



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:43 AM UTC

PDB ID : 3OWA / pdb_00003owa
Title : Crystal Structure of Acyl-CoA Dehydrogenase complexed with FAD from Bacillus anthracis
Authors : Kim, Y.; Maltseva, N.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2010-09-17
Resolution : 1.97 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

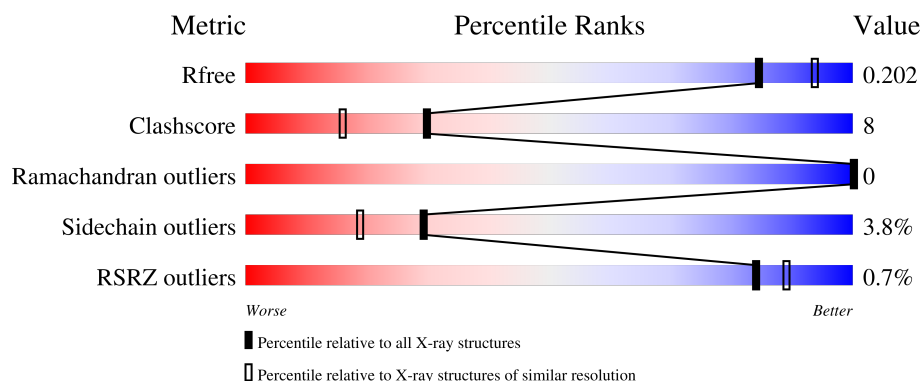
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	597	 80% 16% ..
1	B	597	 % 84% 11% . .
1	C	597	 % 84% 13% ..
1	D	597	 % 83% 13% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	A	602	-	-	X	-
3	1PE	B	602	-	-	X	-
3	1PE	D	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20926 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 Acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	Se	0	13	0
			4653	2960	786	889	3	15			
1	B	572	Total	C	N	O	S	Se	0	8	0
			4508	2865	758	869	3	13			
1	C	587	Total	C	N	O	S	Se	0	14	0
			4689	2978	790	901	3	17			
1	D	582	Total	C	N	O	S	Se	0	5	0
			4567	2901	773	876	3	14			

There are 12 discrepancies between the modelled and reference sequences:

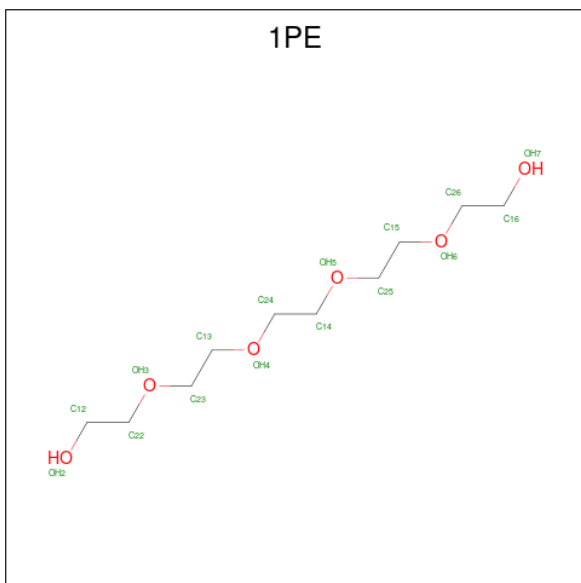
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q81XJ1
A	-1	ASN	-	expression tag	UNP Q81XJ1
A	0	ALA	-	expression tag	UNP Q81XJ1
B	-2	SER	-	expression tag	UNP Q81XJ1
B	-1	ASN	-	expression tag	UNP Q81XJ1
B	0	ALA	-	expression tag	UNP Q81XJ1
C	-2	SER	-	expression tag	UNP Q81XJ1
C	-1	ASN	-	expression tag	UNP Q81XJ1
C	0	ALA	-	expression tag	UNP Q81XJ1
D	-2	SER	-	expression tag	UNP Q81XJ1
D	-1	ASN	-	expression tag	UNP Q81XJ1
D	0	ALA	-	expression tag	UNP Q81XJ1

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



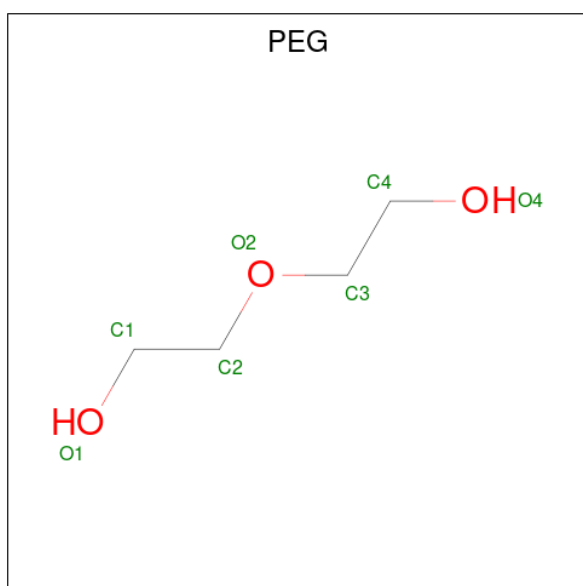
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $\text{C}_{10}\text{H}_{22}\text{O}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

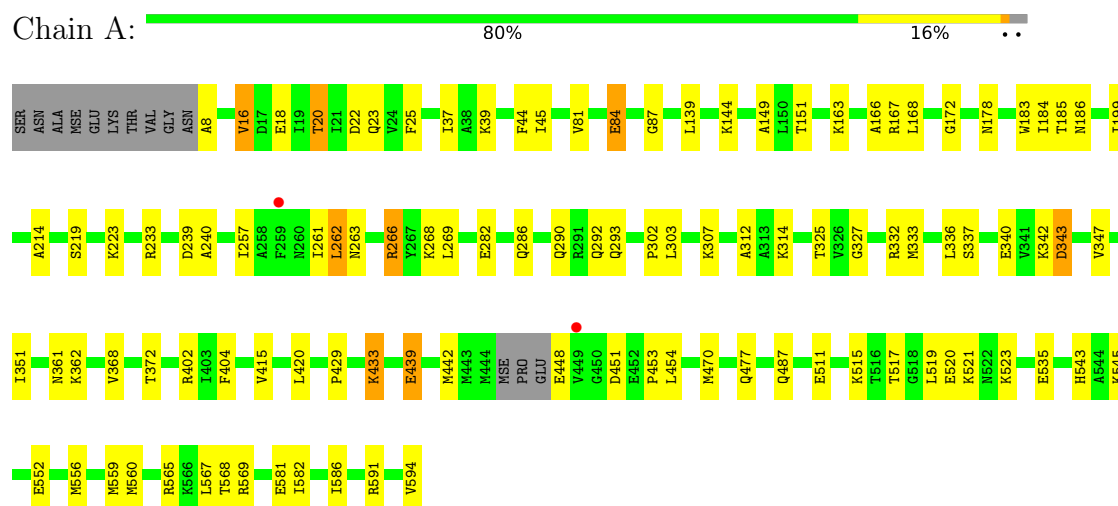
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	530	Total	O	0	0
			530	530		
7	B	517	Total	O	0	0
			517	517		
7	C	612	Total	O	0	0
			612	612		
7	D	488	Total	O	0	0
			488	488		

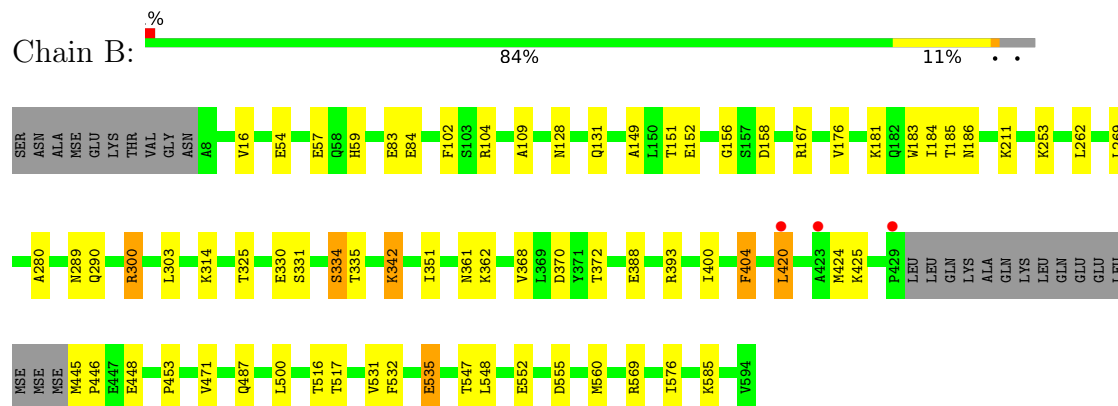
3 Residue-property plots

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.

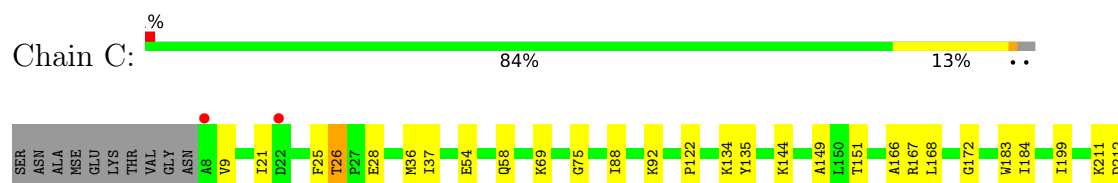
• Molecule 1: Acyl-CoA dehydrogenase

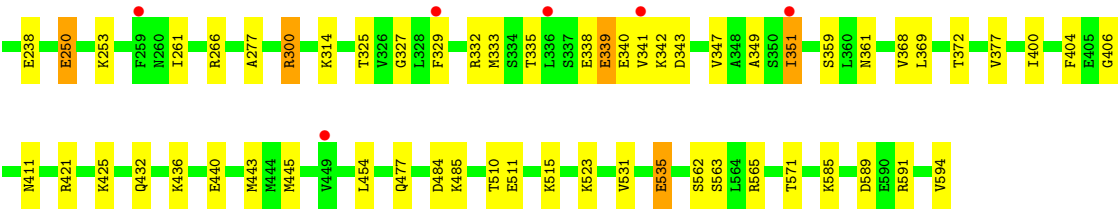


• Molecule 1: Acyl-CoA dehydrogenase

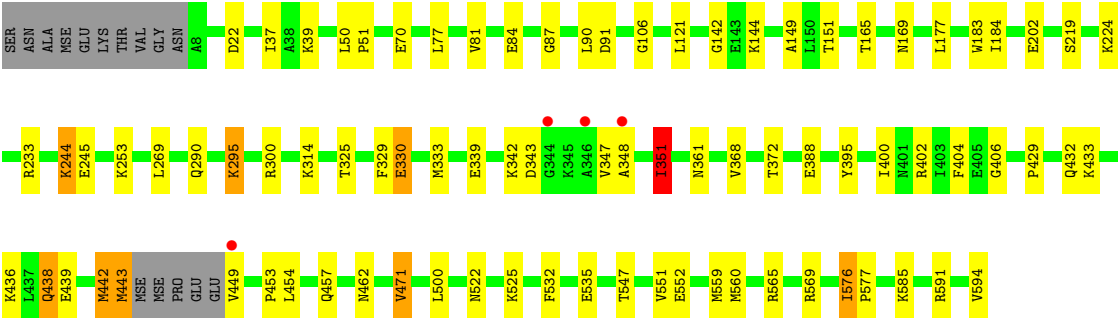
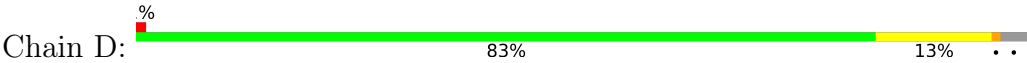


• Molecule 1: Acyl-CoA dehydrogenase





● Molecule 1: Acyl-CoA dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.61Å 98.03Å 107.74Å 92.80° 106.63° 105.30°	Depositor
Resolution (Å)	50.00 – 1.97 50.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.9 (50.00-1.97) 97.2 (50.00-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0109, PHENIX	Depositor
R, R_{free}	0.162 , 0.201 0.164 , 0.202	Depositor DCC
R_{free} test set	9842 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20926	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 1PE, FAD, SO4, PEG

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	0.89	1/4706 (0.0%)	0.92	0/6304
1	B	0.85	1/4566 (0.0%)	0.89	0/6131
1	C	0.91	1/4744 (0.0%)	0.92	0/6358
1	D	0.87	2/4620 (0.0%)	0.93	3/6194 (0.0%)
All	All	0.88	5/18636 (0.0%)	0.92	3/24987 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	576	ILE	CA-CB	7.34	1.58	1.54
1	C	377	VAL	CA-CB	6.47	1.61	1.54
1	A	415	VAL	CA-CB	5.51	1.57	1.54
1	B	576	ILE	CA-CB	5.29	1.57	1.54
1	D	395	TYR	C-O	-5.05	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	351	ILE	CB-CA-C	-5.65	102.02	111.29
1	D	121	LEU	CA-C-N	-5.03	113.46	119.05
1	D	121	LEU	C-N-CA	-5.03	113.46	119.05

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	4653	0	4733	78	0
1	B	4508	0	4554	77	0
1	C	4689	0	4739	81	0
1	D	4567	0	4638	70	0
2	A	53	0	30	5	0
2	B	53	0	31	8	0
2	C	53	0	31	7	0
2	D	53	0	31	6	0
3	A	16	0	22	9	0
3	B	16	0	22	13	0
3	C	16	0	22	4	0
3	D	16	0	22	13	0
4	A	7	0	10	0	0
4	B	7	0	10	0	0
4	C	7	0	10	0	0
4	D	7	0	10	1	0
5	A	6	0	8	1	0
5	B	24	0	32	6	0
5	C	18	0	24	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	530	0	0	24	0
7	B	517	0	0	23	0
7	C	612	0	0	28	0
7	D	488	0	0	22	0
All	All	20926	0	18979	321	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 8.

All (321) 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)
2:B:601:FAD:C5'	2:B:601:FAD:C4'	1.79	1.58
1:D:439:GLU:O	1:D:442:MSE:HG3	1.61	1.01
1:C:329[A]:PHE:CE1	1:C:351:ILE:HD12	1.97	0.99
1:B:300[B]:ARG:HH11	1:B:300[B]:ARG:CG	1.77	0.97
1:B:300[B]:ARG:HH11	1:B:300[B]:ARG:HG3	1.31	0.94
1:B:314:LYS:HZ3	3:B:602:1PE:H251	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:1PE:H232	7:B:1369:HOH:O	1.70	0.90
1:D:532:PHE:HE1	3:D:602:1PE:H231	1.35	0.88
1:D:532:PHE:CE1	3:D:602:1PE:H231	2.10	0.85
1:D:330:GLU:HG2	7:D:1227:HOH:O	1.75	0.85
3:C:602:1PE:H142	7:C:1925:HOH:O	1.76	0.85
5:A:604:GOL:H31	7:A:2071:HOH:O	1.77	0.84
1:C:75:GLY:HA3	1:C:88:ILE:HD11	1.60	0.83
1:C:75:GLY:CA	1:C:88:ILE:HD11	2.09	0.83
1:D:551:VAL:HG12	1:D:552:GLU:HG3	1.61	0.83
1:A:314:LYS:HZ1	3:A:602:1PE:H141	1.45	0.82
1:C:591:ARG:HD3	7:C:2027:HOH:O	1.80	0.81
1:B:84:GLU:HG2	1:B:342:LYS:HE3	1.61	0.81
2:B:601:FAD:C5'	2:B:601:FAD:C3'	2.59	0.80
2:B:601:FAD:H2'	2:B:601:FAD:H9	1.63	0.78
1:B:531:VAL:O	1:B:535:GLU:HG2	1.84	0.77
1:D:565:ARG:O	1:D:569:ARG:HG3	1.84	0.77
1:D:535:GLU:HB2	3:D:602:1PE:H222	1.67	0.77
1:B:314:LYS:NZ	3:B:602:1PE:H251	1.99	0.76
1:D:471:VAL:HG13	1:D:547:THR:HG21	1.68	0.75
1:C:562[B]:SER:O	1:C:565[B]:ARG:HG3	1.85	0.75
1:B:314:LYS:NZ	3:B:602:1PE:H162	2.02	0.74
1:B:535:GLU:HB3	7:B:1945:HOH:O	1.85	0.74
1:D:224:LYS:NZ	7:D:1982:HOH:O	2.22	0.73
1:C:329[A]:PHE:CE1	1:C:351:ILE:CD1	2.71	0.73
1:D:522:ASN:OD1	1:D:525:LYS:HE3	1.87	0.73
1:C:368:VAL:O	1:C:372[A]:THR:HG23	1.87	0.73
1:D:439:GLU:O	1:D:442:MSE:CG	2.36	0.73
1:C:300:ARG:NH1	7:C:1172:HOH:O	2.22	0.72
1:C:443:MSE:SE	1:C:445:MSE:HE2	2.39	0.72
1:D:429:PRO:O	1:D:433:LYS:HG2	1.89	0.72
1:A:314:LYS:NZ	3:A:602:1PE:H131	2.04	0.72
1:A:163:LYS:HE2	7:A:1763:HOH:O	1.90	0.71
2:B:601:FAD:H2'	2:B:601:FAD:C9	2.21	0.70
1:C:523:LYS:HG3	7:C:1843:HOH:O	1.90	0.69
1:A:183:TRP:O	2:A:601:FAD:N5	2.25	0.69
1:B:453:PRO:HA	7:B:1219:HOH:O	1.92	0.69
1:A:565:ARG:O	1:A:569:ARG:HG3	1.92	0.68
7:A:619:HOH:O	5:B:607:GOL:H12	1.93	0.68
1:A:84:GLU:OE1	1:A:342:LYS:HG3	1.95	0.67
1:A:581:GLU:HG3	7:A:795:HOH:O	1.95	0.66
1:A:556:MSE:HE3	7:A:2011:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:HG3	7:A:1915:HOH:O	1.94	0.66
1:C:349:ALA:HA	7:C:1337:HOH:O	1.97	0.65
1:D:388:GLU:HG3	7:D:2137:HOH:O	1.96	0.65
1:A:293:GLN:HE22	1:B:156:GLY:H	1.42	0.65
1:C:343:ASP:HB3	7:C:1341:HOH:O	1.95	0.65
1:B:300[B]:ARG:HG3	1:B:300[B]:ARG:NH1	2.05	0.65
1:B:149:ALA:HA	1:B:184:ILE:HD12	1.79	0.65
1:D:314:LYS:HZ2	3:D:602:1PE:H232	1.62	0.65
1:A:16:VAL:HG13	1:A:433:LYS:HG2	1.78	0.64
1:D:368:VAL:O	1:D:372:THR:HG23	1.98	0.63
1:C:406:GLY:CA	7:C:1927:HOH:O	2.46	0.63
1:B:331:SER:HB2	7:B:1713:HOH:O	1.98	0.63
1:B:54:GLU:HG2	7:B:1385:HOH:O	1.99	0.62
1:C:75:GLY:HA3	1:C:88:ILE:CD1	2.30	0.62
1:C:329[B]:PHE:HD2	1:C:329[B]:PHE:O	1.82	0.61
1:A:314:LYS:HZ2	3:A:602:1PE:H131	1.63	0.61
1:A:470:MSE:CE	1:A:567:LEU:HD12	2.30	0.61
1:A:556:MSE:HB3	7:A:2011:HOH:O	2.00	0.61
1:D:576:ILE:HB	1:D:577:PRO:HD3	1.82	0.61
1:C:421[A]:ARG:HE	1:C:425:LYS:HZ2	1.49	0.61
1:C:440:GLU:HG3	1:C:445:MSE:HE3	1.82	0.61
1:B:300[B]:ARG:NH1	7:B:1957:HOH:O	2.33	0.61
1:B:167:ARG:HH11	1:B:176:VAL:HG21	1.65	0.60
1:A:269[B]:LEU:HD22	1:A:362:LYS:HG2	1.83	0.60
1:C:211:LYS:HE3	7:C:1246:HOH:O	2.01	0.60
1:C:21:ILE:HD13	1:C:515:LYS:HD2	1.84	0.59
1:C:212:ASP:HB2	7:C:1515:HOH:O	2.00	0.59
1:A:314:LYS:NZ	3:A:602:1PE:H141	2.15	0.59
1:C:406:GLY:HA2	7:C:1927:HOH:O	2.03	0.59
1:D:333:MSE:SE	1:D:347:VAL:HG13	2.53	0.59
1:D:406:GLY:CA	7:D:1657:HOH:O	2.52	0.58
1:D:432:GLN:O	1:D:436:LYS:HG3	2.03	0.58
1:A:293:GLN:NE2	1:B:156:GLY:H	2.01	0.58
1:A:552:GLU:OE1	1:A:560:MSE:HG3	2.04	0.58
1:C:144:LYS:HE2	7:C:1771:HOH:O	2.03	0.58
1:C:400:ILE:HD11	2:C:601:FAD:C8M	2.33	0.58
1:C:406:GLY:N	7:C:1927:HOH:O	2.37	0.58
1:A:263:ASN:ND2	7:A:1542:HOH:O	2.37	0.58
1:D:438:GLN:HG3	7:D:2076:HOH:O	2.04	0.58
1:A:582:ILE:HG12	7:A:1571:HOH:O	2.04	0.57
1:A:343:ASP:C	1:A:343:ASP:OD1	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:604:GOL:H2	7:C:1644:HOH:O	2.05	0.57
1:B:532:PHE:HE1	3:B:602:1PE:H252	1.68	0.57
1:D:400:ILE:HD11	2:D:601:FAD:C8M	2.34	0.57
1:A:470:MSE:HE1	1:A:567:LEU:HD12	1.87	0.57
1:B:552:GLU:HB2	1:B:560:MSE:CE	2.35	0.57
1:A:149:ALA:HA	1:A:184:ILE:HD12	1.87	0.57
1:C:369:LEU:HA	1:C:372[B]:THR:HG22	1.85	0.56
1:A:511:GLU:O	1:A:515:LYS:HG3	2.04	0.56
1:B:314:LYS:HZ3	3:B:602:1PE:H162	1.67	0.56
1:B:446:PRO:HG2	1:B:569:ARG:NH1	2.19	0.56
1:B:585:LYS:HE3	7:B:1781:HOH:O	2.05	0.56
1:C:338:GLU:HA	1:C:341:VAL:HG12	1.87	0.56
1:A:543:HIS:HD2	7:A:2009:HOH:O	1.89	0.56
1:C:515:LYS:HE3	7:C:1330:HOH:O	2.04	0.56
1:A:333:MSE:SE	1:A:347:VAL:HG13	2.55	0.56
1:D:348:ALA:O	1:D:351:ILE:HD12	2.06	0.56
1:B:128:ASN:H	1:B:131:GLN:NE2	2.03	0.56
1:D:552:GLU:OE1	1:D:560:MSE:HG3	2.06	0.56
2:A:601:FAD:H2'	2:A:601:FAD:H9	1.87	0.55
1:C:26:THR:CG2	1:C:28:GLU:H	2.18	0.55
1:D:454:LEU:HA	1:D:457:GLN:HE21	1.69	0.55
1:B:300[B]:ARG:HH11	1:B:300[B]:ARG:HG2	1.69	0.55
1:A:20:THR:HG22	1:A:23:GLN:HG3	1.88	0.55
1:A:303:LEU:HG	1:B:487:GLN:HB3	1.88	0.55
1:B:300[A]:ARG:NH1	7:B:630:HOH:O	2.39	0.55
1:B:368:VAL:O	1:B:372[A]:THR:HG23	2.07	0.55
1:B:388[B]:GLU:CD	1:B:388[B]:GLU:H	2.15	0.55
1:B:552:GLU:HB2	1:B:560:MSE:HE1	1.89	0.54
1:B:269:LEU:C	1:B:269:LEU:HD23	2.33	0.54
1:B:314:LYS:HZ1	3:B:602:1PE:H222	1.72	0.54
1:C:400:ILE:HD11	2:C:601:FAD:HM83	1.90	0.54
1:A:84:GLU:CD	1:A:342:LYS:HG3	2.33	0.54
1:B:183:TRP:O	2:B:601:FAD:N5	2.41	0.54
1:B:128:ASN:H	1:B:131:GLN:HE21	1.56	0.54
1:C:333:MSE:HE1	7:C:932:HOH:O	2.07	0.54
1:C:342:LYS:HA	7:C:1794:HOH:O	2.07	0.54
1:C:400:ILE:CD1	2:C:601:FAD:HM83	2.38	0.53
1:D:342:LYS:HD3	1:D:342:LYS:N	2.23	0.53
1:B:289:ASN:HB3	5:B:608:GOL:H2	1.91	0.53
1:C:421[A]:ARG:HH11	1:C:425:LYS:HZ1	1.57	0.53
1:A:290[A]:GLN:HG2	7:A:1115:HOH:O	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLY:HA2	1:C:88:ILE:HD11	1.90	0.53
1:A:292:GLN:HB2	7:B:1846:HOH:O	2.08	0.53
1:C:329[A]:PHE:CZ	1:C:351:ILE:CD1	2.92	0.53
1:C:26:THR:HG23	1:C:28:GLU:H	1.73	0.52
1:D:314:LYS:HZ1	3:D:602:1PE:H252	1.73	0.52
1:A:487:GLN:HB3	1:B:303:LEU:HG	1.91	0.52
1:C:58:GLN:HG2	7:C:937:HOH:O	2.08	0.52
1:A:535:GLU:HG3	7:A:1987:HOH:O	2.10	0.52
1:D:84:GLU:OE2	1:D:342:LYS:HG3	2.10	0.52
1:B:57:GLU:HG3	7:B:1707:HOH:O	2.10	0.52
1:A:183:TRP:O	2:A:601:FAD:C4X	2.58	0.52
1:B:185:THR:O	1:B:186:ASN:HB2	2.10	0.51
5:B:607:GOL:H11	7:B:673:HOH:O	2.10	0.51
1:D:165:THR:O	1:D:177:LEU:HA	2.09	0.51
1:D:406:GLY:HA2	7:D:1657:HOH:O	2.09	0.51
1:A:185:THR:O	1:A:186:ASN:HB2	2.09	0.51
1:D:314:LYS:HE3	3:D:602:1PE:H252	1.93	0.51
1:A:8:ALA:HB3	1:A:332:ARG:HH11	1.76	0.51
1:B:516:THR:HG22	1:B:517:THR:HG23	1.91	0.51
1:B:290[A]:GLN:HG2	7:B:718:HOH:O	2.10	0.51
1:D:183:TRP:O	2:D:601:FAD:N5	2.44	0.51
1:C:134:LYS:HE3	1:C:135:TYR:CZ	2.45	0.51
1:D:591:ARG:HD3	7:D:1998:HOH:O	2.10	0.51
3:D:602:1PE:H151	7:D:1484:HOH:O	2.11	0.51
1:A:144[B]:LYS:NZ	7:A:2112:HOH:O	2.43	0.51
1:C:421[A]:ARG:HH11	1:C:425:LYS:NZ	2.09	0.51
1:A:262:LEU:HD22	1:A:266:ARG:HD3	1.93	0.50
1:B:314:LYS:HD3	3:B:602:1PE:H141	1.92	0.50
1:C:339:GLU:HG2	1:C:340:GLU:N	2.26	0.50
1:C:134:LYS:HE2	7:C:677:HOH:O	2.11	0.50
1:C:183:TRP:O	2:C:601:FAD:N5	2.45	0.50
1:A:20:THR:HG23	1:A:22:ASP:H	1.77	0.50
1:C:314:LYS:NZ	3:C:602:1PE:H122	2.26	0.50
1:B:420[B]:LEU:HD13	1:B:420[B]:LEU:C	2.37	0.50
1:D:169:ASN:HA	7:D:1230:HOH:O	2.11	0.50
1:D:453:PRO:HA	7:D:1475:HOH:O	2.12	0.50
1:A:453:PRO:O	1:A:454:LEU:HB2	2.11	0.49
1:A:545:LYS:HD3	7:B:1536:HOH:O	2.11	0.49
1:D:343:ASP:HB3	7:D:1251:HOH:O	2.12	0.49
1:B:471:VAL:HG13	1:B:547:THR:HG21	1.94	0.49
1:D:290[B]:GLN:HG2	7:D:635:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:LEU:HA	1:D:457:GLN:NE2	2.27	0.49
1:B:548:LEU:HD22	1:B:560:MSE:HE3	1.94	0.49
1:B:335:THR:HG21	7:B:633:HOH:O	2.11	0.49
1:C:369:LEU:O	1:C:372[B]:THR:HG22	2.12	0.49
1:D:400:ILE:CD1	2:D:601:FAD:HM83	2.43	0.49
1:D:314:LYS:NZ	3:D:602:1PE:H122	2.27	0.49
1:A:39:LYS:HE2	7:A:1926:HOH:O	2.12	0.49
1:C:300:ARG:NH2	7:C:689:HOH:O	2.40	0.49
1:A:25:PHE:HB3	1:A:327:GLY:HA3	1.94	0.49
1:D:300[A]:ARG:NH1	7:D:1273:HOH:O	2.32	0.48
1:C:183:TRP:O	2:C:601:FAD:C4X	2.61	0.48
1:B:314:LYS:HZ1	3:B:602:1PE:H162	1.78	0.48
1:C:122:PRO:HG3	1:C:261:ILE:HG13	1.96	0.48
1:D:314:LYS:NZ	3:D:602:1PE:H261	2.27	0.48
1:A:337:SER:OG	1:A:340:GLU:HG3	2.12	0.48
1:D:400:ILE:HD11	2:D:601:FAD:HM83	1.95	0.48
1:D:351:ILE:HD13	7:D:1249:HOH:O	2.12	0.48
1:C:266:ARG:NE	1:C:411:ASN:OD1	2.47	0.48
1:C:325:THR:CB	1:C:361:ASN:HD21	2.27	0.48
1:A:178:ASN:ND2	1:A:239:ASP:H	2.11	0.48
1:B:370:ASP:OD2	5:B:607:GOL:H11	2.14	0.48
1:B:104:ARG:O	1:B:104:ARG:HG3	2.14	0.47
3:A:602:1PE:H261	7:A:1389:HOH:O	2.13	0.47
2:B:601:FAD:H9	2:B:601:FAD:C2'	2.34	0.47
1:C:26:THR:HG21	7:C:702:HOH:O	2.14	0.47
1:A:314:LYS:HZ2	3:A:602:1PE:C13	2.27	0.47
1:C:329[B]:PHE:O	1:C:329[B]:PHE:CD2	2.66	0.47
1:D:219:SER:O	1:D:233:ARG:HD3	2.14	0.47
1:A:368:VAL:O	1:A:372:THR:HG23	2.14	0.47
1:C:69:LYS:CE	7:C:624:HOH:O	2.61	0.47
1:C:531:VAL:O	1:C:535:GLU:HG2	2.15	0.47
1:A:44:PHE:HD1	1:A:45:ILE:HD12	1.80	0.47
1:B:300[B]:ARG:CG	1:B:300[B]:ARG:NH1	2.50	0.47
1:C:332:ARG:NH1	7:C:1653:HOH:O	2.44	0.46
1:A:219:SER:O	1:A:233:ARG:HD3	2.15	0.46
3:B:602:1PE:C23	7:B:1369:HOH:O	2.47	0.46
1:C:168[A]:LEU:HG	1:C:172:GLY:HA2	1.97	0.46
1:D:151:THR:OG1	2:D:601:FAD:H1'1	2.16	0.46
1:D:149:ALA:HA	1:D:184:ILE:HD12	1.97	0.46
1:A:535:GLU:HB2	3:A:602:1PE:H162	1.98	0.46
1:D:81:VAL:HB	1:D:87:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:OG1	2:A:601:FAD:H1'1	2.16	0.45
1:B:393:ARG:HD3	5:B:606:GOL:O3	2.16	0.45
1:D:325:THR:CB	1:D:361:ASN:HD21	2.29	0.45
1:A:336:LEU:HA	1:A:340:GLU:OE1	2.16	0.45
1:C:484:ASP:OD1	1:C:485:LYS:HD3	2.17	0.45
3:C:602:1PE:H252	3:C:602:1PE:H262	1.77	0.45
1:D:295:LYS:NZ	7:D:1758:HOH:O	2.50	0.45
1:D:84:GLU:OE1	1:D:342:LYS:HE2	2.17	0.45
3:A:602:1PE:H151	3:A:602:1PE:H161	1.72	0.45
1:B:532:PHE:CE1	3:B:602:1PE:H252	2.50	0.45
1:D:314:LYS:HZ1	3:D:602:1PE:H261	1.82	0.45
7:A:1705:HOH:O	1:C:238:GLU:CD	2.58	0.45
1:B:290[A]:GLN:OE1	5:B:608:GOL:H11	2.17	0.45
1:B:330:GLU:HG2	7:B:1907:HOH:O	2.17	0.45
1:C:149:ALA:HA	1:C:184:ILE:HD12	1.99	0.45
1:C:69:LYS:HE3	7:C:624:HOH:O	2.17	0.45
1:D:402:ARG:NH2	7:D:1424:HOH:O	2.49	0.45
1:A:214:ALA:O	1:A:240:ALA:HA	2.16	0.45
1:B:535:GLU:HG2	1:B:535:GLU:H	1.58	0.44
1:C:421[A]:ARG:HD3	7:C:1586:HOH:O	2.17	0.44
1:D:329:PHE:CE1	1:D:351:ILE:HG13	2.52	0.44
1:C:454:LEU:HD11	1:C:510:THR:HG22	1.99	0.44
1:A:257:ILE:O	1:A:261:ILE:HG12	2.18	0.44
1:A:325:THR:CB	1:A:361:ASN:HD21	2.29	0.44
1:B:269:LEU:HD22	1:B:362:LYS:HG2	1.99	0.44
1:B:300[B]:ARG:HD3	1:B:300[B]:ARG:N	2.33	0.44
1:B:388[B]:GLU:CD	1:B:388[B]:GLU:N	2.74	0.44
1:A:293:GLN:NE2	1:B:158:ASP:H	2.15	0.44
1:A:293:GLN:HE21	1:B:158:ASP:H	1.66	0.44
1:B:325:THR:CB	1:B:361:ASN:HD21	2.30	0.44
1:B:445:MSE:HG3	1:B:446:PRO:HD2	1.99	0.44
1:C:585:LYS:HE2	1:C:589:ASP:OD2	2.18	0.44
1:A:439:GLU:O	1:A:442:MSE:HG3	2.17	0.44
1:C:314:LYS:HZ3	3:C:602:1PE:H122	1.83	0.44
1:C:571:THR:HB	7:C:1944:HOH:O	2.18	0.44
1:C:144:LYS:NZ	7:C:806:HOH:O	2.44	0.43
1:B:362:LYS:HE3	1:B:404[B]:PHE:O	2.19	0.43
1:A:429:PRO:O	1:A:433:LYS:HB2	2.18	0.43
1:C:92:LYS:NZ	7:C:1471:HOH:O	2.47	0.43
2:C:601:FAD:H62A	4:D:603:PEG:H22	1.83	0.43
1:B:152:GLU:OE2	1:B:181:LYS:NZ	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:602:1PE:C15	7:B:1747:HOH:O	2.66	0.43
1:C:277:ALA:HA	1:C:372[B]:THR:HG21	2.00	0.43
1:C:329[B]:PHE:CD2	1:C:329[B]:PHE:C	2.96	0.43
1:A:591[B]:ARG:NH2	7:A:1769:HOH:O	2.50	0.43
2:A:601:FAD:H2'	2:A:601:FAD:C9	2.48	0.43
1:A:8:ALA:HB1	7:A:1641:HOH:O	2.19	0.42
1:B:362:LYS:C	1:B:362:LYS:HD3	2.44	0.42
1:C:166:ALA:O	1:C:199:ILE:HA	2.18	0.42
1:A:81:VAL:O	1:A:87:GLY:HA3	2.19	0.42
1:D:532:PHE:CD1	3:D:602:1PE:H121	2.54	0.42
1:A:168[A]:LEU:HG	1:A:172:GLY:HA2	2.00	0.42
1:A:282:GLU:O	1:A:286:GLN:HG3	2.19	0.42
1:C:75:GLY:CA	1:C:88:ILE:CD1	2.92	0.42
1:D:70:GLU:HG2	7:D:2040:HOH:O	2.18	0.42
1:D:269:LEU:C	1:D:269:LEU:HD23	2.44	0.42
1:D:339:GLU:HG3	7:D:1606:HOH:O	2.19	0.42
1:D:453:PRO:O	1:D:454:LEU:HB2	2.19	0.42
1:B:253:LYS:HG2	7:B:779:HOH:O	2.18	0.42
1:D:442:MSE:H	1:D:442:MSE:HG2	1.53	0.42
1:A:223[B]:LYS:HE2	7:A:836:HOH:O	2.20	0.42
1:A:312:ALA:CB	1:A:586:ILE:HD11	2.49	0.42
1:A:351:ILE:HG23	7:A:798:HOH:O	2.20	0.42
1:B:59:HIS:HE1	7:B:873:HOH:O	2.02	0.42
1:B:151:THR:OG1	2:B:601:FAD:H1'1	2.20	0.42
1:C:26:THR:HG22	1:C:28:GLU:N	2.35	0.42
1:D:585:LYS:HE3	7:D:662:HOH:O	2.18	0.42
1:C:511:GLU:OE2	1:C:515:LYS:NZ	2.38	0.42
1:B:183:TRP:O	2:B:601:FAD:C4X	2.68	0.42
1:A:517:THR:HG22	1:A:521:LYS:HD2	2.02	0.42
1:B:585:LYS:HE2	7:B:1444:HOH:O	2.20	0.42
1:C:36[B]:MSE:HE2	1:C:36[B]:MSE:HB3	1.89	0.42
1:A:263:ASN:ND2	7:A:1384:HOH:O	2.52	0.41
1:A:470:MSE:CE	1:A:567:LEU:CD1	2.98	0.41
1:D:443:MSE:H	1:D:443:MSE:HG2	1.72	0.41
1:A:453:PRO:HA	7:A:1529:HOH:O	2.19	0.41
1:A:517:THR:HG22	1:A:517:THR:O	2.20	0.41
1:D:244:LYS:H	1:D:244:LYS:HG3	1.64	0.41
1:C:25:PHE:HB3	1:C:327:GLY:HA3	2.01	0.41
1:D:400:ILE:HD11	2:D:601:FAD:HM81	2.00	0.41
1:C:69:LYS:HE2	7:C:624:HOH:O	2.20	0.41
1:C:151:THR:OG1	2:C:601:FAD:H1'1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421[A]:ARG:HE	1:C:425:LYS:NZ	2.17	0.41
1:D:106:GLY:C	7:D:1516:HOH:O	2.64	0.41
1:B:16:VAL:O	1:B:16:VAL:HG12	2.20	0.41
1:B:351:ILE:HG23	7:B:1026:HOH:O	2.21	0.41
3:D:602:1PE:H232	3:D:602:1PE:H122	1.69	0.41
1:A:307:LYS:NZ	7:A:644:HOH:O	2.51	0.41
1:C:535:GLU:HG2	1:C:535:GLU:H	1.68	0.41
1:A:314:LYS:HZ1	3:A:602:1PE:C14	2.25	0.41
1:B:211:LYS:HD3	7:B:1203:HOH:O	2.21	0.41
1:B:280:ALA:HB3	1:B:372[B]:THR:HG22	2.03	0.41
1:B:331:SER:O	1:B:334:SER:HB2	2.21	0.41
1:D:532:PHE:HD1	3:D:602:1PE:H121	1.85	0.41
1:A:302:PRO:HB2	1:B:487:GLN:HB2	2.02	0.41
3:B:602:1PE:H232	3:B:602:1PE:H242	1.85	0.41
1:A:166:ALA:O	1:A:199:ILE:HA	2.22	0.40
1:D:50:LEU:N	1:D:51:PRO:CD	2.84	0.40
1:B:102:PHE:O	1:B:109:ALA:HB2	2.20	0.40
1:C:250:GLU:HB3	1:C:253:LYS:HD2	2.03	0.40
1:D:37:ILE:HD13	1:D:90:LEU:HD13	2.02	0.40
1:A:139:LEU:HD23	1:A:144[B]:LYS:O	2.21	0.40
1:B:400:ILE:O	1:B:400:ILE:HG13	2.20	0.40
1:B:425:LYS:HA	7:B:1602:HOH:O	2.20	0.40
1:A:402:ARG:NH2	7:A:1971:HOH:O	2.54	0.40
1:D:406:GLY:N	7:D:1657:HOH:O	2.54	0.40
1:C:300:ARG:NH1	1:C:300:ARG:HA	2.36	0.40
1:C:347:VAL:O	1:C:351:ILE:HG22	2.21	0.40
1:D:77:LEU:HD12	1:D:142:GLY:HA3	2.02	0.40
1:D:565:ARG:NH1	7:D:2030:HOH:O	2.52	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	593/597 (99%)	588 (99%)	5 (1%)	0	100	100
1	B	576/597 (96%)	566 (98%)	10 (2%)	0	100	100
1	C	599/597 (100%)	594 (99%)	5 (1%)	0	100	100
1	D	583/597 (98%)	575 (99%)	8 (1%)	0	100	100
All	All	2351/2388 (98%)	2323 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	493/474 (104%)	470 (95%)	23 (5%)	23	12
1	B	477/474 (101%)	462 (97%)	15 (3%)	35	26
1	C	497/474 (105%)	477 (96%)	20 (4%)	28	17
1	D	483/474 (102%)	462 (96%)	21 (4%)	26	14
All	All	1950/1896 (103%)	1871 (96%)	79 (4%)	29	16

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	18	GLU
1	A	20	THR
1	A	37	ILE
1	A	84	GLU
1	A	167	ARG
1	A	262	LEU
1	A	266	ARG
1	A	268	LYS
1	A	343	ASP
1	A	404[A]	PHE
1	A	404[B]	PHE
1	A	420	LEU

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Mol	Chain	Res	Type
1	A	433	LYS
1	A	439	GLU
1	A	448	GLU
1	A	451	ASP
1	A	477	GLN
1	A	519	LEU
1	A	520	GLU
1	A	559	MSE
1	A	568	THR
1	A	594	VAL
1	B	83	GLU
1	B	262	LEU
1	B	300[A]	ARG
1	B	300[B]	ARG
1	B	334	SER
1	B	342	LYS
1	B	404[A]	PHE
1	B	404[B]	PHE
1	B	420[A]	LEU
1	B	420[B]	LEU
1	B	424	MSE
1	B	448	GLU
1	B	500	LEU
1	B	535	GLU
1	B	555	ASP
1	C	9	VAL
1	C	26	THR
1	C	37	ILE
1	C	54[A]	GLU
1	C	54[B]	GLU
1	C	167	ARG
1	C	250	GLU
1	C	300	ARG
1	C	335	THR
1	C	339	GLU
1	C	351	ILE
1	C	359	SER
1	C	404	PHE
1	C	432[A]	GLN
1	C	432[B]	GLN
1	C	436	LYS
1	C	477	GLN

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Mol	Chain	Res	Type
1	C	535	GLU
1	C	563	SER
1	C	594	VAL
1	D	22	ASP
1	D	39	LYS
1	D	91	ASP
1	D	144	LYS
1	D	202	GLU
1	D	244	LYS
1	D	245	GLU
1	D	253	LYS
1	D	295	LYS
1	D	330	GLU
1	D	351	ILE
1	D	404	PHE
1	D	438	GLN
1	D	442	MSE
1	D	443	MSE
1	D	449	VAL
1	D	462	ASN
1	D	471	VAL
1	D	500	LEU
1	D	559	MSE
1	D	594	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	263	ASN
1	A	293	GLN
1	A	361	ASN
1	A	411	ASN
1	A	435	GLN
1	A	463	ASN
1	B	131	GLN
1	B	203	HIS
1	B	255	HIS
1	B	260	ASN
1	B	289	ASN
1	B	463	ASN
1	C	462	ASN

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Mol	Chain	Res	Type
1	C	463	ASN
1	C	477	GLN
1	D	289	ASN
1	D	361	ASN
1	D	457	GLN
1	D	538	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	B	601	-	58,58,58	2.93	6 (10%)	85,89,89	1.87	19 (22%)
5	GOL	C	605	-	5,5,5	0.37	0	5,5,5	0.32	0
2	FAD	D	601	-	58,58,58	1.16	7 (12%)	85,89,89	1.65	17 (20%)
2	FAD	A	601	-	58,58,58	2.26	9 (15%)	85,89,89	1.75	20 (23%)
5	GOL	B	607	-	5,5,5	0.37	0	5,5,5	0.65	0
2	FAD	C	601	-	58,58,58	1.29	10 (17%)	85,89,89	1.66	17 (20%)
4	PEG	B	603	-	6,6,6	0.54	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	D	603	-	6,6,6	0.64	0	5,5,5	0.35	0
4	PEG	C	603	-	6,6,6	0.54	0	5,5,5	0.26	0
5	GOL	A	604	-	5,5,5	0.37	0	5,5,5	0.73	0
3	1PE	B	602	-	15,15,15	0.78	0	14,14,14	0.77	1 (7%)
3	1PE	D	602	-	15,15,15	0.68	0	14,14,14	0.60	0
3	1PE	C	602	-	15,15,15	0.63	0	14,14,14	0.79	0
3	1PE	A	602	-	15,15,15	0.74	0	14,14,14	0.73	0
5	GOL	B	606	-	5,5,5	0.38	0	5,5,5	0.43	0
4	PEG	A	603	-	6,6,6	0.46	0	5,5,5	0.32	0
6	SO4	B	604	-	4,4,4	0.26	0	6,6,6	0.15	0
6	SO4	A	606	-	4,4,4	0.30	0	6,6,6	0.10	0
5	GOL	C	606	-	5,5,5	0.41	0	5,5,5	0.58	0
5	GOL	C	604	-	5,5,5	0.39	0	5,5,5	0.37	0
5	GOL	B	608	-	5,5,5	0.37	0	5,5,5	0.55	0
5	GOL	B	605	-	5,5,5	0.41	0	5,5,5	0.48	0

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	B	601	-	-	5/34/50/50	0/6/6/6
5	GOL	C	605	-	-	4/4/4/4	-
2	FAD	D	601	-	-	4/34/50/50	0/6/6/6
2	FAD	A	601	-	-	7/34/50/50	0/6/6/6
5	GOL	B	607	-	-	4/4/4/4	-
2	FAD	C	601	-	-	4/34/50/50	0/6/6/6
4	PEG	B	603	-	-	1/4/4/4	-
4	PEG	D	603	-	-	4/4/4/4	-
4	PEG	C	603	-	-	1/4/4/4	-
5	GOL	A	604	-	-	2/4/4/4	-
3	1PE	B	602	-	-	10/13/13/13	-
3	1PE	D	602	-	-	9/13/13/13	-
3	1PE	C	602	-	-	8/13/13/13	-
3	1PE	A	602	-	-	10/13/13/13	-
5	GOL	B	606	-	-	3/4/4/4	-
4	PEG	A	603	-	-	2/4/4/4	-
5	GOL	C	606	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	604	-	-	0/4/4/4	-
5	GOL	B	608	-	-	2/4/4/4	-
5	GOL	B	605	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C5'-C4'	20.44	1.79	1.51
2	A	601	FAD	C4'-C3'	-11.90	1.32	1.53
2	A	601	FAD	C2'-C3'	8.13	1.67	1.53
2	B	601	FAD	C4X-N5	3.81	1.39	1.30
2	A	601	FAD	C4X-N5	3.59	1.38	1.30
2	D	601	FAD	C4X-N5	3.50	1.38	1.30
2	A	601	FAD	PA-O3P	3.47	1.63	1.59
2	C	601	FAD	C4X-N5	3.43	1.38	1.30
2	A	601	FAD	C2A-N3A	3.20	1.39	1.33
2	D	601	FAD	P-O3P	3.08	1.62	1.59
2	C	601	FAD	P-O3P	3.07	1.62	1.59
2	A	601	FAD	C2A-N1A	2.93	1.39	1.33
2	C	601	FAD	C1'-C2'	2.73	1.56	1.52
2	B	601	FAD	C2A-N1A	2.71	1.38	1.33
2	B	601	FAD	C8A-N7A	2.61	1.36	1.31
2	C	601	FAD	PA-O3P	2.54	1.62	1.59
2	B	601	FAD	C2A-N3A	2.52	1.38	1.33
2	C	601	FAD	C5A-N7A	-2.47	1.34	1.39
2	D	601	FAD	C10-N1	2.47	1.38	1.33
2	C	601	FAD	C1'-N10	2.32	1.53	1.47
2	D	601	FAD	C2A-N1A	2.31	1.38	1.33
2	A	601	FAD	C5A-N7A	-2.25	1.35	1.39
2	A	601	FAD	C10-N1	2.21	1.37	1.33
2	D	601	FAD	C2A-N3A	2.13	1.37	1.33
2	C	601	FAD	C2A-N1A	2.12	1.37	1.33
2	C	601	FAD	C2A-N3A	2.09	1.37	1.33
2	C	601	FAD	C8A-N7A	2.09	1.35	1.31
2	C	601	FAD	C5'-C4'	2.07	1.54	1.51
2	B	601	FAD	C10-N1	2.04	1.37	1.33
2	D	601	FAD	C5'-C4'	2.03	1.54	1.51
2	D	601	FAD	C5A-N7A	-2.03	1.35	1.39
2	A	601	FAD	C1'-N10	2.03	1.52	1.47

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	N3A-C2A-N1A	-6.04	119.44	128.58
2	D	601	FAD	N3A-C2A-N1A	-5.89	119.66	128.58
2	B	601	FAD	O4'-C4'-C5'	5.69	122.54	109.99
2	C	601	FAD	N3A-C2A-N1A	-5.53	120.21	128.58
2	A	601	FAD	N3A-C2A-N1A	-5.11	120.85	128.58
2	B	601	FAD	C5'-C4'-C3'	-4.73	103.30	112.22
2	A	601	FAD	O2'-C2'-C3'	4.62	120.06	109.25
2	B	601	FAD	O5'-C5'-C4'	4.51	121.40	109.36
2	A	601	FAD	C5'-C4'-C3'	4.40	120.51	112.22
2	A	601	FAD	C5A-C4A-N3A	-4.15	121.00	126.72
2	D	601	FAD	C5A-C4A-N3A	-4.10	121.08	126.72
2	D	601	FAD	N9A-C8A-N7A	-3.89	108.42	113.94
2	B	601	FAD	C5A-C4A-N3A	-3.82	121.45	126.72
2	C	601	FAD	C5X-C9A-N10	3.72	121.33	117.97
2	B	601	FAD	C5X-C9A-N10	3.43	121.07	117.97
2	B	601	FAD	C2A-N3A-C4A	3.43	120.20	111.83
2	D	601	FAD	C2A-N3A-C4A	3.43	120.20	111.83
2	B	601	FAD	N9A-C8A-N7A	-3.38	109.14	113.94
2	A	601	FAD	C5X-C9A-N10	3.37	121.02	117.97
2	C	601	FAD	C4X-C10-N10	3.35	121.28	116.48
2	B	601	FAD	C9A-C5X-N5	-3.25	119.00	122.45
2	D	601	FAD	C4-N3-C2	-3.24	119.89	125.64
2	D	601	FAD	C4X-C10-N10	3.24	121.11	116.48
2	C	601	FAD	C4-N3-C2	-3.23	119.91	125.64
2	A	601	FAD	C4X-C10-N10	3.21	121.08	116.48
2	A	601	FAD	N9A-C8A-N7A	-3.14	109.48	113.94
2	D	601	FAD	C5A-N7A-C8A	3.13	108.37	103.45
2	A	601	FAD	O3'-C3'-C2'	-3.10	101.88	108.93
2	C	601	FAD	C5A-C4A-N3A	-3.10	122.45	126.72
2	C	601	FAD	C9A-C5X-N5	-3.08	119.19	122.45
2	D	601	FAD	C10-C4X-N5	-3.04	118.60	124.81
2	C	601	FAD	C10-C4X-N5	-3.04	118.60	124.81
2	C	601	FAD	O2P-P-O3P	3.04	115.48	107.27
2	A	601	FAD	C2A-N3A-C4A	3.02	119.20	111.83
2	C	601	FAD	O3P-P-O1P	-2.98	101.75	110.70
2	A	601	FAD	C5A-N7A-C8A	2.95	108.09	103.45
2	C	601	FAD	O2A-PA-O3P	2.95	115.24	107.27
2	B	601	FAD	C4X-C10-N10	2.94	120.70	116.48
2	C	601	FAD	N9A-C8A-N7A	-2.89	109.84	113.94
2	C	601	FAD	C4-C4X-C10	2.76	121.66	116.93
2	B	601	FAD	C5A-N7A-C8A	2.69	107.67	103.45
2	C	601	FAD	C4X-C10-N1	-2.68	118.02	124.59
2	A	601	FAD	C4A-C5A-N7A	-2.66	107.54	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	N3A-C4A-N9A	2.63	131.64	127.17
2	A	601	FAD	C8M-C8-C9	-2.61	114.97	119.57
2	C	601	FAD	C2A-N3A-C4A	2.61	118.21	111.83
2	A	601	FAD	C4-N3-C2	-2.59	121.03	125.64
2	B	601	FAD	O2'-C2'-C3'	2.58	115.30	109.25
2	A	601	FAD	N3A-C4A-N9A	2.58	131.56	127.17
2	A	601	FAD	C4-C4X-C10	2.58	121.35	116.93
2	A	601	FAD	C10-C4X-N5	-2.55	119.61	124.81
2	A	601	FAD	C9A-C5X-N5	-2.51	119.80	122.45
2	D	601	FAD	C4X-C10-N1	-2.50	118.47	124.59
2	D	601	FAD	C4-C4X-C10	2.45	121.13	116.93
2	B	601	FAD	C10-C4X-N5	-2.43	119.86	124.81
2	B	601	FAD	C4-N3-C2	-2.40	121.38	125.64
2	D	601	FAD	O2-C2-N1	-2.38	117.85	121.80
2	C	601	FAD	C2A-N1A-C6A	2.30	122.50	118.73
2	A	601	FAD	C4X-C10-N1	-2.29	118.97	124.59
2	B	601	FAD	C4A-C5A-N7A	-2.29	107.96	110.58
2	C	601	FAD	C5A-N7A-C8A	2.27	107.02	103.45
2	D	601	FAD	C4A-C5A-N7A	-2.20	108.06	110.58
2	B	601	FAD	O2-C2-N1	-2.16	118.21	121.80
2	D	601	FAD	C4X-C4-N3	2.12	118.66	113.25
2	B	601	FAD	O3P-P-O1P	-2.09	104.40	110.70
3	B	602	1PE	OH4-C13-C23	2.08	119.85	110.35
2	A	601	FAD	O2P-P-O3P	2.07	112.86	107.27
2	B	601	FAD	N3A-C4A-N9A	2.06	130.67	127.17
2	C	601	FAD	C5X-N5-C4X	2.03	121.38	118.09
2	D	601	FAD	C9A-C5X-N5	-2.03	120.31	122.45
2	D	601	FAD	C4A-N9A-C8A	2.02	107.86	105.74
2	B	601	FAD	C8M-C8-C9	-2.01	116.03	119.57
2	A	601	FAD	C6-C5X-C9A	2.01	121.80	119.05
2	D	601	FAD	C5X-C9A-N10	2.00	119.78	117.97

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C2'-C1'-N10-C10
2	A	601	FAD	C1'-C2'-C3'-O3'
2	A	601	FAD	C1'-C2'-C3'-C4'
2	A	601	FAD	O2'-C2'-C3'-O3'
2	A	601	FAD	O2'-C2'-C3'-C4'
2	B	601	FAD	C2'-C1'-N10-C10

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Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	B	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	C	601	FAD	C1'-C2'-C3'-C4'
2	C	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	C1'-C2'-C3'-O3'
2	D	601	FAD	C1'-C2'-C3'-C4'
2	D	601	FAD	O2'-C2'-C3'-O3'
2	D	601	FAD	O2'-C2'-C3'-C4'
5	B	605	GOL	O1-C1-C2-C3
5	B	607	GOL	O1-C1-C2-C3
5	B	608	GOL	C1-C2-C3-O3
5	C	605	GOL	O1-C1-C2-C3
5	C	605	GOL	C1-C2-C3-O3
5	C	605	GOL	O2-C2-C3-O3
5	C	606	GOL	O1-C1-C2-C3
3	D	602	1PE	C12-C22-OH3-C23
3	A	602	1PE	C14-C24-OH4-C13
3	A	602	1PE	C16-C26-OH6-C15
3	B	602	1PE	C23-C13-OH4-C24
3	C	602	1PE	C25-C15-OH6-C26
3	A	602	1PE	C15-C25-OH5-C14
2	C	601	FAD	O2'-C2'-C3'-O3'
3	B	602	1PE	OH4-C13-C23-OH3
3	C	602	1PE	OH6-C15-C25-OH5
3	D	602	1PE	OH5-C14-C24-OH4
3	B	602	1PE	C25-C15-OH6-C26
3	D	602	1PE	OH4-C13-C23-OH3
5	A	604	GOL	O1-C1-C2-O2
5	B	605	GOL	O1-C1-C2-O2
3	B	602	1PE	OH2-C12-C22-OH3
3	C	602	1PE	OH2-C12-C22-OH3
4	A	603	PEG	O2-C3-C4-O4
3	A	602	1PE	OH5-C14-C24-OH4
3	A	602	1PE	OH6-C15-C25-OH5
3	A	602	1PE	OH2-C12-C22-OH3
4	D	603	PEG	O2-C3-C4-O4
5	A	604	GOL	O1-C1-C2-C3
5	B	606	GOL	C1-C2-C3-O3
5	B	607	GOL	C1-C2-C3-O3
4	B	603	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	B	602	1PE	OH6-C15-C25-OH5
5	B	607	GOL	O1-C1-C2-O2
5	C	605	GOL	O1-C1-C2-O2
5	C	606	GOL	O1-C1-C2-O2
2	A	601	FAD	O4'-C4'-C5'-O5'
3	D	602	1PE	OH6-C15-C25-OH5
3	B	602	1PE	OH5-C14-C24-OH4
3	A	602	1PE	OH7-C16-C26-OH6
3	D	602	1PE	OH7-C16-C26-OH6
4	A	603	PEG	O1-C1-C2-O2
5	B	607	GOL	O2-C2-C3-O3
3	C	602	1PE	OH5-C14-C24-OH4
5	B	606	GOL	O1-C1-C2-O2
4	C	603	PEG	O2-C3-C4-O4
3	D	602	1PE	C14-C24-OH4-C13
2	C	601	FAD	C1'-C2'-C3'-O3'
3	B	602	1PE	C16-C26-OH6-C15
3	A	602	1PE	C12-C22-OH3-C23
2	A	601	FAD	C3'-C4'-C5'-O5'
4	D	603	PEG	C1-C2-O2-C3
3	B	602	1PE	C14-C24-OH4-C13
3	C	602	1PE	C16-C26-OH6-C15
3	D	602	1PE	OH2-C12-C22-OH3
4	D	603	PEG	O1-C1-C2-O2
5	B	606	GOL	O2-C2-C3-O3
5	B	608	GOL	O2-C2-C3-O3
3	B	602	1PE	C24-C14-OH5-C25
3	D	602	1PE	C23-C13-OH4-C24
3	C	602	1PE	OH4-C13-C23-OH3
3	A	602	1PE	OH4-C13-C23-OH3
3	D	602	1PE	C24-C14-OH5-C25
3	A	602	1PE	C25-C15-OH6-C26
3	C	602	1PE	C12-C22-OH3-C23
3	C	602	1PE	OH7-C16-C26-OH6
4	D	603	PEG	C4-C3-O2-C2
3	B	602	1PE	C15-C25-OH5-C14

There are no ring outliers.

14 monomers are involved in 73 short contacts:

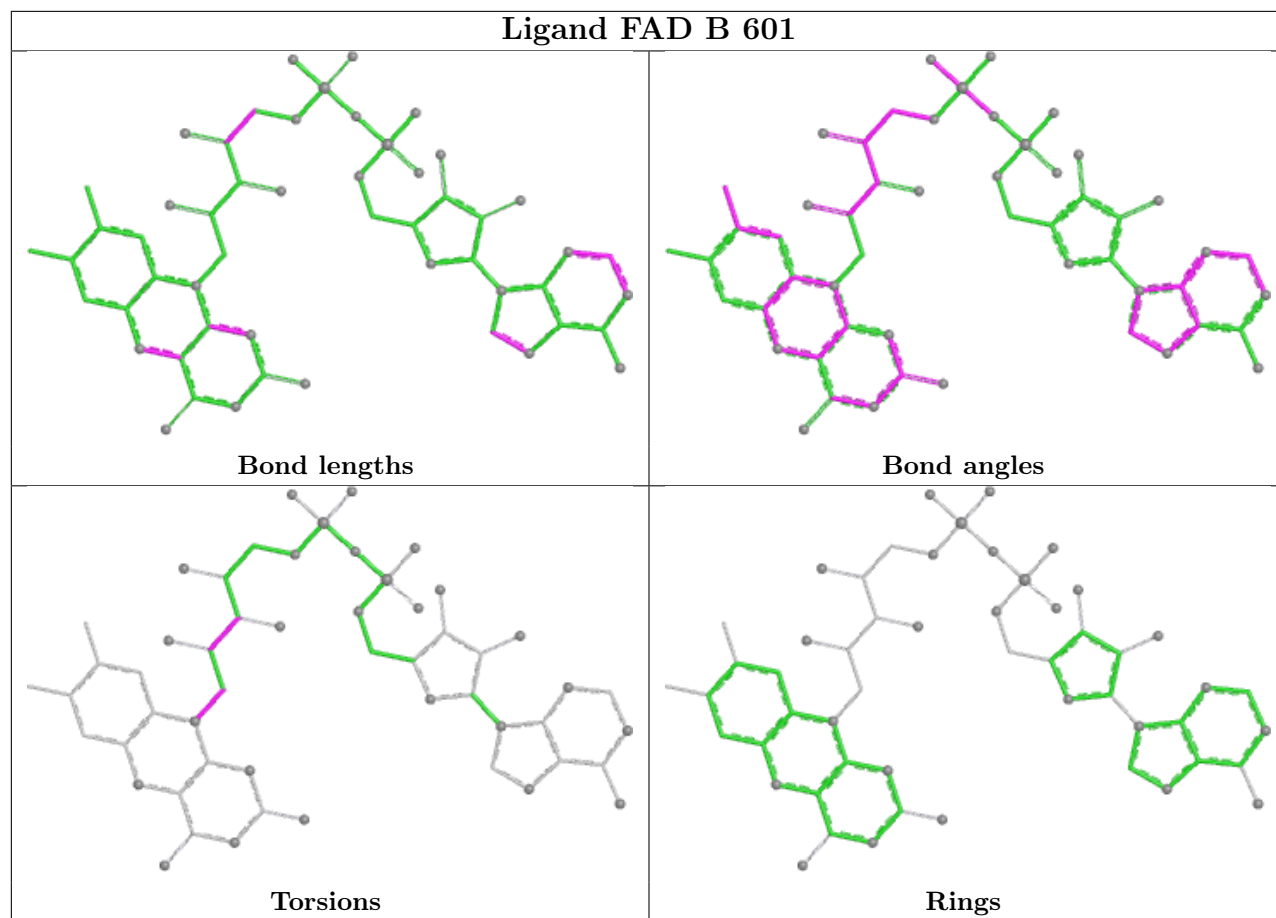
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	8	0

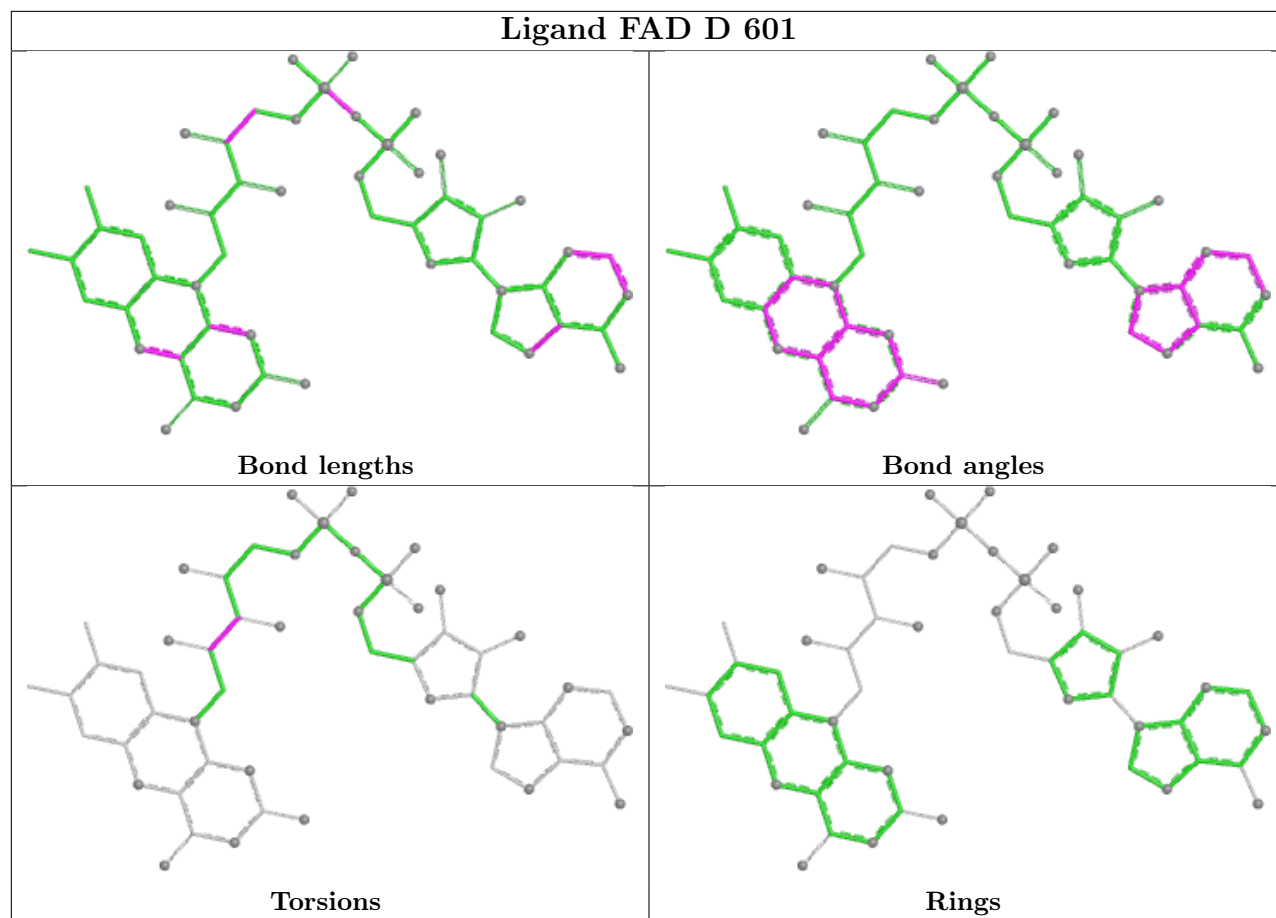
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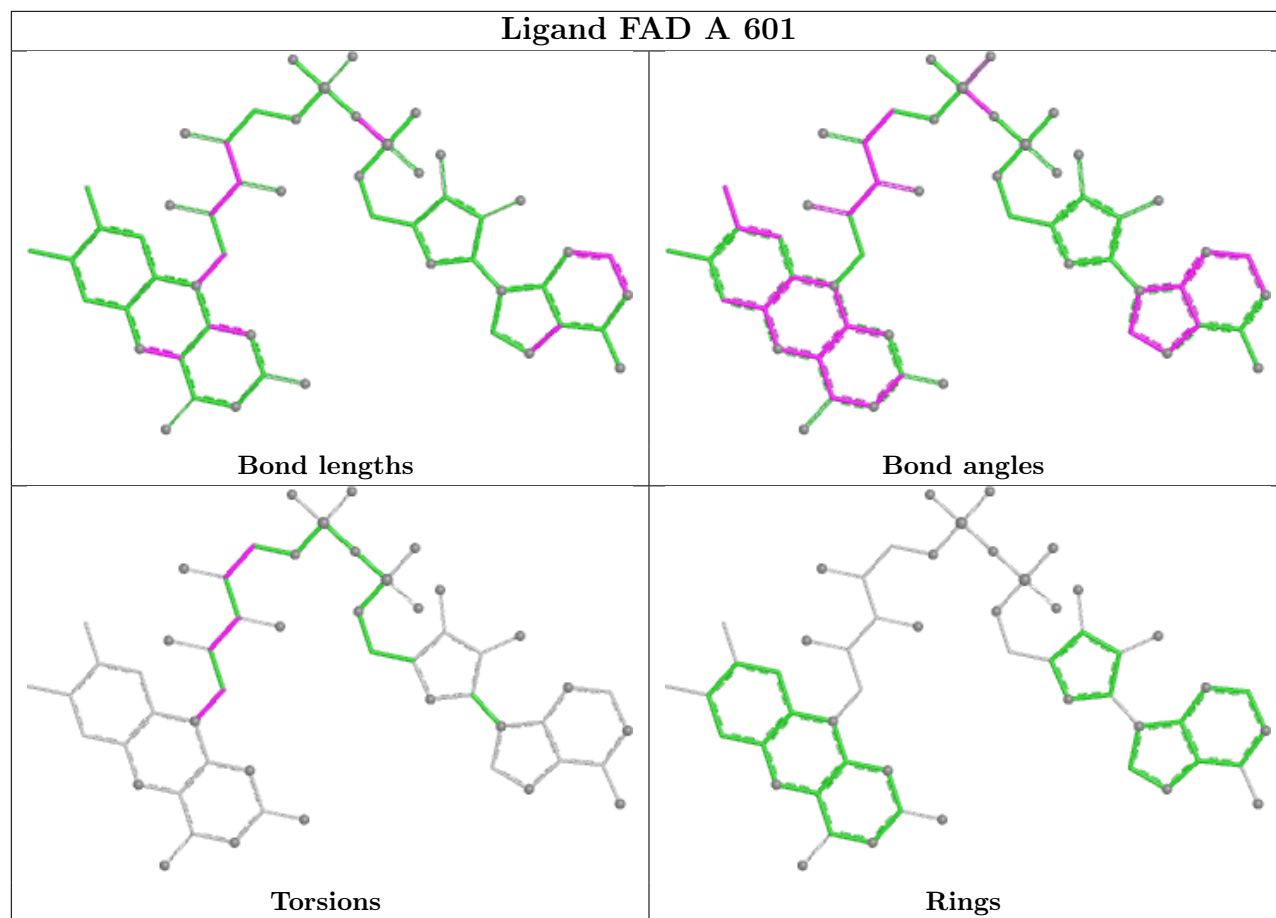
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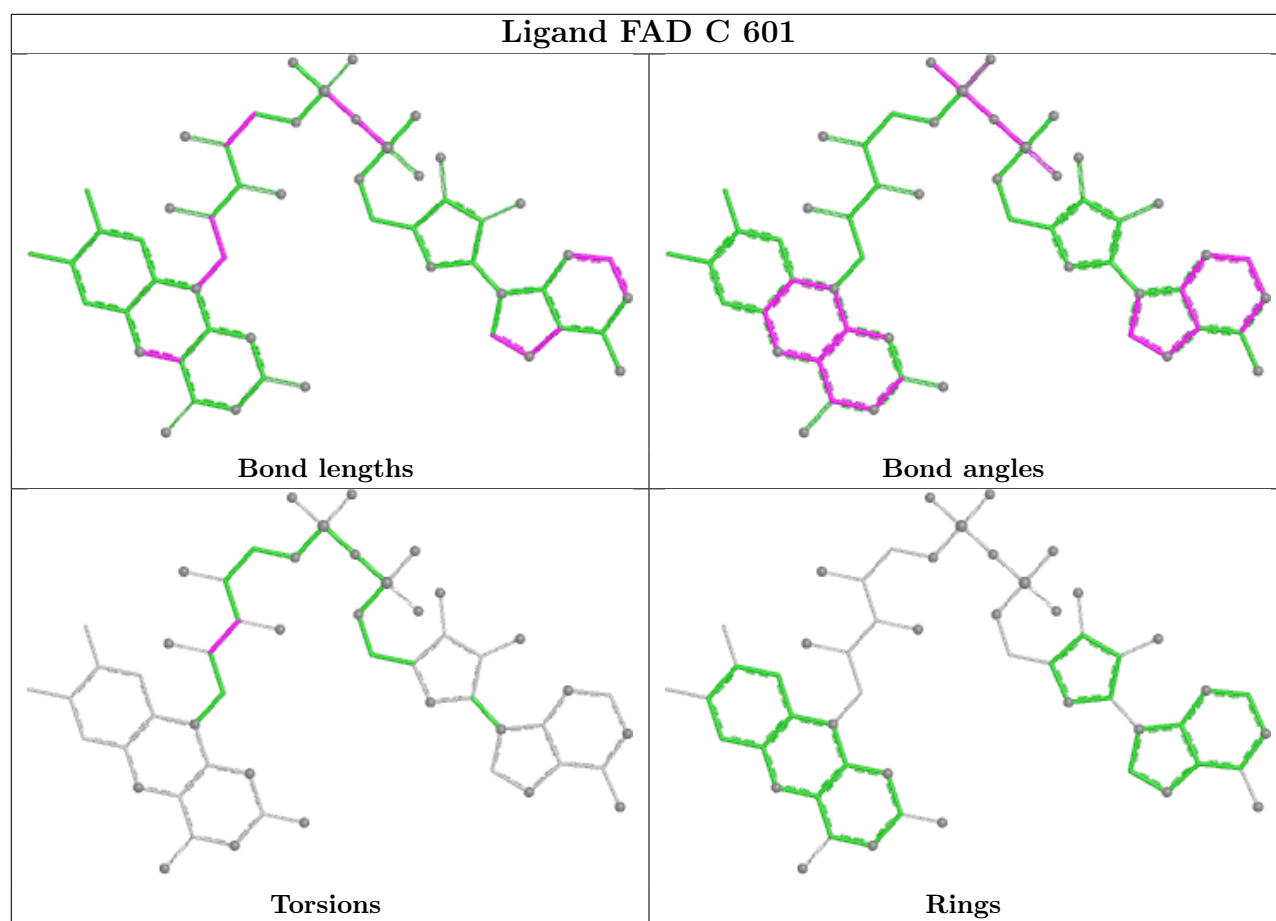
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FAD	6	0
2	A	601	FAD	5	0
5	B	607	GOL	3	0
2	C	601	FAD	7	0
4	D	603	PEG	1	0
5	A	604	GOL	1	0
3	B	602	1PE	13	0
3	D	602	1PE	13	0
3	C	602	1PE	4	0
3	A	602	1PE	9	0
5	B	606	GOL	1	0
5	C	604	GOL	1	0
5	B	608	GOL	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	569/597 (95%)	-0.21	2 (0%) 88 92	13, 40, 77, 126	13 (2%)
1	B	559/597 (93%)	-0.24	3 (0%) 87 91	12, 41, 69, 98	8 (1%)
1	C	571/597 (95%)	-0.25	8 (1%) 73 81	12, 38, 66, 107	13 (2%)
1	D	568/597 (95%)	-0.08	4 (0%) 84 89	18, 46, 79, 109	5 (0%)
All	All	2267/2388 (94%)	-0.19	17 (0%) 84 89	12, 41, 74, 126	39 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	259[A]	PHE	4.0
1	C	336	LEU	3.8
1	C	449	VAL	3.4
1	B	423	ALA	3.3
1	B	420[A]	LEU	3.2
1	C	351	ILE	2.9
1	D	449	VAL	2.9
1	C	341	VAL	2.7
1	A	259	PHE	2.6
1	A	449	VAL	2.5
1	C	8	ALA	2.4
1	C	329[A]	PHE	2.2
1	C	22	ASP	2.2
1	D	344	GLY	2.2
1	D	348	ALA	2.1
1	D	346	ALA	2.0
1	B	429	PRO	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

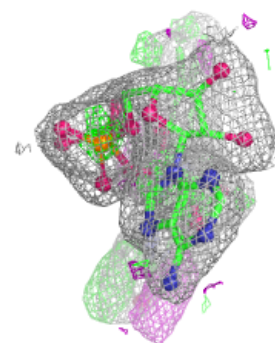
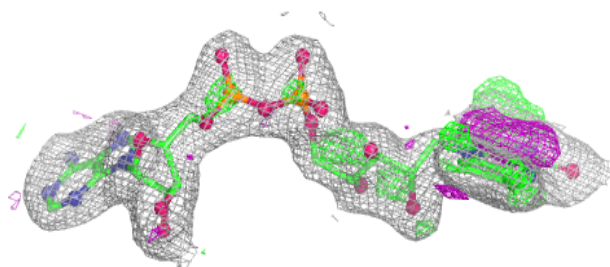
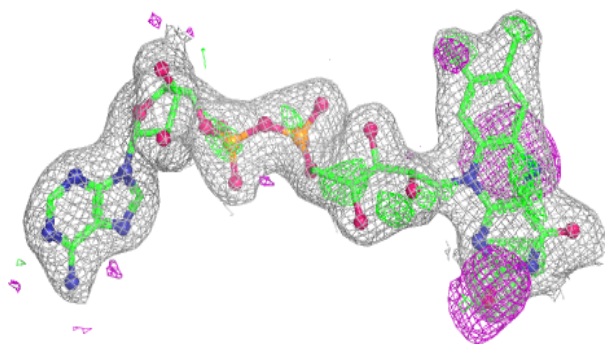
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	C	605	6/6	0.79	0.12	98,99,99,99	0
5	GOL	B	607	6/6	0.80	0.15	82,84,85,85	0
5	GOL	A	604	6/6	0.82	0.11	85,86,87,87	0
6	SO4	A	606	5/5	0.84	0.08	183,183,183,183	0
5	GOL	B	608	6/6	0.86	0.09	78,83,84,85	0
3	1PE	D	602	16/16	0.86	0.15	70,72,74,74	0
4	PEG	C	603	7/7	0.86	0.13	72,72,74,74	0
5	GOL	B	605	6/6	0.87	0.11	81,82,84,85	0
4	PEG	A	603	7/7	0.88	0.14	67,67,70,73	0
6	SO4	B	604	5/5	0.88	0.07	119,119,120,120	0
4	PEG	B	603	7/7	0.89	0.15	74,75,76,76	0
3	1PE	B	602	16/16	0.89	0.15	71,73,75,76	0
3	1PE	C	602	16/16	0.89	0.14	65,71,74,74	0
4	PEG	D	603	7/7	0.90	0.12	67,69,71,73	0
5	GOL	B	606	6/6	0.92	0.10	80,80,81,81	0
3	1PE	A	602	16/16	0.92	0.12	68,72,77,78	0
5	GOL	C	606	6/6	0.93	0.12	62,67,67,67	0
2	FAD	B	601	53/53	0.94	0.09	29,37,44,46	0
2	FAD	A	601	53/53	0.94	0.09	28,34,42,46	0
5	GOL	C	604	6/6	0.95	0.12	87,88,88,89	0
2	FAD	D	601	53/53	0.95	0.09	32,38,44,46	0
2	FAD	C	601	53/53	0.95	0.08	23,32,37,39	0

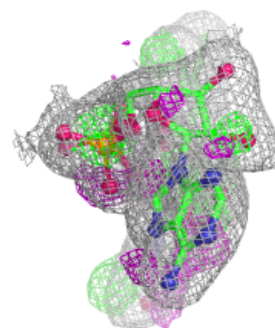
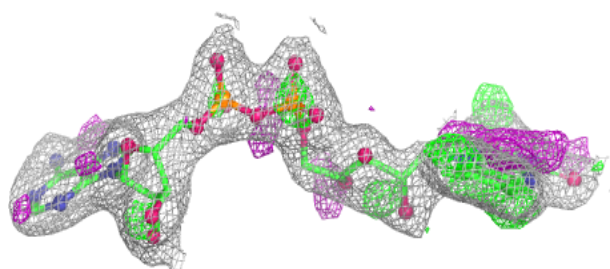
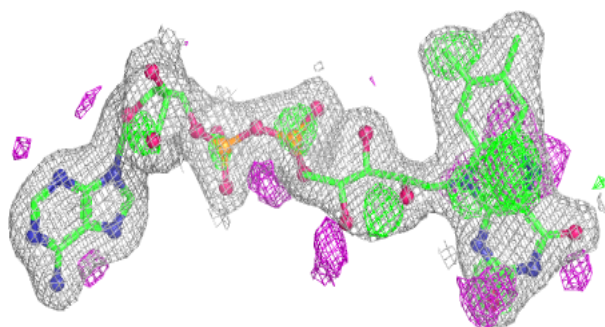
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 601:

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

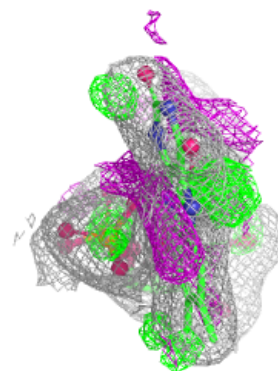
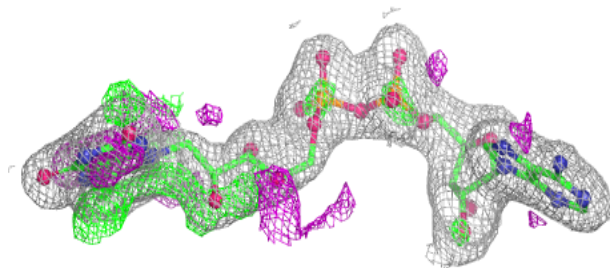
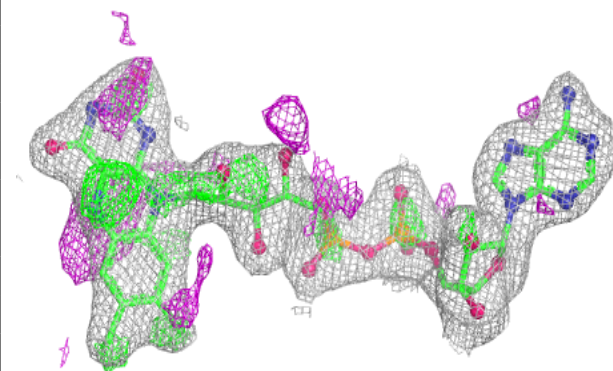
**Electron density around FAD A 601:**

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

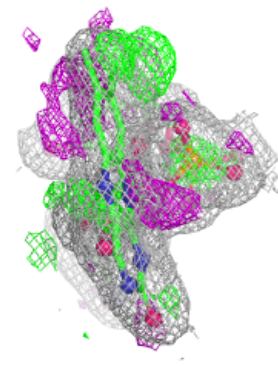
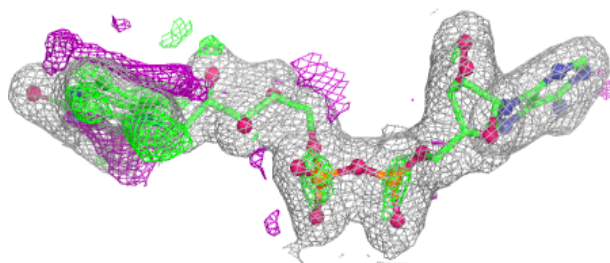
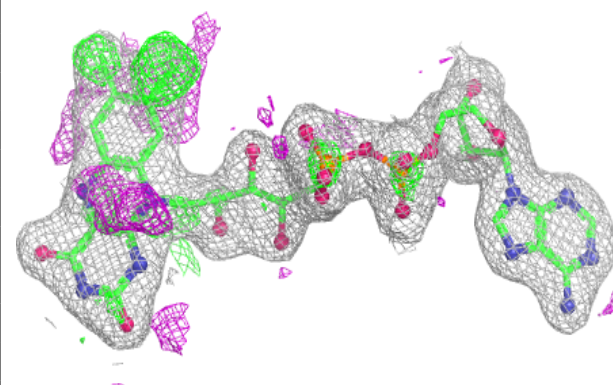


Electron density around FAD D 601:

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

**Electron density around FAD C 601:**

$2mF_o-DF_c$ (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.