



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 AM UTC

PDB ID : 6RVH / pdb_00006rvh
Title : NADH-dependent Coenzyme A Disulfide Reductase soaked with Menadione
Authors : Koepke, J.; Preu, J.
Deposited on : 2019-05-31
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

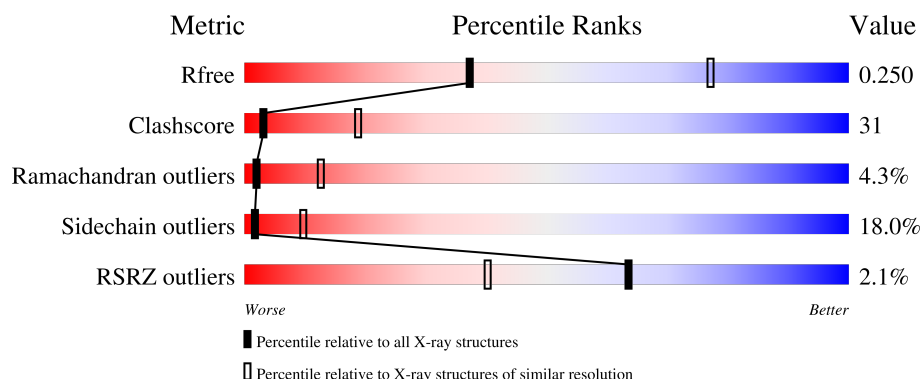
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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
4	VK3	D	503	-	-	-	X

2 Entry composition [i](#)

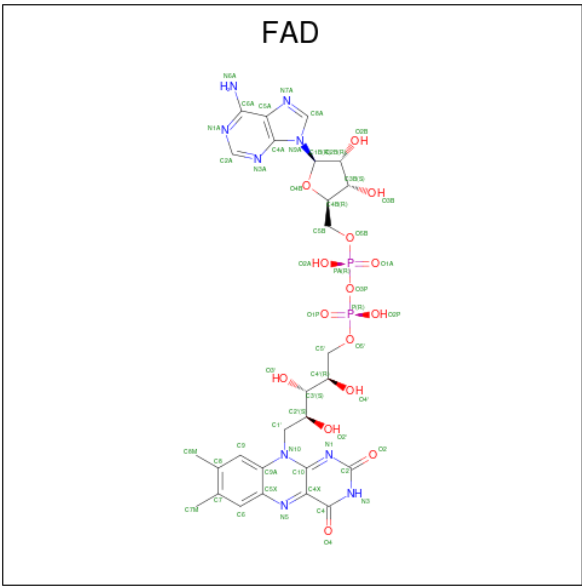
There are 5 unique types of molecules in this entry. The entry contains 14105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).



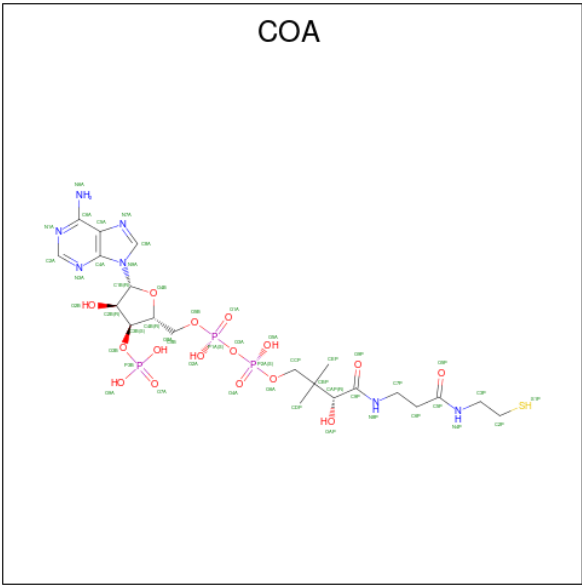
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
2	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

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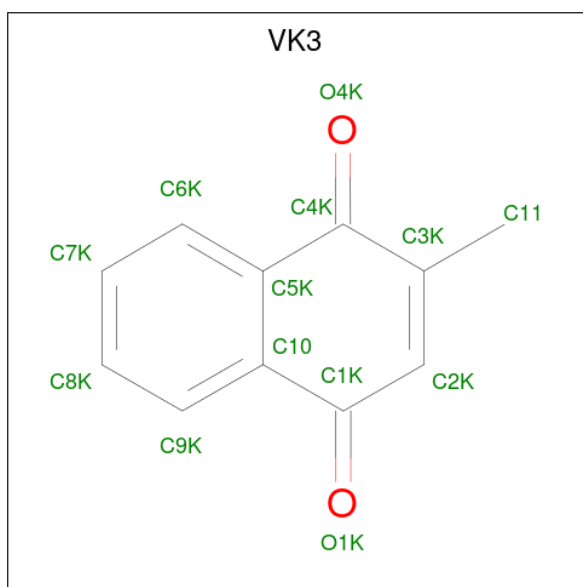
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

- Molecule 4 is MENADIONE (CCD ID: VK3) (formula: C₁₁H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	11	2		
4	B	1	Total	C	O	0	0
			13	11	2		
4	C	1	Total	C	O	0	0
			13	11	2		
4	D	1	Total	C	O	0	0
			13	11	2		

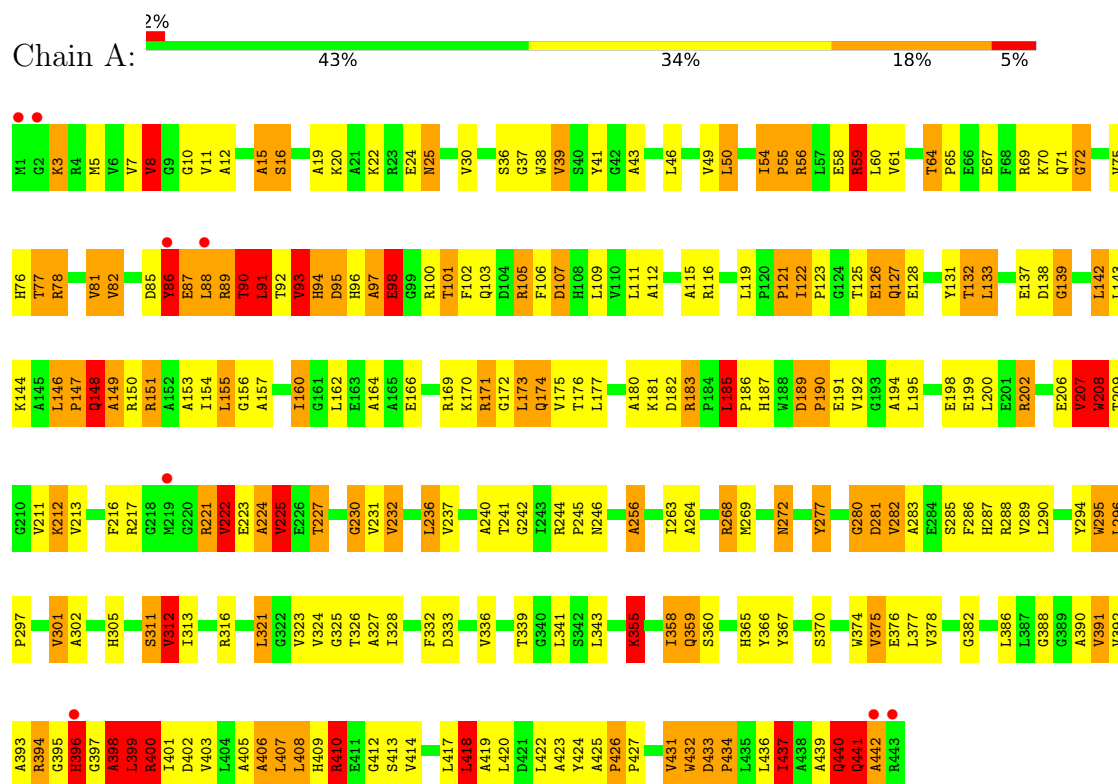
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	35	Total	O	0	0
			35	35		
5	C	36	Total	O	0	0
			36	36		
5	D	30	Total	O	0	0
			30	30		

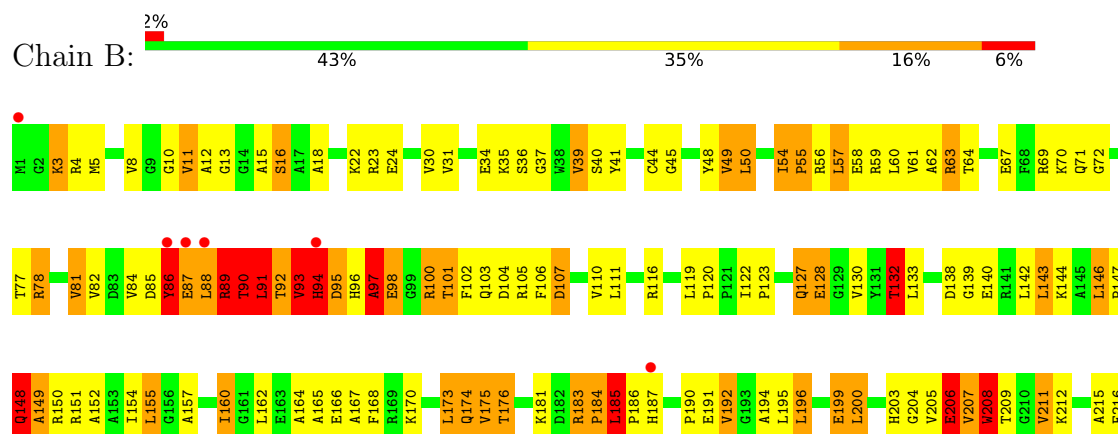
3 Residue-property plots

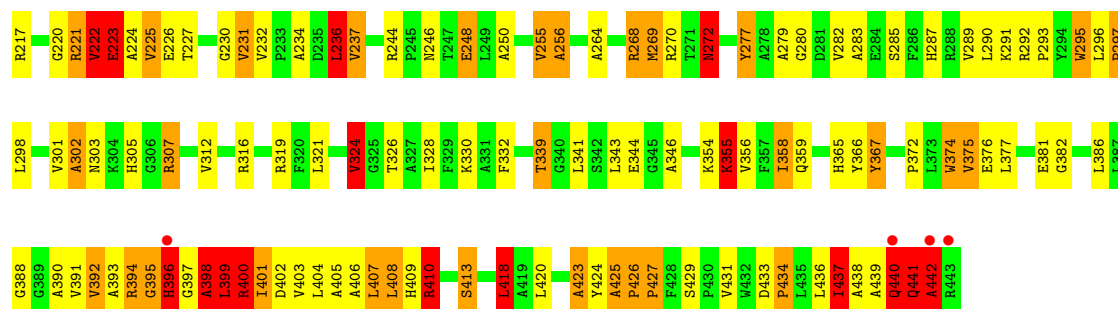
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: NADH oxidase

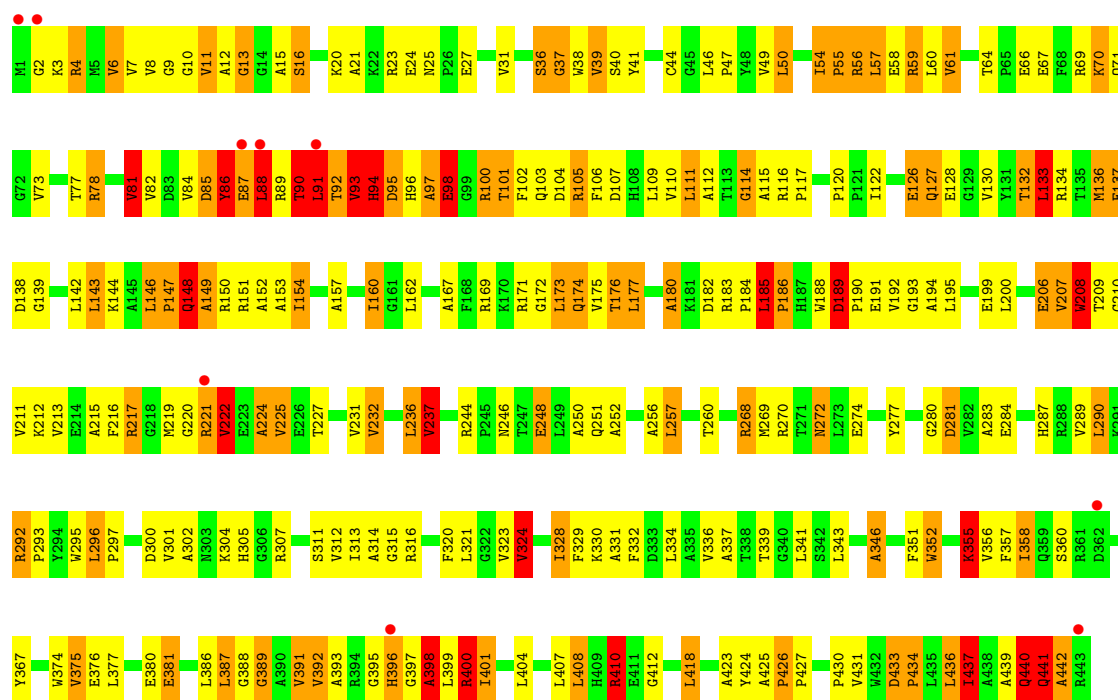


• Molecule 1: NADH oxidase

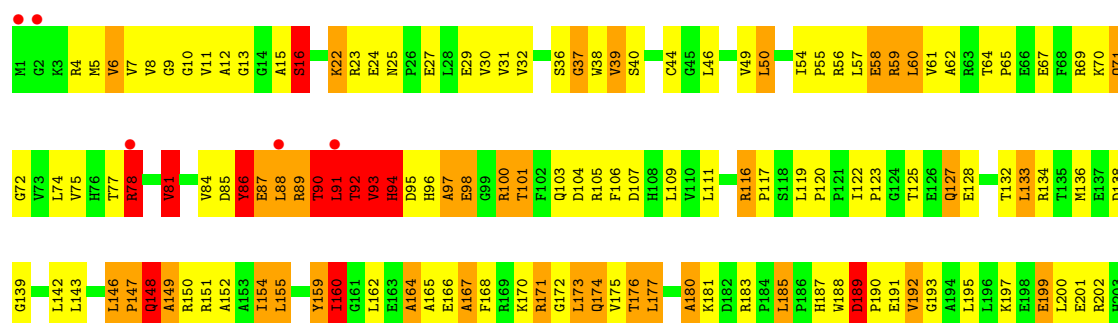


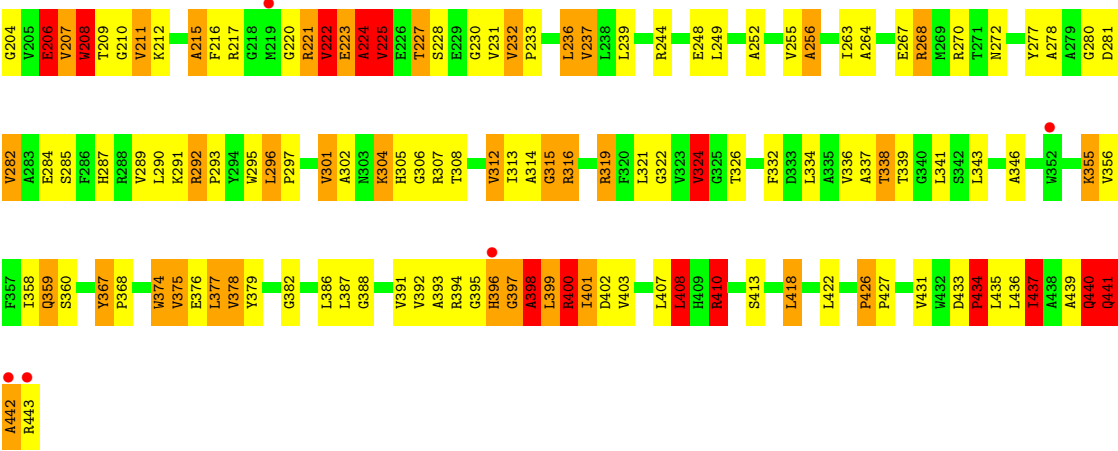


● Molecule 1: NADH oxidase



● 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	159.95Å 159.95Å 255.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.35 – 3.00 58.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (58.35-3.00) 95.0 (58.35-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.29	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.215 , 0.259 0.207 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14105	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: COA, FAD, VK3

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	2.13	107/3451 (3.1%)	1.91	106/4686 (2.3%)
1	B	1.97	75/3451 (2.2%)	1.92	108/4686 (2.3%)
1	C	1.98	73/3450 (2.1%)	1.87	102/4683 (2.2%)
1	D	1.92	61/3449 (1.8%)	1.92	128/4683 (2.7%)
All	All	2.00	316/13801 (2.3%)	1.91	444/18738 (2.4%)

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	5
1	D	0	6
All	All	0	24

All (316) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ILE	CA-CB	-14.26	1.43	1.54
1	B	93	VAL	CA-CB	12.88	1.72	1.54
1	A	406	ALA	CA-CB	-12.38	1.33	1.53
1	A	437	ILE	CA-CB	12.37	1.70	1.54
1	D	396	HIS	C-O	12.21	1.40	1.24
1	B	398	ALA	CA-CB	-12.06	1.33	1.53
1	A	378	VAL	CA-CB	11.78	1.69	1.54
1	D	93	VAL	CA-CB	11.65	1.70	1.54
1	B	438	ALA	CA-CB	-11.56	1.33	1.53
1	A	440	GLN	C-O	11.35	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	HIS	C-O	10.87	1.38	1.24
1	A	398	ALA	CA-CB	-10.10	1.36	1.53
1	C	396	HIS	C-O	10.03	1.37	1.24
1	D	441	GLN	CA-C	9.81	1.66	1.52
1	B	396	HIS	C-O	9.70	1.36	1.24
1	A	87	GLU	CA-C	9.51	1.68	1.53
1	B	264	ALA	CA-CB	-9.30	1.38	1.53
1	A	156	GLY	C-O	-9.30	1.11	1.23
1	D	293	PRO	C-O	9.25	1.34	1.23
1	C	337	ALA	CA-CB	-9.25	1.39	1.53
1	D	96	HIS	CA-C	9.19	1.64	1.52
1	C	87	GLU	CA-C	9.18	1.67	1.53
1	A	390	ALA	CA-CB	-9.14	1.36	1.54
1	A	399	LEU	N-CA	9.09	1.57	1.46
1	B	437	ILE	CA-CB	9.05	1.65	1.54
1	A	264	ALA	CA-CB	-8.99	1.40	1.53
1	D	395	GLY	C-O	-8.70	1.12	1.23
1	B	398	ALA	CA-C	8.64	1.64	1.52
1	A	112	ALA	CA-C	-8.55	1.43	1.53
1	B	87	GLU	CA-C	8.53	1.66	1.53
1	C	441	GLN	CA-C	8.43	1.64	1.52
1	B	297	PRO	CA-C	-8.40	1.44	1.53
1	B	255	VAL	CA-CB	-8.32	1.43	1.54
1	B	440	GLN	C-O	8.32	1.34	1.24
1	A	408	LEU	CA-CB	-8.25	1.40	1.53
1	C	120	PRO	CA-C	8.24	1.57	1.52
1	C	215	ALA	CA-CB	-8.21	1.39	1.53
1	A	77	THR	CA-CB	-8.15	1.39	1.53
1	A	289	VAL	CA-CB	-8.06	1.44	1.54
1	D	97	ALA	CA-CB	8.05	1.67	1.53
1	A	208	TRP	CA-C	8.03	1.64	1.52
1	A	405	ALA	CA-CB	-8.00	1.40	1.53
1	B	97	ALA	N-CA	7.99	1.56	1.46
1	D	154	ILE	CA-CB	-7.98	1.44	1.54
1	C	185	LEU	CA-C	7.97	1.58	1.53
1	C	290	LEU	CA-C	7.97	1.64	1.52
1	C	7	VAL	CA-CB	-7.79	1.44	1.53
1	A	396	HIS	N-CA	7.73	1.56	1.46
1	A	409	HIS	CA-C	7.73	1.63	1.52
1	C	440	GLN	C-O	7.72	1.33	1.24
1	D	97	ALA	N-CA	7.68	1.56	1.46
1	A	180	ALA	CA-CB	-7.67	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	256	ALA	C-O	7.64	1.33	1.23
1	C	96	HIS	CA-C	7.63	1.62	1.52
1	C	331	ALA	CA-CB	-7.61	1.41	1.53
1	A	43	ALA	CA-CB	-7.58	1.39	1.53
1	C	423	ALA	CA-CB	-7.56	1.42	1.53
1	B	203	HIS	CA-C	-7.53	1.43	1.52
1	B	425	ALA	C-O	-7.42	1.14	1.24
1	D	422	LEU	C-O	7.41	1.33	1.23
1	B	429	SER	CA-C	7.40	1.60	1.52
1	D	6	VAL	CA-CB	-7.37	1.45	1.54
1	D	167	ALA	CA-CB	-7.32	1.42	1.53
1	B	302	ALA	CA-CB	-7.31	1.41	1.53
1	A	109	LEU	CA-C	-7.22	1.44	1.52
1	C	115	ALA	CA-CB	-7.20	1.40	1.54
1	B	167	ALA	CA-CB	-7.18	1.42	1.53
1	A	115	ALA	CA-C	-7.12	1.43	1.52
1	C	283	ALA	C-O	7.11	1.32	1.24
1	B	165	ALA	CA-CB	-7.09	1.42	1.53
1	A	375	VAL	CA-CB	7.08	1.63	1.55
1	C	237	VAL	CA-CB	-7.08	1.45	1.54
1	D	291	LYS	CA-C	7.03	1.62	1.53
1	A	97	ALA	N-CA	6.98	1.55	1.46
1	D	71	GLN	CA-C	-6.97	1.43	1.53
1	D	192	VAL	CA-CB	-6.97	1.46	1.54
1	C	213	VAL	CA-CB	-6.95	1.45	1.54
1	D	322	GLY	C-O	6.93	1.30	1.23
1	B	291	LYS	CA-C	6.92	1.62	1.53
1	B	57	LEU	CA-C	6.88	1.61	1.52
1	C	304	LYS	CA-C	6.88	1.61	1.52
1	D	441	GLN	CA-CB	6.85	1.65	1.53
1	B	407	LEU	C-O	-6.85	1.16	1.24
1	A	8	VAL	CA-C	6.83	1.60	1.53
1	A	286	PHE	C-O	-6.83	1.15	1.24
1	A	126	GLU	CB-CG	6.77	1.72	1.52
1	C	441	GLN	CG-CD	6.76	1.69	1.52
1	B	98	GLU	C-O	6.75	1.31	1.24
1	C	93	VAL	CA-C	6.75	1.61	1.52
1	D	87	GLU	CA-C	6.69	1.63	1.53
1	A	164	ALA	CA-CB	-6.68	1.43	1.53
1	A	407	LEU	CA-C	-6.66	1.44	1.52
1	D	437	ILE	CA-CB	6.66	1.62	1.54
1	B	155	LEU	CA-C	6.66	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	ALA	CA-CB	-6.66	1.43	1.53
1	C	167	ALA	CA-CB	-6.65	1.43	1.53
1	D	278	ALA	CA-CB	-6.64	1.42	1.53
1	B	164	ALA	CA-C	6.64	1.61	1.52
1	D	120	PRO	C-O	6.63	1.30	1.24
1	C	70	LYS	CA-C	6.61	1.61	1.52
1	A	400	ARG	CA-C	6.58	1.62	1.52
1	A	225	VAL	CA-CB	6.56	1.63	1.54
1	C	9	GLY	C-O	-6.52	1.15	1.23
1	C	356	VAL	CA-CB	6.50	1.64	1.54
1	D	120	PRO	CA-C	6.48	1.56	1.52
1	A	157	ALA	CA-CB	-6.48	1.42	1.53
1	A	313	ILE	CA-CB	6.46	1.62	1.54
1	C	97	ALA	N-CA	6.46	1.54	1.46
1	C	281	ASP	CA-C	-6.45	1.43	1.52
1	C	375	VAL	CA-CB	6.44	1.62	1.55
1	D	224	ALA	CA-CB	-6.41	1.45	1.53
1	D	346	ALA	CA-CB	6.41	1.63	1.53
1	A	417	LEU	C-O	-6.41	1.16	1.24
1	B	200	LEU	C-O	6.40	1.31	1.24
1	D	338	THR	CA-C	6.40	1.60	1.52
1	C	400	ARG	CA-C	6.38	1.61	1.52
1	B	31	VAL	CA-CB	6.37	1.63	1.54
1	B	184	PRO	C-O	6.36	1.31	1.23
1	A	151	ARG	CA-C	6.36	1.59	1.52
1	C	85	ASP	C-O	-6.34	1.15	1.24
1	B	420	LEU	CA-C	-6.33	1.44	1.52
1	D	39	VAL	CA-C	6.32	1.60	1.52
1	B	442	ALA	CA-C	6.31	1.61	1.52
1	A	72	GLY	C-O	6.29	1.33	1.24
1	B	30	VAL	C-O	6.29	1.31	1.24
1	B	324	VAL	C-O	-6.28	1.16	1.24
1	B	279	ALA	CA-C	6.26	1.60	1.52
1	C	401	ILE	C-O	-6.23	1.16	1.24
1	C	112	ALA	CA-CB	-6.22	1.47	1.53
1	D	16	SER	C-O	6.17	1.31	1.24
1	C	143	LEU	CA-C	-6.14	1.44	1.52
1	B	355	LYS	CA-C	6.13	1.60	1.52
1	A	426	PRO	C-O	-6.13	1.17	1.24
1	A	202	ARG	C-O	-6.11	1.16	1.24
1	A	256	ALA	CA-CB	-6.11	1.43	1.53
1	B	185	LEU	C-O	-6.10	1.21	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	390	ALA	CA-CB	-6.09	1.42	1.54
1	D	324	VAL	CA-CB	-6.08	1.47	1.54
1	C	396	HIS	N-CA	6.08	1.54	1.46
1	C	250	ALA	CA-C	6.05	1.60	1.52
1	B	440	GLN	CD-NE2	6.02	1.45	1.33
1	C	154	ILE	CA-CB	-6.00	1.47	1.54
1	D	377	LEU	CA-C	5.96	1.59	1.52
1	A	192	VAL	CA-CB	-5.96	1.47	1.54
1	A	7	VAL	CA-CB	-5.96	1.46	1.53
1	A	155	LEU	CA-C	-5.93	1.45	1.52
1	A	283	ALA	CA-CB	-5.92	1.44	1.53
1	A	97	ALA	CA-CB	5.91	1.63	1.53
1	C	207	VAL	CA-CB	5.90	1.61	1.53
1	B	86	TYR	CB-CG	5.90	1.64	1.51
1	A	98	GLU	N-CA	5.88	1.53	1.46
1	D	431	VAL	C-O	-5.88	1.17	1.24
1	C	232	VAL	C-O	-5.88	1.17	1.24
1	D	32	VAL	CA-CB	5.88	1.61	1.54
1	A	378	VAL	CA-C	-5.87	1.45	1.52
1	A	294	TYR	C-O	-5.85	1.16	1.23
1	D	398	ALA	N-CA	5.84	1.53	1.46
1	A	433	ASP	CA-C	5.83	1.59	1.53
1	C	186	PRO	CA-C	-5.83	1.41	1.52
1	C	13	GLY	C-O	5.83	1.30	1.23
1	A	393	ALA	CA-CB	-5.82	1.43	1.53
1	B	91	LEU	N-CA	5.82	1.53	1.46
1	A	82	VAL	CA-CB	-5.78	1.46	1.54
1	A	301	VAL	CA-CB	5.77	1.62	1.54
1	A	156	GLY	CA-C	-5.76	1.43	1.51
1	D	284	GLU	CA-C	-5.75	1.45	1.52
1	A	160	ILE	CA-C	-5.75	1.46	1.52
1	C	93	VAL	CA-CB	5.74	1.62	1.54
1	C	389	GLY	C-O	5.74	1.30	1.24
1	C	180	ALA	CA-CB	-5.71	1.44	1.53
1	D	7	VAL	CA-C	5.71	1.60	1.52
1	C	97	ALA	CA-CB	5.70	1.63	1.53
1	D	224	ALA	CA-C	-5.70	1.48	1.52
1	A	323	VAL	CA-CB	-5.69	1.46	1.54
1	C	355	LYS	CA-C	-5.68	1.45	1.52
1	B	168	PHE	C-O	5.68	1.30	1.24
1	D	164	ALA	CA-CB	5.67	1.62	1.53
1	A	305	HIS	CA-C	-5.66	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	437	ILE	CA-CB	5.66	1.60	1.54
1	C	391	VAL	CA-C	-5.66	1.45	1.52
1	B	48	TYR	CA-C	5.64	1.60	1.52
1	C	355	LYS	C-O	-5.63	1.17	1.23
1	B	89	ARG	C-O	5.63	1.31	1.24
1	A	187	HIS	CA-C	-5.63	1.44	1.52
1	B	289	VAL	C-O	5.61	1.29	1.23
1	C	283	ALA	CA-CB	-5.61	1.43	1.53
1	A	375	VAL	CA-C	-5.60	1.45	1.52
1	B	396	HIS	N-CA	5.60	1.53	1.46
1	D	337	ALA	CA-CB	-5.59	1.45	1.53
1	A	30	VAL	CA-CB	5.58	1.61	1.54
1	C	21	ALA	CA-CB	5.58	1.62	1.53
1	A	112	ALA	CA-CB	-5.58	1.47	1.53
1	B	326	THR	C-O	5.57	1.30	1.23
1	D	326	THR	CA-CB	-5.57	1.44	1.53
1	A	5	MET	CA-C	-5.56	1.45	1.52
1	D	62	ALA	CA-CB	-5.55	1.45	1.53
1	A	240	ALA	CA-CB	-5.54	1.44	1.53
1	D	304	LYS	N-CA	-5.52	1.39	1.46
1	D	152	ALA	CA-CB	-5.51	1.45	1.53
1	B	222	VAL	CA-CB	5.51	1.61	1.54
1	A	183	ARG	C-O	-5.51	1.18	1.24
1	A	109	LEU	C-O	5.50	1.30	1.24
1	C	86	TYR	CB-CG	5.50	1.63	1.51
1	C	130	VAL	CA-CB	-5.50	1.47	1.54
1	B	18	ALA	CA-CB	-5.49	1.44	1.53
1	C	132	THR	CA-C	-5.49	1.46	1.52
1	C	6	VAL	CA-CB	-5.48	1.47	1.54
1	D	338	THR	CA-CB	-5.48	1.45	1.53
1	A	327	ALA	C-O	-5.43	1.17	1.23
1	B	282	VAL	CA-C	5.43	1.59	1.53
1	B	130	VAL	CA-CB	-5.42	1.47	1.54
1	C	122	ILE	CA-CB	-5.42	1.50	1.54
1	A	121	PRO	CA-C	-5.42	1.47	1.53
1	A	425	ALA	CA-CB	-5.41	1.44	1.53
1	A	91	LEU	N-CA	5.41	1.53	1.46
1	C	56	ARG	C-O	-5.41	1.17	1.24
1	A	59	ARG	C-O	-5.40	1.17	1.24
1	A	311	SER	CA-C	5.40	1.59	1.52
1	B	97	ALA	CA-CB	5.40	1.62	1.53
1	B	426	PRO	C-O	-5.39	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	THR	CA-CB	-5.39	1.44	1.53
1	C	328	ILE	CA-CB	-5.39	1.45	1.55
1	A	312	VAL	C-O	-5.38	1.17	1.24
1	A	359	GLN	CA-CB	-5.38	1.45	1.53
1	B	413	SER	CA-C	-5.37	1.45	1.52
1	C	105	ARG	CA-C	-5.36	1.46	1.52
1	B	425	ALA	CA-CB	-5.36	1.45	1.53
1	A	441	GLN	CA-C	5.35	1.59	1.52
1	D	16	SER	CA-C	5.35	1.60	1.52
1	B	208	TRP	CG-CD1	5.34	1.50	1.36
1	A	76	HIS	CA-C	-5.34	1.47	1.53
1	D	398	ALA	CA-CB	-5.34	1.44	1.53
1	A	194	ALA	CA-CB	-5.33	1.45	1.53
1	D	378	VAL	CA-CB	-5.32	1.47	1.54
1	A	25	ASN	C-O	-5.32	1.18	1.24
1	C	401	ILE	CA-CB	5.31	1.61	1.54
1	B	187	HIS	C-O	-5.31	1.17	1.24
1	B	303	ASN	C-O	-5.31	1.18	1.24
1	D	39	VAL	C-O	5.30	1.29	1.23
1	B	374	TRP	CA-CB	-5.30	1.45	1.53
1	A	256	ALA	C-O	5.30	1.30	1.23
1	A	295	TRP	CA-CB	5.29	1.61	1.53
1	A	295	TRP	CA-C	-5.29	1.46	1.52
1	C	437	ILE	CA-C	5.29	1.59	1.52
1	B	440	GLN	CA-CB	5.28	1.62	1.53
1	B	152	ALA	C-O	5.28	1.29	1.23
1	B	49	VAL	C-O	5.28	1.30	1.24
1	B	236	LEU	C-O	5.27	1.29	1.24
1	D	264	ALA	CA-C	-5.27	1.46	1.52
1	D	316	ARG	C-O	-5.26	1.17	1.23
1	C	252	ALA	CA-CB	5.26	1.61	1.53
1	A	313	ILE	CA-C	-5.26	1.46	1.52
1	C	425	ALA	CA-CB	-5.26	1.45	1.53
1	D	401	ILE	CA-C	-5.26	1.45	1.52
1	A	86	TYR	CB-CG	5.25	1.63	1.51
1	B	175	VAL	CA-CB	-5.25	1.47	1.54
1	A	115	ALA	CA-CB	-5.25	1.44	1.53
1	A	212	LYS	C-O	-5.24	1.17	1.24
1	C	194	ALA	CA-CB	-5.24	1.45	1.53
1	D	168	PHE	CA-C	-5.24	1.46	1.52
1	A	333	ASP	CA-C	-5.23	1.45	1.52
1	A	326	THR	CA-CB	5.22	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	VAL	CA-C	-5.21	1.46	1.52
1	D	78	ARG	NE-CZ	5.21	1.38	1.33
1	A	391	VAL	CA-CB	5.20	1.62	1.54
1	A	15	ALA	CA-C	5.20	1.60	1.52
1	B	250	ALA	CA-C	-5.20	1.46	1.52
1	C	111	LEU	CA-C	5.20	1.59	1.52
1	C	157	ALA	CA-CB	-5.20	1.44	1.53
1	A	440	GLN	CD-NE2	5.20	1.44	1.33
1	C	11	VAL	CA-CB	-5.19	1.48	1.54
1	B	11	VAL	CA-CB	-5.17	1.47	1.54
1	B	291	LYS	CE-NZ	5.17	1.64	1.49
1	D	215	ALA	CA-CB	-5.16	1.45	1.53
1	A	213	VAL	CA-CB	-5.15	1.47	1.54
1	A	153	ALA	C-O	-5.14	1.17	1.24
1	D	180	ALA	CA-CB	-5.14	1.45	1.53
1	D	393	ALA	CA-CB	-5.14	1.45	1.53
1	B	358	ILE	C-O	5.14	1.30	1.23
1	D	399	LEU	N-CA	5.13	1.56	1.46
1	D	160	ILE	CA-CB	5.12	1.59	1.54
1	B	392	VAL	CA-C	-5.12	1.46	1.52
1	A	414	VAL	CA-CB	-5.11	1.47	1.54
1	C	268	ARG	NE-CZ	5.11	1.38	1.33
1	D	228	SER	CA-C	5.11	1.59	1.52
1	C	2	GLY	C-O	5.11	1.30	1.23
1	C	153	ALA	C-O	-5.11	1.18	1.24
1	B	48	TYR	C-O	5.10	1.30	1.24
1	B	277	TYR	CA-C	5.10	1.59	1.53
1	B	205	VAL	CA-CB	-5.10	1.48	1.54
1	B	395	GLY	C-O	-5.09	1.18	1.23
1	A	38	TRP	CA-C	-5.09	1.46	1.52
1	A	49	VAL	CA-CB	-5.09	1.47	1.54
1	D	155	LEU	CA-C	5.09	1.59	1.52
1	A	137	GLU	N-CA	-5.09	1.40	1.46
1	A	321	LEU	C-O	-5.09	1.17	1.24
1	C	208	TRP	C-O	-5.08	1.17	1.24
1	B	256	ALA	CA-CB	5.08	1.61	1.53
1	A	242	GLY	C-O	-5.07	1.17	1.23
1	B	56	ARG	CA-C	5.07	1.59	1.52
1	B	295	TRP	C-O	-5.05	1.17	1.24
1	A	46	LEU	CA-C	5.05	1.59	1.52
1	D	9	GLY	C-O	-5.05	1.17	1.23
1	D	408	LEU	C-O	-5.05	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	387	LEU	C-O	-5.04	1.17	1.24
1	A	95	ASP	CA-C	-5.04	1.46	1.52
1	A	224	ALA	CA-CB	-5.03	1.45	1.53
1	A	241	THR	CA-CB	5.02	1.59	1.53
1	A	19	ALA	CA-CB	5.01	1.61	1.53
1	A	245	PRO	CA-C	5.01	1.58	1.52
1	A	296	LEU	CA-C	-5.01	1.46	1.52
1	D	443	ARG	CB-CG	5.01	1.67	1.52
1	C	11	VAL	C-O	-5.01	1.19	1.24
1	A	424	TYR	CA-C	-5.01	1.46	1.52
1	A	397	GLY	CA-C	5.00	1.58	1.51
1	C	351	PHE	C-O	5.00	1.29	1.23

All (444) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	VAL	N-CA-C	-13.13	99.95	112.29
1	D	400	ARG	N-CA-C	-11.25	99.51	113.01
1	B	400	ARG	N-CA-C	-11.11	99.67	113.01
1	C	54	ILE	CA-C-N	10.53	133.00	119.84
1	C	54	ILE	C-N-CA	10.53	133.00	119.84
1	B	13	GLY	N-CA-C	-10.47	99.82	112.49
1	B	95	ASP	N-CA-C	10.15	124.27	109.14
1	A	288	ARG	N-CA-C	10.06	124.81	112.54
1	A	398	ALA	N-CA-C	-9.98	89.55	110.80
1	C	11	VAL	N-CA-C	9.75	119.61	110.74
1	D	160	ILE	N-CA-C	-9.71	99.24	110.21
1	C	146	LEU	CA-C-N	-9.70	110.43	120.03
1	C	146	LEU	C-N-CA	-9.70	110.43	120.03
1	D	396	HIS	O-C-N	9.69	134.89	122.39
1	A	160	ILE	N-CA-C	-9.62	96.13	109.21
1	B	289	VAL	N-CA-C	-9.62	102.53	111.67
1	A	102	PHE	N-CA-C	9.54	122.31	108.86
1	D	396	HIS	CA-C-N	9.19	133.79	122.03
1	D	396	HIS	C-N-CA	9.19	133.79	122.03
1	D	96	HIS	N-CA-C	9.17	123.88	108.20
1	A	396	HIS	O-C-N	9.07	134.10	122.39
1	B	396	HIS	O-C-N	9.04	134.85	122.37
1	D	292	ARG	N-CA-C	9.02	116.10	108.07
1	A	207	VAL	N-CA-C	8.92	119.52	106.85
1	B	54	ILE	CA-C-N	8.88	130.94	119.84
1	B	54	ILE	C-N-CA	8.88	130.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	304	LYS	N-CA-C	-8.76	101.67	111.14
1	C	143	LEU	N-CA-C	-8.76	102.73	113.41
1	C	396	HIS	O-C-N	8.75	133.68	122.39
1	D	201	GLU	N-CA-C	-8.72	100.97	111.69
1	A	95	ASP	N-CA-C	8.68	121.90	108.96
1	D	410	ARG	CA-C-N	-8.66	110.19	122.41
1	D	410	ARG	C-N-CA	-8.66	110.19	122.41
1	C	95	ASP	N-CA-C	8.58	121.92	109.14
1	D	324	VAL	N-CA-C	-8.43	105.11	113.20
1	A	54	ILE	CA-C-N	8.41	130.36	119.84
1	A	54	ILE	C-N-CA	8.41	130.36	119.84
1	B	410	ARG	CA-C-N	-8.40	109.62	122.05
1	B	410	ARG	C-N-CA	-8.40	109.62	122.05
1	D	174	GLN	CA-C-N	-8.39	111.48	123.06
1	D	174	GLN	C-N-CA	-8.39	111.48	123.06
1	B	107	ASP	N-CA-C	-8.33	103.70	114.04
1	D	232	VAL	N-CA-C	8.20	115.67	107.55
1	C	120	PRO	CA-C-O	8.16	127.17	120.73
1	B	395	GLY	N-CA-C	8.08	122.53	111.54
1	D	232	VAL	CA-C-N	-8.04	111.48	119.76
1	D	232	VAL	C-N-CA	-8.04	111.48	119.76
1	D	282	VAL	N-CA-C	-7.97	104.94	112.83
1	C	100	ARG	N-CA-C	7.94	120.58	109.31
1	C	185	LEU	CA-C-N	7.91	127.63	119.56
1	C	185	LEU	C-N-CA	7.91	127.63	119.56
1	A	410	ARG	CA-C-N	-7.88	111.11	122.77
1	A	410	ARG	C-N-CA	-7.88	111.11	122.77
1	A	172	GLY	N-CA-C	7.83	125.73	115.47
1	A	282	VAL	N-CA-C	-7.81	105.10	112.83
1	B	185	LEU	CA-C-N	7.80	127.47	119.82
1	B	185	LEU	C-N-CA	7.80	127.47	119.82
1	B	160	ILE	N-CA-C	-7.78	98.81	109.55
1	B	164	ALA	N-CA-C	7.77	119.38	111.07
1	C	206	GLU	CA-C-N	-7.75	112.57	123.11
1	C	206	GLU	C-N-CA	-7.75	112.57	123.11
1	A	82	VAL	CB-CA-C	-7.71	100.78	111.65
1	D	96	HIS	N-CA-CB	-7.70	97.67	110.37
1	C	189	ASP	CA-C-N	7.65	127.29	119.56
1	C	189	ASP	C-N-CA	7.65	127.29	119.56
1	A	107	ASP	N-CA-C	-7.65	103.79	113.43
1	A	397	GLY	CA-C-N	7.61	136.08	121.54
1	A	397	GLY	C-N-CA	7.61	136.08	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	GLU	N-CA-C	-7.56	102.97	111.14
1	B	394	ARG	N-CA-C	-7.54	102.73	112.23
1	A	122	ILE	CA-C-O	7.50	124.16	119.51
1	D	223	GLU	CA-C-N	-7.45	112.51	121.90
1	D	223	GLU	C-N-CA	-7.45	112.51	121.90
1	A	394	ARG	N-CA-C	-7.44	102.54	111.69
1	A	437	ILE	N-CA-C	-7.43	103.05	110.62
1	B	404	LEU	N-CA-C	-7.34	103.36	111.36
1	B	146	LEU	CA-C-N	-7.32	112.24	119.78
1	B	146	LEU	C-N-CA	-7.32	112.24	119.78
1	D	54	ILE	CA-C-N	7.30	128.97	119.84
1	D	54	ILE	C-N-CA	7.30	128.97	119.84
1	C	174	GLN	CA-C-N	-7.28	111.76	122.68
1	C	174	GLN	C-N-CA	-7.28	111.76	122.68
1	D	146	LEU	CA-C-N	-7.28	112.83	120.03
1	D	146	LEU	C-N-CA	-7.28	112.83	120.03
1	A	133	LEU	CB-CA-C	-7.26	99.04	111.23
1	B	35	LYS	N-CA-C	7.24	119.18	111.28
1	D	224	ALA	N-CA-C	7.19	122.05	111.34
1	D	90	THR	CB-CA-C	-7.17	96.15	110.42
1	D	119	LEU	CA-C-N	-7.17	114.50	119.66
1	D	119	LEU	C-N-CA	-7.17	114.50	119.66
1	A	378	VAL	N-CA-C	-7.12	97.35	107.75
1	D	206	GLU	CA-C-N	-7.10	113.45	123.11
1	D	206	GLU	C-N-CA	-7.10	113.45	123.11
1	A	422	LEU	N-CA-C	7.10	119.69	110.53
1	D	36	SER	CA-C-N	-7.10	109.89	122.16
1	D	36	SER	C-N-CA	-7.10	109.89	122.16
1	B	174	GLN	CA-C-N	-7.09	113.27	123.06
1	B	174	GLN	C-N-CA	-7.09	113.27	123.06
1	D	13	GLY	N-CA-C	-7.08	103.70	112.77
1	C	94	HIS	N-CA-C	-7.03	97.78	109.24
1	A	402	ASP	N-CA-C	-7.02	103.64	111.71
1	C	208	TRP	CA-CB-CG	7.02	126.94	113.60
1	B	437	ILE	CA-CB-CG2	7.00	122.41	110.50
1	C	296	LEU	CA-C-N	7.00	128.59	119.84
1	C	296	LEU	C-N-CA	7.00	128.59	119.84
1	C	91	LEU	CA-CB-CG	7.00	140.79	116.30
1	D	426	PRO	CA-C-N	-7.00	112.98	120.47
1	D	426	PRO	C-N-CA	-7.00	112.98	120.47
1	D	437	ILE	N-CA-CB	6.98	120.03	110.54
1	D	312	VAL	N-CA-C	6.98	117.12	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	GLU	N-CA-C	-6.97	104.04	112.54
1	A	96	HIS	N-CA-C	6.94	120.27	107.99
1	D	81	VAL	CB-CA-C	6.91	119.17	111.08
1	A	119	LEU	N-CA-C	6.90	119.62	109.62
1	C	412	GLY	N-CA-C	-6.89	103.32	112.82
1	B	204	GLY	CA-C-N	-6.87	113.08	122.91
1	B	204	GLY	C-N-CA	-6.87	113.08	122.91
1	D	120	PRO	CA-C-N	6.84	128.39	119.84
1	D	120	PRO	C-N-CA	6.84	128.39	119.84
1	C	410	ARG	N-CA-C	-6.83	101.32	110.55
1	D	160	ILE	CA-C-N	-6.83	108.01	121.41
1	D	160	ILE	C-N-CA	-6.83	108.01	121.41
1	C	90	THR	OG1-CB-CG2	6.81	122.91	109.30
1	B	206	GLU	CA-C-N	-6.79	113.87	123.10
1	B	206	GLU	C-N-CA	-6.79	113.87	123.10
1	B	394	ARG	CA-C-N	6.75	127.20	120.31
1	B	394	ARG	C-N-CA	6.75	127.20	120.31
1	C	336	VAL	N-CA-C	6.73	117.33	107.37
1	A	36	SER	CA-C-N	-6.65	108.61	121.78
1	A	36	SER	C-N-CA	-6.65	108.61	121.78
1	D	185	LEU	CA-C-N	6.65	126.79	119.87
1	D	185	LEU	C-N-CA	6.65	126.79	119.87
1	B	192	VAL	CA-C-O	-6.62	114.20	121.29
1	B	418	LEU	N-CA-C	6.62	118.49	111.28
1	D	393	ALA	N-CA-C	-6.62	99.61	108.74
1	C	182	ASP	N-CA-C	6.61	120.60	112.54
1	A	146	LEU	CA-C-N	-6.61	113.14	120.14
1	A	146	LEU	C-N-CA	-6.61	113.14	120.14
1	D	95	ASP	N-CA-C	6.61	119.22	109.24
1	C	96	HIS	N-CA-CB	-6.60	99.66	110.42
1	C	36	SER	CA-C-N	-6.60	108.48	121.41
1	C	36	SER	C-N-CA	-6.60	108.48	121.41
1	C	127	GLN	N-CA-C	6.59	124.85	110.80
1	B	94	HIS	N-CA-C	-6.59	98.46	109.07
1	B	437	ILE	N-CA-CB	6.58	118.25	110.55
1	A	96	HIS	CA-C-O	-6.56	113.44	120.46
1	B	128	GLU	N-CA-C	6.55	121.48	112.90
1	D	207	VAL	N-CA-C	6.54	117.06	107.37
1	D	410	ARG	N-CA-C	-6.53	102.11	110.53
1	C	397	GLY	N-CA-C	6.50	128.59	113.18
1	C	437	ILE	N-CA-CB	6.49	117.72	110.51
1	D	232	VAL	CA-C-O	6.47	124.17	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	ARG	CA-C-N	6.47	127.92	119.84
1	D	116	ARG	C-N-CA	6.47	127.92	119.84
1	D	204	GLY	CA-C-N	-6.46	114.79	122.93
1	D	204	GLY	C-N-CA	-6.46	114.79	122.93
1	A	440	GLN	O-C-N	6.45	131.17	122.59
1	B	119	LEU	CA-C-N	-6.41	115.04	119.66
1	B	119	LEU	C-N-CA	-6.41	115.04	119.66
1	C	160	ILE	N-CA-C	-6.41	100.49	109.21
1	D	301	VAL	N-CA-C	6.41	117.19	110.72
1	D	91	LEU	CA-CB-CG	6.39	138.65	116.30
1	D	296	LEU	CA-C-N	6.37	127.81	119.84
1	D	296	LEU	C-N-CA	6.37	127.81	119.84
1	B	132	THR	CA-C-N	-6.36	113.52	123.13
1	B	132	THR	C-N-CA	-6.36	113.52	123.13
1	C	410	ARG	CA-C-N	-6.36	112.16	122.34
1	C	410	ARG	C-N-CA	-6.36	112.16	122.34
1	C	300	ASP	N-CA-C	-6.36	104.43	111.36
1	C	257	LEU	N-CA-C	-6.35	99.95	110.17
1	B	160	ILE	CA-C-N	-6.34	108.98	121.41
1	B	160	ILE	C-N-CA	-6.34	108.98	121.41
1	D	422	LEU	N-CA-C	6.34	119.10	110.35
1	C	250	ALA	N-CA-C	6.34	118.19	111.28
1	A	91	LEU	CA-CB-CG	6.32	138.43	116.30
1	D	164	ALA	N-CA-C	6.32	117.83	111.07
1	D	119	LEU	N-CA-C	6.31	118.63	109.04
1	B	96	HIS	CA-C-O	-6.31	113.98	120.54
1	A	174	GLN	CA-C-N	-6.30	112.08	122.67
1	A	174	GLN	C-N-CA	-6.30	112.08	122.67
1	C	324	VAL	N-CA-C	-6.30	107.15	113.20
1	C	397	GLY	CA-C-N	6.29	133.55	121.54
1	C	397	GLY	C-N-CA	6.29	133.55	121.54
1	D	437	ILE	N-CA-C	-6.25	104.25	110.62
1	D	336	VAL	N-CA-C	6.24	116.84	107.80
1	A	333	ASP	N-CA-C	-6.23	105.26	112.92
1	B	367	TYR	CA-C-N	6.23	127.62	119.84
1	B	367	TYR	C-N-CA	6.23	127.62	119.84
1	D	100	ARG	N-CA-C	6.22	118.14	109.31
1	A	390	ALA	CA-C-N	-6.21	113.76	122.71
1	A	390	ALA	C-N-CA	-6.21	113.76	122.71
1	C	232	VAL	N-CA-C	6.20	114.71	107.77
1	C	437	ILE	CA-CB-CG2	6.17	120.98	110.50
1	B	91	LEU	CA-CB-CG	6.14	137.79	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	ALA	CA-C-N	6.11	126.67	120.38
1	B	425	ALA	C-N-CA	6.11	126.67	120.38
1	D	422	LEU	CA-C-O	6.11	128.79	121.88
1	D	91	LEU	N-CA-C	-6.09	97.84	110.80
1	A	187	HIS	N-CA-C	-6.07	105.45	112.92
1	A	208	TRP	CA-CB-CG	6.07	125.14	113.60
1	D	86	TYR	N-CA-C	6.05	123.68	110.80
1	B	397	GLY	N-CA-C	6.04	127.48	113.18
1	B	207	VAL	N-CA-C	6.03	116.30	106.72
1	A	198	GLU	N-CA-C	-6.01	104.65	111.14
1	B	154	ILE	CA-C-N	-6.00	114.44	122.42
1	B	154	ILE	C-N-CA	-6.00	114.44	122.42
1	C	102	PHE	N-CA-C	6.00	116.48	108.38
1	D	292	ARG	CA-C-N	-6.00	113.79	119.85
1	D	292	ARG	C-N-CA	-6.00	113.79	119.85
1	C	160	ILE	CA-C-N	-5.99	109.68	121.41
1	C	160	ILE	C-N-CA	-5.99	109.68	121.41
1	C	114	GLY	N-CA-C	5.97	121.75	111.47
1	C	91	LEU	N-CA-C	-5.97	98.09	110.80
1	D	248	GLU	N-CA-C	-5.97	104.69	111.14
1	C	207	VAL	N-CA-C	5.96	116.19	107.37
1	C	305	HIS	CA-C-N	5.96	126.43	119.94
1	C	305	HIS	C-N-CA	5.96	126.43	119.94
1	D	315	GLY	N-CA-C	5.96	123.88	115.30
1	B	230	GLY	CA-C-N	-5.95	115.19	123.10
1	B	230	GLY	C-N-CA	-5.95	115.19	123.10
1	C	283	ALA	N-CA-C	5.94	119.16	109.59
1	C	82	VAL	CB-CA-C	-5.94	104.45	111.94
1	D	397	GLY	N-CA-C	5.93	119.96	111.12
1	D	375	VAL	CA-C-O	-5.92	113.98	120.43
1	B	63	ARG	NE-CZ-NH1	-5.91	115.59	121.50
1	C	172	GLY	N-CA-C	5.91	123.19	115.40
1	C	110	VAL	N-CA-C	5.90	116.30	107.51
1	C	346	ALA	N-CA-C	-5.90	104.98	111.82
1	A	367	TYR	CA-C-N	5.89	126.23	119.93
1	A	367	TYR	C-N-CA	5.89	126.23	119.93
1	B	395	GLY	CA-C-O	-5.89	116.28	121.58
1	A	190	PRO	CA-C-N	5.88	128.08	120.44
1	A	190	PRO	C-N-CA	5.88	128.08	120.44
1	C	86	TYR	N-CA-C	5.87	123.30	110.80
1	B	282	VAL	CB-CA-C	5.87	119.92	111.88
1	C	352	TRP	CA-C-N	-5.86	114.14	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	352	TRP	C-N-CA	-5.86	114.14	122.94
1	A	432	TRP	CA-C-N	-5.86	112.01	120.51
1	A	432	TRP	C-N-CA	-5.86	112.01	120.51
1	A	224	ALA	N-CA-C	5.86	123.28	110.80
1	A	401	ILE	N-CA-C	-5.85	103.47	111.89
1	C	90	THR	CB-CA-C	-5.84	98.79	110.42
1	D	159	TYR	CB-CA-C	5.84	119.95	110.96
1	D	232	VAL	CB-CA-C	-5.83	104.16	111.04
1	D	374	TRP	CA-C-N	-5.83	114.30	122.75
1	D	374	TRP	C-N-CA	-5.83	114.30	122.75
1	B	248	GLU	N-CA-C	-5.83	104.83	111.07
1	D	97	ALA	N-CA-CB	5.83	120.34	110.49
1	C	98	GLU	CB-CA-C	5.83	119.63	110.19
1	B	211	VAL	CB-CA-C	-5.82	102.15	110.83
1	D	211	VAL	CB-CA-C	-5.82	102.16	110.83
1	B	427	PRO	N-CA-C	5.82	122.12	114.27
1	D	394	ARG	N-CA-C	-5.80	104.92	112.23
1	B	402	ASP	N-CA-C	-5.79	105.31	112.38
1	A	325	GLY	CA-C-O	5.78	125.45	118.86
1	B	96	HIS	N-CA-CB	-5.77	100.85	110.37
1	A	119	LEU	CA-C-N	-5.77	114.44	120.38
1	A	119	LEU	C-N-CA	-5.77	114.44	120.38
1	A	296	LEU	CA-C-N	5.75	127.03	119.84
1	A	296	LEU	C-N-CA	5.75	127.03	119.84
1	A	433	ASP	CA-C-N	5.74	127.02	119.84
1	A	433	ASP	C-N-CA	5.74	127.02	119.84
1	D	382	GLY	CA-C-N	5.74	127.97	120.28
1	D	382	GLY	C-N-CA	5.74	127.97	120.28
1	C	433	ASP	CA-C-N	5.74	127.01	119.84
1	C	433	ASP	C-N-CA	5.74	127.01	119.84
1	B	144	LYS	N-CA-C	-5.72	104.68	111.03
1	D	308	THR	N-CA-C	-5.72	104.66	111.69
1	C	393	ALA	N-CA-C	-5.71	100.26	108.60
1	C	292	ARG	N-CA-C	5.71	113.15	108.07
1	C	426	PRO	N-CA-C	5.71	117.67	110.70
1	D	37	GLY	CA-C-O	5.71	124.60	118.95
1	C	237	VAL	CA-C-N	5.70	131.04	123.00
1	C	237	VAL	C-N-CA	5.70	131.04	123.00
1	A	105	ARG	N-CA-C	-5.68	100.87	109.85
1	D	401	ILE	O-C-N	5.68	127.61	121.87
1	B	307	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	A	185	LEU	CA-C-N	5.67	126.93	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	LEU	C-N-CA	5.67	126.93	119.84
1	D	90	THR	OG1-CB-CG2	5.66	120.63	109.30
1	D	267	GLU	N-CA-C	-5.66	106.33	113.18
1	B	423	ALA	O-C-N	5.65	129.66	123.22
1	D	367	TYR	CA-C-N	5.65	126.90	119.84
1	D	367	TYR	C-N-CA	5.65	126.90	119.84
1	A	418	LEU	N-CA-C	5.65	117.44	111.28
1	A	98	GLU	CA-CB-CG	-5.64	102.83	114.10
1	C	98	GLU	CA-C-O	5.63	126.38	120.36
1	B	40	SER	N-CA-C	5.62	119.15	111.39
1	A	355	LYS	CA-C-N	-5.62	114.62	122.71
1	A	355	LYS	C-N-CA	-5.62	114.62	122.71
1	A	431	VAL	CA-C-O	5.61	126.31	120.25
1	D	147	PRO	CA-C-O	-5.58	114.94	122.08
1	D	29	GLU	N-CA-C	-5.57	100.10	108.96
1	A	91	LEU	N-CA-CB	5.56	119.89	110.49
1	B	396	HIS	CA-C-N	5.55	132.29	121.41
1	B	396	HIS	C-N-CA	5.55	132.29	121.41
1	A	410	ARG	O-C-N	-5.55	115.88	122.65
1	C	437	ILE	N-CA-C	-5.55	104.53	110.36
1	B	223	GLU	CA-C-N	-5.54	110.95	121.54
1	B	223	GLU	C-N-CA	-5.54	110.95	121.54
1	C	185	LEU	CB-CA-C	5.51	115.89	110.71
1	A	280	GLY	CA-C-O	5.51	125.49	120.53
1	A	398	ALA	O-C-N	5.50	129.91	122.59
1	A	426	PRO	CB-CA-C	5.50	117.63	110.92
1	B	392	VAL	O-C-N	5.50	129.12	123.18
1	B	366	TYR	N-CA-C	5.50	119.83	113.18
1	B	102	PHE	N-CA-C	5.49	115.78	108.38
1	B	440	GLN	O-C-N	5.49	129.89	122.59
1	D	6	VAL	N-CA-C	5.48	115.99	107.99
1	A	182	ASP	N-CA-C	5.48	119.22	112.54
1	C	148	GLN	CB-CA-C	-5.47	104.81	111.82
1	D	171	ARG	CG-CD-NE	-5.47	99.96	112.00
1	C	283	ALA	CA-C-O	5.47	126.51	120.71
1	B	399	LEU	N-CA-CB	5.46	119.78	110.50
1	C	395	GLY	N-CA-C	5.46	126.11	113.18
1	A	412	GLY	N-CA-C	-5.45	104.36	113.02
1	C	224	ALA	N-CA-C	5.43	122.37	110.80
1	D	252	ALA	N-CA-C	-5.43	104.60	111.11
1	C	323	VAL	CB-CA-C	-5.42	103.76	111.19
1	C	96	HIS	N-CA-C	5.42	117.56	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	VAL	N-CA-C	5.41	115.68	108.11
1	D	410	ARG	O-C-N	-5.41	116.00	122.65
1	A	339	THR	CA-CB-CG2	5.41	119.69	110.50
1	A	370	SER	N-CA-C	-5.40	101.86	109.96
1	A	394	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	D	147	PRO	CA-C-N	-5.40	114.47	122.35
1	D	147	PRO	C-N-CA	-5.40	114.47	122.35
1	C	4	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	A	183	ARG	CA-C-N	-5.39	114.41	119.85
1	A	183	ARG	C-N-CA	-5.39	114.41	119.85
1	D	22	LYS	N-CA-C	-5.38	105.52	111.71
1	A	8	VAL	N-CA-C	5.38	115.33	108.12
1	A	190	PRO	O-C-N	5.38	129.45	122.24
1	B	183	ARG	CA-C-N	-5.38	114.70	120.03
1	B	183	ARG	C-N-CA	-5.38	114.70	120.03
1	B	199	GLU	N-CA-C	5.38	117.89	111.71
1	C	436	LEU	N-CA-C	5.38	116.82	111.07
1	C	169	ARG	N-CA-C	-5.37	105.50	111.36
1	D	256	ALA	N-CA-C	5.37	118.10	110.10
1	A	147	PRO	N-CA-C	-5.37	102.72	111.68
1	A	382	GLY	CA-C-N	5.36	127.72	120.38
1	A	382	GLY	C-N-CA	5.36	127.72	120.38
1	A	336	VAL	N-CA-C	5.34	115.55	107.80
1	B	82	VAL	CB-CA-C	-5.34	105.40	111.55
1	B	397	GLY	CA-C-N	5.34	131.75	121.54
1	B	397	GLY	C-N-CA	5.34	131.75	121.54
1	B	127	GLN	N-CA-C	5.34	117.77	109.60
1	D	154	ILE	CB-CA-C	-5.33	103.17	110.96
1	B	339	THR	OG1-CB-CG2	-5.33	98.63	109.30
1	C	381	GLU	N-CA-C	5.33	116.78	111.07
1	D	107	ASP	N-CA-C	-5.33	106.71	113.43
1	B	394	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	A	232	VAL	N-CA-C	5.32	113.73	107.77
1	D	152	ALA	N-CA-C	5.32	118.49	109.76
1	D	189	ASP	CA-C-N	5.31	124.92	119.56
1	D	189	ASP	C-N-CA	5.31	124.92	119.56
1	B	346	ALA	N-CA-C	-5.31	105.61	111.71
1	A	171	ARG	N-CA-C	5.30	119.30	113.21
1	C	133	LEU	CB-CA-C	-5.29	102.73	111.51
1	C	398	ALA	CA-C-N	5.29	131.21	121.70
1	C	398	ALA	C-N-CA	5.29	131.21	121.70
1	D	239	LEU	N-CA-C	5.28	116.91	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	174	GLN	N-CA-CB	5.26	118.10	109.95
1	D	94	HIS	N-CA-C	-5.25	100.67	109.24
1	D	375	VAL	CA-C-N	5.25	131.04	122.07
1	D	375	VAL	C-N-CA	5.25	131.04	122.07
1	A	225	VAL	N-CA-CB	5.24	119.88	111.23
1	B	297	PRO	CA-C-O	-5.24	115.57	121.97
1	B	269	MET	CG-SD-CE	5.23	112.41	100.90
1	B	86	TYR	N-CA-C	5.23	121.95	110.80
1	A	98	GLU	CG-CD-OE1	5.23	130.42	118.40
1	A	241	THR	CB-CA-C	-5.23	102.72	111.13
1	D	403	VAL	N-CA-C	-5.23	105.30	111.00
1	C	87	GLU	N-CA-C	5.22	118.69	107.67
1	C	147	PRO	N-CA-C	-5.22	103.58	111.41
1	C	290	LEU	N-CA-C	5.22	119.13	112.87
1	A	281	ASP	CA-C-N	-5.22	114.32	122.09
1	A	281	ASP	C-N-CA	-5.22	114.32	122.09
1	D	284	GLU	N-CA-C	-5.22	102.76	110.48
1	D	89	ARG	O-C-N	5.21	129.52	122.59
1	B	110	VAL	N-CA-CB	5.21	118.02	111.46
1	D	49	VAL	N-CA-C	-5.21	106.06	111.58
1	A	72	GLY	CA-C-N	-5.20	116.36	123.12
1	A	72	GLY	C-N-CA	-5.20	116.36	123.12
1	C	248	GLU	N-CA-CB	5.20	117.61	110.07
1	B	120	PRO	CA-C-N	5.20	126.34	119.84
1	B	120	PRO	C-N-CA	5.20	126.34	119.84
1	A	336	VAL	CA-C-N	-5.20	115.14	122.94
1	A	336	VAL	C-N-CA	-5.20	115.14	122.94
1	D	377	LEU	N-CA-CB	-5.20	102.30	110.77
1	D	98	GLU	N-CA-C	5.19	117.08	108.20
1	D	98	GLU	CB-CA-C	5.18	119.08	110.78
1	C	57	LEU	N-CA-C	5.18	118.38	111.75
1	B	330	LYS	CD-CE-NZ	5.17	128.45	111.90
1	B	303	ASN	N-CA-C	5.16	116.91	111.28
1	A	86	TYR	N-CA-C	5.16	121.79	110.80
1	D	231	VAL	N-CA-C	5.15	115.39	108.17
1	B	426	PRO	N-CA-C	5.15	116.99	110.70
1	D	30	VAL	CB-CA-C	-5.15	104.60	110.73
1	C	231	VAL	CA-C-N	-5.15	117.67	123.02
1	C	231	VAL	C-N-CA	-5.15	117.67	123.02
1	A	137	GLU	N-CA-C	-5.14	105.59	111.14
1	D	98	GLU	CA-CB-CG	-5.14	103.82	114.10
1	D	397	GLY	CA-C-N	5.14	131.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	397	GLY	C-N-CA	5.14	131.35	121.54
1	C	410	ARG	O-C-N	-5.13	117.00	122.85
1	D	96	HIS	CA-C-O	-5.12	115.22	120.54
1	A	437	ILE	CB-CA-C	5.11	119.04	112.14
1	B	152	ALA	N-CA-C	5.11	118.40	110.17
1	A	323	VAL	N-CA-CB	-5.10	106.02	112.60
1	B	429	SER	O-C-N	-5.09	117.87	121.84
1	A	189	ASP	CA-C-N	5.09	124.75	119.56
1	A	189	ASP	C-N-CA	5.09	124.75	119.56
1	A	213	VAL	N-CA-C	5.09	116.07	108.54
1	B	208	TRP	O-C-N	-5.08	116.55	122.96
1	B	143	LEU	CA-C-N	5.08	127.54	120.63
1	B	143	LEU	C-N-CA	5.08	127.54	120.63
1	B	382	GLY	CA-C-N	5.08	127.09	120.28
1	B	382	GLY	C-N-CA	5.08	127.09	120.28
1	D	399	LEU	N-CA-CB	5.08	119.13	110.50
1	A	231	VAL	N-CA-C	5.07	115.16	107.75
1	C	81	VAL	CB-CA-C	5.07	116.71	111.23
1	B	5	MET	CA-C-O	5.07	125.78	120.36
1	A	56	ARG	N-CA-C	5.07	118.07	109.76
1	C	357	PHE	CA-C-N	-5.07	114.68	122.68
1	C	357	PHE	C-N-CA	-5.07	114.68	122.68
1	D	208	TRP	CA-CB-CG	5.06	123.22	113.60
1	A	399	LEU	N-CA-CB	5.06	119.04	110.49
1	B	192	VAL	O-C-N	5.06	127.15	121.94
1	A	437	ILE	CA-CB-CG2	5.05	119.09	110.50
1	C	88	LEU	CB-CA-C	5.05	119.70	110.10
1	D	92	THR	N-CA-C	-5.05	100.04	110.80
1	B	62	ALA	CA-C-O	5.04	126.15	120.00
1	B	405	ALA	CA-C-N	5.03	127.33	120.54
1	B	405	ALA	C-N-CA	5.03	127.33	120.54
1	D	40	SER	N-CA-C	5.02	118.25	111.17
1	B	272	ASN	N-CA-C	5.02	116.75	111.28
1	D	338	THR	N-CA-C	5.02	117.52	110.14
1	D	148	GLN	CB-CA-C	-5.02	104.81	111.63
1	A	230	GLY	N-CA-C	5.01	120.22	112.45
1	B	36	SER	CA-C-N	-5.01	111.59	121.41
1	B	36	SER	C-N-CA	-5.01	111.59	121.41
1	C	248	GLU	N-CA-C	-5.01	105.73	111.14
1	A	64	THR	N-CA-C	-5.00	103.85	110.40

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	GLN	Peptide
1	A	396	HIS	Peptide
1	A	398	ALA	Peptide
1	A	440	GLN	Peptide
1	A	90	THR	Peptide
1	A	91	LEU	Peptide
1	A	93	VAL	Peptide
1	A	98	GLU	Peptide
1	B	396	HIS	Peptide
1	B	398	ALA	Peptide
1	B	440	GLN	Peptide
1	B	90	THR	Peptide
1	B	91	LEU	Peptide
1	C	396	HIS	Peptide
1	C	440	GLN	Peptide
1	C	90	THR	Peptide
1	C	91	LEU	Peptide
1	C	98	GLU	Peptide
1	D	224	ALA	Peptide
1	D	396	HIS	Peptide
1	D	398	ALA	Peptide
1	D	440	GLN	Peptide
1	D	90	THR	Peptide
1	D	91	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3379	0	3407	213	0
1	B	3379	0	3407	229	0
1	C	3378	0	3402	222	0
1	D	3377	0	3402	221	0
2	A	53	0	31	3	0
2	B	53	0	31	5	0
2	C	53	0	31	5	0
2	D	53	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	31	4	0
3	B	48	0	31	10	0
3	C	48	0	30	11	0
3	D	48	0	31	5	0
4	A	13	0	8	4	0
4	B	13	0	8	1	0
4	C	13	0	8	2	0
4	D	13	0	8	2	0
5	A	35	0	0	10	0
5	B	35	0	0	14	0
5	C	36	0	0	25	0
5	D	30	0	0	22	0
All	All	14105	0	13897	872	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 31.

All (872) 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:A:439:ALA:O	1:A:441:GLN:HB2	1.11	1.28
1:D:439:ALA:O	1:D:441:GLN:HB2	1.30	1.28
1:C:439:ALA:O	1:C:441:GLN:HB2	1.21	1.26
1:B:439:ALA:O	1:B:441:GLN:HB2	1.02	1.19
1:A:396:HIS:ND1	1:B:396:HIS:CE1	2.12	1.17
1:A:90:THR:HA	1:A:92:THR:HG21	1.27	1.17
1:D:379:TYR:HA	5:D:606:HOH:O	1.45	1.14
1:B:90:THR:HA	1:B:92:THR:CG2	1.78	1.14
3:C:502:COA:H61	5:C:635:HOH:O	1.48	1.11
1:B:149:ALA:CB	1:B:150:ARG:HA	1.79	1.11
1:B:439:ALA:O	1:B:441:GLN:CB	1.98	1.11
1:A:90:THR:HA	1:A:92:THR:CG2	1.81	1.10
1:A:396:HIS:CE1	1:B:396:HIS:ND1	2.18	1.10
1:D:149:ALA:CB	1:D:150:ARG:HA	1.83	1.08
1:C:149:ALA:CB	1:C:150:ARG:HA	1.84	1.08
1:A:149:ALA:HB3	1:A:150:ARG:HA	1.33	1.07
1:B:85:ASP:C	1:B:92:THR:HG22	1.80	1.06
1:A:439:ALA:O	1:A:441:GLN:CB	2.04	1.06
1:D:74:LEU:HB2	5:D:609:HOH:O	1.55	1.05
1:B:90:THR:HA	1:B:92:THR:HG21	1.33	1.03
1:A:440:GLN:NE2	1:A:440:GLN:HA	1.74	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ALA:HB3	1:B:150:ARG:HA	1.35	1.03
1:D:37:GLY:HA2	1:D:77:THR:HB	1.34	1.03
1:A:91:LEU:O	1:A:92:THR:OG1	1.75	1.02
1:B:37:GLY:HA2	1:B:77:THR:HB	1.40	1.02
1:D:440:GLN:HA	1:D:440:GLN:NE2	1.72	1.02
1:C:149:ALA:HB3	1:C:150:ARG:HA	1.39	1.01
1:A:147:PRO:O	1:A:148:GLN:HB2	1.56	1.01
1:A:149:ALA:CB	1:A:150:ARG:HA	1.91	1.00
1:C:440:GLN:NE2	5:C:602:HOH:O	1.94	1.00
1:D:149:ALA:HB3	1:D:150:ARG:HA	1.41	0.99
1:B:90:THR:HG23	1:B:92:THR:OG1	1.60	0.99
1:B:86:TYR:N	1:B:92:THR:HG22	1.76	0.98
1:B:91:LEU:O	1:B:92:THR:OG1	1.81	0.98
1:C:85:ASP:H	1:C:92:THR:HA	1.25	0.98
1:C:439:ALA:O	1:C:441:GLN:CB	2.11	0.97
1:D:85:ASP:H	1:D:92:THR:HA	1.31	0.96
1:D:217:ARG:HB3	1:D:224:ALA:HB3	1.46	0.95
1:A:37:GLY:HA2	1:A:77:THR:HB	1.45	0.95
1:A:91:LEU:HD12	1:A:92:THR:H	1.33	0.94
1:A:217:ARG:HB3	1:A:224:ALA:HB3	1.47	0.94
1:A:85:ASP:H	1:A:92:THR:HA	1.32	0.94
1:C:440:GLN:NE2	1:C:440:GLN:HA	1.82	0.94
1:A:224:ALA:O	1:A:232:VAL:O	1.87	0.92
1:A:398:ALA:H	1:A:399:LEU:HB2	1.32	0.92
1:C:37:GLY:HA2	1:C:77:THR:HB	1.51	0.92
1:B:440:GLN:HA	1:B:440:GLN:NE2	1.84	0.91
1:D:147:PRO:O	1:D:148:GLN:HB2	1.67	0.91
1:A:85:ASP:C	1:A:92:THR:HG22	1.96	0.91
1:D:91:LEU:HD12	1:D:92:THR:H	1.32	0.91
1:B:192:VAL:O	5:B:601:HOH:O	1.88	0.91
1:B:217:ARG:HB3	1:B:224:ALA:HB3	1.52	0.91
1:A:396:HIS:ND1	1:B:396:HIS:ND1	2.15	0.91
1:B:85:ASP:H	1:B:92:THR:HA	1.34	0.90
1:A:343:LEU:HD22	1:A:355:LYS:HB3	1.50	0.89
1:A:86:TYR:N	1:A:92:THR:HG22	1.86	0.89
1:A:90:THR:HG23	1:A:92:THR:OG1	1.71	0.89
1:C:398:ALA:HA	1:C:400:ARG:H	1.37	0.88
1:B:90:THR:CG2	1:B:92:THR:OG1	2.22	0.88
1:D:439:ALA:O	1:D:441:GLN:CB	2.19	0.87
1:B:196:LEU:HB2	5:B:601:HOH:O	1.73	0.86
1:D:386:LEU:HA	5:D:606:HOH:O	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:VAL:HA	5:D:609:HOH:O	1.75	0.85
1:C:87:GLU:HA	1:C:88:LEU:C	2.02	0.85
1:D:236:LEU:HD12	1:D:236:LEU:C	2.02	0.85
1:D:358:ILE:C	1:D:358:ILE:HD12	2.01	0.84
1:B:224:ALA:O	1:B:232:VAL:O	1.95	0.84
1:B:50:LEU:HD12	1:B:143:LEU:HD13	1.60	0.83
1:B:87:GLU:HA	1:B:88:LEU:C	2.03	0.83
1:D:343:LEU:HD22	1:D:355:LYS:HB3	1.59	0.83
1:A:398:ALA:H	1:A:399:LEU:CB	1.92	0.83
1:B:147:PRO:O	1:B:148:GLN:HB2	1.78	0.83
1:C:437:ILE:C	1:C:437:ILE:HD12	2.02	0.83
1:A:94:HIS:CD2	1:A:94:HIS:N	2.42	0.83
1:C:91:LEU:HD12	1:C:92:THR:H	1.41	0.83
1:C:343:LEU:HD22	1:C:355:LYS:HB3	1.61	0.82
1:B:410:ARG:HH11	1:B:410:ARG:HG2	1.43	0.82
1:B:196:LEU:CB	5:B:601:HOH:O	2.24	0.82
1:D:440:GLN:HA	1:D:440:GLN:HE21	1.44	0.81
1:C:399:LEU:N	5:C:604:HOH:O	2.07	0.81
1:D:398:ALA:O	5:D:601:HOH:O	1.98	0.81
1:B:90:THR:HA	1:B:92:THR:HG23	1.62	0.81
1:C:50:LEU:HD12	1:C:143:LEU:HD13	1.61	0.81
1:A:396:HIS:ND1	1:B:396:HIS:HE1	1.76	0.80
1:D:341:LEU:O	1:D:388:GLY:HA3	1.81	0.80
1:A:440:GLN:HA	1:A:440:GLN:HE21	1.43	0.80
1:D:287:HIS:HD2	1:D:289:VAL:H	1.29	0.80
1:C:225:VAL:N	5:C:601:HOH:O	1.83	0.80
1:B:91:LEU:HD12	1:B:92:THR:H	1.47	0.79
1:C:440:GLN:O	1:C:441:GLN:O	2.01	0.79
1:A:91:LEU:C	1:A:92:THR:OG1	2.26	0.79
1:C:436:LEU:HD12	5:C:610:HOH:O	1.82	0.79
1:D:87:GLU:HA	1:D:88:LEU:C	2.08	0.78
1:A:437:ILE:O	1:A:441:GLN:HB3	1.83	0.78
1:B:85:ASP:C	1:B:92:THR:CG2	2.56	0.78
1:C:94:HIS:N	1:C:94:HIS:CD2	2.48	0.78
1:B:91:LEU:HD13	1:B:103:GLN:OE1	1.83	0.78
1:C:147:PRO:O	1:C:148:GLN:HB2	1.83	0.78
1:B:410:ARG:HH11	1:B:410:ARG:CG	1.96	0.78
1:D:127:GLN:HG2	1:D:220:GLY:HA2	1.66	0.77
1:C:90:THR:HG21	1:C:106:PHE:H	1.47	0.77
1:C:440:GLN:O	5:C:603:HOH:O	2.01	0.77
1:A:90:THR:CG2	1:A:92:THR:OG1	2.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB1	1:A:173:LEU:HD22	1.67	0.77
1:C:217:ARG:HB3	1:C:224:ALA:HB3	1.67	0.77
3:A:502:COA:H31	1:B:431:VAL:HG21	1.67	0.76
1:B:272:ASN:HD22	1:B:272:ASN:H	1.31	0.76
1:D:256:ALA:H	1:D:272:ASN:ND2	1.84	0.76
1:B:236:LEU:C	1:B:236:LEU:HD12	2.11	0.76
1:B:343:LEU:HD22	1:B:355:LYS:HB3	1.67	0.76
1:C:236:LEU:C	1:C:236:LEU:HD12	2.10	0.76
1:D:410:ARG:HH11	1:D:410:ARG:CG	1.99	0.75
1:D:187:HIS:ND1	5:D:605:HOH:O	2.20	0.75
1:B:44:CYS:O	5:B:602:HOH:O	2.05	0.75
1:B:341:LEU:O	1:B:388:GLY:HA3	1.86	0.74
1:C:8:VAL:HG13	1:C:81:VAL:HG13	1.69	0.74
1:C:440:GLN:HA	5:C:602:HOH:O	1.86	0.74
1:D:98:GLU:HA	1:D:98:GLU:OE2	1.87	0.74
1:C:352:TRP:NE1	5:C:607:HOH:O	2.20	0.74
1:A:256:ALA:H	1:A:272:ASN:ND2	1.86	0.74
1:B:437:ILE:O	1:B:441:GLN:HB3	1.87	0.74
1:C:149:ALA:HB1	1:C:150:ARG:HA	1.69	0.73
3:B:503:COA:N1A	5:B:603:HOH:O	2.21	0.73
1:C:224:ALA:O	1:C:232:VAL:O	2.07	0.73
1:D:224:ALA:O	1:D:232:VAL:O	2.07	0.73
1:A:202:ARG:NH2	5:A:604:HOH:O	2.21	0.73
1:B:295:TRP:CE2	1:B:297:PRO:HG3	2.23	0.72
1:C:91:LEU:HD13	1:C:103:GLN:OE1	1.89	0.72
1:D:11:VAL:HG23	2:D:501:FAD:H4B	1.70	0.72
1:A:98:GLU:HA	1:A:98:GLU:OE2	1.89	0.72
1:C:339:THR:HG22	1:C:401:ILE:HD11	1.71	0.72
1:A:272:ASN:ND2	1:A:272:ASN:H	1.88	0.72
1:C:149:ALA:CB	1:C:150:ARG:CA	2.63	0.72
1:B:173:LEU:HD23	1:B:173:LEU:N	2.05	0.72
1:A:295:TRP:CE2	1:A:297:PRO:HG3	2.25	0.71
1:B:196:LEU:N	5:B:601:HOH:O	2.23	0.71
1:B:426:PRO:HB2	1:B:427:PRO:HD3	1.70	0.71
1:B:91:LEU:C	1:B:92:THR:OG1	2.34	0.71
1:D:440:GLN:NE2	1:D:440:GLN:CA	2.53	0.71
1:D:208:TRP:HB3	1:D:211:VAL:HG21	1.72	0.71
1:B:149:ALA:CB	1:B:150:ARG:CA	2.64	0.71
1:A:121:PRO:HG3	1:D:149:ALA:HB3	1.71	0.71
1:C:174:GLN:O	5:C:605:HOH:O	2.09	0.70
1:A:94:HIS:N	1:A:94:HIS:HD2	1.86	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ALA:HB1	3:B:503:COA:H142	1.73	0.70
1:D:397:GLY:O	5:D:602:HOH:O	2.09	0.70
1:B:359:GLN:HB2	1:B:374:TRP:CD1	2.27	0.70
1:D:256:ALA:H	1:D:272:ASN:HD21	1.40	0.70
1:B:34:GLU:HG2	1:B:39:VAL:HG23	1.74	0.69
1:D:148:GLN:O	1:D:149:ALA:O	2.10	0.69
1:A:90:THR:HA	1:A:92:THR:HG23	1.73	0.69
3:D:502:COA:H72	4:D:503:VK3:H9K1	1.73	0.69
1:A:10:GLY:O	1:A:39:VAL:HG22	1.92	0.69
1:C:191:GLU:OE2	1:C:355:LYS:HE3	1.92	0.69
1:B:86:TYR:O	1:B:89:ARG:HA	1.92	0.69
1:B:208:TRP:HB3	1:B:211:VAL:HG21	1.74	0.69
1:B:98:GLU:OE2	1:B:98:GLU:HA	1.92	0.69
1:B:92:THR:HB	1:B:106:PHE:HE2	1.57	0.69
1:B:94:HIS:N	1:B:94:HIS:CD2	2.60	0.69
1:A:396:HIS:HE1	1:B:396:HIS:ND1	1.84	0.69
1:C:127:GLN:HG2	1:C:220:GLY:HA2	1.75	0.69
1:A:24:GLU:HG2	1:A:316:ARG:HG3	1.75	0.69
1:C:381:GLU:N	5:C:608:HOH:O	2.26	0.69
1:C:410:ARG:CG	1:C:410:ARG:HH11	2.05	0.68
1:A:91:LEU:HD12	1:A:92:THR:N	2.06	0.68
1:D:91:LEU:CD1	1:D:92:THR:H	2.05	0.68
1:A:208:TRP:HB3	1:A:211:VAL:HG21	1.74	0.68
1:D:94:HIS:N	1:D:94:HIS:CD2	2.60	0.68
1:D:197:LYS:NZ	5:D:610:HOH:O	2.26	0.68
1:C:256:ALA:H	1:C:272:ASN:ND2	1.92	0.68
1:D:12:ALA:O	1:D:16:SER:HB2	1.93	0.68
1:A:92:THR:HB	1:A:106:PHE:HE2	1.57	0.68
1:B:139:GLY:O	1:B:143:LEU:HB2	1.93	0.68
1:C:358:ILE:HD12	1:C:358:ILE:C	2.19	0.68
1:D:100:ARG:C	1:D:101:THR:HG22	2.17	0.68
1:C:272:ASN:H	1:C:272:ASN:HD22	1.41	0.67
1:B:91:LEU:C	1:B:92:THR:HG1	1.99	0.67
1:D:91:LEU:HD13	1:D:103:GLN:OE1	1.94	0.67
1:D:149:ALA:HB1	1:D:150:ARG:HA	1.72	0.67
1:A:50:LEU:HD12	1:A:143:LEU:HD13	1.76	0.67
1:D:91:LEU:HD12	1:D:92:THR:N	2.08	0.67
1:A:406:ALA:O	5:A:602:HOH:O	2.12	0.67
1:B:12:ALA:O	1:B:16:SER:HB2	1.95	0.67
1:B:410:ARG:HG2	1:B:410:ARG:NH1	2.06	0.67
1:D:295:TRP:CE2	1:D:297:PRO:HG3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:CG	1:A:316:ARG:HG3	2.24	0.67
1:C:94:HIS:N	1:C:94:HIS:HD2	1.91	0.67
1:D:410:ARG:HH11	1:D:410:ARG:HG2	1.59	0.67
1:B:162:LEU:HD13	1:B:196:LEU:HD22	1.76	0.67
4:A:503:VK3:H9K1	3:B:503:COA:H72	1.76	0.67
1:B:441:GLN:O	1:B:442:ALA:O	2.12	0.66
1:C:441:GLN:O	1:C:442:ALA:O	2.13	0.66
1:D:149:ALA:CB	1:D:150:ARG:CA	2.68	0.66
1:A:410:ARG:N	5:A:602:HOH:O	2.27	0.66
1:D:171:ARG:NH2	5:D:608:HOH:O	2.24	0.66
1:D:287:HIS:CD2	1:D:289:VAL:H	2.13	0.66
1:B:149:ALA:HB1	1:B:150:ARG:HA	1.74	0.66
1:C:440:GLN:HA	1:C:440:GLN:HE21	1.60	0.66
1:B:116:ARG:HH22	1:B:244:ARG:HH11	1.43	0.66
1:B:287:HIS:HD2	1:B:290:LEU:H	1.41	0.66
1:C:11:VAL:HG23	2:C:501:FAD:H4B	1.76	0.66
1:D:116:ARG:CZ	1:D:244:ARG:HD2	2.26	0.66
1:D:398:ALA:C	5:D:601:HOH:O	2.39	0.66
1:A:149:ALA:CB	1:A:173:LEU:HD22	2.26	0.66
1:B:92:THR:HB	1:B:106:PHE:CE2	2.31	0.66
1:C:272:ASN:ND2	1:C:272:ASN:H	1.94	0.66
1:A:92:THR:HB	1:A:106:PHE:CE2	2.31	0.66
1:A:441:GLN:O	1:A:442:ALA:O	2.14	0.65
1:B:176:THR:HB	1:B:206:GLU:HB2	1.76	0.65
1:A:256:ALA:H	1:A:272:ASN:HD21	1.44	0.65
1:A:86:TYR:O	1:A:89:ARG:HA	1.95	0.65
1:C:183:ARG:HD3	1:C:190:PRO:HA	1.78	0.65
1:D:386:LEU:CA	5:D:606:HOH:O	2.40	0.65
1:A:244:ARG:NH2	5:A:609:HOH:O	2.30	0.65
1:B:287:HIS:CD2	1:B:290:LEU:H	2.15	0.65
1:D:90:THR:HG23	1:D:92:THR:CB	2.27	0.65
1:A:3:LYS:HB3	1:A:107:ASP:OD2	1.96	0.64
1:C:410:ARG:HH11	1:C:410:ARG:HG2	1.61	0.64
1:B:116:ARG:CZ	1:B:244:ARG:HD2	2.28	0.64
1:B:399:LEU:C	1:B:401:ILE:H	2.05	0.64
1:B:11:VAL:CG2	2:B:502:FAD:H4B	2.28	0.64
1:D:216:PHE:CD1	1:D:225:VAL:HG22	2.32	0.64
1:A:149:ALA:CB	1:A:150:ARG:CA	2.70	0.64
1:B:256:ALA:H	1:B:272:ASN:ND2	1.96	0.64
1:B:11:VAL:HG23	2:B:502:FAD:H4B	1.79	0.64
1:C:295:TRP:CE2	1:C:297:PRO:HG3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ASP:OD1	1:D:88:LEU:HD23	1.98	0.63
1:D:359:GLN:HB2	1:D:374:TRP:CD1	2.33	0.63
1:A:64:THR:OG1	1:A:67:GLU:HG3	1.99	0.63
1:A:87:GLU:HA	1:A:88:LEU:C	2.24	0.63
1:D:50:LEU:HD12	1:D:143:LEU:HD13	1.80	0.63
1:A:11:VAL:HG23	2:A:501:FAD:H4B	1.80	0.63
1:A:398:ALA:HA	1:A:400:ARG:H	1.63	0.63
1:C:98:GLU:OE2	1:C:98:GLU:HA	1.97	0.63
1:A:395:GLY:HA2	1:B:396:HIS:NE2	2.14	0.63
1:A:272:ASN:H	1:A:272:ASN:HD22	1.46	0.62
1:A:287:HIS:CD2	1:A:290:LEU:H	2.17	0.62
1:B:358:ILE:C	1:B:358:ILE:HD12	2.23	0.62
1:B:191:GLU:OE2	1:B:355:LYS:HE3	1.99	0.62
1:B:440:GLN:HA	1:B:440:GLN:HE21	1.61	0.62
1:D:236:LEU:HD12	1:D:237:VAL:N	2.13	0.62
1:A:268:ARG:HG2	1:A:312:VAL:HG21	1.80	0.62
1:D:397:GLY:C	5:D:602:HOH:O	2.42	0.62
1:A:85:ASP:C	1:A:92:THR:CG2	2.70	0.62
1:D:154:ILE:HB	1:D:177:LEU:HD23	1.82	0.62
1:C:256:ALA:H	1:C:272:ASN:HD21	1.48	0.62
1:D:387:LEU:N	5:D:606:HOH:O	2.33	0.62
1:B:403:VAL:O	1:B:406:ALA:HB3	2.00	0.62
1:D:65:PRO:HB3	1:D:75:VAL:CG2	2.30	0.62
1:C:154:ILE:HB	1:C:177:LEU:HD23	1.82	0.61
1:A:147:PRO:O	1:A:148:GLN:CB	2.37	0.61
1:D:11:VAL:CG2	2:D:501:FAD:H4B	2.30	0.61
1:D:56:ARG:CZ	1:D:59:ARG:HH11	2.12	0.61
1:A:162:LEU:HD22	1:A:200:LEU:HD11	1.83	0.61
1:D:208:TRP:HB3	1:D:211:VAL:CG2	2.30	0.61
1:C:380:GLU:HG2	5:C:608:HOH:O	2.00	0.61
1:A:81:VAL:HA	1:A:95:ASP:HB3	1.81	0.61
1:D:149:ALA:HB1	1:D:173:LEU:HD22	1.82	0.61
1:B:208:TRP:HB3	1:B:211:VAL:CG2	2.30	0.61
1:D:441:GLN:O	1:D:442:ALA:O	2.19	0.61
1:B:398:ALA:HA	1:B:400:ARG:H	1.66	0.61
1:C:8:VAL:HG13	1:C:81:VAL:CG1	2.31	0.61
1:C:117:PRO:HD3	1:C:134:ARG:HG2	1.83	0.61
1:B:86:TYR:N	1:B:92:THR:CG2	2.57	0.60
1:B:280:GLY:HA2	1:B:302:ALA:HA	1.83	0.60
1:D:84:VAL:O	1:D:86:TYR:HD1	1.84	0.60
1:D:280:GLY:HA2	1:D:302:ALA:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD13	1:A:103:GLN:OE1	2.01	0.60
1:A:123:PRO:HD3	1:D:172:GLY:CA	2.31	0.60
1:C:90:THR:CG2	1:C:106:PHE:H	2.13	0.60
1:C:401:ILE:HB	5:C:604:HOH:O	2.01	0.60
1:A:15:ALA:HB1	3:A:502:COA:H142	1.83	0.60
1:D:90:THR:HG22	1:D:91:LEU:O	2.01	0.60
1:A:116:ARG:CZ	1:A:244:ARG:HD2	2.31	0.60
1:B:64:THR:OG1	1:B:67:GLU:HG3	2.02	0.60
1:B:221:ARG:O	1:B:222:VAL:HB	2.00	0.60
1:C:36:SER:O	1:C:38:TRP:N	2.34	0.60
1:C:180:ALA:O	1:C:210:GLY:HA2	2.00	0.60
1:A:440:GLN:NE2	1:A:440:GLN:CA	2.60	0.60
1:C:91:LEU:CD1	1:C:92:THR:H	2.13	0.60
1:D:339:THR:HG22	1:D:401:ILE:HD11	1.82	0.60
1:D:23:ARG:NH2	3:D:502:COA:O5A	2.34	0.60
1:A:208:TRP:HB3	1:A:211:VAL:CG2	2.32	0.60
1:C:137:GLU:OE1	5:C:606:HOH:O	2.16	0.60
1:C:139:GLY:O	1:C:143:LEU:HB2	2.02	0.60
1:A:91:LEU:CD1	1:A:92:THR:H	2.09	0.60
1:D:23:ARG:HH22	3:D:502:COA:P2A	2.25	0.60
1:D:180:ALA:O	1:D:210:GLY:HA2	2.02	0.59
1:A:90:THR:CA	1:A:92:THR:CG2	2.71	0.59
1:A:398:ALA:N	1:A:399:LEU:HB2	2.12	0.59
1:C:116:ARG:CZ	1:C:244:ARG:HD2	2.32	0.59
1:D:191:GLU:OE2	1:D:355:LYS:HE3	2.02	0.59
1:D:87:GLU:HA	1:D:88:LEU:O	2.02	0.59
1:D:173:LEU:HD23	1:D:173:LEU:N	2.18	0.59
1:B:401:ILE:HG13	1:B:401:ILE:O	2.01	0.59
1:B:222:VAL:HG12	5:B:609:HOH:O	2.02	0.59
1:C:40:SER:OG	3:C:502:COA:H141	2.02	0.59
1:D:164:ALA:O	1:D:167:ALA:HB3	2.03	0.59
1:A:121:PRO:CG	1:D:149:ALA:HB3	2.33	0.59
1:B:123:PRO:HG2	1:B:215:ALA:HB2	1.85	0.59
1:B:399:LEU:C	1:B:401:ILE:N	2.56	0.58
1:D:166:GLU:HA	1:D:332:PHE:CZ	2.38	0.58
1:D:268:ARG:HH22	1:D:270:ARG:NH1	2.01	0.58
1:A:97:ALA:O	1:A:98:GLU:CD	2.46	0.58
1:C:85:ASP:N	1:C:92:THR:HA	2.08	0.58
1:D:410:ARG:HG2	1:D:410:ARG:NH1	2.18	0.58
1:C:418:LEU:HD13	1:C:439:ALA:HB3	1.84	0.58
1:B:4:ARG:NH1	1:B:104:ASP:OD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:VAL:O	1:C:86:TYR:HD1	1.86	0.58
1:D:85:ASP:N	1:D:92:THR:HA	2.12	0.58
1:D:189:ASP:OD2	1:D:376:GLU:OE2	2.22	0.58
1:D:440:GLN:O	5:D:604:HOH:O	2.17	0.58
1:C:87:GLU:HA	1:C:88:LEU:O	2.04	0.58
1:C:418:LEU:HD22	1:C:439:ALA:HB1	1.86	0.58
1:B:87:GLU:HA	1:B:88:LEU:O	2.03	0.57
1:D:64:THR:OG1	1:D:67:GLU:HG3	2.03	0.57
1:D:149:ALA:CB	1:D:173:LEU:HD22	2.34	0.57
1:A:191:GLU:OE2	1:A:355:LYS:HE3	2.04	0.57
1:B:183:ARG:HD3	1:B:190:PRO:HA	1.86	0.57
1:B:84:VAL:O	1:B:86:TYR:HD1	1.87	0.57
1:C:352:TRP:CD1	5:C:607:HOH:O	2.56	0.57
1:A:200:LEU:HD23	1:A:332:PHE:HE2	1.70	0.57
4:C:503:VK3:H8K1	5:C:635:HOH:O	2.03	0.57
1:D:399:LEU:C	1:D:401:ILE:H	2.12	0.57
1:A:225:VAL:N	5:A:601:HOH:O	2.08	0.57
1:D:86:TYR:O	1:D:89:ARG:HA	2.05	0.57
1:D:399:LEU:N	5:D:601:HOH:O	2.37	0.57
1:D:433:ASP:O	1:D:436:LEU:N	2.38	0.57
1:B:94:HIS:N	1:B:94:HIS:HD2	2.02	0.57
1:C:10:GLY:O	1:C:39:VAL:HG22	2.05	0.57
1:A:437:ILE:HD12	1:A:437:ILE:C	2.30	0.56
1:A:185:LEU:N	1:A:186:PRO:CD	2.68	0.56
1:B:24:GLU:HG2	1:B:316:ARG:HG3	1.86	0.56
1:B:91:LEU:CD1	1:B:92:THR:H	2.15	0.56
1:A:77:THR:O	1:A:78:ARG:HB2	2.04	0.56
1:B:292:ARG:HB2	1:B:293:PRO:CD	2.36	0.56
1:C:69:ARG:C	1:C:71:GLN:H	2.13	0.56
1:C:221:ARG:O	1:C:222:VAL:HB	2.06	0.56
1:B:166:GLU:HG2	1:B:170:LYS:HE3	1.87	0.56
1:C:56:ARG:NH1	5:C:612:HOH:O	2.38	0.56
1:A:236:LEU:HD12	1:A:236:LEU:C	2.30	0.56
1:C:410:ARG:HG2	1:C:410:ARG:NH1	2.21	0.56
1:D:90:THR:O	5:D:603:HOH:O	2.17	0.56
1:C:251:GLN:HB2	5:C:613:HOH:O	2.04	0.56
1:A:431:VAL:HG21	3:B:503:COA:H31	1.86	0.56
1:B:437:ILE:C	1:B:437:ILE:HD12	2.31	0.56
1:B:283:ALA:HB3	1:B:305:HIS:CE1	2.41	0.56
1:A:86:TYR:N	1:A:92:THR:CG2	2.66	0.56
1:A:358:ILE:HD12	1:A:358:ILE:C	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ALA:HB1	1:B:162:LEU:HD21	1.88	0.56
1:B:183:ARG:HG3	1:B:184:PRO:O	2.06	0.56
1:B:433:ASP:O	1:B:436:LEU:N	2.38	0.56
1:A:121:PRO:CG	1:D:149:ALA:CB	2.84	0.55
1:B:221:ARG:O	1:B:222:VAL:CB	2.54	0.55
1:A:419:ALA:HB1	1:B:409:HIS:CE1	2.41	0.55
1:D:162:LEU:HD22	1:D:200:LEU:HD11	1.89	0.55
1:A:11:VAL:CG2	2:A:501:FAD:H4B	2.37	0.55
1:D:401:ILE:HG23	1:D:402:ASP:N	2.22	0.55
1:B:196:LEU:HD12	5:B:601:HOH:O	2.06	0.55
1:D:94:HIS:N	1:D:94:HIS:HD2	2.02	0.55
1:D:418:LEU:HD13	1:D:439:ALA:HB3	1.89	0.55
1:C:183:ARG:CD	1:C:190:PRO:HA	2.36	0.55
1:D:176:THR:HB	1:D:206:GLU:HB2	1.89	0.55
1:C:11:VAL:CG2	2:C:501:FAD:H4B	2.35	0.55
1:C:236:LEU:HD12	1:C:237:VAL:N	2.21	0.55
1:D:97:ALA:O	1:D:98:GLU:CD	2.50	0.55
1:D:116:ARG:NH2	1:D:244:ARG:HD2	2.22	0.55
1:B:90:THR:CA	1:B:92:THR:HG23	2.34	0.55
1:C:90:THR:HG23	1:C:92:THR:CB	2.36	0.55
1:D:183:ARG:HD3	1:D:190:PRO:HA	1.88	0.55
1:A:91:LEU:N	1:A:92:THR:HG23	2.21	0.55
1:C:15:ALA:HB1	3:C:502:COA:H142	1.89	0.55
1:D:91:LEU:O	1:D:92:THR:CB	2.55	0.55
1:D:139:GLY:O	1:D:143:LEU:HB2	2.07	0.55
1:A:69:ARG:C	1:A:71:GLN:H	2.15	0.54
1:C:268:ARG:HH22	1:C:270:ARG:NH1	2.04	0.54
1:A:287:HIS:HE1	5:A:620:HOH:O	1.90	0.54
1:B:200:LEU:HD23	1:B:332:PHE:HE2	1.72	0.54
1:B:398:ALA:H	1:B:399:LEU:HB3	1.72	0.54
1:C:90:THR:HG22	1:C:91:LEU:O	2.07	0.54
3:A:502:COA:H72	4:B:501:VK3:H9K1	1.89	0.54
1:B:418:LEU:HD13	1:B:439:ALA:HB3	1.89	0.54
1:A:395:GLY:HA2	1:B:396:HIS:HE2	1.73	0.54
1:B:8:VAL:HG13	1:B:81:VAL:HG13	1.89	0.54
1:A:151:ARG:HE	1:A:174:GLN:HE21	1.54	0.54
1:A:328:ILE:HG22	1:B:423:ALA:HB1	1.90	0.54
1:B:426:PRO:CB	1:B:427:PRO:HD3	2.38	0.54
1:D:324:VAL:HG21	1:D:408:LEU:HB3	1.89	0.54
1:A:8:VAL:HG13	1:A:81:VAL:HG13	1.89	0.54
1:C:208:TRP:HB3	1:C:211:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:502:COA:H72	4:C:503:VK3:H9K1	1.90	0.54
1:B:10:GLY:O	1:B:39:VAL:HG22	2.08	0.54
1:D:148:GLN:O	1:D:149:ALA:C	2.50	0.54
1:B:92:THR:O	1:B:93:VAL:O	2.26	0.54
1:D:202:ARG:NH2	5:D:613:HOH:O	2.40	0.54
1:D:90:THR:HG21	1:D:106:PHE:H	1.73	0.54
1:B:149:ALA:CB	1:B:173:LEU:HD22	2.38	0.53
1:B:155:LEU:N	1:B:155:LEU:HD12	2.24	0.53
1:A:94:HIS:CD2	1:A:94:HIS:H	2.23	0.53
1:A:100:ARG:C	1:A:101:THR:HG22	2.33	0.53
1:A:128:GLU:HB3	1:A:221:ARG:HA	1.89	0.53
1:A:268:ARG:O	1:A:269:MET:HB2	2.07	0.53
1:A:341:LEU:O	1:A:388:GLY:HA3	2.08	0.53
1:A:418:LEU:HD13	1:A:439:ALA:HB3	1.89	0.53
1:B:116:ARG:NH2	1:B:244:ARG:HD2	2.23	0.53
1:C:217:ARG:HD2	1:C:224:ALA:HB2	1.90	0.53
1:C:410:ARG:CG	1:C:410:ARG:NH1	2.71	0.53
1:A:91:LEU:O	1:A:105:ARG:HA	2.08	0.53
1:D:410:ARG:CG	1:D:410:ARG:NH1	2.68	0.53
1:B:85:ASP:CA	1:B:92:THR:HG22	2.38	0.53
1:C:174:GLN:C	5:C:605:HOH:O	2.51	0.53
1:D:84:VAL:HA	1:D:93:VAL:H	1.74	0.53
1:A:90:THR:CG2	1:A:106:PHE:H	2.22	0.53
1:B:49:VAL:HG11	1:B:57:LEU:HD12	1.90	0.53
1:B:90:THR:HG21	1:B:106:PHE:O	2.07	0.53
1:C:149:ALA:HB3	1:C:150:ARG:CA	2.27	0.53
1:A:359:GLN:HB2	1:A:374:TRP:CD1	2.44	0.53
1:A:403:VAL:O	1:A:406:ALA:HB3	2.08	0.53
1:C:398:ALA:H	1:C:399:LEU:CB	2.22	0.53
1:C:50:LEU:CD2	1:C:133:LEU:HD11	2.38	0.53
1:C:64:THR:OG1	1:C:67:GLU:HG3	2.09	0.53
1:C:208:TRP:HB3	1:C:211:VAL:HG21	1.91	0.53
1:A:12:ALA:O	1:A:16:SER:HB2	2.09	0.53
1:B:166:GLU:HA	1:B:332:PHE:CZ	2.44	0.53
1:A:69:ARG:O	1:A:71:GLN:N	2.42	0.52
1:A:295:TRP:C	1:A:297:PRO:HD3	2.34	0.52
1:D:216:PHE:HD1	1:D:225:VAL:HG22	1.71	0.52
1:C:85:ASP:OD1	1:C:88:LEU:HB3	2.09	0.52
1:C:162:LEU:HD23	1:C:177:LEU:HD11	1.90	0.52
1:C:56:ARG:CZ	1:C:59:ARG:HH11	2.23	0.52
1:D:88:LEU:O	1:D:89:ARG:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HD11	1:B:375:VAL:HG13	1.90	0.52
1:A:121:PRO:HG3	1:D:149:ALA:CB	2.38	0.52
1:A:437:ILE:O	1:A:441:GLN:CB	2.56	0.52
1:D:4:ARG:NH1	1:D:104:ASP:OD2	2.43	0.52
1:D:188:TRP:O	1:D:189:ASP:C	2.52	0.52
1:A:90:THR:HG21	1:A:106:PHE:O	2.10	0.52
1:B:97:ALA:O	1:B:98:GLU:CD	2.53	0.52
1:B:63:ARG:NH1	5:B:610:HOH:O	2.39	0.52
1:C:36:SER:O	1:C:37:GLY:C	2.51	0.52
1:D:57:LEU:O	1:D:60:LEU:HB2	2.10	0.52
1:D:399:LEU:C	1:D:401:ILE:N	2.61	0.52
1:A:90:THR:HG21	1:A:106:PHE:H	1.73	0.52
1:B:292:ARG:HB2	1:B:293:PRO:HD2	1.92	0.52
1:C:152:ALA:HA	1:C:236:LEU:O	2.09	0.52
1:A:90:THR:CA	1:A:92:THR:HG23	2.40	0.51
1:C:307:ARG:NH1	3:C:502:COA:O8A	2.35	0.51
1:D:84:VAL:O	1:D:86:TYR:CD1	2.63	0.51
1:D:122:ILE:HG23	1:D:215:ALA:HA	1.91	0.51
1:A:116:ARG:NH2	1:A:244:ARG:HD2	2.25	0.51
1:B:90:THR:HG21	1:B:106:PHE:H	1.75	0.51
1:C:23:ARG:HH22	3:C:502:COA:P2A	2.32	0.51
1:D:437:ILE:O	1:D:441:GLN:HB3	2.09	0.51
1:C:4:ARG:NH1	1:C:104:ASP:OD2	2.44	0.51
1:C:346:ALA:HB1	1:C:387:LEU:HD13	1.93	0.51
1:C:437:ILE:C	1:C:437:ILE:CD1	2.75	0.51
1:B:149:ALA:HB1	1:B:173:LEU:HD22	1.92	0.51
1:D:56:ARG:CZ	1:D:59:ARG:NH1	2.73	0.51
1:D:236:LEU:C	1:D:236:LEU:CD1	2.79	0.51
1:A:440:GLN:O	1:A:441:GLN:O	2.28	0.51
1:C:144:LYS:O	1:C:147:PRO:HD2	2.11	0.51
1:C:269:MET:HE3	1:C:320:PHE:HB3	1.92	0.51
1:C:341:LEU:O	1:C:388:GLY:HA3	2.10	0.51
1:A:440:GLN:C	1:A:441:GLN:O	2.54	0.51
1:B:116:ARG:NH2	1:B:244:ARG:HH11	2.09	0.51
1:B:236:LEU:HD12	1:B:237:VAL:N	2.24	0.51
1:D:151:ARG:HE	1:D:174:GLN:HE21	1.59	0.51
1:D:386:LEU:HD23	1:D:413:SER:C	2.35	0.51
1:A:22:LYS:HE2	1:A:72:GLY:HA3	1.93	0.51
1:B:440:GLN:NE2	1:B:440:GLN:CA	2.68	0.51
1:C:149:ALA:HB1	1:C:150:ARG:CA	2.37	0.51
1:D:338:THR:O	1:D:339:THR:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:LYS:HE3	1:B:381:GLU:OE2	2.11	0.51
1:A:91:LEU:C	1:A:92:THR:HG1	2.08	0.51
1:A:151:ARG:HG2	5:A:612:HOH:O	2.11	0.51
1:B:196:LEU:CG	5:B:601:HOH:O	2.53	0.51
1:C:41:TYR:CD2	1:C:136:MET:HG2	2.45	0.51
1:D:221:ARG:O	1:D:222:VAL:HB	2.10	0.51
1:D:358:ILE:HD12	1:D:358:ILE:O	2.10	0.51
1:C:69:ARG:O	1:C:71:GLN:N	2.44	0.50
1:C:302:ALA:HB2	2:C:501:FAD:H5'2	1.92	0.50
1:D:360:SER:HB3	1:D:434:PRO:HG3	1.92	0.50
1:A:151:ARG:HE	1:A:174:GLN:NE2	2.08	0.50
1:C:176:THR:HB	1:C:206:GLU:HB2	1.93	0.50
1:D:25:ASN:OD1	1:D:27:GLU:HB2	2.10	0.50
1:A:169:ARG:HB3	1:C:219:MET:HG3	1.92	0.50
1:B:123:PRO:HG2	1:B:215:ALA:CB	2.41	0.50
1:C:437:ILE:O	1:C:441:GLN:HB3	2.12	0.50
1:D:24:GLU:HG2	1:D:316:ARG:HG3	1.93	0.50
1:D:77:THR:O	1:D:78:ARG:HB2	2.11	0.50
1:C:398:ALA:HA	1:C:400:ARG:N	2.16	0.50
1:C:84:VAL:O	1:C:86:TYR:CD1	2.65	0.50
1:D:100:ARG:C	1:D:101:THR:CG2	2.84	0.50
1:D:426:PRO:HB2	1:D:427:PRO:HD3	1.93	0.50
1:D:304:LYS:O	1:D:305:HIS:C	2.54	0.50
1:D:437:ILE:HD12	1:D:437:ILE:C	2.37	0.50
1:C:41:TYR:HA	1:C:61:VAL:HA	1.93	0.49
1:A:423:ALA:HB1	1:B:328:ILE:HG22	1.93	0.49
1:A:432:TRP:O	1:A:433:ASP:C	2.53	0.49
1:B:86:TYR:O	1:B:89:ARG:CA	2.59	0.49
1:B:91:LEU:HD12	1:B:92:THR:N	2.20	0.49
1:C:12:ALA:O	1:C:16:SER:HB2	2.12	0.49
1:C:401:ILE:N	5:C:604:HOH:O	2.36	0.49
1:D:187:HIS:HB2	5:D:605:HOH:O	2.11	0.49
3:D:502:COA:C7P	4:D:503:VK3:H9K1	2.40	0.49
1:B:272:ASN:HD22	1:B:272:ASN:N	2.07	0.49
1:C:216:PHE:HA	5:C:601:HOH:O	2.12	0.49
1:A:386:LEU:HD23	1:A:413:SER:C	2.36	0.49
1:C:24:GLU:HG2	1:C:316:ARG:HG3	1.93	0.49
1:B:216:PHE:CD1	1:B:225:VAL:HG22	2.46	0.49
1:C:189:ASP:OD2	1:C:376:GLU:OE2	2.30	0.49
1:B:122:ILE:HG23	1:B:215:ALA:HA	1.95	0.49
1:D:166:GLU:HG2	1:D:170:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:HIS:CD2	1:D:290:LEU:H	2.31	0.49
1:C:400:ARG:HD3	1:C:433:ASP:OD1	2.12	0.49
1:D:199:GLU:HG3	1:D:334:LEU:HG	1.95	0.49
1:D:440:GLN:HA	5:D:614:HOH:O	2.13	0.49
1:B:255:VAL:HA	1:B:272:ASN:HD21	1.78	0.49
1:B:272:ASN:H	1:B:272:ASN:ND2	2.05	0.49
1:A:263:ILE:HD12	1:A:282:VAL:HG22	1.94	0.49
1:A:396:HIS:CE1	1:B:396:HIS:CE1	2.79	0.49
1:B:90:THR:HG22	1:B:92:THR:OG1	2.10	0.49
1:C:221:ARG:O	1:C:222:VAL:CB	2.60	0.49
1:C:287:HIS:CD2	1:C:290:LEU:H	2.31	0.49
1:C:440:GLN:O	1:C:441:GLN:C	2.55	0.48
1:D:85:ASP:OD1	1:D:88:LEU:HB3	2.13	0.48
1:A:200:LEU:HD23	1:A:332:PHE:CE2	2.47	0.48
1:B:69:ARG:C	1:B:71:GLN:H	2.22	0.48
1:B:86:TYR:H	1:B:92:THR:HG22	1.72	0.48
1:D:69:ARG:C	1:D:71:GLN:H	2.21	0.48
3:A:502:COA:H141	3:A:502:COA:O9P	2.14	0.48
1:B:41:TYR:HA	1:B:61:VAL:HA	1.95	0.48
1:B:84:VAL:HA	1:B:93:VAL:H	1.77	0.48
1:B:277:TYR:CD1	1:B:277:TYR:N	2.81	0.48
1:D:90:THR:HA	1:D:92:THR:CB	2.44	0.48
1:D:147:PRO:O	1:D:148:GLN:CB	2.43	0.48
1:D:200:LEU:HD23	1:D:332:PHE:HE2	1.78	0.48
1:D:272:ASN:HD22	1:D:272:ASN:H	1.61	0.48
1:A:287:HIS:HD2	1:A:290:LEU:H	1.59	0.48
1:D:302:ALA:HB2	2:D:501:FAD:H5'2	1.95	0.48
1:A:85:ASP:CA	1:A:92:THR:HG22	2.43	0.48
1:A:423:ALA:HB1	1:B:328:ILE:CG2	2.43	0.48
1:C:287:HIS:HD2	1:C:289:VAL:H	1.61	0.48
1:A:221:ARG:O	1:A:222:VAL:HB	2.14	0.48
1:B:97:ALA:O	1:B:98:GLU:OE1	2.31	0.48
1:B:386:LEU:HD23	1:B:413:SER:C	2.38	0.48
1:C:81:VAL:HA	1:C:95:ASP:HB3	1.95	0.48
1:D:58:GLU:C	1:D:60:LEU:H	2.21	0.48
1:C:12:ALA:CB	3:C:502:COA:HN4	2.27	0.48
1:A:41:TYR:HA	1:A:61:VAL:HA	1.96	0.48
1:B:88:LEU:O	1:B:89:ARG:HB2	2.14	0.47
1:B:90:THR:CA	1:B:92:THR:CG2	2.70	0.47
1:D:221:ARG:O	1:D:222:VAL:CB	2.62	0.47
1:D:398:ALA:HA	1:D:400:ARG:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:O	1:A:91:LEU:N	2.47	0.47
1:C:97:ALA:O	1:C:98:GLU:CD	2.57	0.47
1:D:367:TYR:CE1	1:D:427:PRO:HG3	2.49	0.47
1:D:386:LEU:C	5:D:606:HOH:O	2.57	0.47
1:A:183:ARG:CD	1:A:190:PRO:HA	2.44	0.47
1:B:15:ALA:HB1	3:B:503:COA:CEP	2.42	0.47
1:B:440:GLN:C	1:B:441:GLN:O	2.58	0.47
1:C:401:ILE:CB	5:C:604:HOH:O	2.59	0.47
1:D:166:GLU:HA	1:D:332:PHE:CE1	2.49	0.47
1:B:183:ARG:CD	1:B:190:PRO:HA	2.44	0.47
1:C:138:ASP:O	1:C:139:GLY:C	2.57	0.47
1:A:97:ALA:O	1:A:98:GLU:OE1	2.33	0.47
1:A:296:LEU:N	1:A:297:PRO:HD3	2.28	0.47
1:C:398:ALA:CA	1:C:400:ARG:H	2.20	0.47
1:D:24:GLU:HB3	1:D:314:ALA:CB	2.44	0.47
1:D:123:PRO:HG2	1:D:215:ALA:HB2	1.96	0.47
1:D:408:LEU:HD12	1:D:408:LEU:HA	1.68	0.47
1:A:65:PRO:HB3	1:A:75:VAL:CG2	2.45	0.47
1:B:339:THR:O	1:B:388:GLY:HA2	2.13	0.47
1:C:50:LEU:HD22	1:C:133:LEU:HD11	1.96	0.47
1:D:81:VAL:HG22	1:D:249:LEU:HD21	1.96	0.47
1:B:343:LEU:O	1:B:344:GLU:C	2.56	0.47
1:B:408:LEU:HA	1:B:408:LEU:HD12	1.59	0.47
1:C:386:LEU:HB3	1:C:408:LEU:CD1	2.45	0.47
1:C:430:PRO:HD2	1:C:434:PRO:HD3	1.96	0.47
1:D:263:ILE:CD1	1:D:282:VAL:HG22	2.45	0.47
1:D:263:ILE:HD12	1:D:282:VAL:HG22	1.95	0.47
1:D:277:TYR:CD1	1:D:277:TYR:N	2.82	0.47
1:D:321:LEU:HD23	1:D:321:LEU:HA	1.66	0.47
1:D:401:ILE:CG2	1:D:402:ASP:N	2.76	0.47
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.73	0.47
1:A:396:HIS:H	1:B:396:HIS:CE1	2.32	0.47
1:C:66:GLU:HB2	5:C:622:HOH:O	2.14	0.47
1:C:100:ARG:C	1:C:101:THR:HG22	2.40	0.47
1:C:367:TYR:CE1	1:C:427:PRO:HG3	2.49	0.47
1:D:200:LEU:HD23	1:D:332:PHE:CE2	2.50	0.47
1:B:24:GLU:CG	1:B:316:ARG:HG3	2.45	0.47
1:B:91:LEU:O	1:B:105:ARG:HA	2.14	0.47
1:C:114:GLY:O	1:C:246:ASN:HB2	2.15	0.47
1:B:356:VAL:O	1:B:376:GLU:HA	2.15	0.47
1:C:57:LEU:HG	1:C:136:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:GLN:C	1:C:441:GLN:O	2.58	0.47
1:A:420:LEU:HD22	1:B:406:ALA:HA	1.95	0.46
1:B:23:ARG:HH22	3:B:503:COA:P2A	2.38	0.46
1:B:148:GLN:O	1:B:149:ALA:O	2.33	0.46
1:B:223:GLU:HA	1:B:234:ALA:O	2.15	0.46
1:A:88:LEU:O	1:A:89:ARG:HB2	2.15	0.46
1:B:132:THR:O	1:B:138:ASP:HB3	2.15	0.46
1:B:324:VAL:HG21	1:B:408:LEU:HB3	1.98	0.46
1:C:173:LEU:N	1:C:173:LEU:HD23	2.31	0.46
1:C:281:ASP:CG	2:C:501:FAD:H5'1	2.40	0.46
1:A:20:LYS:NZ	5:A:613:HOH:O	2.48	0.46
1:B:226:GLU:HA	1:B:231:VAL:HG22	1.97	0.46
1:C:127:GLN:HB3	1:C:128:GLU:H	1.50	0.46
1:D:91:LEU:O	1:D:105:ARG:HA	2.16	0.46
1:D:272:ASN:ND2	1:D:272:ASN:H	2.13	0.46
1:A:328:ILE:HD13	1:A:328:ILE:HG21	1.51	0.46
1:A:360:SER:HB3	1:A:434:PRO:HG3	1.97	0.46
1:B:100:ARG:C	1:B:101:THR:HG22	2.40	0.46
1:B:256:ALA:H	1:B:272:ASN:HD21	1.60	0.46
1:B:268:ARG:HH22	1:B:270:ARG:NH1	2.13	0.46
1:C:25:ASN:OD1	1:C:27:GLU:HB2	2.16	0.46
1:D:89:ARG:O	1:D:91:LEU:N	2.48	0.46
1:D:255:VAL:HA	1:D:272:ASN:HD21	1.79	0.46
1:A:127:GLN:HB3	1:A:128:GLU:H	1.47	0.46
1:B:127:GLN:HG2	1:B:220:GLY:HA2	1.98	0.46
1:C:41:TYR:CE2	1:C:136:MET:HG2	2.51	0.46
1:C:280:GLY:HA2	1:C:302:ALA:HA	1.97	0.46
1:C:313:ILE:C	1:C:315:GLY:H	2.23	0.46
1:C:424:TYR:CD1	1:C:431:VAL:HA	2.51	0.46
1:D:10:GLY:O	1:D:39:VAL:HG22	2.15	0.46
1:A:93:VAL:C	1:A:94:HIS:HD2	2.24	0.46
1:C:408:LEU:HA	1:C:408:LEU:HD12	1.58	0.46
1:B:393:ALA:HB1	1:B:395:GLY:H	1.80	0.46
1:D:6:VAL:O	1:D:109:LEU:HD12	2.15	0.46
1:A:217:ARG:N	5:A:601:HOH:O	2.19	0.46
1:C:91:LEU:O	1:C:105:ARG:HA	2.16	0.46
1:C:185:LEU:N	1:C:186:PRO:CD	2.79	0.46
1:D:398:ALA:HB2	5:D:602:HOH:O	2.16	0.46
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.70	0.46
1:A:365:HIS:H	4:A:503:VK3:C6K	2.29	0.46
1:A:410:ARG:HH11	1:A:410:ARG:CG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:HD13	1:D:133:LEU:HD22	1.98	0.46
1:A:366:TYR:CE1	1:B:45:GLY:HA3	2.52	0.45
1:C:188:TRP:O	1:C:189:ASP:C	2.59	0.45
1:C:352:TRP:CE2	5:C:607:HOH:O	2.56	0.45
1:D:183:ARG:CD	1:D:190:PRO:HA	2.46	0.45
1:B:50:LEU:HD12	1:B:50:LEU:HA	1.72	0.45
1:B:151:ARG:HE	1:B:174:GLN:NE2	2.14	0.45
1:B:398:ALA:HA	1:B:400:ARG:N	2.30	0.45
1:B:440:GLN:O	1:B:441:GLN:O	2.35	0.45
1:C:296:LEU:HD12	1:C:296:LEU:HA	1.68	0.45
1:C:358:ILE:HD12	1:C:358:ILE:O	2.15	0.45
1:D:378:VAL:O	5:D:606:HOH:O	2.21	0.45
1:A:170:LYS:HG2	1:C:219:MET:HE3	1.98	0.45
1:C:24:GLU:HG2	1:C:316:ARG:CG	2.46	0.45
1:C:189:ASP:HA	1:C:190:PRO:HD3	1.62	0.45
1:C:200:LEU:HD23	1:C:332:PHE:HE2	1.82	0.45
1:D:149:ALA:HB1	1:D:150:ARG:CA	2.43	0.45
1:D:281:ASP:CG	2:D:501:FAD:H5'1	2.42	0.45
1:D:358:ILE:C	1:D:358:ILE:CD1	2.75	0.45
1:A:123:PRO:HD3	1:D:172:GLY:HA3	1.97	0.45
1:C:6:VAL:HG22	1:C:31:VAL:CG1	2.46	0.45
1:D:128:GLU:HB3	1:D:221:ARG:HA	1.98	0.45
1:D:398:ALA:H	1:D:399:LEU:HB3	1.81	0.45
1:A:139:GLY:O	1:A:143:LEU:HB2	2.16	0.45
1:B:128:GLU:HB3	1:B:221:ARG:HA	1.99	0.45
1:C:251:GLN:CD	1:C:257:LEU:HD11	2.42	0.45
1:C:426:PRO:HB2	1:C:427:PRO:HD3	1.98	0.45
1:A:208:TRP:HE3	1:A:208:TRP:N	2.15	0.45
1:A:441:GLN:HG2	1:B:307:ARG:NH2	2.32	0.45
1:C:407:LEU:O	1:C:410:ARG:O	2.34	0.45
1:D:256:ALA:N	1:D:272:ASN:HD21	2.13	0.45
1:A:149:ALA:CA	1:A:173:LEU:HD22	2.47	0.45
1:A:281:ASP:N	5:A:611:HOH:O	2.47	0.45
1:B:85:ASP:N	1:B:92:THR:HA	2.15	0.45
1:B:185:LEU:N	1:B:186:PRO:CD	2.79	0.45
1:A:149:ALA:HB1	1:A:173:LEU:CD2	2.41	0.45
1:B:77:THR:O	1:B:78:ARG:HB2	2.16	0.45
1:B:166:GLU:CG	1:B:170:LYS:HE3	2.47	0.45
1:B:424:TYR:CD1	1:B:425:ALA:N	2.84	0.45
1:D:268:ARG:HG2	1:D:312:VAL:HG21	1.98	0.45
1:A:86:TYR:H	1:A:92:THR:HG22	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:O	1:A:82:VAL:HG12	2.15	0.44
1:C:20:LYS:HE3	1:C:311:SER:OG	2.18	0.44
1:D:407:LEU:HA	1:D:407:LEU:HD23	1.72	0.44
1:B:200:LEU:HD23	1:B:332:PHE:CE2	2.52	0.44
1:B:81:VAL:HA	1:B:95:ASP:HB3	1.99	0.44
1:B:151:ARG:HE	1:B:174:GLN:HE21	1.65	0.44
1:B:367:TYR:N	5:B:605:HOH:O	2.50	0.44
1:C:399:LEU:C	1:C:401:ILE:H	2.26	0.44
1:C:437:ILE:HD12	1:C:437:ILE:O	2.15	0.44
1:D:50:LEU:HD12	1:D:50:LEU:HA	1.69	0.44
1:D:287:HIS:HD2	1:D:289:VAL:N	2.05	0.44
1:C:268:ARG:HG2	1:C:312:VAL:HG21	1.99	0.44
1:A:277:TYR:CD1	1:A:277:TYR:N	2.86	0.44
1:A:436:LEU:O	1:A:437:ILE:C	2.56	0.44
1:C:95:ASP:OD1	1:C:95:ASP:N	2.50	0.44
1:C:199:GLU:HG3	1:C:334:LEU:HG	1.99	0.44
1:A:90:THR:HG22	1:A:92:THR:OG1	2.17	0.44
1:A:407:LEU:HA	1:A:407:LEU:HD23	1.79	0.44
1:A:8:VAL:HG13	1:A:81:VAL:CG1	2.48	0.44
1:A:88:LEU:O	1:A:89:ARG:CB	2.64	0.44
1:C:436:LEU:O	1:C:437:ILE:C	2.60	0.44
1:A:86:TYR:O	1:A:89:ARG:CA	2.64	0.44
1:A:217:ARG:HD2	1:A:224:ALA:HB2	2.00	0.44
1:B:49:VAL:HG11	1:B:57:LEU:CD1	2.47	0.44
1:D:151:ARG:HE	1:D:174:GLN:NE2	2.14	0.44
1:A:144:LYS:O	1:A:147:PRO:HD2	2.18	0.44
1:C:54:ILE:HA	1:C:55:PRO:HD2	1.69	0.44
1:C:91:LEU:HD12	1:C:92:THR:N	2.20	0.44
1:B:88:LEU:O	1:B:89:ARG:CB	2.63	0.43
1:B:192:VAL:O	1:B:195:LEU:HB2	2.18	0.43
1:B:295:TRP:CZ2	1:B:297:PRO:HG3	2.53	0.43
3:B:503:COA:C2A	5:B:603:HOH:O	2.63	0.43
1:C:330:LYS:HE2	1:C:332:PHE:O	2.18	0.43
1:D:324:VAL:CG2	1:D:408:LEU:HB3	2.47	0.43
1:A:92:THR:O	1:A:93:VAL:O	2.35	0.43
1:A:122:ILE:HA	1:A:123:PRO:HD2	1.81	0.43
1:A:24:GLU:HG3	1:A:316:ARG:CG	2.47	0.43
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.59	0.43
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.80	0.43
1:C:277:TYR:CD1	1:C:277:TYR:N	2.86	0.43
1:A:54:ILE:HA	1:A:55:PRO:HD2	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:CG	1:A:312:VAL:HG21	2.48	0.43
1:B:54:ILE:HA	1:B:55:PRO:HD2	1.68	0.43
1:B:84:VAL:O	1:B:86:TYR:CD1	2.71	0.43
1:C:3:LYS:HB3	1:C:107:ASP:OD2	2.18	0.43
1:C:12:ALA:HB2	3:C:502:COA:HN4	1.82	0.43
1:C:23:ARG:NH2	3:C:502:COA:O5A	2.51	0.43
1:C:328:ILE:HG12	1:C:329:PHE:N	2.32	0.43
1:C:398:ALA:H	1:C:399:LEU:HB2	1.84	0.43
1:D:90:THR:CG2	1:D:106:PHE:H	2.31	0.43
1:D:165:ALA:O	1:D:166:GLU:C	2.61	0.43
1:A:149:ALA:CB	1:A:173:LEU:CD2	2.95	0.43
1:C:324:VAL:HG21	1:C:408:LEU:HB3	2.01	0.43
1:C:380:GLU:CG	5:C:608:HOH:O	2.64	0.43
1:A:24:GLU:HG3	1:A:316:ARG:HG3	1.98	0.43
1:A:154:ILE:HB	1:A:177:LEU:HD23	2.00	0.43
1:A:207:VAL:O	1:A:207:VAL:HG22	2.17	0.43
1:A:280:GLY:HA2	1:A:302:ALA:HA	2.01	0.43
1:B:433:ASP:O	1:B:434:PRO:C	2.58	0.43
1:C:360:SER:HB3	1:C:434:PRO:HG3	2.01	0.43
1:A:85:ASP:N	1:A:92:THR:HA	2.15	0.43
1:A:216:PHE:CD1	1:A:225:VAL:HG22	2.54	0.43
1:B:91:LEU:N	1:B:92:THR:HG23	2.33	0.43
1:B:127:GLN:HB3	1:B:128:GLU:H	1.48	0.43
1:C:195:LEU:HA	1:C:195:LEU:HD23	1.80	0.43
1:A:155:LEU:N	1:A:155:LEU:HD12	2.33	0.43
1:C:15:ALA:O	1:C:16:SER:C	2.61	0.43
1:D:159:TYR:O	1:D:160:ILE:C	2.58	0.43
1:D:192:VAL:O	1:D:193:GLY:C	2.62	0.43
1:C:224:ALA:O	1:C:225:VAL:HG23	2.18	0.43
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.81	0.43
1:B:268:ARG:O	1:B:269:MET:HB2	2.19	0.43
1:B:367:TYR:CE1	1:B:427:PRO:HG3	2.53	0.42
1:C:3:LYS:HB3	1:C:107:ASP:CB	2.49	0.42
1:D:296:LEU:HD12	1:D:296:LEU:HA	1.79	0.42
1:A:149:ALA:HB1	1:A:150:ARG:HA	1.94	0.42
1:A:365:HIS:H	4:A:503:VK3:H6K1	1.85	0.42
1:B:280:GLY:HA3	2:B:502:FAD:O2P	2.19	0.42
1:B:90:THR:CG2	1:B:106:PHE:H	2.31	0.42
1:B:143:LEU:HD12	1:B:143:LEU:HA	1.84	0.42
1:C:328:ILE:HG21	1:C:328:ILE:HD13	1.68	0.42
1:D:6:VAL:HG22	1:D:31:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:HG22	1:A:138:ASP:CG	2.44	0.42
1:B:139:GLY:O	1:B:140:GLU:C	2.63	0.42
1:C:85:ASP:OD1	1:C:88:LEU:HD23	2.19	0.42
1:C:94:HIS:CD2	1:C:94:HIS:H	2.31	0.42
1:D:195:LEU:HA	1:D:195:LEU:HD23	1.71	0.42
1:A:396:HIS:NE2	1:B:395:GLY:HA2	2.34	0.42
1:B:195:LEU:HA	1:B:195:LEU:HD23	1.73	0.42
1:A:85:ASP:OD1	1:A:88:LEU:HB3	2.18	0.42
1:B:166:GLU:HA	1:B:332:PHE:CE1	2.55	0.42
1:C:374:TRP:CE3	1:C:392:VAL:HG22	2.55	0.42
1:D:15:ALA:HB1	3:D:502:COA:H142	2.02	0.42
1:B:23:ARG:NH2	3:B:503:COA:O5A	2.53	0.42
1:C:270:ARG:NH2	5:C:619:HOH:O	2.53	0.42
1:D:123:PRO:HG2	1:D:215:ALA:CB	2.50	0.42
1:D:171:ARG:HH11	1:D:171:ARG:HD2	1.62	0.42
1:B:386:LEU:HA	1:B:386:LEU:HD13	1.81	0.42
1:C:24:GLU:CG	1:C:316:ARG:CG	2.98	0.42
1:C:116:ARG:NH2	1:C:248:GLU:OE1	2.53	0.42
1:D:155:LEU:N	1:D:155:LEU:HD12	2.34	0.42
1:A:217:ARG:HB3	1:A:224:ALA:CB	2.33	0.42
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.94	0.42
1:B:328:ILE:HG21	1:B:328:ILE:HD13	1.77	0.41
1:D:22:LYS:HE2	1:D:72:GLY:HA3	2.01	0.41
1:D:87:GLU:CA	1:D:88:LEU:C	2.88	0.41
1:D:227:THR:HG23	1:D:230:GLY:O	2.20	0.41
1:D:268:ARG:HD3	1:D:319:ARG:NH2	2.35	0.41
1:A:189:ASP:OD2	1:A:376:GLU:OE2	2.38	0.41
1:B:3:LYS:HB3	1:B:107:ASP:HB2	2.03	0.41
1:B:248:GLU:OE1	5:B:604:HOH:O	2.22	0.41
1:D:134:ARG:HA	1:D:134:ARG:HD2	1.91	0.41
1:A:69:ARG:C	1:A:71:GLN:N	2.76	0.41
1:A:131:TYR:CG	1:A:142:LEU:HD13	2.55	0.41
1:A:227:THR:HG23	1:A:230:GLY:O	2.21	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.64	0.41
1:A:426:PRO:N	1:A:427:PRO:CD	2.83	0.41
1:C:151:ARG:HE	1:C:174:GLN:HE21	1.67	0.41
1:D:5:MET:SD	1:D:313:ILE:HG21	2.60	0.41
1:D:117:PRO:HD3	1:D:134:ARG:HG2	2.01	0.41
1:D:313:ILE:C	1:D:315:GLY:H	2.29	0.41
1:A:56:ARG:CZ	1:A:59:ARG:HH11	2.33	0.41
1:D:92:THR:O	1:D:93:VAL:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ARG:O	1:D:244:ARG:HG3	2.20	0.41
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.64	0.41
1:D:8:VAL:HG13	1:D:81:VAL:HG13	2.01	0.41
1:D:232:VAL:O	1:D:233:PRO:C	2.56	0.41
1:A:189:ASP:HA	1:A:190:PRO:HD3	1.84	0.41
1:B:302:ALA:CB	2:B:502:FAD:H5'2	2.50	0.41
1:D:306:GLY:O	1:D:307:ARG:C	2.61	0.41
1:D:426:PRO:N	1:D:427:PRO:CD	2.84	0.41
1:A:166:GLU:HA	1:A:332:PHE:CZ	2.55	0.41
1:C:37:GLY:H	1:C:78:ARG:H	1.67	0.41
1:A:151:ARG:NE	1:A:174:GLN:HE21	2.19	0.41
1:A:162:LEU:CD2	1:A:200:LEU:HD11	2.50	0.41
1:B:296:LEU:HG	1:B:298:LEU:HD12	2.03	0.41
1:B:398:ALA:N	1:B:399:LEU:CB	2.84	0.41
1:C:13:GLY:N	2:C:501:FAD:O1P	2.50	0.41
1:C:23:ARG:NH1	3:C:502:COA:O8A	2.53	0.41
1:C:109:LEU:HA	1:C:109:LEU:HD12	1.75	0.41
1:C:389:GLY:HA3	1:C:404:LEU:HD13	2.03	0.41
1:D:138:ASP:O	1:D:139:GLY:C	2.62	0.41
1:D:302:ALA:CB	2:D:501:FAD:H5'2	2.51	0.41
1:A:272:ASN:HD22	1:A:272:ASN:N	2.17	0.41
1:A:281:ASP:CG	2:A:501:FAD:H5'1	2.45	0.41
4:A:503:VK3:H9K1	3:B:503:COA:C7P	2.46	0.41
1:B:11:VAL:HG21	2:B:502:FAD:H4B	2.03	0.41
1:B:92:THR:O	1:B:93:VAL:C	2.60	0.41
1:B:162:LEU:HD22	1:B:200:LEU:HD11	2.03	0.41
1:B:216:PHE:HD1	1:B:225:VAL:HG22	1.86	0.41
1:C:46:LEU:HB2	1:C:47:PRO:HD3	2.03	0.41
1:C:192:VAL:O	1:C:193:GLY:C	2.58	0.41
1:C:269:MET:O	1:C:277:TYR:HB3	2.20	0.41
1:C:321:LEU:HA	1:C:321:LEU:HD23	1.53	0.41
1:C:398:ALA:H	1:C:399:LEU:HB3	1.85	0.41
1:C:418:LEU:HD22	1:C:439:ALA:CB	2.50	0.41
1:D:88:LEU:O	1:D:89:ARG:HB2	2.21	0.41
1:D:122:ILE:O	1:D:125:THR:OG1	2.31	0.41
1:D:295:TRP:CZ2	1:D:297:PRO:HG3	2.55	0.41
1:D:307:ARG:HH11	1:D:307:ARG:HD2	1.60	0.41
1:A:86:TYR:HB2	1:A:87:GLU:H	1.19	0.41
1:B:365:HIS:C	5:B:605:HOH:O	2.63	0.41
1:C:49:VAL:HG11	1:C:57:LEU:CD1	2.51	0.41
1:A:89:ARG:O	1:A:90:THR:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LYS:HE2	1:B:72:GLY:HA3	2.02	0.40
1:C:25:ASN:OD1	1:C:25:ASN:C	2.63	0.40
1:C:260:THR:H	1:C:260:THR:HG23	1.59	0.40
1:A:256:ALA:N	1:A:272:ASN:HD21	2.15	0.40
1:B:296:LEU:HD12	1:B:296:LEU:HA	1.84	0.40
3:B:503:COA:H31	3:B:503:COA:H62	1.86	0.40
1:C:69:ARG:C	1:C:71:GLN:N	2.78	0.40
1:C:184:PRO:HG2	1:C:193:GLY:O	2.21	0.40
1:C:292:ARG:HB2	1:C:293:PRO:CD	2.51	0.40
1:D:38:TRP:CE3	1:D:136:MET:HE2	2.56	0.40
1:D:216:PHE:CE1	1:D:225:VAL:HG22	2.56	0.40
1:D:367:TYR:HA	1:D:368:PRO:HD3	1.91	0.40
1:A:440:GLN:HB3	1:A:441:GLN:H	1.70	0.40
1:B:100:ARG:HB2	1:B:101:THR:H	1.60	0.40
1:B:191:GLU:O	1:B:194:ALA:HB3	2.22	0.40
1:C:66:GLU:HA	1:C:66:GLU:OE1	2.21	0.40
1:C:128:GLU:HB3	1:C:221:ARG:HA	2.03	0.40
1:C:426:PRO:N	1:C:427:PRO:CD	2.84	0.40
1:D:69:ARG:C	1:D:71:GLN:N	2.80	0.40
1:A:25:ASN:OD1	1:A:25:ASN:C	2.64	0.40
1:C:23:ARG:NH2	3:C:502:COA:P2A	2.94	0.40
1:C:136:MET:HE3	1:C:136:MET:HB3	1.99	0.40
1:C:219:MET:HE3	1:C:219:MET:HB3	1.88	0.40
1:C:307:ARG:HH11	1:C:307:ARG:HD2	1.70	0.40
1:D:92:THR:CB	1:D:106:PHE:CE2	3.04	0.40
1:A:183:ARG:HD3	1:A:190:PRO:HA	2.04	0.40
1:B:148:GLN:O	1:B:149:ALA:C	2.64	0.40
1:B:400:ARG:HH11	1:B:400:ARG:HD3	1.79	0.40
1:C:114:GLY:HA2	1:C:281:ASP:HB2	2.03	0.40
1:C:260:THR:HG23	1:C:284:GLU:OE1	2.21	0.40
1:C:313:ILE:C	1:C:315:GLY:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/443 (100%)	378 (86%)	44 (10%)	19 (4%)	2	12
1	B	441/443 (100%)	381 (86%)	40 (9%)	20 (4%)	2	12
1	C	441/443 (100%)	385 (87%)	38 (9%)	18 (4%)	2	13
1	D	441/443 (100%)	386 (88%)	36 (8%)	19 (4%)	2	12
All	All	1764/1772 (100%)	1530 (87%)	158 (9%)	76 (4%)	2	12

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	A	149	ALA
1	A	398	ALA
1	A	441	GLN
1	A	442	ALA
1	B	90	THR
1	B	149	ALA
1	B	222	VAL
1	B	440	GLN
1	B	441	GLN
1	B	442	ALA
1	C	70	LYS
1	C	149	ALA
1	C	441	GLN
1	C	442	ALA
1	D	86	TYR
1	D	90	THR
1	D	149	ALA
1	D	222	VAL
1	D	440	GLN
1	D	441	GLN
1	D	442	ALA
1	A	55	PRO
1	A	70	LYS
1	A	86	TYR
1	A	93	VAL
1	A	222	VAL
1	A	399	LEU
1	A	440	GLN
1	B	86	TYR

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Mol	Chain	Res	Type
1	C	88	LEU
1	C	90	THR
1	C	93	VAL
1	C	222	VAL
1	C	225	VAL
1	C	314	ALA
1	C	398	ALA
1	C	440	GLN
1	D	88	LEU
1	A	148	GLN
1	A	223	GLU
1	B	55	PRO
1	B	88	LEU
1	B	89	ARG
1	B	223	GLU
1	B	246	ASN
1	B	399	LEU
1	D	92	THR
1	D	127	GLN
1	A	88	LEU
1	A	89	ARG
1	A	225	VAL
1	B	70	LYS
1	B	148	GLN
1	C	55	PRO
1	C	92	THR
1	D	55	PRO
1	D	70	LYS
1	D	189	ASP
1	D	223	GLU
1	D	398	ALA
1	D	435	LEU
1	A	246	ASN
1	B	92	THR
1	B	93	VAL
1	B	97	ALA
1	B	225	VAL
1	B	398	ALA
1	C	86	TYR
1	C	89	ARG
1	C	189	ASP
1	D	93	VAL

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Mol	Chain	Res	Type
1	D	225	VAL
1	D	434	PRO
1	C	37	GLY
1	A	139	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%)	275 (81%)	63 (19%)	1	9
1	B	338/338 (100%)	276 (82%)	62 (18%)	2	9
1	C	337/338 (100%)	279 (83%)	58 (17%)	2	11
1	D	337/338 (100%)	277 (82%)	60 (18%)	2	10
All	All	1350/1352 (100%)	1107 (82%)	243 (18%)	2	10

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	8	VAL
1	A	16	SER
1	A	39	VAL
1	A	50	LEU
1	A	58	GLU
1	A	59	ARG
1	A	60	LEU
1	A	78	ARG
1	A	81	VAL
1	A	86	TYR
1	A	91	LEU
1	A	93	VAL
1	A	94	HIS
1	A	101	THR
1	A	111	LEU
1	A	126	GLU

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Mol	Chain	Res	Type
1	A	132	THR
1	A	133	LEU
1	A	142	LEU
1	A	146	LEU
1	A	148	GLN
1	A	160	ILE
1	A	171	ARG
1	A	173	LEU
1	A	175	VAL
1	A	176	THR
1	A	181	LYS
1	A	185	LEU
1	A	199	GLU
1	A	206	GLU
1	A	207	VAL
1	A	208	TRP
1	A	209	THR
1	A	212	LYS
1	A	221	ARG
1	A	222	VAL
1	A	227	THR
1	A	236	LEU
1	A	237	VAL
1	A	268	ARG
1	A	272	ASN
1	A	277	TYR
1	A	285	SER
1	A	301	VAL
1	A	311	SER
1	A	312	VAL
1	A	324	VAL
1	A	355	LYS
1	A	358	ILE
1	A	375	VAL
1	A	377	LEU
1	A	391	VAL
1	A	392	VAL
1	A	394	ARG
1	A	400	ARG
1	A	408	LEU
1	A	410	ARG
1	A	418	LEU

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Mol	Chain	Res	Type
1	A	434	PRO
1	A	437	ILE
1	A	440	GLN
1	A	441	GLN
1	B	3	LYS
1	B	16	SER
1	B	39	VAL
1	B	50	LEU
1	B	58	GLU
1	B	59	ARG
1	B	60	LEU
1	B	78	ARG
1	B	81	VAL
1	B	91	LEU
1	B	93	VAL
1	B	94	HIS
1	B	100	ARG
1	B	101	THR
1	B	111	LEU
1	B	132	THR
1	B	133	LEU
1	B	142	LEU
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	181	LYS
1	B	185	LEU
1	B	196	LEU
1	B	199	GLU
1	B	206	GLU
1	B	207	VAL
1	B	208	TRP
1	B	209	THR
1	B	212	LYS
1	B	221	ARG
1	B	222	VAL
1	B	227	THR
1	B	231	VAL
1	B	236	LEU

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Mol	Chain	Res	Type
1	B	237	VAL
1	B	268	ARG
1	B	272	ASN
1	B	285	SER
1	B	301	VAL
1	B	312	VAL
1	B	319	ARG
1	B	324	VAL
1	B	355	LYS
1	B	372	PRO
1	B	375	VAL
1	B	377	LEU
1	B	391	VAL
1	B	392	VAL
1	B	394	ARG
1	B	400	ARG
1	B	401	ILE
1	B	408	LEU
1	B	410	ARG
1	B	418	LEU
1	B	434	PRO
1	B	437	ILE
1	B	440	GLN
1	B	441	GLN
1	C	16	SER
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	78	ARG
1	C	81	VAL
1	C	86	TYR
1	C	91	LEU
1	C	93	VAL
1	C	94	HIS
1	C	101	THR
1	C	111	LEU
1	C	126	GLU
1	C	132	THR

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Mol	Chain	Res	Type
1	C	133	LEU
1	C	136	MET
1	C	142	LEU
1	C	146	LEU
1	C	148	GLN
1	C	160	ILE
1	C	171	ARG
1	C	173	LEU
1	C	175	VAL
1	C	176	THR
1	C	177	LEU
1	C	185	LEU
1	C	207	VAL
1	C	208	TRP
1	C	209	THR
1	C	212	LYS
1	C	217	ARG
1	C	221	ARG
1	C	222	VAL
1	C	227	THR
1	C	236	LEU
1	C	237	VAL
1	C	272	ASN
1	C	274	GLU
1	C	301	VAL
1	C	324	VAL
1	C	355	LYS
1	C	358	ILE
1	C	375	VAL
1	C	377	LEU
1	C	391	VAL
1	C	392	VAL
1	C	400	ARG
1	C	408	LEU
1	C	410	ARG
1	C	418	LEU
1	C	434	PRO
1	C	437	ILE
1	C	440	GLN
1	C	441	GLN
1	D	16	SER
1	D	44	CYS

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Mol	Chain	Res	Type
1	D	50	LEU
1	D	58	GLU
1	D	59	ARG
1	D	60	LEU
1	D	61	VAL
1	D	78	ARG
1	D	81	VAL
1	D	86	TYR
1	D	91	LEU
1	D	93	VAL
1	D	94	HIS
1	D	101	THR
1	D	111	LEU
1	D	132	THR
1	D	133	LEU
1	D	142	LEU
1	D	146	LEU
1	D	148	GLN
1	D	160	ILE
1	D	173	LEU
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	206	GLU
1	D	207	VAL
1	D	208	TRP
1	D	209	THR
1	D	212	LYS
1	D	221	ARG
1	D	222	VAL
1	D	225	VAL
1	D	227	THR
1	D	236	LEU
1	D	237	VAL
1	D	268	ARG
1	D	285	SER
1	D	292	ARG
1	D	301	VAL
1	D	319	ARG

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Mol	Chain	Res	Type
1	D	324	VAL
1	D	355	LYS
1	D	356	VAL
1	D	359	GLN
1	D	375	VAL
1	D	377	LEU
1	D	391	VAL
1	D	392	VAL
1	D	400	ARG
1	D	408	LEU
1	D	410	ARG
1	D	418	LEU
1	D	434	PRO
1	D	437	ILE
1	D	440	GLN
1	D	441	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	148	GLN
1	A	174	GLN
1	A	272	ASN
1	A	287	HIS
1	A	409	HIS
1	A	441	GLN
1	B	71	GLN
1	B	76	HIS
1	B	174	GLN
1	B	272	ASN
1	B	287	HIS
1	B	396	HIS
1	C	71	GLN
1	C	94	HIS
1	C	148	GLN
1	C	272	ASN
1	C	287	HIS
1	C	359	GLN
1	D	94	HIS
1	D	148	GLN
1	D	174	GLN

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Mol	Chain	Res	Type
1	D	251	GLN
1	D	272	ASN
1	D	287	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	COA	B	503	1	47,50,50	1.62	5 (10%)	69,75,75	2.42	21 (30%)
4	VK3	C	503	-	14,14,14	2.08	2 (14%)	20,20,20	2.28	6 (30%)
4	VK3	B	501	-	14,14,14	2.12	3 (21%)	20,20,20	2.63	11 (55%)
4	VK3	D	503	-	14,14,14	2.29	4 (28%)	20,20,20	2.74	8 (40%)
3	COA	C	502	1	47,50,50	1.68	9 (19%)	69,75,75	2.43	23 (33%)
2	FAD	C	501	-	58,58,58	2.81	24 (41%)	85,89,89	2.26	29 (34%)
4	VK3	A	503	-	14,14,14	2.20	3 (21%)	20,20,20	2.86	11 (55%)
2	FAD	B	502	-	58,58,58	3.12	28 (48%)	85,89,89	2.38	34 (40%)
2	FAD	D	501	-	58,58,58	2.78	27 (46%)	85,89,89	2.28	31 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	501	-	58,58,58	2.83	26 (44%)	85,89,89	2.24	26 (30%)
3	COA	A	502	1	47,50,50	1.76	7 (14%)	69,75,75	2.48	23 (33%)
3	COA	D	502	1	47,50,50	1.80	7 (14%)	69,75,75	2.35	24 (34%)

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
3	COA	B	503	1	-	20/48/64/64	0/3/3/3
4	VK3	C	503	-	-	-	0/2/2/2
4	VK3	B	501	-	-	-	0/2/2/2
4	VK3	D	503	-	-	-	0/2/2/2
3	COA	C	502	1	-	19/48/64/64	0/3/3/3
2	FAD	C	501	-	-	15/34/50/50	0/6/6/6
4	VK3	A	503	-	-	-	0/2/2/2
2	FAD	B	502	-	-	16/34/50/50	0/6/6/6
2	FAD	D	501	-	-	18/34/50/50	0/6/6/6
2	FAD	A	501	-	-	17/34/50/50	0/6/6/6
3	COA	A	502	1	-	19/48/64/64	0/3/3/3
3	COA	D	502	1	-	19/48/64/64	0/3/3/3

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C5A-C4A	9.10	1.55	1.39
2	A	501	FAD	PA-O3P	9.02	1.69	1.59
2	A	501	FAD	C5A-C4A	8.84	1.54	1.39
2	B	502	FAD	PA-O3P	8.84	1.69	1.59
2	D	501	FAD	C5A-C4A	8.74	1.54	1.39
2	B	502	FAD	C5A-C4A	8.46	1.54	1.39
2	C	501	FAD	C9A-C5X	7.44	1.53	1.41
2	D	501	FAD	C9A-C5X	6.94	1.52	1.41
2	B	502	FAD	C9A-C5X	6.93	1.52	1.41
2	A	501	FAD	C9A-C5X	6.69	1.51	1.41
4	D	503	VK3	C10-C5K	6.48	1.51	1.40
4	A	503	VK3	C10-C5K	6.47	1.51	1.40
4	C	503	VK3	C10-C5K	6.28	1.50	1.40
4	B	501	VK3	C10-C5K	6.27	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	COA	C5A-C4A	6.24	1.50	1.39
2	B	502	FAD	C5'-C4'	6.06	1.60	1.51
3	A	502	COA	C4A-N3A	5.77	1.45	1.34
2	B	502	FAD	C4A-N3A	5.62	1.44	1.34
2	A	501	FAD	C4A-N3A	5.57	1.44	1.34
3	D	502	COA	C5A-C4A	5.39	1.48	1.39
2	C	501	FAD	P-O3P	5.38	1.65	1.59
3	A	502	COA	C5A-C4A	5.37	1.48	1.39
2	D	501	FAD	PA-O3P	5.37	1.65	1.59
2	B	502	FAD	C8-C7	5.34	1.53	1.40
3	D	502	COA	P1A-O3A	5.31	1.65	1.59
3	C	502	COA	C5A-C4A	5.29	1.48	1.39
3	D	502	COA	P2A-O3A	5.22	1.65	1.59
2	C	501	FAD	C4A-N3A	5.22	1.44	1.34
2	C	501	FAD	PA-O3P	5.02	1.64	1.59
2	C	501	FAD	C8-C7	4.94	1.52	1.40
2	A	501	FAD	P-O3P	4.63	1.64	1.59
2	B	502	FAD	P-O3P	4.60	1.64	1.59
2	D	501	FAD	C2A-N1A	4.59	1.42	1.33
3	A	502	COA	C5A-C6A	4.57	1.53	1.41
2	B	502	FAD	C5A-C6A	4.51	1.53	1.41
2	C	501	FAD	C2A-N1A	4.48	1.41	1.33
2	D	501	FAD	C4A-N3A	4.48	1.42	1.34
2	D	501	FAD	O2-C2	4.40	1.33	1.24
2	B	502	FAD	C2A-N1A	4.36	1.41	1.33
3	B	503	COA	C5A-C6A	4.32	1.53	1.41
2	D	501	FAD	C5A-C6A	4.26	1.52	1.41
2	D	501	FAD	C2A-N3A	4.25	1.41	1.33
2	B	502	FAD	C4X-C10	4.18	1.56	1.44
2	B	502	FAD	C10-N10	4.17	1.46	1.37
2	C	501	FAD	C4X-N5	4.13	1.39	1.30
2	C	501	FAD	C10-N10	4.05	1.46	1.37
2	A	501	FAD	C8A-N7A	4.01	1.39	1.31
2	A	501	FAD	C4X-N5	3.86	1.39	1.30
2	B	502	FAD	C10-N1	3.83	1.41	1.33
2	C	501	FAD	C1B-N9A	3.77	1.56	1.46
2	A	501	FAD	C1B-N9A	3.77	1.56	1.46
2	D	501	FAD	C8-C7	3.77	1.50	1.40
3	D	502	COA	C5A-C6A	3.76	1.51	1.41
2	A	501	FAD	C5A-C6A	3.71	1.51	1.41
2	B	502	FAD	C8A-N7A	3.68	1.38	1.31
2	D	501	FAD	C9A-N10	3.68	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C4X-C10	3.67	1.55	1.44
3	C	502	COA	C5A-N7A	-3.60	1.32	1.39
2	D	501	FAD	C5'-C4'	3.60	1.56	1.51
2	D	501	FAD	C10-N10	3.58	1.45	1.37
2	C	501	FAD	C5A-C6A	3.53	1.50	1.41
3	B	503	COA	C8A-N7A	3.52	1.38	1.31
2	A	501	FAD	C5'-C4'	3.47	1.56	1.51
2	A	501	FAD	C8-C7	3.46	1.49	1.40
2	A	501	FAD	C10-N10	3.42	1.44	1.37
2	A	501	FAD	C4X-C10	3.40	1.54	1.44
2	D	501	FAD	C4X-C10	3.36	1.54	1.44
2	B	502	FAD	C4'-C3'	3.35	1.59	1.53
3	C	502	COA	C2A-N3A	3.34	1.39	1.33
2	C	501	FAD	C8A-N7A	3.34	1.38	1.31
2	C	501	FAD	C2A-N3A	3.32	1.39	1.33
3	B	503	COA	P1A-O3A	3.30	1.63	1.59
2	B	502	FAD	O3B-C3B	3.25	1.51	1.43
2	C	501	FAD	O3B-C3B	3.18	1.50	1.43
2	D	501	FAD	P-O3P	3.17	1.62	1.59
3	C	502	COA	P3B-O3B	3.14	1.65	1.59
2	A	501	FAD	C2A-N1A	3.13	1.39	1.33
2	D	501	FAD	C8A-N7A	3.13	1.37	1.31
2	B	502	FAD	C2A-N3A	3.08	1.39	1.33
3	B	503	COA	C6A-N6A	3.08	1.42	1.34
2	B	502	FAD	O4'-C4'	3.06	1.49	1.43
2	D	501	FAD	O4-C4	3.04	1.29	1.23
2	A	501	FAD	C8A-N9A	2.98	1.42	1.37
2	D	501	FAD	C1B-N9A	2.96	1.54	1.46
2	D	501	FAD	C4X-N5	2.93	1.37	1.30
2	A	501	FAD	O4'-C4'	2.92	1.49	1.43
2	B	502	FAD	C4X-N5	2.83	1.36	1.30
3	C	502	COA	C5A-C6A	2.83	1.48	1.41
2	C	501	FAD	C8A-N9A	2.82	1.42	1.37
3	C	502	COA	O2B-C2B	-2.79	1.36	1.43
2	C	501	FAD	C4X-C4	2.74	1.54	1.44
2	C	501	FAD	C10-N1	2.72	1.38	1.33
4	D	503	VK3	C2K-C3K	2.72	1.41	1.35
3	A	502	COA	C8A-N7A	2.71	1.36	1.31
2	C	501	FAD	C6-C7	2.70	1.43	1.39
2	B	502	FAD	O2-C2	2.68	1.29	1.24
2	B	502	FAD	O4-C4	2.62	1.28	1.23
3	A	502	COA	C8A-N9A	-2.61	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C3B-C4B	2.58	1.59	1.53
2	B	502	FAD	C1B-N9A	2.56	1.53	1.46
3	A	502	COA	C6A-N6A	2.55	1.40	1.34
2	C	501	FAD	O4-C4	2.54	1.28	1.23
2	D	501	FAD	C10-N1	2.53	1.38	1.33
3	A	502	COA	C6A-N1A	2.49	1.42	1.35
2	C	501	FAD	C9A-N10	2.49	1.45	1.41
3	D	502	COA	C2A-N1A	2.46	1.38	1.33
2	A	501	FAD	O4-C4	2.40	1.28	1.23
3	C	502	COA	C8A-N7A	2.38	1.36	1.31
2	A	501	FAD	PA-O1A	2.38	1.59	1.50
2	D	501	FAD	C4'-C3'	2.37	1.57	1.53
2	B	502	FAD	C4A-N9A	2.36	1.42	1.37
2	B	502	FAD	C3B-C4B	2.36	1.59	1.53
2	A	501	FAD	C9A-N10	2.35	1.45	1.41
2	D	501	FAD	O3B-C3B	2.35	1.48	1.43
2	B	502	FAD	C6A-N1A	2.34	1.42	1.35
2	A	501	FAD	C6A-N1A	2.33	1.42	1.35
3	D	502	COA	C5A-N7A	-2.33	1.34	1.39
2	B	502	FAD	C2-N3	2.33	1.44	1.39
2	D	501	FAD	C2B-C1B	2.32	1.60	1.53
2	B	502	FAD	PA-O1A	2.31	1.58	1.50
4	D	503	VK3	C5K-C4K	2.31	1.52	1.48
3	D	502	COA	OAP-CAP	2.31	1.46	1.42
2	B	502	FAD	C4X-C4	2.31	1.53	1.44
4	D	503	VK3	C3K-C4K	2.30	1.51	1.48
2	D	501	FAD	C6A-N1A	2.29	1.42	1.35
2	D	501	FAD	O2B-C2B	2.29	1.48	1.43
2	D	501	FAD	C1'-N10	2.28	1.53	1.47
2	A	501	FAD	C4X-C4	2.27	1.52	1.44
2	B	502	FAD	PA-O5B	2.26	1.68	1.59
2	C	501	FAD	O4B-C1B	2.25	1.47	1.42
4	C	503	VK3	C2K-C3K	2.23	1.40	1.35
4	B	501	VK3	C2K-C3K	2.22	1.40	1.35
2	A	501	FAD	C4'-C3'	2.21	1.57	1.53
3	C	502	COA	O9P-C9P	2.15	1.27	1.23
2	A	501	FAD	C4A-N9A	2.13	1.42	1.37
4	B	501	VK3	C2K-C1K	-2.11	1.40	1.44
4	A	503	VK3	C2K-C3K	2.10	1.39	1.35
2	A	501	FAD	C10-N1	2.08	1.37	1.33
2	D	501	FAD	C8A-N9A	2.08	1.41	1.37
3	C	502	COA	C9P-N8P	2.08	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C6A-N6A	2.07	1.39	1.34
4	A	503	VK3	C10-C1K	2.05	1.51	1.48
2	D	501	FAD	PA-O5B	2.03	1.67	1.59
2	A	501	FAD	O3B-C3B	2.02	1.48	1.43
2	C	501	FAD	C1'-N10	2.01	1.52	1.47

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	COA	C5A-C4A-N3A	-8.53	114.98	126.72
3	B	503	COA	C5A-C4A-N3A	-8.30	115.29	126.72
3	A	502	COA	C5A-C4A-N3A	-7.67	116.16	126.72
2	D	501	FAD	O4B-C1B-N9A	7.37	122.24	108.09
3	D	502	COA	C7P-C6P-C5P	-7.32	100.20	112.39
2	B	502	FAD	O4B-C1B-N9A	7.17	121.86	108.09
3	D	502	COA	C5A-C4A-N3A	-7.06	117.00	126.72
3	B	503	COA	C7P-C6P-C5P	-6.97	100.78	112.39
2	A	501	FAD	O4B-C1B-N9A	6.97	121.47	108.09
3	B	503	COA	N3A-C4A-N9A	6.97	139.01	127.17
3	A	502	COA	N3A-C4A-N9A	6.67	138.51	127.17
2	B	502	FAD	N3A-C4A-N9A	6.52	138.25	127.17
2	B	502	FAD	C5A-C4A-N3A	-6.51	117.75	126.72
2	C	501	FAD	O4B-C1B-N9A	6.36	120.31	108.09
3	A	502	COA	C7P-C6P-C5P	-6.14	102.16	112.39
3	A	502	COA	N3A-C2A-N1A	-6.09	119.36	128.58
2	A	501	FAD	O2-C2-N1	-6.01	111.82	121.80
2	D	501	FAD	N3A-C4A-N9A	5.83	137.09	127.17
2	C	501	FAD	O2-C2-N1	-5.83	112.12	121.80
3	C	502	COA	N3A-C4A-N9A	5.79	137.02	127.17
2	A	501	FAD	N3A-C4A-N9A	5.75	136.95	127.17
3	A	502	COA	C2A-N3A-C4A	5.74	125.84	111.83
4	D	503	VK3	C6K-C5K-C10	-5.67	112.90	119.26
4	D	503	VK3	C11-C3K-C4K	5.64	127.20	117.83
3	C	502	COA	C2A-N3A-C4A	5.57	125.44	111.83
2	A	501	FAD	N3A-C2A-N1A	-5.21	120.69	128.58
3	C	502	COA	O2B-C2B-C1B	-5.17	92.32	110.10
4	A	503	VK3	C11-C3K-C4K	5.16	126.41	117.83
2	A	501	FAD	C5A-C4A-N3A	-5.15	119.63	126.72
3	B	503	COA	C2A-N3A-C4A	5.12	124.35	111.83
2	C	501	FAD	N3A-C4A-N9A	5.10	135.84	127.17
3	C	502	COA	C7P-C6P-C5P	-5.08	103.93	112.39
3	D	502	COA	N3A-C4A-N9A	5.07	135.79	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	COA	O2A-P1A-O3A	5.07	120.97	107.27
3	C	502	COA	C7P-N8P-C9P	4.95	131.43	122.55
2	B	502	FAD	O2-C2-N1	-4.91	113.65	121.80
3	D	502	COA	O5A-P2A-O4A	4.84	134.97	112.44
2	D	501	FAD	C5A-C4A-N3A	-4.71	120.24	126.72
4	D	503	VK3	C5K-C10-C1K	-4.70	116.76	120.25
2	C	501	FAD	O2'-C2'-C3'	-4.69	98.27	109.25
2	D	501	FAD	N6A-C6A-N1A	4.65	128.74	118.38
4	A	503	VK3	C5K-C10-C1K	-4.65	116.79	120.25
4	C	503	VK3	C11-C3K-C4K	4.62	125.51	117.83
4	B	501	VK3	O1K-C1K-C2K	-4.60	114.52	121.88
3	A	502	COA	C4A-C5A-N7A	-4.48	105.45	110.58
4	C	503	VK3	C6K-C5K-C10	-4.48	114.24	119.26
4	D	503	VK3	C6K-C5K-C4K	4.45	126.59	120.10
2	D	501	FAD	C4A-N9A-C8A	4.43	110.39	105.74
2	D	501	FAD	O2'-C2'-C3'	-4.42	98.90	109.25
4	A	503	VK3	O1K-C1K-C2K	-4.34	114.94	121.88
2	C	501	FAD	C5A-C4A-N3A	-4.34	120.75	126.72
3	C	502	COA	O4B-C1B-C2B	-4.32	97.36	106.62
3	A	502	COA	C7P-N8P-C9P	4.30	130.27	122.55
3	B	503	COA	C4A-N9A-C8A	4.30	110.25	105.74
4	C	503	VK3	C6K-C5K-C4K	4.29	126.36	120.10
4	A	503	VK3	C8K-C7K-C6K	4.27	125.51	120.24
4	B	501	VK3	C6K-C5K-C4K	4.26	126.31	120.10
2	C	501	FAD	N6A-C6A-N1A	4.24	127.81	118.38
3	D	502	COA	O6A-CCP-CBP	-4.22	103.77	110.55
2	A	501	FAD	N6A-C6A-N1A	4.20	127.72	118.38
2	A	501	FAD	C2A-N1A-C6A	4.19	125.61	118.73
2	C	501	FAD	O3B-C3B-C4B	4.18	123.08	111.08
4	A	503	VK3	C7K-C8K-C9K	-4.16	115.11	120.24
3	D	502	COA	O4B-C1B-C2B	-4.14	97.76	106.62
4	B	501	VK3	C5K-C10-C1K	-4.08	117.21	120.25
4	A	503	VK3	C6K-C5K-C4K	4.03	125.97	120.10
2	A	501	FAD	C4'-C3'-C2'	-4.02	106.89	113.57
2	C	501	FAD	C4-C4X-N5	3.99	123.73	118.21
2	D	501	FAD	C9A-N10-C10	-3.95	114.73	120.75
2	B	502	FAD	N6A-C6A-N1A	3.92	127.11	118.38
2	A	501	FAD	C2A-N3A-C4A	3.92	121.40	111.83
4	B	501	VK3	C11-C3K-C4K	3.90	124.31	117.83
3	A	502	COA	C4A-N9A-C8A	3.82	109.75	105.74
3	D	502	COA	C3B-C2B-C1B	3.80	108.24	99.89
3	C	502	COA	C5A-C6A-N6A	-3.80	113.89	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FAD	C5A-C6A-N6A	-3.79	113.91	123.29
3	C	502	COA	N3A-C2A-N1A	-3.78	122.86	128.58
3	D	502	COA	O6A-P2A-O4A	-3.77	94.00	108.94
3	D	502	COA	C2A-N3A-C4A	3.75	120.99	111.83
2	B	502	FAD	O4B-C4B-C3B	3.75	112.59	105.15
2	C	501	FAD	C4X-C10-N10	3.69	121.77	116.48
2	B	502	FAD	O5'-C5'-C4'	3.68	119.18	109.36
2	B	502	FAD	C2A-N3A-C4A	3.62	120.68	111.83
3	A	502	COA	C5A-N7A-C8A	3.61	109.12	103.45
3	A	502	COA	CDP-CBP-CCP	-3.61	102.27	108.22
2	C	501	FAD	O3'-C3'-C4'	3.59	117.09	108.93
3	B	503	COA	C7P-N8P-C9P	3.55	128.93	122.55
3	D	502	COA	C4A-C5A-N7A	-3.54	106.53	110.58
2	A	501	FAD	C4-C4X-N5	3.53	123.09	118.21
3	B	503	COA	C4A-C5A-N7A	-3.52	106.55	110.58
3	B	503	COA	O3A-P1A-O1A	-3.51	100.16	110.70
4	B	501	VK3	O4K-C4K-C3K	-3.50	116.45	120.33
2	B	502	FAD	O3B-C3B-C4B	3.50	121.14	111.08
2	B	502	FAD	N3A-C2A-N1A	-3.49	123.31	128.58
2	C	501	FAD	C3B-C2B-C1B	3.48	108.04	101.46
2	C	501	FAD	C4'-C3'-C2'	-3.46	107.81	113.57
2	D	501	FAD	O4-C4-N3	3.46	126.61	120.11
4	C	503	VK3	C5K-C10-C1K	-3.42	117.71	120.25
2	C	501	FAD	N3A-C2A-N1A	-3.40	123.43	128.58
3	A	502	COA	CEP-CBP-CDP	3.38	115.94	109.20
2	B	502	FAD	C5X-C9A-N10	3.33	120.98	117.97
2	D	501	FAD	C4X-C10-N10	3.32	121.23	116.48
2	B	502	FAD	C4A-C5A-N7A	-3.32	106.79	110.58
2	C	501	FAD	C9A-N10-C10	-3.30	115.72	120.75
2	D	501	FAD	O2-C2-N3	3.29	124.89	118.58
3	D	502	COA	O4B-C1B-N9A	3.27	114.37	108.09
3	C	502	COA	O5P-C5P-C6P	-3.27	116.10	122.02
2	B	502	FAD	C5A-N7A-C8A	3.27	108.58	103.45
2	A	501	FAD	C5A-C6A-N6A	-3.26	115.21	123.29
4	B	501	VK3	C10-C1K-C2K	3.25	123.10	116.55
4	C	503	VK3	C11-C3K-C2K	-3.25	114.58	121.96
2	C	501	FAD	C5A-C6A-N6A	-3.24	115.25	123.29
2	D	501	FAD	C5X-C9A-N10	3.24	120.90	117.97
2	A	501	FAD	O2-C2-N3	3.23	124.79	118.58
2	C	501	FAD	O2-C2-N3	3.23	124.78	118.58
2	B	502	FAD	C9A-N10-C10	-3.19	115.89	120.75
2	B	502	FAD	C4A-N9A-C8A	3.19	109.09	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	C2A-N1A-C6A	3.17	123.93	118.73
4	A	503	VK3	C11-C3K-C2K	-3.14	114.81	121.96
3	C	502	COA	C3B-C2B-C1B	3.13	106.77	99.89
3	C	502	COA	C2B-C3B-C4B	-3.12	97.78	103.24
4	B	501	VK3	C10-C5K-C4K	-3.08	117.41	120.71
2	B	502	FAD	C4'-C3'-C2'	-3.07	108.45	113.57
2	D	501	FAD	O4B-C4B-C3B	3.07	111.25	105.15
4	D	503	VK3	C11-C3K-C2K	-3.05	115.02	121.96
2	D	501	FAD	O3B-C3B-C4B	3.05	119.83	111.08
2	A	501	FAD	C2'-C1'-N10	3.04	124.59	110.20
2	D	501	FAD	C9A-C9-C8	3.04	125.34	119.22
3	C	502	COA	O6A-CCP-CBP	-3.02	105.69	110.55
2	A	501	FAD	O3'-C3'-C4'	3.02	115.80	108.93
2	B	502	FAD	O3'-C3'-C2'	3.01	115.77	108.93
2	D	501	FAD	O4-C4-C4X	-3.00	118.60	126.53
2	A	501	FAD	O3B-C3B-C4B	3.00	119.71	111.08
2	B	502	FAD	O2-C2-N3	2.97	124.28	118.58
2	D	501	FAD	O5'-C5'-C4'	2.95	117.24	109.36
3	C	502	COA	CAP-C9P-N8P	-2.95	110.89	116.48
3	B	503	COA	O5A-P2A-O4A	2.95	126.15	112.44
3	B	503	COA	C3B-C2B-C1B	2.93	106.32	99.89
2	A	501	FAD	C3B-C2B-C1B	2.91	106.96	101.46
2	B	502	FAD	C2'-C1'-N10	2.90	123.91	110.20
3	B	503	COA	O6A-CCP-CBP	-2.90	105.89	110.55
2	D	501	FAD	C5A-C4A-N9A	-2.89	102.66	105.81
2	D	501	FAD	O2B-C2B-C1B	2.89	120.05	110.10
4	A	503	VK3	C6K-C5K-C10	-2.88	116.03	119.26
4	B	501	VK3	C8K-C7K-C6K	2.86	123.77	120.24
3	B	503	COA	O4B-C4B-C3B	2.86	110.96	104.92
3	D	502	COA	O2A-P1A-O3A	2.86	115.01	107.27
2	A	501	FAD	C4X-C10-N10	2.86	120.57	116.48
2	D	501	FAD	O2P-P-O5'	2.84	120.46	107.57
2	D	501	FAD	C10-N1-C2	2.84	123.00	116.85
3	A	502	COA	C2A-N1A-C6A	2.83	123.38	118.73
3	B	503	COA	N9A-C8A-N7A	-2.82	109.93	113.94
3	A	502	COA	C6A-C5A-N7A	2.79	137.46	132.09
2	B	502	FAD	C4X-C10-N10	2.79	120.47	116.48
4	A	503	VK3	C10-C1K-C2K	2.76	122.11	116.55
2	C	501	FAD	O3P-PA-O1A	2.76	119.00	110.70
2	C	501	FAD	O2P-P-O3P	-2.75	99.83	107.27
2	B	502	FAD	C5A-C6A-N6A	-2.72	116.55	123.29
2	A	501	FAD	C9A-N10-C10	-2.71	116.61	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	VK3	C11-C3K-C2K	-2.71	115.79	121.96
3	B	503	COA	N3A-C2A-N1A	-2.71	124.49	128.58
3	C	502	COA	CEP-CBP-CCP	2.68	112.65	108.22
2	C	501	FAD	C7M-C7-C8	2.68	126.22	120.76
4	D	503	VK3	C3K-C2K-C1K	2.67	126.75	123.25
3	C	502	COA	O5A-P2A-O4A	2.67	124.86	112.44
3	D	502	COA	CEP-CBP-CCP	2.66	112.62	108.22
4	B	501	VK3	C6K-C5K-C10	-2.66	116.28	119.26
2	B	502	FAD	C2A-N1A-C6A	2.64	123.07	118.73
2	B	502	FAD	O4B-C4B-C5B	-2.63	100.91	109.33
2	C	501	FAD	C2'-C1'-N10	2.63	122.62	110.20
3	B	503	COA	C5A-N7A-C8A	2.62	107.56	103.45
2	D	501	FAD	C2'-C1'-N10	2.61	122.53	110.20
2	C	501	FAD	C1'-C2'-C3'	2.60	116.70	109.66
2	B	502	FAD	O4-C4-N3	2.60	125.00	120.11
2	B	502	FAD	O3'-C3'-C4'	2.59	114.82	108.93
2	D	501	FAD	C1'-C2'-C3'	2.59	116.67	109.66
2	D	501	FAD	C5A-N7A-C8A	2.58	107.50	103.45
2	C	501	FAD	C10-C4X-N5	-2.56	119.57	124.81
2	D	501	FAD	O2-C2-N1	-2.54	117.57	121.80
3	D	502	COA	C2B-C3B-C4B	-2.54	98.78	103.24
3	B	503	COA	C1B-N9A-C8A	-2.54	121.46	127.09
3	A	502	COA	N9A-C8A-N7A	-2.53	110.35	113.94
4	A	503	VK3	C10-C5K-C4K	-2.53	118.00	120.71
2	C	501	FAD	O5'-C5'-C4'	2.52	116.08	109.36
3	D	502	COA	C6A-C5A-C4A	2.51	120.60	117.18
2	A	501	FAD	C1'-C2'-C3'	2.50	116.45	109.66
2	C	501	FAD	C2A-N3A-C4A	2.50	117.94	111.83
3	A	502	COA	O9P-C9P-N8P	2.50	128.26	122.98
3	A	502	COA	O3A-P2A-O4A	-2.49	103.20	110.70
2	A	501	FAD	O4B-C4B-C3B	2.49	110.09	105.15
3	D	502	COA	P3B-O3B-C3B	2.48	130.06	123.43
3	A	502	COA	O2B-C2B-C1B	-2.47	101.59	110.10
3	D	502	COA	CDP-CBP-CCP	2.47	112.30	108.22
4	D	503	VK3	C7K-C8K-C9K	-2.47	117.19	120.24
2	A	501	FAD	O3P-PA-O1A	2.44	118.05	110.70
3	A	502	COA	O5B-C5B-C4B	-2.43	100.72	108.99
3	A	502	COA	O9A-P3B-O8A	2.43	116.90	107.80
2	B	502	FAD	C10-C4X-N5	-2.40	119.91	124.81
3	C	502	COA	C4A-C5A-N7A	-2.39	107.84	110.58
2	C	501	FAD	C4X-C10-N1	-2.39	118.73	124.59
2	B	502	FAD	O4'-C4'-C5'	2.37	115.20	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	VK3	C7K-C6K-C5K	2.36	124.07	119.80
2	C	501	FAD	C5X-C9A-N10	2.36	120.11	117.97
2	B	502	FAD	C4-C4X-N5	2.35	121.46	118.21
3	C	502	COA	O8A-P3B-O7A	2.35	120.00	110.83
2	B	502	FAD	C1'-C2'-C3'	2.33	115.97	109.66
2	A	501	FAD	C5X-C9A-N10	2.30	120.05	117.97
2	A	501	FAD	O3'-C3'-C2'	2.29	114.13	108.93
2	A	501	FAD	C10-C4X-N5	-2.29	120.14	124.81
3	A	502	COA	CAP-C9P-N8P	-2.27	112.17	116.48
2	D	501	FAD	C2A-N3A-C4A	2.27	117.37	111.83
2	B	502	FAD	O2B-C2B-C1B	2.27	117.91	110.10
3	D	502	COA	C7P-N8P-C9P	2.26	126.60	122.55
3	D	502	COA	O9P-C9P-CAP	2.24	127.14	120.89
2	B	502	FAD	C9-C9A-N10	-2.23	118.85	121.85
2	D	501	FAD	O3'-C3'-C4'	2.23	113.99	108.93
2	D	501	FAD	O3P-P-O1P	-2.23	104.01	110.70
3	C	502	COA	O4B-C1B-N9A	2.22	112.36	108.09
2	C	501	FAD	C5A-C4A-N9A	-2.22	103.39	105.81
2	C	501	FAD	C10-N1-C2	2.20	121.61	116.85
2	A	501	FAD	C5A-C4A-N9A	-2.19	103.42	105.81
3	C	502	COA	P3B-O3B-C3B	2.19	129.28	123.43
2	D	501	FAD	C1'-N10-C9A	2.19	124.89	120.63
3	A	502	COA	O3A-P1A-O1A	-2.19	104.12	110.70
3	C	502	COA	N6A-C6A-N1A	2.17	123.21	118.38
3	D	502	COA	N6A-C6A-N1A	2.16	123.19	118.38
3	D	502	COA	O8A-P3B-O7A	2.14	119.19	110.83
3	B	503	COA	CDP-CBP-CCP	2.13	111.75	108.22
3	C	502	COA	C5A-C6A-N1A	2.12	122.90	117.51
3	D	502	COA	C6P-C5P-N4P	2.12	120.20	116.34
2	B	502	FAD	C3B-C2B-C1B	2.11	105.45	101.46
3	D	502	COA	O2B-C2B-C1B	-2.11	102.85	110.10
2	B	502	FAD	C1B-N9A-C8A	-2.10	122.42	127.09
3	D	502	COA	OAP-CAP-CBP	-2.10	105.32	110.18
2	A	501	FAD	C4X-C10-N1	-2.09	119.46	124.59
3	B	503	COA	N6A-C6A-N1A	2.09	123.03	118.38
4	C	503	VK3	C7K-C6K-C5K	2.08	123.55	119.80
3	B	503	COA	O4B-C1B-N9A	2.07	112.06	108.09
2	D	501	FAD	N9A-C8A-N7A	-2.05	111.03	113.94
2	B	502	FAD	O2'-C2'-C3'	-2.04	104.47	109.25
4	A	503	VK3	C8K-C9K-C10	2.03	123.46	119.80
3	A	502	COA	OAP-CAP-CBP	-2.03	105.49	110.18
4	B	501	VK3	C7K-C8K-C9K	-2.02	117.74	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	COA	O3B-C3B-C2B	-2.02	104.44	111.68
3	C	502	COA	C5A-C4A-N9A	2.01	108.00	105.81
3	A	502	COA	O2A-P1A-O1A	2.01	121.78	112.44
2	D	501	FAD	C3B-C2B-C1B	2.00	105.25	101.46

There are no chirality outliers.

All (143) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	A	502	COA	CCP-O6A-P2A-O3A
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	A	502	COA	CAP-C9P-N8P-C7P
3	A	502	COA	C6P-C5P-N4P-C3P
3	A	502	COA	O5P-C5P-N4P-C3P
3	B	503	COA	CCP-O6A-P2A-O3A
3	B	503	COA	CCP-O6A-P2A-O5A
3	B	503	COA	CDP-CBP-CCP-O6A
3	B	503	COA	CEP-CBP-CCP-O6A
3	B	503	COA	CAP-CBP-CCP-O6A
3	B	503	COA	CAP-C9P-N8P-C7P
3	B	503	COA	C6P-C5P-N4P-C3P
3	B	503	COA	O5P-C5P-N4P-C3P
3	C	502	COA	CCP-O6A-P2A-O3A
3	C	502	COA	CCP-O6A-P2A-O5A
3	C	502	COA	CDP-CBP-CCP-O6A
3	C	502	COA	CEP-CBP-CCP-O6A
3	C	502	COA	CAP-CBP-CCP-O6A
3	C	502	COA	CAP-C9P-N8P-C7P
3	C	502	COA	C5P-C6P-C7P-N8P
3	C	502	COA	C6P-C5P-N4P-C3P
3	D	502	COA	O4B-C4B-C5B-O5B
3	D	502	COA	CCP-O6A-P2A-O3A
3	D	502	COA	CCP-O6A-P2A-O5A
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	D	502	COA	CAP-C9P-N8P-C7P
3	D	502	COA	C5P-C6P-C7P-N8P
3	D	502	COA	S1P-C2P-C3P-N4P
3	C	502	COA	O9P-C9P-N8P-C7P
3	D	502	COA	O9P-C9P-N8P-C7P
3	A	502	COA	O9P-C9P-N8P-C7P
3	B	503	COA	O9P-C9P-N8P-C7P
3	D	502	COA	C6P-C5P-N4P-C3P
3	B	503	COA	O4B-C4B-C5B-O5B
3	C	502	COA	O4B-C4B-C5B-O5B
3	C	502	COA	O5P-C5P-N4P-C3P
3	D	502	COA	O5P-C5P-N4P-C3P

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Mol	Chain	Res	Type	Atoms
2	C	501	FAD	O2'-C2'-C3'-O3'
2	D	501	FAD	O2'-C2'-C3'-O3'
3	B	503	COA	C4B-C3B-O3B-P3B
3	A	502	COA	C3B-C4B-C5B-O5B
3	B	503	COA	C3B-C4B-C5B-O5B
3	D	502	COA	C3B-C4B-C5B-O5B
2	A	501	FAD	O2'-C2'-C3'-O3'
3	C	502	COA	C3B-C4B-C5B-O5B
3	B	503	COA	C2B-C3B-O3B-P3B
2	B	502	FAD	O2'-C2'-C3'-O3'
3	A	502	COA	C3B-O3B-P3B-O7A
3	B	503	COA	P1A-O3A-P2A-O4A
3	D	502	COA	P2A-O3A-P1A-O1A
3	D	502	COA	N8P-C9P-CAP-CBP
2	D	501	FAD	O2'-C2'-C3'-C4'
2	A	501	FAD	PA-O3P-P-O5'
2	B	502	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
3	A	502	COA	C5P-C6P-C7P-N8P
3	D	502	COA	C2B-C3B-O3B-P3B
3	A	502	COA	P2A-O3A-P1A-O2A
3	B	503	COA	P2A-O3A-P1A-O2A
3	B	503	COA	P1A-O3A-P2A-O5A
3	D	502	COA	P2A-O3A-P1A-O2A
3	D	502	COA	P1A-O3A-P2A-O5A
2	C	501	FAD	O2'-C2'-C3'-C4'
3	C	502	COA	C3B-O3B-P3B-O7A
3	A	502	COA	S1P-C2P-C3P-N4P
3	B	503	COA	S1P-C2P-C3P-N4P
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	C5B-O5B-PA-O1A
2	C	501	FAD	C5B-O5B-PA-O2A
2	D	501	FAD	C5B-O5B-PA-O2A
3	A	502	COA	P1A-O3A-P2A-O4A
3	A	502	COA	P1A-O3A-P2A-O5A
3	B	503	COA	P2A-O3A-P1A-O1A
3	C	502	COA	P1A-O3A-P2A-O5A
3	A	502	COA	N8P-C9P-CAP-CBP
2	B	502	FAD	O4B-C1B-N9A-C8A
3	B	503	COA	C3B-O3B-P3B-O7A
3	D	502	COA	C3B-O3B-P3B-O7A

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Mol	Chain	Res	Type	Atoms
2	B	502	FAD	P-O3P-PA-O2A
3	C	502	COA	P2A-O3A-P1A-O1A
2	A	501	FAD	O4B-C1B-N9A-C8A
2	D	501	FAD	O4B-C1B-N9A-C8A
2	A	501	FAD	C2B-C1B-N9A-C8A
2	A	501	FAD	P-O3P-PA-O1A
2	A	501	FAD	P-O3P-PA-O2A
2	C	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	PA-O3P-P-O2P
3	C	502	COA	P1A-O3A-P2A-O4A
2	B	502	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	O4B-C4B-C5B-O5B
3	B	503	COA	C5P-C6P-C7P-N8P
2	B	502	FAD	C2B-C1B-N9A-C8A
3	C	502	COA	C2P-C3P-N4P-C5P
3	C	502	COA	S1P-C2P-C3P-N4P
2	A	501	FAD	PA-O3P-P-O2P
2	B	502	FAD	P-O3P-PA-O1A
2	B	502	FAD	PA-O3P-P-O2P
2	C	501	FAD	PA-O3P-P-O1P
2	C	501	FAD	PA-O3P-P-O2P
3	A	502	COA	P2A-O3A-P1A-O1A
3	C	502	COA	P2A-O3A-P1A-O2A

There are no ring outliers.

12 monomers are involved in 51 short contacts:

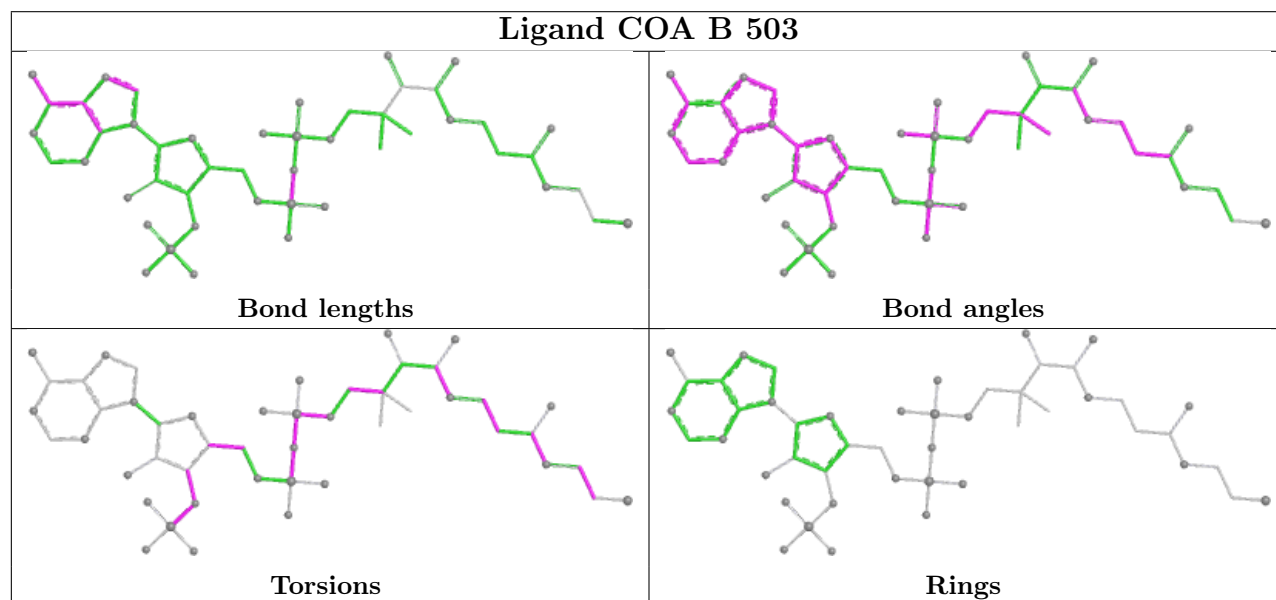
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	COA	10	0
4	C	503	VK3	2	0
4	B	501	VK3	1	0
4	D	503	VK3	2	0
3	C	502	COA	11	0
2	C	501	FAD	5	0
4	A	503	VK3	4	0
2	B	502	FAD	5	0
2	D	501	FAD	5	0
2	A	501	FAD	3	0
3	A	502	COA	4	0

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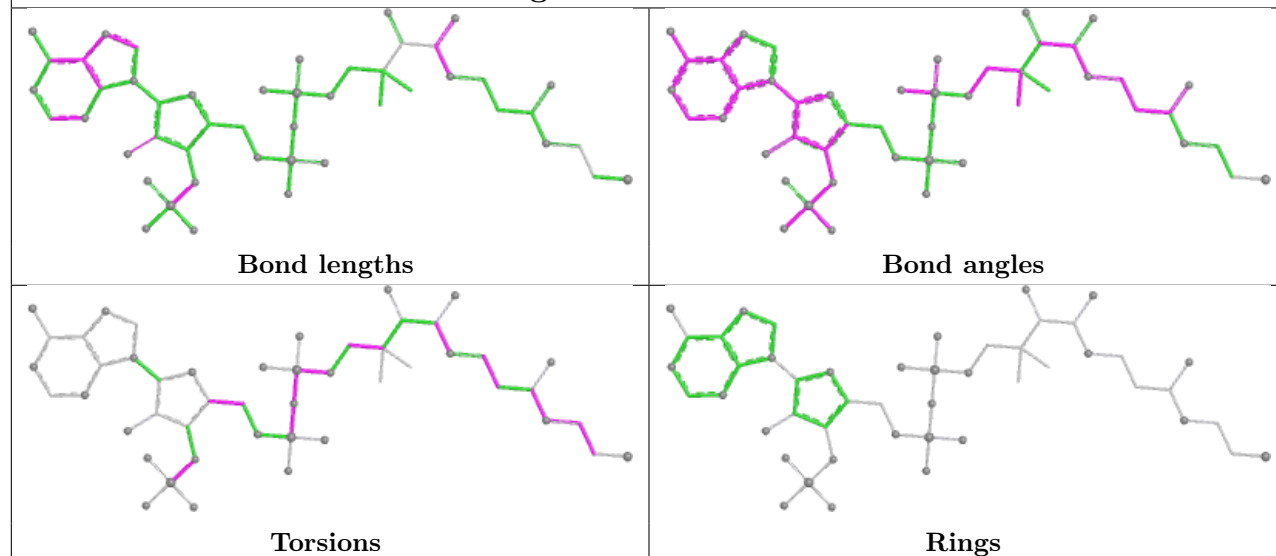
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	COA	5	0

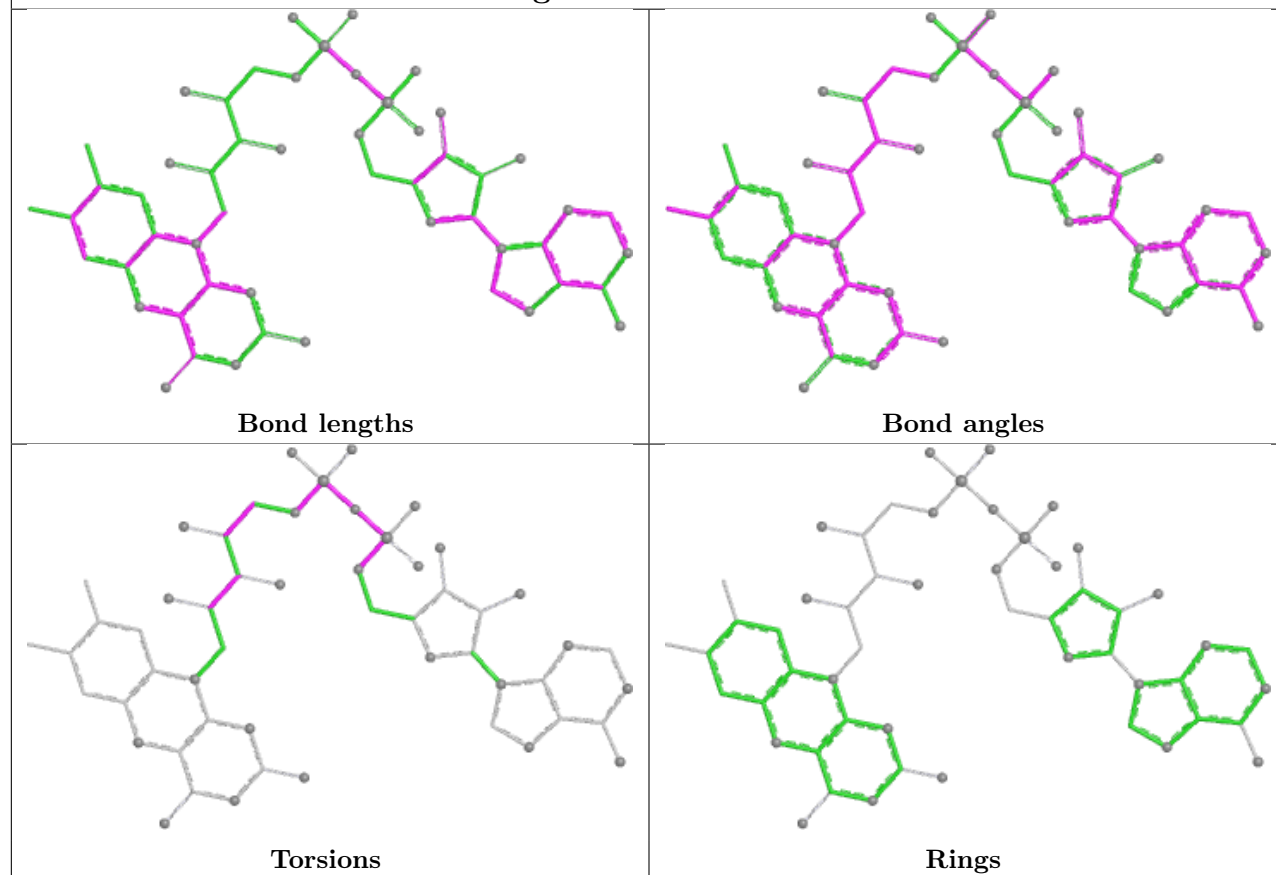
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

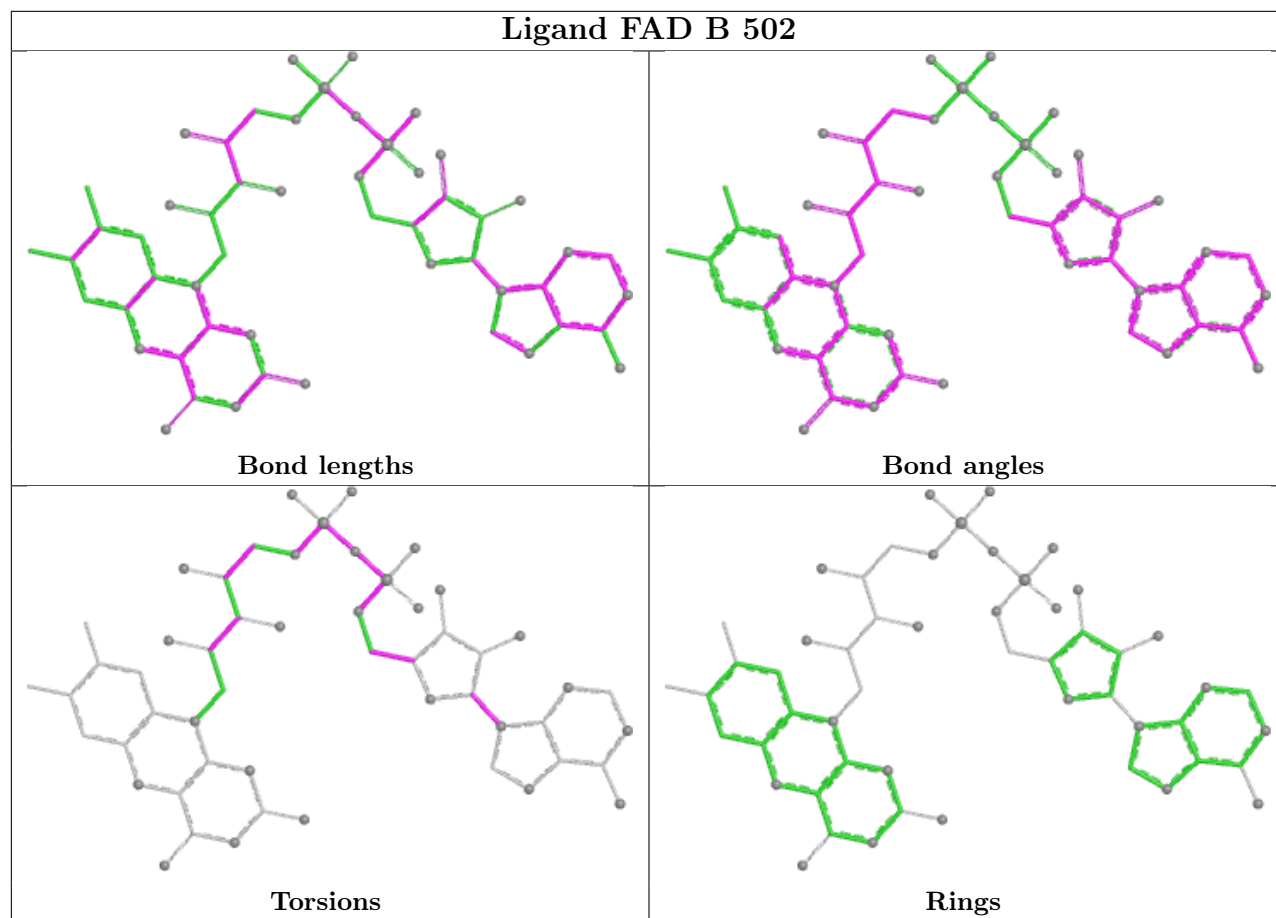


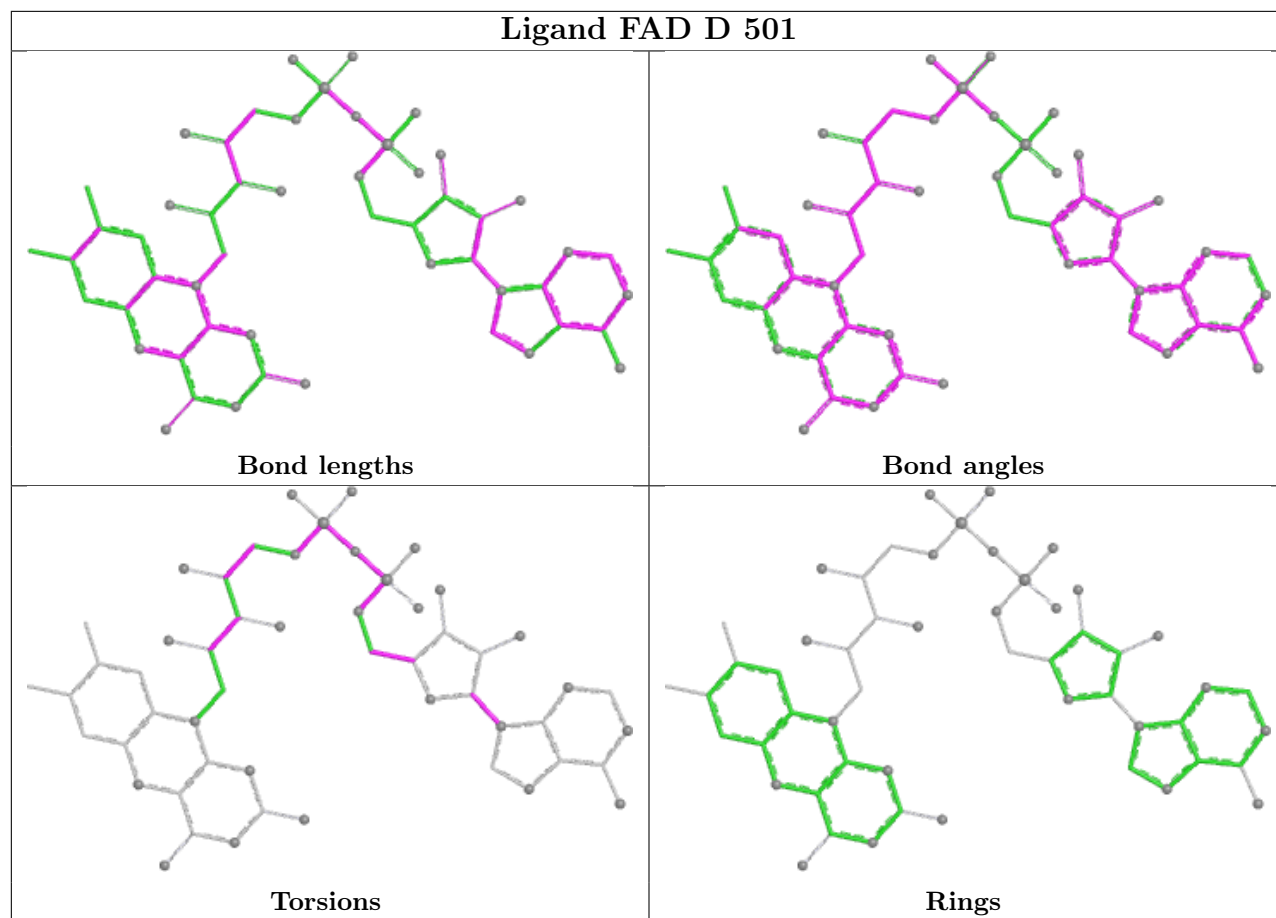
Ligand COA C 502



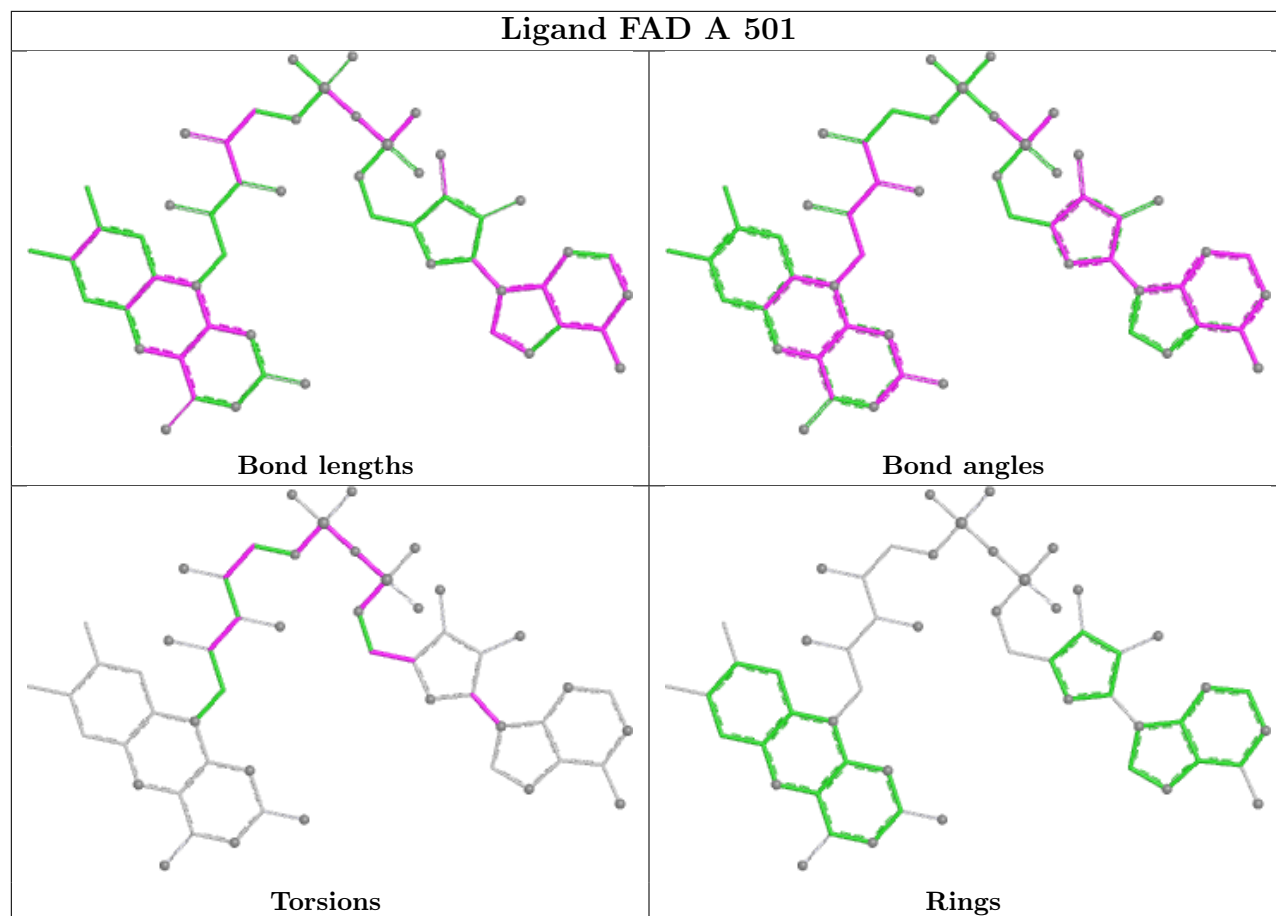
Ligand FAD C 501



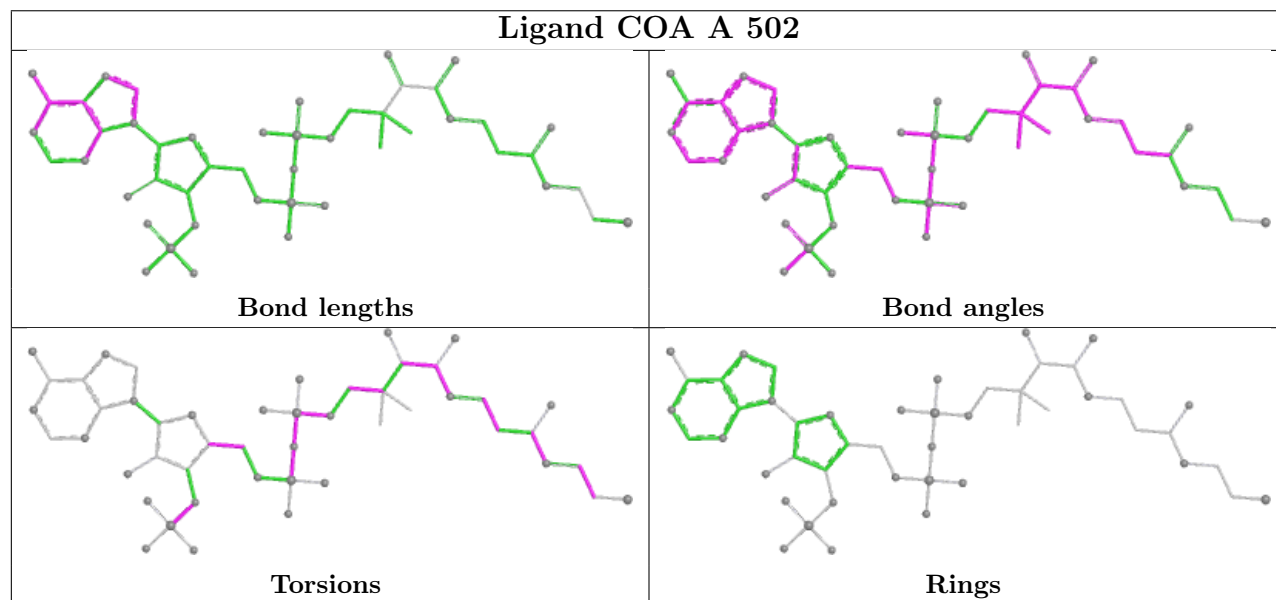


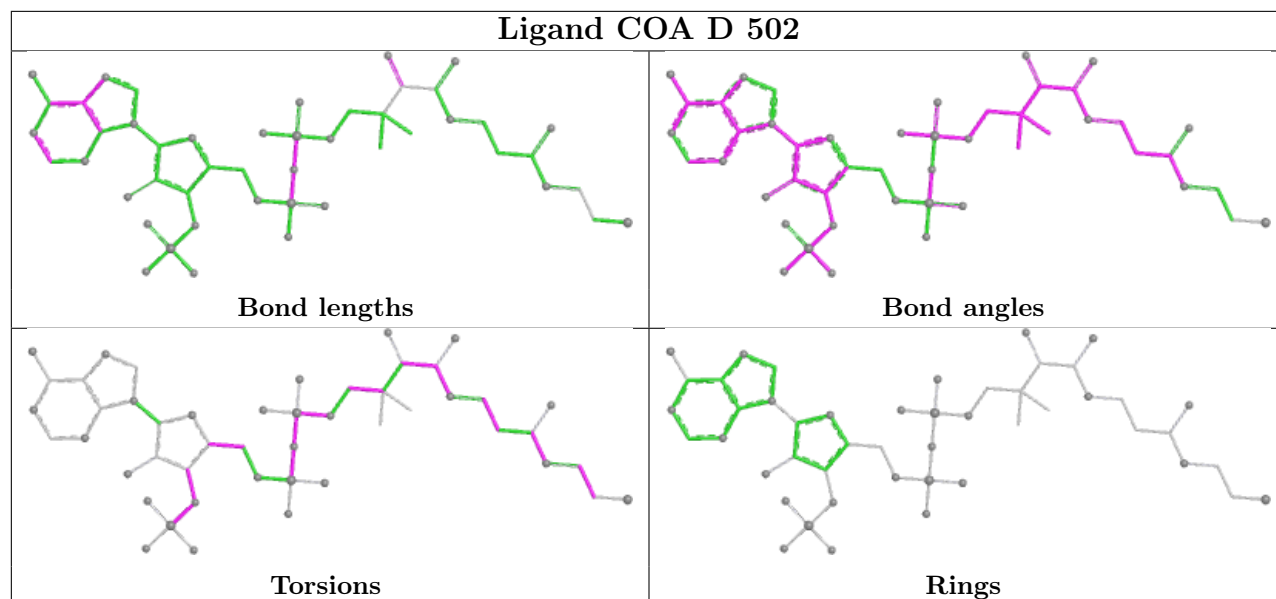


Ligand FAD A 501



Ligand COA A 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%)	-0.08	8 (1%) 67 44	28, 47, 74, 134	0
1	B	443/443 (100%)	-0.04	10 (2%) 61 38	29, 48, 75, 137	0
1	C	443/443 (100%)	-0.08	9 (2%) 65 41	28, 48, 74, 136	0
1	D	443/443 (100%)	-0.05	10 (2%) 61 38	27, 49, 76, 137	0
All	All	1772/1772 (100%)	-0.06	37 (2%) 63 40	27, 48, 76, 137	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.1
1	D	1	MET	6.0
1	A	1	MET	4.6
1	A	396	HIS	4.4
1	D	88	LEU	4.2
1	D	396	HIS	4.2
1	C	1	MET	3.8
1	C	396	HIS	3.7
1	D	443	ARG	3.6
1	B	396	HIS	3.5
1	D	442	ALA	3.5
1	B	86	TYR	3.2
1	A	2	GLY	3.2
1	D	91	LEU	3.1
1	A	86	TYR	3.0
1	C	88	LEU	3.0
1	B	88	LEU	2.9
1	A	88	LEU	2.8
1	C	362	ASP	2.8
1	D	2	GLY	2.7
1	C	221	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	443	ARG	2.6
1	B	440	GLN	2.4
1	A	443	ARG	2.4
1	C	443	ARG	2.4
1	B	94	HIS	2.3
1	C	91	LEU	2.3
1	A	219	MET	2.3
1	B	442	ALA	2.3
1	B	187	HIS	2.2
1	D	352	TRP	2.2
1	D	78	ARG	2.1
1	C	2	GLY	2.1
1	C	87	GLU	2.1
1	A	442	ALA	2.1
1	B	87	GLU	2.0
1	D	219	MET	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
4	VK3	D	503	13/13	0.51	0.44	80,101,140,141	0
4	VK3	A	503	13/13	0.65	0.33	80,100,137,143	0
4	VK3	B	501	13/13	0.72	0.34	79,106,136,140	0
4	VK3	C	503	13/13	0.75	0.31	81,103,139,139	0
2	FAD	B	502	53/53	0.80	0.19	55,83,109,156	0
2	FAD	D	501	53/53	0.84	0.18	54,81,111,141	0
2	FAD	C	501	53/53	0.86	0.17	50,79,108,131	0

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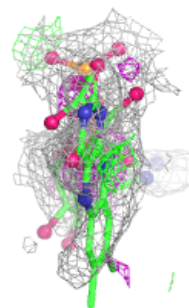
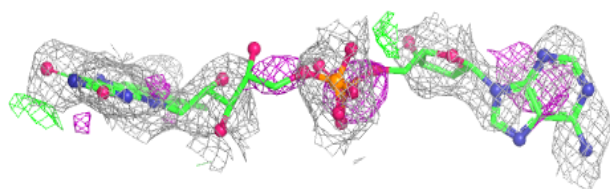
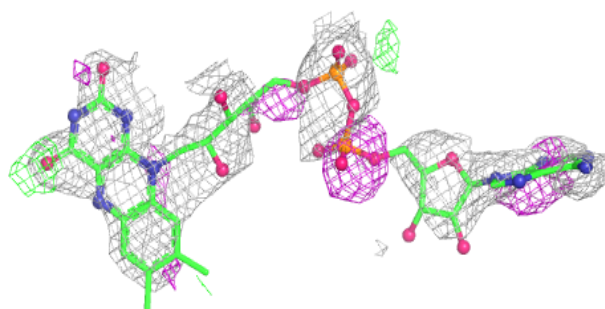
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	501	53/53	0.87	0.16	54,81,113,152	0
3	COA	A	502	48/48	0.94	0.09	38,52,70,94	0
3	COA	B	503	48/48	0.95	0.09	39,52,75,91	0
3	COA	C	502	48/48	0.96	0.09	37,52,74,99	0
3	COA	D	502	48/48	0.96	0.09	36,52,73,94	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.

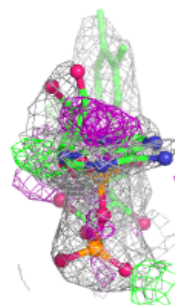
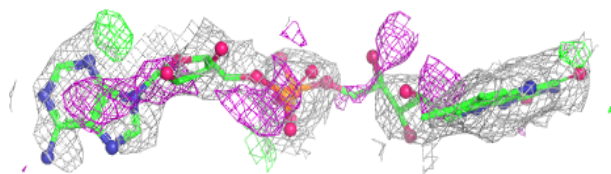
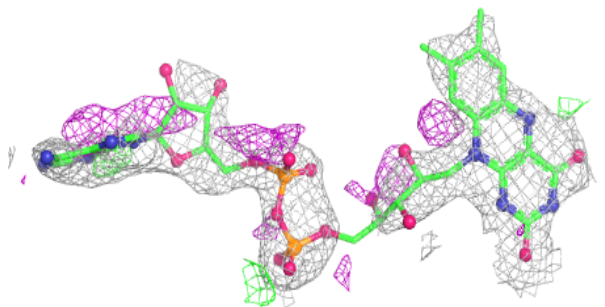
Electron density around FAD B 502:

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

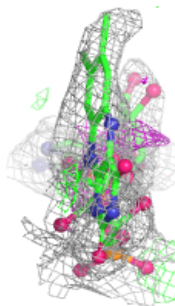
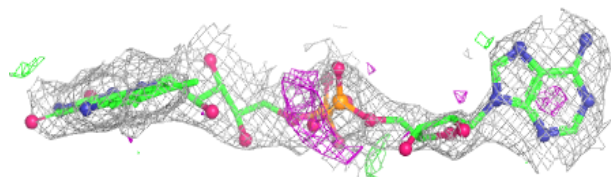
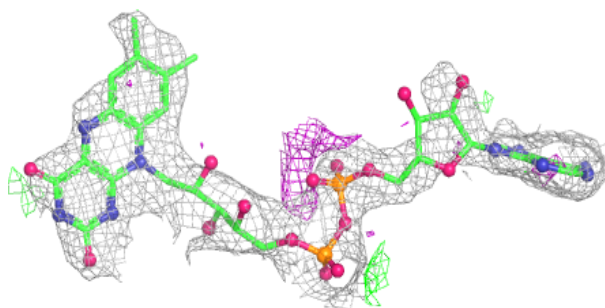


Electron density around FAD D 501:

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

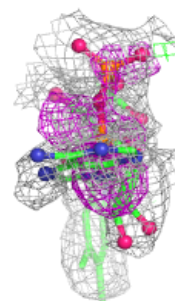
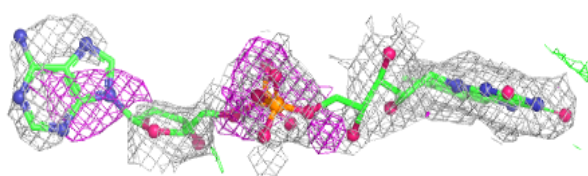
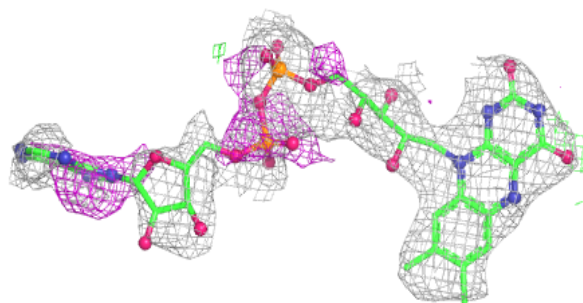
**Electron density around FAD C 501:**

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

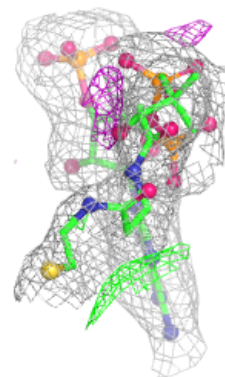
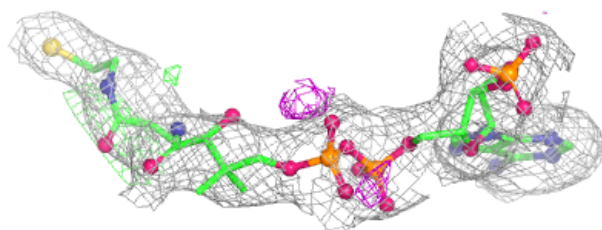
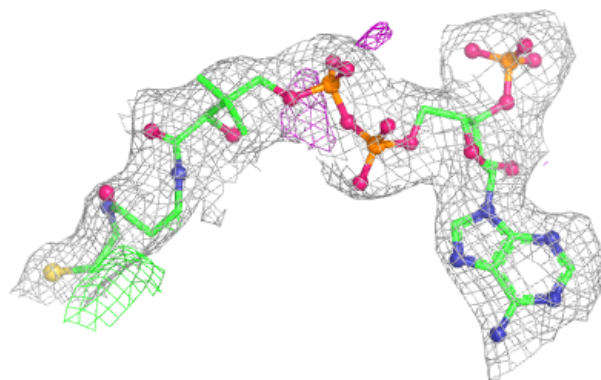


Electron density around FAD A 501:

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

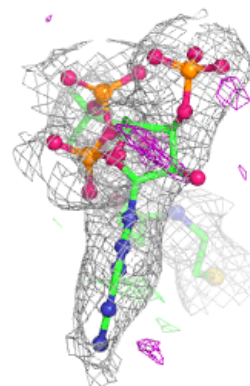
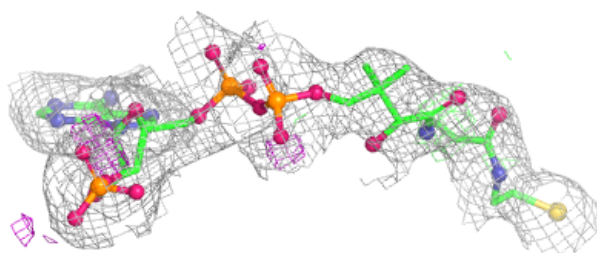
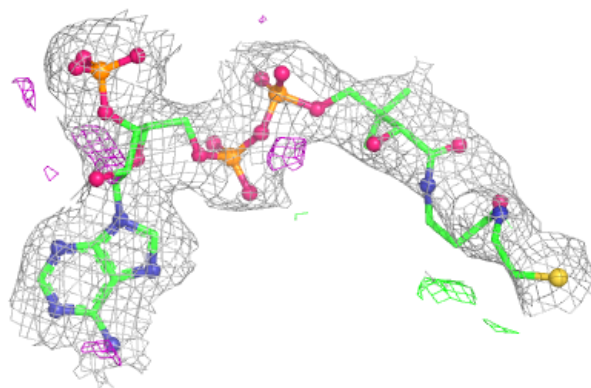
**Electron density around COA A 502:**

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

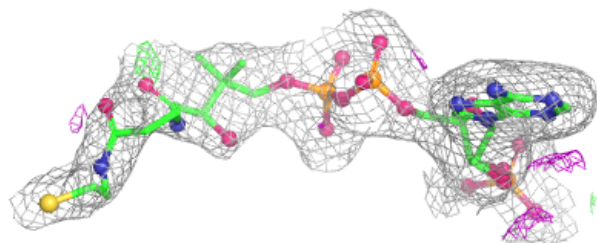
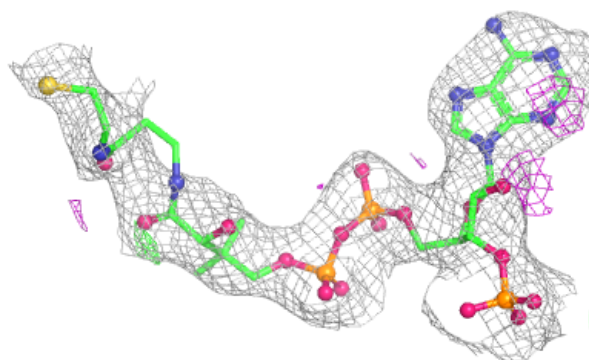


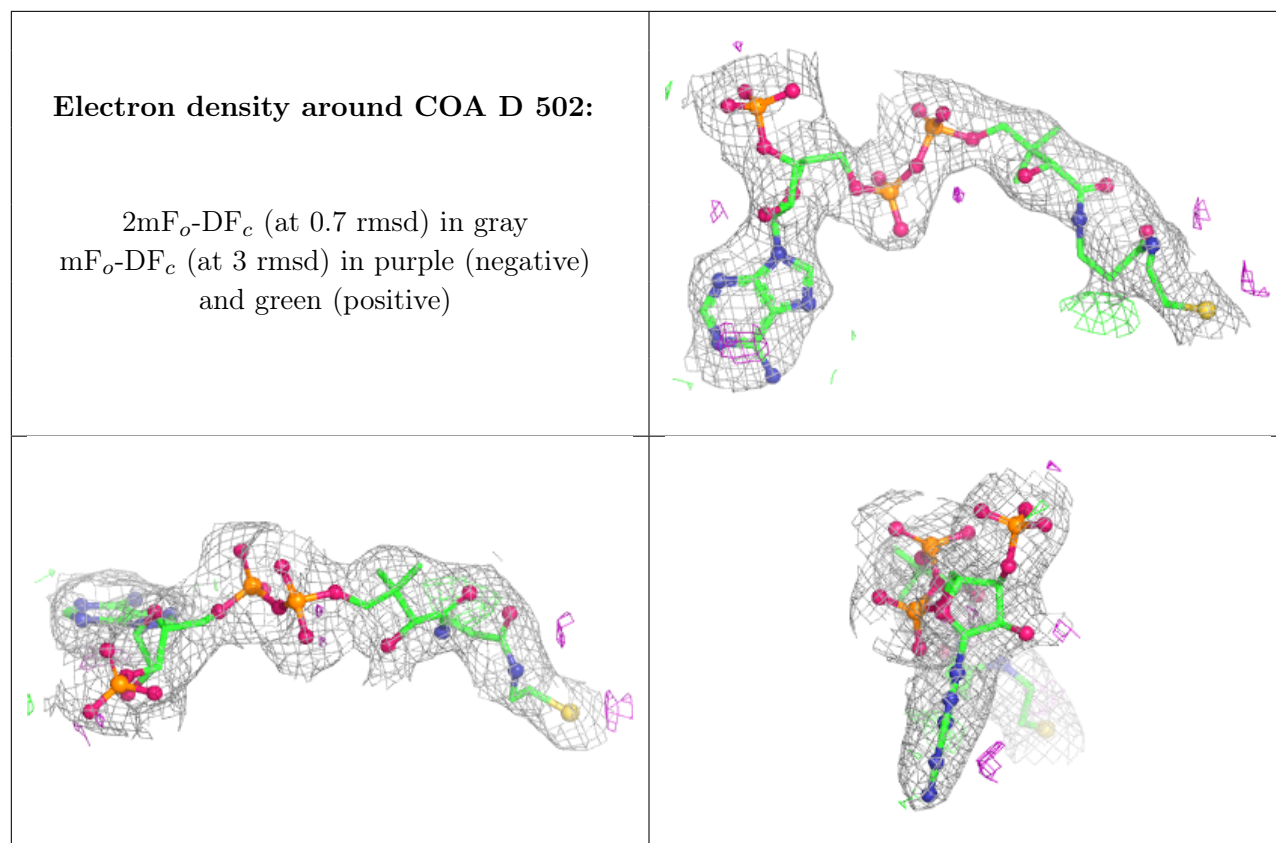
Electron density around COA B 503:

$2mF_o - DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.