Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 04:00 AM EDT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

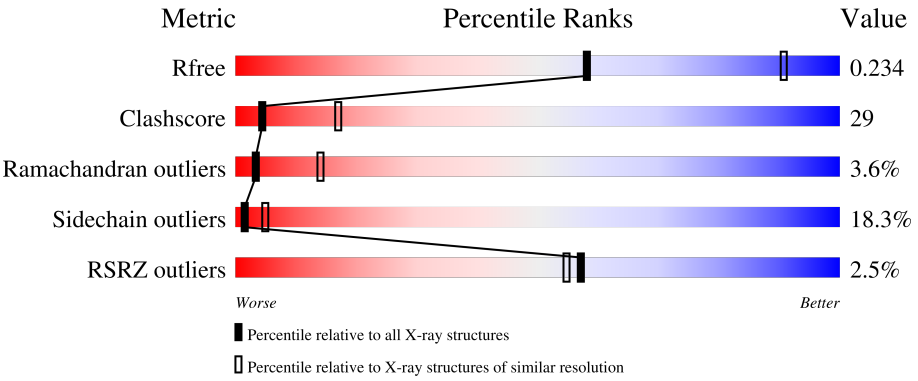
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 55% 31% 9% 5%
1	B	443	3% 53% 32% 11% 5%
1	C	443	3% 56% 29% 12% .
1	D	443	2% 48% 36% 11% 5%

2 Entry composition (i)

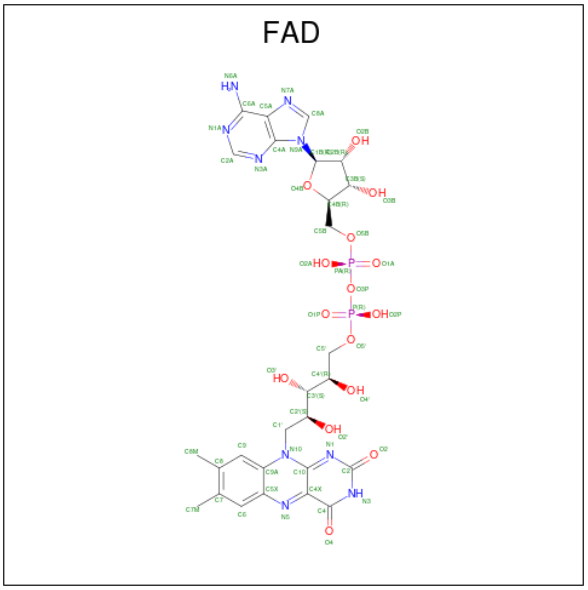
There are 4 unique types of molecules in this entry. The entry contains 13974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH oxidase.

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

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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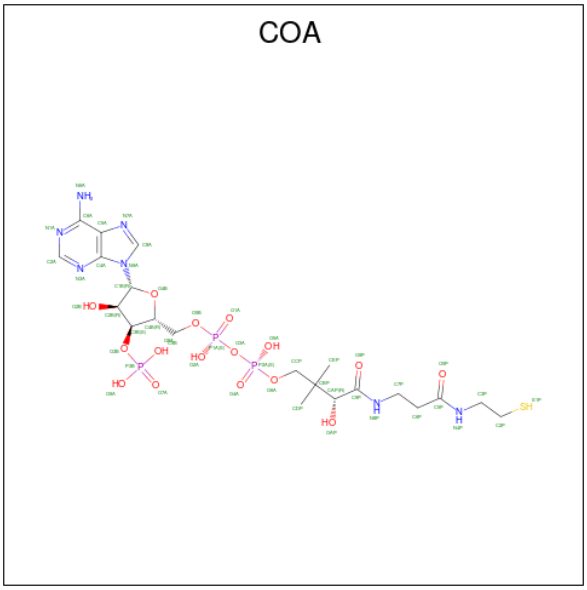
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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 water.

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

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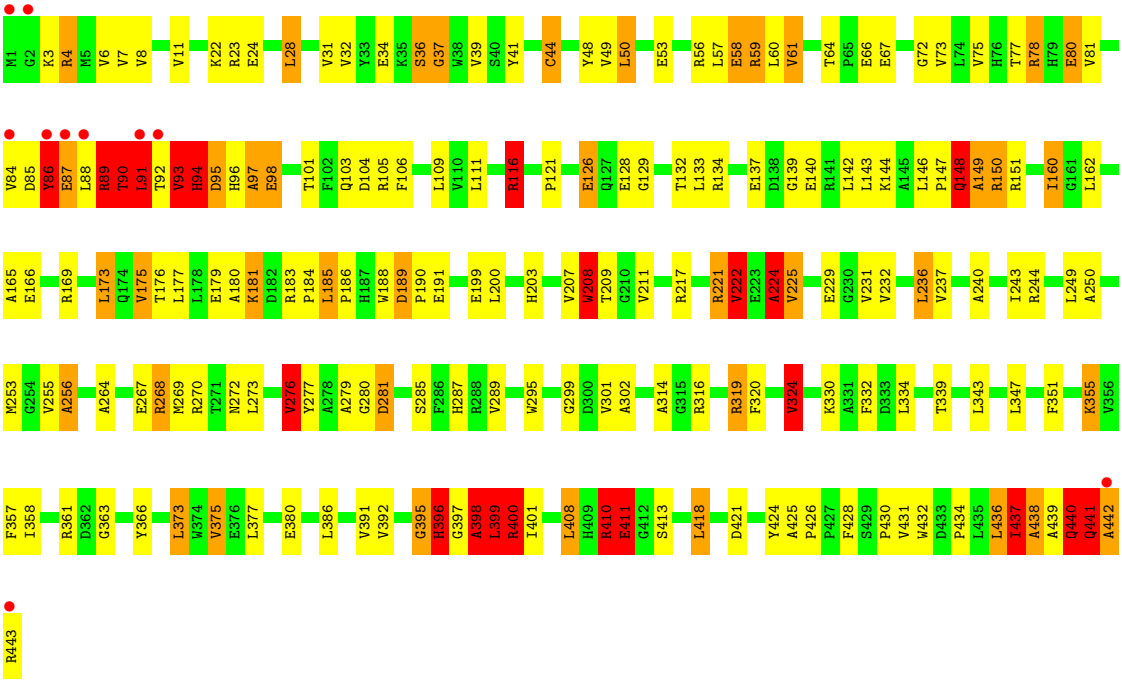
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	11	Total O 11 11	0	0

3 Residue-property plots (i)

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

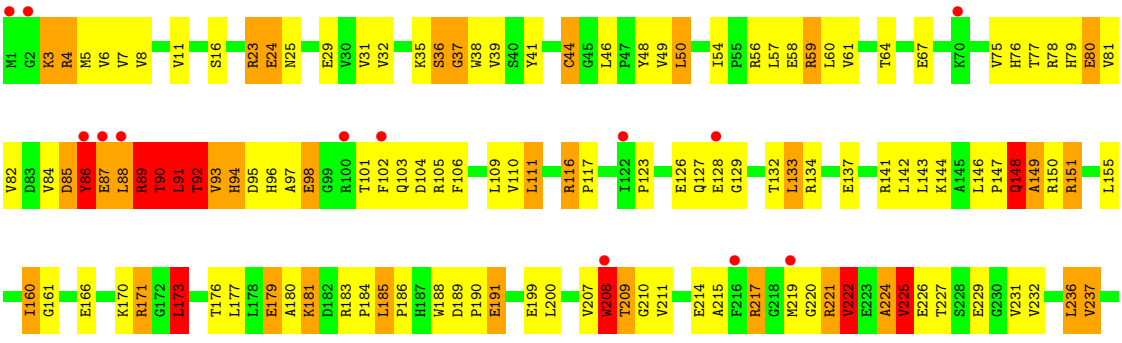
• Molecule 1: NADH oxidase

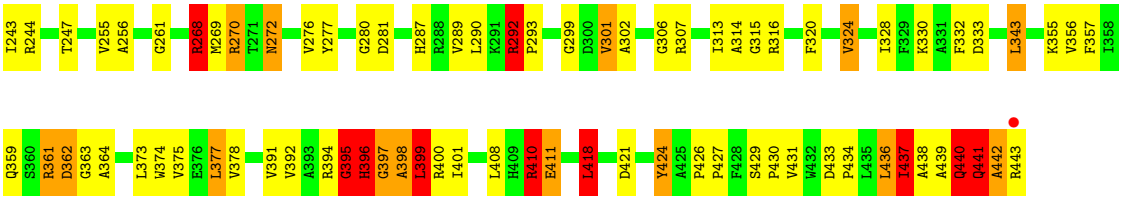
Chain A:



• Molecule 1: NADH oxidase

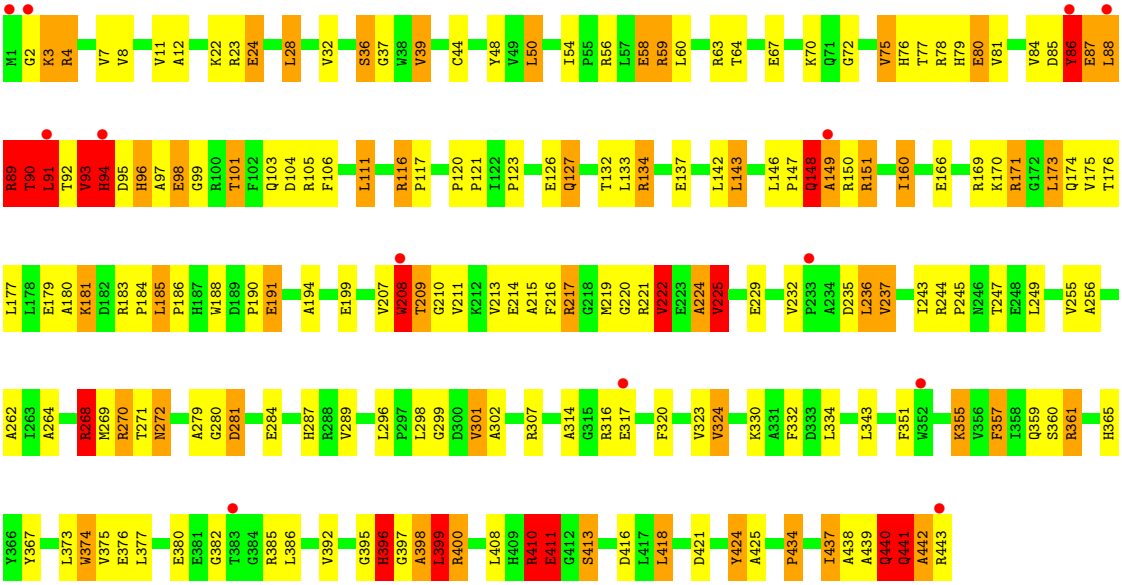
Chain B:





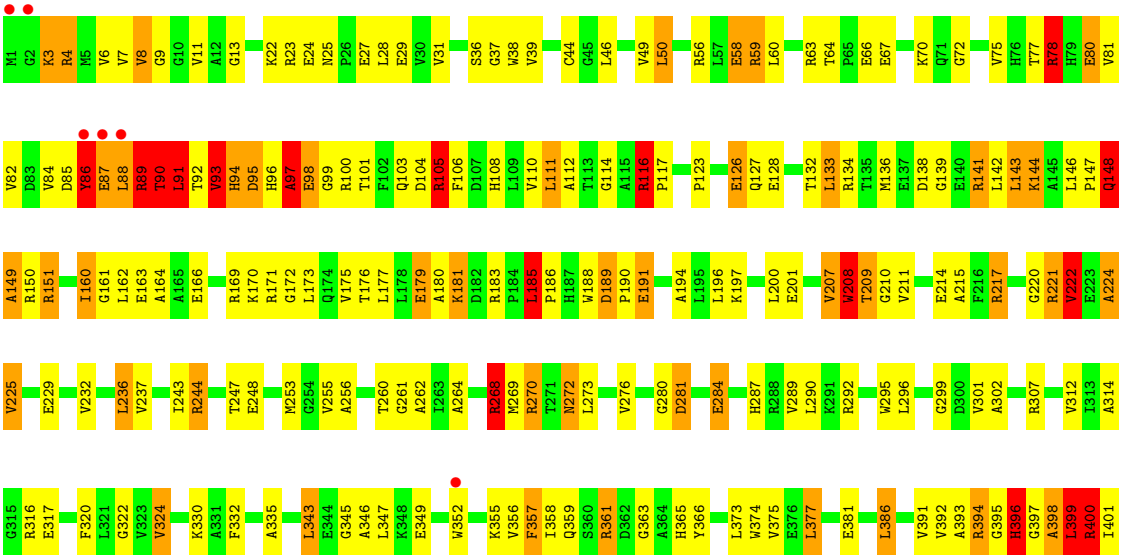
• Molecule 1: NADH oxidase

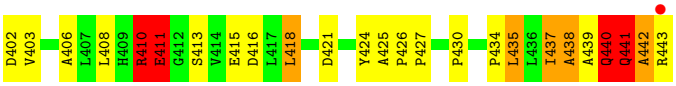
Chain C:



• Molecule 1: NADH oxidase

Chain D:




D402
V403
A406
L407
L408
H409
R410
E411
G412
S413
V414
E415
D416
L417
L418
D421
Y424
A425
P426
P427
P430
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	159.98Å 159.98Å 256.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.38 – 2.90 58.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (58.38-2.90) 98.2 (58.38-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.30	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.207 , 0.244 0.200 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å^2)	72.7	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13974	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, COA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.68	51/3451 (1.5%)	1.46	50/4686 (1.1%)
1	B	1.66	37/3451 (1.1%)	1.46	36/4686 (0.8%)
1	C	1.59	38/3450 (1.1%)	1.43	43/4683 (0.9%)
1	D	1.63	44/3449 (1.3%)	1.44	51/4683 (1.1%)
All	All	1.64	170/13801 (1.2%)	1.45	180/18738 (1.0%)

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

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

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	GLU	CG-CD	11.35	1.69	1.51
1	A	98	GLU	CG-CD	11.18	1.68	1.51
1	C	86	TYR	CB-CG	10.23	1.67	1.51
1	A	208	TRP	CG-CD1	10.14	1.50	1.36
1	A	86	TYR	CB-CG	10.06	1.66	1.51
1	B	440	GLN	C-O	10.03	1.42	1.23
1	C	440	GLN	C-O	9.86	1.42	1.23
1	D	97	ALA	CA-CB	9.65	1.72	1.52
1	D	396	HIS	C-O	9.53	1.41	1.23
1	C	396	HIS	C-O	9.43	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	351	PHE	CE1-CZ	9.18	1.54	1.37
1	D	440	GLN	C-O	8.96	1.40	1.23
1	B	86	TYR	CB-CG	8.81	1.64	1.51
1	A	440	GLN	C-O	8.80	1.40	1.23
1	B	137	GLU	CG-CD	8.76	1.65	1.51
1	B	208	TRP	CG-CD1	8.75	1.49	1.36
1	C	98	GLU	CG-CD	8.53	1.64	1.51
1	D	208	TRP	CG-CD1	8.40	1.48	1.36
1	C	87	GLU	CD-OE1	8.39	1.34	1.25
1	B	396	HIS	C-O	8.01	1.38	1.23
1	A	87	GLU	CD-OE2	7.99	1.34	1.25
1	B	441	GLN	CG-CD	7.92	1.69	1.51
1	D	317	GLU	CG-CD	7.83	1.63	1.51
1	D	191	GLU	CD-OE2	7.80	1.34	1.25
1	C	137	GLU	CG-CD	7.75	1.63	1.51
1	B	86	TYR	CD1-CE1	7.73	1.50	1.39
1	D	163	GLU	CG-CD	7.72	1.63	1.51
1	C	87	GLU	CD-OE2	7.60	1.34	1.25
1	A	441	GLN	CG-CD	7.41	1.68	1.51
1	A	256	ALA	CA-CB	-7.37	1.36	1.52
1	C	86	TYR	CD1-CE1	7.35	1.50	1.39
1	C	86	TYR	CE1-CZ	7.34	1.48	1.38
1	D	295	TRP	CB-CG	-7.29	1.37	1.50
1	C	441	GLN	CG-CD	7.25	1.67	1.51
1	C	97	ALA	CA-CB	7.23	1.67	1.52
1	C	24	GLU	CD-OE2	7.22	1.33	1.25
1	D	440	GLN	CD-NE2	7.18	1.50	1.32
1	B	191	GLU	CD-OE2	7.17	1.33	1.25
1	D	441	GLN	CG-CD	7.08	1.67	1.51
1	C	93	VAL	CA-CB	7.06	1.69	1.54
1	C	411	GLU	CG-CD	7.04	1.62	1.51
1	D	29	GLU	CG-CD	6.97	1.62	1.51
1	A	264	ALA	CA-CB	-6.97	1.37	1.52
1	A	86	TYR	CD1-CE1	6.95	1.49	1.39
1	A	86	TYR	CG-CD1	6.94	1.48	1.39
1	D	191	GLU	CD-OE1	6.93	1.33	1.25
1	A	87	GLU	CD-OE1	6.89	1.33	1.25
1	B	98	GLU	CD-OE1	6.89	1.33	1.25
1	D	98	GLU	CG-CD	6.89	1.62	1.51
1	C	194	ALA	CA-CB	-6.86	1.38	1.52
1	B	226	GLU	CG-CD	6.78	1.62	1.51
1	C	86	TYR	CG-CD2	6.75	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	ALA	CA-CB	6.73	1.66	1.52
1	B	87	GLU	CD-OE1	6.68	1.33	1.25
1	B	191	GLU	CD-OE1	6.66	1.32	1.25
1	D	90	THR	CB-CG2	6.65	1.74	1.52
1	B	222	VAL	CA-CB	6.62	1.68	1.54
1	D	86	TYR	CE1-CZ	6.58	1.47	1.38
1	D	86	TYR	CB-CG	6.57	1.61	1.51
1	C	58	GLU	CG-CD	6.56	1.61	1.51
1	B	301	VAL	CB-CG1	-6.47	1.39	1.52
1	C	374	TRP	CE3-CZ3	6.47	1.49	1.38
1	D	87	GLU	CB-CG	6.44	1.64	1.52
1	B	208	TRP	CD2-CE2	6.43	1.49	1.41
1	C	191	GLU	CD-OE1	6.41	1.32	1.25
1	B	137	GLU	CD-OE1	6.40	1.32	1.25
1	A	126	GLU	CG-CD	6.40	1.61	1.51
1	D	179	GLU	CG-CD	6.38	1.61	1.51
1	B	86	TYR	CG-CD2	6.34	1.47	1.39
1	B	440	GLN	CD-NE2	6.32	1.48	1.32
1	C	86	TYR	CG-CD1	6.28	1.47	1.39
1	A	48	TYR	CE2-CZ	6.27	1.46	1.38
1	A	86	TYR	CE1-CZ	6.24	1.46	1.38
1	B	424	TYR	CE2-CZ	6.23	1.46	1.38
1	A	53	GLU	CD-OE2	6.22	1.32	1.25
1	A	98	GLU	CB-CG	6.20	1.64	1.52
1	A	93	VAL	CB-CG2	-6.19	1.39	1.52
1	C	357	PHE	CD1-CE1	6.18	1.51	1.39
1	C	208	TRP	CG-CD1	6.17	1.45	1.36
1	D	381	GLU	C-O	6.14	1.35	1.23
1	B	86	TYR	CG-CD1	6.12	1.47	1.39
1	A	440	GLN	CA-CB	6.10	1.67	1.53
1	B	24	GLU	CD-OE1	6.08	1.32	1.25
1	C	317	GLU	CG-CD	6.08	1.61	1.51
1	C	440	GLN	CA-CB	6.08	1.67	1.53
1	C	264	ALA	CA-CB	-6.07	1.39	1.52
1	C	411	GLU	CB-CG	6.03	1.63	1.52
1	A	437	ILE	CA-CB	6.00	1.68	1.54
1	D	163	GLU	CD-OE1	5.95	1.32	1.25
1	A	97	ALA	CA-CB	5.88	1.64	1.52
1	A	137	GLU	CD-OE1	5.82	1.32	1.25
1	A	208	TRP	CD2-CE2	5.82	1.48	1.41
1	A	58	GLU	CG-CD	5.81	1.60	1.51
1	D	268	ARG	CZ-NH1	5.81	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	GLU	CA-C	5.81	1.68	1.52
1	D	86	TYR	CD1-CE1	5.78	1.48	1.39
1	C	441	GLN	CB-CG	5.77	1.68	1.52
1	B	35	LYS	CB-CG	-5.74	1.37	1.52
1	B	87	GLU	CD-OE2	5.74	1.31	1.25
1	C	137	GLU	CD-OE1	5.72	1.31	1.25
1	C	24	GLU	CG-CD	5.71	1.60	1.51
1	A	380	GLU	CG-CD	5.70	1.60	1.51
1	D	349	GLU	CD-OE1	5.69	1.31	1.25
1	A	150	ARG	CG-CD	5.68	1.66	1.51
1	D	58	GLU	CG-CD	5.65	1.60	1.51
1	B	87	GLU	CB-CG	5.62	1.62	1.52
1	C	421	ASP	CB-CG	5.60	1.63	1.51
1	A	166	GLU	CD-OE1	5.59	1.31	1.25
1	A	277	TYR	CD1-CE1	-5.57	1.31	1.39
1	C	410	ARG	CG-CD	5.56	1.65	1.51
1	B	231	VAL	CB-CG1	5.55	1.64	1.52
1	D	322	GLY	C-O	5.55	1.32	1.23
1	A	95	ASP	CB-CG	-5.54	1.40	1.51
1	C	397	GLY	CA-C	5.51	1.60	1.51
1	D	105	ARG	CZ-NH1	5.49	1.40	1.33
1	A	366	TYR	CE2-CZ	5.46	1.45	1.38
1	D	179	GLU	CD-OE1	5.45	1.31	1.25
1	D	264	ALA	CA-CB	-5.44	1.41	1.52
1	A	165	ALA	CA-CB	5.43	1.63	1.52
1	D	349	GLU	CD-OE2	5.42	1.31	1.25
1	D	86	TYR	CD2-CE2	5.39	1.47	1.39
1	D	126	GLU	CG-CD	5.39	1.60	1.51
1	A	97	ALA	N-CA	5.39	1.57	1.46
1	A	295	TRP	CG-CD1	-5.38	1.29	1.36
1	A	73	VAL	CB-CG2	5.37	1.64	1.52
1	A	351	PHE	CE1-CZ	5.36	1.47	1.37
1	B	89	ARG	CG-CD	5.35	1.65	1.51
1	D	357	PHE	CD2-CE2	5.34	1.50	1.39
1	A	188	TRP	CZ3-CH2	5.34	1.48	1.40
1	D	86	TYR	CG-CD2	5.34	1.46	1.39
1	B	179	GLU	CG-CD	5.34	1.59	1.51
1	D	357	PHE	CE1-CZ	5.33	1.47	1.37
1	D	441	GLN	C-O	5.31	1.33	1.23
1	B	378	VAL	CB-CG1	-5.30	1.41	1.52
1	B	29	GLU	CD-OE2	5.30	1.31	1.25
1	B	86	TYR	CE1-CZ	5.29	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	ALA	CA-CB	-5.29	1.41	1.52
1	D	66	GLU	CD-OE1	5.27	1.31	1.25
1	D	87	GLU	CD-OE1	5.27	1.31	1.25
1	B	86	TYR	CD2-CE2	5.25	1.47	1.39
1	A	86	TYR	CD2-CE2	5.23	1.47	1.39
1	B	225	VAL	CA-CB	5.23	1.65	1.54
1	A	438	ALA	CA-CB	-5.23	1.41	1.52
1	A	93	VAL	CA-CB	5.22	1.65	1.54
1	A	324	VAL	CB-CG2	-5.21	1.42	1.52
1	B	437	ILE	CA-CB	5.21	1.66	1.54
1	A	250	ALA	CA-CB	-5.20	1.41	1.52
1	D	8	VAL	CB-CG1	5.20	1.63	1.52
1	D	335	ALA	CA-CB	5.17	1.63	1.52
1	D	366	TYR	CG-CD1	5.16	1.45	1.39
1	B	207	VAL	CA-CB	5.16	1.65	1.54
1	D	49	VAL	CB-CG2	-5.16	1.42	1.52
1	A	279	ALA	CA-CB	5.15	1.63	1.52
1	A	410	ARG	CG-CD	5.11	1.64	1.51
1	D	411	GLU	CG-CD	5.10	1.59	1.51
1	A	357	PHE	CD1-CE1	5.09	1.49	1.39
1	A	411	GLU	CG-CD	5.07	1.59	1.51
1	C	87	GLU	CA-C	5.06	1.66	1.52
1	C	2	GLY	C-O	5.05	1.31	1.23
1	C	279	ALA	CA-CB	5.05	1.63	1.52
1	A	276	VAL	CB-CG1	-5.05	1.42	1.52
1	A	324	VAL	CB-CG1	-5.04	1.42	1.52
1	A	355	LYS	CB-CG	-5.04	1.39	1.52
1	D	415	GLU	CG-CD	5.03	1.59	1.51
1	C	213	VAL	CB-CG2	-5.02	1.42	1.52
1	A	396	HIS	C-O	5.02	1.32	1.23
1	D	284	GLU	CD-OE2	5.01	1.31	1.25
1	A	222	VAL	CA-CB	5.01	1.65	1.54
1	C	367	TYR	CB-CG	-5.01	1.44	1.51
1	A	295	TRP	CB-CG	-5.00	1.41	1.50

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	397	GLY	N-CA-C	13.68	147.29	113.10
1	C	87	GLU	OE1-CD-OE2	10.31	135.67	123.30
1	A	134	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	A	268	ARG	NE-CZ-NH2	-10.04	115.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	268	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	C	4	ARG	NE-CZ-NH1	-9.83	115.39	120.30
1	C	397	GLY	N-CA-C	9.15	135.98	113.10
1	D	4	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	A	347	LEU	CB-CG-CD2	8.59	125.60	111.00
1	D	36	SER	C-N-CA	-8.59	104.27	122.30
1	D	141	ARG	NE-CZ-NH1	-8.43	116.09	120.30
1	C	385	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	C	160	ILE	C-N-CA	-8.32	104.82	122.30
1	B	421	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	D	268	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	160	ILE	C-N-CA	-8.12	105.25	122.30
1	C	217	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	B	141	ARG	NE-CZ-NH1	-7.87	116.37	120.30
1	C	36	SER	C-N-CA	-7.87	105.78	122.30
1	B	160	ILE	C-N-CA	-7.82	105.88	122.30
1	D	217	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	D	160	ILE	C-N-CA	-7.80	105.91	122.30
1	A	98	GLU	OE1-CD-OE2	-7.76	113.98	123.30
1	C	396	HIS	CA-C-N	-7.75	100.70	116.20
1	A	28	LEU	CB-CG-CD2	-7.74	97.84	111.00
1	B	87	GLU	OE1-CD-OE2	7.66	132.49	123.30
1	A	89	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	C	421	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	B	91	LEU	CA-CB-CG	7.41	132.33	115.30
1	A	421	ASP	CB-CG-OD2	-7.37	111.66	118.30
1	D	208	TRP	CA-CB-CG	7.34	127.64	113.70
1	B	268	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	C	91	LEU	CA-CB-CG	7.22	131.90	115.30
1	C	440	GLN	CA-C-N	-7.18	101.40	117.20
1	C	208	TRP	CA-CB-CG	7.13	127.24	113.70
1	A	208	TRP	CA-CB-CG	7.09	127.17	113.70
1	A	397	GLY	N-CA-C	7.06	130.75	113.10
1	D	397	GLY	N-CA-C	7.06	130.74	113.10
1	B	36	SER	C-N-CA	-7.03	107.55	122.30
1	C	91	LEU	N-CA-C	-7.01	92.06	111.00
1	D	87	GLU	OE1-CD-OE2	6.99	131.69	123.30
1	D	396	HIS	CA-C-N	-6.99	102.23	116.20
1	A	36	SER	C-N-CA	-6.93	107.74	122.30
1	C	96	HIS	N-CA-CB	-6.91	98.17	110.60
1	C	134	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	C	171	ARG	NE-CZ-NH1	-6.88	116.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	160	ILE	N-CA-C	-6.88	92.43	111.00
1	D	244	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	400	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	97	ALA	N-CA-CB	6.79	119.60	110.10
1	D	394	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	395	GLY	N-CA-C	6.71	129.88	113.10
1	C	94	HIS	N-CA-C	-6.70	92.91	111.00
1	A	116	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	C	89	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	C	98	GLU	CA-CB-CG	-6.58	98.92	113.40
1	D	307	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	B	343	LEU	CB-CG-CD2	-6.53	99.90	111.00
1	B	91	LEU	N-CA-C	-6.49	93.49	111.00
1	B	395	GLY	N-CA-C	6.45	129.22	113.10
1	C	316	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	87	GLU	OE1-CD-OE2	6.34	130.91	123.30
1	C	160	ILE	N-CA-C	-6.33	93.91	111.00
1	C	396	HIS	O-C-N	6.33	133.96	123.20
1	D	396	HIS	O-C-N	6.32	133.94	123.20
1	C	307	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	B	217	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	A	319	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	A	399	LEU	CB-CA-C	-6.27	98.29	110.20
1	D	397	GLY	C-N-CA	6.26	137.34	121.70
1	A	89	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	D	189	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	C	4	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	A	98	GLU	CG-CD-OE1	6.05	130.41	118.30
1	A	93	VAL	CB-CA-C	6.04	122.89	111.40
1	B	440	GLN	CA-C-N	-6.04	103.90	117.20
1	B	89	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	292	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	C	63	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	C	440	GLN	O-C-N	5.93	132.19	122.70
1	B	208	TRP	CA-CB-CG	5.92	124.95	113.70
1	A	93	VAL	CG1-CB-CG2	-5.86	101.53	110.90
1	B	97	ALA	N-CA-CB	5.86	118.30	110.10
1	D	96	HIS	N-CA-CB	-5.85	100.08	110.60
1	B	96	HIS	N-CA-CB	-5.83	100.10	110.60
1	B	333	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	86	TYR	CB-CG-CD1	5.79	124.47	121.00
1	A	222	VAL	CG1-CB-CG2	-5.77	101.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	398	ALA	CB-CA-C	5.73	118.69	110.10
1	B	307	ARG	NE-CZ-NH1	-5.71	117.45	120.30
1	B	399	LEU	CB-CG-CD2	5.68	120.65	111.00
1	B	173	LEU	CB-CG-CD1	-5.67	101.36	111.00
1	A	96	HIS	N-CA-CB	-5.67	100.40	110.60
1	C	235	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	A	91	LEU	O-C-N	5.66	131.76	122.70
1	B	436	LEU	CA-CB-CG	-5.65	102.30	115.30
1	A	160	ILE	N-CA-C	-5.64	95.77	111.00
1	A	91	LEU	CA-C-N	-5.62	104.83	117.20
1	D	217	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	400	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	97	ALA	N-CA-CB	5.59	117.92	110.10
1	C	424	TYR	CA-CB-CG	-5.59	102.79	113.40
1	D	138	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	281	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	421	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	400	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	90	THR	N-CA-C	-5.55	96.02	111.00
1	A	91	LEU	CA-CB-CG	5.54	128.05	115.30
1	D	343	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	C	386	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	A	373	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	D	410	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	421	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	402	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	395	GLY	C-N-CA	5.50	135.46	121.70
1	B	437	ILE	CB-CA-C	5.50	122.60	111.60
1	B	410	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	134	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	B	171	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	B	292	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	410	ARG	O-C-N	-5.46	113.96	122.70
1	A	441	GLN	CA-CB-CG	5.46	125.41	113.40
1	A	436	LEU	CA-CB-CG	-5.42	102.83	115.30
1	D	440	GLN	CA-C-N	-5.41	105.30	117.20
1	B	88	LEU	CB-CG-CD1	5.38	120.15	111.00
1	A	281	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	C	268	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	395	GLY	N-CA-C	5.36	126.49	113.10
1	A	98	GLU	CA-CB-CG	-5.34	101.65	113.40
1	A	410	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	89	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	225	VAL	N-CA-CB	5.33	123.22	111.50
1	A	225	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	B	189	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	D	307	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	93	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	D	441	GLN	CA-CB-CG	5.30	125.06	113.40
1	D	191	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	A	95	ASP	CB-CG-OD1	-5.29	113.53	118.30
1	D	4	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	D	435	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	D	116	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	28	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	D	224	ALA	N-CA-C	5.26	125.19	111.00
1	A	396	HIS	CA-C-N	-5.25	105.69	116.20
1	A	437	ILE	CA-CB-CG2	5.25	121.41	110.90
1	B	85	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	C	397	GLY	CA-C-O	5.24	130.03	120.60
1	D	185	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	189	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	440	GLN	O-C-N	5.21	131.03	122.70
1	C	134	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	D	91	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	224	ALA	N-CA-C	5.18	125.00	111.00
1	B	440	GLN	O-C-N	5.18	131.00	122.70
1	C	90	THR	N-CA-C	-5.18	97.00	111.00
1	C	316	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	4	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	5	MET	CG-SD-CE	5.18	108.48	100.20
1	D	281	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	D	78	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	421	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	109	LEU	CB-CG-CD1	5.14	119.73	111.00
1	D	63	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	D	134	ARG	CG-CD-NE	-5.12	101.04	111.80
1	D	395	GLY	N-CA-C	5.11	125.87	113.10
1	D	95	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	D	399	LEU	CB-CA-C	-5.09	100.53	110.20
1	B	98	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	D	128	GLU	C-N-CA	-5.06	111.67	122.30
1	B	307	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	D	196	LEU	CB-CG-CD2	-5.04	102.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	347	LEU	CB-CG-CD2	5.04	119.58	111.00
1	B	23	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	224	ALA	N-CA-C	5.04	124.60	111.00
1	D	93	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	A	94	HIS	N-CA-C	-5.02	97.44	111.00
1	D	296	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	A	440	GLN	CA-C-N	-5.02	106.15	117.20
1	D	98	GLU	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ALA	Peptide
1	A	240	ALA	Peptide
1	A	37	GLY	Peptide
1	A	396	HIS	Peptide
1	A	398	ALA	Peptide
1	A	399	LEU	Peptide
1	A	440	GLN	Peptide
1	A	90	THR	Peptide
1	B	161	GLY	Peptide
1	B	37	GLY	Peptide
1	B	396	HIS	Peptide
1	B	440	GLN	Peptide
1	B	90	THR	Peptide
1	C	127	GLN	Peptide
1	C	224	ALA	Peptide
1	C	396	HIS	Peptide
1	C	399	LEU	Peptide
1	C	440	GLN	Peptide
1	C	89	ARG	Peptide
1	C	90	THR	Peptide
1	C	99	GLY	Peptide
1	D	396	HIS	Peptide
1	D	440	GLN	Peptide
1	D	90	THR	Peptide
1	D	99	GLY	Peptide

5.2 Too-close contacts (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	212	0
1	B	3379	0	3407	233	0
1	C	3378	0	3402	171	0
1	D	3377	0	3402	204	0
2	A	53	0	31	9	0
2	B	53	0	31	8	0
2	C	53	0	31	10	0
2	D	53	0	31	7	0
3	A	48	0	31	6	0
3	B	48	0	31	7	0
3	C	48	0	31	4	0
3	D	48	0	31	3	0
4	A	14	0	0	7	0
4	B	17	0	0	19	0
4	C	15	0	0	11	0
4	D	11	0	0	9	0
All	All	13974	0	13866	799	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 29.

All (799) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HA	4:B:604:HOH:O	1.29	1.29
1:D:439:ALA:O	1:D:441:GLN:HB2	1.11	1.26
1:B:439:ALA:O	1:B:441:GLN:CB	1.89	1.21
1:A:149:ALA:CB	1:A:150:ARG:HA	1.75	1.17
1:C:439:ALA:O	1:C:441:GLN:HB2	0.99	1.16
1:A:439:ALA:O	1:A:441:GLN:HB2	0.98	1.16
1:A:90:THR:HA	1:A:92:THR:HG23	1.22	1.16
1:A:437:ILE:HD12	1:A:437:ILE:C	1.58	1.15
1:B:149:ALA:CB	1:B:150:ARG:HA	1.73	1.15
1:A:439:ALA:O	1:A:441:GLN:CB	1.95	1.15
1:C:439:ALA:O	1:C:441:GLN:CB	1.95	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:O	1:A:92:THR:HG22	1.47	1.12
1:C:149:ALA:HB1	1:C:150:ARG:HA	1.13	1.12
1:D:147:PRO:O	1:D:148:GLN:HB2	1.48	1.11
1:C:410:ARG:HG2	1:C:410:ARG:HH11	1.06	1.11
1:D:410:ARG:HG2	1:D:410:ARG:HH11	0.98	1.10
1:A:398:ALA:H	1:A:399:LEU:HB2	1.14	1.10
1:B:439:ALA:O	1:B:441:GLN:HB2	0.92	1.08
1:B:437:ILE:C	1:B:437:ILE:HD12	1.72	1.07
1:A:147:PRO:O	1:A:148:GLN:HB2	1.55	1.05
1:C:147:PRO:O	1:C:148:GLN:HB2	1.55	1.04
1:D:398:ALA:H	1:D:399:LEU:HB2	1.18	1.04
1:B:410:ARG:HH11	1:B:410:ARG:HG2	1.12	1.03
1:A:85:ASP:C	1:A:92:THR:HG22	1.79	1.02
1:A:149:ALA:HB1	1:A:150:ARG:HA	1.06	1.02
1:B:85:ASP:O	1:B:92:THR:HG22	1.58	1.02
1:D:149:ALA:HB1	1:D:150:ARG:HA	1.06	1.01
1:C:149:ALA:CB	1:C:150:ARG:HA	1.89	1.01
1:C:50:LEU:HD12	1:C:143:LEU:HD13	1.40	1.00
1:D:149:ALA:CB	1:D:150:ARG:HA	1.88	1.00
1:D:439:ALA:O	1:D:441:GLN:CB	2.08	1.00
1:A:410:ARG:HG2	1:A:410:ARG:HH11	1.22	0.99
1:B:149:ALA:HB1	1:B:150:ARG:CA	1.92	0.99
1:B:441:GLN:O	1:B:442:ALA:O	1.79	0.98
1:A:217:ARG:HB3	1:A:224:ALA:HB3	1.46	0.97
1:A:129:GLY:N	4:A:602:HOH:O	1.93	0.97
1:D:225:VAL:N	4:D:601:HOH:O	1.97	0.97
1:B:149:ALA:HB1	1:B:150:ARG:HA	0.96	0.96
1:C:217:ARG:HB3	1:C:224:ALA:HB3	1.47	0.96
1:D:440:GLN:HA	1:D:440:GLN:NE2	1.81	0.96
1:B:90:THR:OG1	4:B:601:HOH:O	1.84	0.96
1:A:37:GLY:HA2	1:A:77:THR:HB	1.46	0.95
1:C:437:ILE:C	1:C:437:ILE:HD12	1.87	0.95
1:D:116:ARG:NH1	1:D:244:ARG:HD2	1.82	0.94
1:C:410:ARG:HG2	1:C:410:ARG:NH1	1.81	0.94
1:D:410:ARG:HG2	1:D:410:ARG:NH1	1.77	0.94
1:B:37:GLY:HA2	1:B:77:THR:HB	1.48	0.93
1:D:50:LEU:HD12	1:D:143:LEU:HD13	1.48	0.93
1:D:149:ALA:HB1	1:D:150:ARG:CA	1.98	0.92
1:D:441:GLN:O	1:D:442:ALA:O	1.87	0.92
1:A:90:THR:HA	1:A:92:THR:CG2	1.99	0.92
1:A:396:HIS:CE1	1:B:396:HIS:ND1	2.38	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:HIS:CE1	1:B:396:HIS:CE1	2.58	0.91
1:C:86:TYR:CE1	1:C:88:LEU:HD22	2.05	0.91
1:A:269:MET:HE3	1:A:320:PHE:HB3	1.52	0.91
1:B:236:LEU:C	1:B:236:LEU:HD12	1.90	0.91
1:B:147:PRO:O	1:B:148:GLN:HB2	1.69	0.90
1:D:437:ILE:HD12	1:D:437:ILE:C	1.90	0.90
1:B:129:GLY:N	4:B:602:HOH:O	1.92	0.89
1:D:11:VAL:HG23	2:D:501:FAD:H4B	1.54	0.89
1:D:208:TRP:HB3	1:D:211:VAL:HG21	1.56	0.88
1:B:90:THR:HA	1:B:92:THR:HG23	1.53	0.88
1:D:123:PRO:HG2	1:D:215:ALA:HB2	1.55	0.88
1:C:398:ALA:H	1:C:399:LEU:HB2	1.39	0.88
1:D:94:HIS:N	1:D:94:HIS:CD2	2.41	0.87
1:B:92:THR:OG1	1:B:93:VAL:HG23	1.73	0.87
1:B:217:ARG:HB3	1:B:224:ALA:HB3	1.54	0.87
1:C:440:GLN:HA	1:C:440:GLN:NE2	1.91	0.86
1:B:85:ASP:C	1:B:92:THR:HG22	1.95	0.86
1:C:441:GLN:O	1:C:442:ALA:O	1.92	0.85
1:D:398:ALA:N	1:D:399:LEU:HB2	1.91	0.85
1:C:116:ARG:NH1	1:C:244:ARG:HD2	1.92	0.85
1:A:86:TYR:CE1	1:A:88:LEU:HD22	2.11	0.84
1:A:149:ALA:HB1	1:A:150:ARG:CA	2.01	0.84
1:C:410:ARG:HH11	1:C:410:ARG:CG	1.88	0.84
1:B:410:ARG:HG2	1:B:410:ARG:NH1	1.89	0.84
1:C:208:TRP:HB3	1:C:211:VAL:HG21	1.58	0.84
1:A:440:GLN:NE2	1:A:440:GLN:HA	1.93	0.84
1:A:116:ARG:NH1	1:A:244:ARG:HD2	1.92	0.84
1:A:121:PRO:HG2	1:D:149:ALA:HB2	1.57	0.83
1:A:149:ALA:CB	1:A:150:ARG:CA	2.56	0.83
1:A:410:ARG:HG2	1:A:410:ARG:NH1	1.91	0.83
1:A:441:GLN:O	1:A:442:ALA:O	1.97	0.83
1:A:221:ARG:O	1:A:221:ARG:HD3	1.79	0.82
1:B:149:ALA:CB	1:B:150:ARG:CA	2.55	0.82
1:A:396:HIS:ND1	1:B:396:HIS:CE1	2.47	0.82
1:A:396:HIS:CG	1:B:396:HIS:CE1	2.68	0.82
1:A:121:PRO:HG2	1:D:149:ALA:CB	2.09	0.82
1:A:94:HIS:CD2	1:A:94:HIS:N	2.46	0.81
1:C:440:GLN:HA	4:C:602:HOH:O	1.80	0.81
1:B:437:ILE:HD12	1:B:438:ALA:N	1.95	0.81
1:B:94:HIS:N	1:B:94:HIS:CD2	2.44	0.81
1:B:270:ARG:HH11	1:B:270:ARG:HB2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLY:C	1:B:397:GLY:HA2	2.02	0.81
1:D:217:ARG:HB3	1:D:224:ALA:HB3	1.63	0.81
1:A:89:ARG:O	4:A:603:HOH:O	1.98	0.80
1:D:50:LEU:HD12	1:D:143:LEU:CD1	2.11	0.80
1:C:85:ASP:H	1:C:92:THR:HA	1.46	0.80
1:C:398:ALA:H	1:C:399:LEU:CB	1.93	0.80
1:B:224:ALA:O	1:B:232:VAL:O	2.00	0.80
1:B:270:ARG:CB	1:B:270:ARG:NH1	2.45	0.80
1:B:50:LEU:HD12	1:B:143:LEU:HD13	1.64	0.79
1:C:440:GLN:NE2	4:C:602:HOH:O	2.16	0.79
1:B:208:TRP:HB3	1:B:211:VAL:HG21	1.63	0.79
1:D:86:TYR:CE1	1:D:88:LEU:HD22	2.16	0.79
1:A:398:ALA:H	1:A:399:LEU:CB	1.94	0.79
1:A:398:ALA:N	1:A:399:LEU:HB2	1.96	0.79
1:D:50:LEU:CD1	1:D:143:LEU:HD13	2.12	0.78
1:D:248:GLU:HB2	4:D:602:HOH:O	1.80	0.78
1:A:85:ASP:H	1:A:92:THR:HA	1.48	0.78
1:D:256:ALA:H	1:D:272:ASN:ND2	1.81	0.78
1:D:440:GLN:HA	1:D:440:GLN:HE21	1.47	0.78
1:D:224:ALA:O	1:D:232:VAL:O	2.01	0.78
1:A:150:ARG:NH2	4:A:601:HOH:O	1.87	0.78
1:D:211:VAL:HG22	1:D:229:GLU:HG3	1.66	0.78
1:A:211:VAL:HG22	1:A:229:GLU:HG3	1.65	0.77
1:A:396:HIS:CE1	1:B:396:HIS:CG	2.72	0.77
1:B:116:ARG:NH1	1:B:244:ARG:HD2	1.99	0.77
1:B:359:GLN:HB2	1:B:374:TRP:CD1	2.19	0.77
1:C:87:GLU:HA	1:C:88:LEU:C	2.04	0.77
1:C:94:HIS:N	1:C:94:HIS:CD2	2.52	0.77
1:A:270:ARG:HB2	1:A:270:ARG:HH11	1.48	0.77
1:A:92:THR:OG1	1:A:93:VAL:HG23	1.84	0.77
1:C:50:LEU:CD1	1:C:143:LEU:HD13	2.15	0.77
1:A:50:LEU:HD12	1:A:143:LEU:HD13	1.66	0.77
1:D:149:ALA:HA	1:D:173:LEU:HD22	1.66	0.77
1:A:11:VAL:HG23	2:A:501:FAD:H4B	1.67	0.77
1:D:147:PRO:O	1:D:148:GLN:CB	2.30	0.77
1:B:183:ARG:HG3	1:B:184:PRO:O	1.84	0.77
1:B:398:ALA:H	1:B:399:LEU:CB	1.99	0.76
1:C:37:GLY:HA2	1:C:77:THR:HB	1.67	0.76
1:C:270:ARG:HH11	1:C:270:ARG:CB	1.97	0.76
1:B:440:GLN:HA	4:B:603:HOH:O	1.84	0.76
1:B:6:VAL:HG22	1:B:31:VAL:CG1	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:HA	1:B:92:THR:CG2	2.15	0.76
1:C:50:LEU:HD12	1:C:143:LEU:CD1	2.16	0.76
1:D:37:GLY:HA2	1:D:77:THR:HB	1.68	0.76
1:B:270:ARG:HH11	1:B:270:ARG:CB	1.98	0.76
1:B:395:GLY:O	1:B:397:GLY:HA2	1.86	0.76
1:D:94:HIS:N	1:D:94:HIS:HD2	1.83	0.75
1:B:437:ILE:O	1:B:441:GLN:HB3	1.87	0.75
1:A:437:ILE:HD12	1:A:438:ALA:N	2.02	0.75
1:B:91:LEU:O	4:B:601:HOH:O	2.04	0.75
1:C:256:ALA:H	1:C:272:ASN:ND2	1.85	0.75
1:B:86:TYR:CE1	1:B:88:LEU:HD22	2.21	0.74
1:B:11:VAL:HG23	2:B:501:FAD:H4B	1.68	0.74
1:A:437:ILE:C	1:A:437:ILE:CD1	2.48	0.74
1:B:396:HIS:N	1:B:397:GLY:HA2	2.01	0.74
1:A:85:ASP:O	1:A:92:THR:CG2	2.34	0.74
1:A:50:LEU:HD12	1:A:143:LEU:CD1	2.17	0.74
1:B:123:PRO:HG2	1:B:215:ALA:HB2	1.68	0.74
1:B:50:LEU:HD12	1:B:143:LEU:CD1	2.17	0.73
1:A:147:PRO:O	1:A:148:GLN:CB	2.36	0.73
1:B:87:GLU:HA	1:B:88:LEU:C	2.08	0.73
1:D:56:ARG:NH2	1:D:59:ARG:HH11	1.87	0.73
1:D:418:LEU:HD13	1:D:439:ALA:HB3	1.69	0.73
1:B:440:GLN:NE2	4:B:603:HOH:O	2.22	0.72
1:D:270:ARG:HH11	1:D:270:ARG:HB2	1.54	0.72
1:B:128:GLU:N	4:B:602:HOH:O	2.21	0.72
1:B:64:THR:OG1	1:B:67:GLU:HG3	1.90	0.72
1:C:149:ALA:HA	1:C:173:LEU:HD22	1.70	0.72
1:B:440:GLN:O	4:B:603:HOH:O	2.07	0.72
1:D:116:ARG:NH2	4:D:602:HOH:O	2.22	0.72
1:D:90:THR:OG1	1:D:91:LEU:O	2.04	0.72
1:A:442:ALA:HB2	3:B:502:COA:H1B	1.71	0.72
1:C:270:ARG:HH11	1:C:270:ARG:HB2	1.54	0.71
1:D:410:ARG:HH11	1:D:410:ARG:CG	1.92	0.71
1:A:270:ARG:HH11	1:A:270:ARG:CB	2.04	0.71
1:B:94:HIS:N	1:B:94:HIS:HD2	1.89	0.71
1:D:255:VAL:HA	1:D:272:ASN:HD21	1.55	0.71
1:D:343:LEU:HD22	1:D:355:LYS:HB3	1.72	0.71
1:C:8:VAL:HG13	1:C:81:VAL:HG13	1.72	0.71
1:C:343:LEU:HD22	1:C:355:LYS:HB3	1.72	0.71
1:D:86:TYR:HD1	1:D:86:TYR:H	1.39	0.71
1:D:437:ILE:O	1:D:441:GLN:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ARG:CB	1:A:270:ARG:NH1	2.54	0.70
1:D:127:GLN:HG2	1:D:220:GLY:HA2	1.73	0.70
1:A:410:ARG:HH11	1:A:410:ARG:CG	1.99	0.70
1:D:85:ASP:H	1:D:92:THR:HA	1.57	0.70
1:A:98:GLU:HA	1:A:98:GLU:OE2	1.92	0.70
1:A:191:GLU:OE2	1:A:355:LYS:HE3	1.92	0.70
1:A:437:ILE:O	1:A:441:GLN:HB3	1.92	0.69
1:A:150:ARG:NH1	4:A:601:HOH:O	2.22	0.69
1:D:6:VAL:HG22	1:D:31:VAL:CG1	2.22	0.69
1:D:22:LYS:HE2	1:D:72:GLY:HA3	1.74	0.69
1:A:94:HIS:N	1:A:94:HIS:HD2	1.90	0.69
1:B:149:ALA:HA	1:B:173:LEU:HD22	1.73	0.69
1:C:440:GLN:HA	1:C:440:GLN:HE21	1.56	0.69
1:B:343:LEU:HD22	1:B:355:LYS:HB3	1.74	0.69
1:C:255:VAL:HA	1:C:272:ASN:HD21	1.58	0.68
1:A:398:ALA:HA	1:A:400:ARG:H	1.58	0.68
1:B:211:VAL:HG22	1:B:229:GLU:HG3	1.73	0.68
1:D:87:GLU:HA	1:D:88:LEU:C	2.13	0.68
1:B:7:VAL:O	4:B:604:HOH:O	2.11	0.68
1:B:256:ALA:H	1:B:272:ASN:ND2	1.91	0.68
1:D:270:ARG:HH11	1:D:270:ARG:CB	2.07	0.67
1:A:396:HIS:HE1	1:B:396:HIS:H	1.42	0.67
1:B:269:MET:HE3	1:B:320:PHE:HB3	1.76	0.67
1:A:440:GLN:HA	1:A:440:GLN:HE21	1.59	0.67
1:D:85:ASP:OD1	1:D:88:LEU:HD23	1.95	0.67
1:B:270:ARG:HB2	1:B:270:ARG:NH1	2.08	0.67
1:D:269:MET:HE2	1:D:320:PHE:HB3	1.75	0.67
1:C:80:GLU:N	4:C:603:HOH:O	2.20	0.67
1:C:211:VAL:HG22	1:C:229:GLU:HG3	1.75	0.67
1:B:398:ALA:H	1:B:399:LEU:HB2	1.59	0.66
1:B:272:ASN:HD22	1:B:272:ASN:H	1.41	0.66
1:C:270:ARG:CB	1:C:270:ARG:NH1	2.59	0.66
1:D:269:MET:CE	1:D:320:PHE:HB3	2.25	0.66
1:B:437:ILE:C	1:B:437:ILE:CD1	2.58	0.66
1:D:98:GLU:HA	1:D:98:GLU:OE2	1.94	0.66
1:C:398:ALA:HA	1:C:400:ARG:H	1.60	0.66
1:A:256:ALA:H	1:A:272:ASN:ND2	1.94	0.66
1:C:94:HIS:N	1:C:94:HIS:HD2	1.93	0.66
1:B:48:TYR:HB2	1:B:54:ILE:HD12	1.77	0.65
1:A:91:LEU:CG	1:A:92:THR:H	2.05	0.65
1:B:4:ARG:NH1	1:B:104:ASP:OD2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:VAL:CG2	2:D:501:FAD:H4B	2.24	0.65
1:C:380:GLU:HG2	4:C:601:HOH:O	1.97	0.65
1:C:64:THR:OG1	1:C:67:GLU:HG3	1.97	0.65
1:D:92:THR:O	1:D:104:ASP:O	2.14	0.65
1:A:287:HIS:HD2	1:A:289:VAL:H	1.45	0.65
1:C:270:ARG:NH1	1:C:270:ARG:HB3	2.12	0.65
1:B:7:VAL:CA	4:B:604:HOH:O	2.46	0.64
1:B:37:GLY:CA	1:B:77:THR:HB	2.23	0.64
1:B:398:ALA:H	1:B:399:LEU:HB3	1.63	0.64
1:A:396:HIS:CD2	1:B:396:HIS:CE1	2.86	0.64
1:D:180:ALA:O	1:D:210:GLY:HA2	1.97	0.64
1:B:440:GLN:HA	1:B:440:GLN:NE2	2.13	0.64
1:D:270:ARG:CB	1:D:270:ARG:NH1	2.61	0.64
1:B:373:LEU:HD22	1:B:434:PRO:HG2	1.80	0.64
1:A:208:TRP:HB3	1:A:211:VAL:HG21	1.80	0.64
1:B:183:ARG:NH1	1:B:188:TRP:O	2.31	0.63
1:B:50:LEU:CD1	1:B:143:LEU:HD13	2.29	0.63
1:C:357:PHE:HD1	1:C:376:GLU:HB2	1.64	0.63
1:D:123:PRO:HG2	1:D:215:ALA:CB	2.28	0.63
1:A:183:ARG:HD3	1:A:190:PRO:HA	1.81	0.63
1:A:272:ASN:H	1:A:272:ASN:HD22	1.46	0.63
1:D:281:ASP:OD1	2:D:501:FAD:H5'1	1.99	0.63
1:D:330:LYS:HE2	1:D:332:PHE:O	1.98	0.63
1:D:440:GLN:NE2	1:D:440:GLN:CA	2.60	0.63
1:D:56:ARG:NH2	1:D:59:ARG:NH1	2.46	0.63
1:C:183:ARG:NH1	1:C:188:TRP:O	2.32	0.62
1:A:22:LYS:HE2	1:A:72:GLY:HA3	1.82	0.62
1:C:11:VAL:HG23	2:C:501:FAD:H4B	1.79	0.62
1:D:224:ALA:C	4:D:601:HOH:O	2.32	0.62
1:A:149:ALA:HA	1:A:173:LEU:HD22	1.81	0.62
1:A:50:LEU:CD1	1:A:143:LEU:HD13	2.28	0.62
1:A:87:GLU:HA	1:A:88:LEU:C	2.20	0.62
1:C:98:GLU:OE2	1:C:98:GLU:HA	1.97	0.62
1:C:262:ALA:HB3	1:C:284:GLU:HG2	1.82	0.62
1:A:396:HIS:H	1:B:396:HIS:HE1	1.46	0.61
1:D:94:HIS:CD2	1:D:94:HIS:H	2.16	0.61
1:D:287:HIS:HD2	1:D:289:VAL:H	1.47	0.61
1:A:255:VAL:HA	1:A:272:ASN:HD21	1.64	0.61
1:B:7:VAL:HB	4:B:604:HOH:O	2.00	0.61
1:B:85:ASP:H	1:B:92:THR:HA	1.65	0.61
1:C:418:LEU:HD13	1:C:439:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:CYS:HA	2:B:501:FAD:C5X	2.30	0.61
1:B:221:ARG:O	1:B:221:ARG:HD3	2.00	0.61
1:B:123:PRO:HG2	1:B:215:ALA:CB	2.30	0.61
1:D:44:CYS:HA	2:D:501:FAD:C5X	2.31	0.61
1:A:396:HIS:CE1	1:B:396:HIS:H	2.19	0.61
1:D:209:THR:O	1:D:211:VAL:HG23	2.00	0.61
1:D:426:PRO:HB2	1:D:427:PRO:HD3	1.83	0.61
1:A:44:CYS:HA	2:A:501:FAD:C5X	2.30	0.60
1:A:90:THR:CA	1:A:92:THR:HG23	2.13	0.60
1:A:281:ASP:OD1	2:A:501:FAD:H5'1	2.01	0.60
1:B:76:HIS:HB3	1:B:79:HIS:CE1	2.36	0.60
1:D:64:THR:OG1	1:D:67:GLU:HG3	2.00	0.60
1:C:382:GLY:N	4:C:601:HOH:O	2.09	0.60
1:B:11:VAL:CG2	2:B:501:FAD:H4B	2.31	0.60
1:B:144:LYS:O	1:B:147:PRO:HD2	2.02	0.60
1:D:247:THR:HG21	1:D:261:GLY:O	2.00	0.60
1:A:373:LEU:HD22	1:A:434:PRO:HG2	1.83	0.60
1:D:418:LEU:HD13	1:D:439:ALA:CB	2.32	0.60
1:D:8:VAL:HG13	1:D:81:VAL:HG13	1.82	0.60
1:D:214:GLU:O	1:D:215:ALA:HB2	2.01	0.60
1:D:398:ALA:HA	1:D:400:ARG:H	1.67	0.60
1:A:90:THR:OG1	1:A:91:LEU:O	2.04	0.59
1:D:179:GLU:OE2	1:D:181:LYS:HG2	2.01	0.59
1:D:377:LEU:HD22	1:D:438:ALA:HB1	1.84	0.59
1:A:224:ALA:O	1:A:232:VAL:O	2.20	0.59
1:B:81:VAL:HA	1:B:95:ASP:HB3	1.84	0.59
1:C:398:ALA:N	1:C:399:LEU:HB2	2.15	0.59
1:A:236:LEU:HD12	1:A:236:LEU:C	2.23	0.59
1:A:37:GLY:CA	1:A:77:THR:HB	2.24	0.59
1:A:270:ARG:HB2	1:A:270:ARG:NH1	2.16	0.59
1:B:200:LEU:HD23	1:B:332:PHE:HE1	1.68	0.59
1:D:149:ALA:HA	1:D:173:LEU:CD2	2.32	0.59
1:A:64:THR:OG1	1:A:67:GLU:HG3	2.02	0.59
1:A:126:GLU:HA	1:A:126:GLU:OE1	2.02	0.59
1:C:44:CYS:HA	2:C:501:FAD:C5X	2.32	0.59
1:D:437:ILE:HD12	1:D:438:ALA:N	2.17	0.59
1:B:104:ASP:OD1	1:B:105:ARG:N	2.34	0.59
1:A:84:VAL:HG13	1:A:92:THR:HB	1.83	0.59
1:B:85:ASP:H	1:B:92:THR:HB	1.68	0.59
1:B:88:LEU:O	1:B:89:ARG:HB2	2.03	0.59
1:C:147:PRO:O	1:C:148:GLN:CB	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LEU:HD22	1:C:434:PRO:HG2	1.84	0.59
1:A:49:VAL:HG11	1:A:57:LEU:HD13	1.85	0.58
1:B:85:ASP:N	1:B:92:THR:HB	2.18	0.58
1:D:91:LEU:CG	1:D:92:THR:H	2.14	0.58
1:B:49:VAL:HG11	1:B:57:LEU:HD13	1.86	0.58
1:B:85:ASP:O	1:B:92:THR:CG2	2.44	0.58
1:B:277:TYR:CD1	1:B:277:TYR:N	2.71	0.58
1:B:362:ASP:OD2	4:B:605:HOH:O	2.17	0.58
1:C:104:ASP:OD1	1:C:105:ARG:N	2.35	0.58
1:B:23:ARG:NH2	3:B:502:COA:O5A	2.36	0.58
1:B:236:LEU:C	1:B:236:LEU:CD1	2.68	0.58
1:C:437:ILE:O	1:C:441:GLN:HB3	2.02	0.58
1:C:224:ALA:O	1:C:232:VAL:O	2.22	0.58
1:D:262:ALA:HB3	1:D:284:GLU:HG2	1.85	0.58
1:C:272:ASN:H	1:C:272:ASN:HD22	1.52	0.58
1:B:84:VAL:HG13	1:B:92:THR:HB	1.85	0.57
1:B:127:GLN:HG2	1:B:220:GLY:HA2	1.86	0.57
1:A:91:LEU:HD13	1:A:103:GLN:OE1	2.05	0.57
1:B:91:LEU:HD13	1:B:103:GLN:OE1	2.04	0.57
1:B:180:ALA:O	1:B:210:GLY:HA2	2.05	0.57
1:D:149:ALA:CB	1:D:150:ARG:CA	2.66	0.57
1:B:200:LEU:HD23	1:B:332:PHE:CE1	2.39	0.57
1:A:121:PRO:CG	1:D:149:ALA:CB	2.82	0.57
1:B:86:TYR:O	1:B:89:ARG:HA	2.04	0.57
1:B:255:VAL:HA	1:B:272:ASN:HD21	1.69	0.57
1:B:7:VAL:N	4:B:604:HOH:O	2.35	0.57
1:C:268:ARG:HH12	1:C:270:ARG:HH22	1.53	0.56
1:C:411:GLU:OE2	1:C:411:GLU:HA	2.05	0.56
1:B:173:LEU:HD23	1:B:173:LEU:N	2.20	0.56
1:C:149:ALA:CB	1:C:150:ARG:CA	2.73	0.56
1:A:56:ARG:NH2	1:A:59:ARG:NH1	2.52	0.56
1:B:128:GLU:CA	4:B:602:HOH:O	2.51	0.56
1:B:155:LEU:N	1:B:155:LEU:HD12	2.20	0.56
1:C:56:ARG:NH2	1:C:59:ARG:HH11	2.03	0.56
1:C:123:PRO:HG2	1:C:215:ALA:HB2	1.86	0.56
1:C:281:ASP:OD1	2:C:501:FAD:H5'1	2.06	0.56
1:D:56:ARG:HH21	1:D:59:ARG:NH1	2.01	0.56
1:D:236:LEU:HD12	1:D:236:LEU:C	2.26	0.56
1:B:7:VAL:CB	4:B:604:HOH:O	2.54	0.56
1:B:399:LEU:C	1:B:401:ILE:N	2.58	0.56
1:A:23:ARG:NH2	3:A:502:COA:O5A	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:HIS:N	1:B:397:GLY:CA	2.69	0.56
1:C:287:HIS:HD2	1:C:289:VAL:H	1.54	0.56
1:D:183:ARG:NH1	1:D:188:TRP:O	2.38	0.56
1:B:269:MET:HE3	1:B:320:PHE:CB	2.35	0.56
1:A:34:GLU:OE2	1:A:36:SER:HB3	2.06	0.56
1:B:94:HIS:CD2	1:B:94:HIS:H	2.21	0.56
1:C:280:GLY:HA2	1:C:302:ALA:HA	1.87	0.56
1:A:169:ARG:CD	1:A:175:VAL:HG13	2.36	0.56
1:A:203:HIS:HD2	1:C:219:MET:SD	2.29	0.56
1:C:96:HIS:N	4:C:603:HOH:O	2.35	0.56
1:D:6:VAL:HG22	1:D:31:VAL:HG13	1.87	0.56
1:C:269:MET:HE1	1:C:320:PHE:CD2	2.41	0.56
1:A:4:ARG:NH1	1:A:104:ASP:OD2	2.38	0.55
1:D:81:VAL:HA	1:D:95:ASP:HB3	1.88	0.55
1:A:24:GLU:CG	1:A:316:ARG:HG3	2.36	0.55
1:D:424:TYR:O	1:D:425:ALA:HB2	2.06	0.55
1:A:86:TYR:CD1	1:A:88:LEU:HD22	2.41	0.55
1:B:236:LEU:HD12	1:B:237:VAL:N	2.21	0.55
1:B:440:GLN:O	1:B:441:GLN:O	2.23	0.55
1:D:269:MET:HE3	1:D:320:PHE:CD2	2.40	0.55
1:B:185:LEU:N	1:B:186:PRO:CD	2.69	0.55
1:B:399:LEU:C	1:B:401:ILE:H	2.09	0.55
1:B:361:ARG:CZ	1:B:361:ARG:HB3	2.37	0.55
1:C:180:ALA:O	1:C:210:GLY:HA2	2.07	0.55
1:C:185:LEU:N	1:C:186:PRO:HD3	2.22	0.55
1:B:217:ARG:O	1:B:222:VAL:HA	2.06	0.55
1:C:91:LEU:HD13	1:C:103:GLN:OE1	2.06	0.55
1:C:209:THR:O	1:C:211:VAL:HG23	2.06	0.55
1:C:359:GLN:HB2	1:C:374:TRP:CD1	2.42	0.55
1:B:185:LEU:N	1:B:186:PRO:HD3	2.22	0.55
1:C:91:LEU:CG	1:C:92:THR:H	2.16	0.54
1:C:4:ARG:NH1	1:C:104:ASP:OD2	2.40	0.54
1:D:224:ALA:CA	4:D:601:HOH:O	2.55	0.54
1:A:81:VAL:HG22	1:A:249:LEU:HD21	1.88	0.54
1:D:411:GLU:HA	1:D:411:GLU:OE2	2.08	0.54
1:D:37:GLY:CA	1:D:77:THR:HB	2.37	0.54
1:C:37:GLY:CA	1:C:77:THR:HB	2.37	0.54
1:C:96:HIS:HB3	4:C:603:HOH:O	2.06	0.54
1:C:183:ARG:HG3	1:C:184:PRO:O	2.08	0.54
1:B:85:ASP:H	1:B:92:THR:CB	2.19	0.54
1:A:396:HIS:CD2	1:B:396:HIS:NE2	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:CYS:HB3	2:B:501:FAD:C4X	2.37	0.54
1:B:281:ASP:OD1	2:B:501:FAD:H5'1	2.08	0.54
1:C:86:TYR:O	1:C:89:ARG:HA	2.07	0.54
1:A:183:ARG:HG3	1:A:184:PRO:O	2.08	0.54
1:D:91:LEU:HD13	1:D:103:GLN:OE1	2.07	0.54
1:D:150:ARG:CZ	1:D:151:ARG:HH22	2.21	0.54
1:A:343:LEU:HD22	1:A:355:LYS:HB3	1.90	0.53
1:A:85:ASP:N	1:A:92:THR:HB	2.23	0.53
1:C:56:ARG:NH2	1:C:59:ARG:NH1	2.57	0.53
1:A:85:ASP:H	1:A:92:THR:CA	2.18	0.53
1:D:358:ILE:C	1:D:358:ILE:HD12	2.29	0.53
1:B:270:ARG:NH1	1:B:270:ARG:HB3	2.19	0.53
1:A:140:GLU:CD	4:A:608:HOH:O	2.47	0.53
1:C:299:GLY:HA3	3:C:502:COA:C2P	2.38	0.53
1:A:121:PRO:CB	1:D:172:GLY:O	2.57	0.53
1:B:398:ALA:HA	1:B:400:ARG:H	1.73	0.53
1:C:236:LEU:C	1:C:236:LEU:HD12	2.29	0.53
1:B:31:VAL:O	1:B:31:VAL:HG13	2.08	0.53
1:B:398:ALA:N	1:B:399:LEU:HB2	2.24	0.53
1:D:273:LEU:HB2	1:D:276:VAL:CG2	2.38	0.53
1:A:6:VAL:HG22	1:A:31:VAL:CG1	2.39	0.53
1:A:128:GLU:N	4:A:602:HOH:O	2.40	0.53
1:C:299:GLY:HA3	3:C:502:COA:H22	1.90	0.53
1:D:91:LEU:HG	1:D:92:THR:H	1.74	0.53
1:A:431:VAL:HG21	3:B:502:COA:H32	1.91	0.52
1:B:90:THR:CA	1:B:92:THR:HG23	2.35	0.52
1:B:126:GLU:OE1	1:B:126:GLU:HA	2.09	0.52
1:C:8:VAL:HG13	1:C:81:VAL:CG1	2.38	0.52
1:A:273:LEU:HB2	1:A:276:VAL:CG2	2.40	0.52
1:B:183:ARG:HD3	1:B:190:PRO:HA	1.91	0.52
1:C:281:ASP:N	2:C:501:FAD:O2P	2.34	0.52
1:C:330:LYS:HE2	1:C:332:PHE:O	2.08	0.52
1:A:162:LEU:HD22	1:A:200:LEU:HD11	1.91	0.52
1:D:400:ARG:HG2	1:D:435:LEU:HD11	1.90	0.52
1:A:437:ILE:HD12	1:A:437:ILE:O	2.05	0.52
1:B:363:GLY:H	1:B:430:PRO:HD3	1.75	0.52
1:C:85:ASP:OD1	1:C:88:LEU:HD23	2.08	0.52
1:C:360:SER:HB3	1:C:434:PRO:HG3	1.90	0.52
1:A:169:ARG:HD3	1:A:175:VAL:HG13	1.92	0.52
1:A:396:HIS:NE2	1:B:396:HIS:CD2	2.78	0.52
1:A:396:HIS:NE2	1:B:396:HIS:NE2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:HIS:HD2	1:B:289:VAL:H	1.56	0.52
1:A:92:THR:HG1	1:A:106:PHE:HE2	1.57	0.52
1:B:49:VAL:HG22	1:B:54:ILE:HB	1.92	0.52
1:A:56:ARG:NH2	1:A:59:ARG:HH11	2.07	0.52
1:A:396:HIS:NE2	1:B:396:HIS:CE1	2.78	0.52
1:B:302:ALA:CB	2:B:501:FAD:H5'2	2.40	0.52
1:A:92:THR:O	1:A:104:ASP:O	2.28	0.52
1:B:86:TYR:H	1:B:86:TYR:HD1	1.57	0.52
1:A:339:THR:HG22	1:A:401:ILE:HD11	1.91	0.51
1:C:81:VAL:HA	1:C:95:ASP:HB3	1.92	0.51
1:D:299:GLY:HA2	2:D:501:FAD:H4'	1.93	0.51
1:B:4:ARG:HD3	1:B:105:ARG:O	2.10	0.51
1:D:4:ARG:NH1	1:D:104:ASP:OD2	2.43	0.51
1:A:185:LEU:N	1:A:186:PRO:CD	2.73	0.51
1:B:247:THR:HG21	1:B:261:GLY:O	2.10	0.51
1:C:86:TYR:CD1	1:C:88:LEU:HD22	2.45	0.51
1:D:270:ARG:NH1	1:D:270:ARG:HB3	2.24	0.51
1:B:23:ARG:HH22	3:B:502:COA:P2A	2.34	0.51
1:D:272:ASN:HD22	1:D:272:ASN:H	1.57	0.51
1:B:80:GLU:HG2	1:B:82:VAL:HG22	1.92	0.51
1:B:411:GLU:HA	1:B:411:GLU:OE2	2.10	0.51
1:C:191:GLU:OE2	1:C:355:LYS:HE3	2.10	0.51
1:A:49:VAL:HG11	1:A:57:LEU:CD1	2.40	0.51
1:C:88:LEU:O	1:C:89:ARG:CB	2.58	0.51
1:A:270:ARG:NH1	1:A:270:ARG:HB3	2.26	0.51
1:B:256:ALA:H	1:B:272:ASN:HD21	1.55	0.51
1:C:7:VAL:HB	1:C:32:VAL:HG22	1.93	0.51
1:D:88:LEU:O	1:D:89:ARG:CB	2.58	0.51
1:D:9:GLY:HA3	1:D:112:ALA:O	2.11	0.50
1:A:440:GLN:NE2	1:A:440:GLN:CA	2.70	0.50
1:B:24:GLU:CG	1:B:316:ARG:HG3	2.41	0.50
1:B:85:ASP:H	1:B:92:THR:CA	2.24	0.50
1:D:85:ASP:HA	1:D:88:LEU:HD23	1.92	0.50
1:D:88:LEU:O	1:D:89:ARG:HB2	2.10	0.50
1:C:302:ALA:HB2	2:C:501:FAD:H5'2	1.94	0.50
1:B:91:LEU:HD12	1:B:92:THR:HA	1.92	0.50
1:B:400:ARG:HD3	1:B:433:ASP:OD1	2.12	0.50
1:C:87:GLU:HA	1:C:88:LEU:O	2.12	0.50
1:C:357:PHE:CD1	1:C:376:GLU:HB2	2.44	0.50
1:C:424:TYR:CD1	1:C:425:ALA:N	2.79	0.50
1:D:24:GLU:HG2	1:D:316:ARG:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:HD3	1:A:221:ARG:C	2.32	0.50
1:C:440:GLN:NE2	1:C:440:GLN:CA	2.71	0.50
1:B:377:LEU:HD22	1:B:438:ALA:HB1	1.93	0.50
1:C:298:LEU:HB2	1:C:301:VAL:HG13	1.92	0.50
1:C:185:LEU:N	1:C:186:PRO:CD	2.75	0.50
1:D:144:LYS:O	1:D:147:PRO:HD2	2.12	0.50
1:B:92:THR:O	1:B:104:ASP:O	2.30	0.50
1:C:126:GLU:HA	1:C:126:GLU:OE1	2.12	0.50
1:D:373:LEU:HD22	1:D:434:PRO:HG2	1.93	0.50
1:C:256:ALA:H	1:C:272:ASN:HD21	1.60	0.49
1:B:86:TYR:O	1:B:89:ARG:CA	2.61	0.49
1:B:150:ARG:CZ	1:B:151:ARG:HH22	2.25	0.49
1:B:287:HIS:CD2	1:B:290:LEU:H	2.30	0.49
1:B:424:TYR:CD1	1:B:431:VAL:HA	2.48	0.49
1:C:440:GLN:O	1:C:441:GLN:O	2.30	0.49
1:D:7:VAL:HG13	1:D:110:VAL:HB	1.94	0.49
1:D:352:TRP:NE1	4:D:604:HOH:O	2.42	0.49
1:B:179:GLU:OE2	1:B:181:LYS:HG2	2.13	0.49
1:B:440:GLN:C	1:B:441:GLN:O	2.51	0.49
1:C:22:LYS:HE2	1:C:72:GLY:HA3	1.95	0.49
1:B:313:ILE:C	1:B:315:GLY:H	2.15	0.49
1:C:56:ARG:HH21	1:C:59:ARG:NH1	2.11	0.49
2:C:501:FAD:O2'	2:C:501:FAD:H9	2.13	0.49
1:A:86:TYR:O	1:A:89:ARG:HA	2.13	0.49
1:C:88:LEU:O	1:C:89:ARG:HB2	2.12	0.49
1:C:96:HIS:CA	4:C:603:HOH:O	2.60	0.49
1:B:268:ARG:HH12	1:B:270:ARG:HH22	1.60	0.49
1:B:398:ALA:N	1:B:399:LEU:CB	2.72	0.49
1:A:267:GLU:OE2	1:A:319:ARG:NH1	2.40	0.49
1:A:189:ASP:HB3	1:A:190:PRO:CD	2.42	0.49
1:A:11:VAL:CG2	2:A:501:FAD:H4B	2.41	0.49
1:D:27:GLU:OE2	1:D:27:GLU:HA	2.13	0.49
1:A:91:LEU:O	1:A:92:THR:HG23	2.13	0.48
1:B:92:THR:HG1	1:B:106:PHE:HE2	1.60	0.48
1:B:287:HIS:HD2	1:B:290:LEU:H	1.61	0.48
1:B:98:GLU:OE2	1:B:98:GLU:HA	2.11	0.48
1:D:200:LEU:HD23	1:D:332:PHE:HE1	1.77	0.48
1:A:23:ARG:NH2	3:A:502:COA:P2A	2.86	0.48
1:B:92:THR:OG1	1:B:93:VAL:N	2.45	0.48
1:B:214:GLU:O	1:B:215:ALA:HB2	2.14	0.48
1:C:361:ARG:HD3	1:C:365:HIS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:NH1	4:A:610:HOH:O	2.46	0.48
1:A:203:HIS:CD2	1:C:219:MET:SD	3.07	0.48
1:A:272:ASN:ND2	1:A:272:ASN:H	2.12	0.48
1:B:24:GLU:HG2	1:B:316:ARG:HG3	1.96	0.48
1:B:426:PRO:N	1:B:427:PRO:CD	2.77	0.48
1:D:24:GLU:HG3	1:D:316:ARG:CZ	2.43	0.48
1:D:363:GLY:H	1:D:430:PRO:HD3	1.79	0.48
1:A:426:PRO:HG3	1:B:44:CYS:HB2	1.96	0.48
1:B:330:LYS:HE2	1:B:332:PHE:O	2.14	0.48
1:C:299:GLY:HA2	2:C:501:FAD:H4'	1.95	0.48
1:D:207:VAL:HG22	1:D:207:VAL:O	2.14	0.48
1:A:324:VAL:HG21	1:A:408:LEU:HB3	1.95	0.48
1:D:191:GLU:O	1:D:194:ALA:HB3	2.14	0.48
1:D:260:THR:HG23	1:D:284:GLU:OE1	2.13	0.48
1:D:359:GLN:HB2	1:D:374:TRP:CD1	2.48	0.48
1:D:25:ASN:HB2	1:D:314:ALA:HB1	1.96	0.48
1:D:191:GLU:OE2	1:D:355:LYS:HE3	2.14	0.48
2:A:501:FAD:H9	2:A:501:FAD:O2'	2.14	0.47
1:A:273:LEU:HB2	1:A:276:VAL:HG21	1.95	0.47
1:D:183:ARG:HD3	1:D:190:PRO:HA	1.95	0.47
1:A:23:ARG:HH22	3:A:502:COA:P2A	2.37	0.47
1:B:8:VAL:HG13	1:B:81:VAL:HG13	1.97	0.47
1:B:80:GLU:O	1:B:95:ASP:HB2	2.14	0.47
1:B:225:VAL:HG12	1:B:227:THR:CG2	2.43	0.47
1:B:299:GLY:HA2	2:B:501:FAD:H4'	1.96	0.47
1:A:24:GLU:HG2	1:A:316:ARG:HG3	1.97	0.47
1:A:128:GLU:HG3	1:A:221:ARG:NH2	2.29	0.47
1:D:185:LEU:N	1:D:186:PRO:CD	2.78	0.47
1:A:424:TYR:CD1	1:A:425:ALA:N	2.83	0.47
1:D:403:VAL:O	1:D:406:ALA:HB3	2.15	0.47
1:B:16:SER:HB2	1:B:306:GLY:HA3	1.97	0.47
1:D:38:TRP:CE3	1:D:136:MET:HE2	2.50	0.47
1:A:85:ASP:H	1:A:92:THR:CB	2.27	0.47
1:A:139:GLY:O	1:A:143:LEU:HB2	2.14	0.47
1:A:396:HIS:CE1	1:B:396:HIS:CD2	3.02	0.47
1:A:396:HIS:ND1	1:B:396:HIS:ND1	2.58	0.47
1:A:418:LEU:HD13	1:A:439:ALA:HB3	1.96	0.47
1:C:296:LEU:HD23	1:C:323:VAL:HG11	1.96	0.47
1:C:440:GLN:C	1:C:441:GLN:O	2.52	0.47
1:D:3:LYS:HE2	1:D:3:LYS:HB3	1.66	0.47
1:D:80:GLU:HG2	1:D:82:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LEU:HD23	1:D:332:PHE:CE1	2.50	0.47
1:D:224:ALA:N	4:D:601:HOH:O	2.48	0.47
1:D:273:LEU:HB2	1:D:276:VAL:HG21	1.97	0.47
1:A:37:GLY:HA2	1:A:77:THR:CB	2.32	0.47
1:B:88:LEU:O	1:B:89:ARG:CB	2.62	0.47
1:A:85:ASP:H	1:A:92:THR:HB	1.80	0.47
1:B:299:GLY:HA3	3:B:502:COA:C2P	2.44	0.47
1:B:441:GLN:C	1:B:442:ALA:O	2.52	0.47
1:A:81:VAL:HA	1:A:95:ASP:HB3	1.96	0.47
1:A:92:THR:OG1	1:A:106:PHE:HE2	1.97	0.47
1:D:256:ALA:H	1:D:272:ASN:HD21	1.58	0.47
1:D:352:TRP:CD1	4:D:604:HOH:O	2.68	0.47
1:A:173:LEU:N	1:A:173:LEU:HD23	2.30	0.46
3:A:502:COA:N8P	3:A:502:COA:O5P	2.43	0.46
1:B:147:PRO:O	1:B:148:GLN:CB	2.52	0.46
1:C:268:ARG:NH1	1:C:270:ARG:HH22	2.13	0.46
1:C:424:TYR:O	1:C:425:ALA:HB2	2.15	0.46
1:B:23:ARG:NH2	3:B:502:COA:P2A	2.89	0.46
1:A:436:LEU:HD23	1:A:436:LEU:HA	1.69	0.46
1:A:85:ASP:C	1:A:92:THR:CG2	2.67	0.46
1:C:179:GLU:OE2	1:C:181:LYS:HG2	2.16	0.46
1:D:185:LEU:N	1:D:186:PRO:HD3	2.30	0.46
1:A:269:MET:HE3	1:A:320:PHE:CB	2.34	0.46
1:B:85:ASP:OD1	1:B:88:LEU:HB3	2.15	0.46
1:C:437:ILE:HD12	1:C:438:ALA:N	2.28	0.46
1:D:217:ARG:O	1:D:222:VAL:HA	2.16	0.46
1:A:183:ARG:CD	1:A:190:PRO:HA	2.45	0.46
1:B:56:ARG:NH2	1:B:59:ARG:HH11	2.13	0.46
1:B:117:PRO:HD3	1:B:134:ARG:HG2	1.97	0.46
1:C:302:ALA:CB	2:C:501:FAD:H5'2	2.45	0.46
1:A:88:LEU:O	1:A:89:ARG:HB2	2.14	0.46
1:B:209:THR:O	1:B:211:VAL:HG23	2.16	0.46
1:C:117:PRO:HD3	1:C:134:ARG:HG2	1.97	0.46
1:D:440:GLN:O	1:D:441:GLN:O	2.34	0.46
1:B:272:ASN:ND2	1:B:272:ASN:H	2.12	0.46
1:C:86:TYR:O	1:C:89:ARG:CA	2.63	0.46
1:D:361:ARG:HB3	1:D:361:ARG:CZ	2.46	0.46
1:D:398:ALA:CA	1:D:399:LEU:HB2	2.45	0.46
1:A:179:GLU:OE2	1:A:181:LYS:HG2	2.16	0.46
1:B:111:LEU:HD12	1:B:111:LEU:HA	1.60	0.46
1:A:169:ARG:HB3	1:C:219:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:O	1:B:149:ALA:O	2.34	0.46
1:B:183:ARG:CD	1:B:190:PRO:HA	2.46	0.46
1:C:245:PRO:HB2	1:C:247:THR:HG23	1.98	0.46
1:D:270:ARG:HB2	1:D:270:ARG:NH1	2.26	0.46
1:D:287:HIS:CD2	1:D:290:LEU:H	2.34	0.46
1:D:373:LEU:HD12	1:D:393:ALA:HB2	1.97	0.46
1:A:316:ARG:HG2	1:A:316:ARG:HH11	1.81	0.45
1:C:76:HIS:HB3	1:C:79:HIS:CE1	2.51	0.45
1:D:162:LEU:CD2	1:D:200:LEU:HD11	2.46	0.45
1:B:86:TYR:CD1	1:B:88:LEU:HD22	2.51	0.45
1:D:399:LEU:C	1:D:401:ILE:H	2.20	0.45
1:D:426:PRO:CB	1:D:427:PRO:HD3	2.45	0.45
1:A:330:LYS:HE2	1:A:332:PHE:O	2.17	0.45
1:B:36:SER:O	1:B:38:TRP:N	2.49	0.45
1:C:48:TYR:HB2	1:C:54:ILE:HD12	1.98	0.45
1:D:80:GLU:O	1:D:95:ASP:HB2	2.16	0.45
1:A:199:GLU:HG3	1:A:334:LEU:HG	1.98	0.45
1:A:418:LEU:HD12	1:A:418:LEU:HA	1.66	0.45
1:C:181:LYS:HG2	1:C:181:LYS:H	1.40	0.45
1:C:217:ARG:O	1:C:222:VAL:HA	2.17	0.45
1:D:86:TYR:CD1	1:D:86:TYR:N	2.75	0.45
1:A:34:GLU:OE2	1:A:36:SER:CB	2.65	0.45
1:A:88:LEU:O	1:A:89:ARG:CB	2.64	0.45
1:A:396:HIS:HE1	1:B:396:HIS:N	2.13	0.45
1:C:86:TYR:H	1:C:86:TYR:HD1	1.58	0.45
1:C:101:THR:HG22	4:C:606:HOH:O	2.17	0.45
1:C:214:GLU:O	1:C:215:ALA:HB2	2.17	0.45
1:D:86:TYR:CD1	1:D:88:LEU:HD22	2.51	0.45
1:A:181:LYS:HG2	1:A:181:LYS:H	1.52	0.45
1:A:299:GLY:HA2	2:A:501:FAD:H4'	1.97	0.45
1:A:440:GLN:C	1:A:441:GLN:O	2.55	0.45
1:B:287:HIS:CD2	1:B:289:VAL:H	2.34	0.45
1:C:169:ARG:CD	1:C:175:VAL:HG13	2.47	0.45
1:C:85:ASP:OD1	1:C:88:LEU:HB3	2.17	0.45
1:B:324:VAL:HG21	1:B:408:LEU:HB3	1.99	0.45
1:C:28:LEU:HA	1:C:28:LEU:HD23	1.77	0.45
1:C:280:GLY:HA3	2:C:501:FAD:O2P	2.16	0.45
1:C:199:GLU:HG3	1:C:334:LEU:HG	1.99	0.45
1:D:92:THR:CB	1:D:106:PHE:HE2	2.30	0.45
1:A:24:GLU:HG3	1:A:316:ARG:HG3	1.97	0.44
1:A:41:TYR:HA	1:A:61:VAL:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HA	1:A:173:LEU:CD2	2.46	0.44
1:B:356:VAL:HG22	1:B:357:PHE:N	2.31	0.44
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.79	0.44
1:C:92:THR:CB	1:C:106:PHE:HE2	2.30	0.44
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.64	0.44
1:A:316:ARG:HG2	1:A:316:ARG:NH1	2.32	0.44
1:B:105:ARG:CB	4:B:601:HOH:O	2.65	0.44
1:B:191:GLU:OE2	1:B:355:LYS:HE3	2.17	0.44
1:C:183:ARG:HD3	1:C:190:PRO:HA	1.99	0.44
1:A:121:PRO:CG	1:D:149:ALA:HB1	2.46	0.44
1:B:56:ARG:NH2	1:B:59:ARG:NH1	2.65	0.44
1:D:189:ASP:HB3	1:D:190:PRO:CD	2.46	0.44
1:A:93:VAL:C	1:A:94:HIS:HD2	2.21	0.44
1:D:280:GLY:HA3	2:D:501:FAD:O2P	2.17	0.44
1:B:3:LYS:HB3	1:B:3:LYS:HE2	1.74	0.44
1:C:151:ARG:HG2	1:C:174:GLN:HG3	2.00	0.44
1:C:398:ALA:N	1:C:399:LEU:CB	2.72	0.44
1:A:56:ARG:HH21	1:A:59:ARG:NH1	2.14	0.44
1:B:25:ASN:HB2	1:B:314:ALA:HB1	1.99	0.44
1:C:86:TYR:O	1:C:89:ARG:N	2.51	0.44
1:D:126:GLU:OE1	1:D:126:GLU:HA	2.18	0.44
1:D:424:TYR:CD1	1:D:425:ALA:N	2.86	0.44
1:D:441:GLN:C	1:D:442:ALA:O	2.56	0.44
1:B:143:LEU:HD12	1:B:143:LEU:HA	1.79	0.44
1:D:28:LEU:HD23	1:D:28:LEU:HA	1.84	0.44
1:A:432:TRP:HB3	1:A:437:ILE:HG22	1.99	0.44
1:D:25:ASN:OD1	1:D:25:ASN:C	2.54	0.44
1:D:116:ARG:HH12	1:D:244:ARG:HD2	1.77	0.44
1:B:76:HIS:HB3	1:B:79:HIS:ND1	2.32	0.44
1:D:97:ALA:HB1	1:D:98:GLU:H	1.57	0.44
1:A:28:LEU:HA	1:A:28:LEU:HD23	1.86	0.43
1:C:96:HIS:CB	4:C:603:HOH:O	2.65	0.43
1:A:90:THR:CB	1:A:92:THR:HG23	2.48	0.43
1:B:46:LEU:HD13	1:B:133:LEU:HD22	2.00	0.43
1:C:50:LEU:HD12	1:C:50:LEU:HA	1.74	0.43
1:D:23:ARG:HH22	3:D:502:COA:P2A	2.41	0.43
1:A:94:HIS:CD2	1:A:94:HIS:H	2.30	0.43
1:A:185:LEU:N	1:A:186:PRO:HD3	2.34	0.43
1:C:143:LEU:O	1:C:147:PRO:HD3	2.18	0.43
1:C:373:LEU:HD23	1:C:373:LEU:C	2.39	0.43
1:D:302:ALA:CB	2:D:501:FAD:H5'2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HB	1:A:32:VAL:HG22	2.01	0.43
1:D:299:GLY:HA3	3:D:502:COA:H22	2.00	0.43
1:A:200:LEU:HD23	1:A:332:PHE:CE1	2.54	0.43
1:B:280:GLY:HA3	2:B:501:FAD:O2P	2.19	0.43
1:D:77:THR:O	1:D:78:ARG:HB2	2.18	0.43
1:A:91:LEU:HD12	1:A:92:THR:CA	2.49	0.43
1:B:7:VAL:C	4:B:604:HOH:O	2.57	0.43
1:C:116:ARG:HH12	1:C:244:ARG:HD2	1.81	0.43
1:C:216:PHE:CE1	1:C:225:VAL:HG22	2.54	0.43
1:C:271:THR:HB	4:C:609:HOH:O	2.18	0.43
1:D:141:ARG:HH11	1:D:141:ARG:HD2	1.61	0.43
1:D:386:LEU:HD13	1:D:386:LEU:HA	1.76	0.43
1:D:399:LEU:C	1:D:401:ILE:N	2.69	0.43
1:B:91:LEU:CG	1:B:92:THR:H	2.31	0.43
1:B:410:ARG:HH11	1:B:410:ARG:CG	2.05	0.43
1:D:197:LYS:O	1:D:201:GLU:HB2	2.19	0.43
1:B:7:VAL:HG13	1:B:110:VAL:HB	2.01	0.43
1:B:94:HIS:HA	1:B:102:PHE:O	2.19	0.43
1:D:161:GLY:H	1:D:164:ALA:H	1.67	0.43
1:B:94:HIS:CG	1:B:103:GLN:HE22	2.37	0.43
1:D:8:VAL:HG13	1:D:81:VAL:CG1	2.49	0.43
1:D:85:ASP:OD1	1:D:88:LEU:CD2	2.65	0.43
1:D:299:GLY:HA3	3:D:502:COA:C2P	2.47	0.43
1:D:398:ALA:CA	1:D:399:LEU:CB	2.97	0.43
1:A:80:GLU:O	1:A:95:ASP:HB2	2.19	0.42
1:D:86:TYR:O	1:D:89:ARG:N	2.52	0.42
1:A:37:GLY:H	1:A:78:ARG:H	1.67	0.42
1:B:292:ARG:HB2	1:B:293:PRO:HD2	2.00	0.42
1:D:25:ASN:CB	1:D:314:ALA:HB1	2.49	0.42
1:A:253:MET:HG3	1:A:255:VAL:HG23	2.01	0.42
1:B:23:ARG:NH1	3:B:502:COA:O8A	2.53	0.42
1:D:112:ALA:HB1	4:D:605:HOH:O	2.18	0.42
1:B:91:LEU:HD12	1:B:92:THR:CA	2.50	0.42
1:B:269:MET:CE	1:B:320:PHE:HB3	2.48	0.42
1:C:127:GLN:HG2	1:C:220:GLY:HA2	2.01	0.42
1:D:356:VAL:HG12	1:D:377:LEU:HB2	2.02	0.42
1:D:361:ARG:HD3	1:D:365:HIS:HA	2.02	0.42
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.93	0.42
1:C:39:VAL:HG11	1:C:75:VAL:HG21	2.02	0.42
1:C:166:GLU:OE2	1:C:170:LYS:HE3	2.18	0.42
1:C:23:ARG:HH22	3:C:502:COA:P2A	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:TYR:HB2	1:C:87:GLU:H	1.22	0.42
1:C:120:PRO:HA	1:C:121:PRO:HD3	1.80	0.42
1:D:413:SER:O	1:D:416:ASP:HB2	2.19	0.42
1:B:429:SER:HA	1:B:430:PRO:HD2	1.84	0.42
1:D:345:GLY:O	1:D:346:ALA:C	2.58	0.42
1:B:86:TYR:O	1:B:89:ARG:N	2.53	0.42
1:B:219:MET:HB2	4:B:608:HOH:O	2.20	0.42
1:A:358:ILE:HD11	1:A:375:VAL:HG13	2.02	0.42
1:A:363:GLY:H	1:A:430:PRO:HD3	1.84	0.42
1:B:155:LEU:N	1:B:155:LEU:CD1	2.82	0.42
1:C:81:VAL:HG22	1:C:249:LEU:HD21	2.01	0.42
1:D:3:LYS:HD3	1:D:108:HIS:NE2	2.35	0.42
1:D:166:GLU:HG2	1:D:170:LYS:HE3	2.00	0.42
1:A:92:THR:OG1	1:A:106:PHE:CE2	2.69	0.42
1:C:24:GLU:HB3	1:C:314:ALA:CB	2.50	0.42
1:D:24:GLU:HG2	1:D:316:ARG:CG	2.49	0.42
1:D:31:VAL:HG13	1:D:31:VAL:O	2.20	0.42
1:C:398:ALA:H	1:C:399:LEU:HB3	1.77	0.41
1:A:428:PHE:CD2	1:B:328:ILE:HD13	2.55	0.41
2:A:501:FAD:H2'	3:A:502:COA:S1P	2.59	0.41
1:B:313:ILE:HG21	1:B:313:ILE:HD13	1.69	0.41
1:C:123:PRO:HG2	1:C:215:ALA:CB	2.48	0.41
1:C:413:SER:O	1:C:416:ASP:HB2	2.20	0.41
1:C:437:ILE:HD12	1:C:437:ILE:O	2.20	0.41
1:D:87:GLU:HA	1:D:88:LEU:O	2.19	0.41
1:D:268:ARG:HG2	1:D:312:VAL:HG21	2.02	0.41
1:A:92:THR:HG21	1:A:106:PHE:CE2	2.55	0.41
1:B:166:GLU:OE2	1:B:170:LYS:HE3	2.20	0.41
1:C:222:VAL:O	1:C:222:VAL:CG1	2.67	0.41
1:C:236:LEU:HD12	1:C:237:VAL:N	2.35	0.41
1:D:81:VAL:HA	1:D:95:ASP:CB	2.50	0.41
1:A:8:VAL:HG13	1:A:81:VAL:HG13	2.02	0.41
1:A:86:TYR:O	1:A:89:ARG:CA	2.68	0.41
1:A:189:ASP:HA	1:A:190:PRO:HD3	1.74	0.41
1:D:269:MET:HE3	1:D:320:PHE:HB3	2.01	0.41
1:A:44:CYS:SG	4:B:609:HOH:O	2.61	0.41
1:A:92:THR:OG1	1:A:93:VAL:N	2.52	0.41
2:A:501:FAD:H8A	2:A:501:FAD:H2B	1.96	0.41
1:B:41:TYR:HA	1:B:61:VAL:HA	2.02	0.41
1:B:87:GLU:HA	1:B:88:LEU:O	2.20	0.41
1:C:199:GLU:OE1	1:C:332:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:TYR:HB2	1:D:87:GLU:H	1.32	0.41
1:A:411:GLU:OE2	1:A:411:GLU:HA	2.19	0.41
1:A:86:TYR:HD1	1:A:86:TYR:H	1.66	0.41
1:A:91:LEU:C	1:A:92:THR:HG23	2.41	0.41
1:A:144:LYS:O	1:A:147:PRO:HD2	2.21	0.41
1:A:169:ARG:HG2	1:A:175:VAL:CG1	2.50	0.41
1:A:280:GLY:HA2	1:A:302:ALA:HA	2.02	0.41
1:A:299:GLY:HA3	3:A:502:COA:H22	2.03	0.41
1:A:302:ALA:CB	2:A:501:FAD:H5'2	2.51	0.41
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.87	0.41
1:C:216:PHE:CE1	1:C:237:VAL:HG21	2.55	0.41
1:D:93:VAL:C	1:D:94:HIS:HD2	2.24	0.41
1:D:111:LEU:HD12	1:D:111:LEU:HA	1.85	0.41
1:D:268:ARG:CG	1:D:312:VAL:HG21	2.51	0.41
1:B:166:GLU:HA	1:B:332:PHE:CZ	2.56	0.41
1:C:3:LYS:HB3	1:C:3:LYS:HE2	1.66	0.41
1:C:90:THR:OG1	1:C:91:LEU:O	2.12	0.41
1:D:207:VAL:O	1:D:207:VAL:CG2	2.68	0.41
1:A:24:GLU:HG3	1:A:316:ARG:CG	2.51	0.41
1:A:97:ALA:HB1	1:A:98:GLU:H	1.55	0.41
1:B:105:ARG:HH11	1:B:105:ARG:HD3	1.60	0.41
1:B:418:LEU:HD13	1:B:439:ALA:HB3	2.03	0.41
1:C:12:ALA:N	2:C:501:FAD:O1P	2.49	0.41
1:C:84:VAL:HA	1:C:93:VAL:H	1.86	0.41
1:C:269:MET:CE	1:C:320:PHE:HB3	2.51	0.41
1:D:46:LEU:HD13	1:D:133:LEU:HD22	2.02	0.41
1:D:105:ARG:HH11	1:D:105:ARG:HD3	1.72	0.41
1:D:114:GLY:HA2	1:D:281:ASP:HB2	2.02	0.41
1:D:139:GLY:O	1:D:143:LEU:HB2	2.21	0.41
1:D:253:MET:HG3	1:D:255:VAL:HG23	2.03	0.41
1:D:356:VAL:HG22	1:D:357:PHE:N	2.35	0.41
1:B:50:LEU:HD12	1:B:50:LEU:HA	1.79	0.41
1:C:4:ARG:HH11	1:C:4:ARG:HD3	1.57	0.41
1:D:221:ARG:O	1:D:222:VAL:HG12	2.21	0.40
1:A:24:GLU:HB3	1:A:314:ALA:CB	2.51	0.40
1:A:64:THR:C	1:A:66:GLU:N	2.75	0.40
1:A:86:TYR:O	1:A:89:ARG:N	2.55	0.40
1:A:91:LEU:HD12	1:A:92:THR:HA	2.04	0.40
1:A:143:LEU:HA	1:A:143:LEU:HD12	1.77	0.40
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.82	0.40
1:B:211:VAL:HG22	1:B:229:GLU:CG	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:ILE:C	1:C:437:ILE:CD1	2.69	0.40
1:D:84:VAL:HA	1:D:93:VAL:H	1.86	0.40
1:B:398:ALA:CA	1:B:399:LEU:CB	2.99	0.40
1:A:148:GLN:O	1:A:149:ALA:O	2.40	0.40
1:C:23:ARG:NH2	3:C:502:COA:P2A	2.94	0.40
1:C:111:LEU:HD12	1:C:111:LEU:HA	1.89	0.40
1:D:169:ARG:CD	1:D:175:VAL:HG13	2.52	0.40
1:D:287:HIS:CD2	1:D:289:VAL:H	2.32	0.40
1:D:324:VAL:HG21	1:D:408:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (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%)	393 (89%)	33 (8%)	15 (3%)	3	15
1	B	441/443 (100%)	379 (86%)	46 (10%)	16 (4%)	3	14
1	C	441/443 (100%)	391 (89%)	35 (8%)	15 (3%)	3	15
1	D	441/443 (100%)	381 (86%)	42 (10%)	18 (4%)	3	11
All	All	1764/1772 (100%)	1544 (88%)	156 (9%)	64 (4%)	3	14

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	TYR
1	A	91	LEU
1	A	148	GLN
1	A	149	ALA
1	A	398	ALA
1	A	441	GLN

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Mol	Chain	Res	Type
1	A	442	ALA
1	B	86	TYR
1	B	89	ARG
1	B	148	GLN
1	B	149	ALA
1	B	398	ALA
1	B	440	GLN
1	B	441	GLN
1	B	442	ALA
1	C	86	TYR
1	C	148	GLN
1	C	149	ALA
1	C	398	ALA
1	C	441	GLN
1	C	442	ALA
1	D	86	TYR
1	D	91	LEU
1	D	148	GLN
1	D	149	ALA
1	D	398	ALA
1	D	441	GLN
1	D	442	ALA
1	A	89	ARG
1	A	399	LEU
1	A	440	GLN
1	C	89	ARG
1	C	399	LEU
1	C	440	GLN
1	D	89	ARG
1	D	399	LEU
1	D	400	ARG
1	D	440	GLN
1	B	222	VAL
1	C	222	VAL
1	D	97	ALA
1	D	222	VAL
1	A	222	VAL
1	B	225	VAL
1	B	364	ALA
1	B	399	LEU
1	C	70	LYS
1	C	88	LEU

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Mol	Chain	Res	Type
1	D	88	LEU
1	A	93	VAL
1	A	225	VAL
1	A	400	ARG
1	B	93	VAL
1	B	418	LEU
1	C	225	VAL
1	D	93	VAL
1	D	225	VAL
1	D	438	ALA
1	B	92	THR
1	C	93	VAL
1	B	395	GLY
1	C	324	VAL
1	D	13	GLY
1	A	395	GLY

5.3.2 Protein sidechains (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%)	276 (82%)	62 (18%)	1 5
1	B	338/338 (100%)	276 (82%)	62 (18%)	1 5
1	C	337/338 (100%)	277 (82%)	60 (18%)	2 5
1	D	337/338 (100%)	274 (81%)	63 (19%)	1 5
All	All	1350/1352 (100%)	1103 (82%)	247 (18%)	1 5

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	39	VAL
1	A	44	CYS
1	A	50	LEU
1	A	58	GLU

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Mol	Chain	Res	Type
1	A	59	ARG
1	A	60	LEU
1	A	61	VAL
1	A	75	VAL
1	A	78	ARG
1	A	80	GLU
1	A	86	TYR
1	A	90	THR
1	A	91	LEU
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	148	GLN
1	A	151	ARG
1	A	160	ILE
1	A	173	LEU
1	A	175	VAL
1	A	176	THR
1	A	177	LEU
1	A	181	LYS
1	A	185	LEU
1	A	207	VAL
1	A	208	TRP
1	A	209	THR
1	A	221	ARG
1	A	222	VAL
1	A	231	VAL
1	A	236	LEU
1	A	237	VAL
1	A	243	ILE
1	A	268	ARG
1	A	276	VAL
1	A	285	SER
1	A	301	VAL
1	A	324	VAL
1	A	361	ARG

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Mol	Chain	Res	Type
1	A	375	VAL
1	A	377	LEU
1	A	386	LEU
1	A	391	VAL
1	A	392	VAL
1	A	396	HIS
1	A	408	LEU
1	A	410	ARG
1	A	411	GLU
1	A	413	SER
1	A	418	LEU
1	A	437	ILE
1	A	440	GLN
1	A	441	GLN
1	A	443	ARG
1	B	3	LYS
1	B	4	ARG
1	B	39	VAL
1	B	44	CYS
1	B	50	LEU
1	B	58	GLU
1	B	59	ARG
1	B	60	LEU
1	B	75	VAL
1	B	78	ARG
1	B	80	GLU
1	B	86	TYR
1	B	90	THR
1	B	91	LEU
1	B	92	THR
1	B	94	HIS
1	B	101	THR
1	B	111	LEU
1	B	116	ARG
1	B	132	THR
1	B	133	LEU
1	B	142	LEU
1	B	146	LEU
1	B	148	GLN
1	B	151	ARG
1	B	160	ILE
1	B	171	ARG

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Mol	Chain	Res	Type
1	B	173	LEU
1	B	176	THR
1	B	177	LEU
1	B	181	LYS
1	B	185	LEU
1	B	199	GLU
1	B	208	TRP
1	B	209	THR
1	B	221	ARG
1	B	222	VAL
1	B	236	LEU
1	B	237	VAL
1	B	243	ILE
1	B	268	ARG
1	B	270	ARG
1	B	272	ASN
1	B	276	VAL
1	B	292	ARG
1	B	301	VAL
1	B	324	VAL
1	B	361	ARG
1	B	362	ASP
1	B	375	VAL
1	B	377	LEU
1	B	391	VAL
1	B	392	VAL
1	B	394	ARG
1	B	396	HIS
1	B	410	ARG
1	B	411	GLU
1	B	418	LEU
1	B	437	ILE
1	B	440	GLN
1	B	441	GLN
1	B	443	ARG
1	C	3	LYS
1	C	36	SER
1	C	39	VAL
1	C	50	LEU
1	C	58	GLU
1	C	59	ARG
1	C	60	LEU

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Mol	Chain	Res	Type
1	C	75	VAL
1	C	78	ARG
1	C	80	GLU
1	C	86	TYR
1	C	90	THR
1	C	91	LEU
1	C	94	HIS
1	C	101	THR
1	C	111	LEU
1	C	116	ARG
1	C	132	THR
1	C	133	LEU
1	C	142	LEU
1	C	143	LEU
1	C	146	LEU
1	C	148	GLN
1	C	151	ARG
1	C	160	ILE
1	C	171	ARG
1	C	173	LEU
1	C	176	THR
1	C	177	LEU
1	C	181	LYS
1	C	185	LEU
1	C	207	VAL
1	C	208	TRP
1	C	209	THR
1	C	221	ARG
1	C	222	VAL
1	C	236	LEU
1	C	237	VAL
1	C	243	ILE
1	C	268	ARG
1	C	270	ARG
1	C	272	ASN
1	C	301	VAL
1	C	324	VAL
1	C	355	LYS
1	C	361	ARG
1	C	375	VAL
1	C	377	LEU
1	C	392	VAL

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Mol	Chain	Res	Type
1	C	396	HIS
1	C	408	LEU
1	C	410	ARG
1	C	411	GLU
1	C	413	SER
1	C	418	LEU
1	C	434	PRO
1	C	437	ILE
1	C	440	GLN
1	C	441	GLN
1	C	443	ARG
1	D	3	LYS
1	D	39	VAL
1	D	50	LEU
1	D	58	GLU
1	D	59	ARG
1	D	60	LEU
1	D	70	LYS
1	D	75	VAL
1	D	78	ARG
1	D	80	GLU
1	D	86	TYR
1	D	90	THR
1	D	91	LEU
1	D	94	HIS
1	D	100	ARG
1	D	101	THR
1	D	105	ARG
1	D	111	LEU
1	D	116	ARG
1	D	117	PRO
1	D	132	THR
1	D	133	LEU
1	D	142	LEU
1	D	143	LEU
1	D	144	LYS
1	D	146	LEU
1	D	148	GLN
1	D	151	ARG
1	D	160	ILE
1	D	171	ARG
1	D	176	THR

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Mol	Chain	Res	Type
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	236	LEU
1	D	237	VAL
1	D	243	ILE
1	D	268	ARG
1	D	270	ARG
1	D	272	ASN
1	D	301	VAL
1	D	324	VAL
1	D	361	ARG
1	D	375	VAL
1	D	377	LEU
1	D	386	LEU
1	D	391	VAL
1	D	392	VAL
1	D	394	ARG
1	D	396	HIS
1	D	400	ARG
1	D	410	ARG
1	D	411	GLU
1	D	418	LEU
1	D	437	ILE
1	D	440	GLN
1	D	441	GLN
1	D	443	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	96	HIS
1	A	203	HIS
1	A	272	ASN
1	A	287	HIS
1	A	396	HIS

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Mol	Chain	Res	Type
1	A	440	GLN
1	A	441	GLN
1	B	94	HIS
1	B	96	HIS
1	B	272	ASN
1	B	287	HIS
1	B	396	HIS
1	B	440	GLN
1	C	94	HIS
1	C	96	HIS
1	C	272	ASN
1	C	287	HIS
1	C	440	GLN
1	D	94	HIS
1	D	96	HIS
1	D	272	ASN
1	D	287	HIS
1	D	440	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	COA	C	502	1	41,50,50	1.22	5 (12%)	52,75,75	2.02	17 (32%)
2	FAD	C	501	-	53,58,58	3.07	24 (45%)	68,89,89	1.75	20 (29%)
3	COA	D	502	1	41,50,50	0.80	0	52,75,75	2.02	15 (28%)
2	FAD	A	501	-	53,58,58	2.93	27 (50%)	68,89,89	1.83	17 (25%)
3	COA	A	502	1	41,50,50	1.47	8 (19%)	52,75,75	2.12	15 (28%)
2	FAD	D	501	-	53,58,58	2.99	24 (45%)	68,89,89	1.70	16 (23%)
2	FAD	B	501	-	53,58,58	3.33	27 (50%)	68,89,89	2.03	22 (32%)
3	COA	B	502	1	41,50,50	1.41	5 (12%)	52,75,75	1.79	16 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	C	502	1	-	19/44/64/64	0/3/3/3
2	FAD	C	501	-	-	15/30/50/50	0/6/6/6
3	COA	D	502	1	-	16/44/64/64	0/3/3/3
2	FAD	A	501	-	-	13/30/50/50	0/6/6/6
3	COA	A	502	1	-	15/44/64/64	0/3/3/3
2	FAD	D	501	-	-	15/30/50/50	0/6/6/6
2	FAD	B	501	-	-	15/30/50/50	0/6/6/6
3	COA	B	502	1	-	18/44/64/64	0/3/3/3

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FAD	C9A-C5X	9.39	1.56	1.41
2	C	501	FAD	C9A-C5X	8.38	1.55	1.41
2	B	501	FAD	C4A-N3A	8.20	1.47	1.35
2	D	501	FAD	C9A-C5X	7.59	1.53	1.41
2	A	501	FAD	C9A-C5X	7.59	1.53	1.41
2	C	501	FAD	C4A-N3A	7.23	1.45	1.35
2	C	501	FAD	C2A-N3A	7.12	1.43	1.32
2	C	501	FAD	C5A-C4A	6.91	1.59	1.40
2	D	501	FAD	C4A-N3A	6.84	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C2A-N3A	6.81	1.43	1.32
2	B	501	FAD	C2A-N3A	6.79	1.43	1.32
2	D	501	FAD	C5A-C4A	6.75	1.58	1.40
2	D	501	FAD	C2A-N3A	6.39	1.42	1.32
2	D	501	FAD	C2A-N1A	6.36	1.45	1.33
2	A	501	FAD	C5A-C4A	6.30	1.57	1.40
2	B	501	FAD	C5A-C4A	6.16	1.57	1.40
2	C	501	FAD	C2A-N1A	6.06	1.45	1.33
2	B	501	FAD	C2A-N1A	5.58	1.44	1.33
2	A	501	FAD	C4A-N3A	5.35	1.43	1.35
2	A	501	FAD	C2B-C1B	5.30	1.61	1.53
2	B	501	FAD	C8-C7	5.29	1.54	1.40
2	B	501	FAD	C4X-N5	5.23	1.40	1.30
2	B	501	FAD	O4B-C1B	5.16	1.48	1.41
2	D	501	FAD	C2B-C1B	5.07	1.61	1.53
2	C	501	FAD	C8-C7	5.05	1.53	1.40
2	A	501	FAD	C8-C7	4.86	1.53	1.40
3	B	502	COA	C2A-N3A	4.75	1.39	1.32
2	D	501	FAD	C4X-N5	4.74	1.40	1.30
2	C	501	FAD	C4X-N5	4.73	1.39	1.30
2	A	501	FAD	C2A-N1A	4.65	1.42	1.33
2	C	501	FAD	O2-C2	4.50	1.32	1.24
2	C	501	FAD	O4-C4	4.41	1.32	1.23
2	D	501	FAD	C8-C7	4.31	1.51	1.40
2	B	501	FAD	O4-C4	4.21	1.31	1.23
2	B	501	FAD	C4X-C10	4.20	1.56	1.44
2	A	501	FAD	C4X-N5	4.12	1.38	1.30
2	B	501	FAD	O3B-C3B	4.00	1.52	1.43
2	B	501	FAD	C10-N10	3.92	1.45	1.37
2	D	501	FAD	C4X-C10	3.86	1.55	1.44
2	B	501	FAD	C5'-C4'	3.85	1.57	1.51
2	A	501	FAD	C5'-C4'	3.79	1.57	1.51
3	A	502	COA	C2B-C1B	-3.76	1.48	1.53
2	A	501	FAD	C10-N1	3.73	1.40	1.33
2	C	501	FAD	C2B-C1B	3.71	1.59	1.53
2	D	501	FAD	C10-N10	3.71	1.45	1.37
2	A	501	FAD	O2-C2	3.70	1.31	1.24
2	A	501	FAD	C10-N10	3.69	1.45	1.37
2	B	501	FAD	C6A-C5A	3.63	1.56	1.43
2	C	501	FAD	C10-N10	3.62	1.45	1.37
2	D	501	FAD	C9A-N10	3.60	1.47	1.41
2	A	501	FAD	PA-O1A	3.58	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FAD	C6A-C5A	3.58	1.56	1.43
2	B	501	FAD	C10-N1	3.58	1.40	1.33
2	B	501	FAD	C6-C7	3.57	1.44	1.39
2	B	501	FAD	C2B-C1B	3.52	1.59	1.53
2	B	501	FAD	C9A-N10	3.45	1.47	1.41
2	D	501	FAD	O4B-C1B	3.43	1.45	1.41
2	A	501	FAD	C4X-C10	3.41	1.54	1.44
2	C	501	FAD	C4X-C10	3.40	1.54	1.44
2	D	501	FAD	C6A-C5A	3.39	1.55	1.43
2	A	501	FAD	O4-C4	3.22	1.29	1.23
2	A	501	FAD	C9A-N10	3.22	1.46	1.41
2	D	501	FAD	C10-N1	3.18	1.39	1.33
2	C	501	FAD	C9A-N10	3.17	1.46	1.41
3	A	502	COA	C2A-N3A	3.06	1.37	1.32
2	C	501	FAD	C6A-C5A	2.91	1.54	1.43
2	D	501	FAD	O4-C4	2.88	1.29	1.23
2	C	501	FAD	C10-N1	2.86	1.39	1.33
2	B	501	FAD	C3B-C4B	2.84	1.60	1.53
2	B	501	FAD	C6-C5X	2.83	1.44	1.40
3	A	502	COA	O5P-C5P	-2.76	1.17	1.23
2	B	501	FAD	PA-O1A	2.76	1.60	1.50
3	B	502	COA	C5A-C4A	2.75	1.48	1.40
2	A	501	FAD	O3B-C3B	2.73	1.49	1.43
2	D	501	FAD	PA-O1A	2.72	1.60	1.50
2	C	501	FAD	C5'-C4'	2.70	1.55	1.51
3	A	502	COA	C6P-C5P	-2.69	1.46	1.51
2	C	501	FAD	C8A-N7A	2.68	1.39	1.34
2	D	501	FAD	O2B-C2B	2.67	1.49	1.43
3	C	502	COA	C5A-C4A	2.66	1.48	1.40
2	A	501	FAD	C9-C9A	2.64	1.43	1.39
2	D	501	FAD	C4X-C4	2.63	1.54	1.44
2	B	501	FAD	C4X-C4	2.61	1.54	1.44
3	B	502	COA	C2B-C1B	-2.58	1.49	1.53
2	C	501	FAD	C3B-C4B	2.57	1.59	1.53
2	D	501	FAD	C5'-C4'	2.57	1.55	1.51
2	A	501	FAD	C6-C7	2.56	1.43	1.39
3	C	502	COA	O4B-C1B	2.56	1.44	1.41
2	D	501	FAD	C6-C7	2.55	1.43	1.39
2	C	501	FAD	O3B-C3B	2.54	1.49	1.43
2	A	501	FAD	O4B-C1B	2.51	1.44	1.41
2	C	501	FAD	PA-O1A	2.51	1.59	1.50
2	C	501	FAD	C6-C7	2.49	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	COA	C2A-N3A	2.47	1.36	1.32
2	C	501	FAD	O4B-C1B	2.44	1.44	1.41
2	A	501	FAD	C4X-C4	2.42	1.53	1.44
3	A	502	COA	C5A-N7A	-2.41	1.31	1.39
3	B	502	COA	O9P-C9P	-2.39	1.18	1.23
2	D	501	FAD	C6-C5X	2.35	1.43	1.40
2	B	501	FAD	O4'-C4'	2.34	1.48	1.43
3	A	502	COA	O4B-C1B	2.30	1.44	1.41
2	A	501	FAD	O4'-C4'	2.27	1.48	1.43
2	A	501	FAD	C6A-N6A	2.26	1.42	1.34
2	D	501	FAD	C9-C8	2.26	1.42	1.39
2	A	501	FAD	PA-O5B	2.23	1.68	1.59
2	B	501	FAD	C9-C8	2.18	1.42	1.39
3	C	502	COA	C6A-N6A	2.16	1.41	1.34
2	D	501	FAD	O2-C2	2.13	1.28	1.24
3	A	502	COA	P3B-O8A	-2.13	1.46	1.54
3	C	502	COA	P3B-O3B	2.10	1.63	1.59
3	B	502	COA	P3B-O8A	-2.09	1.46	1.54
2	B	501	FAD	O2-C2	2.08	1.28	1.24
2	D	501	FAD	O3B-C3B	2.07	1.47	1.43
2	B	501	FAD	C8A-N7A	2.05	1.38	1.34
2	A	501	FAD	C8A-N7A	2.05	1.38	1.34
2	A	501	FAD	C2-N1	2.05	1.41	1.36
2	B	501	FAD	C4'-C3'	2.04	1.57	1.53
3	A	502	COA	C2A-N1A	2.03	1.37	1.33
2	C	501	FAD	O2B-C2B	2.03	1.47	1.43
2	C	501	FAD	C6-C5X	2.01	1.43	1.40

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	COA	O4B-C1B-C2B	-6.65	97.20	106.93
3	B	502	COA	O4B-C1B-C2B	-5.39	99.05	106.93
2	A	501	FAD	N6A-C6A-N1A	5.31	129.60	118.57
3	D	502	COA	CDP-CBP-CCP	5.24	116.78	108.23
2	B	501	FAD	C5X-C9A-N10	5.19	123.31	117.95
2	B	501	FAD	N6A-C6A-N1A	4.63	128.19	118.57
3	A	502	COA	C4A-C5A-N7A	-4.61	104.60	109.40
3	D	502	COA	OAP-CAP-CBP	-4.33	100.06	110.25
3	C	502	COA	CDP-CBP-CCP	4.32	115.28	108.23
2	D	501	FAD	N6A-C6A-N1A	4.25	127.39	118.57
3	A	502	COA	CDP-CBP-CAP	4.24	116.17	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	FAD	N6A-C6A-N1A	4.22	127.33	118.57
3	D	502	COA	CEP-CBP-CAP	4.20	116.10	108.82
2	C	501	FAD	C5X-C9A-N10	4.18	122.27	117.95
3	C	502	COA	C3P-N4P-C5P	-4.17	115.09	122.84
2	B	501	FAD	C3B-C2B-C1B	4.16	107.25	100.98
3	A	502	COA	O2B-C2B-C1B	-4.07	95.84	110.85
3	A	502	COA	C7P-N8P-C9P	-4.06	115.35	122.59
2	A	501	FAD	O4B-C4B-C3B	4.04	113.10	105.11
2	B	501	FAD	O3'-C3'-C4'	4.00	118.46	108.81
3	A	502	COA	C7P-C6P-C5P	-3.95	105.77	112.36
2	B	501	FAD	O2-C2-N1	-3.91	115.35	121.83
3	B	502	COA	CEP-CBP-CAP	3.87	115.54	108.82
3	D	502	COA	N3A-C2A-N1A	-3.82	122.71	128.68
2	A	501	FAD	C3B-C2B-C1B	3.81	106.71	100.98
2	A	501	FAD	C5A-C6A-N6A	-3.75	114.65	120.35
3	C	502	COA	N6A-C6A-N1A	3.75	126.36	118.57
3	C	502	COA	CEP-CBP-CCP	-3.74	102.12	108.23
3	C	502	COA	CEP-CBP-CAP	3.71	115.25	108.82
3	D	502	COA	O6A-CCP-CBP	-3.70	104.60	110.55
2	D	501	FAD	O4B-C4B-C3B	3.70	112.43	105.11
3	D	502	COA	O4B-C1B-C2B	-3.66	101.57	106.93
2	B	501	FAD	C9A-N10-C10	-3.64	115.09	120.77
2	C	501	FAD	C9A-C5X-N5	-3.63	118.48	122.43
3	D	502	COA	O2A-P1A-O1A	3.52	129.66	112.24
3	A	502	COA	C6P-C7P-N8P	3.51	118.98	111.90
3	C	502	COA	O2A-P1A-O1A	3.47	129.41	112.24
2	C	501	FAD	O3B-C3B-C4B	3.43	120.95	111.05
3	A	502	COA	C1B-N9A-C4A	3.41	132.63	126.64
2	A	501	FAD	C10-N1-C2	3.38	123.66	116.90
2	B	501	FAD	O4-C4-C4X	-3.38	117.64	126.60
2	D	501	FAD	C9A-C5X-N5	-3.37	118.77	122.43
2	C	501	FAD	O4B-C4B-C3B	3.35	111.74	105.11
2	B	501	FAD	O4B-C4B-C3B	3.34	111.73	105.11
2	B	501	FAD	C5A-C6A-N6A	-3.34	115.28	120.35
2	A	501	FAD	O3'-C3'-C4'	3.31	116.81	108.81
3	B	502	COA	O9P-C9P-N8P	-3.26	116.00	122.99
2	B	501	FAD	O4-C4-N3	3.20	126.26	120.12
3	D	502	COA	O9A-P3B-O7A	3.17	123.11	110.68
2	D	501	FAD	C5X-C9A-N10	3.17	121.23	117.95
3	C	502	COA	O6A-CCP-CBP	-3.17	105.46	110.55
2	B	501	FAD	O3B-C3B-C4B	3.08	119.97	111.05
2	D	501	FAD	O2'-C2'-C1'	3.00	117.06	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	COA	O9A-P3B-O7A	2.98	122.35	110.68
2	C	501	FAD	O4-C4-N3	2.98	125.83	120.12
3	C	502	COA	O4B-C1B-C2B	-2.91	102.67	106.93
3	D	502	COA	C7P-N8P-C9P	-2.91	117.39	122.59
3	C	502	COA	C7P-N8P-C9P	-2.88	117.45	122.59
2	C	501	FAD	O5'-C5'-C4'	2.87	117.03	109.36
3	C	502	COA	C5A-C6A-N6A	-2.87	115.99	120.35
3	B	502	COA	C7P-N8P-C9P	-2.86	117.48	122.59
3	A	502	COA	C3B-C2B-C1B	2.84	106.18	99.89
3	A	502	COA	O6A-CCP-CBP	-2.80	106.05	110.55
2	A	501	FAD	C4X-C10-N1	-2.79	118.26	124.73
2	D	501	FAD	C2A-N1A-C6A	2.78	123.52	118.75
2	A	501	FAD	O5'-C5'-C4'	2.77	116.76	109.36
2	D	501	FAD	O5'-C5'-C4'	2.72	116.61	109.36
3	A	502	COA	O5P-C5P-C6P	-2.69	117.10	122.02
3	B	502	COA	C3P-N4P-C5P	-2.68	117.85	122.84
3	C	502	COA	O5B-P1A-O1A	-2.67	98.62	109.07
2	D	501	FAD	C5X-N5-C4X	2.67	122.51	118.07
2	B	501	FAD	C9A-C5X-N5	-2.66	119.54	122.43
3	C	502	COA	N3A-C2A-N1A	-2.66	124.52	128.68
3	D	502	COA	C4A-C5A-N7A	-2.66	106.63	109.40
2	A	501	FAD	O4-C4-C4X	-2.65	119.57	126.60
2	A	501	FAD	O3B-C3B-C4B	2.65	118.70	111.05
3	B	502	COA	O5A-P2A-O4A	2.64	125.29	112.24
2	C	501	FAD	O2P-P-O5'	2.58	119.74	107.75
2	D	501	FAD	O2P-P-O5'	2.55	119.58	107.75
2	A	501	FAD	O2P-P-O5'	2.54	119.54	107.75
3	B	502	COA	C4A-C5A-N7A	-2.54	106.75	109.40
3	B	502	COA	O3B-P3B-O7A	-2.53	99.62	109.39
3	A	502	COA	CEP-CBP-CCP	-2.53	104.11	108.23
3	D	502	COA	C2P-C3P-N4P	-2.52	106.54	112.31
2	A	501	FAD	C9A-N10-C10	-2.51	116.86	120.77
3	A	502	COA	N6A-C6A-N1A	2.51	123.78	118.57
3	D	502	COA	O5A-P2A-O4A	2.49	124.54	112.24
2	A	501	FAD	O2B-C2B-C1B	2.46	119.94	110.85
2	C	501	FAD	O4-C4-C4X	-2.46	120.08	126.60
2	D	501	FAD	C3B-C2B-C1B	2.44	104.66	100.98
2	D	501	FAD	C5A-C6A-N1A	-2.44	114.83	120.35
2	C	501	FAD	C3B-C2B-C1B	2.43	104.64	100.98
2	C	501	FAD	C5A-C6A-N6A	-2.39	116.72	120.35
2	C	501	FAD	O2B-C2B-C1B	2.39	119.68	110.85
3	B	502	COA	N6A-C6A-N1A	2.38	123.52	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	COA	CAP-C9P-N8P	2.37	121.29	116.58
2	A	501	FAD	C4-C4X-N5	2.35	121.57	118.23
2	A	501	FAD	C4X-C10-N10	2.34	119.91	116.48
2	C	501	FAD	C9A-N10-C10	-2.34	117.11	120.77
2	B	501	FAD	O5'-C5'-C4'	2.34	115.61	109.36
3	C	502	COA	O5A-P2A-O4A	2.33	123.77	112.24
2	D	501	FAD	O2-C2-N1	-2.32	117.98	121.83
3	B	502	COA	C5A-C6A-N6A	-2.32	116.83	120.35
2	D	501	FAD	O3'-C3'-C4'	2.31	114.39	108.81
2	C	501	FAD	O4'-C4'-C3'	2.30	114.69	109.10
2	C	501	FAD	C8M-C8-C9	-2.28	115.27	119.49
2	C	501	FAD	C10-N1-C2	2.28	121.46	116.90
2	B	501	FAD	N3A-C2A-N1A	-2.26	125.15	128.68
2	B	501	FAD	C4X-C10-N1	-2.25	119.52	124.73
2	B	501	FAD	C1'-N10-C9A	2.24	124.25	120.51
2	D	501	FAD	O2B-C2B-C1B	2.24	119.12	110.85
3	B	502	COA	CAP-C9P-N8P	2.23	121.01	116.58
3	B	502	COA	C3B-C2B-C1B	2.22	104.81	99.89
2	B	501	FAD	C4A-C5A-N7A	-2.21	107.10	109.40
3	C	502	COA	O2B-C2B-C3B	-2.21	104.90	111.17
3	A	502	COA	O2A-P1A-O1A	2.20	123.10	112.24
3	B	502	COA	O2B-C2B-C3B	-2.19	104.93	111.17
2	C	501	FAD	O2A-PA-O1A	2.19	123.09	112.24
2	C	501	FAD	C2A-N1A-C6A	2.16	122.45	118.75
3	B	502	COA	O2A-P1A-O1A	2.16	122.91	112.24
2	D	501	FAD	C9A-C9-C8	2.15	123.62	119.30
3	C	502	COA	C1B-N9A-C4A	2.14	130.40	126.64
2	B	501	FAD	C8M-C8-C9	-2.13	115.55	119.49
3	B	502	COA	C6P-C7P-N8P	2.13	116.20	111.90
3	B	502	COA	N3A-C2A-N1A	-2.13	125.35	128.68
2	C	501	FAD	C6-C5X-C9A	2.11	121.93	118.94
2	B	501	FAD	C10-N1-C2	2.11	121.11	116.90
2	B	501	FAD	O3B-C3B-C2B	2.07	118.52	111.82
2	D	501	FAD	N3A-C2A-N1A	-2.07	125.45	128.68
3	A	502	COA	C6P-C5P-N4P	2.05	119.88	116.42
3	D	502	COA	C1B-N9A-C4A	2.05	130.24	126.64
3	D	502	COA	C6P-C5P-N4P	2.03	119.84	116.42
3	D	502	COA	C7P-C6P-C5P	-2.03	108.98	112.36
2	A	501	FAD	C5A-C6A-N1A	-2.03	115.75	120.35
2	C	501	FAD	O2P-P-O1P	2.03	122.26	112.24
2	B	501	FAD	O2P-P-O5'	2.01	117.10	107.75
2	A	501	FAD	O2-C2-N3	2.01	122.56	118.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FAD	P-O5'-C5'	2.00	133.43	121.68

There are no chirality outliers.

All (126) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	A	502	COA	O4B-C4B-C5B-O5B
3	A	502	COA	C5B-O5B-P1A-O3A
3	A	502	COA	CCP-O6A-P2A-O4A
3	A	502	COA	CCP-O6A-P2A-O5A
3	A	502	COA	CEP-CBP-CCP-O6A
3	A	502	COA	CAP-CBP-CCP-O6A
3	B	502	COA	C3B-C4B-C5B-O5B
3	B	502	COA	C5B-O5B-P1A-O1A
3	B	502	COA	C5B-O5B-P1A-O3A
3	B	502	COA	CCP-O6A-P2A-O4A
3	B	502	COA	CAP-CBP-CCP-O6A
3	C	502	COA	C3B-O3B-P3B-O7A
3	C	502	COA	C3B-C4B-C5B-O5B
3	C	502	COA	C5B-O5B-P1A-O1A
3	C	502	COA	C5B-O5B-P1A-O3A
3	C	502	COA	CCP-O6A-P2A-O4A
3	C	502	COA	CAP-CBP-CCP-O6A
3	D	502	COA	C3B-C4B-C5B-O5B
3	D	502	COA	O4B-C4B-C5B-O5B
3	D	502	COA	C5B-O5B-P1A-O2A
3	D	502	COA	C5B-O5B-P1A-O3A
3	D	502	COA	CCP-O6A-P2A-O4A
3	D	502	COA	CAP-CBP-CCP-O6A
3	B	502	COA	O4B-C4B-C5B-O5B
3	C	502	COA	O4B-C4B-C5B-O5B
3	C	502	COA	C4B-C3B-O3B-P3B
3	A	502	COA	CDP-CBP-CCP-O6A
3	B	502	COA	CDP-CBP-CCP-O6A
3	B	502	COA	CEP-CBP-CCP-O6A
3	C	502	COA	CDP-CBP-CCP-O6A
3	C	502	COA	CEP-CBP-CCP-O6A
3	D	502	COA	CDP-CBP-CCP-O6A
3	A	502	COA	O5P-C5P-N4P-C3P
3	C	502	COA	C2B-C3B-O3B-P3B
3	A	502	COA	C6P-C5P-N4P-C3P
3	D	502	COA	CEP-CBP-CCP-O6A
3	B	502	COA	O5P-C5P-N4P-C3P
3	B	502	COA	P2A-O3A-P1A-O1A
3	D	502	COA	P2A-O3A-P1A-O1A
3	D	502	COA	O5P-C5P-N4P-C3P
3	D	502	COA	C6P-C5P-N4P-C3P
2	A	501	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
2	B	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	D	501	FAD	PA-O3P-P-O5'
3	B	502	COA	C6P-C5P-N4P-C3P
3	C	502	COA	O5P-C5P-N4P-C3P
3	C	502	COA	C6P-C5P-N4P-C3P
2	A	501	FAD	C5B-O5B-PA-O3P
3	D	502	COA	CCP-O6A-P2A-O3A
3	A	502	COA	P2A-O3A-P1A-O1A
3	A	502	COA	P2A-O3A-P1A-O2A
3	B	502	COA	P2A-O3A-P1A-O2A
3	D	502	COA	P2A-O3A-P1A-O2A
2	A	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	C5'-O5'-P-O1P
2	D	501	FAD	C5'-O5'-P-O1P
3	A	502	COA	C5B-O5B-P1A-O1A
3	A	502	COA	C5B-O5B-P1A-O2A
3	B	502	COA	C5B-O5B-P1A-O2A
3	B	502	COA	CCP-O6A-P2A-O5A
3	C	502	COA	C5B-O5B-P1A-O2A
3	C	502	COA	CCP-O6A-P2A-O5A
3	D	502	COA	C5B-O5B-P1A-O1A
3	D	502	COA	CCP-O6A-P2A-O5A
3	C	502	COA	P1A-O3A-P2A-O5A
3	B	502	COA	C2B-C3B-O3B-P3B
2	D	501	FAD	O4B-C4B-C5B-O5B
3	B	502	COA	C5P-C6P-C7P-N8P
2	A	501	FAD	O4B-C4B-C5B-O5B
3	D	502	COA	C2B-C3B-O3B-P3B
2	D	501	FAD	C5B-O5B-PA-O3P
3	A	502	COA	CCP-O6A-P2A-O3A
3	B	502	COA	CCP-O6A-P2A-O3A
3	C	502	COA	C3B-O3B-P3B-O8A
3	C	502	COA	CCP-O6A-P2A-O3A
2	B	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	PA-O3P-P-O2P
2	B	501	FAD	P-O3P-PA-O2A
2	B	501	FAD	PA-O3P-P-O2P
2	C	501	FAD	P-O3P-PA-O1A
2	C	501	FAD	P-O3P-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	D	501	FAD	P-O3P-PA-O1A
2	D	501	FAD	P-O3P-PA-O2A
3	C	502	COA	P2A-O3A-P1A-O2A
2	C	501	FAD	O4B-C4B-C5B-O5B
3	B	502	COA	C4B-C3B-O3B-P3B
2	D	501	FAD	C2'-C1'-N10-C10

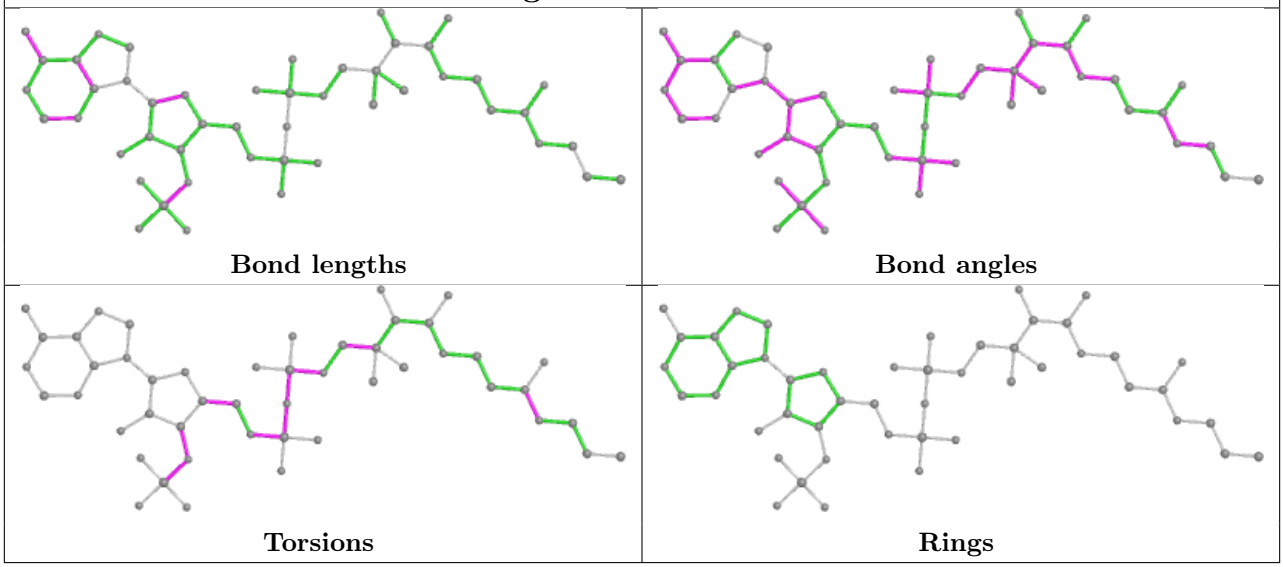
There are no ring outliers.

8 monomers are involved in 53 short contacts:

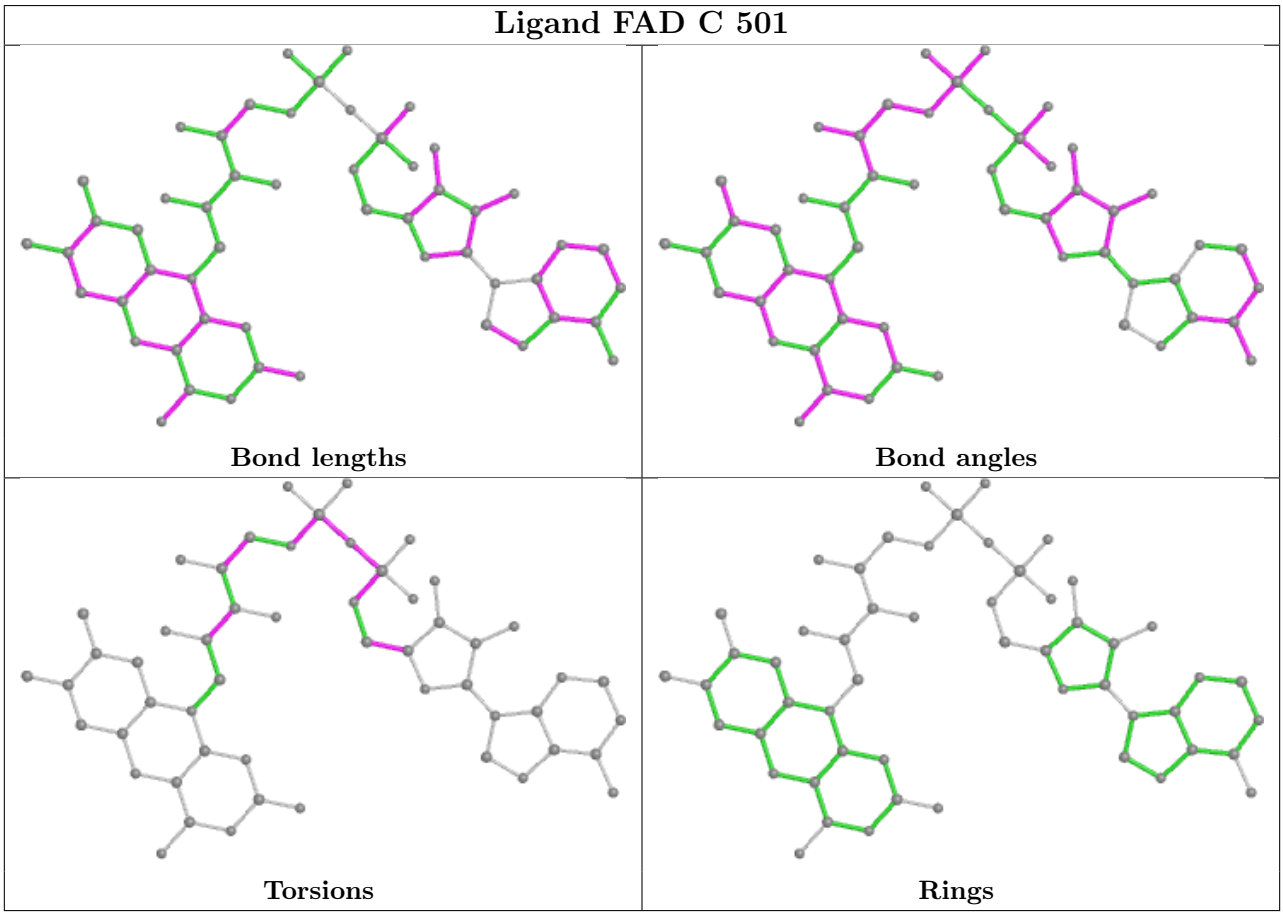
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	COA	4	0
2	C	501	FAD	10	0
3	D	502	COA	3	0
2	A	501	FAD	9	0
3	A	502	COA	6	0
2	D	501	FAD	7	0
2	B	501	FAD	8	0
3	B	502	COA	7	0

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

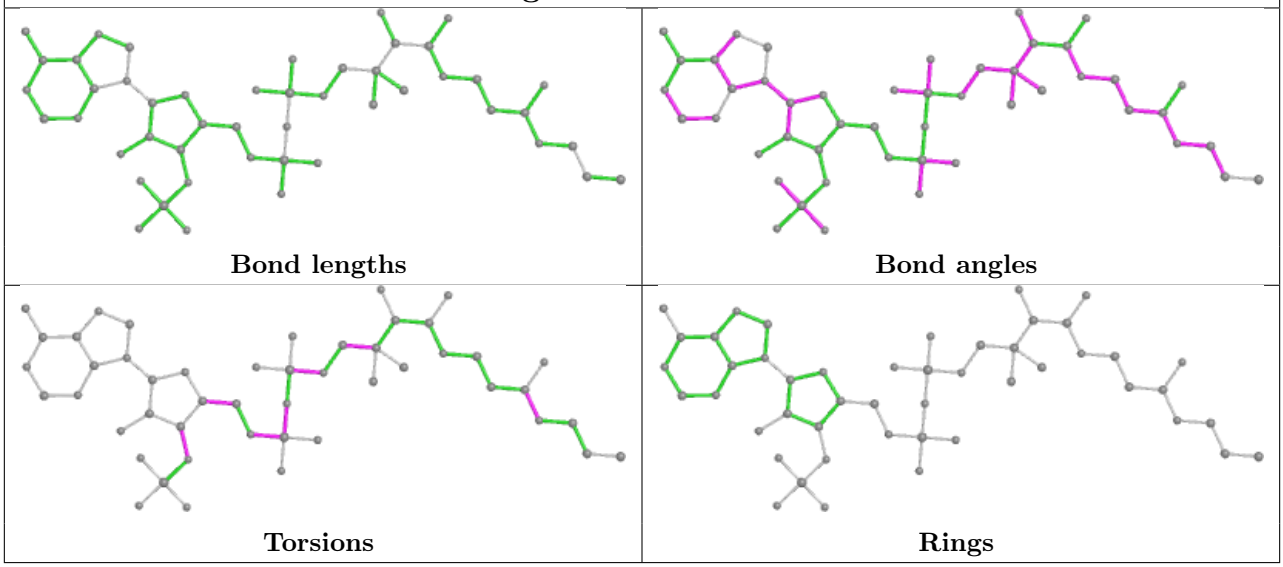
Ligand COA C 502



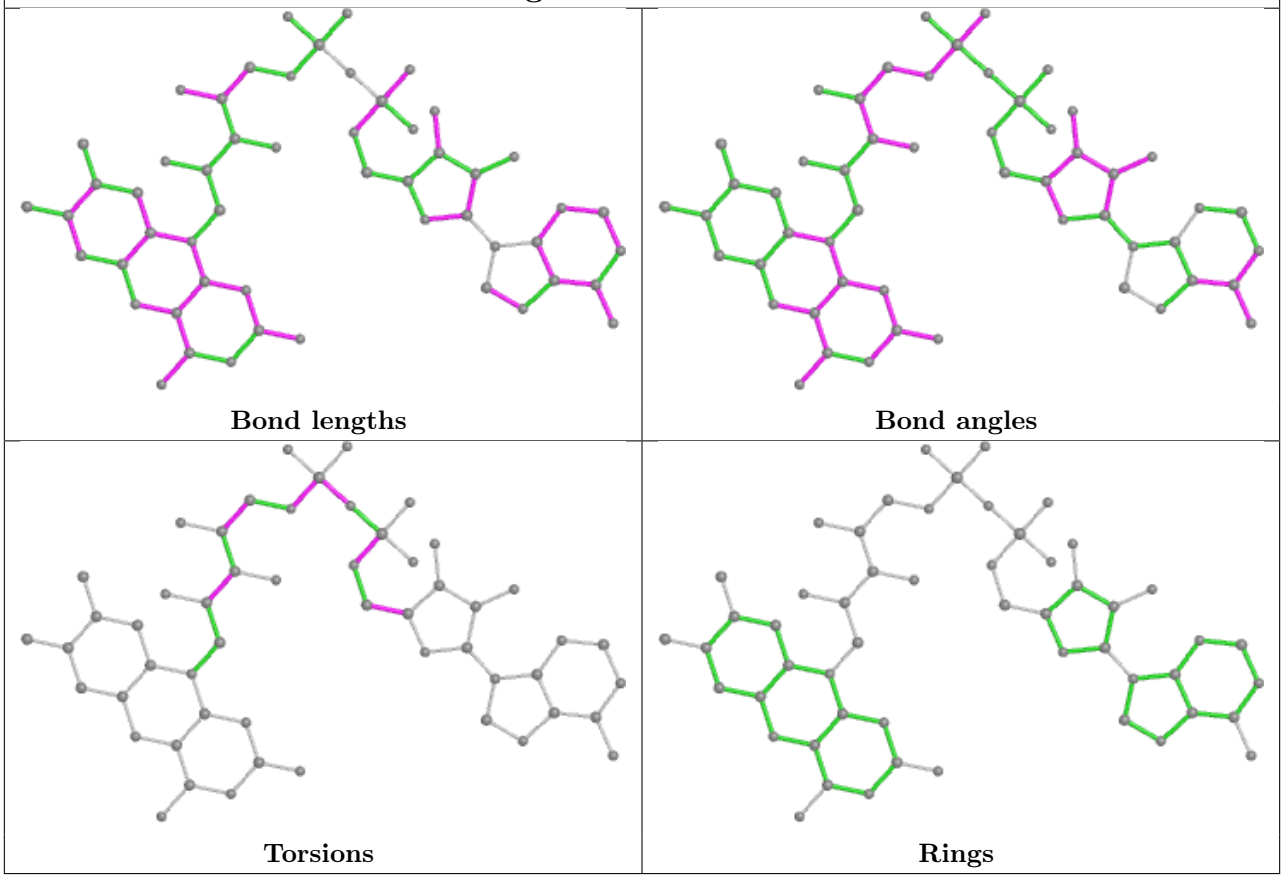
Ligand FAD C 501



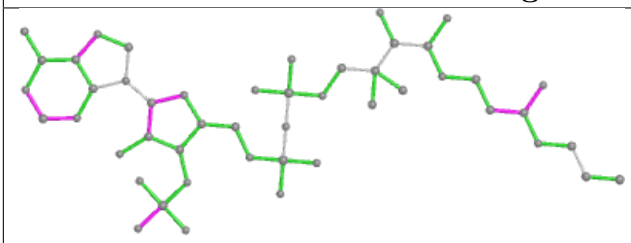
Ligand COA D 502



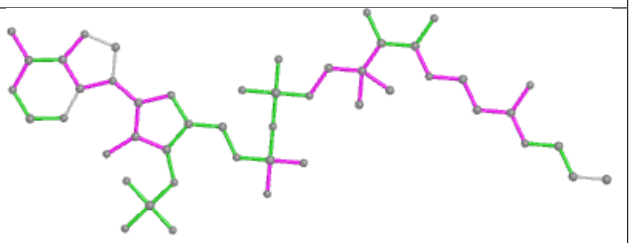
Ligand FAD A 501



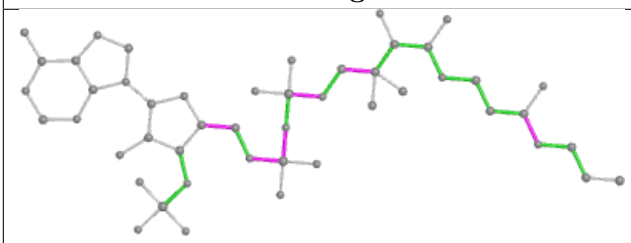
Ligand COA A 502



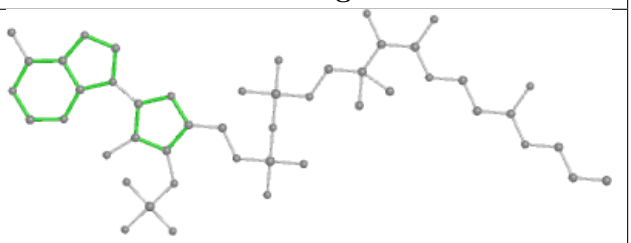
Bond lengths



Bond angles

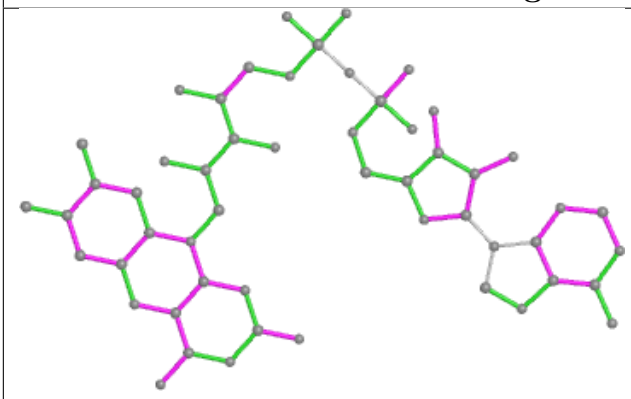


Torsions

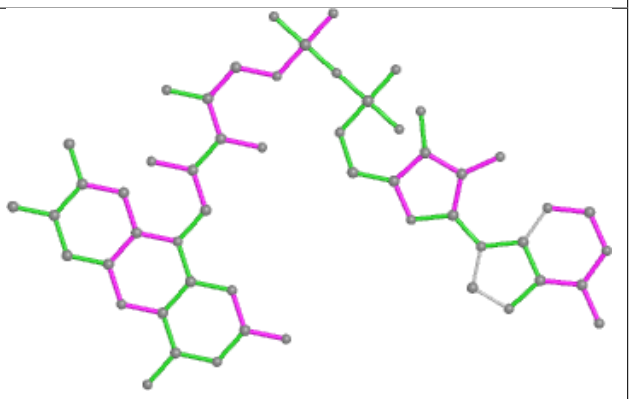


Rings

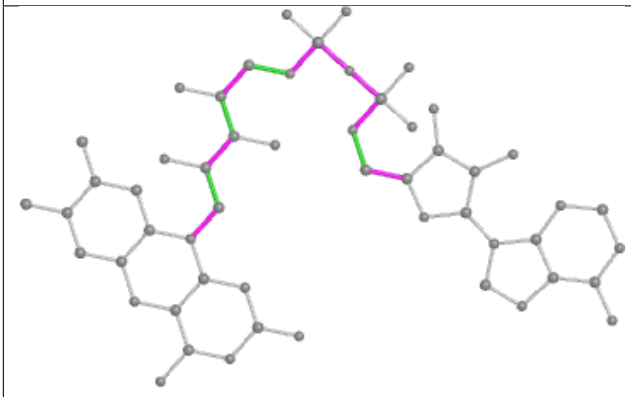
Ligand FAD D 501



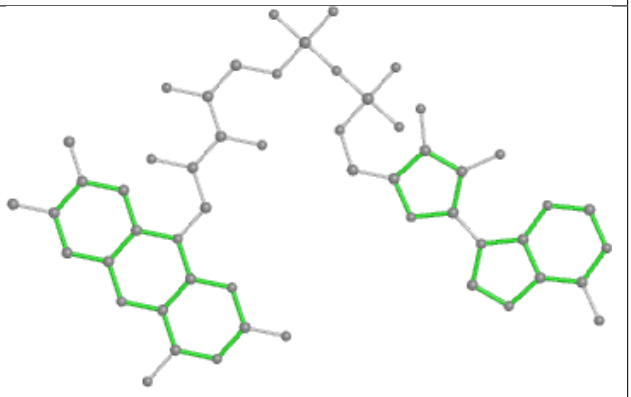
Bond lengths



Bond angles

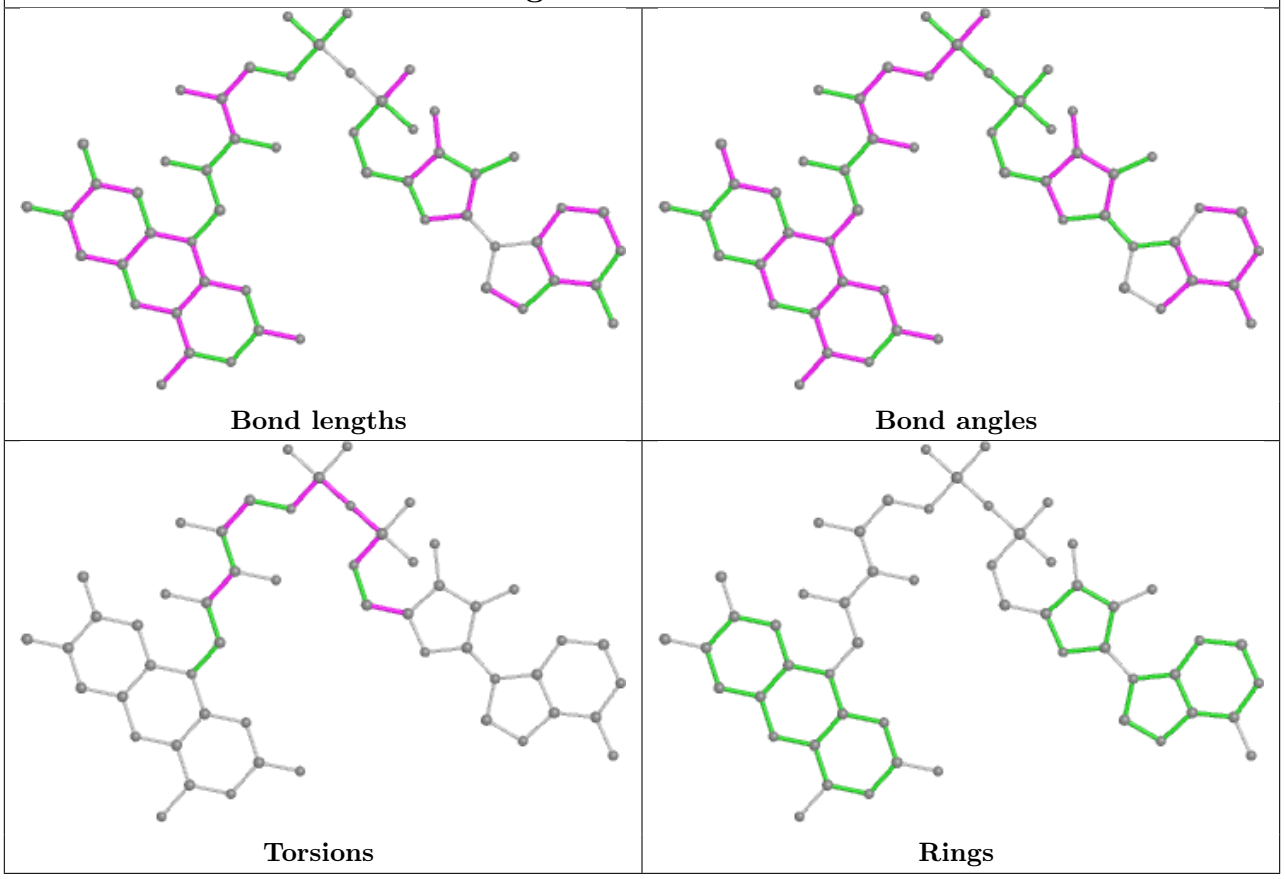


Torsions

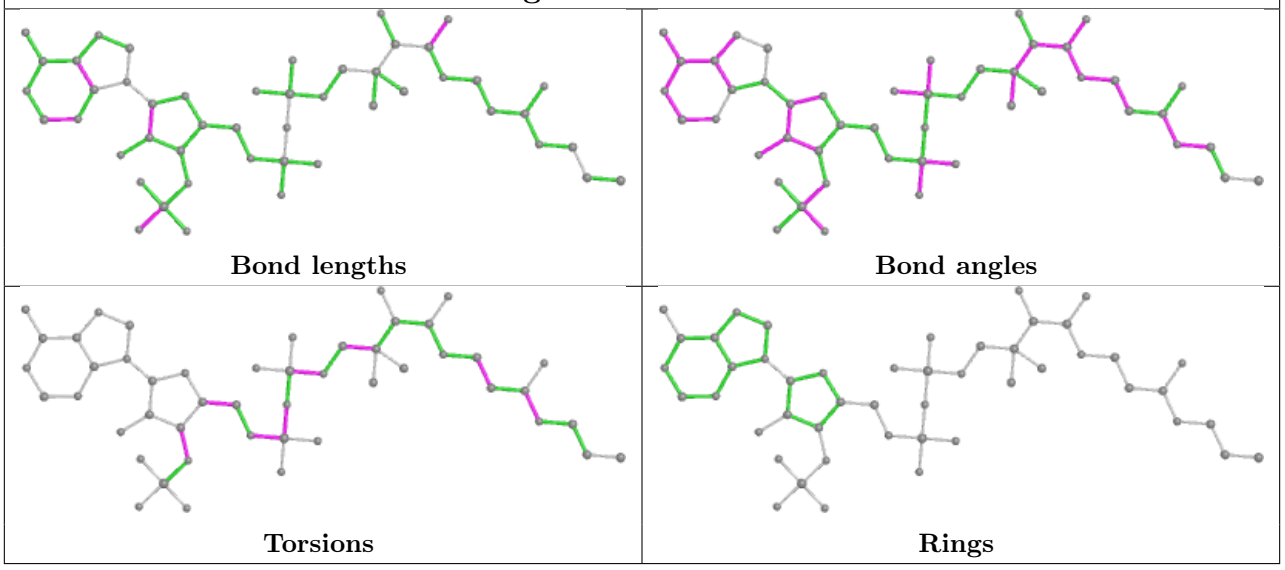


Rings

Ligand FAD B 501



Ligand COA B 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.31	10 (2%)	60	58	48, 66, 92, 140	0
1	B	443/443 (100%)	0.33	14 (3%)	47	43	46, 68, 94, 139	0
1	C	443/443 (100%)	0.15	13 (2%)	51	47	46, 67, 92, 141	0
1	D	443/443 (100%)	0.13	7 (1%)	72	71	46, 68, 93, 140	0
All	All	1772/1772 (100%)	0.23	44 (2%)	57	55	46, 67, 93, 141	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	11.0
1	A	1	MET	10.6
1	C	1	MET	10.0
1	D	1	MET	8.7
1	C	2	GLY	7.7
1	A	443	ARG	6.0
1	D	443	ARG	5.7
1	D	2	GLY	5.6
1	B	443	ARG	5.2
1	B	2	GLY	5.1
1	A	88	LEU	4.9
1	A	91	LEU	4.8
1	A	2	GLY	4.6
1	C	88	LEU	4.1
1	C	443	ARG	3.8
1	B	88	LEU	3.8
1	D	88	LEU	3.7
1	D	86	TYR	3.7
1	C	86	TYR	3.5
1	B	87	GLU	3.5
1	B	86	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	442	ALA	3.4
1	A	84	VAL	3.3
1	A	86	TYR	3.0
1	B	102	PHE	2.9
1	B	216	PHE	2.7
1	C	352	TRP	2.6
1	D	87	GLU	2.5
1	B	100	ARG	2.5
1	D	352	TRP	2.4
1	B	128	GLU	2.4
1	C	94	HIS	2.3
1	B	70	LYS	2.2
1	C	383	THR	2.2
1	A	87	GLU	2.2
1	C	149	ALA	2.2
1	B	219	MET	2.1
1	C	91	LEU	2.1
1	B	208	TRP	2.1
1	C	233	PRO	2.1
1	C	317	GLU	2.1
1	B	122	ILE	2.1
1	A	92	THR	2.0
1	C	208	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.

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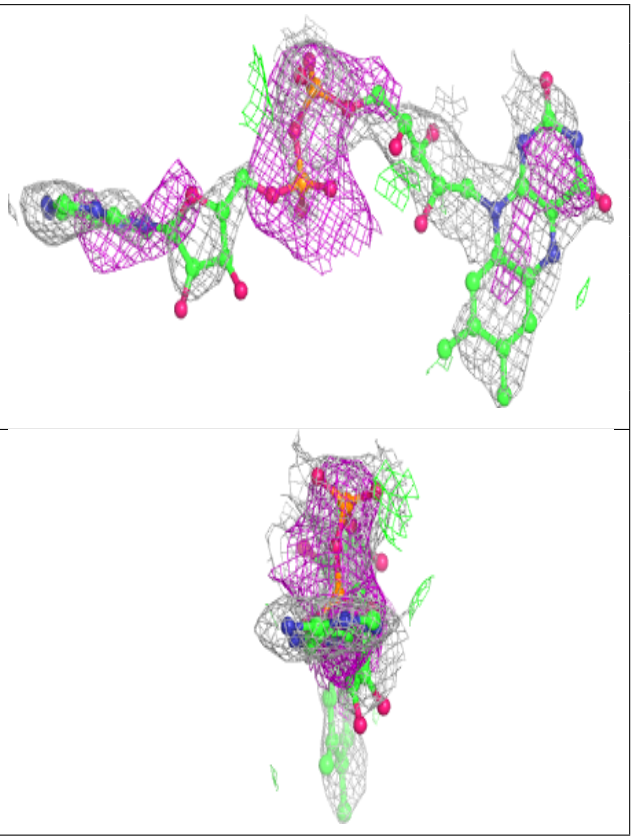
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

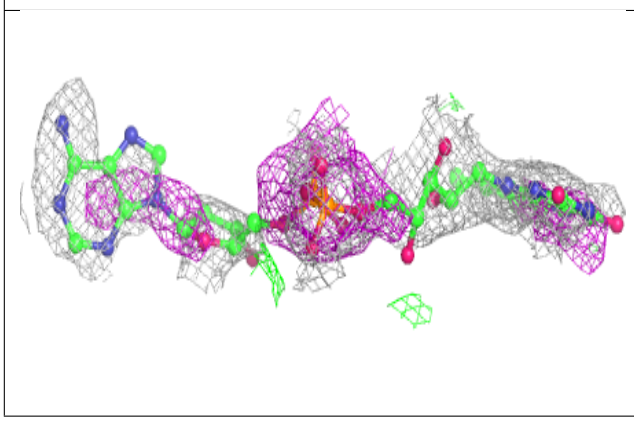
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	B	501	53/53	0.80	0.52	65,104,124,161	0
2	FAD	A	501	53/53	0.84	0.47	71,103,120,158	0
2	FAD	D	501	53/53	0.86	0.40	71,103,126,159	0
2	FAD	C	501	53/53	0.87	0.34	71,104,124,153	0
3	COA	A	502	48/48	0.96	0.17	53,70,80,106	0
3	COA	C	502	48/48	0.96	0.16	56,69,82,121	0
3	COA	D	502	48/48	0.97	0.15	57,69,84,119	0
3	COA	B	502	48/48	0.98	0.17	57,68,79,115	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 501:

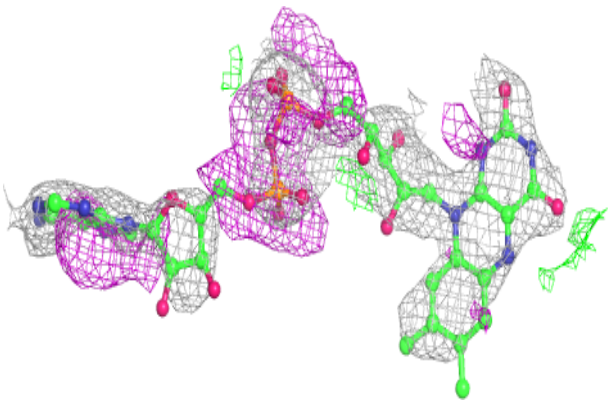
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

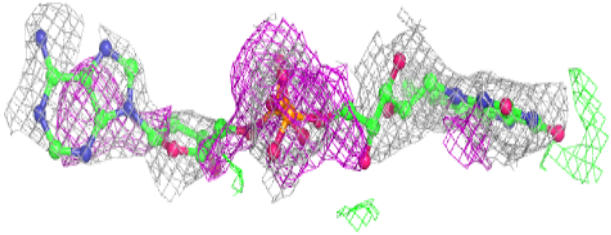


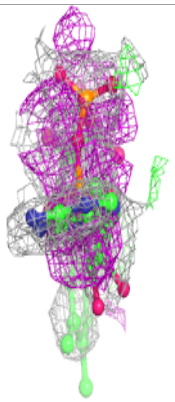


Electron density around FAD A 501:

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

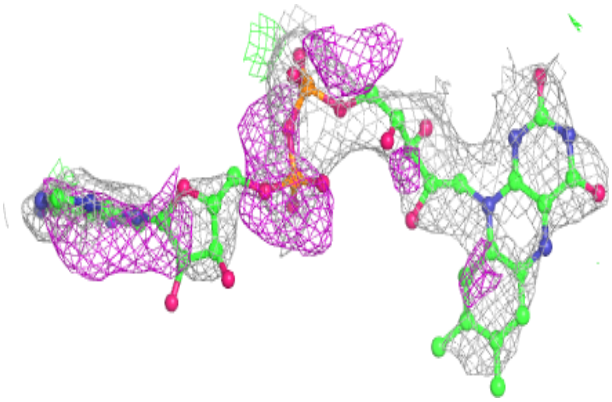


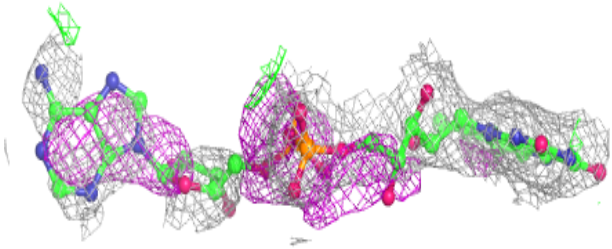


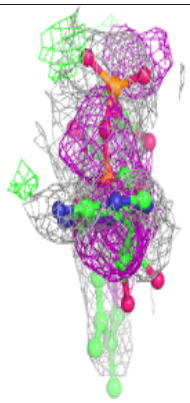


Electron density around FAD D 501:

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

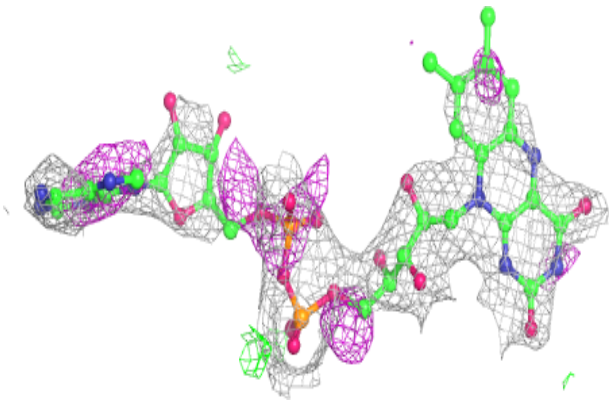


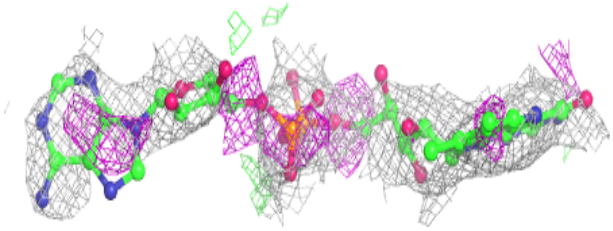


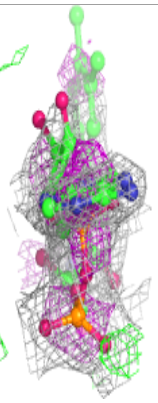


Electron density around FAD C 501:

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

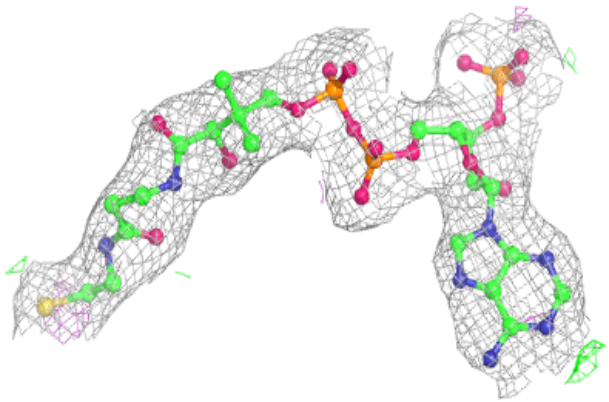


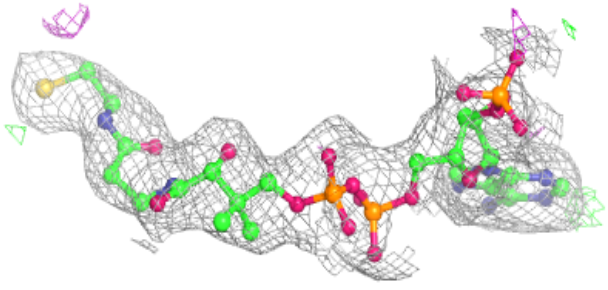


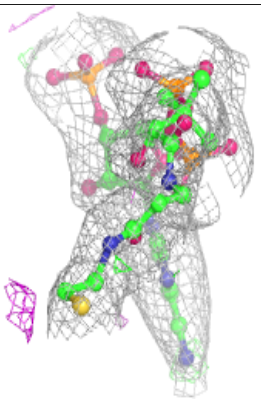


Electron density around COA A 502:

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

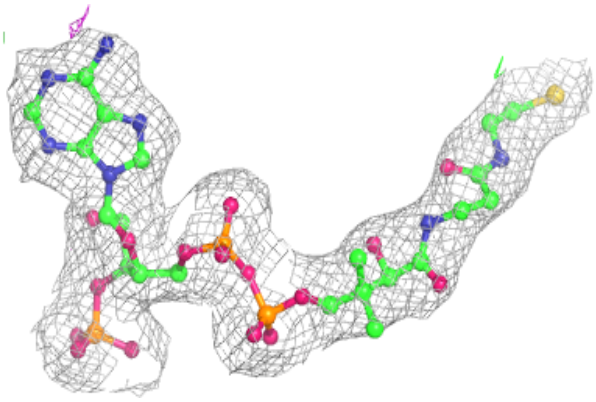


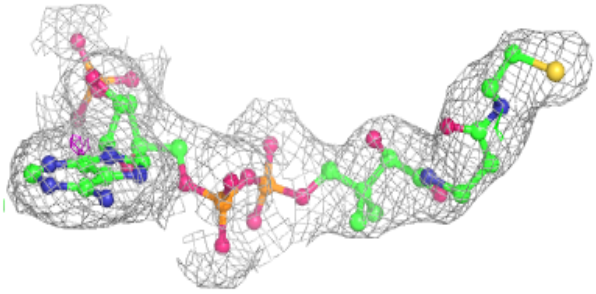


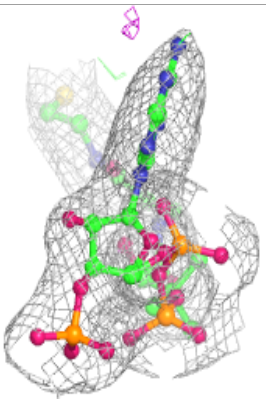


Electron density around COA C 502:

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

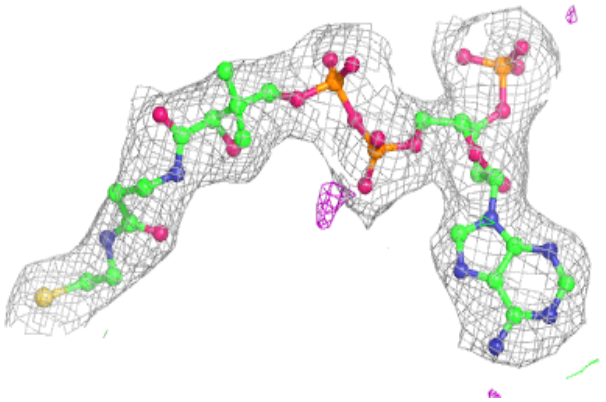


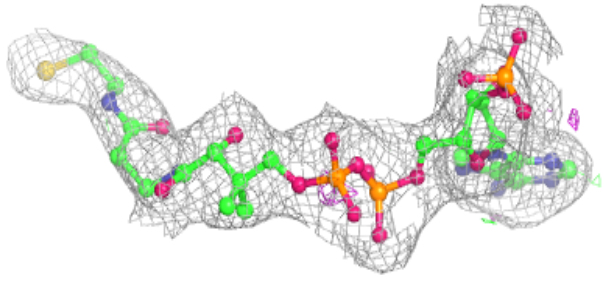


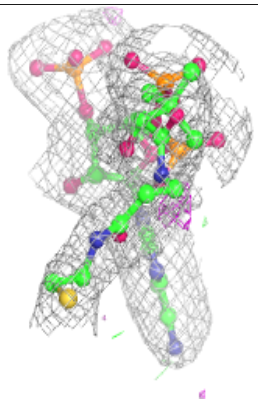


Electron density around COA D 502:

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

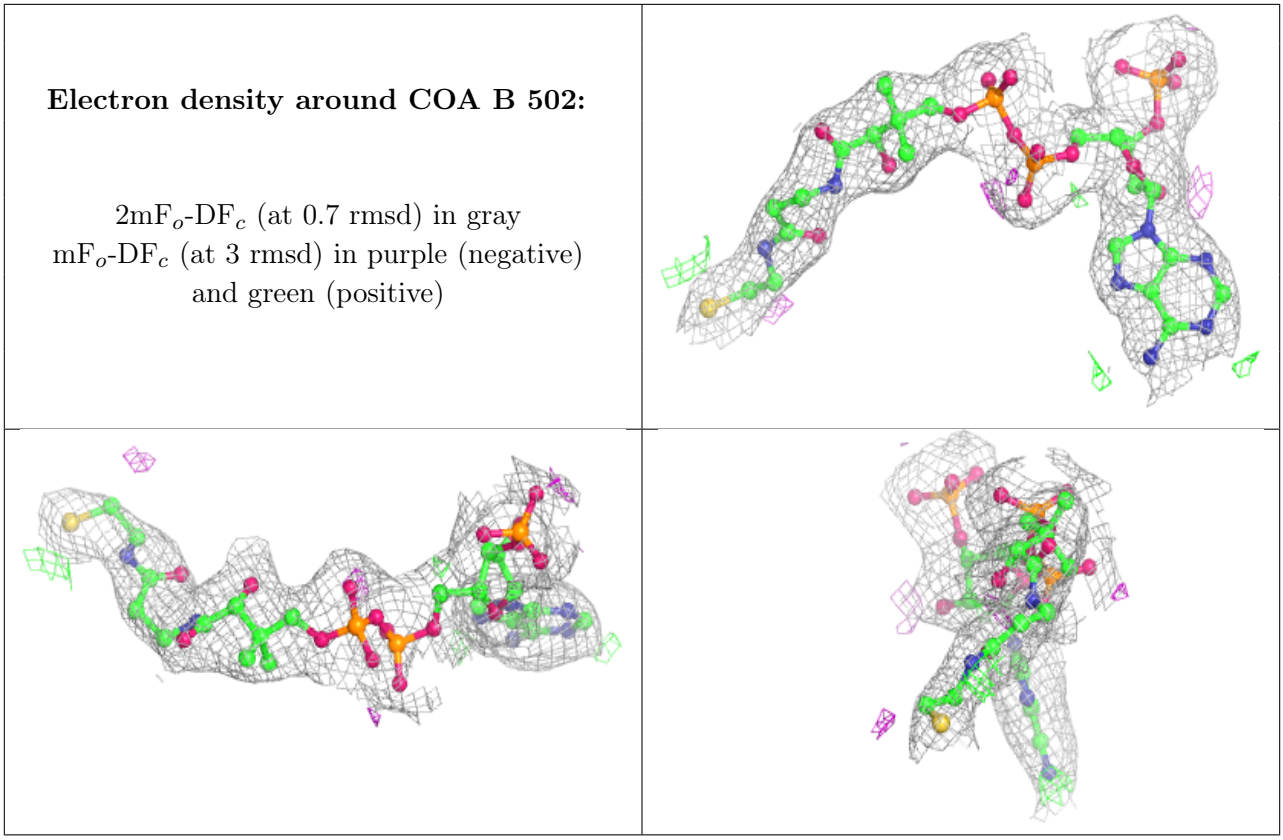






Electron density around COA B 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.