Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 12:52 pm BST

PDB ID	:	6RVH
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 (i) symbol.

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

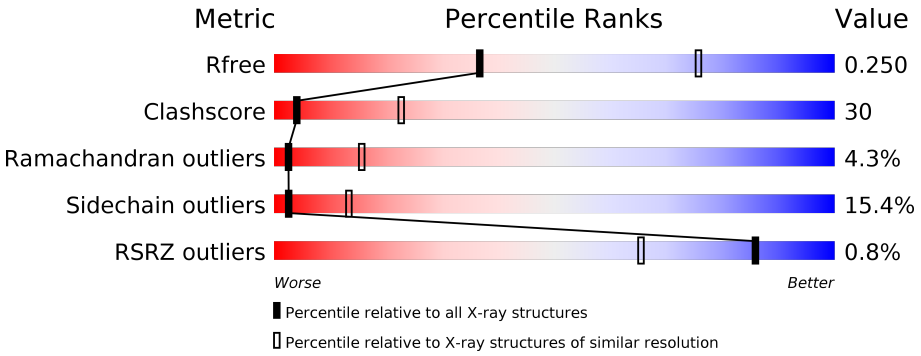
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on 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 <=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	54% 30% 12% 5%
1	B	443	51% 33% 13%
1	C	443	49% 37% 12%
1	D	443	49% 36% 12%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	VK3	A	503	-	-	-	X
4	VK3	B	501	-	-	-	X
4	VK3	C	503	-	-	-	X
4	VK3	D	503	-	-	-	X

2 Entry composition

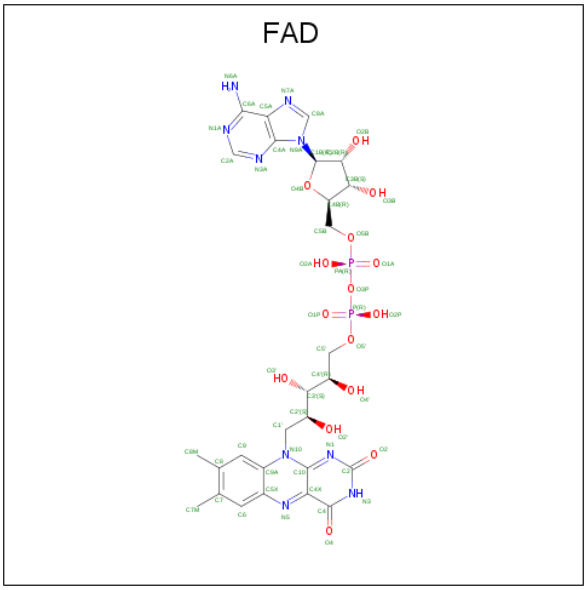
There are 5 unique types of molecules in this entry. The entry contains 14105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by author).



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

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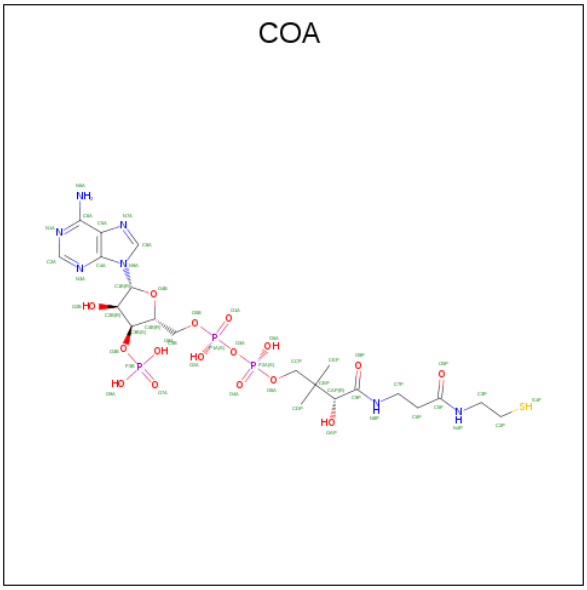
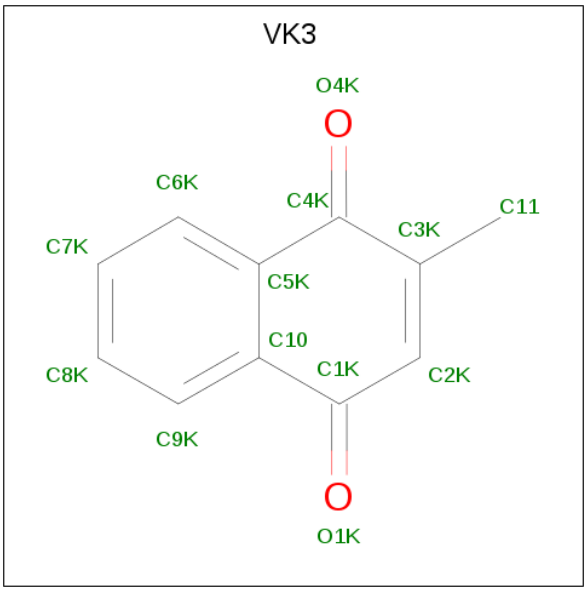
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 4 is MENADIONE (three-letter code: VK3) (formula: $C_{11}H_8O_2$).



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

- Molecule 5 is water.

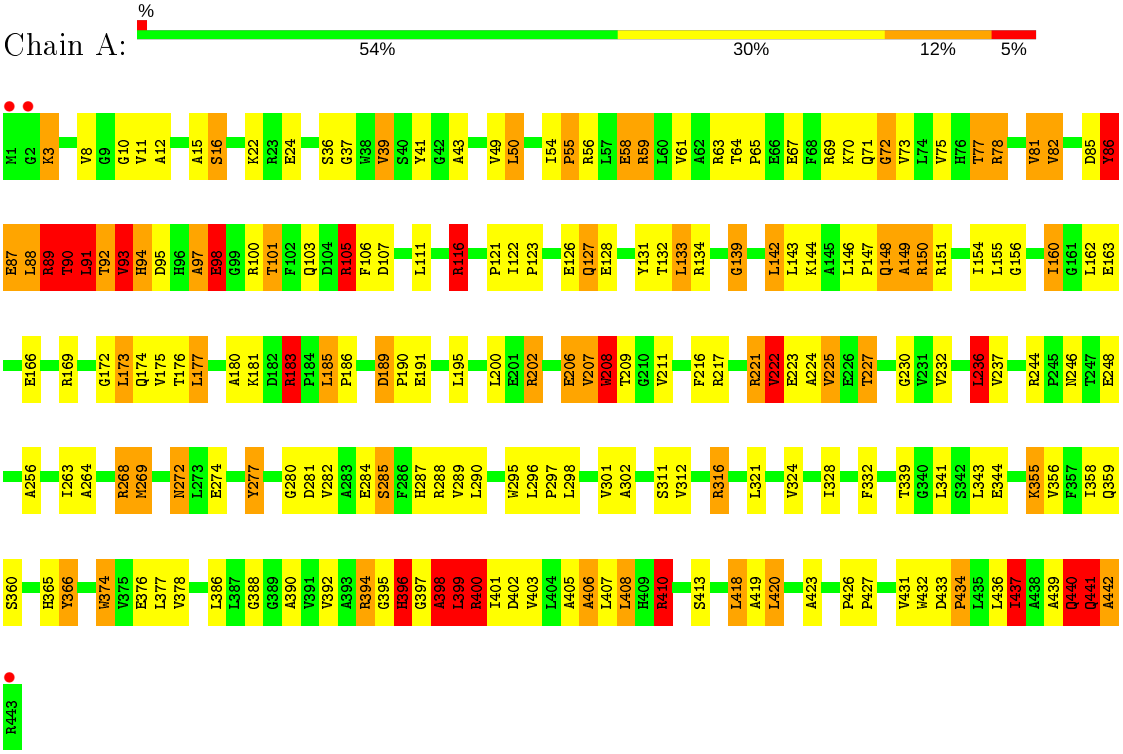
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	35	Total O 35 35	0	0
5	B	35	Total O 35 35	0	0
5	C	36	Total O 36 36	0	0
5	D	30	Total O 30 30	0	0

3 Residue-property plots (i)

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

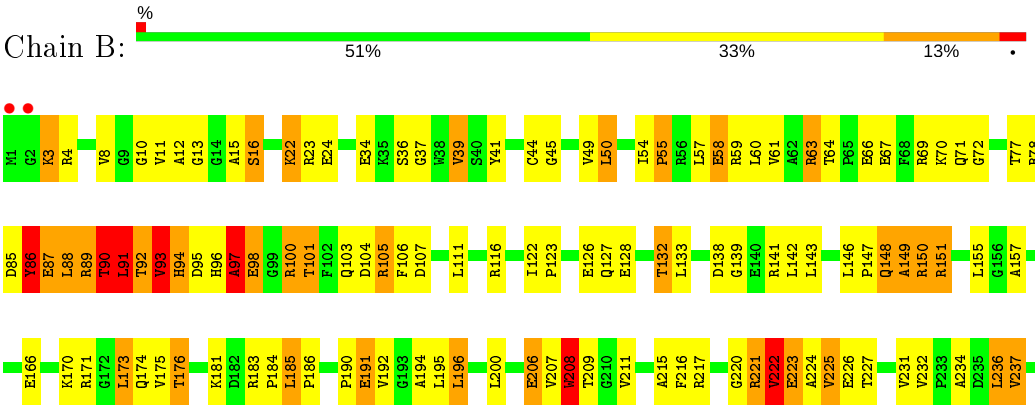
- Molecule 1: NADH oxidase

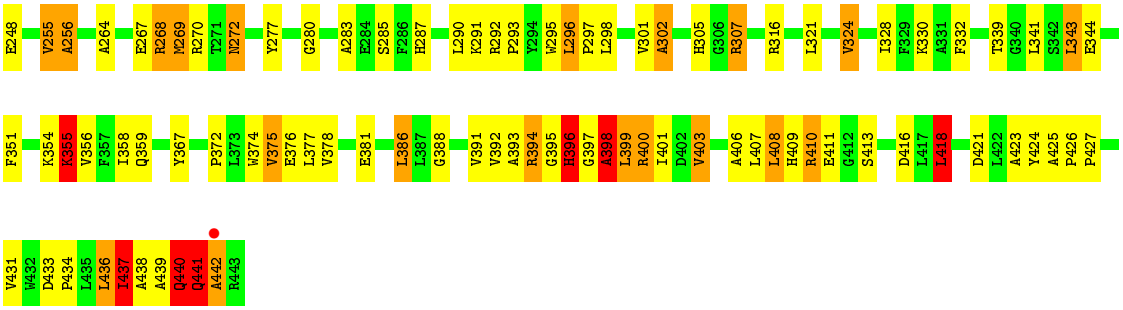
Chain A:



- Molecule 1: NADH oxidase

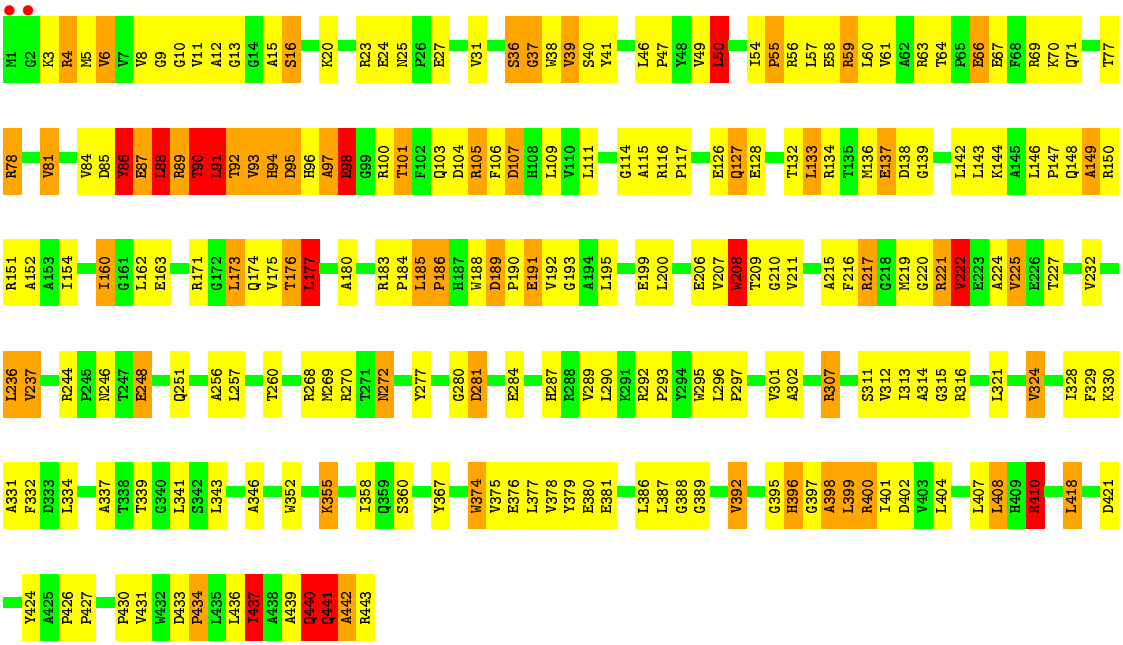
Chain B:





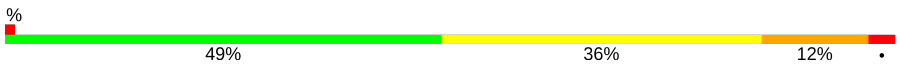
• Molecule 1: NADH oxidase

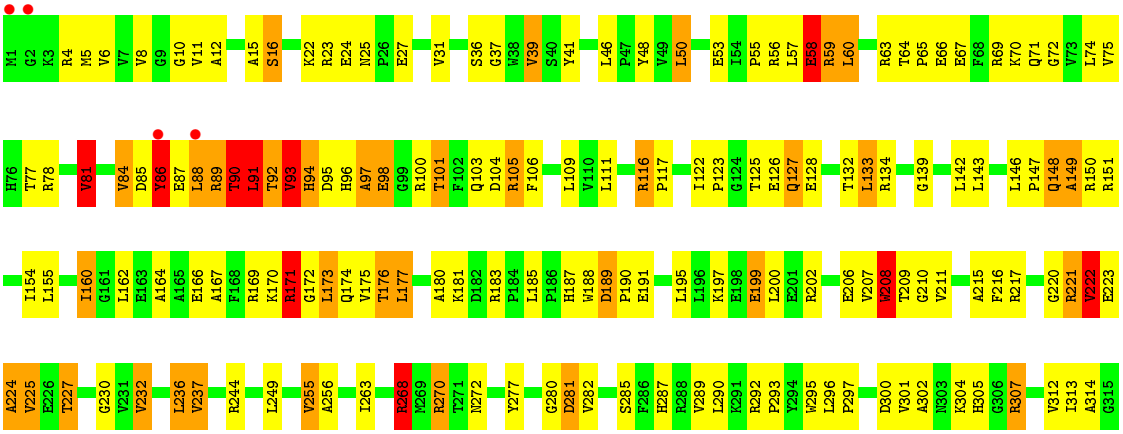
Chain C:

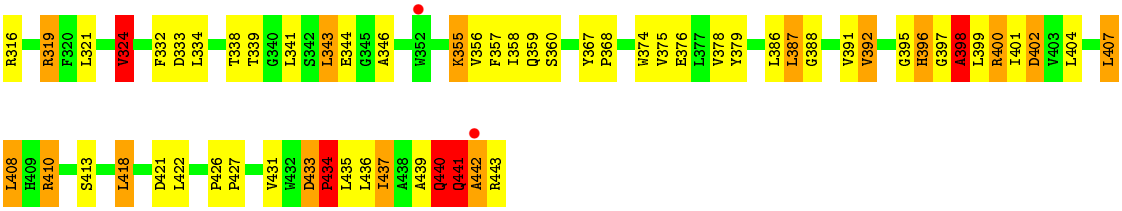


• Molecule 1: NADH oxidase

Chain D:






R316
R319
F320
L321
V324
F332
D333
L334
T338
T339
G340
L341
S342
L343
E344
G345
A346
W352
K355
V356
F357
I358
Q359
S360
Y367
P368
W374
V375
E376
L377
V378
Y379
L386
L387
G388
V391
V392
G395
H396
G397
A398
L399
R400
I401
D402
V403
L404
L407
L408
H409
R410
S413
L418
D421
L422
P426
P427
V431
W432
D433
P434
L435
L436
I437
A438
A439
Q440
Q441
A442
R443

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.215 , 0.259 0.206 , 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)	0.33 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, VK3, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.69	50/3451 (1.4%)	1.53	50/4686 (1.1%)
1	B	1.60	36/3451 (1.0%)	1.48	35/4686 (0.7%)
1	C	1.63	32/3450 (0.9%)	1.45	32/4683 (0.7%)
1	D	1.59	37/3449 (1.1%)	1.44	28/4683 (0.6%)
All	All	1.63	155/13801 (1.1%)	1.47	145/18738 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	5
1	C	0	5
1	D	0	6
All	All	0	24

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLU	CB-CG	10.85	1.72	1.52
1	B	208	TRP	CG-CD1	9.69	1.50	1.36
1	B	398	ALA	CA-CB	-9.22	1.33	1.52
1	D	396	HIS	C-O	8.88	1.40	1.23
1	B	438	ALA	CA-CB	-8.84	1.33	1.52
1	A	406	ALA	CA-CB	-8.79	1.33	1.52
1	B	86	TYR	CD1-CE1	8.72	1.52	1.39
1	B	86	TYR	CB-CG	8.65	1.64	1.51
1	D	41	TYR	CD2-CE2	8.24	1.51	1.39
1	B	93	VAL	CA-CB	8.20	1.72	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	98	GLU	CG-CD	8.17	1.64	1.51
1	C	126	GLU	CG-CD	8.13	1.64	1.51
1	C	86	TYR	CB-CG	8.07	1.63	1.51
1	D	126	GLU	CB-CG	8.05	1.67	1.52
1	A	396	HIS	C-O	7.94	1.38	1.23
1	C	126	GLU	CB-CG	7.90	1.67	1.52
1	A	440	GLN	C-O	7.86	1.38	1.23
1	C	441	GLN	CG-CD	7.79	1.69	1.51
1	A	356	VAL	CB-CG1	-7.71	1.36	1.52
1	A	86	TYR	CB-CG	7.71	1.63	1.51
1	A	156	GLY	C-O	-7.67	1.11	1.23
1	A	398	ALA	CA-CB	-7.64	1.36	1.52
1	A	390	ALA	CA-CB	-7.54	1.36	1.52
1	A	208	TRP	CG-CD1	7.54	1.47	1.36
1	D	93	VAL	CA-CB	7.41	1.70	1.54
1	C	396	HIS	C-O	7.36	1.37	1.23
1	C	163	GLU	CG-CD	7.29	1.62	1.51
1	D	84	VAL	CB-CG1	-7.21	1.37	1.52
1	D	395	GLY	C-O	-7.17	1.12	1.23
1	B	396	HIS	C-O	7.12	1.36	1.23
1	A	126	GLU	CG-CD	7.08	1.62	1.51
1	D	208	TRP	CB-CG	7.05	1.62	1.50
1	D	66	GLU	CG-CD	7.04	1.62	1.51
1	D	97	ALA	CA-CB	6.96	1.67	1.52
1	D	86	TYR	CD1-CE1	6.93	1.49	1.39
1	B	126	GLU	CB-CG	6.82	1.65	1.52
1	A	378	VAL	CA-CB	6.80	1.69	1.54
1	C	208	TRP	CG-CD1	6.71	1.46	1.36
1	B	86	TYR	CD2-CE2	6.62	1.49	1.39
1	B	264	ALA	CA-CB	-6.62	1.38	1.52
1	A	437	ILE	CA-CB	6.56	1.70	1.54
1	A	86	TYR	CD1-CE1	6.54	1.49	1.39
1	A	58	GLU	CG-CD	6.52	1.61	1.51
1	A	98	GLU	CG-CD	6.48	1.61	1.51
1	D	98	GLU	CD-OE1	6.45	1.32	1.25
1	C	163	GLU	CD-OE1	6.44	1.32	1.25
1	A	208	TRP	CD2-CE2	6.43	1.49	1.41
1	B	66	GLU	CG-CD	6.42	1.61	1.51
1	A	86	TYR	CG-CD1	6.40	1.47	1.39
1	A	98	GLU	CD-OE2	-6.35	1.18	1.25
1	B	291	LYS	CE-NZ	6.33	1.64	1.49
1	C	86	TYR	CD1-CE1	6.24	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	TRP	CG-CD1	6.20	1.45	1.36
1	C	337	ALA	CA-CB	-6.19	1.39	1.52
1	A	344	GLU	CG-CD	6.15	1.61	1.51
1	D	66	GLU	CB-CG	6.07	1.63	1.52
1	A	73	VAL	CB-CG2	-6.06	1.40	1.52
1	D	58	GLU	CG-CD	6.06	1.61	1.51
1	A	274	GLU	CG-CD	6.04	1.61	1.51
1	B	86	TYR	CE1-CZ	6.03	1.46	1.38
1	A	378	VAL	CB-CG1	-6.02	1.40	1.52
1	B	208	TRP	CB-CG	6.01	1.61	1.50
1	C	215	ALA	CA-CB	-5.99	1.39	1.52
1	A	43	ALA	CA-CB	-5.98	1.39	1.52
1	A	264	ALA	CA-CB	-5.98	1.40	1.52
1	B	87	GLU	CD-OE1	5.98	1.32	1.25
1	A	87	GLU	CA-C	5.97	1.68	1.52
1	A	72	GLY	C-O	5.96	1.33	1.23
1	C	378	VAL	CB-CG1	-5.95	1.40	1.52
1	C	248	GLU	CG-CD	5.90	1.60	1.51
1	A	206	GLU	CD-OE2	5.89	1.32	1.25
1	A	402	ASP	CB-CG	5.87	1.64	1.51
1	B	441	GLN	CG-CD	5.86	1.64	1.51
1	D	81	VAL	CB-CG2	5.85	1.65	1.52
1	B	440	GLN	C-O	5.85	1.34	1.23
1	C	374	TRP	CE3-CZ3	5.81	1.48	1.38
1	A	441	GLN	CG-CD	5.79	1.64	1.51
1	C	115	ALA	CA-CB	-5.79	1.40	1.52
1	A	408	LEU	CA-CB	-5.79	1.40	1.53
1	C	402	ASP	CB-CG	5.79	1.64	1.51
1	A	399	LEU	N-CA	5.78	1.57	1.46
1	A	49	VAL	CB-CG1	-5.78	1.40	1.52
1	D	126	GLU	CG-CD	5.78	1.60	1.51
1	B	126	GLU	CG-CD	5.74	1.60	1.51
1	B	58	GLU	CG-CD	5.73	1.60	1.51
1	A	86	TYR	CD2-CE2	5.72	1.48	1.39
1	B	411	GLU	CG-CD	5.70	1.60	1.51
1	A	366	TYR	CE1-CZ	5.68	1.46	1.38
1	A	285	SER	CB-OG	5.65	1.49	1.42
1	B	267	GLU	CG-CD	5.64	1.60	1.51
1	B	86	TYR	CG-CD1	5.62	1.46	1.39
1	B	163	GLU	CD-OE1	5.61	1.31	1.25
1	D	441	GLN	CG-CD	5.61	1.64	1.51
1	D	392	VAL	CB-CG1	-5.60	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	GLU	CG-CD	5.57	1.60	1.51
1	D	293	PRO	C-O	5.55	1.34	1.23
1	A	405	ALA	CA-CB	-5.54	1.40	1.52
1	C	379	TYR	CD1-CE1	5.54	1.47	1.39
1	D	443	ARG	CB-CG	5.54	1.67	1.52
1	D	39	VAL	CB-CG2	-5.53	1.41	1.52
1	D	402	ASP	CB-CG	5.52	1.63	1.51
1	C	6	VAL	CB-CG1	-5.51	1.41	1.52
1	C	186	PRO	CA-C	-5.50	1.41	1.52
1	D	232	VAL	CB-CG2	5.50	1.64	1.52
1	B	378	VAL	CB-CG2	-5.49	1.41	1.52
1	A	284	GLU	CG-CD	5.49	1.60	1.51
1	C	440	GLN	C-O	5.45	1.33	1.23
1	A	441	GLN	CB-CG	5.44	1.67	1.52
1	C	87	GLU	CA-C	5.42	1.67	1.52
1	D	346	ALA	CA-CB	5.42	1.63	1.52
1	A	180	ALA	CA-CB	-5.41	1.41	1.52
1	A	86	TYR	CE1-CZ	5.41	1.45	1.38
1	D	422	LEU	C-O	5.39	1.33	1.23
1	B	86	TYR	CG-CD2	5.39	1.46	1.39
1	D	86	TYR	CB-CG	5.38	1.59	1.51
1	C	9	GLY	C-O	-5.33	1.15	1.23
1	A	248	GLU	CG-CD	5.33	1.59	1.51
1	C	208	TRP	CB-CG	5.31	1.59	1.50
1	D	344	GLU	CD-OE2	5.30	1.31	1.25
1	D	53	GLU	CG-CD	5.28	1.59	1.51
1	B	355	LYS	CE-NZ	5.26	1.62	1.49
1	A	97	ALA	CA-CB	5.24	1.63	1.52
1	B	255	VAL	CA-CB	-5.23	1.43	1.54
1	B	440	GLN	CD-NE2	5.22	1.45	1.32
1	A	77	THR	CA-CB	-5.20	1.39	1.53
1	D	324	VAL	CB-CG2	-5.20	1.42	1.52
1	C	86	TYR	CE1-CZ	5.18	1.45	1.38
1	A	163	GLU	CD-OE1	5.18	1.31	1.25
1	C	66	GLU	CG-CD	5.14	1.59	1.51
1	B	256	ALA	C-O	5.14	1.33	1.23
1	B	330	LYS	CD-CE	5.14	1.64	1.51
1	A	289	VAL	CA-CB	-5.12	1.44	1.54
1	A	374	TRP	CE3-CZ3	5.12	1.47	1.38
1	C	89	ARG	CG-CD	5.11	1.64	1.51
1	D	199	GLU	CD-OE2	5.11	1.31	1.25
1	D	431	VAL	CB-CG1	-5.11	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	GLU	CG-CD	5.10	1.59	1.51
1	D	443	ARG	CG-CD	5.10	1.64	1.51
1	C	98	GLU	CG-CD	5.09	1.59	1.51
1	B	351	PHE	CG-CD2	5.08	1.46	1.38
1	B	97	ALA	N-CA	5.08	1.56	1.46
1	C	97	ALA	CA-CB	5.08	1.63	1.52
1	C	331	ALA	CA-CB	-5.07	1.41	1.52
1	A	156	GLY	CA-C	-5.06	1.43	1.51
1	B	87	GLU	CA-C	5.05	1.66	1.52
1	D	441	GLN	CA-CB	5.05	1.65	1.53
1	C	443	ARG	CG-CD	5.04	1.64	1.51
1	A	89	ARG	CB-CG	5.03	1.66	1.52
1	D	255	VAL	CB-CG2	-5.03	1.42	1.52
1	B	302	ALA	CA-CB	-5.03	1.41	1.52
1	D	89	ARG	CB-CG	5.03	1.66	1.52
1	D	48	TYR	CB-CG	5.02	1.59	1.51
1	C	191	GLU	CG-CD	5.02	1.59	1.51
1	A	90	THR	CB-CG2	5.01	1.68	1.52
1	B	403	VAL	CB-CG1	-5.01	1.42	1.52

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	91	LEU	CA-CB-CG	11.08	140.79	115.30
1	D	91	LEU	CA-CB-CG	10.15	138.65	115.30
1	A	91	LEU	CA-CB-CG	10.06	138.43	115.30
1	B	91	LEU	CA-CB-CG	9.78	137.79	115.30
1	B	63	ARG	NE-CZ-NH1	-9.41	115.59	120.30
1	B	307	ARG	NE-CZ-NH1	-8.95	115.83	120.30
1	A	410	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	C	421	ASP	CB-CG-OD2	-8.86	110.32	118.30
1	A	189	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	D	95	ASP	CB-CG-OD1	-8.39	110.75	118.30
1	C	4	ARG	NE-CZ-NH1	-8.39	116.11	120.30
1	A	134	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	398	ALA	N-CA-C	-7.95	89.55	111.00
1	A	105	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	269	MET	CG-SD-CE	7.63	112.41	100.20
1	C	402	ASP	CB-CG-OD2	7.61	125.15	118.30
1	B	151	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	394	ARG	NE-CZ-NH2	7.51	124.06	120.30
1	A	402	ASP	CB-CG-OD2	7.47	125.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	394	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	A	105	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	97	ALA	N-CA-CB	7.31	120.34	110.10
1	A	63	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	B	330	LYS	CD-CE-NZ	7.28	128.45	111.70
1	D	96	HIS	N-CA-CB	-7.19	97.67	110.60
1	A	420	LEU	CB-CG-CD1	-7.18	98.80	111.00
1	A	183	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	C	177	LEU	CA-CB-CG	7.07	131.57	115.30
1	A	98	GLU	OE1-CD-OE2	-6.99	114.91	123.30
1	A	400	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	C	208	TRP	CA-CB-CG	6.97	126.94	113.70
1	D	396	HIS	O-C-N	6.88	134.89	123.20
1	B	396	HIS	O-C-N	6.85	134.85	123.20
1	C	89	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	410	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	D	433	ASP	CB-CG-OD2	6.82	124.44	118.30
1	D	160	ILE	C-N-CA	-6.80	108.01	122.30
1	A	92	THR	CA-CB-CG2	-6.69	103.04	112.40
1	D	270	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	C	36	SER	C-N-CA	-6.58	108.48	122.30
1	D	343	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	A	36	SER	C-N-CA	-6.52	108.61	122.30
1	A	396	HIS	CA-C-N	-6.50	103.20	116.20
1	B	63	ARG	NE-CZ-NH2	6.49	123.54	120.30
1	B	87	GLU	OE1-CD-OE2	6.47	131.07	123.30
1	A	116	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	391	VAL	CG1-CB-CG2	6.45	121.22	110.90
1	B	386	LEU	CB-CG-CD1	-6.44	100.06	111.00
1	A	396	HIS	O-C-N	6.41	134.10	123.20
1	D	116	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	202	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	160	ILE	C-N-CA	-6.34	108.98	122.30
1	A	402	ASP	OD1-CG-OD2	-6.27	111.38	123.30
1	C	396	HIS	CA-C-N	-6.27	103.67	116.20
1	C	95	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	C	307	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	D	396	HIS	CA-C-N	-6.22	103.76	116.20
1	B	396	HIS	CA-C-N	-6.22	103.76	116.20
1	C	397	GLY	N-CA-C	6.20	128.59	113.10
1	B	416	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	396	HIS	O-C-N	6.16	133.68	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	87	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	D	407	LEU	CB-CG-CD2	-6.12	100.59	111.00
1	C	410	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	96	HIS	N-CA-CB	-6.08	99.66	110.60
1	A	98	GLU	CG-CD-OE1	6.06	130.42	118.30
1	A	398	ALA	CB-CA-C	6.05	119.17	110.10
1	A	208	TRP	CA-CB-CG	6.02	125.14	113.70
1	C	160	ILE	C-N-CA	-6.01	109.68	122.30
1	A	126	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	A	288	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	307	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	B	150	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	151	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	36	SER	C-N-CA	-5.91	109.89	122.30
1	C	5	MET	CG-SD-CE	5.90	109.64	100.20
1	A	150	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	298	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	A	133	LEU	CB-CA-C	-5.88	99.04	110.20
1	A	402	ASP	CB-CG-OD1	5.86	123.58	118.30
1	C	63	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	C	97	ALA	N-CA-CB	5.84	118.28	110.10
1	A	269	MET	CG-SD-CE	5.80	109.49	100.20
1	A	89	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	399	LEU	CB-CG-CD2	5.76	120.80	111.00
1	B	397	GLY	N-CA-C	5.75	127.48	113.10
1	B	437	ILE	CA-CB-CG2	5.75	122.41	110.90
1	A	397	GLY	C-N-CA	5.75	136.08	121.70
1	B	437	ILE	CG1-CB-CG2	-5.72	98.81	111.40
1	D	90	THR	CB-CA-C	-5.72	96.15	111.60
1	B	93	VAL	CG1-CB-CG2	-5.68	101.81	110.90
1	B	343	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	D	171	ARG	CG-CD-NE	-5.64	99.96	111.80
1	C	90	THR	OG1-CB-CG2	5.61	122.91	110.00
1	A	440	GLN	CA-C-N	-5.60	104.88	117.20
1	A	82	VAL	CB-CA-C	-5.59	100.78	111.40
1	B	421	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	22	LYS	CD-CE-NZ	-5.58	98.87	111.70
1	D	63	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	160	ILE	N-CA-C	-5.51	96.13	111.00
1	D	421	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	191	GLU	OE1-CD-OE2	5.48	129.87	123.30
1	D	396	HIS	C-N-CA	5.47	133.79	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	281	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	B	96	HIS	N-CA-CB	-5.42	100.85	110.60
1	D	404	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	A	202	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	97	ALA	N-CA-CB	5.38	117.64	110.10
1	A	177	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	A	401	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	D	300	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	141	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	13	GLY	N-CA-C	-5.31	99.82	113.10
1	A	440	GLN	O-C-N	5.30	131.17	122.70
1	A	436	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	B	91	LEU	CB-CG-CD1	5.27	119.95	111.00
1	C	281	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	D	333	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	398	ALA	CB-CA-C	5.25	117.97	110.10
1	B	296	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	A	339	THR	CA-CB-CG2	5.21	119.69	112.40
1	C	395	GLY	N-CA-C	5.21	126.11	113.10
1	D	89	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	387	LEU	CB-CG-CD2	5.18	119.81	111.00
1	C	443	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	127	GLN	N-CA-C	5.13	124.85	111.00
1	D	169	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	A	288	ARG	N-CA-C	5.11	124.81	111.00
1	B	436	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	B	36	SER	C-N-CA	-5.10	111.59	122.30
1	A	236	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	150	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	378	VAL	N-CA-C	-5.05	97.35	111.00
1	B	418	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	A	172	GLY	N-CA-C	5.05	125.73	113.10
1	A	316	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	437	ILE	CA-CB-CG2	5.04	120.98	110.90
1	C	171	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	C	107	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	268	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	50	LEU	CB-CG-CD2	5.03	119.54	111.00
1	C	421	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	208	TRP	CA-CB-CG	5.01	123.22	113.70
1	A	356	VAL	CG1-CB-CG2	-5.01	102.89	110.90
1	C	88	LEU	CB-CA-C	5.00	119.70	110.20

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3379	0	3407	204	0
1	B	3379	0	3407	223	0
1	C	3378	0	3402	213	0
1	D	3377	0	3402	211	0
2	A	53	0	31	2	0
2	B	53	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	5	0
2	D	53	0	31	5	0
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	9	0
5	B	35	0	0	13	0
5	C	36	0	0	25	0
5	D	30	0	0	22	0
All	All	14105	0	13897	839	0

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

All (839) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:GLY:HA2	1:D:77:THR:HB	1.34	1.03
1:A:440:GLN:HA	1:A:440:GLN:NE2	1.74	1.03
1:B:149:ALA:HB3	1:B:150:ARG:HA	1.35	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:B:85:ASP:C	1:B:92:THR:HG22	1.80	1.02
1:D:440:GLN:NE2	1:D:440:GLN:HA	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:217:ARG:HB3	1:A:224:ALA:HB3	1.47	0.94
1:A:91:LEU:HD12	1:A:92:THR:H	1.33	0.94
1:A:85:ASP:H	1:A:92:THR:HA	1.32	0.94
1:C:440:GLN:HA	1:C:440:GLN:NE2	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:NE2	1:B:440:GLN:HA	1.84	0.92
1:D:147:PRO:O	1:D:148:GLN:HB2	1.67	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:A:85:ASP:C	1:A:92:THR:HG22	1.96	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:31:VAL:HA	5:D:609:HOH:O	1.75	0.85
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: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: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:HE21	1:D:440:GLN:HA	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:C:87:GLU:HA	1:C:88:LEU:C	2.02	0.80
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:D:358:ILE:HD12	1:D:358:ILE:C	2.01	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:D:236:LEU:C	1:D:236:LEU:HD12	2.02	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:C:436:LEU:HD12	5:C:610:HOH:O	1.82	0.79
1:A:437:ILE:O	1:A:441:GLN:HB3	1.83	0.78
1:C:94:HIS:CD2	1:C:94:HIS:N	2.48	0.78
1:B:91:LEU:HD13	1:B:103:GLN:OE1	1.83	0.78
1:B:87:GLU:HA	1:B:88:LEU:C	2.03	0.78
1:C:437:ILE:HD12	1:C:437:ILE:C	2.02	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:149:ALA:HB1	1:A:173:LEU:HD22	1.67	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: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:H	1:B:272:ASN:HD22	1.31	0.76
1:D:256:ALA:H	1:D:272:ASN:ND2	1.84	0.76
1:B:343:LEU:HD22	1:B:355:LYS:HB3	1.67	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:440:GLN:HA	5:C:602:HOH:O	1.86	0.74
1:C:8:VAL:HG13	1:C:81:VAL:HG13	1.69	0.74
1:A:91:LEU:C	1:A:92:THR:OG1	2.26	0.74
1:D:98:GLU:OE2	1:D:98:GLU:HA	1.87	0.74
1:C:352:TRP:NE1	5:C:607:HOH:O	2.20	0.74
1:D:87:GLU:HA	1:D:88:LEU:C	2.08	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:B:85:ASP:C	1:B:92:THR:CG2	2.56	0.73
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:H	1:A:272:ASN:ND2	1.88	0.72
1:C:149:ALA:CB	1:C:150:ARG:CA	2.63	0.72
1:B:173:LEU:N	1:B:173:LEU:HD23	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: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:C:236:LEU:HD12	1:C:236:LEU:C	2.10	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:B:236:LEU:C	1:B:236:LEU:HD12	2.11	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:208:TRP:HB3	1:B:211:VAL:HG21	1.74	0.69
1:B:86:TYR:O	1:B:89:ARG:HA	1.92	0.69
1:B:98:GLU:OE2	1:B:98:GLU:HA	1.92	0.69
1:B:94:HIS:CD2	1:B:94:HIS:N	2.60	0.69
1:B:92:THR:HB	1:B:106:PHE:HE2	1.57	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:272:ASN:H	1:C:272:ASN:HD22	1.41	0.67
1:D:149:ALA:HB1	1:D:150:ARG:HA	1.72	0.67
1:D:91:LEU:HD13	1:D:103:GLN:OE1	1.94	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:NH1	1:B:410:ARG:HG2	2.06	0.67
1:D:295:TRP:CE2	1:D:297:PRO:HG3	2.30	0.67
1:A:24:GLU:CG	1:A:316:ARG:HG3	2.24	0.67
1:C:94:HIS:HD2	1:C:94:HIS:N	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:ARG:HG2	1:D:410:ARG:HH11	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:91:LEU:C	1:B:92:THR:OG1	2.34	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: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:H	1:C:272:ASN:ND2	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:HG2	1:C:410:ARG:HH11	1.61	0.64
1:B:116:ARG:CZ	1:B:244:ARG:HD2	2.28	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
1:D:85:ASP:OD1	1:D:88:LEU:HD23	1.98	0.63
1:D:100:ARG:C	1:D:101:THR:HG22	2.17	0.63
1:D:359:GLN:HB2	1:D:374:TRP:CD1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:OG1	1:A:67:GLU:HG3	1.99	0.63
1:D:50:LEU:HD12	1:D:143:LEU:HD13	1.80	0.63
1:A:398:ALA:HA	1:A:400:ARG:H	1.63	0.63
1:A:11:VAL:HG23	2:A:501:FAD:H4B	1.80	0.63
1:C:98:GLU:OE2	1:C:98:GLU:HA	1.97	0.63
1:C:358:ILE:HD12	1:C:358:ILE:C	2.19	0.63
1:A:395:GLY:HA2	1:B:396:HIS:NE2	2.14	0.63
1:A:272:ASN:HD22	1:A:272:ASN:H	1.46	0.62
1:A:287:HIS:CD2	1:A:290:LEU:H	2.17	0.62
1:B:191:GLU:OE2	1:B:355:LYS:HE3	1.99	0.62
1:B:440:GLN:HE21	1:B:440:GLN:HA	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:B:221:ARG:O	1:B:222:VAL:HB	2.00	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:117:PRO:HD3	1:C:134:ARG:HG2	1.83	0.61
1:C:8:VAL:HG13	1:C:81:VAL:CG1	2.31	0.61
1:B:280:GLY:HA2	1:B:302:ALA:HA	1.83	0.60
1:B:86:TYR:N	1:B:92:THR:CG2	2.57	0.60
1:D:280:GLY:HA2	1:D:302:ALA:HA	1.82	0.60
1:D:84:VAL:O	1:D:86:TYR:HD1	1.84	0.60
1:A:91:LEU:HD13	1:A:103:GLN:OE1	2.01	0.60
1:C:401:ILE:HB	5:C:604:HOH:O	2.01	0.60
1:C:90:THR:CG2	1:C:106:PHE:H	2.13	0.60
1:A:123:PRO:HD3	1:D:172:GLY:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ALA:C	5:D:601:HOH:O	2.39	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:C:180:ALA:O	1:C:210:GLY:HA2	2.00	0.60
1:C:36:SER:O	1:C:38:TRP:N	2.34	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:B:399:LEU:C	1:B:401:ILE:H	2.05	0.59
1:D:180:ALA:O	1:D:210:GLY:HA2	2.02	0.59
1:A:398:ALA:N	1:A:399:LEU:HB2	2.12	0.59
1:A:90:THR:CA	1:A:92:THR:CG2	2.71	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:173:LEU:N	1:D:173:LEU:HD23	2.18	0.59
1:D:87:GLU:HA	1:D:88:LEU:O	2.02	0.59
1:B:401:ILE:O	1:B:401:ILE:HG13	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:A:87:GLU:HA	1:A:88:LEU:C	2.24	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:C:352:TRP:CE2	5:C:607:HOH:O	2.56	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
1:B:358:ILE:HD12	1:B:358:ILE:C	2.23	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:LEU:HD22	1:C:439:ALA:HB1	1.86	0.58
1:C:87:GLU:HA	1:C:88:LEU:O	2.04	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:A:85:ASP:C	1:A:92:THR:CG2	2.70	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:A:225:VAL:N	5:A:601:HOH:O	2.08	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:D:86:TYR:O	1:D:89:ARG:HA	2.05	0.57
1:B:94:HIS:HD2	1:B:94:HIS:N	2.02	0.57
1:C:10:GLY:O	1:C:39:VAL:HG22	2.05	0.57
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:C:221:ARG:O	1:C:222:VAL:HB	2.06	0.56
1:D:397:GLY:C	5:D:602:HOH:O	2.42	0.56
1:B:292:ARG:HB2	1:B:293:PRO:CD	2.36	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:C:410:ARG:NH1	1:C:410:ARG:HG2	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: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: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:399:LEU:C	1:B:401:ILE:N	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:418:LEU:HD13	1:D:439:ALA:HB3	1.89	0.55
1:D:94:HIS:N	1:D:94:HIS:HD2	2.02	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: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:139:GLY:O	1:D:143:LEU:HB2	2.07	0.55
1:D:91:LEU:O	1:D:92:THR:CB	2.55	0.55
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
1:B:418:LEU:HD13	1:B:439:ALA:HB3	1.89	0.54
3:A:502:COA:H72	4:B:501:VK3:H9K1	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
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: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:399:LEU:C	1:D:401:ILE:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:HD12	1:B:155:LEU:N	2.24	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:A:94:HIS:CD2	1:A:94:HIS:H	2.23	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:NH1	1:D:410:ARG:CG	2.68	0.53
1:B:85:ASP:CA	1:B:92:THR:HG22	2.38	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:A:97:ALA:O	1:A:98:GLU:CD	2.46	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:B:236:LEU:HD12	1:B:237:VAL:N	2.24	0.53
1:C:398:ALA:H	1:C:399:LEU:CB	2.22	0.53
1:C:208:TRP:HB3	1:C:211:VAL:HG21	1.91	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: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:D:216:PHE:HD1	1:D:225:VAL:HG22	1.71	0.52
1:D:221:ARG:O	1:D:222:VAL:HB	2.10	0.52
1:C:162:LEU:HD23	1:C:177:LEU:HD11	1.90	0.52
1:C:85:ASP:OD1	1:C:88:LEU:HB3	2.09	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
1:A:236:LEU:HD12	1:A:236:LEU:C	2.30	0.52
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:A:90:THR:HG21	1:A:106:PHE:O	2.10	0.52
1:A:437:ILE:HD12	1:A:437:ILE:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:NH1	5:B:610:HOH:O	2.39	0.52
1:D:57:LEU:O	1:D:60:LEU:HB2	2.10	0.52
1:A:90:THR:HG21	1:A:106:PHE:H	1.73	0.52
1:C:69:ARG:C	1:C:71:GLN:H	2.13	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:122:ILE:HG23	1:D:215:ALA:HA	1.91	0.51
1:D:84:VAL:O	1:D:86:TYR:CD1	2.63	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:B:149:ALA:HB1	1:B:173:LEU:HD22	1.92	0.51
1:D:358:ILE:HD12	1:D:358:ILE:O	2.10	0.51
1:D:56:ARG:CZ	1:D:59:ARG:NH1	2.73	0.51
1:A:440:GLN:O	1:A:441:GLN:O	2.28	0.51
1:B:437:ILE:HD12	1:B:437:ILE:C	2.31	0.51
1:C:144:LYS:O	1:C:147:PRO:HD2	2.11	0.51
1:C:341:LEU:O	1:C:388:GLY:HA3	2.10	0.51
1:B:116:ARG:NH2	1:B:244:ARG:HH11	2.09	0.51
1:D:151:ARG:HE	1:D:174:GLN:HE21	1.59	0.51
1:A:22:LYS:HE2	1:A:72:GLY:HA3	1.93	0.51
1:A:358:ILE:HD12	1:A:358:ILE:C	2.31	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
1:B:354:LYS:HE3	1:B:381:GLU:OE2	2.11	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:C:302:ALA:HB2	2:C:501:FAD:H5'2	1.92	0.50
1:C:69:ARG:O	1:C:71:GLN:N	2.44	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:B:123:PRO:HG2	1:B:215:ALA:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:HB3	1:C:219:MET:HG3	1.92	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:D:97:ALA:O	1:D:98:GLU:CD	2.50	0.50
1:C:398:ALA:HA	1:C:400:ARG:N	2.16	0.50
1:D:399:LEU:C	1:D:401:ILE:N	2.61	0.50
1:C:84:VAL:O	1:C:86:TYR:CD1	2.65	0.50
1:D:426:PRO:HB2	1:D:427:PRO:HD3	1.93	0.50
1:A:69:ARG:C	1:A:71:GLN:H	2.15	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: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:N	1:B:272:ASN:HD22	2.07	0.49
1:C:216:PHE:HA	5:C:601:HOH:O	2.12	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:148:GLN:O	1:D:149:ALA:C	2.50	0.49
1:D:166:GLU:HG2	1:D:170:LYS:HE3	1.94	0.49
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:ND2	1:B:272:ASN:H	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: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:86:TYR:H	1:B:92:THR:HG22	1.72	0.48
3:A:502:COA:H141	3:A:502:COA:O9P	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:TYR:N	1:B:277:TYR:CD1	2.81	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: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:H	1:D:272:ASN:HD22	1.61	0.48
1:D:90:THR:HA	1:D:92:THR:CB	2.44	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:423:ALA:HB1	1:B:328:ILE:CG2	2.43	0.48
1:A:85:ASP:CA	1:A:92:THR:HG22	2.43	0.48
1:C:287:HIS:HD2	1:C:289:VAL:H	1.61	0.48
1:A:100:ARG:C	1:A:101:THR:HG22	2.33	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:C:57:LEU:HG	1:C:136:MET:HE3	1.96	0.48
1:A:295:TRP:C	1:A:297:PRO:HD3	2.34	0.48
1:C:81:VAL:HA	1:C:95:ASP:HB3	1.95	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
1:A:89:ARG:O	1:A:91:LEU:N	2.47	0.47
1:D:367:TYR:CE1	1:D:427:PRO:HG3	2.49	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: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:D:188:TRP:O	1:D:189:ASP:C	2.52	0.47
1:D:401:ILE:CG2	1:D:402:ASP:N	2.76	0.47
1:A:296:LEU:N	1:A:297:PRO:HD3	2.28	0.47
1:A:97:ALA:O	1:A:98:GLU:OE1	2.33	0.47
1:C:398:ALA:CA	1:C:400:ARG:H	2.20	0.47
1:D:123:PRO:HG2	1:D:215:ALA:HB2	1.96	0.47
1:D:24:GLU:HB3	1:D:314:ALA:CB	2.44	0.47
1:D:408:LEU:HA	1:D:408:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ALA:O	1:B:98:GLU:CD	2.53	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:408:LEU:HD12	1:B:408:LEU:HA	1.59	0.47
1:C:430:PRO:HD2	1:C:434:PRO:HD3	1.96	0.47
1:D:277:TYR:N	1:D:277:TYR:CD1	2.82	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:C:386:LEU:HB3	1:C:408:LEU:CD1	2.45	0.47
1:D:321:LEU:HD23	1:D:321:LEU:HA	1.66	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:367:TYR:CE1	1:C:427:PRO:HG3	2.49	0.47
1:C:66:GLU:HB2	5:C:622:HOH:O	2.14	0.47
1:D:200:LEU:HD23	1:D:332:PHE:CE2	2.50	0.47
1:B:91:LEU:O	1:B:105:ARG:HA	2.14	0.47
1:B:24:GLU:CG	1:B:316:ARG:HG3	2.45	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:437:ILE:C	1:C:437:ILE:CD1	2.75	0.47
1:C:57:LEU:HG	1:C:136:MET:CE	2.45	0.47
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: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:A:88:LEU:O	1:A:89:ARG:HB2	2.15	0.46
1:A:440:GLN:C	1:A:441:GLN:O	2.54	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: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:C:437:ILE:HD12	1:C:437:ILE:O	2.15	0.46
1:D:91:LEU:O	1:D:105:ARG:HA	2.16	0.46
1:D:272:ASN:H	1:D:272:ASN:ND2	2.13	0.46
1:D:386:LEU:HD23	1:D:413:SER:C	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HA	1:D:272:ASN:HD21	1.79	0.46
1:D:89:ARG:O	1:D:91:LEU:N	2.48	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: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:C:408:LEU:HD12	1:C:408:LEU:HA	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:D:236:LEU:CD1	1:D:236:LEU:C	2.79	0.46
1:A:217:ARG:N	5:A:601:HOH:O	2.19	0.46
1:C:174:GLN:C	5:C:605:HOH:O	2.51	0.46
1:C:185:LEU:N	1:C:186:PRO:CD	2.79	0.46
1:C:91:LEU:O	1:C:105:ARG:HA	2.16	0.46
1:D:398:ALA:HB2	5:D:602:HOH:O	2.16	0.46
1:A:410:ARG:HH11	1:A:410:ARG:CG	2.29	0.46
1:A:365:HIS:H	4:A:503:VK3:C6K	2.29	0.46
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.70	0.46
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:36:SER:O	1:C:37:GLY:C	2.51	0.45
1:D:183:ARG:CD	1:D:190:PRO:HA	2.46	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:B:50:LEU:HA	1:B:50:LEU:HD12	1.72	0.45
1:C:296:LEU:HA	1:C:296:LEU:HD12	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:88:LEU:O	1:A:89:ARG:CB	2.64	0.45
1:C:189:ASP:HA	1:C:190:PRO:HD3	1.62	0.45
1:C:24:GLU:HG2	1:C:316:ARG:CG	2.46	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: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:A:123:PRO:HD3	1:D:172:GLY:HA3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLU:HB3	1:B:221:ARG:HA	1.99	0.45
1:C:426:PRO:HB2	1:C:427:PRO:HD3	1.98	0.45
1:D:304:LYS:O	1:D:305:HIS:C	2.54	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:D:437:ILE:HD12	1:D:437:ILE:C	2.37	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:185:LEU:N	1:B:186:PRO:CD	2.79	0.45
1:B:85:ASP:N	1:B:92:THR:HA	2.15	0.45
1:A:149:ALA:HB1	1:A:173:LEU:CD2	2.41	0.45
1:A:432:TRP:O	1:A:433:ASP:C	2.53	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
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:HD23	1:D:407:LEU:HA	1.72	0.44
1:B:200:LEU:HD23	1:B:332:PHE:CE2	2.52	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:B:81:VAL:HA	1:B:95:ASP:HB3	1.99	0.44
1:D:287:HIS:HD2	1:D:289:VAL:N	2.05	0.44
1:D:50:LEU:HA	1:D:50:LEU:HD12	1.69	0.44
1:A:386:LEU:HD23	1:A:413:SER:C	2.36	0.44
1:C:268:ARG:HG2	1:C:312:VAL:HG21	1.99	0.44
1:A:277:TYR:N	1:A:277:TYR:CD1	2.86	0.44
1:C:199:GLU:HG3	1:C:334:LEU:HG	1.99	0.44
1:C:95:ASP:OD1	1:C:95:ASP:N	2.50	0.44
1:A:407:LEU:HA	1:A:407:LEU:HD23	1.79	0.44
1:A:90:THR:HG22	1:A:92:THR:OG1	2.17	0.44
1:A:8:VAL:HG13	1:A:81:VAL:CG1	2.48	0.44
1:A:217:ARG:HD2	1:A:224:ALA:HB2	2.00	0.44
1:A:86:TYR:O	1:A:89:ARG:CA	2.64	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:D:69:ARG:C	1:D:71:GLN:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LYS:O	1:A:147:PRO:HD2	2.18	0.44
1:B:69:ARG:C	1:B:71:GLN:H	2.22	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: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:B:88:LEU:O	1:B:89:ARG:CB	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:122:ILE:HA	1:A:123:PRO:HD2	1.81	0.43
1:A:92:THR:O	1:A:93:VAL:O	2.35	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:N	1:C:277:TYR:CD1	2.86	0.43
1:C:440:GLN:O	1:C:441:GLN:C	2.55	0.43
1:A:268:ARG:CG	1:A:312:VAL:HG21	2.48	0.43
1:A:54:ILE:HA	1:A:55:PRO:HD2	1.68	0.43
1:B:386:LEU:HD23	1:B:413:SER:C	2.38	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: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:C:23:ARG:NH2	3:C:502:COA:O5A	2.51	0.43
1:D:90:THR:CG2	1:D:106:PHE:H	2.31	0.43
1:A:149:ALA:CB	1:A:173:LEU:CD2	2.95	0.43
1:C:380:GLU:CG	5:C:608:HOH:O	2.64	0.43
1:C:324:VAL:HG21	1:C:408:LEU:HB3	2.01	0.43
1:D:58:GLU:C	1:D:60:LEU:H	2.21	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:A:24:GLU:HG3	1:A:316:ARG:HG3	1.98	0.43
1:C:360:SER:HB3	1:C:434:PRO:HG3	2.01	0.43
1:A:216:PHE:CD1	1:A:225:VAL:HG22	2.54	0.43
1:A:85:ASP:N	1:A:92:THR:HA	2.15	0.43
1:B:127:GLN:HB3	1:B:128:GLU:H	1.48	0.43
1:B:91:LEU:N	1:B:92:THR:HG23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.80	0.43
1:A:155:LEU:N	1:A:155:LEU:HD12	2.33	0.43
1:D:386:LEU:C	5:D:606:HOH:O	2.57	0.43
1:C:224:ALA:O	1:C:225:VAL:HG23	2.18	0.43
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.81	0.43
1:B:268:ARG:O	1:B:269:MET:HB2	2.19	0.43
1:B:440:GLN:C	1:B:441:GLN:O	2.58	0.43
1:C:97:ALA:O	1:C:98:GLU:CD	2.57	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:C:138:ASP:O	1:C:139:GLY:C	2.57	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:D:358:ILE:C	1:D:358:ILE:CD1	2.75	0.42
1:B:90:THR:CG2	1:B:106:PHE:H	2.31	0.42
1:B:143:LEU:HA	1:B:143:LEU:HD12	1.84	0.42
1:C:328:ILE:HD13	1:C:328:ILE:HG21	1.68	0.42
1:D:6:VAL:HG22	1:D:31:VAL:CG1	2.50	0.42
1:C:100:ARG:C	1:C:101:THR:HG22	2.40	0.42
1:C:85:ASP:OD1	1:C:88:LEU:HD23	2.19	0.42
1:C:94:HIS:H	1:C:94:HIS:CD2	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:B:343:LEU:O	1:B:344:GLU:C	2.56	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:C:440:GLN:C	1:C:441:GLN:O	2.58	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:116:ARG:NH2	1:C:248:GLU:OE1	2.53	0.42
1:C:24:GLU:CG	1:C:316:ARG:CG	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.94	0.42
1:B:328:ILE:HD13	1:B:328:ILE:HG21	1.77	0.41
1:C:281:ASP:CG	2:C:501:FAD:H5'1	2.40	0.41
1:D:22:LYS:HE2	1:D:72:GLY:HA3	2.01	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: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:HA	1:A:321:LEU:HD23	1.64	0.41
1:A:426:PRO:N	1:A:427:PRO:CD	2.83	0.41
1:B:100:ARG:C	1:B:101:THR:HG22	2.40	0.41
1:C:151:ARG:HE	1:C:174:GLN:HE21	1.67	0.41
1:D:117:PRO:HD3	1:D:134:ARG:HG2	2.01	0.41
1:D:5:MET:SD	1:D:313:ILE:HG21	2.60	0.41
1:A:56:ARG:CZ	1:A:59:ARG:HH11	2.33	0.41
1:D:244:ARG:O	1:D:244:ARG:HG3	2.20	0.41
1:D:92:THR:O	1:D:93:VAL:O	2.38	0.41
1:A:93:VAL:C	1:A:94:HIS:HD2	2.24	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: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: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:109:LEU:HA	1:C:109:LEU:HD12	1.75	0.41
1:C:23:ARG:NH1	3:C:502:COA:O8A	2.53	0.41
1:C:389:GLY:HA3	1:C:404:LEU:HD13	2.03	0.41
1:C:13:GLY:N	2:C:501:FAD:O1P	2.50	0.41
1:D:302:ALA:CB	2:D:501:FAD:H5'2	2.51	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:C:188:TRP:O	1:C:189:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ILE:C	1:C:315:GLY:H	2.23	0.41
1:C:418:LEU:HD22	1:C:439:ALA:CB	2.50	0.41
1:C:46:LEU:HB2	1:C:47:PRO:HD3	2.03	0.41
1:D:281:ASP:CG	2:D:501:FAD:H5'1	2.42	0.41
1:D:307:ARG:HH11	1:D:307:ARG:HD2	1.60	0.41
1:D:88:LEU:O	1:D:89:ARG:HB2	2.21	0.41
1:A:272:ASN:N	1:A:272:ASN:HD22	2.17	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: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: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:A:86:TYR:HB2	1:A:87:GLU:H	1.19	0.41
1:C:49:VAL:HG11	1:C:57:LEU:CD1	2.51	0.41
1:B:22:LYS:HE2	1:B:72:GLY:HA3	2.02	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: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: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:128:GLU:HB3	1:C:221:ARG:HA	2.03	0.40
1:C:251:GLN:CD	1:C:257:LEU:HD11	2.42	0.40
1:C:426:PRO:N	1:C:427:PRO:CD	2.84	0.40
1:C:66:GLU:HA	1:C:66:GLU:OE1	2.21	0.40
1:D:356:VAL:CG2	1:D:357:PHE:N	2.82	0.40
1:C:192:VAL:O	1:C:193:GLY:C	2.58	0.40
1:C:307:ARG:HD2	1:C:307:ARG:HH11	1.70	0.40
1:C:23:ARG:NH2	3:C:502:COA:P2A	2.94	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: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

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	15
1	B	441/443 (100%)	381 (86%)	40 (9%)	20 (4%)	2	14
1	C	441/443 (100%)	385 (87%)	38 (9%)	18 (4%)	3	16
1	D	441/443 (100%)	386 (88%)	36 (8%)	19 (4%)	2	15
All	All	1764/1772 (100%)	1530 (87%)	158 (9%)	76 (4%)	2	15

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	D	225	VAL
1	D	434	PRO
1	C	37	GLY
1	A	139	GLY

5.3.2 Protein sidechains (i)

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%)	284 (84%)	54 (16%)	2	12
1	B	338/338 (100%)	284 (84%)	54 (16%)	2	12
1	C	337/338 (100%)	288 (86%)	49 (14%)	3	15
1	D	337/338 (100%)	286 (85%)	51 (15%)	3	14
All	All	1350/1352 (100%)	1142 (85%)	208 (15%)	2	13

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	16	SER
1	A	39	VAL
1	A	50	LEU
1	A	58	GLU
1	A	59	ARG
1	A	78	ARG

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Mol	Chain	Res	Type
1	A	81	VAL
1	A	86	TYR
1	A	93	VAL
1	A	94	HIS
1	A	101	THR
1	A	105	ARG
1	A	111	LEU
1	A	116	ARG
1	A	132	THR
1	A	133	LEU
1	A	142	LEU
1	A	146	LEU
1	A	160	ILE
1	A	173	LEU
1	A	175	VAL
1	A	176	THR
1	A	181	LYS
1	A	183	ARG
1	A	185	LEU
1	A	206	GLU
1	A	207	VAL
1	A	208	TRP
1	A	209	THR
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	324	VAL
1	A	355	LYS
1	A	377	LEU
1	A	392	VAL
1	A	394	ARG
1	A	400	ARG
1	A	408	LEU
1	A	410	ARG

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Mol	Chain	Res	Type
1	A	418	LEU
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	81	VAL
1	B	94	HIS
1	B	100	ARG
1	B	101	THR
1	B	105	ARG
1	B	111	LEU
1	B	132	THR
1	B	133	LEU
1	B	142	LEU
1	B	146	LEU
1	B	160	ILE
1	B	171	ARG
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	206	GLU
1	B	207	VAL
1	B	208	TRP
1	B	209	THR
1	B	221	ARG
1	B	222	VAL
1	B	227	THR
1	B	236	LEU
1	B	237	VAL
1	B	244	ARG
1	B	268	ARG
1	B	272	ASN

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Mol	Chain	Res	Type
1	B	285	SER
1	B	301	VAL
1	B	324	VAL
1	B	355	LYS
1	B	372	PRO
1	B	375	VAL
1	B	377	LEU
1	B	392	VAL
1	B	394	ARG
1	B	400	ARG
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	50	LEU
1	C	58	GLU
1	C	59	ARG
1	C	60	LEU
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	105	ARG
1	C	111	LEU
1	C	132	THR
1	C	133	LEU
1	C	142	LEU
1	C	146	LEU
1	C	160	ILE
1	C	173	LEU
1	C	175	VAL
1	C	176	THR
1	C	177	LEU
1	C	185	LEU

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Mol	Chain	Res	Type
1	C	207	VAL
1	C	208	TRP
1	C	209	THR
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	301	VAL
1	C	324	VAL
1	C	355	LYS
1	C	375	VAL
1	C	377	LEU
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	50	LEU
1	D	58	GLU
1	D	59	ARG
1	D	60	LEU
1	D	81	VAL
1	D	86	TYR
1	D	93	VAL
1	D	94	HIS
1	D	101	THR
1	D	105	ARG
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

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Mol	Chain	Res	Type
1	D	171	ARG
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	207	VAL
1	D	208	TRP
1	D	209	THR
1	D	221	ARG
1	D	222	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
1	D	324	VAL
1	D	355	LYS
1	D	375	VAL
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	174	GLN
1	A	272	ASN
1	A	287	HIS
1	A	409	HIS

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Mol	Chain	Res	Type
1	A	441	GLN
1	B	94	HIS
1	B	174	GLN
1	B	203	HIS
1	B	272	ASN
1	B	287	HIS
1	B	396	HIS
1	B	441	GLN
1	C	94	HIS
1	C	174	GLN
1	C	272	ASN
1	C	287	HIS
1	D	94	HIS
1	D	174	GLN
1	D	272	ASN
1	D	287	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\|>2$
4	VK3	D	503	-	14,14,14	2.26	4 (28%)	20,20,20	3.03	7 (35%)
2	FAD	C	501	-	51,58,58	3.58	19 (37%)	60,89,89	2.77	22 (36%)
2	FAD	A	501	-	51,58,58	3.30	23 (45%)	60,89,89	2.72	20 (33%)
3	COA	B	503	1	41,50,50	1.30	6 (14%)	52,75,75	1.80	10 (19%)
4	VK3	B	501	-	14,14,14	2.09	3 (21%)	20,20,20	2.73	10 (50%)
3	COA	C	502	1	41,50,50	1.57	7 (17%)	52,75,75	2.25	16 (30%)
3	COA	A	502	1	41,50,50	1.67	5 (12%)	52,75,75	2.05	14 (26%)
3	COA	D	502	1	41,50,50	1.16	5 (12%)	52,75,75	2.25	18 (34%)
4	VK3	A	503	-	14,14,14	2.15	3 (21%)	20,20,20	3.00	10 (50%)
4	VK3	C	503	-	14,14,14	2.05	2 (14%)	20,20,20	2.51	5 (25%)
2	FAD	B	502	-	51,58,58	3.86	25 (49%)	60,89,89	2.93	24 (40%)
2	FAD	D	501	-	51,58,58	3.51	22 (43%)	60,89,89	3.05	20 (33%)

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
4	VK3	D	503	-	-	-	0/2/2/2
2	FAD	C	501	-	-	14/30/50/50	0/6/6/6
2	FAD	A	501	-	-	14/30/50/50	0/6/6/6
3	COA	B	503	1	-	19/44/64/64	0/3/3/3
4	VK3	B	501	-	-	-	0/2/2/2
3	COA	C	502	1	-	18/44/64/64	0/3/3/3
3	COA	A	502	1	-	19/44/64/64	0/3/3/3
3	COA	D	502	1	-	19/44/64/64	0/3/3/3
4	VK3	A	503	-	-	-	0/2/2/2
4	VK3	C	503	-	-	-	0/2/2/2
2	FAD	B	502	-	-	13/30/50/50	0/6/6/6
2	FAD	D	501	-	-	17/30/50/50	0/6/6/6

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	FAD	C4X-C10	17.68	1.56	1.38
2	C	501	FAD	C4X-C10	16.18	1.55	1.38
2	A	501	FAD	C4X-C10	15.37	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C4X-C10	15.27	1.54	1.38
2	C	501	FAD	C4-C4X	7.71	1.54	1.41
3	A	502	COA	C4A-N3A	6.92	1.45	1.35
2	B	502	FAD	C4-C4X	6.77	1.53	1.41
2	B	502	FAD	C4A-N3A	6.72	1.44	1.35
2	A	501	FAD	C4-C4X	6.70	1.52	1.41
2	D	501	FAD	C9A-N10	6.67	1.47	1.38
2	A	501	FAD	C4A-N3A	6.65	1.44	1.35
4	D	503	VK3	C10-C5K	6.36	1.51	1.40
4	A	503	VK3	C10-C5K	6.35	1.51	1.40
2	C	501	FAD	C4A-N3A	6.18	1.44	1.35
4	C	503	VK3	C10-C5K	6.16	1.50	1.40
4	B	501	VK3	C10-C5K	6.16	1.50	1.40
2	B	502	FAD	C10-N1	6.02	1.41	1.33
2	B	502	FAD	C5'-C4'	5.84	1.60	1.51
2	D	501	FAD	C2A-N3A	5.82	1.41	1.32
2	C	501	FAD	C5A-C4A	5.44	1.55	1.40
2	C	501	FAD	C9A-C5X	5.27	1.53	1.42
2	A	501	FAD	C5A-C4A	5.26	1.54	1.40
2	D	501	FAD	C4-C4X	5.24	1.50	1.41
2	D	501	FAD	C5A-C4A	5.20	1.54	1.40
2	B	502	FAD	C8-C7	5.19	1.53	1.40
2	D	501	FAD	C4A-N3A	5.18	1.42	1.35
2	C	501	FAD	C9A-N10	5.15	1.45	1.38
2	D	501	FAD	C1'-N10	5.02	1.53	1.48
2	B	502	FAD	C5A-C4A	5.01	1.54	1.40
2	A	501	FAD	C9A-N10	4.97	1.45	1.38
2	D	501	FAD	C9A-C5X	4.87	1.52	1.42
2	B	502	FAD	C9A-C5X	4.87	1.52	1.42
3	C	502	COA	C2A-N3A	4.82	1.39	1.32
2	C	501	FAD	C8-C7	4.80	1.52	1.40
2	C	501	FAD	C2A-N3A	4.80	1.39	1.32
2	A	501	FAD	C9A-C5X	4.67	1.51	1.42
2	D	501	FAD	C2B-C1B	4.63	1.60	1.53
2	D	501	FAD	C4-N3	4.61	1.41	1.33
2	B	502	FAD	C2A-N3A	4.54	1.39	1.32
2	C	501	FAD	C4X-N5	4.44	1.39	1.33
2	D	501	FAD	C2A-N1A	4.39	1.42	1.33
2	C	501	FAD	O4B-C1B	4.39	1.47	1.41
2	C	501	FAD	C1'-N10	4.37	1.52	1.48
2	C	501	FAD	C2A-N1A	4.29	1.41	1.33
2	B	502	FAD	C1'-N10	4.29	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	C10-N1	4.26	1.38	1.33
2	B	502	FAD	C4-N3	4.19	1.40	1.33
2	B	502	FAD	C2A-N1A	4.18	1.41	1.33
2	B	502	FAD	C9A-N10	4.09	1.44	1.38
2	A	501	FAD	C4X-N5	4.03	1.39	1.33
2	D	501	FAD	C10-N1	3.94	1.38	1.33
3	B	503	COA	O4B-C1B	3.73	1.46	1.41
2	D	501	FAD	C8-C7	3.66	1.50	1.40
3	B	503	COA	C5A-C4A	3.51	1.50	1.40
2	D	501	FAD	C5'-C4'	3.47	1.56	1.51
2	B	502	FAD	O3B-C3B	3.41	1.51	1.43
2	B	502	FAD	C2B-C1B	3.38	1.58	1.53
2	A	501	FAD	C8-C7	3.36	1.49	1.40
2	A	501	FAD	C5'-C4'	3.34	1.56	1.51
2	C	501	FAD	O3B-C3B	3.33	1.50	1.43
2	D	501	FAD	O4B-C1B	3.28	1.45	1.41
2	A	501	FAD	C10-N1	3.24	1.37	1.33
3	C	502	COA	C2B-C1B	-3.15	1.49	1.53
2	C	501	FAD	C4-N3	3.13	1.38	1.33
2	B	502	FAD	C4'-C3'	3.09	1.59	1.53
3	A	502	COA	C2B-C1B	-3.08	1.49	1.53
2	A	501	FAD	C1'-N10	3.07	1.51	1.48
3	B	503	COA	C2A-N3A	3.05	1.37	1.32
3	C	502	COA	P3B-O3B	3.03	1.65	1.59
2	B	502	FAD	O4'-C4'	3.02	1.49	1.43
2	A	501	FAD	C2A-N1A	3.00	1.39	1.33
2	B	502	FAD	C2-N3	2.98	1.44	1.38
3	C	502	COA	O2B-C2B	-2.94	1.36	1.43
3	D	502	COA	C5A-C4A	2.94	1.48	1.40
3	A	502	COA	C5A-C4A	2.92	1.48	1.40
2	A	501	FAD	O4'-C4'	2.89	1.49	1.43
3	C	502	COA	C5A-C4A	2.87	1.48	1.40
3	D	502	COA	C2A-N3A	2.81	1.36	1.32
3	A	502	COA	C6A-C5A	2.81	1.53	1.43
2	A	501	FAD	C2A-N3A	2.78	1.36	1.32
2	B	502	FAD	C6A-C5A	2.76	1.53	1.43
2	A	501	FAD	C4-N3	2.74	1.37	1.33
4	D	503	VK3	C2K-C3K	2.73	1.41	1.35
2	A	501	FAD	O4B-C1B	2.73	1.44	1.41
3	A	502	COA	C2A-N3A	2.70	1.36	1.32
2	A	501	FAD	C8A-N7A	2.63	1.39	1.34
2	D	501	FAD	C4X-N5	2.63	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	COA	C6A-C5A	2.62	1.53	1.43
2	C	501	FAD	C2B-C1B	2.61	1.57	1.53
2	D	501	FAD	C2-N3	2.60	1.43	1.38
2	D	501	FAD	C6A-C5A	2.58	1.52	1.43
2	C	501	FAD	C3B-C4B	2.56	1.59	1.53
2	B	502	FAD	O4B-C1B	2.56	1.44	1.41
2	B	502	FAD	C4X-N5	2.48	1.36	1.33
2	D	501	FAD	O3B-C3B	2.46	1.48	1.43
2	D	501	FAD	O2B-C2B	2.39	1.48	1.43
3	D	502	COA	C2A-N1A	2.36	1.38	1.33
4	D	503	VK3	C5K-C4K	2.35	1.52	1.48
2	B	502	FAD	C3B-C4B	2.34	1.59	1.53
2	A	501	FAD	C2B-C1B	2.32	1.57	1.53
4	D	503	VK3	C3K-C4K	2.31	1.51	1.48
2	A	501	FAD	PA-O1A	2.30	1.59	1.50
2	B	502	FAD	C8A-N7A	2.28	1.38	1.34
4	C	503	VK3	C2K-C3K	2.25	1.40	1.35
3	C	502	COA	C9P-N8P	2.25	1.38	1.33
2	D	501	FAD	C5X-N5	2.24	1.39	1.35
4	B	501	VK3	C2K-C3K	2.24	1.40	1.35
2	B	502	FAD	PA-O1A	2.24	1.58	1.50
3	D	502	COA	OAP-CAP	2.23	1.46	1.42
3	B	503	COA	C6A-N6A	2.21	1.42	1.34
2	B	502	FAD	PA-O5B	2.21	1.68	1.59
2	C	501	FAD	C6-C7	2.20	1.43	1.37
3	D	502	COA	C6A-C5A	2.20	1.51	1.43
2	D	501	FAD	C4'-C3'	2.17	1.57	1.53
2	A	501	FAD	C6A-C5A	2.17	1.51	1.43
2	A	501	FAD	O3B-C3B	2.12	1.48	1.43
4	A	503	VK3	C2K-C3K	2.12	1.39	1.35
3	B	503	COA	C8A-N7A	2.11	1.38	1.34
3	C	502	COA	O9P-C9P	2.08	1.27	1.23
2	A	501	FAD	C6-C5X	-2.08	1.38	1.41
4	B	501	VK3	C2K-C1K	-2.05	1.40	1.44
2	A	501	FAD	C4'-C3'	2.02	1.57	1.53
2	C	501	FAD	C6A-C5A	2.02	1.50	1.43
4	A	503	VK3	C10-C1K	2.00	1.51	1.48

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FAD	C4-N3-C2	14.20	127.13	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	FAD	C4-N3-C2	13.18	126.27	115.14
2	A	501	FAD	C4-N3-C2	11.18	124.58	115.14
2	C	501	FAD	C4-N3-C2	9.70	123.33	115.14
2	D	501	FAD	C1'-N10-C9A	8.38	124.89	118.29
4	D	503	VK3	C11-C3K-C4K	8.17	127.20	117.72
4	A	503	VK3	C11-C3K-C4K	7.49	126.41	117.72
3	D	502	COA	C7P-C6P-C5P	-7.30	100.20	112.36
2	C	501	FAD	C1'-N10-C9A	7.29	124.03	118.29
2	B	502	FAD	C4X-C4-N3	-7.16	113.64	123.43
3	B	503	COA	C7P-C6P-C5P	-6.95	100.78	112.36
4	C	503	VK3	C11-C3K-C4K	6.71	125.51	117.72
3	C	502	COA	O4B-C1B-C2B	-6.54	97.36	106.93
2	D	501	FAD	C4X-C4-N3	-6.32	114.79	123.43
3	D	502	COA	O4B-C1B-C2B	-6.27	97.76	106.93
3	A	502	COA	C7P-C6P-C5P	-6.12	102.16	112.36
2	A	501	FAD	C4X-C4-N3	-6.04	115.17	123.43
3	A	502	COA	N3A-C2A-N1A	-5.96	119.36	128.68
4	D	503	VK3	C6K-C5K-C10	-5.72	112.90	119.26
2	A	501	FAD	C1'-N10-C9A	5.68	122.77	118.29
4	B	501	VK3	C11-C3K-C4K	5.68	124.31	117.72
2	D	501	FAD	C9A-N10-C10	-5.48	114.73	121.91
2	B	502	FAD	C1'-N10-C9A	5.25	122.42	118.29
2	A	501	FAD	N3A-C2A-N1A	-5.11	120.69	128.68
3	C	502	COA	C7P-C6P-C5P	-5.06	103.93	112.36
2	C	501	FAD	C4X-C4-N3	-5.05	116.52	123.43
3	C	502	COA	O2B-C2B-C1B	-5.02	92.32	110.85
3	C	502	COA	C7P-N8P-C9P	4.96	131.43	122.59
4	D	503	VK3	C5K-C10-C1K	-4.92	116.76	120.21
2	C	501	FAD	C4-C4X-C10	-4.91	116.70	119.95
2	D	501	FAD	N6A-C6A-N1A	4.90	128.74	118.57
4	A	503	VK3	C5K-C10-C1K	-4.87	116.79	120.21
2	A	501	FAD	C4-C4X-C10	-4.80	116.77	119.95
2	C	501	FAD	C9A-N10-C10	-4.72	115.72	121.91
2	C	501	FAD	C3B-C2B-C1B	4.69	108.04	100.98
2	B	502	FAD	C9A-N10-C10	-4.60	115.89	121.91
3	D	502	COA	O5A-P2A-O4A	4.60	134.97	112.24
4	C	503	VK3	C6K-C5K-C10	-4.52	114.24	119.26
2	B	502	FAD	C5X-C9A-N10	4.50	120.98	117.72
2	C	501	FAD	C4-C4X-N5	4.49	123.73	118.60
2	C	501	FAD	O2'-C2'-C3'	-4.45	98.27	109.10
2	C	501	FAD	N6A-C6A-N1A	4.45	127.81	118.57
4	D	503	VK3	C6K-C5K-C4K	4.43	126.59	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FAD	N6A-C6A-N1A	4.41	127.72	118.57
2	D	501	FAD	C5X-C9A-N10	4.39	120.90	117.72
4	B	501	VK3	O1K-C1K-C2K	-4.35	114.52	121.79
3	A	502	COA	C7P-N8P-C9P	4.31	130.27	122.59
4	B	501	VK3	C5K-C10-C1K	-4.27	117.21	120.21
4	C	503	VK3	C6K-C5K-C4K	4.27	126.36	120.10
3	C	502	COA	C5A-C6A-N6A	-4.26	113.89	120.35
2	D	501	FAD	C5A-C6A-N6A	-4.24	113.91	120.35
4	B	501	VK3	C6K-C5K-C4K	4.24	126.31	120.10
3	D	502	COA	O6A-CCP-CBP	-4.22	103.77	110.55
2	B	502	FAD	C4X-N5-C5X	4.21	120.98	116.77
2	D	501	FAD	O2'-C2'-C3'	-4.19	98.90	109.10
2	C	501	FAD	O3B-C3B-C4B	4.16	123.08	111.05
2	B	502	FAD	N6A-C6A-N1A	4.11	127.11	118.57
4	A	503	VK3	O1K-C1K-C2K	-4.10	114.94	121.79
2	A	501	FAD	C9A-N10-C10	-4.04	116.61	121.91
2	A	501	FAD	C2A-N1A-C6A	4.01	125.61	118.75
4	A	503	VK3	C6K-C5K-C4K	4.00	125.97	120.10
2	A	501	FAD	C3B-C2B-C1B	3.97	106.96	100.98
2	A	501	FAD	C4-C4X-N5	3.93	123.09	118.60
3	D	502	COA	O6A-P2A-O4A	-3.86	94.00	109.07
3	A	502	COA	C4A-C5A-N7A	-3.79	105.45	109.40
2	B	502	FAD	O4B-C4B-C3B	3.78	112.59	105.11
3	D	502	COA	C3B-C2B-C1B	3.77	108.24	99.89
3	C	502	COA	N3A-C2A-N1A	-3.72	122.86	128.68
2	B	502	FAD	O5'-C5'-C4'	3.68	119.18	109.36
3	A	502	COA	CDP-CBP-CCP	-3.65	102.27	108.23
2	A	501	FAD	C4X-N5-C5X	3.65	120.42	116.77
2	B	502	FAD	C1'-N10-C10	3.63	121.66	118.41
4	C	503	VK3	C5K-C10-C1K	-3.57	117.71	120.21
3	B	503	COA	C7P-N8P-C9P	3.55	128.93	122.59
2	D	501	FAD	C4-C4X-C10	-3.53	117.61	119.95
4	A	503	VK3	C8K-C7K-C6K	3.49	125.51	120.19
2	B	502	FAD	O3B-C3B-C4B	3.49	121.14	111.05
2	B	502	FAD	N3A-C2A-N1A	-3.44	123.31	128.68
2	C	501	FAD	O3'-C3'-C4'	3.43	117.09	108.81
4	B	501	VK3	O4K-C4K-C3K	-3.40	116.45	120.33
2	A	501	FAD	C5A-C6A-N6A	-3.38	115.21	120.35
2	C	501	FAD	N3A-C2A-N1A	-3.36	123.43	128.68
2	C	501	FAD	C5A-C6A-N6A	-3.35	115.25	120.35
4	A	503	VK3	C7K-C8K-C9K	-3.33	115.11	120.19
3	A	502	COA	CEP-CBP-CDP	3.32	115.94	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	FAD	C4X-N5-C5X	3.30	120.07	116.77
2	C	501	FAD	C5X-C9A-N10	3.30	120.11	117.72
4	C	503	VK3	C11-C3K-C2K	-3.28	114.58	121.87
3	C	502	COA	O5P-C5P-C6P	-3.23	116.10	122.02
2	A	501	FAD	C5X-C9A-N10	3.22	120.05	117.72
4	A	503	VK3	C11-C3K-C2K	-3.18	114.81	121.87
4	B	501	VK3	C10-C1K-C2K	3.16	123.10	116.63
2	A	501	FAD	C4'-C3'-C2'	-3.11	106.89	113.36
3	C	502	COA	C3B-C2B-C1B	3.10	106.77	99.89
2	D	501	FAD	O4B-C4B-C3B	3.10	111.25	105.11
4	D	503	VK3	C11-C3K-C2K	-3.08	115.02	121.87
3	C	502	COA	C2B-C3B-C4B	-3.07	97.78	103.22
2	D	501	FAD	O3B-C3B-C4B	3.04	119.83	111.05
2	C	501	FAD	C2A-N1A-C6A	3.03	123.93	118.75
4	B	501	VK3	C10-C5K-C4K	-3.02	117.41	120.68
3	C	502	COA	O6A-CCP-CBP	-3.02	105.69	110.55
2	A	501	FAD	O3B-C3B-C4B	3.00	119.71	111.05
2	B	502	FAD	C3B-C2B-C1B	2.97	105.45	100.98
2	D	501	FAD	O5'-C5'-C4'	2.95	117.24	109.36
4	A	503	VK3	C6K-C5K-C10	-2.91	116.03	119.26
3	B	503	COA	C3B-C2B-C1B	2.90	106.32	99.89
3	B	503	COA	O6A-CCP-CBP	-2.90	105.89	110.55
2	A	501	FAD	O3'-C3'-C4'	2.89	115.80	108.81
2	B	502	FAD	O3'-C3'-C2'	2.88	115.77	108.81
3	C	502	COA	CAP-C9P-N8P	-2.86	110.89	116.58
3	B	503	COA	O4B-C4B-C3B	2.84	110.96	104.87
2	D	501	FAD	C3B-C2B-C1B	2.84	105.25	100.98
3	B	503	COA	O5A-P2A-O4A	2.81	126.15	112.24
3	D	502	COA	C4A-C5A-N7A	-2.75	106.53	109.40
4	B	501	VK3	C11-C3K-C2K	-2.74	115.79	121.87
2	D	501	FAD	O2P-P-O5'	2.74	120.46	107.75
3	B	503	COA	C4A-C5A-N7A	-2.73	106.55	109.40
3	C	502	COA	CEP-CBP-CCP	2.71	112.65	108.23
3	A	502	COA	C2A-N1A-C6A	2.70	123.38	118.75
3	D	502	COA	CEP-CBP-CCP	2.69	112.62	108.23
4	B	501	VK3	C6K-C5K-C10	-2.68	116.28	119.26
3	B	503	COA	N3A-C2A-N1A	-2.68	124.49	128.68
2	C	501	FAD	C7M-C7-C8	2.68	126.22	120.74
4	A	503	VK3	C10-C1K-C2K	2.68	122.11	116.63
2	C	501	FAD	C4'-C3'-C2'	-2.67	107.81	113.36
2	B	502	FAD	O4B-C4B-C5B	-2.57	100.91	109.37
4	D	503	VK3	C3K-C2K-C1K	2.55	126.75	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	COA	O5A-P2A-O4A	2.55	124.86	112.24
2	B	502	FAD	C2A-N1A-C6A	2.52	123.07	118.75
2	C	501	FAD	O5'-C5'-C4'	2.52	116.08	109.36
2	A	501	FAD	O4B-C4B-C3B	2.52	110.09	105.11
3	A	502	COA	O2B-C2B-C1B	-2.51	101.59	110.85
2	B	502	FAD	C4A-C5A-N7A	-2.51	106.79	109.40
3	D	502	COA	C2B-C3B-C4B	-2.50	98.78	103.22
2	B	502	FAD	C4-C4X-N5	2.50	121.46	118.60
2	B	502	FAD	C5A-C6A-N6A	-2.50	116.55	120.35
3	D	502	COA	CDP-CBP-CCP	2.49	112.30	108.23
2	D	501	FAD	O2B-C2B-C1B	2.49	120.05	110.85
2	B	502	FAD	O3'-C3'-C4'	2.49	114.82	108.81
4	A	503	VK3	C10-C5K-C4K	-2.48	118.00	120.68
2	C	501	FAD	C1'-C2'-C3'	2.47	116.70	109.79
2	D	501	FAD	C1'-C2'-C3'	2.46	116.67	109.79
3	A	502	COA	O9P-C9P-N8P	2.45	128.26	122.99
2	C	501	FAD	C10-C4X-N5	-2.44	119.57	121.26
3	A	502	COA	O9A-P3B-O8A	2.42	116.90	107.64
3	A	502	COA	O5B-C5B-C4B	-2.40	100.72	108.99
2	A	501	FAD	C1'-C2'-C3'	2.38	116.45	109.79
3	C	502	COA	O8A-P3B-O7A	2.38	120.00	110.68
2	B	502	FAD	C4'-C3'-C2'	-2.36	108.45	113.36
2	B	502	FAD	O4'-C4'-C5'	2.35	115.20	109.92
4	B	501	VK3	C8K-C7K-C6K	2.35	123.77	120.19
2	D	501	FAD	C4X-N5-C5X	2.34	119.11	116.77
3	D	502	COA	C7P-N8P-C9P	2.25	126.60	122.59
4	D	503	VK3	C7K-C6K-C5K	2.25	124.07	119.81
3	D	502	COA	C6P-C5P-N4P	2.25	120.20	116.42
3	C	502	COA	C1B-N9A-C4A	2.24	130.57	126.64
3	C	502	COA	N6A-C6A-N1A	2.24	123.21	118.57
3	D	502	COA	N6A-C6A-N1A	2.22	123.19	118.57
3	A	502	COA	CAP-C9P-N8P	-2.22	112.17	116.58
2	B	502	FAD	C1'-C2'-C3'	2.21	115.97	109.79
2	A	501	FAD	O3'-C3'-C2'	2.20	114.13	108.81
3	D	502	COA	C1B-N9A-C4A	2.20	130.51	126.64
2	A	501	FAD	C1'-N10-C10	2.19	120.37	118.41
2	B	502	FAD	O4B-C1B-C2B	2.18	110.11	106.93
3	D	502	COA	O8A-P3B-O7A	2.17	119.19	110.68
3	D	502	COA	O2B-C2B-C1B	-2.17	102.85	110.85
3	B	503	COA	CDP-CBP-CCP	2.16	111.75	108.23
3	B	503	COA	N6A-C6A-N1A	2.15	123.03	118.57
2	D	501	FAD	O3'-C3'-C4'	2.15	113.99	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FAD	C1'-N10-C10	2.14	120.33	118.41
3	A	502	COA	C6P-C5P-N4P	-2.13	112.84	116.42
3	D	502	COA	OAP-CAP-CBP	-2.09	105.32	110.25
3	D	502	COA	C5A-C6A-N1A	-2.09	115.61	120.35
2	D	501	FAD	C7-C6-C5X	2.06	124.13	121.22
3	A	502	COA	OAP-CAP-CBP	-2.02	105.49	110.25
2	C	501	FAD	C1'-N10-C10	2.02	120.22	118.41

There are no chirality outliers.

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	PA-O3P-P-O5'
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
3	B	503	COA	C3B-O3B-P3B-O7A
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	B	503	COA	S1P-C2P-C3P-N4P
3	C	502	COA	C3B-O3B-P3B-O7A
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

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Mol	Chain	Res	Type	Atoms
3	C	502	COA	C5P-C6P-C7P-N8P
3	C	502	COA	C6P-C5P-N4P-C3P
3	A	502	COA	C3B-O3B-P3B-O7A
3	A	502	COA	O4B-C4B-C5B-O5B
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	A	502	COA	S1P-C2P-C3P-N4P
3	D	502	COA	C3B-O3B-P3B-O7A
3	D	502	COA	O4B-C4B-C5B-O5B
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
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	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
3	C	502	COA	O9P-C9P-N8P-C7P
3	D	502	COA	O9P-C9P-N8P-C7P
3	D	502	COA	C6P-C5P-N4P-C3P
3	B	503	COA	O9P-C9P-N8P-C7P
3	A	502	COA	O9P-C9P-N8P-C7P

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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	C3B-C4B-C5B-O5B
3	B	503	COA	O4B-C4B-C5B-O5B
3	C	502	COA	O4B-C4B-C5B-O5B
3	A	502	COA	C3B-C4B-C5B-O5B
3	D	502	COA	C3B-C4B-C5B-O5B
3	C	502	COA	O5P-C5P-N4P-C3P
3	D	502	COA	O5P-C5P-N4P-C3P
3	C	502	COA	C3B-C4B-C5B-O5B
3	B	503	COA	C4B-C3B-O3B-P3B
2	A	501	FAD	O2'-C2'-C3'-O3'
3	B	503	COA	C2B-C3B-O3B-P3B
2	B	502	FAD	O2'-C2'-C3'-O3'
3	B	503	COA	P1A-O3A-P2A-O4A
3	D	502	COA	P2A-O3A-P1A-O1A
3	D	502	COA	N8P-C9P-CAP-CBP
3	C	502	COA	S1P-C2P-C3P-N4P
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	D	502	COA	CCP-O6A-P2A-O3A
3	B	503	COA	P2A-O3A-P1A-O2A
3	B	503	COA	P1A-O3A-P2A-O5A
3	A	502	COA	P2A-O3A-P1A-O2A
3	D	502	COA	P2A-O3A-P1A-O2A
3	D	502	COA	P1A-O3A-P2A-O5A
2	C	501	FAD	C5B-O5B-PA-O1A
2	C	501	FAD	C5B-O5B-PA-O2A
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O2A
2	D	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	O2'-C2'-C3'-C4'
3	B	503	COA	P2A-O3A-P1A-O1A
3	C	502	COA	P1A-O3A-P2A-O5A
3	A	502	COA	P1A-O3A-P2A-O4A
3	A	502	COA	P1A-O3A-P2A-O5A
3	A	502	COA	N8P-C9P-CAP-CBP
2	B	502	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	501	FAD	O4B-C4B-C5B-O5B
3	C	502	COA	P2A-O3A-P1A-O1A
2	B	502	FAD	P-O3P-PA-O2A
2	A	501	FAD	O4B-C4B-C5B-O5B
3	C	502	COA	C2P-C3P-N4P-C5P
2	C	501	FAD	C5'-O5'-P-O3P
2	A	501	FAD	C5'-O5'-P-O3P
3	A	502	COA	C3B-O3B-P3B-O8A
2	B	502	FAD	C5'-O5'-P-O3P
2	D	501	FAD	C5'-O5'-P-O3P
2	C	501	FAD	P-O3P-PA-O1A
2	A	501	FAD	P-O3P-PA-O1A
2	A	501	FAD	P-O3P-PA-O2A
3	C	502	COA	P1A-O3A-P2A-O4A
2	D	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	PA-O3P-P-O2P
2	B	502	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

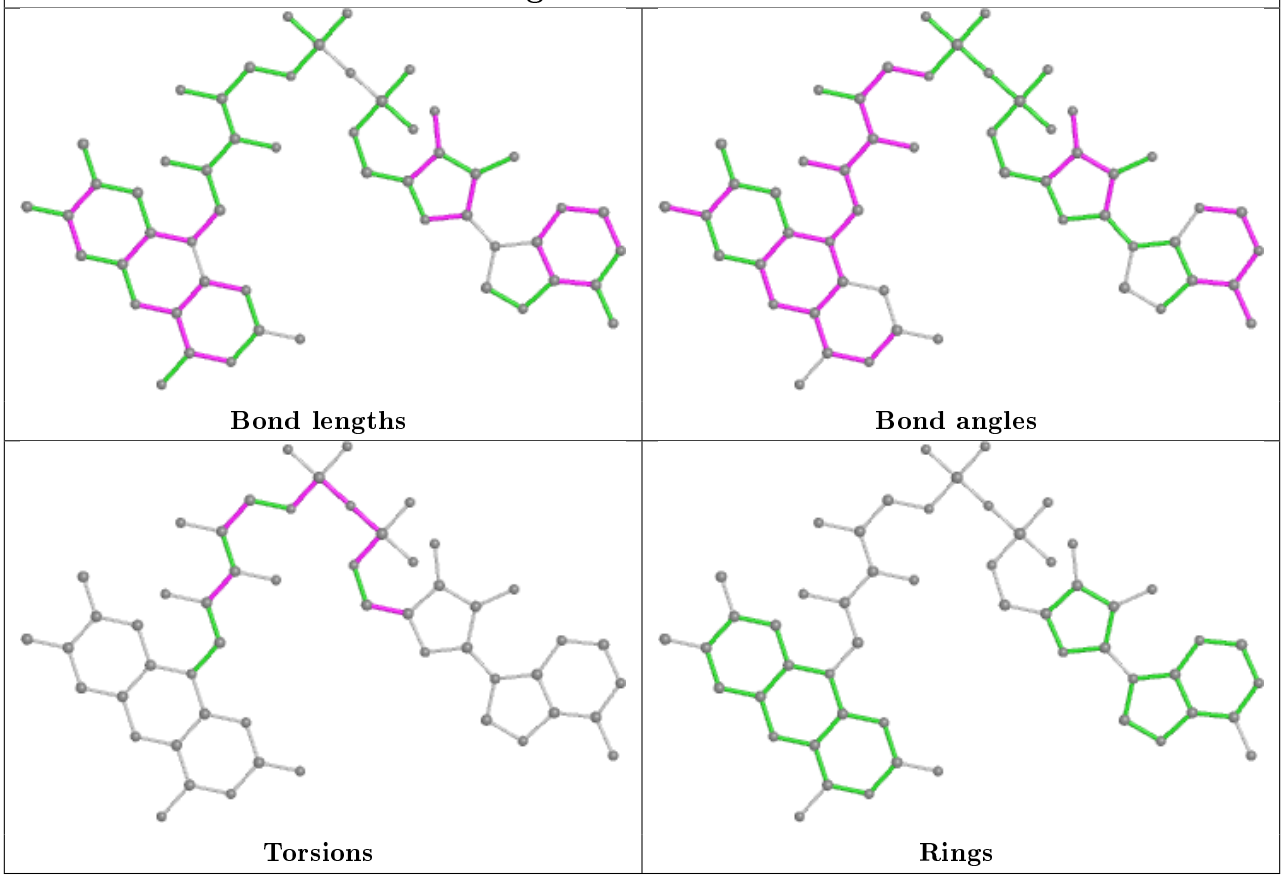
12 monomers are involved in 50 short contacts:

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

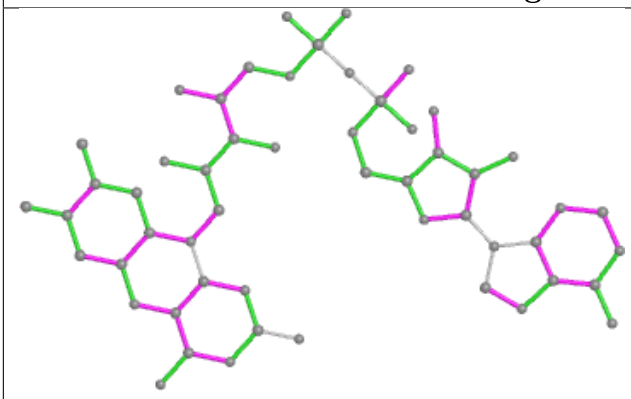
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

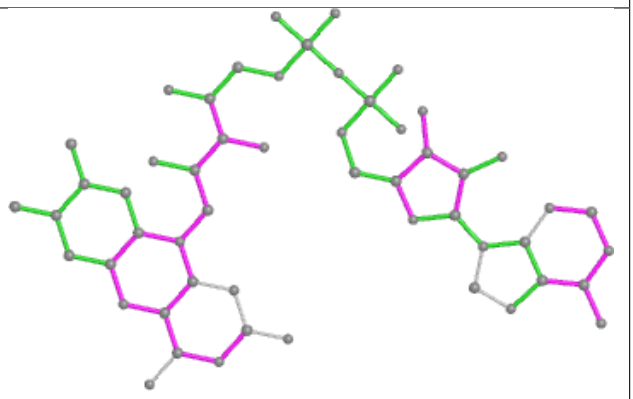
Ligand FAD C 501



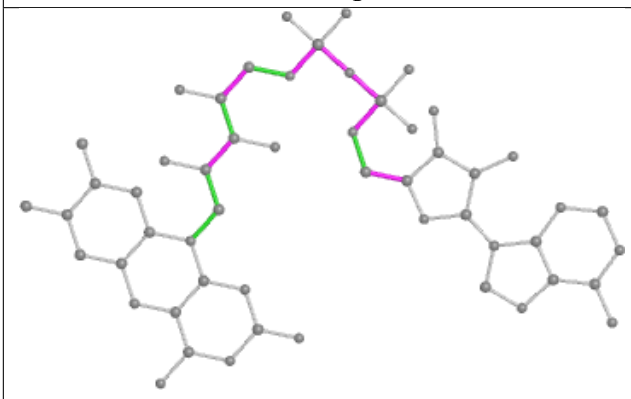
Ligand FAD A 501



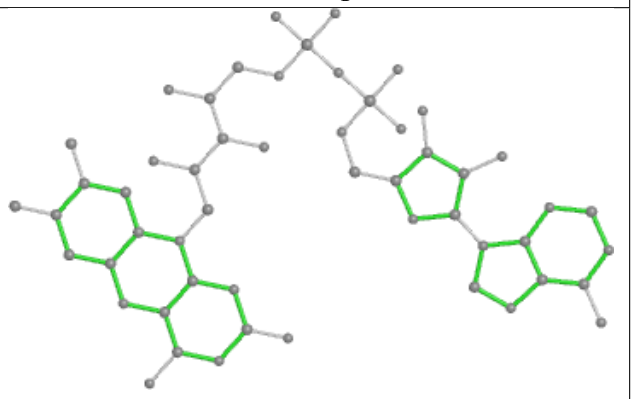
Bond lengths



Bond angles

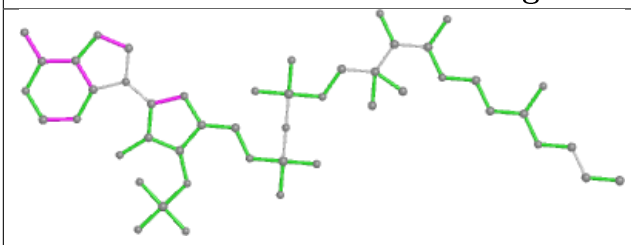


Torsions

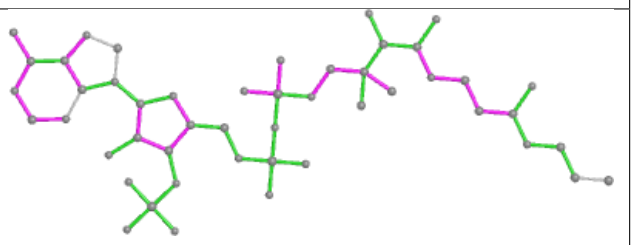


Rings

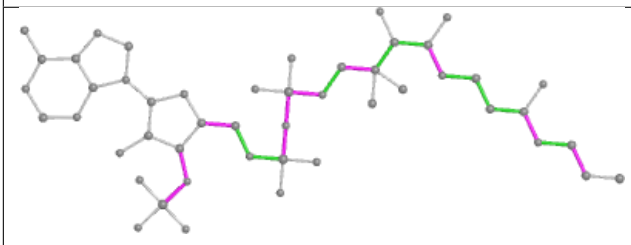
Ligand COA B 503



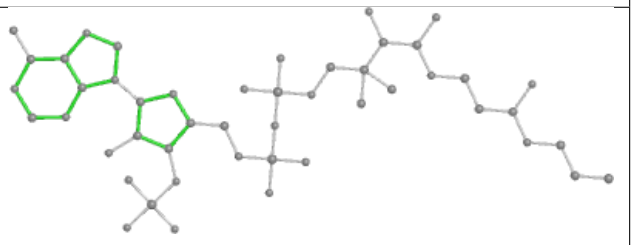
Bond lengths



Bond angles

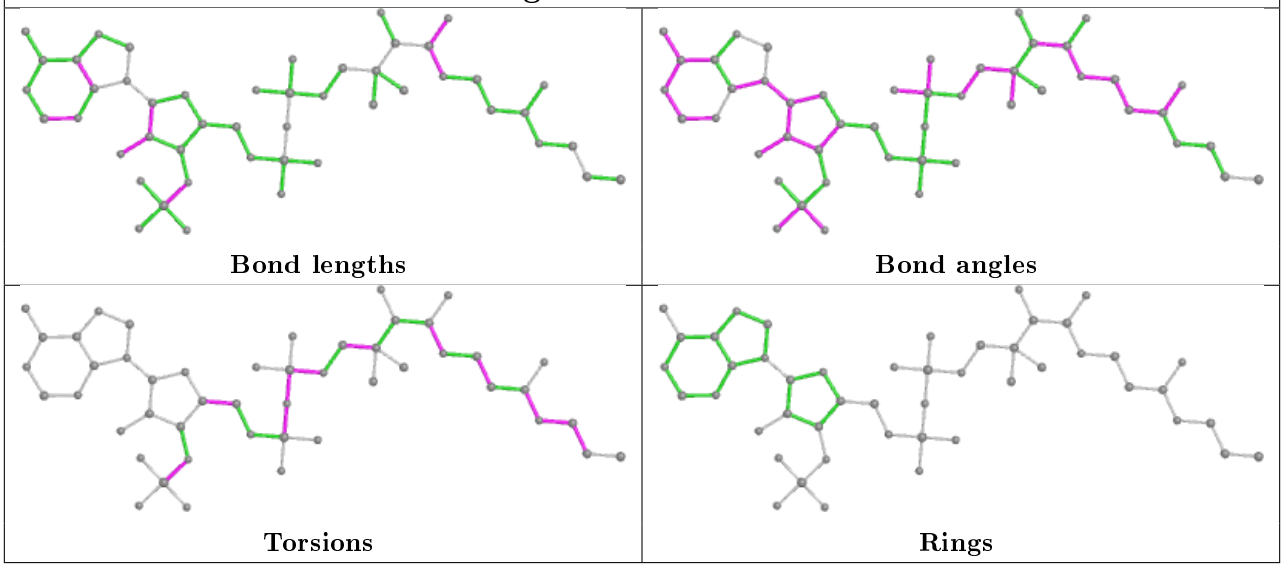


Torsions

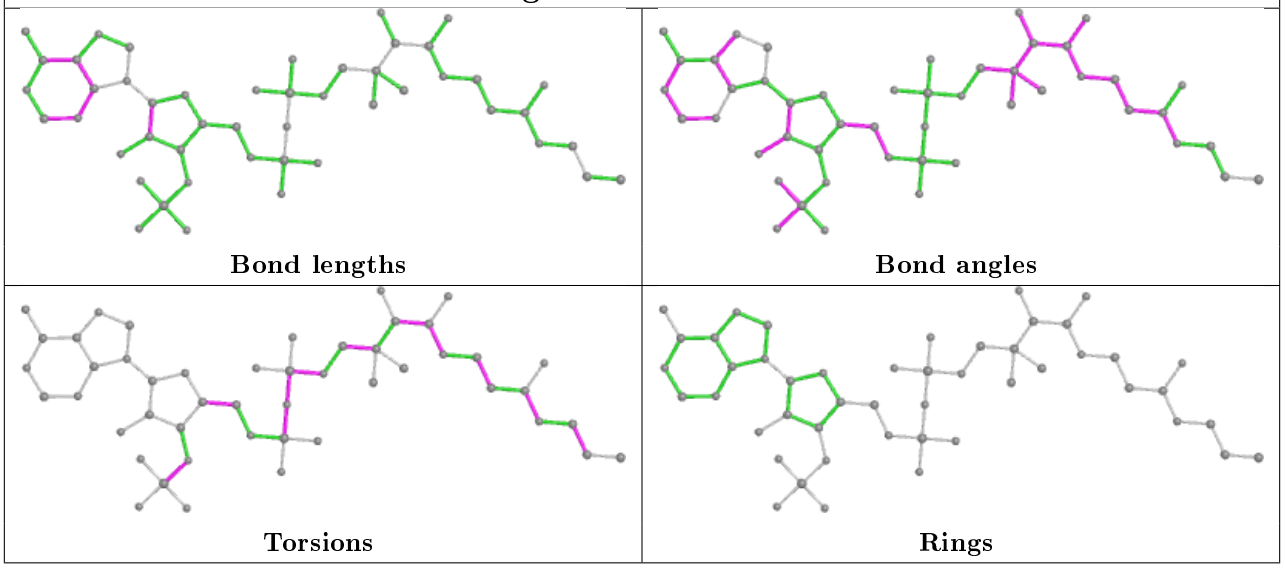


Rings

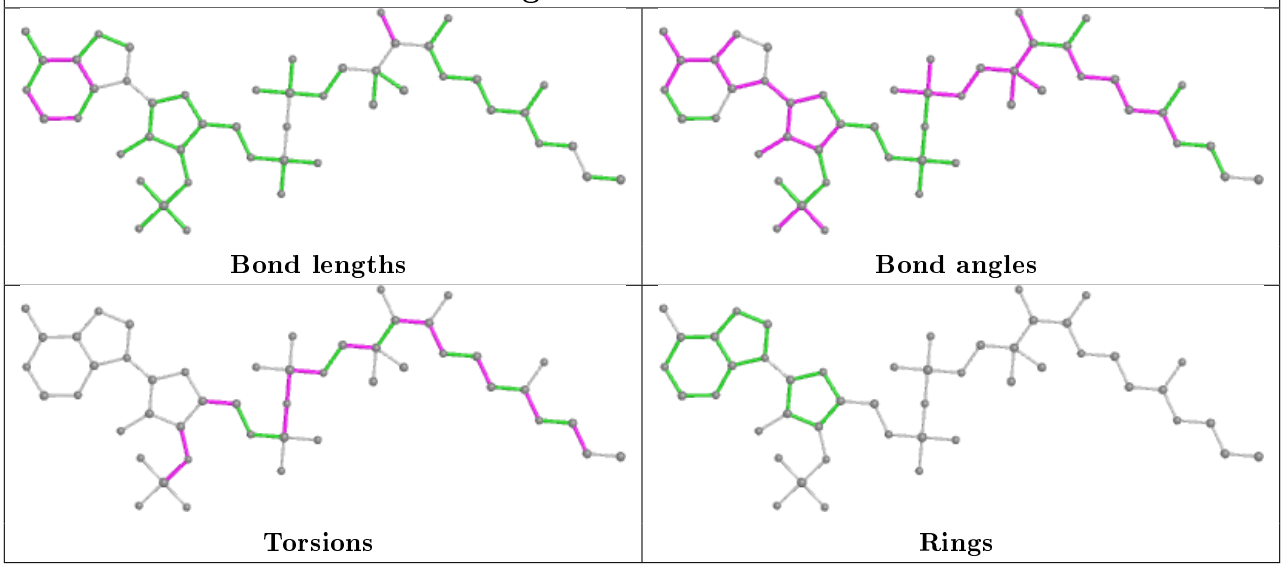
Ligand COA C 502



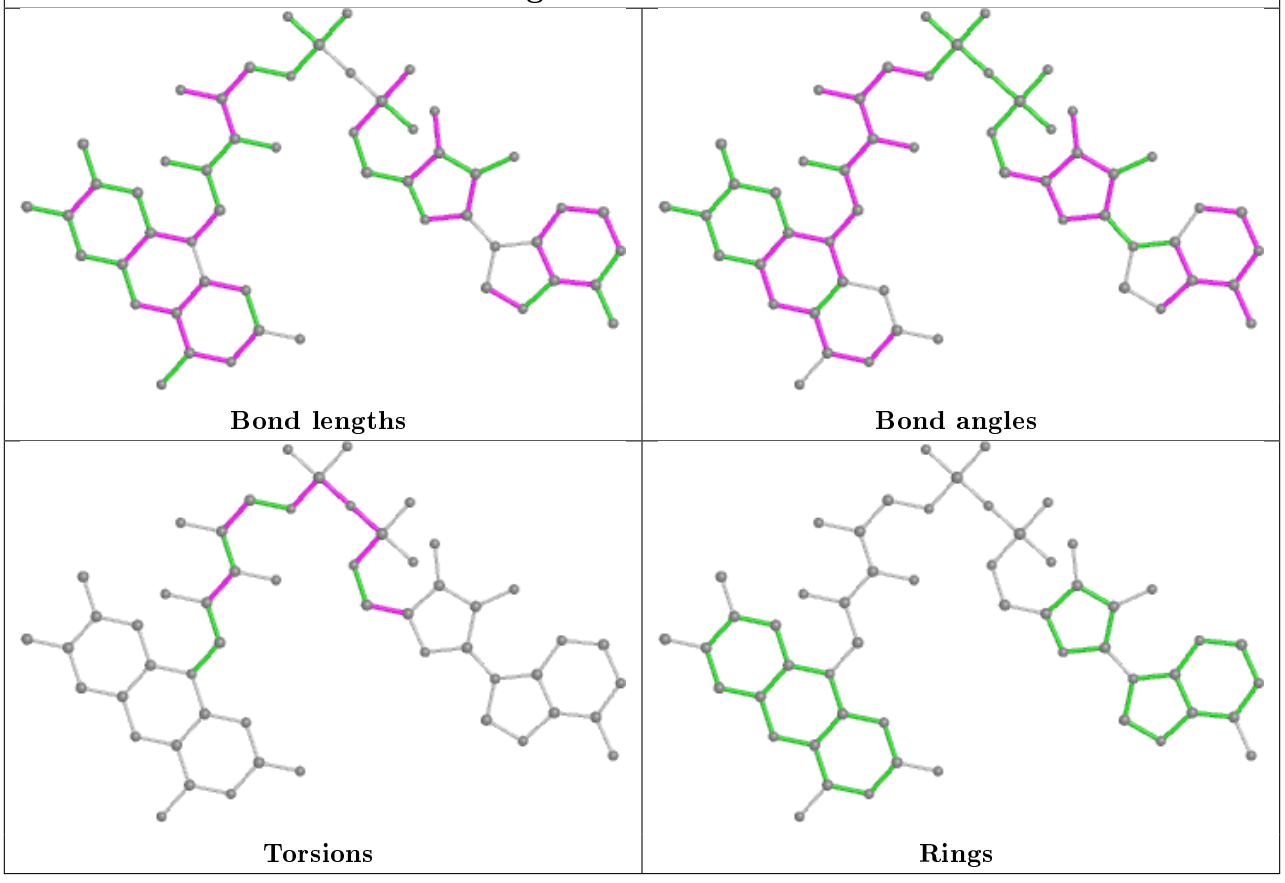
Ligand COA A 502



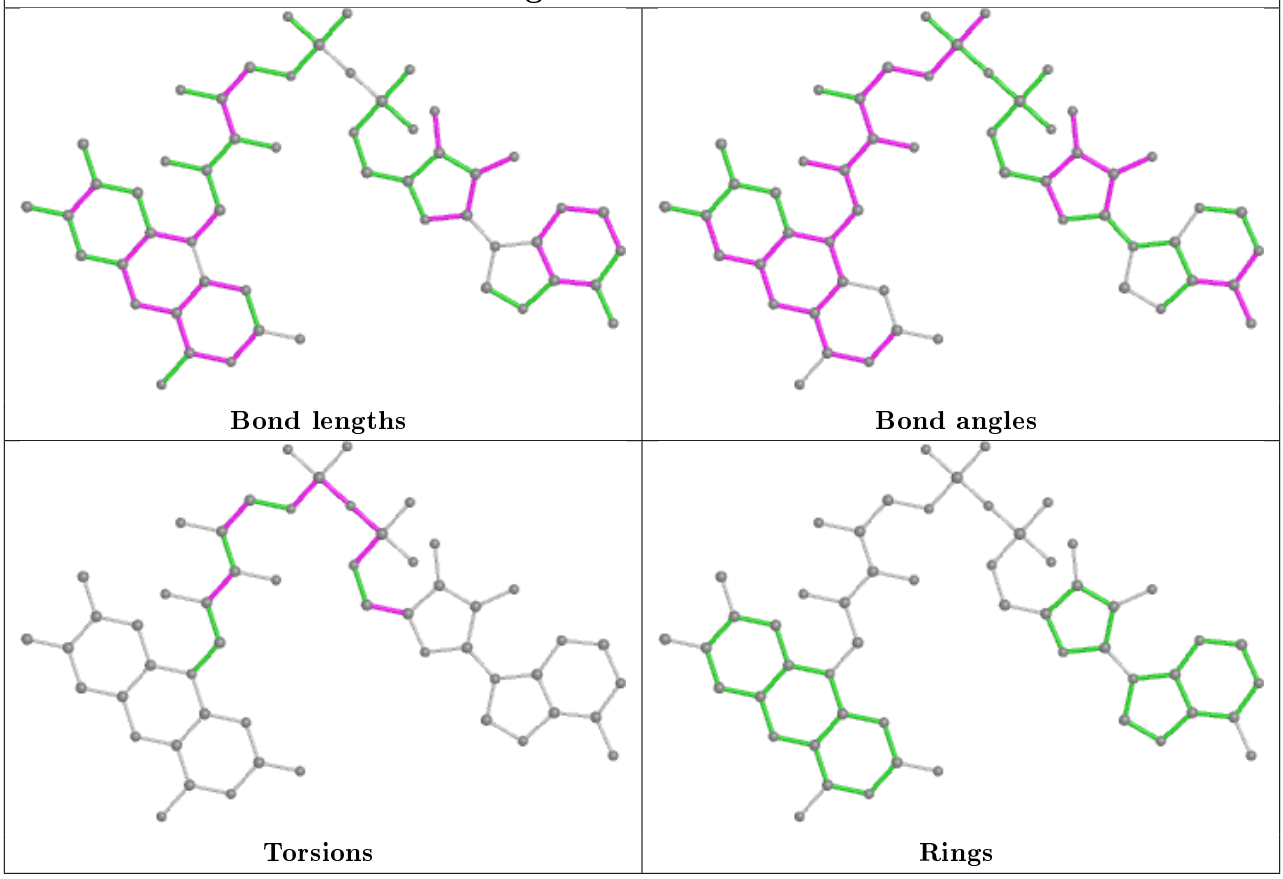
Ligand COA D 502



Ligand FAD B 502



Ligand FAD D 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.27	3 (0%)	87	69	28, 47, 74, 134	0
1	B	443/443 (100%)	-0.20	3 (0%)	87	69	29, 48, 75, 137	0
1	C	443/443 (100%)	-0.30	2 (0%)	91	75	28, 48, 74, 136	0
1	D	443/443 (100%)	-0.32	6 (1%)	75	49	27, 49, 76, 137	0
All	All	1772/1772 (100%)	-0.27	14 (0%)	86	65	27, 48, 76, 137	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	7.6
1	D	1	MET	6.0
1	C	1	MET	6.0
1	A	1	MET	4.4
1	B	2	GLY	4.2
1	C	2	GLY	3.7
1	D	88	LEU	3.1
1	B	442	ALA	3.1
1	D	442	ALA	2.8
1	D	352	TRP	2.6
1	D	2	GLY	2.4
1	D	86	TYR	2.2
1	A	2	GLY	2.1
1	A	443	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

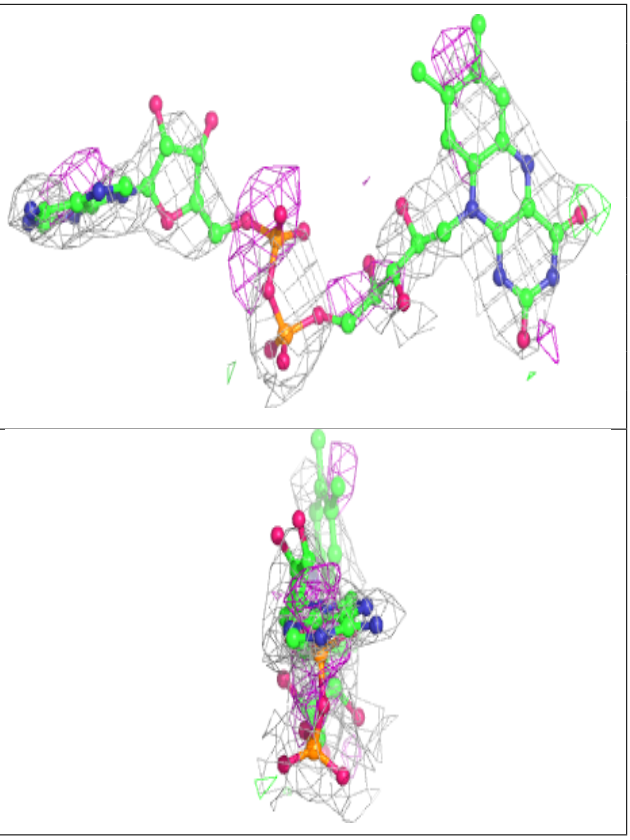
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.59	0.58	80,101,140,141	0
4	VK3	B	501	13/13	0.69	0.57	79,106,136,140	0
4	VK3	A	503	13/13	0.69	0.48	80,100,137,143	0
4	VK3	C	503	13/13	0.70	0.51	81,103,139,139	0
2	FAD	B	502	53/53	0.83	0.47	55,83,109,156	0
2	FAD	A	501	53/53	0.88	0.38	54,81,113,152	0
2	FAD	D	501	53/53	0.89	0.30	54,81,111,141	0
2	FAD	C	501	53/53	0.90	0.26	50,79,108,131	0
3	COA	A	502	48/48	0.96	0.18	38,52,70,94	0
3	COA	D	502	48/48	0.96	0.18	36,52,73,94	0
3	COA	B	503	48/48	0.97	0.18	39,52,75,91	0
3	COA	C	502	48/48	0.97	0.17	37,52,74,99	0

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

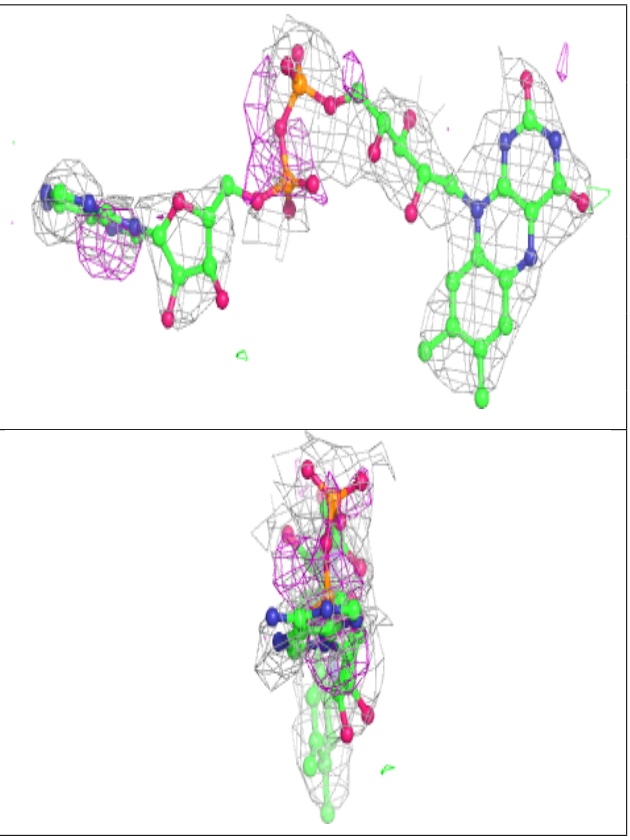
Electron density around FAD B 502:

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



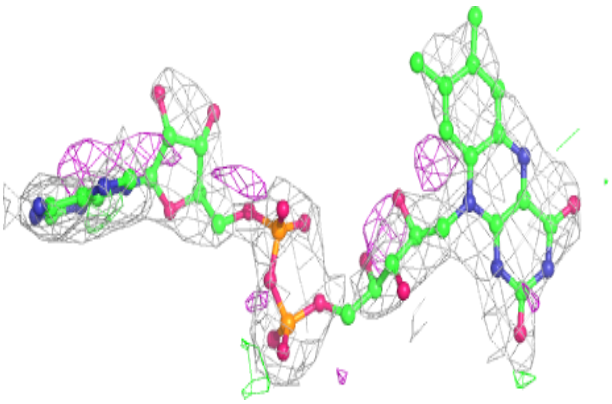
Electron density around FAD A 501:

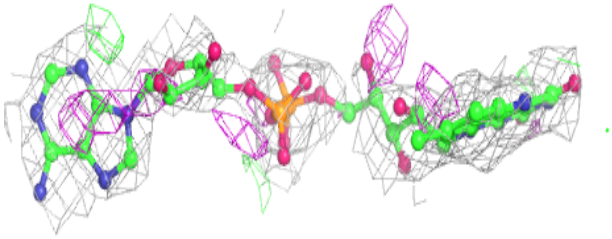
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

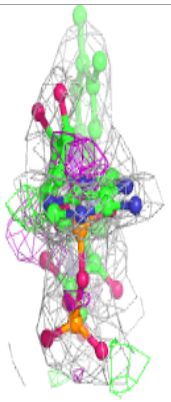


Electron density around FAD D 501:

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

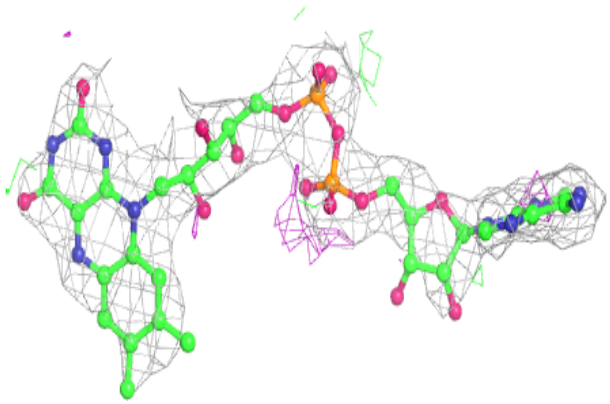


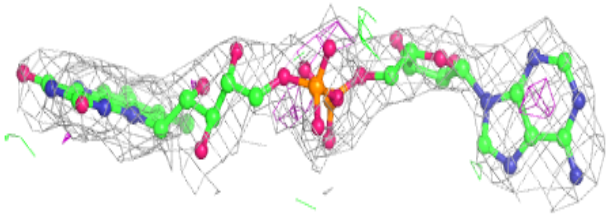


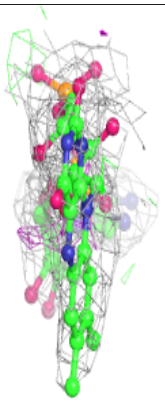


Electron density around FAD C 501:

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

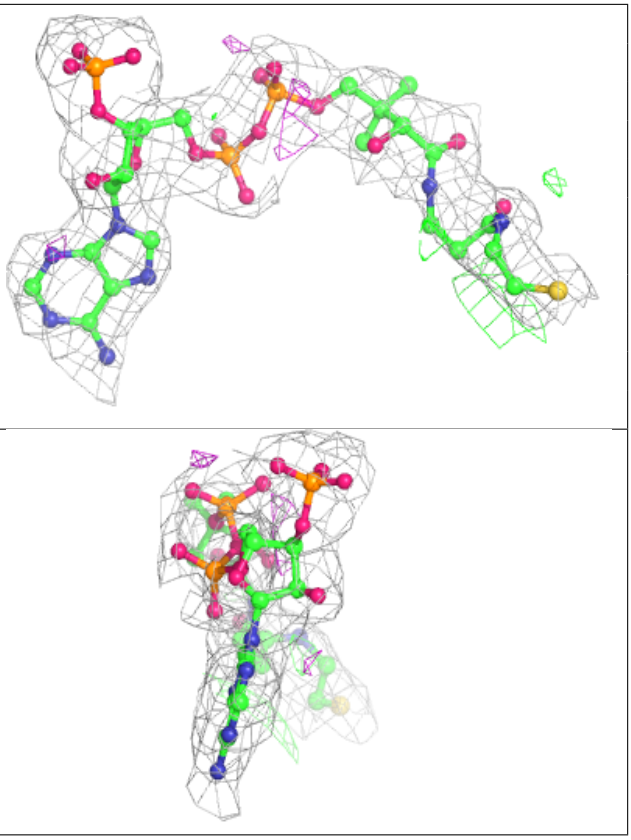






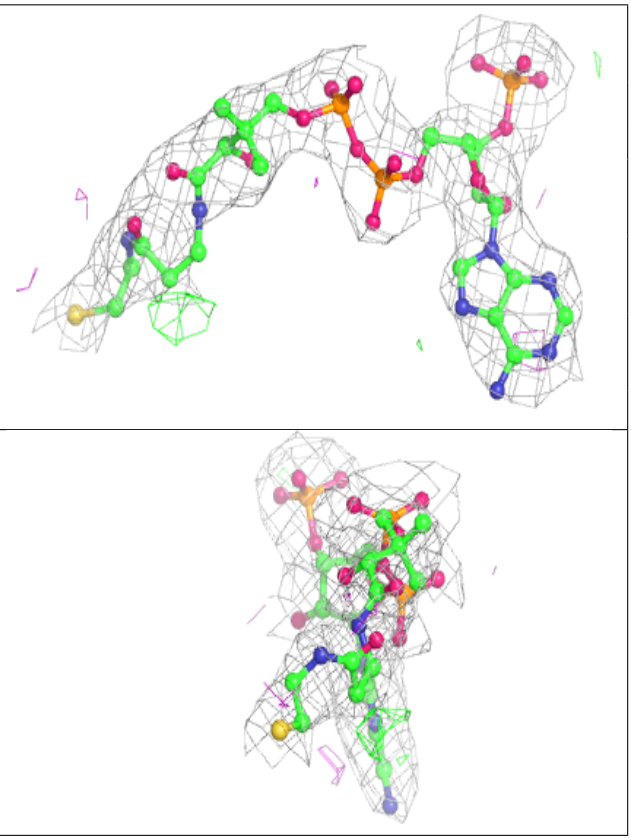
Electron density around COA A 502:

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



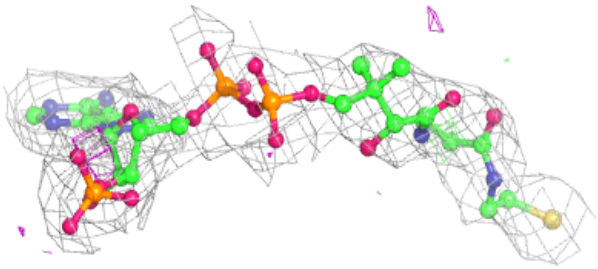
Electron density around COA D 502:

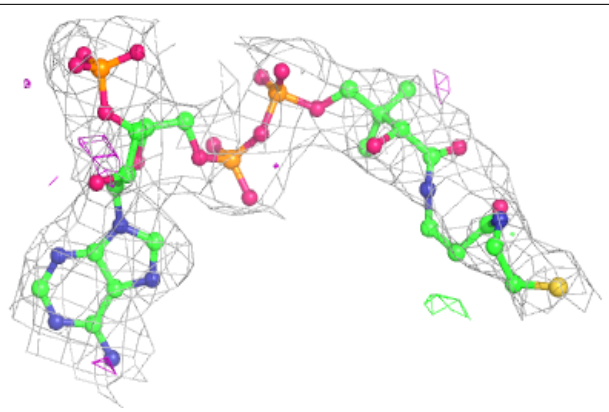
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around COA B 503:

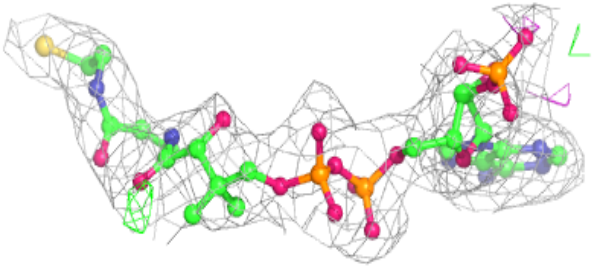
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

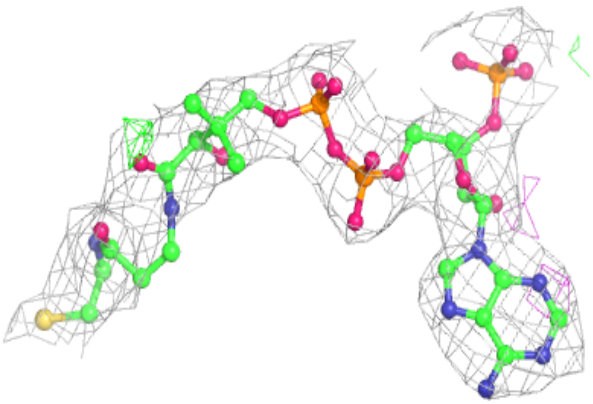


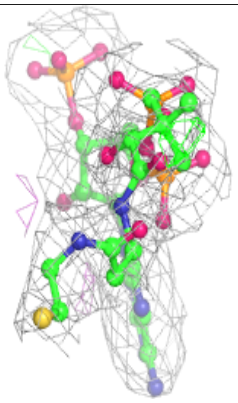


Electron density around COA C 502:

$2mF_o$-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.