



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:51 PM UTC

PDB ID : 3QD9 / pdb_00003qd9
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

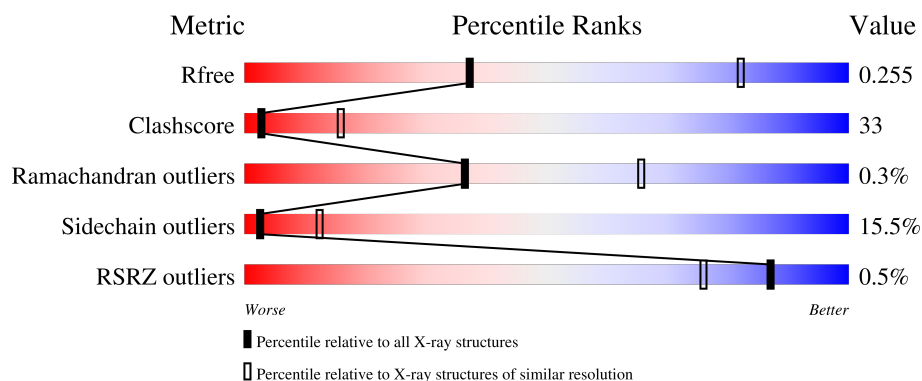
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	470	41%32%9%•17%
1	B	470	% 39%34%9%•17%
1	C	470	39%33%9%18%
1	D	470	% 37%36%8%•18%

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:

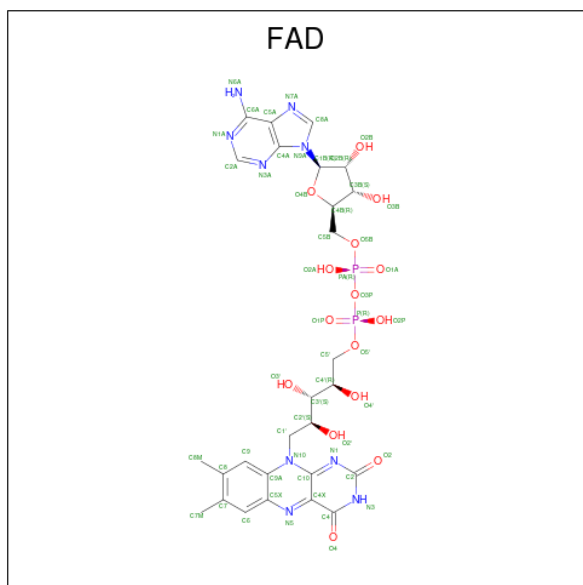
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	GLY	-	expression tag	UNP Q585M6
A	17	SER	-	expression tag	UNP Q585M6
A	18	HIS	-	expression tag	UNP Q585M6
A	19	MET	-	expression tag	UNP Q585M6
A	72	SER	CYS	engineered mutation	UNP Q585M6
A	353	SER	CYS	engineered mutation	UNP Q585M6
B	16	GLY	-	expression 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

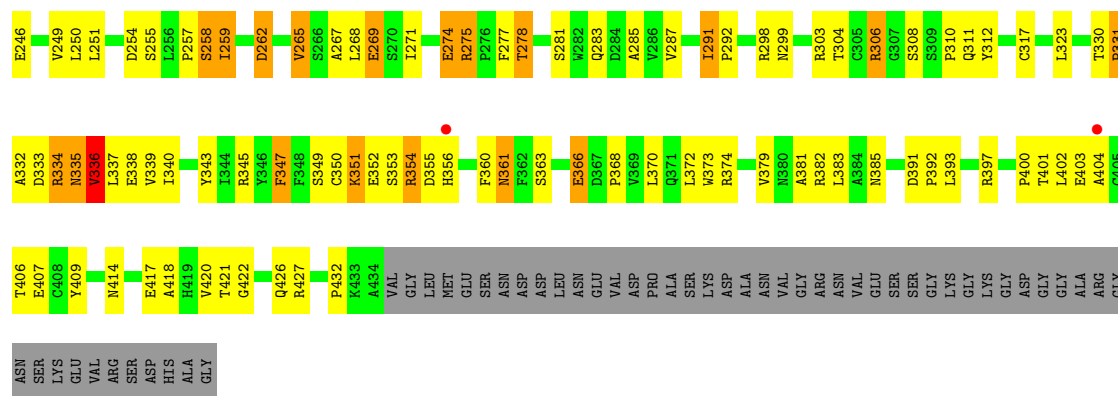
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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		

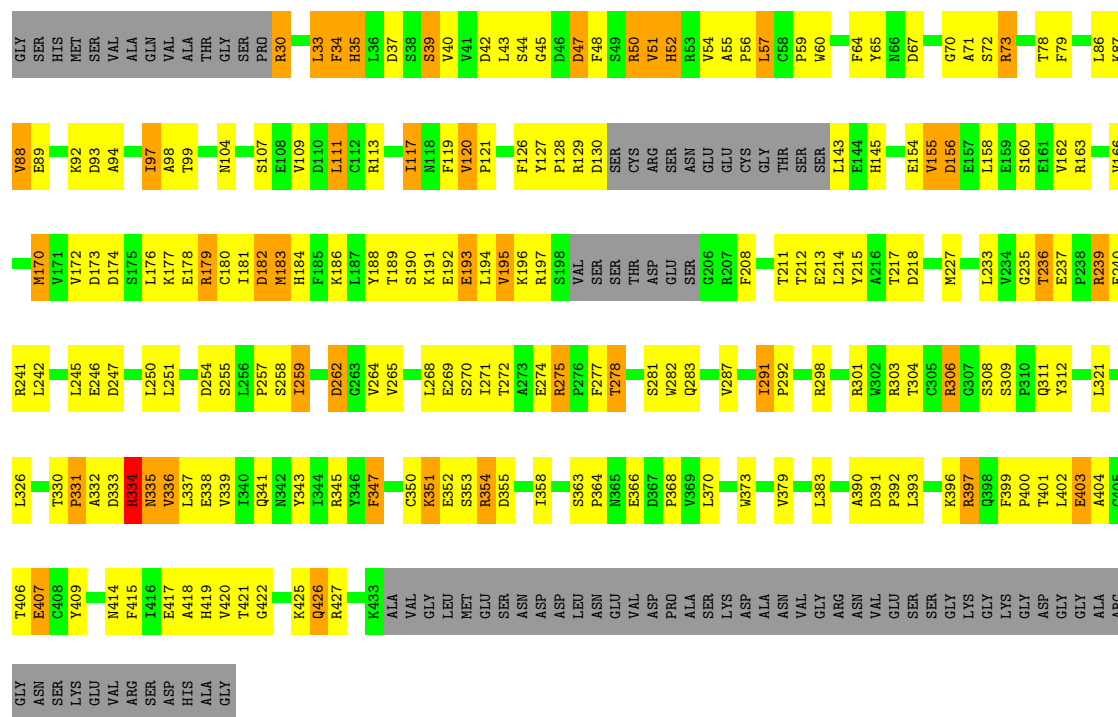
- Molecule 3 is water.

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		



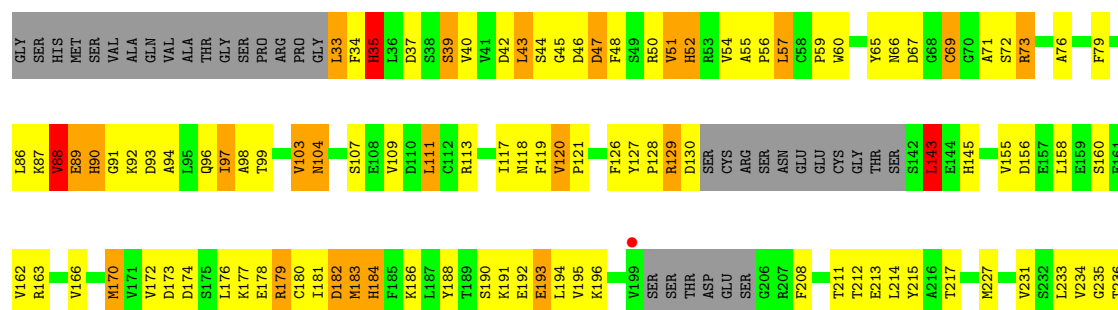
• Molecule 1: QSOX from *Trypanosoma brucei* (TbQSOX)

Chain C: 39% 33% 9% 18%



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

Chain D: 37% 36% 8% 18%



ARG	ASN	VAL	GLU	SER	SER	GLY	LYS	GLY	LYS	GLY	ASP	GLY	GLY	ALA	ARG	GLY	ASN	SER	LYS	GLU	VAL	ARG	SER	ASP	HIS	ALA	GLY																																	
L383	A384	R385		D391	P392	L393		R397	Q398	F399	P400	T401	L402	E403	A404	C405	T406	E407	C408	Y409		N414	F415	I416	E417	A418	H419	V420	T421	G422		Q426	R427		K433	ALA	VAL	GLY	LEU	MET	GLU	SER	ASN	ASP	ASP	LEU	ASN	GLU	VAL	ASP	PRO	ALA	SER	LYS	ASP	ALA	ASN	VAL	GLY	
E237	F236	R239	E240	R241	L242		L245	E246	D247	F248	V249	L250	L251	V252	K253	D254	S255	L256	P257	S258	I259	G260	A261	D262		V265	S266	A267	L268	E269	S270	L271		E274	R275	P276	F277	T278		S281	W282	Q283	D284	A285	V286	V287		L291	P297	R298		R301	W302	R303	T304	C305	R306	G307		
S308		Q311	Y312	R313		W320	L321	L322	L323	H324	A325	L326		T330	P331	A332	D333	R334	R335	V336	L337	E338	V339	I340		Y343	I344	R345	Y346	F347		C350	R351	E352	S353	R354	D355	H356		F360		S363		E366	D367	P368		V369	L370	I371	L372	W373	R374	A375	H376		Y379	R380	A381	R382

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.04Å 120.31Å 106.22Å 90.00° 105.44° 90.00°	Depositor
Resolution (Å)	38.11 – 3.30 38.11 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.11-3.30) 98.5 (38.11-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_629)	Depositor
R, R_{free}	0.190 , 0.249 0.206 , 0.255	Depositor DCC
R_{free} test set	2939 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12535	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

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	0.98	9/3143 (0.3%)	1.25	39/4270 (0.9%)
1	B	1.03	12/3181 (0.4%)	1.24	31/4318 (0.7%)
1	C	0.98	6/3150 (0.2%)	1.22	31/4275 (0.7%)
1	D	0.92	9/3144 (0.3%)	1.22	21/4266 (0.5%)
All	All	0.98	36/12618 (0.3%)	1.23	122/17129 (0.7%)

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 (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	HIS	CE1-NE2	13.51	1.46	1.32
1	D	103	VAL	C-O	10.06	1.35	1.24
1	A	90	HIS	CE1-NE2	9.81	1.42	1.32
1	C	89	GLU	CA-C	-8.30	1.45	1.53
1	A	53	ARG	NE-CZ	8.03	1.41	1.33
1	A	271	ILE	CA-C	-7.94	1.44	1.52
1	B	35	HIS	ND1-CE1	7.67	1.40	1.32
1	D	90	HIS	CE1-NE2	7.63	1.40	1.32
1	B	35	HIS	CG-CD2	6.97	1.43	1.35
1	B	237	GLU	CD-OE2	6.69	1.38	1.25
1	D	104	ASN	CG-ND2	-6.42	1.19	1.33
1	B	35	HIS	CD2-NE2	-6.41	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	298	ARG	CZ-NH1	6.34	1.41	1.32
1	D	184	HIS	CE1-NE2	-6.04	1.26	1.32
1	C	89	GLU	CB-CG	-5.94	1.34	1.52
1	A	52	HIS	CD2-NE2	-5.91	1.31	1.37
1	C	426	GLN	CD-NE2	-5.78	1.21	1.33
1	D	52	HIS	CD2-NE2	-5.75	1.31	1.37
1	B	89	GLU	CA-C	-5.75	1.47	1.53
1	A	35	HIS	ND1-CE1	5.72	1.38	1.32
1	D	184	HIS	CG-ND1	-5.59	1.32	1.38
1	D	35	HIS	ND1-CE1	5.58	1.38	1.32
1	B	52	HIS	ND1-CE1	5.57	1.38	1.32
1	D	184	HIS	ND1-CE1	5.45	1.38	1.32
1	C	50	ARG	CZ-NH1	5.44	1.40	1.32
1	A	426	GLN	CD-OE1	5.37	1.33	1.23
1	B	335	ASN	CG-ND2	-5.37	1.22	1.33
1	B	145	HIS	CD2-NE2	-5.34	1.31	1.37
1	C	52	HIS	ND1-CE1	5.28	1.37	1.32
1	A	53	ARG	CZ-NH1	5.26	1.40	1.32
1	B	274	GLU	CB-CG	-5.26	1.36	1.52
1	B	361	ASN	CG-ND2	-5.22	1.22	1.33
1	A	120	VAL	CA-CB	-5.22	1.47	1.54
1	A	335	ASN	CG-ND2	-5.17	1.22	1.33
1	B	92	LYS	CA-C	-5.14	1.46	1.53
1	C	52	HIS	CD2-NE2	-5.02	1.32	1.37

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ILE	CG1-CB-CG2	-14.38	67.57	110.70
1	A	271	ILE	N-CA-CB	11.46	124.40	110.31
1	C	89	GLU	CA-CB-CG	11.04	136.19	114.10
1	B	363	SER	CA-C-N	-11.01	110.53	121.65
1	B	363	SER	C-N-CA	-11.01	110.53	121.65
1	D	363	SER	CA-C-N	-10.37	111.18	121.65
1	D	363	SER	C-N-CA	-10.37	111.18	121.65
1	C	363	SER	CA-C-N	-8.83	109.99	121.91
1	C	363	SER	C-N-CA	-8.83	109.99	121.91
1	A	363	SER	CA-C-N	-8.75	110.09	121.91
1	A	363	SER	C-N-CA	-8.75	110.09	121.91
1	A	271	ILE	CB-CA-C	-8.47	98.72	111.33
1	C	274	GLU	CA-CB-CG	8.39	130.88	114.10
1	A	292	PRO	CA-C-O	-8.17	115.26	121.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	PRO	CA-C-O	-7.76	115.57	121.31
1	B	274	GLU	CA-CB-CG	7.65	129.40	114.10
1	A	347	PHE	N-CA-C	7.62	123.52	113.30
1	D	366	GLU	CB-CG-CD	-7.62	99.65	112.60
1	C	274	GLU	CB-CA-C	-7.59	94.90	110.38
1	A	88	VAL	N-CA-C	-7.51	98.43	108.35
1	B	89	GLU	CB-CA-C	-7.46	98.65	112.00
1	B	89	GLU	CA-CB-CG	7.44	128.98	114.10
1	B	274	GLU	CB-CA-C	-7.39	94.54	109.99
1	D	104	ASN	CB-CG-OD1	-7.34	106.12	120.80
1	B	366	GLU	N-CA-C	7.34	120.52	109.95
1	D	347	PHE	N-CA-C	7.21	122.96	113.30
1	C	88	VAL	N-CA-C	-7.09	98.99	108.35
1	C	89	GLU	CB-CG-CD	-7.04	100.64	112.60
1	B	347	PHE	N-CA-C	7.02	122.70	113.30
1	C	30	ARG	CA-C-N	7.01	126.26	118.97
1	C	30	ARG	C-N-CA	7.01	126.26	118.97
1	B	174	ASP	N-CA-C	-6.93	103.72	112.93
1	A	174	ASP	N-CA-C	-6.90	103.75	112.93
1	B	52	HIS	CB-CG-CD2	-6.85	122.29	131.20
1	D	88	VAL	N-CA-C	-6.84	99.32	108.35
1	C	347	PHE	N-CA-C	6.81	122.43	113.30
1	A	335	ASN	N-CA-CB	6.80	121.98	110.49
1	D	35	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	A	335	ASN	CB-CA-C	-6.74	97.01	110.42
1	D	174	ASP	N-CA-C	-6.71	104.01	112.93
1	B	35	HIS	CB-CG-CD2	-6.68	122.52	131.20
1	A	335	ASN	N-CA-C	6.58	124.81	110.80
1	C	195	VAL	CA-C-N	-6.57	112.30	122.16
1	C	195	VAL	C-N-CA	-6.57	112.30	122.16
1	C	52	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	D	52	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	A	364	PRO	CA-C-O	-6.53	116.48	121.31
1	A	35	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	A	52	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	A	92	LYS	CD-CE-NZ	6.32	132.12	111.90
1	A	52	HIS	CB-CG-ND1	6.27	132.11	122.70
1	B	30	ARG	CA-C-N	6.27	127.68	119.84
1	B	30	ARG	C-N-CA	6.27	127.68	119.84
1	D	52	HIS	CB-CG-ND1	6.25	132.07	122.70
1	A	271	ILE	CA-CB-CG1	6.24	121.00	110.40
1	B	292	PRO	CA-C-O	-6.19	116.73	121.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	GLU	CB-CG-CD	-6.19	102.08	112.60
1	B	88	VAL	N-CA-C	-6.17	100.20	108.35
1	B	89	GLU	N-CA-CB	6.15	119.86	110.39
1	D	274	GLU	CA-CB-CG	6.13	126.36	114.10
1	B	145	HIS	CB-CG-CD2	-6.12	123.25	131.20
1	A	328	VAL	N-CA-C	6.11	116.89	110.72
1	C	334	ARG	CG-CD-NE	-6.09	98.59	112.00
1	A	274	GLU	CA-CB-CG	6.05	126.19	114.10
1	B	92	LYS	CB-CA-C	-6.02	101.63	111.68
1	C	364	PRO	CA-C-O	-5.99	116.88	121.31
1	A	259	ILE	N-CA-C	-5.98	106.91	112.83
1	B	145	HIS	CB-CG-ND1	5.97	131.65	122.70
1	C	339	VAL	N-CA-C	5.94	116.60	110.36
1	A	339	VAL	CB-CA-C	-5.93	104.11	111.70
1	A	339	VAL	N-CA-C	5.86	116.32	110.23
1	C	52	HIS	CB-CG-ND1	5.79	131.39	122.70
1	B	274	GLU	CB-CG-CD	-5.77	102.80	112.60
1	C	339	VAL	CB-CA-C	-5.76	104.50	111.88
1	A	366	GLU	CB-CG-CD	-5.76	102.81	112.60
1	A	396	LYS	N-CA-C	5.75	119.06	112.57
1	D	184	HIS	CG-CD2-NE2	5.73	112.93	107.20
1	B	52	HIS	CB-CG-ND1	5.66	131.19	122.70
1	A	397	ARG	N-CA-C	5.64	118.19	110.24
1	C	174	ASP	N-CA-C	-5.62	105.20	112.68
1	B	335	ASN	N-CA-C	5.62	122.76	110.80
1	D	35	HIS	CB-CG-ND1	5.61	131.12	122.70
1	A	201	SER	N-CA-C	5.60	117.36	108.79
1	A	366	GLU	N-CA-C	5.60	117.75	109.69
1	C	366	GLU	CB-CG-CD	-5.57	103.12	112.60
1	B	259	ILE	N-CA-C	-5.55	107.33	112.83
1	C	92	LYS	CB-CA-C	-5.54	102.43	111.68
1	C	368	PRO	N-CA-C	-5.49	104.88	113.78
1	A	237	GLU	CB-CG-CD	-5.48	103.29	112.60
1	C	366	GLU	N-CA-C	5.45	117.54	109.69
1	A	237	GLU	CB-CA-C	-5.45	100.62	108.84
1	D	89	GLU	N-CA-CB	-5.44	101.30	110.49
1	D	143	LEU	N-CA-C	5.43	118.07	109.50
1	A	35	HIS	CB-CG-ND1	5.39	130.79	122.70
1	C	396	LYS	N-CA-C	5.36	118.63	112.57
1	B	368	PRO	N-CA-C	-5.36	105.10	113.78
1	D	91	GLY	N-CA-C	-5.35	101.65	110.80
1	A	206	GLY	N-CA-C	5.35	117.22	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	GLU	CB-CG-CD	-5.32	103.55	112.60
1	C	397	ARG	N-CA-C	5.32	117.80	110.35
1	A	92	LYS	CG-CD-CE	5.32	123.54	111.30
1	D	92	LYS	CB-CA-C	-5.30	102.83	111.68
1	A	191	LYS	CD-CE-NZ	5.26	128.74	111.90
1	D	368	PRO	N-CA-C	-5.25	105.27	113.78
1	D	366	GLU	N-CA-CB	-5.22	102.99	110.87
1	C	259	ILE	N-CA-C	-5.21	107.67	112.83
1	D	69	CYS	N-CA-C	5.21	118.04	109.76
1	A	237	GLU	N-CA-C	5.20	118.06	110.10
1	B	335	ASN	CB-CA-C	-5.20	100.08	110.42
1	C	331	PRO	N-CA-C	-5.14	103.38	111.34
1	A	92	LYS	CB-CG-CD	-5.13	99.50	111.30
1	C	335	ASN	N-CA-C	5.13	121.72	110.80
1	A	368	PRO	N-CA-C	-5.12	105.49	113.78
1	C	236	THR	N-CA-C	5.12	119.21	112.92
1	D	184	HIS	CB-CG-ND1	5.11	130.36	122.70
1	B	334	ARG	CG-CD-NE	-5.09	100.81	112.00
1	B	237	GLU	CB-CG-CD	-5.06	104.00	112.60
1	A	237	GLU	CA-CB-CG	5.06	124.21	114.10
1	A	89	GLU	N-CA-CB	-5.04	101.97	110.49
1	B	432	PRO	N-CA-C	5.04	120.48	113.98
1	B	339	VAL	CB-CA-C	-5.03	105.53	111.97
1	B	331	PRO	N-CA-C	-5.03	103.55	111.34

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 ⓘ

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3102	0	2986	194	2
1	C	3072	0	2957	201	2
1	D	3067	0	2959	222	0
2	A	53	0	31	9	0
2	B	53	0	31	2	0
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	804	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 33.

All (804) 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:HA	1:C:193:GLU:OE1	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:OE1	1:D:193:GLU:HA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HH11	1:D:73:ARG:CG	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: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:D:354:ARG:C	1:D:354:ARG:HD2	2.08	0.78
1:A:73:ARG:NH2	1:A:311:GLN:O	2.16	0.78
1:C:73:ARG:HG2	1:C:73:ARG:HH11	1.49	0.78
1:C:334:ARG:O	1:C:335:ASN:HB2	1.83	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:HG2	1:A:239:ARG:HH11	1.50	0.76
1:D:402:LEU:HA	1:D:409:TYR:CE2	2.18	0.76
1:A:193:GLU:OE1	1:A:193:GLU:CA	2.34	0.76
1:B:354:ARG:C	1:B:354:ARG:HD2	2.10	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:D:354:ARG:C	1:D:354:ARG:CD	2.60	0.74
1:A:73:ARG:HH11	1:A:73:ARG:HG2	1.53	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLU:HG2	1:A:353:SER:N	2.02	0.74
1:C:73:ARG:HH11	1:C:73:ARG:CG	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
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:C:354:ARG:HD2	1:C:354:ARG:C	2.15	0.72
1:A:34:PHE:CD2	1:A:40:VAL:HG11	2.22	0.72
1:C:35:HIS:O	1:C:35:HIS:CD2	2.43	0.72
1:C:143:LEU:N	1:C:143:LEU:HD23	2.05	0.72
1:D:354:ARG:HD2	1:D:355:ASP:N	2.05	0.72
1:B:94:ALA:O	1:B:97:ILE:HG23	1.90	0.71
1:A:170:MET:HE2	1:A:170:MET:HA	1.72	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:HH11	1:C:239:ARG:CG	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: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:B:354:ARG:C	1:B:354:ARG:CD	2.65	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ARG:HD2	1:A:354:ARG:C	2.20	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
1:B:34:PHE:CD2	1:B:40:VAL:HG11	2.30	0.65
2:D:501:FAD:O2A	2:D:501:FAD:O3'	2.14	0.65
1:A:306:ARG:NH1	1:A:306:ARG:HG3	2.11	0.65
1:C:30:ARG:N	1:C:298:ARG:HH21	1.91	0.65
1:C:33:LEU:C	1:C:34:PHE:HD1	2.04	0.65
1:C:184:HIS:NE2	1:C:188:TYR:CE2	2.65	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:33:LEU:HD22	1:D:34:PHE:CE1	2.32	0.65
1:D:306:ARG:NH1	1:D:306:ARG:HG3	2.11	0.65
1:D:73:ARG:CG	1:D:73:ARG:NH1	2.53	0.65
1:A:418:ALA:O	1:D:382:ARG:HD2	1.96	0.65
1:B:73:ARG:CG	1:B:73:ARG:NH1	2.48	0.65
1:D:129:ARG:O	1:D:130:ASP:HB2	1.96	0.65
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:B:128:PRO:HG2	1:B:170:MET:HE1	1.79	0.64
1:C:214:LEU:HA	1:C:304:THR:HG21	1.80	0.64
1:C:354:ARG:C	1:C:354:ARG:CD	2.69	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:OE1	1:C:193:GLU:CA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PHE:N	1:C:34:PHE:CD1	2.67	0.63
1:D:129:ARG:HH11	1:D:129:ARG:CG	2.10	0.62
1:B:119:PHE:CD2	1:B:351:LYS:HB2	2.33	0.62
1:A:354:ARG:C	1:A:354:ARG:CD	2.72	0.62
1:B:34:PHE:HE2	1:B:79:PHE:HD2	1.47	0.62
1:B:120:VAL:HB	1:B:121:PRO:HA	1.81	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
1:C:301:ARG:HG3	1:C:301:ARG:HH11	1.65	0.62
1:A:45:GLY:HA3	1:A:50:ARG:HH22	1.65	0.62
1:A:214:LEU:HA	1:A:304:THR:HG21	1.80	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:C:35:HIS:CD2	1:C:35:HIS:C	2.77	0.61
1:A:208:PHE:CD1	1:A:308:SER:HA	2.35	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:D:45:GLY:HA3	1:D:50:ARG:HH22	1.66	0.61
1:D:278:THR:HG23	1:D:281:SER:HB3	1.81	0.61
1:A:301:ARG:HG3	1:A:301:ARG:HH11	1.64	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:B:170:MET:HE2	1:B:170:MET:HA	1.83	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:HG2	1:B:239:ARG:HH11	1.64	0.60
1:C:182:ASP:OD1	1:C:183:MET:N	2.35	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HD11	1:A:330:THR:HG23	1.84	0.59
1:A:403:GLU:CD	1:A:403:GLU:H	2.10	0.59
1:B:31:PRO:HG2	1:B:32:GLY:H	1.66	0.59
1:B:34:PHE:N	1:B:34:PHE:HD1	1.99	0.59
1:B:34:PHE:N	1:B:34:PHE:CD1	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
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:42:ASP:OD2	1:B:191:LYS:NZ	2.34	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:D:193:GLU:OE1	1:D:193:GLU:CA	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:B:403:GLU:CD	1:B:403:GLU:H	2.11	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:33:LEU:C	1:B:34:PHE:HD1	2.11	0.58
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:HG3	1:C:179:ARG:HH11	1.69	0.58
1:C:128:PRO:HG2	1:C:170:MET:HE1	1.85	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:CD1	1:A:34:PHE:N	2.70	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:O	1:C:35:HIS:HD2	1.87	0.58
1:D:127:TYR:HB2	1:D:128:PRO:HD2	1.86	0.58
1:D:403:GLU:CD	1:D:403:GLU:H	2.12	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:170:MET:HA	1:C:170:MET:HE2	1.86	0.57
1:C:183:MET:HG3	1:C:184:HIS:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:SER:HB3	1:A:87:LYS:HE2	1.87	0.57
1:A:306:ARG:HG3	1:A:306:ARG:HH11	1.68	0.57
1:B:55:ALA:HB3	1:B:56:PRO:HD3	1.86	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
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
1:C:334:ARG:NH1	1:C:334:ARG:HG3	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: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:B:39:SER:HB3	1:B:87:LYS:HE2	1.87	0.56
1:C:119:PHE:CD2	1:C:351:LYS:HB2	2.40	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:54:VAL:CG1	1:D:57:LEU:HD12	2.36	0.56
1:D:356:HIS:CE1	2:D:501:FAD:O4	2.58	0.56
1:D:255:SER:O	1:D:257:PRO:HD3	2.06	0.56
1:C:47:ASP:C	1:C:47:ASP:OD1	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HH11	1:B:73:ARG:HG3	1.69	0.55
1:C:335:ASN:O	1:C:336:VAL:C	2.49	0.55
1:D:213:GLU:O	1:D:304:THR:CG2	2.55	0.55
1:D:239:ARG:HH11	1:D:239:ARG:CG	2.19	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:A:33:LEU:C	1:A:34:PHE:HD1	2.15	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:HD2	1:A:376:HIS:O	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:D:60:TRP:CZ3	1:D:99:THR:HB	2.42	0.54
1:D:393:LEU:HD12	1:D:393:LEU:N	2.22	0.54
1:A:242:LEU:O	1:A:246:GLU:HG3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ARG:HG3	1:D:306:ARG:HH11	1.73	0.54
1:B:128:PRO:CG	1:B:170:MET:HE1	2.38	0.54
1:C:393:LEU:HD12	1:C:393:LEU:N	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
1:D:60:TRP:CE3	1:D:99:THR:HB	2.44	0.53
1:D:173:ASP:HB2	1:D:176:LEU:CB	2.34	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:45:GLY:HA3	1:C:50:ARG:HH22	1.74	0.53
1:C:345:ARG:O	1:C:354:ARG:NH1	2.41	0.53
1:B:278:THR:HG23	1:B:281:SER:HB3	1.90	0.53
1:C:227:MET:HE3	1:C:282:TRP:HZ2	1.74	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:B:47:ASP:C	1:B:47:ASP:OD1	2.50	0.53
1:C:86:LEU:O	1:C:184:HIS:CE1	2.62	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:47:ASP:OD1	1:A:47:ASP:C	2.52	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:39:SER:CB	1:D:87:LYS:HE2	2.39	0.52
1:D:170:MET:HE2	1:D:170:MET:HA	1.90	0.52
1:D:183:MET:HG3	1:D:184:HIS:H	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:ARG:HH21	1:A:311:GLN:C	2.12	0.52
1:A:301:ARG:HG3	1:A:301:ARG:NH1	2.24	0.52
1:B:59:PRO:HG2	1:B:98:ALA:HA	1.91	0.52
1:B:251:LEU:HD11	1:B:330:THR:HG23	1.90	0.52
1:A:262:ASP:OD1	1:A:262:ASP:N	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
1:B:332:ALA:O	1:B:333:ASP:HB2	2.09	0.52
1:A:38:SER:HA	1:A:191:LYS:HD3	1.92	0.52
1:A:184:HIS:CD2	1:A:188:TYR:CZ	2.98	0.52
1:A:312:TYR:HB3	1:A:391:ASP:HB2	1.91	0.52
1:B:31:PRO:O	1:B:35:HIS:HB3	2.10	0.52
1:B:52:HIS:HB3	1:B:55:ALA:HB2	1.92	0.52
1:B:213:GLU:O	1:B:304:THR:HG22	2.09	0.52
1:B:392:PRO:HB2	1:B:393:LEU:HD12	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:47:ASP:OD1	1:D:47:ASP:C	2.53	0.52
1:D:312:TYR:HB3	1:D:391:ASP:HB2	1.91	0.52
1:B:48:PHE:O	1:B:55:ALA:HB3	2.10	0.51
1:B:370:LEU:HD21	1:B:417:GLU:HB3	1.92	0.51
1:C:128:PRO:CG	1:C:170:MET:HE1	2.41	0.51
1:C:403:GLU:H	1:C:403:GLU:CD	2.19	0.51
1:D:277:PHE:C	1:D:277:PHE:CD2	2.87	0.51
1:A:335:ASN:O	1:A:336:VAL:C	2.51	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:HD12	1:A:393:LEU:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:PHE:C	1:C:277:PHE:CD2	2.88	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:60:TRP:CZ3	1:C:99:THR:HB	2.46	0.51
1:C:301:ARG:HG3	1:C:301:ARG:NH1	2.25	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:71:ALA:HB3	1:B:352:GLU:OE1	2.10	0.51
1:B:330:THR:OG1	1:B:336:VAL:HG11	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:30:ARG:NE	1:B:31:PRO:HD2	2.25	0.50
1:B:283:GLN:O	1:B:287:VAL:HG23	2.10	0.50
1:A:60:TRP:CZ3	1:A:99:THR:HB	2.46	0.50
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:D:227:MET:HE3	1:D:282:TRP:HZ2	1.77	0.50
1:A:409:TYR:CE1	1:A:415:PHE:CE2	2.99	0.50
1:A:60:TRP:CE3	1:A:99:THR:HB	2.47	0.50
1:A:235:GLY:O	1:A:241:ARG:HD3	2.11	0.50
1:A:345:ARG:O	1:A:354:ARG:NH1	2.43	0.50
1:A:352:GLU:HG2	1:A:353:SER:H	1.75	0.50
1:B:89:GLU:HB2	1:B:90:HIS:ND1	2.26	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:C:166:VAL:HG13	1:C:170:MET:HG3	1.93	0.50
1:A:354:ARG:HD2	1:A:355:ASP:CA	2.41	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:67:ASP:O	1:D:73:ARG:NH1	2.44	0.50
1:D:242:LEU:O	1:D:246:GLU:HG3	2.12	0.50
1:A:376:HIS:HE1	2:A:501:FAD:C5B	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:143:LEU:CD2	2.72	0.49
1:D:107:SER:C	1:D:109:VAL:H	2.19	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:54:VAL:HG13	1:B:57:LEU:HD12	1.94	0.49
1:B:173:ASP:CB	1:B:176:LEU:H	2.24	0.49
1:D:128:PRO:HG2	1:D:170:MET:HE1	1.93	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:D:93:ASP:O	1:D:94:ALA:C	2.56	0.49
1:A:330:THR:OG1	1:A:336:VAL:CG1	2.61	0.49
1:B:277:PHE:C	1:B:277:PHE:CD2	2.91	0.49
1:C:403:GLU:O	1:C:404:ALA:C	2.56	0.49
1:D:239:ARG:HG2	1:D:239:ARG:HH11	1.77	0.49
1:B:65:TYR:HB2	1:B:72:SER:HB3	1.94	0.49
1:B:353:SER:HB3	2:B:501:FAD:N5	2.28	0.49
1:C:120:VAL:CB	1:C:121:PRO:HA	2.42	0.49
1:A:46:ASP:OD1	1:A:46:ASP:O	2.31	0.49
1:A:180:CYS:O	1:A:184:HIS:HB3	2.12	0.49
1:A:208:PHE:C	1:A:208:PHE:CD2	2.91	0.48
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:93:ASP:OD1	1:C:163:ARG:NH1	2.46	0.48
1:C:126:PHE:CE2	1:C:145:HIS:HB3	2.48	0.48
1:C:196:LYS:O	1:C:197:ARG:NE	2.46	0.48
1:C:208:PHE:CD2	1:C:208:PHE:C	2.90	0.48
1:D:237:GLU:O	1:D:241:ARG:NH1	2.46	0.48
1:D:374:ARG:NH1	1:D:374:ARG:HG3	2.27	0.48
1:D:399:PHE:CD1	1:D:400:PRO:HA	2.49	0.48
1:B:184:HIS:NE2	1:B:188:TYR:CZ	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:A:374:ARG:NH1	2.28	0.48
1:B:246:GLU:HG2	1:B:268:LEU:HD23	1.96	0.48
1:C:55:ALA:HB3	1:C:56:PRO:HD3	1.94	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: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:A:107:SER:C	1:A:109:VAL:H	2.21	0.48
1:B:195:VAL:HA	1:B:198:SER:HB2	1.96	0.48
1:D:52:HIS:CE1	1:D:183:MET:HB2	2.49	0.48
1:D:173:ASP:HB3	1:D:176:LEU:H	1.79	0.48
1:B:72:SER:OG	1:B:120:VAL:HG23	2.14	0.48
1:B:111:LEU:HD12	1:B:111:LEU:C	2.39	0.48
1:A:55:ALA:HB3	1:A:56:PRO:HD3	1.94	0.48
1:B:335:ASN:O	1:B:336:VAL:C	2.56	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: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
1:B:255:SER:OG	1:B:330:THR:HA	2.14	0.47
1:C:182:ASP:CG	1:C:183:MET:N	2.73	0.47
1:C:215:TYR:CE2	1:C:303:ARG:NH2	2.81	0.47
1:A:48:PHE:HA	1:A:51:VAL:HG12	1.96	0.47
1:A:186:LYS:O	1:A:190:SER:HB3	2.14	0.47
1:A:277:PHE:C	1:A:277:PHE:CD2	2.92	0.47
1:A:397:ARG:HD3	1:A:401:THR:HG22	1.95	0.47
1:C:107:SER:C	1:C:109:VAL:H	2.22	0.47
1:A:403:GLU:OE2	1:A:403:GLU:N	2.47	0.47
1:C:65:TYR:HB2	1:C:72:SER:HB3	1.96	0.47
1:C:111:LEU:HD12	1:C:111:LEU:O	2.14	0.47
1:A:126:PHE:CE2	1:A:145:HIS:HB3	2.50	0.47
1:A:259:ILE:O	1:A:259:ILE:HG23	2.15	0.47
1:A:332:ALA:O	1:A:333:ASP:HB2	2.15	0.47
1:A:419:HIS:CE1	1:D:360:PHE:CE1	3.02	0.47
2:A:501:FAD:O2A	2:A:501:FAD:O3'	2.21	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:O	1:B:337:LEU:N	2.47	0.47
1:D:52:HIS:CE1	1:D:54:VAL:HG23	2.49	0.47
1:A:173:ASP:CB	1:A:176:LEU:H	2.27	0.47
1:A:421:THR:HG23	1:D:382:ARG:CG	2.44	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:60:TRP:CZ2	1:D:183:MET:HE1	2.49	0.47
1:D:259:ILE:O	1:D:291:ILE:HG23	2.13	0.47
1:D:400:PRO:HB2	1:D:404:ALA:HB3	1.97	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:CG	1:A:73:ARG:NH1	2.62	0.47
1:B:360:PHE:CD1	1:C:419:HIS:CE1	3.03	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:D:397:ARG:HD3	1:D:401:THR:HG22	1.97	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:70:GLY:O	1:C:73:ARG:HB2	2.15	0.47
1:C:237:GLU:O	1:C:241:ARG:NH1	2.48	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
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:259:ILE:O	1:C:259:ILE:HG23	2.14	0.46
1:C:275:ARG:NH2	1:C:281:SER:HB2	2.17	0.46
1:D:73:ARG:HH21	1:D:312:TYR:HA	1.80	0.46
1:D:179:ARG:CG	1:D:179:ARG:HH11	2.29	0.46
1:D:255:SER:OG	1:D:330:THR:HA	2.15	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:A:86:LEU:O	1:A:184:HIS:HE1	1.95	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:48:PHE:HA	1:D:51:VAL:HG12	1.96	0.46
1:D:179:ARG:HG3	1:D:179:ARG:HH11	1.79	0.46
1:D:254:ASP:CG	1:D:334:ARG:NH2	2.73	0.46
1:D:403:GLU:OE2	1:D:403:GLU:N	2.49	0.46
1:B:179:ARG:HG3	1:B:179:ARG:NH1	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:63:LEU:HD11	1:A:121:PRO:HB2	1.96	0.46
1:A:189:THR:O	1:A:192:GLU:HB3	2.16	0.46
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.47	0.46
1:B:269:GLU:H	1:B:269:GLU:HG3	1.63	0.46
1:C:52:HIS:CE1	1:C:54:VAL:HG23	2.51	0.46
1:C:194:LEU:O	1:C:197:ARG:HG2	2.15	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:D:350:CYS:HB3	1:D:352:GLU:OE2	2.16	0.46
1:B:418:ALA:O	1:B:421:THR:HG22	2.15	0.46
1:C:34:PHE:HE2	1:C:79:PHE:CD2	2.34	0.46
1:C:173:ASP:CB	1:C:176:LEU:H	2.29	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:48:PHE:HA	1:C:51:VAL:HG12	1.97	0.45
1:C:283:GLN:O	1:C:287:VAL:HG23	2.15	0.45
1:D:46:ASP:OD1	1:D:46:ASP:O	2.34	0.45
1:A:43:LEU:N	1:A:43:LEU:HD23	2.30	0.45
1:A:343:TYR:CE1	1:A:347:PHE:HB2	2.51	0.45
1:B:48:PHE:HA	1:B:51:VAL:HG12	1.98	0.45
1:B:335:ASN:CB	1:B:338:GLU:HB3	2.31	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:46:ASP:OD1	1:B:46:ASP:O	2.34	0.45
1:B:78:THR:HG23	1:B:155:VAL:HG22	1.98	0.45
1:B:251:LEU:HD13	1:B:334:ARG:HG3	1.96	0.45
1:A:65:TYR:HB2	1:A:72:SER:HB3	1.98	0.45
1:A:403:GLU:O	1:A:404:ALA:C	2.59	0.45
1:B:60:TRP:CZ2	1:B:183:MET:HE1	2.52	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:O	1:D:111:LEU:HD12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:60:TRP:CE3	1:B:99:THR:HB	2.51	0.45
1:B:173:ASP:HB2	1:B:176:LEU:CB	2.39	0.45
1:C:194:LEU:HD23	1:C:194:LEU:HA	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:35:HIS:O	1:D:35:HIS:ND1	2.50	0.45
1:D:306:ARG:HH11	1:D:306:ARG:CG	2.30	0.45
1:B:259:ILE:O	1:B:259:ILE:HG23	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:D:335:ASN:O	1:D:336:VAL:C	2.60	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:93:ASP:O	1:B:94:ALA:C	2.60	0.44
1:B:311:GLN:OE1	1:B:311:GLN:N	2.45	0.44
1:B:350:CYS:HB3	1:B:352:GLU:OE2	2.17	0.44
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.66	0.44
1:D:33:LEU:HD13	1:D:65:TYR:CE1	2.52	0.44
1:D:48:PHE:CE2	1:D:60:TRP:CD1	3.05	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:A:52:HIS:CE1	1:A:54:VAL:HG23	2.52	0.44
1:A:376:HIS:O	1:A:376:HIS:CD2	2.70	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:OD1	1:D:262:ASP:N	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:D:403:GLU:O	1:D:404:ALA:C	2.61	0.44
1:A:182:ASP:OD1	1:A:183:MET:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PHE:CD2	1:B:208:PHE:C	2.96	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:73:ARG:NE	1:A:311:GLN:O	2.49	0.44
1:A:396:LYS:CE	2:A:501:FAD:H5'2	2.48	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:71:ALA:CB	1:C:352:GLU:OE1	2.63	0.44
1:C:235:GLY:O	1:C:241:ARG:HD3	2.17	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:64:PHE:HB2	1:B:122:ARG:HB3	2.00	0.44
1:B:275:ARG:HD2	1:B:275:ARG:HA	1.67	0.44
1:D:320:TRP:O	1:D:321:LEU:C	2.61	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: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:B:254:ASP:CG	1:B:334:ARG:NH2	2.76	0.43
1:C:189:THR:O	1:C:192:GLU:HB3	2.17	0.43
1:D:215:TYR:CE1	1:D:303:ARG:NH2	2.86	0.43
1:A:71:ALA:HB2	1:A:352:GLU:OE1	2.18	0.43
1:A:418:ALA:CB	1:D:356:HIS:HD2	2.31	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:HD23	1:D:194:LEU:HA	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:HD23	1:D:326:LEU:HA	1.75	0.43
1:D:332:ALA:O	1:D:333:ASP:HB2	2.18	0.43
1:D:352:GLU:HG2	1:D:353:SER:OG	2.18	0.43
1:B:215:TYR:CE2	1:B:303:ARG:NH2	2.86	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:LEU:HD11	1:C:73:ARG:HD3	2.01	0.43
1:D:128:PRO:CG	1:D:170:MET:HE1	2.49	0.43
1:D:208:PHE:CD2	1:D:208:PHE:C	2.97	0.43
1:D:301:ARG:HG3	1:D:301:ARG:NH1	2.33	0.43
1:A:111:LEU:HD12	1:A:111:LEU:C	2.44	0.43
2:A:501:FAD:H9	2:A:501:FAD:H1'1	1.74	0.43
1:B:48:PHE:O	1:B:51:VAL:HG12	2.18	0.43
1:C:48:PHE:O	1:C:51:VAL:CG1	2.67	0.43
1:C:111:LEU:HD12	1:C:111:LEU:C	2.44	0.43
1:B:374:ARG:HG3	1:B:374:ARG:HH11	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:C9A	2:A:501:FAD:O2'	2.67	0.42
1:B:43:LEU:HB2	1:B:103:VAL:HG22	2.00	0.42
1:D:370:LEU:O	1:D:373:TRP:HB3	2.20	0.42
1:A:374:ARG:HG3	1:A:374:ARG:HH11	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:O	1:C:195:VAL:HG12	2.20	0.41
1:D:344:ILE:O	1:D:345:ARG:C	2.62	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:D:336:VAL:O	1:D:337:LEU:C	2.62	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:48:PHE:O	1:C:51:VAL:HG12	2.20	0.41
1:C:246:GLU:HG2	1:C:268:LEU:HD23	2.01	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:67:ASP:O	1:C:73:ARG:NH1	2.53	0.41
1:C:390:ALA:O	1:C:392:PRO:HD3	2.20	0.41
1:D:34:PHE:CE1	1:D:76:ALA:HB1	2.55	0.41
1:D:402:LEU:CA	1:D:409:TYR:HE2	2.33	0.41
1:A:48:PHE:O	1:A:51:VAL:HG12	2.20	0.41
1:A:311:GLN:OE1	1:A:311:GLN:N	2.45	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
1:D:253:LYS:HD2	1:D:262:ASP:HA	2.03	0.41
1:A:122:ARG:HA	1:A:122:ARG:HD2	1.82	0.41
1:B:29:PRO:HA	1:B:298:ARG:NH2	2.36	0.41
1:B:267:ALA:HB2	1:B:285:ALA:HB1	2.02	0.41
1:C:391:ASP:OD1	1:C:391:ASP:C	2.62	0.41
1:A:34:PHE:CE2	1:A:79:PHE:HD2	2.35	0.41
1:A:390:ALA:O	1:A:392:PRO:HD3	2.21	0.41
1:C:269:GLU:H	1:C:269:GLU:HG3	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:HD2	1:D:275:ARG:HA	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:C9A	2:D:501:FAD:O2'	2.68	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:370:LEU:HA	1:A:370:LEU:HD12	1.77	0.41
1:A:418:ALA:HB1	1:D:356:HIS:CD2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ASP:OD1	1:A:432:PRO:CD	2.68	0.41
1:B:385:ASN:HD21	1:C:425:LYS:HE2	1.84	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:154:GLU:O	1:C:155:VAL:C	2.62	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:C:227:MET:HE2	1:C:264:VAL:HG11	2.03	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:30:ARG:HG3	1:B:299:ASN:OD1	2.21	0.40
1:B:173:ASP:HB3	1:B:176:LEU:H	1.85	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:118:ASN:OD1	1:D:118:ASN:C	2.64	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:B:354:ARG:NH1	1:B:354:ARG:HG2	2.36	0.40
1:C:334:ARG:O	1:C:335:ASN:CB	2.59	0.40
1:C:352:GLU:HG2	1:C:353:SER:H	1.84	0.40
1:D:127:TYR:C	1:D:143:LEU:HD13	2.46	0.40
1:D:335:ASN:C	1:D:336:VAL:CG2	2.94	0.40
1:B:86:LEU:O	1:B:184:HIS:HE1	2.00	0.40
1:C:34:PHE:CE2	1:C:79:PHE:HD2	2.37	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: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:D:88:VAL:HB	1:D:96:GLN:CD	2.46	0.40
1:D:111:LEU:HD12	1:D:111:LEU:C	2.47	0.40
1:D:227:MET:HE1	1:D:245:LEU:HD11	2.03	0.40
1:A:35:HIS:ND1	1:A:35:HIS:C	2.76	0.40
1:B:70:GLY:O	1:B:73:ARG:HB2	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:LEU:HD12	1:B:372:LEU:HA	1.89	0.40
1:D:255:SER:C	1:D:257:PRO:HD3	2.46	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%)	36	65
1	B	384/470 (82%)	360 (94%)	23 (6%)	1 (0%)	36	65
1	C	379/470 (81%)	355 (94%)	23 (6%)	1 (0%)	36	65
1	D	378/470 (80%)	352 (93%)	25 (7%)	1 (0%)	36	65
All	All	1523/1880 (81%)	1425 (94%)	94 (6%)	4 (0%)	36	65

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%)	280 (85%)	48 (15%)	3	14
1	B	335/400 (84%)	280 (84%)	55 (16%)	2	11
1	C	332/400 (83%)	282 (85%)	50 (15%)	3	13
1	D	333/400 (83%)	280 (84%)	53 (16%)	2	12
All	All	1328/1600 (83%)	1122 (84%)	206 (16%)	2	12

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	PHE
1	A	35	HIS
1	A	39	SER
1	A	43	LEU
1	A	44	SER
1	A	47	ASP
1	A	51	VAL
1	A	57	LEU
1	A	73	ARG
1	A	88	VAL
1	A	89	GLU
1	A	97	ILE
1	A	111	LEU
1	A	117	ILE
1	A	155	VAL
1	A	156	ASP
1	A	160	SER
1	A	170	MET
1	A	172	VAL
1	A	178	GLU
1	A	182	ASP
1	A	183	MET
1	A	193	GLU
1	A	211	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	217	THR
1	A	233	LEU
1	A	236	THR
1	A	239	ARG
1	A	250	LEU
1	A	258	SER
1	A	262	ASP
1	A	265	VAL
1	A	271	ILE
1	A	274	GLU
1	A	275	ARG
1	A	278	THR
1	A	291	ILE
1	A	306	ARG
1	A	317	CYS
1	A	335	ASN
1	A	351	LYS
1	A	354	ARG
1	A	374	ARG
1	A	403	GLU
1	A	406	THR
1	A	407	GLU
1	A	414	ASN
1	A	420	VAL
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	51	VAL
1	B	57	LEU
1	B	73	ARG
1	B	88	VAL
1	B	89	GLU
1	B	97	ILE
1	B	111	LEU
1	B	117	ILE
1	B	120	VAL
1	B	143	LEU
1	B	155	VAL
1	B	156	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	160	SER
1	B	170	MET
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	196	LYS
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	265	VAL
1	B	269	GLU
1	B	271	ILE
1	B	275	ARG
1	B	278	THR
1	B	291	ILE
1	B	306	ARG
1	B	310	PRO
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	B	420	VAL
1	C	33	LEU
1	C	34	PHE
1	C	35	HIS
1	C	39	SER
1	C	43	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	44	SER
1	C	47	ASP
1	C	51	VAL
1	C	57	LEU
1	C	73	ARG
1	C	88	VAL
1	C	97	ILE
1	C	111	LEU
1	C	117	ILE
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	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	265	VAL
1	C	271	ILE
1	C	275	ARG
1	C	278	THR
1	C	291	ILE
1	C	306	ARG
1	C	334	ARG
1	C	351	LYS
1	C	354	ARG
1	C	403	GLU
1	C	406	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	407	GLU
1	C	414	ASN
1	C	420	VAL
1	D	33	LEU
1	D	35	HIS
1	D	39	SER
1	D	43	LEU
1	D	44	SER
1	D	47	ASP
1	D	51	VAL
1	D	57	LEU
1	D	73	ARG
1	D	88	VAL
1	D	89	GLU
1	D	90	HIS
1	D	97	ILE
1	D	111	LEU
1	D	117	ILE
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	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	265	VAL
1	D	269	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	271	ILE
1	D	274	GLU
1	D	275	ARG
1	D	278	THR
1	D	291	ILE
1	D	306	ARG
1	D	351	LYS
1	D	354	ARG
1	D	374	ARG
1	D	403	GLU
1	D	406	THR
1	D	407	GLU
1	D	414	ASN
1	D	420	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	GLN
1	B	371	GLN
1	C	356	HIS
1	C	371	GLN
1	D	335	ASN
1	D	371	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	501	-	58,58,58	1.78	14 (24%)	85,89,89	1.76	18 (21%)
2	FAD	C	501	-	58,58,58	1.15	6 (10%)	85,89,89	1.76	21 (24%)
2	FAD	A	501	-	58,58,58	1.25	6 (10%)	85,89,89	2.01	25 (29%)
2	FAD	D	501	-	58,58,58	1.47	7 (12%)	85,89,89	2.00	25 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	501	-	-	8/34/50/50	0/6/6/6
2	FAD	C	501	-	-	7/34/50/50	0/6/6/6
2	FAD	A	501	-	-	11/34/50/50	0/6/6/6
2	FAD	D	501	-	-	10/34/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	PA-O3P	-6.95	1.52	1.59
2	D	501	FAD	P-O3P	5.17	1.65	1.59
2	C	501	FAD	C4X-N5	3.92	1.39	1.30
2	A	501	FAD	C4X-N5	3.78	1.38	1.30
2	D	501	FAD	C4X-N5	3.71	1.38	1.30
2	B	501	FAD	PA-O2A	-3.60	1.38	1.55
2	B	501	FAD	C4X-N5	3.53	1.38	1.30
2	D	501	FAD	C10-N1	3.52	1.40	1.33
2	D	501	FAD	PA-O3P	3.22	1.63	1.59
2	D	501	FAD	C2A-N3A	3.17	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C8A-N7A	3.05	1.37	1.31
2	C	501	FAD	C10-N1	3.04	1.39	1.33
2	A	501	FAD	C8A-N7A	2.99	1.37	1.31
2	A	501	FAD	C9A-N10	-2.96	1.36	1.41
2	D	501	FAD	C2A-N1A	2.95	1.39	1.33
2	B	501	FAD	P-O3P	2.93	1.62	1.59
2	B	501	FAD	PA-O1A	-2.91	1.40	1.50
2	A	501	FAD	C2A-N1A	2.70	1.38	1.33
2	C	501	FAD	C2A-N3A	2.68	1.38	1.33
2	B	501	FAD	C10-N1	2.61	1.38	1.33
2	B	501	FAD	C9A-N10	-2.61	1.36	1.41
2	C	501	FAD	C9A-N10	-2.58	1.36	1.41
2	B	501	FAD	C1'-C2'	2.57	1.56	1.52
2	B	501	FAD	C2A-N1A	2.53	1.38	1.33
2	B	501	FAD	O4B-C4B	-2.39	1.39	1.45
2	D	501	FAD	C8A-N7A	2.31	1.36	1.31
2	B	501	FAD	C9-C8	-2.24	1.36	1.39
2	B	501	FAD	PA-O5B	-2.24	1.50	1.59
2	A	501	FAD	PA-O2A	-2.16	1.45	1.55
2	A	501	FAD	C1'-C2'	2.12	1.55	1.52
2	C	501	FAD	C5'-C4'	2.10	1.54	1.51
2	B	501	FAD	C2A-N3A	2.03	1.37	1.33
2	C	501	FAD	P-O2P	-2.01	1.46	1.55

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	N3A-C2A-N1A	-6.27	119.09	128.58
2	A	501	FAD	O2A-PA-O3P	5.71	122.72	107.27
2	B	501	FAD	C5A-C4A-N3A	-5.18	119.58	126.72
2	C	501	FAD	N3A-C2A-N1A	-5.01	121.00	128.58
2	D	501	FAD	C5A-C4A-N3A	-4.97	119.87	126.72
2	D	501	FAD	C1'-C2'-C3'	4.85	122.80	109.66
2	B	501	FAD	N3A-C2A-N1A	-4.75	121.39	128.58
2	A	501	FAD	C1'-C2'-C3'	4.62	122.17	109.66
2	D	501	FAD	N3A-C2A-N1A	-4.61	121.61	128.58
2	A	501	FAD	C5A-C4A-N3A	-4.52	120.49	126.72
2	D	501	FAD	C4'-C3'-C2'	4.52	121.08	113.57
2	C	501	FAD	N9A-C8A-N7A	-4.49	107.57	113.94
2	C	501	FAD	C5A-C4A-N3A	-4.42	120.63	126.72
2	B	501	FAD	C4A-C5A-N7A	-4.18	105.80	110.58
2	B	501	FAD	N9A-C8A-N7A	-4.15	108.05	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C5A-N7A-C8A	4.06	109.83	103.45
2	D	501	FAD	C5X-C9A-N10	4.05	121.63	117.97
2	D	501	FAD	N9A-C8A-N7A	-3.80	108.54	113.94
2	A	501	FAD	C2A-N3A-C4A	3.77	121.04	111.83
2	C	501	FAD	C9-C9A-N10	-3.73	116.84	121.85
2	C	501	FAD	C1'-C2'-C3'	3.71	119.71	109.66
2	D	501	FAD	O4-C4-C4X	-3.63	116.96	126.53
2	A	501	FAD	C9-C9A-N10	-3.61	117.00	121.85
2	D	501	FAD	C4-N3-C2	-3.61	119.23	125.64
2	A	501	FAD	N9A-C8A-N7A	-3.59	108.84	113.94
2	A	501	FAD	C4-C4X-N5	3.56	123.12	118.21
2	C	501	FAD	C5A-N7A-C8A	3.55	109.03	103.45
2	D	501	FAD	N3A-C4A-N9A	3.51	133.13	127.17
2	B	501	FAD	C4-N3-C2	-3.47	119.48	125.64
2	D	501	FAD	C4X-C4-N3	3.36	121.81	113.25
2	A	501	FAD	C4X-C10-N10	3.35	121.28	116.48
2	B	501	FAD	C2A-N3A-C4A	3.30	119.89	111.83
2	C	501	FAD	N3A-C4A-N9A	3.30	132.78	127.17
2	B	501	FAD	C1'-C2'-C3'	3.27	118.51	109.66
2	D	501	FAD	C2A-N3A-C4A	3.26	119.80	111.83
2	D	501	FAD	C5A-N7A-C8A	3.26	108.57	103.45
2	B	501	FAD	C5X-C9A-N10	3.25	120.90	117.97
2	B	501	FAD	C9-C9A-N10	-3.23	117.51	121.85
2	C	501	FAD	C2A-N3A-C4A	3.23	119.72	111.83
2	B	501	FAD	C5A-C4A-N9A	3.15	109.24	105.81
2	C	501	FAD	C4A-N9A-C8A	3.13	109.03	105.74
2	D	501	FAD	O2P-P-O3P	3.08	115.60	107.27
2	C	501	FAD	C4'-C3'-C2'	3.05	118.65	113.57
2	A	501	FAD	C5A-N7A-C8A	2.99	108.15	103.45
2	D	501	FAD	C9A-C5X-N5	-2.96	119.31	122.45
2	D	501	FAD	O3P-PA-O1A	2.93	119.53	110.70
2	A	501	FAD	O4B-C4B-C5B	-2.88	100.12	109.33
2	A	501	FAD	O2-C2-N1	-2.82	117.11	121.80
2	C	501	FAD	C4X-C10-N10	2.79	120.47	116.48
2	B	501	FAD	O2-C2-N1	-2.71	117.29	121.80
2	B	501	FAD	O4-C4-C4X	-2.69	119.42	126.53
2	C	501	FAD	C4-C4X-N5	2.68	121.91	118.21
2	A	501	FAD	C2'-C1'-N10	-2.67	97.59	110.20
2	A	501	FAD	O2-C2-N3	2.65	123.66	118.58
2	A	501	FAD	C10-C4X-N5	-2.63	119.43	124.81
2	D	501	FAD	C2B-C1B-N9A	-2.62	106.78	113.30
2	A	501	FAD	N3A-C4A-N9A	2.58	131.55	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FAD	C6A-C5A-C4A	2.55	120.66	117.18
2	C	501	FAD	C5X-C9A-N10	2.52	120.25	117.97
2	B	501	FAD	C6A-C5A-C4A	2.52	120.61	117.18
2	A	501	FAD	C4-N3-C2	-2.50	121.21	125.64
2	B	501	FAD	C4X-C4-N3	2.49	119.58	113.25
2	C	501	FAD	C2'-C1'-N10	-2.47	98.52	110.20
2	C	501	FAD	C4A-C5A-N7A	-2.46	107.77	110.58
2	C	501	FAD	C4X-C4-N3	2.46	119.50	113.25
2	A	501	FAD	C5X-C9A-N10	2.45	120.18	117.97
2	C	501	FAD	O4-C4-C4X	-2.45	120.07	126.53
2	A	501	FAD	C4X-C4-N3	2.45	119.48	113.25
2	A	501	FAD	O3B-C3B-C4B	2.41	117.99	111.08
2	D	501	FAD	C4X-C10-N1	-2.36	118.80	124.59
2	B	501	FAD	N3A-C4A-N9A	2.36	131.17	127.17
2	A	501	FAD	C6-C5X-N5	2.32	122.30	118.44
2	D	501	FAD	C4A-C5A-N7A	-2.30	107.95	110.58
2	D	501	FAD	C10-N1-C2	2.22	121.66	116.85
2	A	501	FAD	C4A-C5A-N7A	-2.20	108.07	110.58
2	C	501	FAD	C10-C4X-N5	-2.19	120.34	124.81
2	D	501	FAD	C3B-C2B-C1B	2.18	105.59	101.46
2	B	501	FAD	C4X-C10-N10	2.17	119.59	116.48
2	D	501	FAD	O4'-C4'-C3'	2.15	114.29	109.25
2	D	501	FAD	O4'-C4'-C5'	-2.13	105.29	109.99
2	C	501	FAD	O2B-C2B-C1B	-2.10	102.87	110.10
2	D	501	FAD	C4A-N9A-C8A	2.09	107.94	105.74
2	A	501	FAD	O2P-P-O3P	2.08	112.90	107.27
2	D	501	FAD	O2'-C2'-C1'	-2.08	101.65	110.20
2	A	501	FAD	O4-C4-C4X	-2.05	121.13	126.53
2	C	501	FAD	C4-N3-C2	-2.04	122.03	125.64
2	B	501	FAD	C2'-C1'-N10	-2.01	100.72	110.20
2	A	501	FAD	O4B-C1B-N9A	2.00	111.94	108.09
2	C	501	FAD	O4B-C1B-N9A	2.00	111.94	108.09

There are no chirality outliers.

All (36) 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	C5B-O5B-PA-O3P
2	A	501	FAD	C2'-C3'-C4'-O4'
2	A	501	FAD	C2'-C3'-C4'-C5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	O4'-C4'-C5'-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	D	501	FAD	C5B-O5B-PA-O1A
2	D	501	FAD	C5B-O5B-PA-O3P
2	B	501	FAD	C2'-C3'-C4'-O4'
2	D	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	O3'-C3'-C4'-O4'
2	B	501	FAD	O3'-C3'-C4'-O4'
2	D	501	FAD	C3B-C4B-C5B-O5B
2	A	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	C2'-C3'-C4'-C5'
2	B	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
2	A	501	FAD	C3'-C4'-C5'-O5'
2	D	501	FAD	C2B-C1B-N9A-C8A
2	B	501	FAD	C5'-O5'-P-O1P
2	C	501	FAD	C5'-O5'-P-O1P
2	C	501	FAD	C5'-O5'-P-O3P
2	D	501	FAD	C5B-O5B-PA-O2A
2	D	501	FAD	C5'-O5'-P-O1P
2	D	501	FAD	C5'-O5'-P-O3P
2	A	501	FAD	PA-O3P-P-O1P
2	C	501	FAD	PA-O3P-P-O2P
2	D	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	PA-O3P-P-O2P

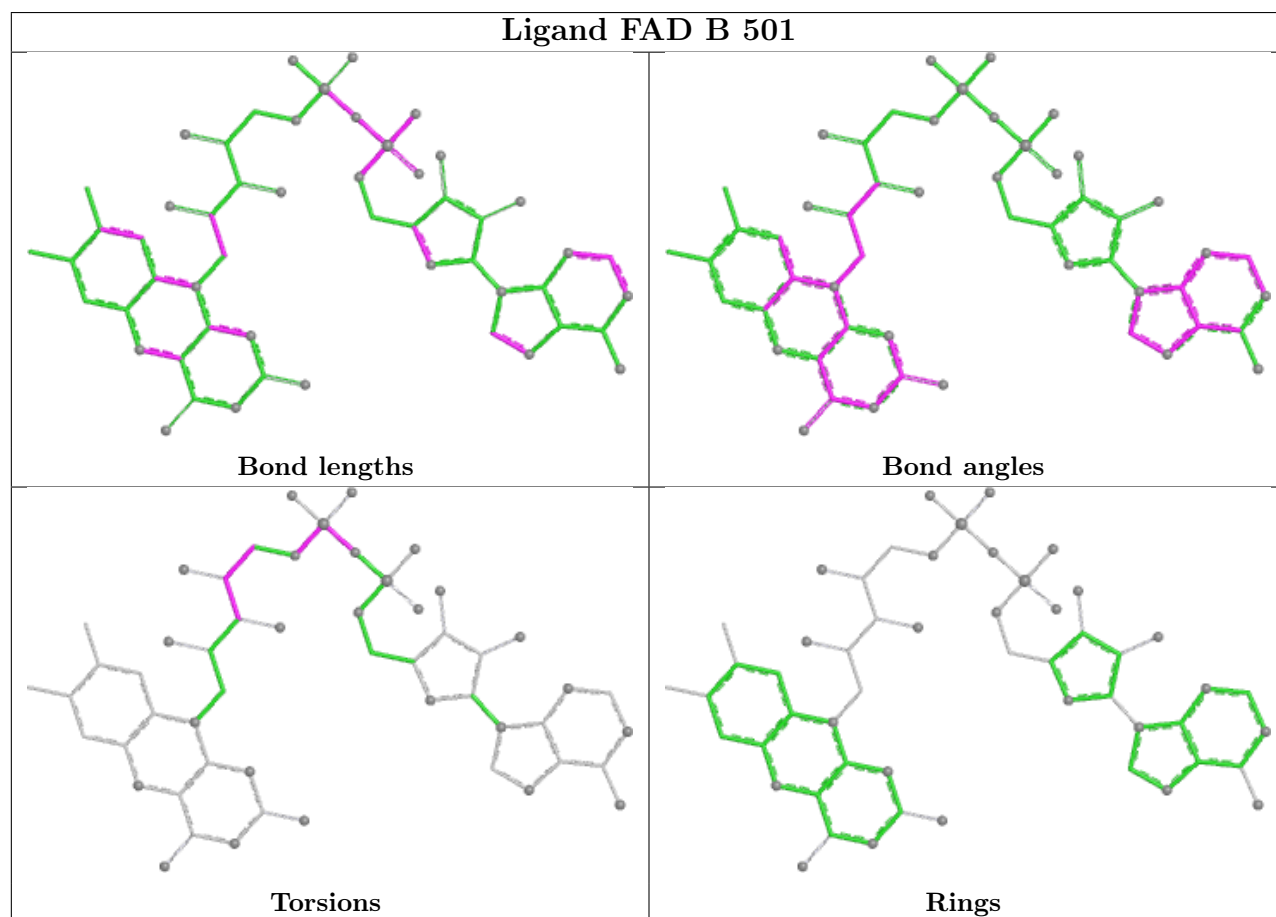
There are no ring outliers.

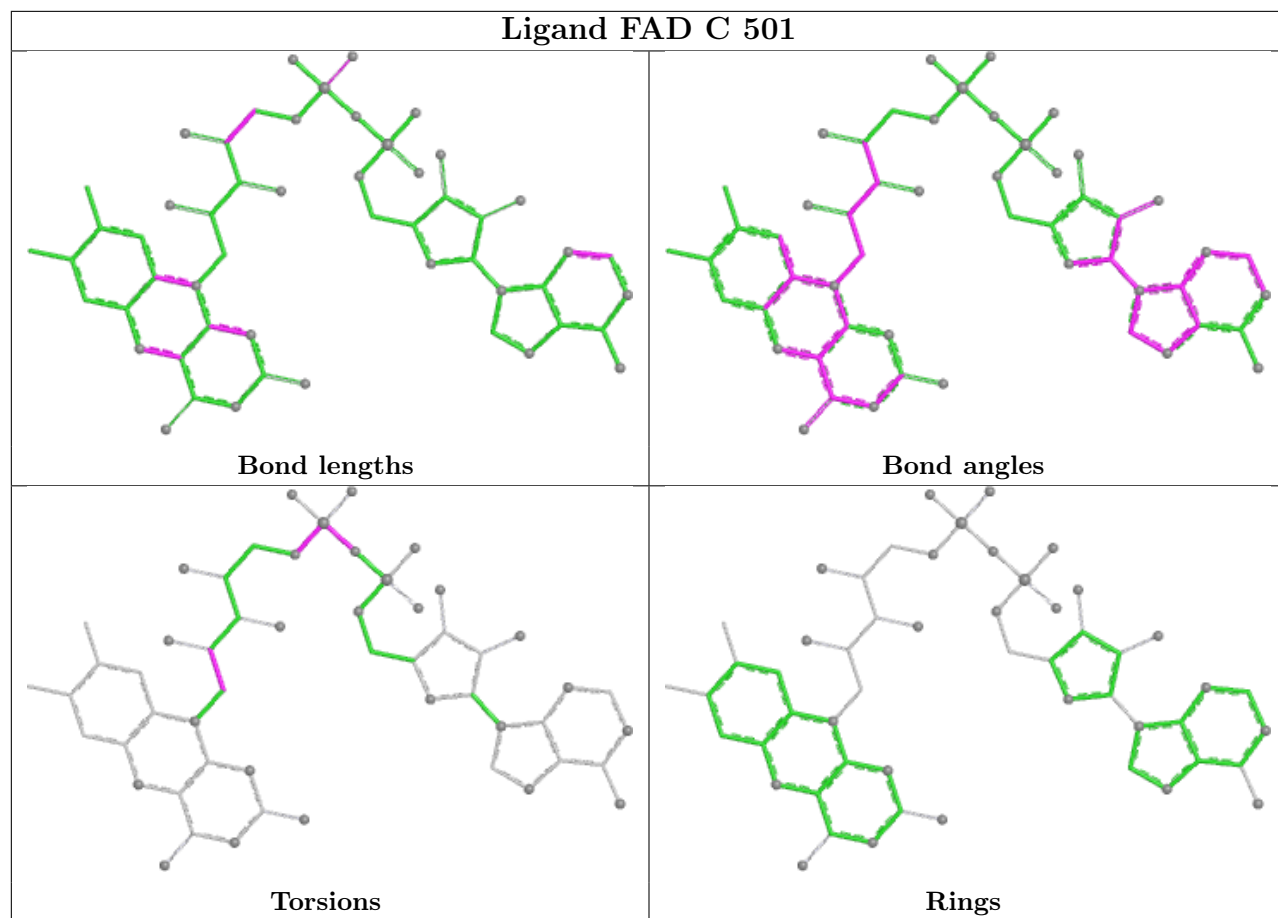
4 monomers are involved in 25 short contacts:

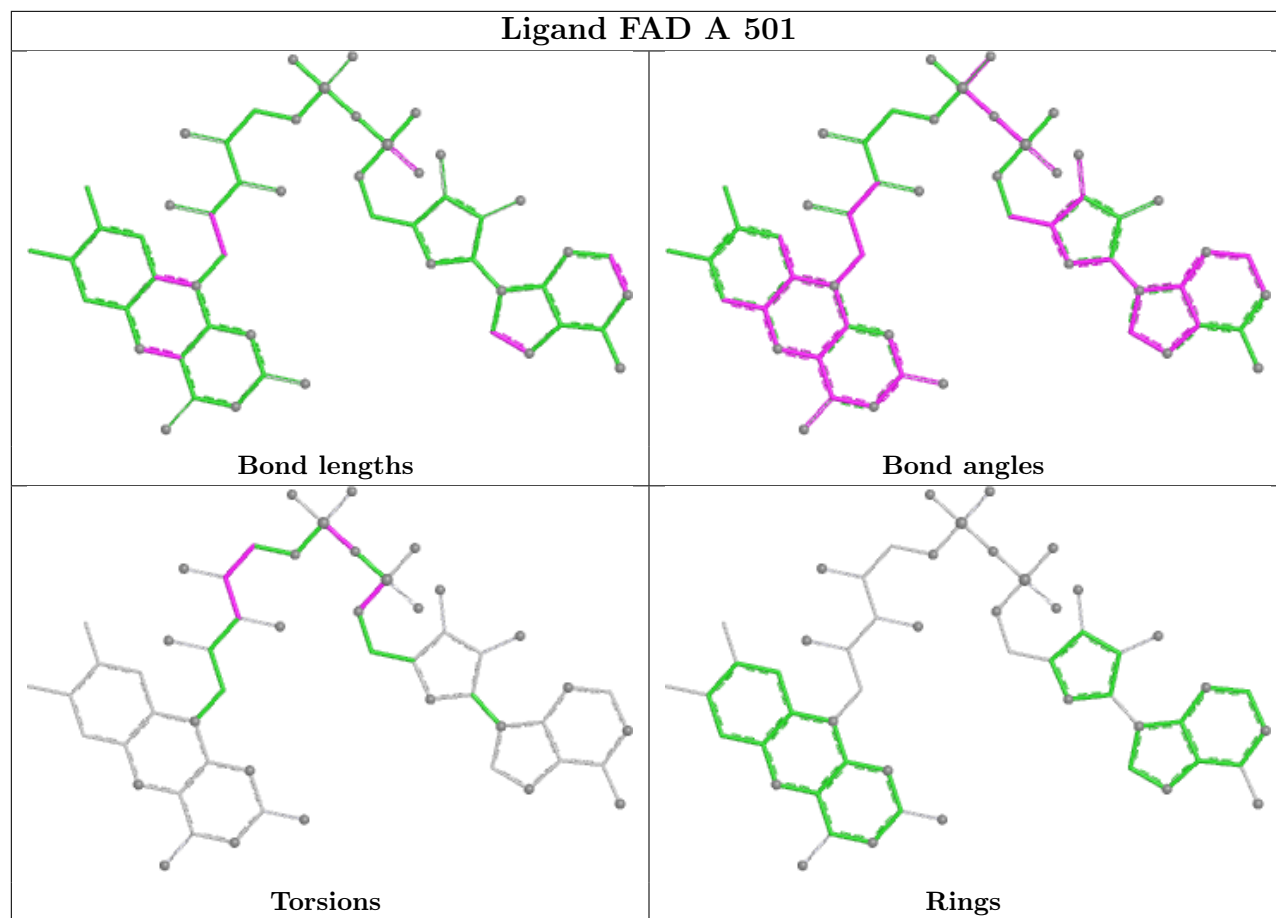
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FAD	2	0
2	C	501	FAD	2	0
2	A	501	FAD	9	0
2	D	501	FAD	12	0

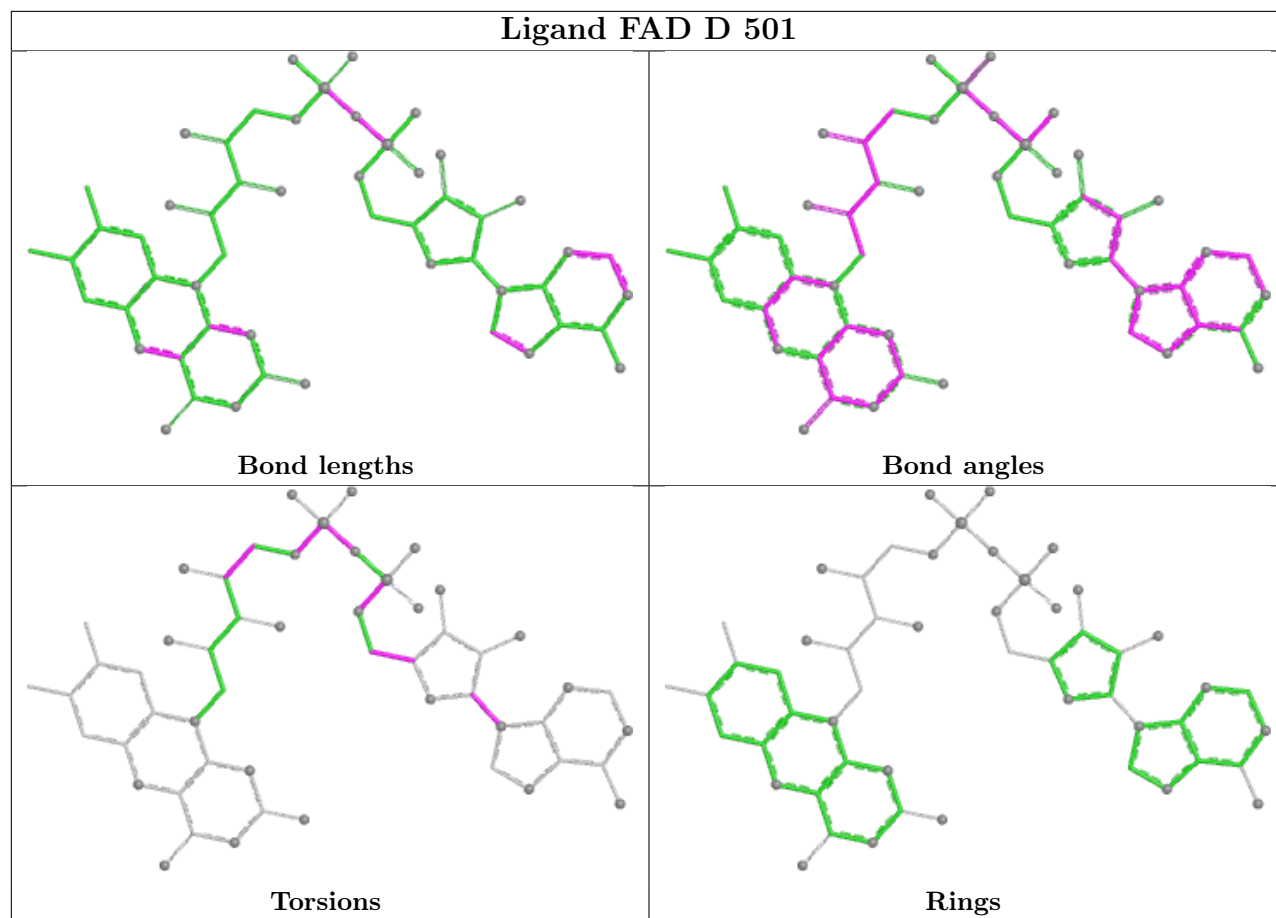
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/470 (82%)	-0.04	0 100 100	42, 82, 149, 216	0
1	B	390/470 (82%)	-0.02	4 (1%) 79 63	29, 81, 145, 223	0
1	C	385/470 (81%)	-0.05	0 100 100	38, 83, 147, 248	0
1	D	384/470 (81%)	0.29	4 (1%) 79 63	55, 97, 151, 204	0
All	All	1547/1880 (82%)	0.04	8 (0%) 87 76	29, 86, 149, 248	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	HIS	3.6
1	B	88	VAL	3.5
1	B	96	GLN	2.9
1	B	404	ALA	2.9
1	D	356	HIS	2.6
1	D	297	PRO	2.6
1	D	259	ILE	2.4
1	D	199	VAL	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

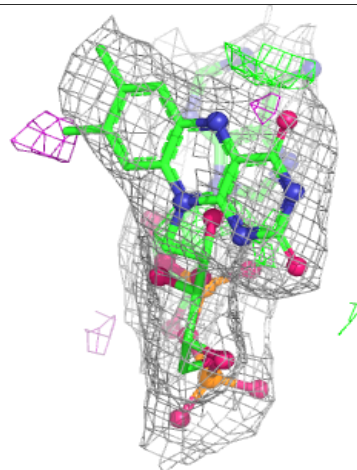
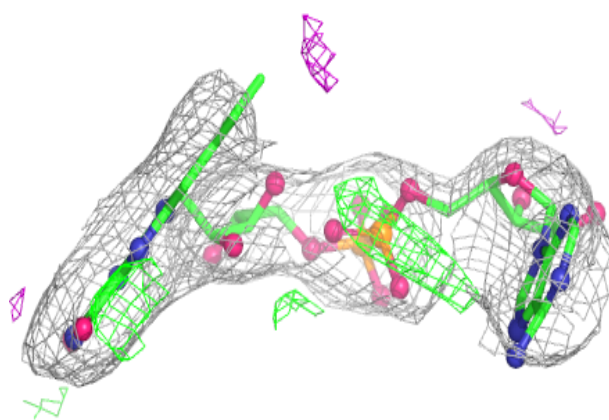
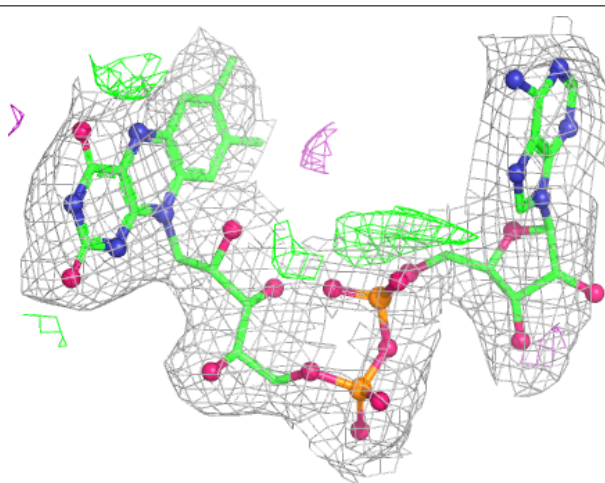
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	D	501	53/53	0.93	0.09	18,70,98,107	0
2	FAD	B	501	53/53	0.95	0.09	0,42,66,150	0
2	FAD	C	501	53/53	0.97	0.06	7,48,77,99	0
2	FAD	A	501	53/53	0.97	0.07	21,53,79,103	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.

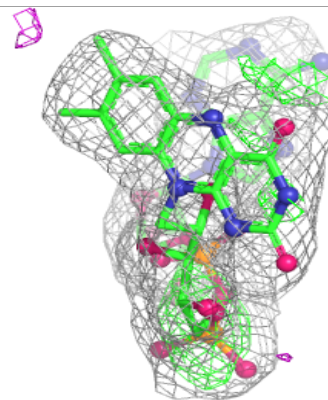
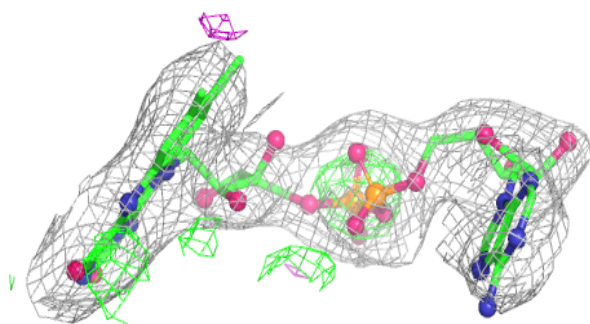
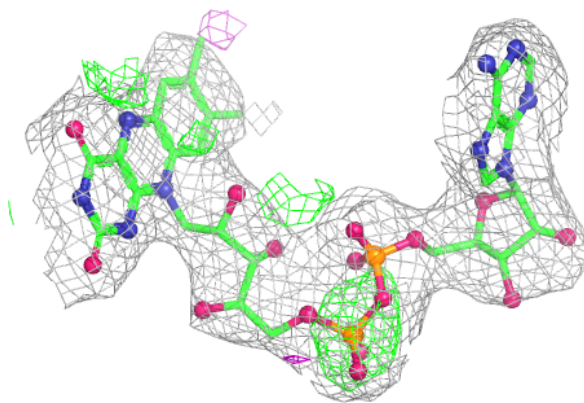
Electron density around FAD D 501:

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



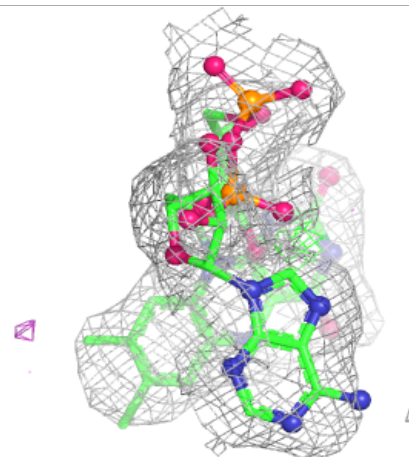
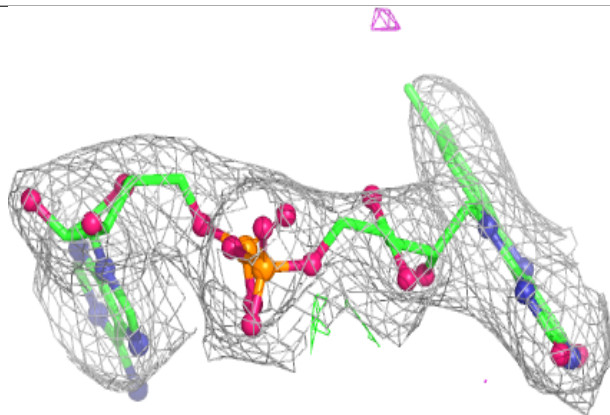
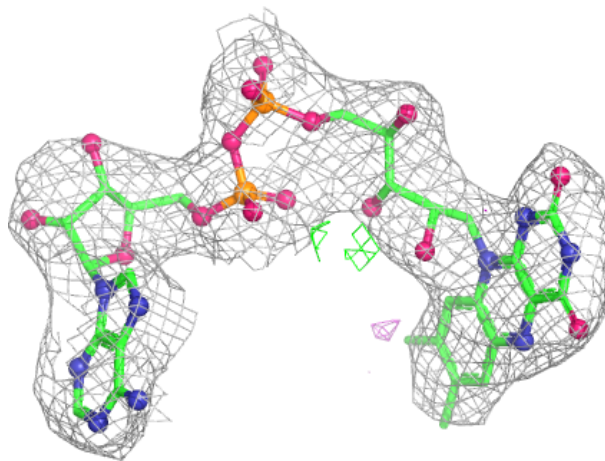
Electron density around FAD B 501:

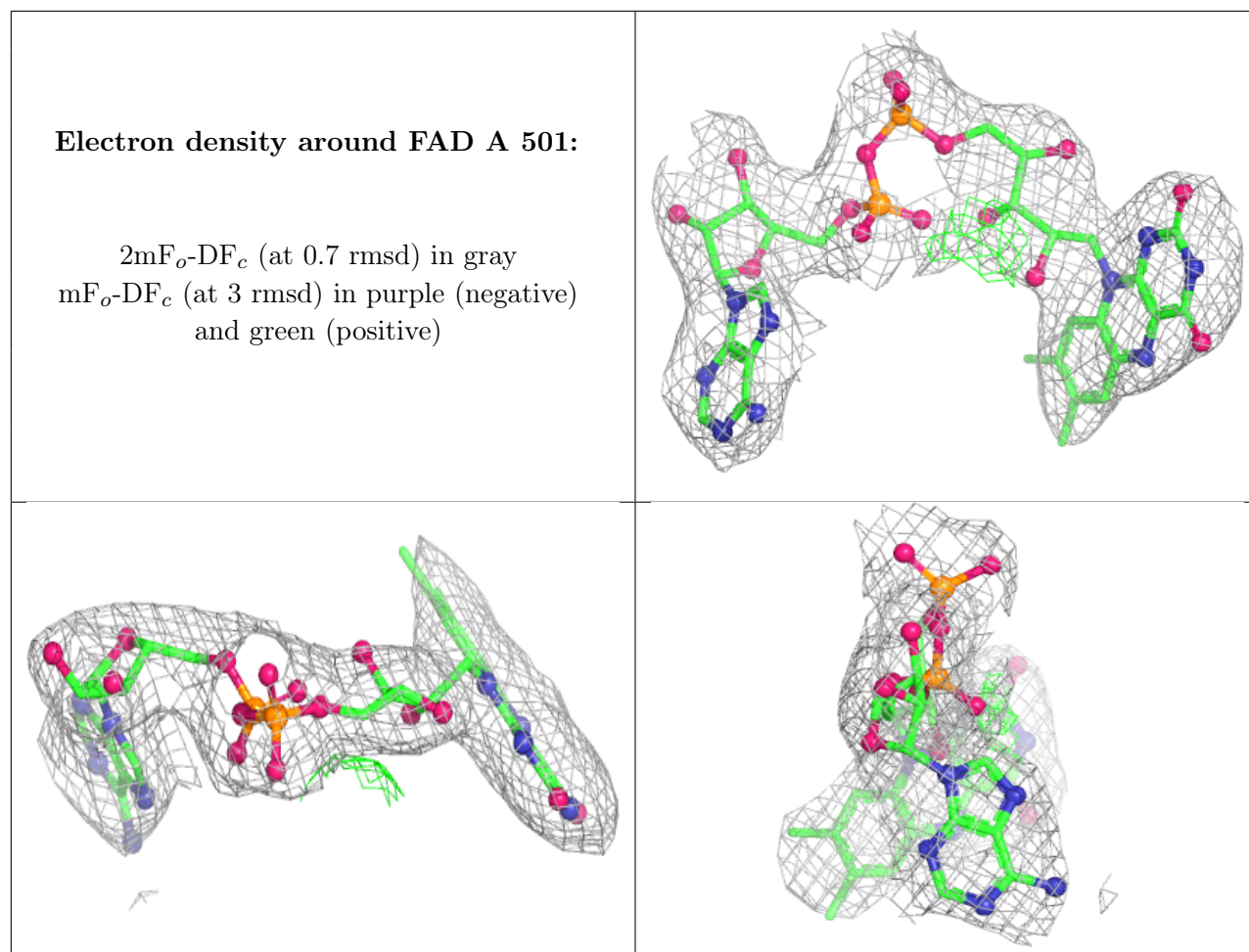
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FAD C 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 [i](#)

There are no such residues in this entry.