



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:29 PM UTC

PDB ID : 7KHO / pdb_00007kho
Title : NicA2 variant N462V in complex with (S)-nicotine
Authors : Tararina, M.A.; Allen, K.N.
Deposited on : 2020-10-21
Resolution : 2.69 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

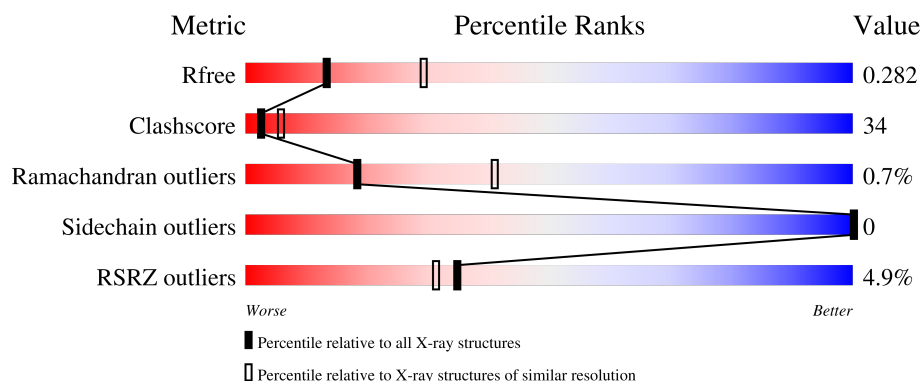
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	490	 3% 51% 36% 12%
1	B	490	 2% 55% 33% 12%
1	C	490	 4% 42% 45% 12%
1	D	490	 7% 39% 42% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FAD	D	502	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13600 atoms, of which 112 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 Amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3353	2127	582	632	12			
1	B	432	Total	C	N	O	S	0	0	0
			3353	2127	582	632	12			
1	C	432	Total	C	N	O	S	0	0	0
			3353	2127	582	632	12			
1	D	405	Total	C	N	O	S	0	0	0
			3152	2002	544	594	12			

There are 36 discrepancies between the modelled and reference sequences:

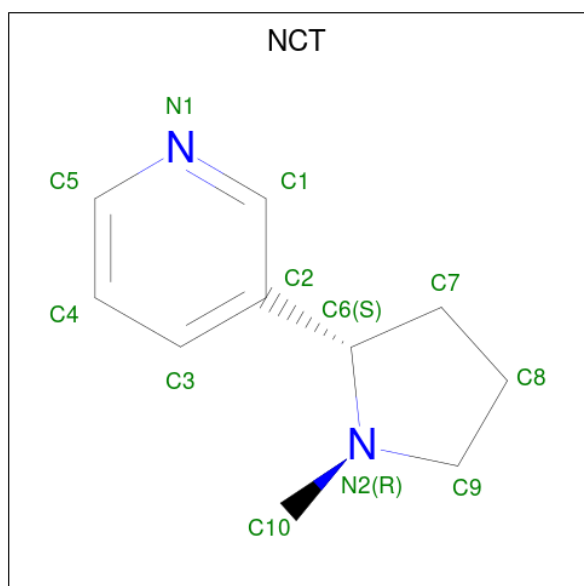
Chain	Residue	Modelled	Actual	Comment	Reference
A	462	VAL	ASN	engineered mutation	UNP F8G0P2
A	483	LEU	-	expression tag	UNP F8G0P2
A	484	GLU	-	expression tag	UNP F8G0P2
A	485	HIS	-	expression tag	UNP F8G0P2
A	486	HIS	-	expression tag	UNP F8G0P2
A	487	HIS	-	expression tag	UNP F8G0P2
A	488	HIS	-	expression tag	UNP F8G0P2
A	489	HIS	-	expression tag	UNP F8G0P2
A	490	HIS	-	expression tag	UNP F8G0P2
B	462	VAL	ASN	engineered mutation	UNP F8G0P2
B	483	LEU	-	expression tag	UNP F8G0P2
B	484	GLU	-	expression tag	UNP F8G0P2
B	485	HIS	-	expression tag	UNP F8G0P2
B	486	HIS	-	expression tag	UNP F8G0P2
B	487	HIS	-	expression tag	UNP F8G0P2
B	488	HIS	-	expression tag	UNP F8G0P2
B	489	HIS	-	expression tag	UNP F8G0P2
B	490	HIS	-	expression tag	UNP F8G0P2
C	462	VAL	ASN	engineered mutation	UNP F8G0P2
C	483	LEU	-	expression tag	UNP F8G0P2
C	484	GLU	-	expression tag	UNP F8G0P2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	485	HIS	-	expression tag	UNP F8G0P2
C	486	HIS	-	expression tag	UNP F8G0P2
C	487	HIS	-	expression tag	UNP F8G0P2
C	488	HIS	-	expression tag	UNP F8G0P2
C	489	HIS	-	expression tag	UNP F8G0P2
C	490	HIS	-	expression tag	UNP F8G0P2
D	462	VAL	ASN	engineered mutation	UNP F8G0P2
D	483	LEU	-	expression tag	UNP F8G0P2
D	484	GLU	-	expression tag	UNP F8G0P2
D	485	HIS	-	expression tag	UNP F8G0P2
D	486	HIS	-	expression tag	UNP F8G0P2
D	487	HIS	-	expression tag	UNP F8G0P2
D	488	HIS	-	expression tag	UNP F8G0P2
D	489	HIS	-	expression tag	UNP F8G0P2
D	490	HIS	-	expression tag	UNP F8G0P2

- Molecule 2 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (CCD ID: NCT) (formula: $C_{10}H_{14}N_2$) (labeled as "Ligand of Interest" by depositor).



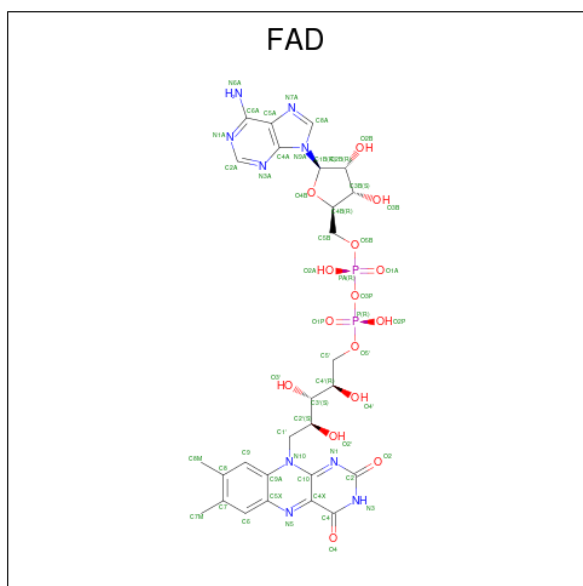
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			12	10	2		
2	B	1	Total	C	N	0	0
			12	10	2		
2	C	1	Total	C	N	0	0
			12	10	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	N	0	0
			12	10	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 81	C 27	H 28	N 9	O 15	P 2	0	0
3	B	1	Total 81	C 27	H 28	N 9	O 15	P 2	0	0
3	C	1	Total 81	C 27	H 28	N 9	O 15	P 2	0	0
3	D	1	Total 81	C 27	H 28	N 9	O 15	P 2	0	0

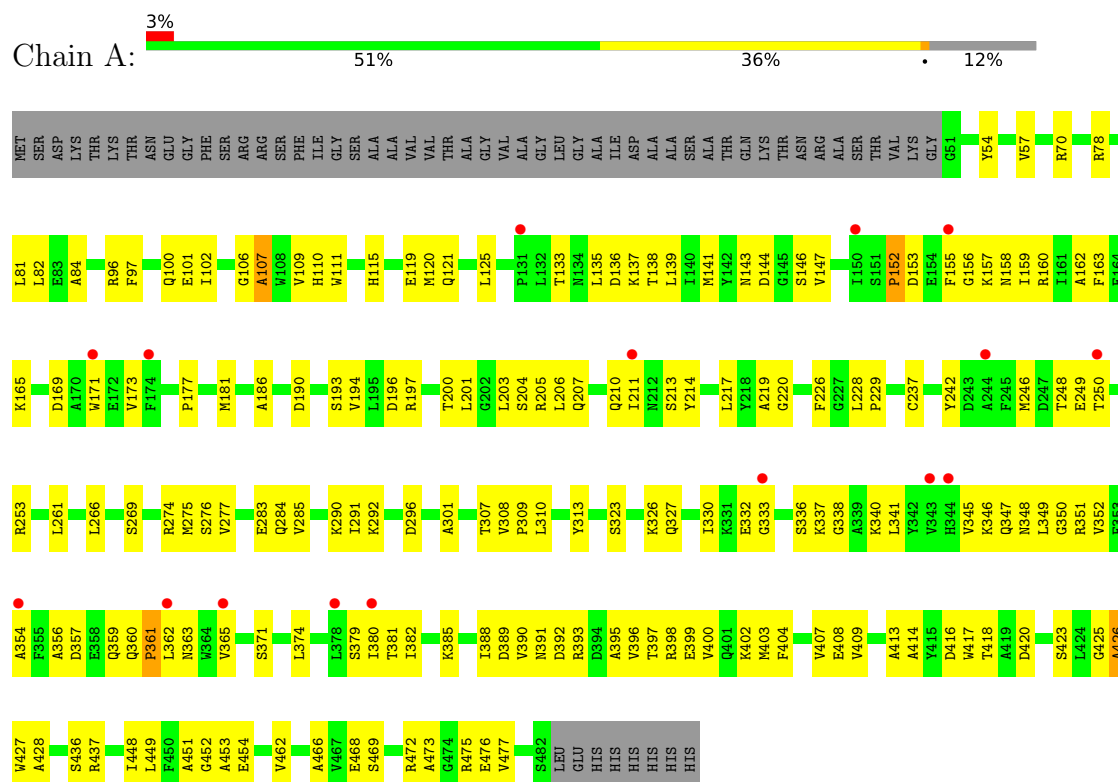
- Molecule 4 is water.

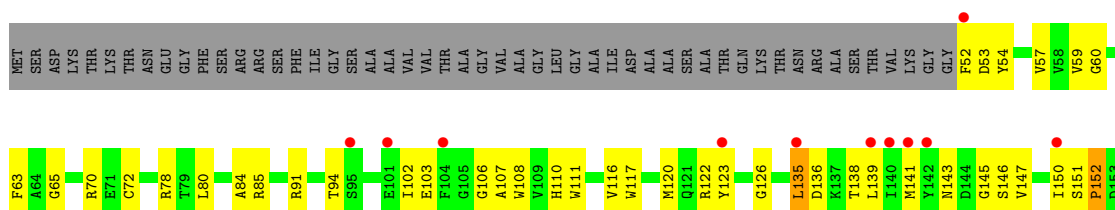
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	8	Total O 8 8	0	0
4	C	2	Total O 2 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Amine oxidase





A444	E154	T312	S379	G250	E154
E445	F155	Y313	I380	V231	F155
G446	G156	K314	T381	L232	G156
R447	K157	H315	R384	F235	K157
I448	N158	I316	K385	A236	N158
L449	I159	S323	E386	C237	I159
F450	R160	K326	T387	Y242	R160
A453	I161	I327	I388	D247	I161
E454	A162	Q327	D389	T248	A162
G458	F163	R328	V390	E249	F163
W459	E164	F329	N391	T250	E164
V462	I172	I330	D392	H251	I172
I463	V173	K331	R393	Q255	V173
D464	F174	E332	D394	I262	F174
A473	P175	G333	ALA	N263	P175
G474	R176	Q334	VAL	T267	R176
R475	P177	I335	THR	D268	P177
E476	M181	S336	ARG	S269	M181
V477	R185	K337	E399	E272	R185
K478	A186	G338	V400	V273	A186
Q479	R187	A339	K401	R274	R187
L480	E188	K340	Q402	S276	E188
L481	L189	I341	M403	V279	L189
S482	D190	Y342	F404	V282	D190
LEU	V194	VAL	P405	E283	V194
GLU	L195	HIS	G406	Q284	L195
HIS	I196	VAL	V407	V285	I196
HIS	R197	HIS	GLU	N286	R197
HIS	I198	VAL	VAL	G287	I198
HIS	K199	LYS	LEU	G288	K199
HIS	T200	ASN	GLY	V289	T200
HIS	L201	LEU	THR	K290	L201
HIS	G202	ARG	A413	I291	G202
HIS	L203	VAL	Y415	K292	L203
S204	S204	F353	T418	D296	S204
R205	R205	A354	A419	E297	R205
L206	L206	F355	D420	I298	L206
Q207	Q207	A356	S423	T299	Q207
Q208	Q208	D357	A426	T300	Q208
I211	I211	E358	W427	A301	I211
Y214	Y214	Q359	A428	G302	Y214
M215	M215	Q360	Y430	V303	M215
A216	A216	P361	G431	V304	A216
L217	L217	L362	Q434	V308	L217
Y218	Y218	K363	L435	P309	Y218
A219	A219	W364	S436	L310	A219
T222	T222	V365	R437	ILE	T222
T223	T223	Q366	L438	GLY	T223
F226	F226	T367	K439	LEU	F226
G227	G227	Y370	R441	D440	G227
L228	L228	S371	D442	L441	L228
P229	P229	ASP	A443	Q442	P229
		GLU			
		LEU			
		THR			
		ILE			
		LEU			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.40Å 134.56Å 168.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 2.69 39.60 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.7 (39.60-2.69) 90.9 (39.60-2.69)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.236 , 0.286 0.235 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.839	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13600	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, NCT

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	0.13	0/3424	0.37	2/4638 (0.0%)
1	B	0.17	0/3424	0.38	0/4638
1	C	0.17	1/3424 (0.0%)	0.38	0/4638
1	D	0.18	0/3218	0.43	0/4352
All	All	0.17	1/13490 (0.0%)	0.39	2/18266 (0.0%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	345	VAL	CB-CG2	5.08	1.69	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	ALA	CB-CA-C	-5.96	107.77	116.53
1	A	426	ALA	CA-C-O	5.15	121.58	118.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	135	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3353	0	3299	216	0
1	B	3353	0	3299	155	2
1	C	3353	0	3299	267	0
1	D	3152	0	3081	289	2
2	A	12	0	14	1	0
2	B	12	0	14	5	0
2	C	12	0	14	4	0
2	D	12	0	14	1	0
3	A	53	28	31	9	0
3	B	53	28	31	6	0
3	C	53	28	31	5	0
3	D	53	28	29	13	0
4	A	7	0	0	0	0
4	B	8	0	0	0	0
4	C	2	0	0	0	0
All	All	13488	112	13156	914	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 34.

All (914) 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:362:LEU:HD12	1:D:403:MET:SD	1.75	1.26
1:D:362:LEU:HD12	1:D:403:MET:CE	1.68	1.22
1:D:362:LEU:CD1	1:D:403:MET:SD	2.35	1.14
1:C:274:ARG:HG2	1:D:274:ARG:HG2	1.23	1.13
1:D:362:LEU:CD1	1:D:403:MET:HE3	1.80	1.12
1:C:346:LYS:HB2	1:C:410:LEU:HD21	1.30	1.11
1:A:141:MET:SD	1:A:360:GLN:OE1	2.09	1.11
1:D:150:ILE:HD11	1:D:155:PHE:HB2	1.34	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:HD3	1:C:201:LEU:HB3	1.30	1.07
1:D:289:VAL:HG21	1:D:304:VAL:HG23	1.31	1.07
1:A:274:ARG:HG2	1:B:274:ARG:HG2	1.30	1.06
1:C:135:LEU:HD13	1:C:351:ARG:HB3	1.34	1.06
1:C:185:ARG:HA	1:C:188:GLU:HG2	1.32	1.06
1:D:291:ILE:HD11	1:D:304:VAL:HG21	1.33	1.05
1:D:203:LEU:HB3	1:D:207:GLN:HG3	1.40	1.03
1:A:361:PRO:HG2	1:A:362:LEU:HD12	1.38	1.03
1:C:137:LYS:HB2	1:C:352:VAL:HG12	1.41	1.02
1:D:362:LEU:CD1	1:D:403:MET:CE	2.34	1.02
1:A:165:LYS:HB3	1:A:201:LEU:HD21	1.46	0.97
1:C:345:VAL:CG2	1:C:376:THR:HB	1.97	0.95
1:C:194:VAL:HG11	1:C:215:MET:HG3	1.46	0.95
1:D:287:GLY:O	1:D:447:ARG:NE	2.00	0.94
1:D:399:GLU:HG2	1:D:402:LYS:HE3	1.49	0.93
1:D:361:PRO:HD2	1:D:362:LEU:HD23	1.49	0.93
1:D:201:LEU:HD23	1:D:203:LEU:HD11	1.46	0.93
1:B:349:LEU:H	1:B:376:THR:HG21	1.34	0.92
1:C:345:VAL:CG2	1:C:376:THR:CB	2.50	0.90
1:D:362:LEU:HD11	1:D:403:MET:HE3	1.49	0.89
1:D:402:LYS:HE2	1:D:402:LYS:H	1.35	0.89
1:D:173:VAL:HG22	1:D:185:ARG:HG2	1.55	0.89
1:A:143:ASN:HD22	1:A:359:GLN:HG2	1.37	0.88
1:B:186:ALA:HA	1:B:189:LEU:HD12	1.54	0.87
1:A:121:GLN:O	1:C:475:ARG:NH1	2.07	0.86
1:D:150:ILE:HD11	1:D:155:PHE:CB	2.04	0.86
1:B:354:ALA:HB3	1:B:365:VAL:HG22	1.57	0.86
1:C:91:ARG:N	3:C:502:FAD:O2A	2.08	0.86
1:D:52:PHE:HE1	1:D:288:GLY:HA3	1.38	0.85
1:A:390:VAL:HG11	1:A:414:ALA:HB2	1.59	0.85
1:D:323:SER:OG	1:D:326:LYS:N	2.09	0.85
1:C:221:GLU:HG3	1:C:222:THR:H	1.40	0.84
1:A:365:VAL:HG22	1:A:380:ILE:HG12	1.60	0.84
1:A:347:GLN:HE22	1:A:408:GLU:H	1.25	0.84
1:B:354:ALA:HB3	1:B:365:VAL:CG2	2.08	0.84
1:D:394:ASP:OD2	1:D:400:VAL:HG12	1.78	0.83
1:D:162:ALA:HA	1:D:203:LEU:HD21	1.58	0.83
1:A:285:VAL:HG21	1:A:290:LYS:HE2	1.59	0.83
1:C:401:GLN:HB3	1:C:407:VAL:HG22	1.59	0.83
1:A:396:VAL:O	1:A:400:VAL:HG12	1.78	0.82
1:B:70:ARG:HG2	1:B:70:ARG:HH11	1.44	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:VAL:HG21	1:C:376:THR:CB	2.09	0.82
1:B:339:ALA:HB3	1:B:382:ILE:HD11	1.60	0.82
1:B:194:VAL:HG22	1:B:226:PHE:HB3	1.62	0.82
1:A:203:LEU:HB3	1:A:207:GLN:HG3	1.60	0.81
1:D:359:GLN:O	1:D:360:GLN:HG3	1.79	0.81
1:C:282:VAL:HG13	1:C:291:ILE:HD13	1.62	0.81
1:D:197:ARG:O	1:D:200:THR:HG22	1.80	0.81
1:D:195:LEU:HA	1:D:198:ILE:HD12	1.60	0.81
1:D:135:LEU:HG	1:D:136:ASP:H	1.45	0.80
1:D:203:LEU:HB3	1:D:207:GLN:CG	2.11	0.80
1:D:341:LEU:HG	1:D:414:ALA:HB2	1.62	0.79
1:C:181:MET:HE2	1:C:181:MET:HA	1.64	0.79
1:A:427:TRP:CE2	2:A:501:NCT:HC71	2.18	0.79
1:C:345:VAL:HG21	1:C:376:THR:HB	1.61	0.79
1:C:345:VAL:HG22	1:C:376:THR:HB	1.63	0.79
1:D:150:ILE:CD1	1:D:155:PHE:HB2	2.13	0.79
1:C:56:VAL:HG13	1:C:79:THR:HG23	1.65	0.78
1:B:324:LYS:O	1:B:324:LYS:HD3	1.82	0.78
1:C:194:VAL:HG12	1:C:198:ILE:HD11	1.63	0.78
1:A:159:ILE:HD13	1:A:210:GLN:HB3	1.64	0.78
1:D:145:GLY:HA2	1:D:360:GLN:HE22	1.48	0.78
1:D:194:VAL:O	1:D:198:ILE:HG13	1.84	0.77
1:B:427:TRP:CD2	2:B:501:NCT:HC71	2.19	0.77
1:C:167:CYS:HA	1:C:232:LEU:HD13	1.66	0.77
1:D:399:GLU:CG	1:D:402:LYS:HE3	2.15	0.77
1:C:212:ASN:OD1	1:C:223:THR:HG21	1.85	0.77
1:C:345:VAL:HG22	1:C:376:THR:CB	2.13	0.77
1:B:361:PRO:HA	1:B:387:THR:HG21	1.68	0.76
1:C:133:THR:HG22	1:C:134:ASN:H	1.51	0.76
1:D:80:LEU:HD12	1:D:272:GLU:O	1.84	0.76
1:D:222:THR:HB	1:D:358:GLU:OE1	1.85	0.76
1:A:57:VAL:HG11	1:A:291:ILE:HD13	1.67	0.76
1:A:165:LYS:CB	1:A:201:LEU:HD21	2.15	0.76
1:C:181:MET:SD	1:C:187:ARG:HG2	2.24	0.76
1:D:197:ARG:O	1:D:201:LEU:HD13	1.85	0.76
1:A:214:TYR:HE2	1:A:246:MET:HE1	1.51	0.76
1:C:466:ALA:O	1:C:469:SER:OG	2.04	0.75
1:D:190:ASP:HA	1:D:229:PRO:HG2	1.68	0.75
1:A:133:THR:H	1:A:351:ARG:NH1	1.85	0.75
1:C:127:VAL:CG2	1:C:252:TYR:HB3	2.17	0.75
1:B:348:ASN:HA	1:B:376:THR:CG2	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:PRO:O	1:D:155:PHE:HB3	1.88	0.74
1:C:346:LYS:CB	1:C:410:LEU:HD21	2.15	0.73
1:D:141:MET:CE	1:D:362:LEU:HD11	2.17	0.73
1:C:326:LYS:O	1:C:330:ILE:HG23	1.89	0.73
1:C:282:VAL:HG13	1:C:291:ILE:CD1	2.19	0.73
1:C:304:VAL:CG1	1:C:448:ILE:HD13	2.19	0.73
1:D:185:ARG:CZ	1:D:189:LEU:HD11	2.19	0.73
1:C:130:ASP:OD1	1:C:253:ARG:NH1	2.22	0.73
1:B:190:ASP:HA	1:B:229:PRO:HG2	1.71	0.73
1:C:150:ILE:HG22	1:C:151:SER:H	1.53	0.73
1:D:309:PRO:HD3	3:D:502:FAD:H51A	1.70	0.73
1:D:303:VAL:HG23	1:D:447:ARG:O	1.89	0.72
1:D:385:LYS:HE2	1:D:389:ASP:HA	1.71	0.72
1:D:390:VAL:HG21	1:D:414:ALA:CB	2.18	0.72
1:A:165:LYS:HB3	1:A:201:LEU:HD11	1.71	0.72
1:A:397:THR:HG23	1:A:409:VAL:CG1	2.19	0.72
1:D:323:SER:HB3	1:D:445:GLU:OE2	1.90	0.72
1:A:110:HIS:CG	1:A:248:THR:HG22	2.25	0.72
1:B:110:HIS:CG	1:B:248:THR:HG22	2.25	0.72
1:A:143:ASN:HB3	1:A:359:GLN:HG2	1.71	0.71
1:A:109:VAL:HG21	1:A:120:MET:HE1	1.72	0.71
1:C:185:ARG:CA	1:C:188:GLU:HG2	2.14	0.71
1:B:347:GLN:O	1:B:376:THR:HG23	1.91	0.71
1:A:214:TYR:OH	1:A:249:GLU:OE1	2.08	0.70
1:C:351:ARG:HA	1:C:367:THR:HG21	1.74	0.70
1:D:399:GLU:HA	1:D:402:LYS:HZ1	1.56	0.70
1:C:190:ASP:HA	1:C:229:PRO:HG2	1.74	0.70
1:C:345:VAL:HG22	1:C:376:THR:CA	2.22	0.70
1:D:337:LYS:O	1:D:384:ARG:HA	1.91	0.70
1:C:337:LYS:NZ	1:C:386:GLU:H	1.90	0.70
1:D:473:ALA:O	1:D:477:VAL:HG23	1.92	0.70
1:A:158:ASN:HD22	1:A:206:LEU:HD23	1.56	0.69
1:C:127:VAL:HG21	1:C:252:TYR:HB3	1.73	0.69
1:C:273:VAL:HG11	1:D:275:MET:HE3	1.74	0.69
1:A:143:ASN:HB3	1:A:359:GLN:CG	2.22	0.69
1:C:83:GLU:OE1	3:C:502:FAD:O2B	2.05	0.69
1:B:184:GLU:HA	1:B:187:ARG:NE	2.08	0.69
1:C:385:LYS:NZ	1:C:389:ASP:HA	2.06	0.69
1:A:332:GLU:OE1	1:A:437:ARG:NH2	2.26	0.69
1:D:94:THR:HG22	1:D:103:GLU:OE1	1.92	0.69
1:A:310:LEU:HA	1:A:313:TYR:HD2	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLY:H	1:A:469:SER:HB2	1.57	0.68
1:A:204:SER:HB3	1:A:207:GLN:HG2	1.74	0.68
1:B:346:LYS:HB2	1:B:410:LEU:HD21	1.75	0.68
1:D:362:LEU:HD23	1:D:362:LEU:H	1.56	0.68
1:C:195:LEU:HA	1:C:198:ILE:HD12	1.75	0.68
1:D:427:TRP:CD2	2:D:501:NCT:HC71	2.28	0.68
1:B:214:TYR:HB2	1:B:355:PHE:CZ	2.29	0.68
1:A:214:TYR:CE2	1:A:246:MET:HE1	2.29	0.68
1:D:399:GLU:HA	1:D:402:LYS:NZ	2.09	0.68
1:D:52:PHE:CE1	1:D:288:GLY:HA3	2.25	0.68
1:C:337:LYS:HZ1	1:C:386:GLU:HB3	1.58	0.68
1:A:143:ASN:ND2	1:A:359:GLN:HG2	2.09	0.68
1:B:215:MET:SD	1:B:231:VAL:HG11	2.34	0.68
1:D:150:ILE:HD11	1:D:155:PHE:CA	2.23	0.68
1:A:57:VAL:HG23	1:A:301:ALA:HB2	1.74	0.68
1:C:371:SER:HB3	1:C:374:LEU:HB3	1.75	0.68
1:D:341:LEU:HD12	1:D:390:VAL:HG11	1.76	0.68
1:D:361:PRO:HD2	1:D:362:LEU:CD2	2.24	0.67
1:B:184:GLU:HA	1:B:187:ARG:HE	1.59	0.67
1:D:150:ILE:HD12	1:D:151:SER:O	1.94	0.67
1:A:163:PHE:HD2	1:A:211:ILE:HD11	1.58	0.67
1:B:141:MET:HE1	1:B:402:LYS:HZ2	1.60	0.67
1:C:167:CYS:HA	1:C:232:LEU:CD1	2.24	0.67
1:A:392:ASP:O	1:A:396:VAL:HG13	1.94	0.67
1:B:137:LYS:HD3	1:B:139:LEU:HD21	1.76	0.67
1:D:204:SER:H	1:D:207:GLN:CD	2.02	0.67
1:A:165:LYS:HB3	1:A:201:LEU:CD2	2.23	0.67
1:D:198:ILE:HA	1:D:201:LEU:HD22	1.77	0.67
1:D:102:ILE:HB	1:D:342:TYR:CD2	2.30	0.67
1:B:303:VAL:HG23	1:B:447:ARG:O	1.95	0.66
1:D:145:GLY:HA2	1:D:360:GLN:NE2	2.10	0.66
1:D:217:LEU:O	1:D:427:TRP:HZ2	1.77	0.66
1:C:139:LEU:HD12	1:C:403:MET:HG2	1.77	0.66
1:A:310:LEU:HA	1:A:313:TYR:CD2	2.31	0.66
1:A:350:GLY:O	1:A:352:VAL:HG23	1.96	0.66
1:B:389:ASP:OD2	1:B:392:ASP:HB3	1.96	0.66
1:A:219:ALA:HB2	1:A:226:PHE:CG	2.31	0.66
1:A:416:ASP:OD1	1:A:418:THR:OG1	2.10	0.66
1:B:171:TRP:HB3	1:B:172:GLU:OE1	1.95	0.66
1:D:106:GLY:HA2	3:D:502:FAD:C4X	2.26	0.66
1:A:348:ASN:C	1:A:349:LEU:HD23	2.21	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:VAL:HG22	1:D:120:MET:HE2	1.77	0.66
1:A:361:PRO:HG2	1:A:362:LEU:CD1	2.19	0.66
1:C:188:GLU:HG3	1:C:189:LEU:N	2.10	0.66
1:C:139:LEU:CD2	1:C:149:SER:HB3	2.26	0.66
1:C:433:GLY:O	1:C:437:ARG:HD3	1.94	0.66
1:A:362:LEU:HD12	1:A:362:LEU:H	1.62	0.65
1:C:194:VAL:CG1	1:C:215:MET:HG3	2.24	0.65
1:C:481:LEU:O	1:C:482:SER:HB2	1.96	0.65
1:A:347:GLN:OE1	1:A:407:VAL:HA	1.96	0.65
1:B:427:TRP:CD1	2:B:501:NCT:HC81	2.31	0.65
1:A:390:VAL:CG1	1:A:414:ALA:HB2	2.26	0.65
1:B:70:ARG:HG2	1:B:70:ARG:NH1	2.11	0.65
1:B:194:VAL:O	1:B:198:ILE:HG13	1.97	0.65
1:C:165:LYS:HG2	1:C:201:LEU:HD22	1.79	0.65
1:D:135:LEU:HG	1:D:136:ASP:N	2.11	0.65
1:A:466:ALA:O	1:A:469:SER:OG	2.12	0.65
1:B:351:ARG:HH21	1:B:366:GLN:HG2	1.62	0.65
1:C:345:VAL:HG21	1:C:376:THR:OG1	1.96	0.65
1:D:362:LEU:CD1	1:D:403:MET:CG	2.75	0.65
1:C:144:ASP:OD2	1:C:146:SER:HB2	1.97	0.65
1:D:185:ARG:O	1:D:189:LEU:HD13	1.96	0.65
1:C:473:ALA:O	1:C:477:VAL:HG23	1.97	0.65
1:C:143:ASN:OD1	1:C:357:ASP:HB3	1.97	0.64
1:B:194:VAL:CG2	1:B:226:PHE:HB3	2.27	0.64
1:C:197:ARG:O	1:C:200:THR:OG1	2.15	0.64
1:B:143:ASN:OD1	1:B:357:ASP:HB3	1.97	0.64
1:A:347:GLN:OE1	1:A:407:VAL:HG12	1.97	0.64
1:D:94:THR:HG22	1:D:103:GLU:CD	2.23	0.64
1:D:362:LEU:HD13	1:D:403:MET:CB	2.27	0.64
1:D:362:LEU:HD13	1:D:403:MET:SD	2.36	0.64
1:D:103:GLU:O	1:D:340:LYS:HE3	1.97	0.64
1:C:190:ASP:HA	1:C:229:PRO:CG	2.28	0.63
1:A:70:ARG:HA	1:A:269:SER:HB3	1.80	0.63
1:B:282:VAL:HG13	1:B:291:ILE:HD13	1.79	0.63
1:A:473:ALA:O	1:A:477:VAL:HG23	1.99	0.63
1:C:345:VAL:HG22	1:C:376:THR:N	2.14	0.63
1:D:194:VAL:HG11	1:D:215:MET:HG3	1.81	0.63
1:A:197:ARG:HE	1:A:228:LEU:HD21	1.64	0.63
1:C:350:GLY:HA2	1:C:370:TYR:CE1	2.34	0.63
1:A:143:ASN:HB3	1:A:359:GLN:CD	2.24	0.62
1:D:361:PRO:HB3	1:D:388:ILE:CG2	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ASP:HB3	1:D:423:SER:OG	1.99	0.62
1:A:390:VAL:HG11	1:A:414:ALA:CB	2.29	0.62
1:D:194:VAL:HG23	1:D:226:PHE:O	1.99	0.62
1:D:329:PHE:CE1	1:D:434:GLN:HG2	2.34	0.62
1:C:83:GLU:OE2	1:C:83:GLU:HA	1.98	0.62
1:C:304:VAL:HG12	1:C:448:ILE:HD13	1.81	0.62
1:C:246:MET:O	1:C:249:GLU:HB2	1.99	0.62
1:C:273:VAL:CG1	1:D:275:MET:HB2	2.29	0.62
1:C:169:ASP:O	1:C:173:VAL:HG12	1.99	0.62
1:D:102:ILE:HB	1:D:342:TYR:CE2	2.34	0.62
1:D:390:VAL:HG21	1:D:414:ALA:HB3	1.80	0.62
1:B:219:ALA:HB2	1:B:226:PHE:CG	2.35	0.62
1:C:274:ARG:NH1	1:C:299:ILE:HD11	2.15	0.61
1:C:284:GLN:OE1	1:C:447:ARG:N	2.31	0.61
1:D:314:LYS:HG3	1:D:315:HIS:ND1	2.15	0.61
1:D:326:LYS:HE3	1:D:450:PHE:CD1	2.35	0.61
1:C:401:GLN:HA	1:C:404:PHE:H	1.66	0.61
1:D:475:ARG:O	1:D:479:GLN:HG3	2.00	0.61
1:B:84:ALA:O	1:B:276:SER:HA	1.99	0.61
1:C:139:LEU:HD22	1:C:149:SER:HB3	1.82	0.61
1:C:231:VAL:C	1:C:232:LEU:HD23	2.25	0.61
1:A:385:LYS:HE3	1:A:416:ASP:OD2	1.99	0.61
1:A:397:THR:HG23	1:A:409:VAL:HG13	1.82	0.61
1:D:57:VAL:HG23	1:D:301:ALA:HB2	1.82	0.61
1:A:138:THR:C	1:A:139:LEU:HD12	2.24	0.61
1:D:313:TYR:HA	1:D:316:ILE:HD13	1.80	0.61
1:D:428:ALA:CB	1:D:454:GLU:HG3	2.31	0.61
1:A:97:PHE:CD1	1:A:413:ALA:HB2	2.35	0.61
1:D:428:ALA:HB2	1:D:454:GLU:HG3	1.81	0.61
1:D:364:TRP:O	1:D:380:ILE:HA	2.01	0.61
1:C:337:LYS:HZ1	1:C:386:GLU:H	1.49	0.61
1:D:361:PRO:CB	1:D:388:ILE:HG21	2.30	0.61
1:B:135:LEU:HD23	1:B:351:ARG:HG3	1.83	0.60
1:C:223:THR:HG23	1:C:358:GLU:OE1	2.01	0.60
1:A:100:GLN:OE1	1:A:100:GLN:HA	1.99	0.60
1:C:420:ASP:O	1:C:424:LEU:HD12	2.01	0.60
1:C:137:LYS:CB	1:C:352:VAL:HG12	2.25	0.60
1:D:141:MET:HE2	1:D:403:MET:HG3	1.83	0.60
1:A:362:LEU:HD11	1:A:399:GLU:HB3	1.83	0.60
1:D:341:LEU:HD12	1:D:390:VAL:CG1	2.31	0.60
1:D:141:MET:HE3	1:D:362:LEU:HD11	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HB3	1:A:207:GLN:CG	2.31	0.60
1:B:141:MET:HE1	1:B:402:LYS:NZ	2.15	0.60
1:B:196:ASP:O	1:B:200:THR:HG23	2.00	0.60
1:C:427:TRP:CD2	2:C:501:NCT:HC71	2.37	0.60
1:D:401:GLN:HG3	1:D:407:VAL:CG2	2.31	0.60
1:B:462:VAL:HB	3:B:502:FAD:O2	2.01	0.60
1:D:362:LEU:HD13	1:D:403:MET:HB2	1.83	0.60
1:A:347:GLN:NE2	1:A:408:GLU:H	1.95	0.59
1:C:84:ALA:O	1:C:276:SER:HA	2.02	0.59
1:D:366:GLN:CG	1:D:367:THR:H	2.15	0.59
1:B:116:VAL:HG22	1:B:120:MET:HE2	1.84	0.59
1:B:166:LEU:HD12	1:B:211:ILE:CG1	2.31	0.59
1:C:221:GLU:HG3	1:C:222:THR:N	2.14	0.59
1:D:190:ASP:HA	1:D:229:PRO:CG	2.33	0.59
1:A:228:LEU:HB3	1:A:229:PRO:HD3	1.84	0.59
1:C:98:ALA:HB1	1:C:344:HIS:HD2	1.67	0.59
1:C:197:ARG:HG3	1:C:201:LEU:HD11	1.84	0.59
1:C:242:TYR:CE2	1:C:246:MET:HE2	2.37	0.59
1:B:166:LEU:HD12	1:B:211:ILE:HG12	1.83	0.59
1:B:173:VAL:HG11	1:B:189:LEU:CD1	2.32	0.59
1:B:185:ARG:O	1:B:189:LEU:HD12	2.02	0.59
1:C:137:LYS:HB2	1:C:352:VAL:CG1	2.27	0.59
1:C:217:LEU:HD21	1:C:381:THR:CG2	2.31	0.59
1:D:117:TRP:HA	1:D:120:MET:HE3	1.85	0.59
1:D:289:VAL:CG2	1:D:304:VAL:HG23	2.19	0.59
1:C:428:ALA:CB	1:C:454:GLU:HG3	2.31	0.59
1:A:371:SER:HB3	1:A:374:LEU:HD12	1.84	0.59
1:C:389:ASP:OD2	1:C:392:ASP:HB2	2.03	0.59
1:A:158:ASN:HD22	1:A:206:LEU:CD2	2.14	0.59
1:A:162:ALA:HB2	1:A:207:GLN:HB2	1.84	0.59
1:A:356:ALA:HB3	1:A:363:ASN:HA	1.85	0.59
1:B:385:LYS:NZ	1:B:389:ASP:HA	2.17	0.59
1:C:56:VAL:CG1	1:C:79:THR:HG23	2.32	0.59
1:D:328:ARG:O	1:D:332:GLU:HG3	2.03	0.59
1:A:109:VAL:CG2	1:A:120:MET:HE1	2.32	0.59
1:D:162:ALA:HA	1:D:203:LEU:CD2	2.31	0.59
1:B:212:ASN:OD1	1:B:223:THR:HG21	2.02	0.59
1:C:194:VAL:HG12	1:C:198:ILE:CD1	2.30	0.59
1:C:219:ALA:HB2	1:C:226:PHE:CG	2.38	0.59
1:C:219:ALA:HB2	1:C:226:PHE:CD2	2.38	0.59
1:D:279:VAL:HG12	3:D:502:FAD:N1A	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PRO:CA	1:B:387:THR:HG21	2.32	0.58
1:C:91:ARG:NH1	1:C:309:PRO:HG3	2.18	0.58
1:C:122:ARG:HD2	1:C:123:TYR:CZ	2.38	0.58
1:C:181:MET:SD	1:C:436:SER:HA	2.43	0.58
1:C:431:GLY:N	1:C:434:GLN:OE1	2.28	0.58
1:D:402:LYS:HE2	1:D:402:LYS:N	2.11	0.58
1:C:188:GLU:HG3	1:C:189:LEU:H	1.68	0.58
1:A:428:ALA:HB2	1:A:454:GLU:HG3	1.86	0.58
1:A:70:ARG:HA	1:A:269:SER:CB	2.34	0.58
1:A:462:VAL:HB	3:A:502:FAD:O2	2.04	0.57
1:D:194:VAL:CG2	1:D:226:PHE:HB3	2.33	0.57
1:D:247:ASP:OD1	1:D:251:HIS:ND1	2.36	0.57
1:B:173:VAL:CG1	1:B:186:ALA:HB2	2.34	0.57
1:C:441:LEU:HD12	1:C:441:LEU:O	2.04	0.57
1:D:362:LEU:HD23	1:D:362:LEU:N	2.18	0.57
1:B:197:ARG:O	1:B:201:LEU:HG	2.04	0.57
1:C:347:GLN:OE1	1:C:408:GLU:N	2.32	0.57
1:A:156:GLY:O	1:A:159:ILE:HG22	2.04	0.57
1:B:348:ASN:HA	1:B:376:THR:HG23	1.86	0.57
1:B:462:VAL:HB	3:B:502:FAD:C2	2.34	0.57
1:D:141:MET:SD	1:D:145:GLY:O	2.61	0.57
1:A:309:PRO:HD3	3:A:502:FAD:H51A	1.87	0.57
1:B:184:GLU:N	1:B:187:ARG:HH21	2.03	0.57
1:D:214:TYR:HE1	1:D:364:TRP:HZ3	1.52	0.57
1:A:109:VAL:HG21	1:A:120:MET:CE	2.35	0.57
1:A:462:VAL:HA	3:A:502:FAD:H1'2	1.87	0.57
1:C:440:ASP:OD1	1:C:440:ASP:N	2.36	0.57
1:D:173:VAL:HG22	1:D:185:ARG:CG	2.33	0.57
1:D:195:LEU:HB2	1:D:223:THR:HG22	1.86	0.57
1:C:80:LEU:HD12	1:C:272:GLU:HB3	1.87	0.56
1:A:84:ALA:O	1:A:276:SER:HA	2.05	0.56
1:A:125:LEU:HD12	1:A:261:LEU:HD13	1.87	0.56
1:D:404:PHE:HD2	1:D:405:PRO:HD2	1.70	0.56
1:B:385:LYS:NZ	1:B:390:VAL:H	2.02	0.56
1:C:345:VAL:CG2	1:C:376:THR:N	2.68	0.56
1:C:396:VAL:O	1:C:400:VAL:HG23	2.05	0.56
1:D:177:PRO:HB2	1:D:237:CYS:SG	2.46	0.56
1:D:194:VAL:HG21	1:D:226:PHE:CD2	2.39	0.56
1:D:291:ILE:HD11	1:D:304:VAL:CG2	2.23	0.56
1:C:361:PRO:HB3	1:C:388:ILE:HB	1.87	0.56
1:C:184:GLU:CD	1:C:184:GLU:H	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ARG:HH22	1:D:423:SER:HB3	1.71	0.56
1:D:217:LEU:HD11	1:D:381:THR:CG2	2.35	0.56
1:A:462:VAL:HB	3:A:502:FAD:C2	2.35	0.56
1:B:190:ASP:CA	1:B:229:PRO:HG2	2.36	0.56
1:D:53:ASP:HB2	1:D:300:THR:O	2.06	0.56
1:B:122:ARG:HD2	1:B:123:TYR:CE2	2.41	0.56
1:C:351:ARG:HG2	1:C:367:THR:HG21	1.88	0.56
1:A:194:VAL:HG12	1:A:228:LEU:HA	1.88	0.56
1:A:392:ASP:HB2	1:A:395:ALA:HB3	1.88	0.56
1:C:150:ILE:HG22	1:C:151:SER:N	2.21	0.56
1:D:199:LYS:NZ	1:D:208:GLN:HE22	2.04	0.56
1:D:334:GLN:HG2	1:D:335:LEU:H	1.71	0.56
1:D:335:LEU:HD22	1:D:431:GLY:CA	2.36	0.56
1:B:302:GLY:O	1:B:447:ARG:HD3	2.07	0.55
1:C:323:SER:HB3	1:C:445:GLU:OE1	2.06	0.55
1:D:194:VAL:HG23	1:D:226:PHE:HB3	1.87	0.55
1:A:143:ASN:CB	1:A:359:GLN:HG2	2.35	0.55
1:B:352:VAL:HG22	1:B:367:THR:OG1	2.05	0.55
1:D:203:LEU:HD23	1:D:207:GLN:NE2	2.21	0.55
1:A:147:VAL:HG23	1:A:147:VAL:O	2.07	0.55
1:C:212:ASN:CG	1:C:223:THR:HG21	2.31	0.55
1:C:350:GLY:HA2	1:C:370:TYR:CD1	2.42	0.55
1:D:401:GLN:HG3	1:D:407:VAL:HG22	1.88	0.55
1:B:200:THR:C	1:B:201:LEU:HD23	2.31	0.55
1:B:402:LYS:NZ	1:B:402:LYS:HB3	2.22	0.55
1:D:361:PRO:HB3	1:D:388:ILE:HG21	1.88	0.55
1:B:135:LEU:HD23	1:B:351:ARG:CG	2.37	0.55
1:B:177:PRO:HB2	1:B:237:CYS:SG	2.46	0.55
1:A:220:GLY:HA3	1:A:336:SER:HA	1.89	0.55
1:C:167:CYS:CA	1:C:232:LEU:HD13	2.36	0.55
1:C:323:SER:O	1:C:327:GLN:HG3	2.05	0.55
1:D:356:ALA:HB2	1:D:362:LEU:HG	1.87	0.55
1:A:340:LYS:HD2	1:A:380:ILE:O	2.06	0.55
1:C:91:ARG:HH12	1:C:309:PRO:HG3	1.72	0.55
1:D:203:LEU:CD2	1:D:207:GLN:HG3	2.35	0.55
1:A:196:ASP:O	1:A:200:THR:HG23	2.06	0.55
1:C:347:GLN:O	1:C:349:LEU:HD22	2.07	0.55
1:A:158:ASN:ND2	1:A:206:LEU:HD23	2.22	0.55
1:A:397:THR:OG1	1:A:409:VAL:HG21	2.06	0.55
1:D:107:ALA:HB3	1:D:108:TRP:CE3	2.42	0.55
1:A:143:ASN:HD22	1:A:359:GLN:H	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:CG	1:A:197:ARG:HH12	2.15	0.54
1:C:354:ALA:HB3	1:C:365:VAL:HB	1.89	0.54
1:A:204:SER:H	1:A:207:GLN:CD	2.15	0.54
1:A:204:SER:HB3	1:A:207:GLN:CG	2.37	0.54
1:C:67:THR:OG1	1:C:265:MET:HE1	2.07	0.54
1:D:70:ARG:HA	1:D:269:SER:CB	2.38	0.54
1:D:160:ARG:O	1:D:164:GLU:HG3	2.08	0.54
1:C:133:THR:H	1:C:351:ARG:NH1	2.04	0.54
1:A:177:PRO:HB2	1:A:237:CYS:SG	2.47	0.54
1:B:462:VAL:HA	3:B:502:FAD:H1'2	1.89	0.54
1:C:57:VAL:HG23	1:C:301:ALA:CB	2.38	0.54
1:B:220:GLY:HA3	1:B:336:SER:HA	1.89	0.54
1:B:401:GLN:HG2	1:B:407:VAL:HG22	1.90	0.54
1:B:441:LEU:HG	1:B:455:THR:HG22	1.90	0.54
1:C:370:TYR:HB3	1:C:376:THR:HG23	1.89	0.54
1:A:323:SER:O	1:A:327:GLN:HG3	2.06	0.54
1:C:337:LYS:CG	1:C:418:THR:HG21	2.37	0.54
1:D:185:ARG:HD2	1:D:188:GLU:OE2	2.07	0.54
1:D:360:GLN:HB3	1:D:361:PRO:CD	2.38	0.54
1:B:426:ALA:HB1	1:B:427:TRP:CE3	2.44	0.53
1:C:343:VAL:CG1	1:C:409:VAL:HG13	2.38	0.53
1:D:203:LEU:HD23	1:D:207:GLN:HE21	1.73	0.53
1:A:57:VAL:HG23	1:A:301:ALA:CB	2.38	0.53
1:B:186:ALA:HA	1:B:189:LEU:CD1	2.34	0.53
1:C:228:LEU:HB3	1:C:229:PRO:HD3	1.90	0.53
1:C:339:ALA:HB1	1:C:415:TYR:O	2.08	0.53
1:C:117:TRP:HA	1:C:120:MET:HE3	1.90	0.53
1:D:138:THR:HG21	1:D:155:PHE:CG	2.43	0.53
1:A:213:SER:HB2	1:A:356:ALA:O	2.07	0.53
1:B:165:LYS:HE3	1:B:203:LEU:CD2	2.39	0.53
1:C:428:ALA:HB2	1:C:454:GLU:HG3	1.91	0.53
1:A:389:ASP:CG	1:A:391:ASN:HB3	2.33	0.53
1:C:330:ILE:HG13	1:C:331:LYS:N	2.22	0.53
1:C:459:TRP:HB3	1:C:462:VAL:CG2	2.39	0.53
1:D:85:ARG:HH21	1:D:420:ASP:CG	2.16	0.53
1:B:360:GLN:HA	1:B:360:GLN:NE2	2.23	0.53
1:B:427:TRP:CE3	2:B:501:NCT:HC71	2.43	0.53
1:A:389:ASP:HB3	1:A:392:ASP:OD2	2.09	0.53
1:B:66:ALA:CB	1:B:265:MET:HE3	2.39	0.53
1:D:218:TYR:O	1:D:427:TRP:NE1	2.40	0.53
1:A:136:ASP:O	1:A:137:LYS:HG2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:GLN:O	1:D:255:GLN:HG3	2.09	0.53
1:A:190:ASP:CA	1:A:229:PRO:HG2	2.38	0.53
1:A:141:MET:HE3	1:A:403:MET:HE2	1.91	0.52
1:C:54:TYR:CZ	1:C:80:LEU:HD13	2.44	0.52
1:C:135:LEU:CD1	1:C:351:ARG:HB3	2.24	0.52
1:C:97:PHE:HB2	1:C:102:ILE:HD13	1.91	0.52
1:B:186:ALA:CA	1:B:189:LEU:HD12	2.34	0.52
1:B:310:LEU:HA	1:B:313:TYR:HD2	1.74	0.52
1:C:138:THR:C	1:C:139:LEU:HD23	2.35	0.52
1:C:479:GLN:OE1	1:C:479:GLN:HA	2.08	0.52
1:D:84:ALA:O	1:D:276:SER:HA	2.08	0.52
1:A:190:ASP:CB	1:A:229:PRO:HG2	2.39	0.52
1:D:364:TRP:HE1	1:D:366:GLN:NE2	2.06	0.52
1:A:346:LYS:HB3	1:A:347:GLN:HE21	1.75	0.52
1:A:452:GLY:H	1:A:469:SER:CB	2.22	0.52
1:B:138:THR:HG21	1:B:152:PRO:HA	1.91	0.52
1:A:379:SER:C	1:A:380:ILE:HG13	2.34	0.52
1:D:437:ARG:HB3	1:D:440:ASP:OD1	2.10	0.52
1:A:133:THR:H	1:A:351:ARG:HH12	1.54	0.52
1:D:110:HIS:CG	1:D:248:THR:HG22	2.44	0.52
1:D:126:GLY:O	1:D:255:GLN:HG2	2.10	0.52
1:C:79:THR:HB	1:C:271:ALA:HB2	1.92	0.52
1:D:287:GLY:O	1:D:447:ARG:CZ	2.58	0.52
1:C:368:HIS:ND1	1:C:377:ILE:HB	2.24	0.52
1:B:362:LEU:HD22	1:B:380:ILE:HG21	1.92	0.51
1:A:169:ASP:O	1:A:173:VAL:HG23	2.09	0.51
1:B:172:GLU:OE1	1:B:172:GLU:N	2.43	0.51
1:B:284:GLN:HG2	1:B:448:ILE:HD11	1.91	0.51
1:B:290:LYS:HG2	1:B:300:THR:HG22	1.91	0.51
1:D:156:GLY:HA2	1:D:159:ILE:CG2	2.41	0.51
1:D:235:PHE:HE1	1:D:242:TYR:HA	1.74	0.51
1:D:361:PRO:HB3	1:D:387:THR:HG22	1.93	0.51
1:B:173:VAL:HG11	1:B:189:LEU:HD13	1.92	0.51
1:D:434:GLN:HG3	1:D:437:ARG:NH2	2.26	0.51
1:A:57:VAL:CG2	1:A:301:ALA:HB2	2.41	0.51
1:B:385:LYS:HZ1	1:B:389:ASP:HA	1.73	0.51
1:C:116:VAL:HG22	1:C:120:MET:HE2	1.92	0.51
1:C:171:TRP:CZ3	1:C:172:GLU:HG2	2.46	0.51
1:D:70:ARG:HA	1:D:269:SER:HB3	1.93	0.51
1:A:352:VAL:HG11	1:A:404:PHE:CE1	2.46	0.51
1:C:217:LEU:HD21	1:C:381:THR:HG21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:TYR:CE1	1:D:364:TRP:HZ3	2.29	0.51
1:C:156:GLY:HA2	1:C:159:ILE:HG22	1.92	0.51
1:B:309:PRO:HD3	3:B:502:FAD:H51A	1.93	0.51
1:C:345:VAL:CG2	1:C:376:THR:OG1	2.58	0.51
1:D:326:LYS:O	1:D:330:ILE:HD12	2.11	0.51
1:B:160:ARG:NH1	1:B:164:GLU:OE1	2.44	0.51
1:B:473:ALA:O	1:B:477:VAL:HG23	2.11	0.51
1:D:284:GLN:OE1	1:D:446:GLY:HA3	2.10	0.50
1:D:366:GLN:HG2	1:D:367:THR:H	1.76	0.50
1:D:462:VAL:HB	3:D:502:FAD:O2	2.11	0.50
1:A:393:ARG:NH2	1:A:409:VAL:O	2.43	0.50
1:C:120:MET:HG2	1:C:125:LEU:HB2	1.93	0.50
1:C:277:VAL:HG22	1:D:272:GLU:HG3	1.93	0.50
1:D:282:VAL:HG11	1:D:448:ILE:HD11	1.91	0.50
1:D:289:VAL:HG21	1:D:304:VAL:CG2	2.22	0.50
1:A:393:ARG:HA	1:A:396:VAL:HG22	1.94	0.50
1:A:249:GLU:HG3	1:A:250:THR:HG23	1.91	0.50
1:B:310:LEU:HA	1:B:313:TYR:CD2	2.46	0.50
1:D:52:PHE:HE1	1:D:288:GLY:CA	2.17	0.50
1:D:72:CYS:SG	1:D:477:VAL:HG11	2.52	0.50
1:D:282:VAL:CG1	1:D:448:ILE:HD11	2.41	0.50
1:C:141:MET:HA	1:C:146:SER:O	2.12	0.50
1:D:187:ARG:HH11	1:D:187:ARG:HB3	1.76	0.50
1:D:190:ASP:CA	1:D:229:PRO:HG2	2.39	0.50
1:B:188:GLU:OE1	1:B:191:LYS:NZ	2.38	0.50
1:C:57:VAL:HG23	1:C:301:ALA:HB2	1.94	0.50
1:D:190:ASP:OD2	1:D:436:SER:OG	2.22	0.50
1:D:439:LYS:HD3	1:D:442:GLN:OE1	2.11	0.50
1:A:125:LEU:CD1	1:A:261:LEU:HD13	2.42	0.50
1:B:140:ILE:HD12	1:B:210:GLN:HG3	1.94	0.50
1:D:361:PRO:CD	1:D:362:LEU:HD23	2.32	0.50
1:A:143:ASN:ND2	1:A:359:GLN:H	2.10	0.50
1:B:166:LEU:HD12	1:B:211:ILE:HD11	1.94	0.50
1:B:345:VAL:HG22	1:B:376:THR:O	2.11	0.50
1:C:194:VAL:HG11	1:C:215:MET:CG	2.30	0.50
1:D:204:SER:H	1:D:207:GLN:CG	2.25	0.50
1:D:401:GLN:CD	1:D:401:GLN:H	2.19	0.50
1:A:354:ALA:HB3	1:A:365:VAL:HB	1.93	0.50
1:A:389:ASP:OD2	1:A:391:ASN:HB3	2.12	0.50
1:B:72:CYS:SG	1:B:477:VAL:HG11	2.52	0.50
1:C:295:ASP:OD2	1:D:78:ARG:NH2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ARG:NH1	1:D:454:GLU:OE1	2.38	0.50
1:D:194:VAL:HG12	1:D:198:ILE:HD11	1.93	0.50
1:A:141:MET:HE2	1:A:147:VAL:CG1	2.42	0.49
1:A:190:ASP:HA	1:A:229:PRO:HG2	1.94	0.49
1:A:347:GLN:CD	1:A:347:GLN:H	2.19	0.49
1:C:139:LEU:HD12	1:C:403:MET:CG	2.42	0.49
1:A:341:LEU:HD13	1:A:390:VAL:CG1	2.42	0.49
1:A:217:LEU:HD11	1:A:381:THR:CG2	2.43	0.49
1:C:195:LEU:HB2	1:C:223:THR:OG1	2.12	0.49
1:D:85:ARG:NH1	3:D:502:FAD:O2B	2.45	0.49
1:D:282:VAL:HG11	1:D:448:ILE:CD1	2.42	0.49
1:C:337:LYS:HG3	1:C:418:THR:HG21	1.94	0.49
1:B:211:ILE:HD11	1:B:215:MET:HE3	1.94	0.49
1:C:108:TRP:NE1	1:C:253:ARG:HG3	2.27	0.49
1:C:334:GLN:HB2	1:C:429:ALA:O	2.13	0.49
1:D:290:LYS:HG2	1:D:300:THR:HG22	1.94	0.49
1:D:481:LEU:O	1:D:482:SER:CB	2.59	0.49
1:A:70:ARG:HH22	1:A:119:GLU:CD	2.20	0.49
1:C:326:LYS:HE3	1:C:450:PHE:CE2	2.48	0.49
1:D:219:ALA:HB2	1:D:226:PHE:CG	2.47	0.49
1:A:139:LEU:HD12	1:A:139:LEU:N	2.28	0.49
1:A:153:ASP:OD2	1:A:153:ASP:N	2.44	0.49
1:A:217:LEU:HD11	1:A:381:THR:HG21	1.95	0.49
1:B:190:ASP:HA	1:B:229:PRO:CG	2.42	0.49
1:A:110:HIS:ND1	1:A:248:THR:HG22	2.28	0.49
1:A:389:ASP:C	1:A:391:ASN:N	2.70	0.49
1:D:143:ASN:HA	1:D:359:GLN:HB2	1.95	0.49
1:D:150:ILE:HG12	1:D:206:LEU:HD11	1.95	0.49
1:A:397:THR:HG23	1:A:409:VAL:HG11	1.92	0.49
1:B:159:ILE:HD13	1:B:210:GLN:HB3	1.94	0.49
1:C:297:GLU:HG2	1:C:298:ILE:N	2.27	0.49
1:D:217:LEU:O	1:D:427:TRP:CZ2	2.63	0.49
1:A:165:LYS:HB3	1:A:201:LEU:CD1	2.40	0.49
1:B:173:VAL:HG12	1:B:186:ALA:HB2	1.95	0.49
1:B:326:LYS:O	1:B:330:ILE:HG13	2.13	0.49
1:C:337:LYS:HZ1	1:C:386:GLU:CB	2.26	0.49
1:D:393:ARG:O	1:D:394:ASP:HB2	2.13	0.49
1:A:326:LYS:O	1:A:330:ILE:HG13	2.12	0.48
1:A:346:LYS:HD3	1:A:408:GLU:OE1	2.12	0.48
1:A:219:ALA:HB2	1:A:226:PHE:CD2	2.48	0.48
1:D:459:TRP:HB2	1:D:464:ASP:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LYS:HA	1:B:410:LEU:HD11	1.94	0.48
1:C:65:GLY:HA2	1:C:307:THR:HG21	1.95	0.48
1:C:190:ASP:CA	1:C:229:PRO:HG2	2.42	0.48
1:D:57:VAL:HG23	1:D:301:ALA:CB	2.43	0.48
1:D:328:ARG:HG2	1:D:332:GLU:OE1	2.14	0.48
1:A:310:LEU:HG	1:A:333:GLY:HA2	1.96	0.48
1:B:141:MET:HB2	1:B:147:VAL:HG22	1.96	0.48
1:B:393:ARG:HG3	1:B:412:THR:HG23	1.96	0.48
1:C:160:ARG:HG3	1:C:160:ARG:HH11	1.78	0.48
1:C:189:LEU:HD11	1:C:197:ARG:HH22	1.79	0.48
1:D:151:SER:HB3	1:D:154:GLU:HG3	1.94	0.48
1:D:356:ALA:CB	1:D:362:LEU:HG	2.44	0.48
1:A:308:VAL:HB	3:A:502:FAD:C8A	2.44	0.48
1:A:360:GLN:HE22	1:A:402:LYS:NZ	2.11	0.48
1:C:193:SER:OG	1:C:432:VAL:HG22	2.14	0.48
1:C:207:GLN:O	1:C:211:ILE:HG22	2.14	0.48
1:C:345:VAL:HG22	1:C:376:THR:C	2.39	0.48
1:C:394:ASP:O	1:C:398:ARG:HD3	2.12	0.48
1:A:136:ASP:C	1:A:137:LYS:HG2	2.38	0.48
1:A:205:ARG:HG3	1:A:206:LEU:H	1.79	0.48
1:C:193:SER:HB3	1:C:226:PHE:O	2.14	0.48
1:C:421:PRO:HA	1:C:424:LEU:CD1	2.43	0.48
1:D:323:SER:HG	1:D:326:LYS:N	2.09	0.48
1:D:334:GLN:OE1	1:D:336:SER:HB3	2.14	0.48
1:A:201:LEU:O	1:A:201:LEU:HG	2.12	0.48
1:B:66:ALA:HB1	1:B:265:MET:HE3	1.95	0.48
1:A:177:PRO:HD2	1:C:111:TRP:CZ2	2.48	0.47
1:A:283:GLU:HG2	1:A:285:VAL:HG13	1.96	0.47
1:B:337:LYS:HA	1:B:418:THR:HG22	1.94	0.47
1:D:283:GLU:HG2	1:D:285:VAL:HG13	1.96	0.47
1:A:82:LEU:HD23	1:A:274:ARG:HB2	1.95	0.47
1:A:171:TRP:CZ3	1:C:243:ASP:HB3	2.49	0.47
1:A:194:VAL:HG22	1:A:226:PHE:HB3	1.96	0.47
1:C:167:CYS:CB	1:C:232:LEU:HD13	2.44	0.47
1:C:217:LEU:O	1:C:427:TRP:HZ2	1.97	0.47
1:B:289:VAL:HG21	1:B:304:VAL:HG12	1.95	0.47
1:D:313:TYR:HB2	1:D:330:ILE:HG23	1.95	0.47
1:A:97:PHE:HB3	1:A:102:ILE:HD13	1.97	0.47
1:A:307:THR:HG22	1:A:451:ALA:HB3	1.97	0.47
1:B:115:HIS:CE1	1:B:468:GLU:HB2	2.49	0.47
1:B:365:VAL:HG12	1:B:380:ILE:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLY:HA2	3:D:502:FAD:N5	2.30	0.47
1:D:282:VAL:HG22	1:D:291:ILE:CD1	2.44	0.47
1:B:91:ARG:HA	1:B:417:TRP:CZ3	2.50	0.47
1:B:133:THR:OG1	1:B:134:ASN:N	2.46	0.47
1:B:287:GLY:O	1:B:447:ARG:NH1	2.48	0.47
1:B:339:ALA:HB3	1:B:382:ILE:CD1	2.37	0.47
1:C:63:PHE:CE1	1:C:261:LEU:HD23	2.50	0.47
1:C:160:ARG:HG3	1:C:242:TYR:CD1	2.50	0.47
1:C:215:MET:SD	1:C:231:VAL:HG21	2.55	0.47
1:C:335:LEU:HD21	1:C:430:TYR:C	2.39	0.47
1:C:364:TRP:HB3	1:C:381:THR:HB	1.97	0.47
1:A:345:VAL:HG12	1:A:409:VAL:HA	1.97	0.47
1:B:79:THR:HB	1:B:271:ALA:HB2	1.95	0.47
1:C:221:GLU:HA	1:C:384:ARG:HD3	1.97	0.47
1:D:361:PRO:HB2	1:D:388:ILE:HG21	1.96	0.47
1:A:275:MET:O	1:A:277:VAL:HG23	2.15	0.47
1:B:192:SER:O	1:B:432:VAL:HG13	2.15	0.47
1:C:428:ALA:HB1	1:C:454:GLU:HG3	1.96	0.47
1:C:166:LEU:HD12	1:C:166:LEU:O	2.14	0.47
1:D:217:LEU:HD11	1:D:381:THR:HG22	1.95	0.47
1:A:181:MET:SD	1:A:436:SER:HB3	2.55	0.46
1:A:201:LEU:HB3	1:A:203:LEU:HD11	1.96	0.46
1:B:213:SER:HB2	1:B:356:ALA:O	2.14	0.46
1:C:190:ASP:O	1:C:433:GLY:N	2.47	0.46
1:D:60:GLY:O	1:D:65:GLY:HA3	2.14	0.46
1:D:143:ASN:OD1	1:D:357:ASP:HB3	2.16	0.46
1:D:156:GLY:HA2	1:D:159:ILE:HG22	1.96	0.46
1:D:282:VAL:HG22	1:D:291:ILE:HD12	1.95	0.46
1:D:309:PRO:HG3	3:D:502:FAD:O1A	2.16	0.46
1:A:141:MET:HA	1:A:146:SER:O	2.16	0.46
1:C:385:LYS:HZ1	1:C:389:ASP:HA	1.77	0.46
1:D:206:LEU:C	1:D:206:LEU:HD23	2.39	0.46
1:D:323:SER:OG	1:D:326:LYS:HB2	2.15	0.46
1:D:407:VAL:HG23	1:D:407:VAL:O	2.15	0.46
1:A:96:ARG:NH1	1:B:255:GLN:HG2	2.31	0.46
1:A:160:ARG:HG3	1:A:242:TYR:CD2	2.50	0.46
1:B:85:ARG:HH21	1:B:420:ASP:CG	2.24	0.46
1:B:197:ARG:NH2	1:B:228:LEU:HD21	2.29	0.46
1:C:358:GLU:O	1:C:384:ARG:NH2	2.37	0.46
1:C:361:PRO:CB	1:C:388:ILE:HB	2.46	0.46
1:C:83:GLU:OE2	3:C:502:FAD:H1B	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:VAL:HG13	1:C:409:VAL:CG1	2.46	0.46
1:D:459:TRP:HB3	1:D:462:VAL:CG2	2.46	0.46
1:B:88:LEU:HD13	1:B:266:LEU:CD1	2.44	0.46
1:C:244:ALA:O	1:C:248:THR:HG23	2.15	0.46
1:C:325:GLY:HA3	1:C:440:ASP:OD2	2.16	0.46
1:D:218:TYR:OH	1:D:249:GLU:OE2	2.23	0.46
1:A:107:ALA:O	1:A:253:ARG:HG2	2.16	0.46
1:A:190:ASP:HA	1:A:229:PRO:CG	2.45	0.46
1:C:285:VAL:HG12	1:C:286:ASN:N	2.31	0.46
1:C:410:LEU:N	1:C:410:LEU:HD22	2.31	0.46
1:D:185:ARG:NE	1:D:189:LEU:HD11	2.29	0.46
1:D:362:LEU:HD11	1:D:403:MET:CE	2.25	0.46
1:A:309:PRO:HD3	3:A:502:FAD:C5B	2.46	0.46
1:C:151:SER:O	1:C:153:ASP:N	2.48	0.46
1:D:195:LEU:HB2	1:D:223:THR:CG2	2.46	0.46
1:A:111:TRP:CZ2	1:C:177:PRO:HD2	2.50	0.46
1:C:91:ARG:HB2	3:C:502:FAD:H3'	1.98	0.46
1:D:138:THR:O	1:D:139:LEU:HG	2.15	0.46
1:D:197:ARG:HA	1:D:200:THR:HG22	1.97	0.46
1:B:360:GLN:OE1	1:B:402:LYS:HE2	2.16	0.46
1:C:79:THR:HB	1:C:271:ALA:CB	2.46	0.46
1:C:328:ARG:O	1:C:332:GLU:HG3	2.15	0.46
1:D:328:ARG:HA	1:D:331:LYS:HG2	1.97	0.46
1:D:401:GLN:HG3	1:D:407:VAL:HG21	1.97	0.46
1:D:141:MET:SD	1:D:360:GLN:OE1	2.74	0.46
1:D:198:ILE:CD1	1:D:223:THR:HG21	2.46	0.46
1:D:312:THR:HG21	3:D:502:FAD:N7A	2.30	0.46
1:D:326:LYS:HE3	1:D:450:PHE:CE1	2.51	0.46
1:A:158:ASN:OD1	1:A:207:GLN:NE2	2.49	0.45
1:B:166:LEU:HD12	1:B:211:ILE:CD1	2.45	0.45
1:A:173:VAL:HG12	1:A:186:ALA:HB2	1.98	0.45
1:B:67:THR:O	1:B:71:GLU:HG2	2.16	0.45
1:D:309:PRO:HD3	3:D:502:FAD:C5B	2.42	0.45
1:C:70:ARG:NH2	1:C:119:GLU:OE2	2.37	0.45
1:C:343:VAL:HG12	1:C:409:VAL:HG13	1.98	0.45
1:C:345:VAL:HG22	1:C:376:THR:O	2.17	0.45
1:C:427:TRP:CG	2:C:501:NCT:HC71	2.51	0.45
1:D:214:TYR:OH	1:D:249:GLU:OE2	2.32	0.45
1:C:362:LEU:HD23	1:C:362:LEU:N	2.31	0.45
1:D:162:ALA:HB1	1:D:211:ILE:HB	1.98	0.45
1:D:228:LEU:HG	1:D:232:LEU:CD1	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:O	1:B:159:ILE:HG22	2.17	0.45
1:D:80:LEU:HD13	1:D:272:GLU:CD	2.41	0.45
1:D:126:GLY:N	1:D:255:GLN:HG2	2.32	0.45
1:D:141:MET:SD	1:D:147:VAL:HG22	2.56	0.45
1:A:379:SER:O	1:A:380:ILE:HG13	2.17	0.45
1:C:329:PHE:HE2	1:C:437:ARG:O	2.00	0.45
1:D:141:MET:HE2	1:D:141:MET:HB2	1.64	0.45
1:D:354:ALA:HB1	1:D:403:MET:HE1	1.99	0.45
1:A:193:SER:OG	1:A:194:VAL:N	2.49	0.45
1:A:362:LEU:HD12	1:A:362:LEU:N	2.29	0.45
1:B:417:TRP:HB3	1:B:425:GLY:O	2.17	0.45
1:D:389:ASP:C	1:D:391:ASN:H	2.24	0.45
1:D:462:VAL:HA	3:D:502:FAD:N1	2.31	0.45
1:A:133:THR:O	1:A:351:ARG:NH1	2.50	0.45
1:A:338:GLY:HA2	1:A:382:ILE:O	2.17	0.45
1:A:428:ALA:CB	1:A:454:GLU:HG3	2.47	0.45
1:C:477:VAL:O	1:C:481:LEU:HD12	2.16	0.45
1:D:141:MET:HG3	1:D:146:SER:O	2.17	0.45
1:A:81:LEU:C	1:A:81:LEU:HD23	2.42	0.45
1:A:393:ARG:O	1:A:397:THR:OG1	2.32	0.45
1:C:98:ALA:CB	1:C:344:HIS:HD2	2.28	0.45
1:C:203:LEU:HD12	1:C:203:LEU:H	1.81	0.45
1:B:356:ALA:HB3	1:B:363:ASN:HA	1.98	0.44
1:C:63:PHE:HE1	1:C:261:LEU:HD23	1.81	0.44
1:A:292:LYS:HE3	1:A:296:ASP:OD1	2.16	0.44
1:A:361:PRO:HB2	1:A:388:ILE:HB	1.99	0.44
1:A:385:LYS:HZ3	1:A:390:VAL:H	1.66	0.44
1:A:426:ALA:HB1	1:A:427:TRP:CE3	2.53	0.44
1:A:472:ARG:HG3	1:A:475:ARG:HH22	1.82	0.44
1:C:193:SER:OG	1:C:432:VAL:CG2	2.66	0.44
1:C:335:LEU:H	1:C:335:LEU:HD23	1.82	0.44
1:D:361:PRO:CA	1:D:387:THR:HG21	2.48	0.44
1:C:316:ILE:HD11	3:C:502:FAD:N6A	2.32	0.44
1:C:326:LYS:HE2	1:C:445:GLU:OE1	2.18	0.44
1:A:157:LYS:HA	1:A:157:LYS:HD3	1.69	0.44
1:A:393:ARG:O	1:A:396:VAL:HG22	2.16	0.44
1:A:404:PHE:O	1:A:407:VAL:HG22	2.18	0.44
1:B:402:LYS:O	1:B:402:LYS:HG2	2.16	0.44
1:D:328:ARG:O	1:D:331:LYS:HG3	2.18	0.44
1:B:106:GLY:HA2	3:B:502:FAD:C4X	2.48	0.44
1:D:80:LEU:HD13	1:D:272:GLU:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:TRP:CG	1:D:250:THR:HA	2.53	0.44
1:D:122:ARG:O	1:D:123:TYR:CG	2.71	0.44
1:B:418:THR:HA	1:B:425:GLY:N	2.32	0.44
1:D:335:LEU:HD22	1:D:431:GLY:HA2	1.99	0.44
1:D:404:PHE:O	1:D:407:VAL:HG13	2.18	0.44
1:A:284:GLN:CD	1:A:448:ILE:HG13	2.43	0.44
1:A:361:PRO:CB	1:A:388:ILE:HB	2.48	0.44
1:B:70:ARG:HD3	1:B:123:TYR:OH	2.17	0.44
1:B:214:TYR:O	1:B:217:LEU:HB3	2.18	0.44
1:C:160:ARG:HG3	1:C:242:TYR:CE1	2.53	0.44
1:C:277:VAL:CG2	1:D:272:GLU:HG3	2.47	0.44
1:A:100:GLN:CD	1:A:101:GLU:H	2.25	0.44
1:B:351:ARG:HH22	1:B:366:GLN:HE21	1.66	0.44
1:C:98:ALA:HB3	1:C:377:ILE:HD11	1.99	0.44
1:C:171:TRP:CH2	1:C:172:GLU:HG2	2.53	0.44
1:C:218:TYR:CD2	2:C:501:NCT:HC82	2.53	0.44
1:D:63:PHE:CD2	1:D:262:ILE:HD11	2.52	0.44
1:D:155:PHE:O	1:D:159:ILE:HG22	2.18	0.44
1:A:144:ASP:CG	1:A:146:SER:HG	2.26	0.44
1:A:213:SER:HB3	1:A:357:ASP:OD1	2.17	0.44
1:C:98:ALA:HB1	1:C:344:HIS:CD2	2.51	0.44
1:C:138:THR:HG23	1:C:138:THR:O	2.17	0.44
1:C:231:VAL:HG22	1:C:232:LEU:HD23	1.99	0.44
1:C:393:ARG:NH2	1:C:410:LEU:O	2.51	0.44
1:D:426:ALA:HB1	1:D:427:TRP:CE3	2.53	0.44
1:C:206:LEU:C	1:C:206:LEU:HD13	2.42	0.43
1:C:427:TRP:CE2	2:C:501:NCT:HC71	2.52	0.43
1:D:156:GLY:O	1:D:159:ILE:CG2	2.66	0.43
1:D:228:LEU:N	1:D:229:PRO:CD	2.81	0.43
1:A:115:HIS:CE1	1:A:468:GLU:HB2	2.53	0.43
1:A:138:THR:HG23	1:A:152:PRO:HG3	2.00	0.43
1:D:111:TRP:HA	1:D:117:TRP:CD2	2.53	0.43
1:D:311:ASN:OD1	1:D:334:GLN:N	2.48	0.43
1:B:219:ALA:HB2	1:B:226:PHE:CD2	2.52	0.43
1:B:451:ALA:HB1	1:B:469:SER:HB2	1.99	0.43
1:D:107:ALA:HB3	1:D:108:TRP:CZ3	2.54	0.43
1:A:165:LYS:HD3	1:A:201:LEU:HD11	2.00	0.43
1:B:166:LEU:CD1	1:B:211:ILE:HD11	2.47	0.43
1:C:83:GLU:OE2	1:C:83:GLU:CA	2.66	0.43
1:C:274:ARG:HH12	1:C:299:ILE:HD11	1.82	0.43
1:D:362:LEU:CD1	1:D:403:MET:CB	2.95	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:LEU:CD1	1:D:403:MET:HB2	2.47	0.43
1:A:341:LEU:HD13	1:A:390:VAL:HG13	1.99	0.43
1:A:409:VAL:O	1:A:409:VAL:HG23	2.17	0.43
1:B:150:ILE:HG22	1:B:151:SER:N	2.34	0.43
1:D:326:LYS:HE2	1:D:443:ALA:O	2.19	0.43
1:D:439:LYS:HD3	1:D:439:LYS:HA	1.89	0.43
1:C:160:ARG:HG3	1:C:160:ARG:NH1	2.33	0.43
1:C:337:LYS:NZ	1:C:386:GLU:HB3	2.29	0.43
1:D:222:THR:CB	1:D:358:GLU:OE1	2.62	0.43
1:B:427:TRP:CG	2:B:501:NCT:HC81	2.53	0.43
1:A:97:PHE:CB	1:A:102:ILE:HD13	2.49	0.43
1:B:427:TRP:CE2	2:B:501:NCT:HC71	2.54	0.43
1:C:156:GLY:HA2	1:C:159:ILE:CG2	2.49	0.43
1:C:228:LEU:N	1:C:229:PRO:CD	2.82	0.43
1:C:280:THR:O	1:C:316:ILE:HA	2.19	0.43
1:C:321:ALA:HB1	1:C:327:GLN:NE2	2.33	0.43
1:C:328:ARG:HD3	1:C:332:GLU:OE2	2.19	0.43
1:D:141:MET:CE	1:D:403:MET:HG3	2.48	0.43
1:B:71:GLU:OE1	1:B:71:GLU:HA	2.17	0.43
1:D:279:VAL:CG2	1:D:291:ILE:HG23	2.49	0.43
1:A:190:ASP:HB2	1:A:229:PRO:HG2	2.00	0.43
1:A:313:TYR:HB2	1:A:330:ILE:HG23	2.01	0.43
1:A:349:LEU:HD23	1:A:349:LEU:N	2.34	0.43
1:A:385:LYS:HE3	1:A:416:ASP:CG	2.44	0.43
1:C:337:LYS:HG2	1:C:418:THR:HG21	2.00	0.43
1:D:59:VAL:HG11	1:D:279:VAL:HG11	2.00	0.43
1:A:205:ARG:HG3	1:A:206:LEU:N	2.33	0.42
1:A:360:GLN:HE22	1:A:402:LYS:HZ1	1.67	0.42
1:A:389:ASP:OD2	1:A:391:ASN:CB	2.66	0.42
1:C:106:GLY:O	1:C:258:THR:HG21	2.19	0.42
1:C:374:LEU:HD23	1:C:375:GLY:C	2.44	0.42
1:D:138:THR:HG21	1:D:155:PHE:CB	2.49	0.42
1:A:217:LEU:O	1:A:427:TRP:HZ2	2.01	0.42
1:B:326:LYS:NZ	1:B:441:LEU:O	2.52	0.42
1:C:132:LEU:O	1:C:133:THR:OG1	2.33	0.42
1:C:326:LYS:NZ	1:C:441:LEU:O	2.52	0.42
1:D:138:THR:C	1:D:139:LEU:HD12	2.43	0.42
1:D:156:GLY:O	1:D:159:ILE:HG23	2.20	0.42
1:D:295:ASP:O	1:D:296:ASP:HB2	2.18	0.42
1:D:312:THR:HG22	1:D:316:ILE:HD11	2.01	0.42
1:D:364:TRP:HE1	1:D:366:GLN:HE21	1.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ALA:HB1	1:A:469:SER:HB2	2.01	0.42
1:B:162:ALA:HB1	1:B:211:ILE:HB	2.01	0.42
1:C:54:TYR:O	1:C:301:ALA:HA	2.20	0.42
1:C:151:SER:C	1:C:153:ASP:H	2.27	0.42
1:D:157:LYS:HD2	1:D:157:LYS:HA	1.56	0.42
1:D:199:LYS:CE	1:D:208:GLN:HE22	2.32	0.42
1:A:135:LEU:HD13	1:A:351:ARG:HB3	2.02	0.42
1:B:57:VAL:O	1:B:304:VAL:HA	2.20	0.42
1:B:220:GLY:O	1:B:337:LYS:HG2	2.20	0.42
1:C:57:VAL:O	1:C:304:VAL:HA	2.19	0.42
1:D:181:MET:HE3	1:D:435:LEU:HG	2.01	0.42
1:D:366:GLN:HB3	1:D:379:SER:HB3	2.01	0.42
1:D:380:ILE:N	1:D:380:ILE:HD12	2.33	0.42
1:D:481:LEU:O	1:D:482:SER:HB2	2.20	0.42
1:C:337:LYS:HZ1	1:C:386:GLU:N	2.15	0.42
1:D:326:LYS:NZ	1:D:440:ASP:O	2.45	0.42
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.90	0.42
1:B:57:VAL:HG23	1:B:301:ALA:HB2	2.00	0.42
1:B:309:PRO:HD3	3:B:502:FAD:C5B	2.49	0.42
1:C:345:VAL:O	1:C:345:VAL:HG23	2.18	0.42
1:D:462:VAL:HA	3:D:502:FAD:H1'2	2.02	0.42
1:A:106:GLY:HA2	3:A:502:FAD:C4X	2.50	0.42
1:B:384:ARG:O	1:B:387:THR:OG1	2.21	0.42
1:D:54:TYR:CZ	1:D:80:LEU:HD22	2.55	0.42
1:D:263:ASN:O	1:D:267:THR:OG1	2.25	0.42
1:D:337:LYS:HA	1:D:418:THR:HG22	2.01	0.42
1:B:109:VAL:HG21	1:B:120:MET:HE1	2.01	0.42
1:B:173:VAL:HG13	1:B:186:ALA:HB2	2.01	0.42
1:C:91:ARG:NH1	1:C:309:PRO:HB3	2.35	0.42
1:C:197:ARG:CG	1:C:201:LEU:HD11	2.50	0.42
1:A:284:GLN:O	1:A:285:VAL:HG13	2.20	0.42
1:C:347:GLN:OE1	1:C:407:VAL:HA	2.18	0.42
1:D:150:ILE:HD11	1:D:155:PHE:HA	1.98	0.42
1:D:427:TRP:HB3	3:D:502:FAD:H1'1	2.02	0.42
1:D:453:ALA:HB2	3:D:502:FAD:H5'2	2.00	0.42
1:A:137:LYS:HA	1:A:137:LYS:HE2	2.02	0.42
1:A:141:MET:HE2	1:A:147:VAL:HG11	2.02	0.42
1:C:387:THR:O	1:C:387:THR:HG22	2.19	0.42
1:A:345:VAL:HA	1:A:408:GLU:O	2.20	0.41
1:B:195:LEU:HB2	1:B:223:THR:OG1	2.20	0.41
1:B:298:ILE:HD12	1:B:298:ILE:C	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLU:HG3	1:B:450:PHE:CE1	2.54	0.41
1:C:185:ARG:O	1:C:188:GLU:CG	2.68	0.41
1:C:228:LEU:O	1:C:231:VAL:HG12	2.20	0.41
1:C:307:THR:HA	1:C:451:ALA:O	2.19	0.41
1:C:331:LYS:HD3	1:C:331:LYS:HA	1.60	0.41
1:D:157:LYS:O	1:D:161:ILE:HG12	2.20	0.41
1:A:417:TRP:HB3	1:A:425:GLY:O	2.20	0.41
1:B:452:GLY:H	1:B:469:SER:CB	2.32	0.41
1:C:215:MET:HE2	1:C:215:MET:HA	2.01	0.41
1:C:340:LYS:HG3	1:C:380:ILE:O	2.19	0.41
1:A:362:LEU:HD11	1:A:399:GLU:CB	2.49	0.41
1:A:420:ASP:HB3	1:A:423:SER:OG	2.20	0.41
1:B:189:LEU:C	1:B:191:LYS:N	2.79	0.41
1:C:133:THR:HG22	1:C:134:ASN:N	2.26	0.41
1:D:59:VAL:HG12	1:D:308:VAL:CG1	2.50	0.41
1:D:172:GLU:O	1:D:175:PRO:HD3	2.20	0.41
1:C:368:HIS:O	1:C:369:ASP:OD2	2.37	0.41
1:D:339:ALA:HB1	1:D:415:TYR:O	2.21	0.41
1:A:313:TYR:CB	1:A:330:ILE:HG23	2.51	0.41
1:A:337:LYS:HE2	1:A:337:LYS:HB2	1.70	0.41
1:B:74:LEU:HD23	1:B:74:LEU:HA	1.92	0.41
1:C:74:LEU:HD23	1:C:74:LEU:HA	1.78	0.41
1:C:206:LEU:O	1:C:206:LEU:HD22	2.20	0.41
1:C:336:SER:HB3	1:C:427:TRP:O	2.21	0.41
1:D:203:LEU:CB	1:D:207:GLN:HE21	2.34	0.41
1:D:228:LEU:HG	1:D:232:LEU:HD11	2.03	0.41
1:D:326:LYS:HG2	1:D:440:ASP:O	2.21	0.41
1:A:144:ASP:OD1	1:A:146:SER:OG	2.36	0.41
1:B:291:ILE:O	1:B:298:ILE:HA	2.20	0.41
1:B:452:GLY:H	1:B:469:SER:HB2	1.85	0.41
1:C:116:VAL:HG12	1:C:464:ASP:OD1	2.21	0.41
1:D:122:ARG:HG3	1:D:122:ARG:HH11	1.85	0.41
1:D:430:TYR:OH	1:D:454:GLU:O	2.35	0.41
1:A:78:ARG:HE	1:A:78:ARG:HB3	1.61	0.41
1:A:100:GLN:OE1	1:A:100:GLN:CA	2.68	0.41
1:C:147:VAL:O	1:C:147:VAL:HG13	2.21	0.41
1:C:173:VAL:O	1:C:173:VAL:HG22	2.19	0.41
1:C:190:ASP:OD1	1:C:229:PRO:HG2	2.20	0.41
1:D:150:ILE:HD12	1:D:150:ILE:C	2.46	0.41
1:A:152:PRO:O	1:A:155:PHE:N	2.53	0.41
1:C:327:GLN:O	1:C:330:ILE:HG12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:LYS:HG3	1:D:298:ILE:HD11	2.02	0.41
1:A:453:ALA:HB2	3:A:502:FAD:H5'2	2.02	0.41
1:B:91:ARG:O	1:B:105:GLY:HA3	2.21	0.41
1:B:184:GLU:CA	1:B:187:ARG:HH21	2.34	0.41
1:B:277:VAL:O	1:B:277:VAL:HG12	2.21	0.41
1:C:191:LYS:HD2	1:C:191:LYS:HA	1.81	0.41
1:C:222:THR:HG22	1:C:358:GLU:CD	2.45	0.41
1:C:222:THR:HA	1:C:358:GLU:OE1	2.21	0.41
1:C:273:VAL:HG12	1:D:275:MET:HB2	1.99	0.41
1:D:379:SER:C	1:D:380:ILE:HD12	2.45	0.41
1:A:352:VAL:HG11	1:A:404:PHE:CZ	2.56	0.41
1:A:398:ARG:CZ	1:A:398:ARG:HB3	2.50	0.41
1:B:298:ILE:HD12	1:B:298:ILE:O	2.21	0.41
1:C:309:PRO:HG2	1:C:423:SER:HA	2.03	0.41
1:C:449:LEU:HD12	1:C:477:VAL:HG22	2.02	0.41
1:D:228:LEU:O	1:D:231:VAL:CG1	2.68	0.41
1:D:303:VAL:HG23	1:D:447:ARG:C	2.46	0.41
1:A:392:ASP:HB2	1:A:395:ALA:CB	2.50	0.40
1:B:166:LEU:O	1:B:166:LEU:HD23	2.21	0.40
1:C:356:ALA:HB3	1:C:363:ASN:HA	2.03	0.40
1:D:323:SER:O	1:D:327:GLN:HB2	2.21	0.40
1:A:106:GLY:HA2	3:A:502:FAD:N5	2.36	0.40
1:B:349:LEU:H	1:B:376:THR:CG2	2.17	0.40
1:C:185:ARG:O	1:C:188:GLU:HG3	2.21	0.40
1:C:295:ASP:O	1:C:296:ASP:HB2	2.19	0.40
1:C:318:PHE:CD1	1:C:322:LEU:HD11	2.56	0.40
1:D:290:LYS:CG	1:D:300:THR:HG22	2.52	0.40
1:A:54:TYR:O	1:A:301:ALA:HA	2.20	0.40
1:A:385:LYS:HZ3	1:A:389:ASP:HA	1.86	0.40
1:A:449:LEU:HD22	1:A:476:GLU:OE2	2.20	0.40
1:C:154:GLU:HA	1:C:157:LYS:HB2	2.03	0.40
1:D:197:ARG:HA	1:D:197:ARG:HD3	1.90	0.40
1:D:360:GLN:C	1:D:387:THR:HG21	2.47	0.40
1:B:289:VAL:HG21	1:B:304:VAL:CG1	2.50	0.40
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.86	0.40
1:C:345:VAL:CG2	1:C:345:VAL:O	2.69	0.40
1:C:449:LEU:CD1	1:C:477:VAL:HG22	2.52	0.40
1:D:329:PHE:HE2	1:D:437:ARG:O	2.04	0.40
1:D:360:GLN:HB3	1:D:361:PRO:HD2	2.03	0.40
1:A:147:VAL:O	1:A:147:VAL:CG2	2.70	0.40
1:C:214:TYR:CE1	1:C:218:TYR:HE1	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:VAL:O	1:C:375:GLY:HA3	2.21	0.40
1:D:138:THR:HG21	1:D:155:PHE:HB2	2.03	0.40
1:D:361:PRO:HB3	1:D:388:ILE:HG22	2.02	0.40
1:D:384:ARG:O	1:D:387:THR:HB	2.22	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:71:GLU:OE2	1:D:122:ARG:NH1[2_554]	2.08	0.12
1:B:75:GLN:NE2	1:D:268:ASP:OD1[2_554]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/490 (88%)	407 (95%)	20 (5%)	3 (1%)	18	41
1	B	430/490 (88%)	404 (94%)	25 (6%)	1 (0%)	43	68
1	C	430/490 (88%)	401 (93%)	27 (6%)	2 (0%)	24	48
1	D	395/490 (81%)	359 (91%)	31 (8%)	5 (1%)	9	25
All	All	1685/1960 (86%)	1571 (93%)	103 (6%)	11 (1%)	18	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	323	SER
1	A	361	PRO
1	B	107	ALA
1	D	390	VAL
1	A	107	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	152	PRO
1	D	205	ARG
1	D	286	ASN
1	C	369	ASP
1	C	361	PRO
1	D	152	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/390 (89%)	347 (100%)	0	100	100
1	B	347/390 (89%)	347 (100%)	0	100	100
1	C	347/390 (89%)	347 (100%)	0	100	100
1	D	325/390 (83%)	325 (100%)	0	100	100
All	All	1366/1560 (88%)	1366 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	143	ASN
1	A	286	ASN
1	A	347	GLN
1	A	360	GLN
1	A	368	HIS
1	B	100	GLN
1	B	327	GLN
1	C	344	HIS
1	C	391	ASN
1	D	207	GLN
1	D	208	GLN
1	D	479	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 ⓘ

8 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	NCT	C	501	-	13,13,13	1.28	1 (7%)	17,17,17	0.72	0
3	FAD	D	502	-	58,58,58	2.44	12 (20%)	85,89,89	2.88	31 (36%)
2	NCT	D	501	-	13,13,13	1.27	1 (7%)	17,17,17	0.72	0
2	NCT	A	501	-	13,13,13	1.27	1 (7%)	17,17,17	0.75	0
3	FAD	A	502	-	58,58,58	2.18	7 (12%)	85,89,89	1.88	22 (25%)
2	NCT	B	501	-	13,13,13	1.23	1 (7%)	17,17,17	0.90	0
3	FAD	C	502	-	58,58,58	2.20	7 (12%)	85,89,89	2.31	23 (27%)
3	FAD	B	502	-	58,58,58	2.21	7 (12%)	85,89,89	2.06	22 (25%)

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	NCT	C	501	-	-	1/4/14/14	0/2/2/2
3	FAD	D	502	-	1/1/9/9	8/34/50/50	0/6/6/6
2	NCT	D	501	-	-	1/4/14/14	0/2/2/2
2	NCT	A	501	-	-	0/4/14/14	0/2/2/2
3	FAD	A	502	-	-	9/34/50/50	0/6/6/6
2	NCT	B	501	-	-	1/4/14/14	0/2/2/2
3	FAD	C	502	-	-	12/34/50/50	0/6/6/6
3	FAD	B	502	-	-	6/34/50/50	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	FAD	P-O3P	-11.61	1.47	1.59
3	D	502	FAD	P-O3P	-11.59	1.47	1.59
3	A	502	FAD	P-O3P	-11.43	1.47	1.59
3	B	502	FAD	P-O3P	-11.27	1.47	1.59
3	B	502	FAD	PA-O3P	8.51	1.68	1.59
3	A	502	FAD	PA-O3P	8.37	1.68	1.59
3	D	502	FAD	PA-O3P	8.32	1.68	1.59
3	C	502	FAD	PA-O3P	8.27	1.68	1.59
3	D	502	FAD	C4X-N5	4.37	1.40	1.30
3	B	502	FAD	C4X-N5	4.31	1.40	1.30
2	C	501	NCT	C7-C6	4.29	1.65	1.54
2	A	501	NCT	C7-C6	4.27	1.65	1.54
2	D	501	NCT	C7-C6	4.25	1.65	1.54
3	C	502	FAD	C4X-N5	4.21	1.39	1.30
3	A	502	FAD	C4X-N5	4.17	1.39	1.30
3	D	502	FAD	C1'-N10	4.10	1.57	1.47
2	B	501	NCT	C7-C6	4.07	1.64	1.54
3	D	502	FAD	O2'-C2'	-3.94	1.35	1.43
3	D	502	FAD	C2'-C3'	3.49	1.59	1.53
3	D	502	FAD	C10-N1	3.26	1.39	1.33
3	B	502	FAD	C10-N1	3.02	1.39	1.33
3	C	502	FAD	C10-N1	2.93	1.39	1.33
3	A	502	FAD	C10-N1	2.87	1.39	1.33
3	D	502	FAD	C1'-C2'	-2.65	1.48	1.52
3	D	502	FAD	C8A-N7A	2.60	1.36	1.31
3	C	502	FAD	C2A-N1A	2.58	1.38	1.33
3	B	502	FAD	C2A-N1A	2.58	1.38	1.33
3	A	502	FAD	C2A-N1A	2.56	1.38	1.33
3	D	502	FAD	C2A-N1A	2.53	1.38	1.33
3	B	502	FAD	C8A-N7A	2.50	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	FAD	C8A-N7A	2.49	1.36	1.31
3	C	502	FAD	C8A-N7A	2.48	1.36	1.31
3	C	502	FAD	C2A-N3A	2.27	1.38	1.33
3	B	502	FAD	C2A-N3A	2.23	1.37	1.33
3	A	502	FAD	C2A-N3A	2.21	1.37	1.33
3	D	502	FAD	C2A-N3A	2.20	1.37	1.33
3	D	502	FAD	O3'-C3'	-2.15	1.37	1.43

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	FAD	C1'-C2'-C3'	15.46	151.59	109.66
3	C	502	FAD	C4'-C3'-C2'	12.35	134.12	113.57
3	D	502	FAD	C5'-C4'-C3'	-8.57	96.04	112.22
3	B	502	FAD	C4'-C3'-C2'	8.48	127.68	113.57
3	D	502	FAD	C9A-C5X-N5	-7.04	114.98	122.45
3	D	502	FAD	N3A-C2A-N1A	-6.38	118.92	128.58
3	A	502	FAD	N3A-C2A-N1A	-6.35	118.98	128.58
3	C	502	FAD	N3A-C2A-N1A	-6.32	119.02	128.58
3	B	502	FAD	N3A-C2A-N1A	-6.29	119.06	128.58
3	D	502	FAD	C9A-N10-C10	-5.13	112.94	120.75
3	B	502	FAD	C9A-C5X-N5	-5.01	117.14	122.45
3	A	502	FAD	C4'-C3'-C2'	4.77	121.50	113.57
3	A	502	FAD	C9A-C5X-N5	-4.59	117.58	122.45
3	C	502	FAD	C5'-C4'-C3'	-4.59	103.56	112.22
3	C	502	FAD	C9A-C5X-N5	-4.43	117.75	122.45
3	D	502	FAD	C4-N3-C2	-4.39	117.84	125.64
3	A	502	FAD	O2'-C2'-C3'	4.33	119.38	109.25
3	D	502	FAD	C4'-C3'-C2'	4.23	120.60	113.57
3	C	502	FAD	C5A-C4A-N3A	-3.96	121.26	126.72
3	B	502	FAD	C5A-C4A-N3A	-3.91	121.34	126.72
3	D	502	FAD	C5A-C4A-N3A	-3.79	121.50	126.72
3	C	502	FAD	O3'-C3'-C2'	-3.79	100.32	108.93
3	A	502	FAD	C5A-C4A-N3A	-3.78	121.52	126.72
3	B	502	FAD	C4-N3-C2	-3.70	119.07	125.64
3	A	502	FAD	C4-N3-C2	-3.68	119.11	125.64
3	B	502	FAD	C5'-C4'-C3'	-3.61	105.42	112.22
3	C	502	FAD	C4-N3-C2	-3.57	119.30	125.64
3	B	502	FAD	O3'-C3'-C4'	-3.55	100.87	108.93
3	D	502	FAD	O4-C4-C4X	-3.53	117.21	126.53
3	D	502	FAD	C2A-N3A-C4A	3.52	120.43	111.83
3	B	502	FAD	C2A-N3A-C4A	3.48	120.33	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	FAD	C2A-N3A-C4A	3.48	120.32	111.83
3	A	502	FAD	C2A-N3A-C4A	3.44	120.23	111.83
3	D	502	FAD	O3'-C3'-C2'	-3.33	101.36	108.93
3	A	502	FAD	O3'-C3'-C4'	-3.26	101.51	108.93
3	D	502	FAD	C2B-C1B-N9A	3.19	121.24	113.30
3	D	502	FAD	C4X-C4-N3	3.19	121.36	113.25
3	C	502	FAD	O4-C4-C4X	-3.18	118.13	126.53
3	A	502	FAD	O4-C4-C4X	-3.14	118.26	126.53
3	B	502	FAD	O2'-C2'-C1'	3.12	123.03	110.20
3	B	502	FAD	O4-C4-C4X	-3.09	118.37	126.53
3	D	502	FAD	C4X-C10-N1	-3.02	117.19	124.59
3	D	502	FAD	C5A-N7A-C8A	3.01	108.18	103.45
3	A	502	FAD	C5A-N7A-C8A	2.89	108.00	103.45
3	B	502	FAD	C5A-N7A-C8A	2.89	107.98	103.45
3	D	502	FAD	N9A-C8A-N7A	-2.88	109.85	113.94
3	C	502	FAD	C5A-N7A-C8A	2.87	107.96	103.45
3	D	502	FAD	C4A-C5A-N7A	-2.81	107.37	110.58
3	A	502	FAD	N9A-C8A-N7A	-2.80	109.97	113.94
3	C	502	FAD	O2'-C2'-C3'	2.78	115.76	109.25
3	D	502	FAD	C5X-C9A-N10	2.77	120.47	117.97
3	C	502	FAD	N9A-C8A-N7A	-2.70	110.11	113.94
3	C	502	FAD	O3'-C3'-C4'	-2.69	102.82	108.93
3	B	502	FAD	N9A-C8A-N7A	-2.68	110.14	113.94
3	A	502	FAD	C5'-C4'-C3'	-2.67	107.19	112.22
3	B	502	FAD	C4X-C4-N3	2.66	120.03	113.25
3	D	502	FAD	O4'-C4'-C5'	2.66	115.85	109.99
3	C	502	FAD	C4X-C4-N3	2.64	119.98	113.25
3	C	502	FAD	O2'-C2'-C1'	2.64	121.06	110.20
3	B	502	FAD	C4A-C5A-N7A	-2.62	107.59	110.58
3	C	502	FAD	C10-C4X-N5	-2.62	119.47	124.81
3	A	502	FAD	C4X-C4-N3	2.61	119.90	113.25
3	A	502	FAD	C2A-N1A-C6A	2.60	123.00	118.73
3	D	502	FAD	C4-C4X-C10	2.57	121.35	116.93
3	A	502	FAD	C4A-C5A-N7A	-2.57	107.64	110.58
3	C	502	FAD	C2A-N1A-C6A	2.55	122.92	118.73
3	B	502	FAD	C10-C4X-N5	-2.55	119.61	124.81
3	B	502	FAD	C2A-N1A-C6A	2.52	122.86	118.73
3	D	502	FAD	C2A-N1A-C6A	2.52	122.86	118.73
3	A	502	FAD	C10-C4X-N5	-2.51	119.69	124.81
3	C	502	FAD	O2P-P-O3P	2.50	114.04	107.27
3	C	502	FAD	C4A-C5A-N7A	-2.50	107.73	110.58
3	A	502	FAD	O2'-C2'-C1'	2.47	120.36	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	FAD	O2A-PA-O3P	-2.46	100.63	107.27
3	D	502	FAD	C5A-C4A-N9A	2.45	108.48	105.81
3	D	502	FAD	C8M-C8-C9	-2.45	115.26	119.57
3	D	502	FAD	C1'-N10-C9A	2.41	125.31	120.63
3	D	502	FAD	O3'-C3'-C4'	2.40	114.39	108.93
3	B	502	FAD	C5A-C4A-N9A	2.29	108.31	105.81
3	B	502	FAD	C5X-N5-C4X	2.28	121.78	118.09
3	D	502	FAD	O2P-P-O3P	2.25	113.34	107.27
3	D	502	FAD	C8M-C8-C7	2.21	125.28	120.76
3	A	502	FAD	O2P-P-O3P	2.21	113.24	107.27
3	D	502	FAD	O2'-C2'-C3'	-2.20	104.11	109.25
3	B	502	FAD	O2'-C2'-C3'	2.19	114.38	109.25
3	C	502	FAD	C5A-C4A-N9A	2.15	108.16	105.81
3	A	502	FAD	C5A-C4A-N9A	2.15	108.15	105.81
3	D	502	FAD	O2A-PA-O3P	-2.13	101.52	107.27
3	A	502	FAD	O2A-PA-O3P	-2.10	101.58	107.27
3	A	502	FAD	C5X-N5-C4X	2.10	121.48	118.09
3	D	502	FAD	C1B-N9A-C8A	2.05	131.65	127.09
3	C	502	FAD	C6A-C5A-C4A	2.05	119.98	117.18
3	B	502	FAD	C4-C4X-C10	2.03	120.41	116.93
3	D	502	FAD	C2'-C1'-N10	2.03	119.78	110.20
3	B	502	FAD	O2A-PA-O3P	-2.02	101.81	107.27
3	A	502	FAD	C4-C4X-C10	2.01	120.38	116.93
3	C	502	FAD	N3A-C4A-N9A	2.01	130.58	127.17
3	B	502	FAD	O2P-P-O3P	2.00	112.69	107.27

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	502	FAD	C2'

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	FAD	N10-C1'-C2'-O2'
3	A	502	FAD	C1'-C2'-C3'-O3'
3	A	502	FAD	C1'-C2'-C3'-C4'
3	A	502	FAD	O4'-C4'-C5'-O5'
3	B	502	FAD	C1'-C2'-C3'-O3'
3	B	502	FAD	C1'-C2'-C3'-C4'
3	B	502	FAD	O4'-C4'-C5'-O5'
3	C	502	FAD	C5B-O5B-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	502	FAD	C5B-O5B-PA-O2A
3	C	502	FAD	C5B-O5B-PA-O3P
3	C	502	FAD	N10-C1'-C2'-O2'
3	C	502	FAD	C1'-C2'-C3'-O3'
3	C	502	FAD	C1'-C2'-C3'-C4'
3	D	502	FAD	N10-C1'-C2'-O2'
3	D	502	FAD	C1'-C2'-C3'-O3'
3	D	502	FAD	O2'-C2'-C3'-O3'
3	D	502	FAD	O2'-C2'-C3'-C4'
3	D	502	FAD	O4'-C4'-C5'-O5'
3	C	502	FAD	O2'-C2'-C3'-C4'
3	C	502	FAD	O2'-C2'-C3'-O3'
3	A	502	FAD	C3'-C4'-C5'-O5'
3	D	502	FAD	C3'-C4'-C5'-O5'
3	A	502	FAD	PA-O3P-P-O5'
3	D	502	FAD	PA-O3P-P-O5'
2	B	501	NCT	C1-C2-C6-N2
3	B	502	FAD	C5B-O5B-PA-O3P
3	D	502	FAD	C5B-O5B-PA-O3P
3	C	502	FAD	PA-O3P-P-O2P
3	A	502	FAD	O4B-C4B-C5B-O5B
3	B	502	FAD	O4B-C4B-C5B-O5B
3	B	502	FAD	C3B-C4B-C5B-O5B
3	A	502	FAD	P-O3P-PA-O1A
3	A	502	FAD	C3B-C4B-C5B-O5B
2	C	501	NCT	C1-C2-C6-N2
2	D	501	NCT	C1-C2-C6-N2
3	C	502	FAD	C4'-C5'-O5'-P
3	C	502	FAD	P-O3P-PA-O2A
3	C	502	FAD	PA-O3P-P-O1P

There are no ring outliers.

8 monomers are involved in 44 short contacts:

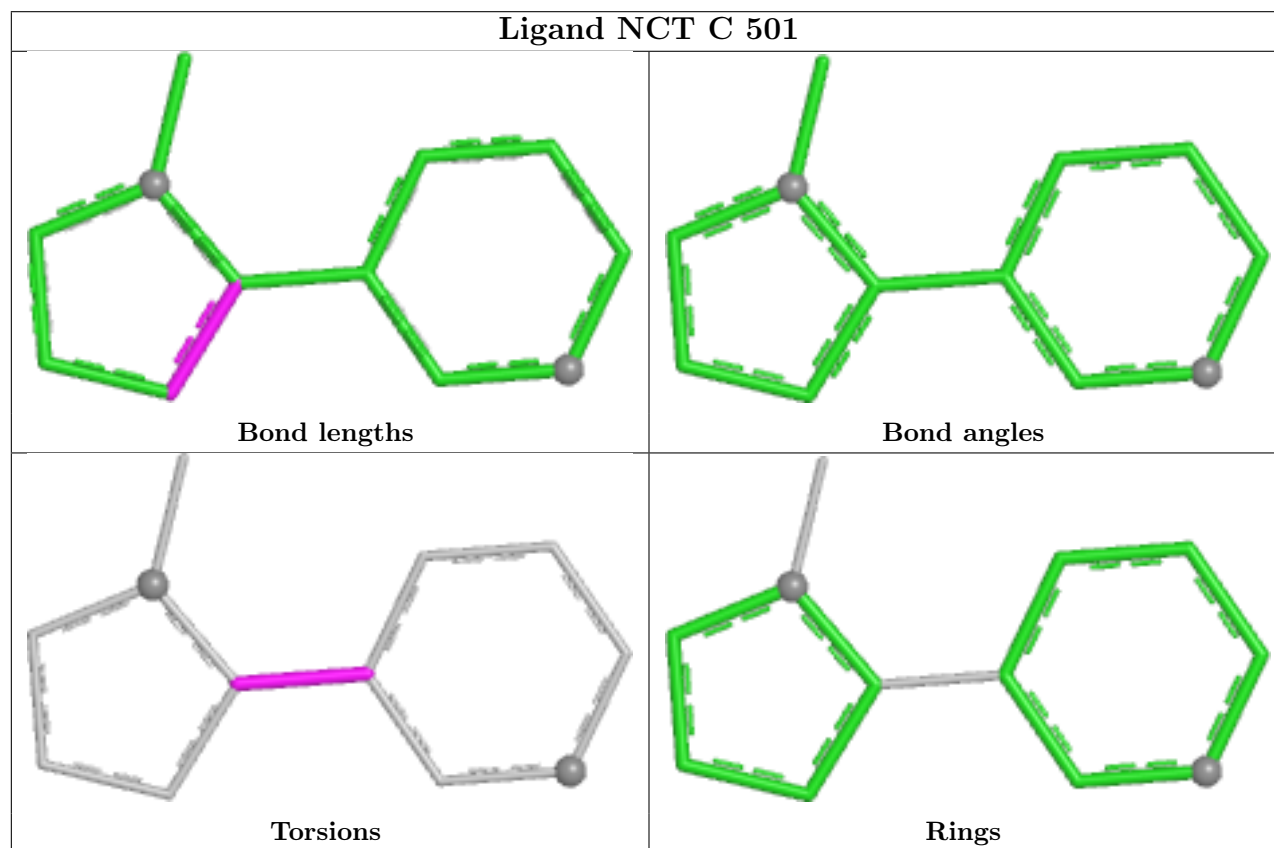
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NCT	4	0
3	D	502	FAD	13	0
2	D	501	NCT	1	0
2	A	501	NCT	1	0
3	A	502	FAD	9	0
2	B	501	NCT	5	0
3	C	502	FAD	5	0

Continued on next page...

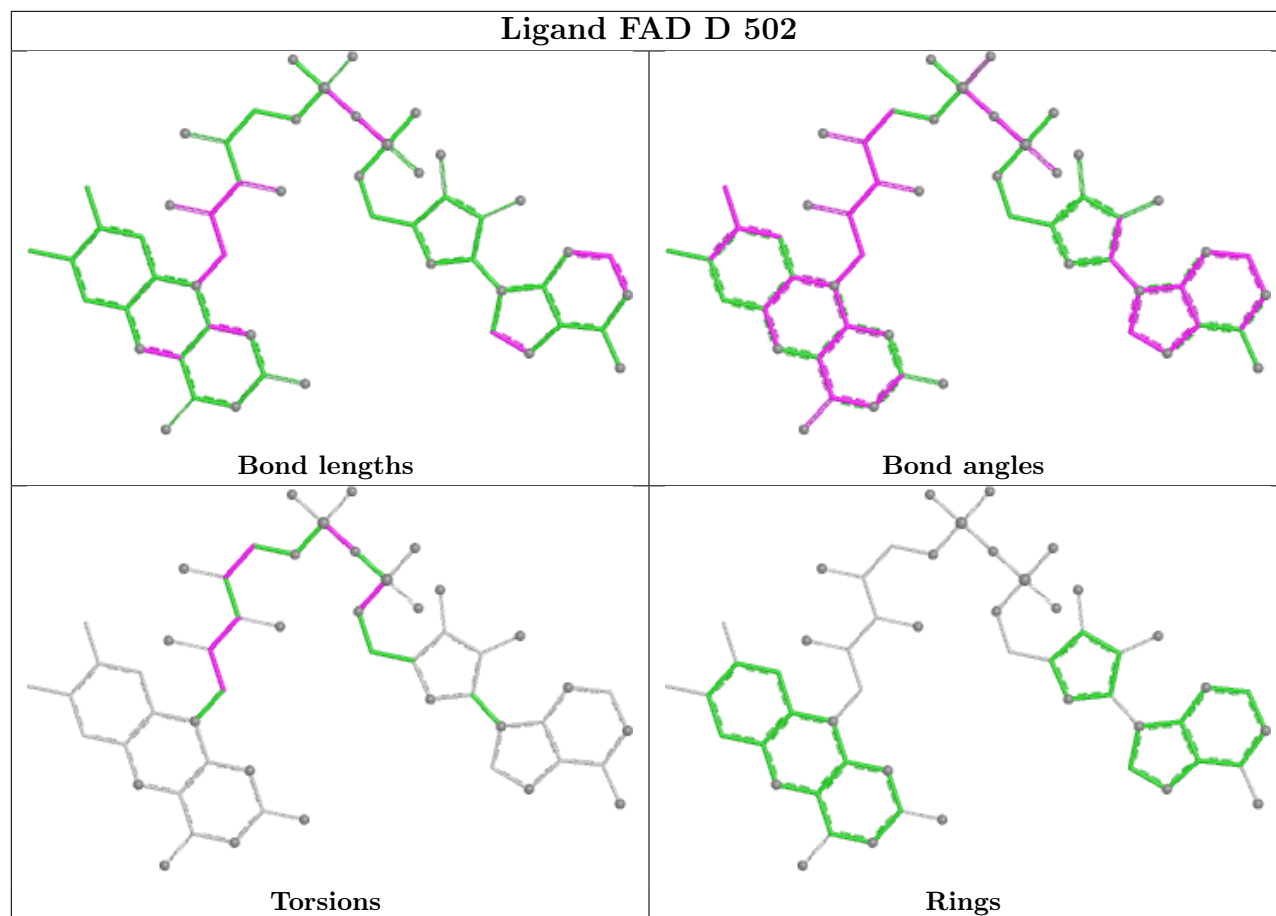
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	FAD	6	0

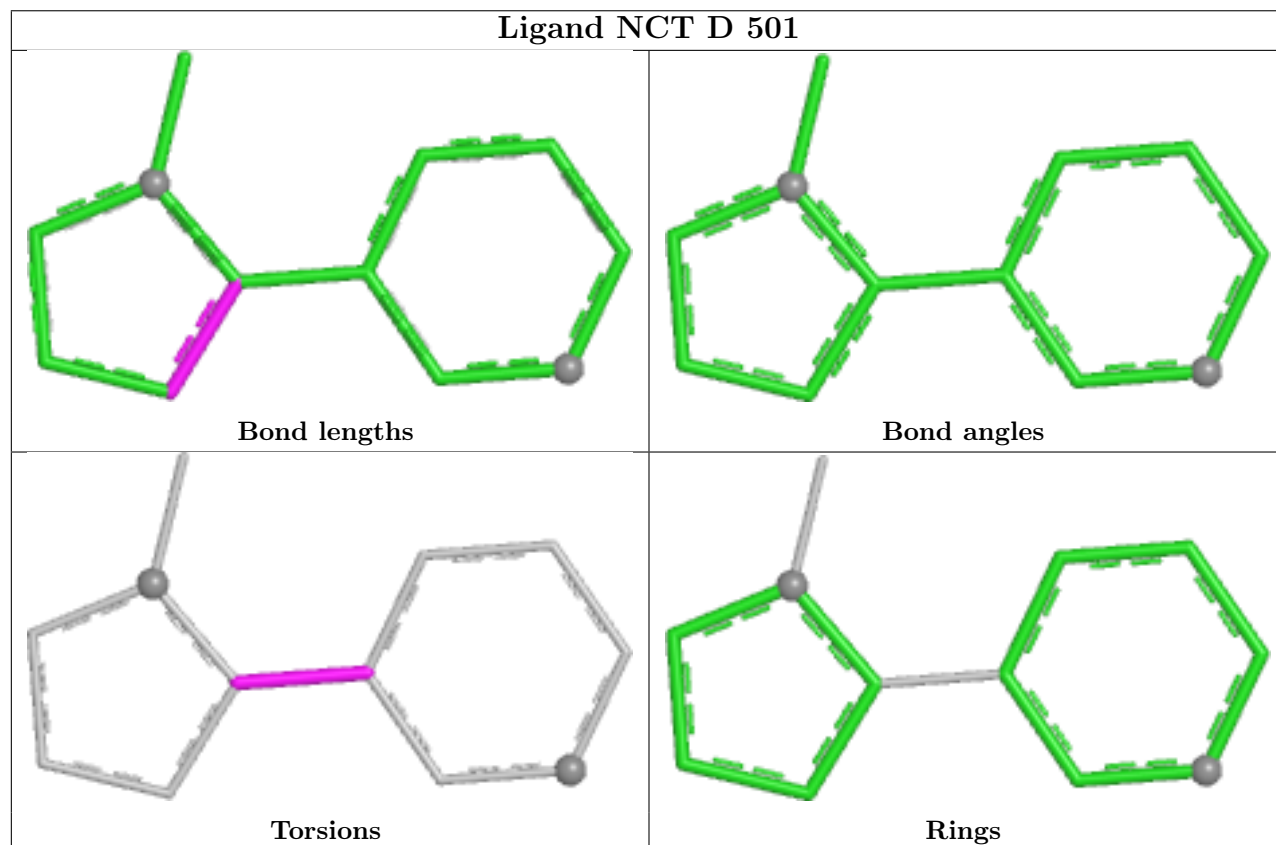
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



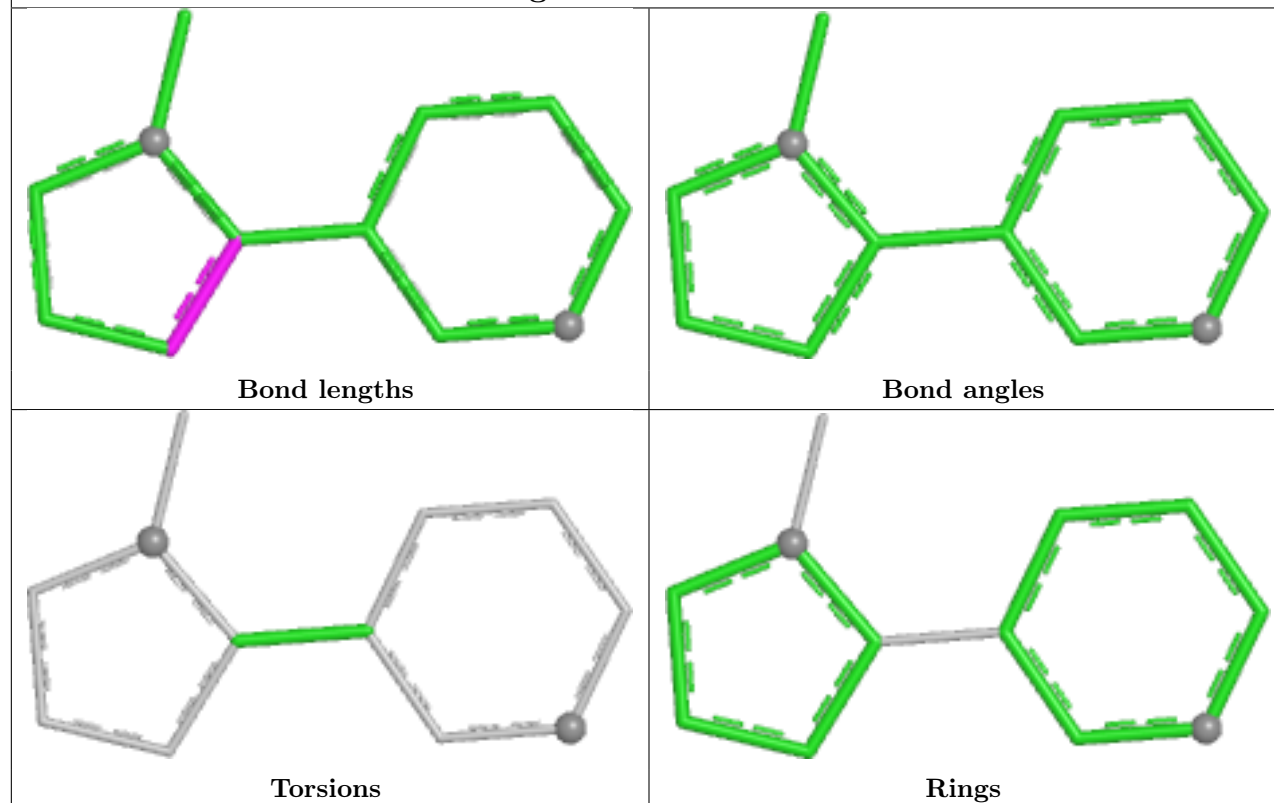
Ligand FAD D 502



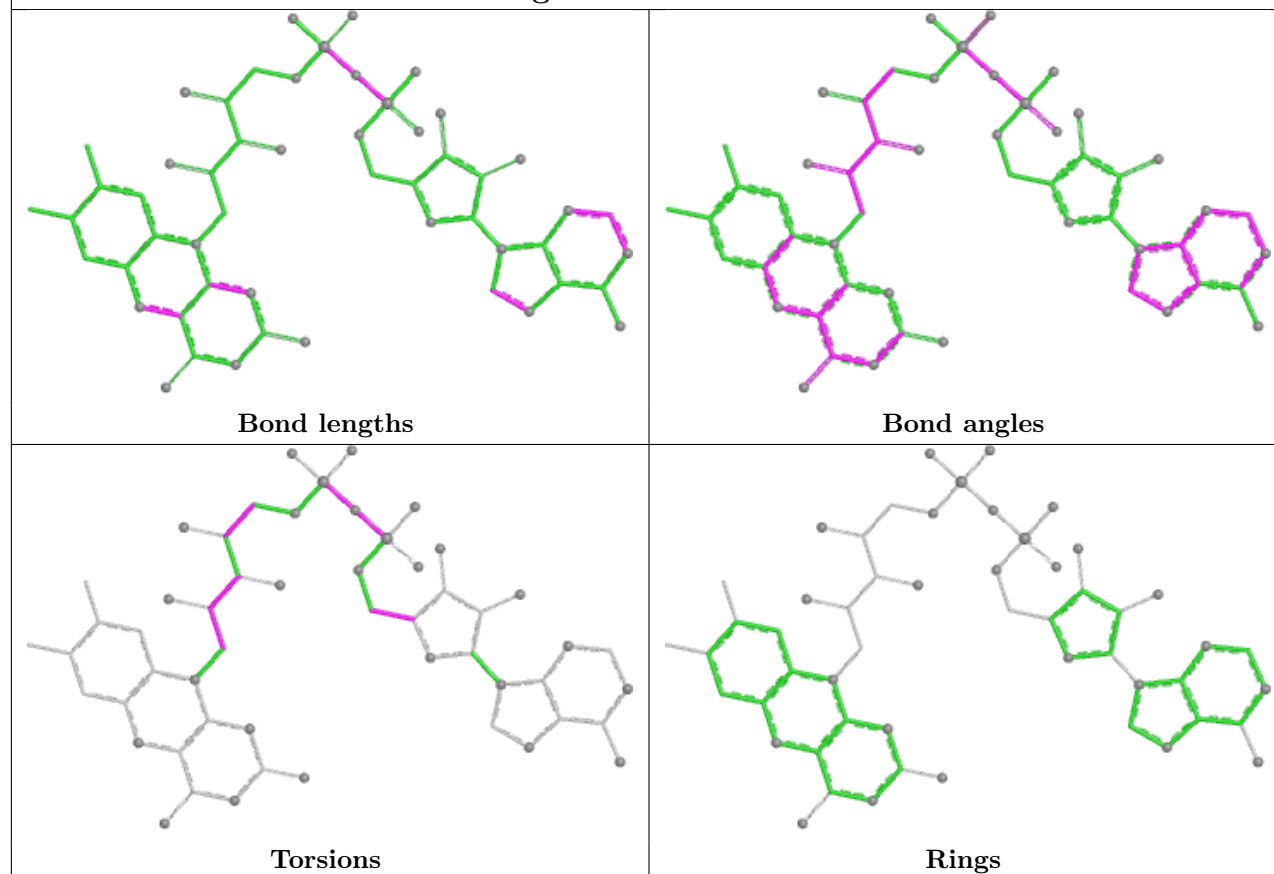
Ligand NCT D 501



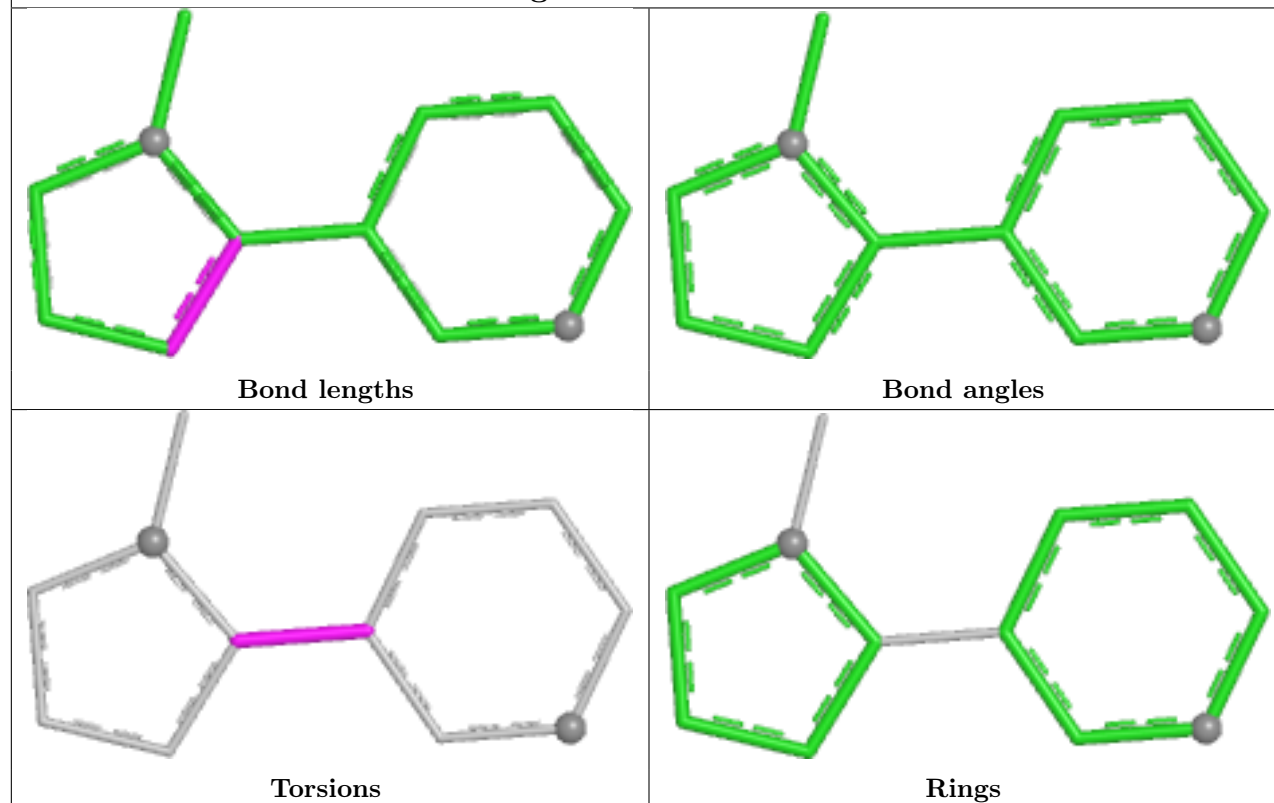
Ligand NCT A 501



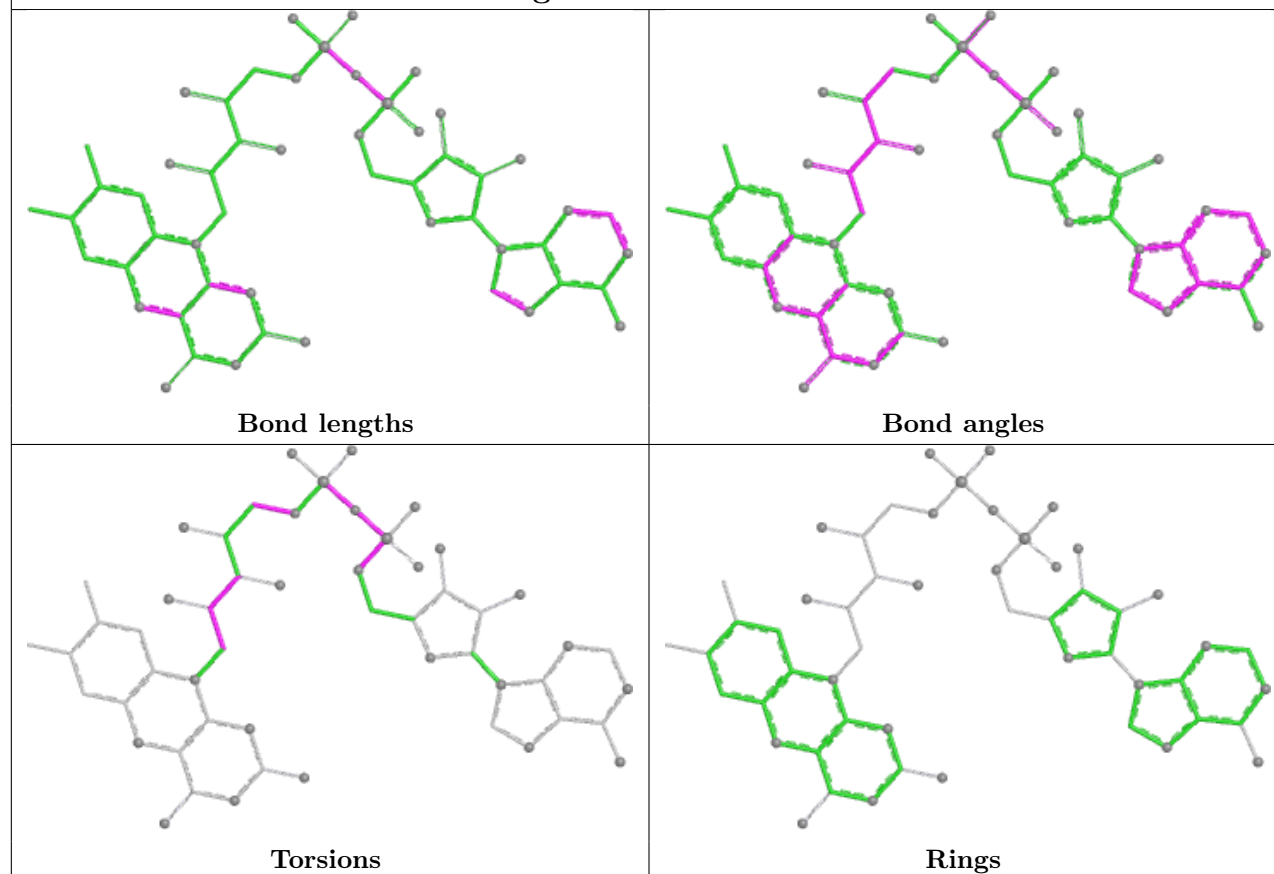
Ligand FAD A 502

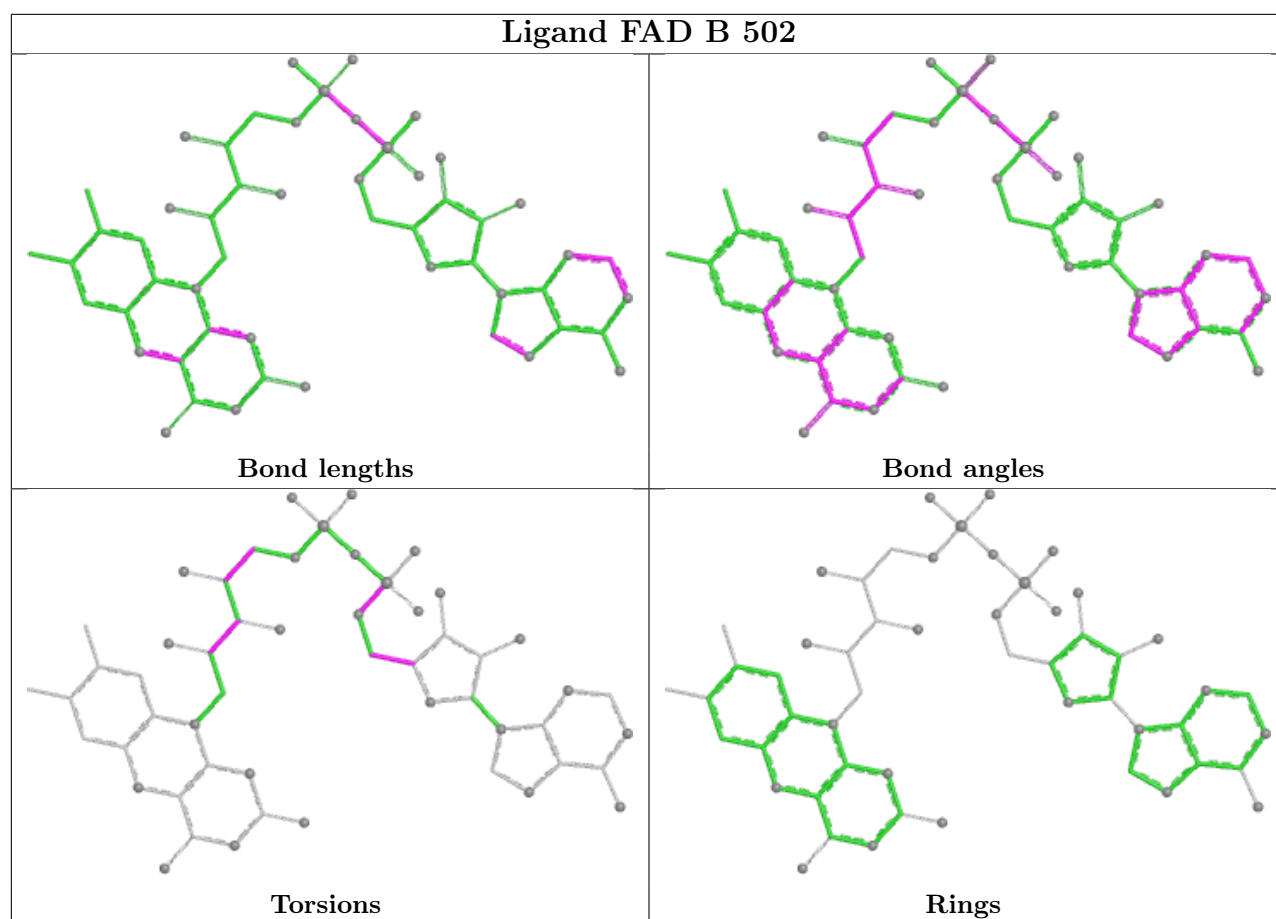


Ligand NCT B 501



Ligand FAD C 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/490 (88%)	0.45	16 (3%) 45 41	38, 66, 101, 113	0
1	B	432/490 (88%)	0.29	11 (2%) 58 55	36, 61, 82, 110	0
1	C	432/490 (88%)	0.71	22 (5%) 33 29	40, 75, 110, 121	0
1	D	405/490 (82%)	0.68	35 (8%) 16 13	41, 72, 112, 120	0
All	All	1701/1960 (86%)	0.53	84 (4%) 35 31	36, 68, 104, 121	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	107	ALA	5.2
1	C	231	VAL	4.5
1	D	139	LEU	4.3
1	A	378	LEU	4.1
1	D	362	LEU	4.1
1	D	406	GLY	3.9
1	A	244	ALA	3.5
1	D	135	LEU	3.4
1	C	131	PRO	3.4
1	B	132	LEU	3.4
1	C	244	ALA	3.4
1	D	404	PHE	3.3
1	D	142	TYR	3.3
1	A	362	LEU	3.1
1	D	388	ILE	3.1
1	D	390	VAL	2.8
1	D	371	SER	2.8
1	B	214	TYR	2.8
1	B	285	VAL	2.8
1	C	482	SER	2.8
1	C	375	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	282	VAL	2.8
1	A	131	PRO	2.7
1	A	150	ILE	2.7
1	A	343	VAL	2.7
1	D	342	TYR	2.7
1	C	174	PHE	2.7
1	B	146	SER	2.7
1	D	123	TYR	2.6
1	C	365	VAL	2.6
1	D	413	ALA	2.6
1	C	114	PRO	2.6
1	B	211	ILE	2.6
1	C	200	THR	2.5
1	D	407	VAL	2.5
1	B	360	GLN	2.5
1	C	294	ASP	2.5
1	A	174	PHE	2.5
1	D	353	PHE	2.5
1	C	230	GLY	2.4
1	C	374	LEU	2.4
1	D	363	ASN	2.4
1	C	407	VAL	2.4
1	B	131	PRO	2.4
1	B	227	GLY	2.4
1	A	211	ILE	2.4
1	D	211	ILE	2.3
1	D	140	ILE	2.3
1	C	249	GLU	2.3
1	A	365	VAL	2.3
1	D	365	VAL	2.3
1	D	52	PHE	2.3
1	C	152	PRO	2.3
1	A	380	ILE	2.2
1	D	355	PHE	2.2
1	D	405	PRO	2.2
1	A	171	TRP	2.2
1	A	155	PHE	2.2
1	D	104	PHE	2.2
1	A	250	THR	2.2
1	C	378	LEU	2.2
1	C	403	MET	2.2
1	D	150	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	155	PHE	2.2
1	C	302	GLY	2.2
1	D	101	GLU	2.1
1	D	141	MET	2.1
1	D	159	ILE	2.1
1	D	403	MET	2.1
1	D	370	TYR	2.1
1	C	377	ILE	2.1
1	A	354	ALA	2.1
1	B	171	TRP	2.1
1	D	364	TRP	2.1
1	B	215	MET	2.1
1	D	95	SER	2.1
1	D	354	ALA	2.0
1	D	356	ALA	2.0
1	C	232	LEU	2.0
1	A	344	HIS	2.0
1	D	202	GLY	2.0
1	B	170	ALA	2.0
1	A	333	GLY	2.0
1	D	458	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

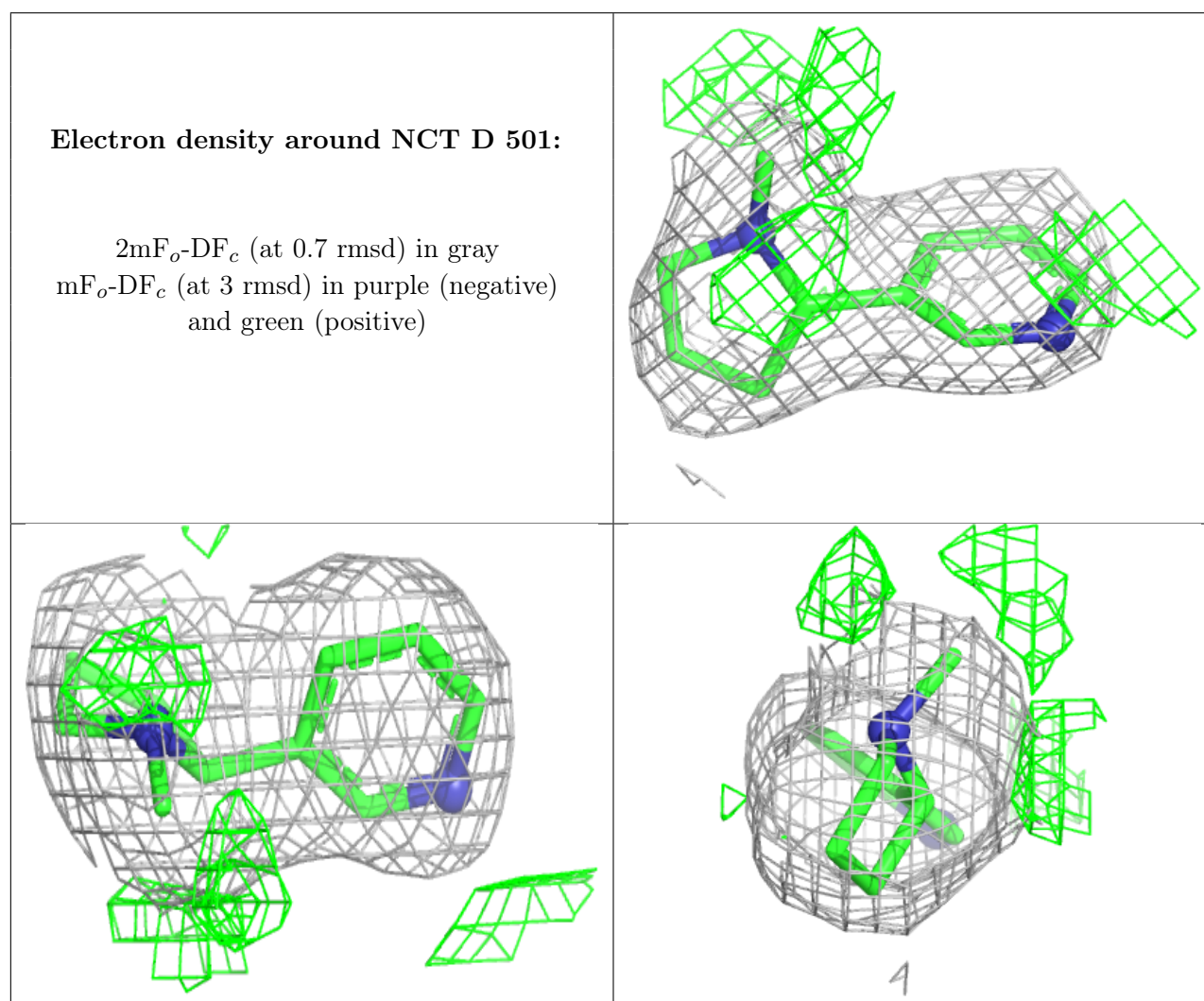
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NCT	D	501	12/12	0.85	0.18	63,76,82,82	0
2	NCT	B	501	12/12	0.86	0.16	61,66,69,70	0

Continued on next page...

Continued from previous page...

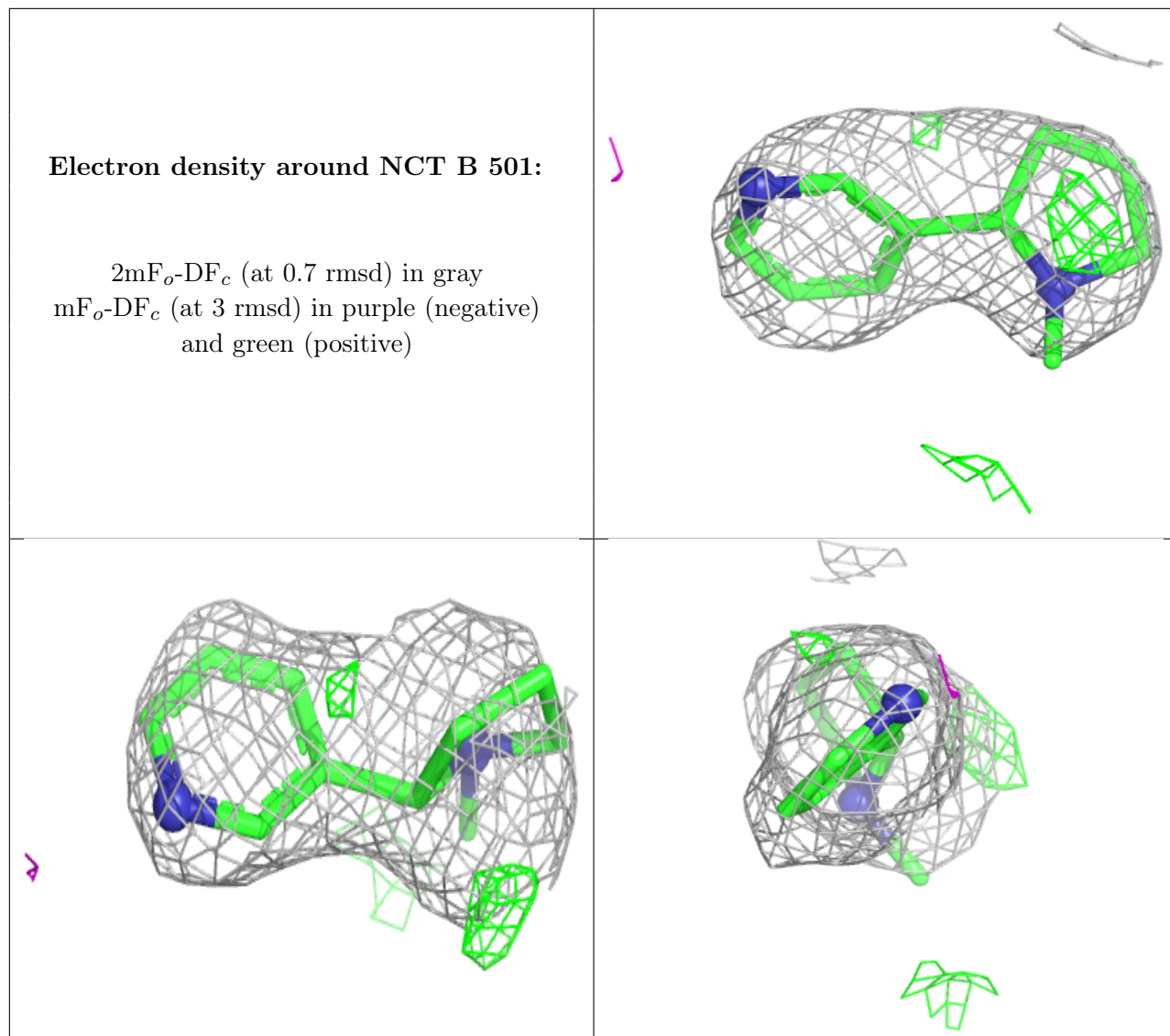
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	C	502	53/53	0.89	0.10	45,60,75,80	0
2	NCT	C	501	12/12	0.91	0.13	70,75,80,80	0
3	FAD	D	502	53/53	0.92	0.10	39,57,80,86	0
2	NCT	A	501	12/12	0.93	0.13	60,65,69,70	0
3	FAD	B	502	53/53	0.94	0.08	30,49,61,68	0
3	FAD	A	502	53/53	0.95	0.08	36,52,68,71	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.



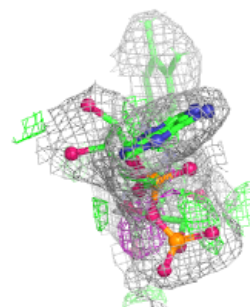
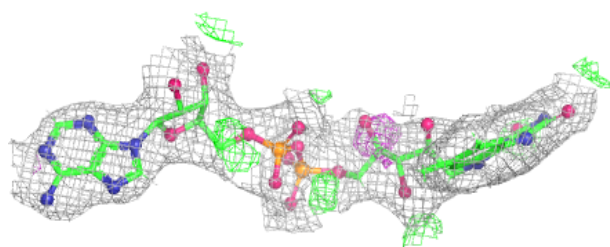
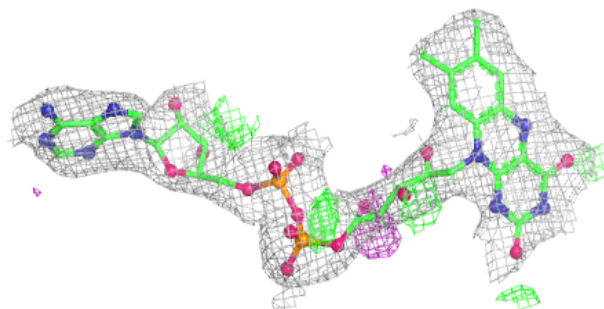
Electron density around NCT B 501:

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

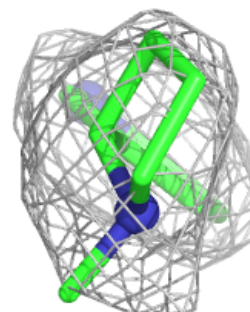
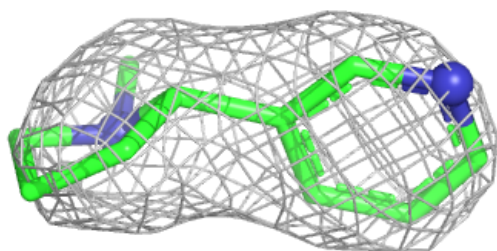
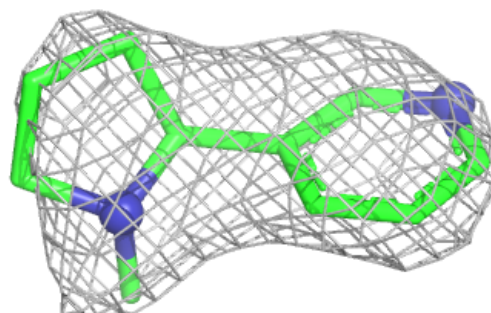


Electron density around FAD C 502:

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

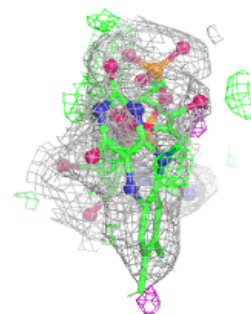
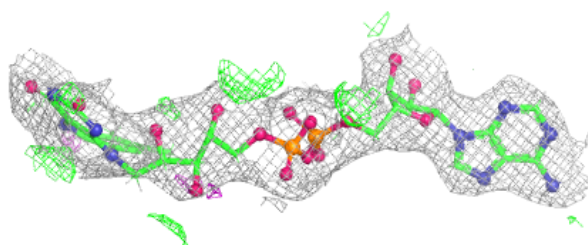
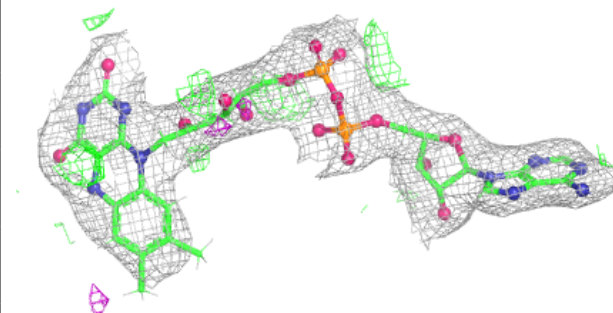
**Electron density around NCT C 501:**

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

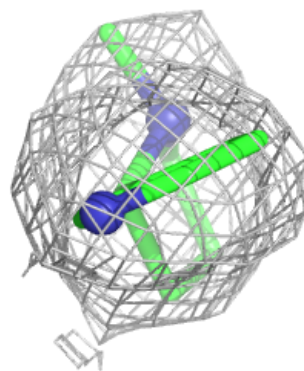
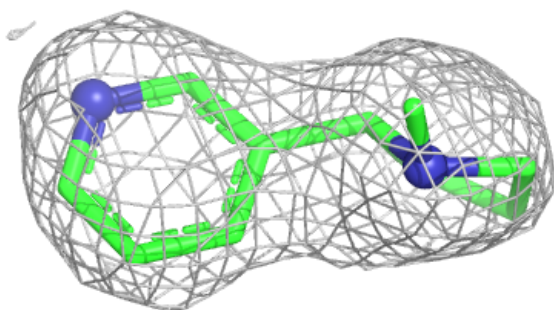
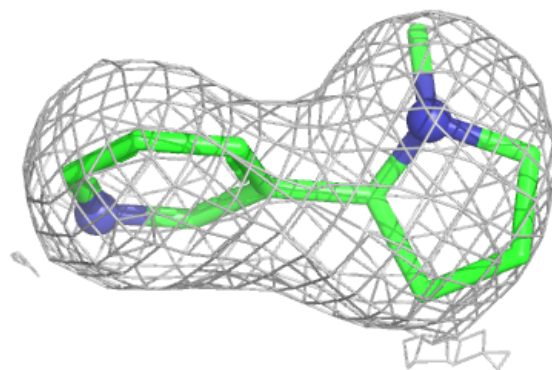


Electron density around FAD D 502:

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

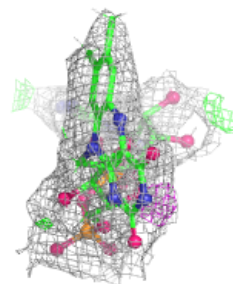
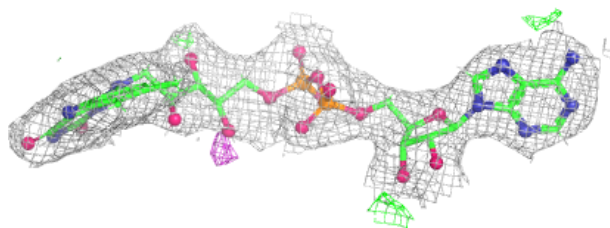
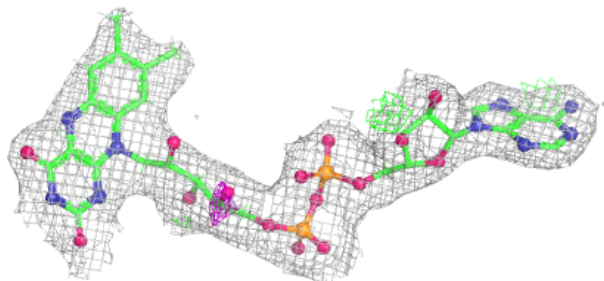
**Electron density around NCT A 501:**

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

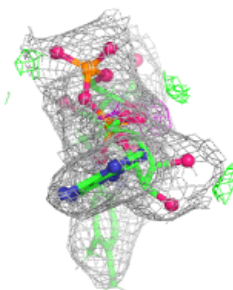
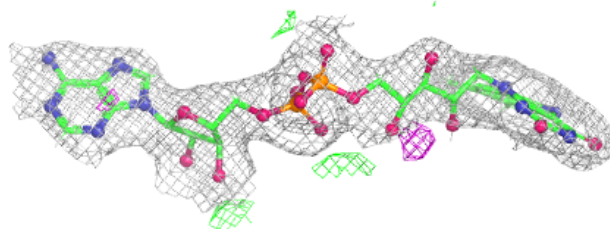
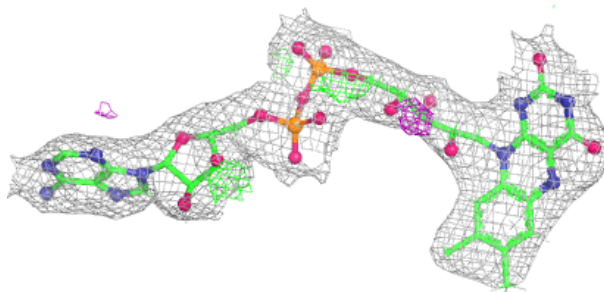


Electron density around FAD B 502:

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

**Electron density around FAD A 502:**

$2mF_o-DF_c$ (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.