



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:21 PM UTC

PDB ID : 3GD3 / pdb_00003gd3
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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

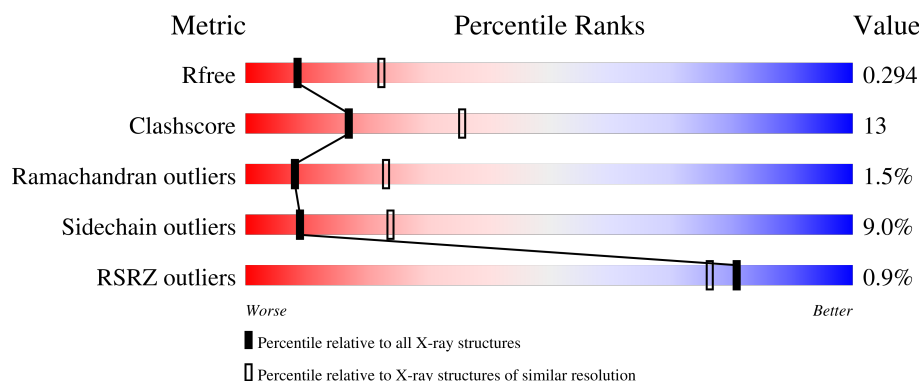
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 $\leq 5\%$. 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	535	2% 53% 29% 13%
1	B	535	64% 23% 11%
1	C	535	60% 23% 13%
1	D	535	2% 62% 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.

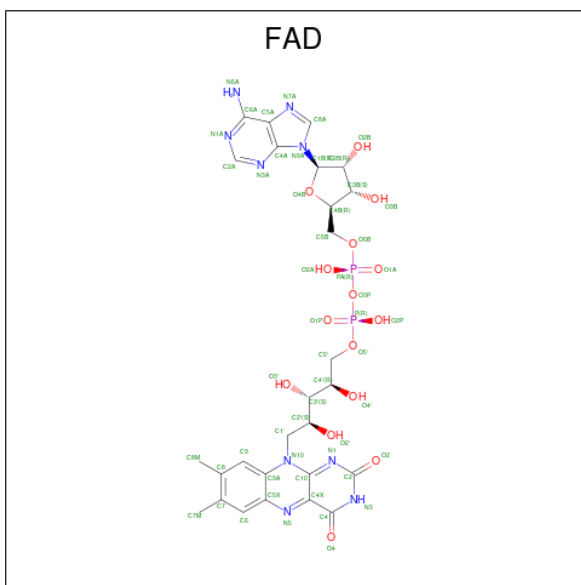
- Molecule 1 is a protein called Apoptosis-inducing factor 1, mitochondrial.

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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

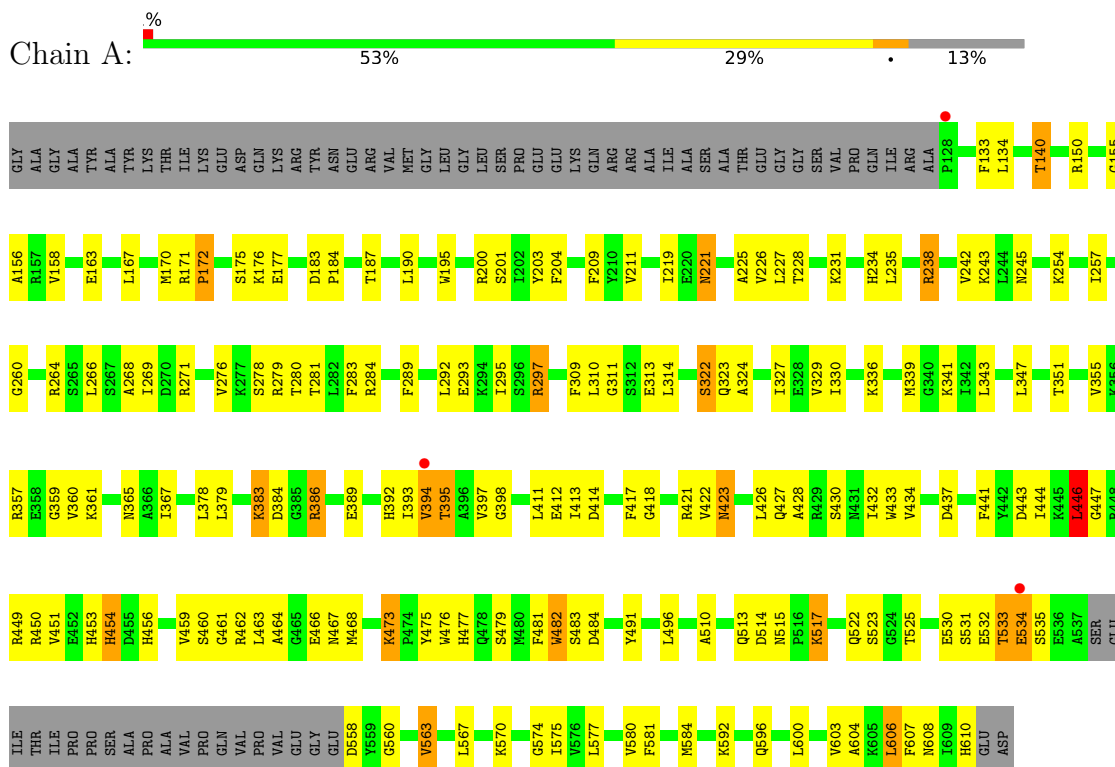
- Molecule 4 is water.

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

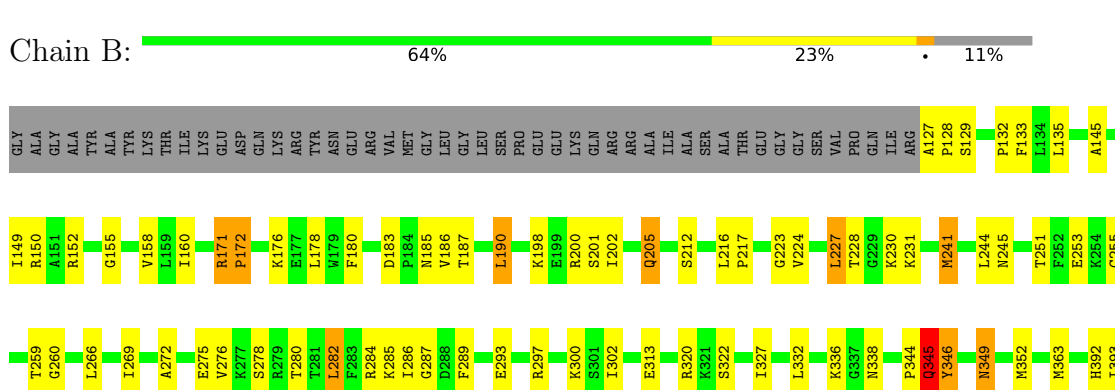
3 Residue-property plots

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

- Molecule 1: Apoptosis-inducing factor 1, mitochondrial



- Molecule 1: Apoptosis-inducing factor 1, mitochondrial





- Molecule 2: Apoptosis-inducing factor 1, mitochondrial

Chain E:  89% 11%



- 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 46.64 – 2.95	Depositor EDS
% Data completeness (in resolution range)	83.4 (46.64-2.95) 82.9 (46.64-2.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
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)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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 [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	0.63	0/3634	0.93	3/4909 (0.1%)
1	B	0.58	0/3728	0.93	6/5040 (0.1%)
1	C	0.60	2/3664 (0.1%)	0.90	6/4950 (0.1%)
1	D	0.59	0/3649	0.90	3/4929 (0.1%)
All	All	0.60	2/14675 (0.0%)	0.91	18/19828 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	532	GLU	C-N	9.67	1.47	1.33
1	C	152	ARG	C-N	6.01	1.39	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	PRO	N-CA-C	7.39	119.71	110.70
1	C	470	GLY	N-CA-C	6.54	122.86	115.08
1	A	172	PRO	N-CA-C	6.38	118.48	110.70
1	B	532	GLU	CA-C-N	5.90	132.81	121.54
1	B	532	GLU	C-N-CA	5.90	132.81	121.54
1	D	172	PRO	N-CA-C	5.75	117.72	110.70
1	C	449	ARG	N-CA-C	5.42	116.23	108.74
1	C	172	PRO	N-CA-C	5.36	117.23	110.70
1	B	205	GLN	CA-C-N	5.14	125.67	120.38
1	B	205	GLN	C-N-CA	5.14	125.67	120.38
1	C	451	VAL	N-CA-C	5.14	116.05	108.45
1	A	473	LYS	CA-C-N	5.13	125.86	120.11
1	A	473	LYS	C-N-CA	5.13	125.86	120.11
1	D	480	MET	N-CA-C	5.11	117.75	109.06
1	B	562	GLY	N-CA-C	5.08	118.11	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	LYS	CA-C-N	5.06	125.50	120.14
1	C	473	LYS	C-N-CA	5.06	125.50	120.14
1	D	283	PHE	N-CA-C	5.02	116.59	108.41

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	3564	0	3589	115	0
1	B	3656	0	3676	95	0
1	C	3594	0	3618	95	0
1	D	3579	0	3600	74	0
2	E	40	0	11	0	0
2	F	45	0	14	0	0
3	A	53	0	30	2	0
3	B	53	0	30	3	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	373	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (373) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:339:MET:HE1	1:C:351:THR:HG21	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:430:SER:HG	1:D:425:GLU:CD	2.12	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
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:C:412:GLU:CD	1:C:421:ARG:HD2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:175:SER:OG	1:A:313:GLU:OE2	2.27	0.52
1:B:278:SER:C	1:B:280:THR:H	2.18	0.52
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
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:D:154:PRO:O	1:D:155:GLY:C	2.52	0.51
1:A:443:ASP:O	1:A:447:GLY:N	2.28	0.51
1:C:197:GLY:O	1:C:198:LYS:C	2.53	0.51
1:C:271:ARG:HH11	1:C:271:ARG:CG	2.17	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:A:423:ASN:C	1:A:423:ASN:HD22	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:SER:C	1:A:324:ALA:H	2.19	0.50
1:A:454:HIS:CD2	1:A:454:HIS:C	2.88	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:B:344:PRO:O	1:B:345:GLN:C	2.56	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:313:GLU:OE1	1:A:483:SER:OG	2.26	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:339:MET:HE2	1:A:343:LEU:HD11	1.96	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: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:266:LEU:O	1:C:267:SER:C	2.59	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:A:604:ALA:C	1:A:606:LEU:H	2.23	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
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: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:A:604:ALA:C	1:A:606:LEU:N	2.73	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:B:286:ILE:O	1:B:287:GLY:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:LYS:H	1:D:245:ASN:ND2	2.14	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:A:309:PHE:CE2	1:A:339:MET:HE3	2.52	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:172:PRO:HB3	1:B:176:LYS:HZ1	1.82	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:C:584:MET:O	1:C:585:PRO:C	2.60	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:259:THR:C	3:B:1611:FAD:H52A	2.42	0.44
1:B:266:LEU:HB3	1:B:269:ILE:HD12	1.98	0.44
1:C:536:GLU:O	1:C:537:ALA:C	2.60	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:C:423:ASN:C	1:C:423:ASN:HD22	2.26	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:170:MET:HE1	1:A:200:ARG:NH2	2.32	0.44
1:A:195:TRP:O	1:A:517:LYS:HD2	2.17	0.44
1:A:279:ARG:CB	1:A:378:LEU:HD11	2.48	0.44
1:A:475:TYR:C	1:A:475:TYR:CD2	2.96	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:178:LEU:HB3	1:B:289:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:357:ARG:C	1:A:359:GLY:H	2.25	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:C:309:PHE:O	1:C:310:LEU:C	2.62	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:C:351:THR:C	1:C:353:GLU:N	2.77	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:A:264:ARG:HG3	1:A:398:GLY:C	2.45	0.42
1:C:143:PHE:CE2	1:C:204:PHE:HB3	2.55	0.42
1:C:511:THR:HG22	1:C:514:ASP:CG	2.45	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:D:131:VAL:HG22	1:D:133:PHE:H	1.85	0.41
1:A:481:PHE:CG	1:A:482:TRP:N	2.88	0.41
1:C:461:GLY:O	1:C:462:ARG:C	2.63	0.41
1:D:492:GLU:CB	1:D:577:LEU:HB2	2.42	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:PHE:CD2	1:A:209:PHE:C	2.98	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:B:423:ASN:C	1:B:423:ASN:HD22	2.28	0.41
1:D:170:MET:HE1	1:D:200:ARG:NH1	2.35	0.41
1:D:566:TYR:HB2	1:D:574:GLY:HA3	2.01	0.41
1:D:581:PHE:C	1:D:583:ARG:H	2.28	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: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:278:SER:C	1:A:280:THR:H	2.28	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: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:367:ILE:O	1:C:383:LYS:N	2.53	0.40
1:A:175:SER:HB3	3:A:1611:FAD:HM73	2.02	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:310:LEU:O	1:A:311:GLY:C	2.64	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
1:B:467:ASN:HA	1:B:471:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	5	15
1	B	472/535 (88%)	426 (90%)	41 (9%)	5 (1%)	11	29
1	C	463/535 (86%)	410 (89%)	48 (10%)	5 (1%)	11	29
1	D	461/535 (86%)	417 (90%)	36 (8%)	8 (2%)	7	20
All	All	1855/2140 (87%)	1659 (89%)	168 (9%)	28 (2%)	8	23

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
1	B	284	ARG

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Mol	Chain	Res	Type
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%)	343 (90%)	36 (10%)	8	22
1	B	390/435 (90%)	360 (92%)	30 (8%)	12	30
1	C	383/435 (88%)	346 (90%)	37 (10%)	8	21
1	D	381/435 (88%)	346 (91%)	35 (9%)	8	23
All	All	1533/1740 (88%)	1395 (91%)	138 (9%)	9	24

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	LEU
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	276	VAL
1	A	297	ARG
1	A	322	SER
1	A	341	LYS
1	A	379	LEU
1	A	383	LYS
1	A	386	ARG
1	A	389	GLU
1	A	394	VAL
1	A	395	THR
1	A	397	VAL
1	A	413	ILE
1	A	423	ASN
1	A	432	ILE
1	A	446	LEU
1	A	451	VAL
1	A	454	HIS
1	A	466	GLU
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	592	LYS
1	A	596	GLN
1	A	606	LEU
1	B	129	SER
1	B	158	VAL
1	B	171	ARG
1	B	187	THR
1	B	190	LEU
1	B	198	LYS
1	B	202	ILE
1	B	205	GLN
1	B	212	SER
1	B	224	VAL
1	B	227	LEU
1	B	228	THR
1	B	241	MET

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Mol	Chain	Res	Type
1	B	275	GLU
1	B	282	LEU
1	B	285	LYS
1	B	300	LYS
1	B	336	LYS
1	B	345	GLN
1	B	346	TYR
1	B	349	ASN
1	B	423	ASN
1	B	446	LEU
1	B	451	VAL
1	B	476	TRP
1	B	494	ILE
1	B	506	VAL
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	219	ILE
1	C	220	GLU
1	C	226	VAL
1	C	227	LEU
1	C	266	LEU
1	C	271	ARG
1	C	275	GLU
1	C	276	VAL
1	C	294	LYS
1	C	332	LEU
1	C	345	GLN
1	C	353	GLU
1	C	367	ILE
1	C	380	ILE
1	C	394	VAL
1	C	402	ASN
1	C	415	SER

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Mol	Chain	Res	Type
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
1	C	500	SER
1	C	511	THR
1	C	541	THR
1	C	563	VAL
1	C	593	ASP
1	D	129	SER
1	D	152	ARG
1	D	158	VAL
1	D	167	LEU
1	D	186	VAL
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	232	VAL
1	D	241	MET
1	D	282	LEU
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	371	VAL
1	D	400	GLU
1	D	413	ILE
1	D	429	ARG
1	D	432	ILE
1	D	443	ASP

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Mol	Chain	Res	Type
1	D	446	LEU
1	D	494	ILE
1	D	497	VAL
1	D	573	VAL
1	D	599	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	240	ASN
1	A	249	GLN
1	A	338	ASN
1	A	365	ASN
1	A	402	ASN
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	478	GLN
1	A	596	GLN
1	A	610	HIS
1	B	205	GLN
1	B	234	HIS
1	B	240	ASN
1	B	245	ASN
1	B	338	ASN
1	B	365	ASN
1	B	369	GLN
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	515	ASN
1	B	579	ASN
1	B	610	HIS
1	C	205	GLN
1	C	245	ASN

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Mol	Chain	Res	Type
1	C	249	GLN
1	C	323	GLN
1	C	365	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	240	ASN
1	D	402	ASN
1	D	456	HIS
1	D	467	ASN
1	D	477	HIS
1	D	579	ASN
1	D	596	GLN
1	D	610	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	1611	-	58,58,58	2.22	12 (20%)	85,89,89	2.91	22 (25%)
3	FAD	C	1611	-	58,58,58	2.25	11 (18%)	85,89,89	2.95	20 (23%)
3	FAD	B	1611	-	58,58,58	2.28	13 (22%)	85,89,89	2.99	23 (27%)
3	FAD	D	1611	-	58,58,58	2.24	12 (20%)	85,89,89	3.04	22 (25%)

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	A	1611	-	-	5/34/50/50	0/6/6/6
3	FAD	C	1611	-	-	10/34/50/50	0/6/6/6
3	FAD	B	1611	-	-	11/34/50/50	0/6/6/6
3	FAD	D	1611	-	-	11/34/50/50	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1611	FAD	C6-C7	-9.67	1.26	1.39
3	B	1611	FAD	C6-C7	-9.64	1.26	1.39
3	D	1611	FAD	C6-C7	-9.38	1.26	1.39
3	C	1611	FAD	C6-C5X	-9.24	1.25	1.40
3	A	1611	FAD	C6-C5X	-9.07	1.26	1.40
3	B	1611	FAD	C6-C5X	-9.00	1.26	1.40
3	A	1611	FAD	C6-C7	-9.00	1.27	1.39
3	D	1611	FAD	C6-C5X	-8.91	1.26	1.40
3	B	1611	FAD	C5A-C4A	5.26	1.48	1.39
3	A	1611	FAD	C9A-C5X	5.20	1.49	1.41
3	D	1611	FAD	C5A-C4A	5.12	1.48	1.39
3	C	1611	FAD	C5A-C4A	5.02	1.48	1.39
3	A	1611	FAD	C5A-C4A	4.80	1.47	1.39
3	B	1611	FAD	C9A-C5X	4.73	1.48	1.41
3	D	1611	FAD	C9A-C5X	4.55	1.48	1.41
3	C	1611	FAD	C9A-C5X	4.44	1.48	1.41
3	C	1611	FAD	C5X-N5	-3.05	1.33	1.39
3	A	1611	FAD	C5X-N5	-3.05	1.33	1.39
3	B	1611	FAD	C9-C8	3.00	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1611	FAD	C5X-N5	-2.95	1.34	1.39
3	B	1611	FAD	P-O3P	2.87	1.62	1.59
3	D	1611	FAD	C5X-N5	-2.74	1.34	1.39
3	D	1611	FAD	PA-O3P	2.52	1.62	1.59
3	D	1611	FAD	P-O3P	2.50	1.62	1.59
3	D	1611	FAD	C10-N10	2.49	1.42	1.37
3	D	1611	FAD	C9-C8	2.48	1.43	1.39
3	D	1611	FAD	C8A-N7A	2.46	1.36	1.31
3	A	1611	FAD	C5A-N7A	-2.46	1.34	1.39
3	C	1611	FAD	C8A-N7A	2.44	1.36	1.31
3	A	1611	FAD	C10-N10	2.39	1.42	1.37
3	C	1611	FAD	C5A-N7A	-2.38	1.34	1.39
3	D	1611	FAD	C4X-N5	2.38	1.35	1.30
3	C	1611	FAD	C9-C8	2.27	1.42	1.39
3	B	1611	FAD	C8A-N7A	2.24	1.36	1.31
3	B	1611	FAD	PA-O3P	2.24	1.61	1.59
3	C	1611	FAD	C4A-N9A	-2.23	1.33	1.37
3	A	1611	FAD	C8A-N7A	2.21	1.35	1.31
3	B	1611	FAD	C4A-N9A	-2.21	1.33	1.37
3	A	1611	FAD	C4X-N5	2.20	1.35	1.30
3	D	1611	FAD	C9-C9A	2.14	1.43	1.39
3	C	1611	FAD	C4X-N5	2.11	1.35	1.30
3	A	1611	FAD	C4A-N9A	-2.11	1.33	1.37
3	B	1611	FAD	C9-C9A	2.08	1.43	1.39
3	A	1611	FAD	C9-C8	2.06	1.42	1.39
3	B	1611	FAD	C10-N10	2.05	1.41	1.37
3	B	1611	FAD	C5A-N7A	-2.04	1.35	1.39
3	C	1611	FAD	C10-N10	2.04	1.41	1.37
3	A	1611	FAD	C8A-N9A	-2.02	1.34	1.37

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1611	FAD	C5X-C6-C7	16.29	151.00	120.83
3	B	1611	FAD	C5X-C6-C7	16.10	150.66	120.83
3	C	1611	FAD	C5X-C6-C7	16.03	150.52	120.83
3	A	1611	FAD	C5X-C6-C7	15.41	149.38	120.83
3	D	1611	FAD	C6-C5X-C9A	-10.72	104.32	119.05
3	C	1611	FAD	C6-C5X-C9A	-10.49	104.64	119.05
3	B	1611	FAD	C6-C5X-C9A	-10.41	104.75	119.05
3	A	1611	FAD	C6-C5X-C9A	-10.05	105.25	119.05
3	A	1611	FAD	C6-C7-C8	-8.79	106.79	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1611	FAD	C6-C7-C8	-8.56	107.13	119.69
3	D	1611	FAD	C6-C7-C8	-8.51	107.20	119.69
3	C	1611	FAD	C6-C7-C8	-8.43	107.31	119.69
3	D	1611	FAD	C6-C5X-N5	8.26	132.16	118.44
3	C	1611	FAD	C6-C5X-N5	8.12	131.92	118.44
3	A	1611	FAD	C6-C5X-N5	8.08	131.86	118.44
3	B	1611	FAD	C6-C5X-N5	7.62	131.09	118.44
3	D	1611	FAD	C5A-C4A-N3A	-6.45	117.83	126.72
3	C	1611	FAD	C5A-C4A-N3A	-5.94	118.54	126.72
3	A	1611	FAD	C5A-C4A-N3A	-5.57	119.05	126.72
3	B	1611	FAD	C5A-C4A-N3A	-5.32	119.39	126.72
3	D	1611	FAD	N3A-C4A-N9A	4.93	135.55	127.17
3	A	1611	FAD	N3A-C4A-N9A	4.45	134.74	127.17
3	D	1611	FAD	C4A-C5A-N7A	-4.44	105.51	110.58
3	C	1611	FAD	N3A-C4A-N9A	4.22	134.34	127.17
3	B	1611	FAD	C9-C9A-N10	4.19	127.49	121.85
3	B	1611	FAD	N3A-C4A-N9A	4.14	134.21	127.17
3	C	1611	FAD	C4A-C5A-N7A	-4.13	105.86	110.58
3	B	1611	FAD	N3A-C2A-N1A	-4.09	122.39	128.58
3	A	1611	FAD	N3A-C2A-N1A	-4.06	122.44	128.58
3	C	1611	FAD	C7M-C7-C6	3.93	126.50	119.57
3	C	1611	FAD	N3A-C2A-N1A	-3.87	122.72	128.58
3	D	1611	FAD	N3A-C2A-N1A	-3.86	122.74	128.58
3	D	1611	FAD	C2A-N3A-C4A	3.77	121.05	111.83
3	B	1611	FAD	C4X-C10-N10	3.76	121.87	116.48
3	A	1611	FAD	C7M-C7-C6	3.76	126.20	119.57
3	A	1611	FAD	C4A-C5A-N7A	-3.76	106.29	110.58
3	D	1611	FAD	C7M-C7-C6	3.65	126.00	119.57
3	B	1611	FAD	C7M-C7-C6	3.55	125.83	119.57
3	B	1611	FAD	C4A-C5A-N7A	-3.55	106.53	110.58
3	D	1611	FAD	C9-C9A-N10	3.45	126.49	121.85
3	C	1611	FAD	C2A-N3A-C4A	3.45	120.25	111.83
3	A	1611	FAD	C4X-C4-N3	3.33	121.72	113.25
3	B	1611	FAD	C4'-C3'-C2'	-3.27	108.12	113.57
3	A	1611	FAD	C4-N3-C2	-3.27	119.83	125.64
3	A	1611	FAD	C2A-N3A-C4A	3.25	119.77	111.83
3	C	1611	FAD	C4X-C10-N10	3.22	121.09	116.48
3	D	1611	FAD	C5A-N7A-C8A	3.19	108.46	103.45
3	D	1611	FAD	C4X-C10-N10	3.16	121.01	116.48
3	C	1611	FAD	C9-C9A-N10	3.14	126.07	121.85
3	B	1611	FAD	C2A-N3A-C4A	3.10	119.41	111.83
3	B	1611	FAD	C7M-C7-C8	3.08	127.04	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1611	FAD	C7M-C7-C8	3.06	127.01	120.76
3	B	1611	FAD	C4-N3-C2	-3.05	120.22	125.64
3	A	1611	FAD	C9-C9A-N10	3.01	125.91	121.85
3	D	1611	FAD	C7M-C7-C8	2.96	126.80	120.76
3	A	1611	FAD	O4-C4-C4X	-2.96	118.72	126.53
3	A	1611	FAD	C4A-N9A-C8A	2.94	108.83	105.74
3	D	1611	FAD	C4A-N9A-C8A	2.84	108.72	105.74
3	B	1611	FAD	C5X-C9A-N10	-2.76	115.47	117.97
3	A	1611	FAD	C4X-C10-N10	2.73	120.40	116.48
3	D	1611	FAD	C4X-C4-N3	2.66	120.02	113.25
3	C	1611	FAD	C7M-C7-C8	2.66	126.19	120.76
3	A	1611	FAD	C5A-N7A-C8A	2.64	107.60	103.45
3	B	1611	FAD	C4X-C4-N3	2.63	119.96	113.25
3	C	1611	FAD	C5A-N7A-C8A	2.62	107.57	103.45
3	C	1611	FAD	C4X-C4-N3	2.60	119.88	113.25
3	C	1611	FAD	C4-N3-C2	-2.59	121.05	125.64
3	B	1611	FAD	C4A-N9A-C8A	2.48	108.34	105.74
3	B	1611	FAD	O4-C4-C4X	-2.43	120.11	126.53
3	B	1611	FAD	C10-N1-C2	2.41	122.06	116.85
3	D	1611	FAD	C4-N3-C2	-2.32	121.53	125.64
3	D	1611	FAD	N9A-C8A-N7A	-2.29	110.69	113.94
3	C	1611	FAD	O4-C4-C4X	-2.26	120.57	126.53
3	B	1611	FAD	C5A-N7A-C8A	2.24	106.97	103.45
3	B	1611	FAD	C4X-C10-N1	-2.23	119.12	124.59
3	A	1611	FAD	O2A-PA-O1A	2.19	122.61	112.44
3	A	1611	FAD	C4X-C10-N1	-2.17	119.27	124.59
3	C	1611	FAD	C4A-N9A-C8A	2.17	108.01	105.74
3	D	1611	FAD	O4-C4-C4X	-2.15	120.85	126.53
3	A	1611	FAD	C10-N1-C2	2.14	121.47	116.85
3	D	1611	FAD	C6A-C5A-N7A	2.14	136.21	132.09
3	C	1611	FAD	C10-N1-C2	2.12	121.44	116.85
3	D	1611	FAD	C10-N1-C2	2.11	121.42	116.85
3	B	1611	FAD	C2A-N1A-C6A	2.08	122.15	118.73
3	C	1611	FAD	C9A-N10-C10	-2.06	117.61	120.75
3	D	1611	FAD	C4X-C10-N1	-2.03	119.62	124.59
3	A	1611	FAD	N9A-C8A-N7A	-2.02	111.07	113.94

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1611	FAD	C5B-O5B-PA-O1A

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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

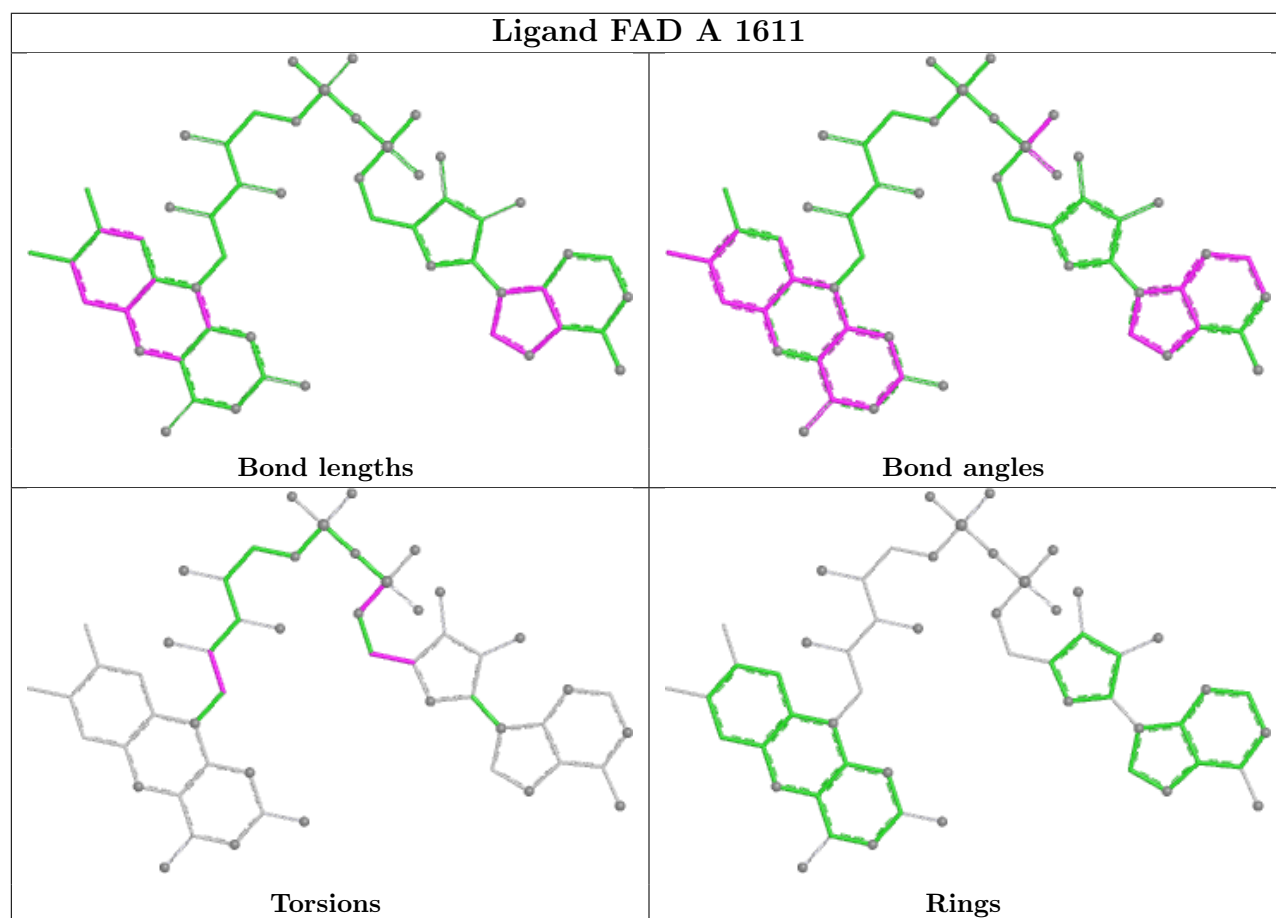
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1611	FAD	2	0

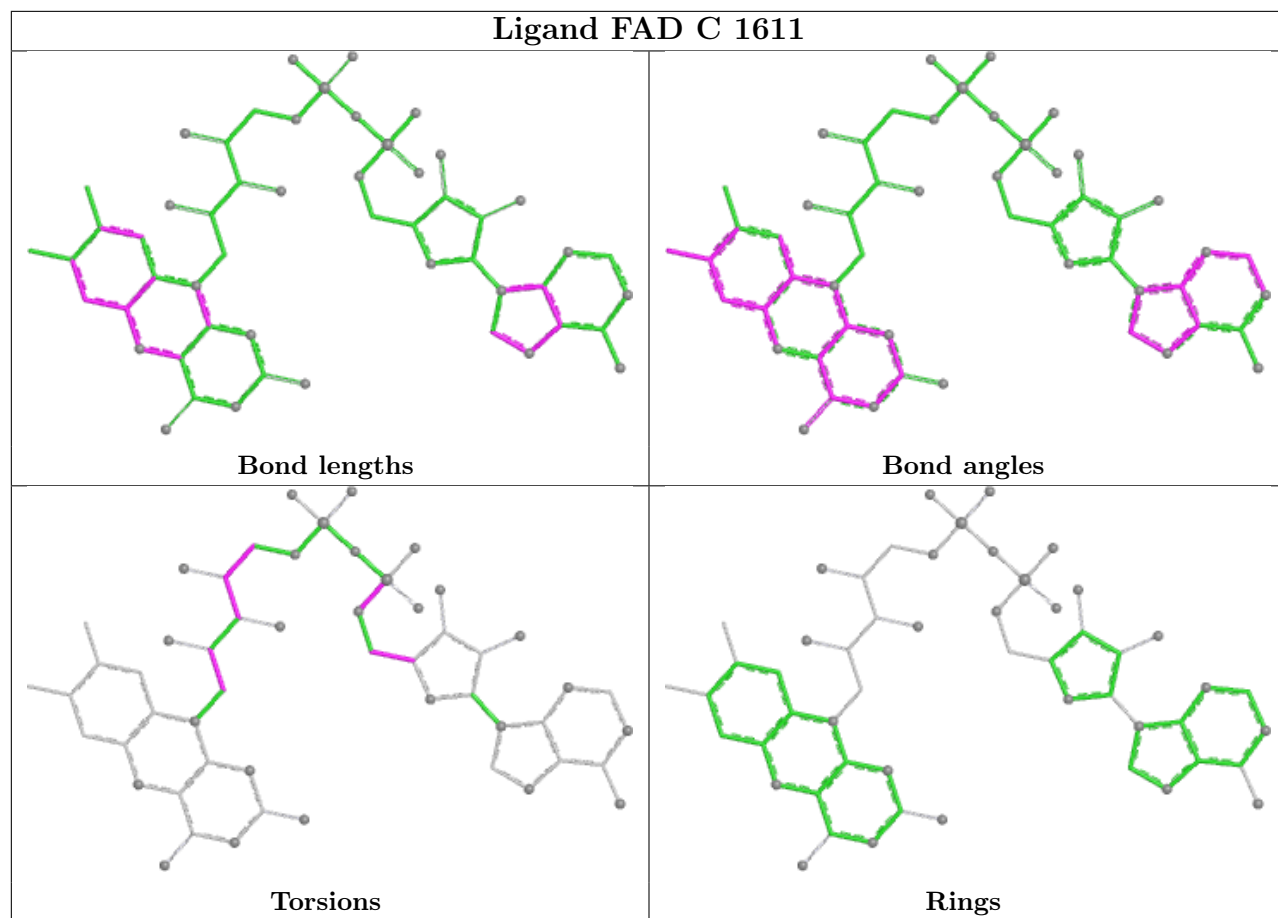
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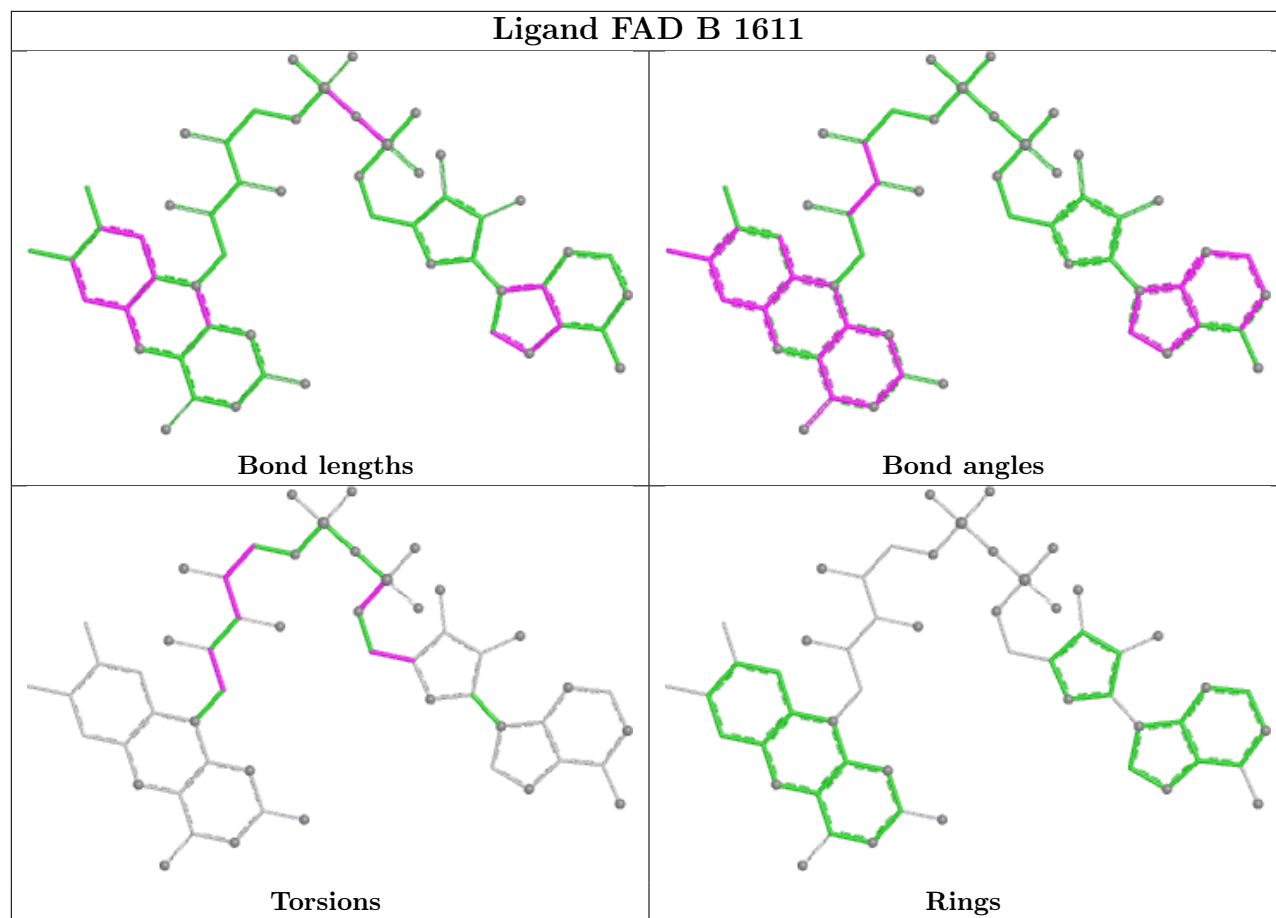
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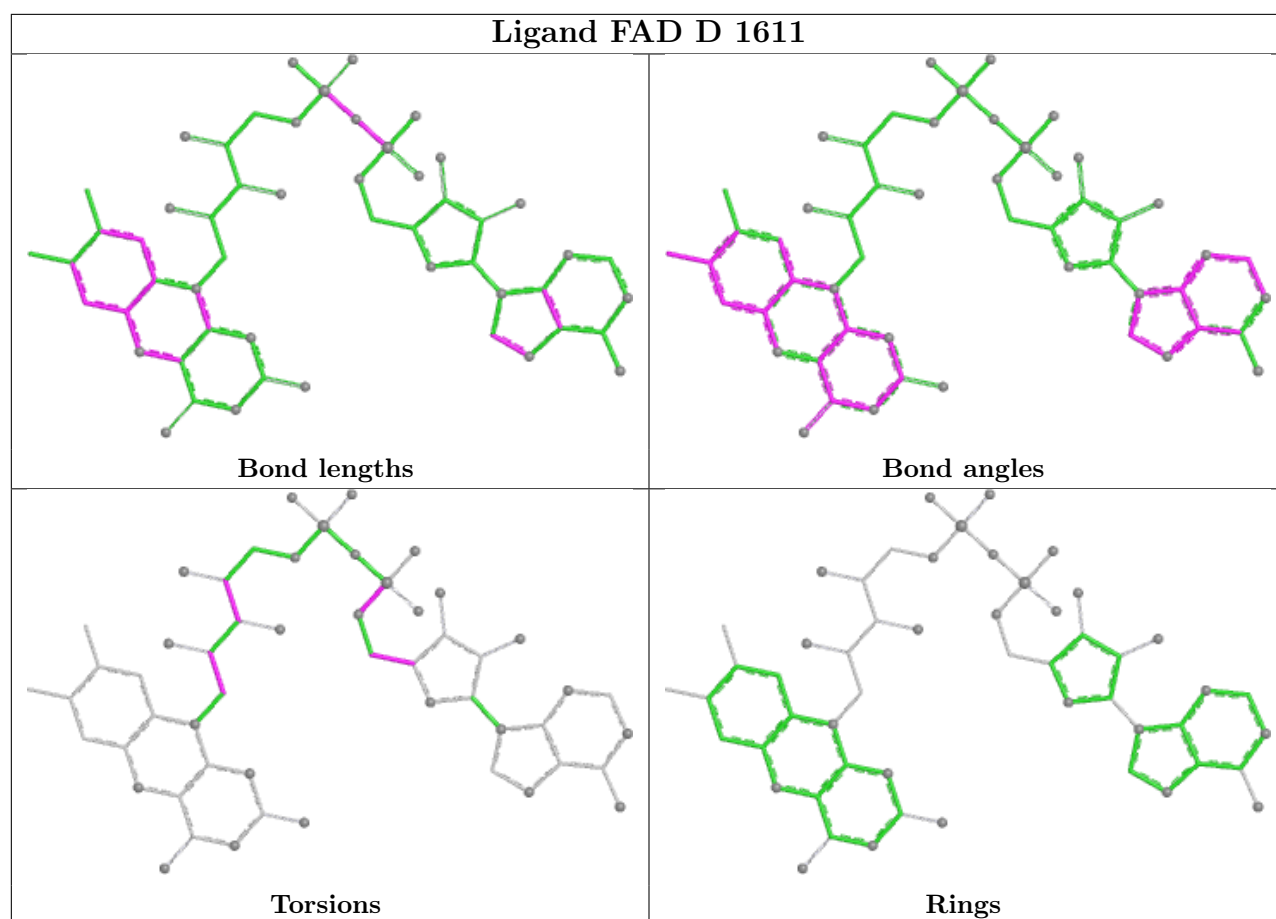
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1611	FAD	3	0
3	D	1611	FAD	1	0

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 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.









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	463/535 (86%)	-0.11	3 (0%) 85 82	50, 78, 109, 124	0
1	B	476/535 (88%)	-0.13	1 (0%) 91 90	60, 98, 149, 196	0
1	C	467/535 (87%)	-0.03	1 (0%) 91 90	62, 94, 137, 163	0
1	D	465/535 (86%)	0.25	11 (2%) 59 51	73, 154, 224, 263	0
2	E	0/9	-	-	-	-
2	F	0/9	-	-	-	-
All	All	1871/2158 (86%)	-0.01	16 (0%) 81 76	50, 95, 196, 263	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	LEU	4.5
1	D	305	ILE	3.4
1	D	303	THR	2.9
1	A	394	VAL	2.6
1	D	283	PHE	2.5
1	A	534	GLU	2.4
1	D	395	THR	2.4
1	A	128	PRO	2.4
1	D	319	GLY	2.3
1	C	444	ILE	2.2
1	D	152	ARG	2.1
1	B	610	HIS	2.1
1	D	388	VAL	2.1
1	D	167	LEU	2.1
1	D	315	ALA	2.0
1	D	394	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

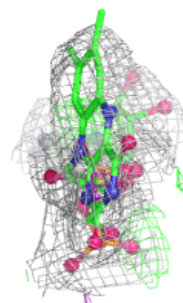
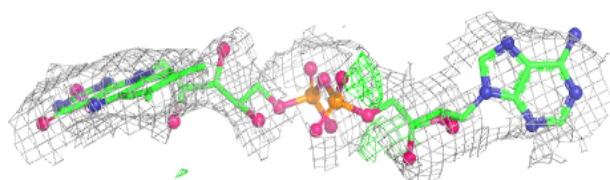
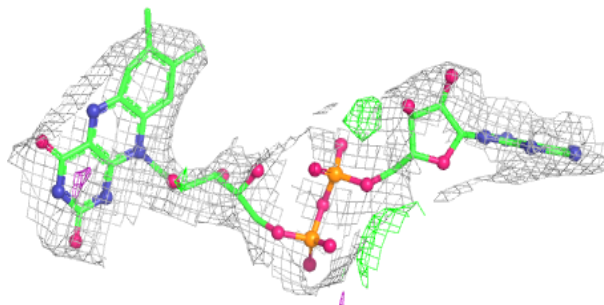
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	D	1611	53/53	0.89	0.10	87,90,111,111	0
3	FAD	C	1611	53/53	0.93	0.09	77,78,81,82	0
3	FAD	A	1611	53/53	0.94	0.08	58,64,76,77	0
3	FAD	B	1611	53/53	0.94	0.06	60,63,69,70	0

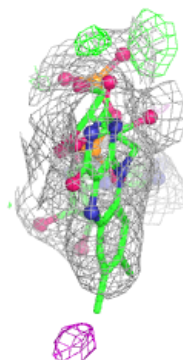
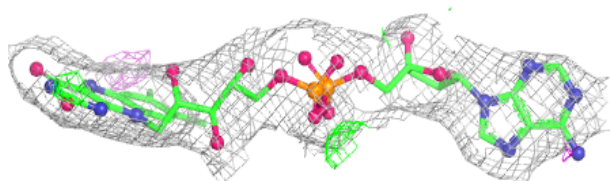
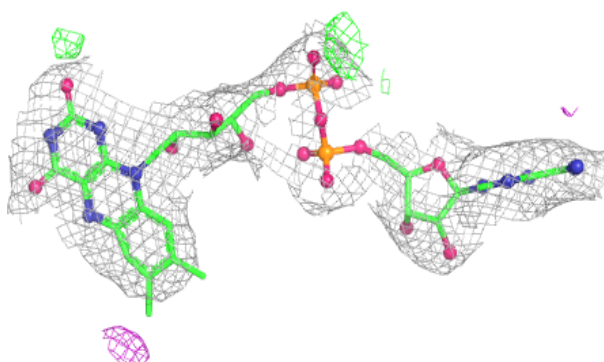
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD D 1611:

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

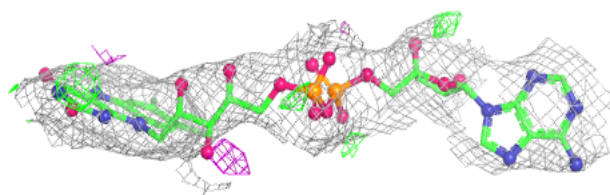
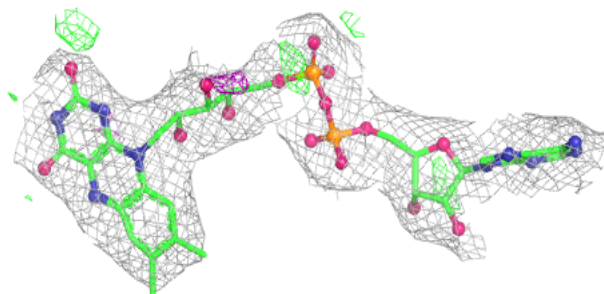
**Electron density around FAD C 1611:**

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

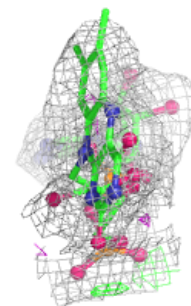
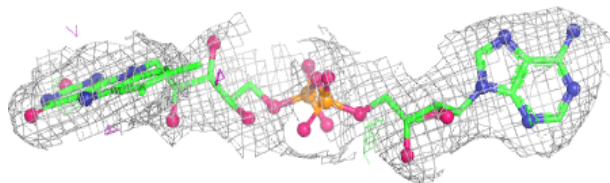
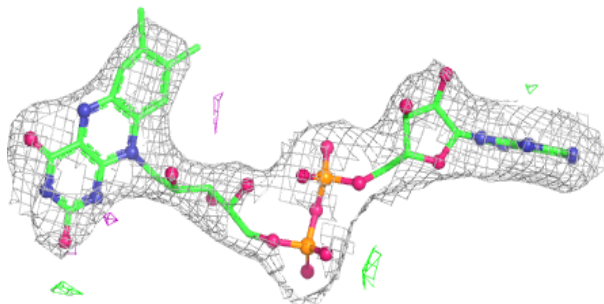


Electron density around FAD A 1611:

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

**Electron density around FAD B 1611:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.