



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:05 am BST

PDB ID : 4BC9
Title : MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATE SYN-
THASE: WILD-TYPE, ADDUCT WITH CYANOETHYL
Authors : Nenci, S.; Piano, V.; Rosati, S.; Aliverti, A.; Pandini, V.; Fraaije, M.W.; Heck,
A.J.R.; Edmondson, D.E.; Mattevi, A.
Deposited on : 2012-10-01
Resolution : 2.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

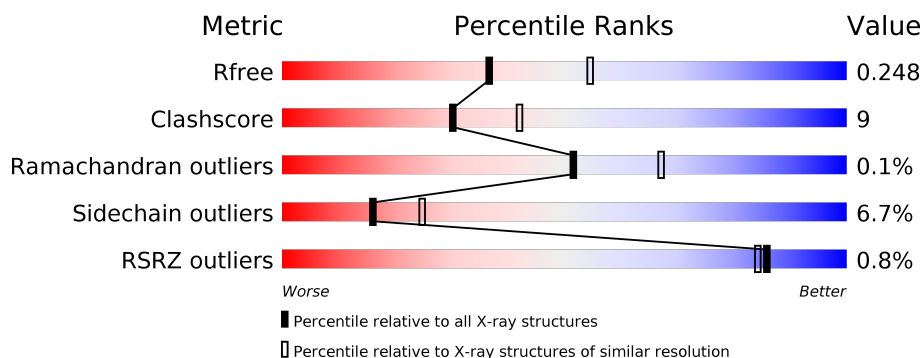
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	658	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	658	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>18%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	658	<div> <div></div> <div> <div>64%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	658	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>19%</div> <div>•</div> <div>16%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CNV	B	998	-	-	X	-
2	CNV	C	998	-	-	X	-

2 Entry composition [i](#)

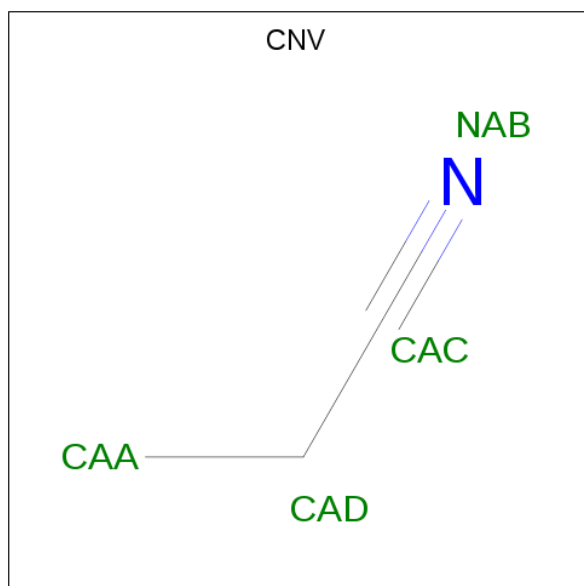
There are 5 unique types of molecules in this entry. The entry contains 17839 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	1	0
			4365	2773	754	813	25			
1	B	542	Total	C	N	O	S	0	0	0
			4259	2705	737	793	24			
1	C	552	Total	C	N	O	S	0	1	0
			4331	2745	750	812	24			
1	D	550	Total	C	N	O	S	0	1	0
			4321	2739	752	806	24			

- Molecule 2 is propanenitrile (three-letter code: CNV) (formula: C₃H₅N).



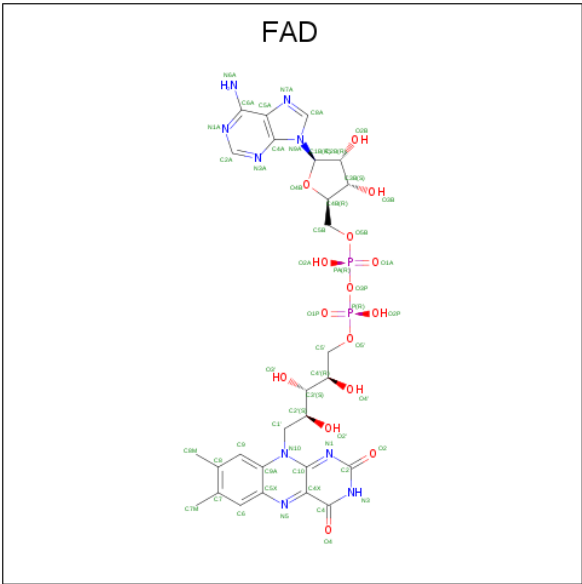
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			4	3	1		
2	B	1	Total	C	N	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	N	0	0
			4	3	1		
2	D	1	Total	C	N	0	0
			4	3	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

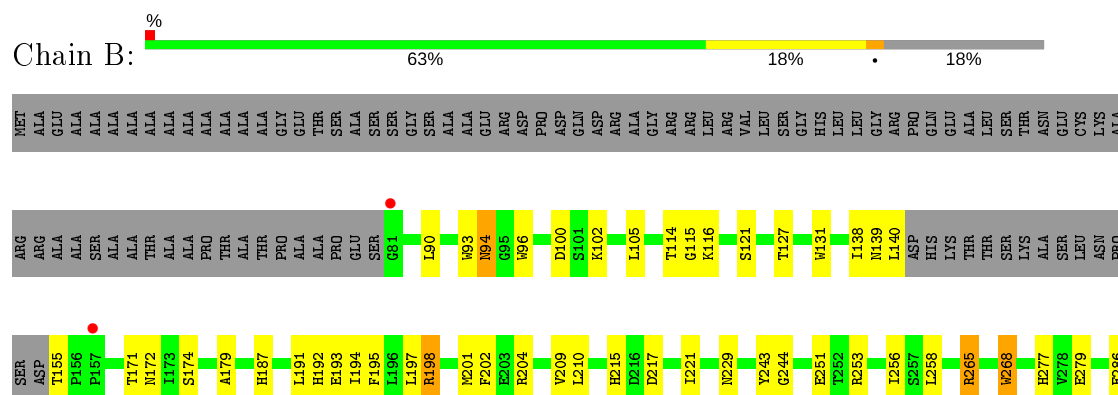


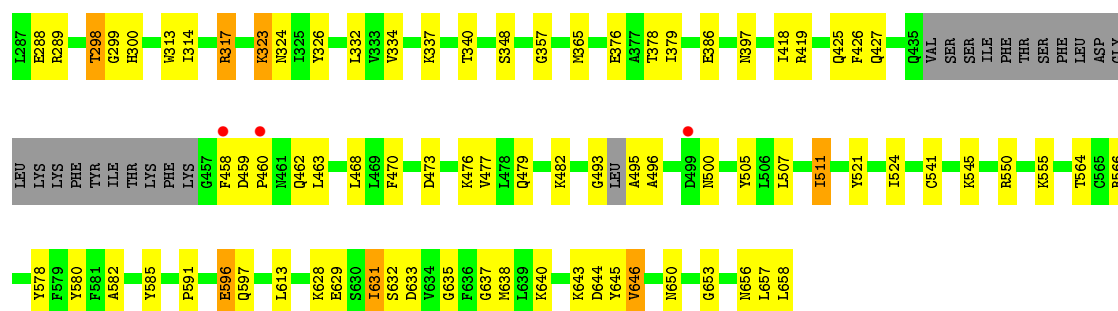
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		
5	B	73	Total	O	0	0
			73	73		
5	C	91	Total	O	0	0
			91	91		
5	D	66	Total	O	0	0
			66	66		

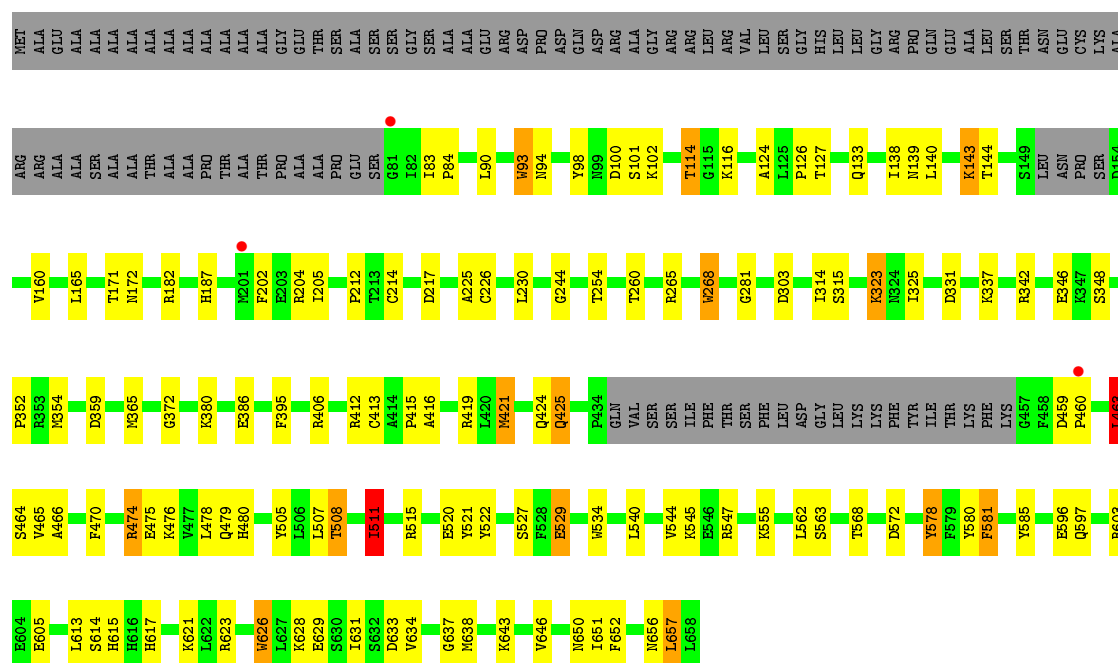
- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL





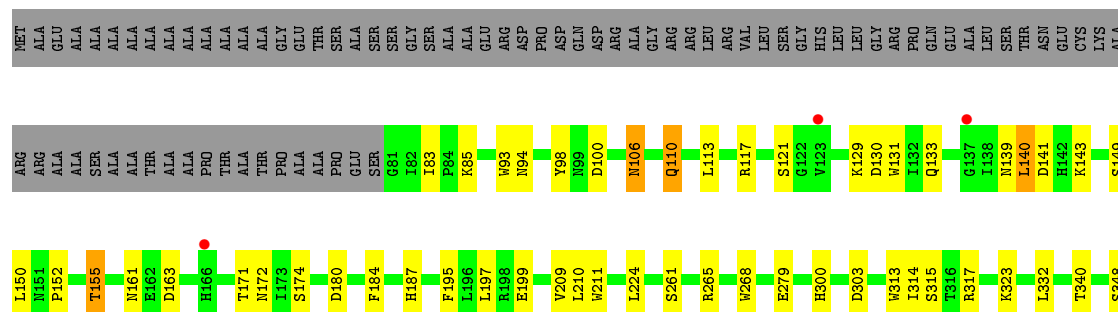
- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

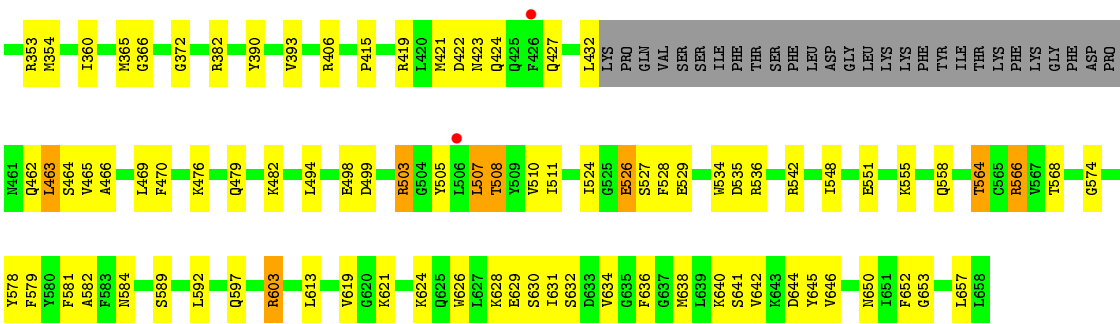
Chain C: 64% 17% 16%



- Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

Chain D: 63% 19% 16%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.91Å 98.62Å 106.28Å 90.92° 89.84° 95.66°	Depositor
Resolution (Å)	54.06 – 2.41 54.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.6 (54.06-2.41) 97.7 (54.00-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.186 , 0.248 0.187 , 0.248	Depositor DCC
R_{free} test set	1014 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17839	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: CNV, SO4, 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	0.73	2/4465 (0.0%)	0.82	2/6038 (0.0%)
1	B	0.75	5/4354 (0.1%)	0.82	2/5888 (0.0%)
1	C	0.73	4/4430 (0.1%)	0.82	4/5993 (0.1%)
1	D	0.73	6/4420 (0.1%)	0.79	1/5981 (0.0%)
All	All	0.74	17/17669 (0.1%)	0.81	9/23900 (0.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	626	TRP	CD2-CE2	7.13	1.50	1.41
1	B	268	TRP	CD2-CE2	6.93	1.49	1.41
1	B	313	TRP	CD2-CE2	6.31	1.49	1.41
1	B	96	TRP	CD2-CE2	6.29	1.48	1.41
1	C	534	TRP	CD2-CE2	6.18	1.48	1.41
1	C	626	TRP	CD2-CE2	6.18	1.48	1.41
1	C	268	TRP	CD2-CE2	6.07	1.48	1.41
1	B	93	TRP	CD2-CE2	5.84	1.48	1.41
1	D	268	TRP	CD2-CE2	5.81	1.48	1.41
1	D	313	TRP	CD2-CE2	5.80	1.48	1.41
1	D	211	TRP	CD2-CE2	5.70	1.48	1.41
1	D	534	TRP	CD2-CE2	5.58	1.48	1.41
1	B	131	TRP	CD2-CE2	5.30	1.47	1.41
1	A	93	TRP	CD2-CE2	5.24	1.47	1.41
1	D	131	TRP	CD2-CE2	5.13	1.47	1.41
1	A	211	TRP	CD2-CE2	5.04	1.47	1.41
1	C	93	TRP	CD2-CE2	5.03	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	603	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	C	623	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	463	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	317	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	631	ILE	N-CA-C	-5.23	96.89	111.00
1	A	317	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	572	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	422	ASP	CB-CG-OD1	5.13	122.91	118.30
1	B	631	ILE	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4365	0	4289	85	0
1	B	4259	0	4174	84	0
1	C	4331	0	4236	89	0
1	D	4321	0	4239	81	0
2	A	4	0	3	0	0
2	B	4	0	3	2	0
2	C	4	0	3	5	0
2	D	4	0	3	1	0
3	A	53	0	31	1	0
3	B	53	0	31	2	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	A	90	0	0	5	0
5	B	73	0	0	3	0
5	C	91	0	0	3	0
5	D	66	0	0	0	0
All	All	17839	0	17074	322	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 9.

All (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:HIS:HD2	1:A:616:HIS:CD2	1.77	1.03
1:D:503:ARG:HH11	1:D:503:ARG:HG3	1.23	1.01
1:A:615:HIS:CD2	1:A:616:HIS:HD2	1.82	0.97
1:C:144:THR:HG22	1:C:520:GLU:HA	1.48	0.94
1:C:505:TYR:O	1:C:508:THR:HG23	1.68	0.93
1:B:139:ASN:O	1:B:140:LEU:HB2	1.68	0.93
1:A:596:GLU:HB2	5:A:2084:HOH:O	1.69	0.91
1:C:419:ARG:HH22	1:C:508:THR:CG2	1.86	0.88
1:A:615:HIS:HD2	1:A:616:HIS:HD2	0.93	0.88
1:B:555:LYS:HE3	1:B:597:GLN:HE21	1.42	0.84
1:B:555:LYS:HE3	1:B:597:GLN:NE2	1.92	0.84
1:B:555:LYS:CE	1:B:597:GLN:HE21	1.91	0.83
1:B:192:HIS:HB3	1:B:243:TYR:OH	1.79	0.82
1:A:439:ILE:HG12	1:D:535:ASP:HB2	1.63	0.80
1:C:628:LYS:O	1:C:631:ILE:O	2.01	0.78
1:C:144:THR:CG2	1:C:520:GLU:HA	2.13	0.78
1:A:187:HIS:HD2	1:A:188:GLY:O	1.68	0.77
1:B:596:GLU:HG2	1:B:597:GLN:N	1.99	0.76
1:C:419:ARG:HH22	1:C:508:THR:HG21	1.48	0.76
1:B:425:GLN:NE2	1:B:566:ARG:HD3	2.01	0.75
1:A:215:HIS:HD2	1:A:375:THR:OG1	1.69	0.74
1:C:139:ASN:O	1:C:140:LEU:HB2	1.89	0.73
1:B:495:ALA:N	5:B:2054:HOH:O	2.21	0.73
1:B:100:ASP:O	1:B:114:THR:HG22	1.90	0.71
1:A:243:TYR:HE2	1:A:622:LEU:HD13	1.53	0.71
1:C:421:MET:HE2	1:C:465:VAL:HB	1.71	0.71
1:B:277:HIS:HD2	1:B:378:THR:OG1	1.73	0.70
1:D:603:ARG:HH11	1:D:603:ARG:HG2	1.57	0.69
1:C:421:MET:CE	1:C:465:VAL:HB	2.22	0.69
1:C:656:ASN:O	1:C:657:LEU:HB2	1.92	0.69
1:B:115:GLY:O	1:B:121:SER:HB3	1.93	0.68
1:D:507:LEU:O	1:D:511:ILE:HD12	1.92	0.68
1:C:419:ARG:HH22	1:C:508:THR:HG22	1.57	0.68
1:B:277:HIS:HE1	1:B:376:GLU:OE1	1.78	0.67
1:A:243:TYR:CE2	1:A:622:LEU:HD13	2.29	0.66
1:B:650:ASN:HD21	1:B:653:GLY:HA2	1.60	0.66
1:A:423:ASN:HD21	1:A:427:GLN:HE21	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ARG:NH1	1:B:505:TYR:CE1	2.64	0.66
1:B:340:THR:HB	1:B:646:VAL:HG13	1.77	0.65
1:B:541:CYS:O	1:B:545:LYS:HG3	1.98	0.64
1:C:638:MET:HG2	1:D:642:VAL:HG13	1.78	0.64
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.79	0.63
1:B:507:LEU:O	1:B:511:ILE:HD12	1.99	0.63
1:A:615:HIS:CD2	1:A:616:HIS:CD2	2.69	0.63
1:B:192:HIS:CB	1:B:243:TYR:OH	2.48	0.62
1:C:421:MET:HB2	1:C:425:GLN:HB3	1.81	0.61
1:D:423:ASN:HD21	1:D:427:GLN:NE2	1.98	0.61
1:A:81:GLY:HA3	1:A:286:GLU:OE1	2.01	0.61
1:A:557:VAL:HA	1:A:588:ILE:HD11	1.83	0.60
1:C:133:GLN:HG2	1:C:138:ILE:O	2.01	0.60
1:A:571:TYR:OH	1:A:615:HIS:HE1	1.84	0.60
1:B:473:ASP:HB2	1:B:476:LYS:HD3	1.84	0.60
1:C:634:VAL:HG12	1:C:638:MET:HE2	1.84	0.60
1:B:94:ASN:HD22	1:B:94:ASN:H	1.48	0.59
1:B:251:GLU:OE2	1:B:253:ARG:NE	2.33	0.59
1:B:314:ILE:HG23	1:B:365:MET:HG2	1.85	0.59
1:D:603:ARG:NH1	1:D:603:ARG:HG2	2.16	0.58
1:D:390:TYR:O	1:D:498:GLU:HG3	2.03	0.58
1:D:152:PRO:HA	1:D:155:THR:HG23	1.86	0.58
1:D:650:ASN:HD21	1:D:653:GLY:HA2	1.67	0.58
1:D:187:HIS:CE1	1:D:197:LEU:HD11	2.38	0.58
5:A:2051:HOH:O	1:B:632:SER:HB2	2.03	0.58
1:C:359:ASP:H	1:D:317[B]:ARG:NH2	2.02	0.57
1:A:251:GLU:OE2	1:A:253:ARG:HB2	2.05	0.57
1:C:93:TRP:CE2	1:C:94:ASN:HB3	2.40	0.57
1:A:419:ARG:O	1:A:466:ALA:HA	2.05	0.56
1:A:534:TRP:HH2	1:A:570:THR:HG22	1.70	0.56
1:A:230:LEU:HD22	1:A:254:THR:HB	1.87	0.56
1:A:82:ILE:HG12	1:A:264:ASN:ND2	2.21	0.56
1:D:419:ARG:O	1:D:466:ALA:HA	2.06	0.56
1:C:182:ARG:HB3	1:C:205:ILE:HD12	1.87	0.55
1:C:421:MET:O	1:C:464:SER:HB2	2.07	0.55
1:C:419:ARG:NH2	1:C:508:THR:CG2	2.65	0.55
1:C:613:LEU:HD21	1:C:626:TRP:HB2	1.89	0.55
1:C:143:LYS:HB3	1:C:521:TYR:CE1	2.42	0.55
1:A:505:TYR:O	1:A:508:THR:HG23	2.07	0.55
1:A:215:HIS:CD2	1:A:375:THR:OG1	2.56	0.54
1:B:286:GLU:OE2	1:B:289:ARG:NH2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:O	1:B:172:ASN:HB2	2.06	0.54
1:C:540:LEU:O	1:C:544:VAL:HG23	2.06	0.54
1:D:424:GLN:HB2	1:D:564:THR:CG2	2.38	0.54
1:C:419:ARG:NH2	1:C:508:THR:HG22	2.22	0.54
1:A:248:PRO:HG2	1:A:655:ARG:HG3	1.90	0.54
1:B:215:HIS:CE1	1:B:337:LYS:HD2	2.42	0.54
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.90	0.54
1:D:130:ASP:HA	1:D:133:GLN:HE21	1.73	0.53
1:B:288:GLU:OE1	1:B:298:THR:HB	2.08	0.53
1:D:422:ASP:OD1	1:D:564:THR:HG22	2.08	0.53
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.43	0.53
1:B:555:LYS:CE	1:B:597:GLN:NE2	2.61	0.53
1:B:640:LYS:HE3	1:B:644:ASP:OD2	2.08	0.53
1:D:421:MET:HE2	1:D:465:VAL:HB	1.90	0.53
1:A:192:HIS:CD2	1:A:592:LEU:CD1	2.92	0.52
1:A:630:SER:HA	1:B:348:SER:OG	2.08	0.52
1:D:139:ASN:O	1:D:140:LEU:HB2	2.09	0.52
1:D:603:ARG:CG	1:D:603:ARG:HH11	2.22	0.52
1:B:244:GLY:HA2	1:B:656:ASN:HD21	1.75	0.52
1:D:503:ARG:HH11	1:D:503:ARG:CG	2.08	0.52
1:D:93:TRP:HA	1:D:184:PHE:CE2	2.44	0.52
1:B:277:HIS:CD2	1:B:378:THR:OG1	2.57	0.52
1:C:413:CYS:O	1:C:480:HIS:NE2	2.37	0.52
1:D:113:LEU:HD23	1:D:121:SER:HA	1.92	0.52
1:D:340:THR:HB	1:D:646:VAL:HG13	1.90	0.52
1:C:547:ARG:NH1	1:C:605:GLU:OE1	2.37	0.52
1:C:631:ILE:HB	1:D:360:ILE:HD13	1.91	0.52
1:D:551:GLU:O	1:D:555:LYS:HD2	2.09	0.51
1:B:127:THR:O	1:B:127:THR:HG22	2.10	0.51
1:C:323:LYS:HD2	1:C:323:LYS:C	2.30	0.51
1:C:331:ASP:O	1:C:380:LYS:HE3	2.11	0.51
1:B:299:GLY:HA3	1:B:326:TYR:CG	2.45	0.51
1:C:101:SER:HA	1:C:114:THR:HG22	1.93	0.51
1:B:217:ASP:O	1:B:221:ILE:HG13	2.10	0.50
1:D:303:ASP:HB2	2:D:998:CNV:HAA1	1.94	0.50
1:C:337:LYS:HE2	1:C:346:GLU:OE2	2.11	0.50
1:A:628:LYS:O	1:A:631:ILE:O	2.30	0.50
1:C:226:CYS:SG	1:C:651:ILE:HD13	2.52	0.50
1:C:144:THR:HG22	1:C:520:GLU:CA	2.31	0.50
1:D:503:ARG:NH1	1:D:503:ARG:HG3	2.02	0.50
1:B:210:LEU:HD13	1:B:256:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HG3	1:A:140:LEU:HD22	1.93	0.50
1:B:138:ILE:HD13	1:B:521:TYR:HB3	1.94	0.50
1:B:458:PHE:HB2	1:B:463:LEU:HD12	1.93	0.50
1:C:204:ARG:HD2	5:C:2016:HOH:O	2.11	0.50
1:A:425:GLN:OE1	1:A:566:ARG:HD3	2.11	0.49
1:B:314:ILE:O	1:B:365:MET:HA	2.11	0.49
1:A:423:ASN:HD21	1:A:427:GLN:NE2	2.06	0.49
1:A:526:GLU:HB3	1:A:595:PHE:HZ	1.77	0.49
1:A:372:GLY:HA2	1:A:652:PHE:CZ	2.46	0.49
1:C:100:ASP:O	1:C:114:THR:HG22	2.12	0.49
1:A:528:PHE:HZ	1:A:548:ILE:HD11	1.76	0.49
1:C:171:THR:O	1:C:172:ASN:HB2	2.11	0.49
2:B:998:CNV:CAC	3:B:999:FAD:C10	2.91	0.49
1:C:372:GLY:HA2	1:C:652:PHE:CZ	2.48	0.49
1:A:481:GLU:O	1:A:485:TYR:HD2	1.95	0.49
1:A:442:SER:HB3	1:D:542:ARG:NH1	2.28	0.49
1:B:496:ALA:O	1:B:500:ASN:ND2	2.42	0.49
1:A:541:CYS:O	1:A:545:LYS:HG3	2.12	0.49
1:B:298:THR:CG2	1:B:300:HIS:H	2.26	0.49
1:B:585:TYR:CD1	1:B:591:PRO:HG3	2.48	0.49
1:A:167:GLU:OE2	1:A:228:TYR:OH	2.20	0.48
1:B:277:HIS:CE1	1:B:376:GLU:OE1	2.63	0.48
1:C:419:ARG:O	1:C:466:ALA:HA	2.13	0.48
1:A:194:ILE:O	1:A:198:ARG:HG3	2.14	0.48
1:D:634:VAL:O	1:D:638:MET:HG3	2.12	0.48
1:B:425:GLN:HE22	1:B:566:ARG:HD3	1.77	0.48
1:C:412:ARG:CZ	1:D:382:ARG:HD3	2.43	0.48
1:D:619:VAL:HB	1:D:657:LEU:HD23	1.95	0.48
1:C:160:VAL:HG22	1:C:254:THR:HG21	1.96	0.48
5:A:2055:HOH:O	1:B:317:ARG:NH2	2.47	0.48
1:D:98:TYR:CD2	1:D:117:ARG:HD3	2.49	0.48
1:D:503:ARG:O	1:D:507:LEU:HB2	2.13	0.48
1:A:539:ASP:OD1	1:A:542:ARG:NH2	2.47	0.47
1:C:214:CYS:O	1:C:217:ASP:HB2	2.14	0.47
1:A:432:LEU:HD13	1:A:507:LEU:HD21	1.95	0.47
1:D:93:TRP:CE2	1:D:94:ASN:HB3	2.49	0.47
1:C:124:ALA:O	1:C:126:PRO:HD3	2.15	0.47
1:C:348:SER:HB3	1:D:629:GLU:O	2.14	0.47
2:B:998:CNV:CAC	3:B:999:FAD:C9A	2.92	0.47
1:C:621:LYS:HG3	1:C:656:ASN:HD22	1.80	0.47
1:A:164:PHE:HB2	1:A:228:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ARG:NH2	1:A:526:GLU:OE1	2.47	0.47
1:D:640:LYS:HE2	1:D:644:ASP:OD1	2.15	0.47
1:D:100:ASP:OD2	1:D:117:ARG:NH2	2.40	0.47
1:B:323:LYS:C	1:B:323:LYS:HD2	2.36	0.46
1:C:421:MET:HE1	1:C:465:VAL:HB	1.97	0.46
1:A:319:SER:HA	1:A:328:ASN:HD22	1.80	0.46
1:C:139:ASN:O	1:C:140:LEU:CB	2.62	0.46
1:A:160:VAL:HG11	1:A:165:LEU:HD13	1.97	0.46
1:A:88:GLN:CD	1:A:88:GLN:H	2.18	0.46
1:C:562:LEU:O	1:C:581:PHE:HA	2.15	0.46
1:C:585:TYR:CD1	1:C:585:TYR:O	2.68	0.46
1:D:555:LYS:HE2	1:D:597:GLN:HB2	1.97	0.46
1:A:421[A]:MET:HB2	1:A:425:GLN:HB3	1.96	0.46
1:A:529:GLU:OE1	1:A:617:HIS:CG	2.69	0.46
1:B:209:VAL:C	1:B:210:LEU:HD12	2.35	0.46
1:C:545:LYS:HD2	1:C:563:SER:O	2.16	0.46
1:C:83:ILE:HA	1:C:84:PRO:HD3	1.83	0.46
5:C:2055:HOH:O	1:D:632:SER:HB2	2.15	0.46
1:B:100:ASP:C	1:B:100:ASP:OD1	2.54	0.46
1:B:244:GLY:HA2	1:B:656:ASN:ND2	2.31	0.46
1:B:419:ARG:NH1	1:B:505:TYR:CD1	2.83	0.46
1:B:94:ASN:HA	1:B:197:LEU:HD13	1.98	0.46
1:C:578:TYR:OH	2:C:998:CNV:NAB	2.49	0.46
1:A:133:GLN:HG2	1:D:536:ARG:NH2	2.30	0.46
1:B:94:ASN:HD22	1:B:94:ASN:N	2.11	0.46
1:C:507:LEU:O	1:C:511:ILE:HD12	2.16	0.46
1:C:527:SER:HB3	1:C:580:TYR:HD2	1.81	0.46
1:C:93:TRP:CD2	1:C:94:ASN:HB3	2.50	0.46
1:D:640:LYS:HA	1:D:640:LYS:HD2	1.77	0.46
1:C:415:PRO:HB3	1:C:470:PHE:CE1	2.50	0.45
1:D:300:HIS:HB2	1:D:332:LEU:CD1	2.46	0.45
1:A:192:HIS:CD2	1:A:592:LEU:HD11	2.51	0.45
1:A:417:SER:HB3	1:A:469:LEU:HB3	1.97	0.45
1:B:204:ARG:NH2	1:B:253:ARG:O	2.49	0.45
1:A:592:LEU:HB2	5:A:2083:HOH:O	2.15	0.45
1:D:650:ASN:ND2	1:D:650:ASN:O	2.49	0.45
1:C:260:THR:O	1:C:281:GLY:HA3	2.16	0.45
1:D:628:LYS:HE2	1:D:636:PHE:CD1	2.52	0.45
1:A:571:TYR:HA	4:A:1659:SO4:O3	2.17	0.45
1:B:258:LEU:HD23	1:B:258:LEU:C	2.37	0.45
1:D:83:ILE:HB	1:D:261:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:GLY:HA2	1:B:638:MET:CE	2.47	0.45
1:B:265:ARG:HG2	1:B:279:GLU:OE1	2.17	0.45
1:C:421:MET:HB3	1:C:425:GLN:HG2	1.98	0.45
1:D:419:ARG:NH2	1:D:566:ARG:HH21	2.15	0.45
1:B:194:ILE:O	1:B:198:ARG:HG3	2.16	0.45
1:B:397:ASN:HA	1:B:462:GLN:O	2.17	0.45
1:B:116:LYS:HA	1:B:116:LYS:HD3	1.83	0.44
1:A:366:GLY:O	1:B:357:GLY:HA2	2.17	0.44
1:C:212:PRO:HB3	1:C:217:ASP:HB3	2.00	0.44
1:A:319:SER:HA	1:A:328:ASN:ND2	2.32	0.44
1:B:628:LYS:O	1:B:631:ILE:O	2.35	0.44
1:C:325:ILE:HD11	1:C:416:ALA:HB2	2.00	0.44
1:D:424:GLN:CB	1:D:564:THR:CG2	2.95	0.44
1:D:469:LEU:HD12	1:D:470:PHE:N	2.32	0.44
1:D:650:ASN:O	1:D:650:ASN:CG	2.55	0.44
1:A:386:GLU:HB2	1:A:472:GLY:O	2.18	0.44
1:B:493:GLY:C	5:B:2054:HOH:O	2.55	0.44
1:D:526:GLU:HG3	1:D:527:SER:N	2.33	0.44
1:A:545:LYS:HD2	1:A:563:SER:O	2.17	0.44
1:C:314:ILE:HG23	1:C:365:MET:HG2	2.00	0.43
1:D:315:SER:O	1:D:366:GLY:HA2	2.18	0.43
1:B:643:LYS:NZ	1:B:650:ASN:HD22	2.16	0.43
1:D:195:PHE:CD1	1:D:592:LEU:HD11	2.53	0.43
1:D:542:ARG:HE	1:D:542:ARG:HB3	1.51	0.43
1:B:564:THR:HG22	1:B:580:TYR:HB3	2.00	0.43
1:C:303:ASP:HB2	2:C:998:CNV:HAA1	2.00	0.43
1:A:138:ILE:CD1	1:A:140:LEU:HD12	2.49	0.43
1:A:191:LEU:HD12	1:A:595:PHE:CD2	2.54	0.43
1:B:470:PHE:HB3	1:B:477:VAL:HG13	2.01	0.43
1:C:165:LEU:HA	1:C:165:LEU:HD12	1.90	0.43
1:D:621:LYS:HG2	1:D:624:LYS:HD2	2.01	0.43
1:A:284:GLY:HA2	1:A:313:TRP:HH2	1.84	0.43
1:B:323:LYS:HD2	1:B:324:ASN:N	2.34	0.43
1:D:171:THR:O	1:D:172:ASN:HB2	2.18	0.43
1:D:187:HIS:CD2	1:D:197:LEU:HD11	2.53	0.43
1:D:415:PRO:HB3	1:D:470:PHE:CE2	2.54	0.43
1:A:94:ASN:HA	1:A:197:LEU:HD13	2.00	0.43
1:C:225:ALA:HA	1:C:230:LEU:HD12	2.00	0.43
1:C:629:GLU:O	1:D:348:SER:HB3	2.19	0.43
1:D:463:LEU:O	1:D:463:LEU:HD23	2.19	0.43
1:A:185:ARG:HG2	1:A:235:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LYS:NZ	1:A:486:ASP:OD2	2.49	0.43
1:C:100:ASP:O	1:C:114:THR:CG2	2.66	0.43
1:C:419:ARG:NH2	1:C:508:THR:HG21	2.25	0.43
1:C:90:LEU:HD23	1:C:98:TYR:HE1	1.84	0.43
1:A:265:ARG:HD2	1:A:279:GLU:OE1	2.18	0.42
1:B:524:ILE:O	1:B:582:ALA:HA	2.18	0.42
1:C:395:PHE:O	1:C:463:LEU:HB2	2.19	0.42
1:C:265:ARG:HD3	5:C:2019:HOH:O	2.19	0.42
1:C:474:ARG:NH1	1:C:478:LEU:HD11	2.33	0.42
1:C:555:LYS:HZ2	1:C:597:GLN:HB3	1.84	0.42
1:D:424:GLN:CB	1:D:564:THR:HG23	2.49	0.42
1:A:138:ILE:HD12	1:A:140:LEU:HD12	1.99	0.42
1:A:390:TYR:CE2	1:A:469:LEU:HD13	2.55	0.42
1:B:555:LYS:HE2	1:B:597:GLN:HB2	1.99	0.42
1:C:529:GLU:OE1	1:C:615:HIS:N	2.33	0.42
1:A:299:GLY:HA3	1:A:326:TYR:CD2	2.54	0.42
1:A:613:LEU:HD11	1:A:623:ARG:HB3	2.00	0.42
1:B:629:GLU:HG3	5:B:2068:HOH:O	2.18	0.42
1:D:93:TRP:NE1	1:D:94:ASN:ND2	2.68	0.42
1:A:527:SER:HB3	1:A:580:TYR:HD2	1.85	0.42
1:C:522:TYR:HA	1:C:585:TYR:CE2	2.54	0.42
1:A:645:TYR:CZ	1:B:637:GLY:HA3	2.55	0.42
1:A:171:THR:O	1:A:172:ASN:HB2	2.20	0.42
1:B:555:LYS:HE2	1:B:597:GLN:CB	2.50	0.42
1:D:106:ASN:HD21	1:D:110:GLN:H	1.68	0.42
1:D:527:SER:HA	1:D:579:PHE:O	2.20	0.42
1:A:555:LYS:HE2	1:A:597:GLN:HB3	2.01	0.42
1:B:459:ASP:C	1:B:459:ASP:OD1	2.59	0.42
1:B:418:ILE:HG13	1:B:468:LEU:CD2	2.50	0.41
1:C:637:GLY:HA3	1:D:645:TYR:CZ	2.55	0.41
1:A:119:PRO:CG	1:A:506:LEU:HD22	2.50	0.41
1:B:229:ASN:O	1:B:253:ARG:HD2	2.20	0.41
1:D:528:PHE:HZ	1:D:548:ILE:HD11	1.85	0.41
1:B:628:LYS:HD3	1:B:633:ASP:OD1	2.20	0.41
1:A:165:LEU:HA	1:A:165:LEU:HD12	1.74	0.41
1:A:524:ILE:HG21	1:A:524:ILE:HD13	1.79	0.41
1:B:193:GLU:HG3	1:B:243:TYR:CE2	2.56	0.41
1:C:303:ASP:OD2	2:C:998:CNV:HAA1	2.21	0.41
1:C:585:TYR:HD1	1:C:585:TYR:O	2.03	0.41
1:D:421:MET:O	1:D:464:SER:HB2	2.20	0.41
1:D:499:ASP:HB3	1:D:503:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:GLY:HA3	1:B:645:TYR:CZ	2.55	0.41
1:A:164:PHE:HB2	1:A:228:TYR:CG	2.56	0.41
1:A:571:TYR:OH	1:A:615:HIS:CE1	2.70	0.41
1:C:615:HIS:O	1:D:353:ARG:NH1	2.52	0.41
1:A:524:ILE:O	1:A:582:ALA:HA	2.20	0.41
1:B:268:TRP:CZ2	1:B:277:HIS:HB2	2.56	0.41
1:C:212:PRO:CB	1:C:217:ASP:HB3	2.50	0.41
1:C:459:ASP:HA	1:C:460:PRO:HD3	1.91	0.41
1:D:463:LEU:HD23	1:D:463:LEU:C	2.41	0.41
1:A:372:GLY:HA2	1:A:652:PHE:CE1	2.56	0.41
1:C:643:LYS:NZ	1:C:650:ASN:HD22	2.19	0.41
1:D:555:LYS:HE3	1:D:597:GLN:OE1	2.21	0.41
1:A:243:TYR:HA	5:A:2018:HOH:O	2.21	0.41
1:A:438:SER:O	1:A:441:THR:HG22	2.21	0.41
1:A:479:GLN:HE22	1:B:479:GLN:HE22	1.69	0.41
1:A:187:HIS:CD2	1:A:188:GLY:O	2.59	0.40
1:A:555:LYS:HE2	1:A:597:GLN:CB	2.51	0.40
1:B:155:THR:HG21	1:B:179:ALA:HB1	2.03	0.40
1:A:281:GLY:O	1:A:309:THR:HG22	2.21	0.40
1:A:459:ASP:HA	1:A:460:PRO:HD3	1.95	0.40
3:A:999:FAD:N1	3:A:999:FAD:H3'	2.36	0.40
1:B:298:THR:HG22	1:B:300:HIS:H	1.84	0.40
1:C:578:TYR:OH	2:C:998:CNV:CAC	2.70	0.40
1:D:265:ARG:HB2	1:D:279:GLU:OE1	2.22	0.40
1:C:479:GLN:OE1	1:D:479:GLN:NE2	2.54	0.40
1:D:524:ILE:O	1:D:582:ALA:HA	2.21	0.40
1:B:332:LEU:HB3	1:B:379:ILE:HG23	2.03	0.40
1:C:352:PRO:HG3	1:D:574:GLY:C	2.42	0.40
1:C:617:HIS:NE2	2:C:998:CNV:NAB	2.69	0.40
1:D:393:VAL:O	1:D:465:VAL:HG13	2.22	0.40
1:D:505:TYR:O	1:D:508:THR:OG1	2.33	0.40
1:C:187:HIS:HB3	1:C:202:PHE:CZ	2.56	0.40
1:C:244:GLY:HA2	1:C:656:ASN:HD21	1.86	0.40
1:C:540:LEU:HD23	1:C:540:LEU:C	2.42	0.40
1:C:342:ARG:HG3	1:D:634:VAL:HG22	2.03	0.40
1:D:372:GLY:HA2	1:D:652:PHE:CZ	2.57	0.40
1:B:187:HIS:HB3	1:B:202:PHE:CZ	2.56	0.40
1:D:161:ASN:OD1	1:D:163:ASP:N	2.54	0.40
1:D:209:VAL:C	1:D:210:LEU:HD12	2.42	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	550/658 (84%)	527 (96%)	23 (4%)	0	100	100
1	B	534/658 (81%)	509 (95%)	24 (4%)	1 (0%)	47	61
1	C	547/658 (83%)	527 (96%)	19 (4%)	1 (0%)	47	61
1	D	547/658 (83%)	529 (97%)	17 (3%)	1 (0%)	47	61
All	All	2178/2632 (83%)	2092 (96%)	83 (4%)	3 (0%)	51	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	558	GLN
1	B	460	PRO
1	C	511	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	469/545 (86%)	439 (94%)	30 (6%)	17	27
1	B	456/545 (84%)	431 (94%)	25 (6%)	21	33
1	C	464/545 (85%)	435 (94%)	29 (6%)	18	27
1	D	463/545 (85%)	423 (91%)	40 (9%)	10	15
All	All	1852/2180 (85%)	1728 (93%)	124 (7%)	16	25

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	102	LYS
1	A	116	LYS
1	A	138	ILE
1	A	140	LEU
1	A	174	SER
1	A	191	LEU
1	A	195	PHE
1	A	323	LYS
1	A	354	MET
1	A	406	ARG
1	A	419	ARG
1	A	439	ILE
1	A	441	THR
1	A	462	GLN
1	A	468	LEU
1	A	476	LYS
1	A	508	THR
1	A	510	VAL
1	A	511	ILE
1	A	515	ARG
1	A	516	ASP
1	A	535	ASP
1	A	550	ARG
1	A	578	TYR
1	A	588	ILE
1	A	592	LEU
1	A	631	ILE
1	A	646	VAL
1	A	657	LEU
1	B	90	LEU
1	B	94	ASN
1	B	102	LYS
1	B	105	LEU
1	B	174	SER
1	B	191	LEU
1	B	195	PHE
1	B	198	ARG
1	B	201	MET
1	B	265	ARG
1	B	298	THR
1	B	323	LYS
1	B	334	VAL

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Mol	Chain	Res	Type
1	B	386	GLU
1	B	426	PHE
1	B	427	GLN
1	B	482	LYS
1	B	511	ILE
1	B	550	ARG
1	B	578	TYR
1	B	596	GLU
1	B	613	LEU
1	B	646	VAL
1	B	657	LEU
1	B	658	LEU
1	C	102	LYS
1	C	114	THR
1	C	116	LYS
1	C	127	THR
1	C	143	LYS
1	C	315	SER
1	C	323	LYS
1	C	354	MET
1	C	386	GLU
1	C	406	ARG
1	C	421	MET
1	C	424	GLN
1	C	425	GLN
1	C	463	LEU
1	C	474	ARG
1	C	475	GLU
1	C	476	LYS
1	C	508	THR
1	C	511	ILE
1	C	515	ARG
1	C	529	GLU
1	C	568	THR
1	C	578	TYR
1	C	581	PHE
1	C	596	GLU
1	C	614	SER
1	C	633	ASP
1	C	646	VAL
1	C	657	LEU
1	D	85	LYS

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Mol	Chain	Res	Type
1	D	106	ASN
1	D	110	GLN
1	D	129	LYS
1	D	140	LEU
1	D	141	ASP
1	D	143	LYS
1	D	149	SER
1	D	150	LEU
1	D	155	THR
1	D	174	SER
1	D	180	ASP
1	D	199	GLU
1	D	224	LEU
1	D	323	LYS
1	D	354	MET
1	D	406	ARG
1	D	432	LEU
1	D	462	GLN
1	D	463	LEU
1	D	476	LYS
1	D	482	LYS
1	D	494	LEU
1	D	503	ARG
1	D	507	LEU
1	D	508	THR
1	D	510	VAL
1	D	526	GLU
1	D	529	GLU
1	D	564	THR
1	D	566	ARG
1	D	568	THR
1	D	578	TYR
1	D	581	PHE
1	D	584	ASN
1	D	589	SER
1	D	603	ARG
1	D	613	LEU
1	D	630	SER
1	D	641	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	172	ASN
1	A	187	HIS
1	A	192	HIS
1	A	215	HIS
1	A	290	GLN
1	A	328	ASN
1	A	335	HIS
1	A	423	ASN
1	A	479	GLN
1	A	500	ASN
1	A	615	HIS
1	A	616	HIS
1	B	94	ASN
1	B	110	GLN
1	B	133	GLN
1	B	177	GLN
1	B	277	HIS
1	B	362	HIS
1	B	423	ASN
1	B	597	GLN
1	B	650	ASN
1	B	656	ASN
1	C	139	ASN
1	C	177	GLN
1	C	400	GLN
1	C	479	GLN
1	C	500	ASN
1	C	597	GLN
1	C	650	ASN
1	C	656	ASN
1	D	106	ASN
1	D	133	GLN
1	D	151	ASN
1	D	189	HIS
1	D	427	GLN
1	D	479	GLN
1	D	500	ASN
1	D	650	ASN
1	D	656	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 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	CNV	B	998	3	3,3,3	1.50	1 (33%)	2,2,2	0.60	0
3	FAD	A	999	2	51,58,58	2.18	8 (15%)	60,89,89	2.30	13 (21%)
3	FAD	C	999	2	51,58,58	1.89	9 (17%)	60,89,89	2.31	15 (25%)
4	SO4	D	1659	-	4,4,4	0.64	0	6,6,6	0.45	0
2	CNV	D	998	3	3,3,3	0.41	0	2,2,2	0.78	0
4	SO4	B	1659	-	4,4,4	0.50	0	6,6,6	0.49	0
4	SO4	A	1659	-	4,4,4	0.45	0	6,6,6	0.39	0
2	CNV	C	998	3	3,3,3	1.67	1 (33%)	2,2,2	0.57	0
2	CNV	A	998	3	3,3,3	0.66	0	2,2,2	0.60	0
3	FAD	B	999	2	51,58,58	2.21	7 (13%)	60,89,89	2.21	14 (23%)
3	FAD	D	999	2	51,58,58	2.11	11 (21%)	60,89,89	2.14	16 (26%)

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	CNV	B	998	3	-	0/1/1/1	-
3	FAD	A	999	2	-	2/30/50/50	0/6/6/6
3	FAD	C	999	2	-	3/30/50/50	0/6/6/6
2	CNV	D	998	3	-	0/1/1/1	-
2	CNV	C	998	3	-	0/1/1/1	-
2	CNV	A	998	3	-	0/1/1/1	-
3	FAD	B	999	2	-	3/30/50/50	0/6/6/6
3	FAD	D	999	2	-	2/30/50/50	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	FAD	C4X-C10	10.11	1.48	1.38
3	A	999	FAD	C4X-C10	9.97	1.48	1.38
3	C	999	FAD	C4X-C10	8.20	1.47	1.38
3	D	999	FAD	C4X-C10	7.22	1.46	1.38
3	B	999	FAD	C5X-N5	6.81	1.46	1.35
3	D	999	FAD	C4X-N5	5.85	1.41	1.33
3	A	999	FAD	C5X-N5	5.72	1.44	1.35
3	A	999	FAD	C9A-N10	5.15	1.45	1.38
3	D	999	FAD	C5X-N5	4.91	1.43	1.35
3	B	999	FAD	C4-C4X	4.71	1.49	1.41
3	D	999	FAD	C9A-N10	4.65	1.44	1.38
3	C	999	FAD	C9A-N10	4.51	1.44	1.38
3	A	999	FAD	C9A-C5X	4.14	1.50	1.42
3	A	999	FAD	C8-C7	3.98	1.50	1.40
3	C	999	FAD	C4-C4X	3.90	1.48	1.41
3	D	999	FAD	C4-C4X	3.88	1.48	1.41
3	B	999	FAD	C8-C7	3.80	1.50	1.40
3	B	999	FAD	C9A-C5X	3.80	1.50	1.42
3	D	999	FAD	C8-C7	3.68	1.50	1.40
3	C	999	FAD	C5X-N5	3.57	1.41	1.35
3	A	999	FAD	C4-C4X	3.38	1.47	1.41
3	C	999	FAD	C8-C7	3.34	1.49	1.40
3	D	999	FAD	C9A-C5X	3.33	1.49	1.42
3	B	999	FAD	C9A-N10	3.04	1.42	1.38
3	B	999	FAD	C5A-C4A	2.89	1.48	1.40
2	C	998	CNV	CAC-NAB	2.84	1.25	1.14
3	D	999	FAD	C5A-C4A	2.80	1.48	1.40
3	C	999	FAD	C9A-C5X	2.80	1.48	1.42
2	B	998	CNV	CAC-NAB	2.46	1.24	1.14
3	C	999	FAD	C2A-N3A	2.34	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	999	FAD	C5A-C4A	2.30	1.47	1.40
3	D	999	FAD	C4-N3	2.20	1.36	1.33
3	A	999	FAD	C4X-N5	2.15	1.36	1.33
3	C	999	FAD	C4-N3	2.14	1.36	1.33
3	A	999	FAD	C10-N1	2.11	1.36	1.33
3	D	999	FAD	C5'-C4'	2.10	1.54	1.51
3	D	999	FAD	C2-N3	-2.03	1.34	1.38

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	FAD	C4-N3-C2	10.22	123.77	115.14
3	C	999	FAD	C1'-N10-C9A	9.20	125.53	118.29
3	B	999	FAD	C4-N3-C2	9.04	122.77	115.14
3	D	999	FAD	C4-N3-C2	8.39	122.23	115.14
3	C	999	FAD	C4-N3-C2	7.75	121.69	115.14
3	A	999	FAD	C4-C4X-C10	-6.46	115.68	119.95
3	B	999	FAD	C4-C4X-C10	-6.23	115.83	119.95
3	D	999	FAD	C1'-N10-C9A	6.08	123.08	118.29
3	C	999	FAD	C4X-N5-C5X	6.03	122.79	116.77
3	A	999	FAD	C1'-N10-C9A	5.37	122.52	118.29
3	B	999	FAD	C1'-N10-C9A	5.15	122.35	118.29
3	C	999	FAD	C4X-C4-N3	-5.11	116.44	123.43
3	A	999	FAD	C4X-N5-C5X	4.55	121.32	116.77
3	D	999	FAD	C4-C4X-C10	-4.31	117.09	119.95
3	B	999	FAD	C4-C4X-N5	4.22	123.42	118.60
3	A	999	FAD	C5X-C9A-N10	4.22	120.77	117.72
3	B	999	FAD	C4X-N5-C5X	4.19	120.96	116.77
3	D	999	FAD	C4X-C4-N3	-4.11	117.81	123.43
3	C	999	FAD	C4A-C5A-N7A	-3.89	105.35	109.40
3	D	999	FAD	N3A-C2A-N1A	-3.88	122.61	128.68
3	B	999	FAD	C5X-C9A-N10	3.68	120.38	117.72
3	D	999	FAD	C4X-N5-C5X	3.68	120.44	116.77
3	D	999	FAD	C4-C4X-N5	3.66	122.78	118.60
3	B	999	FAD	N3A-C2A-N1A	-3.54	123.15	128.68
3	A	999	FAD	C9A-C5X-N5	-3.47	116.94	122.36
3	B	999	FAD	C4X-C4-N3	-3.19	119.06	123.43
3	A	999	FAD	C4X-C4-N3	-3.18	119.08	123.43
3	A	999	FAD	N3A-C2A-N1A	-3.04	123.92	128.68
3	D	999	FAD	C2A-N1A-C6A	2.89	123.69	118.75
3	C	999	FAD	C9A-N10-C10	-2.88	118.13	121.91
3	A	999	FAD	C4-C4X-N5	2.87	121.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	FAD	C9A-C5X-N5	-2.80	117.98	122.36
3	A	999	FAD	C4A-C5A-N7A	-2.67	106.62	109.40
3	C	999	FAD	N3A-C2A-N1A	-2.65	124.54	128.68
3	C	999	FAD	O2'-C2'-C3'	2.64	115.53	109.10
3	C	999	FAD	O2'-C2'-C1'	-2.63	103.27	109.59
3	C	999	FAD	C9A-C5X-N5	-2.57	118.33	122.36
3	B	999	FAD	C2A-N1A-C6A	2.53	123.08	118.75
3	C	999	FAD	P-O3P-PA	-2.50	124.23	132.83
3	D	999	FAD	C1B-N9A-C4A	-2.50	122.25	126.64
3	D	999	FAD	O3'-C3'-C4'	2.49	114.82	108.81
3	A	999	FAD	P-O3P-PA	-2.48	124.30	132.83
3	C	999	FAD	C1'-N10-C10	-2.46	116.20	118.41
3	D	999	FAD	P-O3P-PA	-2.42	124.52	132.83
3	D	999	FAD	N6A-C6A-N1A	2.37	123.50	118.57
3	A	999	FAD	C6-C5X-N5	2.37	121.66	119.05
3	B	999	FAD	C5'-C4'-C3'	2.36	116.76	112.20
3	B	999	FAD	C9A-N10-C10	-2.30	118.89	121.91
3	D	999	FAD	C5X-C9A-N10	2.30	119.38	117.72
3	B	999	FAD	O3B-C3B-C2B	-2.20	104.69	111.82
3	D	999	FAD	C9A-C5X-N5	-2.19	118.93	122.36
3	D	999	FAD	O2P-P-O1P	2.16	122.94	112.24
3	C	999	FAD	C3B-C2B-C1B	2.15	104.22	100.98
3	C	999	FAD	C5X-C9A-N10	2.09	119.23	117.72
3	A	999	FAD	C9A-N10-C10	-2.07	119.20	121.91
3	B	999	FAD	P-O3P-PA	-2.05	125.80	132.83
3	C	999	FAD	C4-C4X-C10	-2.03	118.61	119.95
3	D	999	FAD	C3B-C2B-C1B	2.01	104.00	100.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

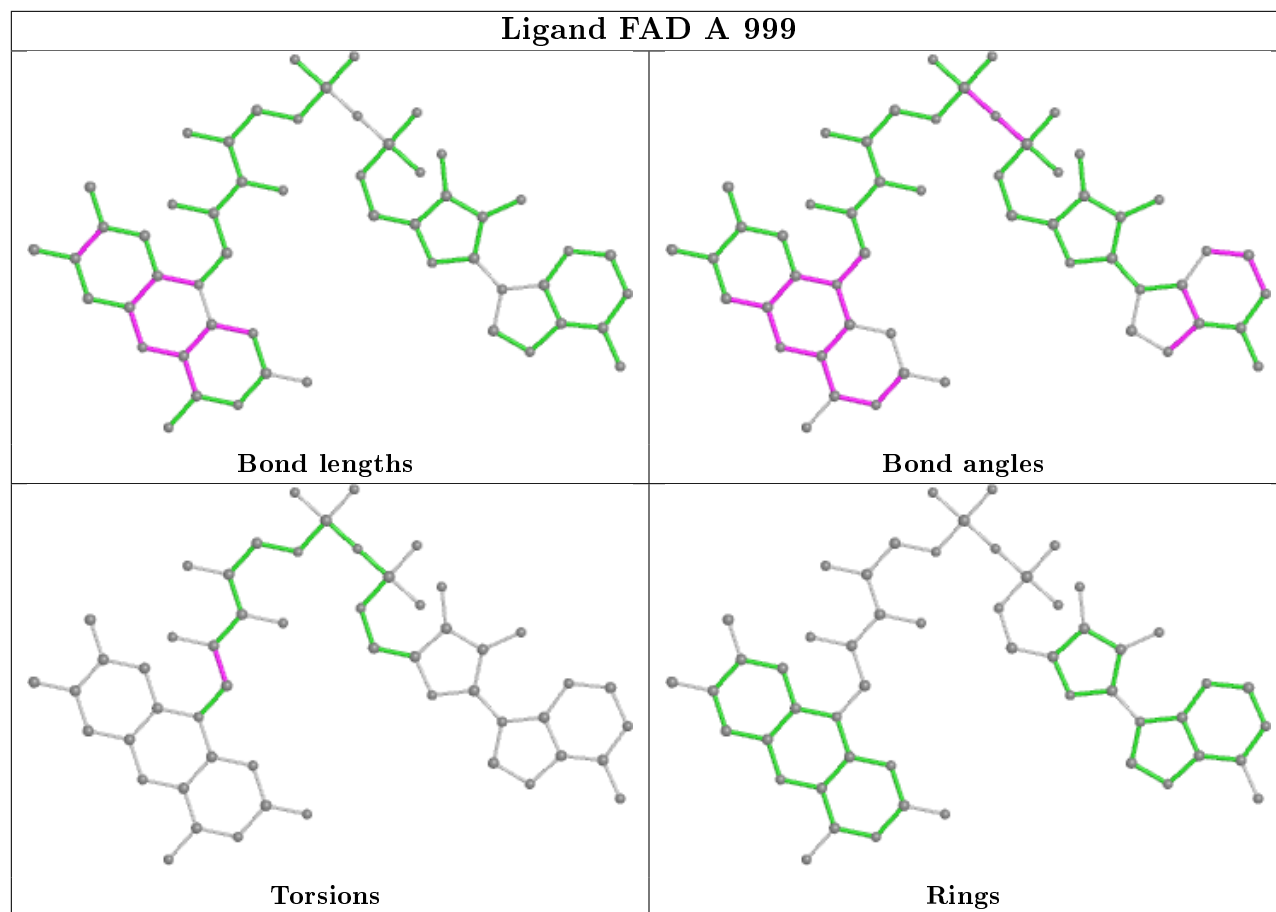
Mol	Chain	Res	Type	Atoms
3	A	999	FAD	N10-C1'-C2'-O2'
3	C	999	FAD	N10-C1'-C2'-O2'
3	B	999	FAD	N10-C1'-C2'-O2'
3	D	999	FAD	N10-C1'-C2'-O2'
3	D	999	FAD	N10-C1'-C2'-C3'
3	A	999	FAD	N10-C1'-C2'-C3'
3	C	999	FAD	N10-C1'-C2'-C3'
3	B	999	FAD	N10-C1'-C2'-C3'
3	C	999	FAD	C2'-C3'-C4'-C5'
3	B	999	FAD	C5'-O5'-P-O1P

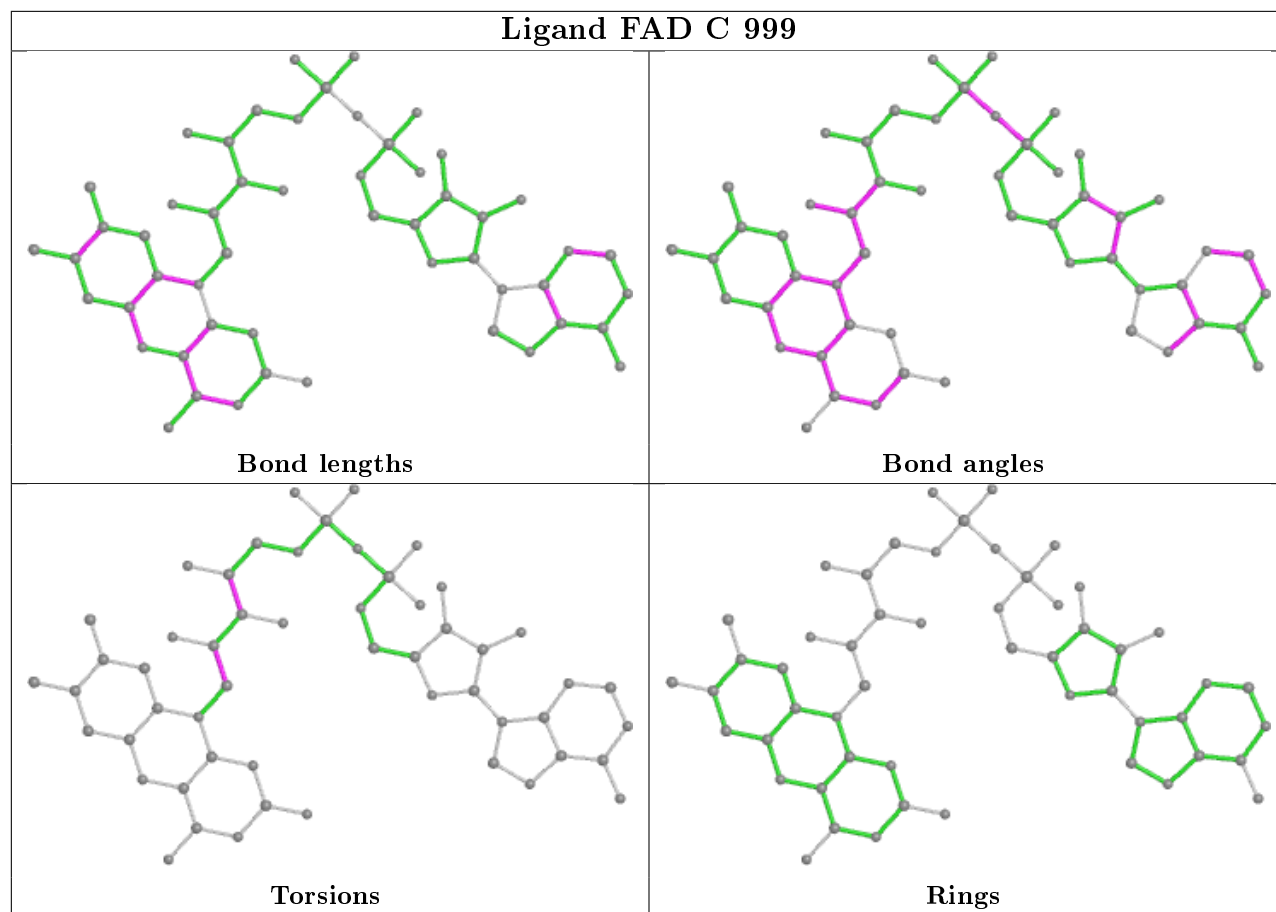
There are no ring outliers.

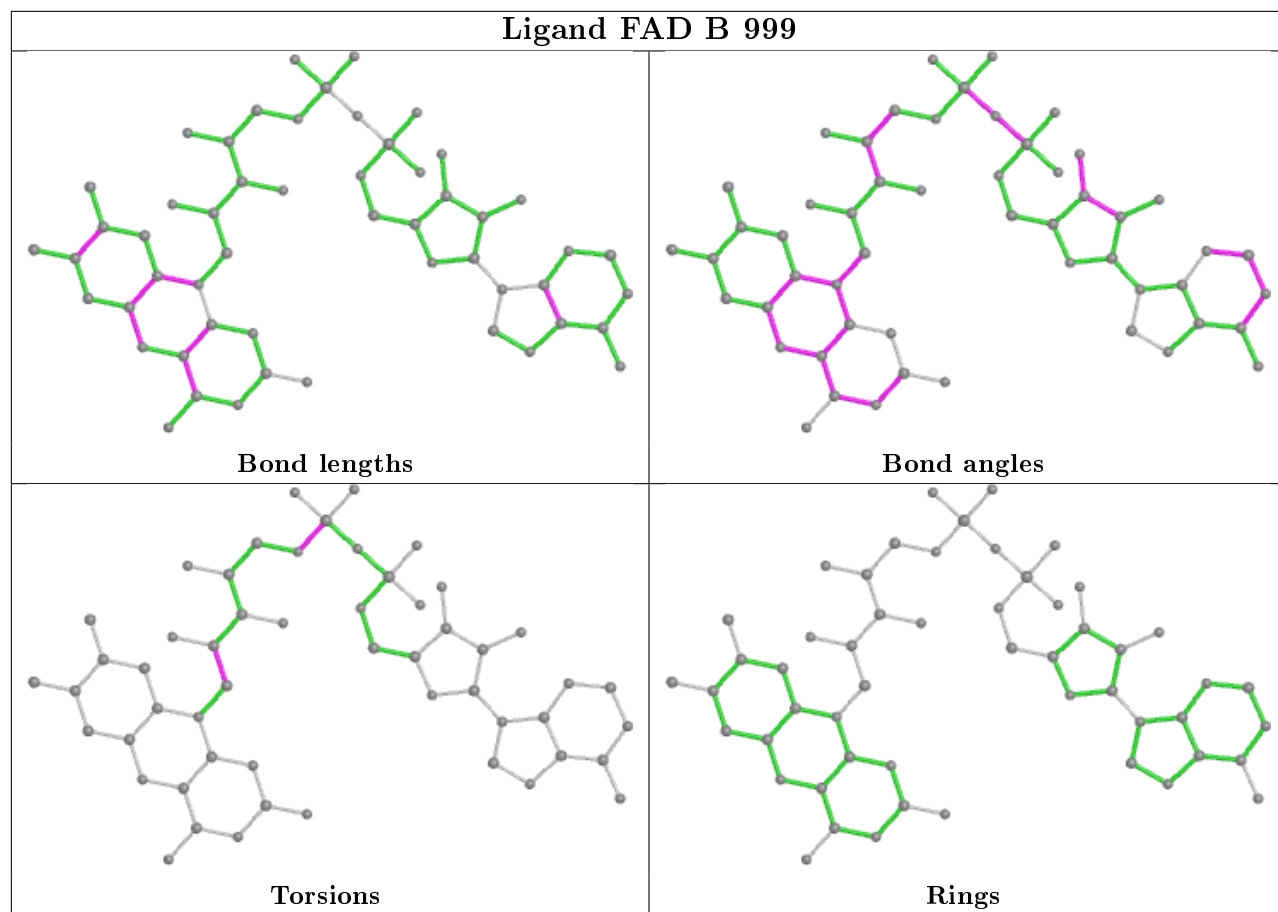
6 monomers are involved in 10 short contacts:

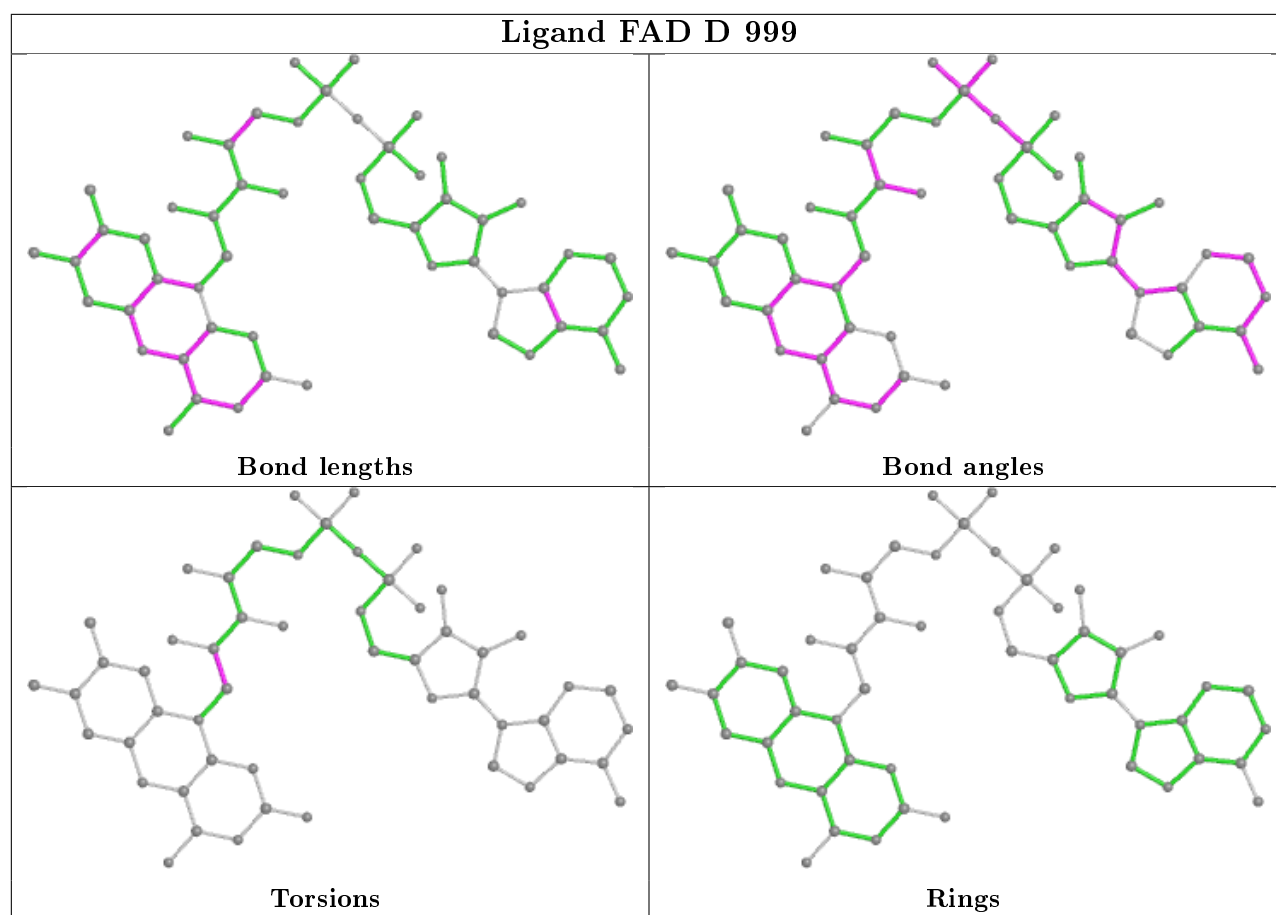
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	998	CNV	2	0
3	A	999	FAD	1	0
2	D	998	CNV	1	0
4	A	1659	SO4	1	0
2	C	998	CNV	5	0
3	B	999	FAD	2	0

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

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	555/658 (84%)	-0.36	5 (0%) 84 82	17, 30, 58, 89	0
1	B	542/658 (82%)	-0.38	5 (0%) 84 82	15, 31, 60, 91	0
1	C	552/658 (83%)	-0.45	3 (0%) 91 89	16, 31, 59, 84	0
1	D	550/658 (83%)	-0.34	5 (0%) 84 82	16, 34, 61, 79	0
All	All	2199/2632 (83%)	-0.38	18 (0%) 86 84	15, 31, 60, 91	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	PRO	3.6
1	B	458	PHE	3.6
1	C	460	PRO	2.7
1	D	137	GLY	2.5
1	A	172	ASN	2.4
1	D	506	LEU	2.4
1	B	81	GLY	2.4
1	C	201	MET	2.2
1	A	434	PRO	2.2
1	D	166	HIS	2.2
1	D	426	PHE	2.2
1	A	589	SER	2.2
1	C	81	GLY	2.1
1	D	123	VAL	2.1
1	A	83	ILE	2.1
1	B	157	PRO	2.1
1	A	436	VAL	2.0
1	B	499	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

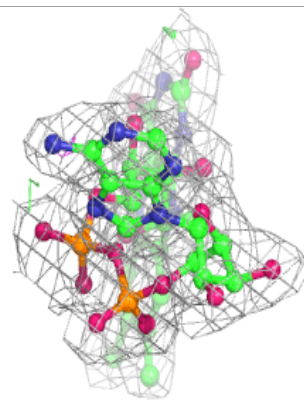
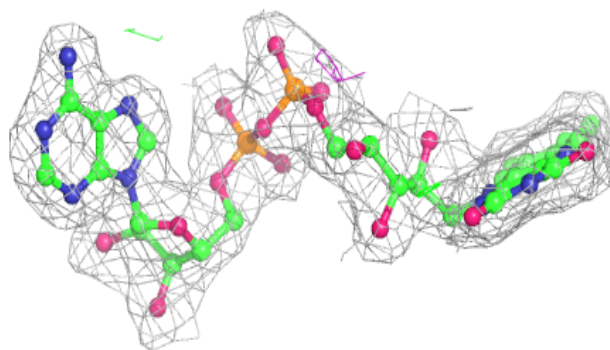
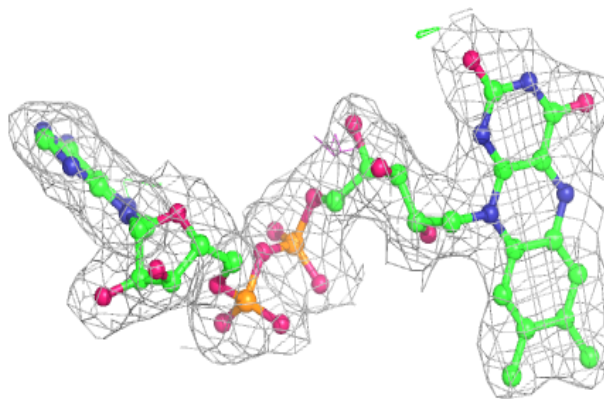
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	1659	5/5	0.92	0.17	53,57,61,63	0
4	SO4	A	1659	5/5	0.94	0.15	50,51,62,63	0
2	CNV	D	998	4/4	0.96	0.13	38,40,44,45	0
2	CNV	B	998	4/4	0.96	0.12	28,28,31,32	0
4	SO4	D	1659	5/5	0.96	0.11	40,46,53,54	0
2	CNV	A	998	4/4	0.96	0.13	24,28,33,34	0
2	CNV	C	998	4/4	0.97	0.12	23,24,27,31	0
3	FAD	A	999	53/53	0.98	0.11	14,19,23,25	0
3	FAD	C	999	53/53	0.98	0.11	14,17,20,22	0
3	FAD	B	999	53/53	0.98	0.10	16,21,27,30	0
3	FAD	D	999	53/53	0.98	0.12	15,22,26,27	0

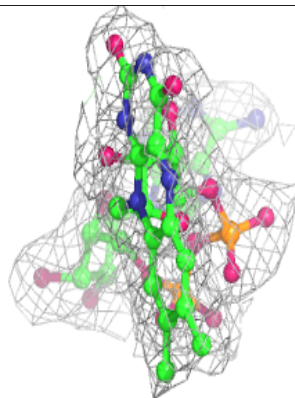
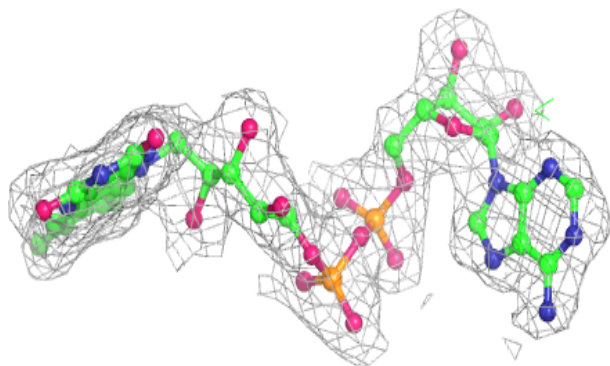
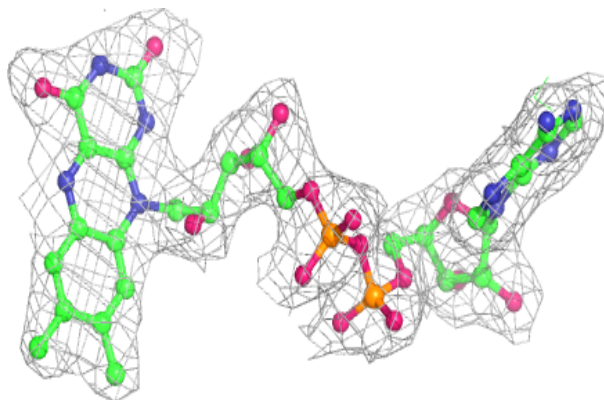
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 999:

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

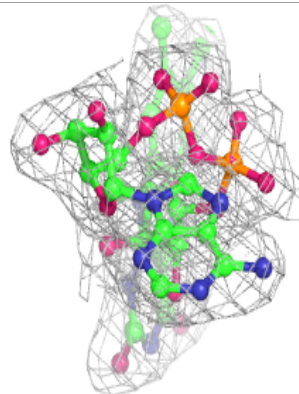
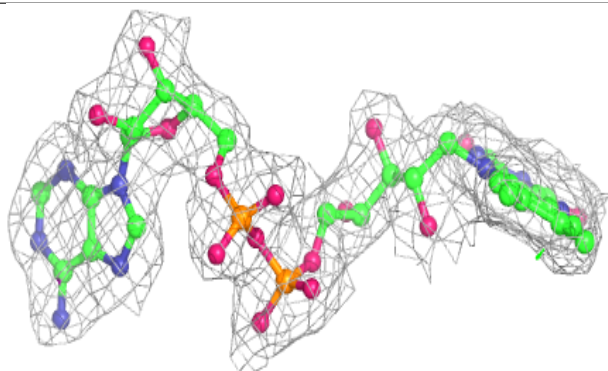
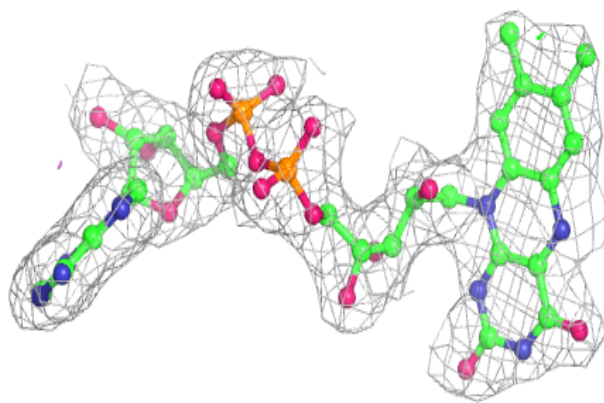
**Electron density around FAD C 999:**

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

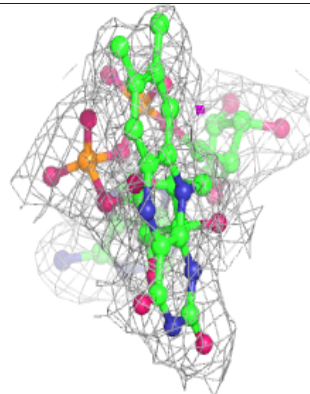
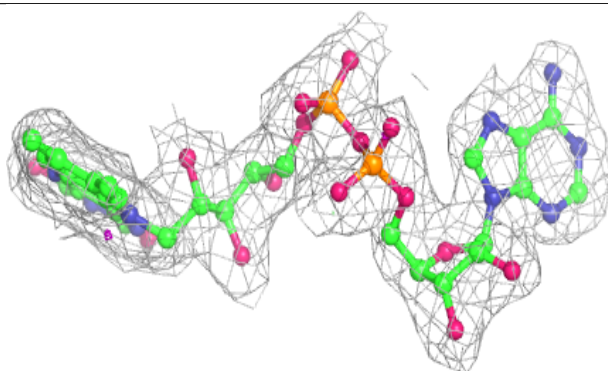
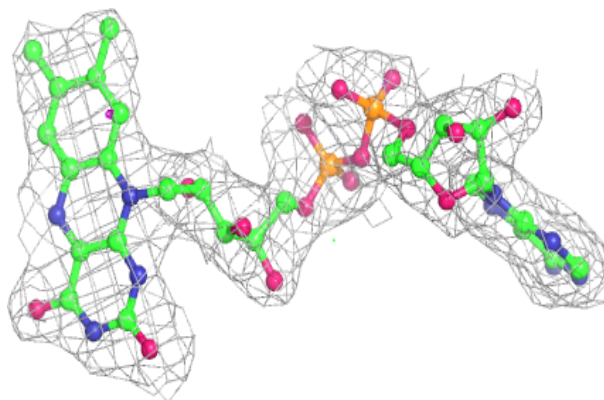


Electron density around FAD B 999:

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

**Electron density around FAD D 999:**

$2mF_o-DF_c$ (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.