



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:17 pm BST

PDB ID : 3QD9  
Title : C72S/C353S mutant of Trypanosoma brucei QSOX containing an interdomain disulfide  
Authors : Alon, A.; Fass, D.  
Deposited on : 2011-01-18  
Resolution : 3.30 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](mailto: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

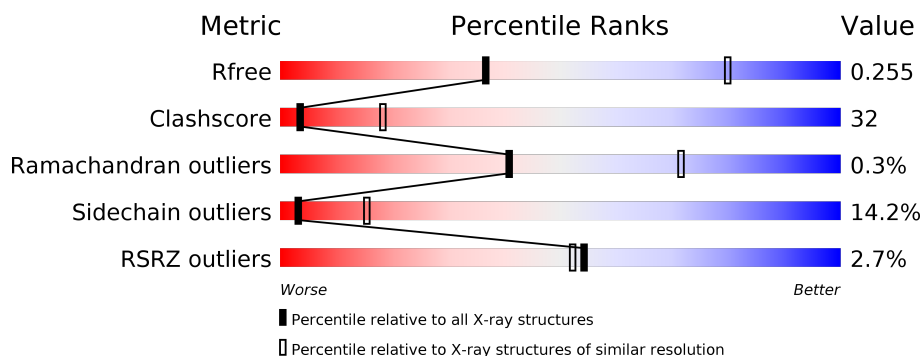
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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  $\geq 3$ , 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	470	<div> <div>2%</div> <div> <div></div> <div>43%</div> <div>33%</div> <div>7%</div> <div>17%</div> </div> </div>
1	B	470	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>34%</div> <div>7%</div> <div>17%</div> </div> </div>
1	C	470	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>33%</div> <div>6%</div> <div>18%</div> </div> </div>
1	D	470	<div> <div>3%</div> <div> <div></div> <div>40%</div> <div>35%</div> <div>7%</div> <div>18%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12535 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 QSOX from Trypanosoma brucei (TbQSOX).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3065	1952	530	569	14			
1	B	390	Total	C	N	O	S	0	0	0
			3102	1974	542	572	14			
1	C	385	Total	C	N	O	S	0	0	0
			3072	1955	537	566	14			
1	D	384	Total	C	N	O	S	0	0	0
			3067	1953	534	566	14			

There are 24 discrepancies between the modelled and reference sequences:

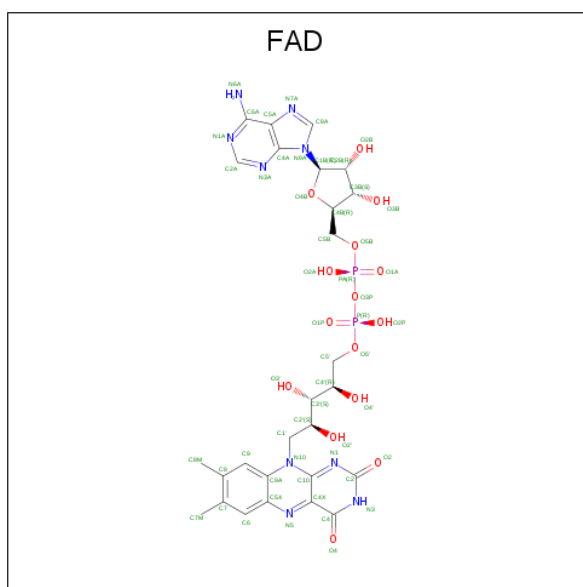
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	EXPRESSION TAG	UNP Q585M6
A	17	SER	-	EXPRESSION TAG	UNP Q585M6
A	18	HIS	-	EXPRESSION TAG	UNP Q585M6
A	19	MET	-	EXPRESSION TAG	UNP Q585M6
A	72	SER	CYS	ENGINEERED MUTATION	UNP Q585M6
A	353	SER	CYS	ENGINEERED MUTATION	UNP Q585M6
B	16	GLY	-	EXPRESSION TAG	UNP Q585M6
B	17	SER	-	EXPRESSION TAG	UNP Q585M6
B	18	HIS	-	EXPRESSION TAG	UNP Q585M6
B	19	MET	-	EXPRESSION TAG	UNP Q585M6
B	72	SER	CYS	ENGINEERED MUTATION	UNP Q585M6
B	353	SER	CYS	ENGINEERED MUTATION	UNP Q585M6
C	16	GLY	-	EXPRESSION TAG	UNP Q585M6
C	17	SER	-	EXPRESSION TAG	UNP Q585M6
C	18	HIS	-	EXPRESSION TAG	UNP Q585M6
C	19	MET	-	EXPRESSION TAG	UNP Q585M6
C	72	SER	CYS	ENGINEERED MUTATION	UNP Q585M6
C	353	SER	CYS	ENGINEERED MUTATION	UNP Q585M6
D	16	GLY	-	EXPRESSION TAG	UNP Q585M6
D	17	SER	-	EXPRESSION TAG	UNP Q585M6
D	18	HIS	-	EXPRESSION TAG	UNP Q585M6

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	19	MET	-	EXPRESSION TAG	UNP Q585M6
D	72	SER	CYS	ENGINEERED MUTATION	UNP Q585M6
D	353	SER	CYS	ENGINEERED MUTATION	UNP Q585M6

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



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

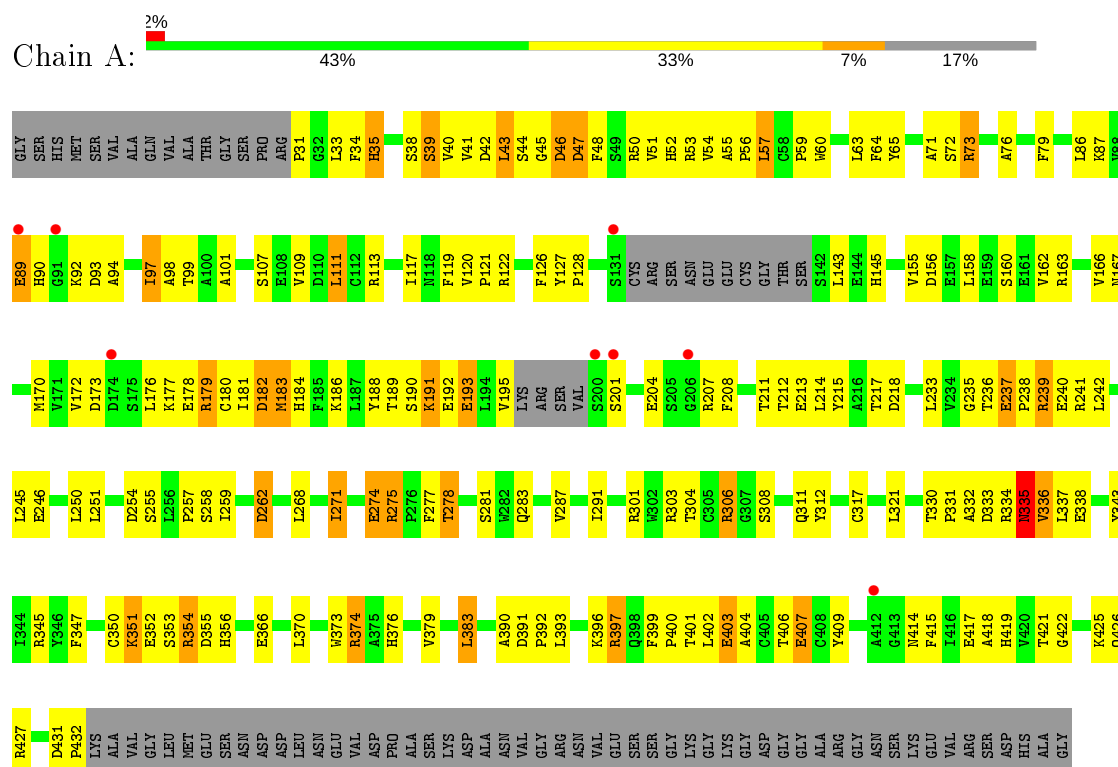
- Molecule 3 is water.

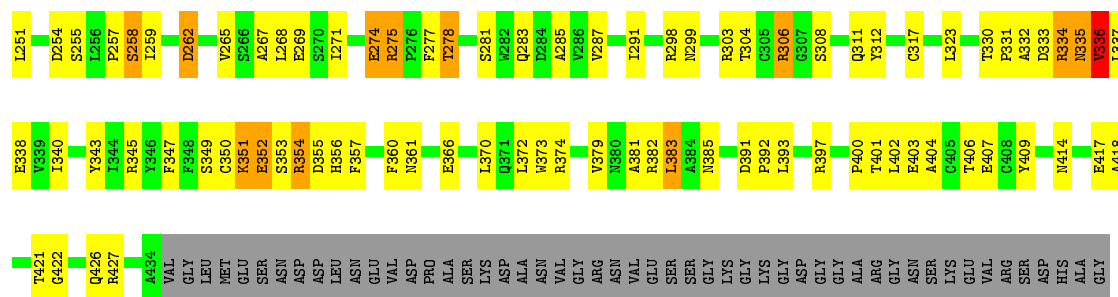
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	7	Total	O	0	0
			7	7		
3	C	5	Total	O	0	0
			5	5		

### 3 Residue-property plots [i](#)

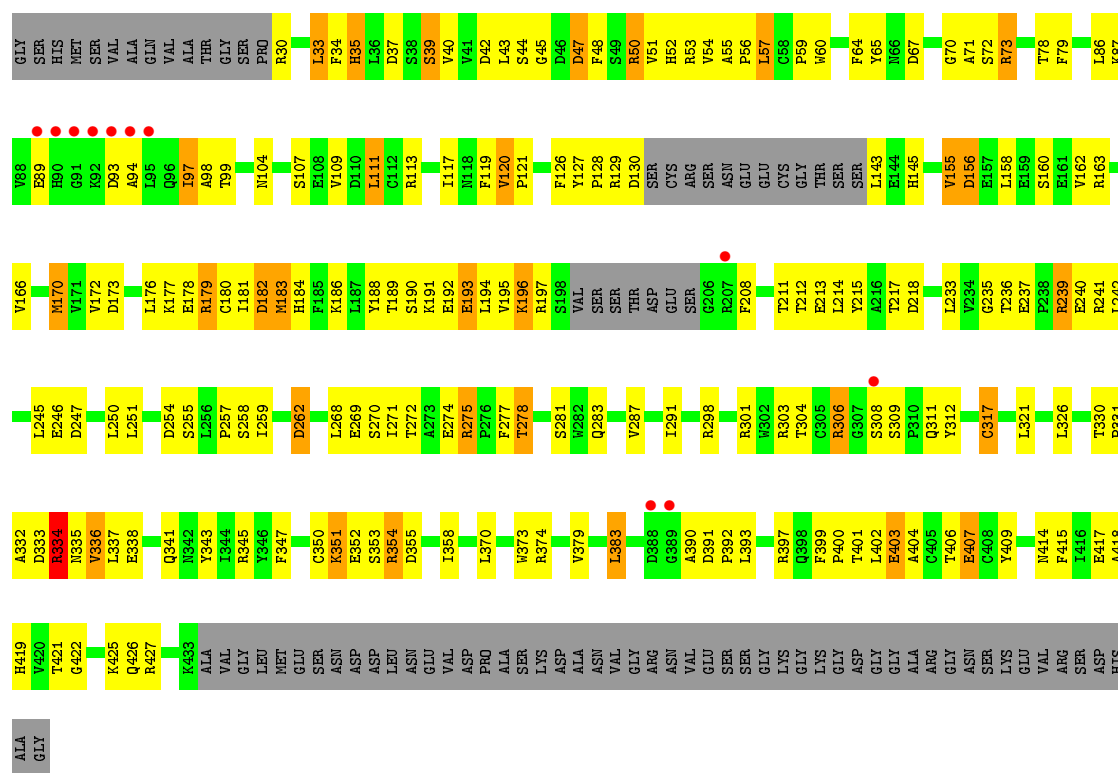
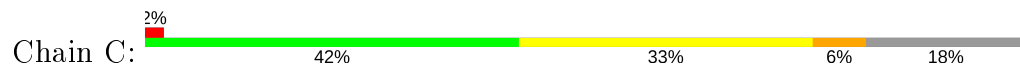
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: QSOX from *Trypanosoma brucei* (TbQSOX)

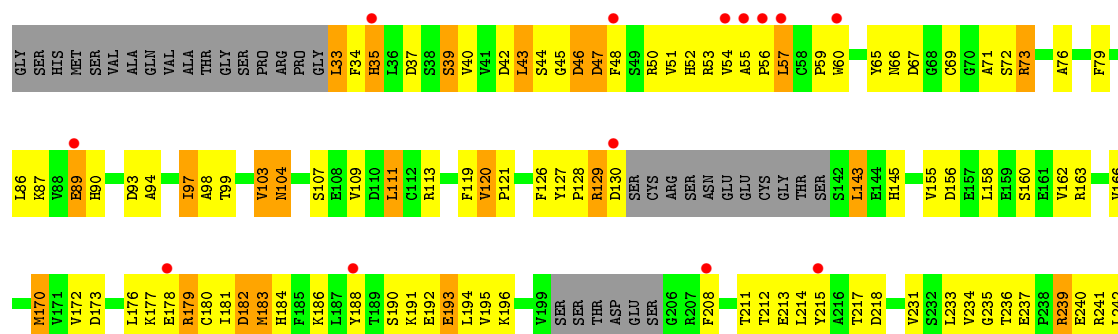
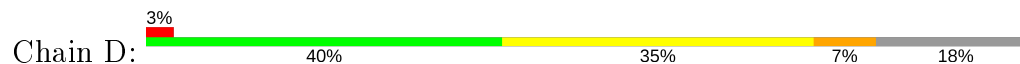


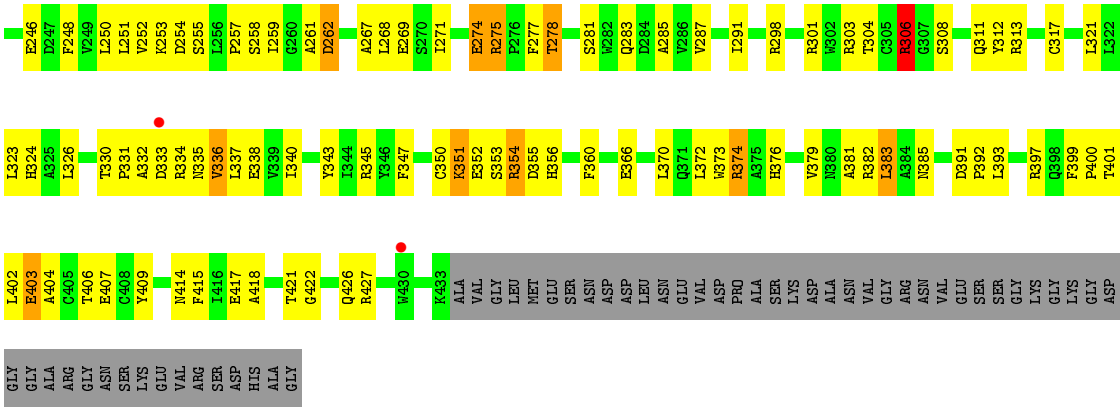


- Molecule 1: QSOX from *Trypanosoma brucei* (TbQSOX)



- Molecule 1: QSOX from *Trypanosoma brucei* (TbQSOX)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.04Å 120.31Å 106.22Å 90.00° 105.44° 90.00°	Depositor
Resolution (Å)	38.11 – 3.30 40.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.11-3.30) 98.5 (40.75-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.17 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_629)	Depositor
R, $R_{free}$	0.190 , 0.249 0.205 , 0.255	Depositor DCC
$R_{free}$ test set	2939 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 89.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	3/3143 (0.1%)	0.96	16/4270 (0.4%)
1	B	0.81	7/3181 (0.2%)	0.91	15/4318 (0.3%)
1	C	0.79	5/3150 (0.2%)	0.89	9/4275 (0.2%)
1	D	0.73	4/3144 (0.1%)	0.90	10/4266 (0.2%)
All	All	0.77	19/12618 (0.2%)	0.91	50/17129 (0.3%)

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	B	0	1
1	D	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	GLU	CD-OE2	11.28	1.38	1.25
1	C	89	GLU	CB-CG	-9.21	1.34	1.52
1	B	274	GLU	CB-CG	-8.15	1.36	1.52
1	B	89	GLU	CB-CG	-7.11	1.38	1.52
1	A	53	ARG	NE-CZ	6.79	1.41	1.33
1	C	274	GLU	CB-CG	-6.70	1.39	1.52
1	D	298	ARG	CZ-NH1	6.59	1.41	1.33
1	C	317	CYS	CB-SG	-6.58	1.71	1.82
1	D	103	VAL	C-O	6.22	1.35	1.23
1	B	193	GLU	CG-CD	6.06	1.61	1.51
1	B	35	HIS	CE1-NE2	5.83	1.46	1.32
1	A	237	GLU	CD-OE2	5.74	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	50	ARG	CZ-NH1	5.63	1.40	1.33
1	A	53	ARG	CZ-NH1	5.44	1.40	1.33
1	B	237	GLU	CD-OE1	5.29	1.31	1.25
1	D	104	ASN	CG-ND2	-5.23	1.19	1.32
1	C	53	ARG	CZ-NH2	5.10	1.39	1.33
1	B	352	GLU	CD-OE1	-5.09	1.20	1.25
1	D	366	GLU	CB-CG	-5.00	1.42	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ILE	CG1-CB-CG2	-19.92	67.57	111.40
1	A	53	ARG	NE-CZ-NH1	12.17	126.39	120.30
1	C	89	GLU	CA-CB-CG	10.36	136.19	113.40
1	A	53	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	D	298	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	D	306	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	92	LYS	CD-CE-NZ	8.88	132.12	111.70
1	D	298	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	C	274	GLU	CA-CB-CG	7.94	130.88	113.40
1	C	50	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	274	GLU	CB-CA-C	-7.93	94.54	110.40
1	D	306	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	C	274	GLU	CB-CA-C	-7.75	94.90	110.40
1	D	104	ASN	CB-CG-OD1	-7.74	106.12	121.60
1	B	193	GLU	OE1-CD-OE2	7.68	132.51	123.30
1	B	334	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	334	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	191	LYS	CD-CE-NZ	7.41	128.74	111.70
1	B	274	GLU	CA-CB-CG	7.27	129.40	113.40
1	B	89	GLU	CA-CB-CG	7.08	128.98	113.40
1	B	50	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	B	50	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	335	ASN	CB-CA-C	-6.69	97.01	110.40
1	A	237	GLU	OE1-CD-OE2	6.49	131.09	123.30
1	A	271	ILE	CB-CA-C	-6.44	98.72	111.60
1	A	335	ASN	N-CA-CB	6.32	121.98	110.60
1	C	334	ARG	CG-CD-NE	-6.29	98.59	111.80
1	C	53	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	A	397	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	C	334	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	383	LEU	CA-CB-CG	-5.94	101.63	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ILE	N-CA-CB	5.92	124.40	110.80
1	D	274	GLU	CA-CB-CG	5.89	126.36	113.40
1	B	89	GLU	CB-CA-C	-5.87	98.65	110.40
1	A	274	GLU	CA-CB-CG	5.81	126.19	113.40
1	C	383	LEU	CA-CB-CG	-5.63	102.36	115.30
1	B	239	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	D	53	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	366	GLU	CB-CG-CD	-5.39	99.65	114.20
1	A	271	ILE	CA-CB-CG1	5.26	121.00	111.00
1	B	334	ARG	CG-CD-NE	-5.24	100.81	111.80
1	B	383	LEU	CA-CB-CG	-5.22	103.29	115.30
1	B	237	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	D	383	LEU	CA-CB-CG	-5.18	103.38	115.30
1	D	89	GLU	N-CA-CB	-5.17	101.30	110.60
1	B	335	ASN	CB-CA-C	-5.16	100.08	110.40
1	B	89	GLU	N-CA-CB	5.14	119.86	110.60
1	A	366	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	A	335	ASN	N-CA-C	5.12	124.81	111.00
1	C	89	GLU	CB-CG-CD	-5.02	100.64	114.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	108	GLU	Mainchain
1	D	104	ASN	Sidechain

## 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	3065	0	2920	198	0
1	B	3102	0	2986	190	2
1	C	3072	0	2957	196	2
1	D	3067	0	2959	205	0
2	A	53	0	31	9	0
2	B	53	0	31	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	2	0
2	D	53	0	31	12	0
3	A	5	0	0	1	0
3	B	7	0	0	3	0
3	C	5	0	0	0	0
All	All	12535	0	11946	778	2

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 32.

All (778) 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:D:376:HIS:CE1	2:D:501:FAD:H52A	1.70	1.25
1:D:376:HIS:HE1	2:D:501:FAD:H52A	1.01	1.06
1:C:193:GLU:OE1	1:C:193:GLU:HA	1.51	1.06
1:A:193:GLU:HA	1:A:193:GLU:OE1	1.52	1.05
1:B:258:SER:HA	3:B:602:HOH:O	1.55	1.04
1:D:193:GLU:HA	1:D:193:GLU:OE1	1.57	1.00
1:C:129:ARG:HG3	1:C:143:LEU:HA	1.43	0.97
1:B:335:ASN:HB3	1:B:338:GLU:HB3	1.47	0.96
1:D:330:THR:HG22	1:D:331:PRO:O	1.65	0.96
1:D:335:ASN:HB3	1:D:338:GLU:HB3	1.47	0.95
1:C:335:ASN:HB3	1:C:338:GLU:HB3	1.47	0.93
1:B:330:THR:HG22	1:B:331:PRO:O	1.66	0.93
1:C:34:PHE:HD2	1:C:40:VAL:HG11	1.32	0.93
1:B:73:ARG:HH11	1:B:73:ARG:CG	1.80	0.92
1:C:330:THR:HG22	1:C:331:PRO:O	1.69	0.91
1:C:275:ARG:HH22	1:C:281:SER:HB2	1.36	0.90
1:A:34:PHE:HD2	1:A:40:VAL:HG11	1.34	0.89
1:A:330:THR:HG22	1:A:331:PRO:O	1.71	0.89
1:B:193:GLU:OE1	1:B:193:GLU:HA	1.69	0.89
1:D:173:ASP:HB2	1:D:176:LEU:HB3	1.54	0.88
1:A:335:ASN:HB2	1:A:338:GLU:HB3	1.56	0.87
1:A:275:ARG:HH22	1:A:281:SER:HB2	1.39	0.86
1:C:30:ARG:N	1:C:298:ARG:NH2	2.24	0.86
1:D:73:ARG:HG2	1:D:73:ARG:HH11	1.39	0.86
1:B:71:ALA:HB2	1:B:352:GLU:OE1	1.76	0.86
1:D:34:PHE:HD2	1:D:40:VAL:HG11	1.39	0.85
1:C:370:LEU:HD13	1:C:421:THR:HB	1.59	0.85
1:B:73:ARG:HH11	1:B:73:ARG:HG2	1.41	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:NH1	1:C:239:ARG:HG2	1.91	0.84
1:B:177:LYS:O	1:B:181:ILE:HG13	1.79	0.82
1:D:71:ALA:HB2	1:D:352:GLU:OE1	1.78	0.82
1:D:71:ALA:CB	1:D:352:GLU:OE1	2.27	0.82
1:C:173:ASP:HB2	1:C:176:LEU:HB3	1.58	0.82
1:B:173:ASP:HB2	1:B:176:LEU:HB3	1.61	0.82
1:C:177:LYS:O	1:C:181:ILE:HG13	1.80	0.82
1:B:370:LEU:HD13	1:B:421:THR:HB	1.60	0.81
1:D:129:ARG:HG2	1:D:129:ARG:HH11	1.45	0.81
1:A:173:ASP:HB2	1:A:176:LEU:HB3	1.61	0.80
1:D:73:ARG:CG	1:D:73:ARG:HH11	1.93	0.80
1:D:370:LEU:HD13	1:D:421:THR:HB	1.63	0.80
1:D:275:ARG:HH22	1:D:281:SER:HB2	1.45	0.79
1:B:170:MET:HA	1:B:170:MET:HE2	1.64	0.79
1:C:129:ARG:CG	1:C:143:LEU:HA	2.11	0.79
1:B:71:ALA:CB	1:B:352:GLU:OE1	2.31	0.79
1:A:370:LEU:HD13	1:A:421:THR:HB	1.64	0.79
1:C:170:MET:HE2	1:C:170:MET:HA	1.63	0.78
1:A:73:ARG:NH2	1:A:311:GLN:O	2.16	0.78
1:D:170:MET:HA	1:D:170:MET:HE2	1.65	0.78
1:C:334:ARG:O	1:C:335:ASN:HB2	1.83	0.78
1:C:73:ARG:HG2	1:C:73:ARG:HH11	1.49	0.78
1:B:275:ARG:HH22	1:B:281:SER:HB2	1.49	0.77
1:D:177:LYS:O	1:D:181:ILE:HG13	1.83	0.77
1:C:239:ARG:HG2	1:C:239:ARG:HH11	1.49	0.77
1:A:177:LYS:O	1:A:181:ILE:HG13	1.84	0.76
1:A:239:ARG:HH11	1:A:239:ARG:HG2	1.50	0.76
1:D:402:LEU:HA	1:D:409:TYR:CE2	2.18	0.76
1:A:193:GLU:CA	1:A:193:GLU:OE1	2.34	0.76
1:A:402:LEU:HA	1:A:409:TYR:CE2	2.21	0.76
1:B:352:GLU:HG2	1:B:353:SER:N	2.01	0.76
1:A:239:ARG:HG2	1:A:239:ARG:NH1	2.02	0.75
1:C:45:GLY:HA3	1:C:50:ARG:NH2	2.01	0.75
1:C:254:ASP:OD1	1:C:334:ARG:NH2	2.18	0.75
1:A:73:ARG:HH11	1:A:73:ARG:CG	1.99	0.75
1:A:352:GLU:HG2	1:A:353:SER:N	2.02	0.74
1:A:73:ARG:HH11	1:A:73:ARG:HG2	1.53	0.74
1:D:354:ARG:C	1:D:354:ARG:HD2	2.08	0.73
1:C:73:ARG:CG	1:C:73:ARG:HH11	2.01	0.73
1:C:402:LEU:HA	1:C:409:TYR:CE2	2.22	0.73
1:D:352:GLU:HG2	1:D:353:SER:N	2.03	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PHE:CD2	1:C:40:VAL:HG11	2.19	0.73
1:C:352:GLU:HG2	1:C:353:SER:N	2.02	0.73
1:C:73:ARG:NH2	1:C:311:GLN:O	2.22	0.72
1:C:215:TYR:CZ	1:C:303:ARG:NH2	2.56	0.72
1:B:34:PHE:HD2	1:B:40:VAL:HG11	1.54	0.72
1:D:45:GLY:HA3	1:D:50:ARG:NH2	2.04	0.72
1:A:34:PHE:CD2	1:A:40:VAL:HG11	2.22	0.72
1:C:143:LEU:HD23	1:C:143:LEU:N	2.05	0.72
1:C:35:HIS:CD2	1:C:35:HIS:O	2.43	0.72
1:D:354:ARG:HD2	1:D:355:ASP:N	2.05	0.72
1:B:354:ARG:HD2	1:B:354:ARG:C	2.10	0.71
1:B:94:ALA:O	1:B:97:ILE:HG23	1.90	0.71
1:B:402:LEU:HA	1:B:409:TYR:CE2	2.25	0.71
1:A:158:LEU:O	1:A:162:VAL:HG23	1.91	0.71
1:D:254:ASP:OD1	1:D:334:ARG:NH2	2.23	0.71
1:C:239:ARG:CG	1:C:239:ARG:HH11	2.04	0.71
1:D:34:PHE:CD2	1:D:40:VAL:HG11	2.26	0.71
1:D:158:LEU:O	1:D:162:VAL:HG23	1.92	0.70
1:D:94:ALA:O	1:D:97:ILE:HG23	1.91	0.70
1:A:128:PRO:HA	1:A:143:LEU:HD22	1.74	0.70
1:D:42:ASP:OD2	1:D:191:LYS:NZ	2.25	0.70
1:D:354:ARG:C	1:D:354:ARG:CD	2.60	0.69
1:D:376:HIS:CE1	2:D:501:FAD:C5B	2.63	0.69
1:A:94:ALA:O	1:A:97:ILE:HG23	1.93	0.69
1:C:94:ALA:O	1:C:97:ILE:HG23	1.92	0.69
1:D:33:LEU:HD22	1:D:34:PHE:HE1	1.58	0.68
1:C:54:VAL:CG1	1:C:57:LEU:HD12	2.23	0.68
1:C:158:LEU:O	1:C:162:VAL:HG23	1.94	0.68
1:B:239:ARG:NH1	1:B:239:ARG:HG2	2.08	0.68
1:A:45:GLY:HA3	1:A:50:ARG:NH2	2.09	0.67
1:C:354:ARG:HD2	1:C:354:ARG:C	2.15	0.67
1:B:183:MET:HG3	1:B:184:HIS:N	2.09	0.67
1:D:120:VAL:CB	1:D:121:PRO:HA	2.25	0.67
1:D:120:VAL:HB	1:D:121:PRO:HA	1.77	0.67
1:D:39:SER:HB3	1:D:87:LYS:HE2	1.76	0.66
1:B:215:TYR:CZ	1:B:303:ARG:NH2	2.63	0.66
1:B:30:ARG:HE	1:B:31:PRO:HD2	1.61	0.66
1:A:418:ALA:CB	1:D:356:HIS:CD2	2.79	0.66
1:A:335:ASN:CB	1:A:338:GLU:HB3	2.25	0.66
1:B:382:ARG:HD2	1:C:418:ALA:O	1.96	0.66
1:B:30:ARG:HG2	1:B:31:PRO:HD2	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PHE:CD2	1:B:40:VAL:HG11	2.30	0.65
1:A:306:ARG:HG3	1:A:306:ARG:NH1	2.11	0.65
1:C:184:HIS:NE2	1:C:188:TYR:CE2	2.65	0.65
1:C:30:ARG:N	1:C:298:ARG:HH21	1.91	0.65
1:D:184:HIS:NE2	1:D:188:TYR:CE2	2.64	0.65
1:A:239:ARG:HH11	1:A:239:ARG:CG	2.10	0.65
1:D:303:ARG:O	1:D:306:ARG:HB3	1.97	0.65
1:B:158:LEU:O	1:B:162:VAL:HG23	1.97	0.65
1:B:30:ARG:CG	1:B:31:PRO:HD2	2.27	0.65
1:B:354:ARG:HD2	1:B:355:ASP:N	2.10	0.65
1:D:306:ARG:NH1	1:D:306:ARG:HG3	2.11	0.65
1:D:33:LEU:HD22	1:D:34:PHE:CE1	2.32	0.65
1:D:73:ARG:CG	1:D:73:ARG:NH1	2.53	0.65
1:B:73:ARG:NH1	1:B:73:ARG:CG	2.48	0.65
1:D:129:ARG:O	1:D:130:ASP:HB2	1.96	0.65
1:A:418:ALA:O	1:D:382:ARG:HD2	1.96	0.65
1:B:354:ARG:C	1:B:354:ARG:CD	2.65	0.64
1:D:334:ARG:O	1:D:335:ASN:HB2	1.96	0.64
1:A:86:LEU:O	1:A:184:HIS:CE1	2.49	0.64
1:D:402:LEU:HA	1:D:409:TYR:HE2	1.61	0.64
1:C:354:ARG:HD2	1:C:355:ASP:N	2.13	0.64
1:C:71:ALA:HB2	1:C:352:GLU:OE1	1.97	0.64
1:D:93:ASP:OD1	1:D:163:ARG:NH1	2.31	0.64
1:C:214:LEU:HA	1:C:304:THR:HG21	1.80	0.64
1:B:184:HIS:NE2	1:B:188:TYR:CE2	2.66	0.64
1:C:275:ARG:HH22	1:C:281:SER:CB	2.11	0.64
1:C:193:GLU:CA	1:C:193:GLU:OE1	2.33	0.63
1:D:392:PRO:HB2	1:D:393:LEU:HD12	1.80	0.63
1:D:208:PHE:CD1	1:D:308:SER:HA	2.34	0.63
1:A:407:GLU:OE2	1:D:374:ARG:HD2	1.99	0.63
1:A:215:TYR:CZ	1:A:303:ARG:NH2	2.67	0.63
1:A:402:LEU:HA	1:A:409:TYR:HE2	1.63	0.63
1:A:254:ASP:OD1	1:A:334:ARG:NH2	2.32	0.63
1:C:34:PHE:N	1:C:34:PHE:CD1	2.67	0.63
1:D:129:ARG:CG	1:D:129:ARG:HH11	2.10	0.62
1:B:119:PHE:CD2	1:B:351:LYS:HB2	2.33	0.62
1:B:120:VAL:HB	1:B:121:PRO:HA	1.81	0.62
1:B:34:PHE:HE2	1:B:79:PHE:HD2	1.47	0.62
1:D:119:PHE:CD2	1:D:351:LYS:HB2	2.34	0.62
1:B:334:ARG:O	1:B:335:ASN:HB2	1.98	0.62
1:C:129:ARG:CZ	1:C:143:LEU:N	2.63	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ARG:HG3	1:C:301:ARG:HH11	1.65	0.62
1:A:214:LEU:HA	1:A:304:THR:HG21	1.80	0.62
1:A:45:GLY:HA3	1:A:50:ARG:HH22	1.65	0.62
1:B:237:GLU:O	1:B:241:ARG:NH1	2.32	0.62
1:B:183:MET:HG3	1:B:184:HIS:H	1.63	0.61
1:D:235:GLY:O	1:D:241:ARG:HD3	1.99	0.61
1:C:54:VAL:HG13	1:C:57:LEU:HD12	1.81	0.61
1:D:212:THR:O	1:D:427:ARG:NH2	2.33	0.61
1:A:184:HIS:NE2	1:A:188:TYR:CE2	2.68	0.61
1:B:239:ARG:HH11	1:B:239:ARG:CG	2.13	0.61
1:A:170:MET:HE2	1:A:170:MET:HA	1.82	0.61
1:A:208:PHE:CD1	1:A:308:SER:HA	2.35	0.61
1:A:354:ARG:C	1:A:354:ARG:HD2	2.20	0.61
1:C:336:VAL:HG23	1:C:337:LEU:H	1.64	0.61
1:A:392:PRO:HB2	1:A:393:LEU:HD12	1.83	0.61
1:C:354:ARG:CD	1:C:354:ARG:C	2.69	0.61
1:D:278:THR:HG23	1:D:281:SER:HB3	1.81	0.61
1:D:45:GLY:HA3	1:D:50:ARG:HH22	1.66	0.61
1:A:301:ARG:HH11	1:A:301:ARG:HG3	1.64	0.61
1:C:33:LEU:C	1:C:34:PHE:HD1	2.04	0.61
1:C:34:PHE:HD1	1:C:34:PHE:N	1.99	0.61
1:B:356:HIS:CD2	1:C:418:ALA:CB	2.84	0.60
1:D:71:ALA:HB3	1:D:352:GLU:OE1	2.02	0.60
1:A:127:TYR:HB2	1:A:128:PRO:HD2	1.83	0.60
1:B:239:ARG:HH11	1:B:239:ARG:HG2	1.64	0.60
1:C:182:ASP:OD1	1:C:183:MET:N	2.35	0.60
2:D:501:FAD:O2A	2:D:501:FAD:O3'	2.14	0.60
1:C:39:SER:HB3	1:C:87:LYS:HE2	1.82	0.60
1:B:127:TYR:HB2	1:B:128:PRO:HD2	1.82	0.60
1:D:370:LEU:HD21	1:D:417:GLU:HB3	1.84	0.60
1:C:251:LEU:HD11	1:C:330:THR:HG23	1.83	0.60
1:C:242:LEU:O	1:C:246:GLU:HG3	2.02	0.60
1:A:183:MET:HG3	1:A:184:HIS:H	1.67	0.60
1:C:127:TYR:HB2	1:C:128:PRO:HD2	1.84	0.59
1:D:239:ARG:NH1	1:D:239:ARG:HG2	2.16	0.59
1:A:251:LEU:HD11	1:A:330:THR:HG23	1.84	0.59
1:B:31:PRO:HG2	1:B:32:GLY:H	1.66	0.59
1:B:34:PHE:HD1	1:B:34:PHE:N	1.99	0.59
1:B:34:PHE:CD1	1:B:34:PHE:N	2.70	0.59
1:B:402:LEU:HA	1:B:409:TYR:HE2	1.66	0.59
1:A:213:GLU:O	1:A:304:THR:CG2	2.51	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:VAL:HG23	1:A:337:LEU:H	1.66	0.59
1:C:213:GLU:O	1:C:304:THR:HG22	2.03	0.59
1:B:86:LEU:O	1:B:184:HIS:CE1	2.55	0.59
1:B:262:ASP:OD1	1:B:262:ASP:N	2.29	0.59
1:B:42:ASP:OD2	1:B:191:LYS:NZ	2.34	0.59
1:D:193:GLU:CA	1:D:193:GLU:OE1	2.40	0.59
1:A:212:THR:O	1:A:427:ARG:NH2	2.35	0.59
1:B:214:LEU:HA	1:B:304:THR:HG21	1.84	0.59
1:D:278:THR:HG23	1:D:281:SER:CB	2.31	0.59
1:B:37:ASP:O	1:B:191:LYS:HE2	2.02	0.59
1:B:254:ASP:OD1	1:B:334:ARG:NH2	2.35	0.58
1:A:354:ARG:HD2	1:A:355:ASP:HA	1.85	0.58
1:D:354:ARG:HD2	1:D:355:ASP:HA	1.84	0.58
1:C:179:ARG:HH11	1:C:179:ARG:HG3	1.69	0.58
1:C:354:ARG:HD2	1:C:355:ASP:HA	1.85	0.58
1:C:179:ARG:HG3	1:C:179:ARG:NH1	2.18	0.58
1:C:208:PHE:CD1	1:C:308:SER:HA	2.38	0.58
1:D:126:PHE:HB3	1:D:143:LEU:HD12	1.86	0.58
1:D:126:PHE:CE2	1:D:145:HIS:HB3	2.38	0.58
1:A:237:GLU:HB3	1:A:238:PRO:HA	1.84	0.58
1:A:396:LYS:NZ	2:A:501:FAD:H5'2	2.18	0.58
1:A:34:PHE:N	1:A:34:PHE:CD1	2.70	0.58
1:A:354:ARG:C	1:A:354:ARG:CD	2.72	0.58
1:A:354:ARG:HD2	1:A:355:ASP:N	2.18	0.58
1:A:376:HIS:CE1	2:A:501:FAD:H51A	2.38	0.58
1:C:35:HIS:HD2	1:C:35:HIS:O	1.87	0.58
1:D:127:TYR:HB2	1:D:128:PRO:HD2	1.86	0.58
1:A:183:MET:HG3	1:A:184:HIS:N	2.19	0.57
1:B:374:ARG:HD2	1:C:407:GLU:OE2	2.04	0.57
1:C:183:MET:HG3	1:C:184:HIS:N	2.19	0.57
1:C:196:LYS:O	1:C:197:ARG:CZ	2.52	0.57
1:C:213:GLU:O	1:C:304:THR:CG2	2.53	0.57
1:D:86:LEU:O	1:D:184:HIS:CE1	2.57	0.57
1:D:213:GLU:O	1:D:304:THR:HG22	2.04	0.57
1:C:73:ARG:CG	1:C:73:ARG:NH1	2.63	0.57
1:D:34:PHE:HE2	1:D:79:PHE:HD2	1.52	0.57
1:A:306:ARG:HH11	1:A:306:ARG:HG3	1.68	0.57
1:A:39:SER:HB3	1:A:87:LYS:HE2	1.87	0.57
1:B:212:THR:O	1:B:427:ARG:NH2	2.37	0.57
1:B:303:ARG:O	1:B:306:ARG:HB3	2.04	0.57
1:B:349:SER:HB3	3:B:607:HOH:O	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ALA:HB3	1:B:56:PRO:HD3	1.86	0.57
1:C:350:CYS:HB3	1:C:352:GLU:OE2	2.04	0.57
1:C:120:VAL:HB	1:C:121:PRO:HA	1.86	0.57
2:A:501:FAD:O2A	2:A:501:FAD:O3'	2.21	0.57
1:C:334:ARG:HG3	1:C:334:ARG:NH1	2.19	0.57
1:D:215:TYR:CZ	1:D:303:ARG:NH2	2.73	0.57
1:A:34:PHE:HE2	1:A:79:PHE:HD2	1.52	0.57
1:D:330:THR:OG1	1:D:336:VAL:HG11	2.04	0.57
1:C:59:PRO:HG2	1:C:98:ALA:HA	1.87	0.57
1:B:129:ARG:O	1:B:130:ASP:OD1	2.23	0.56
1:D:128:PRO:HA	1:D:143:LEU:HD22	1.86	0.56
1:C:35:HIS:CD2	1:C:35:HIS:C	2.77	0.56
1:C:402:LEU:HA	1:C:409:TYR:HE2	1.64	0.56
1:A:422:GLY:O	1:A:426:GLN:HG3	2.04	0.56
1:C:119:PHE:CD2	1:C:351:LYS:HB2	2.40	0.56
1:B:39:SER:HB3	1:B:87:LYS:HE2	1.87	0.56
1:D:418:ALA:O	1:D:421:THR:HG22	2.06	0.56
1:A:278:THR:HG23	1:A:281:SER:OG	2.05	0.56
1:C:278:THR:HG23	1:C:281:SER:OG	2.05	0.56
1:D:214:LEU:HA	1:D:304:THR:HG21	1.88	0.56
1:D:335:ASN:CB	1:D:338:GLU:HB3	2.30	0.56
1:D:356:HIS:NE2	2:D:501:FAD:O4	2.39	0.56
1:A:426:GLN:OE1	1:D:381:ALA:HB2	2.06	0.56
1:B:128:PRO:HA	1:B:143:LEU:HD13	1.87	0.56
1:D:283:GLN:O	1:D:287:VAL:HG23	2.05	0.56
1:C:184:HIS:CD2	1:C:188:TYR:CE2	2.94	0.56
1:D:356:HIS:CE1	2:D:501:FAD:O4	2.58	0.56
1:D:54:VAL:CG1	1:D:57:LEU:HD12	2.36	0.56
1:D:255:SER:O	1:D:257:PRO:HD3	2.06	0.56
1:A:34:PHE:N	1:A:34:PHE:HD1	2.03	0.55
1:B:235:GLY:O	1:B:241:ARG:HD3	2.06	0.55
1:C:215:TYR:CE1	1:C:303:ARG:NH2	2.75	0.55
1:D:402:LEU:HD12	1:D:409:TYR:CD2	2.41	0.55
1:B:208:PHE:CD1	1:B:308:SER:HA	2.42	0.55
1:C:212:THR:O	1:C:427:ARG:NH2	2.40	0.55
1:B:73:ARG:NH1	1:B:73:ARG:HG3	2.21	0.55
1:D:324:HIS:CE1	2:D:501:FAD:C2A	2.90	0.55
1:A:403:GLU:CD	1:A:403:GLU:H	2.10	0.55
1:C:330:THR:OG1	1:C:336:VAL:HG11	2.06	0.55
1:D:195:VAL:HG13	1:D:196:LYS:N	2.21	0.55
1:A:93:ASP:OD1	1:A:163:ARG:NH1	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:PHE:O	1:C:55:ALA:HB3	2.07	0.55
1:D:402:LEU:CD1	1:D:409:TYR:CD2	2.90	0.55
1:A:119:PHE:CD2	1:A:351:LYS:HB2	2.42	0.55
1:B:354:ARG:HD2	1:B:355:ASP:HA	1.89	0.55
1:A:54:VAL:CG1	1:A:57:LEU:HD12	2.37	0.55
1:B:73:ARG:HG3	1:B:73:ARG:HH11	1.69	0.55
1:D:239:ARG:CG	1:D:239:ARG:HH11	2.19	0.55
1:D:213:GLU:O	1:D:304:THR:CG2	2.55	0.55
1:D:330:THR:OG1	1:D:336:VAL:CG1	2.55	0.55
1:A:213:GLU:O	1:A:304:THR:HG22	2.06	0.55
1:A:431:ASP:OD1	1:A:432:PRO:HD2	2.07	0.55
1:D:354:ARG:HD2	1:D:355:ASP:CA	2.36	0.55
1:A:278:THR:HG23	1:A:281:SER:CB	2.37	0.54
1:A:370:LEU:HD21	1:A:417:GLU:HB3	1.89	0.54
1:A:425:LYS:HE2	1:D:385:ASN:HD21	1.73	0.54
1:B:184:HIS:CD2	1:B:188:TYR:CE2	2.95	0.54
1:C:312:TYR:HB3	1:C:391:ASP:HB2	1.89	0.54
1:D:34:PHE:N	1:D:34:PHE:CD1	2.73	0.54
1:A:283:GLN:O	1:A:287:VAL:HG23	2.08	0.54
1:A:350:CYS:HB3	1:A:352:GLU:OE2	2.07	0.54
1:A:376:HIS:O	1:A:376:HIS:HD2	1.91	0.54
1:A:376:HIS:HE1	2:A:501:FAD:H51A	1.73	0.54
1:D:54:VAL:HG13	1:D:57:LEU:HD12	1.90	0.54
1:A:184:HIS:CD2	1:A:188:TYR:CE2	2.95	0.54
1:C:370:LEU:HD21	1:C:417:GLU:HB3	1.90	0.54
1:D:183:MET:HG3	1:D:184:HIS:N	2.23	0.54
1:B:93:ASP:OD1	1:B:163:ARG:NH1	2.40	0.54
1:B:33:LEU:C	1:B:34:PHE:HD1	2.11	0.54
1:D:393:LEU:N	1:D:393:LEU:HD12	2.22	0.54
1:D:60:TRP:CZ3	1:D:99:THR:HB	2.42	0.54
1:A:242:LEU:O	1:A:246:GLU:HG3	2.07	0.54
1:D:306:ARG:HH11	1:D:306:ARG:HG3	1.73	0.54
1:B:403:GLU:H	1:B:403:GLU:CD	2.11	0.54
1:C:393:LEU:N	1:C:393:LEU:HD12	2.23	0.54
1:B:184:HIS:CD2	1:B:188:TYR:CZ	2.96	0.54
1:B:213:GLU:O	1:B:304:THR:CG2	2.56	0.54
1:C:184:HIS:CD2	1:C:188:TYR:CZ	2.96	0.54
1:D:179:ARG:NH1	1:D:179:ARG:HG3	2.22	0.54
1:B:335:ASN:HB3	1:B:338:GLU:CB	2.31	0.53
1:C:34:PHE:HE2	1:C:79:PHE:HD2	1.54	0.53
1:C:354:ARG:HD2	1:C:355:ASP:CA	2.38	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ASP:HB2	1:D:176:LEU:CB	2.34	0.53
1:D:60:TRP:CE3	1:D:99:THR:HB	2.44	0.53
1:C:370:LEU:O	1:C:373:TRP:HB3	2.08	0.53
1:D:278:THR:HG23	1:D:281:SER:OG	2.08	0.53
1:D:335:ASN:HB3	1:D:338:GLU:CB	2.29	0.53
1:A:306:ARG:HH11	1:A:306:ARG:CG	2.22	0.53
1:C:345:ARG:O	1:C:354:ARG:NH1	2.41	0.53
1:C:45:GLY:HA3	1:C:50:ARG:HH22	1.74	0.53
1:B:278:THR:HG23	1:B:281:SER:HB3	1.90	0.53
1:D:343:TYR:CE1	1:D:347:PHE:HB2	2.44	0.53
1:B:45:GLY:HA3	1:B:50:ARG:NH2	2.23	0.53
1:D:48:PHE:O	1:D:55:ALA:HB3	2.08	0.53
1:A:35:HIS:O	1:A:35:HIS:ND1	2.41	0.53
1:D:336:VAL:HG23	1:D:337:LEU:H	1.74	0.53
1:C:86:LEU:O	1:C:184:HIS:CE1	2.62	0.53
1:D:403:GLU:H	1:D:403:GLU:CD	2.12	0.53
1:D:33:LEU:HD13	1:D:65:TYR:CD1	2.44	0.53
1:A:237:GLU:O	1:A:241:ARG:NH1	2.41	0.53
1:C:397:ARG:HD3	1:C:401:THR:HG22	1.91	0.53
1:D:34:PHE:N	1:D:34:PHE:HD1	2.07	0.53
1:D:37:ASP:O	1:D:191:LYS:HE2	2.09	0.53
1:D:59:PRO:HG2	1:D:98:ALA:HA	1.91	0.53
1:B:52:HIS:CE1	1:B:54:VAL:HG23	2.44	0.53
1:D:86:LEU:O	1:D:184:HIS:HE1	1.92	0.53
1:A:120:VAL:HB	1:A:121:PRO:HA	1.90	0.53
1:B:30:ARG:HG2	1:B:31:PRO:CD	2.39	0.52
1:D:183:MET:HG3	1:D:184:HIS:H	1.73	0.52
1:D:39:SER:CB	1:D:87:LYS:HE2	2.39	0.52
1:B:54:VAL:CG1	1:B:57:LEU:HD12	2.39	0.52
1:C:183:MET:HG3	1:C:184:HIS:H	1.73	0.52
1:A:301:ARG:NH1	1:A:301:ARG:HG3	2.24	0.52
1:B:251:LEU:HD11	1:B:330:THR:HG23	1.90	0.52
1:B:59:PRO:HG2	1:B:98:ALA:HA	1.91	0.52
1:A:262:ASP:N	1:A:262:ASP:OD1	2.24	0.52
1:C:392:PRO:HB2	1:C:393:LEU:HD12	1.90	0.52
1:D:109:VAL:O	1:D:113:ARG:HG3	2.10	0.52
1:D:173:ASP:CB	1:D:176:LEU:H	2.22	0.52
1:A:370:LEU:O	1:A:373:TRP:HB3	2.09	0.52
1:B:242:LEU:O	1:B:246:GLU:HG3	2.10	0.52
1:D:52:HIS:HB3	1:D:55:ALA:HB2	1.92	0.52
1:A:54:VAL:HG13	1:A:57:LEU:HD12	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ALA:O	1:B:333:ASP:HB2	2.09	0.52
1:A:184:HIS:CD2	1:A:188:TYR:CZ	2.98	0.52
1:A:38:SER:HA	1:A:191:LYS:HD3	1.92	0.52
1:A:312:TYR:HB3	1:A:391:ASP:HB2	1.91	0.52
1:B:213:GLU:O	1:B:304:THR:HG22	2.09	0.52
1:B:31:PRO:O	1:B:35:HIS:HB3	2.10	0.52
1:B:392:PRO:HB2	1:B:393:LEU:HD12	1.92	0.52
1:B:52:HIS:HB3	1:B:55:ALA:HB2	1.92	0.52
1:C:214:LEU:CD1	1:C:321:LEU:HD22	2.40	0.52
1:B:422:GLY:O	1:B:426:GLN:HG3	2.09	0.52
1:C:52:HIS:CE1	1:C:183:MET:HB2	2.45	0.52
1:A:278:THR:HG23	1:A:281:SER:HB3	1.91	0.52
1:C:60:TRP:CE3	1:C:99:THR:HB	2.44	0.52
1:D:312:TYR:HB3	1:D:391:ASP:HB2	1.91	0.52
1:B:370:LEU:HD21	1:B:417:GLU:HB3	1.92	0.51
1:B:48:PHE:O	1:B:55:ALA:HB3	2.10	0.51
1:B:370:LEU:O	1:B:373:TRP:HB3	2.10	0.51
1:C:54:VAL:HG12	1:C:57:LEU:HD12	1.92	0.51
1:D:184:HIS:NE2	1:D:188:TYR:CZ	2.79	0.51
1:A:393:LEU:N	1:A:393:LEU:HD12	2.25	0.51
1:B:352:GLU:HG2	1:B:353:SER:H	1.73	0.51
1:C:186:LYS:O	1:C:190:SER:HB3	2.11	0.51
1:B:192:GLU:O	1:B:195:VAL:HG12	2.11	0.51
1:C:129:ARG:HG3	1:C:143:LEU:CA	2.31	0.51
1:B:336:VAL:HG23	1:B:337:LEU:H	1.74	0.51
1:B:354:ARG:HD2	1:B:355:ASP:CA	2.40	0.51
1:C:301:ARG:NH1	1:C:301:ARG:HG3	2.25	0.51
1:C:47:ASP:OD1	1:C:47:ASP:C	2.48	0.51
1:C:60:TRP:CZ3	1:C:99:THR:HB	2.46	0.51
1:D:301:ARG:HG3	1:D:301:ARG:HH11	1.76	0.51
1:D:422:GLY:O	1:D:426:GLN:HG3	2.10	0.51
1:B:31:PRO:HG2	1:B:32:GLY:N	2.25	0.51
1:B:330:THR:OG1	1:B:336:VAL:HG11	2.10	0.51
1:B:71:ALA:HB3	1:B:352:GLU:OE1	2.10	0.51
1:C:42:ASP:OD2	1:C:191:LYS:NZ	2.44	0.51
1:D:251:LEU:HD11	1:D:330:THR:HG23	1.93	0.51
1:B:111:LEU:HD12	1:B:111:LEU:O	2.11	0.51
1:C:379:VAL:HG12	1:C:383:LEU:HD12	1.93	0.51
1:B:283:GLN:O	1:B:287:VAL:HG23	2.10	0.50
1:B:30:ARG:NE	1:B:31:PRO:HD2	2.25	0.50
1:A:60:TRP:CZ3	1:A:99:THR:HB	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:SER:O	1:C:257:PRO:HD3	2.11	0.50
1:C:184:HIS:NE2	1:C:188:TYR:CZ	2.80	0.50
1:C:343:TYR:CE1	1:C:347:PHE:HB2	2.46	0.50
1:A:48:PHE:O	1:A:55:ALA:HB3	2.12	0.50
1:B:393:LEU:HD12	1:B:393:LEU:N	2.27	0.50
1:A:409:TYR:CE1	1:A:415:PHE:CE2	2.99	0.50
1:A:235:GLY:O	1:A:241:ARG:HD3	2.11	0.50
1:A:352:GLU:HG2	1:A:353:SER:H	1.75	0.50
1:A:345:ARG:O	1:A:354:ARG:NH1	2.43	0.50
1:A:60:TRP:CE3	1:A:99:THR:HB	2.47	0.50
1:B:255:SER:O	1:B:257:PRO:HD3	2.12	0.50
1:B:259:ILE:O	1:B:291:ILE:HG23	2.11	0.50
1:B:89:GLU:HB2	1:B:90:HIS:ND1	2.26	0.50
1:C:166:VAL:HG13	1:C:170:MET:HG3	1.93	0.50
1:C:335:ASN:O	1:C:336:VAL:C	2.49	0.50
1:A:354:ARG:HD2	1:A:355:ASP:CA	2.41	0.50
1:A:33:LEU:C	1:A:34:PHE:HD1	2.15	0.50
1:B:311:GLN:HA	3:B:604:HOH:O	2.11	0.50
1:C:262:ASP:OD1	1:C:262:ASP:N	2.27	0.50
1:C:422:GLY:O	1:C:426:GLN:HG3	2.12	0.50
1:D:242:LEU:O	1:D:246:GLU:HG3	2.12	0.50
1:D:67:ASP:O	1:D:73:ARG:NH1	2.44	0.50
1:A:376:HIS:HE1	2:A:501:FAD:C5B	2.25	0.50
1:A:330:THR:OG1	1:A:336:VAL:HG11	2.11	0.49
1:B:35:HIS:O	1:B:35:HIS:ND1	2.44	0.49
1:C:143:LEU:CD2	1:C:143:LEU:N	2.72	0.49
1:A:109:VAL:O	1:A:113:ARG:HG3	2.12	0.49
1:A:179:ARG:NH1	1:A:179:ARG:HG3	2.27	0.49
1:D:186:LYS:O	1:D:190:SER:HB3	2.12	0.49
1:D:267:ALA:HB2	1:D:285:ALA:HB1	1.94	0.49
1:D:402:LEU:CA	1:D:409:TYR:CE2	2.95	0.49
1:B:173:ASP:CB	1:B:176:LEU:H	2.24	0.49
1:B:54:VAL:HG13	1:B:57:LEU:HD12	1.94	0.49
1:B:278:THR:HG23	1:B:281:SER:CB	2.43	0.49
1:B:397:ARG:HD3	1:B:401:THR:HG22	1.95	0.49
1:A:419:HIS:CE1	1:D:360:PHE:CD1	3.01	0.49
1:C:52:HIS:HB3	1:C:55:ALA:HB2	1.94	0.49
1:A:330:THR:OG1	1:A:336:VAL:CG1	2.61	0.49
1:D:239:ARG:HG2	1:D:239:ARG:HH11	1.77	0.49
1:B:353:SER:HB3	2:B:501:FAD:N5	2.28	0.49
1:B:65:TYR:HB2	1:B:72:SER:HB3	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:VAL:CB	1:C:121:PRO:HA	2.42	0.49
1:A:180:CYS:O	1:A:184:HIS:HB3	2.12	0.49
1:A:46:ASP:OD1	1:A:46:ASP:O	2.31	0.49
1:B:403:GLU:OE2	1:B:403:GLU:N	2.45	0.48
1:C:179:ARG:HH11	1:C:179:ARG:CG	2.26	0.48
1:A:166:VAL:HG13	1:A:170:MET:HG3	1.95	0.48
1:C:397:ARG:HD3	1:C:401:THR:CG2	2.43	0.48
1:D:246:GLU:HG2	1:D:268:LEU:HD23	1.95	0.48
1:A:111:LEU:HD12	1:A:111:LEU:O	2.13	0.48
1:C:126:PHE:CE2	1:C:145:HIS:HB3	2.48	0.48
1:C:93:ASP:OD1	1:C:163:ARG:NH1	2.46	0.48
1:C:196:LYS:O	1:C:197:ARG:NE	2.46	0.48
1:D:237:GLU:O	1:D:241:ARG:NH1	2.46	0.48
1:D:374:ARG:HG3	1:D:374:ARG:NH1	2.27	0.48
1:D:399:PHE:CD1	1:D:400:PRO:HA	2.49	0.48
1:A:47:ASP:C	1:A:47:ASP:OD1	2.52	0.48
1:B:184:HIS:NE2	1:B:188:TYR:CZ	2.82	0.48
1:B:215:TYR:CE1	1:B:303:ARG:NH2	2.81	0.48
1:C:418:ALA:O	1:C:421:THR:HG22	2.14	0.48
1:D:374:ARG:HG3	1:D:374:ARG:HH11	1.78	0.48
1:A:259:ILE:O	1:A:291:ILE:HG23	2.14	0.48
1:A:374:ARG:NH1	1:A:374:ARG:HG3	2.28	0.48
1:B:246:GLU:HG2	1:B:268:LEU:HD23	1.96	0.48
1:C:214:LEU:HD13	1:C:321:LEU:HD22	1.94	0.48
1:C:330:THR:OG1	1:C:336:VAL:CG1	2.61	0.48
1:C:399:PHE:CD1	1:C:400:PRO:HA	2.49	0.48
1:C:55:ALA:HB3	1:C:56:PRO:HD3	1.94	0.48
1:B:47:ASP:C	1:B:47:ASP:OD1	2.50	0.48
1:B:381:ALA:HB2	1:C:426:GLN:OE1	2.12	0.48
1:A:418:ALA:O	1:A:421:THR:HG22	2.14	0.48
1:B:195:VAL:HA	1:B:198:SER:HB2	1.96	0.48
1:D:173:ASP:HB3	1:D:176:LEU:H	1.79	0.48
1:D:52:HIS:CE1	1:D:183:MET:HB2	2.49	0.48
1:B:72:SER:OG	1:B:120:VAL:HG23	2.14	0.48
1:A:55:ALA:HB3	1:A:56:PRO:HD3	1.94	0.48
1:C:259:ILE:O	1:C:291:ILE:HG23	2.14	0.48
1:C:335:ASN:O	1:C:337:LEU:N	2.47	0.48
1:A:400:PRO:HB2	1:A:404:ALA:HB3	1.96	0.47
1:A:73:ARG:HH21	1:A:311:GLN:C	2.12	0.47
1:C:278:THR:HG23	1:C:281:SER:CB	2.44	0.47
1:A:400:PRO:HB2	1:A:404:ALA:CB	2.44	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:SER:OG	1:B:330:THR:HA	2.14	0.47
1:C:215:TYR:CE2	1:C:303:ARG:NH2	2.81	0.47
1:A:186:LYS:O	1:A:190:SER:HB3	2.14	0.47
1:A:48:PHE:HA	1:A:51:VAL:HG12	1.96	0.47
1:A:397:ARG:HD3	1:A:401:THR:HG22	1.95	0.47
1:A:403:GLU:N	1:A:403:GLU:OE2	2.47	0.47
1:C:111:LEU:HD12	1:C:111:LEU:O	2.14	0.47
1:C:170:MET:HE2	1:C:170:MET:CA	2.40	0.47
1:C:65:TYR:HB2	1:C:72:SER:HB3	1.96	0.47
1:A:126:PHE:CE2	1:A:145:HIS:HB3	2.50	0.47
1:A:259:ILE:HG23	1:A:259:ILE:O	2.15	0.47
1:A:332:ALA:O	1:A:333:ASP:HB2	2.15	0.47
1:B:335:ASN:O	1:B:337:LEU:N	2.47	0.47
1:A:419:HIS:CE1	1:D:360:PHE:CE1	3.02	0.47
1:D:52:HIS:CE1	1:D:54:VAL:HG23	2.49	0.47
1:C:180:CYS:O	1:C:184:HIS:HB3	2.15	0.47
1:C:245:LEU:HB2	1:C:347:PHE:CE1	2.49	0.47
1:D:259:ILE:O	1:D:291:ILE:HG23	2.13	0.47
1:A:421:THR:HG23	1:D:382:ARG:CG	2.44	0.47
1:D:400:PRO:HB2	1:D:404:ALA:HB3	1.97	0.47
1:D:47:ASP:OD1	1:D:47:ASP:C	2.53	0.47
1:A:173:ASP:CB	1:A:176:LEU:H	2.27	0.47
1:B:128:PRO:CA	1:B:143:LEU:HD13	2.45	0.47
1:D:55:ALA:HB3	1:D:56:PRO:HD3	1.96	0.47
1:A:73:ARG:NH1	1:A:73:ARG:CG	2.62	0.47
1:B:357:PHE:CD1	2:B:501:FAD:HM72	2.50	0.47
1:C:129:ARG:NH2	1:C:143:LEU:N	2.63	0.47
1:C:353:SER:HB3	2:C:501:FAD:N5	2.30	0.47
1:B:360:PHE:CD1	1:C:419:HIS:CE1	3.03	0.47
1:D:277:PHE:C	1:D:277:PHE:CD2	2.87	0.47
1:D:397:ARG:HD3	1:D:401:THR:HG22	1.97	0.47
1:A:335:ASN:O	1:A:336:VAL:C	2.51	0.47
1:B:166:VAL:HG13	1:B:170:MET:HG3	1.96	0.47
1:B:323:LEU:HD22	1:B:340:ILE:HG23	1.97	0.47
1:C:237:GLU:O	1:C:241:ARG:NH1	2.48	0.47
1:C:403:GLU:H	1:C:403:GLU:CD	2.19	0.47
1:C:70:GLY:O	1:C:73:ARG:HB2	2.15	0.47
1:D:166:VAL:HG13	1:D:170:MET:HG3	1.96	0.47
1:D:313:ARG:HG2	2:D:501:FAD:O2P	2.14	0.47
1:A:173:ASP:HB2	1:A:176:LEU:CB	2.40	0.46
2:B:501:FAD:H9	2:B:501:FAD:H1'1	1.69	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ILE:HG23	1:C:259:ILE:O	2.14	0.46
1:C:277:PHE:C	1:C:277:PHE:CD2	2.88	0.46
1:D:379:VAL:HG12	1:D:383:LEU:HD12	1.97	0.46
1:D:400:PRO:HB2	1:D:404:ALA:CB	2.45	0.46
1:C:275:ARG:NH2	1:C:281:SER:HB2	2.17	0.46
1:D:179:ARG:CG	1:D:179:ARG:HH11	2.29	0.46
1:D:73:ARG:HH21	1:D:312:TYR:HA	1.80	0.46
1:B:170:MET:CA	1:B:170:MET:HE2	2.41	0.46
1:D:255:SER:OG	1:D:330:THR:HA	2.15	0.46
1:A:86:LEU:O	1:A:184:HIS:HE1	1.95	0.46
1:A:52:HIS:HB3	1:A:55:ALA:HB2	1.96	0.46
1:A:59:PRO:HG2	1:A:98:ALA:HA	1.97	0.46
1:B:109:VAL:O	1:B:113:ARG:HG3	2.16	0.46
1:B:330:THR:OG1	1:B:336:VAL:CG1	2.64	0.46
1:D:179:ARG:HG3	1:D:179:ARG:HH11	1.79	0.46
1:D:403:GLU:OE2	1:D:403:GLU:N	2.49	0.46
1:D:48:PHE:HA	1:D:51:VAL:HG12	1.96	0.46
1:B:179:ARG:HG3	1:B:179:ARG:NH1	2.31	0.46
1:C:37:ASP:O	1:C:191:LYS:HE2	2.15	0.46
1:B:237:GLU:HA	1:B:238:PRO:O	2.16	0.46
1:A:189:THR:O	1:A:192:GLU:HB3	2.16	0.46
1:A:63:LEU:HD11	1:A:121:PRO:HB2	1.96	0.46
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.47	0.46
1:B:269:GLU:HG3	1:B:269:GLU:H	1.63	0.46
1:C:194:LEU:O	1:C:197:ARG:HG2	2.15	0.46
1:C:52:HIS:CE1	1:C:54:VAL:HG23	2.51	0.46
1:D:350:CYS:HB3	1:D:352:GLU:OE2	2.16	0.46
1:D:65:TYR:HB2	1:D:72:SER:HB3	1.97	0.46
1:D:66:ASN:HB2	1:D:120:VAL:HG21	1.98	0.46
1:B:418:ALA:O	1:B:421:THR:HG22	2.15	0.46
1:C:173:ASP:CB	1:C:176:LEU:H	2.29	0.46
1:C:34:PHE:HE2	1:C:79:PHE:CD2	2.34	0.46
1:A:87:LYS:HG2	1:A:188:TYR:CE2	2.51	0.46
1:B:352:GLU:CG	1:B:353:SER:N	2.76	0.46
1:C:72:SER:OG	1:C:120:VAL:HG23	2.16	0.46
1:A:335:ASN:O	1:A:337:LEU:N	2.48	0.45
1:C:283:GLN:O	1:C:287:VAL:HG23	2.15	0.45
1:C:48:PHE:HA	1:C:51:VAL:HG12	1.97	0.45
1:D:46:ASP:O	1:D:46:ASP:OD1	2.34	0.45
1:A:343:TYR:CE1	1:A:347:PHE:HB2	2.51	0.45
1:A:43:LEU:HD23	1:A:43:LEU:N	2.30	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:CB	1:B:338:GLU:HB3	2.31	0.45
1:B:48:PHE:HA	1:B:51:VAL:HG12	1.98	0.45
1:A:303:ARG:O	1:A:306:ARG:HB3	2.17	0.45
1:D:34:PHE:HE2	1:D:79:PHE:CD2	2.34	0.45
1:B:251:LEU:HD13	1:B:334:ARG:HG3	1.96	0.45
1:B:46:ASP:O	1:B:46:ASP:OD1	2.34	0.45
1:B:78:THR:HG23	1:B:155:VAL:HG22	1.98	0.45
1:A:65:TYR:HB2	1:A:72:SER:HB3	1.98	0.45
1:B:180:CYS:O	1:B:184:HIS:HB3	2.16	0.45
1:B:186:LYS:O	1:B:190:SER:HB3	2.17	0.45
1:D:111:LEU:HD12	1:D:111:LEU:O	2.17	0.45
1:D:129:ARG:O	1:D:130:ASP:CB	2.62	0.45
1:A:246:GLU:HG2	1:A:268:LEU:HD23	1.99	0.45
1:A:421:THR:HG23	1:D:382:ARG:HG2	1.98	0.45
1:B:374:ARG:NH1	1:B:374:ARG:HG3	2.32	0.45
1:D:129:ARG:CG	1:D:129:ARG:NH1	2.74	0.45
1:D:195:VAL:CG1	1:D:196:LYS:N	2.80	0.45
1:A:184:HIS:NE2	1:A:188:TYR:CZ	2.85	0.45
1:D:107:SER:C	1:D:109:VAL:H	2.19	0.45
1:B:173:ASP:HB2	1:B:176:LEU:CB	2.39	0.45
1:B:60:TRP:CE3	1:B:99:THR:HB	2.51	0.45
1:C:194:LEU:HA	1:C:194:LEU:HD23	1.55	0.45
1:D:182:ASP:OD1	1:D:183:MET:N	2.50	0.45
1:D:343:TYR:CZ	1:D:347:PHE:HB2	2.52	0.45
1:A:34:PHE:HE2	1:A:79:PHE:CD2	2.33	0.45
1:B:60:TRP:CZ3	1:B:99:THR:HB	2.51	0.45
1:C:303:ARG:O	1:C:306:ARG:HB3	2.17	0.45
1:C:332:ALA:O	1:C:333:ASP:HB2	2.17	0.45
1:D:306:ARG:HH11	1:D:306:ARG:CG	2.30	0.45
1:D:35:HIS:O	1:D:35:HIS:ND1	2.50	0.45
1:B:259:ILE:HG23	1:B:259:ILE:O	2.16	0.45
1:C:129:ARG:NE	1:C:143:LEU:HA	2.31	0.45
1:C:251:LEU:HD13	1:C:334:ARG:HG3	1.99	0.45
1:D:323:LEU:HD22	1:D:340:ILE:HG23	1.99	0.45
1:B:120:VAL:CB	1:B:121:PRO:HA	2.47	0.44
1:D:52:HIS:CE1	1:D:183:MET:CB	3.00	0.44
1:B:312:TYR:HB3	1:B:391:ASP:HB2	1.99	0.44
1:D:184:HIS:CD2	1:D:188:TYR:CE2	3.05	0.44
1:A:215:TYR:CE1	1:A:303:ARG:NH2	2.84	0.44
1:A:379:VAL:HG12	1:A:383:LEU:HD12	1.99	0.44
1:B:311:GLN:N	1:B:311:GLN:OE1	2.45	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:CYS:HB3	1:B:352:GLU:OE2	2.17	0.44
1:C:326:LEU:HA	1:C:326:LEU:HD23	1.66	0.44
1:D:402:LEU:HD13	1:D:409:TYR:CD2	2.53	0.44
1:D:409:TYR:CE1	1:D:415:PHE:CE2	3.05	0.44
1:D:48:PHE:CE2	1:D:60:TRP:CD1	3.05	0.44
1:D:33:LEU:HD13	1:D:65:TYR:CE1	2.52	0.44
1:D:93:ASP:O	1:D:94:ALA:C	2.56	0.44
1:A:376:HIS:CD2	1:A:376:HIS:O	2.70	0.44
1:A:52:HIS:CE1	1:A:54:VAL:HG23	2.52	0.44
1:B:277:PHE:CD2	1:B:277:PHE:C	2.91	0.44
1:C:239:ARG:HG3	1:C:239:ARG:O	2.18	0.44
1:C:403:GLU:O	1:C:404:ALA:C	2.56	0.44
1:C:78:THR:HG23	1:C:155:VAL:HG22	2.00	0.44
1:D:214:LEU:CD1	1:D:321:LEU:HD22	2.48	0.44
1:D:262:ASP:N	1:D:262:ASP:OD1	2.32	0.44
2:D:501:FAD:O2A	2:D:501:FAD:C3'	2.65	0.44
1:A:396:LYS:HZ3	2:A:501:FAD:H5'2	1.82	0.44
1:A:182:ASP:OD1	1:A:183:MET:N	2.50	0.44
1:C:64:PHE:CG	1:C:117:ILE:HD12	2.52	0.44
1:D:402:LEU:HD12	1:D:409:TYR:HD2	1.81	0.44
1:A:208:PHE:C	1:A:208:PHE:CD2	2.91	0.44
1:A:396:LYS:CE	2:A:501:FAD:H5'2	2.48	0.44
1:A:73:ARG:NE	1:A:311:GLN:O	2.49	0.44
1:B:65:TYR:CZ	1:B:104:ASN:HB2	2.53	0.44
1:B:400:PRO:HB2	1:B:404:ALA:HB3	1.99	0.44
1:C:235:GLY:O	1:C:241:ARG:HD3	2.17	0.44
1:C:71:ALA:CB	1:C:352:GLU:OE1	2.63	0.44
1:A:51:VAL:O	1:A:51:VAL:HG22	2.17	0.44
1:B:195:VAL:HG13	1:B:196:LYS:N	2.33	0.44
1:B:275:ARG:HD2	1:B:275:ARG:HA	1.67	0.44
1:B:64:PHE:HB2	1:B:122:ARG:HB3	2.00	0.44
1:C:208:PHE:CD2	1:C:208:PHE:C	2.90	0.44
1:A:42:ASP:OD2	1:A:191:LYS:NZ	2.51	0.43
1:B:360:PHE:CE1	1:C:419:HIS:CE1	3.06	0.43
1:B:402:LEU:CD1	1:B:409:TYR:CD2	3.01	0.43
1:C:409:TYR:CE1	1:C:415:PHE:CE2	3.06	0.43
1:D:332:ALA:O	1:D:333:ASP:HB2	2.18	0.43
1:A:73:ARG:CZ	1:A:311:GLN:O	2.66	0.43
1:A:352:GLU:CG	1:A:353:SER:N	2.79	0.43
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.84	0.43
1:C:189:THR:O	1:C:192:GLU:HB3	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:TYR:CE1	1:D:303:ARG:NH2	2.86	0.43
1:A:418:ALA:CB	1:D:356:HIS:HD2	2.31	0.43
1:A:71:ALA:HB2	1:A:352:GLU:OE1	2.18	0.43
1:B:182:ASP:OD1	1:B:183:MET:N	2.51	0.43
1:B:343:TYR:CE1	1:B:347:PHE:HB2	2.53	0.43
1:D:194:LEU:HA	1:D:194:LEU:HD23	1.54	0.43
1:A:89:GLU:HB3	1:A:90:HIS:H	1.67	0.43
1:B:50:ARG:HG3	1:B:50:ARG:HH11	1.83	0.43
1:D:326:LEU:HA	1:D:326:LEU:HD23	1.75	0.43
1:D:352:GLU:HG2	1:D:353:SER:OG	2.18	0.43
1:A:107:SER:C	1:A:109:VAL:H	2.21	0.43
1:B:215:TYR:CE2	1:B:303:ARG:NH2	2.86	0.43
1:B:111:LEU:HD12	1:B:111:LEU:C	2.39	0.43
1:C:400:PRO:HB2	1:C:404:ALA:HB3	2.00	0.43
1:D:66:ASN:HB3	1:D:69:CYS:SG	2.58	0.43
1:A:245:LEU:HB2	1:A:347:PHE:CE1	2.54	0.43
1:A:275:ARG:HH22	1:A:281:SER:CB	2.20	0.43
1:A:399:PHE:CD1	1:A:400:PRO:HA	2.54	0.43
1:C:275:ARG:HD2	1:C:275:ARG:HA	1.72	0.43
1:B:335:ASN:O	1:B:336:VAL:C	2.56	0.43
1:C:33:LEU:HD11	1:C:73:ARG:HD3	2.01	0.43
1:D:301:ARG:NH1	1:D:301:ARG:HG3	2.33	0.43
2:A:501:FAD:H1'1	2:A:501:FAD:H9	1.74	0.43
1:B:48:PHE:O	1:B:51:VAL:HG12	2.18	0.43
1:C:107:SER:C	1:C:109:VAL:H	2.22	0.43
1:C:182:ASP:CG	1:C:183:MET:N	2.73	0.43
1:C:48:PHE:O	1:C:51:VAL:CG1	2.67	0.43
1:A:277:PHE:CD2	1:A:277:PHE:C	2.92	0.43
1:B:374:ARG:HH11	1:B:374:ARG:HG3	1.83	0.43
1:B:379:VAL:HG12	1:B:383:LEU:HD12	2.00	0.43
1:A:255:SER:O	1:A:257:PRO:HD3	2.19	0.42
1:B:249:VAL:HG12	1:B:265:VAL:HG23	2.00	0.42
1:C:245:LEU:HB2	1:C:347:PHE:CZ	2.54	0.42
1:D:73:ARG:NH2	1:D:311:GLN:O	2.51	0.42
1:D:427:ARG:HG2	1:D:427:ARG:HH11	1.84	0.42
1:A:201:SER:CB	1:A:204:GLU:H	2.32	0.42
1:A:402:LEU:CA	1:A:409:TYR:CE2	2.99	0.42
1:B:30:ARG:CB	1:B:31:PRO:HD2	2.49	0.42
1:A:120:VAL:CB	1:A:121:PRO:HA	2.50	0.42
2:A:501:FAD:O2'	2:A:501:FAD:C9A	2.67	0.42
1:B:43:LEU:HB2	1:B:103:VAL:HG22	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:LEU:O	1:D:373:TRP:HB3	2.20	0.42
1:A:374:ARG:HH11	1:A:374:ARG:HG3	1.83	0.42
1:C:184:HIS:HE2	1:C:188:TYR:HH	1.67	0.42
1:C:326:LEU:O	1:C:330:THR:OG1	2.37	0.42
1:C:343:TYR:CZ	1:C:347:PHE:HB2	2.54	0.42
1:D:214:LEU:HD13	1:D:321:LEU:HD22	2.01	0.42
1:B:345:ARG:O	1:B:354:ARG:NH1	2.52	0.42
1:B:48:PHE:O	1:B:51:VAL:CG1	2.67	0.42
1:D:43:LEU:HB2	1:D:103:VAL:HG22	2.01	0.42
1:A:34:PHE:CE1	1:A:76:ALA:HB1	2.55	0.42
1:D:180:CYS:O	1:D:184:HIS:HB3	2.20	0.42
1:D:324:HIS:NE2	2:D:501:FAD:C2A	2.83	0.42
1:A:192:GLU:O	1:A:195:VAL:HG12	2.19	0.42
1:A:170:MET:HA	1:A:170:MET:CE	2.47	0.42
1:B:38:SER:HA	1:B:191:LYS:HD3	2.02	0.42
1:C:270:SER:O	1:C:272:THR:HG23	2.20	0.42
1:D:253:LYS:HA	1:D:261:ALA:HB3	2.02	0.42
1:D:353:SER:HB3	2:D:501:FAD:N5	2.34	0.42
1:A:31:PRO:O	1:A:35:HIS:HB3	2.18	0.41
1:A:48:PHE:O	1:A:51:VAL:CG1	2.68	0.41
1:C:192:GLU:O	1:C:195:VAL:HG12	2.20	0.41
1:A:64:PHE:HB2	1:A:122:ARG:HB3	2.01	0.41
1:A:191:LYS:O	1:A:191:LYS:HG2	2.19	0.41
1:B:402:LEU:HD12	1:B:409:TYR:CD2	2.55	0.41
1:C:192:GLU:O	1:C:196:LYS:HD2	2.19	0.41
1:A:120:VAL:HB	1:A:121:PRO:CA	2.50	0.41
1:B:154:GLU:HB2	1:B:157:GLU:HG3	2.02	0.41
1:B:402:LEU:CA	1:B:409:TYR:CE2	3.01	0.41
1:C:246:GLU:HG2	1:C:268:LEU:HD23	2.01	0.41
1:C:48:PHE:O	1:C:51:VAL:HG12	2.20	0.41
1:D:254:ASP:CG	1:D:334:ARG:NH2	2.73	0.41
1:A:33:LEU:HD12	1:A:65:TYR:CD1	2.55	0.41
1:B:194:LEU:O	1:B:198:SER:HB2	2.20	0.41
1:C:390:ALA:O	1:C:392:PRO:HD3	2.20	0.41
1:C:67:ASP:O	1:C:73:ARG:NH1	2.53	0.41
1:D:402:LEU:CA	1:D:409:TYR:HE2	2.33	0.41
1:D:34:PHE:CE1	1:D:76:ALA:HB1	2.55	0.41
1:A:311:GLN:OE1	1:A:311:GLN:N	2.45	0.41
1:A:48:PHE:O	1:A:51:VAL:HG12	2.20	0.41
1:D:34:PHE:CE2	1:D:79:PHE:HD2	2.36	0.41
1:D:248:PHE:O	1:D:252:VAL:HG23	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LYS:HD2	1:D:262:ASP:HA	2.03	0.41
1:A:122:ARG:HD2	1:A:122:ARG:HA	1.82	0.41
1:B:267:ALA:HB2	1:B:285:ALA:HB1	2.02	0.41
1:B:29:PRO:HA	1:B:298:ARG:NH2	2.36	0.41
1:A:278:THR:HG23	1:A:281:SER:HG	1.85	0.41
1:A:390:ALA:O	1:A:392:PRO:HD3	2.21	0.41
1:A:34:PHE:CE2	1:A:79:PHE:HD2	2.35	0.41
1:C:269:GLU:HG3	1:C:269:GLU:H	1.68	0.41
1:C:352:GLU:HG2	1:C:353:SER:OG	2.21	0.41
2:C:501:FAD:H9	2:C:501:FAD:H1'1	1.67	0.41
1:D:275:ARG:HA	1:D:275:ARG:HD2	1.70	0.41
1:D:335:ASN:O	1:D:337:LEU:N	2.54	0.41
1:D:372:LEU:HA	1:D:372:LEU:HD12	1.82	0.41
2:D:501:FAD:O2'	2:D:501:FAD:C9A	2.68	0.41
1:A:370:LEU:HA	1:A:370:LEU:HD12	1.77	0.41
1:B:385:ASN:HD21	1:C:425:LYS:HE2	1.84	0.41
1:A:418:ALA:HB1	1:D:356:HIS:CD2	2.53	0.41
1:A:41:VAL:O	1:A:101:ALA:HA	2.21	0.41
1:A:214:LEU:CD1	1:A:321:LEU:HD22	2.51	0.41
1:A:352:GLU:HG2	1:A:353:SER:OG	2.21	0.41
1:A:431:ASP:OD1	1:A:432:PRO:CD	2.68	0.41
1:C:65:TYR:CZ	1:C:104:ASN:HB2	2.56	0.41
1:C:109:VAL:O	1:C:113:ARG:HG3	2.20	0.41
1:C:400:PRO:HB2	1:C:404:ALA:CB	2.50	0.41
1:D:192:GLU:O	1:D:195:VAL:HG12	2.20	0.41
1:D:234:VAL:HG21	1:D:241:ARG:NH2	2.36	0.41
1:D:345:ARG:O	1:D:354:ARG:NH1	2.53	0.41
1:A:179:ARG:O	1:A:182:ASP:OD1	2.39	0.41
1:B:278:THR:HG23	1:B:281:SER:OG	2.21	0.41
1:A:167:ASN:O	3:A:602:HOH:O	2.22	0.40
1:A:214:LEU:HD13	1:A:321:LEU:HD22	2.03	0.40
1:A:245:LEU:HB2	1:A:347:PHE:CZ	2.56	0.40
1:B:173:ASP:HB3	1:B:176:LEU:H	1.85	0.40
1:B:30:ARG:HG3	1:B:299:ASN:OD1	2.21	0.40
1:B:356:HIS:CD2	1:C:418:ALA:HB1	2.56	0.40
1:C:173:ASP:HB2	1:C:176:LEU:CB	2.39	0.40
1:D:231:VAL:HG22	1:D:347:PHE:CE2	2.55	0.40
1:A:64:PHE:CG	1:A:117:ILE:HD12	2.56	0.40
1:A:403:GLU:O	1:A:404:ALA:C	2.59	0.40
1:B:354:ARG:HG2	1:B:354:ARG:NH1	2.36	0.40
1:C:334:ARG:O	1:C:335:ASN:CB	2.59	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:GLU:HG2	1:C:353:SER:H	1.84	0.40
1:B:86:LEU:O	1:B:184:HIS:HE1	2.00	0.40
1:C:156:ASP:OD1	1:C:156:ASP:N	2.53	0.40
1:C:402:LEU:HD12	1:C:409:TYR:CD2	2.57	0.40
1:C:34:PHE:CE2	1:C:79:PHE:HD2	2.37	0.40
1:A:51:VAL:O	1:A:51:VAL:CG2	2.69	0.40
1:C:309:SER:HB3	1:C:312:TYR:CD1	2.57	0.40
1:C:341:GLN:HG2	1:C:358:ILE:HA	2.04	0.40
1:B:122:ARG:HG2	1:B:122:ARG:NH1	2.36	0.40
1:B:189:THR:O	1:B:192:GLU:HB3	2.22	0.40
1:B:372:LEU:HA	1:B:372:LEU:HD12	1.89	0.40
1:B:70:GLY:O	1:B:73:ARG:HB2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLU:OE2	1:C:247:ASP:OD1[2_655]	1.60	0.60
1:B:275:ARG:NE	1:C:239:ARG:NH1[2_655]	1.90	0.30

## 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	382/470 (81%)	358 (94%)	23 (6%)	1 (0%)	41	71
1	B	384/470 (82%)	360 (94%)	23 (6%)	1 (0%)	41	71
1	C	379/470 (81%)	355 (94%)	23 (6%)	1 (0%)	41	71
1	D	378/470 (80%)	352 (93%)	25 (7%)	1 (0%)	41	71
All	All	1523/1880 (81%)	1425 (94%)	94 (6%)	4 (0%)	41	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	VAL
1	B	336	VAL
1	C	336	VAL
1	D	336	VAL

### 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	328/400 (82%)	282 (86%)	46 (14%)	3	16
1	B	335/400 (84%)	288 (86%)	47 (14%)	3	16
1	C	332/400 (83%)	286 (86%)	46 (14%)	3	16
1	D	333/400 (83%)	283 (85%)	50 (15%)	3	13
All	All	1328/1600 (83%)	1139 (86%)	189 (14%)	3	15

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	39	SER
1	A	43	LEU
1	A	44	SER
1	A	46	ASP
1	A	47	ASP
1	A	57	LEU
1	A	73	ARG
1	A	89	GLU
1	A	97	ILE
1	A	111	LEU
1	A	155	VAL
1	A	156	ASP
1	A	160	SER
1	A	172	VAL
1	A	178	GLU
1	A	179	ARG
1	A	182	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	183	MET
1	A	193	GLU
1	A	207	ARG
1	A	211	THR
1	A	217	THR
1	A	218	ASP
1	A	233	LEU
1	A	236	THR
1	A	239	ARG
1	A	240	GLU
1	A	250	LEU
1	A	258	SER
1	A	262	ASP
1	A	271	ILE
1	A	274	GLU
1	A	275	ARG
1	A	278	THR
1	A	306	ARG
1	A	317	CYS
1	A	335	ASN
1	A	351	LYS
1	A	354	ARG
1	A	356	HIS
1	A	374	ARG
1	A	403	GLU
1	A	406	THR
1	A	407	GLU
1	A	414	ASN
1	B	30	ARG
1	B	34	PHE
1	B	35	HIS
1	B	39	SER
1	B	43	LEU
1	B	44	SER
1	B	47	ASP
1	B	57	LEU
1	B	73	ARG
1	B	89	GLU
1	B	90	HIS
1	B	97	ILE
1	B	108	GLU
1	B	111	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	143	LEU
1	B	155	VAL
1	B	156	ASP
1	B	160	SER
1	B	172	VAL
1	B	178	GLU
1	B	179	ARG
1	B	182	ASP
1	B	183	MET
1	B	193	GLU
1	B	198	SER
1	B	211	THR
1	B	217	THR
1	B	233	LEU
1	B	236	THR
1	B	239	ARG
1	B	240	GLU
1	B	250	LEU
1	B	258	SER
1	B	262	ASP
1	B	271	ILE
1	B	275	ARG
1	B	278	THR
1	B	306	ARG
1	B	317	CYS
1	B	336	VAL
1	B	351	LYS
1	B	354	ARG
1	B	361	ASN
1	B	366	GLU
1	B	406	THR
1	B	407	GLU
1	B	414	ASN
1	C	33	LEU
1	C	35	HIS
1	C	39	SER
1	C	43	LEU
1	C	44	SER
1	C	47	ASP
1	C	57	LEU
1	C	73	ARG
1	C	97	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	111	LEU
1	C	120	VAL
1	C	130	ASP
1	C	155	VAL
1	C	156	ASP
1	C	160	SER
1	C	170	MET
1	C	172	VAL
1	C	178	GLU
1	C	179	ARG
1	C	182	ASP
1	C	183	MET
1	C	193	GLU
1	C	196	LYS
1	C	211	THR
1	C	217	THR
1	C	218	ASP
1	C	233	LEU
1	C	236	THR
1	C	239	ARG
1	C	240	GLU
1	C	250	LEU
1	C	258	SER
1	C	262	ASP
1	C	271	ILE
1	C	275	ARG
1	C	278	THR
1	C	306	ARG
1	C	317	CYS
1	C	334	ARG
1	C	351	LYS
1	C	354	ARG
1	C	374	ARG
1	C	403	GLU
1	C	406	THR
1	C	407	GLU
1	C	414	ASN
1	D	33	LEU
1	D	35	HIS
1	D	39	SER
1	D	43	LEU
1	D	44	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	46	ASP
1	D	47	ASP
1	D	57	LEU
1	D	73	ARG
1	D	89	GLU
1	D	90	HIS
1	D	97	ILE
1	D	111	LEU
1	D	120	VAL
1	D	129	ARG
1	D	143	LEU
1	D	155	VAL
1	D	156	ASP
1	D	160	SER
1	D	170	MET
1	D	172	VAL
1	D	178	GLU
1	D	179	ARG
1	D	182	ASP
1	D	183	MET
1	D	193	GLU
1	D	211	THR
1	D	217	THR
1	D	218	ASP
1	D	233	LEU
1	D	236	THR
1	D	239	ARG
1	D	240	GLU
1	D	250	LEU
1	D	258	SER
1	D	262	ASP
1	D	269	GLU
1	D	271	ILE
1	D	274	GLU
1	D	275	ARG
1	D	278	THR
1	D	306	ARG
1	D	317	CYS
1	D	351	LYS
1	D	354	ARG
1	D	374	ARG
1	D	403	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	406	THR
1	D	407	GLU
1	D	414	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	35	HIS
1	D	361	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FAD	A	501	-	51,58,58	1.46	8 (15%)	60,89,89	2.10	15 (25%)
2	FAD	C	501	-	51,58,58	1.61	8 (15%)	60,89,89	1.90	11 (18%)
2	FAD	B	501	-	51,58,58	1.64	11 (21%)	60,89,89	1.66	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	D	501	-	51,58,58	1.61	6 (11%)	60,89,89	1.94	13 (21%)

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	A	501	-	-	11/30/50/50	0/6/6/6
2	FAD	C	501	-	-	7/30/50/50	0/6/6/6
2	FAD	B	501	-	-	8/30/50/50	0/6/6/6
2	FAD	D	501	-	-	9/30/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C10-N1	5.52	1.40	1.33
2	C	501	FAD	C10-N1	4.76	1.39	1.33
2	D	501	FAD	C2A-N3A	4.64	1.39	1.32
2	C	501	FAD	C4X-N5	4.12	1.39	1.33
2	D	501	FAD	C1'-N10	4.11	1.52	1.48
2	C	501	FAD	C2A-N3A	4.09	1.38	1.32
2	B	501	FAD	C10-N1	4.08	1.38	1.33
2	A	501	FAD	C4X-N5	3.91	1.38	1.33
2	D	501	FAD	C4X-N5	3.79	1.38	1.33
2	C	501	FAD	C4-N3	3.69	1.39	1.33
2	A	501	FAD	C4-N3	3.60	1.39	1.33
2	B	501	FAD	PA-O2A	-3.55	1.38	1.55
2	B	501	FAD	C4X-N5	3.53	1.38	1.33
2	D	501	FAD	C4-N3	3.42	1.39	1.33
2	B	501	FAD	C2A-N3A	3.38	1.37	1.32
2	A	501	FAD	C2A-N3A	3.30	1.37	1.32
2	B	501	FAD	C4-N3	3.07	1.38	1.33
2	B	501	FAD	C6-C5X	-3.04	1.37	1.41
2	A	501	FAD	C10-N1	3.04	1.37	1.33
2	C	501	FAD	C2B-C1B	-2.92	1.49	1.53
2	B	501	FAD	PA-O1A	-2.87	1.40	1.50
2	D	501	FAD	C2A-N1A	2.83	1.39	1.33
2	C	501	FAD	C5X-N5	2.73	1.39	1.35
2	A	501	FAD	C5X-N5	2.65	1.39	1.35
2	A	501	FAD	C2A-N1A	2.59	1.38	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C2A-N1A	2.43	1.38	1.33
2	B	501	FAD	O4B-C4B	-2.38	1.39	1.45
2	B	501	FAD	C2B-C1B	-2.32	1.50	1.53
2	C	501	FAD	C1'-N10	2.15	1.50	1.48
2	B	501	FAD	PA-O5B	-2.14	1.50	1.59
2	A	501	FAD	C2B-C1B	-2.13	1.50	1.53
2	A	501	FAD	PA-O2A	-2.13	1.45	1.55
2	C	501	FAD	C5'-C4'	2.03	1.54	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	C4-N3-C2	8.15	122.03	115.14
2	A	501	FAD	C4-N3-C2	7.19	121.21	115.14
2	A	501	FAD	N3A-C2A-N1A	-6.13	119.09	128.68
2	D	501	FAD	C5X-C9A-N10	5.40	121.63	117.72
2	B	501	FAD	C4-N3-C2	5.14	119.48	115.14
2	D	501	FAD	C1'-N10-C9A	4.92	122.17	118.29
2	C	501	FAD	N3A-C2A-N1A	-4.91	121.00	128.68
2	D	501	FAD	C4-N3-C2	4.85	119.23	115.14
2	B	501	FAD	N3A-C2A-N1A	-4.67	121.39	128.68
2	D	501	FAD	C1'-C2'-C3'	4.66	122.80	109.79
2	D	501	FAD	N3A-C2A-N1A	-4.52	121.61	128.68
2	A	501	FAD	C1'-C2'-C3'	4.43	122.17	109.79
2	B	501	FAD	C5X-C9A-N10	4.40	120.90	117.72
2	A	501	FAD	C4-C4X-N5	3.96	123.12	118.60
2	A	501	FAD	C4-C4X-C10	-3.81	117.43	119.95
2	D	501	FAD	C4'-C3'-C2'	3.71	121.08	113.36
2	C	501	FAD	C1'-C2'-C3'	3.55	119.71	109.79
2	B	501	FAD	P-O3P-PA	-3.52	120.73	132.83
2	C	501	FAD	C5X-C9A-N10	3.50	120.25	117.72
2	B	501	FAD	C4A-C5A-N7A	-3.46	105.80	109.40
2	A	501	FAD	C1'-N10-C9A	3.42	120.98	118.29
2	A	501	FAD	C5X-C9A-N10	3.41	120.18	117.72
2	C	501	FAD	C4-C4X-C10	-3.33	117.75	119.95
2	D	501	FAD	O2'-C2'-C1'	-3.30	101.65	109.59
2	B	501	FAD	C1'-N10-C10	3.20	121.27	118.41
2	B	501	FAD	C1'-C2'-C3'	3.12	118.51	109.79
2	D	501	FAD	C3B-C2B-C1B	3.06	105.59	100.98
2	A	501	FAD	C6-C5X-N5	2.95	122.30	119.05
2	C	501	FAD	C4-C4X-N5	2.90	121.91	118.60
2	A	501	FAD	C4X-C4-N3	-2.89	119.48	123.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	C4X-C4-N3	-2.87	119.50	123.43
2	C	501	FAD	C1'-N10-C9A	2.85	120.54	118.29
2	B	501	FAD	C4X-C4-N3	-2.82	119.58	123.43
2	A	501	FAD	O4B-C4B-C5B	-2.81	100.12	109.37
2	C	501	FAD	P-O3P-PA	-2.76	123.37	132.83
2	A	501	FAD	C10-C4X-N5	-2.64	119.43	121.26
2	D	501	FAD	P-O3P-PA	-2.58	123.98	132.83
2	C	501	FAD	C4'-C3'-C2'	2.54	118.65	113.36
2	D	501	FAD	C4X-N5-C5X	2.48	119.25	116.77
2	A	501	FAD	O3B-C3B-C4B	2.40	117.99	111.05
2	A	501	FAD	C3B-C2B-C1B	2.36	104.54	100.98
2	B	501	FAD	C5A-C6A-N6A	2.35	123.93	120.35
2	D	501	FAD	C9A-N10-C10	-2.34	118.85	121.91
2	A	501	FAD	P-O3P-PA	-2.29	124.98	132.83
2	C	501	FAD	O2B-C2B-C1B	-2.16	102.87	110.85
2	D	501	FAD	O4'-C4'-C3'	2.13	114.29	109.10
2	A	501	FAD	O4B-C1B-C2B	-2.12	103.83	106.93
2	D	501	FAD	O4'-C4'-C5'	-2.06	105.29	109.92

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	C2'-C3'-C4'-O4'
2	A	501	FAD	C2'-C3'-C4'-C5'
2	A	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	N10-C1'-C2'-O2'
2	C	501	FAD	N10-C1'-C2'-C3'
2	C	501	FAD	C5'-O5'-P-O2P
2	B	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	O4'-C4'-C5'-O5'
2	D	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	O3'-C3'-C4'-O4'
2	B	501	FAD	O3'-C3'-C4'-O4'
2	D	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	C2'-C3'-C4'-O4'
2	A	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	C2'-C3'-C4'-C5'

*Continued on next page...*



*Continued from previous page...*

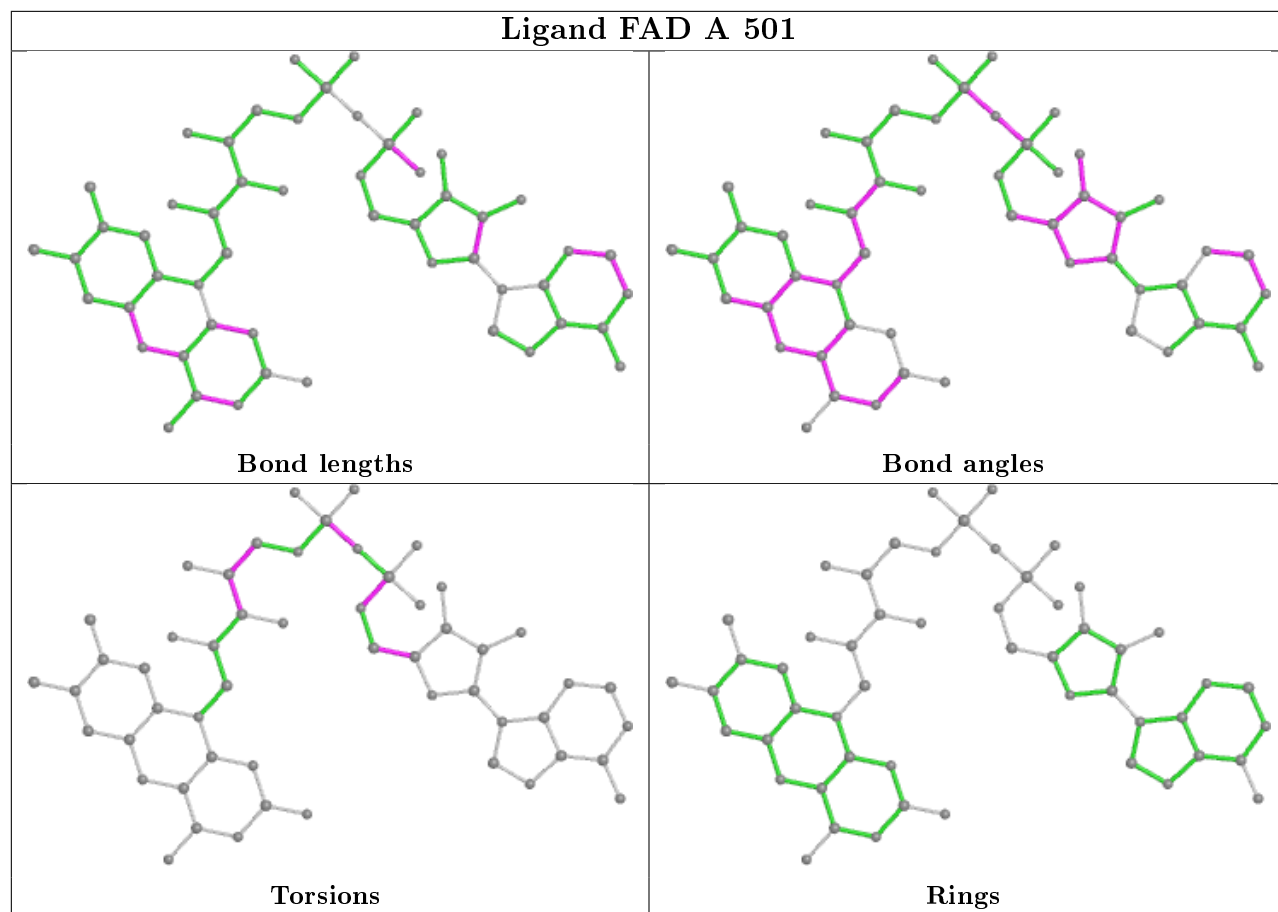
Mol	Chain	Res	Type	Atoms
2	C	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	C5'-O5'-P-O3P
2	D	501	FAD	C5B-O5B-PA-O3P
2	D	501	FAD	C5'-O5'-P-O3P
2	A	501	FAD	C3'-C4'-C5'-O5'
2	C	501	FAD	C5'-O5'-P-O1P
2	D	501	FAD	C5B-O5B-PA-O2A
2	D	501	FAD	C5'-O5'-P-O1P
2	A	501	FAD	C5B-O5B-PA-O3P
2	A	501	FAD	PA-O3P-P-O1P
2	C	501	FAD	PA-O3P-P-O2P
2	B	501	FAD	C5'-O5'-P-O1P
2	A	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4'-C4'-C5'-O5'

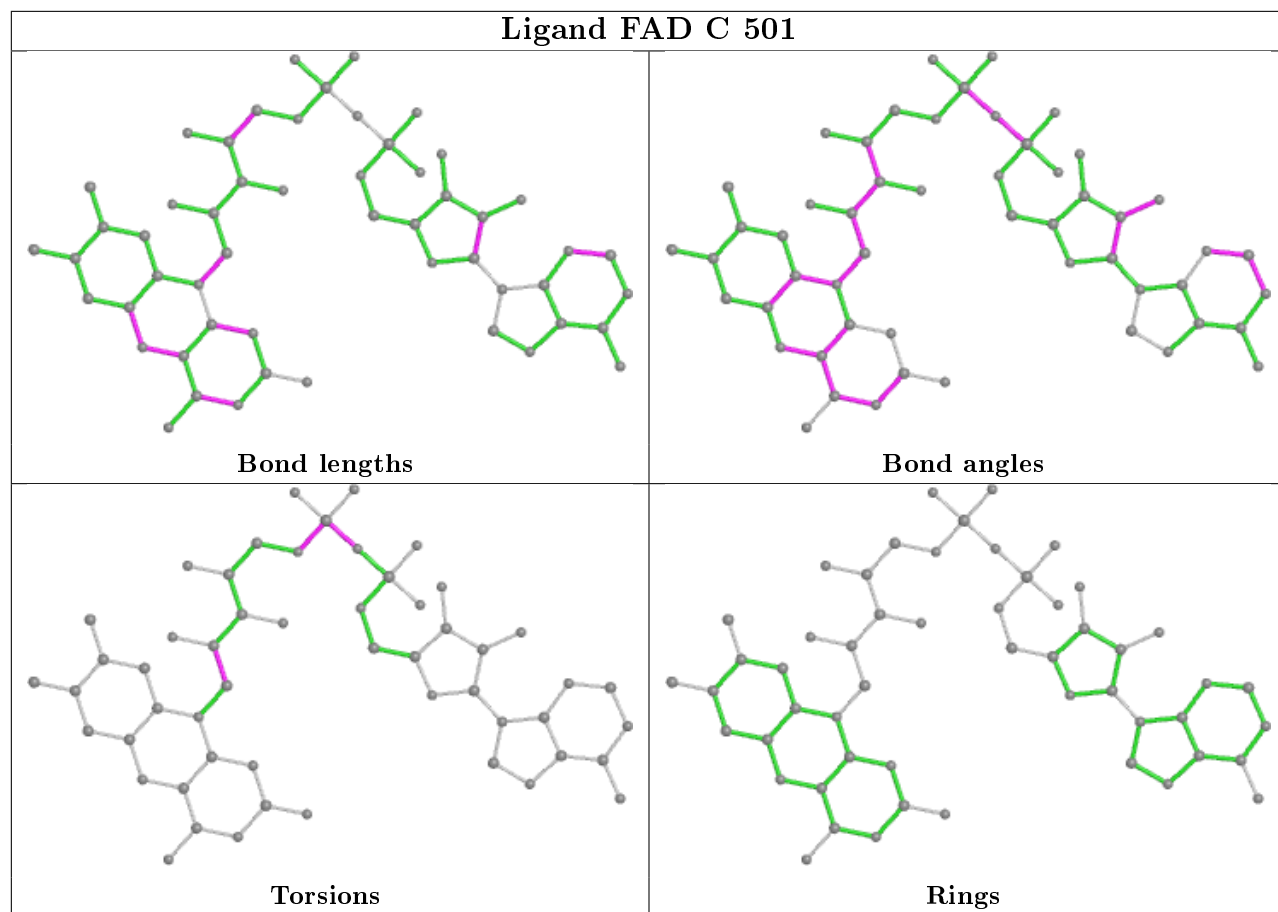
There are no ring outliers.

4 monomers are involved in 26 short contacts:

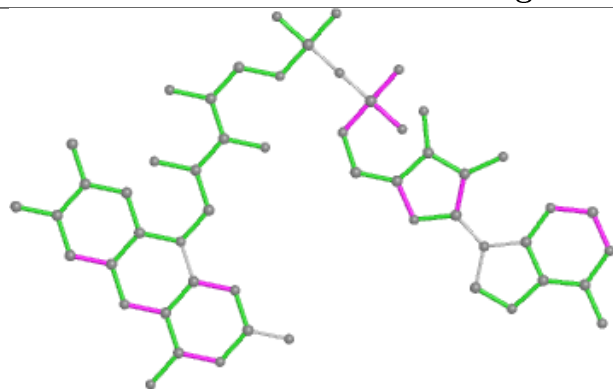
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	9	0
2	C	501	FAD	2	0
2	B	501	FAD	3	0
2	D	501	FAD	12	0

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

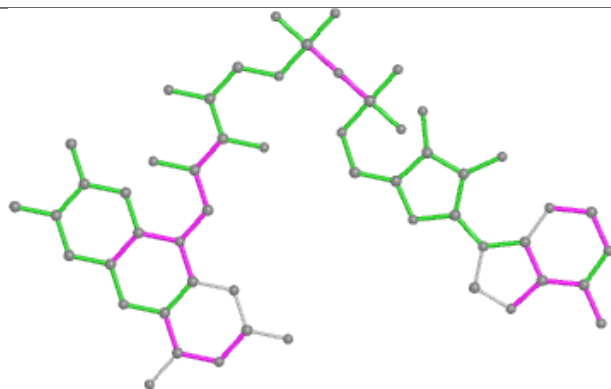




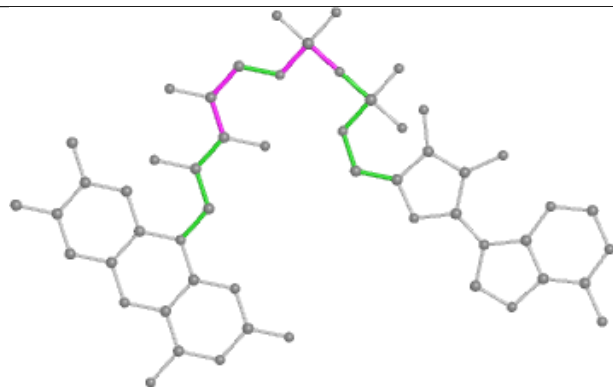
## Ligand FAD B 501



Bond lengths



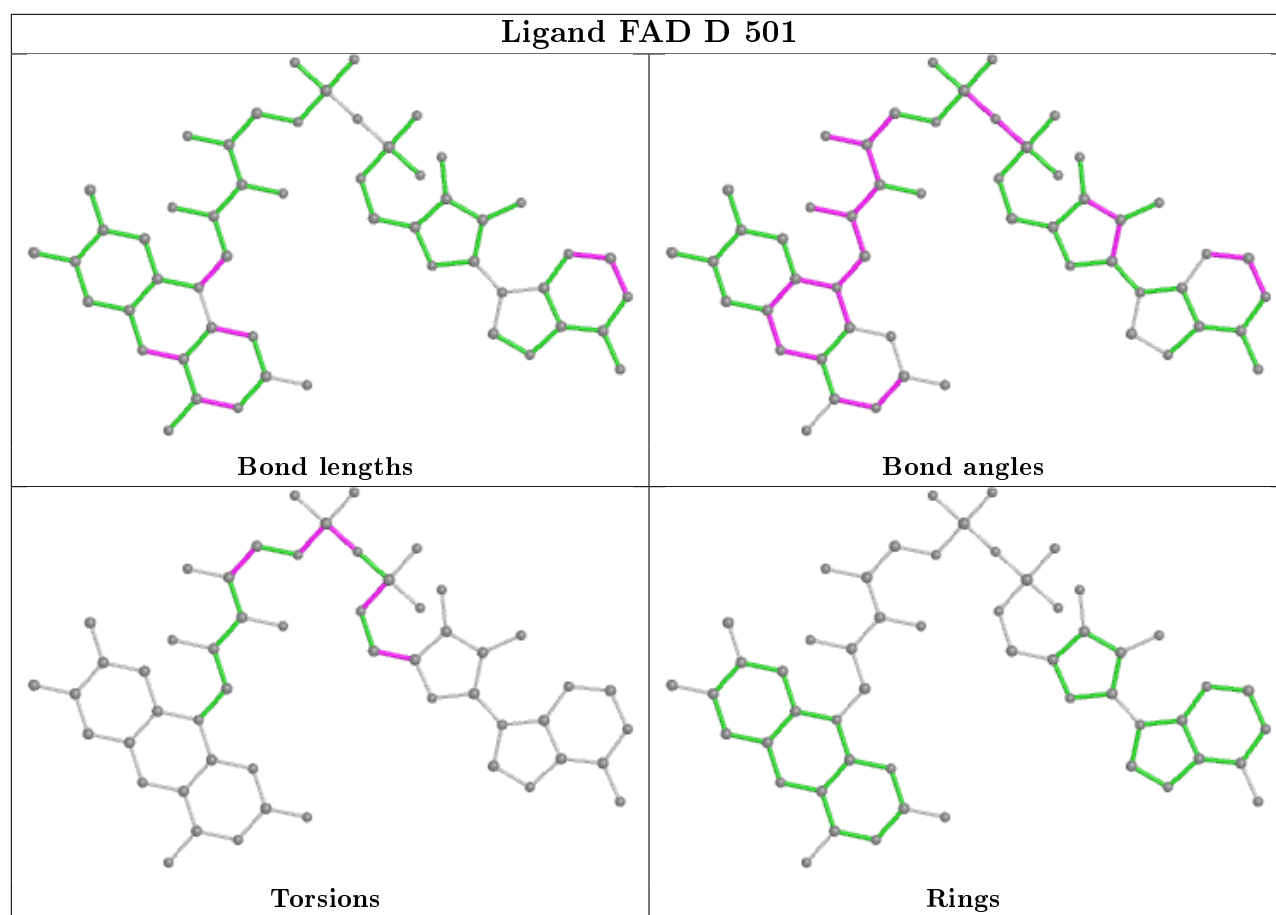
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/470 (82%)	-0.08	8 (2%) 63 62	42, 82, 149, 216	0
1	B	390/470 (82%)	-0.14	8 (2%) 63 62	29, 81, 145, 223	0
1	C	385/470 (81%)	0.00	11 (2%) 51 50	38, 83, 147, 248	0
1	D	384/470 (81%)	0.18	15 (3%) 39 37	55, 97, 151, 204	0
All	All	1547/1880 (82%)	-0.01	42 (2%) 54 52	29, 86, 149, 248	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	SER	5.8
1	A	200	SER	5.4
1	D	35	HIS	4.0
1	C	92	LYS	3.8
1	B	205	SER	3.7
1	A	91	GLY	3.5
1	C	207	ARG	3.3
1	D	57	LEU	3.2
1	C	89	GLU	3.1
1	C	388	ASP	3.1
1	B	88	VAL	3.1
1	A	206	GLY	3.1
1	C	90	HIS	3.0
1	C	95	LEU	3.0
1	B	199	VAL	2.8
1	C	94	ALA	2.8
1	A	174	ASP	2.7
1	D	130	ASP	2.7
1	A	89	GLU	2.7
1	D	55	ALA	2.6
1	D	54	VAL	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	430	TRP	2.4
1	D	333	ASP	2.4
1	A	131	SER	2.4
1	C	389	GLY	2.4
1	C	91	GLY	2.3
1	D	48	PHE	2.3
1	D	56	PRO	2.3
1	D	188	TYR	2.3
1	C	93	ASP	2.3
1	D	89	GLU	2.3
1	D	60	TRP	2.2
1	B	96	GLN	2.2
1	D	208	PHE	2.1
1	D	178	GLU	2.1
1	A	412	ALA	2.1
1	B	92	LYS	2.1
1	C	308	SER	2.1
1	B	208	PHE	2.1
1	D	215	TYR	2.0
1	B	206	GLY	2.0
1	B	90	HIS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	D	501	53/53	0.95	0.17	18,70,98,107	0
2	FAD	B	501	53/53	0.96	0.19	0,42,66,150	0

*Continued on next page...*

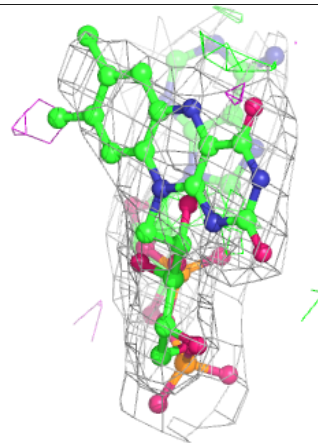
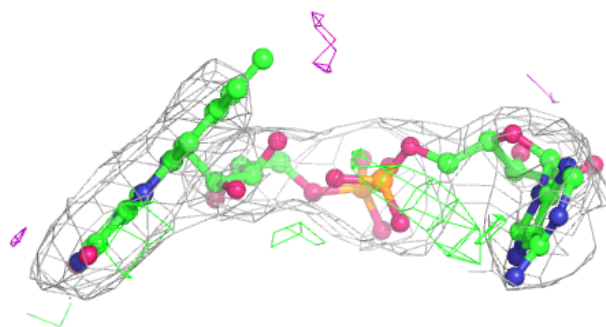
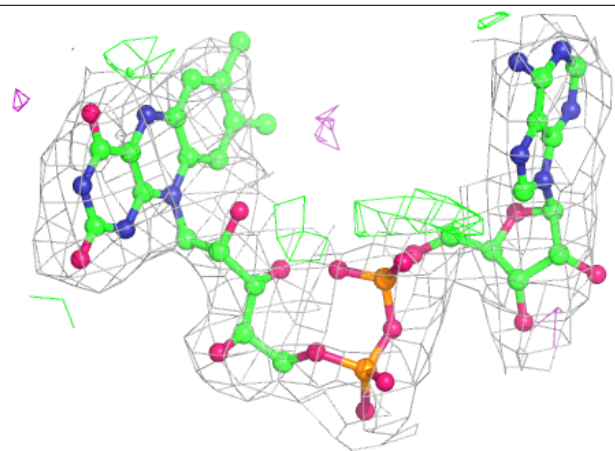
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	501	53/53	0.96	0.20	21,53,79,103	0
2	FAD	C	501	53/53	0.97	0.17	7,48,77,99	0

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

#### Electron density around FAD D 501:

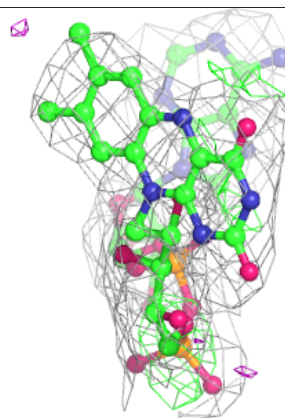
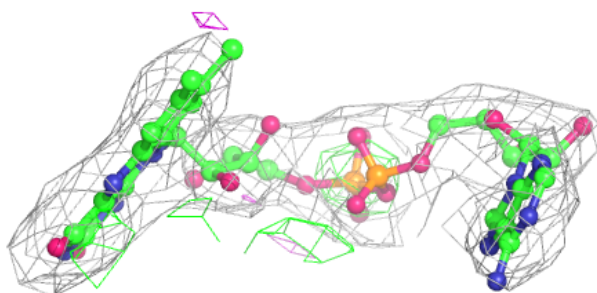
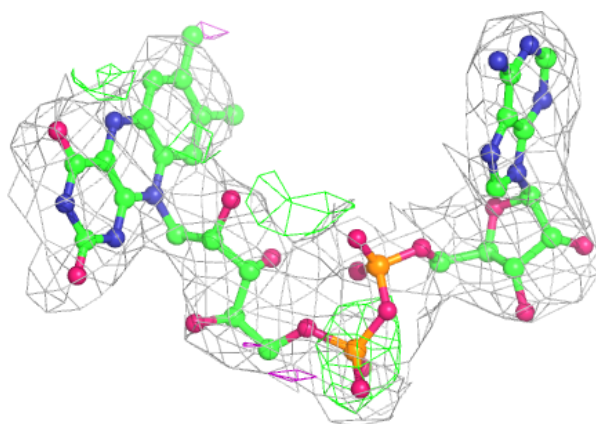
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





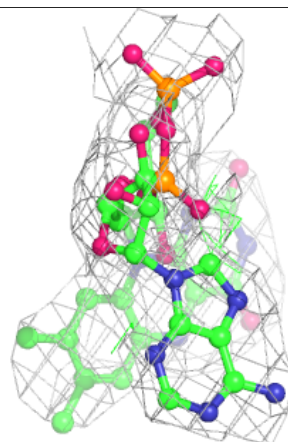
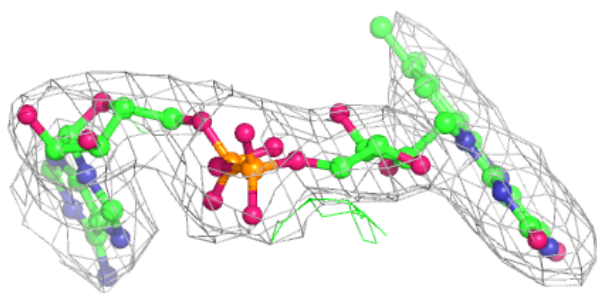
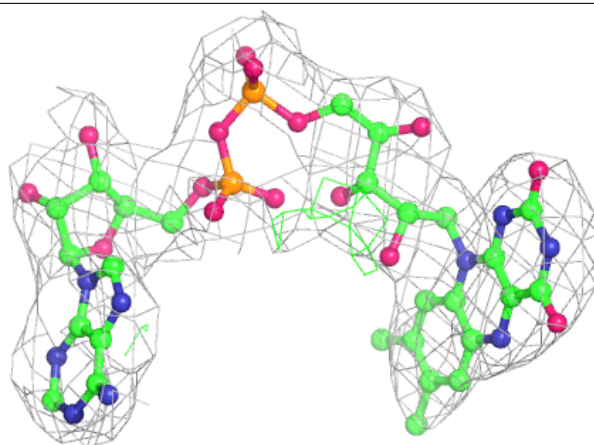
**Electron density around FAD B 501:**

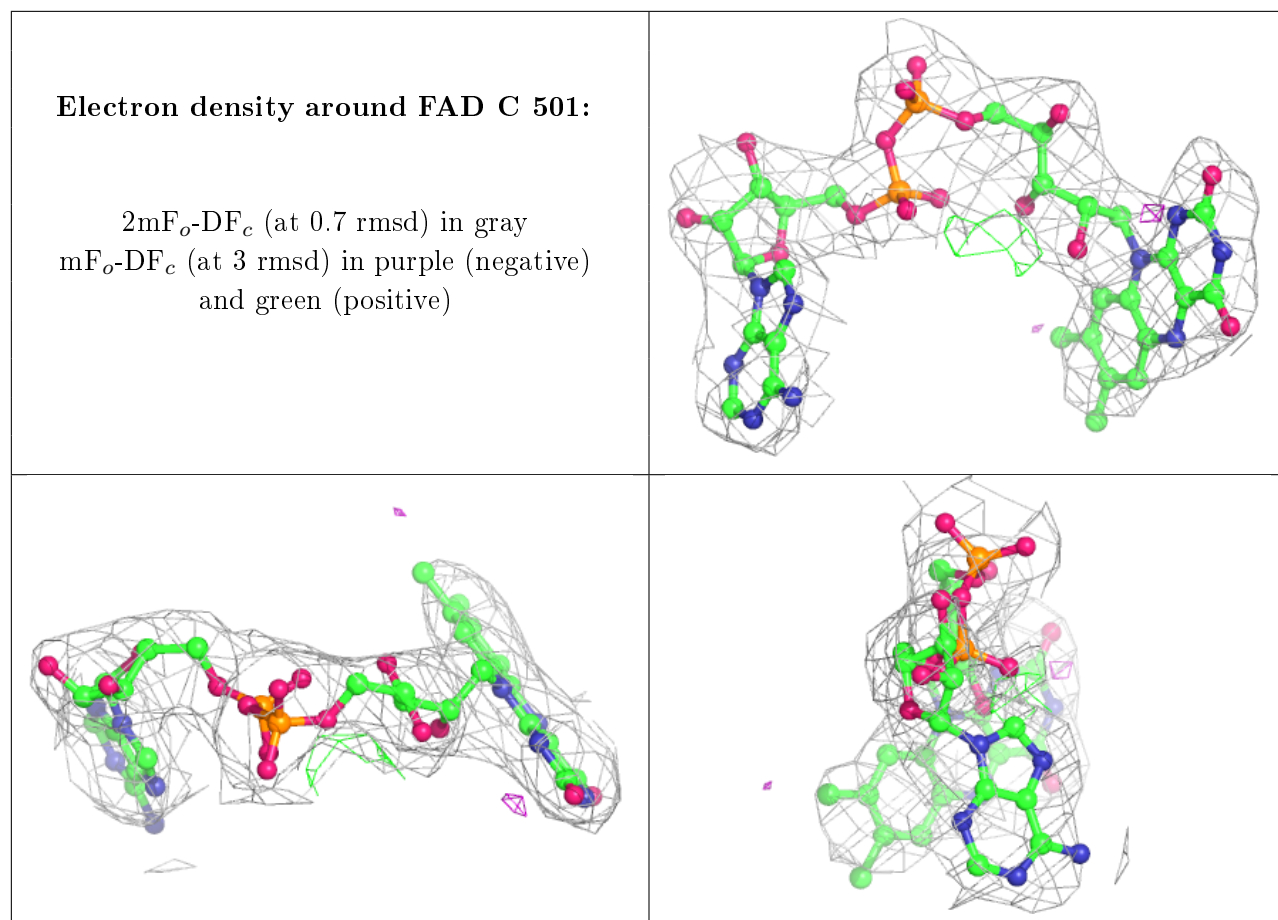
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FAD A 501:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.