



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:51 pm BST

PDB ID : 5YJY
Title : Structure of the Ndi1 protein from *Saccharomyces cerevisiae* in complex with AC0-12.
Authors : Yamasita, T.; Inaoka, D.K.; Shiba, T.; Oohashi, T.; Iwata, S.; Yagi, T.; Kosaka, H.; Harada, S.; Kita, K.; Hirano, K.
Deposited on : 2017-10-11
Resolution : 3.40 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

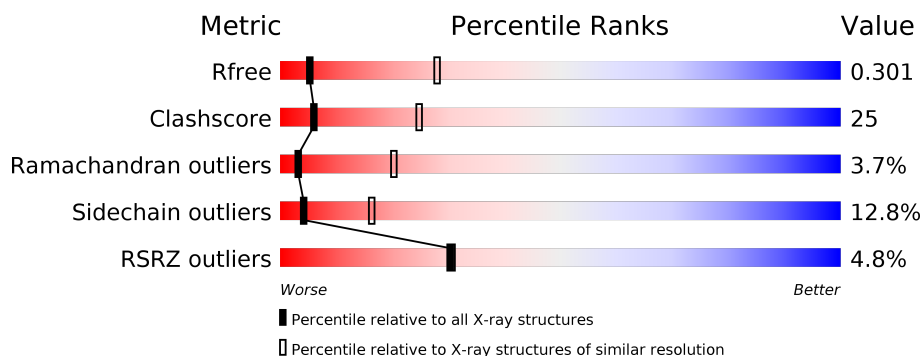
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	485	<div> <div>4%</div> <div> <div></div> <div>49%</div> <div>41%</div> <div>• • 5%</div> </div> </div>
2	B	486	<div> <div>5%</div> <div> <div></div> <div>51%</div> <div>38%</div> <div>6% • •</div> </div> </div>

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.

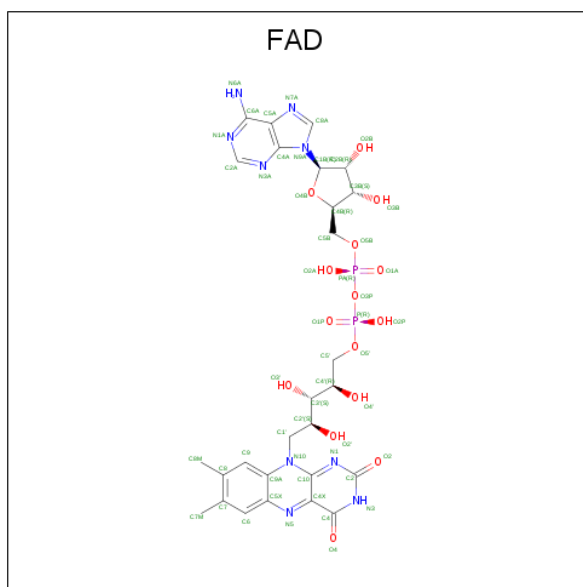
- Molecule 1 is a protein called Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	3	0
			3652	2357	623	667	5			

- Molecule 2 is a protein called Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	465	Total	C	N	O	S	0	4	0
			3684	2381	624	674	5			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by author).



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

Continued on next page...

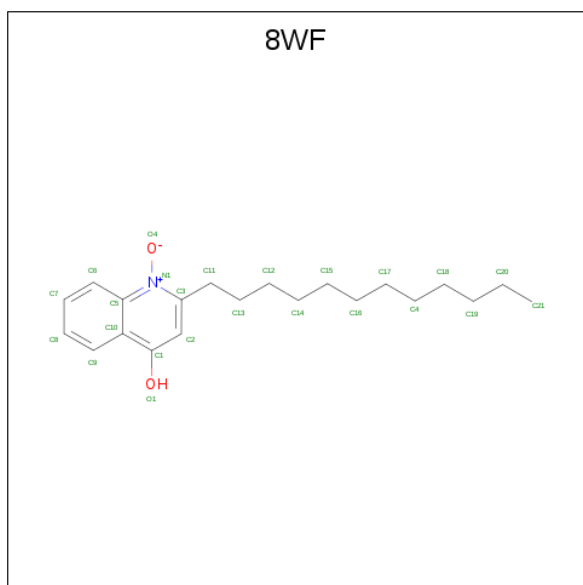
Continued from previous page...

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

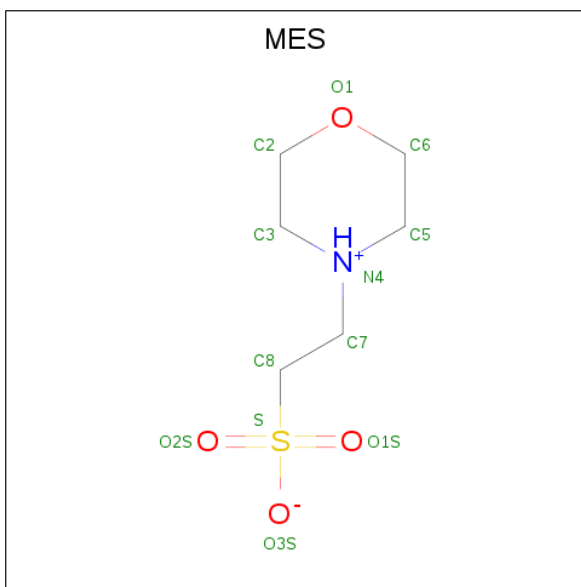
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Mg	0	0
			4	4		
4	A	4	Total	Mg	0	0
			4	4		

- Molecule 5 is 2-dodecyl-1-oxidanidyl-quinolin-1-ium-4-ol (three-letter code: 8WF) (formula: C₂₁H₃₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	16	1	2		
5	B	1	Total	C	N	O	0	0
			19	16	1	2		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).

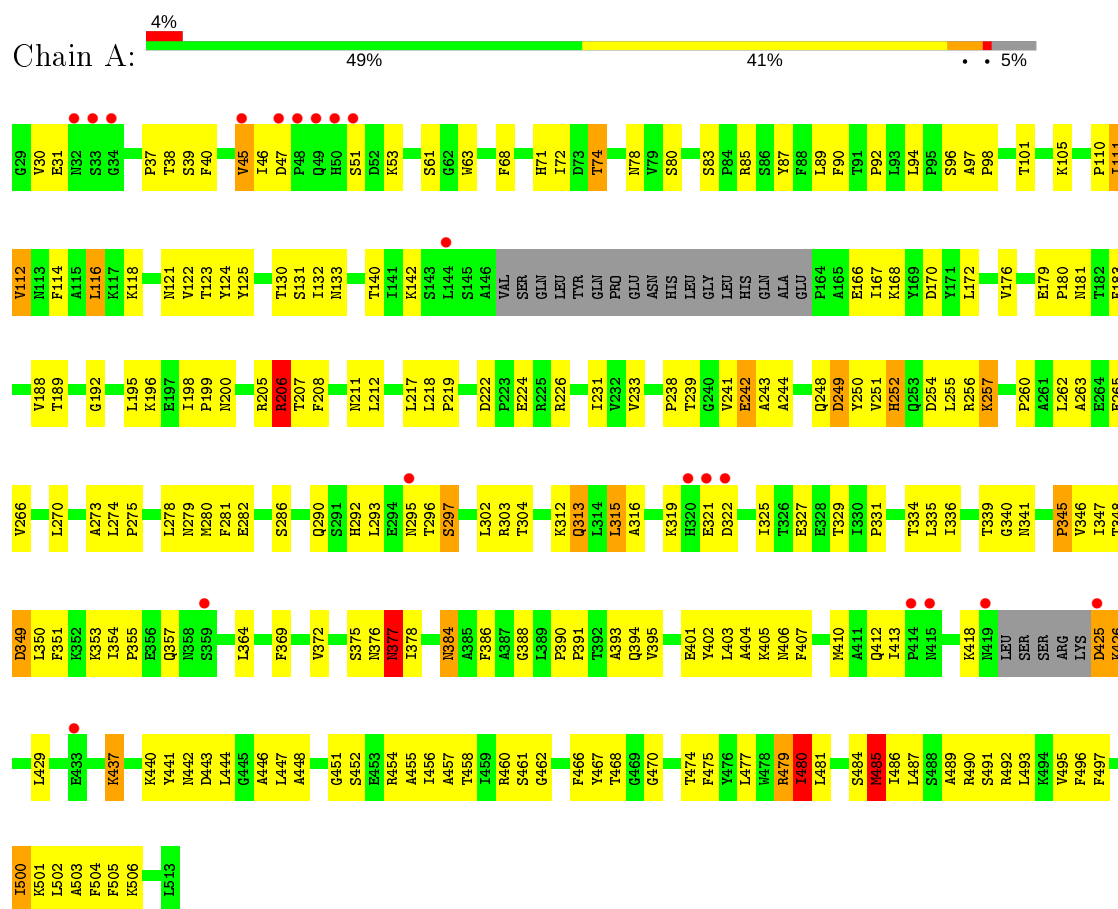


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

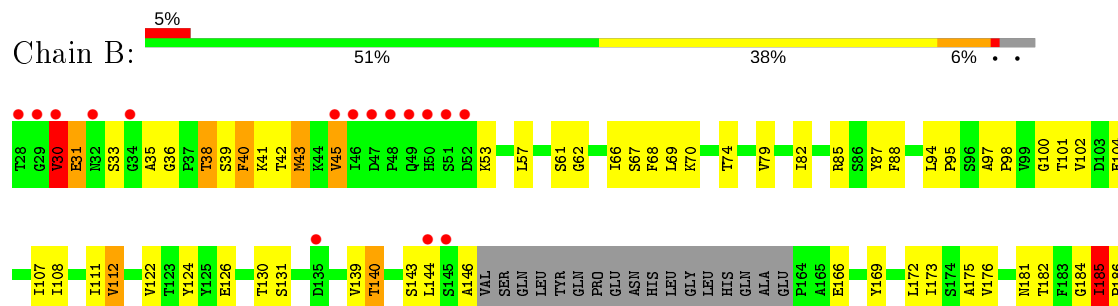
3 Residue-property plots [i](#)

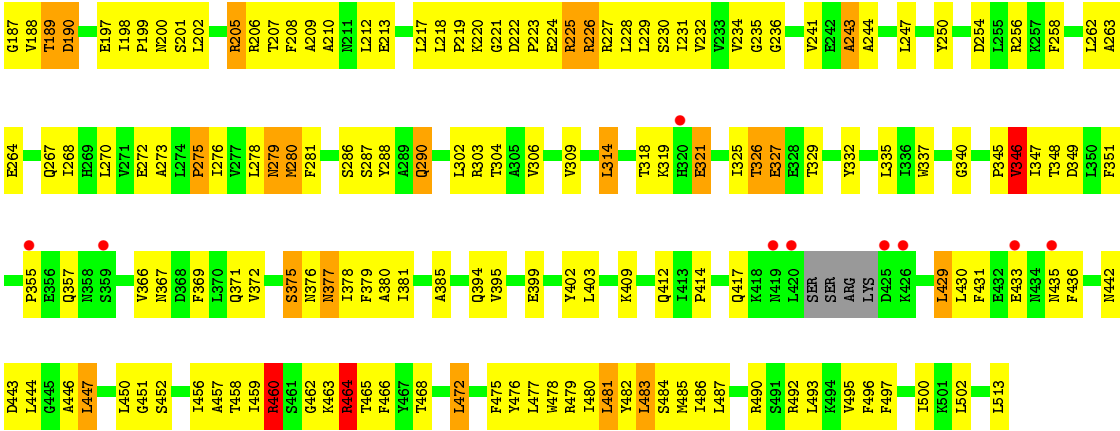
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial



- Molecule 2: Rotenone-insensitive NADH-ubiquinone oxidoreductase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.85Å 115.80Å 166.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 19.95 – 3.40	Depositor EDS
% Data completeness (in resolution range)	82.1 (20.00-3.40) 82.3 (19.95-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 3.44Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.207 , 0.299 0.215 , 0.301	Depositor DCC
R_{free} test set	802 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8985e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 8WF, MG, MES, 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	0.60	0/3733	0.78	1/5046 (0.0%)
2	B	0.64	0/3766	0.83	5/5093 (0.1%)
All	All	0.62	0/7499	0.81	6/10139 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	185	ILE	C-N-CD	-13.96	89.88	120.60
2	B	460	ARG	CB-CA-C	-6.92	96.56	110.40
2	B	205	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	485	MET	N-CA-CB	5.42	120.35	110.60
2	B	464	ARG	N-CA-C	-5.21	96.94	111.00
2	B	205	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	426	LYS	Peptide

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	3652	0	3710	160	0
2	B	3684	0	3749	214	0
3	A	53	0	31	12	0
3	B	53	0	31	7	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	19	0	0	0	0
5	B	19	0	0	4	0
6	A	12	0	13	3	0
6	B	12	0	13	0	0
All	All	7512	0	7547	373	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ARG:HD3	2:B:460:ARG:O	1.20	1.30
2:B:460:ARG:CD	2:B:460:ARG:O	1.84	1.26
2:B:217:LEU:O	2:B:218:LEU:HD23	1.46	1.15
2:B:447:LEU:HD23	2:B:478:TRP:HD1	1.13	1.13
2:B:218:LEU:HD12	2:B:225:ARG:CB	1.84	1.07
2:B:462:GLY:O	2:B:463:LYS:HB2	1.46	1.06
2:B:218:LEU:HD12	2:B:225:ARG:HB2	1.41	1.03
2:B:460:ARG:HB3	2:B:465:THR:HG23	1.40	1.02
2:B:40:PHE:C	2:B:40:PHE:CD1	2.30	1.01
2:B:39:SER:HA	2:B:124:TYR:O	1.61	1.00
2:B:447:LEU:HD23	2:B:478:TRP:CD1	1.98	0.98
2:B:40:PHE:C	2:B:40:PHE:HD1	1.66	0.97
2:B:222:ASP:OD1	2:B:223:PRO:HD2	1.68	0.92
1:A:166:GLU:O	1:A:167:ILE:HD12	1.70	0.92
2:B:447:LEU:CD2	2:B:478:TRP:CD1	2.52	0.91
2:B:447:LEU:CD2	2:B:478:TRP:HD1	1.84	0.91
2:B:464:ARG:NH1	2:B:465:THR:O	2.06	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:PHE:O	2:B:40:PHE:CD1	2.30	0.85
2:B:477:LEU:HD11	2:B:481:LEU:HD22	1.58	0.84
2:B:184:GLY:O	2:B:186:PRO:HD3	1.77	0.83
2:B:460:ARG:C	2:B:460:ARG:HD3	1.98	0.83
2:B:222:ASP:OD1	2:B:223:PRO:CD	2.30	0.80
1:A:87:TYR:HA	1:A:110:PRO:HA	1.62	0.80
2:B:224:GLU:O	2:B:225:ARG:C	2.20	0.79
2:B:235:GLY:O	2:B:270:LEU:HD11	1.83	0.79
2:B:41:LYS:HZ3	2:B:43:MET:HA	1.50	0.76
2:B:102:VAL:HG11	2:B:107:ILE:CG2	2.16	0.76
2:B:217:LEU:O	2:B:218:LEU:CD2	2.30	0.75
1:A:94:LEU:HB3	3:A:601:FAD:HM72	1.68	0.74
2:B:493:LEU:HD11	2:B:497:PHE:CZ	2.22	0.74
1:A:251:VAL:HG21	1:A:266:VAL:HG11	1.70	0.73
2:B:41:LYS:NZ	2:B:43:MET:HA	2.03	0.73
2:B:290:GLN:OE1	2:B:302:LEU:HD11	1.89	0.72
2:B:459:ILE:HG22	2:B:459:ILE:O	1.89	0.72
2:B:429[A]:LEU:CD2	2:B:429[A]:LEU:N	2.51	0.72
2:B:140:THR:HG23	2:B:166:GLU:HG2	1.71	0.72
2:B:218:LEU:HB3	2:B:219:PRO:HD2	1.71	0.72
2:B:224:GLU:O	2:B:227:ARG:N	2.23	0.71
2:B:276:ILE:HD12	2:B:286:SER:HB3	1.72	0.71
2:B:460:ARG:HB3	2:B:465:THR:CG2	2.19	0.71
2:B:460:ARG:HD2	2:B:460:ARG:O	1.87	0.71
2:B:460:ARG:CB	2:B:465:THR:HA	2.22	0.70
2:B:462:GLY:O	2:B:463:LYS:CB	2.30	0.69
2:B:40:PHE:HD1	2:B:41:LYS:N	1.91	0.68
2:B:218:LEU:HD12	2:B:225:ARG:CA	2.24	0.68
1:A:85:ARG:HD2	1:A:87:TYR:CE2	2.28	0.68
2:B:221:GLY:O	2:B:222:ASP:C	2.30	0.67
2:B:275:PRO:O	2:B:302:LEU:HD13	1.94	0.66
1:A:446:ALA:C	1:A:447:LEU:HD23	2.16	0.66
1:A:83:SER:OG	3:A:601:FAD:H1B	1.95	0.66
2:B:326:THR:OG1	2:B:327:GLU:N	2.28	0.66
2:B:187:GLY:O	2:B:190:ASP:N	2.30	0.65
1:A:407:PHE:HA	1:A:410:MET:SD	2.36	0.65
1:A:292:HIS:HA	1:A:295:ASN:HD22	1.62	0.64
2:B:447:LEU:HD22	2:B:478:TRP:CD1	2.31	0.64
2:B:460:ARG:HH11	2:B:460:ARG:CG	2.10	0.64
1:A:390:PRO:O	1:A:395:VAL:HG21	1.98	0.64
2:B:222:ASP:OD1	2:B:224:GLU:N	2.30	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:HD11	1:A:497:PHE:CZ	2.33	0.63
1:A:481:LEU:O	1:A:484:SER:HB2	1.98	0.62
2:B:185:ILE:CG2	2:B:186:PRO:N	2.62	0.62
1:A:222:ASP:OD1	1:A:224:GLU:N	2.32	0.62
1:A:256:ARG:O	1:A:257:LYS:O	2.17	0.62
2:B:87:TYR:CD2	2:B:108:ILE:HG22	2.35	0.62
1:A:443:ASP:OD1	1:A:444:LEU:N	2.33	0.62
2:B:218:LEU:CD1	2:B:225:ARG:CB	2.69	0.62
2:B:205:ARG:NH2	2:B:513:LEU:OXT	2.31	0.61
1:A:377:ASN:N	1:A:377:ASN:HD22	1.98	0.61
2:B:429[A]:LEU:HD23	2:B:429[A]:LEU:N	2.15	0.61
2:B:102:VAL:HG11	2:B:107:ILE:HG23	1.83	0.61
2:B:182:THR:O	2:B:185:ILE:HD12	2.00	0.61
1:A:313:GLN:HB3	1:A:331:PRO:HA	1.83	0.61
1:A:442:ASN:HD21	1:A:462:GLY:H	1.49	0.61
2:B:41:LYS:HZ3	2:B:43:MET:CA	2.14	0.61
2:B:460:ARG:HB3	2:B:465:THR:HA	1.83	0.60
2:B:460:ARG:NH1	2:B:460:ARG:HG2	2.16	0.60
2:B:478:TRP:CZ2	2:B:482:TYR:CE2	2.90	0.60
1:A:486:ILE:HG22	1:A:487:LEU:N	2.16	0.60
2:B:447:LEU:HG	2:B:457:ALA:HB1	1.83	0.60
2:B:208:PHE:CE2	2:B:212:LEU:HD11	2.38	0.59
1:A:83:SER:HG	3:A:601:FAD:H1B	1.65	0.59
2:B:493:LEU:HD11	2:B:497:PHE:CE2	2.38	0.59
1:A:290:GLN:NE2	1:A:302:LEU:HD11	2.18	0.58
1:A:345:PRO:O	1:A:349:ASP:N	2.32	0.58
2:B:481:LEU:O	2:B:484:SER:HB2	2.02	0.58
2:B:176:VAL:C	3:B:601:FAD:H52A	2.24	0.58
1:A:40:PHE:CE2	1:A:124:TYR:HB3	2.38	0.58
2:B:236:GLY:O	2:B:241:VAL:HG23	2.03	0.58
1:A:281:PHE:CZ	1:A:446:ALA:O	2.57	0.58
1:A:278:LEU:HA	1:A:280:MET:SD	2.44	0.58
1:A:275:PRO:O	1:A:302:LEU:HD13	2.03	0.58
2:B:185:ILE:HG22	2:B:186:PRO:N	2.18	0.58
2:B:139:VAL:HG21	2:B:172:LEU:HD11	1.86	0.57
2:B:232:VAL:HG11	2:B:314:LEU:HD21	1.84	0.57
1:A:172:LEU:HD23	1:A:378:ILE:HG23	1.86	0.57
2:B:243:ALA:O	2:B:244:ALA:C	2.43	0.57
1:A:348:THR:HA	1:A:351:PHE:CD2	2.41	0.56
2:B:61:SER:CB	2:B:111:ILE:HD11	2.35	0.56
1:A:341[B]:ASN:N	1:A:341[B]:ASN:OD1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:HA	1:A:124:TYR:O	2.05	0.56
2:B:222:ASP:C	2:B:222:ASP:OD1	2.44	0.56
1:A:71:HIS:O	1:A:404:ALA:HB1	2.06	0.56
1:A:477:LEU:HD11	1:A:481:LEU:HD22	1.89	0.55
1:A:496:PHE:CZ	1:A:500:ILE:HD11	2.41	0.55
2:B:476:TYR:O	2:B:480:ILE:HG12	2.07	0.55
1:A:375:SER:OG	1:A:378:ILE:HD12	2.07	0.55
2:B:40:PHE:HD1	2:B:41:LYS:CA	2.20	0.55
1:A:437:LYS:HD3	1:A:437:LYS:N	2.22	0.55
2:B:41:LYS:HG2	2:B:42:THR:N	2.22	0.55
2:B:479:ARG:O	2:B:483:LEU:HD12	2.07	0.55
1:A:281:PHE:CD2	1:A:456:ILE:HD12	2.42	0.55
1:A:296:THR:O	1:A:297[A]:SER:OG	2.18	0.55
2:B:281:PHE:CE2	2:B:456:ILE:CD1	2.90	0.55
2:B:222:ASP:OD1	2:B:223:PRO:N	2.40	0.54
2:B:429[A]:LEU:HD23	2:B:429[A]:LEU:H	1.73	0.54
1:A:273:ALA:O	1:A:303[A]:ARG:HA	2.07	0.54
2:B:61:SER:HB3	2:B:111:ILE:HD11	1.90	0.54
2:B:230:SER:HB3	2:B:332:TYR:HA	1.89	0.54
1:A:412:GLN:O	1:A:413:ILE:HG13	2.07	0.54
1:A:105:LYS:O	1:A:490:ARG:NH2	2.40	0.54
2:B:94:LEU:HB3	3:B:601:FAD:HM72	1.89	0.54
1:A:74:THR:HG21	1:A:118:LYS:HB3	1.89	0.54
2:B:483:LEU:HA	2:B:486:ILE:HD12	1.89	0.54
2:B:250:TYR:O	2:B:254:ASP:N	2.32	0.54
2:B:466:PHE:CD1	2:B:466:PHE:N	2.73	0.54
2:B:451:GLY:O	2:B:452:SER:C	2.46	0.54
2:B:35:ALA:HA	2:B:146:ALA:HA	1.90	0.53
2:B:496:PHE:CE2	2:B:500:ILE:HD11	2.43	0.53
2:B:367:ASN:OD1	2:B:367:ASN:C	2.47	0.53
1:A:196:LYS:H	1:A:200:ASN:HD22	1.56	0.53
1:A:442:ASN:ND2	1:A:462:GLY:H	2.05	0.53
1:A:491:SER:O	1:A:495:VAL:HG23	2.09	0.53
2:B:472:LEU:HD23	2:B:472:LEU:C	2.29	0.53
2:B:380:ALA:HB1	2:B:385:ALA:HB2	1.91	0.53
1:A:211:ASN:O	1:A:212:LEU:C	2.46	0.53
2:B:223:PRO:HG2	2:B:224:GLU:N	2.23	0.53
2:B:140:THR:HG23	2:B:166:GLU:CG	2.39	0.52
2:B:367:ASN:OD1	2:B:369:PHE:N	2.42	0.52
1:A:350:LEU:HD23	1:A:364:LEU:HD21	1.91	0.52
1:A:426:LYS:HB3	1:A:429:LEU:HD22	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ARG:CB	2:B:465:THR:HG23	2.27	0.52
1:A:486:ILE:CG2	1:A:487:LEU:N	2.73	0.52
1:A:181:ASN:HB3	1:A:183:PHE:CE2	2.44	0.52
1:A:493:LEU:HD11	1:A:497:PHE:CE2	2.45	0.52
2:B:100:GLY:HA2	2:B:102:VAL:O	2.10	0.52
2:B:278:LEU:O	2:B:279:ASN:C	2.47	0.52
2:B:185:ILE:HD13	2:B:337:TRP:HH2	1.75	0.52
1:A:218:LEU:HB3	1:A:219:PRO:HD2	1.92	0.51
1:A:357:GLN:HE21	1:A:372:VAL:HG13	1.74	0.51
1:A:217:LEU:C	1:A:218:LEU:HD23	2.30	0.51
1:A:502:LEU:HA	1:A:505:PHE:O	2.11	0.51
1:A:132:ILE:CD1	1:A:350:LEU:HD22	2.41	0.51
1:A:350:LEU:HD23	1:A:364:LEU:HD11	1.92	0.51
1:A:467:TYR:CD2	1:A:468:THR:N	2.79	0.51
2:B:262:LEU:O	2:B:263:ALA:C	2.49	0.51
1:A:296:THR:O	1:A:297[A]:SER:CB	2.59	0.51
2:B:287:SER:O	2:B:290:GLN:N	2.43	0.51
1:A:394:GLN:HE22	1:A:444:LEU:H	1.58	0.51
2:B:477:LEU:O	2:B:480:ILE:N	2.44	0.51
2:B:287:SER:O	2:B:288:TYR:C	2.48	0.50
2:B:35:ALA:HB1	2:B:143:SER:HB3	1.94	0.50
2:B:460:ARG:HG2	2:B:460:ARG:HH11	1.75	0.50
1:A:496:PHE:CE2	1:A:500:ILE:HD11	2.46	0.50
2:B:199:PRO:O	2:B:200:ASN:C	2.48	0.50
2:B:95:PRO:HD3	3:B:601:FAD:HM72	1.92	0.50
2:B:218:LEU:HB3	2:B:219:PRO:CD	2.41	0.50
2:B:85:ARG:HD2	2:B:87:TYR:CE2	2.47	0.50
1:A:394:GLN:NE2	1:A:444:LEU:H	2.09	0.50
2:B:38:THR:O	2:B:39:SER:C	2.47	0.50
2:B:190:ASP:N	2:B:190:ASP:OD2	2.41	0.50
1:A:244:ALA:HB2	1:A:270:LEU:HD13	1.93	0.49
1:A:492:ARG:O	1:A:495:VAL:HB	2.12	0.49
1:A:251:VAL:CG2	1:A:266:VAL:HG11	2.39	0.49
1:A:481:LEU:O	1:A:485:MET:SD	2.71	0.49
2:B:290:GLN:NE2	2:B:302:LEU:HD11	2.27	0.49
2:B:325:ILE:O	2:B:325:ILE:HG22	2.12	0.49
1:A:335:LEU:HD12	1:A:335:LEU:C	2.33	0.49
1:A:97:ALA:N	1:A:98:PRO:CD	2.76	0.49
2:B:429[A]:LEU:N	2:B:429[A]:LEU:HD22	2.25	0.49
2:B:472:LEU:HA	2:B:475:PHE:HB3	1.95	0.49
1:A:455:ALA:O	1:A:474:THR:HB	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:THR:HG23	3:A:601:FAD:HM73	1.94	0.49
2:B:227:ARG:O	2:B:228:LEU:C	2.51	0.49
2:B:460:ARG:HB2	2:B:465:THR:HA	1.95	0.49
1:A:248:GLN:O	1:A:249:ASP:C	2.50	0.49
1:A:437:LYS:CD	1:A:437:LYS:N	2.75	0.49
2:B:276:ILE:HD12	2:B:286:SER:CB	2.42	0.49
2:B:35:ALA:HB1	2:B:143:SER:CB	2.42	0.49
2:B:483:LEU:O	2:B:492:ARG:NH2	2.45	0.48
2:B:176:VAL:O	3:B:601:FAD:C5B	2.61	0.48
2:B:495:VAL:O	2:B:496:PHE:C	2.48	0.48
2:B:198:ILE:O	2:B:201:SER:HB3	2.12	0.48
2:B:62:GLY:HA2	2:B:85:ARG:HH22	1.78	0.48
1:A:458:THR:HG21	1:A:460:ARG:NH2	2.28	0.48
1:A:489:ALA:O	1:A:492:ARG:N	2.47	0.48
1:A:116:LEU:HD21	2:B:258:PHE:HB3	1.96	0.48
1:A:425:ASP:N	1:A:425:ASP:OD1	2.47	0.48
1:A:248:GLN:HG3	1:A:252:HIS:CD2	2.49	0.48
1:A:412:GLN:C	1:A:413:ILE:HG13	2.34	0.48
2:B:290:GLN:CD	2:B:302:LEU:HD11	2.34	0.48
1:A:243:ALA:O	1:A:244:ALA:C	2.51	0.47
2:B:210:ALA:HA	2:B:213:GLU:OE1	2.14	0.47
1:A:208:PHE:CE1	1:A:231:ILE:HD11	2.49	0.47
1:A:212:LEU:HD23	1:A:262:LEU:HD13	1.96	0.47
1:A:176:VAL:N	1:A:384:ASN:OD1	2.48	0.47
2:B:176:VAL:CG2	2:B:347:ILE:HD11	2.44	0.47
2:B:466:PHE:N	2:B:466:PHE:HD1	2.11	0.47
1:A:451:GLY:O	1:A:452:SER:C	2.53	0.47
1:A:198:ILE:N	1:A:199:PRO:HD2	2.29	0.47
2:B:197:GLU:CB	2:B:199:PRO:HD2	2.45	0.47
1:A:262:LEU:O	1:A:265:GLU:N	2.48	0.47
1:A:205:ARG:O	1:A:206:ARG:O	2.32	0.47
2:B:210:ALA:O	2:B:213:GLU:HB2	2.14	0.47
2:B:485:MET:HE1	5:B:606:8WF:C10	2.45	0.47
2:B:61:SER:C	2:B:66:ILE:HD13	2.35	0.47
1:A:248:GLN:C	1:A:250:TYR:N	2.67	0.47
1:A:345:PRO:O	1:A:348:THR:OG1	2.26	0.47
2:B:139:VAL:HG21	2:B:172:LEU:CD1	2.45	0.47
1:A:457:ALA:HB3	1:A:474:THR:CG2	2.45	0.47
1:A:500:ILE:O	1:A:503:ALA:N	2.48	0.47
2:B:41:LYS:HZ3	2:B:43:MET:HG2	1.79	0.47
2:B:201:SER:O	2:B:202:LEU:C	2.54	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ARG:O	2:B:206:ARG:C	2.52	0.46
2:B:447:LEU:HG	2:B:457:ALA:CB	2.46	0.46
2:B:290:GLN:HE22	2:B:302:LEU:HD11	1.79	0.46
2:B:483:LEU:O	2:B:486:ILE:HB	2.14	0.46
2:B:345:PRO:O	2:B:346:VAL:C	2.53	0.46
2:B:430:LEU:HA	2:B:433:GLU:HB2	1.98	0.46
2:B:493:LEU:HD11	2:B:497:PHE:CE1	2.50	0.46
1:A:238:PRO:HG2	6:A:607:MES:O1S	2.16	0.46
1:A:63:TRP:HD1	3:A:601:FAD:O4'	1.98	0.46
1:A:96:SER:O	1:A:101:THR:HB	2.15	0.46
2:B:309:VAL:HG11	2:B:335:LEU:CD2	2.46	0.46
2:B:176:VAL:O	3:B:601:FAD:H52A	2.15	0.46
2:B:197:GLU:HB3	2:B:199:PRO:HD2	1.97	0.46
2:B:272:GLU:O	2:B:304:THR:N	2.39	0.46
2:B:181:ASN:HB3	2:B:340:GLY:HA3	1.98	0.46
2:B:185:ILE:HG22	2:B:188:VAL:HG23	1.98	0.46
1:A:132:ILE:HD12	1:A:350:LEU:HD22	1.98	0.46
2:B:219:PRO:O	2:B:220:LYS:C	2.51	0.46
2:B:61:SER:HB2	2:B:111:ILE:HD11	1.98	0.46
1:A:188:VAL:O	1:A:192:GLY:N	2.46	0.45
1:A:112:VAL:HG22	1:A:116:LEU:HD22	1.98	0.45
1:A:394:GLN:NE2	1:A:441:TYR:OH	2.50	0.45
1:A:238:PRO:O	1:A:239:THR:C	2.55	0.45
2:B:348:THR:HA	2:B:351:PHE:CD2	2.52	0.45
2:B:40:PHE:CE2	2:B:124:TYR:HB3	2.52	0.45
1:A:233:VAL:HB	1:A:270:LEU:HD12	1.96	0.45
2:B:223:PRO:CG	2:B:224:GLU:N	2.80	0.45
2:B:82:ILE:O	3:B:601:FAD:H2A	2.16	0.45
2:B:94:LEU:N	2:B:95:PRO:CD	2.80	0.45
2:B:218:LEU:CD1	2:B:225:ARG:HB3	2.45	0.45
1:A:179:GLU:HB2	1:A:180:PRO:CD	2.47	0.45
2:B:36:GLY:HA2	2:B:126:GLU:O	2.17	0.45
1:A:248:GLN:O	1:A:250:TYR:N	2.49	0.45
1:A:444:LEU:HA	1:A:460:ARG:O	2.16	0.45
2:B:40:PHE:HD1	2:B:41:LYS:HA	1.82	0.45
2:B:394:GLN:HG3	5:B:606:8WF:C3	2.46	0.45
1:A:354:ILE:HG23	1:A:355:PRO:HD2	1.98	0.45
2:B:225:ARG:O	2:B:229:LEU:HG	2.17	0.45
1:A:125:TYR:CE1	1:A:167:ILE:HG12	2.52	0.45
1:A:479:ARG:O	1:A:480:ILE:C	2.55	0.45
1:A:335:LEU:HD12	1:A:336:ILE:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ILE:HG22	1:A:351:PHE:CZ	2.52	0.44
1:A:111:ILE:O	1:A:114:PHE:HB2	2.18	0.44
2:B:198:ILE:N	2:B:199:PRO:CD	2.80	0.44
2:B:223:PRO:HG2	2:B:224:GLU:H	1.81	0.44
2:B:306:VAL:HG13	2:B:314:LEU:HD13	2.00	0.44
1:A:405:LYS:O	1:A:407:PHE:N	2.51	0.44
1:A:319:LYS:HG3	1:A:325:ILE:HG12	1.98	0.44
2:B:273:ALA:O	2:B:303:ARG:HA	2.18	0.44
2:B:184:GLY:O	2:B:185:ILE:C	2.56	0.44
1:A:348:THR:HA	1:A:351:PHE:CE2	2.52	0.44
1:A:40:PHE:C	1:A:40:PHE:CD1	2.90	0.44
2:B:223:PRO:O	2:B:224:GLU:C	2.52	0.44
2:B:478:TRP:CZ2	2:B:482:TYR:HE2	2.34	0.44
2:B:70:LYS:HD2	2:B:487:LEU:HD23	1.99	0.44
1:A:90:PHE:CD2	1:A:92:PRO:HD2	2.52	0.44
2:B:281:PHE:CE2	2:B:456:ILE:HD11	2.52	0.44
1:A:131:SER:OG	1:A:353:LYS:NZ	2.50	0.43
1:A:256:ARG:O	1:A:257:LYS:C	2.57	0.43
1:A:377:ASN:H	1:A:377:ASN:HD22	1.63	0.43
2:B:62:GLY:HA2	2:B:85:ARG:NH2	2.33	0.43
1:A:63:TRP:HB2	3:A:601:FAD:O5'	2.19	0.43
1:A:375:SER:CB	1:A:378:ILE:HD12	2.48	0.43
1:A:443:ASP:C	1:A:444:LEU:HG	2.39	0.43
1:A:68:PHE:CZ	1:A:72:ILE:HD13	2.54	0.43
2:B:459:ILE:CG2	2:B:459:ILE:O	2.60	0.43
1:A:293:LEU:O	1:A:296:THR:OG1	2.24	0.43
2:B:234:VAL:O	2:B:234:VAL:HG12	2.17	0.43
2:B:431:PHE:HA	2:B:436:PHE:CD2	2.54	0.43
1:A:502:LEU:O	1:A:505:PHE:O	2.37	0.43
2:B:375:SER:OG	2:B:378:ILE:HD12	2.18	0.43
2:B:371:GLN:HG2	2:B:379:PHE:CE2	2.54	0.43
2:B:464:ARG:CG	2:B:466:PHE:HE1	2.31	0.43
2:B:485:MET:HE3	5:B:606:8WF:C1	2.49	0.43
1:A:250:TYR:O	1:A:251:VAL:C	2.57	0.43
2:B:367:ASN:HD21	2:B:371:GLN:CD	2.23	0.43
2:B:487:LEU:HD12	2:B:487:LEU:N	2.34	0.43
2:B:97:ALA:HB1	2:B:104:GLU:HG3	2.00	0.43
1:A:170:ASP:O	1:A:377:ASN:HB2	2.19	0.43
1:A:206:ARG:O	1:A:207:THR:C	2.57	0.43
2:B:414:PRO:HA	2:B:417:GLN:HG2	2.00	0.43
1:A:369:PHE:HA	1:A:402:TYR:OH	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.78	0.42
2:B:231:ILE:N	2:B:267:GLN:O	2.47	0.42
2:B:36:GLY:N	2:B:143:SER:CB	2.82	0.42
1:A:37:PRO:O	1:A:39:SER:N	2.52	0.42
2:B:231:ILE:HB	2:B:268:ILE:HG12	2.00	0.42
2:B:275:PRO:HA	2:B:303:ARG:HG3	2.01	0.42
2:B:97:ALA:O	2:B:98:PRO:C	2.58	0.42
2:B:236:GLY:O	2:B:241:VAL:CG2	2.67	0.42
1:A:37:PRO:HB2	2:B:213:GLU:HG2	2.01	0.42
1:A:241:VAL:O	1:A:242:GLU:C	2.58	0.42
2:B:102:VAL:HG11	2:B:107:ILE:HG21	2.00	0.42
2:B:348:THR:HA	2:B:351:PHE:CE2	2.55	0.42
1:A:315:LEU:HD12	1:A:316:ALA:N	2.35	0.42
1:A:45:VAL:HG23	1:A:121:ASN:HD21	1.85	0.42
3:A:601:FAD:HM83	6:A:607:MES:C2	2.50	0.42
2:B:68:PHE:CE2	2:B:173:ILE:HG13	2.55	0.42
2:B:223:PRO:O	2:B:226:ARG:N	2.53	0.42
1:A:85:ARG:HD2	1:A:87:TYR:CZ	2.55	0.42
2:B:222:ASP:CG	2:B:223:PRO:HD2	2.35	0.42
2:B:218:LEU:CD1	2:B:225:ARG:HB2	2.28	0.42
2:B:232:VAL:O	2:B:335:LEU:HD12	2.20	0.42
2:B:458:THR:CG2	2:B:460:ARG:HG3	2.50	0.42
1:A:447:LEU:O	1:A:448:ALA:HB2	2.19	0.41
2:B:130:THR:OG1	2:B:131:SER:N	2.53	0.41
2:B:30:VAL:HG12	2:B:31:GLU:N	2.35	0.41
1:A:372:VAL:HB	1:A:375:SER:HB3	2.03	0.41
2:B:446:ALA:N	2:B:458:THR:O	2.45	0.41
1:A:364:LEU:O	1:A:386:PHE:N	2.52	0.41
1:A:130:THR:HG21	1:A:142:LYS:HB2	2.02	0.41
1:A:377:ASN:ND2	1:A:377:ASN:N	2.68	0.41
1:A:505:PHE:CE2	2:B:490:ARG:HA	2.56	0.41
1:A:281:PHE:CE2	1:A:456:ILE:HG13	2.56	0.41
1:A:83:SER:HA	3:A:601:FAD:N3A	2.36	0.41
2:B:209:ALA:O	2:B:212:LEU:HB2	2.21	0.41
2:B:403:LEU:HA	2:B:403:LEU:HD12	1.94	0.41
1:A:110:PRO:O	1:A:111:ILE:C	2.58	0.41
1:A:61:SER:HG	3:A:601:FAD:HO3A	1.64	0.41
2:B:345:PRO:O	2:B:348:THR:N	2.54	0.41
1:A:447:LEU:HD11	1:A:481:LEU:HD23	2.03	0.41
2:B:57:LEU:HD22	2:B:169:TYR:HB3	2.02	0.41
2:B:187:GLY:O	2:B:188:VAL:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:THR:OG1	2:B:190:ASP:OD2	2.30	0.41
1:A:401:GLU:O	1:A:402:TYR:C	2.58	0.41
1:A:442:ASN:OD1	1:A:444:LEU:HD21	2.21	0.41
2:B:175:ALA:HB2	2:B:381:ILE:CG1	2.50	0.41
1:A:274:LEU:HB3	1:A:275:PRO:CD	2.50	0.41
2:B:185:ILE:HA	2:B:186:PRO:HD2	1.75	0.41
2:B:357:GLN:HE21	2:B:372:VAL:HG13	1.86	0.41
2:B:502:LEU:HD12	2:B:502:LEU:O	2.21	0.41
1:A:273:ALA:HA	1:A:304:THR:O	2.21	0.40
2:B:247:LEU:O	2:B:250:TYR:HB3	2.21	0.40
2:B:395:VAL:CG1	2:B:399:GLU:OE2	2.69	0.40
1:A:226:ARG:HB3	1:A:226:ARG:NH1	2.35	0.40
1:A:254:ASP:O	1:A:255:LEU:C	2.60	0.40
1:A:403:LEU:O	1:A:407:PHE:HB2	2.21	0.40
1:A:443:ASP:OD1	1:A:443:ASP:C	2.60	0.40
1:A:239:THR:OG1	6:A:607:MES:H81	2.20	0.40
1:A:260:PRO:HA	1:A:263:ALA:HB3	2.03	0.40
1:A:447:LEU:HD23	1:A:447:LEU:N	2.35	0.40
1:A:97:ALA:N	1:A:98:PRO:HD2	2.37	0.40
2:B:219:PRO:CG	2:B:219:PRO:O	2.69	0.40
3:B:601:FAD:HN3	5:B:606:8WF:C9	2.33	0.40
1:A:131:SER:O	1:A:140:THR:N	2.48	0.40
1:A:83:SER:HA	3:A:601:FAD:C2A	2.52	0.40
2:B:218:LEU:HB2	2:B:225:ARG:HD2	2.04	0.40
2:B:74:THR:HG22	2:B:79:VAL:HG21	2.03	0.40
1:A:37:PRO:C	1:A:39:SER:N	2.75	0.40
1:A:393:ALA:N	3:A:601:FAD:H2'	2.36	0.40
1:A:63:TRP:HD1	3:A:601:FAD:HO4'	1.69	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	460/485 (95%)	354 (77%)	84 (18%)	22 (5%)	2	15
2	B	463/486 (95%)	369 (80%)	81 (18%)	13 (3%)	5	24
All	All	923/971 (95%)	723 (78%)	165 (18%)	35 (4%)	3	19

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	206	ARG
1	A	257	LYS
1	A	297[A]	SER
1	A	297[B]	SER
1	A	506	LYS
1	A	38	THR
1	A	111	ILE
1	A	252	HIS
1	A	340	GLY
1	A	377	ASN
1	A	406	ASN
2	B	112	VAL
2	B	280	MET
2	B	443	ASP
1	A	391	PRO
2	B	243	ALA
1	A	322	ASP
1	A	466	PHE
1	A	479	ARG
2	B	43	MET
2	B	45	VAL
1	A	249	ASP
2	B	30	VAL
2	B	346	VAL
2	B	207	THR
2	B	321	GLU
2	B	355	PRO
2	B	377	ASN
1	A	45	VAL
1	A	480	ILE
2	B	275	PRO
1	A	388	GLY
1	A	470	GLY
1	A	345	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/412 (95%)	344 (88%)	47 (12%)	5	19
2	B	396/413 (96%)	342 (86%)	54 (14%)	3	14
All	All	787/825 (95%)	686 (87%)	101 (13%)	4	16

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	46	ILE
1	A	47	ASP
1	A	51	SER
1	A	53	LYS
1	A	74	THR
1	A	78	ASN
1	A	80	SER
1	A	89	LEU
1	A	112	VAL
1	A	116	LEU
1	A	122	VAL
1	A	123	THR
1	A	133	ASN
1	A	168	LYS
1	A	189	THR
1	A	195	LEU
1	A	206	ARG
1	A	242	GLU
1	A	279	ASN
1	A	282	GLU
1	A	286	SER
1	A	312	LYS
1	A	313	GLN
1	A	315	LEU
1	A	321	GLU
1	A	327	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	329	THR
1	A	334	THR
1	A	339	THR
1	A	346	VAL
1	A	349	ASP
1	A	376	ASN
1	A	377	ASN
1	A	384	ASN
1	A	418	LYS
1	A	425	ASP
1	A	437	LYS
1	A	440	LYS
1	A	454	ARG
1	A	461	SER
1	A	475	PHE
1	A	480	ILE
1	A	485	MET
1	A	500	ILE
1	A	501	LYS
1	A	504	PHE
2	B	30	VAL
2	B	31	GLU
2	B	33	SER
2	B	38	THR
2	B	40	PHE
2	B	45	VAL
2	B	53	LYS
2	B	67	SER
2	B	69	LEU
2	B	88	PHE
2	B	101	THR
2	B	112	VAL
2	B	122	VAL
2	B	140	THR
2	B	144	LEU
2	B	185	ILE
2	B	189	THR
2	B	190	ASP
2	B	225	ARG
2	B	226	ARG
2	B	256	ARG
2	B	264	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	279	ASN
2	B	280	MET
2	B	290	GLN
2	B	314	LEU
2	B	318	THR
2	B	319	LYS
2	B	321	GLU
2	B	326	THR
2	B	327	GLU
2	B	329	THR
2	B	346	VAL
2	B	349	ASP
2	B	366	VAL
2	B	375	SER
2	B	376	ASN
2	B	377	ASN
2	B	402	TYR
2	B	409	LYS
2	B	412	GLN
2	B	429[A]	LEU
2	B	429[B]	LEU
2	B	435	ASN
2	B	442	ASN
2	B	444	LEU
2	B	447	LEU
2	B	450	LEU
2	B	460	ARG
2	B	464	ARG
2	B	468	THR
2	B	472	LEU
2	B	481	LEU
2	B	483	LEU

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

Mol	Chain	Res	Type
1	A	137	ASN
1	A	193	HIS
1	A	200	ASN
1	A	248	GLN
1	A	279	ASN
1	A	290	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	295	ASN
1	A	320	HIS
1	A	377	ASN
1	A	394	GLN
1	A	415	ASN
1	A	442	ASN
2	B	71	HIS
2	B	133	ASN
2	B	137	ASN
2	B	267	GLN
2	B	376	ASN
2	B	377	ASN
2	B	384	ASN
2	B	442	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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
6	MES	B	607	-	12,12,12	2.24	1 (8%)	14,16,16	1.27	1 (7%)
5	8WF	A	606	-	20,20,25	2.87	4 (20%)	18,26,31	1.30	2 (11%)
6	MES	A	607	-	12,12,12	2.37	1 (8%)	14,16,16	0.96	1 (7%)
3	FAD	B	601	4	51,58,58	2.03	7 (13%)	60,89,89	2.35	17 (28%)
3	FAD	A	601	4	51,58,58	1.67	6 (11%)	60,89,89	2.22	15 (25%)
5	8WF	B	606	-	20,20,25	2.81	4 (20%)	18,26,31	1.16	1 (5%)

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
6	MES	B	607	-	-	1/6/14/14	0/1/1/1
5	8WF	A	606	-	-	3/7/7/12	0/2/2/2
6	MES	A	607	-	-	4/6/14/14	0/1/1/1
3	FAD	B	601	4	-	2/30/50/50	0/6/6/6
3	FAD	A	601	4	-	6/30/50/50	0/6/6/6
5	8WF	B	606	-	-	3/7/7/12	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	FAD	C4X-C10	10.68	1.49	1.38
5	A	606	8WF	O4-N1	-10.60	1.24	1.38
5	B	606	8WF	O4-N1	-10.42	1.24	1.38
3	A	601	FAD	C4X-C10	8.39	1.47	1.38
6	A	607	MES	C8-S	-7.75	1.66	1.77
6	B	607	MES	C8-S	-7.31	1.67	1.77
3	B	601	FAD	C9A-C5X	4.65	1.51	1.42
5	A	606	8WF	C10-C5	4.10	1.49	1.42
5	B	606	8WF	C10-C5	4.06	1.49	1.42
5	A	606	8WF	C1-C10	3.87	1.50	1.42
3	B	601	FAD	C8-C7	3.70	1.50	1.40
5	B	606	8WF	C1-C10	3.62	1.49	1.42
3	A	601	FAD	C4-C4X	3.54	1.47	1.41
3	A	601	FAD	C8-C7	3.11	1.48	1.40
3	A	601	FAD	C9A-C5X	3.08	1.48	1.42
3	B	601	FAD	C4-C4X	3.03	1.46	1.41
5	A	606	8WF	C5-N1	2.87	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	FAD	C9A-N10	2.74	1.42	1.38
3	B	601	FAD	C5A-C4A	2.58	1.47	1.40
3	A	601	FAD	C2A-N3A	2.53	1.36	1.32
3	B	601	FAD	C2A-N3A	2.41	1.36	1.32
3	A	601	FAD	C6-C5X	-2.30	1.38	1.41
5	B	606	8WF	C5-N1	2.28	1.44	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C4-N3-C2	10.61	124.10	115.14
3	A	601	FAD	C4-N3-C2	9.49	123.16	115.14
3	A	601	FAD	C4X-C4-N3	-5.65	115.70	123.43
3	B	601	FAD	C1'-N10-C9A	5.25	122.42	118.29
3	A	601	FAD	C4X-N5-C5X	4.64	121.41	116.77
3	A	601	FAD	C4'-C3'-C2'	-4.38	104.26	113.36
3	B	601	FAD	C4X-C4-N3	-4.34	117.49	123.43
3	B	601	FAD	C9A-N10-C10	-4.28	116.30	121.91
3	B	601	FAD	C4-C4X-C10	-4.13	117.21	119.95
3	B	601	FAD	C4'-C3'-C2'	-3.98	105.08	113.36
3	A	601	FAD	N3A-C2A-N1A	-3.94	122.51	128.68
3	A	601	FAD	C1'-N10-C9A	3.91	121.37	118.29
5	A	606	8WF	O1-C1-C10	3.67	120.90	116.31
3	B	601	FAD	N3A-C2A-N1A	-3.52	123.18	128.68
3	A	601	FAD	C4A-C5A-N7A	-3.52	105.73	109.40
3	B	601	FAD	C5X-C9A-N10	3.36	120.15	117.72
3	B	601	FAD	P-O3P-PA	-3.36	121.30	132.83
5	B	606	8WF	O1-C1-C10	3.33	120.47	116.31
3	B	601	FAD	C1'-N10-C10	3.20	121.28	118.41
3	B	601	FAD	C10-C4X-N5	3.19	123.46	121.26
6	B	607	MES	O1S-S-C8	3.00	110.53	106.92
3	A	601	FAD	C3B-C2B-C1B	-2.90	96.62	100.98
3	A	601	FAD	O3'-C3'-C4'	2.88	115.76	108.81
3	B	601	FAD	C1B-N9A-C4A	-2.84	121.65	126.64
3	A	601	FAD	P-O3P-PA	-2.76	123.36	132.83
3	B	601	FAD	O2P-P-O1P	2.39	124.05	112.24
3	A	601	FAD	C9A-N10-C10	-2.38	118.80	121.91
3	B	601	FAD	O2A-PA-O1A	2.35	123.85	112.24
5	A	606	8WF	C6-C5-C10	-2.34	116.48	119.41
6	A	607	MES	O2S-S-C8	2.34	109.73	106.92
3	A	601	FAD	C1B-N9A-C4A	-2.31	122.59	126.64
3	A	601	FAD	C5'-C4'-C3'	2.23	116.52	112.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	FAD	O2P-P-O1P	2.22	123.20	112.24
3	A	601	FAD	O2B-C2B-C1B	2.18	118.92	110.85
3	B	601	FAD	O4B-C1B-C2B	-2.17	103.76	106.93
3	B	601	FAD	O5B-C5B-C4B	-2.10	101.75	108.99
3	B	601	FAD	C4A-C5A-N7A	-2.06	107.25	109.40

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	607	MES	N4-C7-C8-S
6	A	607	MES	C7-C8-S-O1S
3	A	601	FAD	PA-O3P-P-O5'
6	A	607	MES	C7-C8-S-O3S
5	B	606	8WF	C3-C11-C13-C12
5	A	606	8WF	C14-C15-C16-C17
3	A	601	FAD	O3'-C3'-C4'-C5'
3	A	601	FAD	P-O3P-PA-O1A
5	B	606	8WF	C13-C12-C14-C15
6	A	607	MES	C7-C8-S-O2S
3	A	601	FAD	N10-C1'-C2'-O2'
5	A	606	8WF	C12-C14-C15-C16
3	B	601	FAD	O4B-C4B-C5B-O5B
6	B	607	MES	C8-C7-N4-C5
5	B	606	8WF	C14-C15-C16-C17
3	A	601	FAD	O3'-C3'-C4'-O4'
5	A	606	8WF	C13-C12-C14-C15
3	A	601	FAD	O4B-C4B-C5B-O5B
3	B	601	FAD	C3B-C4B-C5B-O5B

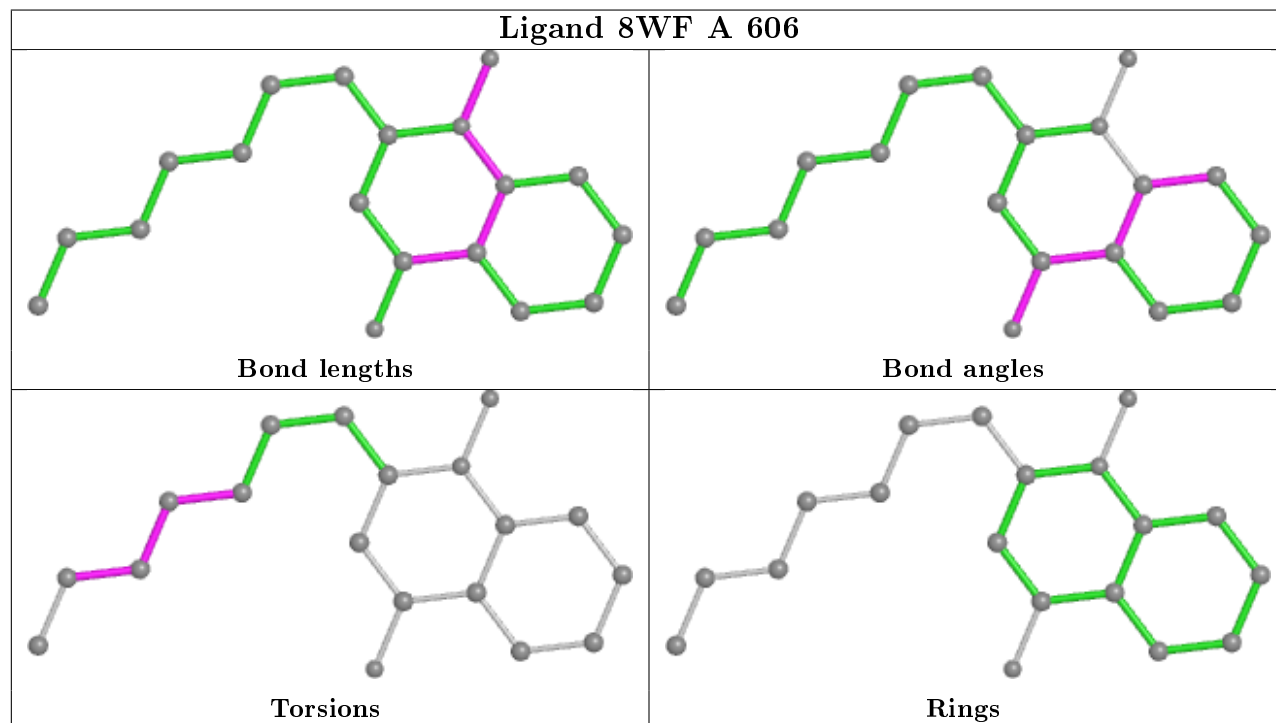
There are no ring outliers.

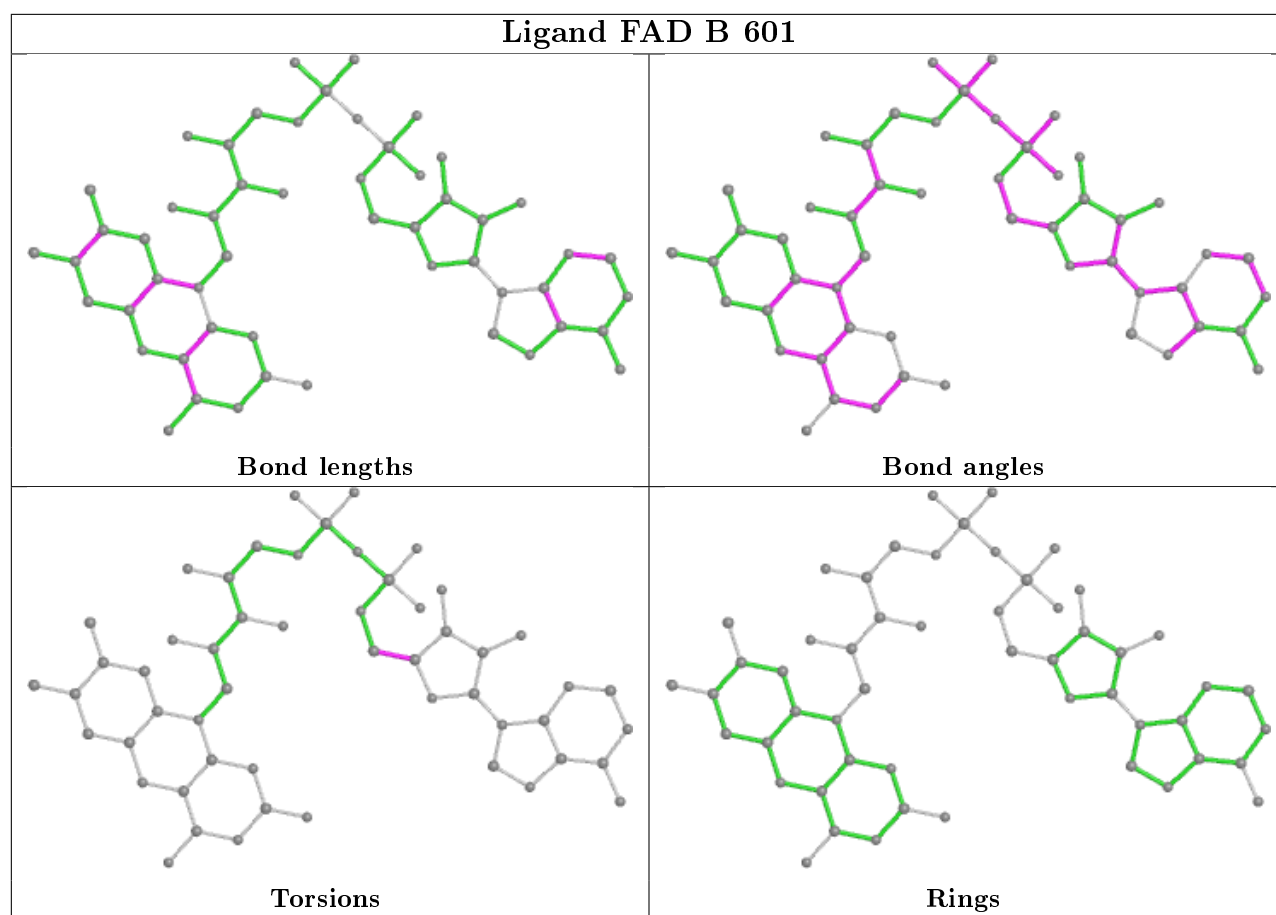
4 monomers are involved in 24 short contacts:

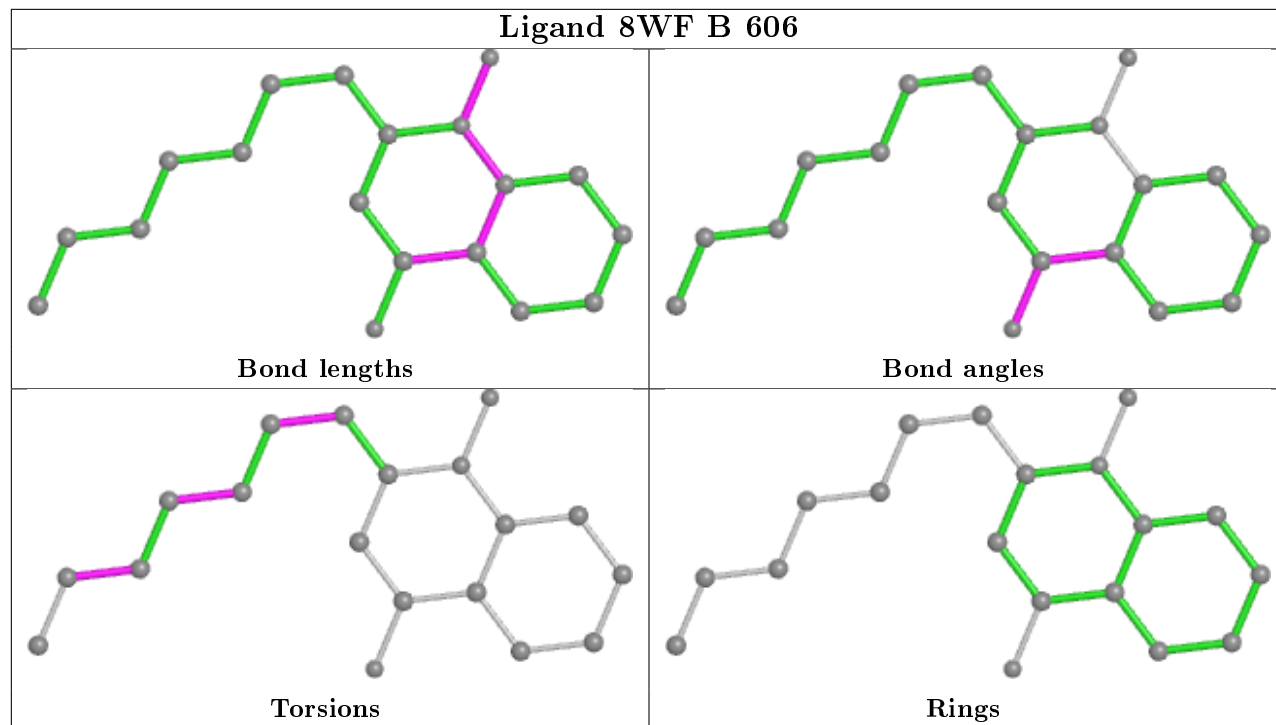
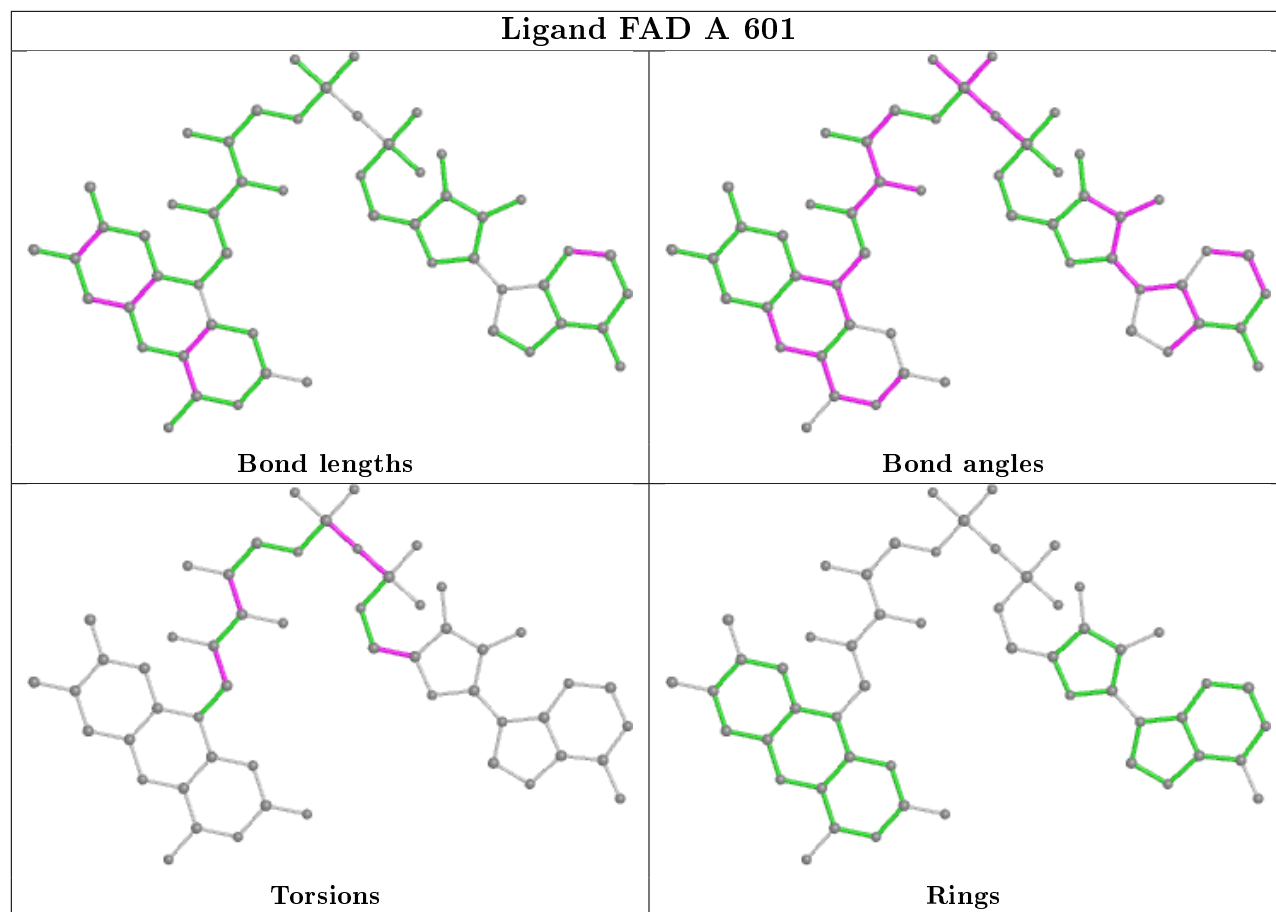
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	607	MES	3	0
3	B	601	FAD	7	0
3	A	601	FAD	12	0
5	B	606	8WF	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	463/485 (95%)	-0.23	20 (4%) 35 35	19, 56, 114, 146	0
2	B	465/486 (95%)	-0.15	25 (5%) 25 26	21, 62, 112, 160	0
All	All	928/971 (95%)	-0.19	45 (4%) 30 31	19, 59, 114, 160	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	46	ILE	8.2
2	B	50	HIS	7.8
1	A	50	HIS	6.0
2	B	29	GLY	5.9
1	A	51	SER	5.3
2	B	30	VAL	5.3
1	A	33	SER	4.6
2	B	47	ASP	4.6
2	B	45	VAL	4.5
2	B	144	LEU	4.5
2	B	359	SER	4.4
2	B	34	GLY	4.3
1	A	34	GLY	4.1
2	B	426	LYS	4.1
2	B	49	GLN	4.0
2	B	425	ASP	4.0
1	A	48	PRO	3.9
2	B	48	PRO	3.9
1	A	414	PRO	3.7
2	B	51	SER	3.7
1	A	47	ASP	3.6
1	A	425	ASP	3.5
1	A	144	LEU	3.2
2	B	145	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	359	SER	3.0
1	A	49	GLN	3.0
1	A	433	GLU	3.0
1	A	419	ASN	2.8
2	B	420	LEU	2.7
1	A	321	GLU	2.7
2	B	435	ASN	2.6
2	B	433	GLU	2.6
2	B	135	ASP	2.6
1	A	32	ASN	2.6
1	A	45	VAL	2.6
1	A	295	ASN	2.5
1	A	415	ASN	2.5
2	B	320	HIS	2.5
1	A	322	ASP	2.4
2	B	28	THR	2.3
2	B	419	ASN	2.2
2	B	355	PRO	2.2
1	A	320	HIS	2.2
2	B	32	ASN	2.1
2	B	52	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.

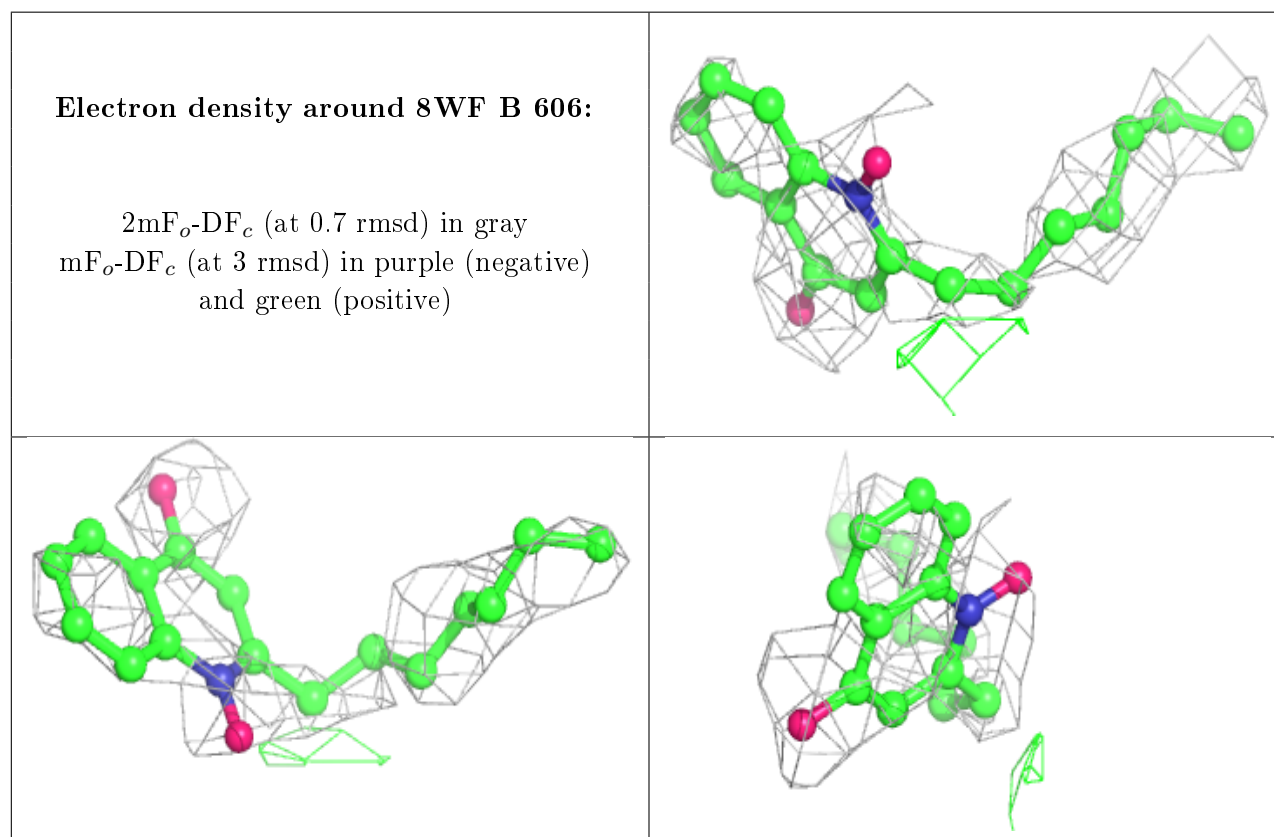
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	8WF	B	606	19/24	0.78	0.34	73,113,129,134	0
5	8WF	A	606	19/24	0.86	0.28	68,87,98,109	0

Continued on next page...

Continued from previous page...

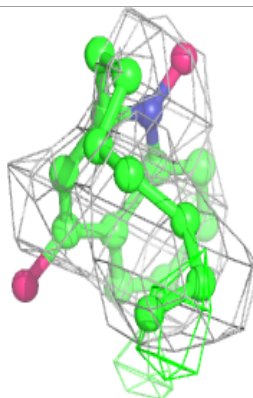
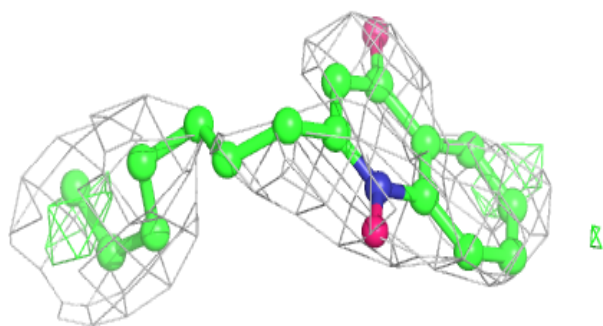
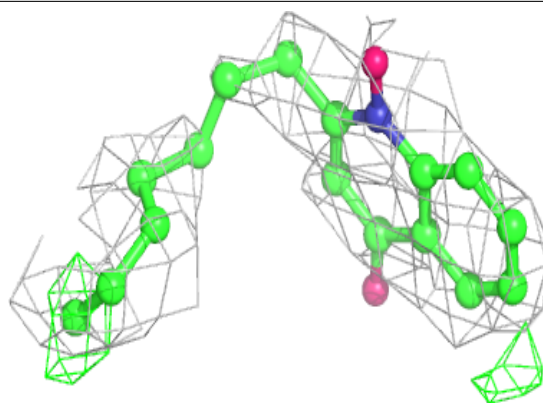
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	A	605	1/1	0.93	0.19	18,18,18,18	0
4	MG	A	602	1/1	0.93	0.44	59,59,59,59	0
6	MES	B	607	12/12	0.94	0.19	76,81,107,108	0
4	MG	B	605	1/1	0.94	0.19	33,33,33,33	0
4	MG	A	604	1/1	0.94	0.19	31,31,31,31	0
6	MES	A	607	12/12	0.95	0.19	68,73,84,85	0
4	MG	B	604	1/1	0.95	0.18	42,42,42,42	0
3	FAD	B	601	53/53	0.97	0.13	25,34,51,57	0
4	MG	B	603	1/1	0.97	0.22	46,46,46,46	0
3	FAD	A	601	53/53	0.98	0.13	19,26,45,50	0
4	MG	B	602	1/1	0.98	0.11	25,25,25,25	0
4	MG	A	603	1/1	0.98	0.18	36,36,36,36	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.

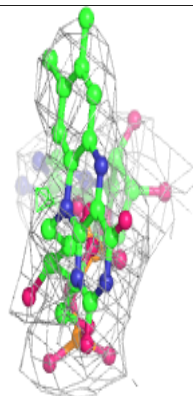
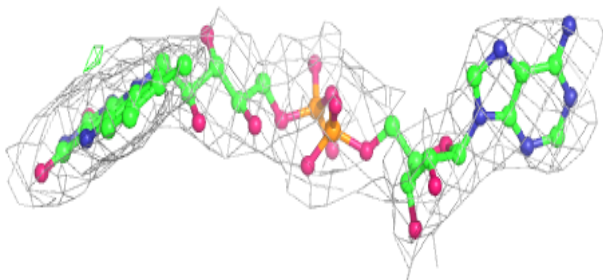
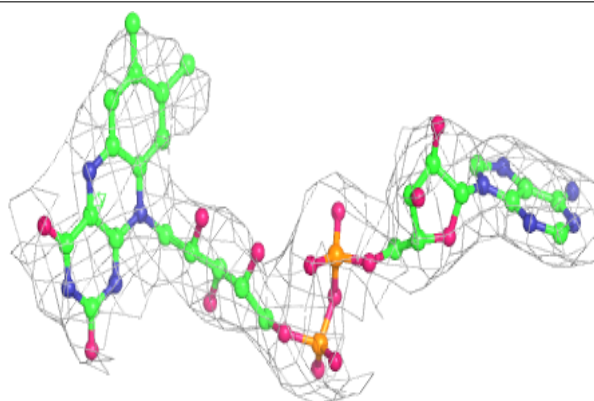


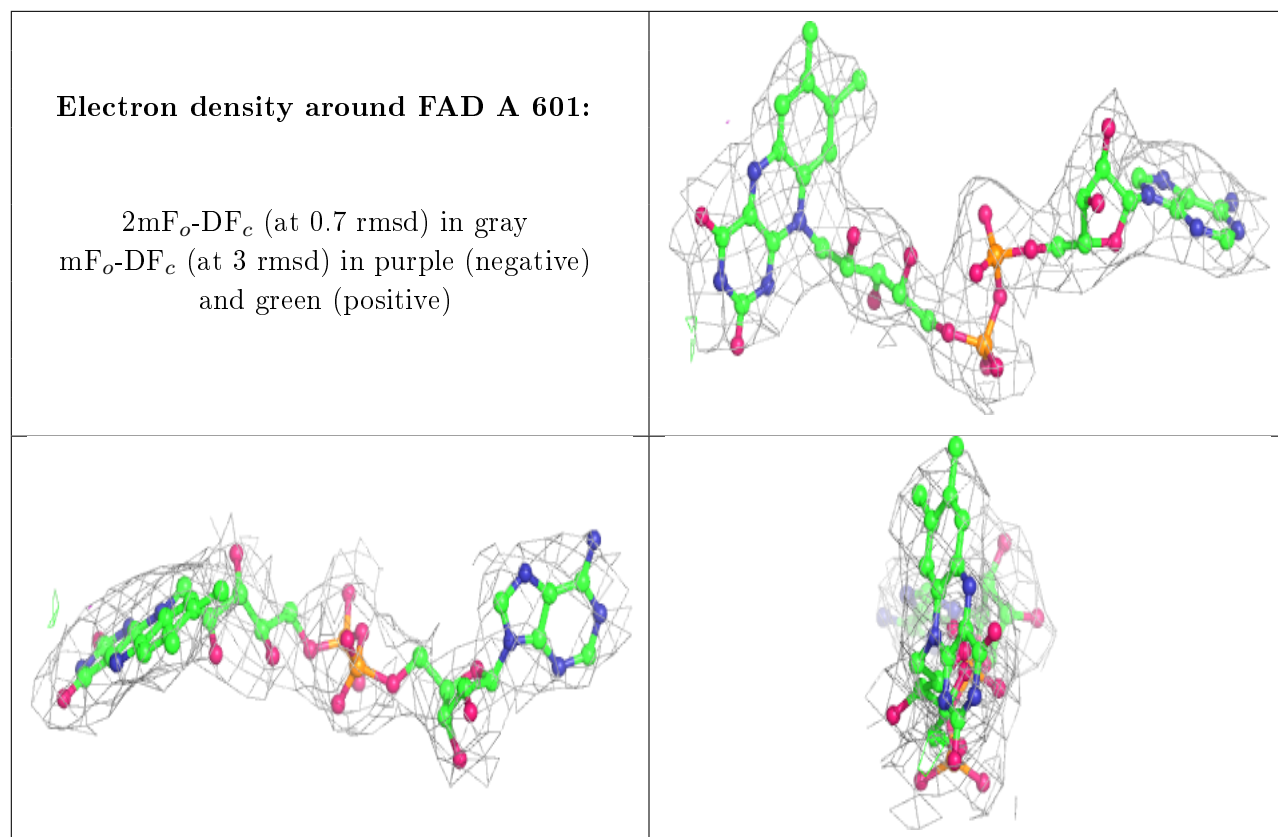
Electron density around 8WF A 606:

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

**Electron density around FAD B 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.