1:B:447:PHE:HD2	1.76	0.49
1:B:268:HIS:NE2	1:B:303:PRO:HD2	2.27	0.49
1:C:30:PRO:HA	1:C:283:ARG:CG	2.42	0.49
1:D:319:GLY:CA	1:D:421:GLY:HA3	2.43	0.49
1:A:259:LEU:HD23	1:A:259:LEU:N	2.27	0.49
1:A:311:GLN:NE2	1:D:320:ARG:NE	2.60	0.49
1:A:309:ARG:HA	1:A:437:ALA:HB1	1.94	0.49
1:C:208:SER:HB2	1:C:428:PRO:HA	1.93	0.49
1:C:333:TRP:CZ2	1:C:365:LEU:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:ILE:HD12	1:D:447:PHE:HD2	1.76	0.49
1:B:319:GLY:CA	1:B:421:GLY:HA3	2.43	0.49
1:A:252:ILE:HG23	1:A:256:LYS:HD2	1.93	0.49
1:A:374:TYR:CZ	1:A:413:THR:HG21	2.48	0.49
1:B:309:ARG:HA	1:B:437:ALA:HB1	1.94	0.49
1:A:319:GLY:CA	1:A:421:GLY:HA3	2.43	0.49
1:D:374:TYR:CZ	1:D:413:THR:HG21	2.48	0.49
1:B:333:TRP:CZ2	1:B:365:LEU:HD13	2.48	0.49
1:A:333:TRP:CZ2	1:A:365:LEU:HD13	2.48	0.49
1:C:374:TYR:CZ	1:C:413:THR:HG21	2.48	0.49
1:A:159:ASP:O	1:A:439:ARG:NH2	2.46	0.49
1:D:342:LEU:HB3	1:D:352:LEU:HB2	1.94	0.49
1:A:111:GLY:O	1:A:112:LYS:HE3	2.13	0.49
1:A:312:LEU:HD22	1:A:437:ALA:HB3	1.95	0.49
1:C:342:LEU:HB3	1:C:352:LEU:HB2	1.94	0.49
1:B:374:TYR:CZ	1:B:413:THR:HG21	2.48	0.48
1:C:111:GLY:O	1:C:112:LYS:HE3	2.13	0.48
1:C:319:GLY:CA	1:C:421:GLY:HA3	2.43	0.48
1:B:381:THR:CB	1:B:383:GLN:HE21	2.25	0.48
1:D:309:ARG:HA	1:D:437:ALA:HB1	1.94	0.48
1:D:374:TYR:CE1	1:D:413:THR:CG2	2.97	0.48
1:D:312:LEU:HD22	1:D:437:ALA:HB3	1.95	0.48
1:A:381:THR:CB	1:A:383:GLN:HE21	2.25	0.48
1:B:374:TYR:CE1	1:B:413:THR:CG2	2.96	0.48
1:C:268:HIS:NE2	1:C:303:PRO:HD2	2.27	0.48
1:C:426:MET:HB3	1:C:430:VAL:HG21	1.95	0.48
1:C:159:ASP:O	1:C:439:ARG:NH2	2.46	0.48
1:B:159:ASP:O	1:B:439:ARG:NH2	2.46	0.48
1:C:312:LEU:HD22	1:C:437:ALA:HB3	1.95	0.48
1:A:48:LYS:HD3	1:A:52:ASP:OD2	2.14	0.48
1:D:159:ASP:O	1:D:439:ARG:NH2	2.46	0.48
1:D:366:ILE:HD11	1:D:368:PHE:HE1	1.73	0.48
1:A:312:LEU:HD21	1:A:438:LEU:HD23	1.96	0.48
1:C:374:TYR:CE1	1:C:413:THR:CG2	2.96	0.48
1:B:32:VAL:HG22	1:B:56:SER:OG	2.14	0.48
1:D:60:VAL:HG21	1:D:261:TRP:CE3	2.49	0.48
1:B:426:MET:HB3	1:B:430:VAL:HG21	1.95	0.47
1:B:342:LEU:HB3	1:B:352:LEU:HB2	1.94	0.47
1:D:111:GLY:O	1:D:112:LYS:HE3	2.13	0.47
1:D:333:TRP:CZ2	1:D:365:LEU:HD13	2.48	0.47
1:D:48:LYS:HD3	1:D:52:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:HG2	1:D:186:GLU:HG2	1.95	0.47
1:B:312:LEU:HD21	1:B:438:LEU:HD23	1.96	0.47
1:B:312:LEU:HD22	1:B:437:ALA:HB3	1.95	0.47
1:C:281:SER:O	1:C:282:LEU:HD13	2.14	0.47
1:C:48:LYS:HD3	1:C:52:ASP:OD2	2.14	0.47
1:A:281:SER:O	1:A:282:LEU:HD13	2.14	0.47
1:A:411:ASP:OD1	1:A:414:GLN:HG2	2.15	0.47
1:B:281:SER:O	1:B:282:LEU:HD13	2.14	0.47
1:B:79:GLY:HA2	1:B:362:LEU:HB2	1.97	0.47
1:C:352:LEU:HA	1:C:352:LEU:HD12	1.76	0.47
1:C:382:PRO:HD2	1:C:383:GLN:NE2	2.29	0.47
1:C:386:GLU:HG3	1:C:407:PHE:CE2	2.50	0.47
1:D:386:GLU:HG3	1:D:407:PHE:CE2	2.50	0.47
1:A:149:LEU:HD22	1:A:212:TRP:CH2	2.50	0.47
1:A:60:VAL:HG21	1:A:261:TRP:CE3	2.49	0.47
1:A:386:GLU:HG3	1:A:407:PHE:CE2	2.50	0.47
1:B:111:GLY:O	1:B:112:LYS:HE3	2.13	0.47
1:C:312:LEU:HD21	1:C:438:LEU:HD23	1.96	0.47
1:D:32:VAL:HG22	1:D:56:SER:OG	2.14	0.47
1:A:32:VAL:HG22	1:A:56:SER:OG	2.14	0.47
1:D:382:PRO:HD2	1:D:383:GLN:NE2	2.30	0.47
1:A:119:ILE:CD1	1:A:124:VAL:HG22	2.42	0.47
1:A:374:TYR:CE1	1:A:413:THR:CG2	2.96	0.47
1:B:60:VAL:HG21	1:B:261:TRP:CE3	2.49	0.47
1:B:411:ASP:OD1	1:B:414:GLN:HG2	2.15	0.47
1:C:36:ILE:HG13	1:C:288:VAL:CG1	2.41	0.47
1:C:32:VAL:HG22	1:C:56:SER:OG	2.14	0.47
1:A:356:THR:CG2	1:A:363:ALA:HA	2.45	0.47
1:D:149:LEU:HD22	1:D:212:TRP:CH2	2.50	0.47
1:A:382:PRO:HD2	1:A:383:GLN:NE2	2.29	0.47
1:B:48:LYS:HD3	1:B:52:ASP:OD2	2.14	0.47
1:A:79:GLY:HA2	1:A:362:LEU:HB2	1.97	0.47
1:B:382:PRO:HD2	1:B:383:GLN:NE2	2.29	0.47
1:C:79:GLY:HA2	1:C:362:LEU:HB2	1.97	0.47
1:D:79:GLY:HA2	1:D:362:LEU:HB2	1.97	0.47
1:B:149:LEU:HD22	1:B:212:TRP:CH2	2.50	0.46
1:C:119:ILE:CD1	1:C:124:VAL:HG22	2.42	0.46
1:B:129:ASP:O	1:B:130:ASP:OD1	2.33	0.46
1:C:411:ASP:OD1	1:C:414:GLN:HG2	2.15	0.46
1:C:286:HIS:HD2	1:C:446:HIS:CE1	2.33	0.46
1:C:149:LEU:HD22	1:C:212:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:VAL:HG21	1:C:261:TRP:CE3	2.49	0.46
1:D:129:ASP:O	1:D:130:ASP:OD1	2.33	0.46
1:D:281:SER:O	1:D:282:LEU:HD13	2.14	0.46
1:D:312:LEU:HD21	1:D:438:LEU:HD23	1.96	0.46
1:D:411:ASP:OD1	1:D:414:GLN:HG2	2.15	0.46
1:A:426:MET:HB3	1:A:430:VAL:HG21	1.95	0.46
1:B:356:THR:CG2	1:B:363:ALA:HA	2.45	0.46
1:D:271:SER:HB2	1:D:283:ARG:NH2	2.31	0.46
1:B:386:GLU:HG3	1:B:407:PHE:CE2	2.50	0.46
1:C:356:THR:CG2	1:C:363:ALA:HA	2.45	0.46
1:D:356:THR:CG2	1:D:363:ALA:HA	2.45	0.46
1:D:426:MET:HB3	1:D:430:VAL:HG21	1.95	0.46
1:A:129:ASP:O	1:A:130:ASP:OD1	2.33	0.46
1:A:36:ILE:HG13	1:A:288:VAL:CG1	2.41	0.46
1:B:271:SER:HB2	1:B:283:ARG:NH2	2.31	0.46
1:B:72:THR:HG21	1:B:240:GLY:HA3	1.98	0.46
1:C:129:ASP:O	1:C:130:ASP:OD1	2.33	0.46
1:D:145:SER:O	1:D:148:ALA:HB3	2.16	0.46
1:D:97:ILE:HG23	1:D:107:MET:HE2	1.98	0.46
1:A:165:PRO:HB2	1:B:144:SER:HB2	1.98	0.46
1:C:169:ALA:HB2	1:D:184:GLU:HB2	1.98	0.46
1:C:72:THR:HG21	1:C:240:GLY:HA3	1.98	0.46
1:A:72:THR:HG21	1:A:240:GLY:HA3	1.98	0.46
1:D:422:PRO:HA	2:D:501:FAD:C8M	2.46	0.46
1:A:422:PRO:HA	2:A:501:FAD:C8M	2.46	0.45
1:B:119:ILE:CD1	1:B:124:VAL:HG22	2.42	0.45
1:C:145:SER:O	1:C:148:ALA:HB3	2.16	0.45
1:B:145:SER:O	1:B:148:ALA:HB3	2.16	0.45
1:B:422:PRO:HA	2:B:501:FAD:C8M	2.46	0.45
1:C:422:PRO:HG2	1:C:423:VAL:HG22	1.98	0.45
1:A:342:LEU:HD22	1:A:352:LEU:HD22	1.99	0.45
1:C:271:SER:HB2	1:C:283:ARG:NH2	2.31	0.45
1:A:66:ILE:HG22	1:A:245:SER:HB3	1.98	0.45
1:D:297:ASN:HD22	1:D:313:GLN:HE21	1.65	0.45
1:C:342:LEU:HD22	1:C:352:LEU:HD22	1.99	0.45
1:D:161:PRO:HG2	1:D:214:TYR:CD1	2.52	0.45
1:A:33:ASP:HB2	1:A:56:SER:O	2.17	0.45
1:C:66:ILE:HG22	1:C:245:SER:HB3	1.98	0.45
1:D:342:LEU:HD22	1:D:352:LEU:HD22	1.99	0.45
1:D:381:THR:CB	1:D:383:GLN:HE21	2.25	0.45
1:D:60:VAL:CG2	1:D:261:TRP:CE3	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:O	1:A:148:ALA:HB3	2.16	0.45
1:C:422:PRO:HA	2:C:501:FAD:C8M	2.46	0.45
1:D:66:ILE:HG22	1:D:245:SER:HB3	1.98	0.45
1:B:66:ILE:HG22	1:B:245:SER:HB3	1.98	0.45
1:B:342:LEU:HD22	1:B:352:LEU:HD22	1.99	0.45
1:C:60:VAL:CG2	1:C:261:TRP:CE3	3.00	0.45
1:A:271:SER:HB2	1:A:283:ARG:NH2	2.31	0.44
1:D:72:THR:HG21	1:D:240:GLY:HA3	1.98	0.44
1:A:201:GLY:O	1:A:371:GLY:HA2	2.17	0.44
1:A:60:VAL:CG2	1:A:261:TRP:CE3	3.00	0.44
1:A:320:ARG:HA	1:A:320:ARG:HD3	1.91	0.44
1:A:422:PRO:HG2	1:A:423:VAL:HG22	1.98	0.44
1:B:297:ASN:HD22	1:B:313:GLN:HE21	1.65	0.44
1:D:422:PRO:HG2	1:D:423:VAL:HG22	1.98	0.44
1:D:33:ASP:HB2	1:D:56:SER:O	2.17	0.44
1:C:185:SER:HB3	1:C:188:VAL:CG2	2.48	0.44
1:B:161:PRO:HG2	1:B:214:TYR:CD1	2.52	0.44
1:B:86:GLY:HA2	2:B:501:FAD:C4X	2.48	0.44
1:C:201:GLY:O	1:C:371:GLY:HA2	2.17	0.44
1:C:297:ASN:HD22	1:C:313:GLN:HE21	1.65	0.44
1:C:41:ILE:HD11	2:C:501:FAD:O4'	2.18	0.44
1:D:201:GLY:O	1:D:371:GLY:HA2	2.17	0.44
1:D:41:ILE:HD11	2:D:501:FAD:O4'	2.18	0.44
1:A:203:ASP:CG	1:A:205:TYR:CD1	2.91	0.44
1:A:161:PRO:HG2	1:A:214:TYR:CD1	2.52	0.44
1:B:60:VAL:CG2	1:B:261:TRP:CE3	3.00	0.44
1:B:41:ILE:HD11	2:B:501:FAD:O4'	2.18	0.44
1:B:33:ASP:HB2	1:B:56:SER:O	2.17	0.44
1:A:86:GLY:HA2	2:A:501:FAD:C4X	2.47	0.44
1:B:201:GLY:O	1:B:371:GLY:HA2	2.17	0.44
1:C:86:GLY:HA2	2:C:501:FAD:C4X	2.47	0.44
1:D:185:SER:HB3	1:D:188:VAL:CG2	2.48	0.44
1:A:286:HIS:HD2	1:A:446:HIS:CE1	2.33	0.44
1:A:41:ILE:HD11	2:A:501:FAD:O4'	2.18	0.44
1:C:203:ASP:CG	1:C:205:TYR:CD1	2.91	0.44
1:C:362:LEU:HD12	1:C:362:LEU:HA	1.81	0.44
1:D:119:ILE:CD1	1:D:124:VAL:HG22	2.42	0.44
1:B:422:PRO:HG2	1:B:423:VAL:HG22	1.98	0.43
1:C:161:PRO:HG2	1:C:214:TYR:CD1	2.52	0.43
1:C:33:ASP:HB2	1:C:56:SER:O	2.17	0.43
1:A:185:SER:HB3	1:A:188:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLY:HA3	1:A:319:GLY:HA3	2.00	0.43
1:B:203:ASP:CG	1:B:205:TYR:CD1	2.91	0.43
1:C:381:THR:HB	1:C:383:GLN:NE2	2.31	0.43
1:A:88:PHE:CZ	1:A:353:LEU:HD23	2.54	0.43
1:B:201:GLY:HA3	1:B:319:GLY:HA3	2.00	0.43
1:D:371:GLY:O	1:D:374:TYR:HB3	2.19	0.43
1:A:222:ILE:N	1:A:222:ILE:CD1	2.50	0.43
1:A:297:ASN:HD22	1:A:313:GLN:HE21	1.65	0.43
1:A:374:TYR:CE1	1:A:413:THR:HG21	2.54	0.43
1:C:66:ILE:CD1	1:C:259:LEU:HD21	2.49	0.43
1:C:88:PHE:CZ	1:C:353:LEU:HD23	2.54	0.43
1:C:97:ILE:HG23	1:C:107:MET:HE2	2.01	0.43
1:D:112:LYS:HA	1:D:112:LYS:HD3	1.83	0.43
1:D:201:GLY:HA3	1:D:319:GLY:HA3	2.00	0.43
1:A:352:LEU:HA	1:A:352:LEU:HD12	1.76	0.43
1:B:32:VAL:HG22	1:B:56:SER:C	2.39	0.43
1:B:356:THR:HG23	1:B:363:ALA:HA	2.00	0.43
1:B:374:TYR:CE1	1:B:413:THR:HG21	2.54	0.43
1:B:58:LEU:HD12	1:B:58:LEU:HA	1.87	0.43
1:C:374:TYR:CE1	1:C:413:THR:HG21	2.54	0.43
1:C:58:LEU:HD12	1:C:58:LEU:HA	1.87	0.43
1:D:374:TYR:CE1	1:D:413:THR:HG21	2.54	0.43
1:A:32:VAL:HG22	1:A:56:SER:C	2.39	0.43
1:B:191:LEU:O	1:B:194:VAL:HG23	2.19	0.43
1:B:88:PHE:CZ	1:B:353:LEU:HD23	2.54	0.43
1:C:112:LYS:HA	1:C:112:LYS:HD3	1.83	0.43
1:D:203:ASP:CG	1:D:205:TYR:CD1	2.92	0.43
1:D:66:ILE:CD1	1:D:259:LEU:HD21	2.49	0.43
1:A:311:GLN:NE2	1:D:320:ARG:HD2	2.33	0.43
1:B:185:SER:HB3	1:B:188:VAL:CG2	2.48	0.43
1:B:371:GLY:O	1:B:374:TYR:HB3	2.19	0.43
1:D:86:GLY:HA2	2:D:501:FAD:C4X	2.48	0.43
1:D:88:PHE:CZ	1:D:353:LEU:HD23	2.53	0.43
1:C:371:GLY:O	1:C:374:TYR:HB3	2.19	0.43
1:C:356:THR:HG23	1:C:363:ALA:HA	2.01	0.43
1:C:383:GLN:N	1:C:383:GLN:CD	2.68	0.43
1:C:374:TYR:CE1	1:C:413:THR:HG23	2.54	0.43
1:B:374:TYR:CE1	1:B:413:THR:HG23	2.54	0.43
1:D:374:TYR:CE1	1:D:413:THR:HG23	2.54	0.43
1:D:383:GLN:CD	1:D:383:GLN:N	2.68	0.43
1:B:352:LEU:HA	1:B:352:LEU:HD12	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ARG:O	1:C:313:GLN:HG3	2.19	0.42
1:C:370:GLY:O	1:C:373:ASN:HB2	2.20	0.42
1:A:371:GLY:O	1:A:374:TYR:HB3	2.19	0.42
1:C:191:LEU:O	1:C:194:VAL:HG23	2.19	0.42
1:C:32:VAL:HG22	1:C:56:SER:C	2.39	0.42
1:A:191:LEU:O	1:A:194:VAL:HG23	2.19	0.42
1:B:280:ARG:HG2	1:B:280:ARG:H	1.48	0.42
1:B:316:ALA:HA	1:B:317:PRO:HD2	1.88	0.42
1:C:97:ILE:HG23	1:C:107:MET:CE	2.50	0.42
1:C:201:GLY:HA3	1:C:319:GLY:HA3	2.00	0.42
1:D:352:LEU:HA	1:D:352:LEU:HD12	1.76	0.42
1:A:280:ARG:H	1:A:280:ARG:HG2	1.48	0.42
1:A:309:ARG:O	1:A:313:GLN:HG3	2.19	0.42
1:D:191:LEU:O	1:D:194:VAL:HG23	2.19	0.42
1:A:238:PHE:CD1	1:A:239:GLY:N	2.88	0.42
1:A:362:LEU:HA	1:A:362:LEU:HD12	1.81	0.42
1:A:97:ILE:HG23	1:A:107:MET:CE	2.49	0.42
1:B:286:HIS:HD2	1:B:446:HIS:CE1	2.33	0.42
1:C:238:PHE:CD1	1:C:239:GLY:N	2.88	0.42
1:D:309:ARG:O	1:D:313:GLN:HG3	2.20	0.42
1:A:75:GLU:O	1:A:76:GLY:O	2.38	0.42
1:B:153:ALA:O	1:B:156:VAL:O	2.38	0.42
1:B:79:GLY:HA3	1:B:362:LEU:HB2	2.01	0.42
1:B:97:ILE:HG23	1:B:107:MET:CE	2.50	0.42
1:C:374:TYR:CZ	1:C:413:THR:CG2	3.03	0.42
1:D:356:THR:HG23	1:D:363:ALA:HA	2.00	0.42
1:A:356:THR:HG23	1:A:363:ALA:HA	2.00	0.42
1:A:374:TYR:CE1	1:A:413:THR:HG23	2.54	0.42
1:B:112:LYS:HD3	1:B:112:LYS:HA	1.83	0.42
1:B:374:TYR:CZ	1:B:413:THR:CG2	3.03	0.42
1:C:307:THR:O	1:C:311:GLN:HG2	2.20	0.42
1:D:32:VAL:HG22	1:D:56:SER:C	2.39	0.42
1:D:285:ARG:O	1:D:444:LYS:HG2	2.20	0.42
1:B:309:ARG:O	1:B:313:GLN:HG3	2.19	0.42
1:B:75:GLU:O	1:B:76:GLY:O	2.38	0.42
1:C:153:ALA:O	1:C:156:VAL:O	2.38	0.42
1:D:153:ALA:O	1:D:156:VAL:O	2.38	0.42
1:D:307:THR:O	1:D:311:GLN:HG2	2.20	0.42
1:D:79:GLY:HA3	1:D:362:LEU:HB2	2.01	0.42
1:D:370:GLY:O	1:D:373:ASN:HB2	2.19	0.42
1:A:79:GLY:HA3	1:A:362:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLU:O	1:C:76:GLY:O	2.38	0.42
1:A:320:ARG:NE	1:D:311:GLN:HE22	2.18	0.42
1:D:97:ILE:HG23	1:D:107:MET:CE	2.50	0.42
1:A:285:ARG:O	1:A:444:LYS:HG2	2.20	0.42
1:A:370:GLY:O	1:A:373:ASN:HB2	2.20	0.42
1:D:312:LEU:HD11	1:D:426:MET:CE	2.50	0.42
1:A:269:ASP:OD2	1:A:271:SER:HB2	2.20	0.41
1:A:316:ALA:HA	1:A:317:PRO:HD2	1.88	0.41
1:D:238:PHE:CD1	1:D:239:GLY:N	2.88	0.41
1:A:366:ILE:HD11	1:A:368:PHE:HE1	1.73	0.41
1:A:381:THR:HB	1:A:383:GLN:NE2	2.31	0.41
1:B:307:THR:O	1:B:311:GLN:HG2	2.20	0.41
1:B:383:GLN:N	1:B:383:GLN:CD	2.68	0.41
1:B:312:LEU:HD11	1:B:426:MET:CE	2.51	0.41
1:C:243:GLN:O	1:C:247:ARG:HB2	2.21	0.41
1:C:269:ASP:OD2	1:C:271:SER:HB2	2.20	0.41
1:D:374:TYR:CZ	1:D:413:THR:CG2	3.03	0.41
1:B:238:PHE:CD1	1:B:239:GLY:N	2.88	0.41
1:B:393:LEU:HB3	1:B:401:ALA:HB1	2.03	0.41
1:D:386:GLU:HG3	1:D:407:PHE:CZ	2.56	0.41
1:A:307:THR:O	1:A:311:GLN:HG2	2.20	0.41
1:A:393:LEU:HB3	1:A:401:ALA:HB1	2.03	0.41
2:A:501:FAD:H1'1	2:A:501:FAD:H9	1.94	0.41
1:B:370:GLY:O	1:B:373:ASN:HB2	2.20	0.41
1:B:381:THR:HB	1:B:383:GLN:NE2	2.31	0.41
1:C:37:ILE:HG23	1:C:263:VAL:HG21	2.02	0.41
1:C:285:ARG:O	1:C:444:LYS:HG2	2.20	0.41
1:C:312:LEU:HD11	1:C:426:MET:CE	2.51	0.41
1:D:269:ASP:OD2	1:D:271:SER:HB2	2.20	0.41
1:A:374:TYR:CZ	1:A:413:THR:CG2	3.03	0.41
1:B:243:GLN:O	1:B:247:ARG:HB2	2.21	0.41
1:B:37:ILE:HG23	1:B:263:VAL:HG21	2.02	0.41
1:C:320:ARG:HA	1:C:320:ARG:HD3	1.91	0.41
1:A:112:LYS:HA	1:A:112:LYS:HD3	1.83	0.41
1:D:243:GLN:O	1:D:247:ARG:HB2	2.21	0.41
1:D:280:ARG:NH1	1:D:280:ARG:HG3	2.36	0.41
1:A:383:GLN:N	1:A:383:GLN:CD	2.68	0.41
1:A:450:THR:HG23	1:A:451:GLU:N	2.36	0.41
1:A:48:LYS:HB2	1:A:248:ILE:HD12	2.02	0.41
1:B:66:ILE:CD1	1:B:259:LEU:HD21	2.49	0.41
1:D:286:HIS:HD2	1:D:446:HIS:CE1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:THR:HG23	1:D:451:GLU:N	2.36	0.41
1:A:186:GLU:OE2	1:A:189:ARG:NH2	2.54	0.41
1:B:311:GLN:HE22	1:C:320:ARG:NE	2.18	0.41
1:B:450:THR:HG23	1:B:451:GLU:N	2.36	0.41
1:C:280:ARG:NH1	1:C:280:ARG:HG3	2.36	0.41
1:C:393:LEU:HB3	1:C:401:ALA:HB1	2.03	0.41
1:C:79:GLY:HA3	1:C:362:LEU:HB2	2.01	0.41
1:B:280:ARG:NH1	1:B:280:ARG:HG3	2.36	0.41
1:B:285:ARG:O	1:B:444:LYS:HG2	2.20	0.41
1:D:48:LYS:HA	1:D:252:ILE:CD1	2.51	0.41
1:A:153:ALA:O	1:A:156:VAL:O	2.38	0.41
1:D:280:ARG:HG2	1:D:280:ARG:H	1.48	0.41
1:D:393:LEU:HB3	1:D:401:ALA:HB1	2.03	0.41
1:A:37:ILE:HG23	1:A:263:VAL:HG21	2.02	0.40
1:B:269:ASP:OD2	1:B:271:SER:HB2	2.20	0.40
1:B:48:LYS:HB2	1:B:248:ILE:HD12	2.02	0.40
1:C:186:GLU:OE2	1:C:189:ARG:NH2	2.54	0.40
1:C:386:GLU:HG2	1:C:390:LEU:HD22	2.03	0.40
1:C:450:THR:HG23	1:C:451:GLU:N	2.36	0.40
1:D:75:GLU:O	1:D:76:GLY:O	2.38	0.40
1:C:312:LEU:HD11	1:C:426:MET:HE1	2.03	0.40
1:A:72:THR:HB	1:A:242:ALA:HB3	2.04	0.40
1:B:320:ARG:NE	1:C:311:GLN:HE22	2.19	0.40
1:B:386:GLU:HG2	1:B:390:LEU:HD22	2.04	0.40
1:D:133:ASP:HA	1:D:134:PRO:HD3	1.86	0.40
1:D:386:GLU:HG2	1:D:390:LEU:HD22	2.03	0.40
1:D:58:LEU:HD12	1:D:58:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

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	447/471 (95%)	422 (94%)	22 (5%)	3 (1%)	22	52
1	B	447/471 (95%)	421 (94%)	23 (5%)	3 (1%)	22	52
1	C	447/471 (95%)	422 (94%)	22 (5%)	3 (1%)	22	52
1	D	447/471 (95%)	422 (94%)	22 (5%)	3 (1%)	22	52
All	All	1788/1884 (95%)	1687 (94%)	89 (5%)	12 (1%)	22	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	GLY
1	B	421	GLY
1	C	421	GLY
1	D	421	GLY
1	A	76	GLY
1	B	76	GLY
1	C	76	GLY
1	D	76	GLY
1	A	422	PRO
1	B	422	PRO
1	C	422	PRO
1	D	422	PRO

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	345/367 (94%)	297 (86%)	48 (14%)	3	10
1	B	345/367 (94%)	297 (86%)	48 (14%)	3	10
1	C	345/367 (94%)	297 (86%)	48 (14%)	3	10
1	D	345/367 (94%)	297 (86%)	48 (14%)	3	10
All	All	1380/1468 (94%)	1188 (86%)	192 (14%)	3	10

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	60	VAL
1	A	63	ASN
1	A	93	HIS
1	A	94	THR
1	A	103	LEU
1	A	130	ASP
1	A	143	LEU
1	A	146	LEU
1	A	156	VAL
1	A	177	THR
1	A	178	TRP
1	A	189	ARG
1	A	194	VAL
1	A	199	LEU
1	A	200	LEU
1	A	222	ILE
1	A	223	GLN
1	A	225	LEU
1	A	234	TRP
1	A	247	ARG
1	A	252	ILE
1	A	255	ASP
1	A	269	ASP
1	A	275	LEU
1	A	280	ARG
1	A	282	LEU
1	A	288	VAL
1	A	289	ILE
1	A	307	THR
1	A	320	ARG
1	A	321	TYR
1	A	325	GLN
1	A	344	ASP
1	A	351	PHE
1	A	352	LEU
1	A	359	THR
1	A	364	THR
1	A	365	LEU
1	A	366	ILE
1	A	382	PRO
1	A	383	GLN
1	A	387	ARG

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Mol	Chain	Res	Type
1	A	390	LEU
1	A	410	THR
1	A	413	THR
1	A	445	VAL
1	A	451	GLU
1	B	41	ILE
1	B	60	VAL
1	B	63	ASN
1	B	93	HIS
1	B	94	THR
1	B	103	LEU
1	B	130	ASP
1	B	143	LEU
1	B	146	LEU
1	B	156	VAL
1	B	177	THR
1	B	178	TRP
1	B	189	ARG
1	B	194	VAL
1	B	199	LEU
1	B	200	LEU
1	B	222	ILE
1	B	223	GLN
1	B	225	LEU
1	B	234	TRP
1	B	247	ARG
1	B	252	ILE
1	B	255	ASP
1	B	269	ASP
1	B	275	LEU
1	B	280	ARG
1	B	282	LEU
1	B	288	VAL
1	B	289	ILE
1	B	307	THR
1	B	320	ARG
1	B	321	TYR
1	B	325	GLN
1	B	344	ASP
1	B	351	PHE
1	B	352	LEU
1	B	359	THR

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Mol	Chain	Res	Type
1	B	364	THR
1	B	365	LEU
1	B	366	ILE
1	B	382	PRO
1	B	383	GLN
1	B	387	ARG
1	B	390	LEU
1	B	410	THR
1	B	413	THR
1	B	445	VAL
1	B	451	GLU
1	C	41	ILE
1	C	60	VAL
1	C	63	ASN
1	C	93	HIS
1	C	94	THR
1	C	103	LEU
1	C	130	ASP
1	C	143	LEU
1	C	146	LEU
1	C	156	VAL
1	C	177	THR
1	C	178	TRP
1	C	189	ARG
1	C	194	VAL
1	C	199	LEU
1	C	200	LEU
1	C	222	ILE
1	C	223	GLN
1	C	225	LEU
1	C	234	TRP
1	C	247	ARG
1	C	252	ILE
1	C	255	ASP
1	C	269	ASP
1	C	275	LEU
1	C	280	ARG
1	C	282	LEU
1	C	288	VAL
1	C	289	ILE
1	C	307	THR
1	C	320	ARG

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Mol	Chain	Res	Type
1	C	321	TYR
1	C	325	GLN
1	C	344	ASP
1	C	351	PHE
1	C	352	LEU
1	C	359	THR
1	C	364	THR
1	C	365	LEU
1	C	366	ILE
1	C	382	PRO
1	C	383	GLN
1	C	387	ARG
1	C	390	LEU
1	C	410	THR
1	C	413	THR
1	C	445	VAL
1	C	451	GLU
1	D	41	ILE
1	D	60	VAL
1	D	63	ASN
1	D	93	HIS
1	D	94	THR
1	D	103	LEU
1	D	130	ASP
1	D	143	LEU
1	D	146	LEU
1	D	156	VAL
1	D	177	THR
1	D	178	TRP
1	D	189	ARG
1	D	194	VAL
1	D	199	LEU
1	D	200	LEU
1	D	222	ILE
1	D	223	GLN
1	D	225	LEU
1	D	234	TRP
1	D	247	ARG
1	D	252	ILE
1	D	255	ASP
1	D	269	ASP
1	D	275	LEU

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Mol	Chain	Res	Type
1	D	280	ARG
1	D	282	LEU
1	D	288	VAL
1	D	289	ILE
1	D	307	THR
1	D	320	ARG
1	D	321	TYR
1	D	325	GLN
1	D	344	ASP
1	D	351	PHE
1	D	352	LEU
1	D	359	THR
1	D	364	THR
1	D	365	LEU
1	D	366	ILE
1	D	382	PRO
1	D	383	GLN
1	D	387	ARG
1	D	390	LEU
1	D	410	THR
1	D	413	THR
1	D	445	VAL
1	D	451	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	93	HIS
1	A	95	HIS
1	A	160	GLN
1	A	192	HIS
1	A	223	GLN
1	A	279	GLN
1	A	286	HIS
1	A	297	ASN
1	A	298	GLN
1	A	311	GLN
1	A	336	GLN
1	A	373	ASN
1	A	383	GLN
1	A	408	HIS

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Mol	Chain	Res	Type
1	A	414	GLN
1	A	446	HIS
1	B	51	HIS
1	B	93	HIS
1	B	95	HIS
1	B	160	GLN
1	B	192	HIS
1	B	223	GLN
1	B	279	GLN
1	B	286	HIS
1	B	297	ASN
1	B	311	GLN
1	B	336	GLN
1	B	373	ASN
1	B	383	GLN
1	B	408	HIS
1	B	414	GLN
1	B	446	HIS
1	C	51	HIS
1	C	93	HIS
1	C	95	HIS
1	C	160	GLN
1	C	192	HIS
1	C	279	GLN
1	C	286	HIS
1	C	297	ASN
1	C	298	GLN
1	C	311	GLN
1	C	336	GLN
1	C	373	ASN
1	C	383	GLN
1	C	408	HIS
1	C	414	GLN
1	C	446	HIS
1	D	51	HIS
1	D	93	HIS
1	D	95	HIS
1	D	160	GLN
1	D	192	HIS
1	D	279	GLN
1	D	286	HIS
1	D	297	ASN

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Mol	Chain	Res	Type
1	D	298	GLN
1	D	311	GLN
1	D	336	GLN
1	D	373	ASN
1	D	383	GLN
1	D	414	GLN
1	D	446	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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
3	CYH	D	502	-	7,7,7	1.11	0	8,8,8	0.44	0
3	CYH	A	502	-	7,7,7	1.12	0	8,8,8	0.44	0
3	CYH	B	502	-	7,7,7	1.12	0	8,8,8	0.43	0
3	CYH	C	502	-	7,7,7	1.12	0	8,8,8	0.44	0
2	FAD	C	501	-	51,58,58	1.44	6 (11%)	60,89,89	2.13	9 (15%)
2	FAD	D	501	-	51,58,58	1.45	6 (11%)	60,89,89	2.12	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	501	-	51,58,58	1.44	6 (11%)	60,89,89	2.12	9 (15%)
2	FAD	B	501	-	51,58,58	1.45	6 (11%)	60,89,89	2.12	9 (15%)

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	CYH	D	502	-	-	-	0/1/1/1
3	CYH	A	502	-	-	-	0/1/1/1
3	CYH	B	502	-	-	-	0/1/1/1
3	CYH	C	502	-	-	-	0/1/1/1
2	FAD	C	501	-	-	1/30/50/50	0/6/6/6
2	FAD	D	501	-	-	1/30/50/50	0/6/6/6
2	FAD	A	501	-	-	1/30/50/50	0/6/6/6
2	FAD	B	501	-	-	1/30/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C4X-N5	5.01	1.40	1.33
2	B	501	FAD	C4X-N5	4.99	1.40	1.33
2	A	501	FAD	C4X-N5	4.97	1.40	1.33
2	C	501	FAD	C4X-N5	4.92	1.40	1.33
2	C	501	FAD	C9A-N10	3.27	1.42	1.38
2	D	501	FAD	C9A-N10	3.24	1.42	1.38
2	A	501	FAD	C9A-N10	3.23	1.42	1.38
2	B	501	FAD	C9A-N10	3.19	1.42	1.38
2	B	501	FAD	C2A-N3A	3.19	1.37	1.32
2	C	501	FAD	C2A-N3A	3.14	1.37	1.32
2	D	501	FAD	C2A-N3A	3.14	1.37	1.32
2	A	501	FAD	C2A-N3A	3.14	1.37	1.32
2	A	501	FAD	C10-N1	3.12	1.37	1.33
2	D	501	FAD	C10-N1	3.07	1.37	1.33
2	B	501	FAD	C10-N1	3.07	1.37	1.33
2	C	501	FAD	C10-N1	3.03	1.37	1.33
2	B	501	FAD	C4-N3	2.77	1.37	1.33
2	A	501	FAD	C4-N3	2.76	1.37	1.33
2	D	501	FAD	C4-N3	2.75	1.37	1.33
2	C	501	FAD	C4-N3	2.73	1.37	1.33
2	C	501	FAD	C4X-C10	2.63	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C4X-C10	2.60	1.41	1.38
2	A	501	FAD	C4X-C10	2.56	1.41	1.38
2	D	501	FAD	C4X-C10	2.53	1.41	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	C4-N3-C2	11.42	124.78	115.14
2	D	501	FAD	C4-N3-C2	11.40	124.77	115.14
2	A	501	FAD	C4-N3-C2	11.40	124.77	115.14
2	B	501	FAD	C4-N3-C2	11.38	124.75	115.14
2	D	501	FAD	C4X-C4-N3	-4.88	116.75	123.43
2	B	501	FAD	C4X-C4-N3	-4.86	116.78	123.43
2	A	501	FAD	C4X-C4-N3	-4.86	116.78	123.43
2	C	501	FAD	C4X-C4-N3	-4.83	116.82	123.43
2	A	501	FAD	C4X-N5-C5X	3.92	120.69	116.77
2	B	501	FAD	C4X-N5-C5X	3.91	120.68	116.77
2	C	501	FAD	C4X-N5-C5X	3.89	120.66	116.77
2	D	501	FAD	C4X-N5-C5X	3.89	120.66	116.77
2	A	501	FAD	O4B-C1B-C2B	-3.89	101.25	106.93
2	D	501	FAD	O4B-C1B-C2B	-3.88	101.26	106.93
2	C	501	FAD	O4B-C1B-C2B	-3.87	101.27	106.93
2	B	501	FAD	O4B-C1B-C2B	-3.86	101.28	106.93
2	C	501	FAD	C1'-N10-C9A	3.73	121.23	118.29
2	A	501	FAD	C1'-N10-C9A	3.72	121.22	118.29
2	B	501	FAD	C1'-N10-C9A	3.71	121.21	118.29
2	D	501	FAD	C1'-N10-C9A	3.68	121.19	118.29
2	C	501	FAD	C4-C4X-C10	-3.53	117.61	119.95
2	B	501	FAD	C4-C4X-C10	-3.41	117.69	119.95
2	A	501	FAD	C4-C4X-C10	-3.40	117.70	119.95
2	D	501	FAD	C4-C4X-C10	-3.32	117.75	119.95
2	B	501	FAD	C5A-C6A-N6A	3.03	124.95	120.35
2	A	501	FAD	C5A-C6A-N6A	3.03	124.95	120.35
2	C	501	FAD	C5A-C6A-N6A	3.02	124.94	120.35
2	D	501	FAD	C5A-C6A-N6A	3.01	124.93	120.35
2	C	501	FAD	C4-C4X-N5	2.52	121.48	118.60
2	A	501	FAD	C4-C4X-N5	2.50	121.45	118.60
2	B	501	FAD	C4-C4X-N5	2.50	121.45	118.60
2	D	501	FAD	C4-C4X-N5	2.45	121.39	118.60
2	C	501	FAD	C5X-C9A-N10	2.11	119.25	117.72
2	B	501	FAD	C5X-C9A-N10	2.10	119.24	117.72
2	A	501	FAD	C5X-C9A-N10	2.08	119.22	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FAD	C5X-C9A-N10	2.06	119.21	117.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

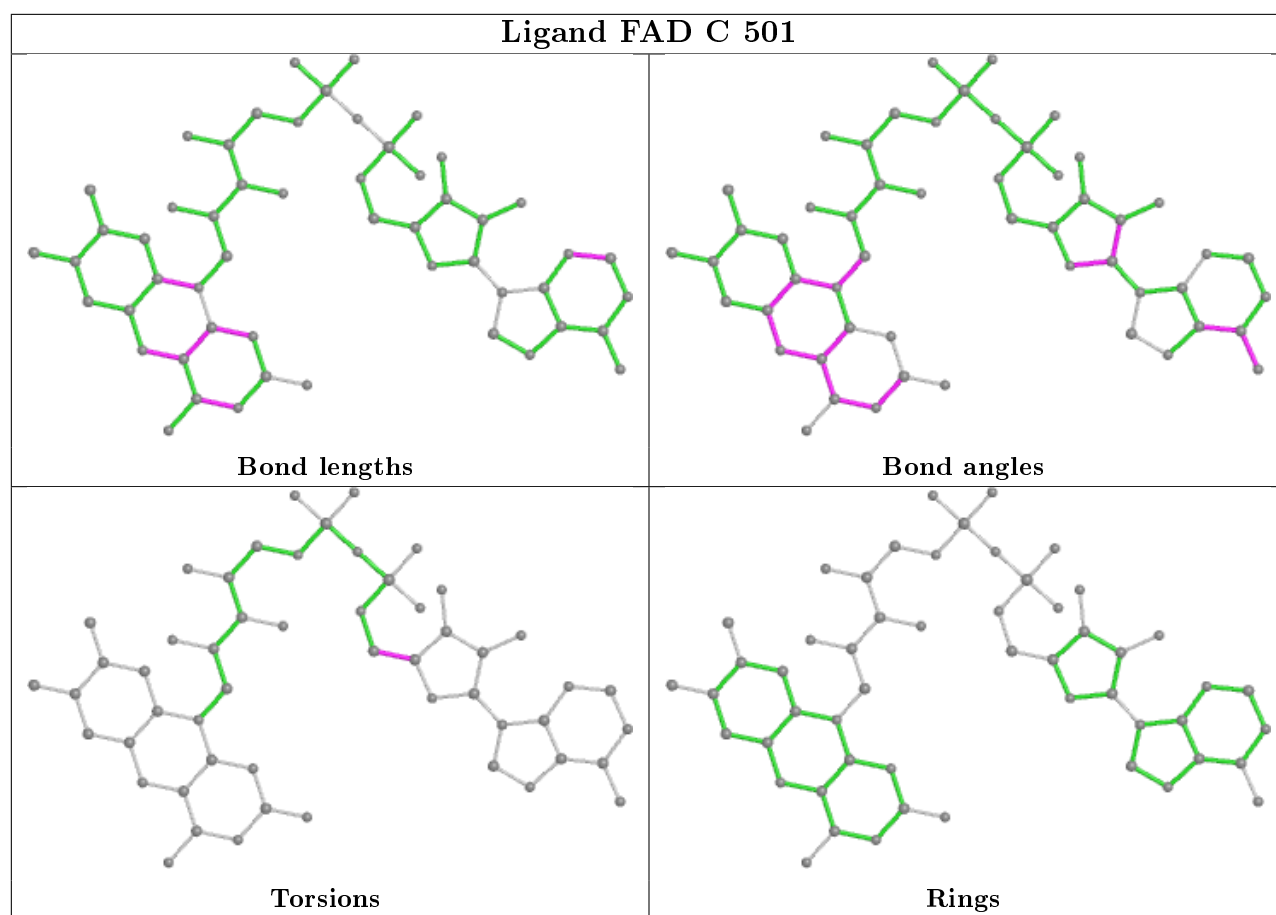
Mol	Chain	Res	Type	Atoms
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

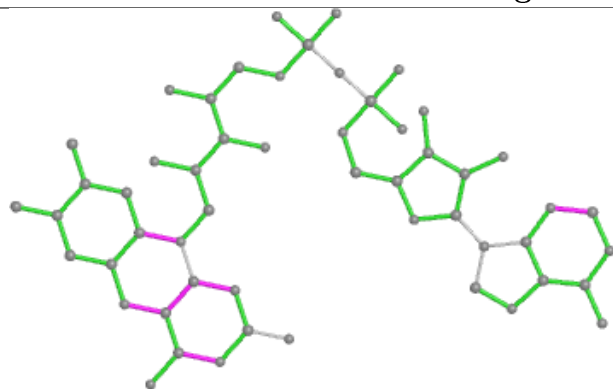
4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	FAD	5	0
2	D	501	FAD	5	0
2	A	501	FAD	6	0
2	B	501	FAD	5	0

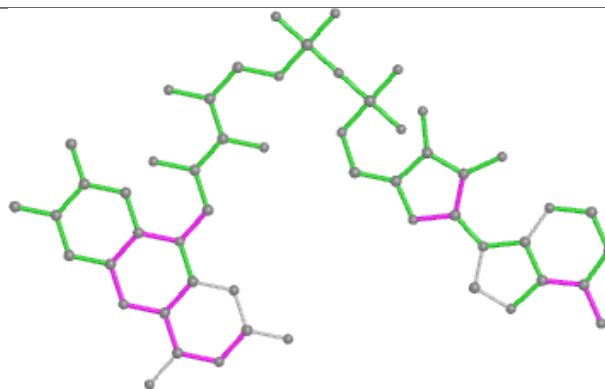
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



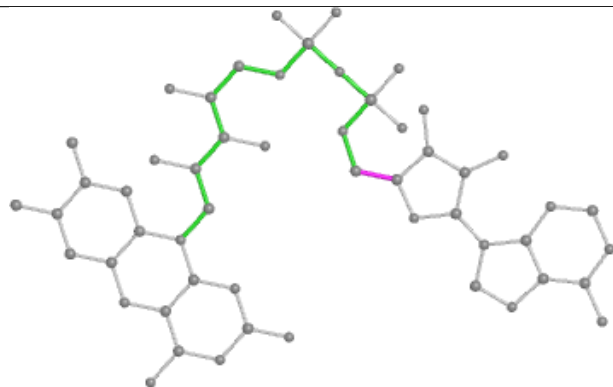
Ligand FAD D 501



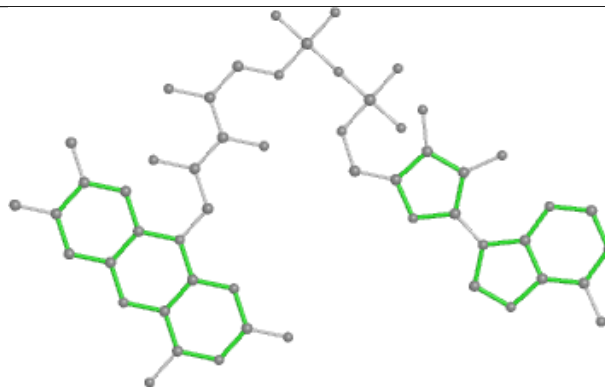
Bond lengths



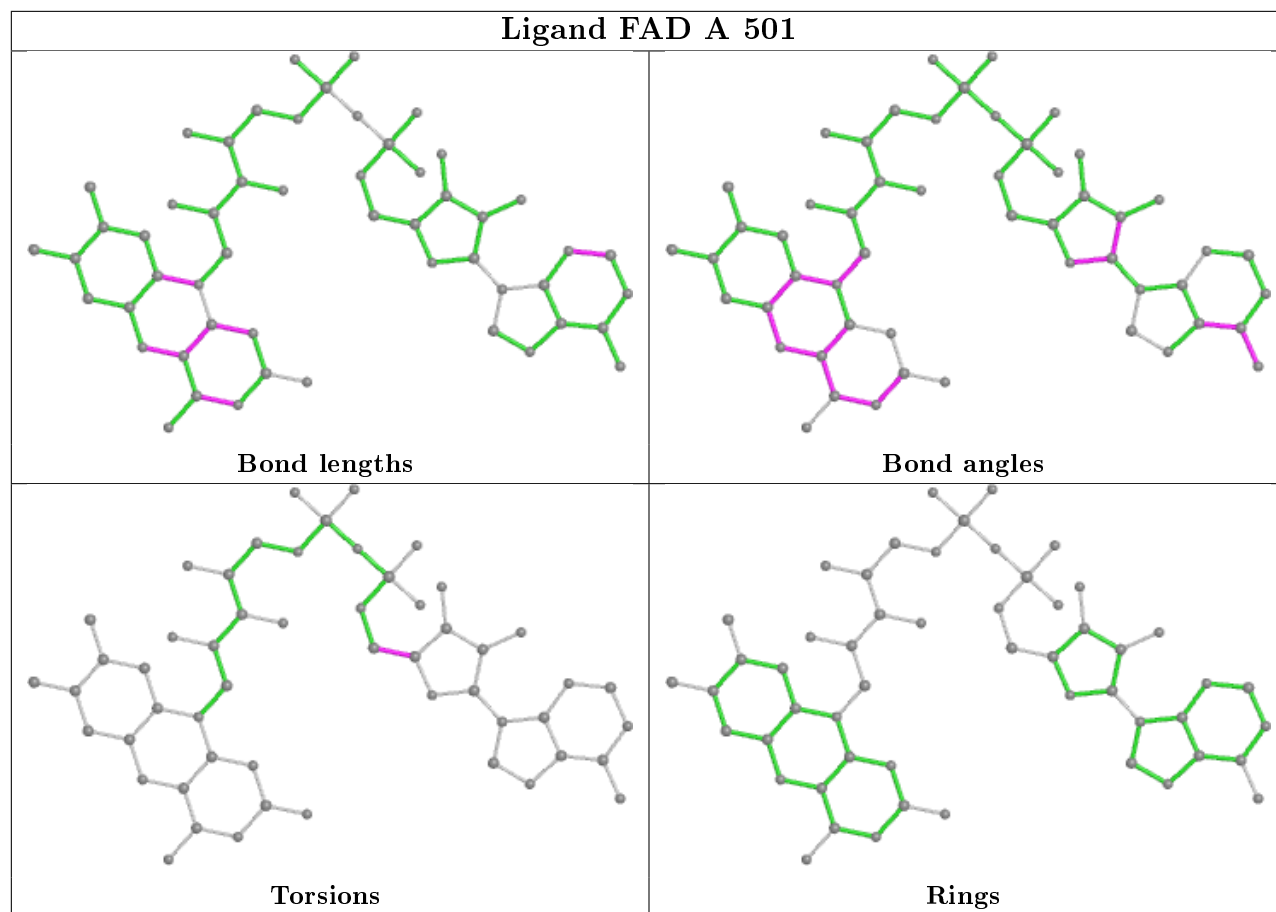
Bond angles

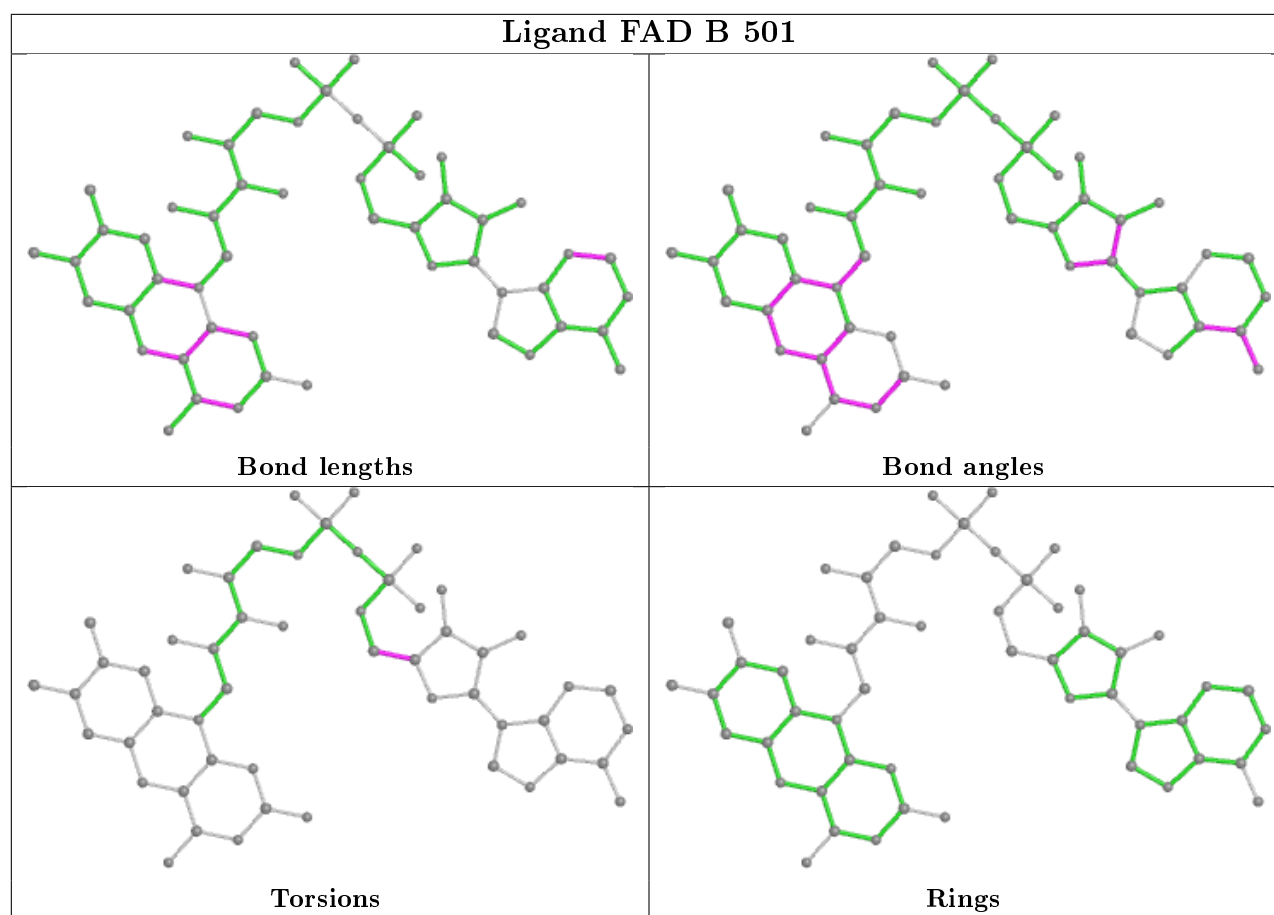


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	449/471 (95%)	-0.01	4 (0%) 84 85	9, 20, 39, 73	0
1	B	449/471 (95%)	0.18	15 (3%) 46 45	9, 20, 39, 73	0
1	C	449/471 (95%)	0.03	4 (0%) 84 85	9, 20, 39, 73	0
1	D	449/471 (95%)	0.01	6 (1%) 77 78	9, 20, 39, 73	0
All	All	1796/1884 (95%)	0.05	29 (1%) 72 73	9, 21, 40, 73	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	GLN	4.3
1	B	130	ASP	4.0
1	C	130	ASP	3.9
1	D	238	PHE	3.9
1	D	77	ALA	3.3
1	A	238	PHE	3.2
1	A	130	ASP	3.1
1	B	56	SER	2.9
1	A	285	ARG	2.6
1	B	252	ILE	2.6
1	B	253	GLY	2.6
1	B	135	ASN	2.5
1	C	387	ARG	2.5
1	D	130	ASP	2.5
1	D	76	GLY	2.4
1	B	53	GLN	2.4
1	B	133	ASP	2.4
1	B	244	VAL	2.4
1	B	32	VAL	2.3
1	B	254	ARG	2.3
1	B	31	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	53	GLN	2.2
1	A	123	ASN	2.2
1	D	56	SER	2.2
1	B	103	LEU	2.1
1	B	279	GLN	2.1
1	B	405	SER	2.1
1	C	270	GLU	2.1
1	B	278	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

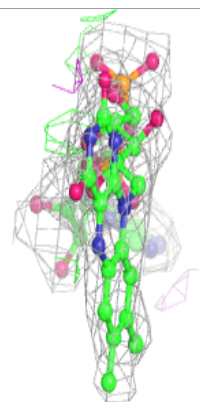
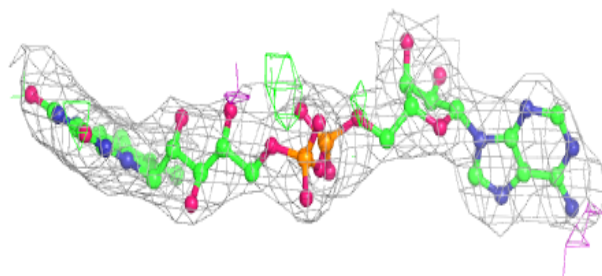
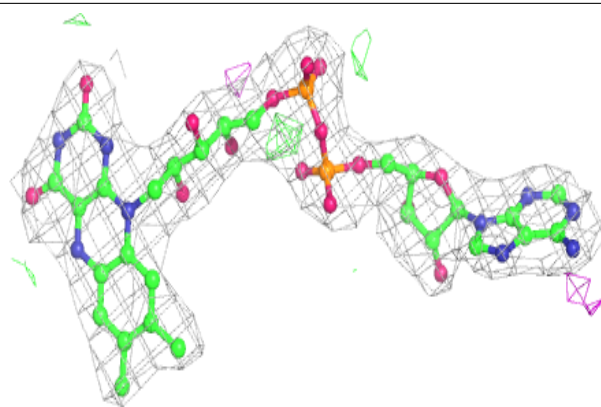
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CYH	D	502	7/7	0.84	0.33	45,47,52,54	0
3	CYH	A	502	7/7	0.90	0.22	45,47,52,54	0
3	CYH	B	502	7/7	0.90	0.22	45,47,52,54	0
3	CYH	C	502	7/7	0.92	0.28	45,47,52,54	0
2	FAD	A	501	53/53	0.95	0.16	10,17,26,28	0
2	FAD	D	501	53/53	0.96	0.20	10,17,26,28	0
2	FAD	C	501	53/53	0.96	0.15	10,17,26,28	0
2	FAD	B	501	53/53	0.96	0.16	10,17,26,28	0

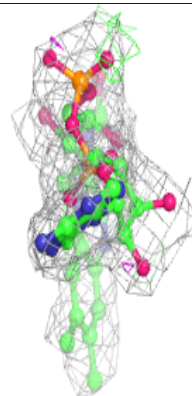
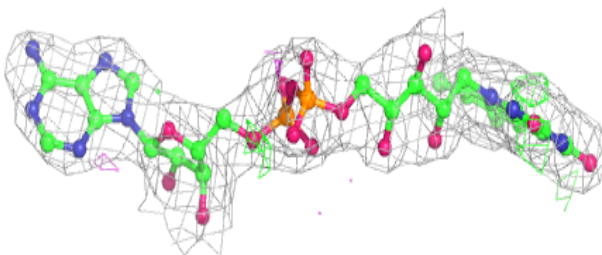
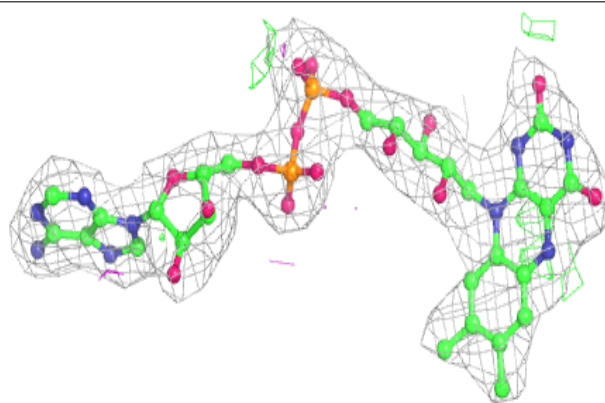
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 501:

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

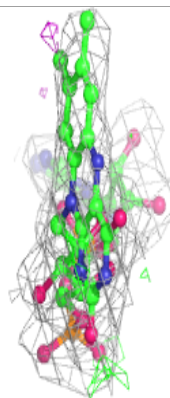
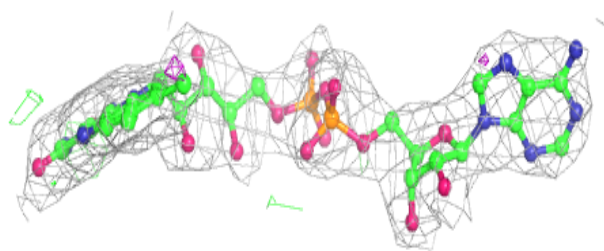
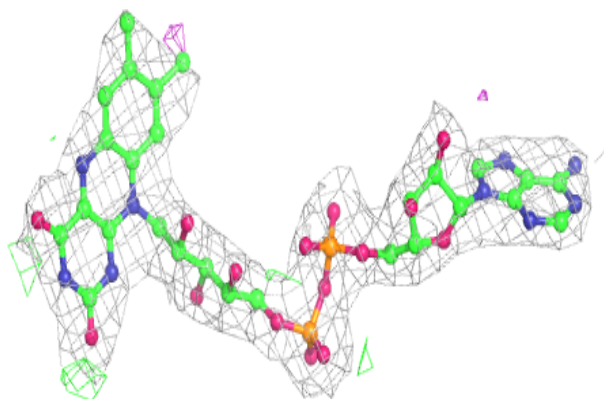
**Electron density around FAD D 501:**

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

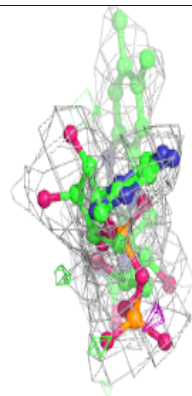
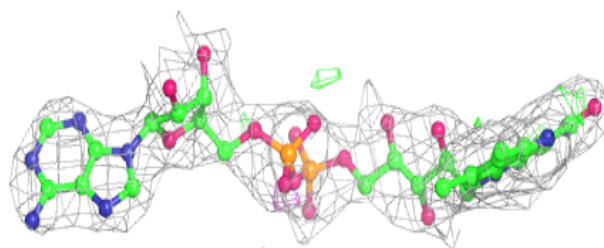
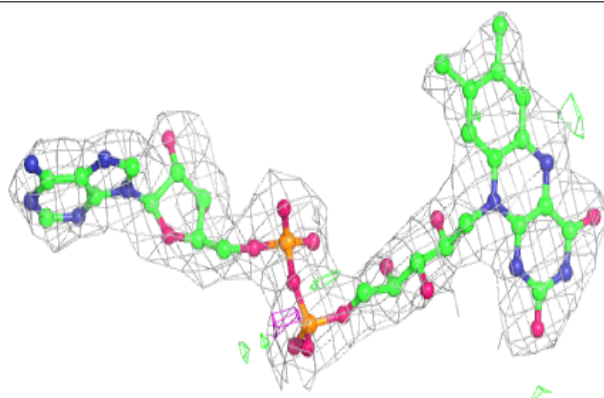


Electron density around FAD C 501:

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

**Electron density around FAD B 501:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.