



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2021 – 11:24 PM EDT

PDB ID : 3JQQ
Title : Crystal structure of the H286K mutant of Ferredoxin-NADP⁺ reductase from Plasmodium falciparum in complex with 2'P-AMP
Authors : Canevari, G.; Milani, M.; Bolognesi, M.
Deposited on : 2009-09-07
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

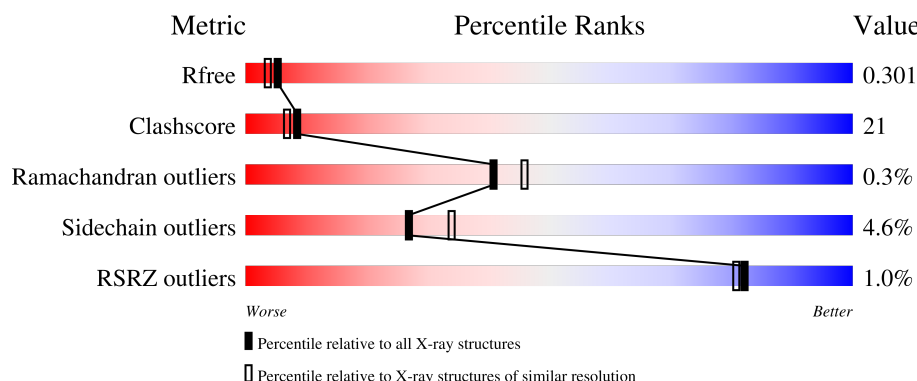
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	316	<div> <div>%</div> <div>61% 20% • 17%</div> </div>
1	B	316	<div> <div>%</div> <div>62% 19% • 17%</div> </div>
1	C	316	<div> <div>%</div> <div>64% 19% • 16%</div> </div>
1	D	316	<div> <div>60% 19% 5% 16%</div> </div>
1	E	316	<div> <div>57% 21% • 20%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	316	<p>2% 51% 28% 20%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14736 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 Ferredoxin NADP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2188	1421	360	398	9			
1	B	263	Total	C	N	O	S	0	0	0
			2207	1436	361	401	9			
1	C	267	Total	C	N	O	S	0	0	0
			2227	1443	367	408	9			
1	D	267	Total	C	N	O	S	0	0	0
			2227	1443	366	409	9			
1	E	253	Total	C	N	O	S	0	0	0
			2121	1382	346	384	9			
1	F	254	Total	C	N	O	S	0	0	0
			2126	1382	348	387	9			

There are 6 discrepancies between the modelled and reference sequences:

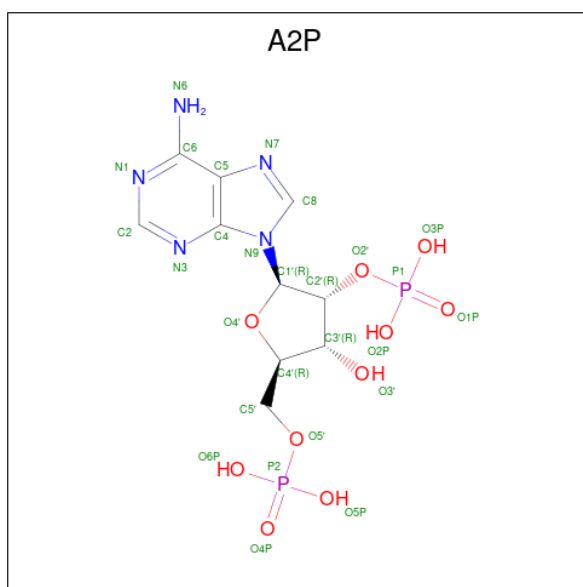
Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LYS	HIS	engineered mutation	UNP C6KT68
B	286	LYS	HIS	engineered mutation	UNP C6KT68
C	286	LYS	HIS	engineered mutation	UNP C6KT68
D	286	LYS	HIS	engineered mutation	UNP C6KT68
E	286	LYS	HIS	engineered mutation	UNP C6KT68
F	286	LYS	HIS	engineered mutation	UNP C6KT68

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is ADENOSINE-2'-5'-DIPHOSPHATE (three-letter code: A2P) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

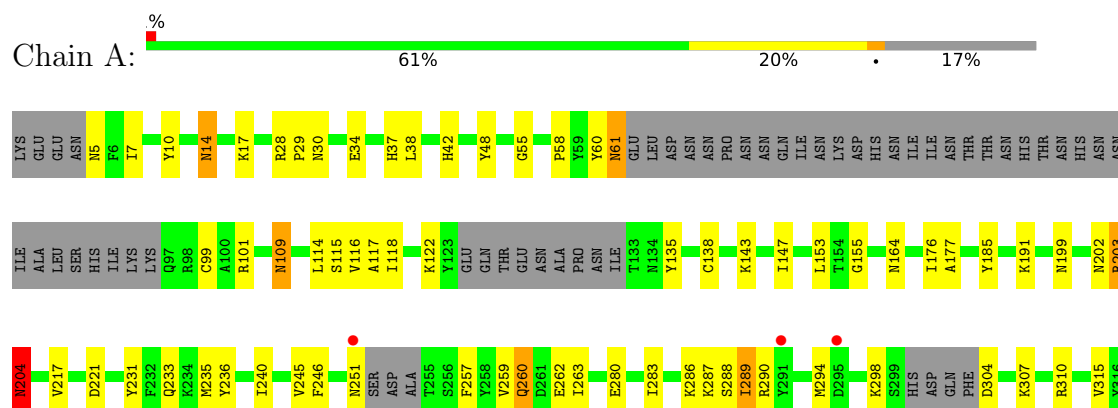
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	194	Total	O	0	0
			194	194		
4	B	223	Total	O	0	0
			223	223		
4	C	221	Total	O	0	0
			221	221		
4	D	198	Total	O	0	0
			198	198		
4	E	152	Total	O	0	0
			152	152		
4	F	172	Total	O	0	0
			172	172		

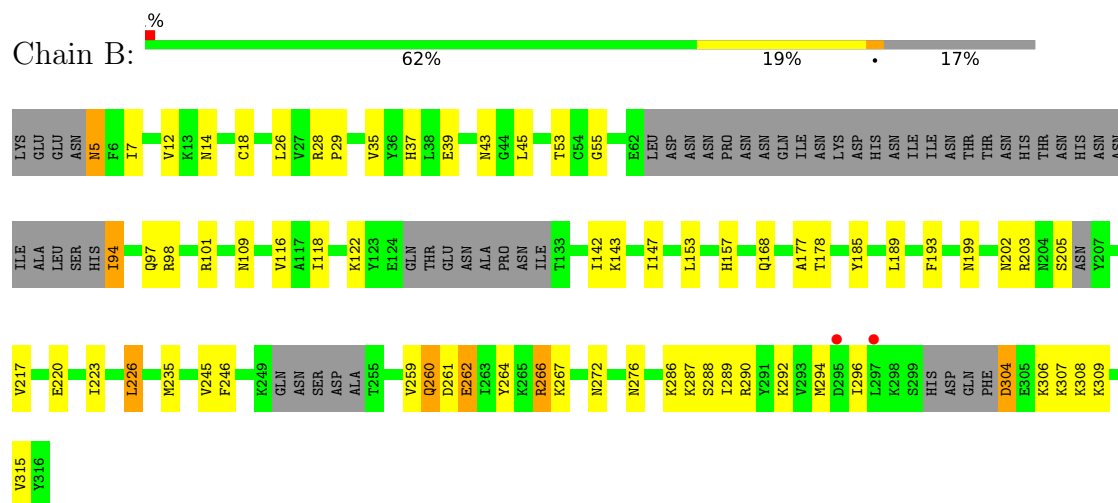
3 Residue-property plots

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.

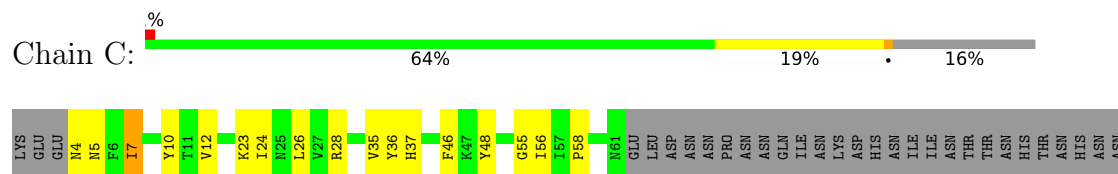
• Molecule 1: Ferredoxin NADP reductase

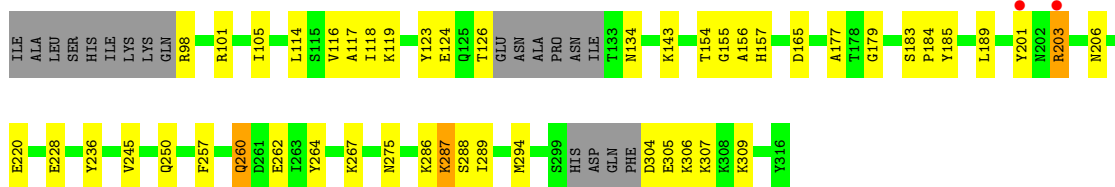


• Molecule 1: Ferredoxin NADP reductase



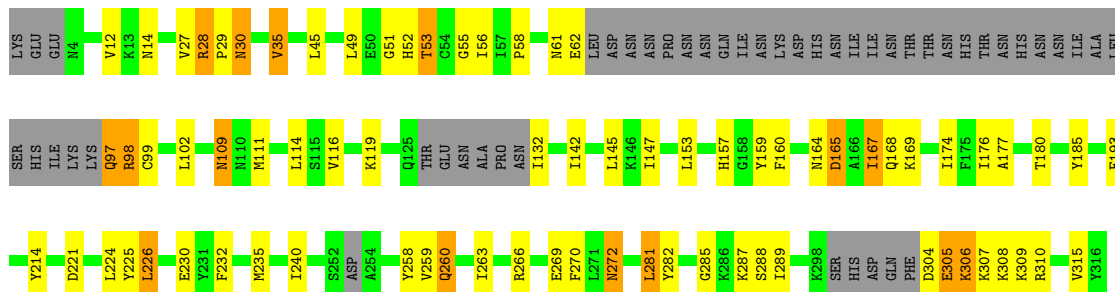
• Molecule 1: Ferredoxin NADP reductase





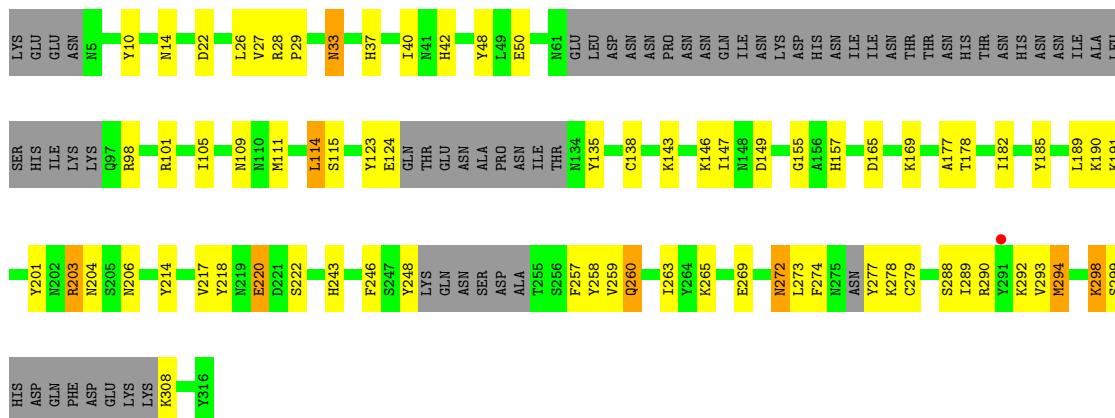
• Molecule 1: Ferredoxin NADP reductase

Chain D: 60% 19% 5% 16%



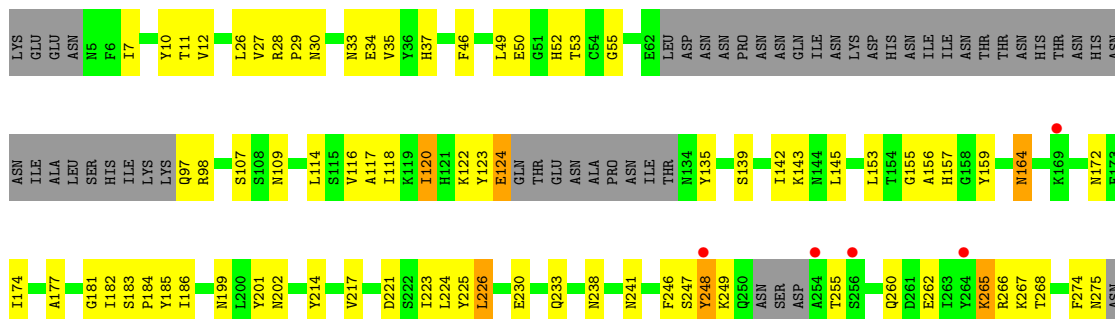
• Molecule 1: Ferredoxin NADP reductase

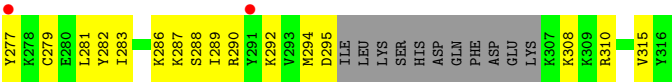
Chain E: 57% 21% 20%



• Molecule 1: Ferredoxin NADP reductase

Chain F: 2% 51% 28% 20%





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.24Å 124.24Å 134.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.12 – 2.20 62.12 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.12-2.20) 100.0 (62.12-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.256 , 0.308 0.254 , 0.301	Depositor DCC
R_{free} test set	5894 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.458 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14736	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4690e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A2P, 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	0.36	0/2240	0.47	0/3019
1	B	0.32	0/2258	0.47	0/3039
1	C	0.41	1/2280 (0.0%)	0.48	0/3076
1	D	0.34	0/2279	0.49	0/3073
1	E	0.32	0/2172	0.46	0/2928
1	F	0.34	0/2177	0.47	0/2934
All	All	0.35	1/13406 (0.0%)	0.47	0/18069

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	TYR	CD2-CE2	-5.62	1.30	1.39

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	2188	0	2154	73	0
1	B	2207	0	2182	81	0
1	C	2227	0	2183	75	0
1	D	2227	0	2178	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2121	0	2083	105	0
1	F	2126	0	2076	134	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
3	A	27	0	11	4	0
3	B	27	0	11	4	0
3	C	27	0	11	5	0
3	D	27	0	11	2	0
3	E	27	0	11	7	0
3	F	27	0	11	1	0
4	A	194	0	0	10	0
4	B	223	0	0	22	0
4	C	221	0	0	12	0
4	D	198	0	0	12	0
4	E	152	0	0	17	0
4	F	172	0	0	24	0
All	All	14736	0	13108	556	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 21.

All (556) 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:E:294:MET:CE	1:E:294:MET:HA	1.60	1.32
1:D:305:GLU:CG	1:D:307:LYS:HG3	1.66	1.25
1:F:294:MET:O	1:F:295:ASP:OD1	1.65	1.12
1:C:305:GLU:HG2	1:C:306:LYS:N	1.44	1.12
1:D:306:LYS:CG	1:D:309:LYS:HD3	1.79	1.12
1:A:203:ARG:HA	1:A:204:ASN:HB2	1.14	1.10
1:E:294:MET:CE	1:E:294:MET:CA	2.30	1.10
1:C:305:GLU:CG	1:C:306:LYS:H	1.68	1.07
1:A:203:ARG:CA	1:A:204:ASN:HB2	1.84	1.07
1:C:26:LEU:HD21	1:C:37:HIS:HB2	1.09	1.06
1:E:294:MET:CA	1:E:294:MET:HE2	1.83	1.06
1:D:306:LYS:HG3	1:D:309:LYS:HD3	1.06	1.05
1:D:305:GLU:HG3	1:D:307:LYS:HG3	1.36	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:ASP:HA	1:E:147:ILE:HD11	1.38	1.03
1:F:260:GLN:OE1	1:F:292:LYS:HG2	1.56	1.03
1:B:118:ILE:HG21	1:B:142:ILE:HD13	1.41	1.02
1:B:168:GLN:HB3	1:E:203:ARG:NH2	1.74	1.02
1:D:97:GLN:HE21	1:D:97:GLN:N	1.57	1.02
1:C:26:LEU:HD12	1:C:35:VAL:CG1	1.91	1.01
1:F:241:ASN:HB2	4:F:903:HOH:O	1.59	1.00
1:D:306:LYS:HG3	1:D:309:LYS:CD	1.91	1.00
1:A:203:ARG:HA	1:A:204:ASN:CB	1.91	1.00
1:C:305:GLU:HG2	1:C:306:LYS:H	0.84	1.00
1:F:248:TYR:HA	1:F:249:LYS:HB3	1.45	0.99
1:C:4:ASN:O	1:C:5:ASN:CG	1.99	0.99
1:E:217:VAL:HG13	4:E:318:HOH:O	1.61	0.99
1:C:26:LEU:CD2	1:C:37:HIS:HB2	1.93	0.98
1:C:26:LEU:HD12	1:C:35:VAL:HG12	1.45	0.98
1:D:147:ILE:HG13	4:D:1239:HOH:O	1.65	0.97
1:E:294:MET:HE3	1:E:294:MET:N	1.80	0.96
1:D:305:GLU:HG2	1:D:307:LYS:HG3	1.47	0.94
1:E:114:LEU:HD12	1:E:114:LEU:O	1.68	0.94
1:F:53:THR:OG1	1:F:157:HIS:HB2	1.68	0.94
1:C:26:LEU:HD21	1:C:37:HIS:CB	2.00	0.92
1:B:118:ILE:HG21	1:B:142:ILE:CD1	1.98	0.92
1:E:248:TYR:HB3	4:E:1197:HOH:O	1.69	0.90
1:F:174:ILE:HG23	1:F:281:LEU:HA	1.54	0.89
1:E:298:LYS:HB2	4:E:1161:HOH:O	1.71	0.89
1:E:294:MET:HA	1:E:294:MET:HE2	0.91	0.88
1:F:46:PHE:CZ	1:F:155:GLY:O	2.27	0.88
1:D:97:GLN:N	1:D:97:GLN:NE2	2.22	0.88
1:A:147:ILE:HD12	1:A:147:ILE:H	1.38	0.88
1:D:53:THR:HG22	1:D:157:HIS:HB2	1.57	0.87
1:B:122:LYS:HE2	4:B:905:HOH:O	1.74	0.87
1:B:309:LYS:HE3	4:B:1211:HOH:O	1.74	0.87
1:F:274:PHE:CD2	1:F:275:ASN:OD1	2.27	0.86
1:D:260:GLN:H	1:D:260:GLN:NE2	1.72	0.86
1:D:260:GLN:H	1:D:260:GLN:HE21	1.20	0.85
1:C:304:ASP:OD1	1:C:307:LYS:HB2	1.76	0.84
1:F:274:PHE:HA	1:F:279:CYS:HB2	1.60	0.83
1:B:118:ILE:HD13	1:B:142:ILE:CD1	2.09	0.83
1:E:177:ALA:HB2	1:E:185:TYR:HE2	1.41	0.83
1:D:305:GLU:OE2	1:D:307:LYS:HE3	1.79	0.82
1:F:226:LEU:HD22	1:F:230:GLU:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:CYS:SG	1:B:153:LEU:HD23	2.19	0.82
1:E:298:LYS:HE2	1:E:298:LYS:O	1.80	0.81
1:F:120:ILE:HG22	1:F:120:ILE:O	1.81	0.81
1:F:267:LYS:HG2	4:F:1183:HOH:O	1.79	0.81
1:E:40:ILE:HB	1:E:114:LEU:CD1	2.11	0.80
1:C:46:PHE:HE1	1:C:154:THR:O	1.65	0.80
1:A:260:GLN:HE22	3:A:416:A2P:H2	1.45	0.79
1:D:147:ILE:HG21	4:D:1239:HOH:O	1.80	0.79
1:B:286:LYS:HD3	4:B:680:HOH:O	1.83	0.79
1:F:266:ARG:HA	4:F:688:HOH:O	1.82	0.78
1:B:94:ILE:HD13	1:B:94:ILE:N	1.98	0.78
1:F:27:VAL:HG13	1:F:35:VAL:CG1	2.14	0.78
1:D:260:GLN:HG2	1:D:289:ILE:HA	1.65	0.77
1:F:11:THR:HG22	1:F:12:VAL:H	1.50	0.77
1:B:260:GLN:HG2	1:B:289:ILE:HA	1.66	0.76
1:F:28:ARG:NH1	1:F:226:LEU:HD12	1.99	0.76
1:C:24:ILE:HD13	4:C:390:HOH:O	1.86	0.76
1:C:46:PHE:CE1	1:C:154:THR:O	2.38	0.76
1:D:305:GLU:HG3	1:D:307:LYS:CG	2.14	0.75
1:C:4:ASN:O	1:C:5:ASN:OD1	2.04	0.75
1:E:22:ASP:CA	1:E:147:ILE:HD11	2.14	0.74
1:F:224:LEU:CD1	4:F:1159:HOH:O	2.35	0.74
1:F:230:GLU:HG2	4:F:930:HOH:O	1.87	0.74
1:C:294:MET:HE2	4:C:1186:HOH:O	1.86	0.73
1:B:43:ASN:HD22	1:C:206:ASN:HD21	1.32	0.73
1:D:306:LYS:C	1:D:308:LYS:N	2.39	0.73
1:E:177:ALA:HB2	1:E:185:TYR:CE2	2.22	0.73
1:D:306:LYS:CG	1:D:309:LYS:CD	2.57	0.73
1:C:10:TYR:O	1:C:155:GLY:N	2.21	0.73
1:B:266:ARG:HD2	4:B:1164:HOH:O	1.89	0.72
1:F:28:ARG:NH2	1:F:223:ILE:O	2.22	0.72
1:B:168:GLN:HB3	1:E:203:ARG:CZ	2.20	0.72
1:E:40:ILE:HB	1:E:114:LEU:HD11	1.70	0.72
1:B:304:ASP:OD1	1:B:304:ASP:C	2.28	0.71
1:F:118:ILE:HD13	1:F:142:ILE:HD13	1.71	0.71
1:D:307:LYS:HD3	1:D:310:ARG:HH21	1.55	0.71
1:F:182:ILE:HD11	1:F:224:LEU:HB2	1.71	0.71
1:B:118:ILE:HD13	1:B:142:ILE:HD13	1.70	0.71
1:F:308:LYS:HG2	4:F:1103:HOH:O	1.90	0.71
1:F:118:ILE:HD13	1:F:142:ILE:CD1	2.21	0.71
1:B:304:ASP:OD2	1:B:308:LYS:NZ	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ASP:O	1:D:305:GLU:HB3	1.91	0.70
1:F:224:LEU:HD11	4:F:1159:HOH:O	1.91	0.70
1:C:177:ALA:HB2	1:C:185:TYR:HE2	1.56	0.70
1:C:26:LEU:HD12	1:C:35:VAL:HG11	1.73	0.70
1:E:114:LEU:HD12	1:E:114:LEU:C	2.12	0.70
1:A:260:GLN:CG	1:A:289:ILE:HA	2.21	0.70
1:A:260:GLN:NE2	3:A:416:A2P:H2	2.06	0.70
1:A:257:PHE:HE2	1:A:262:GLU:HG2	1.56	0.70
1:B:118:ILE:CD1	1:B:142:ILE:HD13	2.21	0.69
3:E:416:A2P:O4P	1:F:287:LYS:HE3	1.92	0.69
1:A:259:VAL:HG12	1:A:260:GLN:HE21	1.56	0.69
1:C:24:ILE:CD1	4:C:390:HOH:O	2.40	0.69
1:E:265:LYS:HA	4:E:1224:HOH:O	1.93	0.69
1:B:118:ILE:HD13	1:B:142:ILE:HD11	1.73	0.69
1:C:12:VAL:HG21	1:D:97:GLN:OE1	1.92	0.69
1:E:290:ARG:HD2	4:E:1315:HOH:O	1.91	0.69
1:E:260:GLN:HG2	1:E:289:ILE:HA	1.75	0.69
1:E:214:TYR:CG	1:E:263:ILE:HD11	2.28	0.68
1:E:293:VAL:HG12	1:E:294:MET:HE3	1.75	0.68
1:D:260:GLN:CG	1:D:289:ILE:HA	2.23	0.68
1:F:118:ILE:CD1	1:F:142:ILE:HD13	2.24	0.68
1:F:294:MET:C	1:F:295:ASP:OD1	2.32	0.68
1:E:293:VAL:C	1:E:294:MET:HE3	2.14	0.67
1:F:248:TYR:HA	1:F:249:LYS:CB	2.14	0.67
1:A:287:LYS:HG3	4:A:915:HOH:O	1.95	0.67
1:E:220:GLU:HG3	1:E:246:PHE:CZ	2.29	0.67
1:B:260:GLN:NE2	3:B:416:A2P:H2	2.09	0.67
1:A:245:VAL:HG22	1:A:262:GLU:HG3	1.77	0.67
1:D:305:GLU:CG	1:D:307:LYS:CG	2.59	0.67
1:A:147:ILE:HD12	1:A:147:ILE:N	2.10	0.67
3:E:416:A2P:O4P	1:F:287:LYS:CE	2.44	0.67
1:A:257:PHE:CE2	1:A:262:GLU:HG2	2.30	0.66
1:B:53:THR:CG2	1:B:157:HIS:HB2	2.26	0.66
1:E:293:VAL:HG12	1:E:294:MET:CE	2.26	0.66
1:F:275:ASN:O	1:F:277:TYR:N	2.28	0.66
1:C:26:LEU:CD1	1:C:35:VAL:HG12	2.24	0.66
1:F:118:ILE:HG21	1:F:142:ILE:HD13	1.79	0.65
1:F:260:GLN:CD	1:F:292:LYS:HG2	2.16	0.65
1:C:305:GLU:OE2	1:C:305:GLU:N	2.29	0.65
1:F:120:ILE:HD11	1:F:143:LYS:HB2	1.77	0.65
1:A:14:ASN:CG	1:A:14:ASN:O	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:LYS:C	1:D:308:LYS:H	1.97	0.65
1:E:165:ASP:HB3	1:E:169:LYS:HG3	1.78	0.65
1:F:11:THR:HG22	1:F:12:VAL:N	2.11	0.65
1:D:62:GLU:N	1:D:62:GLU:OE1	2.30	0.64
1:A:5:ASN:HD22	1:A:7:ILE:HB	1.60	0.64
1:A:191:LYS:NZ	4:A:1272:HOH:O	2.30	0.64
1:E:217:VAL:CG1	1:E:222:SER:HB2	2.27	0.64
1:A:177:ALA:HB2	1:A:185:TYR:HE2	1.62	0.64
1:E:40:ILE:HB	1:E:114:LEU:HD12	1.79	0.64
1:B:260:GLN:CG	1:B:289:ILE:HA	2.27	0.63
1:E:217:VAL:CG1	1:E:218:TYR:N	2.60	0.63
1:E:27:VAL:HG11	1:E:33:ASN:ND2	2.13	0.63
1:E:274:PHE:HA	1:E:279:CYS:HB2	1.81	0.63
1:B:260:GLN:NE2	1:B:260:GLN:H	1.95	0.63
1:D:61:ASN:HB3	1:D:62:GLU:OE1	1.99	0.63
1:C:177:ALA:HB2	1:C:185:TYR:CE2	2.34	0.62
1:D:260:GLN:NE2	3:D:416:A2P:H2	2.13	0.62
1:E:28:ARG:HB3	1:E:29:PRO:HD2	1.82	0.62
1:E:260:GLN:NE2	1:E:260:GLN:H	1.96	0.62
1:C:12:VAL:CG2	1:D:97:GLN:OE1	2.46	0.62
1:C:305:GLU:C	4:C:1308:HOH:O	2.37	0.62
1:D:61:ASN:CB	1:D:62:GLU:OE1	2.47	0.62
1:D:226:LEU:HD22	1:D:230:GLU:HG3	1.81	0.62
1:F:248:TYR:CA	1:F:249:LYS:HB3	2.26	0.62
1:A:260:GLN:HG2	1:A:289:ILE:HA	1.82	0.62
1:F:122:LYS:NZ	4:F:798:HOH:O	2.33	0.62
1:A:236:TYR:O	1:A:240:ILE:HG22	2.00	0.61
1:A:260:GLN:NE2	1:A:260:GLN:H	1.98	0.61
1:C:245:VAL:HG22	1:C:262:GLU:HG3	1.82	0.61
1:E:217:VAL:CG1	1:E:222:SER:CB	2.78	0.61
1:E:298:LYS:HA	4:E:1165:HOH:O	1.98	0.61
1:B:276:ASN:ND2	4:B:1347:HOH:O	2.34	0.61
1:F:281:LEU:HD12	1:F:282:TYR:H	1.66	0.61
1:B:267:LYS:HB2	1:B:296:ILE:HD13	1.82	0.61
1:E:217:VAL:HG12	1:E:218:TYR:N	2.16	0.61
1:F:7:ILE:HA	1:F:156:ALA:HB3	1.83	0.61
1:D:260:GLN:HE22	3:D:416:A2P:H2	1.64	0.61
1:B:53:THR:HG23	1:B:157:HIS:HB2	1.83	0.61
1:E:135:TYR:CD1	4:E:1173:HOH:O	2.52	0.61
1:F:224:LEU:HG	4:F:1159:HOH:O	1.99	0.61
1:F:50:GLU:OE2	1:F:109:ASN:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:241:ASN:CB	4:F:903:HOH:O	2.30	0.60
1:F:260:GLN:CD	1:F:292:LYS:CG	2.69	0.60
1:B:97:GLN:HA	4:B:1237:HOH:O	2.01	0.60
1:E:98:ARG:NH2	1:F:97:GLN:N	2.50	0.60
1:F:28:ARG:HB3	1:F:29:PRO:CD	2.31	0.60
1:F:27:VAL:HG13	1:F:35:VAL:HG11	1.83	0.60
1:C:264:TYR:O	1:C:267:LYS:HB2	2.01	0.60
1:E:214:TYR:CD2	1:E:263:ILE:HD11	2.36	0.60
1:F:177:ALA:HB2	1:F:185:TYR:HE1	1.67	0.60
1:A:259:VAL:O	1:A:263:ILE:HG12	2.01	0.60
1:E:299:SER:HB3	4:E:1240:HOH:O	2.01	0.60
1:F:174:ILE:HD11	1:F:214:TYR:CD1	2.37	0.60
1:B:308:LYS:HG3	4:B:1345:HOH:O	2.02	0.59
1:B:266:ARG:CD	4:B:1164:HOH:O	2.48	0.59
1:D:306:LYS:HG3	1:D:306:LYS:O	2.02	0.59
1:B:7:ILE:HD11	4:B:932:HOH:O	2.01	0.59
1:F:274:PHE:HD2	1:F:275:ASN:OD1	1.86	0.59
1:C:260:GLN:HG3	1:C:289:ILE:HA	1.85	0.59
1:E:155:GLY:O	1:E:157:HIS:CD2	2.56	0.59
1:B:260:GLN:HE22	3:B:416:A2P:H2	1.67	0.59
1:C:7:ILE:HA	1:C:156:ALA:O	2.02	0.59
1:A:10:TYR:HB2	1:A:155:GLY:N	2.18	0.58
1:A:177:ALA:HB2	1:A:185:TYR:CE2	2.37	0.58
1:F:290:ARG:C	4:F:933:HOH:O	2.40	0.58
1:F:281:LEU:HD12	1:F:282:TYR:N	2.19	0.58
1:F:310:ARG:NH2	4:F:1247:HOH:O	2.36	0.58
1:B:267:LYS:CB	1:B:296:ILE:HD13	2.33	0.58
1:A:147:ILE:H	1:A:147:ILE:CD1	2.12	0.58
1:F:10:TYR:HB2	1:F:155:GLY:H	1.68	0.58
1:D:62:GLU:O	1:D:62:GLU:HG2	2.04	0.58
1:D:177:ALA:HB2	1:D:185:TYR:HE1	1.67	0.58
1:A:28:ARG:HB3	1:A:29:PRO:HD2	1.86	0.58
1:E:42:HIS:HD2	1:E:114:LEU:HG	1.68	0.58
1:A:10:TYR:H	1:A:155:GLY:HA3	1.69	0.58
1:C:260:GLN:OE1	3:C:416:A2P:H2	2.04	0.58
1:A:287:LYS:HA	1:A:315:VAL:HG11	1.84	0.58
1:E:101:ARG:HG3	1:E:138:CYS:HB2	1.86	0.58
1:F:30:ASN:HB2	1:F:221:ASP:OD2	2.03	0.57
1:F:224:LEU:CG	4:F:1159:HOH:O	2.53	0.57
1:E:109:ASN:HB2	1:E:191:LYS:NZ	2.20	0.57
1:C:98:ARG:O	1:D:97:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLY:N	1:C:154:THR:OG1	2.38	0.57
1:D:56:ILE:O	1:D:58:PRO:HD3	2.05	0.57
1:F:122:LYS:HE2	1:F:135:TYR:HE2	1.70	0.57
1:B:5:ASN:N	4:B:606:HOH:O	2.37	0.56
1:D:304:ASP:O	1:D:305:GLU:CB	2.53	0.56
1:A:203:ARG:NH2	1:A:235:MET:O	2.38	0.56
4:A:1118:HOH:O	1:B:287:LYS:HD2	2.05	0.56
1:B:267:LYS:HB2	1:B:296:ILE:HG21	1.85	0.56
1:B:309:LYS:HE2	4:B:572:HOH:O	2.05	0.56
1:D:193:PHE:CE2	1:D:240:ILE:HD11	2.40	0.56
1:F:260:GLN:HG2	1:F:292:LYS:HG3	1.87	0.56
1:E:114:LEU:CD1	1:E:114:LEU:C	2.75	0.56
1:E:288:SER:CB	3:E:416:A2P:HN62	2.18	0.56
1:A:147:ILE:HD13	4:A:327:HOH:O	2.05	0.56
1:E:98:ARG:HG3	1:E:98:ARG:O	2.06	0.56
1:E:155:GLY:O	1:E:157:HIS:NE2	2.39	0.56
1:D:28:ARG:NH2	4:D:404:HOH:O	2.39	0.55
1:D:177:ALA:HB2	1:D:185:TYR:CE1	2.41	0.55
1:E:298:LYS:HE2	1:E:298:LYS:HA	1.87	0.55
1:C:257:PHE:HE2	1:C:262:GLU:HG2	1.71	0.55
1:F:159:TYR:N	4:F:629:HOH:O	2.32	0.55
1:E:273:LEU:O	1:E:277:TYR:HB2	2.06	0.55
1:C:306:LYS:N	4:C:1308:HOH:O	2.40	0.55
1:D:305:GLU:C	1:D:307:LYS:H	2.09	0.55
3:C:416:A2P:O2P	1:D:288:SER:OG	2.21	0.55
1:E:42:HIS:CD2	1:E:114:LEU:HG	2.42	0.55
1:E:294:MET:CE	1:E:294:MET:N	2.51	0.55
1:B:266:ARG:NH1	4:B:1329:HOH:O	2.39	0.55
1:D:259:VAL:O	1:D:263:ILE:HG12	2.07	0.55
1:E:290:ARG:CD	4:E:1315:HOH:O	2.52	0.55
1:F:116:VAL:HG12	1:F:118:ILE:HG13	1.87	0.55
1:F:225:TYR:N	4:F:334:HOH:O	2.39	0.55
1:B:5:ASN:N	1:B:5:ASN:OD1	2.39	0.54
1:B:177:ALA:HB2	1:B:185:TYR:HE1	1.73	0.54
1:B:223:ILE:HG21	1:B:226:LEU:HD23	1.90	0.54
1:A:7:ILE:HD11	4:A:363:HOH:O	2.07	0.54
1:E:260:GLN:CG	1:E:289:ILE:HA	2.37	0.54
1:F:248:TYR:HD2	4:F:1171:HOH:O	1.89	0.54
1:D:176:ILE:HD12	1:D:281:LEU:HD21	1.90	0.54
1:E:277:TYR:N	4:E:1275:HOH:O	2.40	0.54
1:E:217:VAL:HG11	1:E:222:SER:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:CD1	1:B:142:ILE:CD1	2.80	0.54
1:B:308:LYS:HE3	4:B:1345:HOH:O	2.07	0.54
1:D:232:PHE:HB3	1:D:240:ILE:HD12	1.90	0.54
1:E:50:GLU:CD	1:E:191:LYS:HD2	2.29	0.54
1:C:260:GLN:CG	1:C:289:ILE:HA	2.38	0.53
1:E:48:TYR:CE2	1:E:105:ILE:HG21	2.43	0.53
1:B:308:LYS:CG	4:B:1345:HOH:O	2.55	0.53
1:F:241:ASN:CG	4:F:903:HOH:O	2.45	0.53
1:F:260:GLN:HG2	1:F:292:LYS:CG	2.39	0.53
1:B:118:ILE:CG2	1:B:142:ILE:HD13	2.28	0.53
1:E:217:VAL:HG12	1:E:222:SER:HB2	1.91	0.53
1:E:298:LYS:HE2	1:E:298:LYS:CA	2.38	0.53
1:F:27:VAL:HG13	1:F:35:VAL:HG12	1.90	0.53
1:F:35:VAL:HG11	1:F:224:LEU:HD21	1.90	0.53
1:F:260:GLN:HG2	1:F:292:LYS:HB2	1.91	0.53
1:A:101:ARG:HG3	1:A:138:CYS:HB2	1.91	0.53
1:B:177:ALA:HB2	1:B:185:TYR:CE1	2.44	0.52
1:E:109:ASN:HB2	1:E:191:LYS:HZ2	1.74	0.52
1:E:259:VAL:HG12	1:E:260:GLN:HE21	1.75	0.52
1:D:114:LEU:HD12	1:D:114:LEU:C	2.30	0.52
1:F:27:VAL:HG21	1:F:33:ASN:O	2.08	0.52
1:F:177:ALA:HB2	1:F:185:TYR:CE1	2.43	0.52
1:C:203:ARG:NH1	4:C:1026:HOH:O	2.43	0.52
1:D:58:PRO:HD2	1:D:99:CYS:O	2.10	0.52
1:A:37:HIS:CE1	1:A:115:SER:HB2	2.45	0.52
1:A:143:LYS:NZ	4:A:784:HOH:O	2.43	0.52
1:D:214:TYR:CG	1:D:263:ILE:HD11	2.45	0.52
1:E:165:ASP:O	1:E:169:LYS:HB2	2.09	0.52
1:F:12:VAL:HG12	1:F:98:ARG:HD3	1.92	0.52
1:A:147:ILE:CD1	4:A:327:HOH:O	2.57	0.52
1:D:306:LYS:HG2	1:D:309:LYS:CD	2.40	0.51
1:A:109:ASN:ND2	4:A:338:HOH:O	2.42	0.51
1:F:260:GLN:OE1	1:F:292:LYS:CG	2.43	0.51
1:E:243:HIS:HA	4:E:1195:HOH:O	2.09	0.51
1:A:288:SER:OG	3:B:416:A2P:O2P	2.27	0.51
1:D:55:GLY:O	1:D:153:LEU:HA	2.10	0.51
1:D:14:ASN:CG	1:D:14:ASN:O	2.49	0.51
1:A:260:GLN:HE22	3:A:416:A2P:C2	2.21	0.51
1:D:12:VAL:HG23	4:D:642:HOH:O	2.11	0.51
1:F:289:ILE:HD11	3:F:416:A2P:H2	1.92	0.51
1:C:10:TYR:H	1:C:155:GLY:HA3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:ASP:HA	1:E:147:ILE:CD1	2.25	0.50
1:E:214:TYR:CD2	1:E:263:ILE:CD1	2.93	0.50
1:E:298:LYS:HE2	1:E:298:LYS:C	2.31	0.50
1:A:10:TYR:HB2	1:A:155:GLY:H	1.75	0.50
1:E:178:THR:HG23	1:E:289:ILE:HD11	1.92	0.50
1:E:143:LYS:HE2	4:E:321:HOH:O	2.11	0.50
1:F:181:GLY:O	1:F:184:PRO:HD2	2.12	0.50
1:F:290:ARG:NE	4:F:1129:HOH:O	2.43	0.50
1:C:116:VAL:HG12	1:C:118:ILE:HG13	1.94	0.50
1:D:281:LEU:HD23	1:D:282:TYR:N	2.26	0.50
1:B:309:LYS:HA	4:B:336:HOH:O	2.10	0.50
1:C:5:ASN:OD1	1:C:5:ASN:O	2.30	0.50
1:B:168:GLN:CB	1:E:203:ARG:NH2	2.62	0.50
1:D:53:THR:CG2	1:D:102:LEU:HD22	2.41	0.50
1:D:285:GLY:O	1:D:315:VAL:HA	2.12	0.50
1:A:199:ASN:HB3	1:A:202:ASN:HD21	1.77	0.50
1:B:220:GLU:HB2	4:B:1126:HOH:O	2.11	0.50
1:E:260:GLN:NE2	3:E:416:A2P:H2	2.26	0.50
1:E:269:GLU:O	1:E:272:ASN:ND2	2.45	0.50
1:A:116:VAL:HG12	1:A:118:ILE:HG13	1.93	0.49
1:F:174:ILE:HD11	1:F:214:TYR:CE1	2.47	0.49
1:D:97:GLN:O	4:D:827:HOH:O	2.20	0.49
1:D:111:MET:HE1	4:D:476:HOH:O	2.11	0.49
1:E:258:TYR:HB3	1:E:260:GLN:HE22	1.77	0.49
1:B:259:VAL:HG12	1:B:260:GLN:HE21	1.78	0.49
1:F:260:GLN:CG	1:F:292:LYS:HB2	2.43	0.49
1:F:277:TYR:N	4:F:1004:HOH:O	2.46	0.49
1:C:126:THR:HB	1:D:159:TYR:HE1	1.77	0.49
1:E:298:LYS:O	1:E:298:LYS:CE	2.55	0.49
1:A:287:LYS:HG2	1:A:315:VAL:HB	1.95	0.49
1:D:167:ILE:HG13	1:D:168:GLN:H	1.77	0.49
1:E:217:VAL:CG1	1:E:218:TYR:H	2.25	0.49
1:F:118:ILE:CD1	1:F:142:ILE:CD1	2.88	0.49
1:F:199:ASN:HB3	1:F:202:ASN:HD22	1.77	0.49
1:F:35:VAL:HG11	1:F:224:LEU:CD2	2.42	0.49
1:B:264:TYR:CD1	1:B:296:ILE:HD11	2.48	0.48
1:E:143:LYS:CE	4:E:321:HOH:O	2.61	0.48
1:F:247:SER:O	1:F:249:LYS:HA	2.12	0.48
1:E:217:VAL:HG11	1:E:222:SER:C	2.33	0.48
1:A:260:GLN:HG3	1:A:289:ILE:HA	1.95	0.48
1:C:116:VAL:CG1	1:C:117:ALA:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:GLU:OE2	4:D:1083:HOH:O	2.20	0.48
1:F:7:ILE:CD1	1:F:159:TYR:CE2	2.96	0.48
1:F:120:ILE:HG21	1:F:122:LYS:HE2	1.94	0.48
1:F:260:GLN:CG	1:F:292:LYS:CG	2.92	0.48
1:D:287:LYS:HA	1:D:315:VAL:HG11	1.95	0.48
1:F:12:VAL:CG1	1:F:98:ARG:HB3	2.43	0.48
1:D:98:ARG:NH1	4:D:1303:HOH:O	2.46	0.48
1:F:143:LYS:O	1:F:143:LYS:HD3	2.13	0.48
1:F:265:LYS:NZ	1:F:265:LYS:HB2	2.29	0.48
1:A:288:SER:O	1:A:289:ILE:C	2.49	0.48
1:C:114:LEU:C	1:C:114:LEU:HD12	2.34	0.48
1:C:155:GLY:O	1:C:157:HIS:CD2	2.66	0.48
1:F:174:ILE:HD11	1:F:214:TYR:HD1	1.79	0.48
1:D:111:MET:CE	4:D:476:HOH:O	2.62	0.48
1:F:268:THR:HG23	4:F:919:HOH:O	2.12	0.48
1:A:176:ILE:HB	1:A:283:ILE:HD13	1.95	0.48
1:A:294:MET:O	1:A:298:LYS:HG2	2.13	0.48
1:C:48:TYR:CE2	1:C:105:ILE:HG21	2.49	0.48
1:C:305:GLU:C	1:C:307:LYS:N	2.67	0.48
1:C:26:LEU:CD2	1:C:37:HIS:CB	2.76	0.47
1:C:275:ASN:HA	4:C:747:HOH:O	2.14	0.47
1:B:260:GLN:HE22	3:B:416:A2P:C2	2.27	0.47
1:D:30:ASN:HB2	1:D:221:ASP:OD2	2.14	0.47
1:C:4:ASN:N	4:C:1108:HOH:O	2.47	0.47
1:A:10:TYR:O	1:A:155:GLY:N	2.46	0.47
1:A:176:ILE:HD12	1:A:283:ILE:CD1	2.45	0.47
1:E:217:VAL:CG1	1:E:222:SER:HB3	2.45	0.47
1:D:307:LYS:HD3	1:D:310:ARG:NH2	2.26	0.47
1:E:26:LEU:HG	1:E:37:HIS:HB2	1.95	0.47
1:F:286:LYS:HB2	1:F:289:ILE:CD1	2.44	0.47
1:F:286:LYS:HB2	1:F:289:ILE:HD13	1.97	0.47
1:D:53:THR:CG2	1:D:157:HIS:HB2	2.37	0.47
1:D:305:GLU:CD	1:D:307:LYS:HE3	2.36	0.47
1:A:55:GLY:O	1:A:153:LEU:HA	2.15	0.46
1:B:272:ASN:O	1:B:276:ASN:HB2	2.15	0.46
1:B:307:LYS:NZ	4:B:986:HOH:O	2.47	0.46
1:E:123:TYR:O	1:E:124:GLU:HB3	2.15	0.46
1:F:283:ILE:HD13	1:F:289:ILE:HG22	1.97	0.46
1:A:245:VAL:CG2	1:A:262:GLU:HG3	2.45	0.46
1:B:26:LEU:HG	1:B:37:HIS:HB2	1.97	0.46
1:B:264:TYR:HD1	1:B:296:ILE:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ASP:OD1	1:B:304:ASP:O	2.33	0.46
1:D:12:VAL:HG12	1:D:12:VAL:O	2.15	0.46
1:D:51:GLY:HA3	1:D:160:PHE:O	2.15	0.46
1:A:251:ASN:HB2	1:B:292:LYS:HE3	1.96	0.46
1:B:245:VAL:HG22	1:B:262:GLU:HG3	1.98	0.46
1:A:288:SER:O	1:A:290:ARG:N	2.48	0.46
1:C:56:ILE:O	1:C:58:PRO:HD3	2.16	0.46
1:C:165:ASP:HA	4:C:982:HOH:O	2.15	0.46
1:A:307:LYS:HG2	1:A:310:ARG:HH21	1.80	0.46
1:B:290:ARG:O	1:B:294:MET:HG2	2.16	0.46
1:F:34:GLU:OE1	1:F:122:LYS:CE	2.64	0.46
1:F:217:VAL:O	1:F:246:PHE:HA	2.15	0.46
1:D:260:GLN:HG3	1:D:289:ILE:HG23	1.98	0.46
1:D:260:GLN:HE21	1:D:260:GLN:N	2.01	0.46
1:F:120:ILE:HD13	1:F:139:SER:HB3	1.96	0.45
1:F:248:TYR:C	1:F:248:TYR:CD2	2.89	0.45
1:F:260:GLN:HG2	1:F:292:LYS:CB	2.45	0.45
1:A:42:HIS:CD2	1:A:114:LEU:HD23	2.51	0.45
1:B:43:ASN:HD22	1:C:206:ASN:ND2	2.07	0.45
1:B:306:LYS:O	1:B:309:LYS:HG2	2.16	0.45
1:D:164:ASN:ND2	1:D:164:ASN:H	2.14	0.45
1:F:49:LEU:O	1:F:52:HIS:HB2	2.17	0.45
1:A:28:ARG:HB3	1:A:29:PRO:CD	2.45	0.45
1:F:226:LEU:CD2	1:F:230:GLU:HG3	2.40	0.45
1:F:292:LYS:HA	1:F:295:ASP:OD2	2.15	0.45
1:C:12:VAL:HB	1:D:97:GLN:OE1	2.17	0.45
1:F:7:ILE:HD13	1:F:159:TYR:CZ	2.51	0.45
1:F:46:PHE:CE1	1:F:155:GLY:O	2.67	0.45
1:A:116:VAL:CG1	1:A:117:ALA:N	2.79	0.45
1:B:288:SER:O	1:B:289:ILE:C	2.54	0.45
1:C:55:GLY:HA2	1:C:101:ARG:O	2.16	0.45
1:D:266:ARG:HG2	1:D:269:GLU:HB2	1.98	0.45
1:D:288:SER:O	1:D:289:ILE:C	2.55	0.45
1:E:259:VAL:CG1	1:E:260:GLN:HE21	2.30	0.45
1:F:120:ILE:HD13	1:F:120:ILE:HG23	1.62	0.45
1:D:226:LEU:CD2	1:D:230:GLU:HG3	2.46	0.45
1:D:258:TYR:HB3	1:D:260:GLN:HE22	1.82	0.45
1:C:26:LEU:HD11	1:C:117:ALA:HB1	1.98	0.45
1:C:287:LYS:HE3	4:D:319:HOH:O	2.17	0.45
1:D:98:ARG:NH2	4:D:1256:HOH:O	2.29	0.45
1:E:27:VAL:HG11	1:E:33:ASN:HD22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:LYS:HA	4:E:1225:HOH:O	2.16	0.45
1:F:114:LEU:C	1:F:114:LEU:HD12	2.37	0.45
1:F:28:ARG:HB3	1:F:29:PRO:HD2	1.99	0.45
1:F:275:ASN:HB3	4:F:1199:HOH:O	2.16	0.45
1:B:28:ARG:HB3	1:B:29:PRO:HD2	1.99	0.45
1:E:214:TYR:CE2	1:E:263:ILE:CD1	3.00	0.45
1:F:262:GLU:O	1:F:265:LYS:HG3	2.17	0.45
1:A:34:GLU:OE2	1:A:143:LYS:HE2	2.17	0.44
1:A:280:GLU:OE1	1:A:310:ARG:HA	2.17	0.44
1:C:185:TYR:O	1:C:189:LEU:HG	2.17	0.44
1:B:94:ILE:N	1:B:94:ILE:CD1	2.70	0.44
1:F:55:GLY:O	1:F:153:LEU:HA	2.18	0.44
1:C:228:GLU:OE1	1:C:228:GLU:N	2.47	0.44
1:F:26:LEU:HG	1:F:37:HIS:HB2	2.00	0.44
1:F:116:VAL:CG1	1:F:117:ALA:N	2.80	0.44
1:F:142:ILE:O	1:F:145:LEU:HB2	2.16	0.44
1:B:12:VAL:O	1:B:98:ARG:NH1	2.50	0.44
1:B:14:ASN:CG	1:B:14:ASN:O	2.54	0.44
1:E:14:ASN:HB3	4:E:753:HOH:O	2.17	0.44
1:F:164:ASN:OD1	1:F:164:ASN:N	2.43	0.44
1:A:122:LYS:HG3	1:A:135:TYR:CD2	2.52	0.44
1:C:143:LYS:NZ	4:C:721:HOH:O	2.48	0.44
1:D:28:ARG:HB3	1:D:29:PRO:HD2	2.00	0.44
1:D:53:THR:HG23	1:D:102:LEU:HD22	1.98	0.44
1:A:231:TYR:CZ	1:A:235:MET:HG3	2.52	0.44
1:C:55:GLY:CA	1:C:154:THR:OG1	2.66	0.44
1:D:142:ILE:O	1:D:145:LEU:HB2	2.17	0.44
1:E:265:LYS:CA	4:E:1224:HOH:O	2.61	0.44
1:F:248:TYR:HD2	1:F:248:TYR:C	2.21	0.44
1:D:61:ASN:HB2	1:D:62:GLU:OE1	2.16	0.44
1:F:28:ARG:HH11	1:F:226:LEU:HD12	1.79	0.44
1:D:27:VAL:HG13	1:D:35:VAL:HG13	1.99	0.44
1:E:214:TYR:CE2	1:E:263:ILE:HD13	2.53	0.44
1:D:235:MET:HA	1:D:235:MET:CE	2.48	0.43
1:B:39:GLU:CG	4:B:449:HOH:O	2.66	0.43
1:C:286:LYS:HG2	3:C:416:A2P:C5	2.47	0.43
1:E:260:GLN:HE22	3:E:416:A2P:H2	1.82	0.43
1:F:287:LYS:HG3	1:F:288:SER:N	2.33	0.43
1:D:305:GLU:C	1:D:307:LYS:N	2.71	0.43
1:D:306:LYS:HG2	1:D:309:LYS:HD3	1.85	0.43
1:F:123:TYR:O	1:F:124:GLU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:O	1:A:109:ASN:ND2	2.51	0.43
1:A:122:LYS:HE2	1:A:135:TYR:HE2	1.83	0.43
1:D:305:GLU:HG3	1:D:307:LYS:H	1.83	0.43
1:C:183:SER:N	1:C:184:PRO:HD2	2.34	0.43
1:E:111:MET:CE	1:E:190:LYS:HD3	2.48	0.43
1:E:206:ASN:N	1:E:206:ASN:HD22	2.15	0.43
1:A:38:LEU:O	1:A:115:SER:HA	2.17	0.43
1:A:55:GLY:HA2	1:A:101:ARG:O	2.19	0.43
1:C:5:ASN:C	1:C:7:ILE:H	2.21	0.43
1:E:185:TYR:O	1:E:189:LEU:HG	2.18	0.43
1:E:217:VAL:HG13	1:E:218:TYR:H	1.82	0.43
1:B:122:LYS:NZ	4:B:1198:HOH:O	2.48	0.43
1:C:220:GLU:CD	1:C:220:GLU:H	2.20	0.43
1:E:294:MET:O	1:E:298:LYS:N	2.45	0.43
1:B:178:THR:HG23	1:B:289:ILE:HD11	1.99	0.43
1:D:49:LEU:O	1:D:52:HIS:HB2	2.19	0.43
1:F:287:LYS:HA	1:F:315:VAL:HG11	2.00	0.43
1:A:58:PRO:HD2	1:A:99:CYS:O	2.19	0.43
1:E:10:TYR:HB2	1:E:155:GLY:N	2.33	0.43
1:F:10:TYR:H	1:F:155:GLY:HA2	1.83	0.43
1:B:217:VAL:O	1:B:246:PHE:HA	2.18	0.43
1:C:119:LYS:NZ	3:C:416:A2P:O5P	2.51	0.43
1:E:146:LYS:O	1:E:149:ASP:HB2	2.18	0.43
1:F:11:THR:CG2	1:F:12:VAL:H	2.27	0.43
1:F:172:ASN:ND2	1:F:277:TYR:HB3	2.34	0.43
1:C:12:VAL:CB	1:D:97:GLN:OE1	2.67	0.42
1:F:233:GLN:HB3	4:F:931:HOH:O	2.18	0.42
1:D:109:ASN:C	1:D:109:ASN:HD22	2.23	0.42
1:F:122:LYS:HE2	1:F:135:TYR:CE2	2.53	0.42
1:A:60:TYR:O	1:A:61:ASN:C	2.57	0.42
1:A:191:LYS:HG3	4:A:371:HOH:O	2.19	0.42
1:B:203:ARG:NH1	1:B:205:SER:O	2.52	0.42
1:C:179:GLY:HA3	4:C:367:HOH:O	2.19	0.42
1:E:257:PHE:HD1	1:F:255:THR:HG22	1.84	0.42
1:F:118:ILE:HG21	1:F:142:ILE:CD1	2.47	0.42
1:F:183:SER:HB2	1:F:184:PRO:HD3	2.01	0.42
1:F:308:LYS:HE2	4:F:1103:HOH:O	2.19	0.42
1:A:17:LYS:HE2	4:A:637:HOH:O	2.20	0.42
1:A:30:ASN:HB2	1:A:221:ASP:OD2	2.20	0.42
1:B:266:ARG:HA	4:B:702:HOH:O	2.19	0.42
1:B:294:MET:HE2	4:B:660:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ARG:HB3	1:D:29:PRO:CD	2.49	0.42
1:A:217:VAL:O	1:A:246:PHE:HA	2.19	0.42
2:C:415:FAD:H1'1	2:C:415:FAD:H9	1.76	0.42
1:D:97:GLN:HA	1:D:98:ARG:NH2	2.35	0.42
1:E:288:SER:OG	3:E:416:A2P:N6	2.53	0.42
1:D:174:ILE:HD13	1:D:270:PHE:CE1	2.55	0.42
1:F:260:GLN:CD	1:F:292:LYS:HG3	2.40	0.42
1:B:199:ASN:HB3	1:B:202:ASN:HD22	1.85	0.42
1:D:147:ILE:CG2	4:D:1239:HOH:O	2.54	0.42
1:E:260:GLN:HE22	3:E:416:A2P:C2	2.33	0.42
1:A:286:LYS:HG3	3:A:416:A2P:C4	2.50	0.41
1:B:261:ASP:OD2	1:B:292:LYS:NZ	2.41	0.41
1:C:288:SER:CB	3:C:416:A2P:HN62	2.33	0.41
1:C:294:MET:CE	4:C:1186:HOH:O	2.56	0.41
1:D:180:THR:HA	1:D:224:LEU:HD12	2.02	0.41
1:E:182:ILE:HD12	1:E:185:TYR:HD2	1.85	0.41
1:C:123:TYR:CZ	1:C:134:ASN:HB2	2.55	0.41
1:F:107:SER:OG	1:F:114:LEU:HA	2.20	0.41
1:F:174:ILE:CG2	1:F:281:LEU:HA	2.38	0.41
1:B:189:LEU:HD22	1:B:193:PHE:HE2	1.85	0.41
1:C:24:ILE:O	1:C:36:TYR:HA	2.20	0.41
1:C:55:GLY:HA3	1:C:154:THR:OG1	2.19	0.41
1:C:155:GLY:O	1:C:157:HIS:NE2	2.54	0.41
1:D:35:VAL:HB	1:D:119:LYS:HA	2.03	0.41
1:D:165:ASP:O	1:D:169:LYS:HB2	2.20	0.41
1:F:172:ASN:HD22	1:F:277:TYR:HB3	1.85	0.41
1:C:23:LYS:O	1:C:24:ILE:HD13	2.20	0.41
1:B:118:ILE:HG21	1:B:142:ILE:HD12	1.95	0.41
1:F:28:ARG:HH22	1:F:223:ILE:HB	1.86	0.41
1:D:109:ASN:C	1:D:109:ASN:ND2	2.74	0.41
1:D:224:LEU:O	1:D:225:TYR:HB2	2.21	0.41
1:F:11:THR:CG2	1:F:12:VAL:N	2.81	0.41
1:A:251:ASN:HB2	1:B:292:LYS:HG3	2.03	0.41
1:A:259:VAL:HG12	1:A:260:GLN:NE2	2.28	0.41
2:A:415:FAD:H1'1	2:A:415:FAD:H9	1.81	0.41
1:B:267:LYS:HB3	1:B:296:ILE:HD13	2.02	0.41
1:B:287:LYS:HA	1:B:315:VAL:HG11	2.03	0.41
1:A:61:ASN:C	1:A:61:ASN:OD1	2.59	0.40
1:B:55:GLY:HA2	1:B:101:ARG:O	2.21	0.40
1:D:269:GLU:HA	1:D:272:ASN:HB2	2.02	0.40
1:E:260:GLN:HB2	1:E:292:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:274:PHE:CE2	1:F:275:ASN:OD1	2.73	0.40
1:C:46:PHE:CZ	1:C:154:THR:O	2.73	0.40
1:E:37:HIS:CE1	1:E:115:SER:HB2	2.56	0.40
1:D:306:LYS:CG	1:D:306:LYS:O	2.68	0.40
1:F:186:ILE:HD13	1:F:186:ILE:HA	1.88	0.40
1:F:260:GLN:CG	1:F:292:LYS:HG3	2.50	0.40
1:F:268:THR:CG2	4:F:919:HOH:O	2.68	0.40
1:B:286:LYS:HA	4:B:825:HOH:O	2.22	0.40
1:E:135:TYR:CE2	1:E:143:LYS:HD2	2.57	0.40
1:E:248:TYR:N	4:E:1197:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/316 (79%)	241 (96%)	8 (3%)	2 (1%)	19	19
1	B	251/316 (79%)	240 (96%)	11 (4%)	0	100	100
1	C	259/316 (82%)	249 (96%)	10 (4%)	0	100	100
1	D	257/316 (81%)	247 (96%)	8 (3%)	2 (1%)	19	19
1	E	241/316 (76%)	236 (98%)	5 (2%)	0	100	100
1	F	242/316 (77%)	231 (96%)	11 (4%)	0	100	100
All	All	1501/1896 (79%)	1444 (96%)	53 (4%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	305	GLU
1	A	204	ASN

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Mol	Chain	Res	Type
1	D	306	LYS
1	A	289	ILE

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	243/295 (82%)	234 (96%)	9 (4%)	34	43
1	B	245/295 (83%)	231 (94%)	14 (6%)	20	24
1	C	246/295 (83%)	237 (96%)	9 (4%)	34	43
1	D	246/295 (83%)	230 (94%)	16 (6%)	17	19
1	E	235/295 (80%)	224 (95%)	11 (5%)	26	33
1	F	234/295 (79%)	226 (97%)	8 (3%)	37	47
All	All	1449/1770 (82%)	1382 (95%)	67 (5%)	27	34

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	61	ASN
1	A	109	ASN
1	A	164	ASN
1	A	203	ARG
1	A	204	ASN
1	A	233	GLN
1	A	260	GLN
1	A	304	ASP
1	B	5	ASN
1	B	35	VAL
1	B	45	LEU
1	B	94	ILE
1	B	109	ASN
1	B	116	VAL
1	B	143	LYS

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Mol	Chain	Res	Type
1	B	147	ILE
1	B	226	LEU
1	B	235	MET
1	B	260	GLN
1	B	262	GLU
1	B	266	ARG
1	B	304	ASP
1	C	7	ILE
1	C	28	ARG
1	C	124	GLU
1	C	201	TYR
1	C	203	ARG
1	C	250	GLN
1	C	260	GLN
1	C	287	LYS
1	C	309	LYS
1	D	28	ARG
1	D	30	ASN
1	D	35	VAL
1	D	45	LEU
1	D	53	THR
1	D	97	GLN
1	D	98	ARG
1	D	109	ASN
1	D	116	VAL
1	D	132	ILE
1	D	165	ASP
1	D	167	ILE
1	D	226	LEU
1	D	260	GLN
1	D	272	ASN
1	D	281	LEU
1	E	33	ASN
1	E	114	LEU
1	E	201	TYR
1	E	203	ARG
1	E	204	ASN
1	E	220	GLU
1	E	260	GLN
1	E	272	ASN
1	E	294	MET
1	E	298	LYS

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Mol	Chain	Res	Type
1	E	308	LYS
1	F	120	ILE
1	F	124	GLU
1	F	164	ASN
1	F	201	TYR
1	F	226	LEU
1	F	238	ASN
1	F	248	TYR
1	F	265	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	8	ASN
1	A	30	ASN
1	A	109	ASN
1	A	144	ASN
1	A	164	ASN
1	A	170	ASN
1	A	204	ASN
1	A	233	GLN
1	A	241	ASN
1	A	250	GLN
1	A	260	GLN
1	A	272	ASN
1	B	5	ASN
1	B	109	ASN
1	B	144	ASN
1	B	161	ASN
1	B	202	ASN
1	B	260	GLN
1	B	272	ASN
1	C	8	ASN
1	C	144	ASN
1	C	161	ASN
1	C	206	ASN
1	C	233	GLN
1	C	241	ASN
1	C	250	GLN
1	D	5	ASN
1	D	8	ASN

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Mol	Chain	Res	Type
1	D	41	ASN
1	D	109	ASN
1	D	164	ASN
1	D	241	ASN
1	D	260	GLN
1	D	272	ASN
1	E	8	ASN
1	E	30	ASN
1	E	33	ASN
1	E	61	ASN
1	E	206	ASN
1	E	241	ASN
1	E	243	HIS
1	E	260	GLN
1	E	272	ASN
1	E	312	HIS
1	F	202	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	D	415	-	51,58,58	1.36	6 (11%)	60,89,89	1.55	8 (13%)
3	A2P	B	416	-	25,29,29	0.95	1 (4%)	31,45,45	1.26	2 (6%)
3	A2P	A	416	-	25,29,29	0.93	1 (4%)	31,45,45	1.21	1 (3%)
3	A2P	C	416	-	25,29,29	0.96	1 (4%)	31,45,45	1.28	2 (6%)
2	FAD	F	415	-	51,58,58	1.33	6 (11%)	60,89,89	1.54	9 (15%)
2	FAD	C	415	-	51,58,58	1.36	6 (11%)	60,89,89	1.57	10 (16%)
2	FAD	E	415	-	51,58,58	1.33	6 (11%)	60,89,89	1.52	9 (15%)
3	A2P	F	416	-	25,29,29	0.93	1 (4%)	31,45,45	1.28	3 (9%)
3	A2P	D	416	-	25,29,29	0.96	1 (4%)	31,45,45	1.24	2 (6%)
2	FAD	B	415	-	51,58,58	1.37	6 (11%)	60,89,89	1.67	9 (15%)
3	A2P	E	416	-	25,29,29	0.95	1 (4%)	31,45,45	1.31	2 (6%)
2	FAD	A	415	-	51,58,58	1.36	6 (11%)	60,89,89	1.59	9 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	415	-	-	1/30/50/50	0/6/6/6
3	A2P	B	416	-	-	3/11/31/31	0/3/3/3
3	A2P	A	416	-	-	2/11/31/31	0/3/3/3
3	A2P	C	416	-	-	2/11/31/31	0/3/3/3
2	FAD	F	415	-	-	3/30/50/50	0/6/6/6
2	FAD	C	415	-	-	4/30/50/50	0/6/6/6
2	FAD	E	415	-	-	0/30/50/50	0/6/6/6
3	A2P	F	416	-	-	2/11/31/31	0/3/3/3
3	A2P	D	416	-	-	2/11/31/31	0/3/3/3
2	FAD	B	415	-	-	4/30/50/50	0/6/6/6
3	A2P	E	416	-	-	0/11/31/31	0/3/3/3
2	FAD	A	415	-	-	2/30/50/50	0/6/6/6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	415	FAD	C2A-N3A	4.34	1.39	1.32
2	C	415	FAD	C2A-N3A	4.01	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	415	FAD	C10-N1	4.00	1.38	1.33
2	A	415	FAD	C10-N1	3.99	1.38	1.33
2	E	415	FAD	C2A-N3A	3.96	1.38	1.32
2	E	415	FAD	C10-N1	3.94	1.38	1.33
2	F	415	FAD	C2A-N3A	3.94	1.38	1.32
2	B	415	FAD	C2A-N3A	3.88	1.38	1.32
2	C	415	FAD	C10-N1	3.83	1.38	1.33
2	F	415	FAD	C10-N1	3.82	1.38	1.33
2	B	415	FAD	C1'-N10	3.77	1.52	1.48
2	A	415	FAD	C2A-N3A	3.76	1.38	1.32
2	C	415	FAD	C4X-N5	3.65	1.38	1.33
2	B	415	FAD	C10-N1	3.63	1.37	1.33
2	A	415	FAD	C4X-N5	3.58	1.38	1.33
2	F	415	FAD	C4X-N5	3.56	1.38	1.33
2	B	415	FAD	C4X-N5	3.50	1.38	1.33
2	E	415	FAD	C4X-N5	3.49	1.38	1.33
2	D	415	FAD	C4X-N5	3.23	1.38	1.33
2	E	415	FAD	C4-N3	3.21	1.38	1.33
2	F	415	FAD	C4-N3	3.14	1.38	1.33
2	D	415	FAD	C1'-N10	3.10	1.51	1.48
2	C	415	FAD	C4-N3	3.07	1.38	1.33
2	A	415	FAD	C4-N3	3.06	1.38	1.33
2	A	415	FAD	C1'-N10	3.03	1.51	1.48
2	B	415	FAD	C4-N3	3.01	1.38	1.33
2	C	415	FAD	C1'-N10	2.95	1.51	1.48
2	F	415	FAD	C1'-N10	2.63	1.50	1.48
2	D	415	FAD	C2A-N1A	2.62	1.38	1.33
2	D	415	FAD	C4-N3	2.55	1.37	1.33
2	C	415	FAD	C2A-N1A	2.55	1.38	1.33
3	F	416	A2P	C5-C4	2.46	1.47	1.40
2	E	415	FAD	C2A-N1A	2.46	1.38	1.33
2	F	415	FAD	C2A-N1A	2.44	1.38	1.33
3	E	416	A2P	C5-C4	2.42	1.47	1.40
3	D	416	A2P	C5-C4	2.41	1.47	1.40
2	B	415	FAD	C2A-N1A	2.39	1.38	1.33
3	B	416	A2P	C5-C4	2.39	1.47	1.40
2	E	415	FAD	C1'-N10	2.36	1.50	1.48
3	C	416	A2P	C5-C4	2.35	1.47	1.40
2	A	415	FAD	C2A-N1A	2.34	1.38	1.33
3	A	416	A2P	C5-C4	2.29	1.47	1.40

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	415	FAD	C4-N3-C2	6.04	120.24	115.14
2	D	415	FAD	C4-N3-C2	5.91	120.13	115.14
2	A	415	FAD	C4-N3-C2	5.90	120.12	115.14
2	F	415	FAD	C4-N3-C2	5.84	120.07	115.14
2	E	415	FAD	C4-N3-C2	5.67	119.93	115.14
2	C	415	FAD	C4-N3-C2	5.65	119.91	115.14
2	A	415	FAD	N3A-C2A-N1A	-5.51	120.06	128.68
2	C	415	FAD	N3A-C2A-N1A	-5.50	120.08	128.68
2	E	415	FAD	N3A-C2A-N1A	-5.49	120.09	128.68
2	F	415	FAD	N3A-C2A-N1A	-5.40	120.24	128.68
2	B	415	FAD	N3A-C2A-N1A	-5.36	120.29	128.68
2	D	415	FAD	N3A-C2A-N1A	-5.29	120.41	128.68
2	B	415	FAD	C1'-N10-C9A	4.31	121.69	118.29
2	B	415	FAD	C5X-C9A-N10	4.23	120.78	117.72
2	C	415	FAD	C5X-C9A-N10	3.83	120.49	117.72
2	A	415	FAD	C5X-C9A-N10	3.68	120.38	117.72
3	F	416	A2P	N3-C2-N1	-3.48	123.24	128.68
2	E	415	FAD	P-O3P-PA	-3.45	120.99	132.83
3	A	416	A2P	N3-C2-N1	-3.45	123.29	128.68
2	B	415	FAD	P-O3P-PA	-3.42	121.08	132.83
2	D	415	FAD	C5X-C9A-N10	3.42	120.19	117.72
3	B	416	A2P	N3-C2-N1	-3.41	123.35	128.68
3	E	416	A2P	N3-C2-N1	-3.38	123.40	128.68
3	D	416	A2P	N3-C2-N1	-3.36	123.42	128.68
2	C	415	FAD	P-O3P-PA	-3.31	121.47	132.83
2	F	415	FAD	C1'-N10-C9A	3.28	120.88	118.29
2	E	415	FAD	C4X-N5-C5X	3.27	120.04	116.77
2	D	415	FAD	C1'-N10-C9A	3.27	120.86	118.29
3	C	416	A2P	N3-C2-N1	-3.26	123.58	128.68
2	F	415	FAD	C5X-C9A-N10	3.14	119.99	117.72
2	F	415	FAD	C4X-N5-C5X	3.10	119.87	116.77
2	A	415	FAD	C1'-N10-C9A	3.10	120.73	118.29
2	D	415	FAD	C4X-N5-C5X	3.08	119.85	116.77
2	F	415	FAD	P-O3P-PA	-3.05	122.36	132.83
2	A	415	FAD	P-O3P-PA	-3.05	122.38	132.83
2	D	415	FAD	P-O3P-PA	-2.97	122.62	132.83
2	C	415	FAD	C4X-N5-C5X	2.91	119.67	116.77
2	A	415	FAD	C4X-N5-C5X	2.87	119.64	116.77
2	D	415	FAD	C4X-C4-N3	-2.84	119.54	123.43
2	E	415	FAD	C5X-C9A-N10	2.80	119.75	117.72
2	B	415	FAD	C9A-N10-C10	-2.79	118.26	121.91
2	B	415	FAD	C4X-C4-N3	-2.77	119.64	123.43
3	E	416	A2P	C4-C5-N7	-2.77	106.52	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	415	FAD	C4X-C4-N3	-2.70	119.73	123.43
2	E	415	FAD	C4X-C4-N3	-2.68	119.77	123.43
3	F	416	A2P	C4-C5-N7	-2.63	106.66	109.40
2	C	415	FAD	C4X-C4-N3	-2.61	119.87	123.43
2	A	415	FAD	C4X-C4-N3	-2.59	119.89	123.43
3	C	416	A2P	C4-C5-N7	-2.58	106.71	109.40
3	B	416	A2P	C4-C5-N7	-2.58	106.71	109.40
2	C	415	FAD	C1'-N10-C10	2.44	120.59	118.41
2	B	415	FAD	C4X-N5-C5X	2.43	119.20	116.77
2	E	415	FAD	C1'-N10-C9A	2.40	120.18	118.29
2	E	415	FAD	C3B-C2B-C1B	2.31	104.45	100.98
2	F	415	FAD	C3B-C2B-C1B	2.30	104.44	100.98
3	D	416	A2P	C4-C5-N7	-2.25	107.06	109.40
2	B	415	FAD	C1'-C2'-C3'	2.20	115.93	109.79
2	C	415	FAD	C1'-N10-C9A	2.18	120.01	118.29
2	D	415	FAD	C9A-N10-C10	-2.18	119.06	121.91
2	A	415	FAD	C9A-N10-C10	-2.18	119.06	121.91
2	C	415	FAD	C9A-N10-C10	-2.12	119.13	121.91
2	A	415	FAD	C3B-C2B-C1B	2.10	104.15	100.98
2	F	415	FAD	C10-C4X-N5	-2.10	119.80	121.26
2	C	415	FAD	C3B-C2B-C1B	2.07	104.10	100.98
3	F	416	A2P	C2-N1-C6	2.07	122.29	118.75
2	E	415	FAD	C10-C4X-N5	-2.07	119.83	121.26

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	415	FAD	C1'-C2'-C3'-C4'
2	C	415	FAD	C1'-C2'-C3'-C4'
3	A	416	A2P	C2'-O2'-P1-O1P
3	B	416	A2P	C2'-O2'-P1-O1P
3	D	416	A2P	C2'-O2'-P1-O1P
3	F	416	A2P	C2'-O2'-P1-O1P
2	B	415	FAD	O2'-C2'-C3'-C4'
2	C	415	FAD	O2'-C2'-C3'-C4'
3	C	416	A2P	C2'-O2'-P1-O1P
2	A	415	FAD	O2'-C2'-C3'-C4'
2	F	415	FAD	O2'-C2'-C3'-C4'
2	C	415	FAD	O2'-C2'-C3'-O3'
3	B	416	A2P	C5'-O5'-P2-O5P
2	F	415	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
3	A	416	A2P	C2'-O2'-P1-O2P
3	B	416	A2P	C2'-O2'-P1-O2P
3	C	416	A2P	C2'-O2'-P1-O3P
3	D	416	A2P	C2'-O2'-P1-O2P
3	F	416	A2P	C2'-O2'-P1-O2P
2	B	415	FAD	O2'-C2'-C3'-O3'
2	A	415	FAD	PA-O3P-P-O2P
2	B	415	FAD	PA-O3P-P-O2P
2	C	415	FAD	PA-O3P-P-O2P
2	D	415	FAD	PA-O3P-P-O2P
2	F	415	FAD	PA-O3P-P-O2P

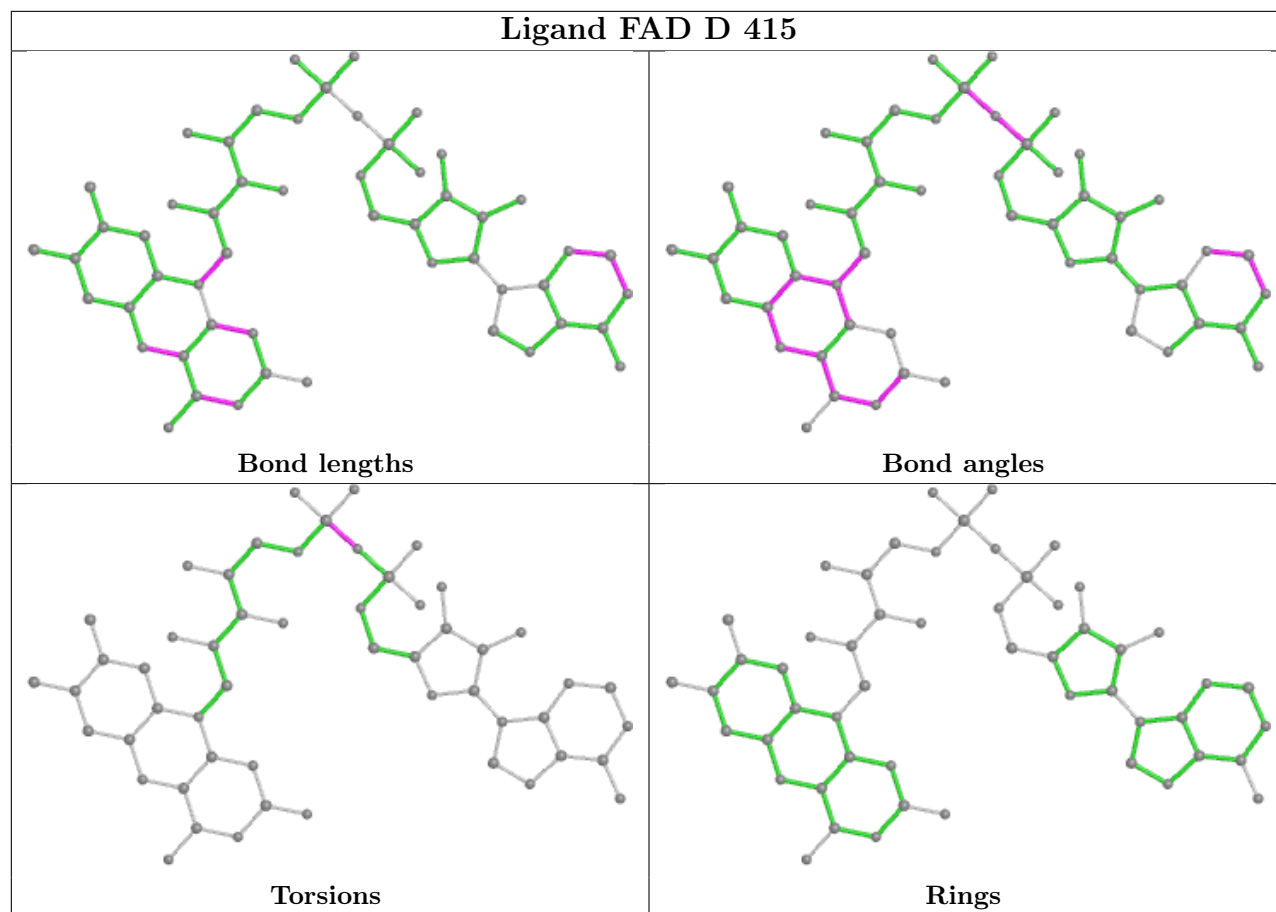
There are no ring outliers.

8 monomers are involved in 25 short contacts:

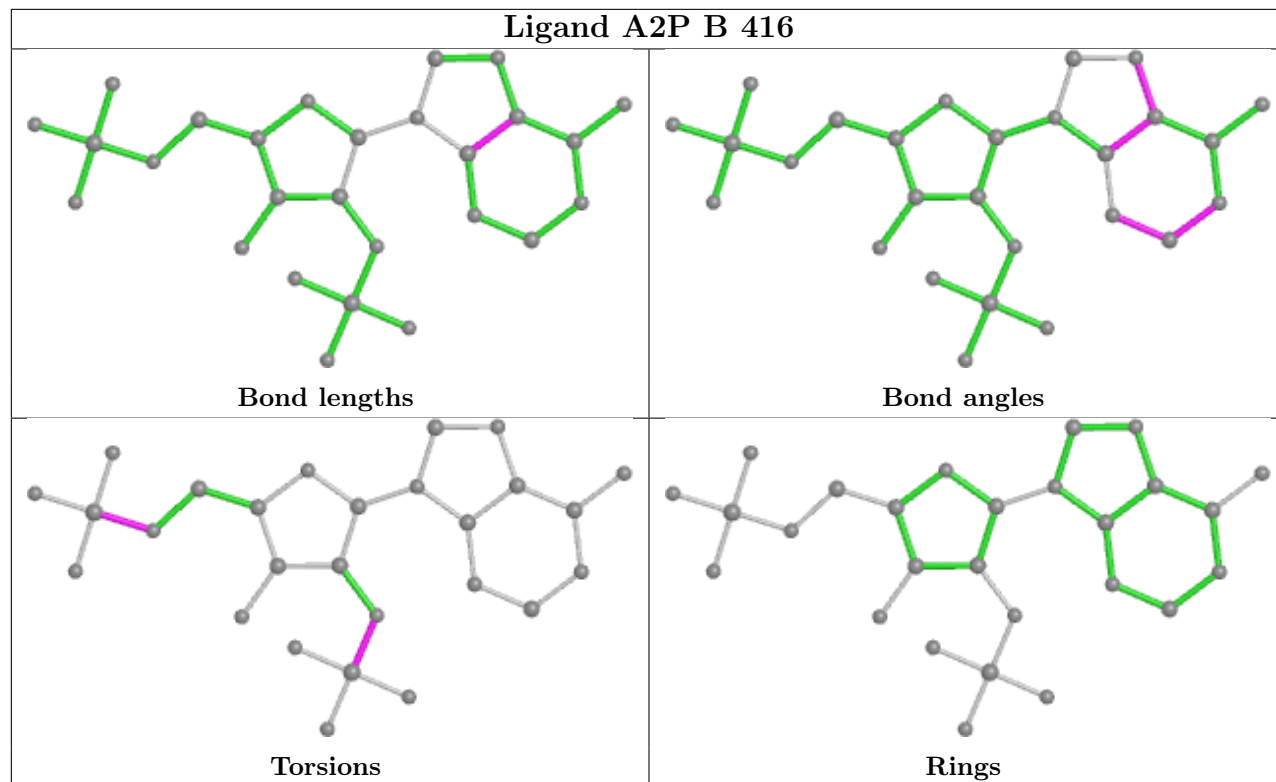
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	416	A2P	4	0
3	A	416	A2P	4	0
3	C	416	A2P	5	0
2	C	415	FAD	1	0
3	F	416	A2P	1	0
3	D	416	A2P	2	0
3	E	416	A2P	7	0
2	A	415	FAD	1	0

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.

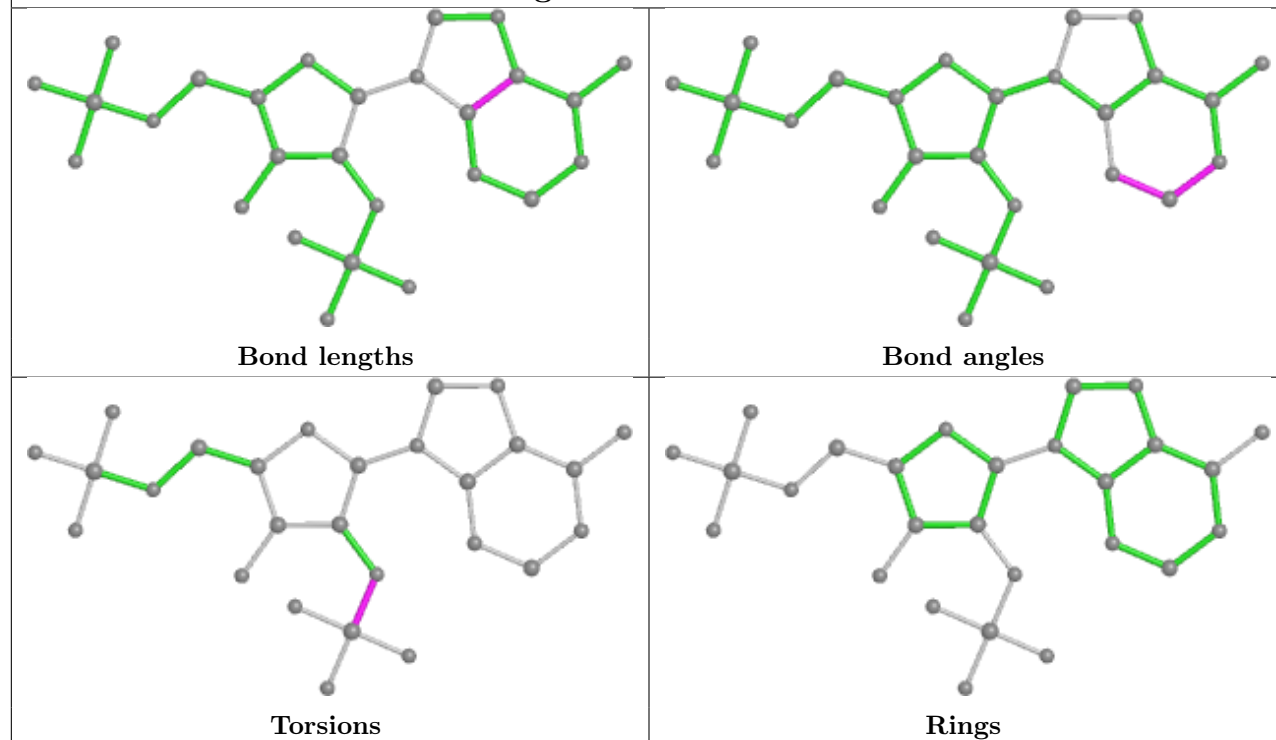
Ligand FAD D 415



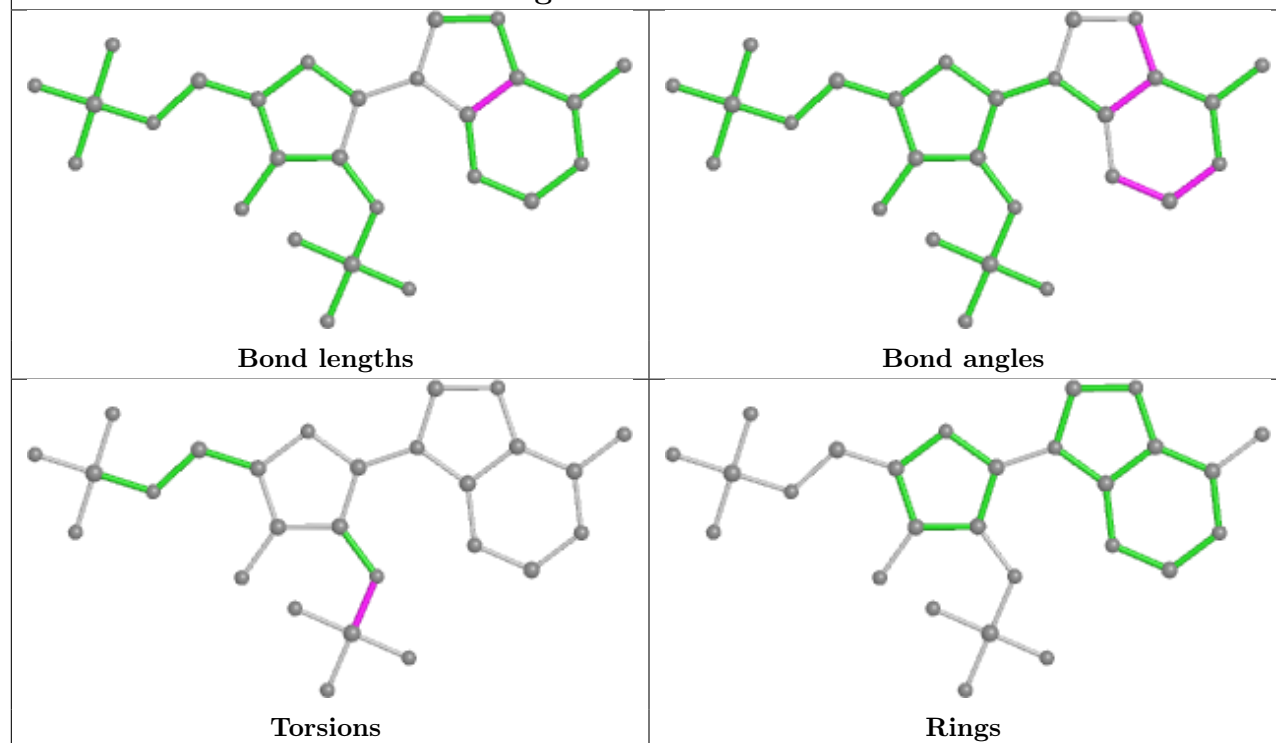
Ligand A2P B 416



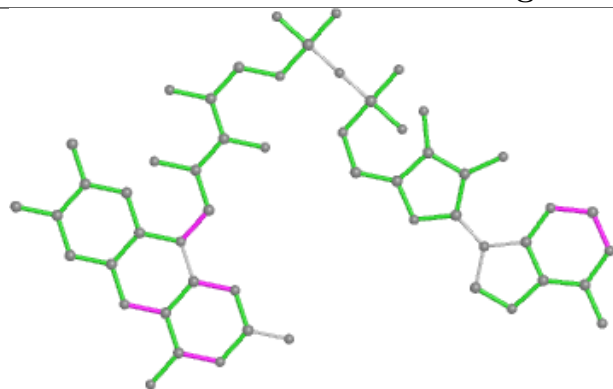
Ligand A2P A 416



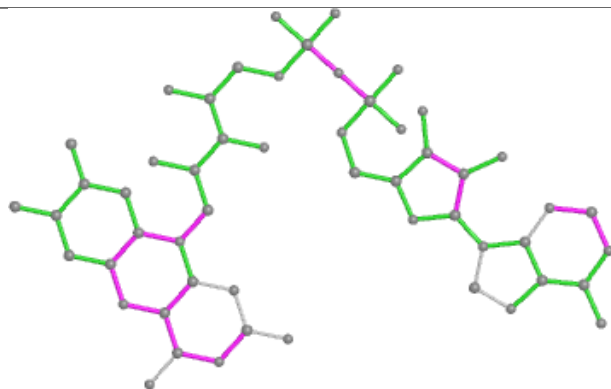
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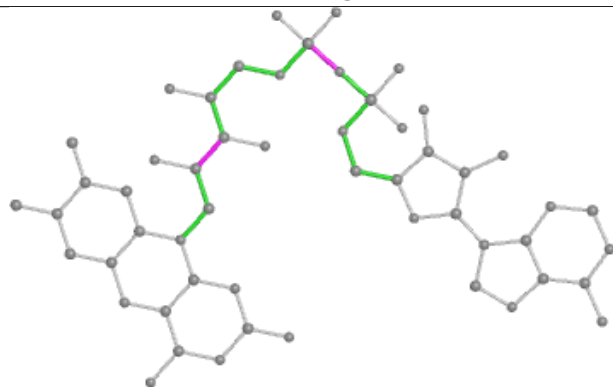
Ligand FAD F 415



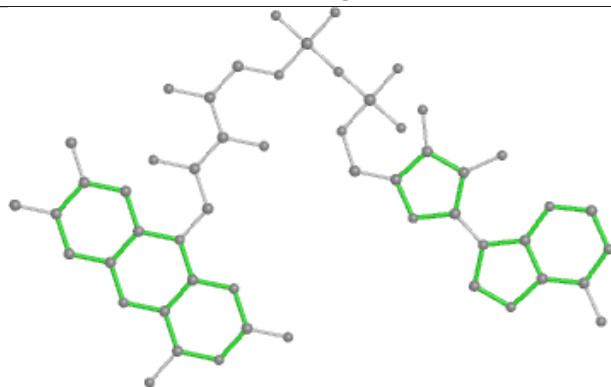
Bond lengths



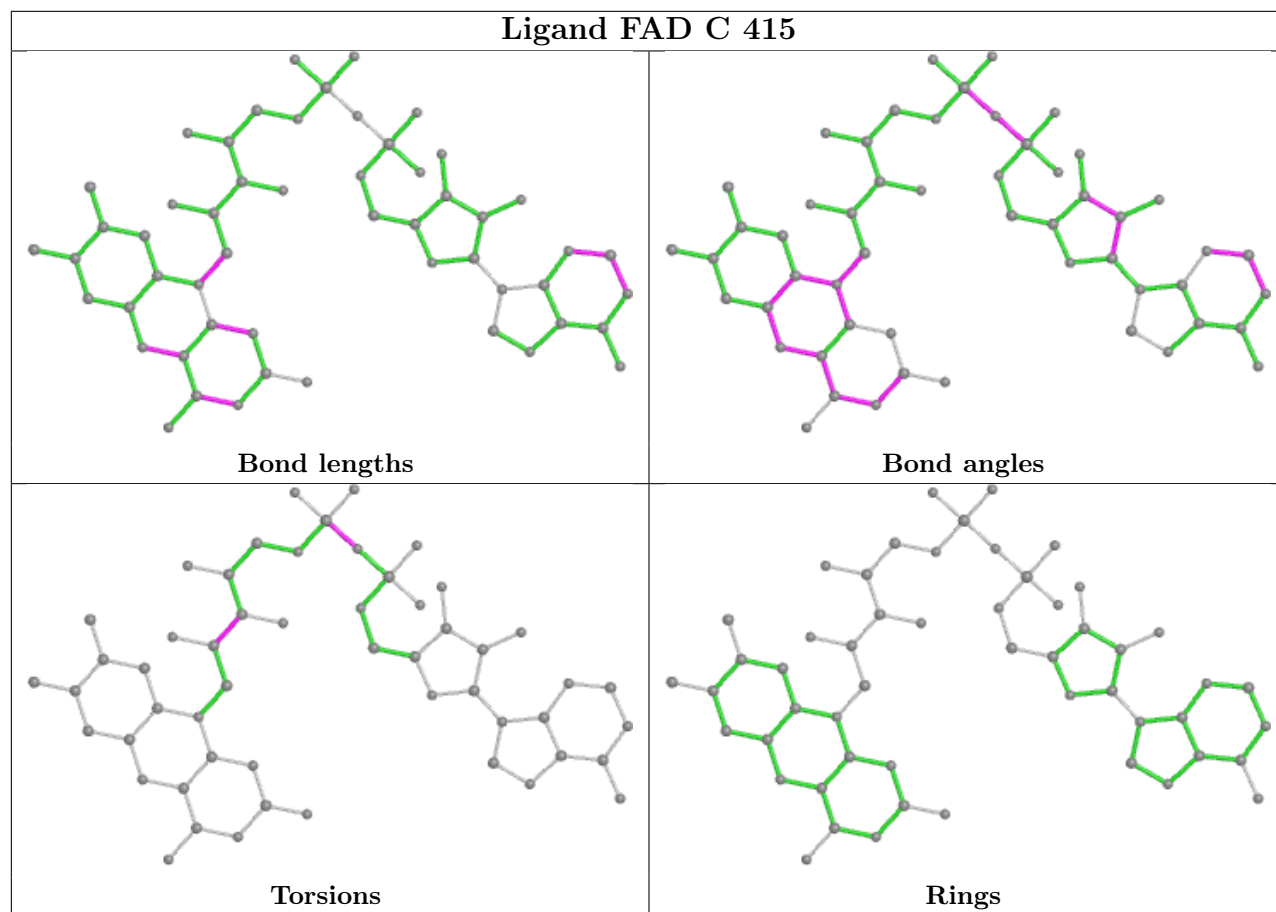
Bond angles



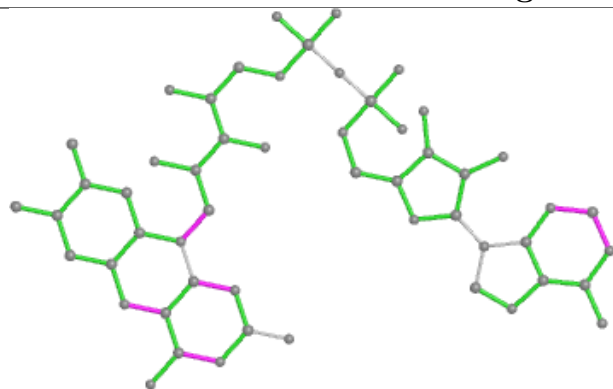
Torsions



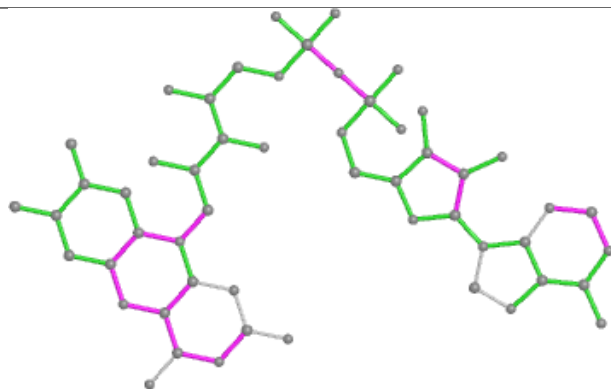
Rings



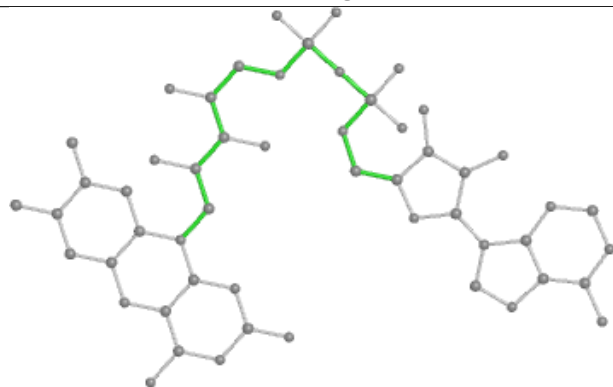
Ligand FAD E 415



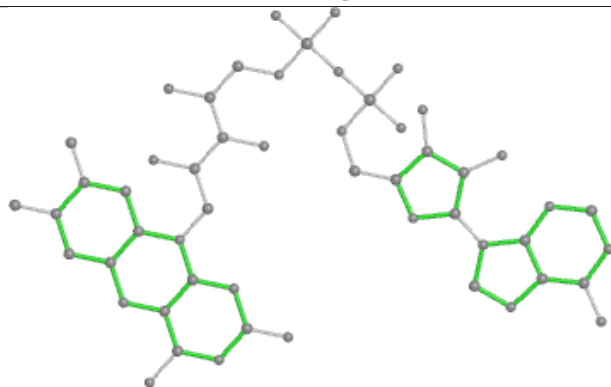
Bond lengths



Bond angles

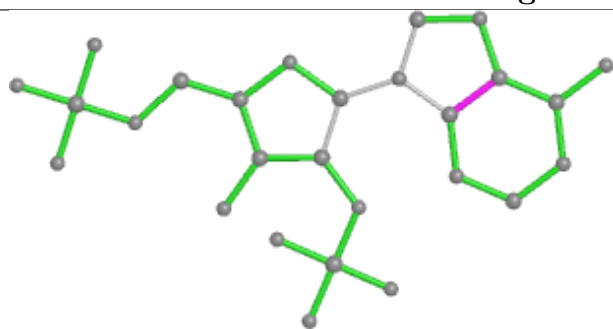


Torsions

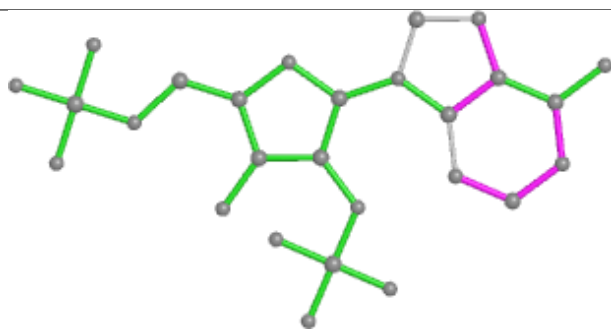


Rings

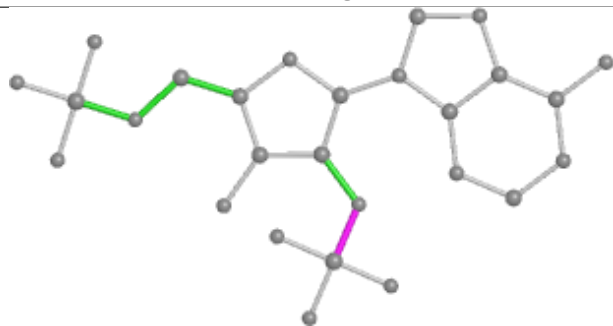
Ligand A2P F 416



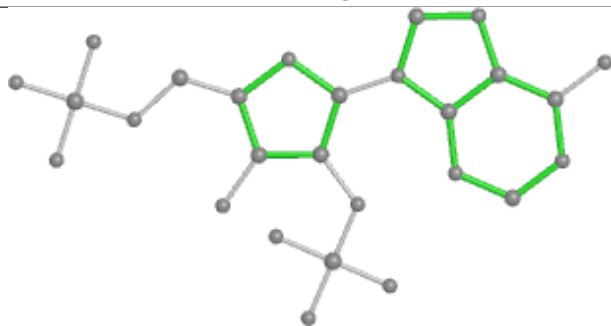
Bond lengths



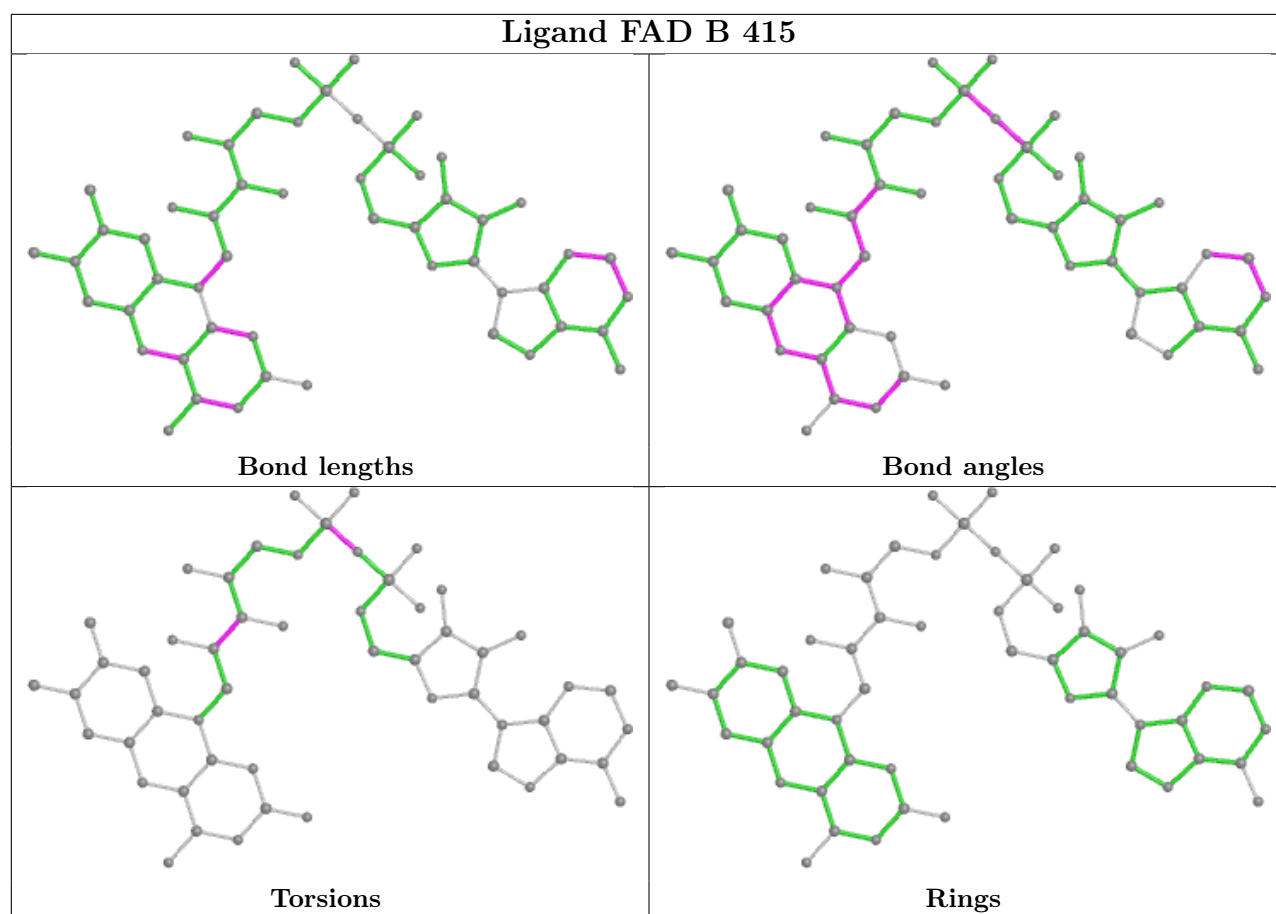
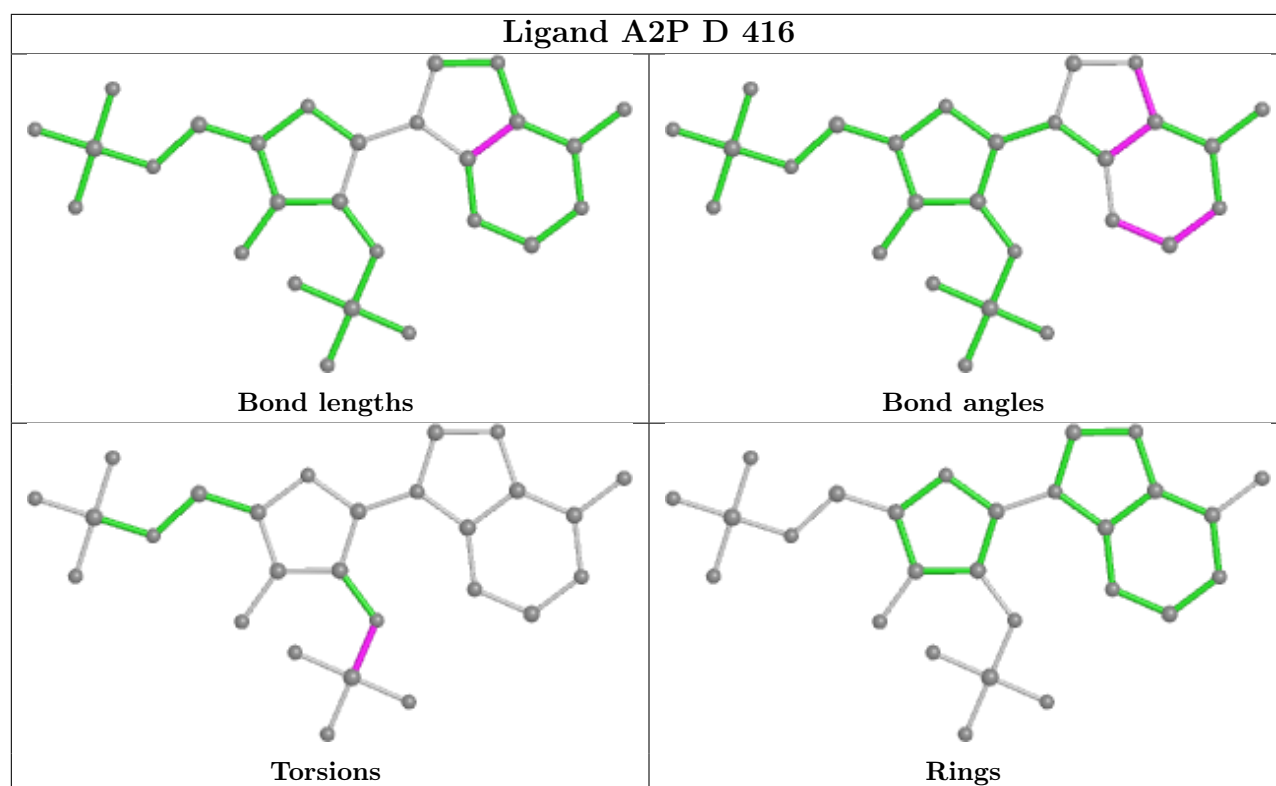
Bond angles



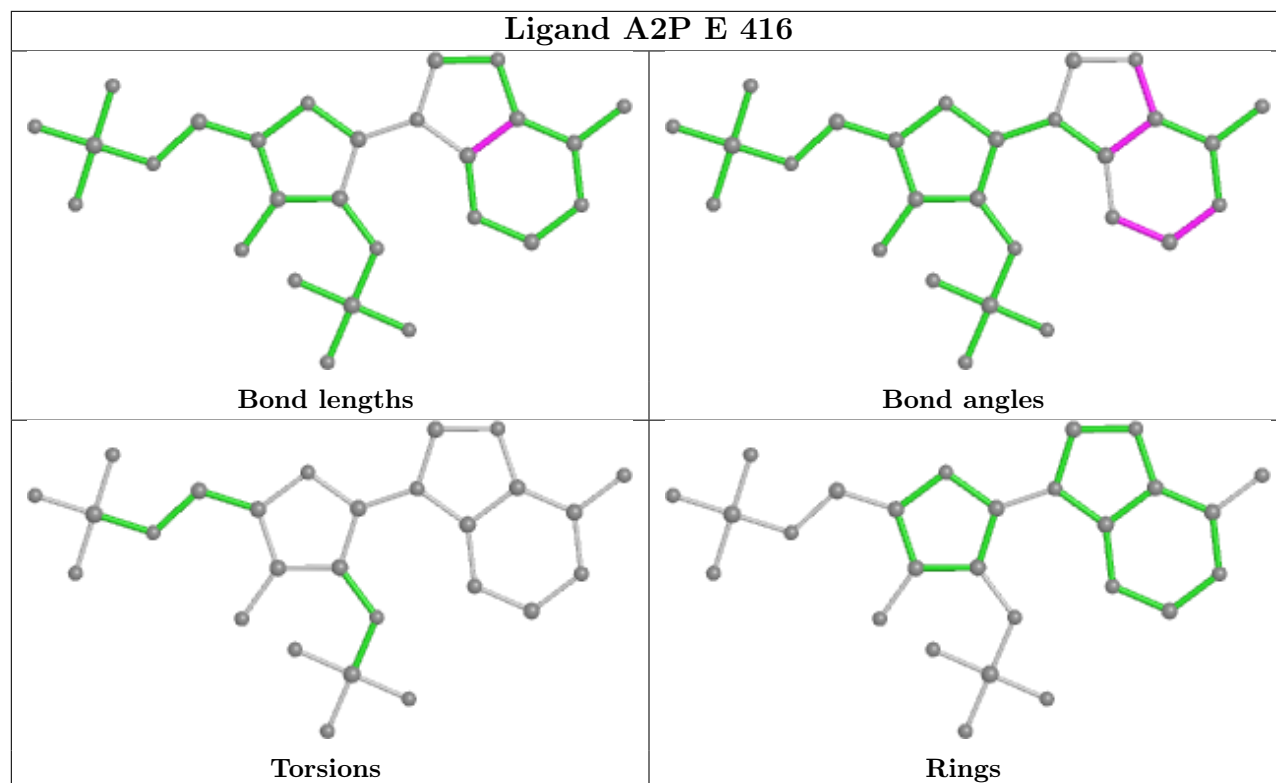
Torsions



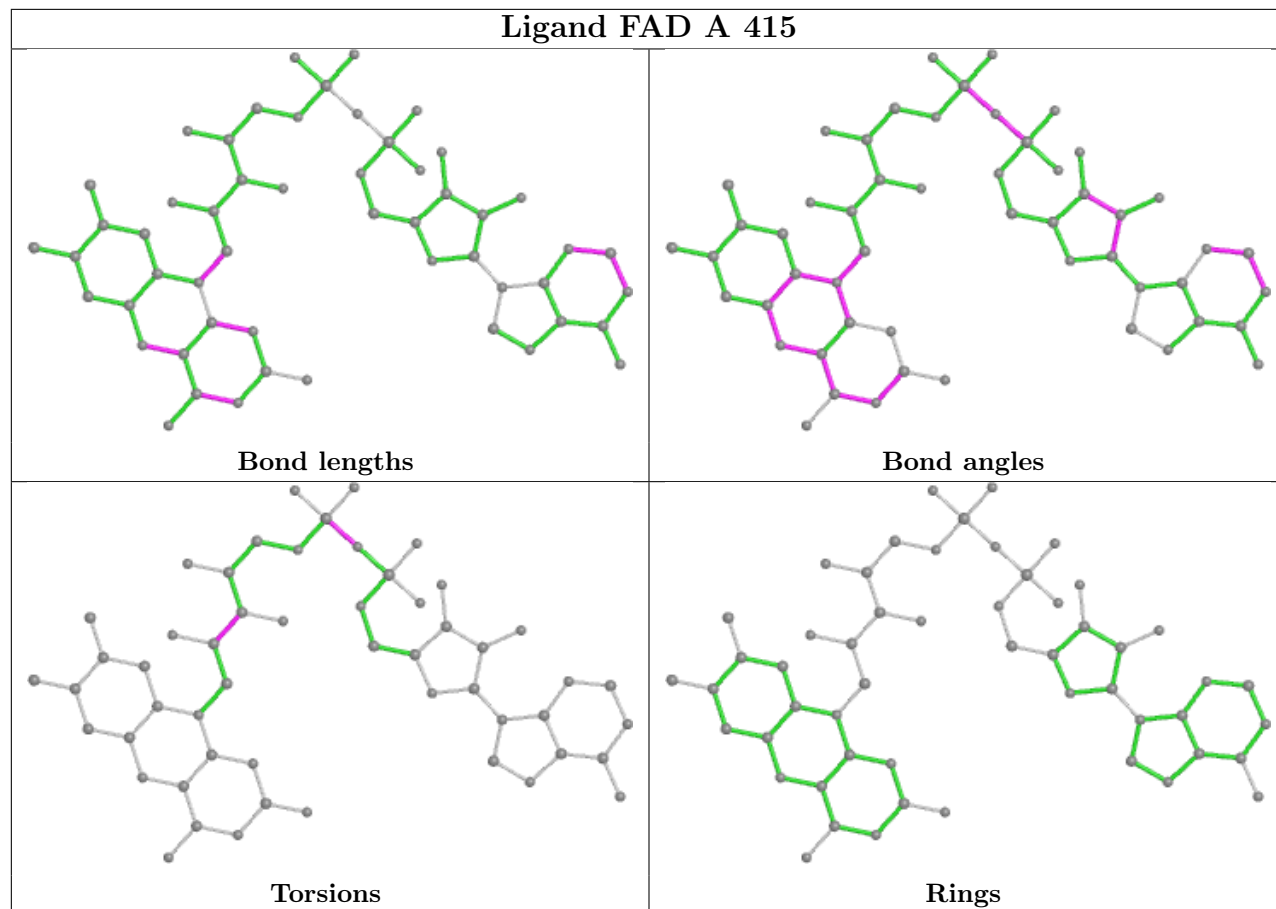
Rings



Ligand A2P E 416



Ligand FAD A 415



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	261/316 (82%)	-0.18	3 (1%) 80 79	17, 27, 47, 56	0
1	B	263/316 (83%)	-0.17	2 (0%) 86 85	17, 30, 53, 67	0
1	C	267/316 (84%)	-0.34	2 (0%) 87 86	14, 25, 44, 54	0
1	D	267/316 (84%)	-0.21	0 100 100	14, 27, 52, 67	0
1	E	253/316 (80%)	0.03	1 (0%) 92 91	29, 42, 67, 74	1 (0%)
1	F	254/316 (80%)	0.17	7 (2%) 53 51	35, 48, 68, 77	0
All	All	1565/1896 (82%)	-0.12	15 (0%) 82 81	14, 35, 61, 77	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	TYR	6.6
1	F	254	ALA	3.5
1	B	295	ASP	3.1
1	F	277	TYR	3.0
1	F	291	TYR	2.7
1	C	201	TYR	2.5
1	A	291	TYR	2.3
1	A	295	ASP	2.3
1	F	248	TYR	2.3
1	A	251	ASN	2.3
1	F	264	TYR	2.3
1	F	169	LYS	2.3
1	F	256	SER	2.2
1	C	203	ARG	2.2
1	B	297	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

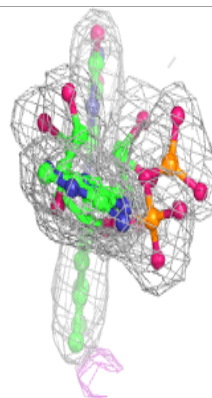
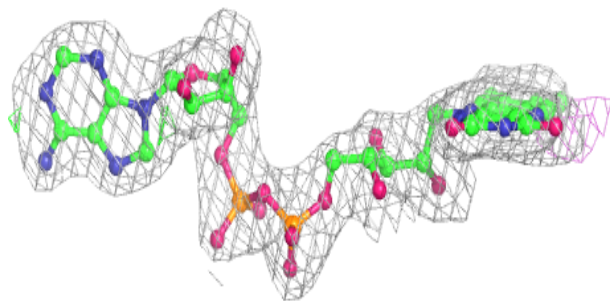
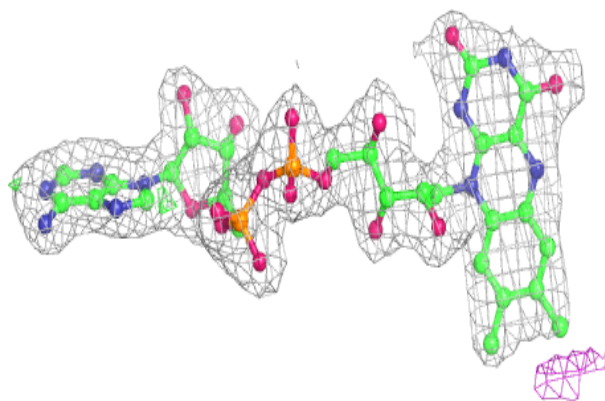
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	F	415	53/53	0.96	0.12	32,34,34,35	0
3	A2P	E	416	27/27	0.96	0.12	32,34,38,38	0
3	A2P	F	416	27/27	0.96	0.12	32,33,36,36	0
2	FAD	A	415	53/53	0.97	0.11	9,16,21,22	0
3	A2P	C	416	27/27	0.97	0.09	16,17,22,23	0
2	FAD	B	415	53/53	0.97	0.10	13,17,22,22	0
2	FAD	E	415	53/53	0.97	0.10	24,29,36,36	0
3	A2P	B	416	27/27	0.98	0.11	18,20,24,24	0
2	FAD	C	415	53/53	0.98	0.09	9,13,17,18	0
3	A2P	D	416	27/27	0.98	0.10	14,16,20,21	0
2	FAD	D	415	53/53	0.98	0.10	11,15,19,20	0
3	A2P	A	416	27/27	0.98	0.12	17,19,23,23	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.

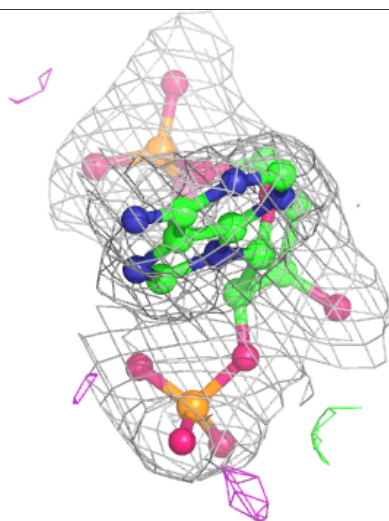
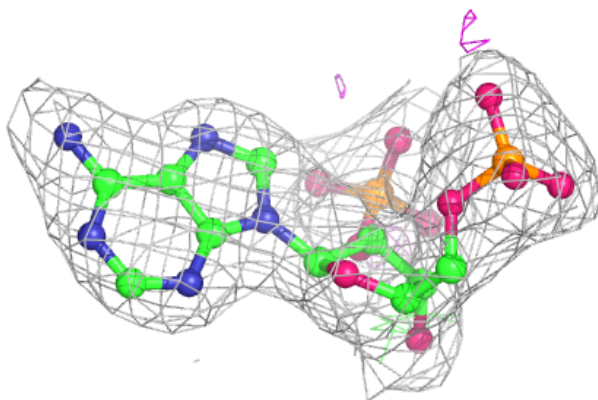
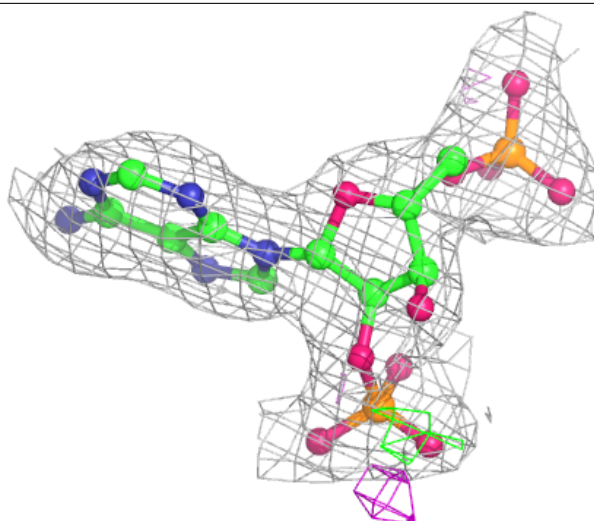
Electron density around FAD F 415:

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



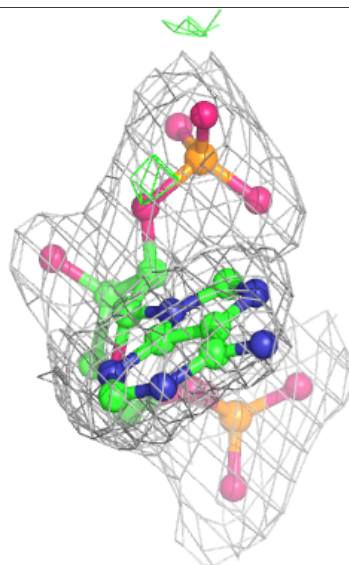
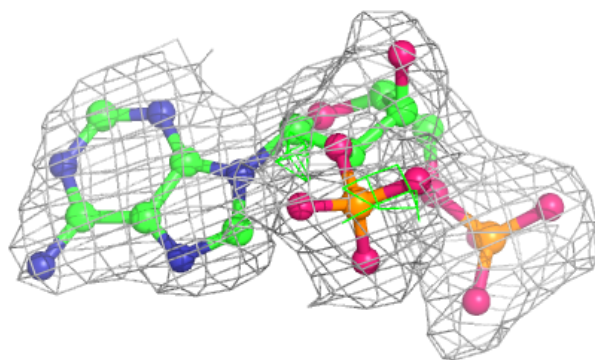
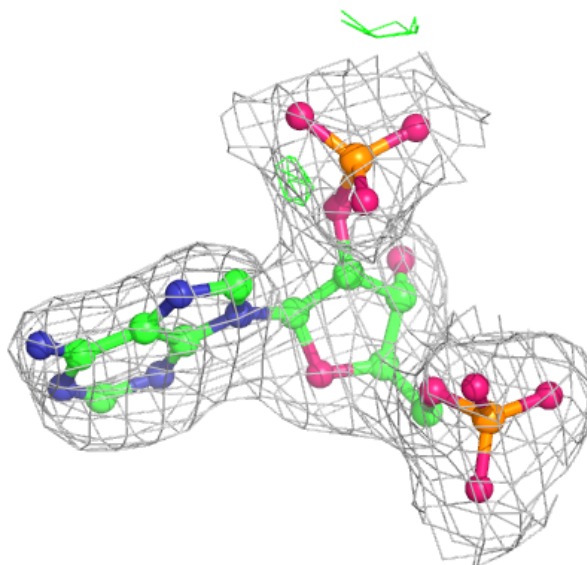
Electron density around A2P E 416:

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



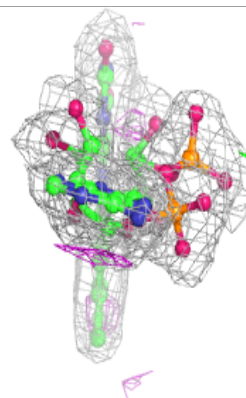
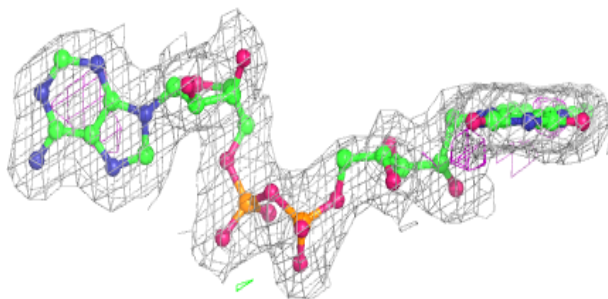
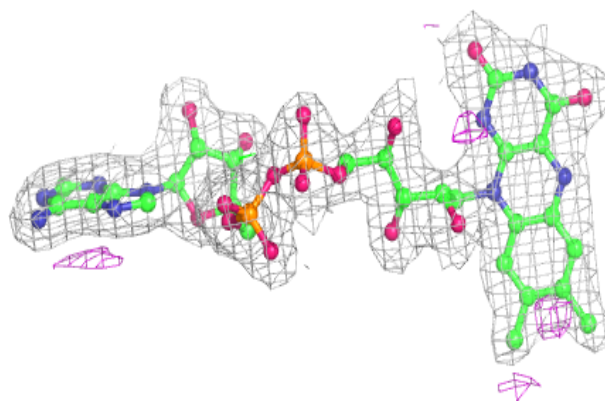
Electron density around A2P F 416:

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

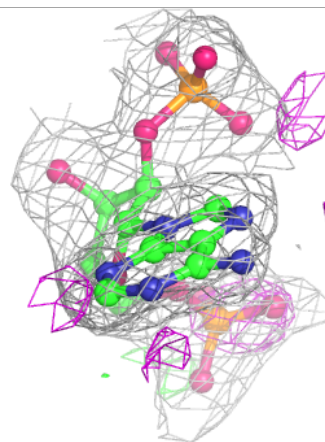
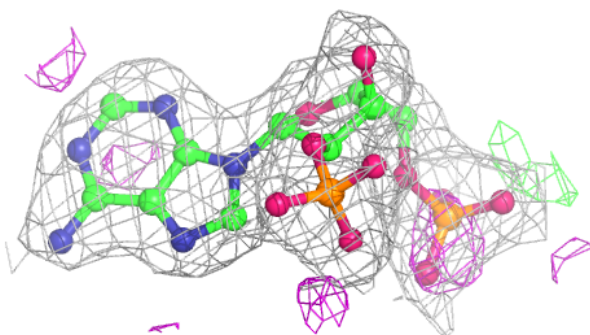
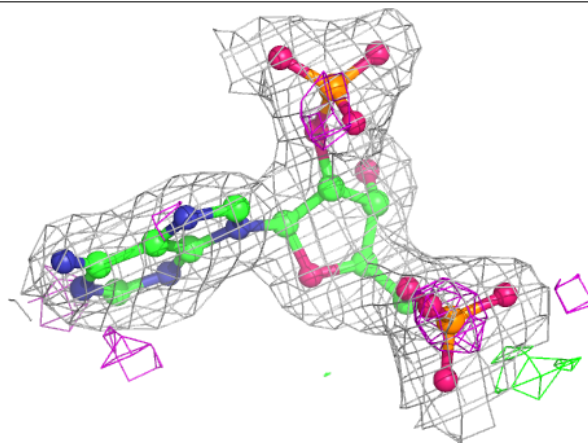


Electron density around FAD A 415:

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

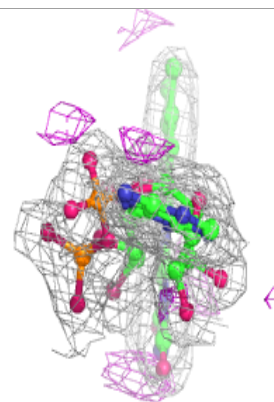
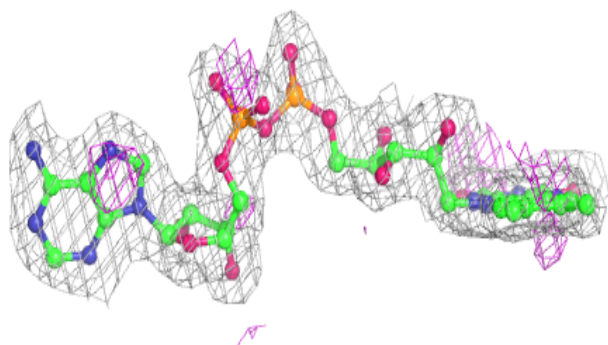
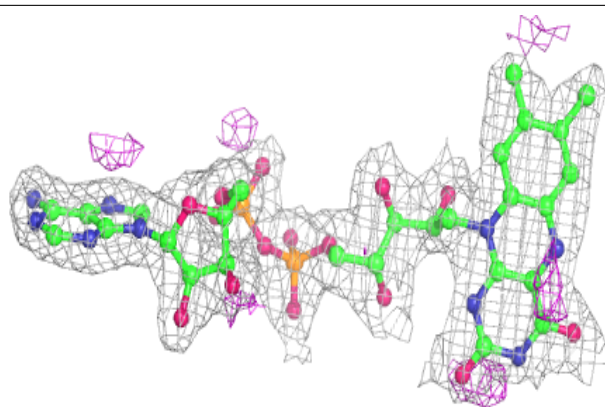
**Electron density around A2P C 416:**

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

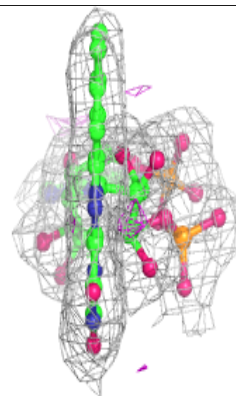
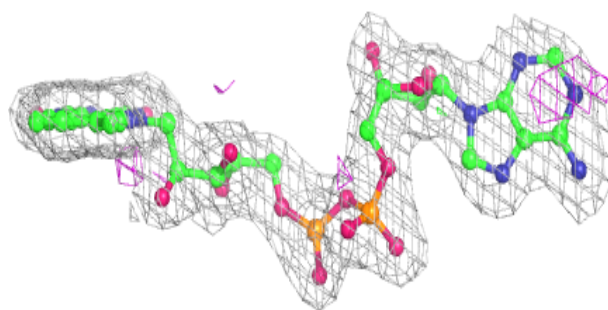
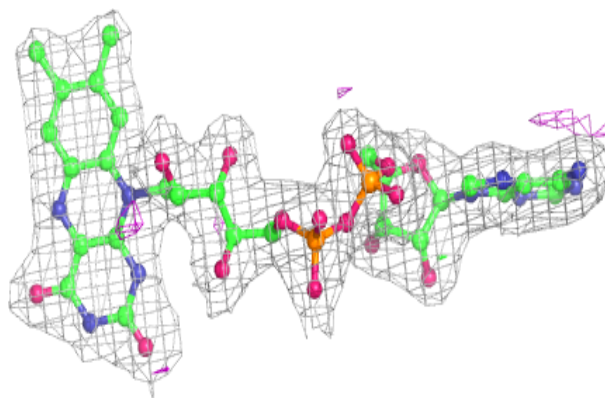


Electron density around FAD B 415:

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

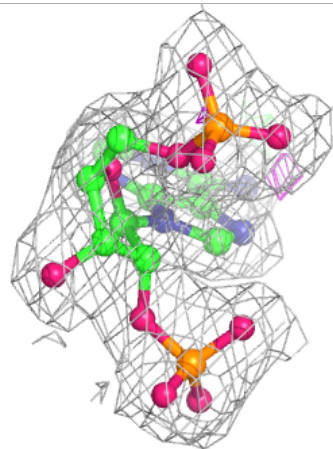
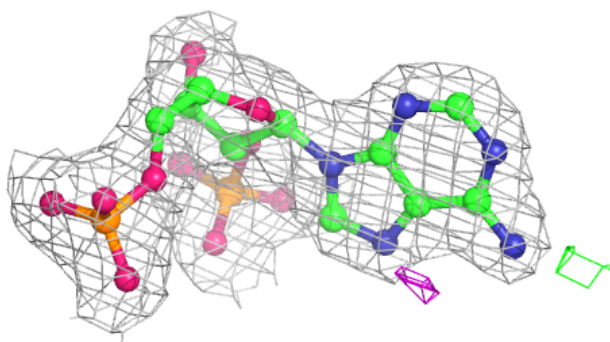
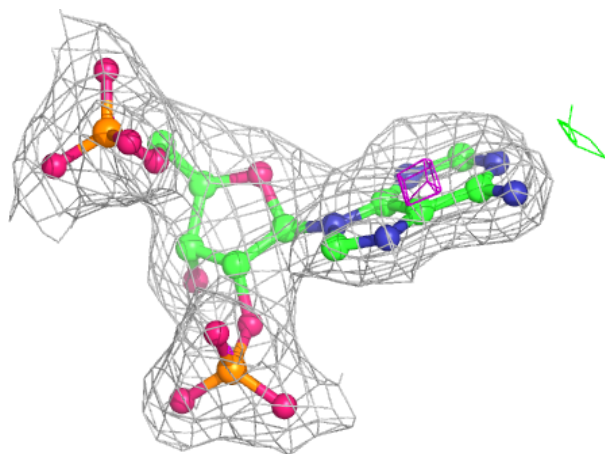
**Electron density around FAD E 415:**

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



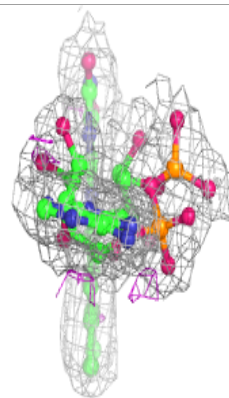
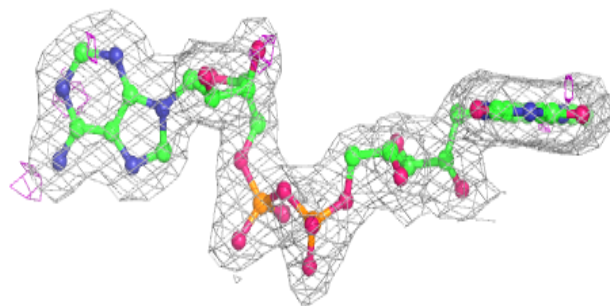
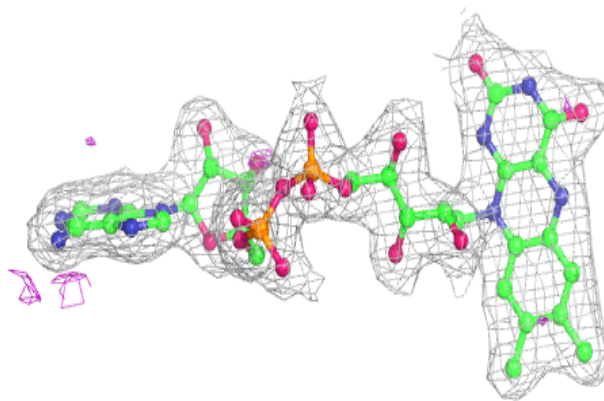
Electron density around A2P B 416:

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



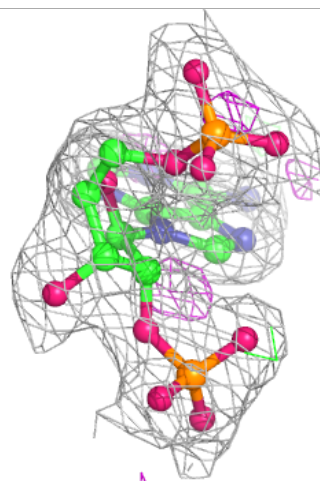
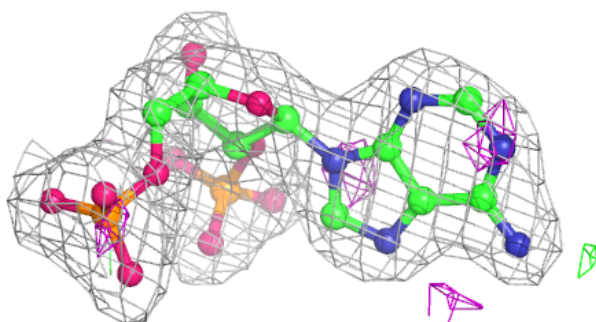
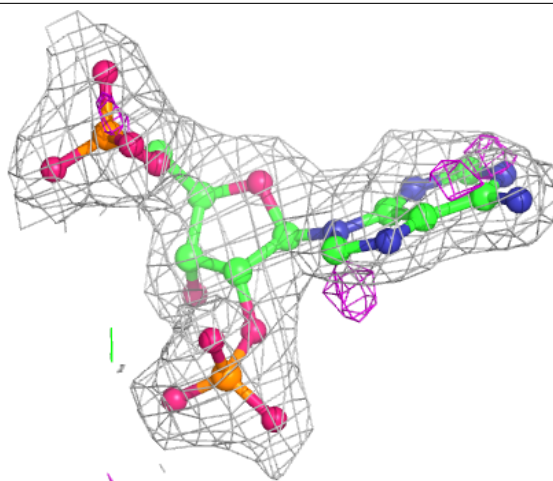
Electron density around FAD C 415:

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



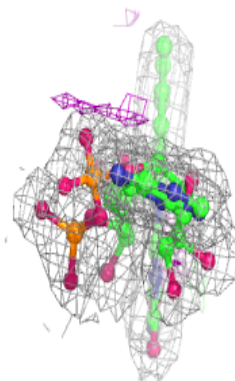
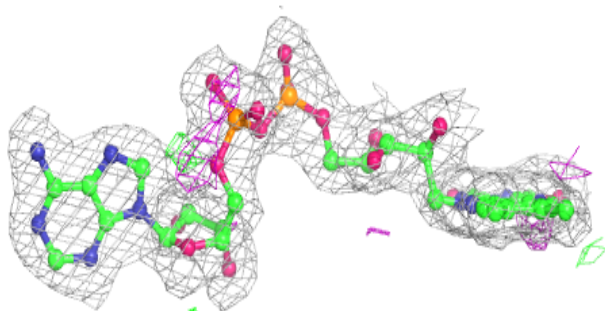
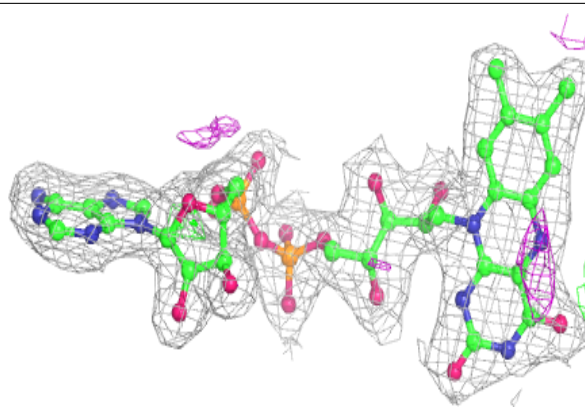
Electron density around A2P D 416:

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

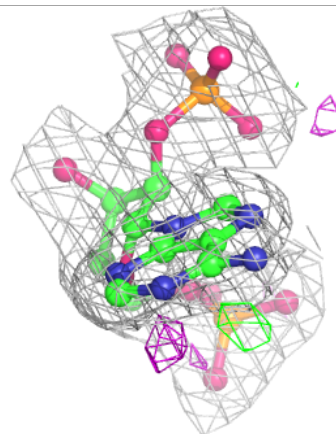
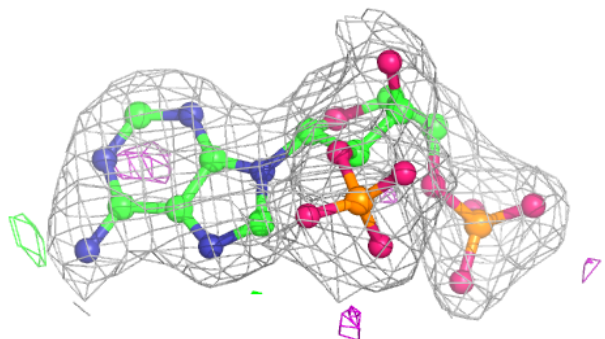
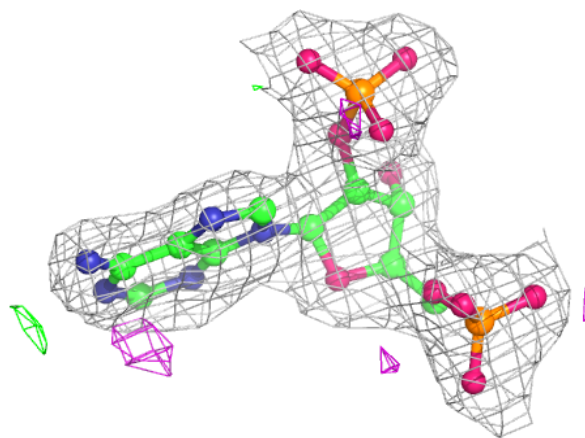


Electron density around FAD D 415:

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

**Electron density around A2P A 416:**

$2mF_o-DF_c$ (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.