WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 04:04 AM EDT

PDB ID	:	3GD3
Title	:	Crystal structure of a naturally folded murine apoptosis inducing factor
Authors	:	Sevrioukova, I.F.
Deposited on	:	2009-02-23
Resolution	:	2.95 Å(reported)

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

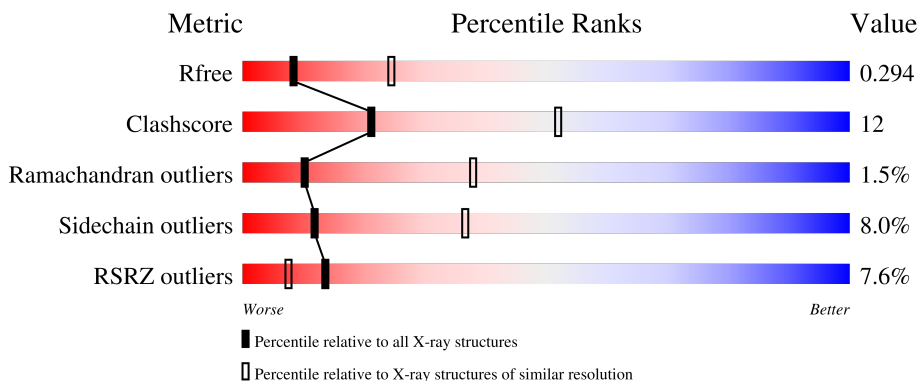|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.95 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.294
Clashscore		12
Ramachandran outliers		1.5%
Sidechain outliers		8.0%
RSRZ outliers		7.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	535	% 56% 27% • 13%
1	B	535	5% 64% 22% • 11%
1	C	535	2% 62% 21% • 13%
1	D	535	19% 63% 21% • 13%
2	E	9	89% 11%

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Mol	Chain	Length	Quality of chain
2	F	9	100%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 14717 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 Apoptosis-inducing factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3564	2255	634	664	11			
1	B	476	Total	C	N	O	S	0	0	0
			3656	2312	647	686	11			
1	C	467	Total	C	N	O	S	0	0	0
			3594	2273	638	672	11			
1	D	465	Total	C	N	O	S	0	0	0
			3579	2263	636	669	11			

- Molecule 2 is a protein called Apoptosis-inducing factor 1, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			40	24	8	8			
2	F	9	Total	C	N	O	0	0	0
			45	27	9	9			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD

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

- Molecule 4 is water.

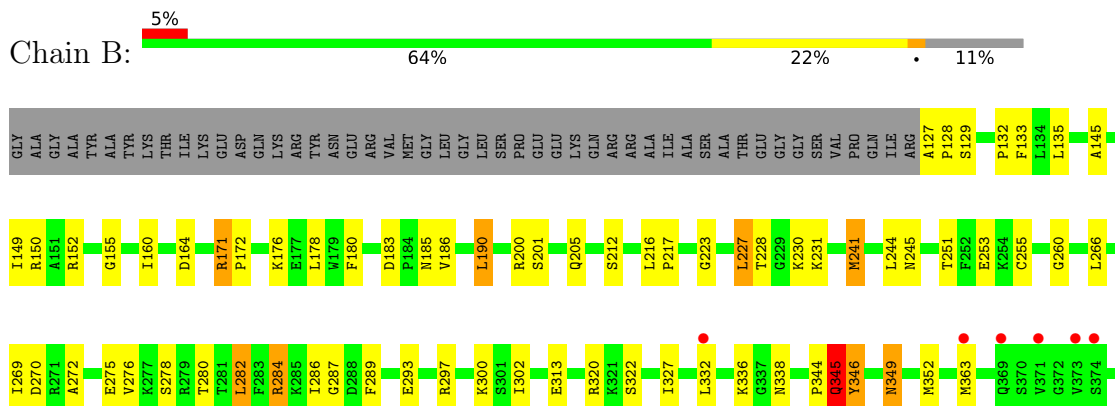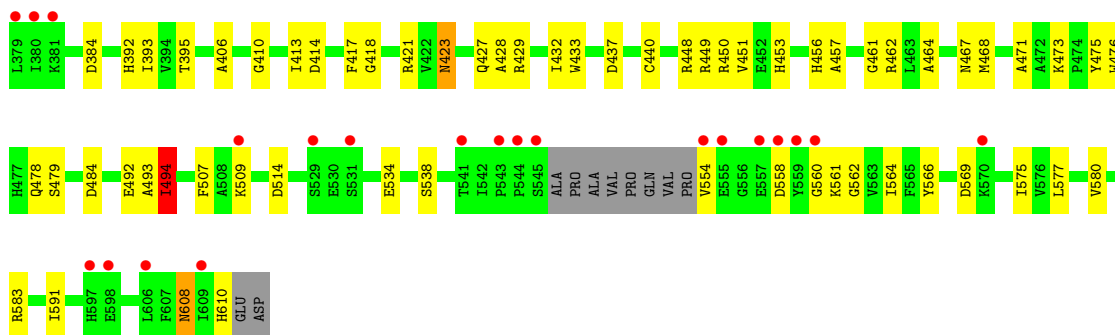| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	3	Total	O	0	0
			3	3		
4	C	7	Total	O	0	0
			7	7		
4	D	4	Total	O	0	0
			4	4		

3 Residue-property plots ⓘ

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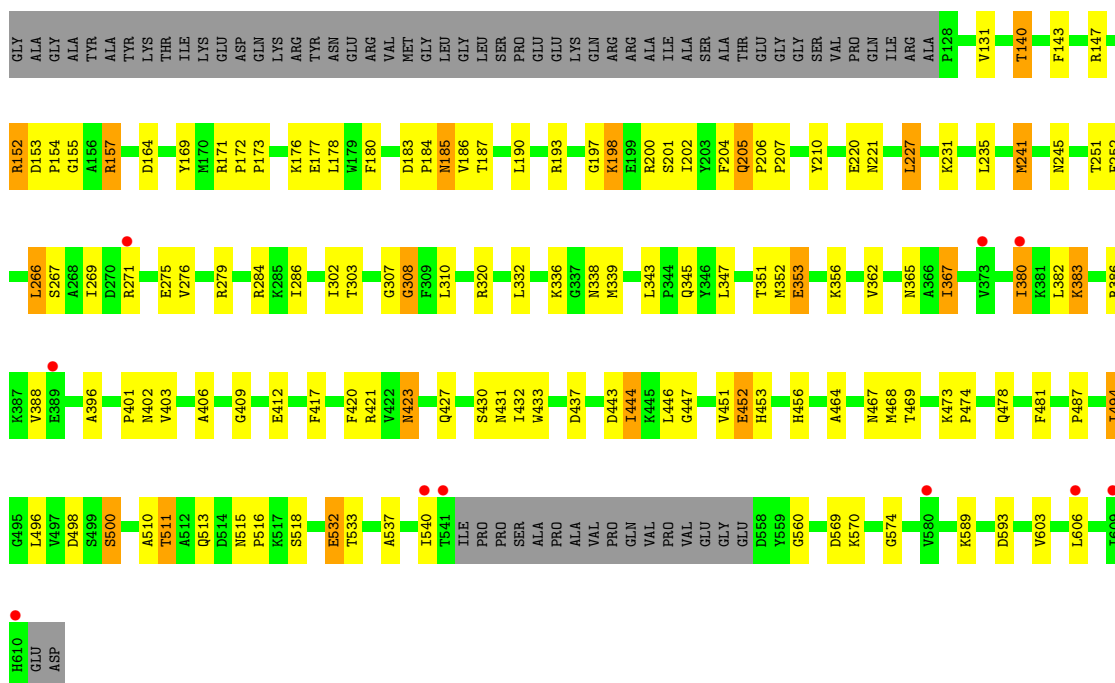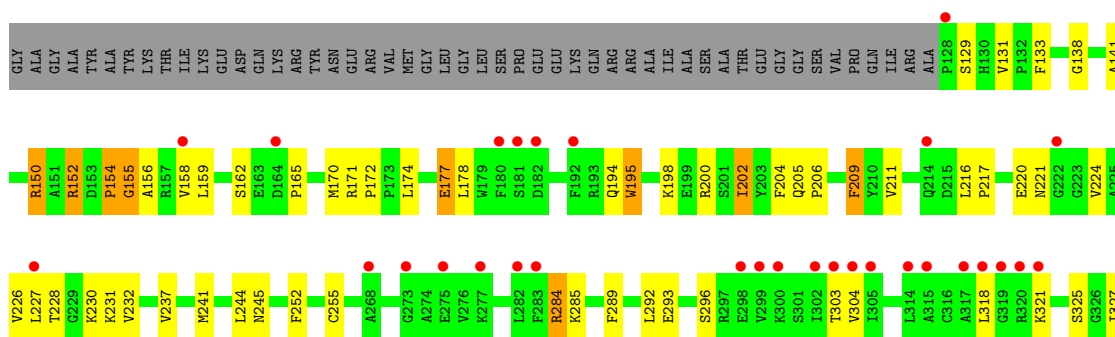
• Molecule 1: Apoptosis-inducing factor 1, mitochondrial

• Molecule 1: Apoptosis-inducing factor 1, mitochondrial

• Molecule 1: Apoptosis-inducing factor 1, mitochondrial

Chain C:

• Molecule 1: Apoptosis-inducing factor 1, mitochondrial

Chain D:

E328 V329 I330 Q331 L332 K336 G337 N338 M339 P344 Q345 Y346 N349 W350 T351 M352 E353 K354 V355 K356 R357 E358 G359 V360 K361 V362 M363 P364 N365 V368 Q369 S370 V371 G372 V373 S374 G375 Q376 R377 L378 L379 I380 K381 L382 K383 V388 H392 I393 V394 T395 I413 D414

G418 G419 F420 E425 L426 Q427 A428 R429 S430 N431 I432 W433 V434 A435 G436 D443 L446 H453 H454 D455 H456 A457 N467 K473 M480 F481 L485 V489 G490 Y491 E492 A493 I494 G495 L496 V497 T503 V504 G505 V506 F507 A508 K509 A510 T511 A512 P516 K517

T520 R528 S529 S538 GLU ILE THR ILE PRO PRO SER ALA PRO ALA VAL PRO GLN VAL PRO VAL GLU GLY E557 D558 Y559 G560 K561 G562 V563 I564 F565 Y566 L567 R568 D569 K570 V573 G574 I575 V576 L577 F581 N582 R583 M584 P585 E595 Q596 H597 E598 D599 L600 N601 E602 V603

A604 K605 L606 F607 N608 I609 H610 GLU ASP

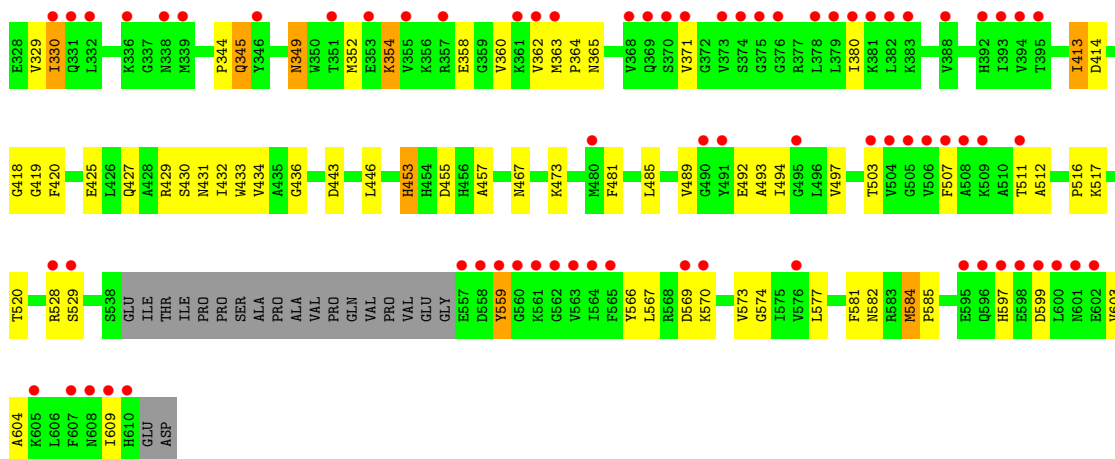• Molecule 2: Apoptosis-inducing factor 1, mitochondrial

Chain E:

89%   11%

X1 X8 UNK

• Molecule 2: Apoptosis-inducing factor 1, mitochondrial

Chain F:

100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.05Å 80.29Å 419.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.64 – 2.95 45.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.4 (46.64-2.95) 81.2 (45.90-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.249 , 0.300 0.237 , 0.294	Depositor DCC
R_{free} test set	2411 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å^2)	85.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.8	EDS
L-test for twinning [2]	$< \lvert L \rvert > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14717	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: 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	0.49	0/3634	0.64	0/4909
1	B	0.45	0/3728	0.59	0/5040
1	C	0.45	1/3664 (0.0%)	0.62	0/4950
1	D	0.46	1/3649 (0.0%)	0.56	0/4929
All	All	0.46	2/14675 (0.0%)	0.61	0/19828

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	532	GLU	C-N	5.73	1.47	1.34
1	D	177	GLU	CD-OE1	5.08	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3564	0	3589	106	0
1	B	3656	0	3676	93	0
1	C	3594	0	3618	89	0
1	D	3579	0	3600	72	0
2	E	40	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	45	0	14	0	0
3	A	53	0	30	2	0
3	B	53	0	30	2	0
3	C	53	0	30	0	0
3	D	53	0	30	1	0
4	A	13	0	0	0	0
4	B	3	0	0	1	0
4	C	7	0	0	1	0
4	D	4	0	0	0	0
All	All	14717	0	14628	354	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 12.

All (354) 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:C:157:ARG:HG2	1:C:157:ARG:HH11	1.11	1.14
1:B:231:LYS:H	1:B:245:ASN:ND2	1.59	0.99
1:C:446:LEU:HD23	1:C:447:GLY:H	1.26	0.98
1:A:533:THR:HG22	1:A:534:GLU:N	1.85	0.91
1:C:231:LYS:H	1:C:245:ASN:ND2	1.68	0.91
1:A:184:PRO:O	1:A:187:THR:HG22	1.72	0.90
1:B:150:ARG:HH11	1:B:155:GLY:H	1.20	0.90
1:D:467:ASN:HD21	1:D:473:LYS:H	0.94	0.89
1:A:467:ASN:HD21	1:A:473:LYS:H	1.19	0.88
1:C:157:ARG:HG2	1:C:157:ARG:NH1	1.88	0.87
1:C:155:GLY:HA2	1:C:221:ASN:O	1.75	0.85
1:C:271:ARG:HG3	1:C:271:ARG:HH11	1.41	0.82
1:D:492:GLU:HB2	1:D:577:LEU:HB2	1.62	0.81
1:A:533:THR:HG22	1:A:534:GLU:H	1.45	0.81
1:D:467:ASN:HD21	1:D:473:LYS:N	1.78	0.81
1:D:467:ASN:ND2	1:D:473:LYS:H	1.77	0.80
1:A:467:ASN:ND2	1:A:473:LYS:H	1.80	0.80
1:C:467:ASN:HD21	1:C:473:LYS:H	1.28	0.79
1:B:467:ASN:HD21	1:B:473:LYS:H	1.30	0.78
1:C:446:LEU:CD2	1:C:447:GLY:H	1.97	0.77
1:D:318:LEU:HB3	1:D:329:VAL:HG21	1.67	0.76
1:A:418:GLY:O	1:A:450:ARG:HD3	1.85	0.75
1:A:533:THR:CG2	1:A:534:GLU:H	1.99	0.75
1:C:464:ALA:O	1:C:468:MET:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ARG:HH21	1:C:152:ARG:HG3	1.51	0.75
1:D:152:ARG:HA	1:D:152:ARG:NE	2.02	0.74
1:A:533:THR:CG2	1:A:534:GLU:N	2.51	0.74
1:B:231:LYS:H	1:B:245:ASN:HD22	1.35	0.74
1:A:257:ILE:HB	1:A:434:VAL:HG22	1.70	0.74
1:C:423:ASN:ND2	1:C:427:GLN:H	1.86	0.74
1:A:477:HIS:CE1	1:A:534:GLU:HB2	2.22	0.73
1:D:177:GLU:OE1	1:D:194:GLN:HA	1.89	0.72
1:D:584:MET:H	1:D:585:PRO:CD	2.02	0.71
1:B:150:ARG:NH1	1:B:155:GLY:H	1.87	0.71
1:C:172:PRO:HB2	1:C:173:PRO:HD3	1.72	0.71
1:B:180:PHE:CE2	1:B:320:ARG:HG3	2.26	0.71
1:C:231:LYS:H	1:C:245:ASN:HD22	1.38	0.70
1:A:140:THR:HG23	1:A:204:PHE:HZ	1.56	0.70
1:A:412:GLU:OE2	1:A:421:ARG:NH2	2.22	0.70
1:B:414:ASP:HA	1:B:421:ARG:NH2	2.05	0.70
1:B:428:ALA:O	1:B:429:ARG:HG2	1.91	0.69
1:C:382:LEU:HD12	1:C:386:ARG:HB2	1.75	0.69
1:A:417:PHE:O	1:A:450:ARG:NE	2.26	0.68
1:B:176:LYS:HD3	1:B:484:ASP:HB2	1.75	0.68
1:C:157:ARG:HH11	1:C:157:ARG:CG	1.95	0.68
1:C:284:ARG:HG3	1:C:284:ARG:HH11	1.58	0.68
1:C:152:ARG:NH2	1:C:469:THR:OG1	2.27	0.68
1:C:176:LYS:O	1:C:178:LEU:N	2.27	0.67
1:A:567:LEU:HD21	1:A:600:LEU:HD11	1.76	0.67
1:B:514:ASP:OD1	1:B:561:LYS:HD2	1.93	0.67
1:B:418:GLY:O	1:B:450:ARG:HD3	1.95	0.67
1:D:152:ARG:HA	1:D:152:ARG:HE	1.59	0.66
1:C:467:ASN:ND2	1:C:473:LYS:H	1.93	0.66
1:A:293:GLU:OE1	1:A:297:ARG:NH2	2.29	0.66
1:A:234:HIS:HB3	1:A:243:LYS:HB2	1.78	0.65
1:B:421:ARG:HH11	1:C:421:ARG:NH1	1.94	0.65
1:B:429:ARG:HH22	1:C:474:PRO:HG3	1.61	0.65
1:C:352:MET:HG2	1:C:362:VAL:HG11	1.79	0.65
1:B:227:LEU:HD22	1:B:230:LYS:HG3	1.79	0.65
1:A:461:GLY:O	1:A:464:ALA:HB3	1.97	0.64
1:C:453:HIS:CE1	1:C:481:PHE:HB2	2.32	0.64
1:B:227:LEU:CD2	1:B:230:LYS:HG3	2.28	0.64
1:A:329:VAL:HG12	1:A:360:VAL:HG13	1.80	0.64
1:B:346:TYR:HD1	1:B:346:TYR:H	1.46	0.64
1:B:410:GLY:HA3	1:C:444:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:CD	1:A:484:ASP:HB2	2.29	0.63
1:A:336:LYS:HG2	1:A:365:ASN:HD21	1.62	0.63
1:B:509:LYS:HE2	1:B:554:VAL:HA	1.80	0.63
1:A:533:THR:HG22	1:A:535:SER:H	1.63	0.63
1:B:346:TYR:HA	1:B:349:ASN:HB2	1.81	0.63
1:A:477:HIS:HE1	1:A:534:GLU:HB2	1.63	0.63
1:B:564:ILE:HG22	1:B:566:TYR:CE1	2.34	0.63
1:B:172:PRO:HB3	1:B:176:LYS:NZ	2.15	0.62
1:C:423:ASN:HD21	1:C:427:GLN:H	1.47	0.62
1:D:481:PHE:HB3	1:D:493:ALA:HB3	1.83	0.61
1:B:200:ARG:HG3	1:B:201:SER:H	1.66	0.61
1:C:478:GLN:HB3	1:C:494:ILE:HD11	1.82	0.61
1:C:157:ARG:NH1	1:C:157:ARG:CG	2.58	0.60
1:C:185:ASN:OD1	1:C:185:ASN:N	2.34	0.60
1:B:255:CYS:HB3	1:B:432:ILE:HD13	1.84	0.60
1:A:163:GLU:HB2	3:A:1611:FAD:O2B	2.02	0.59
1:C:184:PRO:O	1:C:187:THR:HG22	2.02	0.59
1:A:477:HIS:HE1	1:A:534:GLU:CB	2.15	0.59
1:B:183:ASP:HB3	1:B:186:VAL:HG23	1.83	0.59
1:C:200:ARG:HG3	1:C:201:SER:H	1.67	0.59
1:D:174:LEU:HA	1:D:178:LEU:HD12	1.85	0.59
1:D:354:LYS:O	1:D:358:GLU:HG2	2.02	0.59
1:D:131:VAL:HG11	1:D:159:LEU:HD23	1.85	0.58
1:D:138:GLY:HA3	1:D:162:SER:HB2	1.84	0.58
1:A:477:HIS:CE1	1:A:534:GLU:CB	2.85	0.58
1:D:150:ARG:HH11	1:D:156:ALA:H	1.50	0.58
1:B:171:ARG:HG2	1:B:171:ARG:HH11	1.67	0.58
1:B:492:GLU:HB2	1:B:577:LEU:HB2	1.85	0.58
1:A:322:SER:HA	1:A:327:ILE:HG22	1.85	0.58
1:D:414:ASP:O	1:D:418:GLY:HA2	2.04	0.58
1:A:295:ILE:HD13	1:A:392:HIS:CE1	2.38	0.58
1:B:406:ALA:CB	1:B:413:ILE:HD11	2.34	0.58
1:D:455:ASP:HB2	1:D:529:SER:HB2	1.86	0.58
1:D:584:MET:N	1:D:585:PRO:CD	2.67	0.58
1:D:604:ALA:HB1	1:D:609:ILE:HB	1.85	0.58
1:B:554:VAL:HG21	1:B:610:HIS:HE1	1.69	0.57
1:A:574:GLY:O	1:A:575:ILE:HG13	2.05	0.57
1:A:176:LYS:HD2	1:A:484:ASP:HB2	1.87	0.57
1:A:467:ASN:HD21	1:A:473:LYS:N	1.96	0.57
1:B:410:GLY:CA	1:C:444:ILE:HD13	2.34	0.57
1:A:532:GLU:HB3	1:A:584:MET:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LYS:H	1:B:245:ASN:HD21	1.48	0.57
1:C:153:ASP:OD1	1:C:154:PRO:O	2.23	0.56
1:B:171:ARG:HH11	1:B:171:ARG:CG	2.19	0.56
1:B:260:GLY:HA2	1:B:437:ASP:HB2	1.88	0.56
1:A:603:VAL:O	1:A:606:LEU:HB2	2.06	0.56
1:D:220:GLU:O	1:D:221:ASN:HB2	2.05	0.56
1:B:414:ASP:OD1	1:B:417:PHE:N	2.37	0.56
1:B:467:ASN:HD22	1:B:471:ALA:HB3	1.71	0.56
1:C:152:ARG:HH21	1:C:152:ARG:CG	2.19	0.55
1:C:433:TRP:CE3	1:C:468:MET:HG2	2.42	0.55
1:C:511:THR:HG23	1:C:513:GLN:H	1.70	0.55
1:B:322:SER:HA	1:B:327:ILE:HG22	1.89	0.55
1:C:487:PRO:O	1:C:516:PRO:HD2	2.07	0.55
1:C:496:LEU:O	1:C:574:GLY:HA3	2.07	0.55
1:B:176:LYS:HE3	1:B:313:GLU:OE1	2.07	0.55
1:C:193:ARG:HD3	1:C:197:GLY:O	2.07	0.55
1:C:380:ILE:HG13	1:C:388:VAL:HB	1.89	0.55
1:D:584:MET:H	1:D:585:PRO:HD3	1.72	0.55
1:A:459:VAL:HG21	1:A:477:HIS:CD2	2.42	0.54
1:B:269:ILE:HD13	1:B:280:THR:HG21	1.89	0.54
1:C:430:SER:O	1:C:431:ASN:HB2	2.05	0.54
1:A:456:HIS:HD2	1:A:475:TYR:OH	1.90	0.54
1:B:423:ASN:ND2	1:B:427:GLN:H	2.05	0.54
1:D:507:PHE:HB3	1:D:559:TYR:HB3	1.90	0.54
1:B:583:ARG:HH12	1:B:608:ASN:HB2	1.72	0.53
1:B:150:ARG:NH2	1:B:223:GLY:HA2	2.23	0.53
1:B:453:HIS:HD2	1:B:479:SER:OG	1.92	0.53
1:D:205:GLN:HE21	1:D:206:PRO:HD2	1.73	0.53
1:D:453:HIS:CE1	1:D:481:PHE:HB2	2.43	0.53
1:A:453:HIS:CE1	1:A:481:PHE:HB2	2.44	0.53
1:B:478:GLN:HE22	1:B:591:ILE:HB	1.73	0.53
1:D:158:VAL:HB	1:D:224:VAL:HG22	1.91	0.53
1:C:336:LYS:HG2	1:C:365:ASN:HD21	1.73	0.53
1:D:344:PRO:HG3	1:D:503:THR:HG21	1.91	0.53
1:D:150:ARG:NH1	1:D:156:ALA:H	2.06	0.53
1:D:329:VAL:HB	1:D:360:VAL:HG22	1.91	0.52
1:A:231:LYS:HB3	1:A:245:ASN:HD22	1.74	0.52
1:D:303:THR:HG23	1:D:330:ILE:HB	1.91	0.52
1:A:176:LYS:HD3	1:A:484:ASP:HB2	1.90	0.52
1:A:351:THR:O	1:A:355:VAL:HG23	2.09	0.52
1:A:150:ARG:HH11	1:A:156:ALA:N	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ARG:NH1	1:A:155:GLY:H	2.08	0.52
1:B:440:CYS:SG	1:B:448:ARG:HG2	2.49	0.52
1:B:453:HIS:CD2	1:B:479:SER:OG	2.62	0.52
1:A:456:HIS:HB2	1:A:479:SER:OG	2.10	0.51
1:A:608:ASN:OD1	1:A:610:HIS:HE1	1.93	0.51
1:C:510:ALA:HB2	1:C:560:GLY:HA3	1.92	0.51
1:A:443:ASP:O	1:A:447:GLY:N	2.28	0.51
1:A:310:LEU:HD11	3:A:1611:FAD:HM73	1.91	0.51
1:A:430:SER:HG	1:D:425:GLU:CD	2.14	0.51
1:C:271:ARG:HH11	1:C:271:ARG:CG	2.17	0.51
1:C:412:GLU:CD	1:C:421:ARG:HD2	2.31	0.51
1:B:467:ASN:ND2	1:B:473:LYS:H	2.02	0.51
1:A:238:ARG:HB3	1:A:238:ARG:HH21	1.76	0.51
1:A:283:PHE:HE1	1:A:289:PHE:HA	1.76	0.50
1:C:446:LEU:CD2	1:C:447:GLY:N	2.72	0.50
1:C:343:LEU:HD22	1:C:347:LEU:HD23	1.94	0.50
1:A:183:ASP:OD1	1:A:184:PRO:HD2	2.11	0.50
1:C:140:THR:HG23	1:C:204:PHE:HZ	1.77	0.50
1:B:216:LEU:HB3	1:B:217:PRO:HD3	1.93	0.49
1:D:436:GLY:HA2	1:D:457:ALA:HA	1.95	0.49
1:C:437:ASP:OD2	1:C:452:GLU:HA	2.12	0.49
1:D:202:ILE:HG12	1:D:202:ILE:O	2.11	0.49
1:A:525:THR:HG21	1:A:530:GLU:HB2	1.93	0.49
1:C:401:PRO:HG2	4:C:613:HOH:O	2.12	0.49
1:B:421:ARG:NH1	1:C:421:ARG:NH1	2.58	0.49
1:C:284:ARG:HG3	1:C:284:ARG:NH1	2.23	0.49
1:D:511:THR:OG1	1:D:512:ALA:N	2.46	0.49
1:A:283:PHE:CE1	1:A:289:PHE:HA	2.48	0.49
1:A:167:LEU:O	1:A:203:TYR:HD1	1.96	0.49
1:C:569:ASP:O	1:C:570:LYS:HB2	2.13	0.49
1:B:478:GLN:HB3	1:B:494:ILE:HD11	1.94	0.49
1:B:467:ASN:HD21	1:B:473:LYS:N	2.05	0.48
1:A:523:SER:CB	1:A:531:SER:HB2	2.44	0.48
1:B:507:PHE:CD2	1:B:562:GLY:HA3	2.48	0.48
1:D:154:PRO:O	1:D:156:ALA:N	2.46	0.48
1:D:345:GLN:O	1:D:349:ASN:HB2	2.12	0.48
1:A:580:VAL:HG11	1:A:607:PHE:HB3	1.96	0.48
1:C:269:ILE:HG22	1:C:269:ILE:O	2.13	0.48
1:D:232:VAL:HG23	3:D:1611:FAD:N1A	2.29	0.48
1:C:231:LYS:H	1:C:245:ASN:HD21	1.54	0.48
1:C:443:ASP:OD2	1:C:446:LEU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:SER:C	1:B:280:THR:H	2.18	0.48
1:B:338:ASN:ND2	1:B:352:MET:HB2	2.29	0.47
1:D:205:GLN:HG3	1:D:209:PHE:CE2	2.48	0.47
1:A:510:ALA:HB1	1:A:514:ASP:HB2	1.95	0.47
1:C:183:ASP:O	1:C:186:VAL:HB	2.14	0.47
1:C:603:VAL:O	1:C:606:LEU:HB2	2.14	0.47
1:B:132:PRO:HA	1:B:253:GLU:HB2	1.96	0.47
1:B:423:ASN:HD21	1:B:427:GLN:H	1.62	0.47
1:C:338:ASN:O	1:C:339:MET:HB2	2.14	0.47
1:D:154:PRO:O	1:D:155:GLY:C	2.52	0.47
1:A:433:TRP:CE3	1:A:468:MET:HG2	2.49	0.47
1:B:200:ARG:HG3	1:B:201:SER:N	2.30	0.47
1:B:293:GLU:OE2	1:B:297:ARG:NH2	2.48	0.47
1:C:172:PRO:HB2	1:C:173:PRO:CD	2.42	0.47
1:C:200:ARG:HG3	1:C:201:SER:N	2.29	0.47
1:B:200:ARG:CG	1:B:201:SER:N	2.77	0.47
1:C:446:LEU:HD23	1:C:447:GLY:N	2.10	0.47
1:B:135:LEU:HD12	1:B:160:ILE:HG12	1.96	0.47
1:B:280:THR:HA	1:B:393:ILE:O	2.14	0.47
1:B:456:HIS:CD2	1:B:475:TYR:OH	2.68	0.47
1:C:207:PRO:O	1:C:210:TYR:HD2	1.98	0.47
1:D:430:SER:O	1:D:431:ASN:HB2	2.15	0.47
1:D:141:ALA:HA	1:D:457:ALA:O	2.15	0.47
1:A:171:ARG:N	1:A:172:PRO:CD	2.78	0.47
1:C:205:GLN:HE21	1:C:206:PRO:HD2	1.80	0.47
1:A:235:LEU:HD12	1:A:242:VAL:HG12	1.96	0.47
1:A:446:LEU:HD22	1:A:449:ARG:HD2	1.96	0.47
1:A:292:LEU:HD13	1:A:394:VAL:HG21	1.98	0.46
1:D:195:TRP:HB3	1:D:517:LYS:HA	1.96	0.46
1:A:423:ASN:C	1:A:423:ASN:HD22	2.18	0.46
1:C:197:GLY:O	1:C:198:LYS:C	2.53	0.46
1:C:515:ASN:ND2	1:C:518:SER:H	2.13	0.46
1:D:252:PHE:CE1	1:D:255:CYS:HB2	2.50	0.46
1:A:175:SER:OG	1:A:313:GLU:OE2	2.27	0.46
1:B:145:ALA:HA	1:B:461:GLY:O	2.15	0.46
1:B:241:MET:HB3	1:B:251:THR:HG22	1.97	0.46
1:B:332:LEU:HB3	1:B:363:MET:HB2	1.98	0.46
1:C:310:LEU:HB3	1:C:396:ALA:HB1	1.96	0.46
1:C:131:VAL:O	1:C:252:PHE:HA	2.14	0.46
1:B:561:LYS:HE3	1:B:580:VAL:HG22	1.97	0.46
1:D:131:VAL:HG21	1:D:159:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:SER:HB3	1:D:327:ILE:HD12	1.97	0.46
1:B:507:PHE:HD2	1:B:562:GLY:HA3	1.80	0.46
1:C:353:GLU:OE1	1:C:353:GLU:HA	2.16	0.46
1:D:371:VAL:HG13	1:D:380:ILE:HG12	1.98	0.46
1:A:322:SER:C	1:A:324:ALA:H	2.19	0.46
1:A:268:ALA:HA	1:A:271:ARG:NH2	2.30	0.45
1:A:393:ILE:HG22	1:A:395:THR:HG22	1.98	0.45
1:B:133:PHE:CD2	1:B:149:ILE:HD13	2.51	0.45
1:B:171:ARG:CG	1:B:171:ARG:NH1	2.79	0.45
1:A:211:VAL:O	1:A:225:ALA:HA	2.17	0.45
1:C:241:MET:HB3	1:C:251:THR:HG22	1.98	0.45
1:D:170:MET:HB3	1:D:204:PHE:CE1	2.51	0.45
1:D:231:LYS:H	1:D:245:ASN:ND2	2.14	0.45
1:A:454:HIS:CD2	1:A:454:HIS:C	2.88	0.45
1:C:498:ASP:OD2	1:C:500:SER:OG	2.34	0.45
1:A:533:THR:HG22	1:A:535:SER:N	2.29	0.45
1:B:462:ARG:NH2	1:B:534:GLU:OE1	2.49	0.45
1:B:282:LEU:HD23	1:B:395:THR:OG1	2.16	0.45
1:B:479:SER:O	1:B:494:ILE:HG12	2.16	0.45
1:D:597:HIS:NE2	1:D:603:VAL:HG21	2.32	0.45
1:C:271:ARG:HG3	1:C:271:ARG:NH1	2.20	0.45
1:B:583:ARG:NH1	1:B:608:ASN:HB2	2.31	0.45
1:D:414:ASP:O	1:D:418:GLY:N	2.49	0.44
1:D:528:ARG:HD3	1:D:581:PHE:CE2	2.52	0.44
1:B:152:ARG:NE	4:B:613:HOH:O	2.50	0.44
1:B:344:PRO:O	1:B:345:GLN:C	2.56	0.44
1:A:460:SER:O	1:A:464:ALA:N	2.47	0.44
1:B:127:ALA:HA	1:B:128:PRO:HD3	1.87	0.44
1:B:428:ALA:HB3	1:B:432:ILE:HG22	2.00	0.44
1:B:464:ALA:O	1:B:468:MET:HG3	2.17	0.44
1:C:453:HIS:HB2	1:C:456:HIS:HB3	1.99	0.44
1:A:313:GLU:HG2	1:A:484:ASP:O	2.18	0.44
1:A:384:ASP:OD1	1:A:386:ARG:HD3	2.17	0.44
1:B:266:LEU:HB3	1:B:269:ILE:HD12	1.98	0.44
1:D:414:ASP:O	1:D:418:GLY:CA	2.65	0.44
1:A:343:LEU:HD13	1:A:347:LEU:HD23	1.99	0.44
1:A:266:LEU:O	1:A:269:ILE:N	2.42	0.44
1:A:367:ILE:HD12	1:A:383:LYS:HD2	1.99	0.44
1:D:352:MET:HG3	1:D:362:VAL:HG11	1.99	0.44
1:A:279:ARG:HB2	1:A:378:LEU:HD11	1.99	0.44
1:A:195:TRP:O	1:A:517:LYS:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:CB	1:A:378:LEU:HD11	2.48	0.44
1:A:515:ASN:ND2	1:A:517:LYS:HB3	2.33	0.44
1:C:169:TYR:HB2	1:C:202:ILE:HG12	2.00	0.44
1:A:133:PHE:HB2	1:A:158:VAL:HG22	2.00	0.43
1:A:260:GLY:HA2	1:A:437:ASP:HB2	2.00	0.43
1:B:172:PRO:HB3	1:B:176:LYS:HZ3	1.80	0.43
1:B:178:LEU:HB3	1:B:289:PHE:CZ	2.53	0.43
1:D:165:PRO:HA	1:D:228:THR:HB	1.99	0.43
1:A:414:ASP:O	1:A:418:GLY:N	2.50	0.43
1:A:515:ASN:N	1:A:581:PHE:HE1	2.16	0.43
1:A:563:VAL:HB	1:A:577:LEU:HD23	2.00	0.43
1:D:289:PHE:O	1:D:293:GLU:HB2	2.18	0.43
1:D:413:ILE:HG22	1:D:419:GLY:H	1.82	0.43
1:B:427:GLN:HG3	1:B:433:TRP:CE2	2.53	0.43
1:C:302:ILE:HG22	1:C:303:THR:N	2.33	0.43
1:B:150:ARG:HH21	1:B:223:GLY:HA2	1.83	0.43
1:B:183:ASP:OD2	1:B:185:ASN:HB2	2.18	0.43
1:B:451:VAL:HG22	1:B:456:HIS:CG	2.54	0.43
1:C:169:TYR:CE1	1:C:286:ILE:HG13	2.54	0.43
1:C:403:VAL:HG12	1:C:420:PHE:CE1	2.53	0.43
1:A:155:GLY:HA2	1:A:221:ASN:O	2.18	0.43
1:B:457:ALA:HB2	3:B:1611:FAD:H5'2	2.01	0.43
1:A:567:LEU:HD21	1:A:600:LEU:CD1	2.48	0.42
1:A:422:VAL:HG11	1:A:434:VAL:HB	2.01	0.42
1:D:230:LYS:HB3	1:D:244:LEU:HD13	2.01	0.42
1:D:292:LEU:O	1:D:296:SER:N	2.44	0.42
1:A:254:LYS:HD2	1:A:433:TRP:CZ3	2.54	0.42
1:A:464:ALA:O	1:A:468:MET:HG3	2.19	0.42
1:C:180:PHE:HE2	1:C:320:ARG:HG3	1.85	0.42
1:C:356:LYS:HG3	1:C:362:VAL:CG2	2.50	0.42
1:B:231:LYS:O	1:B:244:LEU:HA	2.20	0.42
1:C:540:ILE:HG23	1:C:589:LYS:HG2	2.02	0.42
1:D:485:LEU:HB2	1:D:489:VAL:HB	2.02	0.42
1:C:143:PHE:CE2	1:C:204:PHE:HB3	2.55	0.42
1:C:271:ARG:CG	1:C:271:ARG:NH1	2.81	0.42
1:A:177:GLU:HG3	1:A:195:TRP:CZ2	2.55	0.41
1:C:266:LEU:O	1:C:267:SER:C	2.59	0.41
1:D:131:VAL:HG22	1:D:133:PHE:H	1.85	0.41
1:A:604:ALA:C	1:A:606:LEU:H	2.23	0.41
1:A:481:PHE:CG	1:A:482:TRP:N	2.88	0.41
1:D:492:GLU:CB	1:D:577:LEU:HB2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PHE:CE2	1:A:443:ASP:HB2	2.54	0.41
1:D:216:LEU:HB3	1:D:217:PRO:HD3	2.02	0.41
1:D:363:MET:HA	1:D:364:PRO:HD3	1.90	0.41
1:A:577:LEU:HD21	1:A:607:PHE:CE1	2.56	0.41
1:B:190:LEU:HD12	1:B:190:LEU:HA	1.93	0.41
1:D:566:TYR:HB2	1:D:574:GLY:HA3	2.01	0.41
1:D:584:MET:H	1:D:585:PRO:HD2	1.83	0.41
1:A:453:HIS:CD2	1:A:479:SER:OG	2.74	0.41
1:B:172:PRO:HG3	3:B:1611:FAD:C4X	2.51	0.41
1:A:313:GLU:OE1	1:A:483:SER:OG	2.26	0.41
1:D:155:GLY:HA2	1:D:221:ASN:O	2.21	0.41
1:A:330:ILE:HA	1:A:361:LYS:O	2.21	0.41
1:B:272:ALA:HB1	1:B:276:VAL:HG21	2.02	0.41
1:B:302:ILE:HG23	1:B:392:HIS:HB3	2.02	0.41
1:D:171:ARG:N	1:D:172:PRO:CD	2.84	0.41
1:A:171:ARG:H	1:A:172:PRO:CD	2.34	0.41
1:A:281:THR:OG1	1:A:394:VAL:HG22	2.21	0.41
1:A:426:LEU:HD11	1:A:463:LEU:HD23	2.03	0.41
1:A:604:ALA:C	1:A:606:LEU:N	2.73	0.41
1:B:286:ILE:O	1:B:287:GLY:C	2.59	0.41
1:C:307:GLY:O	1:C:308:GLY:O	2.39	0.41
1:D:228:THR:O	1:D:230:LYS:HG2	2.21	0.41
1:D:427:GLN:HB2	1:D:433:TRP:NE1	2.36	0.41
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.79	0.40
1:C:171:ARG:N	1:C:172:PRO:HD2	2.36	0.40
1:C:339:MET:CE	1:C:351:THR:HG21	2.52	0.40
1:C:532:GLU:O	1:C:533:THR:OG1	2.32	0.40
1:C:367:ILE:O	1:C:383:LYS:N	2.53	0.40
1:B:456:HIS:HD2	1:B:475:TYR:OH	2.04	0.40
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.86	0.40
1:C:235:LEU:O	1:C:409:GLY:HA2	2.20	0.40
1:D:195:TRP:HB2	1:D:520:THR:HG21	2.02	0.40
1:D:420:PHE:HB2	1:D:434:VAL:HG11	2.02	0.40
1:A:226:VAL:HG22	1:A:228:THR:HG23	2.04	0.40
1:A:411:LEU:HD22	1:A:428:ALA:HB1	2.04	0.40
1:A:523:SER:HB3	1:A:531:SER:HB2	2.03	0.40
1:B:493:ALA:O	1:B:494:ILE:HB	2.22	0.40
1:D:569:ASP:O	1:D:570:LYS:HB2	2.22	0.40
1:A:351:THR:OG1	1:A:491:TYR:OH	2.33	0.40
1:A:423:ASN:ND2	1:A:427:GLN:H	2.20	0.40
1:A:608:ASN:OD1	1:A:610:HIS:CE1	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ASN:HA	1:B:471:ALA:HB3	2.04	0.40
1:D:237:VAL:HG11	1:D:429:ARG:CZ	2.51	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	459/535 (86%)	406 (88%)	43 (9%)	10 (2%)	6	28
1	B	472/535 (88%)	426 (90%)	41 (9%)	5 (1%)	14	46
1	C	463/535 (86%)	410 (89%)	48 (10%)	5 (1%)	14	46
1	D	461/535 (86%)	417 (90%)	36 (8%)	8 (2%)	9	34
All	All	1855/2140 (87%)	1659 (89%)	168 (9%)	28 (2%)	10	38

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	446	LEU
1	A	570	LYS
1	C	177	GLU
1	C	537	ALA
1	A	533	THR
1	B	494	ILE
1	B	560	GLY
1	C	308	GLY
1	D	155	GLY
1	D	365	ASN
1	D	559	TYR
1	A	284	ARG

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Mol	Chain	Res	Type
1	B	284	ARG
1	B	538	SER
1	C	198	LYS
1	C	406	ALA
1	D	582	ASN
1	A	462	ARG
1	B	345	GLN
1	D	284	ARG
1	A	323	GLN
1	A	444	ILE
1	A	522	GLN
1	A	560	GLY
1	D	154	PRO
1	D	584	MET
1	D	516	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	379/435 (87%)	345 (91%)	34 (9%)	9	32
1	B	390/435 (90%)	363 (93%)	27 (7%)	15	44
1	C	383/435 (88%)	351 (92%)	32 (8%)	11	35
1	D	381/435 (88%)	351 (92%)	30 (8%)	12	37
All	All	1533/1740 (88%)	1410 (92%)	123 (8%)	12	37

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	THR
1	A	190	LEU
1	A	201	SER
1	A	219	ILE
1	A	227	LEU
1	A	238	ARG

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Mol	Chain	Res	Type
1	A	241	MET
1	A	276	VAL
1	A	297	ARG
1	A	322	SER
1	A	341	LYS
1	A	345	GLN
1	A	379	LEU
1	A	383	LYS
1	A	386	ARG
1	A	389	GLU
1	A	395	THR
1	A	397	VAL
1	A	413	ILE
1	A	423	ASN
1	A	446	LEU
1	A	451	VAL
1	A	454	HIS
1	A	476	TRP
1	A	482	TRP
1	A	496	LEU
1	A	513	GLN
1	A	517	LYS
1	A	534	GLU
1	A	558	ASP
1	A	563	VAL
1	A	569	ASP
1	A	596	GLN
1	A	606	LEU
1	B	129	SER
1	B	164	ASP
1	B	171	ARG
1	B	190	LEU
1	B	205	GLN
1	B	212	SER
1	B	227	LEU
1	B	228	THR
1	B	241	MET
1	B	270	ASP
1	B	275	GLU
1	B	282	LEU
1	B	284	ARG
1	B	300	LYS

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Mol	Chain	Res	Type
1	B	336	LYS
1	B	345	GLN
1	B	346	TYR
1	B	349	ASN
1	B	384	ASP
1	B	423	ASN
1	B	449	ARG
1	B	476	TRP
1	B	494	ILE
1	B	558	ASP
1	B	569	ASP
1	B	575	ILE
1	B	608	ASN
1	C	140	THR
1	C	147	ARG
1	C	152	ARG
1	C	157	ARG
1	C	164	ASP
1	C	185	ASN
1	C	190	LEU
1	C	205	GLN
1	C	220	GLU
1	C	227	LEU
1	C	241	MET
1	C	266	LEU
1	C	275	GLU
1	C	276	VAL
1	C	279	ARG
1	C	332	LEU
1	C	345	GLN
1	C	353	GLU
1	C	367	ILE
1	C	380	ILE
1	C	383	LYS
1	C	402	ASN
1	C	417	PHE
1	C	423	ASN
1	C	432	ILE
1	C	444	ILE
1	C	451	VAL
1	C	452	GLU
1	C	494	ILE

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Mol	Chain	Res	Type
1	C	500	SER
1	C	511	THR
1	C	593	ASP
1	D	129	SER
1	D	150	ARG
1	D	152	ARG
1	D	195	TRP
1	D	198	LYS
1	D	200	ARG
1	D	202	ILE
1	D	209	PHE
1	D	211	VAL
1	D	226	VAL
1	D	227	LEU
1	D	241	MET
1	D	284	ARG
1	D	285	LYS
1	D	304	VAL
1	D	321	LYS
1	D	330	ILE
1	D	345	GLN
1	D	349	ASN
1	D	354	LYS
1	D	413	ILE
1	D	432	ILE
1	D	443	ASP
1	D	446	LEU
1	D	453	HIS
1	D	494	ILE
1	D	497	VAL
1	D	567	LEU
1	D	573	VAL
1	D	599	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	338	ASN
1	A	345	GLN
1	A	365	ASN
1	A	402	ASN

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Mol	Chain	Res	Type
1	A	423	ASN
1	A	453	HIS
1	A	454	HIS
1	A	456	HIS
1	A	467	ASN
1	A	477	HIS
1	A	596	GLN
1	A	610	HIS
1	B	194	GLN
1	B	205	GLN
1	B	234	HIS
1	B	245	ASN
1	B	338	ASN
1	B	365	ASN
1	B	402	ASN
1	B	423	ASN
1	B	453	HIS
1	B	456	HIS
1	B	467	ASN
1	B	478	GLN
1	B	610	HIS
1	C	205	GLN
1	C	245	ASN
1	C	249	GLN
1	C	323	GLN
1	C	365	ASN
1	C	402	ASN
1	C	423	ASN
1	C	453	HIS
1	C	456	HIS
1	C	467	ASN
1	C	513	GLN
1	C	515	ASN
1	C	522	GLN
1	D	205	GLN
1	D	338	ASN
1	D	427	GLN
1	D	456	HIS
1	D	467	ASN
1	D	477	HIS
1	D	579	ASN
1	D	596	GLN

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Mol	Chain	Res	Type
1	D	608	ASN
1	D	610	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	FAD	B	1611	-	53,58,58	2.14	9 (16%)	68,89,89	3.16	19 (27%)
3	FAD	A	1611	-	53,58,58	2.11	7 (13%)	68,89,89	3.07	17 (25%)
3	FAD	C	1611	-	53,58,58	2.13	8 (15%)	68,89,89	3.08	17 (25%)
3	FAD	D	1611	-	53,58,58	2.11	10 (18%)	68,89,89	3.13	16 (23%)

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	FAD	B	1611	-	-	12/30/50/50	0/6/6/6
3	FAD	A	1611	-	-	7/30/50/50	0/6/6/6
3	FAD	C	1611	-	-	10/30/50/50	0/6/6/6
3	FAD	D	1611	-	-	11/30/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1611	FAD	C6-C7	-8.96	1.26	1.39
3	C	1611	FAD	C6-C5X	-8.94	1.25	1.40
3	B	1611	FAD	C6-C7	-8.93	1.26	1.39
3	A	1611	FAD	C6-C5X	-8.77	1.26	1.40
3	B	1611	FAD	C6-C5X	-8.71	1.26	1.40
3	D	1611	FAD	C6-C7	-8.69	1.26	1.39
3	D	1611	FAD	C6-C5X	-8.62	1.26	1.40
3	A	1611	FAD	C6-C7	-8.34	1.27	1.39
3	A	1611	FAD	C9A-C5X	4.99	1.49	1.41
3	B	1611	FAD	C9A-C5X	4.54	1.48	1.41
3	D	1611	FAD	C9A-C5X	4.37	1.48	1.41
3	C	1611	FAD	C9A-C5X	4.26	1.48	1.41
3	C	1611	FAD	C5X-N5	-2.92	1.33	1.39
3	A	1611	FAD	C5X-N5	-2.92	1.33	1.39
3	B	1611	FAD	C5A-C4A	2.85	1.48	1.40
3	B	1611	FAD	C5X-N5	-2.82	1.34	1.39
3	B	1611	FAD	C9-C8	2.81	1.43	1.39
3	D	1611	FAD	C5A-C4A	2.76	1.48	1.40
3	C	1611	FAD	C5A-C4A	2.69	1.48	1.40
3	D	1611	FAD	C4X-N5	2.65	1.35	1.30
3	D	1611	FAD	C5X-N5	-2.63	1.34	1.39
3	A	1611	FAD	C5A-C4A	2.54	1.47	1.40
3	D	1611	FAD	C10-N10	2.46	1.42	1.37
3	A	1611	FAD	C4X-N5	2.45	1.35	1.30
3	A	1611	FAD	C10-N10	2.37	1.42	1.37
3	C	1611	FAD	C4X-N5	2.36	1.35	1.30
3	D	1611	FAD	C9-C8	2.33	1.43	1.39
3	D	1611	FAD	C2A-N3A	2.20	1.35	1.32
3	C	1611	FAD	C9-C8	2.14	1.42	1.39
3	D	1611	FAD	C9-C9A	2.13	1.43	1.39
3	B	1611	FAD	C9-C9A	2.06	1.43	1.39
3	B	1611	FAD	C4X-N5	2.06	1.34	1.30
3	B	1611	FAD	C10-N10	2.03	1.41	1.37
3	C	1611	FAD	C10-N10	2.02	1.41	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1611	FAD	C5X-C6-C7	16.51	151.00	120.71
3	B	1611	FAD	C5X-C6-C7	16.32	150.66	120.71
3	C	1611	FAD	C5X-C6-C7	16.25	150.52	120.71
3	A	1611	FAD	C5X-C6-C7	15.62	149.38	120.71
3	D	1611	FAD	C6-C5X-C9A	-10.33	104.32	118.94
3	C	1611	FAD	C6-C5X-C9A	-10.11	104.64	118.94
3	B	1611	FAD	C6-C5X-C9A	-10.03	104.75	118.94
3	A	1611	FAD	C6-C5X-C9A	-9.68	105.25	118.94
3	A	1611	FAD	C6-C7-C8	-8.99	106.79	119.67
3	B	1611	FAD	C6-C7-C8	-8.75	107.13	119.67
3	D	1611	FAD	C6-C7-C8	-8.70	107.20	119.67
3	C	1611	FAD	C6-C7-C8	-8.62	107.31	119.67
3	D	1611	FAD	C6-C5X-N5	7.82	132.16	118.51
3	C	1611	FAD	C6-C5X-N5	7.68	131.92	118.51
3	A	1611	FAD	C6-C5X-N5	7.65	131.86	118.51
3	B	1611	FAD	C6-C5X-N5	7.20	131.09	118.51
3	B	1611	FAD	C9-C9A-N10	4.18	127.49	121.84
3	B	1611	FAD	N3A-C2A-N1A	-4.02	122.39	128.68
3	A	1611	FAD	N3A-C2A-N1A	-3.99	122.44	128.68
3	A	1611	FAD	P-O3P-PA	-3.90	119.43	132.83
3	C	1611	FAD	N3A-C2A-N1A	-3.81	122.72	128.68
3	D	1611	FAD	N3A-C2A-N1A	-3.80	122.74	128.68
3	C	1611	FAD	C7M-C7-C6	3.79	126.50	119.49
3	D	1611	FAD	C4A-C5A-N7A	-3.73	105.51	109.40
3	B	1611	FAD	C4X-C10-N10	3.69	121.87	116.48
3	A	1611	FAD	C7M-C7-C6	3.63	126.20	119.49
3	D	1611	FAD	C7M-C7-C6	3.52	126.00	119.49
3	C	1611	FAD	P-O3P-PA	-3.51	120.77	132.83
3	D	1611	FAD	C9-C9A-N10	3.44	126.49	121.84
3	B	1611	FAD	C7M-C7-C6	3.43	125.83	119.49
3	C	1611	FAD	C4A-C5A-N7A	-3.40	105.86	109.40
3	A	1611	FAD	C4X-C4-N3	3.36	121.72	113.19
3	C	1611	FAD	C4X-C10-N10	3.16	121.09	116.48
3	A	1611	FAD	C4-N3-C2	-3.15	119.83	125.64
3	C	1611	FAD	C9-C9A-N10	3.13	126.07	121.84
3	D	1611	FAD	C4X-C10-N10	3.10	121.01	116.48
3	B	1611	FAD	C7M-C7-C8	3.08	127.04	120.74
3	A	1611	FAD	C7M-C7-C8	3.06	127.01	120.74
3	A	1611	FAD	C9-C9A-N10	3.01	125.91	121.84
3	A	1611	FAD	C4A-C5A-N7A	-2.99	106.29	109.40
3	A	1611	FAD	O4-C4-C4X	-2.97	118.72	126.60
3	D	1611	FAD	C7M-C7-C8	2.96	126.80	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1611	FAD	C4-N3-C2	-2.93	120.22	125.64
3	B	1611	FAD	C4A-C5A-N7A	-2.75	106.53	109.40
3	D	1611	FAD	P-O3P-PA	-2.69	123.58	132.83
3	D	1611	FAD	C4X-C4-N3	2.69	120.02	113.19
3	A	1611	FAD	C4X-C10-N10	2.68	120.40	116.48
3	B	1611	FAD	C4X-C4-N3	2.67	119.96	113.19
3	C	1611	FAD	C7M-C7-C8	2.66	126.19	120.74
3	C	1611	FAD	C4X-C4-N3	2.63	119.88	113.19
3	B	1611	FAD	O4B-C1B-C2B	-2.61	103.12	106.93
3	B	1611	FAD	C10-N1-C2	2.58	122.06	116.90
3	B	1611	FAD	C4'-C3'-C2'	-2.52	108.12	113.36
3	C	1611	FAD	C4-N3-C2	-2.49	121.05	125.64
3	B	1611	FAD	O4-C4-C4X	-2.45	120.11	126.60
3	B	1611	FAD	C4X-C10-N1	-2.42	119.12	124.73
3	B	1611	FAD	C5X-C9A-N10	-2.40	115.47	117.95
3	A	1611	FAD	C4X-C10-N1	-2.35	119.27	124.73
3	A	1611	FAD	C10-N1-C2	2.29	121.47	116.90
3	C	1611	FAD	O4-C4-C4X	-2.27	120.57	126.60
3	C	1611	FAD	C10-N1-C2	2.27	121.44	116.90
3	D	1611	FAD	C10-N1-C2	2.26	121.42	116.90
3	D	1611	FAD	C4-N3-C2	-2.23	121.53	125.64
3	D	1611	FAD	C4X-C10-N1	-2.20	119.62	124.73
3	D	1611	FAD	O4-C4-C4X	-2.17	120.85	126.60
3	C	1611	FAD	C4X-C10-N1	-2.15	119.74	124.73
3	A	1611	FAD	O2A-PA-O1A	2.10	122.61	112.24
3	B	1611	FAD	P-O3P-PA	-2.05	125.80	132.83
3	C	1611	FAD	C9A-N10-C10	-2.03	117.61	120.77

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1611	FAD	C5B-O5B-PA-O1A
3	A	1611	FAD	N10-C1'-C2'-O2'
3	B	1611	FAD	C5B-O5B-PA-O1A
3	B	1611	FAD	N10-C1'-C2'-O2'
3	B	1611	FAD	N10-C1'-C2'-C3'
3	B	1611	FAD	C2'-C3'-C4'-O4'
3	B	1611	FAD	O3'-C3'-C4'-O4'
3	B	1611	FAD	O3'-C3'-C4'-C5'
3	C	1611	FAD	C5B-O5B-PA-O1A
3	C	1611	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
3	C	1611	FAD	N10-C1'-C2'-C3'
3	C	1611	FAD	C2'-C3'-C4'-O4'
3	C	1611	FAD	O3'-C3'-C4'-O4'
3	C	1611	FAD	O3'-C3'-C4'-C5'
3	C	1611	FAD	O4'-C4'-C5'-O5'
3	D	1611	FAD	C5B-O5B-PA-O1A
3	D	1611	FAD	N10-C1'-C2'-O2'
3	D	1611	FAD	N10-C1'-C2'-C3'
3	D	1611	FAD	C2'-C3'-C4'-C5'
3	D	1611	FAD	O3'-C3'-C4'-C5'
3	D	1611	FAD	O3'-C3'-C4'-O4'
3	A	1611	FAD	O4B-C4B-C5B-O5B
3	A	1611	FAD	C3B-C4B-C5B-O5B
3	B	1611	FAD	O4B-C4B-C5B-O5B
3	B	1611	FAD	C3B-C4B-C5B-O5B
3	C	1611	FAD	O4B-C4B-C5B-O5B
3	C	1611	FAD	C3B-C4B-C5B-O5B
3	D	1611	FAD	O4B-C4B-C5B-O5B
3	D	1611	FAD	C3B-C4B-C5B-O5B
3	D	1611	FAD	C2'-C3'-C4'-O4'
3	B	1611	FAD	C2'-C3'-C4'-C5'
3	C	1611	FAD	C2'-C3'-C4'-C5'
3	B	1611	FAD	C5B-O5B-PA-O3P
3	D	1611	FAD	C5B-O5B-PA-O3P
3	D	1611	FAD	C5B-O5B-PA-O2A
3	B	1611	FAD	O4'-C4'-C5'-O5'
3	A	1611	FAD	C5B-O5B-PA-O3P
3	B	1611	FAD	C5B-O5B-PA-O2A
3	A	1611	FAD	N10-C1'-C2'-C3'
3	A	1611	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1611	FAD	2	0
3	A	1611	FAD	2	0
3	D	1611	FAD	1	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 B 1611

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 1611

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD C 1611

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 1611
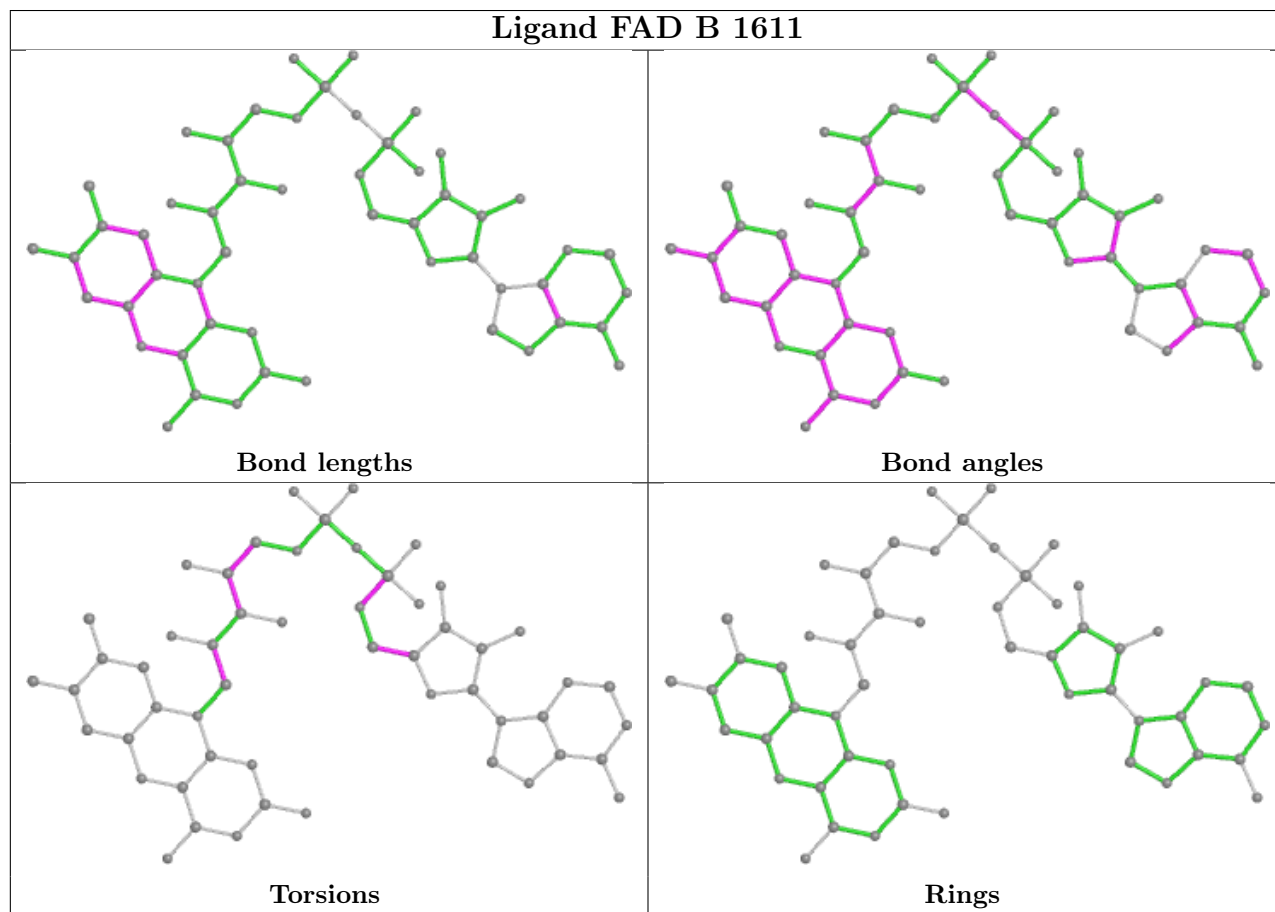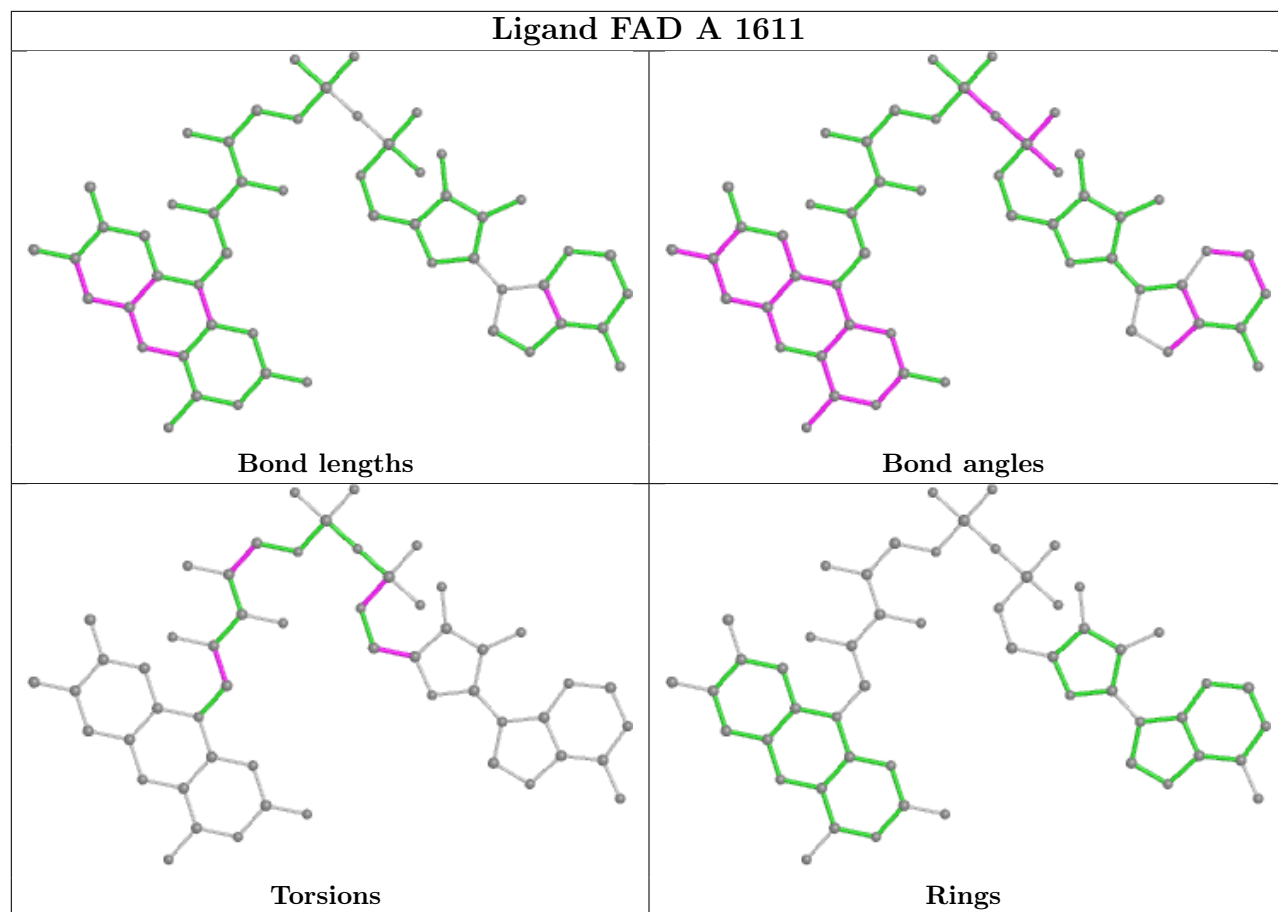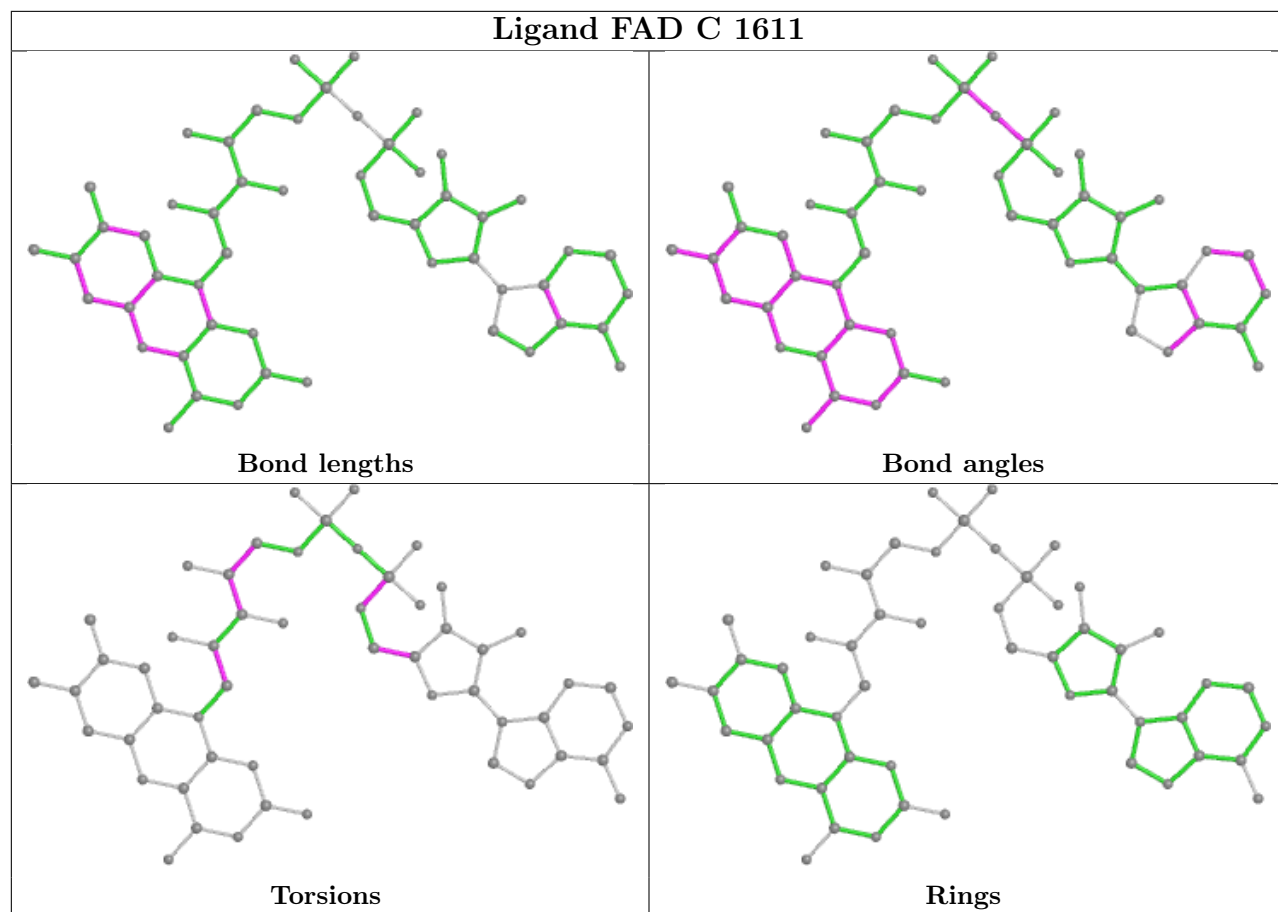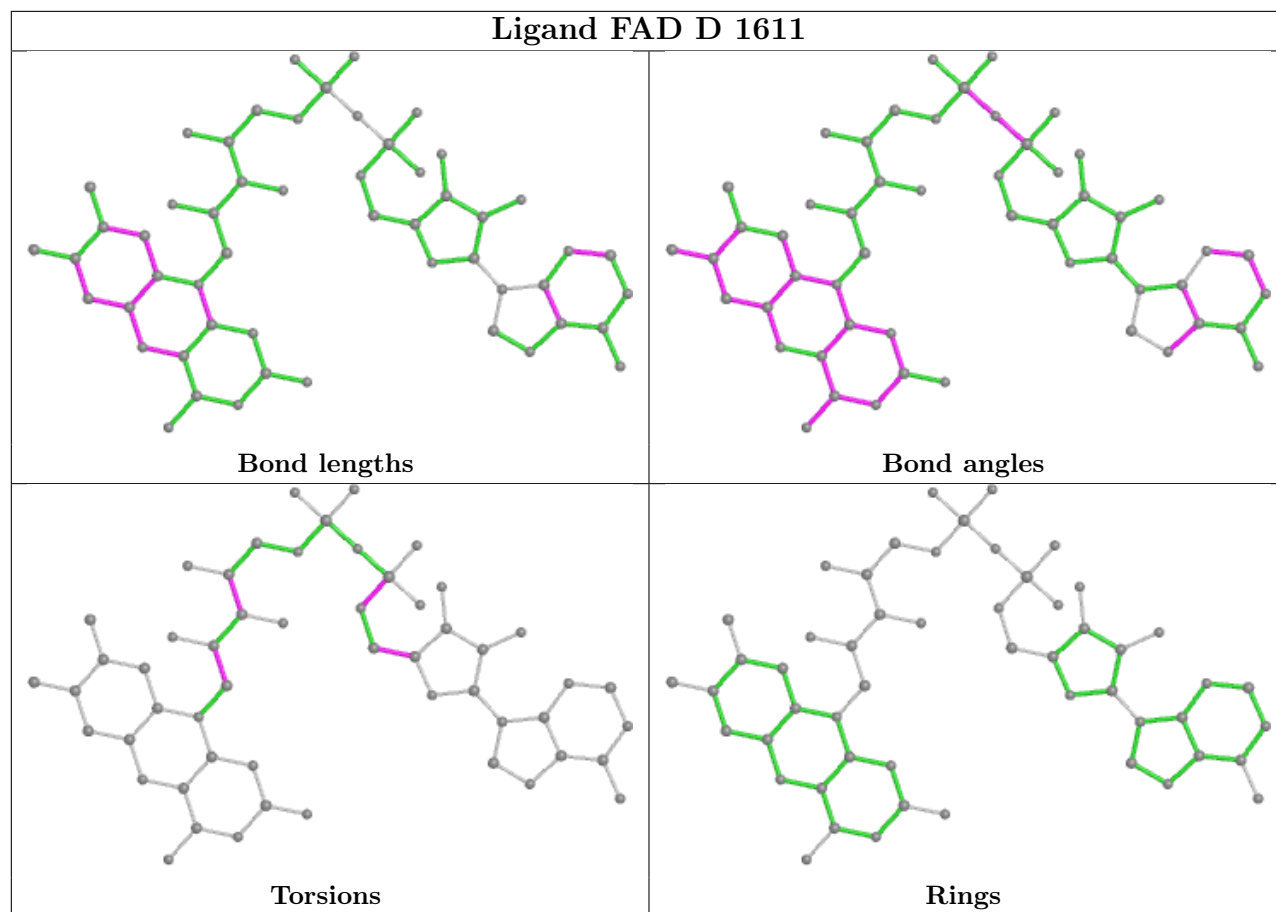
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	463/535 (86%)	0.06	3 (0%)	89	78	50, 78, 109, 124	0
1	B	476/535 (88%)	0.29	27 (5%)	23	14	60, 98, 149, 196	0
1	C	467/535 (87%)	0.11	10 (2%)	63	46	62, 94, 137, 163	0
1	D	465/535 (86%)	1.09	102 (21%)	0	0	73, 154, 224, 263	0
2	E	0/9	-	-			-	-
2	F	0/9	-	-			-	-
All	All	1871/2158 (86%)	0.39	142 (7%)	13	7	50, 95, 196, 263	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	610	HIS	6.9
1	D	562	GLY	6.6
1	D	490	GLY	6.6
1	D	303	THR	6.5
1	D	363	MET	6.4
1	D	506	VAL	6.1
1	B	555	GLU	6.0
1	D	338	ASN	6.0
1	C	541	THR	5.9
1	D	371	VAL	5.9
1	D	319	GLY	5.7
1	D	602	GLU	5.7
1	D	507	PHE	5.5
1	D	374	SER	5.5
1	D	597	HIS	5.4
1	B	554	VAL	5.4
1	B	541	THR	5.3
1	D	563	VAL	5.3
1	D	357	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	381	LYS	5.1
1	D	302	ILE	5.1
1	D	305	ILE	5.0
1	D	504	VAL	4.9
1	B	543	PRO	4.8
1	D	373	VAL	4.8
1	D	565	PHE	4.7
1	D	351	THR	4.7
1	D	607	PHE	4.7
1	B	597	HIS	4.5
1	D	392	HIS	4.3
1	D	570	LYS	4.3
1	D	383	LYS	4.3
1	D	330	ILE	4.2
1	D	395	THR	4.1
1	D	332	LEU	4.1
1	D	369	GLN	4.1
1	B	545	SER	4.1
1	D	353	GLU	4.1
1	B	373	VAL	4.0
1	D	509	LYS	4.0
1	B	598	GLU	4.0
1	D	380	ILE	3.9
1	D	558	ASP	3.9
1	D	491	TYR	3.7
1	C	271	ARG	3.7
1	B	560	GLY	3.7
1	D	382	LEU	3.7
1	D	222	GLY	3.6
1	D	375	GLY	3.6
1	B	557	GLU	3.6
1	D	557	GLU	3.6
1	D	596	GLN	3.6
1	D	595	GLU	3.5
1	D	505	GLY	3.5
1	D	368	VAL	3.5
1	D	576	VAL	3.5
1	D	318	LEU	3.5
1	D	378	LEU	3.5
1	D	227	LEU	3.4
1	B	558	ASP	3.4
1	D	605	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	273	GLY	3.4
1	D	601	ASN	3.4
1	D	314	LEU	3.3
1	D	283	PHE	3.3
1	D	362	VAL	3.3
1	D	275	GLU	3.3
1	D	299	VAL	3.2
1	D	495	GLY	3.2
1	D	394	VAL	3.1
1	D	331	GLN	3.1
1	D	180	PHE	3.1
1	B	371	VAL	3.1
1	D	317	ALA	3.1
1	B	609	ILE	3.1
1	D	361	LYS	3.1
1	D	304	VAL	3.0
1	D	600	LEU	3.0
1	D	300	LYS	3.0
1	D	339	MET	3.0
1	D	608	ASN	2.9
1	B	374	SER	2.9
1	D	569	ASP	2.9
1	D	529	SER	2.9
1	B	379	LEU	2.9
1	D	321	LYS	2.9
1	D	346	TYR	2.9
1	D	370	SER	2.9
1	A	244	LEU	2.9
1	D	182	ASP	2.9
1	D	379	LEU	2.8
1	B	363	MET	2.8
1	D	277	LYS	2.8
1	D	320	ARG	2.8
1	D	158	VAL	2.7
1	B	381	LYS	2.7
1	D	503	THR	2.7
1	C	389	GLU	2.7
1	D	393	ILE	2.7
1	C	373	VAL	2.6
1	D	192	PHE	2.6
1	B	529	SER	2.6
1	D	609	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	268	ALA	2.5
1	D	315	ALA	2.5
1	B	544	PRO	2.5
1	D	559	TYR	2.5
1	D	282	LEU	2.5
1	B	369	GLN	2.4
1	D	561	LYS	2.4
1	B	380	ILE	2.4
1	C	610	HIS	2.4
1	C	380	ILE	2.3
1	D	181	SER	2.3
1	B	606	LEU	2.3
1	D	564	ILE	2.3
1	D	598	GLU	2.3
1	D	336	LYS	2.3
1	D	599	ASP	2.3
1	B	559	TYR	2.3
1	D	298	GLU	2.2
1	C	580	VAL	2.2
1	D	355	VAL	2.2
1	B	509	LYS	2.2
1	B	332	LEU	2.2
1	C	606	LEU	2.2
1	D	508	ALA	2.2
1	A	243	LYS	2.2
1	D	511	THR	2.1
1	D	528	ARG	2.1
1	B	570	LYS	2.1
1	C	540	ILE	2.1
1	D	376	GLY	2.1
1	D	164	ASP	2.1
1	D	214	GLN	2.1
1	D	560	GLY	2.1
1	D	480	MET	2.1
1	B	531	SER	2.0
1	C	609	ILE	2.0
1	D	388	VAL	2.0
1	A	252	PHE	2.0
1	D	128	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	FAD	D	1611	53/53	0.90	0.21	87,90,111,111	0
3	FAD	C	1611	53/53	0.94	0.23	77,78,81,82	0
3	FAD	A	1611	53/53	0.96	0.19	58,64,76,77	0
3	FAD	B	1611	53/53	0.97	0.20	60,63,69,70	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 D 1611:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
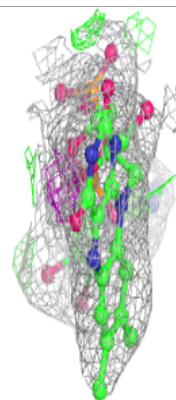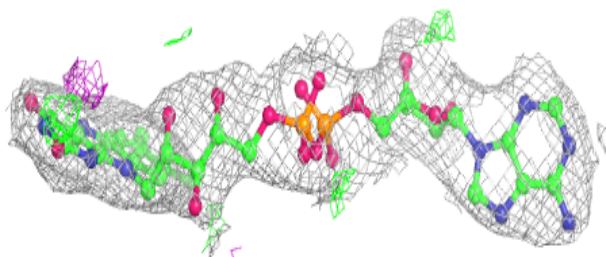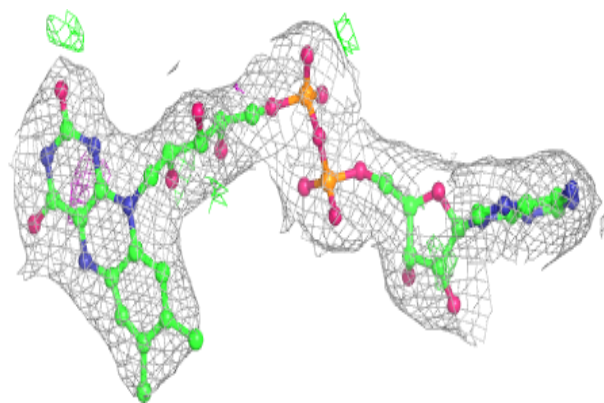and green (positive)
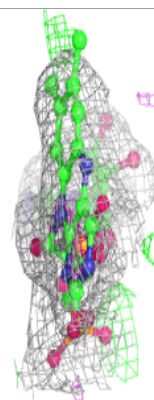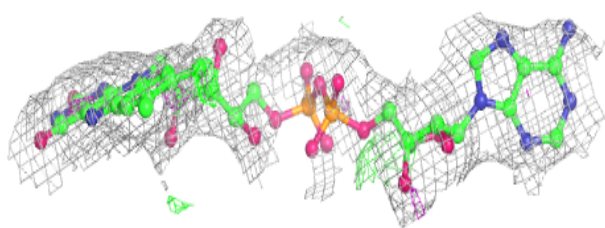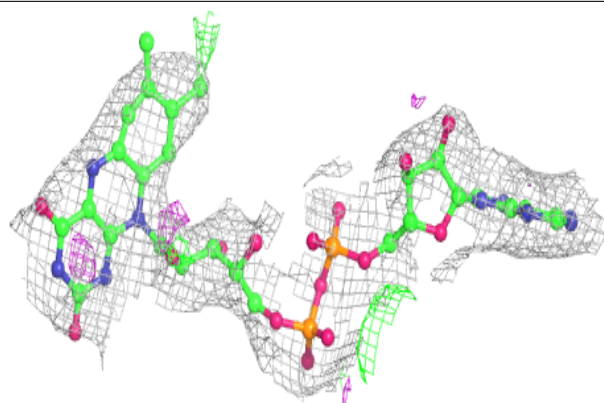
Electron density around FAD C 1611:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
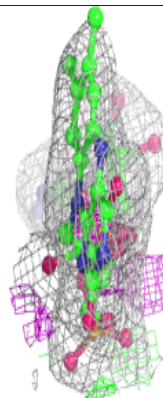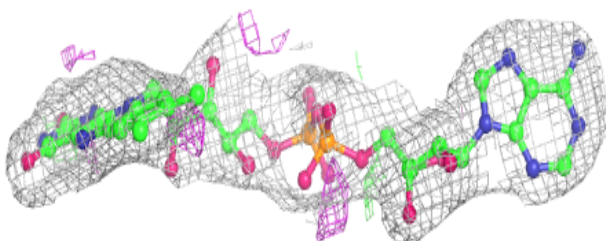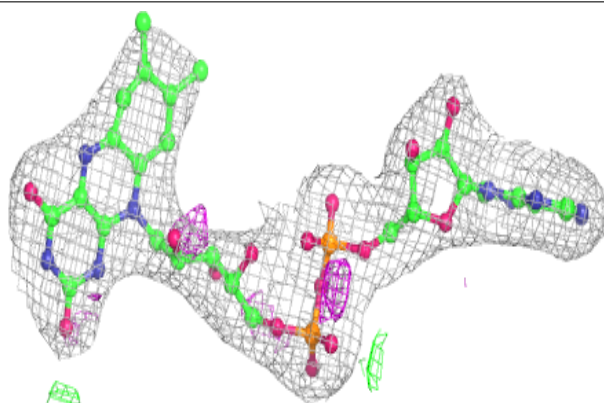$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
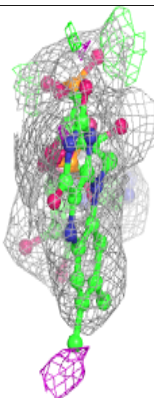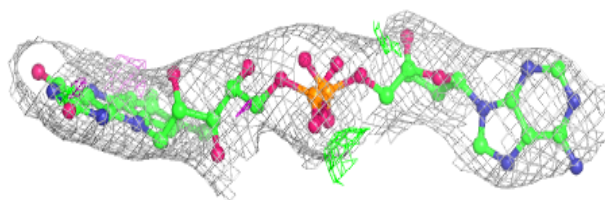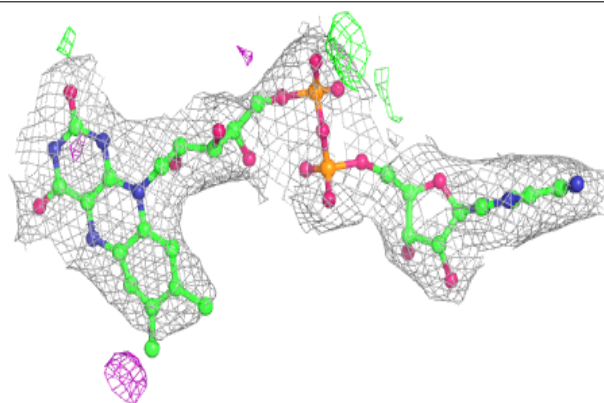
Electron density around FAD A 1611:

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

Electron density around FAD B 1611:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.