



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 04:12 AM UTC

PDB ID : 6RUZ / pdb_00006ruz
Title : NADH-dependent Coenzyme A Disulfide Reductase
Authors : Koepke, J.; Preu, J.
Deposited on : 2019-05-29
Resolution : 2.90 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

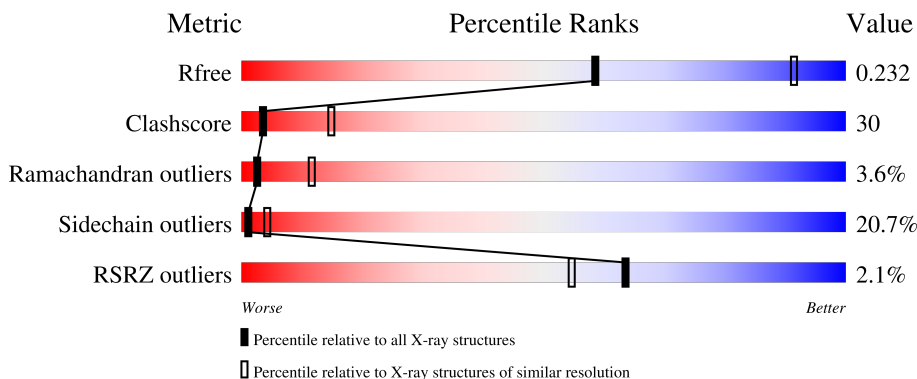
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	443	
1	B	443	
1	C	443	
1	D	443	

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
2	FAD	B	501	-	X	-	-

2 Entry composition [i](#)

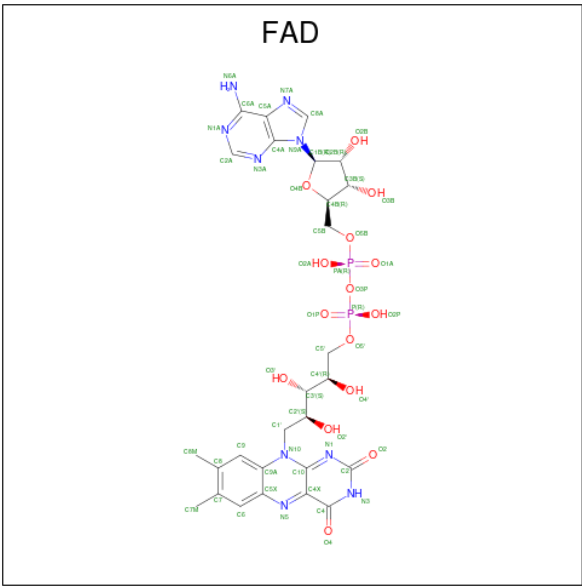
There are 4 unique types of molecules in this entry. The entry contains 13974 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADH oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3379	2147	608	617	7			
1	B	443	Total	C	N	O	S	0	0	0
			3379	2147	608	617	7			
1	C	443	Total	C	N	O	S	0	0	0
			3378	2146	608	617	7			
1	D	443	Total	C	N	O	S	0	0	0
			3377	2146	608	616	7			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



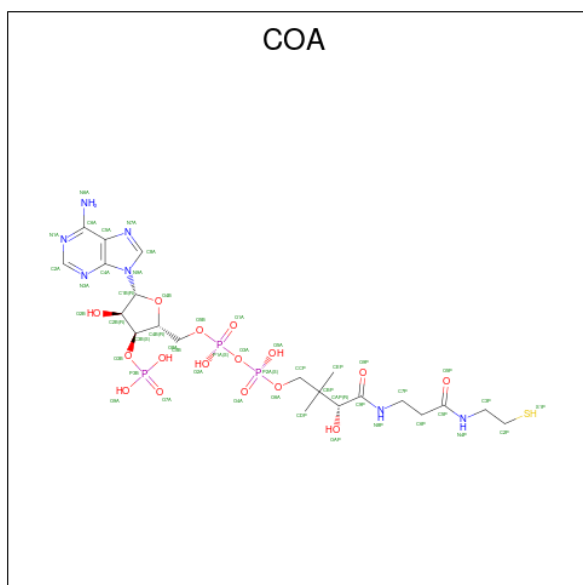
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
2	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	17	Total	O	0	0
			17	17		
4	C	15	Total	O	0	0
			15	15		

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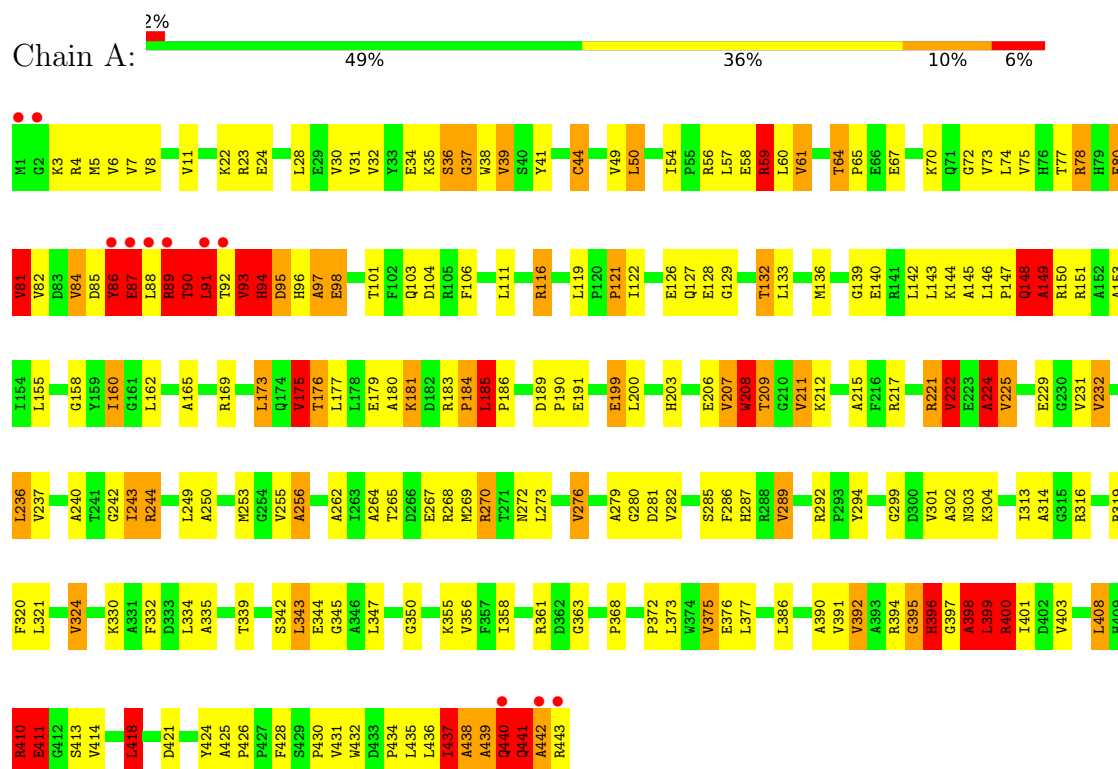
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	11	Total	O	0	0
			11	11		

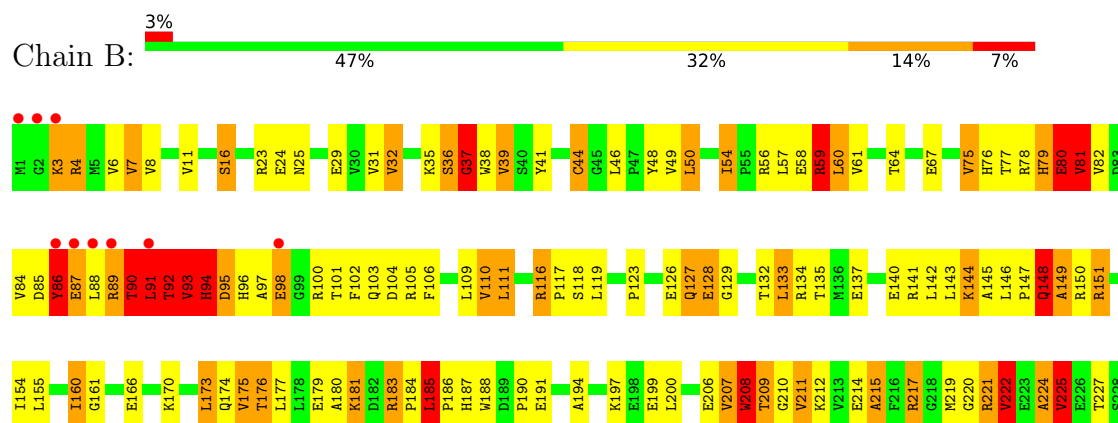
3 Residue-property plots [i](#)

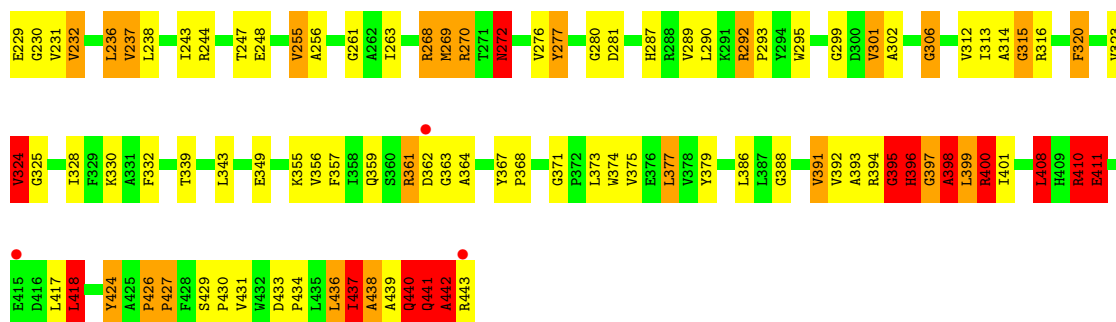
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

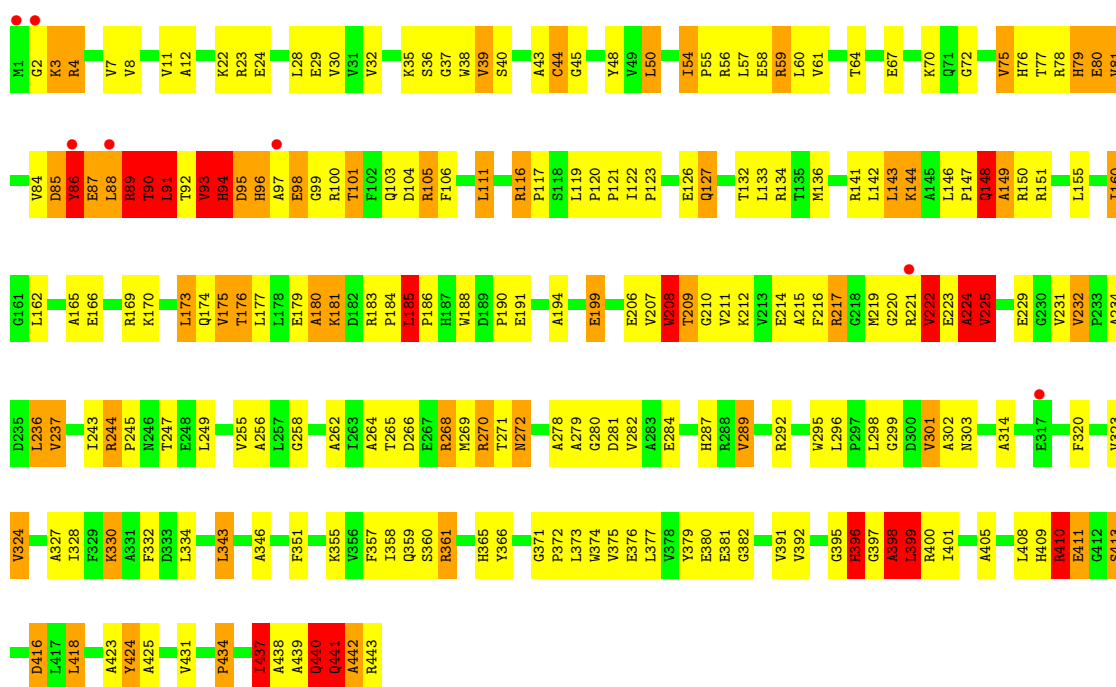


• Molecule 1: NADH oxidase

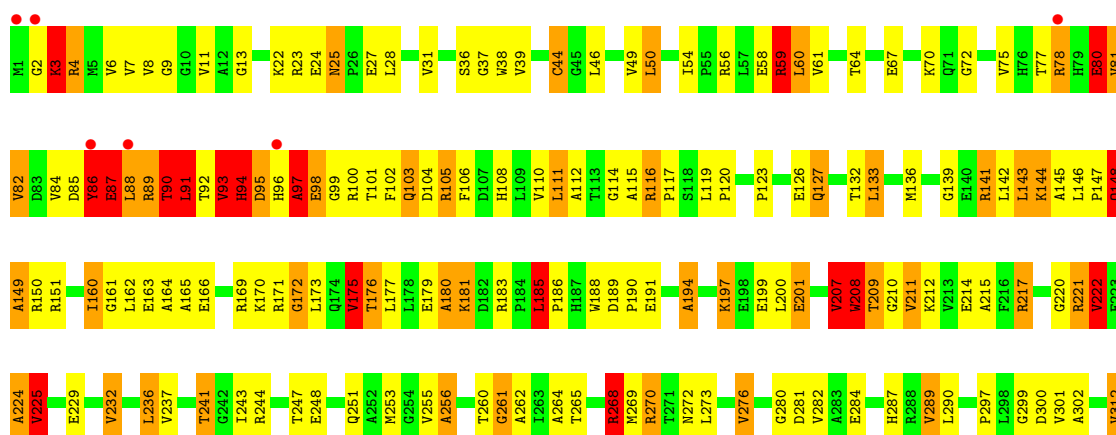


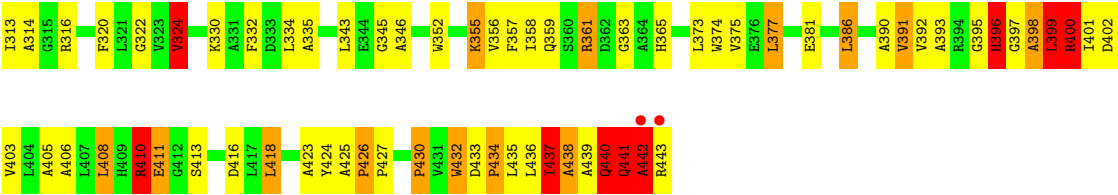


• Molecule 1: NADH oxidase



• Molecule 1: NADH oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.98Å 159.98Å 256.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.38 – 2.90 58.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (58.38-2.90) 98.2 (58.38-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.207 , 0.244 0.197 , 0.232	Depositor DCC
R_{free} test set	2000 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13974	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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, COA

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	2.03	84/3451 (2.4%)	1.87	96/4686 (2.0%)
1	B	1.98	71/3451 (2.1%)	1.85	92/4686 (2.0%)
1	C	1.90	62/3450 (1.8%)	1.82	74/4683 (1.6%)
1	D	1.91	54/3449 (1.6%)	1.83	83/4683 (1.8%)
All	All	1.96	271/13801 (2.0%)	1.84	345/18738 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	5
1	C	0	8
1	D	0	4
All	All	0	25

All (271) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	GLN	C-O	14.62	1.42	1.24
1	C	440	GLN	C-O	14.37	1.42	1.24
1	D	440	GLN	C-O	13.02	1.40	1.24
1	A	440	GLN	C-O	12.78	1.40	1.24
1	D	396	HIS	C-O	12.69	1.41	1.23
1	C	396	HIS	C-O	12.56	1.41	1.23
1	A	437	ILE	CA-CB	11.89	1.68	1.54
1	D	97	ALA	CA-CB	11.38	1.72	1.53
1	B	87	GLU	CA-C	11.29	1.68	1.53
1	B	437	ILE	CA-CB	11.25	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	VAL	CA-CB	11.11	1.69	1.54
1	B	396	HIS	C-O	11.07	1.38	1.24
1	A	256	ALA	CA-CB	-10.69	1.36	1.53
1	B	222	VAL	CA-CB	10.44	1.68	1.54
1	C	194	ALA	CA-CB	-9.87	1.38	1.53
1	C	87	GLU	CA-C	9.82	1.66	1.53
1	B	176	THR	CA-C	9.77	1.64	1.52
1	D	381	GLU	C-O	9.52	1.35	1.24
1	B	207	VAL	CA-CB	9.40	1.65	1.53
1	A	264	ALA	CA-CB	-9.34	1.37	1.53
1	D	322	GLY	C-O	9.32	1.32	1.23
1	A	87	GLU	CA-C	9.23	1.65	1.53
1	B	440	GLN	CA-C	9.14	1.65	1.52
1	C	40	SER	CA-C	9.13	1.64	1.53
1	B	368	PRO	CA-C	-9.13	1.43	1.52
1	A	440	GLN	CA-C	9.08	1.65	1.52
1	D	437	ILE	CA-CB	9.07	1.64	1.54
1	C	96	HIS	CA-C	8.97	1.64	1.52
1	C	264	ALA	CA-CB	-8.91	1.39	1.53
1	A	97	ALA	N-CA	8.47	1.57	1.46
1	A	59	ARG	CA-C	8.44	1.64	1.52
1	A	122	ILE	CA-C	-8.40	1.44	1.52
1	C	97	ALA	CA-CB	8.38	1.67	1.53
1	D	440	GLN	CD-NE2	8.36	1.50	1.33
1	B	225	VAL	CA-CB	8.29	1.65	1.54
1	A	93	VAL	CA-CB	8.28	1.65	1.54
1	C	397	GLY	CA-C	8.27	1.60	1.52
1	A	440	GLN	CA-CB	8.22	1.67	1.53
1	B	185	LEU	C-O	8.22	1.27	1.23
1	C	440	GLN	CA-CB	8.19	1.67	1.53
1	D	82	VAL	CA-CB	-8.08	1.45	1.54
1	A	222	VAL	CA-CB	7.95	1.65	1.54
1	D	120	PRO	CA-C	7.92	1.56	1.51
1	D	441	GLN	CA-C	7.90	1.63	1.52
1	B	440	GLN	N-CA	7.84	1.56	1.46
1	A	96	HIS	CA-C	7.84	1.62	1.52
1	D	264	ALA	CA-CB	-7.80	1.41	1.53
1	B	426	PRO	CA-C	7.80	1.59	1.52
1	B	97	ALA	CA-CB	7.76	1.66	1.53
1	B	154	ILE	CA-CB	-7.75	1.44	1.54
1	A	399	LEU	N-CA	7.74	1.56	1.46
1	B	96	HIS	CA-C	7.74	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	ILE	C-O	-7.68	1.15	1.23
1	A	421	ASP	CA-C	7.57	1.62	1.53
1	A	438	ALA	CA-CB	-7.54	1.41	1.53
1	B	81	VAL	CA-CB	7.53	1.62	1.54
1	D	441	GLN	C-O	7.51	1.33	1.24
1	A	73	VAL	CA-CB	7.50	1.63	1.54
1	A	180	ALA	CA-CB	-7.50	1.41	1.53
1	D	334	LEU	CA-C	-7.49	1.43	1.52
1	B	93	VAL	CA-CB	7.48	1.64	1.54
1	D	440	GLN	CA-C	7.35	1.62	1.52
1	B	440	GLN	CD-NE2	7.34	1.48	1.33
1	A	91	LEU	CA-C	-7.28	1.43	1.52
1	A	158	GLY	C-O	-7.26	1.15	1.23
1	B	29	GLU	C-O	7.26	1.32	1.24
1	A	335	ALA	CA-CB	-7.22	1.43	1.53
1	C	396	HIS	N-CA	7.16	1.55	1.46
1	B	398	ALA	CA-C	7.09	1.62	1.52
1	A	250	ALA	CA-CB	-7.09	1.41	1.53
1	C	225	VAL	N-CA	7.02	1.55	1.46
1	D	87	GLU	CA-C	7.02	1.63	1.53
1	B	339	THR	C-O	7.00	1.32	1.23
1	C	160	ILE	CA-CB	6.98	1.63	1.54
1	C	86	TYR	CB-CG	6.98	1.67	1.51
1	D	396	HIS	N-CA	6.96	1.55	1.46
1	A	397	GLY	CA-C	6.95	1.58	1.52
1	D	93	VAL	CA-CB	6.95	1.64	1.54
1	A	215	ALA	CA-CB	-6.90	1.42	1.53
1	B	441	GLN	CG-CD	6.88	1.69	1.52
1	B	232	VAL	CA-C	-6.88	1.47	1.53
1	A	86	TYR	CB-CG	6.86	1.66	1.51
1	D	225	VAL	C-O	6.86	1.32	1.24
1	C	328	ILE	C-O	-6.85	1.17	1.23
1	A	184	PRO	C-O	6.81	1.31	1.23
1	C	97	ALA	N-CA	6.78	1.54	1.46
1	B	98	GLU	CG-CD	6.77	1.69	1.52
1	A	289	VAL	CA-C	-6.77	1.43	1.52
1	C	372	PRO	C-O	6.74	1.31	1.23
1	B	393	ALA	CA-CB	-6.73	1.43	1.53
1	A	98	GLU	N-CA	6.72	1.55	1.46
1	A	97	ALA	CA-CB	6.71	1.64	1.53
1	A	396	HIS	C-O	6.69	1.32	1.24
1	C	440	GLN	CA-C	6.68	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CG-CD	6.67	1.68	1.52
1	A	207	VAL	C-O	-6.61	1.16	1.24
1	A	398	ALA	CA-CB	-6.59	1.42	1.53
1	D	90	THR	CB-CG2	6.59	1.74	1.52
1	D	160	ILE	CA-CB	6.59	1.62	1.54
1	D	440	GLN	CA-CB	6.56	1.64	1.53
1	A	398	ALA	CA-C	6.53	1.61	1.52
1	A	313	ILE	CA-CB	6.53	1.62	1.54
1	C	441	GLN	CA-C	6.49	1.61	1.52
1	A	225	VAL	CA-CB	6.47	1.63	1.54
1	D	97	ALA	N-CA	6.46	1.54	1.46
1	A	81	VAL	CA-CB	6.46	1.61	1.54
1	C	437	ILE	CA-CB	6.45	1.62	1.54
1	D	180	ALA	CA-CB	-6.45	1.43	1.53
1	D	194	ALA	CA-CB	-6.44	1.43	1.53
1	D	335	ALA	CA-CB	6.44	1.63	1.53
1	A	441	GLN	CG-CD	6.42	1.68	1.52
1	A	411	GLU	CA-C	-6.39	1.45	1.52
1	D	96	HIS	CA-C	6.37	1.61	1.53
1	D	3	LYS	CA-C	6.37	1.62	1.53
1	C	165	ALA	CA-CB	-6.33	1.43	1.53
1	C	366	TYR	CA-C	6.33	1.61	1.52
1	C	94	HIS	CA-C	-6.32	1.45	1.52
1	C	441	GLN	CG-CD	6.28	1.67	1.52
1	A	356	VAL	C-O	-6.26	1.17	1.24
1	B	97	ALA	N-CA	6.23	1.54	1.46
1	D	103	GLN	C-O	6.17	1.31	1.23
1	A	243	ILE	CA-C	-6.16	1.45	1.52
1	A	165	ALA	CA-CB	6.14	1.63	1.53
1	C	441	GLN	C-O	6.14	1.31	1.24
1	B	398	ALA	N-CA	6.14	1.54	1.46
1	D	441	GLN	CG-CD	6.11	1.67	1.52
1	A	390	ALA	C-O	-6.09	1.16	1.23
1	B	442	ALA	CA-CB	-6.07	1.43	1.53
1	B	160	ILE	CA-CB	6.06	1.62	1.54
1	B	323	VAL	CA-C	-6.05	1.46	1.52
1	B	437	ILE	CA-C	6.05	1.60	1.52
1	B	440	GLN	CA-CB	6.05	1.63	1.53
1	B	295	TRP	C-O	-6.04	1.16	1.24
1	C	57	LEU	CA-C	6.04	1.60	1.52
1	B	197	LYS	C-O	6.03	1.31	1.24
1	C	160	ILE	CA-C	-6.03	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	86	TYR	CB-CG	6.01	1.64	1.51
1	C	405	ALA	CA-CB	5.96	1.62	1.53
1	B	60	LEU	CA-C	5.95	1.62	1.52
1	D	400	ARG	CA-C	5.93	1.60	1.52
1	B	417	LEU	C-O	-5.92	1.17	1.24
1	C	278	ALA	C-O	5.88	1.31	1.23
1	C	398	ALA	CA-C	5.87	1.60	1.52
1	C	105	ARG	CA-C	-5.86	1.45	1.52
1	A	410	ARG	CA-C	5.86	1.60	1.52
1	B	248	GLU	CA-C	5.85	1.60	1.52
1	D	440	GLN	N-CA	5.83	1.53	1.46
1	D	115	ALA	C-O	5.83	1.30	1.23
1	D	160	ILE	CA-C	-5.82	1.46	1.52
1	C	141	ARG	CA-C	5.81	1.60	1.52
1	C	278	ALA	CA-C	5.81	1.59	1.52
1	A	343	LEU	N-CA	-5.80	1.39	1.46
1	D	282	VAL	CA-CB	-5.80	1.46	1.54
1	C	232	VAL	C-O	-5.80	1.17	1.24
1	A	96	HIS	C-N	5.80	1.41	1.33
1	B	98	GLU	N-CA	5.79	1.53	1.46
1	C	2	GLY	C-O	5.79	1.31	1.23
1	A	39	VAL	CA-C	5.78	1.59	1.52
1	A	441	GLN	CA-CB	5.78	1.63	1.53
1	C	440	GLN	N-CA	5.77	1.53	1.46
1	B	194	ALA	CA-C	5.76	1.60	1.52
1	A	232	VAL	C-O	-5.76	1.17	1.24
1	D	176	THR	CA-C	5.75	1.59	1.52
1	D	256	ALA	CA-CB	-5.74	1.44	1.53
1	D	265	THR	CA-CB	5.73	1.64	1.53
1	A	91	LEU	N-CA	5.72	1.53	1.46
1	D	232	VAL	C-O	-5.72	1.17	1.24
1	B	398	ALA	CA-CB	-5.71	1.43	1.53
1	D	391	VAL	CA-CB	5.70	1.62	1.54
1	C	330	LYS	C-O	5.66	1.30	1.24
1	B	396	HIS	C-N	5.65	1.41	1.33
1	B	410	ARG	NE-CZ	5.65	1.39	1.33
1	A	225	VAL	N-CA	5.64	1.53	1.46
1	D	297	PRO	CA-C	5.64	1.60	1.52
1	C	98	GLU	N-CA	5.63	1.53	1.46
1	B	93	VAL	CA-C	5.62	1.59	1.52
1	D	268	ARG	CZ-NH1	5.61	1.40	1.32
1	A	440	GLN	CD-NE2	5.61	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	VAL	CA-C	5.60	1.59	1.52
1	A	208	TRP	CG-CD1	5.60	1.50	1.36
1	A	82	VAL	C-O	-5.60	1.17	1.24
1	C	265	THR	CA-C	5.59	1.59	1.52
1	A	209	THR	CA-CB	-5.58	1.44	1.53
1	D	59	ARG	CA-C	5.56	1.60	1.52
1	B	97	ALA	C-O	5.55	1.30	1.24
1	C	431	VAL	CA-CB	5.55	1.62	1.54
1	B	175	VAL	CA-CB	5.53	1.61	1.54
1	D	313	ILE	C-O	-5.52	1.17	1.24
1	A	149	ALA	C-O	5.52	1.30	1.24
1	B	396	HIS	N-CA	5.52	1.52	1.46
1	A	279	ALA	CA-CB	5.51	1.63	1.53
1	B	391	VAL	CA-CB	5.49	1.61	1.54
1	A	441	GLN	C-O	5.48	1.30	1.24
1	C	2	GLY	CA-C	5.48	1.59	1.51
1	B	440	GLN	CD-OE1	5.47	1.33	1.23
1	C	292	ARG	CA-C	5.45	1.59	1.52
1	C	234	ALA	C-O	-5.44	1.17	1.24
1	C	162	LEU	C-O	-5.43	1.17	1.24
1	C	343	LEU	C-O	5.43	1.30	1.24
1	A	368	PRO	CA-C	-5.42	1.47	1.52
1	B	301	VAL	CA-CB	5.42	1.62	1.54
1	A	376	GLU	C-O	-5.41	1.17	1.24
1	B	436	LEU	C-O	5.41	1.30	1.24
1	A	438	ALA	C-O	-5.39	1.17	1.24
1	C	279	ALA	CA-CB	5.39	1.63	1.53
1	C	244	ARG	CA-C	5.39	1.57	1.52
1	C	85	ASP	C-O	-5.38	1.17	1.23
1	C	351	PHE	CE1-CZ	5.38	1.54	1.38
1	A	396	HIS	N-CA	5.38	1.53	1.46
1	B	75	VAL	CA-C	5.37	1.58	1.52
1	A	155	LEU	C-O	-5.37	1.17	1.24
1	C	155	LEU	C-O	-5.36	1.17	1.24
1	D	397	GLY	CA-C	5.34	1.57	1.52
1	D	165	ALA	CA-CB	-5.34	1.45	1.53
1	C	43	ALA	CA-CB	-5.33	1.44	1.53
1	D	430	PRO	CA-C	5.33	1.59	1.52
1	D	105	ARG	CZ-NH1	5.31	1.40	1.32
1	D	148	GLN	N-CA	5.31	1.53	1.46
1	B	269	MET	CA-C	-5.31	1.46	1.52
1	D	405	ALA	CA-CB	5.29	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	GLU	CA-C	5.29	1.59	1.52
1	D	423	ALA	CA-C	-5.28	1.46	1.52
1	C	327	ALA	CA-CB	-5.27	1.44	1.53
1	B	325	GLY	C-O	-5.27	1.16	1.23
1	A	224	ALA	C-O	-5.27	1.17	1.24
1	D	440	GLN	CD-OE1	5.26	1.33	1.23
1	A	400	ARG	CA-C	5.26	1.59	1.52
1	A	303	ASN	CA-C	5.26	1.59	1.52
1	B	215	ALA	C-O	5.24	1.29	1.23
1	C	441	GLN	CB-CG	5.23	1.68	1.52
1	A	232	VAL	CA-C	-5.22	1.48	1.53
1	A	435	LEU	C-O	5.22	1.30	1.24
1	B	137	GLU	CG-CD	5.21	1.65	1.52
1	A	435	LEU	CA-C	5.21	1.59	1.52
1	A	286	PHE	N-CA	-5.20	1.39	1.46
1	A	153	ALA	CA-CB	-5.20	1.45	1.53
1	C	225	VAL	CA-CB	5.20	1.61	1.54
1	A	414	VAL	CA-CB	-5.18	1.48	1.54
1	A	84	VAL	CA-C	5.18	1.59	1.52
1	A	372	PRO	C-O	5.17	1.29	1.23
1	C	223	GLU	CA-C	-5.16	1.45	1.52
1	C	98	GLU	C-O	5.15	1.30	1.24
1	A	265	THR	CA-CB	5.14	1.62	1.53
1	B	217	ARG	C-O	5.14	1.30	1.23
1	A	121	PRO	C-O	-5.14	1.19	1.24
1	B	35	LYS	CB-CG	-5.13	1.37	1.52
1	A	282	VAL	CA-CB	-5.13	1.47	1.54
1	B	176	THR	CA-CB	5.12	1.61	1.53
1	D	442	ALA	C-O	5.12	1.30	1.24
1	A	347	LEU	CG-CD2	5.11	1.69	1.52
1	B	39	VAL	C-O	5.10	1.29	1.24
1	B	59	ARG	CA-C	5.08	1.59	1.52
1	D	2	GLY	CA-C	5.08	1.59	1.51
1	C	98	GLU	CG-CD	5.08	1.64	1.52
1	D	207	VAL	CA-CB	5.08	1.59	1.53
1	B	438	ALA	CA-CB	-5.06	1.45	1.53
1	B	238	LEU	C-O	5.06	1.30	1.24
1	B	151	ARG	CA-C	5.06	1.58	1.52
1	A	321	LEU	CG-CD1	-5.05	1.35	1.52
1	A	36	SER	CA-C	-5.05	1.45	1.52
1	A	39	VAL	C-O	5.05	1.29	1.23
1	B	255	VAL	N-CA	-5.05	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	SER	C-O	5.05	1.29	1.23
1	C	416	ASP	CA-C	-5.04	1.46	1.52
1	B	349	GLU	C-O	-5.04	1.17	1.24
1	C	122	ILE	CA-C	-5.03	1.47	1.52
1	B	263	ILE	CA-CB	-5.02	1.49	1.54
1	A	345	GLY	C-O	-5.02	1.17	1.23
1	C	87	GLU	CD-OE1	5.02	1.34	1.25
1	C	55	PRO	CA-C	5.01	1.59	1.52
1	B	140	GLU	CA-C	5.00	1.59	1.52

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	397	GLY	N-CA-C	17.29	135.98	111.42
1	D	397	GLY	N-CA-C	13.61	130.74	111.42
1	A	397	GLY	N-CA-C	13.43	130.75	111.14
1	D	160	ILE	N-CA-C	-12.34	92.43	109.21
1	B	397	GLY	N-CA-C	11.72	147.29	113.30
1	D	324	VAL	N-CA-C	-11.01	102.63	113.20
1	D	36	SER	CA-C-N	-10.54	104.27	122.09
1	D	36	SER	C-N-CA	-10.54	104.27	122.09
1	C	94	HIS	N-CA-C	-10.04	92.91	109.07
1	A	160	ILE	N-CA-C	-9.98	95.77	109.55
1	B	128	GLU	N-CA-C	9.95	121.72	111.07
1	A	54	ILE	CA-C-N	9.92	129.29	118.97
1	A	54	ILE	C-N-CA	9.92	129.29	118.97
1	A	90	THR	N-CA-C	-9.86	96.02	110.42
1	C	160	ILE	N-CA-C	-9.84	93.91	108.87
1	C	437	ILE	N-CA-C	-9.79	101.33	110.53
1	A	396	HIS	CA-C-N	9.74	130.00	121.82
1	A	396	HIS	C-N-CA	9.74	130.00	121.82
1	C	36	SER	CA-C-N	-9.65	105.78	122.09
1	C	36	SER	C-N-CA	-9.65	105.78	122.09
1	C	396	HIS	CA-C-N	9.57	130.69	122.17
1	C	396	HIS	C-N-CA	9.57	130.69	122.17
1	D	437	ILE	N-CA-C	-9.55	101.04	110.30
1	C	397	GLY	CA-C-O	9.41	130.03	121.47
1	C	396	HIS	O-C-N	9.29	133.96	122.34
1	D	396	HIS	O-C-N	9.28	133.94	122.34
1	A	437	ILE	N-CA-CB	8.84	121.88	110.57
1	C	91	LEU	N-CA-C	-8.80	92.06	110.80
1	A	232	VAL	CA-C-N	-8.77	110.52	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	VAL	C-N-CA	-8.77	110.52	119.99
1	A	289	VAL	N-CA-C	-8.71	103.39	111.67
1	C	90	THR	N-CA-C	-8.70	97.00	109.96
1	B	437	ILE	CB-CA-C	8.63	122.60	111.81
1	B	160	ILE	N-CA-C	-8.59	97.53	109.21
1	B	324	VAL	N-CA-C	-8.58	104.96	113.20
1	D	232	VAL	CA-C-N	-8.51	110.97	119.90
1	D	232	VAL	C-N-CA	-8.51	110.97	119.90
1	C	160	ILE	CA-C-N	-8.46	104.82	121.41
1	C	160	ILE	C-N-CA	-8.46	104.82	121.41
1	B	36	SER	CA-C-N	-8.45	107.55	122.16
1	B	36	SER	C-N-CA	-8.45	107.55	122.16
1	D	437	ILE	N-CA-CB	8.39	119.77	110.62
1	D	397	GLY	CA-C-N	8.27	137.34	121.54
1	D	397	GLY	C-N-CA	8.27	137.34	121.54
1	A	160	ILE	CA-C-N	-8.24	105.25	121.41
1	A	160	ILE	C-N-CA	-8.24	105.25	121.41
1	D	90	THR	N-CA-C	-8.24	98.44	110.64
1	A	185	LEU	CA-C-N	8.22	127.87	119.56
1	A	185	LEU	C-N-CA	8.22	127.87	119.56
1	B	91	LEU	N-CA-C	-8.13	93.49	110.80
1	C	96	HIS	N-CA-C	8.07	122.28	107.99
1	A	96	HIS	N-CA-C	8.02	122.18	107.99
1	B	160	ILE	CA-C-N	-7.92	105.88	121.41
1	B	160	ILE	C-N-CA	-7.92	105.88	121.41
1	D	160	ILE	CA-C-N	-7.91	105.91	121.41
1	D	160	ILE	C-N-CA	-7.91	105.91	121.41
1	A	81	VAL	N-CA-CB	7.87	119.97	111.00
1	D	96	HIS	N-CA-C	7.78	122.94	107.62
1	A	262	ALA	N-CA-C	-7.67	100.19	110.55
1	C	98	GLU	CA-CB-CG	-7.59	98.92	114.10
1	B	388	GLY	CA-C-O	-7.57	114.44	121.63
1	A	394	ARG	N-CA-C	-7.49	102.48	111.69
1	D	145	ALA	N-CA-C	7.48	119.44	111.28
1	C	437	ILE	N-CA-CB	7.46	120.12	110.57
1	C	96	HIS	N-CA-CB	-7.41	98.17	110.47
1	D	208	TRP	CA-CB-CG	7.39	127.64	113.60
1	D	160	ILE	N-CA-CB	7.34	120.32	110.26
1	C	225	VAL	N-CA-CB	7.26	123.22	111.23
1	A	94	HIS	N-CA-C	-7.24	97.44	109.24
1	A	90	THR	CB-CA-C	7.24	119.77	109.71
1	A	395	GLY	CA-C-N	7.23	135.46	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	GLY	C-N-CA	7.23	135.46	122.38
1	C	440	GLN	O-C-N	7.22	132.19	122.59
1	C	208	TRP	CA-CB-CG	7.18	127.24	113.60
1	B	119	LEU	N-CA-C	7.17	120.03	109.42
1	D	437	ILE	CB-CA-C	7.17	120.77	111.81
1	A	208	TRP	CA-CB-CG	7.14	127.17	113.60
1	C	346	ALA	N-CA-C	-7.12	103.52	111.28
1	A	93	VAL	CB-CA-C	7.07	122.89	111.29
1	B	87	GLU	N-CA-C	7.07	118.51	108.54
1	A	395	GLY	N-CA-C	7.04	129.88	113.18
1	B	437	ILE	N-CA-CB	7.04	118.30	110.62
1	D	176	THR	CB-CA-C	7.03	122.04	109.38
1	B	94	HIS	N-CA-C	-7.01	97.81	109.24
1	A	36	SER	CA-C-N	-6.97	107.74	121.41
1	A	36	SER	C-N-CA	-6.97	107.74	121.41
1	B	185	LEU	CA-C-N	6.90	126.60	119.56
1	B	185	LEU	C-N-CA	6.90	126.60	119.56
1	A	91	LEU	O-C-N	6.89	131.76	122.59
1	B	176	THR	CB-CA-C	6.88	121.62	109.72
1	B	324	VAL	CB-CA-C	6.83	117.47	110.70
1	A	368	PRO	CB-CA-C	-6.77	104.18	111.56
1	B	395	GLY	N-CA-C	6.77	129.22	113.18
1	C	95	ASP	N-CA-C	6.77	119.04	108.96
1	D	224	ALA	N-CA-C	6.76	125.19	110.80
1	C	87	GLU	N-CA-C	6.76	118.07	108.54
1	D	395	GLY	CA-C-N	6.75	133.67	122.54
1	D	395	GLY	C-N-CA	6.75	133.67	122.54
1	B	60	LEU	N-CA-C	6.69	121.15	113.19
1	C	185	LEU	CA-C-N	6.67	126.30	119.56
1	C	185	LEU	C-N-CA	6.67	126.30	119.56
1	B	224	ALA	N-CA-C	6.67	125.00	110.80
1	A	292	ARG	N-CA-C	6.65	113.99	108.07
1	B	127	GLN	CA-C-N	6.61	129.03	120.44
1	B	127	GLN	C-N-CA	6.61	129.03	120.44
1	A	403	VAL	N-CA-C	-6.60	104.05	110.72
1	A	437	ILE	N-CA-C	-6.58	104.34	110.53
1	A	294	TYR	CA-C-N	-6.53	114.09	122.77
1	A	294	TYR	C-N-CA	-6.53	114.09	122.77
1	B	315	GLY	N-CA-C	6.52	124.32	114.61
1	C	289	VAL	N-CA-C	-6.52	105.39	111.45
1	C	409	HIS	N-CA-C	6.51	118.17	111.14
1	B	54	ILE	N-CA-C	6.50	113.47	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ARG	O-C-N	-6.49	113.96	122.59
1	D	49	VAL	N-CA-C	-6.49	106.23	111.81
1	C	410	ARG	CA-C-N	-6.48	111.82	120.63
1	C	410	ARG	C-N-CA	-6.48	111.82	120.63
1	A	224	ALA	N-CA-C	6.48	124.60	110.80
1	B	95	ASP	N-CA-C	6.47	118.60	108.96
1	A	89	ARG	CA-C-N	6.47	131.66	121.56
1	A	89	ARG	C-N-CA	6.47	131.66	121.56
1	B	96	HIS	N-CA-C	6.46	119.25	108.20
1	A	87	GLU	N-CA-C	6.45	117.64	108.54
1	A	437	ILE	CB-CA-C	6.45	120.47	112.02
1	A	390	ALA	O-C-N	-6.45	115.41	123.27
1	D	232	VAL	N-CA-C	6.45	113.93	107.55
1	A	437	ILE	CA-CB-CG2	6.42	121.41	110.50
1	B	35	LYS	N-CA-C	6.40	119.25	111.82
1	B	397	GLY	CA-C-N	6.40	133.77	121.54
1	B	397	GLY	C-N-CA	6.40	133.77	121.54
1	D	300	ASP	N-CA-C	-6.40	104.22	111.14
1	C	232	VAL	CA-C-N	-6.40	113.36	119.76
1	C	232	VAL	C-N-CA	-6.40	113.36	119.76
1	C	395	GLY	CA-C-N	6.40	133.10	122.54
1	C	395	GLY	C-N-CA	6.40	133.10	122.54
1	B	410	ARG	CA-C-N	-6.40	111.93	120.63
1	B	410	ARG	C-N-CA	-6.40	111.93	120.63
1	C	397	GLY	CA-C-N	6.40	133.76	121.54
1	C	397	GLY	C-N-CA	6.40	133.76	121.54
1	B	81	VAL	N-CA-CB	6.38	118.10	110.95
1	C	371	GLY	CA-C-N	-6.38	114.06	120.31
1	C	371	GLY	C-N-CA	-6.38	114.06	120.31
1	D	396	HIS	CA-C-N	6.37	127.84	122.17
1	D	396	HIS	C-N-CA	6.37	127.84	122.17
1	A	119	LEU	N-CA-C	6.36	118.83	109.42
1	B	272	ASN	N-CA-C	6.35	119.01	111.71
1	D	440	GLN	O-C-N	6.34	131.03	122.59
1	D	54	ILE	CA-C-N	6.34	127.76	119.84
1	D	54	ILE	C-N-CA	6.34	127.76	119.84
1	B	440	GLN	O-C-N	6.32	131.00	122.59
1	A	145	ALA	N-CA-C	6.32	118.69	111.11
1	D	289	VAL	N-CA-C	-6.31	104.89	111.58
1	A	95	ASP	N-CA-C	6.30	118.35	108.96
1	A	350	GLY	N-CA-C	6.29	124.05	115.30
1	A	396	HIS	O-C-N	6.29	131.05	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	45	GLY	N-CA-C	6.27	121.57	114.67
1	A	410	ARG	CA-C-N	-6.26	110.73	120.88
1	A	410	ARG	C-N-CA	-6.26	110.73	120.88
1	A	225	VAL	N-CA-CB	6.24	121.52	111.23
1	A	98	GLU	CA-CB-CG	-6.22	101.65	114.10
1	B	96	HIS	N-CA-CB	-6.22	100.10	110.37
1	C	54	ILE	CA-C-N	6.22	127.61	119.84
1	C	54	ILE	C-N-CA	6.22	127.61	119.84
1	C	424	TYR	CA-CB-CG	-6.17	102.79	113.90
1	C	160	ILE	N-CA-CB	6.15	119.05	110.56
1	C	105	ARG	N-CA-C	-6.14	100.00	109.52
1	D	96	HIS	N-CA-CB	-6.14	100.08	110.46
1	A	397	GLY	CA-C-O	6.14	128.14	121.57
1	A	96	HIS	CA-C-O	-6.14	113.89	120.46
1	B	400	ARG	N-CA-C	-6.13	104.37	112.34
1	C	295	TRP	CA-C-N	-6.13	115.73	123.15
1	C	295	TRP	C-N-CA	-6.13	115.73	123.15
1	C	4	ARG	NE-CZ-NH1	-6.12	115.39	121.50
1	A	65	PRO	N-CA-C	-6.11	106.52	114.03
1	B	160	ILE	N-CA-CB	6.11	118.62	110.26
1	A	399	LEU	CB-CA-C	-6.09	98.29	110.42
1	B	312	VAL	O-C-N	6.08	127.87	121.91
1	C	79	HIS	CB-CA-C	-6.08	101.44	110.62
1	C	437	ILE	CB-CA-C	6.08	119.99	112.02
1	A	96	HIS	N-CA-CB	-6.07	100.40	110.47
1	C	30	VAL	N-CA-C	6.07	116.35	107.37
1	D	4	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	D	102	PHE	N-CA-C	6.05	116.41	107.88
1	B	54	ILE	CA-C-O	6.02	122.49	119.12
1	D	60	LEU	N-CA-C	5.99	120.43	113.18
1	B	306	GLY	N-CA-C	-5.98	105.26	112.49
1	B	208	TRP	CA-CB-CG	5.98	124.95	113.60
1	D	163	GLU	N-CA-C	-5.97	104.86	111.36
1	B	37	GLY	CA-C-N	-5.96	112.81	122.81
1	B	37	GLY	C-N-CA	-5.96	112.81	122.81
1	A	439	ALA	N-CA-C	5.93	118.80	109.96
1	D	25	ASN	CA-C-N	-5.93	113.87	120.45
1	D	25	ASN	C-N-CA	-5.93	113.87	120.45
1	B	371	GLY	CA-C-N	-5.93	114.16	120.03
1	B	371	GLY	C-N-CA	-5.93	114.16	120.03
1	D	437	ILE	CA-CB-CG2	5.92	120.57	110.50
1	B	367	TYR	N-CA-C	5.91	117.33	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	GLY	N-CA-C	5.88	123.16	115.40
1	A	397	GLY	CA-C-N	5.87	132.74	121.54
1	A	397	GLY	C-N-CA	5.87	132.74	121.54
1	A	64	THR	CA-C-N	-5.85	113.78	119.87
1	A	64	THR	C-N-CA	-5.85	113.78	119.87
1	D	98	GLU	CA-CB-CG	-5.85	102.39	114.10
1	B	86	TYR	CA-C-N	5.84	131.26	123.20
1	B	86	TYR	C-N-CA	5.84	131.26	123.20
1	B	206	GLU	CA-C-N	-5.84	115.16	123.10
1	B	206	GLU	C-N-CA	-5.84	115.16	123.10
1	A	242	GLY	N-CA-C	5.83	117.49	111.95
1	A	342	SER	N-CA-C	-5.83	102.68	110.55
1	C	119	LEU	N-CA-C	5.82	117.32	109.24
1	A	440	GLN	O-C-N	5.81	130.31	122.59
1	A	89	ARG	O-C-N	5.80	130.31	122.59
1	D	251	GLN	N-CA-C	-5.80	105.30	112.90
1	B	396	HIS	O-C-N	5.79	129.38	122.26
1	D	94	HIS	N-CA-C	-5.79	99.81	109.24
1	D	160	ILE	CA-CB-CG2	5.79	120.34	110.50
1	D	197	LYS	N-CA-C	-5.78	105.06	111.36
1	D	324	VAL	CB-CA-C	5.75	116.40	110.70
1	A	91	LEU	CA-C-N	5.75	132.52	121.54
1	A	91	LEU	C-N-CA	5.75	132.52	121.54
1	C	224	ALA	N-CA-C	5.74	123.02	110.80
1	B	426	PRO	N-CA-C	5.72	117.68	110.70
1	A	132	THR	CA-C-N	-5.68	114.01	123.33
1	A	132	THR	C-N-CA	-5.68	114.01	123.33
1	B	54	ILE	CA-C-N	5.68	126.94	119.84
1	B	54	ILE	C-N-CA	5.68	126.94	119.84
1	C	35	LYS	N-CA-C	5.67	119.45	112.54
1	D	119	LEU	N-CA-C	5.67	117.11	109.24
1	D	397	GLY	CA-C-O	5.66	126.62	121.47
1	A	441	GLN	CA-CB-CG	5.66	125.41	114.10
1	A	392	VAL	N-CA-C	5.64	116.00	108.11
1	A	418	LEU	N-CA-C	5.63	118.14	111.33
1	D	175	VAL	CA-C-N	-5.62	114.77	122.93
1	D	175	VAL	C-N-CA	-5.62	114.77	122.93
1	C	395	GLY	N-CA-C	5.62	126.49	113.18
1	A	5	MET	CA-C-O	5.61	126.46	120.46
1	C	206	GLU	CA-C-N	-5.61	115.25	123.10
1	C	206	GLU	C-N-CA	-5.61	115.25	123.10
1	C	282	VAL	N-CA-C	-5.60	107.29	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ALA	CA-C-N	-5.59	115.35	123.06
1	A	390	ALA	C-N-CA	-5.59	115.35	123.06
1	B	379	TYR	N-CA-C	5.58	118.17	109.52
1	A	244	ARG	N-CA-C	-5.56	100.52	109.58
1	B	93	VAL	CB-CA-C	5.55	120.40	111.29
1	D	261	GLY	CA-C-O	5.54	125.35	119.03
1	D	180	ALA	N-CA-C	5.53	117.75	111.11
1	A	35	LYS	N-CA-C	5.52	119.27	112.54
1	B	394	ARG	N-CA-C	-5.51	104.91	111.69
1	C	29	GLU	N-CA-C	-5.50	100.83	109.25
1	D	441	GLN	CA-CB-CG	5.48	125.06	114.10
1	B	32	VAL	N-CA-C	5.46	115.96	107.99
1	D	399	LEU	N-CA-CB	5.45	119.77	110.50
1	B	225	VAL	N-CA-CB	5.43	120.20	111.23
1	A	304	LYS	N-CA-C	-5.42	105.45	111.36
1	D	312	VAL	N-CA-C	-5.42	105.24	110.72
1	C	379	TYR	N-CA-C	5.42	117.65	109.41
1	D	141	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	B	98	GLU	CA-CB-CG	-5.41	103.29	114.10
1	B	145	ALA	N-CA-C	5.41	117.17	111.28
1	B	100	ARG	N-CA-C	5.40	118.42	110.59
1	B	197	LYS	N-CA-C	-5.40	105.29	111.07
1	B	80	GLU	CA-C-N	-5.39	114.25	121.80
1	B	80	GLU	C-N-CA	-5.39	114.25	121.80
1	A	97	ALA	N-CA-CB	5.39	119.60	110.49
1	B	408	LEU	CA-C-O	5.38	126.19	120.10
1	A	127	GLN	CA-C-N	5.36	127.90	120.29
1	A	127	GLN	C-N-CA	5.36	127.90	120.29
1	B	411	GLU	N-CA-CB	5.36	117.75	109.98
1	D	395	GLY	N-CA-C	5.36	125.87	113.18
1	B	135	THR	N-CA-C	5.35	117.40	109.69
1	D	91	LEU	O-C-N	5.35	129.71	122.59
1	A	175	VAL	CA-C-N	-5.34	115.63	123.00
1	A	175	VAL	C-N-CA	-5.34	115.63	123.00
1	A	207	VAL	N-CA-C	5.34	114.43	106.85
1	C	423	ALA	N-CA-C	5.34	118.25	109.76
1	C	87	GLU	OE1-CD-OE2	5.32	135.67	122.90
1	B	230	GLY	CA-C-N	-5.32	115.60	122.99
1	B	230	GLY	C-N-CA	-5.32	115.60	122.99
1	D	185	LEU	CA-C-O	5.31	124.57	120.48
1	C	176	THR	CB-CA-C	5.31	118.93	109.38
1	B	79	HIS	CA-C-N	-5.30	115.73	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	HIS	C-N-CA	-5.30	115.73	122.77
1	C	144	LYS	N-CA-C	5.29	116.73	111.07
1	D	95	ASP	N-CA-C	5.28	116.02	108.74
1	C	100	ARG	N-CA-C	5.28	118.27	110.46
1	D	355	LYS	CA-C-N	-5.27	114.86	122.45
1	D	355	LYS	C-N-CA	-5.27	114.86	122.45
1	D	175	VAL	CA-C-O	5.26	125.46	120.25
1	D	426	PRO	N-CA-C	5.26	117.12	110.70
1	A	206	GLU	CA-C-N	-5.26	115.74	123.10
1	A	206	GLU	C-N-CA	-5.26	115.74	123.10
1	D	410	ARG	O-C-N	-5.25	115.60	122.59
1	D	225	VAL	N-CA-CB	5.25	119.89	111.23
1	C	381	GLU	N-CA-C	5.25	116.69	110.97
1	B	174	GLN	CA-C-N	-5.24	115.71	122.99
1	B	174	GLN	C-N-CA	-5.24	115.71	122.99
1	D	194	ALA	N-CA-C	5.23	117.40	111.02
1	C	93	VAL	CB-CA-C	5.23	119.86	111.29
1	B	427	PRO	CA-C-O	-5.22	111.69	119.00
1	A	98	GLU	CG-CD-OE1	5.22	130.41	118.40
1	D	390	ALA	CA-C-N	-5.22	115.69	122.94
1	D	390	ALA	C-N-CA	-5.22	115.69	122.94
1	A	294	TYR	O-C-N	-5.20	117.65	123.48
1	B	96	HIS	CA-C-O	-5.18	115.16	120.54
1	B	277	TYR	N-CA-C	5.18	118.44	110.42
1	C	303	ASN	N-CA-C	5.17	116.91	111.28
1	C	217	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	D	410	ARG	CA-C-N	-5.15	112.54	120.88
1	D	410	ARG	C-N-CA	-5.15	112.54	120.88
1	B	16	SER	CB-CA-C	-5.14	102.25	110.79
1	C	180	ALA	N-CA-C	5.14	116.69	111.14
1	B	183	ARG	CA-C-N	-5.14	114.66	119.85
1	B	183	ARG	C-N-CA	-5.14	114.66	119.85
1	B	141	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	A	30	VAL	CA-C-N	-5.12	116.43	123.14
1	A	30	VAL	C-N-CA	-5.12	116.43	123.14
1	D	127	GLN	N-CA-C	5.12	116.71	110.41
1	D	207	VAL	N-CA-C	5.12	114.12	106.85
1	B	187	HIS	CB-CA-C	5.12	120.14	109.95
1	C	395	GLY	O-C-N	5.12	129.35	122.70
1	D	217	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	B	110	VAL	CA-C-N	5.09	130.42	122.17
1	B	110	VAL	C-N-CA	5.09	130.42	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	TYR	CA-CB-CG	-5.09	104.74	113.90
1	A	399	LEU	N-CA-CB	5.09	119.09	110.49
1	B	320	PHE	CA-C-N	-5.09	115.08	122.86
1	B	320	PHE	C-N-CA	-5.09	115.08	122.86
1	B	394	ARG	CA-C-N	5.08	131.36	121.41
1	B	394	ARG	C-N-CA	5.08	131.36	121.41
1	D	80	GLU	CA-C-N	-5.06	116.04	122.37
1	D	80	GLU	C-N-CA	-5.06	116.04	122.37
1	D	241	THR	CA-C-N	-5.06	115.84	122.63
1	D	241	THR	C-N-CA	-5.06	115.84	122.63
1	A	176	THR	CB-CA-C	5.06	118.47	109.72
1	D	432	TRP	CA-C-N	-5.05	113.18	120.51
1	D	432	TRP	C-N-CA	-5.05	113.18	120.51
1	B	437	ILE	CA-CB-CG2	5.05	119.08	110.50
1	A	222	VAL	N-CA-CB	5.05	119.56	111.23
1	C	89	ARG	O-C-N	5.04	129.30	122.59
1	D	399	LEU	CB-CA-C	-5.04	100.53	110.10
1	C	57	LEU	N-CA-C	5.04	117.50	111.71
1	C	222	VAL	N-CA-CB	5.02	119.52	111.23
1	C	208	TRP	N-CA-CB	5.02	117.44	109.71
1	A	344	GLU	N-CA-C	-5.01	105.71	111.07
1	A	441	GLN	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ALA	Peptide
1	A	240	ALA	Peptide
1	A	37	GLY	Peptide
1	A	396	HIS	Peptide
1	A	398	ALA	Peptide
1	A	399	LEU	Peptide
1	A	440	GLN	Peptide
1	A	90	THR	Peptide
1	B	161	GLY	Peptide
1	B	37	GLY	Peptide
1	B	396	HIS	Peptide
1	B	440	GLN	Peptide
1	B	90	THR	Peptide
1	C	127	GLN	Peptide
1	C	224	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	C	396	HIS	Peptide
1	C	399	LEU	Peptide
1	C	440	GLN	Peptide
1	C	89	ARG	Peptide
1	C	90	THR	Peptide
1	C	99	GLY	Peptide
1	D	396	HIS	Peptide
1	D	440	GLN	Peptide
1	D	90	THR	Peptide
1	D	99	GLY	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	3379	0	3407	213	0
1	B	3379	0	3407	239	0
1	C	3378	0	3402	179	0
1	D	3377	0	3402	210	0
2	A	53	0	31	9	0
2	B	53	0	31	8	0
2	C	53	0	31	10	0
2	D	53	0	31	7	0
3	A	48	0	31	6	0
3	B	48	0	31	7	0
3	C	48	0	31	4	0
3	D	48	0	31	3	0
4	A	14	0	0	7	0
4	B	17	0	0	20	0
4	C	15	0	0	11	0
4	D	11	0	0	9	0
All	All	13974	0	13866	820	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (820) 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:B:32:VAL:HA	4:B:604:HOH:O	1.29	1.29
1:D:439:ALA:O	1:D:441:GLN:HB2	1.11	1.26
1:B:439:ALA:O	1:B:441:GLN:CB	1.89	1.21
1:A:437:ILE:HD12	1:A:437:ILE:C	1.58	1.20
1:A:149:ALA:CB	1:A:150:ARG:HA	1.75	1.17
1:C:439:ALA:O	1:C:441:GLN:HB2	0.99	1.16
1:A:439:ALA:O	1:A:441:GLN:HB2	0.98	1.16
1:A:90:THR:HA	1:A:92:THR:HG23	1.22	1.16
1:B:149:ALA:CB	1:B:150:ARG:HA	1.73	1.15
1:A:439:ALA:O	1:A:441:GLN:CB	1.95	1.15
1:C:439:ALA:O	1:C:441:GLN:CB	1.95	1.14
1:A:85:ASP:O	1:A:92:THR:HG22	1.47	1.12
1:C:149:ALA:HB1	1:C:150:ARG:HA	1.13	1.12
1:B:437:ILE:C	1:B:437:ILE:HD12	1.72	1.11
1:D:147:PRO:O	1:D:148:GLN:HB2	1.48	1.11
1:C:410:ARG:HG2	1:C:410:ARG:HH11	1.06	1.11
1:D:410:ARG:HG2	1:D:410:ARG:HH11	0.98	1.10
1:A:398:ALA:H	1:A:399:LEU:HB2	1.14	1.10
1:B:439:ALA:O	1:B:441:GLN:HB2	0.92	1.08
1:A:85:ASP:C	1:A:92:THR:HG22	1.79	1.07
1:A:147:PRO:O	1:A:148:GLN:HB2	1.55	1.05
1:C:147:PRO:O	1:C:148:GLN:HB2	1.55	1.04
1:D:398:ALA:H	1:D:399:LEU:HB2	1.18	1.04
1:B:410:ARG:HH11	1:B:410:ARG:HG2	1.12	1.03
1:A:149:ALA:HB1	1:A:150:ARG:HA	1.06	1.02
1:B:85:ASP:O	1:B:92:THR:HG22	1.58	1.02
1:D:149:ALA:HB1	1:D:150:ARG:HA	1.06	1.01
1:C:149:ALA:CB	1:C:150:ARG:HA	1.89	1.01
1:C:50:LEU:HD12	1:C:143:LEU:HD13	1.40	1.00
1:D:149:ALA:CB	1:D:150:ARG:HA	1.88	1.00
1:C:437:ILE:C	1:C:437:ILE:HD12	1.87	1.00
1:D:439:ALA:O	1:D:441:GLN:CB	2.08	1.00
1:A:410:ARG:HG2	1:A:410:ARG:HH11	1.22	0.99
1:B:149:ALA:HB1	1:B:150:ARG:CA	1.92	0.99
1:B:441:GLN:O	1:B:442:ALA:O	1.79	0.98
1:A:217:ARG:HB3	1:A:224:ALA:HB3	1.46	0.97
1:A:129:GLY:N	4:A:602:HOH:O	1.93	0.97
1:D:225:VAL:N	4:D:601:HOH:O	1.97	0.97
1:B:149:ALA:HB1	1:B:150:ARG:HA	0.96	0.96
1:B:236:LEU:C	1:B:236:LEU:HD12	1.90	0.96
1:C:217:ARG:HB3	1:C:224:ALA:HB3	1.47	0.96
1:D:440:GLN:HA	1:D:440:GLN:NE2	1.81	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:OG1	4:B:601:HOH:O	1.84	0.96
1:D:269:MET:HE3	1:D:320:PHE:HB3	1.47	0.96
1:A:37:GLY:HA2	1:A:77:THR:HB	1.46	0.95
1:D:437:ILE:HD12	1:D:437:ILE:C	1.90	0.95
1:D:116:ARG:NH1	1:D:244:ARG:HD2	1.82	0.94
1:C:410:ARG:HG2	1:C:410:ARG:NH1	1.81	0.94
1:D:410:ARG:HG2	1:D:410:ARG:NH1	1.77	0.94
1:B:37:GLY:HA2	1:B:77:THR:HB	1.48	0.93
1:D:50:LEU:HD12	1:D:143:LEU:HD13	1.48	0.93
1:D:149:ALA:HB1	1:D:150:ARG:CA	1.98	0.92
1:D:441:GLN:O	1:D:442:ALA:O	1.87	0.92
1:A:90:THR:HA	1:A:92:THR:CG2	1.99	0.92
1:A:396:HIS:CE1	1:B:396:HIS:ND1	2.38	0.91
1:A:396:HIS:CE1	1:B:396:HIS:CE1	2.58	0.91
1:C:86:TYR:CE1	1:C:88:LEU:HD22	2.05	0.91
1:B:85:ASP:C	1:B:92:THR:HG22	1.95	0.91
1:B:147:PRO:O	1:B:148:GLN:HB2	1.69	0.90
1:A:269:MET:HE3	1:A:320:PHE:HB3	1.54	0.89
1:B:129:GLY:N	4:B:602:HOH:O	1.92	0.89
1:D:11:VAL:HG23	2:D:501:FAD:H4B	1.54	0.89
1:D:208:TRP:HB3	1:D:211:VAL:HG21	1.56	0.88
1:B:90:THR:HA	1:B:92:THR:HG23	1.53	0.88
1:D:123:PRO:HG2	1:D:215:ALA:HB2	1.55	0.88
1:C:398:ALA:H	1:C:399:LEU:HB2	1.39	0.88
1:D:94:HIS:N	1:D:94:HIS:CD2	2.41	0.87
1:B:92:THR:OG1	1:B:93:VAL:HG23	1.73	0.87
1:B:217:ARG:HB3	1:B:224:ALA:HB3	1.54	0.87
1:A:437:ILE:C	1:A:437:ILE:CD1	2.48	0.86
1:C:440:GLN:HA	1:C:440:GLN:NE2	1.91	0.86
1:C:441:GLN:O	1:C:442:ALA:O	1.92	0.85
1:B:395:GLY:C	1:B:397:GLY:HA2	2.02	0.85
1:D:398:ALA:N	1:D:399:LEU:HB2	1.91	0.85
1:C:116:ARG:NH1	1:C:244:ARG:HD2	1.92	0.85
1:A:86:TYR:CE1	1:A:88:LEU:HD22	2.11	0.84
1:A:149:ALA:HB1	1:A:150:ARG:CA	2.01	0.84
1:C:410:ARG:HH11	1:C:410:ARG:CG	1.88	0.84
1:B:410:ARG:HG2	1:B:410:ARG:NH1	1.89	0.84
1:C:208:TRP:HB3	1:C:211:VAL:HG21	1.58	0.84
1:A:440:GLN:NE2	1:A:440:GLN:HA	1.93	0.84
1:A:116:ARG:NH1	1:A:244:ARG:HD2	1.92	0.84
1:A:121:PRO:HG2	1:D:149:ALA:HB2	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:CB	1:A:150:ARG:CA	2.56	0.83
1:A:410:ARG:HG2	1:A:410:ARG:NH1	1.91	0.83
1:A:441:GLN:O	1:A:442:ALA:O	1.97	0.83
1:A:221:ARG:O	1:A:221:ARG:HD3	1.79	0.82
1:B:149:ALA:CB	1:B:150:ARG:CA	2.55	0.82
1:A:396:HIS:ND1	1:B:396:HIS:CE1	2.47	0.82
1:A:396:HIS:CG	1:B:396:HIS:CE1	2.68	0.82
1:A:121:PRO:HG2	1:D:149:ALA:CB	2.09	0.82
1:C:269:MET:HE3	1:C:320:PHE:HB3	1.62	0.82
1:A:94:HIS:CD2	1:A:94:HIS:N	2.46	0.81
1:C:87:GLU:HA	1:C:88:LEU:C	2.04	0.81
1:C:440:GLN:HA	4:C:602:HOH:O	1.80	0.81
1:B:437:ILE:HD12	1:B:438:ALA:N	1.95	0.81
1:B:94:HIS:N	1:B:94:HIS:CD2	2.44	0.81
1:B:270:ARG:HH11	1:B:270:ARG:HB2	1.45	0.81
1:D:217:ARG:HB3	1:D:224:ALA:HB3	1.63	0.81
1:A:89:ARG:O	4:A:603:HOH:O	1.98	0.80
1:D:50:LEU:HD12	1:D:143:LEU:CD1	2.11	0.80
1:C:85:ASP:H	1:C:92:THR:HA	1.46	0.80
1:C:398:ALA:H	1:C:399:LEU:CB	1.93	0.80
1:B:224:ALA:O	1:B:232:VAL:O	2.00	0.80
1:B:270:ARG:CB	1:B:270:ARG:NH1	2.45	0.80
1:B:50:LEU:HD12	1:B:143:LEU:HD13	1.64	0.79
1:C:440:GLN:NE2	4:C:602:HOH:O	2.16	0.79
1:B:208:TRP:HB3	1:B:211:VAL:HG21	1.63	0.79
1:D:86:TYR:CE1	1:D:88:LEU:HD22	2.16	0.79
1:A:398:ALA:H	1:A:399:LEU:CB	1.94	0.79
1:A:398:ALA:N	1:A:399:LEU:HB2	1.96	0.79
1:D:50:LEU:CD1	1:D:143:LEU:HD13	2.12	0.78
1:D:248:GLU:HB2	4:D:602:HOH:O	1.80	0.78
1:A:85:ASP:H	1:A:92:THR:HA	1.48	0.78
1:B:87:GLU:HA	1:B:88:LEU:C	2.08	0.78
1:D:256:ALA:H	1:D:272:ASN:ND2	1.81	0.78
1:D:440:GLN:HA	1:D:440:GLN:HE21	1.47	0.78
1:D:224:ALA:O	1:D:232:VAL:O	2.01	0.78
1:A:150:ARG:NH2	4:A:601:HOH:O	1.87	0.78
1:D:211:VAL:HG22	1:D:229:GLU:HG3	1.66	0.78
1:A:211:VAL:HG22	1:A:229:GLU:HG3	1.65	0.77
1:A:396:HIS:CE1	1:B:396:HIS:CG	2.72	0.77
1:B:116:ARG:NH1	1:B:244:ARG:HD2	1.99	0.77
1:B:359:GLN:HB2	1:B:374:TRP:CD1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:HIS:N	1:C:94:HIS:CD2	2.52	0.77
1:A:270:ARG:HB2	1:A:270:ARG:HH11	1.48	0.77
1:A:92:THR:OG1	1:A:93:VAL:HG23	1.84	0.77
1:C:50:LEU:CD1	1:C:143:LEU:HD13	2.15	0.77
1:A:50:LEU:HD12	1:A:143:LEU:HD13	1.66	0.77
1:D:149:ALA:HA	1:D:173:LEU:HD22	1.66	0.77
1:A:11:VAL:HG23	2:A:501:FAD:H4B	1.67	0.77
1:D:147:PRO:O	1:D:148:GLN:CB	2.30	0.77
1:B:183:ARG:HG3	1:B:184:PRO:O	1.84	0.77
1:B:398:ALA:H	1:B:399:LEU:CB	1.99	0.76
1:C:37:GLY:HA2	1:C:77:THR:HB	1.67	0.76
1:C:270:ARG:HH11	1:C:270:ARG:CB	1.97	0.76
1:B:440:GLN:HA	4:B:603:HOH:O	1.84	0.76
1:B:6:VAL:HG22	1:B:31:VAL:CG1	2.16	0.76
1:B:90:THR:HA	1:B:92:THR:CG2	2.15	0.76
1:C:50:LEU:HD12	1:C:143:LEU:CD1	2.16	0.76
1:D:37:GLY:HA2	1:D:77:THR:HB	1.68	0.76
1:B:270:ARG:HH11	1:B:270:ARG:CB	1.98	0.76
1:D:94:HIS:N	1:D:94:HIS:HD2	1.83	0.75
1:B:437:ILE:O	1:B:441:GLN:HB3	1.87	0.75
1:A:437:ILE:HD12	1:A:438:ALA:N	2.02	0.75
1:B:91:LEU:O	4:B:601:HOH:O	2.04	0.75
1:C:256:ALA:H	1:C:272:ASN:ND2	1.85	0.75
1:D:269:MET:HE3	1:D:320:PHE:CB	2.17	0.74
1:B:86:TYR:CE1	1:B:88:LEU:HD22	2.21	0.74
1:B:11:VAL:HG23	2:B:501:FAD:H4B	1.68	0.74
1:B:395:GLY:O	1:B:397:GLY:HA2	1.86	0.74
1:A:85:ASP:O	1:A:92:THR:CG2	2.34	0.74
1:A:50:LEU:HD12	1:A:143:LEU:CD1	2.17	0.74
1:B:123:PRO:HG2	1:B:215:ALA:HB2	1.68	0.74
1:B:50:LEU:HD12	1:B:143:LEU:CD1	2.17	0.73
1:A:147:PRO:O	1:A:148:GLN:CB	2.36	0.73
1:D:56:ARG:NH2	1:D:59:ARG:HH11	1.87	0.73
1:D:418:LEU:HD13	1:D:439:ALA:HB3	1.69	0.73
1:B:440:GLN:NE2	4:B:603:HOH:O	2.22	0.72
1:D:270:ARG:HH11	1:D:270:ARG:HB2	1.54	0.72
1:D:87:GLU:HA	1:D:88:LEU:C	2.13	0.72
1:B:128:GLU:N	4:B:602:HOH:O	2.21	0.72
1:B:64:THR:OG1	1:B:67:GLU:HG3	1.90	0.72
1:C:149:ALA:HA	1:C:173:LEU:HD22	1.70	0.72
1:B:440:GLN:O	4:B:603:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ARG:NH2	4:D:602:HOH:O	2.22	0.72
1:D:90:THR:OG1	1:D:91:LEU:O	2.04	0.72
1:A:442:ALA:HB2	3:B:502:COA:H1B	1.71	0.72
1:B:396:HIS:N	1:B:397:GLY:HA2	2.01	0.72
1:B:437:ILE:C	1:B:437:ILE:CD1	2.58	0.72
1:C:270:ARG:HH11	1:C:270:ARG:HB2	1.54	0.71
1:D:410:ARG:HH11	1:D:410:ARG:CG	1.92	0.71
1:A:270:ARG:HH11	1:A:270:ARG:CB	2.04	0.71
1:B:94:HIS:N	1:B:94:HIS:HD2	1.89	0.71
1:D:255:VAL:HA	1:D:272:ASN:HD21	1.55	0.71
1:D:343:LEU:HD22	1:D:355:LYS:HB3	1.72	0.71
1:C:8:VAL:HG13	1:C:81:VAL:HG13	1.72	0.71
1:C:343:LEU:HD22	1:C:355:LYS:HB3	1.72	0.71
1:D:86:TYR:HD1	1:D:86:TYR:H	1.39	0.71
1:D:437:ILE:O	1:D:441:GLN:HB3	1.91	0.70
1:A:270:ARG:CB	1:A:270:ARG:NH1	2.54	0.70
1:D:127:GLN:HG2	1:D:220:GLY:HA2	1.73	0.70
1:A:410:ARG:HH11	1:A:410:ARG:CG	1.99	0.70
1:D:85:ASP:H	1:D:92:THR:HA	1.57	0.70
1:A:98:GLU:HA	1:A:98:GLU:OE2	1.92	0.70
1:A:191:GLU:OE2	1:A:355:LYS:HE3	1.92	0.70
1:A:437:ILE:O	1:A:441:GLN:HB3	1.92	0.69
1:A:150:ARG:NH1	4:A:601:HOH:O	2.22	0.69
1:D:6:VAL:HG22	1:D:31:VAL:CG1	2.22	0.69
1:D:22:LYS:HE2	1:D:72:GLY:HA3	1.74	0.69
1:A:94:HIS:N	1:A:94:HIS:HD2	1.90	0.69
1:B:149:ALA:HA	1:B:173:LEU:HD22	1.73	0.69
1:C:440:GLN:HA	1:C:440:GLN:HE21	1.56	0.69
1:B:343:LEU:HD22	1:B:355:LYS:HB3	1.74	0.69
1:C:255:VAL:HA	1:C:272:ASN:HD21	1.58	0.68
1:A:398:ALA:HA	1:A:400:ARG:H	1.58	0.68
1:B:211:VAL:HG22	1:B:229:GLU:HG3	1.73	0.68
1:B:7:VAL:O	4:B:604:HOH:O	2.11	0.68
1:B:256:ALA:H	1:B:272:ASN:ND2	1.91	0.68
1:D:270:ARG:HH11	1:D:270:ARG:CB	2.07	0.67
1:A:396:HIS:HE1	1:B:396:HIS:H	1.42	0.67
1:A:440:GLN:HA	1:A:440:GLN:HE21	1.59	0.67
1:D:85:ASP:OD1	1:D:88:LEU:HD23	1.95	0.67
1:B:270:ARG:HB2	1:B:270:ARG:NH1	2.08	0.67
1:C:80:GLU:N	4:C:603:HOH:O	2.20	0.67
1:C:211:VAL:HG22	1:C:229:GLU:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:HA	1:A:88:LEU:C	2.20	0.67
1:D:224:ALA:C	4:D:601:HOH:O	2.32	0.66
1:B:398:ALA:H	1:B:399:LEU:HB2	1.59	0.66
1:B:272:ASN:HD22	1:B:272:ASN:H	1.41	0.66
1:C:270:ARG:CB	1:C:270:ARG:NH1	2.59	0.66
1:D:98:GLU:HA	1:D:98:GLU:OE2	1.94	0.66
1:B:269:MET:HE3	1:B:320:PHE:HB3	1.77	0.66
1:C:398:ALA:HA	1:C:400:ARG:H	1.60	0.66
1:A:256:ALA:H	1:A:272:ASN:ND2	1.94	0.66
1:C:94:HIS:N	1:C:94:HIS:HD2	1.93	0.66
1:B:48:TYR:HB2	1:B:54:ILE:HD12	1.77	0.65
1:A:91:LEU:CG	1:A:92:THR:H	2.05	0.65
1:B:4:ARG:NH1	1:B:104:ASP:OD2	2.29	0.65
1:D:11:VAL:CG2	2:D:501:FAD:H4B	2.24	0.65
1:C:380:GLU:HG2	4:C:601:HOH:O	1.97	0.65
1:C:64:THR:OG1	1:C:67:GLU:HG3	1.97	0.65
1:D:92:THR:O	1:D:104:ASP:O	2.14	0.65
1:A:287:HIS:HD2	1:A:289:VAL:H	1.45	0.65
1:C:270:ARG:NH1	1:C:270:ARG:HB3	2.12	0.65
1:D:269:MET:CE	1:D:320:PHE:HB3	2.25	0.65
1:B:7:VAL:CA	4:B:604:HOH:O	2.46	0.64
1:B:37:GLY:CA	1:B:77:THR:HB	2.23	0.64
1:B:398:ALA:H	1:B:399:LEU:HB3	1.63	0.64
1:A:396:HIS:CD2	1:B:396:HIS:CE1	2.86	0.64
1:D:180:ALA:O	1:D:210:GLY:HA2	1.97	0.64
1:A:236:LEU:HD12	1:A:236:LEU:C	2.23	0.64
1:B:440:GLN:HA	1:B:440:GLN:NE2	2.13	0.64
1:D:270:ARG:CB	1:D:270:ARG:NH1	2.61	0.64
1:B:373:LEU:HD22	1:B:434:PRO:HG2	1.80	0.64
1:A:208:TRP:HB3	1:A:211:VAL:HG21	1.80	0.64
1:B:183:ARG:NH1	1:B:188:TRP:O	2.31	0.63
1:B:50:LEU:CD1	1:B:143:LEU:HD13	2.29	0.63
1:C:357:PHE:HD1	1:C:376:GLU:HB2	1.64	0.63
1:D:123:PRO:HG2	1:D:215:ALA:CB	2.28	0.63
1:A:183:ARG:HD3	1:A:190:PRO:HA	1.81	0.63
1:A:272:ASN:H	1:A:272:ASN:HD22	1.46	0.63
1:D:281:ASP:OD1	2:D:501:FAD:H5'1	1.99	0.63
1:D:330:LYS:HE2	1:D:332:PHE:O	1.98	0.63
1:D:440:GLN:NE2	1:D:440:GLN:CA	2.60	0.63
1:D:56:ARG:NH2	1:D:59:ARG:NH1	2.46	0.63
1:C:183:ARG:NH1	1:C:188:TRP:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LEU:C	1:B:236:LEU:CD1	2.68	0.62
1:A:22:LYS:HE2	1:A:72:GLY:HA3	1.82	0.62
1:C:11:VAL:HG23	2:C:501:FAD:H4B	1.79	0.62
1:A:149:ALA:HA	1:A:173:LEU:HD22	1.81	0.62
1:A:50:LEU:CD1	1:A:143:LEU:HD13	2.28	0.62
1:C:98:GLU:OE2	1:C:98:GLU:HA	1.97	0.62
1:C:262:ALA:HB3	1:C:284:GLU:HG2	1.82	0.62
1:A:396:HIS:H	1:B:396:HIS:HE1	1.46	0.61
1:D:94:HIS:CD2	1:D:94:HIS:H	2.16	0.61
1:D:287:HIS:HD2	1:D:289:VAL:H	1.47	0.61
1:A:255:VAL:HA	1:A:272:ASN:HD21	1.64	0.61
1:B:7:VAL:HB	4:B:604:HOH:O	2.00	0.61
1:B:85:ASP:H	1:B:92:THR:HA	1.65	0.61
1:C:418:LEU:HD13	1:C:439:ALA:HB3	1.83	0.61
1:B:44:CYS:HA	2:B:501:FAD:C5X	2.30	0.61
1:B:221:ARG:O	1:B:221:ARG:HD3	2.00	0.61
1:B:123:PRO:HG2	1:B:215:ALA:CB	2.30	0.61
1:D:44:CYS:HA	2:D:501:FAD:C5X	2.31	0.61
1:D:236:LEU:HD12	1:D:236:LEU:C	2.26	0.61
1:A:396:HIS:CE1	1:B:396:HIS:H	2.19	0.61
1:D:209:THR:O	1:D:211:VAL:HG23	2.00	0.61
1:D:426:PRO:HB2	1:D:427:PRO:HD3	1.83	0.61
1:A:44:CYS:HA	2:A:501:FAD:C5X	2.30	0.60
1:A:90:THR:CA	1:A:92:THR:HG23	2.13	0.60
1:A:281:ASP:OD1	2:A:501:FAD:H5'1	2.01	0.60
1:B:76:HIS:HB3	1:B:79:HIS:CE1	2.36	0.60
1:D:64:THR:OG1	1:D:67:GLU:HG3	2.00	0.60
1:C:382:GLY:N	4:C:601:HOH:O	2.09	0.60
1:B:11:VAL:CG2	2:B:501:FAD:H4B	2.31	0.60
1:B:144:LYS:O	1:B:147:PRO:HD2	2.02	0.60
1:D:247:THR:HG21	1:D:261:GLY:O	2.00	0.60
1:A:373:LEU:HD22	1:A:434:PRO:HG2	1.83	0.60
1:B:399:LEU:C	1:B:401:ILE:N	2.58	0.60
1:D:418:LEU:HD13	1:D:439:ALA:CB	2.32	0.60
1:D:8:VAL:HG13	1:D:81:VAL:HG13	1.82	0.60
1:D:214:GLU:O	1:D:215:ALA:HB2	2.01	0.60
1:D:398:ALA:HA	1:D:400:ARG:H	1.67	0.60
1:B:399:LEU:C	1:B:401:ILE:H	2.09	0.60
1:A:90:THR:OG1	1:A:91:LEU:O	2.04	0.59
1:D:179:GLU:OE2	1:D:181:LYS:HG2	2.01	0.59
1:D:377:LEU:HD22	1:D:438:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ALA:O	1:A:232:VAL:O	2.20	0.59
1:B:81:VAL:HA	1:B:95:ASP:HB3	1.84	0.59
1:C:398:ALA:N	1:C:399:LEU:HB2	2.15	0.59
1:A:37:GLY:CA	1:A:77:THR:HB	2.24	0.59
1:A:270:ARG:HB2	1:A:270:ARG:NH1	2.16	0.59
1:B:200:LEU:HD23	1:B:332:PHE:HE1	1.68	0.59
1:D:149:ALA:HA	1:D:173:LEU:CD2	2.32	0.59
1:A:64:THR:OG1	1:A:67:GLU:HG3	2.02	0.59
1:C:44:CYS:HA	2:C:501:FAD:C5X	2.32	0.59
1:D:437:ILE:HD12	1:D:438:ALA:N	2.17	0.59
1:B:104:ASP:OD1	1:B:105:ARG:N	2.34	0.59
1:A:84:VAL:HG13	1:A:92:THR:HB	1.83	0.59
1:B:85:ASP:H	1:B:92:THR:HB	1.68	0.59
1:A:85:ASP:C	1:A:92:THR:CG2	2.67	0.59
1:B:88:LEU:O	1:B:89:ARG:HB2	2.03	0.59
1:C:147:PRO:O	1:C:148:GLN:CB	2.38	0.59
1:C:373:LEU:HD22	1:C:434:PRO:HG2	1.84	0.59
1:A:49:VAL:HG11	1:A:57:LEU:HD13	1.85	0.58
1:B:85:ASP:N	1:B:92:THR:HB	2.18	0.58
1:D:91:LEU:CG	1:D:92:THR:H	2.14	0.58
1:B:49:VAL:HG11	1:B:57:LEU:HD13	1.86	0.58
1:A:126:GLU:HA	1:A:126:GLU:OE1	2.02	0.58
1:B:85:ASP:O	1:B:92:THR:CG2	2.44	0.58
1:B:277:TYR:CD1	1:B:277:TYR:N	2.71	0.58
1:B:362:ASP:OD2	4:B:605:HOH:O	2.17	0.58
1:C:104:ASP:OD1	1:C:105:ARG:N	2.35	0.58
1:B:23:ARG:NH2	3:B:502:COA:O5A	2.36	0.58
1:C:437:ILE:O	1:C:441:GLN:HB3	2.02	0.58
1:D:358:ILE:C	1:D:358:ILE:HD12	2.29	0.58
1:C:224:ALA:O	1:C:232:VAL:O	2.22	0.58
1:D:262:ALA:HB3	1:D:284:GLU:HG2	1.85	0.58
1:A:140:GLU:CD	4:A:608:HOH:O	2.47	0.58
1:C:272:ASN:H	1:C:272:ASN:HD22	1.52	0.58
1:C:236:LEU:C	1:C:236:LEU:HD12	2.29	0.57
1:B:84:VAL:HG13	1:B:92:THR:HB	1.85	0.57
1:B:127:GLN:HG2	1:B:220:GLY:HA2	1.86	0.57
1:A:91:LEU:HD13	1:A:103:GLN:OE1	2.05	0.57
1:B:91:LEU:HD13	1:B:103:GLN:OE1	2.04	0.57
1:B:180:ALA:O	1:B:210:GLY:HA2	2.05	0.57
1:D:149:ALA:CB	1:D:150:ARG:CA	2.66	0.57
1:B:200:LEU:HD23	1:B:332:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PRO:CG	1:D:149:ALA:CB	2.82	0.57
1:B:86:TYR:O	1:B:89:ARG:HA	2.04	0.57
1:B:255:VAL:HA	1:B:272:ASN:HD21	1.69	0.57
1:B:7:VAL:N	4:B:604:HOH:O	2.35	0.57
1:C:268:ARG:HH12	1:C:270:ARG:HH22	1.53	0.56
1:C:411:GLU:OE2	1:C:411:GLU:HA	2.05	0.56
1:B:173:LEU:HD23	1:B:173:LEU:N	2.20	0.56
1:C:149:ALA:CB	1:C:150:ARG:CA	2.73	0.56
1:A:56:ARG:NH2	1:A:59:ARG:NH1	2.52	0.56
1:B:128:GLU:CA	4:B:602:HOH:O	2.51	0.56
1:B:155:LEU:N	1:B:155:LEU:HD12	2.20	0.56
1:C:56:ARG:NH2	1:C:59:ARG:HH11	2.03	0.56
1:C:123:PRO:HG2	1:C:215:ALA:HB2	1.86	0.56
1:C:281:ASP:OD1	2:C:501:FAD:H5'1	2.06	0.56
1:D:56:ARG:HH21	1:D:59:ARG:NH1	2.01	0.56
1:B:7:VAL:CB	4:B:604:HOH:O	2.54	0.56
1:A:23:ARG:NH2	3:A:502:COA:O5A	2.39	0.56
1:B:396:HIS:N	1:B:397:GLY:CA	2.69	0.56
1:C:287:HIS:HD2	1:C:289:VAL:H	1.54	0.56
1:D:183:ARG:NH1	1:D:188:TRP:O	2.38	0.56
1:A:34:GLU:OE2	1:A:36:SER:HB3	2.06	0.56
1:B:94:HIS:CD2	1:B:94:HIS:H	2.21	0.56
1:C:280:GLY:HA2	1:C:302:ALA:HA	1.87	0.56
1:A:169:ARG:CD	1:A:175:VAL:HG13	2.36	0.56
1:A:203:HIS:HD2	1:C:219:MET:SD	2.29	0.56
1:C:96:HIS:N	4:C:603:HOH:O	2.35	0.56
1:D:6:VAL:HG22	1:D:31:VAL:HG13	1.87	0.56
1:A:4:ARG:NH1	1:A:104:ASP:OD2	2.38	0.55
1:B:269:MET:HE3	1:B:320:PHE:CB	2.36	0.55
1:D:81:VAL:HA	1:D:95:ASP:HB3	1.88	0.55
1:A:24:GLU:CG	1:A:316:ARG:HG3	2.36	0.55
1:D:424:TYR:O	1:D:425:ALA:HB2	2.06	0.55
1:A:86:TYR:CD1	1:A:88:LEU:HD22	2.41	0.55
1:B:313:ILE:C	1:B:315:GLY:H	2.15	0.55
1:B:440:GLN:O	1:B:441:GLN:O	2.23	0.55
1:B:185:LEU:N	1:B:186:PRO:CD	2.69	0.55
1:B:361:ARG:CZ	1:B:361:ARG:HB3	2.37	0.55
1:C:180:ALA:O	1:C:210:GLY:HA2	2.07	0.55
1:C:185:LEU:N	1:C:186:PRO:HD3	2.22	0.55
1:B:217:ARG:O	1:B:222:VAL:HA	2.06	0.55
1:C:91:LEU:HD13	1:C:103:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:THR:O	1:C:211:VAL:HG23	2.06	0.55
1:C:359:GLN:HB2	1:C:374:TRP:CD1	2.42	0.55
1:A:221:ARG:HD3	1:A:221:ARG:C	2.32	0.55
1:B:185:LEU:N	1:B:186:PRO:HD3	2.22	0.55
1:C:91:LEU:CG	1:C:92:THR:H	2.16	0.54
1:C:4:ARG:NH1	1:C:104:ASP:OD2	2.40	0.54
1:D:224:ALA:CA	4:D:601:HOH:O	2.55	0.54
1:A:81:VAL:HG22	1:A:249:LEU:HD21	1.88	0.54
1:A:439:ALA:C	1:A:441:GLN:HB2	2.09	0.54
1:D:411:GLU:HA	1:D:411:GLU:OE2	2.08	0.54
1:B:236:LEU:HD12	1:B:237:VAL:N	2.21	0.54
1:C:269:MET:HE3	1:C:320:PHE:CB	2.35	0.54
1:D:37:GLY:CA	1:D:77:THR:HB	2.37	0.54
1:C:37:GLY:CA	1:C:77:THR:HB	2.37	0.54
1:C:96:HIS:HB3	4:C:603:HOH:O	2.06	0.54
1:B:440:GLN:C	1:B:441:GLN:O	2.51	0.54
1:C:183:ARG:HG3	1:C:184:PRO:O	2.08	0.54
1:B:85:ASP:H	1:B:92:THR:CB	2.19	0.54
1:A:396:HIS:CD2	1:B:396:HIS:NE2	2.75	0.54
1:B:44:CYS:HB3	2:B:501:FAD:C4X	2.37	0.54
1:B:281:ASP:OD1	2:B:501:FAD:H5'1	2.08	0.54
1:C:86:TYR:O	1:C:89:ARG:HA	2.07	0.54
1:A:183:ARG:HG3	1:A:184:PRO:O	2.08	0.54
1:D:38:TRP:CE3	1:D:136:MET:HE2	2.43	0.54
1:D:91:LEU:HD13	1:D:103:GLN:OE1	2.07	0.54
1:D:150:ARG:CZ	1:D:151:ARG:HH22	2.21	0.54
1:A:343:LEU:HD22	1:A:355:LYS:HB3	1.90	0.53
1:A:85:ASP:N	1:A:92:THR:HB	2.23	0.53
1:C:56:ARG:NH2	1:C:59:ARG:NH1	2.57	0.53
1:A:85:ASP:H	1:A:92:THR:CA	2.18	0.53
1:B:270:ARG:NH1	1:B:270:ARG:HB3	2.19	0.53
1:C:299:GLY:HA3	3:C:502:COA:C2P	2.38	0.53
1:A:121:PRO:CB	1:D:172:GLY:O	2.57	0.53
1:B:398:ALA:HA	1:B:400:ARG:H	1.73	0.53
1:B:31:VAL:O	1:B:31:VAL:HG13	2.08	0.53
1:B:398:ALA:N	1:B:399:LEU:HB2	2.24	0.53
1:D:273:LEU:HB2	1:D:276:VAL:CG2	2.38	0.53
1:A:6:VAL:HG22	1:A:31:VAL:CG1	2.39	0.53
1:A:128:GLU:N	4:A:602:HOH:O	2.40	0.53
1:C:299:GLY:HA3	3:C:502:COA:H22	1.90	0.53
1:D:91:LEU:HG	1:D:92:THR:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:VAL:HG21	3:B:502:COA:H32	1.91	0.52
1:B:90:THR:CA	1:B:92:THR:HG23	2.35	0.52
1:B:126:GLU:OE1	1:B:126:GLU:HA	2.09	0.52
1:C:8:VAL:HG13	1:C:81:VAL:CG1	2.38	0.52
1:A:273:LEU:HB2	1:A:276:VAL:CG2	2.40	0.52
1:B:183:ARG:HD3	1:B:190:PRO:HA	1.91	0.52
1:C:281:ASP:N	2:C:501:FAD:O2P	2.34	0.52
1:C:330:LYS:HE2	1:C:332:PHE:O	2.08	0.52
1:A:162:LEU:HD22	1:A:200:LEU:HD11	1.91	0.52
1:D:400:ARG:HG2	1:D:435:LEU:HD11	1.90	0.52
1:A:437:ILE:HD12	1:A:437:ILE:O	2.05	0.52
1:B:363:GLY:H	1:B:430:PRO:HD3	1.75	0.52
1:C:85:ASP:OD1	1:C:88:LEU:HD23	2.08	0.52
1:C:360:SER:HB3	1:C:434:PRO:HG3	1.90	0.52
1:A:169:ARG:HD3	1:A:175:VAL:HG13	1.92	0.52
1:A:396:HIS:NE2	1:B:396:HIS:CD2	2.78	0.52
1:A:396:HIS:NE2	1:B:396:HIS:NE2	2.57	0.52
1:B:287:HIS:HD2	1:B:289:VAL:H	1.56	0.52
1:A:92:THR:HG1	1:A:106:PHE:HE2	1.57	0.52
1:B:49:VAL:HG22	1:B:54:ILE:HB	1.92	0.52
1:A:56:ARG:NH2	1:A:59:ARG:HH11	2.07	0.52
1:A:396:HIS:NE2	1:B:396:HIS:CE1	2.78	0.52
1:B:302:ALA:CB	2:B:501:FAD:H5'2	2.40	0.52
1:C:440:GLN:C	1:C:441:GLN:O	2.52	0.52
1:A:92:THR:O	1:A:104:ASP:O	2.28	0.52
1:B:86:TYR:H	1:B:86:TYR:HD1	1.57	0.52
1:A:339:THR:HG22	1:A:401:ILE:HD11	1.91	0.51
1:C:81:VAL:HA	1:C:95:ASP:HB3	1.92	0.51
1:D:299:GLY:HA2	2:D:501:FAD:H4'	1.93	0.51
1:D:352:TRP:NE1	4:D:604:HOH:O	2.42	0.51
1:B:441:GLN:C	1:B:442:ALA:O	2.52	0.51
1:B:4:ARG:HD3	1:B:105:ARG:O	2.10	0.51
1:D:4:ARG:NH1	1:D:104:ASP:OD2	2.43	0.51
1:A:185:LEU:N	1:A:186:PRO:CD	2.73	0.51
1:B:247:THR:HG21	1:B:261:GLY:O	2.10	0.51
1:C:86:TYR:CD1	1:C:88:LEU:HD22	2.45	0.51
1:D:270:ARG:NH1	1:D:270:ARG:HB3	2.24	0.51
1:B:23:ARG:HH22	3:B:502:COA:P2A	2.34	0.51
1:D:272:ASN:HD22	1:D:272:ASN:H	1.57	0.51
1:B:80:GLU:HG2	1:B:82:VAL:HG22	1.92	0.51
1:B:411:GLU:HA	1:B:411:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:GLU:OE2	1:C:355:LYS:HE3	2.10	0.51
1:A:49:VAL:HG11	1:A:57:LEU:CD1	2.40	0.51
1:C:88:LEU:O	1:C:89:ARG:CB	2.58	0.51
1:A:270:ARG:NH1	1:A:270:ARG:HB3	2.26	0.51
1:B:256:ALA:H	1:B:272:ASN:HD21	1.55	0.51
1:C:7:VAL:HB	1:C:32:VAL:HG22	1.93	0.51
1:D:88:LEU:O	1:D:89:ARG:CB	2.58	0.51
1:D:399:LEU:C	1:D:401:ILE:N	2.69	0.51
1:D:9:GLY:HA3	1:D:112:ALA:O	2.11	0.50
1:A:440:GLN:NE2	1:A:440:GLN:CA	2.70	0.50
1:B:24:GLU:CG	1:B:316:ARG:HG3	2.41	0.50
1:B:85:ASP:H	1:B:92:THR:CA	2.24	0.50
1:D:85:ASP:HA	1:D:88:LEU:HD23	1.92	0.50
1:D:88:LEU:O	1:D:89:ARG:HB2	2.10	0.50
1:C:302:ALA:HB2	2:C:501:FAD:H5'2	1.94	0.50
1:B:91:LEU:HD12	1:B:92:THR:HA	1.92	0.50
1:B:400:ARG:HD3	1:B:433:ASP:OD1	2.12	0.50
1:C:87:GLU:HA	1:C:88:LEU:O	2.12	0.50
1:C:357:PHE:CD1	1:C:376:GLU:HB2	2.44	0.50
1:C:424:TYR:CD1	1:C:425:ALA:N	2.79	0.50
1:D:24:GLU:HG2	1:D:316:ARG:HG3	1.94	0.50
1:C:440:GLN:NE2	1:C:440:GLN:CA	2.71	0.50
1:B:377:LEU:HD22	1:B:438:ALA:HB1	1.93	0.50
1:C:298:LEU:HB2	1:C:301:VAL:HG13	1.92	0.50
1:C:185:LEU:N	1:C:186:PRO:CD	2.75	0.50
1:D:144:LYS:O	1:D:147:PRO:HD2	2.12	0.50
1:B:92:THR:O	1:B:104:ASP:O	2.30	0.50
1:C:126:GLU:HA	1:C:126:GLU:OE1	2.12	0.50
1:D:373:LEU:HD22	1:D:434:PRO:HG2	1.93	0.50
1:A:440:GLN:C	1:A:441:GLN:O	2.55	0.49
1:C:256:ALA:H	1:C:272:ASN:HD21	1.60	0.49
1:B:86:TYR:O	1:B:89:ARG:CA	2.61	0.49
1:B:150:ARG:CZ	1:B:151:ARG:HH22	2.25	0.49
1:B:287:HIS:CD2	1:B:290:LEU:H	2.30	0.49
1:B:424:TYR:CD1	1:B:431:VAL:HA	2.48	0.49
1:C:440:GLN:O	1:C:441:GLN:O	2.30	0.49
1:D:7:VAL:HG13	1:D:110:VAL:HB	1.94	0.49
1:D:399:LEU:C	1:D:401:ILE:H	2.20	0.49
1:B:179:GLU:OE2	1:B:181:LYS:HG2	2.13	0.49
1:C:22:LYS:HE2	1:C:72:GLY:HA3	1.95	0.49
1:C:56:ARG:HH21	1:C:59:ARG:NH1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:FAD:O2'	2:C:501:FAD:H9	2.13	0.49
1:A:86:TYR:O	1:A:89:ARG:HA	2.13	0.49
1:C:88:LEU:O	1:C:89:ARG:HB2	2.12	0.49
1:C:96:HIS:CA	4:C:603:HOH:O	2.60	0.49
1:B:268:ARG:HH12	1:B:270:ARG:HH22	1.60	0.49
1:B:398:ALA:N	1:B:399:LEU:CB	2.72	0.49
1:A:93:VAL:C	1:A:94:HIS:HD2	2.21	0.49
1:A:267:GLU:OE2	1:A:319:ARG:NH1	2.40	0.49
1:A:189:ASP:HB3	1:A:190:PRO:CD	2.42	0.49
1:A:11:VAL:CG2	2:A:501:FAD:H4B	2.41	0.49
1:D:27:GLU:OE2	1:D:27:GLU:HA	2.13	0.49
1:D:441:GLN:C	1:D:442:ALA:O	2.56	0.49
1:A:91:LEU:O	1:A:92:THR:HG23	2.13	0.48
1:B:287:HIS:HD2	1:B:290:LEU:H	1.61	0.48
1:B:98:GLU:OE2	1:B:98:GLU:HA	2.11	0.48
1:D:25:ASN:C	1:D:25:ASN:OD1	2.54	0.48
1:D:200:LEU:HD23	1:D:332:PHE:HE1	1.77	0.48
1:A:23:ARG:NH2	3:A:502:COA:P2A	2.86	0.48
1:B:92:THR:OG1	1:B:93:VAL:N	2.45	0.48
1:B:214:GLU:O	1:B:215:ALA:HB2	2.14	0.48
1:C:361:ARG:HD3	1:C:365:HIS:HA	1.96	0.48
1:A:78:ARG:NH1	4:A:610:HOH:O	2.46	0.48
1:C:373:LEU:HD23	1:C:373:LEU:C	2.39	0.48
1:A:203:HIS:CD2	1:C:219:MET:SD	3.07	0.48
1:A:272:ASN:ND2	1:A:272:ASN:H	2.12	0.48
1:B:24:GLU:HG2	1:B:316:ARG:HG3	1.96	0.48
1:B:426:PRO:N	1:B:427:PRO:CD	2.77	0.48
1:D:24:GLU:HG3	1:D:316:ARG:CZ	2.43	0.48
1:D:363:GLY:H	1:D:430:PRO:HD3	1.79	0.48
1:A:426:PRO:HG3	1:B:44:CYS:HB2	1.96	0.48
1:B:330:LYS:HE2	1:B:332:PHE:O	2.14	0.48
1:C:299:GLY:HA2	2:C:501:FAD:H4'	1.95	0.48
1:A:38:TRP:CE3	1:A:136:MET:HE2	2.49	0.48
1:A:324:VAL:HG21	1:A:408:LEU:HB3	1.95	0.48
1:D:191:GLU:O	1:D:194:ALA:HB3	2.14	0.48
1:D:260:THR:HG23	1:D:284:GLU:OE1	2.13	0.48
1:D:359:GLN:HB2	1:D:374:TRP:CD1	2.48	0.48
1:D:25:ASN:HB2	1:D:314:ALA:HB1	1.96	0.48
1:D:191:GLU:OE2	1:D:355:LYS:HE3	2.14	0.48
2:A:501:FAD:H9	2:A:501:FAD:O2'	2.14	0.47
1:D:207:VAL:HG22	1:D:207:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HB2	1:A:276:VAL:HG21	1.95	0.47
1:D:183:ARG:HD3	1:D:190:PRO:HA	1.95	0.47
1:A:23:ARG:HH22	3:A:502:COA:P2A	2.37	0.47
1:B:8:VAL:HG13	1:B:81:VAL:HG13	1.97	0.47
1:B:80:GLU:O	1:B:95:ASP:HB2	2.14	0.47
1:B:225:VAL:HG12	1:B:227:THR:CG2	2.43	0.47
1:B:299:GLY:HA2	2:B:501:FAD:H4'	1.96	0.47
1:A:24:GLU:HG2	1:A:316:ARG:HG3	1.97	0.47
1:A:128:GLU:HG3	1:A:221:ARG:NH2	2.29	0.47
1:D:185:LEU:N	1:D:186:PRO:CD	2.78	0.47
1:A:424:TYR:CD1	1:A:425:ALA:N	2.83	0.47
1:D:403:VAL:O	1:D:406:ALA:HB3	2.15	0.47
1:B:16:SER:HB2	1:B:306:GLY:HA3	1.97	0.47
1:A:85:ASP:H	1:A:92:THR:CB	2.27	0.47
1:A:139:GLY:O	1:A:143:LEU:HB2	2.14	0.47
1:A:396:HIS:CE1	1:B:396:HIS:CD2	3.02	0.47
1:A:396:HIS:ND1	1:B:396:HIS:ND1	2.58	0.47
1:A:418:LEU:HD13	1:A:439:ALA:HB3	1.96	0.47
1:C:296:LEU:HD23	1:C:323:VAL:HG11	1.96	0.47
1:D:3:LYS:HE2	1:D:3:LYS:HB3	1.66	0.47
1:D:80:GLU:HG2	1:D:82:VAL:HG22	1.96	0.47
1:D:200:LEU:HD23	1:D:332:PHE:CE1	2.50	0.47
1:D:224:ALA:N	4:D:601:HOH:O	2.48	0.47
1:D:273:LEU:HB2	1:D:276:VAL:HG21	1.97	0.47
1:A:37:GLY:HA2	1:A:77:THR:CB	2.32	0.47
1:B:88:LEU:O	1:B:89:ARG:CB	2.62	0.47
1:D:345:GLY:O	1:D:346:ALA:C	2.58	0.47
1:A:85:ASP:H	1:A:92:THR:HB	1.80	0.47
1:B:299:GLY:HA3	3:B:502:COA:C2P	2.44	0.47
1:A:81:VAL:HA	1:A:95:ASP:HB3	1.96	0.47
1:A:92:THR:OG1	1:A:106:PHE:HE2	1.97	0.47
1:D:256:ALA:H	1:D:272:ASN:HD21	1.58	0.47
1:D:352:TRP:CD1	4:D:604:HOH:O	2.68	0.47
1:A:173:LEU:N	1:A:173:LEU:HD23	2.30	0.46
3:A:502:COA:N8P	3:A:502:COA:O5P	2.43	0.46
1:B:147:PRO:O	1:B:148:GLN:CB	2.52	0.46
1:C:268:ARG:NH1	1:C:270:ARG:HH22	2.13	0.46
1:C:424:TYR:O	1:C:425:ALA:HB2	2.15	0.46
1:B:23:ARG:NH2	3:B:502:COA:P2A	2.89	0.46
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.69	0.46
1:C:179:GLU:OE2	1:C:181:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:N	1:D:186:PRO:HD3	2.30	0.46
1:B:85:ASP:OD1	1:B:88:LEU:HB3	2.15	0.46
1:D:217:ARG:O	1:D:222:VAL:HA	2.16	0.46
1:A:183:ARG:CD	1:A:190:PRO:HA	2.45	0.46
1:B:56:ARG:NH2	1:B:59:ARG:HH11	2.13	0.46
1:B:117:PRO:HD3	1:B:134:ARG:HG2	1.97	0.46
1:C:302:ALA:CB	2:C:501:FAD:H5'2	2.45	0.46
1:A:88:LEU:O	1:A:89:ARG:HB2	2.14	0.46
1:B:209:THR:O	1:B:211:VAL:HG23	2.16	0.46
1:C:117:PRO:HD3	1:C:134:ARG:HG2	1.97	0.46
1:D:440:GLN:O	1:D:441:GLN:O	2.34	0.46
1:B:272:ASN:ND2	1:B:272:ASN:H	2.12	0.46
1:C:86:TYR:O	1:C:89:ARG:CA	2.63	0.46
1:C:437:ILE:HD12	1:C:438:ALA:N	2.28	0.46
1:D:361:ARG:HB3	1:D:361:ARG:CZ	2.46	0.46
1:D:398:ALA:CA	1:D:399:LEU:HB2	2.45	0.46
1:A:91:LEU:C	1:A:92:THR:HG23	2.41	0.46
1:A:179:GLU:OE2	1:A:181:LYS:HG2	2.16	0.46
1:B:111:LEU:HD12	1:B:111:LEU:HA	1.60	0.46
1:D:93:VAL:C	1:D:94:HIS:HD2	2.24	0.46
1:A:169:ARG:HB3	1:C:219:MET:HG3	1.98	0.46
1:B:148:GLN:O	1:B:149:ALA:O	2.34	0.46
1:B:183:ARG:CD	1:B:190:PRO:HA	2.46	0.46
1:C:245:PRO:HB2	1:C:247:THR:HG23	1.98	0.46
1:D:270:ARG:HB2	1:D:270:ARG:NH1	2.26	0.46
1:D:287:HIS:CD2	1:D:290:LEU:H	2.34	0.46
1:D:373:LEU:HD12	1:D:393:ALA:HB2	1.97	0.46
1:A:316:ARG:HG2	1:A:316:ARG:HH11	1.81	0.45
1:C:76:HIS:HB3	1:C:79:HIS:CE1	2.51	0.45
1:D:162:LEU:CD2	1:D:200:LEU:HD11	2.46	0.45
1:B:86:TYR:CD1	1:B:88:LEU:HD22	2.51	0.45
1:D:426:PRO:CB	1:D:427:PRO:HD3	2.45	0.45
1:A:330:LYS:HE2	1:A:332:PHE:O	2.17	0.45
1:B:36:SER:O	1:B:38:TRP:N	2.49	0.45
1:C:48:TYR:HB2	1:C:54:ILE:HD12	1.98	0.45
1:D:80:GLU:O	1:D:95:ASP:HB2	2.16	0.45
1:A:199:GLU:HG3	1:A:334:LEU:HG	1.98	0.45
1:A:269:MET:HE3	1:A:320:PHE:CB	2.38	0.45
1:A:418:LEU:HD12	1:A:418:LEU:HA	1.66	0.45
1:C:181:LYS:HG2	1:C:181:LYS:H	1.40	0.45
1:C:217:ARG:O	1:C:222:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:TYR:CD1	1:D:86:TYR:N	2.75	0.45
1:A:34:GLU:OE2	1:A:36:SER:CB	2.65	0.45
1:A:88:LEU:O	1:A:89:ARG:CB	2.64	0.45
1:A:396:HIS:HE1	1:B:396:HIS:N	2.13	0.45
1:C:86:TYR:H	1:C:86:TYR:HD1	1.58	0.45
1:C:101:THR:HG22	4:C:606:HOH:O	2.17	0.45
1:C:214:GLU:O	1:C:215:ALA:HB2	2.17	0.45
1:D:86:TYR:CD1	1:D:88:LEU:HD22	2.51	0.45
1:A:181:LYS:HG2	1:A:181:LYS:H	1.52	0.45
1:A:299:GLY:HA2	2:A:501:FAD:H4'	1.97	0.45
1:B:287:HIS:CD2	1:B:289:VAL:H	2.34	0.45
1:C:169:ARG:CD	1:C:175:VAL:HG13	2.47	0.45
1:C:85:ASP:OD1	1:C:88:LEU:HB3	2.17	0.45
1:B:324:VAL:HG21	1:B:408:LEU:HB3	1.99	0.45
1:C:28:LEU:HA	1:C:28:LEU:HD23	1.77	0.45
1:C:280:GLY:HA3	2:C:501:FAD:O2P	2.16	0.45
1:C:199:GLU:HG3	1:C:334:LEU:HG	1.99	0.45
1:D:92:THR:CB	1:D:106:PHE:HE2	2.30	0.45
1:A:24:GLU:HG3	1:A:316:ARG:HG3	1.97	0.44
1:A:41:TYR:HA	1:A:61:VAL:HA	1.99	0.44
1:A:149:ALA:HA	1:A:173:LEU:CD2	2.46	0.44
1:B:356:VAL:HG22	1:B:357:PHE:N	2.31	0.44
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.79	0.44
1:C:92:THR:CB	1:C:106:PHE:HE2	2.30	0.44
1:C:441:GLN:C	1:C:442:ALA:O	2.60	0.44
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.64	0.44
1:A:316:ARG:HG2	1:A:316:ARG:NH1	2.32	0.44
1:B:105:ARG:CB	4:B:601:HOH:O	2.65	0.44
1:B:191:GLU:OE2	1:B:355:LYS:HE3	2.17	0.44
1:C:183:ARG:HD3	1:C:190:PRO:HA	1.99	0.44
1:A:121:PRO:CG	1:D:149:ALA:HB1	2.46	0.44
1:B:56:ARG:NH2	1:B:59:ARG:NH1	2.65	0.44
1:D:189:ASP:HB3	1:D:190:PRO:CD	2.46	0.44
1:D:280:GLY:HA3	2:D:501:FAD:O2P	2.17	0.44
1:B:3:LYS:HB3	1:B:3:LYS:HE2	1.74	0.44
1:B:440:GLN:C	4:B:603:HOH:O	2.58	0.44
1:C:151:ARG:HG2	1:C:174:GLN:HG3	2.00	0.44
1:C:398:ALA:N	1:C:399:LEU:CB	2.72	0.44
1:A:56:ARG:HH21	1:A:59:ARG:NH1	2.14	0.44
1:B:25:ASN:HB2	1:B:314:ALA:HB1	1.99	0.44
1:B:92:THR:HG1	1:B:106:PHE:HE2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:TYR:O	1:C:89:ARG:N	2.51	0.44
1:D:424:TYR:CD1	1:D:425:ALA:N	2.86	0.44
1:B:143:LEU:HD12	1:B:143:LEU:HA	1.79	0.44
1:D:28:LEU:HD23	1:D:28:LEU:HA	1.84	0.44
1:A:432:TRP:HB3	1:A:437:ILE:HG22	1.99	0.44
1:D:87:GLU:CA	1:D:88:LEU:C	2.87	0.44
1:D:116:ARG:HH12	1:D:244:ARG:HD2	1.77	0.44
1:B:76:HIS:HB3	1:B:79:HIS:ND1	2.32	0.44
1:D:97:ALA:HB1	1:D:98:GLU:H	1.57	0.44
1:A:28:LEU:HA	1:A:28:LEU:HD23	1.86	0.43
1:B:85:ASP:C	1:B:92:THR:CG2	2.80	0.43
1:C:96:HIS:CB	4:C:603:HOH:O	2.65	0.43
1:C:437:ILE:C	1:C:437:ILE:CD1	2.69	0.43
1:D:89:ARG:O	1:D:90:THR:C	2.61	0.43
1:A:90:THR:CB	1:A:92:THR:HG23	2.48	0.43
1:B:46:LEU:HD13	1:B:133:LEU:HD22	2.00	0.43
1:C:50:LEU:HD12	1:C:50:LEU:HA	1.74	0.43
1:D:23:ARG:HH22	3:D:502:COA:P2A	2.41	0.43
1:A:94:HIS:CD2	1:A:94:HIS:H	2.30	0.43
1:A:185:LEU:N	1:A:186:PRO:HD3	2.34	0.43
1:B:7:VAL:C	4:B:604:HOH:O	2.57	0.43
1:C:143:LEU:O	1:C:147:PRO:HD3	2.18	0.43
1:C:258:GLY:HA3	1:C:284:GLU:CD	2.43	0.43
1:D:302:ALA:CB	2:D:501:FAD:H5'2	2.48	0.43
1:A:7:VAL:HB	1:A:32:VAL:HG22	2.01	0.43
1:D:90:THR:HA	1:D:91:LEU:C	2.43	0.43
1:D:299:GLY:HA3	3:D:502:COA:H22	2.00	0.43
1:A:200:LEU:HD23	1:A:332:PHE:CE1	2.54	0.43
1:B:280:GLY:HA3	2:B:501:FAD:O2P	2.19	0.43
1:D:77:THR:O	1:D:78:ARG:HB2	2.18	0.43
1:A:91:LEU:HD12	1:A:92:THR:CA	2.49	0.43
1:C:116:ARG:HH12	1:C:244:ARG:HD2	1.81	0.43
1:C:216:PHE:CE1	1:C:225:VAL:HG22	2.54	0.43
1:C:271:THR:HB	4:C:609:HOH:O	2.18	0.43
1:D:141:ARG:HH11	1:D:141:ARG:HD2	1.61	0.43
1:D:386:LEU:HD13	1:D:386:LEU:HA	1.76	0.43
1:B:91:LEU:CG	1:B:92:THR:H	2.31	0.43
1:B:410:ARG:HH11	1:B:410:ARG:CG	2.05	0.43
1:D:197:LYS:O	1:D:201:GLU:HB2	2.19	0.43
1:B:7:VAL:HG13	1:B:110:VAL:HB	2.01	0.43
1:B:36:SER:O	1:B:37:GLY:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:HIS:HA	1:B:102:PHE:O	2.19	0.43
1:D:126:GLU:OE1	1:D:126:GLU:HA	2.18	0.43
1:D:161:GLY:H	1:D:164:ALA:H	1.67	0.43
1:B:90:THR:OG1	1:B:91:LEU:O	2.37	0.43
1:B:94:HIS:CG	1:B:103:GLN:HE22	2.37	0.43
1:D:8:VAL:HG13	1:D:81:VAL:CG1	2.49	0.43
1:D:85:ASP:OD1	1:D:88:LEU:CD2	2.65	0.43
1:D:299:GLY:HA3	3:D:502:COA:C2P	2.47	0.43
1:D:398:ALA:CA	1:D:399:LEU:CB	2.97	0.43
1:A:80:GLU:O	1:A:95:ASP:HB2	2.19	0.42
1:C:90:THR:OG1	1:C:91:LEU:O	2.12	0.42
1:D:86:TYR:O	1:D:89:ARG:N	2.52	0.42
1:A:37:GLY:H	1:A:78:ARG:H	1.67	0.42
1:B:292:ARG:HB2	1:B:293:PRO:HD2	2.00	0.42
1:D:25:ASN:CB	1:D:314:ALA:HB1	2.49	0.42
1:A:253:MET:HG3	1:A:255:VAL:HG23	2.01	0.42
1:B:23:ARG:NH1	3:B:502:COA:O8A	2.53	0.42
1:D:112:ALA:HB1	4:D:605:HOH:O	2.18	0.42
1:B:91:LEU:HD12	1:B:92:THR:CA	2.50	0.42
1:B:91:LEU:C	1:B:92:THR:HG23	2.44	0.42
1:B:269:MET:CE	1:B:320:PHE:HB3	2.48	0.42
1:C:127:GLN:HG2	1:C:220:GLY:HA2	2.01	0.42
1:D:356:VAL:HG12	1:D:377:LEU:HB2	2.02	0.42
1:D:361:ARG:HD3	1:D:365:HIS:HA	2.02	0.42
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.93	0.42
1:C:39:VAL:HG11	1:C:75:VAL:HG21	2.02	0.42
1:C:166:GLU:OE2	1:C:170:LYS:HE3	2.18	0.42
1:C:23:ARG:HH22	3:C:502:COA:P2A	2.41	0.42
1:C:86:TYR:HB2	1:C:87:GLU:H	1.22	0.42
1:C:120:PRO:HA	1:C:121:PRO:HD3	1.80	0.42
1:C:358:ILE:HD12	1:C:358:ILE:C	2.45	0.42
1:D:413:SER:O	1:D:416:ASP:HB2	2.19	0.42
1:B:429:SER:HA	1:B:430:PRO:HD2	1.84	0.42
1:B:86:TYR:O	1:B:89:ARG:N	2.53	0.42
1:B:219:MET:HB2	4:B:608:HOH:O	2.20	0.42
1:D:400:ARG:C	1:D:402:ASP:N	2.77	0.42
1:D:440:GLN:C	1:D:441:GLN:O	2.62	0.42
1:A:358:ILE:HD11	1:A:375:VAL:HG13	2.02	0.42
1:A:363:GLY:H	1:A:430:PRO:HD3	1.84	0.42
1:B:155:LEU:N	1:B:155:LEU:CD1	2.82	0.42
1:C:81:VAL:HG22	1:C:249:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LYS:HD3	1:D:108:HIS:NE2	2.35	0.42
1:D:166:GLU:HG2	1:D:170:LYS:HE3	2.00	0.42
1:D:436:LEU:O	1:D:437:ILE:C	2.62	0.42
1:A:92:THR:OG1	1:A:106:PHE:CE2	2.69	0.42
1:C:24:GLU:HB3	1:C:314:ALA:CB	2.50	0.42
1:C:98:GLU:N	1:C:98:GLU:CD	2.78	0.42
1:D:24:GLU:HG2	1:D:316:ARG:CG	2.49	0.42
1:D:31:VAL:HG13	1:D:31:VAL:O	2.20	0.42
1:C:398:ALA:H	1:C:399:LEU:HB3	1.77	0.41
1:A:428:PHE:CD2	1:B:328:ILE:HD13	2.55	0.41
2:A:501:FAD:H2'	3:A:502:COA:S1P	2.59	0.41
1:B:313:ILE:HG21	1:B:313:ILE:HD13	1.69	0.41
1:C:123:PRO:HG2	1:C:215:ALA:CB	2.48	0.41
1:C:413:SER:O	1:C:416:ASP:HB2	2.20	0.41
1:D:87:GLU:HA	1:D:88:LEU:O	2.19	0.41
1:D:268:ARG:HG2	1:D:312:VAL:HG21	2.02	0.41
1:A:92:THR:HG21	1:A:106:PHE:CE2	2.55	0.41
1:B:166:GLU:OE2	1:B:170:LYS:HE3	2.20	0.41
1:C:222:VAL:O	1:C:222:VAL:CG1	2.67	0.41
1:C:236:LEU:HD12	1:C:237:VAL:N	2.35	0.41
1:D:81:VAL:HA	1:D:95:ASP:CB	2.50	0.41
1:A:8:VAL:HG13	1:A:81:VAL:HG13	2.02	0.41
1:A:86:TYR:O	1:A:89:ARG:CA	2.68	0.41
1:A:189:ASP:HA	1:A:190:PRO:HD3	1.74	0.41
1:C:399:LEU:C	1:C:401:ILE:N	2.78	0.41
1:A:44:CYS:SG	4:B:609:HOH:O	2.61	0.41
2:A:501:FAD:H8A	2:A:501:FAD:H2B	1.96	0.41
1:B:41:TYR:HA	1:B:61:VAL:HA	2.02	0.41
1:B:87:GLU:HA	1:B:88:LEU:O	2.20	0.41
1:C:199:GLU:OE1	1:C:332:PHE:HB2	2.20	0.41
1:D:86:TYR:HB2	1:D:87:GLU:H	1.32	0.41
1:A:411:GLU:OE2	1:A:411:GLU:HA	2.19	0.41
1:B:93:VAL:C	1:B:94:HIS:HD2	2.28	0.41
1:D:432:TRP:O	1:D:433:ASP:C	2.62	0.41
1:A:86:TYR:HD1	1:A:86:TYR:H	1.66	0.41
1:A:144:LYS:O	1:A:147:PRO:HD2	2.21	0.41
1:A:169:ARG:HG2	1:A:175:VAL:CG1	2.50	0.41
1:A:280:GLY:HA2	1:A:302:ALA:HA	2.02	0.41
1:A:299:GLY:HA3	3:A:502:COA:H22	2.03	0.41
1:A:302:ALA:CB	2:A:501:FAD:H5'2	2.51	0.41
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:PHE:CE1	1:C:237:VAL:HG21	2.55	0.41
1:D:111:LEU:HD12	1:D:111:LEU:HA	1.85	0.41
1:D:268:ARG:CG	1:D:312:VAL:HG21	2.51	0.41
1:A:441:GLN:C	1:A:442:ALA:O	2.63	0.41
1:B:166:GLU:HA	1:B:332:PHE:CZ	2.56	0.41
1:C:3:LYS:HB3	1:C:3:LYS:HE2	1.66	0.41
1:D:207:VAL:O	1:D:207:VAL:CG2	2.68	0.41
1:A:24:GLU:HG3	1:A:316:ARG:CG	2.51	0.41
1:A:97:ALA:HB1	1:A:98:GLU:H	1.55	0.41
1:B:105:ARG:HH11	1:B:105:ARG:HD3	1.60	0.41
1:B:418:LEU:HD13	1:B:439:ALA:HB3	2.03	0.41
1:C:12:ALA:N	2:C:501:FAD:O1P	2.49	0.41
1:C:38:TRP:CE3	1:C:136:MET:HE2	2.56	0.41
1:C:84:VAL:HA	1:C:93:VAL:H	1.86	0.41
1:C:266:ASP:C	1:C:268:ARG:H	2.29	0.41
1:D:46:LEU:HD13	1:D:133:LEU:HD22	2.02	0.41
1:D:105:ARG:HH11	1:D:105:ARG:HD3	1.72	0.41
1:D:114:GLY:HA2	1:D:281:ASP:HB2	2.02	0.41
1:D:139:GLY:O	1:D:143:LEU:HB2	2.21	0.41
1:D:253:MET:HG3	1:D:255:VAL:HG23	2.03	0.41
1:D:356:VAL:HG22	1:D:357:PHE:N	2.35	0.41
1:B:50:LEU:HD12	1:B:50:LEU:HA	1.79	0.41
1:C:4:ARG:HH11	1:C:4:ARG:HD3	1.57	0.41
1:C:266:ASP:C	1:C:268:ARG:N	2.76	0.41
1:D:221:ARG:O	1:D:222:VAL:HG12	2.21	0.40
1:A:24:GLU:HB3	1:A:314:ALA:CB	2.51	0.40
1:A:86:TYR:O	1:A:89:ARG:N	2.55	0.40
1:A:91:LEU:HD12	1:A:92:THR:HA	2.04	0.40
1:A:143:LEU:HA	1:A:143:LEU:HD12	1.77	0.40
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.82	0.40
1:B:211:VAL:HG22	1:B:229:GLU:CG	2.47	0.40
1:D:84:VAL:HA	1:D:93:VAL:H	1.86	0.40
1:B:398:ALA:CA	1:B:399:LEU:CB	2.99	0.40
1:A:148:GLN:O	1:A:149:ALA:O	2.40	0.40
1:C:23:ARG:NH2	3:C:502:COA:P2A	2.94	0.40
1:C:111:LEU:HD12	1:C:111:LEU:HA	1.89	0.40
1:C:437:ILE:O	1:C:438:ALA:C	2.64	0.40
1:D:169:ARG:CD	1:D:175:VAL:HG13	2.52	0.40
1:D:287:HIS:CD2	1:D:289:VAL:H	2.32	0.40
1:D:324:VAL:HG21	1:D:408:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/443 (100%)	393 (89%)	33 (8%)	15 (3%)	3	12
1	B	441/443 (100%)	379 (86%)	46 (10%)	16 (4%)	2	11
1	C	441/443 (100%)	391 (89%)	35 (8%)	15 (3%)	3	12
1	D	441/443 (100%)	381 (86%)	42 (10%)	18 (4%)	2	9
All	All	1764/1772 (100%)	1544 (88%)	156 (9%)	64 (4%)	2	11

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	TYR
1	A	91	LEU
1	A	148	GLN
1	A	149	ALA
1	A	398	ALA
1	A	441	GLN
1	A	442	ALA
1	B	86	TYR
1	B	89	ARG
1	B	148	GLN
1	B	149	ALA
1	B	398	ALA
1	B	440	GLN
1	B	441	GLN
1	B	442	ALA
1	C	86	TYR
1	C	148	GLN
1	C	149	ALA
1	C	398	ALA
1	C	441	GLN
1	C	442	ALA
1	D	86	TYR

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Mol	Chain	Res	Type
1	D	91	LEU
1	D	148	GLN
1	D	149	ALA
1	D	398	ALA
1	D	441	GLN
1	D	442	ALA
1	A	89	ARG
1	A	399	LEU
1	A	440	GLN
1	C	89	ARG
1	C	399	LEU
1	C	440	GLN
1	D	89	ARG
1	D	399	LEU
1	D	400	ARG
1	D	440	GLN
1	B	222	VAL
1	C	222	VAL
1	D	97	ALA
1	D	222	VAL
1	A	222	VAL
1	B	225	VAL
1	B	364	ALA
1	B	399	LEU
1	C	70	LYS
1	C	88	LEU
1	D	88	LEU
1	A	93	VAL
1	A	225	VAL
1	A	400	ARG
1	B	93	VAL
1	B	418	LEU
1	C	225	VAL
1	D	93	VAL
1	D	225	VAL
1	D	438	ALA
1	B	92	THR
1	C	93	VAL
1	B	395	GLY
1	C	324	VAL
1	D	13	GLY
1	A	395	GLY

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	338/338 (100%)	268 (79%)	70 (21%)	1	4
1	B	338/338 (100%)	269 (80%)	69 (20%)	1	4
1	C	337/338 (100%)	271 (80%)	66 (20%)	1	5
1	D	337/338 (100%)	263 (78%)	74 (22%)	1	3
All	All	1350/1352 (100%)	1071 (79%)	279 (21%)	1	4

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	39	VAL
1	A	44	CYS
1	A	50	LEU
1	A	58	GLU
1	A	59	ARG
1	A	60	LEU
1	A	61	VAL
1	A	70	LYS
1	A	74	LEU
1	A	75	VAL
1	A	78	ARG
1	A	80	GLU
1	A	81	VAL
1	A	86	TYR
1	A	87	GLU
1	A	90	THR
1	A	91	LEU
1	A	94	HIS
1	A	101	THR
1	A	111	LEU
1	A	116	ARG
1	A	132	THR
1	A	133	LEU

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Mol	Chain	Res	Type
1	A	142	LEU
1	A	146	LEU
1	A	148	GLN
1	A	151	ARG
1	A	160	ILE
1	A	173	LEU
1	A	175	VAL
1	A	176	THR
1	A	177	LEU
1	A	181	LYS
1	A	185	LEU
1	A	199	GLU
1	A	207	VAL
1	A	208	TRP
1	A	209	THR
1	A	211	VAL
1	A	212	LYS
1	A	221	ARG
1	A	222	VAL
1	A	231	VAL
1	A	236	LEU
1	A	237	VAL
1	A	243	ILE
1	A	268	ARG
1	A	270	ARG
1	A	276	VAL
1	A	285	SER
1	A	301	VAL
1	A	324	VAL
1	A	361	ARG
1	A	375	VAL
1	A	377	LEU
1	A	386	LEU
1	A	391	VAL
1	A	392	VAL
1	A	396	HIS
1	A	400	ARG
1	A	408	LEU
1	A	410	ARG
1	A	411	GLU
1	A	413	SER
1	A	418	LEU

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Mol	Chain	Res	Type
1	A	437	ILE
1	A	440	GLN
1	A	441	GLN
1	A	443	ARG
1	B	3	LYS
1	B	4	ARG
1	B	7	VAL
1	B	39	VAL
1	B	44	CYS
1	B	50	LEU
1	B	58	GLU
1	B	59	ARG
1	B	60	LEU
1	B	75	VAL
1	B	78	ARG
1	B	80	GLU
1	B	81	VAL
1	B	86	TYR
1	B	90	THR
1	B	91	LEU
1	B	92	THR
1	B	94	HIS
1	B	101	THR
1	B	111	LEU
1	B	116	ARG
1	B	132	THR
1	B	133	LEU
1	B	142	LEU
1	B	144	LYS
1	B	146	LEU
1	B	148	GLN
1	B	160	ILE
1	B	173	LEU
1	B	175	VAL
1	B	176	THR
1	B	177	LEU
1	B	181	LYS
1	B	185	LEU
1	B	199	GLU
1	B	207	VAL
1	B	208	TRP
1	B	209	THR

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Mol	Chain	Res	Type
1	B	211	VAL
1	B	212	LYS
1	B	221	ARG
1	B	222	VAL
1	B	231	VAL
1	B	236	LEU
1	B	237	VAL
1	B	243	ILE
1	B	268	ARG
1	B	270	ARG
1	B	272	ASN
1	B	276	VAL
1	B	292	ARG
1	B	301	VAL
1	B	324	VAL
1	B	361	ARG
1	B	375	VAL
1	B	377	LEU
1	B	386	LEU
1	B	391	VAL
1	B	392	VAL
1	B	396	HIS
1	B	400	ARG
1	B	408	LEU
1	B	410	ARG
1	B	411	GLU
1	B	418	LEU
1	B	437	ILE
1	B	440	GLN
1	B	441	GLN
1	B	443	ARG
1	C	3	LYS
1	C	39	VAL
1	C	44	CYS
1	C	50	LEU
1	C	58	GLU
1	C	59	ARG
1	C	60	LEU
1	C	61	VAL
1	C	75	VAL
1	C	78	ARG
1	C	80	GLU

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Mol	Chain	Res	Type
1	C	81	VAL
1	C	86	TYR
1	C	90	THR
1	C	91	LEU
1	C	94	HIS
1	C	101	THR
1	C	111	LEU
1	C	116	ARG
1	C	132	THR
1	C	133	LEU
1	C	142	LEU
1	C	143	LEU
1	C	144	LYS
1	C	146	LEU
1	C	148	GLN
1	C	160	ILE
1	C	173	LEU
1	C	175	VAL
1	C	176	THR
1	C	177	LEU
1	C	181	LYS
1	C	185	LEU
1	C	199	GLU
1	C	207	VAL
1	C	208	TRP
1	C	209	THR
1	C	212	LYS
1	C	221	ARG
1	C	222	VAL
1	C	225	VAL
1	C	231	VAL
1	C	236	LEU
1	C	237	VAL
1	C	243	ILE
1	C	268	ARG
1	C	270	ARG
1	C	272	ASN
1	C	301	VAL
1	C	324	VAL
1	C	361	ARG
1	C	375	VAL
1	C	377	LEU

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Mol	Chain	Res	Type
1	C	391	VAL
1	C	392	VAL
1	C	396	HIS
1	C	408	LEU
1	C	410	ARG
1	C	411	GLU
1	C	413	SER
1	C	418	LEU
1	C	434	PRO
1	C	437	ILE
1	C	440	GLN
1	C	441	GLN
1	C	443	ARG
1	D	3	LYS
1	D	39	VAL
1	D	44	CYS
1	D	50	LEU
1	D	58	GLU
1	D	59	ARG
1	D	60	LEU
1	D	61	VAL
1	D	70	LYS
1	D	75	VAL
1	D	78	ARG
1	D	80	GLU
1	D	81	VAL
1	D	86	TYR
1	D	87	GLU
1	D	90	THR
1	D	91	LEU
1	D	93	VAL
1	D	94	HIS
1	D	100	ARG
1	D	101	THR
1	D	111	LEU
1	D	116	ARG
1	D	117	PRO
1	D	132	THR
1	D	133	LEU
1	D	142	LEU
1	D	143	LEU
1	D	144	LYS

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Mol	Chain	Res	Type
1	D	146	LEU
1	D	148	GLN
1	D	160	ILE
1	D	171	ARG
1	D	175	VAL
1	D	176	THR
1	D	177	LEU
1	D	181	LYS
1	D	185	LEU
1	D	199	GLU
1	D	201	GLU
1	D	207	VAL
1	D	208	TRP
1	D	209	THR
1	D	211	VAL
1	D	212	LYS
1	D	221	ARG
1	D	222	VAL
1	D	225	VAL
1	D	236	LEU
1	D	237	VAL
1	D	241	THR
1	D	243	ILE
1	D	268	ARG
1	D	270	ARG
1	D	276	VAL
1	D	301	VAL
1	D	324	VAL
1	D	361	ARG
1	D	375	VAL
1	D	377	LEU
1	D	386	LEU
1	D	391	VAL
1	D	392	VAL
1	D	396	HIS
1	D	400	ARG
1	D	408	LEU
1	D	410	ARG
1	D	411	GLU
1	D	418	LEU
1	D	434	PRO
1	D	437	ILE

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Mol	Chain	Res	Type
1	D	440	GLN
1	D	441	GLN
1	D	443	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	94	HIS
1	A	96	HIS
1	A	203	HIS
1	A	272	ASN
1	A	287	HIS
1	A	359	GLN
1	A	396	HIS
1	A	409	HIS
1	A	440	GLN
1	B	94	HIS
1	B	96	HIS
1	B	251	GLN
1	B	272	ASN
1	B	287	HIS
1	B	396	HIS
1	B	440	GLN
1	C	76	HIS
1	C	94	HIS
1	C	96	HIS
1	C	272	ASN
1	C	287	HIS
1	C	440	GLN
1	D	94	HIS
1	D	96	HIS
1	D	272	ASN
1	D	287	HIS
1	D	409	HIS
1	D	440	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	FAD	B	501	-	58,58,58	3.76	33 (56%)	85,89,89	2.41	34 (40%)
2	FAD	A	501	-	58,58,58	3.32	31 (53%)	85,89,89	2.20	26 (30%)
3	COA	C	502	1	47,50,50	1.40	4 (8%)	69,75,75	2.37	23 (33%)
2	FAD	C	501	-	58,58,58	3.38	27 (46%)	85,89,89	2.03	27 (31%)
3	COA	D	502	1	47,50,50	1.10	4 (8%)	69,75,75	2.52	25 (36%)
3	COA	A	502	1	47,50,50	1.68	11 (23%)	69,75,75	2.49	25 (36%)
3	COA	B	502	1	47,50,50	1.57	7 (14%)	69,75,75	2.21	23 (33%)
2	FAD	D	501	-	58,58,58	3.35	27 (46%)	85,89,89	2.03	23 (27%)

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	-	-	15/34/50/50	0/6/6/6
2	FAD	A	501	-	-	15/34/50/50	0/6/6/6
3	COA	C	502	1	-	18/48/64/64	0/3/3/3
2	FAD	C	501	-	-	18/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	D	502	1	-	17/48/64/64	0/3/3/3
3	COA	A	502	1	-	15/48/64/64	0/3/3/3
3	COA	B	502	1	-	18/48/64/64	0/3/3/3
2	FAD	D	501	-	-	15/34/50/50	0/6/6/6

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C5A-C4A	11.28	1.59	1.39
2	D	501	FAD	C5A-C4A	11.04	1.58	1.39
2	B	501	FAD	PA-O3P	10.39	1.70	1.59
2	A	501	FAD	C5A-C4A	10.37	1.57	1.39
2	B	501	FAD	C5A-C4A	10.16	1.57	1.39
2	B	501	FAD	C9A-C5X	9.81	1.56	1.41
2	A	501	FAD	PA-O3P	9.16	1.69	1.59
2	C	501	FAD	C9A-C5X	8.75	1.55	1.41
2	D	501	FAD	PA-O3P	8.48	1.68	1.59
2	D	501	FAD	C9A-C5X	7.93	1.53	1.41
2	A	501	FAD	C9A-C5X	7.92	1.53	1.41
2	C	501	FAD	PA-O3P	7.67	1.67	1.59
2	B	501	FAD	P-O3P	7.16	1.67	1.59
2	B	501	FAD	C4A-N3A	6.71	1.47	1.34
2	D	501	FAD	C2A-N1A	6.64	1.45	1.33
2	C	501	FAD	C2A-N1A	6.33	1.45	1.33
2	C	501	FAD	C4A-N3A	6.00	1.45	1.34
2	D	501	FAD	P-O3P	5.84	1.65	1.59
2	B	501	FAD	C2A-N1A	5.84	1.44	1.33
2	D	501	FAD	C4A-N3A	5.71	1.45	1.34
2	B	501	FAD	C5A-C6A	5.67	1.56	1.41
2	A	501	FAD	C5A-C6A	5.60	1.56	1.41
2	B	501	FAD	C8-C7	5.45	1.54	1.40
2	C	501	FAD	C2A-N3A	5.43	1.43	1.33
2	D	501	FAD	C5A-C6A	5.35	1.55	1.41
2	C	501	FAD	C8-C7	5.20	1.53	1.40
2	A	501	FAD	C2A-N3A	5.15	1.43	1.33
2	B	501	FAD	C2A-N3A	5.14	1.43	1.33
3	B	502	COA	C5A-C4A	5.11	1.48	1.39
2	A	501	FAD	C8-C7	5.01	1.53	1.40
3	C	502	COA	C5A-C4A	4.98	1.48	1.39
2	A	501	FAD	C2A-N1A	4.86	1.42	1.33
2	D	501	FAD	C2A-N3A	4.77	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	P-O3P	4.77	1.64	1.59
2	C	501	FAD	C5A-C6A	4.71	1.54	1.41
2	B	501	FAD	C4X-N5	4.71	1.40	1.30
2	A	501	FAD	C4A-N3A	4.61	1.43	1.34
2	D	501	FAD	C8-C7	4.44	1.51	1.40
2	C	501	FAD	O4-C4	4.43	1.32	1.23
3	A	502	COA	C5A-N7A	-4.43	1.31	1.39
2	C	501	FAD	P-O3P	4.34	1.64	1.59
2	D	501	FAD	C4X-N5	4.27	1.40	1.30
2	C	501	FAD	C4X-N5	4.25	1.39	1.30
2	B	501	FAD	O4-C4	4.23	1.31	1.23
2	B	501	FAD	C4X-C10	4.22	1.56	1.44
2	C	501	FAD	O2-C2	4.15	1.32	1.24
2	C	501	FAD	C8A-N7A	4.06	1.39	1.31
2	B	501	FAD	C5'-C4'	4.00	1.57	1.51
2	B	501	FAD	C1B-N9A	3.99	1.57	1.46
2	B	501	FAD	C10-N10	3.97	1.45	1.37
2	A	501	FAD	C5'-C4'	3.93	1.57	1.51
2	D	501	FAD	C4X-C10	3.88	1.55	1.44
2	B	501	FAD	O3B-C3B	3.81	1.52	1.43
2	B	501	FAD	C6-C7	3.81	1.44	1.39
2	A	501	FAD	C10-N1	3.77	1.40	1.33
2	D	501	FAD	C10-N10	3.75	1.45	1.37
2	A	501	FAD	C10-N10	3.74	1.45	1.37
2	A	501	FAD	C4X-N5	3.70	1.38	1.30
2	A	501	FAD	PA-O1A	3.69	1.63	1.50
2	C	501	FAD	C10-N10	3.66	1.45	1.37
3	A	502	COA	C8A-N9A	-3.66	1.31	1.37
2	D	501	FAD	C9A-N10	3.65	1.47	1.41
3	A	502	COA	C5A-C4A	3.63	1.45	1.39
2	B	501	FAD	C10-N1	3.62	1.40	1.33
2	B	501	FAD	C9A-N10	3.49	1.47	1.41
3	B	502	COA	C5A-C6A	3.49	1.50	1.41
2	B	501	FAD	C6A-N1A	3.49	1.45	1.35
2	B	501	FAD	C8A-N7A	3.47	1.38	1.31
2	A	501	FAD	C8A-N7A	3.47	1.38	1.31
2	A	501	FAD	C4X-C10	3.43	1.54	1.44
3	A	502	COA	C5A-C6A	3.42	1.50	1.41
2	A	501	FAD	O2-C2	3.41	1.31	1.24
2	C	501	FAD	C4X-C10	3.41	1.54	1.44
3	B	502	COA	C2A-N3A	3.27	1.39	1.33
2	D	501	FAD	C8A-N7A	3.26	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C9A-N10	3.26	1.46	1.41
2	A	501	FAD	O4-C4	3.24	1.29	1.23
2	D	501	FAD	C10-N1	3.22	1.39	1.33
2	C	501	FAD	C9A-N10	3.21	1.46	1.41
2	C	501	FAD	C8A-N9A	3.19	1.43	1.37
2	A	501	FAD	C6A-N6A	3.15	1.42	1.34
3	C	502	COA	C5A-C6A	3.15	1.49	1.41
2	D	501	FAD	C6A-N1A	3.04	1.44	1.35
2	C	501	FAD	C6A-N1A	3.04	1.44	1.35
3	C	502	COA	C6A-N6A	3.01	1.41	1.34
2	B	501	FAD	C6-C5X	2.92	1.44	1.40
2	D	501	FAD	O4-C4	2.90	1.29	1.23
3	D	502	COA	C5A-C4A	2.89	1.44	1.39
2	C	501	FAD	C10-N1	2.89	1.39	1.33
2	A	501	FAD	C6A-N1A	2.89	1.43	1.35
2	A	501	FAD	C1B-N9A	2.88	1.54	1.46
2	B	501	FAD	C3B-C4B	2.86	1.60	1.53
2	B	501	FAD	C4A-N9A	2.86	1.43	1.37
2	B	501	FAD	PA-O1A	2.85	1.60	1.50
3	A	502	COA	O5P-C5P	-2.83	1.17	1.23
2	D	501	FAD	PA-O1A	2.81	1.60	1.50
2	C	501	FAD	C5'-C4'	2.80	1.55	1.51
2	A	501	FAD	C6-C7	2.73	1.43	1.39
2	B	501	FAD	O4B-C1B	2.72	1.48	1.42
2	D	501	FAD	C6-C7	2.72	1.43	1.39
2	D	501	FAD	C1B-N9A	2.70	1.53	1.46
2	D	501	FAD	C5'-C4'	2.66	1.55	1.51
2	A	501	FAD	C9-C9A	2.65	1.43	1.39
2	C	501	FAD	C6-C7	2.65	1.43	1.39
2	A	501	FAD	C2B-C1B	2.65	1.61	1.53
2	D	501	FAD	C4X-C4	2.61	1.54	1.44
2	A	501	FAD	O3B-C3B	2.60	1.49	1.43
2	C	501	FAD	PA-O1A	2.59	1.59	1.50
3	B	502	COA	P2A-O3A	-2.59	1.56	1.59
2	B	501	FAD	C4X-C4	2.59	1.54	1.44
2	C	501	FAD	C3B-C4B	2.59	1.59	1.53
2	D	501	FAD	O2B-C2B	2.55	1.49	1.43
3	A	502	COA	C6P-C5P	-2.54	1.46	1.51
2	D	501	FAD	C2B-C1B	2.53	1.61	1.53
3	A	502	COA	CCP-CBP	-2.51	1.48	1.52
3	B	502	COA	O9P-C9P	-2.48	1.18	1.23
3	D	502	COA	C5A-C6A	2.44	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C6-C5X	2.42	1.43	1.40
2	C	501	FAD	O3B-C3B	2.42	1.49	1.43
2	D	501	FAD	C9-C8	2.40	1.42	1.39
2	A	501	FAD	C4X-C4	2.40	1.53	1.44
3	D	502	COA	P2A-O3A	2.38	1.62	1.59
3	B	502	COA	C5A-N7A	-2.37	1.34	1.39
2	B	501	FAD	O4'-C4'	2.37	1.48	1.43
3	A	502	COA	C6A-N6A	2.34	1.40	1.34
2	B	501	FAD	C9-C8	2.32	1.42	1.39
2	A	501	FAD	O4'-C4'	2.30	1.48	1.43
2	C	501	FAD	C1B-N9A	2.28	1.52	1.46
2	A	501	FAD	PA-O5B	2.28	1.68	1.59
2	B	501	FAD	C4'-C3'	2.22	1.57	1.53
2	A	501	FAD	C2-N1	2.20	1.41	1.36
2	B	501	FAD	C6A-N6A	2.20	1.39	1.34
3	A	502	COA	P3B-O8A	-2.20	1.46	1.54
3	D	502	COA	C8A-N9A	-2.20	1.33	1.37
3	B	502	COA	P3B-O8A	-2.16	1.46	1.54
3	C	502	COA	P3B-O3B	2.13	1.63	1.59
3	A	502	COA	C2A-N1A	2.11	1.37	1.33
2	A	501	FAD	C8A-N9A	2.10	1.41	1.37
2	C	501	FAD	C6-C5X	2.07	1.43	1.40
3	A	502	COA	C3B-C4B	-2.06	1.47	1.52
2	B	501	FAD	C8A-N9A	2.05	1.41	1.37
2	D	501	FAD	C8A-N9A	2.01	1.41	1.37
2	B	501	FAD	PA-O5B	2.00	1.67	1.59
2	C	501	FAD	P-O5'	2.00	1.67	1.59

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	COA	C5A-C4A-N3A	-8.70	114.74	126.72
2	A	501	FAD	O4B-C1B-N9A	8.57	124.56	108.09
3	D	502	COA	C5A-C4A-N3A	-8.56	114.92	126.72
3	B	502	COA	C5A-C4A-N3A	-8.04	115.65	126.72
2	D	501	FAD	O4B-C1B-N9A	7.53	122.56	108.09
2	B	501	FAD	O4B-C1B-N9A	7.39	122.28	108.09
3	C	502	COA	N3A-C4A-N9A	7.20	139.41	127.17
3	D	502	COA	N3A-C4A-N9A	6.97	139.03	127.17
2	B	501	FAD	N3A-C4A-N9A	6.86	138.83	127.17
2	C	501	FAD	O4B-C1B-N9A	6.43	120.44	108.09
3	A	502	COA	N3A-C4A-N9A	6.41	138.06	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C5A-C4A-N3A	-6.40	117.90	126.72
3	C	502	COA	C5A-C4A-N3A	-6.36	117.95	126.72
2	A	501	FAD	N3A-C4A-N9A	6.26	137.81	127.17
3	B	502	COA	N3A-C4A-N9A	6.14	137.60	127.17
2	B	501	FAD	C5X-C9A-N10	5.91	123.31	117.97
2	A	501	FAD	C5A-C4A-N3A	-5.68	118.90	126.72
2	C	501	FAD	N3A-C4A-N9A	5.58	136.66	127.17
2	D	501	FAD	N3A-C4A-N9A	5.56	136.62	127.17
3	D	502	COA	C2A-N3A-C4A	5.52	125.32	111.83
3	A	502	COA	C4A-C5A-N7A	-5.23	104.60	110.58
3	D	502	COA	CDP-CBP-CCP	5.18	116.78	108.22
2	A	501	FAD	N6A-C6A-N1A	5.04	129.60	118.38
2	C	501	FAD	C5X-C9A-N10	4.76	122.27	117.97
3	D	502	COA	O3A-P1A-O1A	-4.66	96.68	110.70
2	C	501	FAD	C5A-C4A-N3A	-4.61	120.36	126.72
3	C	502	COA	C4A-N9A-C8A	4.59	110.56	105.74
3	B	502	COA	C2A-N3A-C4A	4.58	123.01	111.83
2	B	501	FAD	N6A-C6A-N1A	4.41	128.19	118.38
3	A	502	COA	O4B-C1B-C2B	-4.40	97.20	106.62
3	D	502	COA	OAP-CAP-CBP	-4.37	100.06	110.18
3	A	502	COA	CDP-CBP-CAP	4.34	116.17	108.77
3	D	502	COA	CEP-CBP-CAP	4.30	116.10	108.77
3	A	502	COA	C2A-N3A-C4A	4.28	122.28	111.83
3	C	502	COA	CDP-CBP-CCP	4.28	115.28	108.22
3	B	502	COA	O2A-P1A-O3A	4.23	118.70	107.27
2	D	501	FAD	C5A-C4A-N3A	-4.21	120.92	126.72
2	B	501	FAD	O3'-C3'-C4'	4.20	118.46	108.93
3	C	502	COA	C3P-N4P-C5P	-4.15	115.09	122.82
3	A	502	COA	O2B-C2B-C1B	-4.14	95.84	110.10
3	A	502	COA	C5A-N7A-C8A	4.12	109.93	103.45
2	D	501	FAD	N6A-C6A-N1A	4.05	127.39	118.38
3	C	502	COA	C2A-N3A-C4A	4.04	121.71	111.83
2	C	501	FAD	N6A-C6A-N1A	4.02	127.33	118.38
3	A	502	COA	C7P-N8P-C9P	-4.00	115.35	122.55
2	A	501	FAD	O4B-C4B-C3B	4.00	113.10	105.15
3	A	502	COA	C7P-C6P-C5P	-3.98	105.77	112.39
3	B	502	COA	CEP-CBP-CAP	3.97	115.54	108.77
2	B	501	FAD	O2-C2-N1	-3.88	115.35	121.80
3	D	502	COA	N3A-C2A-N1A	-3.88	122.71	128.58
3	C	502	COA	CEP-CBP-CAP	3.80	115.25	108.77
3	A	502	COA	C6A-C5A-C4A	3.76	122.31	117.18
2	C	501	FAD	C9A-C5X-N5	-3.74	118.48	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	C9A-N10-C10	-3.71	115.09	120.75
3	D	502	COA	O2A-P1A-O1A	3.70	129.66	112.44
3	D	502	COA	O6A-CCP-CBP	-3.70	104.60	110.55
3	C	502	COA	CEP-CBP-CCP	-3.69	102.12	108.22
2	D	501	FAD	O4B-C4B-C3B	3.66	112.43	105.15
3	C	502	COA	C1B-N9A-C8A	-3.66	118.97	127.09
3	C	502	COA	O2A-P1A-O1A	3.65	129.41	112.44
2	D	501	FAD	C5X-C9A-N10	3.61	121.23	117.97
3	C	502	COA	N6A-C6A-N1A	3.58	126.36	118.38
3	B	502	COA	O4B-C1B-C2B	-3.54	99.05	106.62
2	A	501	FAD	C5A-C6A-N6A	-3.49	114.65	123.29
2	A	501	FAD	O3'-C3'-C4'	3.47	116.81	108.93
2	D	501	FAD	C9A-C5X-N5	-3.47	118.77	122.45
3	D	502	COA	C4A-C5A-N7A	-3.46	106.63	110.58
2	D	501	FAD	C4A-N9A-C8A	3.46	109.37	105.74
2	C	501	FAD	O3B-C3B-C4B	3.44	120.95	111.08
2	B	501	FAD	O4-C4-C4X	-3.37	117.64	126.53
3	B	502	COA	C4A-C5A-N7A	-3.35	106.75	110.58
3	D	502	COA	O2A-P1A-O3A	3.33	116.28	107.27
2	A	501	FAD	C4A-N9A-C8A	3.33	109.23	105.74
2	C	501	FAD	O4B-C4B-C3B	3.32	111.74	105.15
2	B	501	FAD	O4B-C4B-C3B	3.31	111.73	105.15
3	B	502	COA	O9P-C9P-N8P	-3.30	116.00	122.98
3	A	502	COA	C6P-C7P-N8P	3.28	118.98	112.00
2	B	501	FAD	O4-C4-N3	3.27	126.26	120.11
2	B	501	FAD	C5A-N7A-C8A	3.25	108.56	103.45
3	A	502	COA	C1B-N9A-C8A	-3.23	119.92	127.09
2	B	501	FAD	C5A-C6A-N6A	-3.23	115.28	123.29
2	B	501	FAD	C2A-N3A-C4A	3.17	119.58	111.83
3	C	502	COA	O6A-CCP-CBP	-3.17	105.46	110.55
3	D	502	COA	O9A-P3B-O7A	3.15	123.11	110.83
2	A	501	FAD	C10-N1-C2	3.14	123.66	116.85
2	B	501	FAD	C4A-N9A-C8A	3.13	109.03	105.74
3	C	502	COA	O3A-P1A-O1A	-3.12	101.33	110.70
2	B	501	FAD	O3B-C3B-C4B	3.09	119.97	111.08
2	D	501	FAD	C5A-C4A-N9A	-3.07	102.46	105.81
2	B	501	FAD	C3B-C2B-C1B	3.06	107.25	101.46
2	B	501	FAD	C4A-C5A-N7A	-3.05	107.10	110.58
2	C	501	FAD	C4A-N9A-C8A	3.04	108.93	105.74
2	C	501	FAD	O4-C4-N3	3.04	125.83	120.11
3	C	502	COA	O9A-P3B-O7A	2.96	122.35	110.83
3	C	502	COA	C5A-C6A-N6A	-2.95	115.99	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	COA	C5A-C4A-N9A	-2.94	102.61	105.81
3	D	502	COA	C5A-N7A-C8A	2.93	108.06	103.45
2	D	501	FAD	C2A-N1A-C6A	2.91	123.52	118.73
3	A	502	COA	O2A-P1A-O3A	2.90	115.11	107.27
2	C	501	FAD	O5'-C5'-C4'	2.87	117.03	109.36
2	B	501	FAD	O2P-P-O3P	-2.87	99.51	107.27
3	D	502	COA	C7P-N8P-C9P	-2.87	117.39	122.55
3	A	502	COA	C3B-C2B-C1B	2.86	106.18	99.89
2	A	501	FAD	O2B-C2B-C1B	2.86	119.94	110.10
3	C	502	COA	C7P-N8P-C9P	-2.84	117.45	122.55
3	B	502	COA	C7P-N8P-C9P	-2.82	117.48	122.55
3	A	502	COA	O6A-CCP-CBP	-2.80	106.05	110.55
2	C	501	FAD	O2B-C2B-C1B	2.78	119.68	110.10
2	A	501	FAD	C3B-C2B-C1B	2.77	106.71	101.46
2	A	501	FAD	O5'-C5'-C4'	2.77	116.76	109.36
3	A	502	COA	O4B-C1B-N9A	2.76	113.39	108.09
3	B	502	COA	O5A-P2A-O4A	2.76	125.29	112.44
2	B	501	FAD	C9A-C5X-N5	-2.75	119.54	122.45
2	D	501	FAD	C2'-C1'-N10	2.75	123.20	110.20
2	D	501	FAD	C5X-N5-C4X	2.73	122.51	118.09
3	B	502	COA	O3B-P3B-O7A	-2.72	99.62	109.33
2	D	501	FAD	O5'-C5'-C4'	2.72	116.61	109.36
2	D	501	FAD	O3P-P-O1P	-2.71	102.54	110.70
3	A	502	COA	O5P-C5P-C6P	-2.71	117.10	122.02
2	C	501	FAD	O2P-P-O5'	2.69	119.74	107.57
3	C	502	COA	N3A-C2A-N1A	-2.68	124.52	128.58
3	B	502	COA	C3P-N4P-C5P	-2.67	117.85	122.82
2	A	501	FAD	O3B-C3B-C4B	2.65	118.70	111.08
2	C	501	FAD	C5A-C6A-N6A	-2.65	116.72	123.29
2	D	501	FAD	O2P-P-O5'	2.65	119.58	107.57
2	A	501	FAD	O2P-P-O5'	2.64	119.54	107.57
2	B	501	FAD	O3P-P-O1P	-2.64	102.76	110.70
2	A	501	FAD	O4-C4-C4X	-2.64	119.57	126.53
2	C	501	FAD	C5A-C4A-N9A	-2.62	102.96	105.81
2	D	501	FAD	O2B-C2B-C1B	2.62	119.12	110.10
3	D	502	COA	C1B-N9A-C8A	-2.62	121.29	127.09
3	B	502	COA	C5A-C6A-N6A	-2.61	116.83	123.29
3	A	502	COA	O3A-P1A-O1A	-2.60	102.88	110.70
3	C	502	COA	O5B-P1A-O1A	-2.60	98.62	108.94
3	D	502	COA	O5A-P2A-O4A	2.60	124.54	112.44
3	D	502	COA	C4A-N9A-C8A	2.60	108.46	105.74
2	A	501	FAD	C4X-C10-N1	-2.58	118.26	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	COA	C4A-N9A-C1B	2.56	132.63	126.63
2	A	501	FAD	C9A-N10-C10	-2.55	116.86	120.75
3	D	502	COA	C2P-C3P-N4P	-2.54	106.54	112.31
3	C	502	COA	CAP-C9P-N8P	2.53	121.29	116.48
2	B	501	FAD	C2'-C1'-N10	2.51	122.06	110.20
3	B	502	COA	C5A-N7A-C8A	2.50	107.38	103.45
3	A	502	COA	CEP-CBP-CCP	-2.49	104.11	108.22
2	C	501	FAD	O2P-P-O3P	-2.49	100.54	107.27
3	B	502	COA	O3A-P1A-O1A	-2.44	103.35	110.70
2	C	501	FAD	O4-C4-C4X	-2.44	120.08	126.53
2	C	501	FAD	C8M-C8-C9	-2.44	115.27	119.57
3	C	502	COA	O5A-P2A-O4A	2.43	123.77	112.44
2	A	501	FAD	C4-C4X-N5	2.43	121.57	118.21
3	A	502	COA	N6A-C6A-N1A	2.42	123.78	118.38
2	D	501	FAD	O3'-C3'-C4'	2.40	114.39	108.93
2	A	501	FAD	C4X-C10-N10	2.39	119.91	116.48
3	B	502	COA	CAP-C9P-N8P	2.39	121.01	116.48
2	C	501	FAD	C9A-N10-C10	-2.39	117.11	120.75
2	A	501	FAD	O3P-P-O1P	-2.37	103.56	110.70
3	D	502	COA	O4B-C1B-C2B	-2.36	101.57	106.62
2	B	501	FAD	O5'-C5'-C4'	2.34	115.61	109.36
2	B	501	FAD	C5A-C4A-N9A	-2.33	103.27	105.81
2	C	501	FAD	O4'-C4'-C3'	2.32	114.69	109.25
2	A	501	FAD	C5A-C4A-N9A	-2.31	103.29	105.81
3	B	502	COA	N6A-C6A-N1A	2.31	123.52	118.38
2	A	501	FAD	C4A-C5A-N7A	-2.30	107.95	110.58
2	D	501	FAD	O2-C2-N1	-2.30	117.98	121.80
2	A	501	FAD	C2A-N3A-C4A	2.30	117.44	111.83
3	A	502	COA	O2A-P1A-O1A	2.29	123.10	112.44
2	C	501	FAD	O2A-PA-O1A	2.29	123.09	112.44
2	B	501	FAD	C8M-C8-C9	-2.28	115.55	119.57
2	A	501	FAD	O2P-P-O3P	-2.28	101.11	107.27
2	B	501	FAD	N3A-C2A-N1A	-2.27	125.15	128.58
2	C	501	FAD	C2A-N1A-C6A	2.26	122.45	118.73
3	D	502	COA	C5A-C6A-N6A	-2.26	117.70	123.29
3	B	502	COA	O2A-P1A-O1A	2.25	122.91	112.44
3	C	502	COA	O2B-C2B-C3B	-2.25	104.90	111.19
3	B	502	COA	C3B-C2B-C1B	2.24	104.81	99.89
3	B	502	COA	O2B-C2B-C3B	-2.23	104.93	111.19
2	D	501	FAD	C5A-C6A-N6A	-2.22	117.78	123.29
3	C	502	COA	O4B-C1B-N9A	2.22	112.36	108.09
3	D	502	COA	N9A-C8A-N7A	-2.21	110.80	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FAD	C9A-C9-C8	2.19	123.62	119.22
2	A	501	FAD	C5X-C9A-N10	2.19	119.94	117.97
3	D	502	COA	C2B-C1B-N9A	-2.14	107.98	113.30
3	B	502	COA	N3A-C2A-N1A	-2.13	125.35	128.58
2	C	501	FAD	C10-N1-C2	2.13	121.46	116.85
3	B	502	COA	C2B-C1B-N9A	-2.13	108.01	113.30
2	C	501	FAD	O2P-P-O1P	2.11	122.26	112.44
2	B	501	FAD	P-O5'-C5'	2.11	133.43	121.35
3	D	502	COA	O3A-P2A-O4A	-2.10	104.38	110.70
2	B	501	FAD	O2P-P-O5'	2.10	117.10	107.57
2	C	501	FAD	C6-C5X-C9A	2.09	121.93	119.05
2	C	501	FAD	C2B-C1B-N9A	-2.09	108.10	113.30
2	B	501	FAD	O3B-C3B-C2B	2.09	118.52	111.82
3	A	502	COA	N9A-C8A-N7A	-2.09	110.98	113.94
2	B	501	FAD	C1B-N9A-C8A	-2.07	122.50	127.09
2	A	501	FAD	O2-C2-N3	2.07	122.56	118.58
2	D	501	FAD	N3A-C2A-N1A	-2.07	125.45	128.58
2	B	501	FAD	C4X-C10-N1	-2.07	119.52	124.59
2	C	501	FAD	C2'-C1'-N10	2.06	119.92	110.20
3	D	502	COA	C7P-C6P-C5P	-2.05	108.98	112.39
2	B	501	FAD	O2P-P-O1P	2.05	121.98	112.44
2	B	501	FAD	O2'-C2'-C3'	-2.03	104.50	109.25
3	B	502	COA	O3A-P2A-O4A	-2.03	104.60	110.70
2	D	501	FAD	C4-C4X-N5	2.02	121.00	118.21
3	A	502	COA	C2B-C1B-N9A	-2.02	108.29	113.30
2	D	501	FAD	C2A-N3A-C4A	2.01	116.75	111.83
2	B	501	FAD	O2-C2-N3	2.01	122.44	118.58

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C1'-C2'-C3'-O3'
2	A	501	FAD	C1'-C2'-C3'-C4'
2	A	501	FAD	O2'-C2'-C3'-O3'
2	A	501	FAD	O2'-C2'-C3'-C4'
2	A	501	FAD	C3'-C4'-C5'-O5'
2	A	501	FAD	O4'-C4'-C5'-O5'
2	A	501	FAD	C5'-O5'-P-O3P
2	B	501	FAD	C5B-O5B-PA-O1A
2	B	501	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
2	B	501	FAD	C1'-C2'-C3'-O3'
2	B	501	FAD	C1'-C2'-C3'-C4'
2	B	501	FAD	O2'-C2'-C3'-O3'
2	B	501	FAD	O2'-C2'-C3'-C4'
2	B	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	O4'-C4'-C5'-O5'
2	B	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C5'-O5'-P-O3P
2	C	501	FAD	C5B-O5B-PA-O1A
2	C	501	FAD	C5B-O5B-PA-O3P
2	C	501	FAD	C1'-C2'-C3'-O3'
2	C	501	FAD	C1'-C2'-C3'-C4'
2	C	501	FAD	O2'-C2'-C3'-O3'
2	C	501	FAD	O2'-C2'-C3'-C4'
2	C	501	FAD	C3'-C4'-C5'-O5'
2	C	501	FAD	O4'-C4'-C5'-O5'
2	C	501	FAD	C5'-O5'-P-O3P
2	D	501	FAD	C5B-O5B-PA-O1A
2	D	501	FAD	C1'-C2'-C3'-O3'
2	D	501	FAD	C1'-C2'-C3'-C4'
2	D	501	FAD	O2'-C2'-C3'-O3'
2	D	501	FAD	O2'-C2'-C3'-C4'
2	D	501	FAD	C3'-C4'-C5'-O5'
2	D	501	FAD	O4'-C4'-C5'-O5'
2	D	501	FAD	C5'-O5'-P-O3P
3	A	502	COA	O4B-C4B-C5B-O5B
3	A	502	COA	CCP-O6A-P2A-O3A
3	A	502	COA	CCP-O6A-P2A-O4A
3	A	502	COA	CCP-O6A-P2A-O5A
3	A	502	COA	CDP-CBP-CCP-O6A
3	A	502	COA	CEP-CBP-CCP-O6A
3	A	502	COA	CAP-CBP-CCP-O6A
3	B	502	COA	C5B-O5B-P1A-O1A
3	B	502	COA	CCP-O6A-P2A-O3A
3	B	502	COA	CCP-O6A-P2A-O4A
3	B	502	COA	CDP-CBP-CCP-O6A
3	B	502	COA	CEP-CBP-CCP-O6A
3	B	502	COA	CAP-CBP-CCP-O6A
3	C	502	COA	C5B-O5B-P1A-O1A
3	C	502	COA	CCP-O6A-P2A-O3A
3	C	502	COA	CCP-O6A-P2A-O4A
3	C	502	COA	CDP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
3	C	502	COA	CEP-CBP-CCP-O6A
3	C	502	COA	CAP-CBP-CCP-O6A
3	D	502	COA	C3B-C4B-C5B-O5B
3	D	502	COA	O4B-C4B-C5B-O5B
3	D	502	COA	C5B-O5B-P1A-O2A
3	D	502	COA	C5B-O5B-P1A-O3A
3	D	502	COA	CCP-O6A-P2A-O3A
3	D	502	COA	CCP-O6A-P2A-O4A
3	D	502	COA	CDP-CBP-CCP-O6A
3	D	502	COA	CEP-CBP-CCP-O6A
3	D	502	COA	CAP-CBP-CCP-O6A
3	A	502	COA	C3B-C4B-C5B-O5B
3	B	502	COA	C3B-C4B-C5B-O5B
3	B	502	COA	O4B-C4B-C5B-O5B
3	C	502	COA	C3B-C4B-C5B-O5B
3	C	502	COA	O4B-C4B-C5B-O5B
3	C	502	COA	C4B-C3B-O3B-P3B
3	A	502	COA	O5P-C5P-N4P-C3P
3	C	502	COA	C2B-C3B-O3B-P3B
3	A	502	COA	C6P-C5P-N4P-C3P
3	C	502	COA	C3B-O3B-P3B-O7A
3	B	502	COA	P2A-O3A-P1A-O1A
3	D	502	COA	P2A-O3A-P1A-O1A
3	B	502	COA	O5P-C5P-N4P-C3P
3	D	502	COA	O5P-C5P-N4P-C3P
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
3	C	502	COA	O5P-C5P-N4P-C3P
3	B	502	COA	C6P-C5P-N4P-C3P
3	A	502	COA	P2A-O3A-P1A-O1A
3	A	502	COA	P2A-O3A-P1A-O2A
3	B	502	COA	P2A-O3A-P1A-O2A
3	D	502	COA	P2A-O3A-P1A-O2A
3	D	502	COA	C6P-C5P-N4P-C3P
3	C	502	COA	C6P-C5P-N4P-C3P
2	A	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	C5'-O5'-P-O1P
2	D	501	FAD	C5'-O5'-P-O1P

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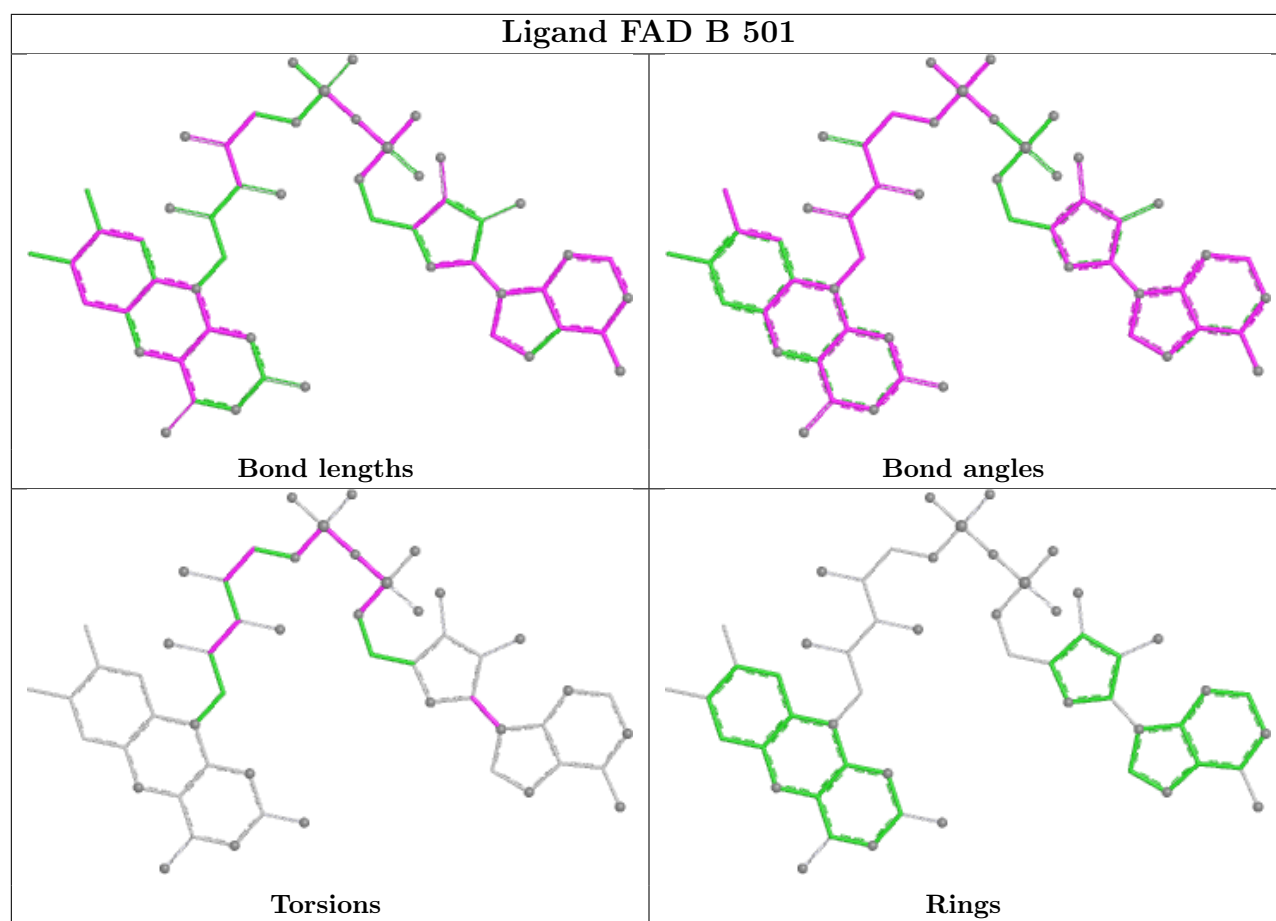
Mol	Chain	Res	Type	Atoms
3	A	502	COA	C5B-O5B-P1A-O1A
3	A	502	COA	C5B-O5B-P1A-O2A
3	A	502	COA	C5B-O5B-P1A-O3A
3	B	502	COA	C5B-O5B-P1A-O2A
3	B	502	COA	C5B-O5B-P1A-O3A
3	B	502	COA	CCP-O6A-P2A-O5A
3	C	502	COA	C5B-O5B-P1A-O2A
3	C	502	COA	C5B-O5B-P1A-O3A
3	C	502	COA	CCP-O6A-P2A-O5A
3	D	502	COA	C5B-O5B-P1A-O1A
3	D	502	COA	CCP-O6A-P2A-O5A
3	C	502	COA	P1A-O3A-P2A-O5A
3	B	502	COA	C2B-C3B-O3B-P3B
2	A	501	FAD	O4B-C1B-N9A-C8A
3	B	502	COA	C5P-C6P-C7P-N8P
2	C	501	FAD	C2'-C3'-C4'-O4'
2	B	501	FAD	O4B-C1B-N9A-C8A
2	C	501	FAD	O4B-C1B-N9A-C8A
2	D	501	FAD	O4B-C1B-N9A-C8A
3	D	502	COA	C2B-C3B-O3B-P3B
2	A	501	FAD	C2B-C1B-N9A-C8A
2	A	501	FAD	PA-O3P-P-O2P
2	B	501	FAD	P-O3P-PA-O2A
2	B	501	FAD	PA-O3P-P-O2P
2	C	501	FAD	P-O3P-PA-O1A
2	C	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	P-O3P-PA-O2A
3	C	502	COA	P2A-O3A-P1A-O2A
3	B	502	COA	C4B-C3B-O3B-P3B
2	C	501	FAD	C2B-C1B-N9A-C8A
2	D	501	FAD	O4B-C4B-C5B-O5B
3	D	502	COA	S1P-C2P-C3P-N4P
2	A	501	FAD	P-O3P-PA-O2A
2	C	501	FAD	PA-O3P-P-O2P
2	D	501	FAD	PA-O3P-P-O2P
2	A	501	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

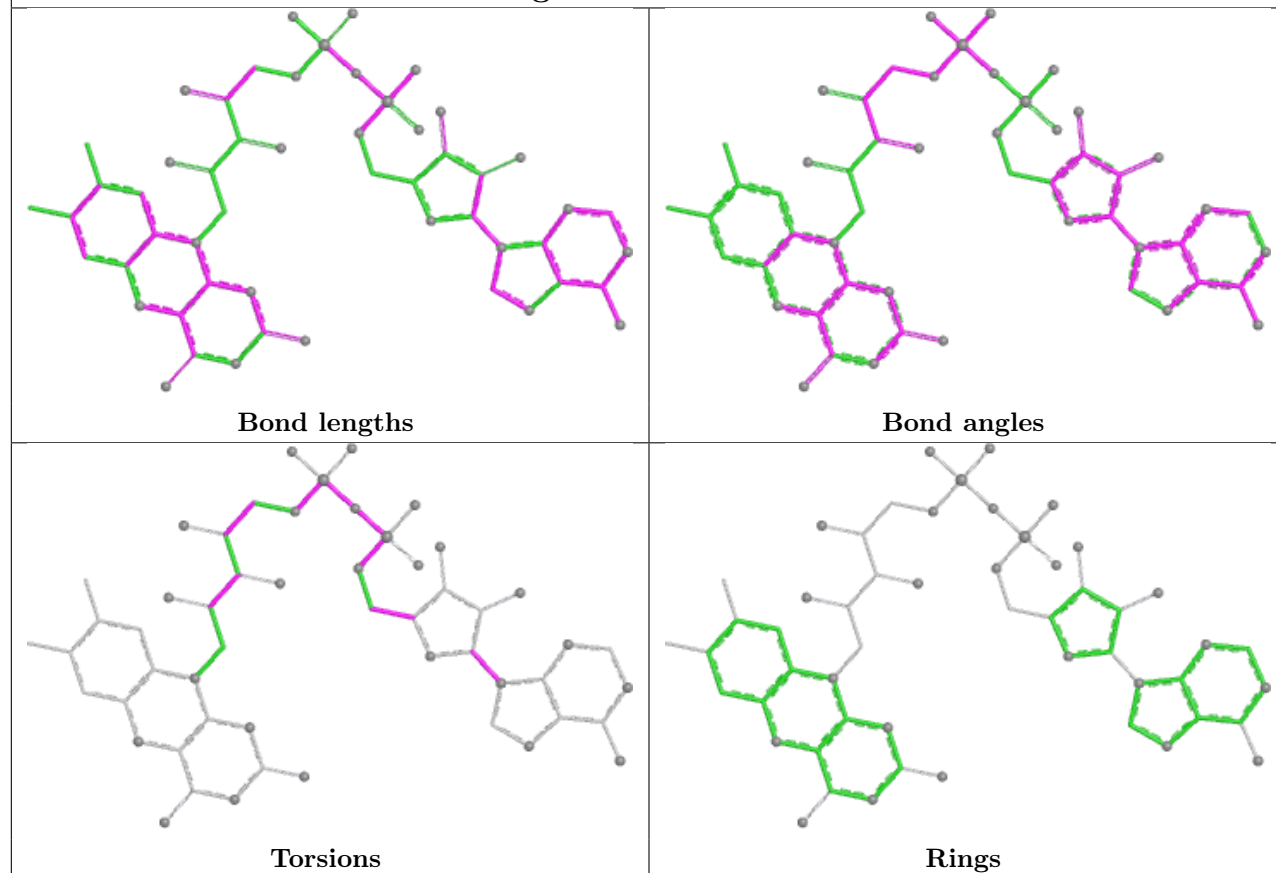
8 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FAD	8	0
2	A	501	FAD	9	0
3	C	502	COA	4	0
2	C	501	FAD	10	0
3	D	502	COA	3	0
3	A	502	COA	6	0
3	B	502	COA	7	0
2	D	501	FAD	7	0

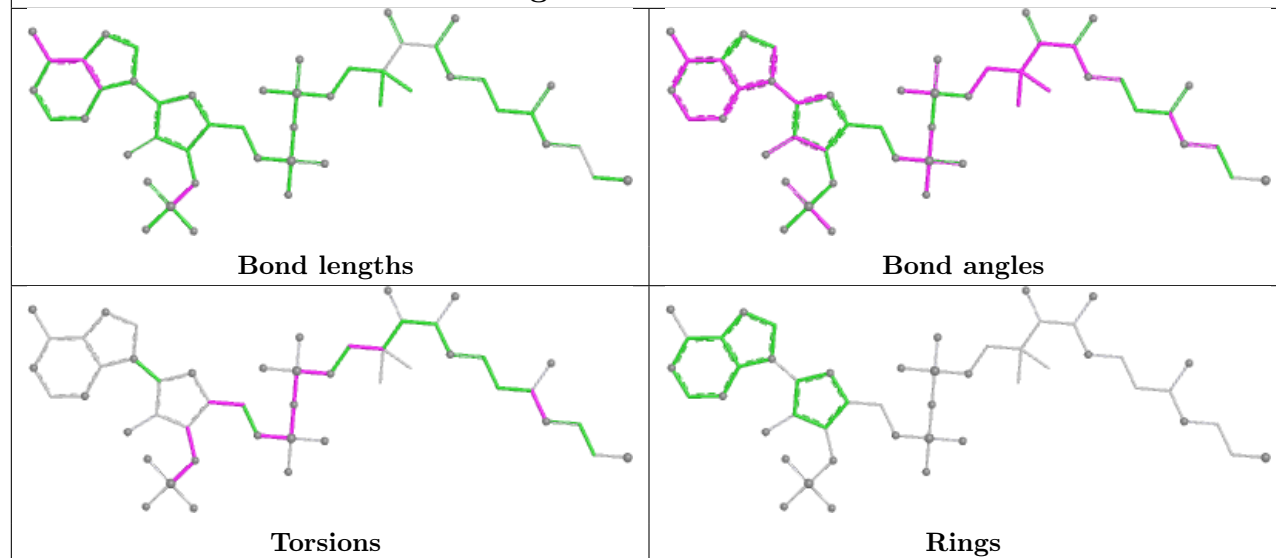
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



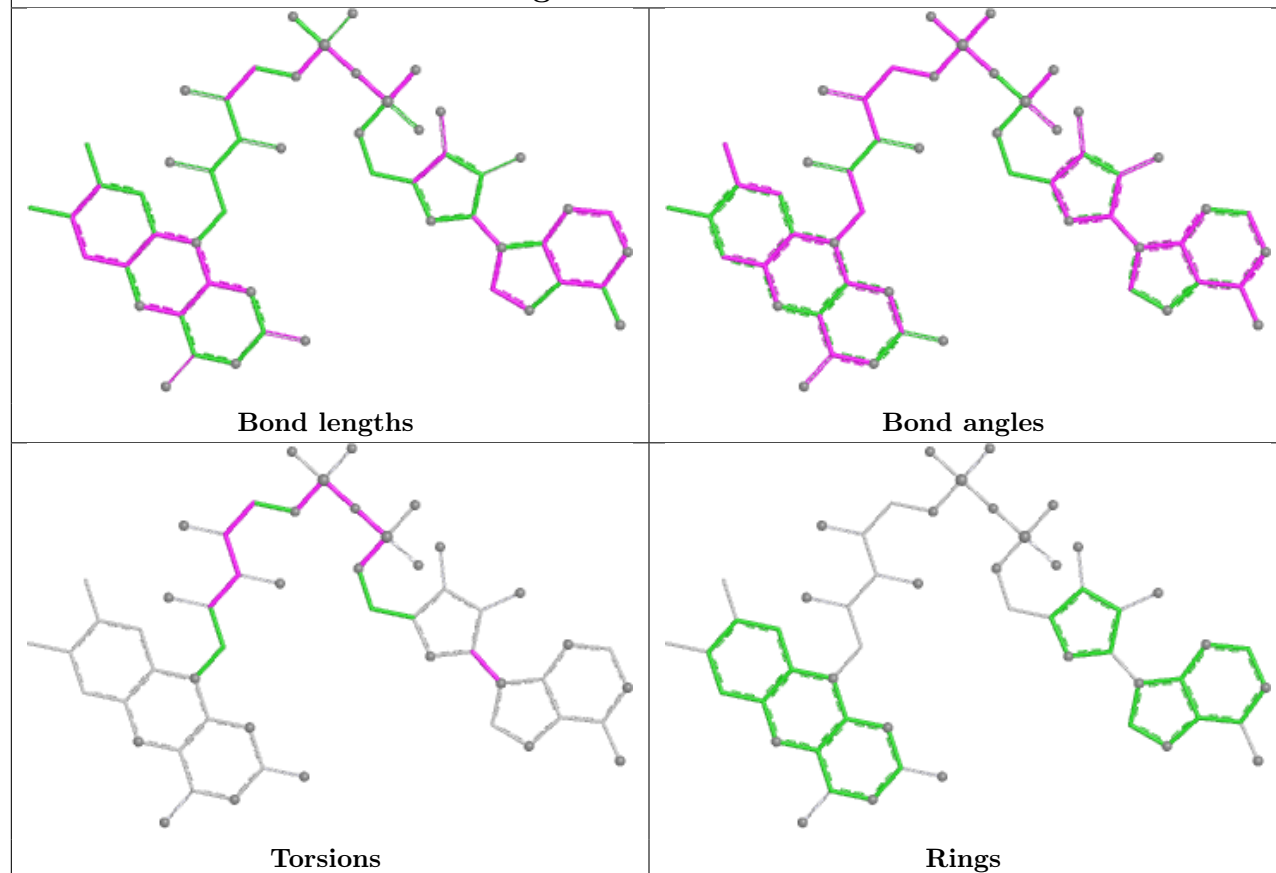
Ligand FAD A 501



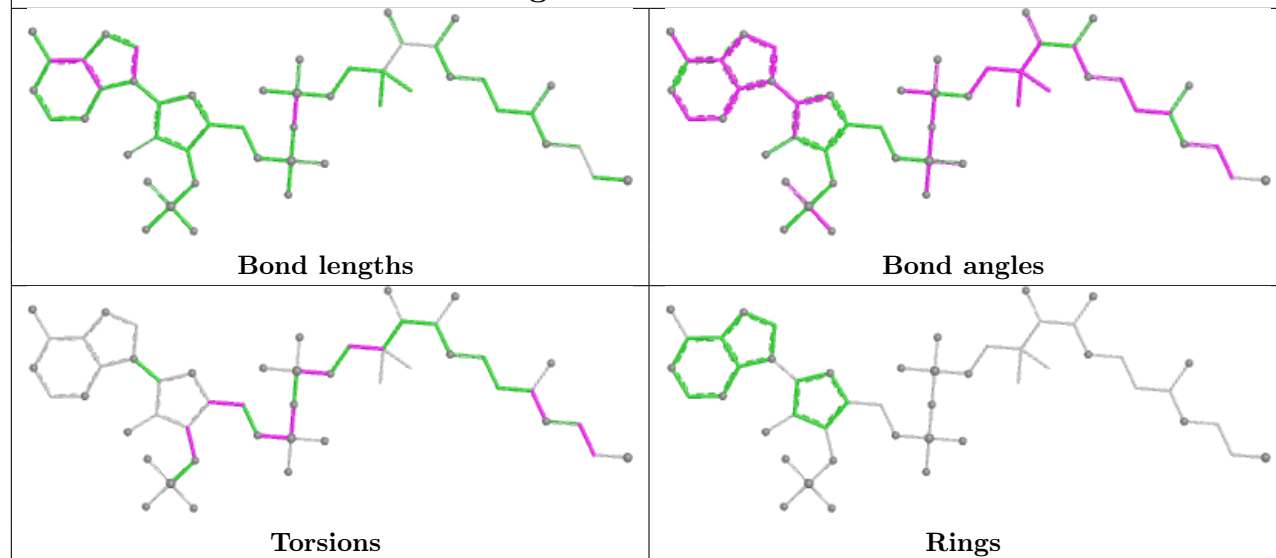
Ligand COA C 502

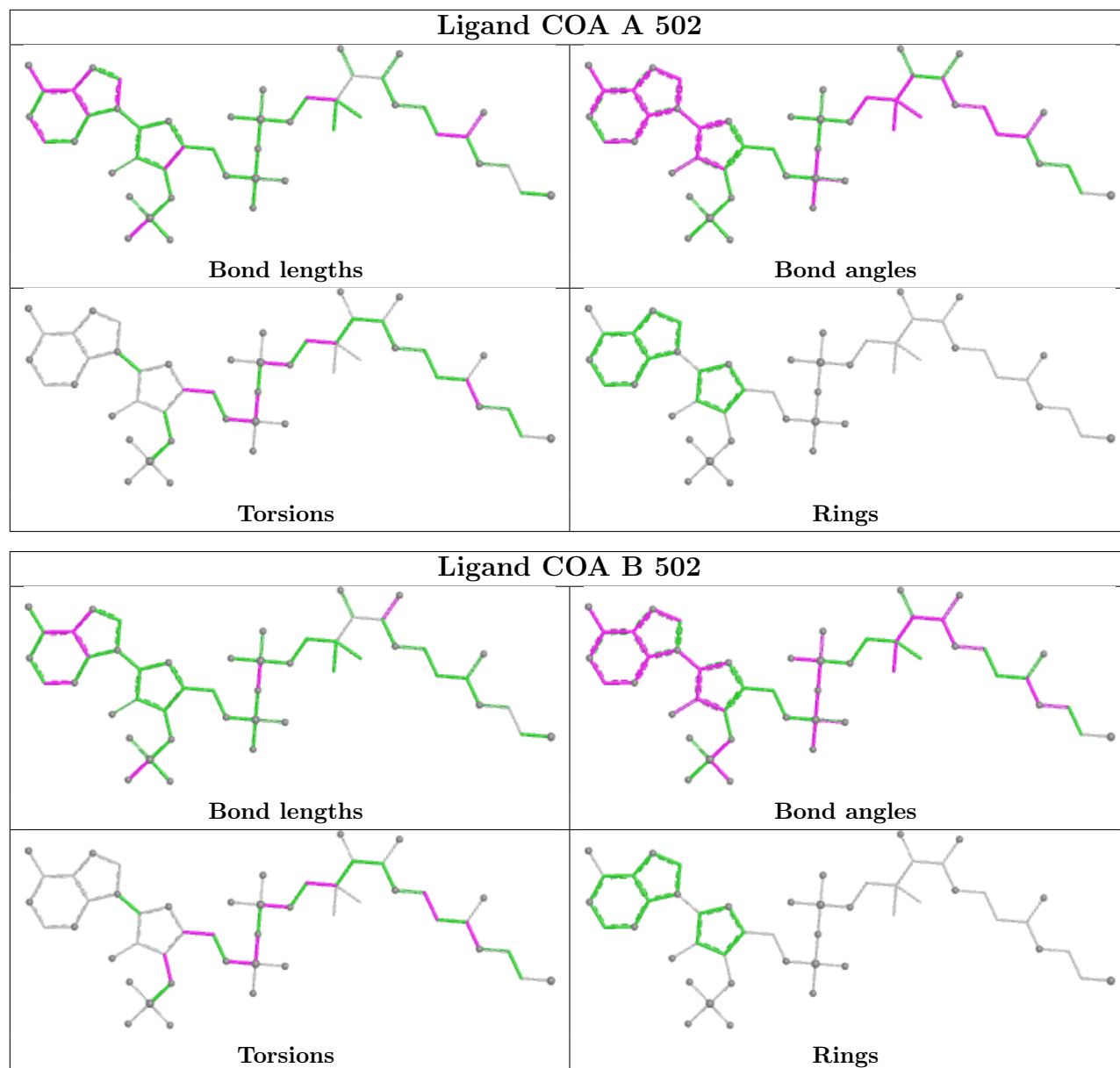


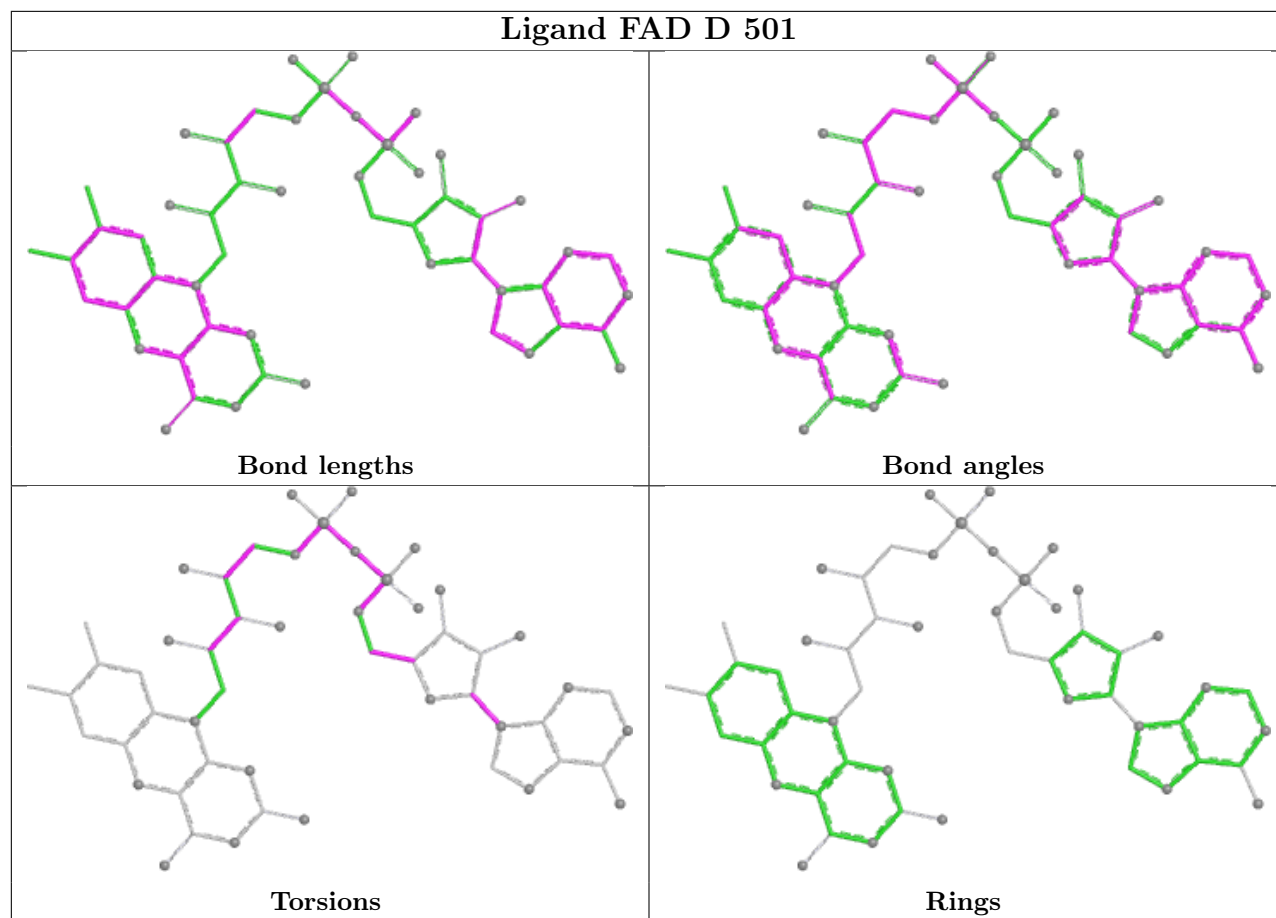
Ligand FAD C 501



Ligand COA D 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	443/443 (100%)	-0.11	11 (2%) 58 48	48, 66, 92, 140	0
1	B	443/443 (100%)	-0.04	12 (2%) 56 47	46, 68, 94, 139	0
1	C	443/443 (100%)	-0.14	7 (1%) 70 62	46, 67, 92, 141	0
1	D	443/443 (100%)	-0.09	8 (1%) 67 59	46, 68, 93, 140	0
All	All	1772/1772 (100%)	-0.10	38 (2%) 63 54	46, 67, 93, 141	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.8
1	B	88	LEU	4.7
1	A	1	MET	4.6
1	B	87	GLU	4.3
1	C	1	MET	4.1
1	B	86	TYR	3.8
1	B	1	MET	3.8
1	A	88	LEU	3.6
1	C	2	GLY	3.6
1	C	88	LEU	3.6
1	A	86	TYR	3.3
1	A	91	LEU	3.2
1	A	92	THR	3.0
1	A	440	GLN	2.9
1	D	443	ARG	2.8
1	A	443	ARG	2.7
1	B	89	ARG	2.6
1	C	317	GLU	2.6
1	C	86	TYR	2.5
1	B	91	LEU	2.4
1	D	88	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	221	ARG	2.3
1	D	2	GLY	2.3
1	D	86	TYR	2.3
1	D	442	ALA	2.2
1	B	415	GLU	2.2
1	B	362	ASP	2.2
1	B	3	LYS	2.2
1	B	443	ARG	2.1
1	D	78	ARG	2.1
1	B	2	GLY	2.1
1	A	442	ALA	2.1
1	D	96	HIS	2.1
1	B	98	GLU	2.1
1	C	97	ALA	2.1
1	A	87	GLU	2.0
1	A	89	ARG	2.0
1	A	2	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.

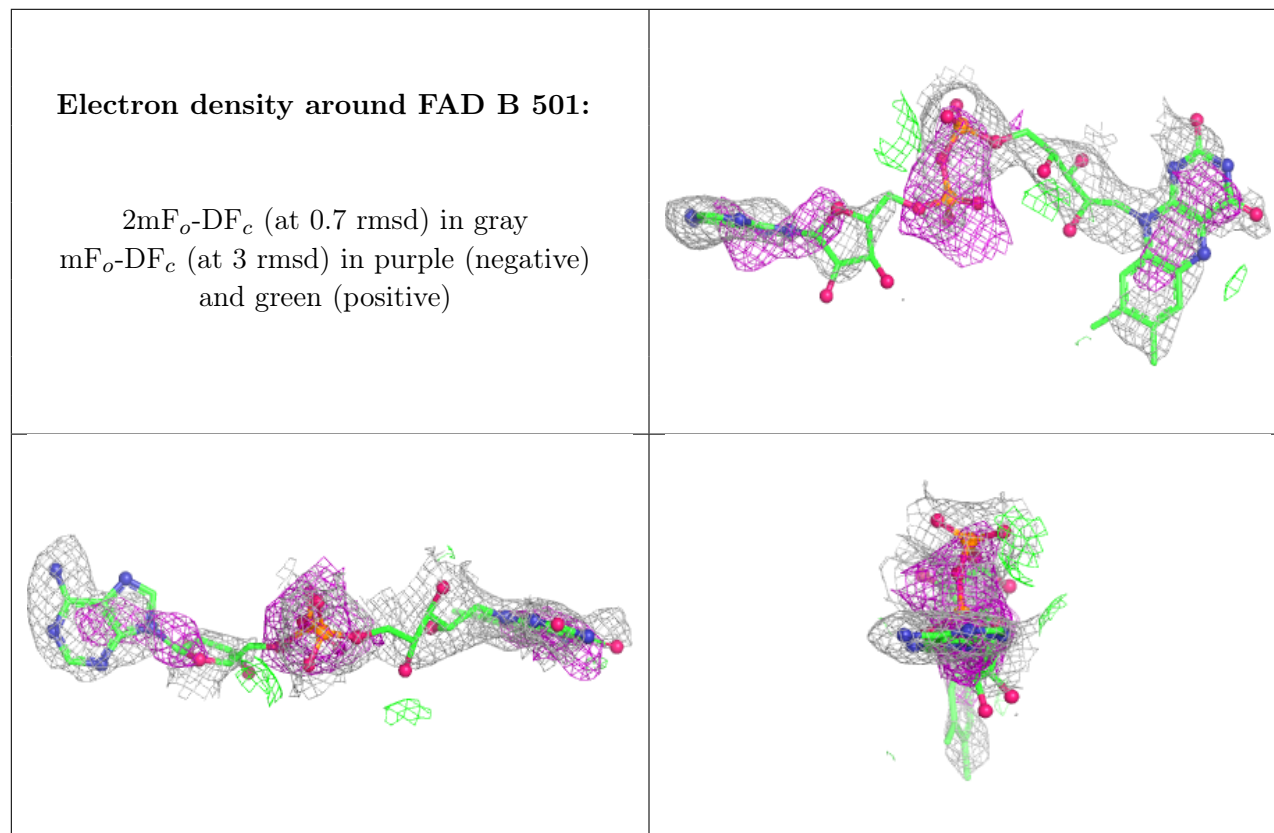
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	501	53/53	0.79	0.18	65,104,124,161	0
2	FAD	A	501	53/53	0.83	0.17	71,103,120,158	0
2	FAD	D	501	53/53	0.86	0.15	71,103,126,159	0
2	FAD	C	501	53/53	0.87	0.15	71,104,124,153	0
3	COA	A	502	48/48	0.96	0.08	53,70,80,106	0
3	COA	B	502	48/48	0.96	0.07	57,68,79,115	0

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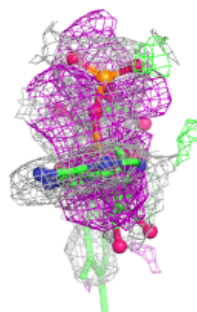
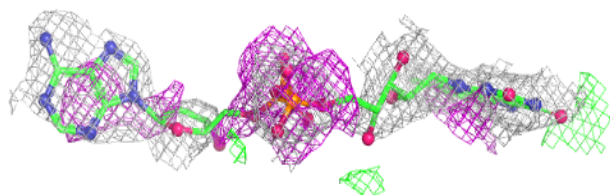
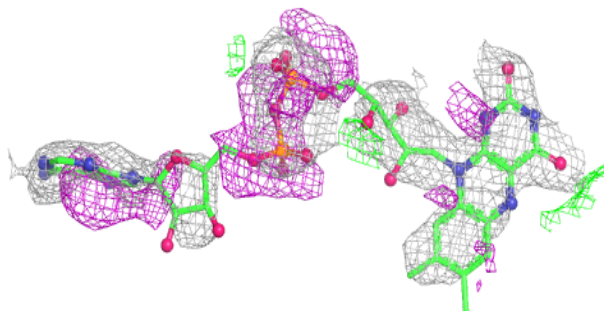
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	COA	C	502	48/48	0.96	0.07	56,69,82,121	0
3	COA	D	502	48/48	0.96	0.07	57,69,84,119	0

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

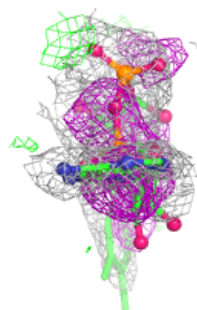
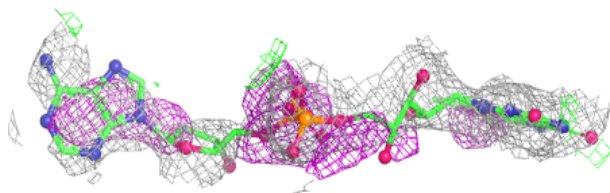
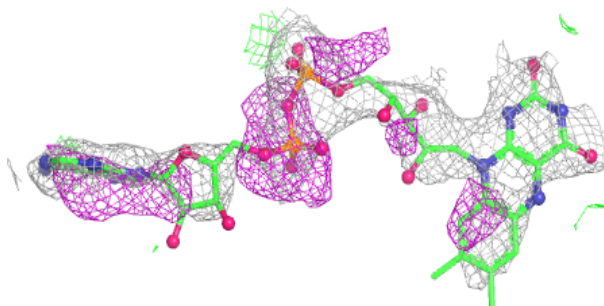


Electron density around FAD A 501:

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

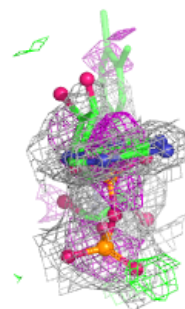
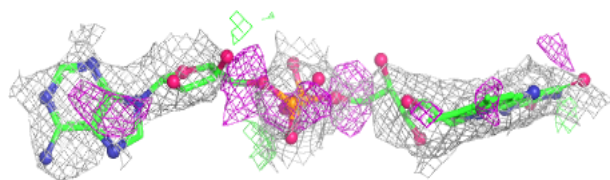
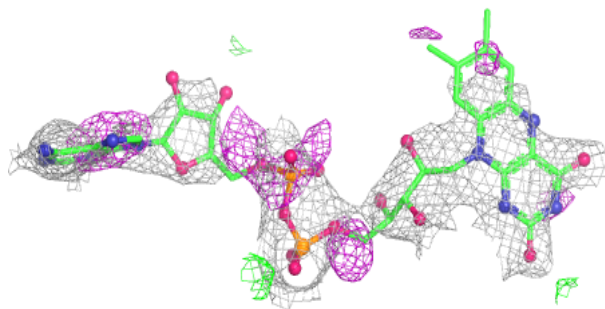
**Electron density around FAD D 501:**

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

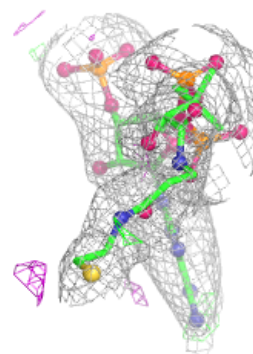
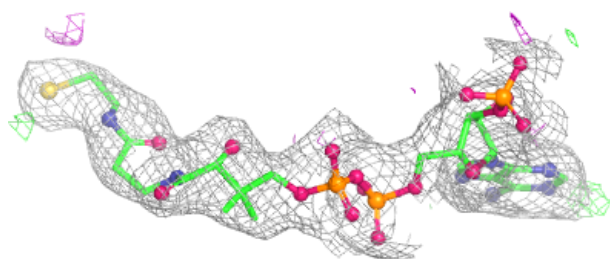
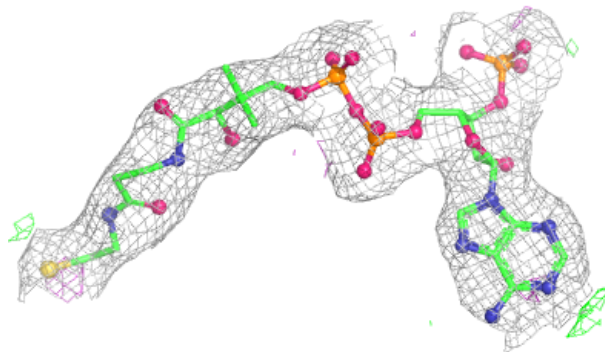


Electron density around FAD C 501:

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

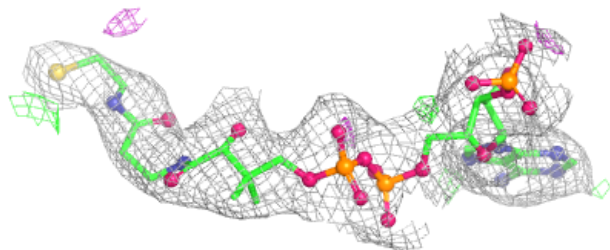
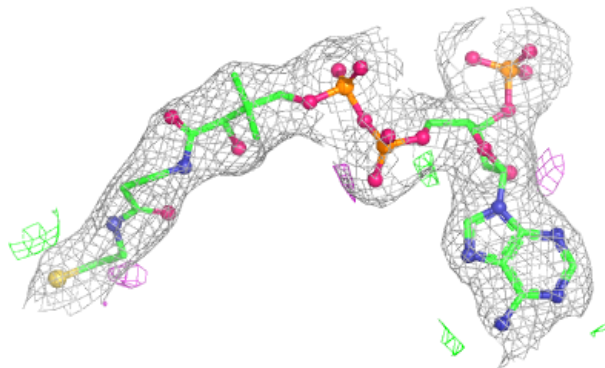
**Electron density around COA A 502:**

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

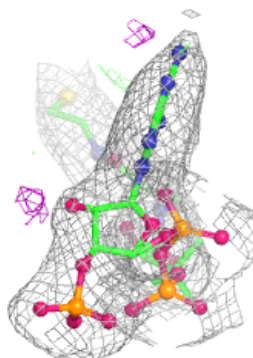
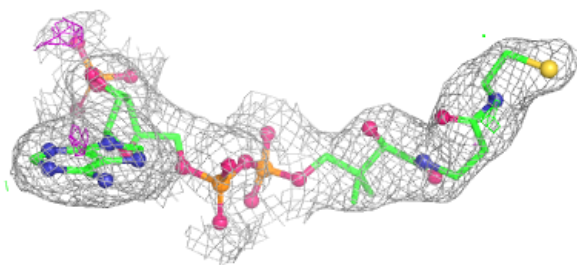
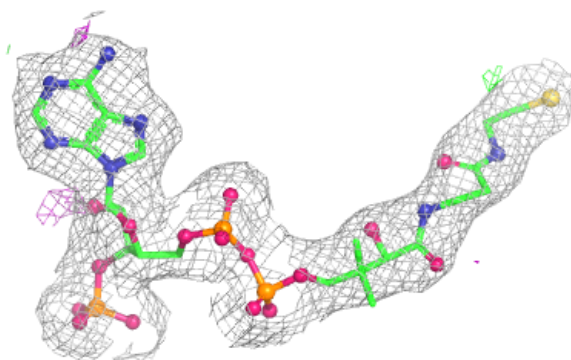


Electron density around COA B 502:

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

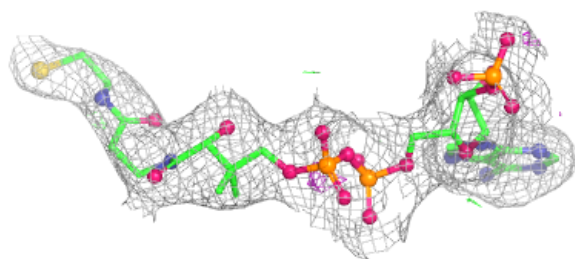
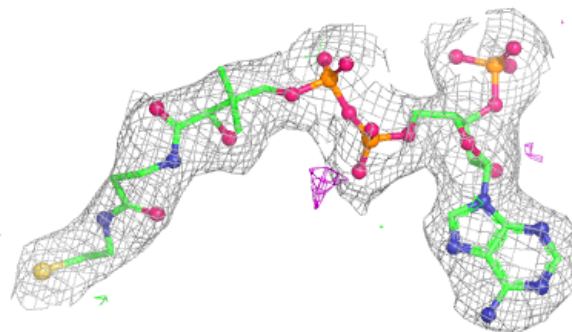
**Electron density around COA C 502:**

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



Electron density around COA 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.