



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 12:09 PM EST

PDB ID : 2LDB
Title : STRUCTURE DETERMINATION AND REFINEMENT OF BACILLUS
STEAROTHERMOPHILUS LACTATE DEHYDROGENASE
Authors : Piontek, K.; Rossmann, M.G.
Deposited on : 1989-03-27
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

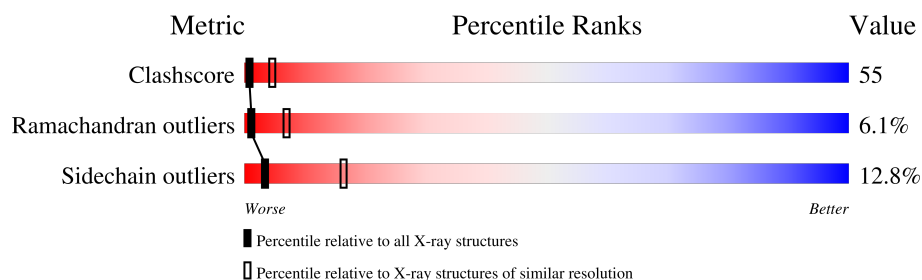
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	317	26% 44% 19% 5% 5%
1	B	317	26% 44% 20% 5% 5%
1	C	317	27% 43% 20% 5% 5%
1	D	317	26% 44% 20% 5% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	3	-	-	X	-
2	SO4	B	7	-	-	X	-
2	SO4	C	11	-	-	X	-
2	SO4	D	332	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9650 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 L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2336	1496	401	431	8			
1	B	301	Total	C	N	O	S	0	0	0
			2336	1496	401	431	8			
1	C	301	Total	C	N	O	S	0	0	0
			2336	1496	401	431	8			
1	D	301	Total	C	N	O	S	0	0	0
			2336	1496	401	431	8			

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



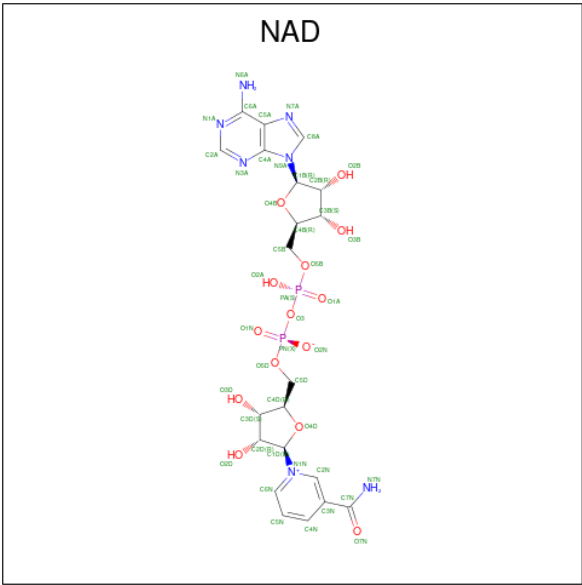
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

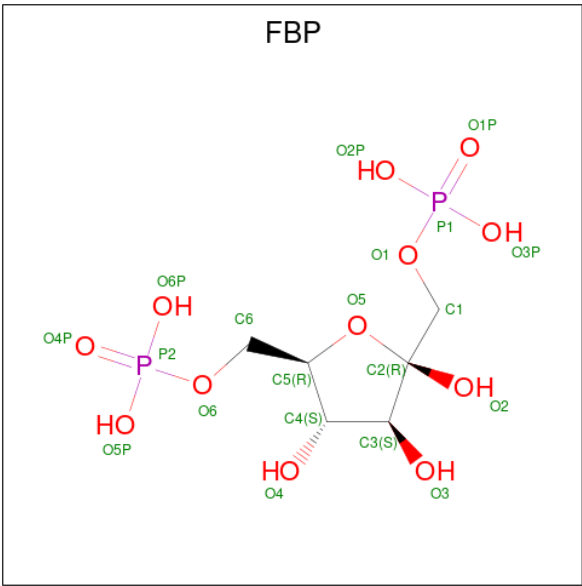
- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula:

C₆H₁₄O₁₂P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is water.

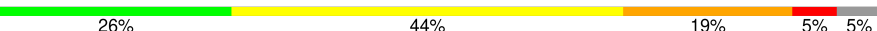
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O	0	0
			47	47		
5	C	3	Total	O	0	0
			3	3		

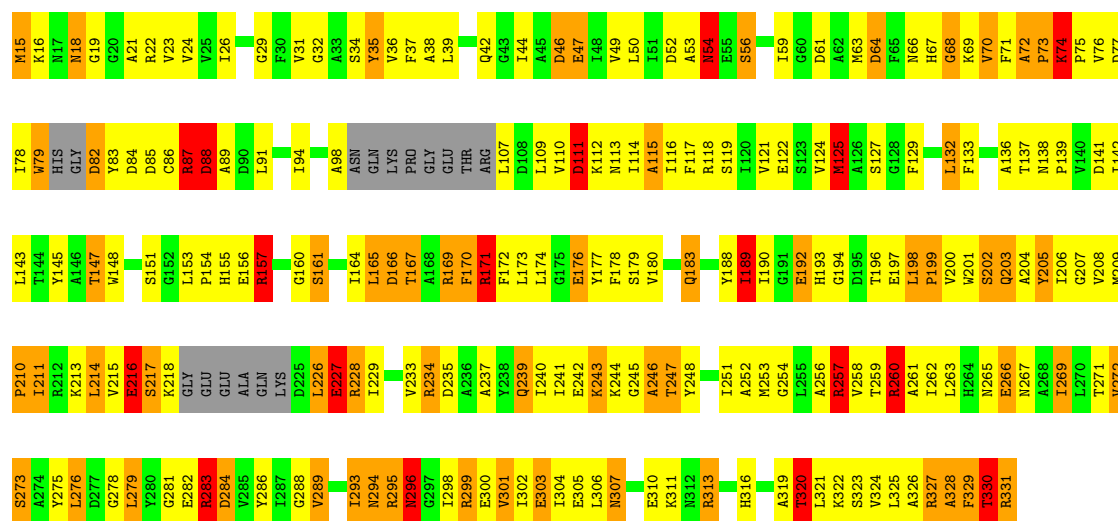
3 Residue-property plots

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

Note EDS was not executed.

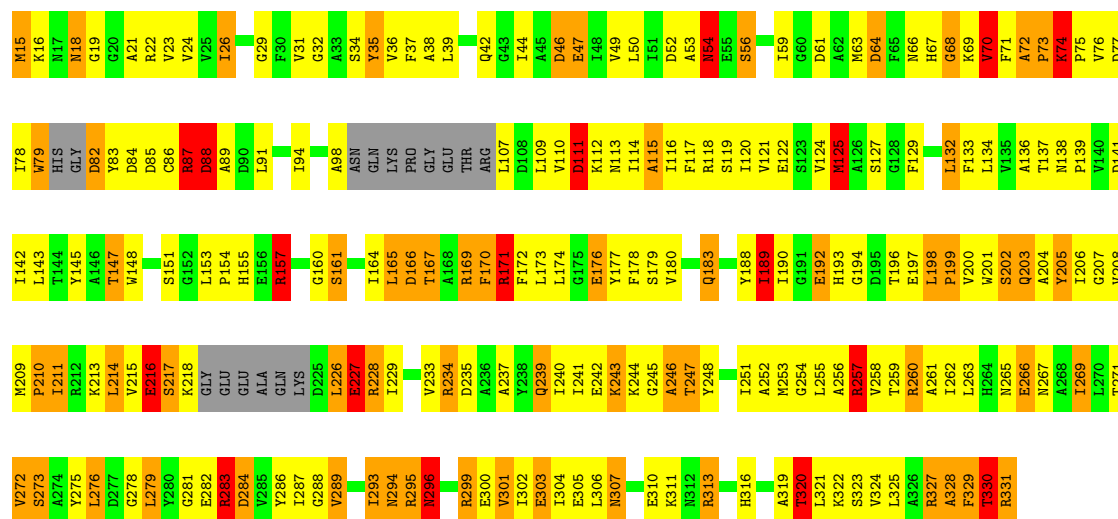
• Molecule 1: L-LACTATE DEHYDROGENASE

Chain A: 

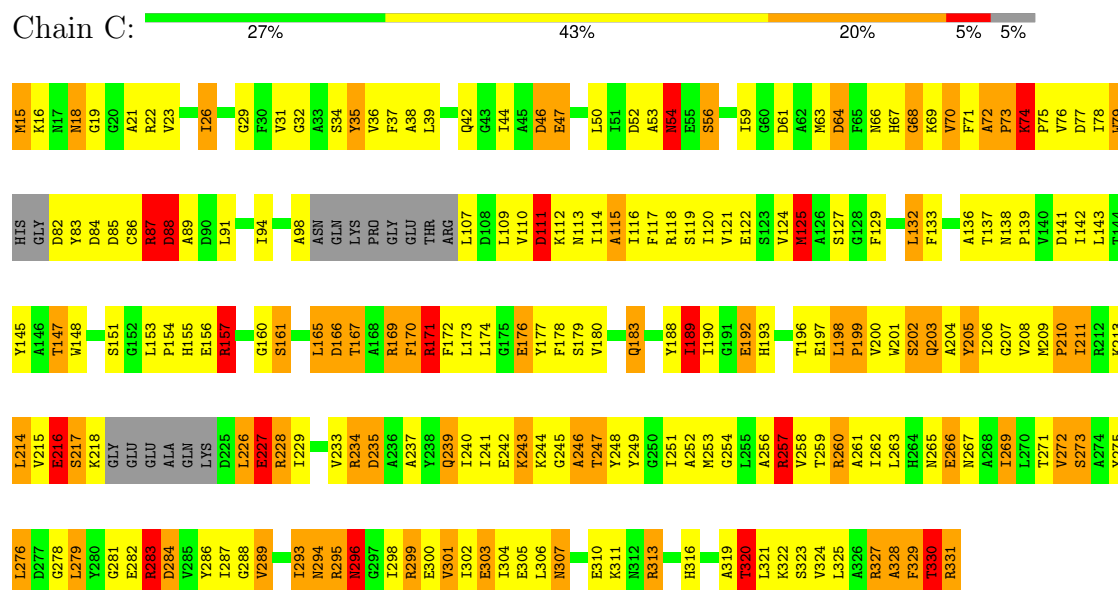


• Molecule 1: L-LACTATE DEHYDROGENASE

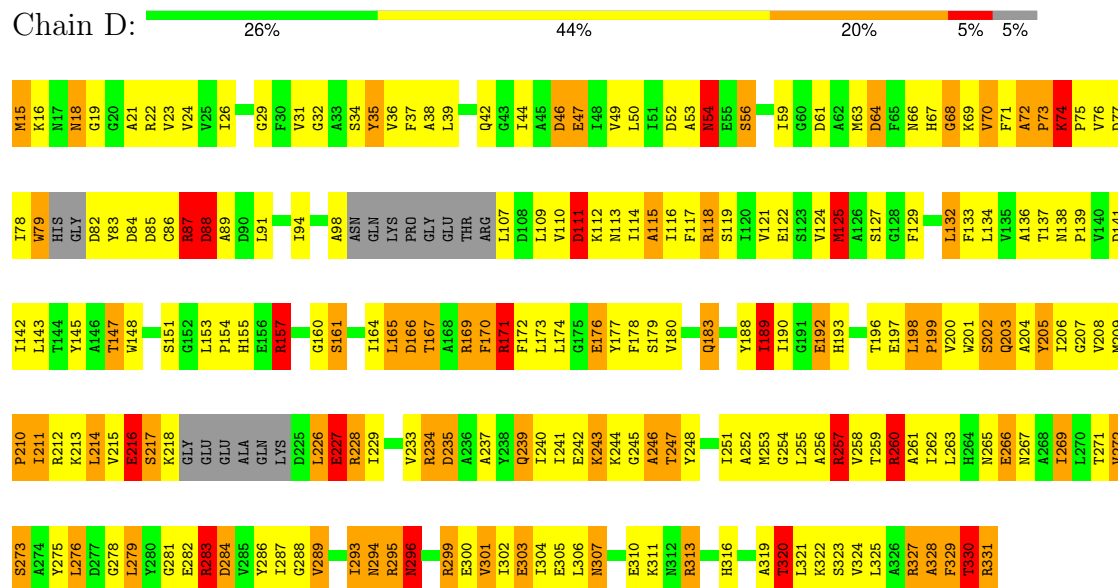
Chain B: 



• Molecule 1: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	86.80 Å 86.80 Å 356.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.260 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9650	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, NAD, SO4

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	1.10	0/2379	2.19	109/3223 (3.4%)
1	B	1.10	1/2379 (0.0%)	2.19	109/3223 (3.4%)
1	C	1.10	0/2379	2.20	111/3223 (3.4%)
1	D	1.10	0/2379	2.19	112/3223 (3.5%)
All	All	1.10	1/9516 (0.0%)	2.19	441/12892 (3.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
1	C	0	9
1	D	0	9
All	All	0	36

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	SER	CB-OG	-5.00	1.35	1.42

All (441) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH1	22.69	131.65	120.30
1	C	118	ARG	NE-CZ-NH1	22.56	131.58	120.30
1	B	118	ARG	NE-CZ-NH1	22.54	131.57	120.30
1	A	118	ARG	NE-CZ-NH1	22.53	131.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	ARG	NE-CZ-NH1	-16.60	112.00	120.30
1	A	260	ARG	NE-CZ-NH1	-16.51	112.05	120.30
1	D	260	ARG	NE-CZ-NH1	-16.49	112.06	120.30
1	B	260	ARG	NE-CZ-NH1	-16.45	112.07	120.30
1	D	211	ILE	C-N-CA	14.57	158.12	121.70
1	B	211	ILE	C-N-CA	14.55	158.08	121.70
1	C	211	ILE	C-N-CA	14.54	158.05	121.70
1	A	211	ILE	C-N-CA	14.54	158.04	121.70
1	B	283	ARG	NE-CZ-NH1	14.48	127.54	120.30
1	A	283	ARG	NE-CZ-NH1	14.39	127.50	120.30
1	D	283	ARG	NE-CZ-NH1	14.36	127.48	120.30
1	C	283	ARG	NE-CZ-NH1	14.34	127.47	120.30
1	A	22	ARG	NE-CZ-NH2	-14.18	113.21	120.30
1	B	22	ARG	NE-CZ-NH2	-14.08	113.26	120.30
1	D	22	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	C	22	ARG	NE-CZ-NH2	-13.98	113.31	120.30
1	B	279	LEU	CA-CB-CG	12.51	144.07	115.30
1	D	279	LEU	CA-CB-CG	12.50	144.06	115.30
1	A	279	LEU	CA-CB-CG	12.50	144.04	115.30
1	C	279	LEU	CA-CB-CG	12.49	144.04	115.30
1	D	77	ASP	CB-CG-OD2	-12.19	107.33	118.30
1	C	77	ASP	CB-CG-OD2	-12.19	107.33	118.30
1	A	77	ASP	CB-CG-OD2	-12.17	107.35	118.30
1	B	77	ASP	CB-CG-OD2	-12.15	107.36	118.30
1	B	260	ARG	CD-NE-CZ	-9.80	109.88	123.60
1	A	260	ARG	CD-NE-CZ	-9.77	109.93	123.60
1	D	260	ARG	CD-NE-CZ	-9.75	109.95	123.60
1	C	260	ARG	CD-NE-CZ	-9.75	109.95	123.60
1	A	111	ASP	CA-CB-CG	9.64	134.61	113.40
1	B	111	ASP	CA-CB-CG	9.64	134.61	113.40
1	C	111	ASP	CA-CB-CG	9.63	134.58	113.40
1	D	111	ASP	CA-CB-CG	9.61	134.55	113.40
1	A	283	ARG	NE-CZ-NH2	-9.51	115.54	120.30
1	B	283	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	B	257	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	D	283	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	A	257	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	C	283	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	C	257	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	D	257	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	D	211	ILE	O-C-N	-8.97	108.35	122.70
1	C	211	ILE	O-C-N	-8.96	108.36	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	118	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	A	211	ILE	O-C-N	-8.95	108.38	122.70
1	B	211	ILE	O-C-N	-8.95	108.38	122.70
1	B	118	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	118	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	171	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	D	257	ARG	CD-NE-CZ	8.93	136.10	123.60
1	A	257	ARG	CD-NE-CZ	8.90	136.06	123.60
1	B	257	ARG	CD-NE-CZ	8.89	136.05	123.60
1	C	257	ARG	CD-NE-CZ	8.89	136.04	123.60
1	A	171	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	D	171	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	C	171	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	A	299	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	C	299	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	D	299	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	D	46	ASP	CB-CG-OD1	8.65	126.08	118.30
1	C	46	ASP	CB-CG-OD1	8.61	126.05	118.30
1	B	46	ASP	CB-CG-OD1	8.60	126.04	118.30
1	A	46	ASP	CB-CG-OD1	8.56	126.00	118.30
1	B	299	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	211	ILE	CA-C-O	8.49	137.93	120.10
1	D	211	ILE	CA-C-O	8.48	137.91	120.10
1	C	211	ILE	CA-C-O	8.48	137.90	120.10
1	B	211	ILE	CA-C-O	8.47	137.90	120.10
1	B	22	ARG	CD-NE-CZ	-8.40	111.85	123.60
1	A	22	ARG	CD-NE-CZ	-8.39	111.86	123.60
1	D	22	ARG	CD-NE-CZ	-8.38	111.87	123.60
1	C	22	ARG	CD-NE-CZ	-8.36	111.89	123.60
1	D	176	GLU	OE1-CD-OE2	7.94	132.83	123.30
1	A	176	GLU	OE1-CD-OE2	7.93	132.81	123.30
1	B	176	GLU	OE1-CD-OE2	7.93	132.81	123.30
1	C	176	GLU	OE1-CD-OE2	7.90	132.78	123.30
1	B	157	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	A	157	ARG	NE-CZ-NH1	-7.77	116.41	120.30
1	D	157	ARG	NE-CZ-NH1	-7.73	116.43	120.30
1	C	157	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	B	46	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	C	46	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	D	46	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	46	ASP	CB-CG-OD2	-7.38	111.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ARG	CD-NE-CZ	-7.28	113.41	123.60
1	D	171	ARG	CD-NE-CZ	-7.23	113.47	123.60
1	A	228	ARG	CD-NE-CZ	-7.23	113.48	123.60
1	C	295	ARG	NE-CZ-NH1	-7.23	116.69	120.30
1	A	171	ARG	CD-NE-CZ	-7.22	113.49	123.60
1	D	228	ARG	CD-NE-CZ	-7.22	113.49	123.60
1	B	228	ARG	CD-NE-CZ	-7.21	113.50	123.60
1	C	228	ARG	CD-NE-CZ	-7.21	113.51	123.60
1	B	171	ARG	CD-NE-CZ	-7.21	113.51	123.60
1	B	295	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	D	295	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	295	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	283	ARG	NH1-CZ-NH2	-6.96	111.74	119.40
1	C	283	ARG	NH1-CZ-NH2	-6.96	111.75	119.40
1	D	283	ARG	NH1-CZ-NH2	-6.96	111.75	119.40
1	B	52	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	283	ARG	NH1-CZ-NH2	-6.93	111.77	119.40
1	C	52	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	52	ASP	CB-CG-OD1	6.86	124.48	118.30
1	A	64	ASP	CB-CG-OD1	-6.85	112.13	118.30
1	D	52	ASP	CB-CG-OD1	6.85	124.47	118.30
1	D	64	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	B	239	GLN	CA-CB-CG	6.79	128.34	113.40
1	C	64	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	A	76	VAL	CB-CA-C	6.79	124.30	111.40
1	B	286	TYR	O-C-N	6.78	133.55	122.70
1	D	286	TYR	O-C-N	6.78	133.54	122.70
1	C	76	VAL	CB-CA-C	6.77	124.27	111.40
1	D	239	GLN	CA-CB-CG	6.77	128.30	113.40
1	B	76	VAL	CB-CA-C	6.77	124.26	111.40
1	C	286	TYR	O-C-N	6.77	133.53	122.70
1	B	64	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	C	239	GLN	CA-CB-CG	6.75	128.26	113.40
1	A	239	GLN	CA-CB-CG	6.75	128.25	113.40
1	D	76	VAL	CB-CA-C	6.74	124.21	111.40
1	A	22	ARG	NH1-CZ-NH2	6.74	126.81	119.40
1	A	286	TYR	O-C-N	6.74	133.48	122.70
1	C	70	VAL	CG1-CB-CG2	6.71	121.63	110.90
1	B	70	VAL	CG1-CB-CG2	6.68	121.58	110.90
1	A	70	VAL	CG1-CB-CG2	6.67	121.58	110.90
1	B	22	ARG	NH1-CZ-NH2	6.67	126.73	119.40
1	B	52	ASP	CB-CG-OD2	-6.66	112.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	VAL	CG1-CB-CG2	6.66	121.56	110.90
1	C	286	TYR	CA-C-O	-6.64	106.15	120.10
1	A	118	ARG	CD-NE-CZ	6.63	132.89	123.60
1	C	52	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	B	286	TYR	CA-C-O	-6.63	106.18	120.10
1	D	286	TYR	CA-C-O	-6.63	106.18	120.10
1	C	118	ARG	CD-NE-CZ	6.63	132.88	123.60
1	D	22	ARG	NH1-CZ-NH2	6.62	126.69	119.40
1	B	118	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	286	TYR	CA-C-O	-6.61	106.22	120.10
1	C	22	ARG	NH1-CZ-NH2	6.60	126.66	119.40
1	D	266	GLU	CA-CB-CG	6.60	127.93	113.40
1	B	266	GLU	CA-CB-CG	6.60	127.92	113.40
1	C	111	ASP	N-CA-CB	6.60	122.47	110.60
1	C	266	GLU	CA-CB-CG	6.60	127.91	113.40
1	D	118	ARG	CD-NE-CZ	6.59	132.83	123.60
1	D	52	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	D	111	ASP	N-CA-CB	6.59	122.47	110.60
1	A	266	GLU	CA-CB-CG	6.59	127.89	113.40
1	B	111	ASP	N-CA-CB	6.59	122.46	110.60
1	A	111	ASP	N-CA-CB	6.58	122.45	110.60
1	A	52	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	C	307	ASN	N-CA-CB	-6.57	98.77	110.60
1	C	166	ASP	CB-CG-OD1	6.57	124.21	118.30
1	D	307	ASN	N-CA-CB	-6.57	98.78	110.60
1	A	170	PHE	O-C-N	6.56	133.19	122.70
1	B	307	ASN	N-CA-CB	-6.55	98.81	110.60
1	A	307	ASN	N-CA-CB	-6.55	98.82	110.60
1	C	170	PHE	O-C-N	6.54	133.16	122.70
1	B	170	PHE	O-C-N	6.53	133.15	122.70
1	D	170	PHE	O-C-N	6.53	133.15	122.70
1	A	166	ASP	CB-CG-OD1	6.52	124.17	118.30
1	D	166	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	166	ASP	CB-CG-OD1	6.48	124.13	118.30
1	D	272	VAL	C-N-CA	6.41	137.73	121.70
1	C	272	VAL	C-N-CA	6.41	137.72	121.70
1	D	203	GLN	CB-CG-CD	6.41	128.26	111.60
1	C	203	GLN	CB-CG-CD	6.41	128.26	111.60
1	A	276	LEU	CA-C-O	6.40	133.54	120.10
1	A	272	VAL	C-N-CA	6.40	137.69	121.70
1	B	203	GLN	CB-CG-CD	6.39	128.22	111.60
1	B	276	LEU	CA-C-O	6.39	133.52	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	276	LEU	CA-C-O	6.39	133.52	120.10
1	C	276	LEU	CA-C-O	6.39	133.52	120.10
1	A	188	TYR	CB-CG-CD1	6.39	124.83	121.00
1	B	272	VAL	C-N-CA	6.39	137.67	121.70
1	A	203	GLN	CB-CG-CD	6.38	128.19	111.60
1	C	256	ALA	CB-CA-C	6.38	119.67	110.10
1	A	279	LEU	CB-CA-C	6.38	122.32	110.20
1	B	279	LEU	CB-CA-C	6.37	122.31	110.20
1	C	188	TYR	CB-CG-CD1	6.37	124.82	121.00
1	B	256	ALA	CB-CA-C	6.37	119.65	110.10
1	D	256	ALA	CB-CA-C	6.37	119.65	110.10
1	A	256	ALA	CB-CA-C	6.36	119.65	110.10
1	C	279	LEU	CB-CA-C	6.35	122.27	110.20
1	B	188	TYR	CB-CG-CD1	6.35	124.81	121.00
1	D	279	LEU	CB-CA-C	6.35	122.26	110.20
1	D	188	TYR	CB-CG-CD1	6.33	124.80	121.00
1	C	169	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	D	169	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	D	118	ARG	NH1-CZ-NH2	-6.28	112.49	119.40
1	B	88	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	B	169	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	C	118	ARG	NH1-CZ-NH2	-6.23	112.55	119.40
1	A	169	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	B	118	ARG	NH1-CZ-NH2	-6.22	112.56	119.40
1	A	118	ARG	NH1-CZ-NH2	-6.21	112.56	119.40
1	C	300	GLU	CA-CB-CG	6.21	127.05	113.40
1	D	300	GLU	CA-CB-CG	6.19	127.03	113.40
1	C	88	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	300	GLU	CA-CB-CG	6.19	127.01	113.40
1	A	300	GLU	CA-CB-CG	6.18	127.00	113.40
1	D	88	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	88	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	141	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	C	227	GLU	CG-CD-OE1	6.15	130.60	118.30
1	C	141	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	171	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	122	GLU	CA-CB-CG	6.13	126.89	113.40
1	B	227	GLU	CG-CD-OE1	6.13	130.56	118.30
1	D	171	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	227	GLU	CG-CD-OE1	6.12	130.55	118.30
1	D	122	GLU	CA-CB-CG	6.12	126.87	113.40
1	D	227	GLU	CG-CD-OE1	6.12	130.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	GLU	CA-CB-CG	6.12	126.86	113.40
1	A	50	LEU	C-N-CA	6.11	136.98	121.70
1	B	50	LEU	C-N-CA	6.11	136.98	121.70
1	C	122	GLU	CA-CB-CG	6.11	126.85	113.40
1	D	141	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	141	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	50	LEU	C-N-CA	6.09	136.93	121.70
1	A	171	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	50	LEU	C-N-CA	6.07	136.88	121.70
1	B	207	GLY	N-CA-C	-6.01	98.07	113.10
1	B	171	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	207	GLY	N-CA-C	-6.01	98.08	113.10
1	C	207	GLY	N-CA-C	-6.00	98.11	113.10
1	D	207	GLY	N-CA-C	-5.98	98.15	113.10
1	D	276	LEU	C-N-CA	5.98	136.64	121.70
1	A	192	GLU	O-C-N	5.98	132.26	122.70
1	B	192	GLU	O-C-N	5.98	132.26	122.70
1	C	192	GLU	O-C-N	5.97	132.25	122.70
1	B	276	LEU	C-N-CA	5.96	136.61	121.70
1	C	234	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	276	LEU	C-N-CA	5.95	136.58	121.70
1	C	276	LEU	C-N-CA	5.95	136.57	121.70
1	D	188	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	D	192	GLU	O-C-N	5.95	132.21	122.70
1	C	188	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	C	276	LEU	CA-C-N	-5.92	104.17	117.20
1	D	266	GLU	OE1-CD-OE2	-5.92	116.20	123.30
1	A	276	LEU	CA-C-N	-5.91	104.19	117.20
1	A	141	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	188	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	C	141	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	266	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	B	276	LEU	CA-C-N	-5.91	104.21	117.20
1	C	266	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	D	276	LEU	CA-C-N	-5.89	104.23	117.20
1	B	266	GLU	OE1-CD-OE2	-5.88	116.24	123.30
1	C	74	LYS	N-CA-C	5.88	126.89	111.00
1	B	125	MET	CG-SD-CE	5.88	109.61	100.20
1	A	125	MET	CG-SD-CE	5.88	109.61	100.20
1	B	141	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	74	LYS	N-CA-C	5.87	126.85	111.00
1	A	74	LYS	N-CA-C	5.87	126.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	125	MET	CG-SD-CE	5.86	109.57	100.20
1	D	141	ASP	CB-CG-OD1	5.86	123.57	118.30
1	D	84	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	B	74	LYS	N-CA-C	5.85	126.80	111.00
1	D	125	MET	CG-SD-CE	5.85	109.56	100.20
1	A	166	ASP	C-N-CA	5.84	136.31	121.70
1	C	115	ALA	N-CA-CB	-5.84	101.92	110.10
1	C	166	ASP	C-N-CA	5.84	136.30	121.70
1	D	331	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	331	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	188	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	B	115	ALA	N-CA-CB	-5.83	101.94	110.10
1	B	166	ASP	C-N-CA	5.82	136.26	121.70
1	D	234	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	D	166	ASP	C-N-CA	5.82	136.25	121.70
1	A	74	LYS	CB-CG-CD	5.82	126.72	111.60
1	A	115	ALA	N-CA-CB	-5.82	101.96	110.10
1	B	74	LYS	CB-CG-CD	5.82	126.72	111.60
1	B	301	VAL	CA-CB-CG1	5.81	119.62	110.90
1	D	74	LYS	CB-CG-CD	5.81	126.72	111.60
1	D	115	ALA	N-CA-CB	-5.81	101.97	110.10
1	A	301	VAL	CA-CB-CG1	5.81	119.61	110.90
1	B	234	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	84	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	303	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	C	74	LYS	CB-CG-CD	5.80	126.67	111.60
1	D	303	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	C	84	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	82	ASP	CA-C-N	-5.78	104.49	117.20
1	B	82	ASP	CA-C-N	-5.77	104.50	117.20
1	C	300	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	B	331	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	84	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	313	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	C	82	ASP	CA-C-N	-5.75	104.54	117.20
1	A	132	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	301	VAL	CA-CB-CG1	5.75	119.53	110.90
1	D	300	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	D	132	LEU	CA-CB-CG	5.75	128.53	115.30
1	A	303	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	B	303	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	D	301	VAL	CA-CB-CG1	5.75	119.52	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	B	300	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	D	82	ASP	CA-C-N	-5.74	104.57	117.20
1	C	132	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	300	GLU	OE1-CD-OE2	-5.73	116.43	123.30
1	B	132	LEU	CA-CB-CG	5.73	128.47	115.30
1	A	234	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	331	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	313	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	B	313	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	47	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	D	111	ASP	CB-CG-OD1	5.64	123.37	118.30
1	B	111	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	111	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	47	GLU	OE1-CD-OE2	5.62	130.04	123.30
1	B	47	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	A	72	ALA	CB-CA-C	5.60	118.50	110.10
1	C	111	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	72	ALA	CB-CA-C	5.59	118.49	110.10
1	C	167	THR	CA-CB-CG2	5.58	120.22	112.40
1	C	72	ALA	CB-CA-C	5.56	118.44	110.10
1	C	47	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	D	72	ALA	CB-CA-C	5.56	118.44	110.10
1	D	235	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	A	167	THR	CA-CB-CG2	5.54	120.16	112.40
1	D	167	THR	CA-CB-CG2	5.54	120.16	112.40
1	B	167	THR	CA-CB-CG2	5.54	120.15	112.40
1	C	235	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	A	235	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	D	74	LYS	CA-CB-CG	5.52	125.55	113.40
1	B	74	LYS	CA-CB-CG	5.52	125.54	113.40
1	A	74	LYS	CA-CB-CG	5.51	125.52	113.40
1	B	235	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	C	74	LYS	CA-CB-CG	5.51	125.51	113.40
1	C	283	ARG	CD-NE-CZ	5.47	131.26	123.60
1	D	283	ARG	CD-NE-CZ	5.47	131.26	123.60
1	B	283	ARG	CD-NE-CZ	5.45	131.23	123.60
1	D	295	ARG	CD-NE-CZ	-5.44	115.98	123.60
1	A	283	ARG	CD-NE-CZ	5.44	131.21	123.60
1	C	23	VAL	CA-CB-CG2	5.43	119.04	110.90
1	C	295	ARG	CD-NE-CZ	-5.43	116.00	123.60
1	B	23	VAL	CA-CB-CG2	5.42	119.04	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	LYS	CB-CA-C	-5.42	99.56	110.40
1	A	74	LYS	CB-CA-C	-5.41	99.58	110.40
1	D	74	LYS	CB-CA-C	-5.41	99.58	110.40
1	D	23	VAL	CA-CB-CG2	5.41	119.02	110.90
1	D	216	GLU	CG-CD-OE2	-5.41	107.49	118.30
1	A	295	ARG	CD-NE-CZ	-5.40	116.03	123.60
1	B	216	GLU	CG-CD-OE2	-5.39	107.51	118.30
1	A	269	ILE	O-C-N	5.39	131.32	122.70
1	B	295	ARG	CD-NE-CZ	-5.39	116.06	123.60
1	A	23	VAL	CA-CB-CG2	5.39	118.98	110.90
1	B	74	LYS	CB-CA-C	-5.39	99.63	110.40
1	B	269	ILE	O-C-N	5.38	131.32	122.70
1	D	269	ILE	O-C-N	5.38	131.31	122.70
1	A	216	GLU	CG-CD-OE2	-5.38	107.55	118.30
1	C	216	GLU	CG-CD-OE2	-5.37	107.56	118.30
1	C	269	ILE	O-C-N	5.37	131.29	122.70
1	D	122	GLU	CB-CG-CD	5.37	128.69	114.20
1	A	257	ARG	CG-CD-NE	5.36	123.06	111.80
1	B	257	ARG	CG-CD-NE	5.36	123.06	111.80
1	B	122	GLU	CB-CG-CD	5.36	128.67	114.20
1	C	257	ARG	CG-CD-NE	5.35	123.04	111.80
1	C	122	GLU	CB-CG-CD	5.35	128.64	114.20
1	A	122	GLU	CB-CG-CD	5.35	128.63	114.20
1	D	257	ARG	CG-CD-NE	5.34	123.02	111.80
1	C	35	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	A	327	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	296	ASN	CA-CB-CG	5.31	125.08	113.40
1	B	296	ASN	CA-CB-CG	5.31	125.07	113.40
1	A	296	ASN	CA-CB-CG	5.30	125.06	113.40
1	D	327	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	313	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	C	327	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	296	ASN	CA-CB-CG	5.28	125.01	113.40
1	D	35	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	D	313	ARG	CD-NE-CZ	-5.25	116.24	123.60
1	B	313	ARG	CD-NE-CZ	-5.24	116.26	123.60
1	B	327	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	82	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	35	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	A	313	ARG	CD-NE-CZ	-5.19	116.33	123.60
1	D	82	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	82	ASP	CB-CG-OD2	-5.18	113.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	D	189	ILE	CA-CB-CG2	5.15	121.20	110.90
1	D	161	SER	CB-CA-C	5.14	119.86	110.10
1	C	161	SER	CB-CA-C	5.13	119.86	110.10
1	C	189	ILE	CA-CB-CG2	5.13	121.17	110.90
1	D	54	ASN	O-C-N	5.13	130.91	122.70
1	D	211	ILE	CB-CA-C	5.13	121.86	111.60
1	A	35	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	C	211	ILE	CB-CA-C	5.12	121.85	111.60
1	C	300	GLU	CB-CG-CD	5.12	128.03	114.20
1	D	300	GLU	CB-CG-CD	5.12	128.04	114.20
1	A	161	SER	CB-CA-C	5.12	119.83	110.10
1	A	300	GLU	CB-CG-CD	5.12	128.02	114.20
1	A	211	ILE	CB-CA-C	5.12	121.83	111.60
1	B	300	GLU	CB-CG-CD	5.12	128.01	114.20
1	D	78	ILE	N-CA-C	-5.12	97.19	111.00
1	B	211	ILE	CB-CA-C	5.11	121.82	111.60
1	B	78	ILE	N-CA-C	-5.11	97.21	111.00
1	A	78	ILE	N-CA-C	-5.11	97.22	111.00
1	A	189	ILE	CA-CB-CG2	5.11	121.11	110.90
1	B	161	SER	CB-CA-C	5.10	119.80	110.10
1	C	54	ASN	O-C-N	5.10	130.87	122.70
1	C	78	ILE	N-CA-C	-5.10	97.22	111.00
1	A	257	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	B	115	ALA	CB-CA-C	5.10	117.74	110.10
1	B	189	ILE	CA-CB-CG2	5.10	121.09	110.90
1	A	115	ALA	CB-CA-C	5.09	117.74	110.10
1	B	54	ASN	O-C-N	5.09	130.84	122.70
1	C	169	ARG	NH1-CZ-NH2	-5.09	113.81	119.40
1	D	35	TYR	CB-CG-CD2	5.09	124.05	121.00
1	C	165	LEU	CB-CA-C	5.08	119.85	110.20
1	D	165	LEU	CB-CA-C	5.08	119.85	110.20
1	B	169	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	D	257	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
1	D	320	THR	CA-CB-CG2	5.07	119.50	112.40
1	B	216	GLU	CG-CD-OE1	5.07	128.44	118.30
1	B	320	THR	CA-CB-CG2	5.07	119.49	112.40
1	D	228	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	54	ASN	O-C-N	5.06	130.80	122.70
1	C	115	ALA	CB-CA-C	5.06	117.69	110.10
1	C	216	GLU	CG-CD-OE1	5.06	128.42	118.30
1	A	216	GLU	CG-CD-OE1	5.06	128.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	GLU	CG-CD-OE1	5.06	128.42	118.30
1	D	115	ALA	CB-CA-C	5.05	117.68	110.10
1	B	165	LEU	CB-CA-C	5.05	119.80	110.20
1	C	320	THR	CA-CB-CG2	5.05	119.47	112.40
1	A	169	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
1	A	320	THR	CA-CB-CG2	5.05	119.47	112.40
1	C	228	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	165	LEU	CB-CA-C	5.04	119.78	110.20
1	B	257	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
1	C	257	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
1	D	212	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	D	169	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
1	C	35	TYR	CB-CG-CD2	5.04	124.02	121.00
1	A	228	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	C	176	GLU	CA-CB-CG	5.01	124.42	113.40
1	B	176	GLU	CA-CB-CG	5.00	124.41	113.40
1	D	176	GLU	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	ARG	Sidechain
1	A	171	ARG	Sidechain
1	A	189	ILE	Mainchain
1	A	205	TYR	Sidechain
1	A	226	LEU	Mainchain
1	A	260	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	47	GLU	Mainchain
1	A	68	GLY	Mainchain
1	B	157	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	189	ILE	Mainchain
1	B	205	TYR	Sidechain
1	B	226	LEU	Mainchain
1	B	260	ARG	Sidechain
1	B	283	ARG	Sidechain
1	B	47	GLU	Mainchain
1	B	68	GLY	Mainchain
1	C	157	ARG	Sidechain
1	C	171	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	189	ILE	Mainchain
1	C	205	TYR	Sidechain
1	C	226	LEU	Mainchain
1	C	260	ARG	Sidechain
1	C	283	ARG	Sidechain
1	C	47	GLU	Mainchain
1	C	68	GLY	Mainchain
1	D	157	ARG	Sidechain
1	D	171	ARG	Sidechain
1	D	189	ILE	Mainchain
1	D	205	TYR	Sidechain
1	D	226	LEU	Mainchain
1	D	260	ARG	Sidechain
1	D	283	ARG	Sidechain
1	D	47	GLU	Mainchain
1	D	68	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2336	0	2327	275	49
1	B	2336	0	2327	278	4
1	C	2336	0	2327	275	10
1	D	2336	0	2327	276	59
2	A	10	0	0	4	0
2	B	10	0	0	4	0
2	C	10	0	0	4	0
2	D	10	0	0	4	0
3	A	44	0	26	8	0
3	B	44	0	26	8	0
3	C	44	0	26	8	0
3	D	44	0	26	8	0
4	C	20	0	10	3	0
4	D	20	0	10	3	0
5	A	47	0	0	1	4
5	C	3	0	0	1	0
All	All	9650	0	9432	1043	63

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 55.

All (1043) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:CD2	1:C:169:ARG:HG2	1.63	1.33
1:B:67:HIS:CD2	1:D:169:ARG:HG2	1.63	1.32
1:B:169:ARG:HG2	1:D:67:HIS:CD2	1.63	1.31
1:A:169:ARG:HG2	1:C:67:HIS:CD2	1.63	1.30
1:B:107:LEU:HD22	1:B:327:ARG:NE	1.54	1.23
1:C:107:LEU:HD22	1:C:327:ARG:NE	1.54	1.22
1:D:107:LEU:HD22	1:D:327:ARG:NE	1.54	1.21
1:A:107:LEU:HD22	1:A:327:ARG:NE	1.54	1.20
1:B:214:LEU:HD12	1:B:215:VAL:N	1.56	1.20
1:C:214:LEU:HD12	1:C:215:VAL:N	1.56	1.20
1:A:214:LEU:HD12	1:A:215:VAL:N	1.56	1.19
1:D:214:LEU:HD12	1:D:215:VAL:N	1.56	1.18
1:D:214:LEU:HD12	1:D:215:VAL:H	0.96	1.09
1:C:214:LEU:HD12	1:C:215:VAL:H	0.96	1.09
1:A:214:LEU:HD12	1:A:215:VAL:H	0.96	1.08
1:A:107:LEU:HD22	1:A:327:ARG:HE	0.93	1.08
1:D:216:GLU:HG3	1:D:217:SER:H	1.13	1.08
1:C:107:LEU:HD22	1:C:327:ARG:HE	0.93	1.08
1:B:216:GLU:HG3	1:B:217:SER:H	1.13	1.07
1:C:216:GLU:HG3	1:C:217:SER:H	1.13	1.06
1:A:216:GLU:HG3	1:A:217:SER:H	1.13	1.06
1:B:214:LEU:HD12	1:B:215:VAL:H	0.96	1.05
1:B:107:LEU:HD22	1:B:327:ARG:HE	0.93	1.04
1:C:15:MET:HE3	1:C:18:ASN:HB3	1.40	1.03
1:C:15:MET:CE	1:C:18:ASN:HB3	1.89	1.03
1:D:107:LEU:HD22	1:D:327:ARG:HE	0.93	1.03
1:D:15:MET:CE	1:D:18:ASN:HB3	1.89	1.02
1:B:15:MET:CE	1:B:18:ASN:HB3	1.89	1.02
1:A:15:MET:CE	1:A:18:ASN:HB3	1.89	1.01
1:A:15:MET:HE3	1:A:18:ASN:HB3	1.43	1.01
1:A:261:ALA:HA	1:A:266:GLU:HG3	1.43	1.00
1:C:112:LYS:O	1:C:115:ALA:HB3	1.62	1.00
1:D:112:LYS:O	1:D:115:ALA:HB3	1.62	1.00
1:D:261:ALA:HA	1:D:266:GLU:HG3	1.43	0.99
1:C:107:LEU:CD2	1:C:327:ARG:HE	1.76	0.99
1:C:183:GLN:NE2	4:C:6:FBP:O3	1.96	0.99
1:D:15:MET:HE3	1:D:18:ASN:HB3	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:CD2	1:B:327:ARG:HE	1.76	0.99
1:D:183:GLN:NE2	4:D:2:FBP:O3	1.96	0.99
1:B:112:LYS:O	1:B:115:ALA:HB3	1.62	0.98
1:A:112:LYS:O	1:A:115:ALA:HB3	1.62	0.98
1:D:107:LEU:CD2	1:D:327:ARG:HE	1.76	0.98
1:A:107:LEU:CD2	1:A:327:ARG:HE	1.76	0.97
1:C:261:ALA:HA	1:C:266:GLU:HG3	1.43	0.97
1:C:237:ALA:O	1:C:241:ILE:HG13	1.65	0.96
1:B:261:ALA:HA	1:B:266:GLU:HG3	1.43	0.96
1:A:237:ALA:O	1:A:241:ILE:HG13	1.65	0.96
1:C:87:ARG:O	1:C:88:ASP:HB2	1.66	0.96
1:D:107:LEU:HB2	1:D:327:ARG:HH21	1.31	0.96
1:B:192:GLU:O	1:B:197:GLU:HB3	1.65	0.96
1:D:192:GLU:O	1:D:197:GLU:HB3	1.65	0.96
1:A:192:GLU:O	1:A:197:GLU:HB3	1.65	0.95
1:D:237:ALA:O	1:D:241:ILE:HG13	1.65	0.95
1:D:87:ARG:O	1:D:88:ASP:HB2	1.66	0.95
1:C:192:GLU:O	1:C:197:GLU:HB3	1.65	0.94
1:D:216:GLU:HG3	1:D:217:SER:N	1.83	0.94
1:D:257:ARG:NH2	1:D:266:GLU:OE2	2.01	0.94
1:A:107:LEU:HB2	1:A:327:ARG:HH21	1.31	0.94
1:B:200:VAL:HG11	1:B:304:ILE:HD12	1.50	0.94
1:B:107:LEU:HB2	1:B:327:ARG:HH21	1.31	0.94
1:B:237:ALA:O	1:B:241:ILE:HG13	1.65	0.94
1:C:107:LEU:HB2	1:C:327:ARG:HH21	1.31	0.94
1:A:87:ARG:O	1:A:88:ASP:HB2	1.66	0.94
1:B:87:ARG:O	1:B:88:ASP:HB2	1.65	0.93
1:C:257:ARG:NH2	1:C:266:GLU:OE2	2.01	0.93
1:B:257:ARG:NH2	1:B:266:GLU:OE2	2.01	0.93
1:B:295:ARG:HH11	1:B:295:ARG:HG2	1.33	0.93
1:A:257:ARG:NH2	1:A:266:GLU:OE2	2.01	0.93
1:C:216:GLU:HG3	1:C:217:SER:N	1.83	0.92
1:B:216:GLU:HG3	1:B:217:SER:N	1.83	0.92
1:C:295:ARG:HG2	1:C:295:ARG:HH11	1.33	0.92
1:A:295:ARG:HG2	1:A:295:ARG:HH11	1.33	0.92
1:D:200:VAL:HG11	1:D:304:ILE:HD12	1.50	0.92
1:A:216:GLU:HG3	1:A:217:SER:N	1.83	0.91
1:C:200:VAL:HG11	1:C:304:ILE:HD12	1.50	0.91
1:D:295:ARG:HG2	1:D:295:ARG:HH11	1.33	0.90
1:A:200:VAL:HG11	1:A:304:ILE:HD12	1.50	0.90
1:B:15:MET:HE3	1:B:18:ASN:HB3	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:HIS:CD2	1:D:169:ARG:CG	2.54	0.90
1:A:169:ARG:CG	1:C:67:HIS:CD2	2.53	0.89
1:A:67:HIS:CD2	1:C:169:ARG:CG	2.54	0.89
1:B:313:ARG:HG2	1:B:313:ARG:HH11	1.37	0.89
1:A:67:HIS:HD2	1:C:169:ARG:HG2	1.38	0.89
1:A:307:ASN:O	1:A:311:LYS:HG3	1.73	0.89
1:C:307:ASN:O	1:C:311:LYS:HG3	1.73	0.89
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.37	0.89
1:B:67:HIS:HD2	1:D:169:ARG:HG2	1.38	0.89
1:D:244:LYS:O	1:D:244:LYS:HG2	1.73	0.89
1:B:169:ARG:HG2	1:D:67:HIS:HD2	1.38	0.89
1:B:169:ARG:CG	1:D:67:HIS:CD2	2.54	0.89
1:D:307:ASN:O	1:D:311:LYS:HG3	1.73	0.88
1:A:283:ARG:H	1:A:322:LYS:HZ2	1.19	0.88
1:B:307:ASN:O	1:B:311:LYS:HG3	1.73	0.88
1:C:313:ARG:HH11	1:C:313:ARG:HG2	1.37	0.88
1:C:160:GLY:HA3	1:C:273:SER:HB3	1.55	0.88
1:B:244:LYS:HG2	1:B:244:LYS:O	1.73	0.88
1:A:160:GLY:HA3	1:A:273:SER:HB3	1.55	0.87
1:C:283:ARG:H	1:C:322:LYS:HZ2	1.19	0.87
1:A:244:LYS:HD3	1:A:246:ALA:O	1.75	0.87
1:B:160:GLY:HA3	1:B:273:SER:HB3	1.55	0.87
1:D:313:ARG:HG2	1:D:313:ARG:HH11	1.37	0.87
1:C:244:LYS:O	1:C:244:LYS:HG2	1.73	0.87
1:A:107:LEU:HD22	1:A:327:ARG:CD	2.04	0.87
1:D:160:GLY:HA3	1:D:273:SER:HB3	1.55	0.86
1:D:107:LEU:HD22	1:D:327:ARG:CD	2.04	0.86
1:B:107:LEU:HD22	1:B:327:ARG:CD	2.04	0.86
1:B:283:ARG:H	1:B:322:LYS:HZ2	1.19	0.86
1:A:244:LYS:O	1:A:244:LYS:HG2	1.73	0.86
1:D:151:SER:OG	1:D:153:LEU:HB2	1.75	0.86
1:D:283:ARG:H	1:D:322:LYS:HZ2	1.20	0.86
1:C:107:LEU:HD22	1:C:327:ARG:CD	2.04	0.86
1:D:244:LYS:HD3	1:D:246:ALA:O	1.75	0.86
1:B:151:SER:OG	1:B:153:LEU:HB2	1.75	0.86
1:B:244:LYS:HD3	1:B:246:ALA:O	1.75	0.85
1:A:183:GLN:HE21	1:A:183:GLN:CA	1.85	0.85
1:C:151:SER:OG	1:C:153:LEU:HB2	1.75	0.85
1:C:183:GLN:CA	1:C:183:GLN:HE21	1.85	0.85
1:A:151:SER:OG	1:A:153:LEU:HB2	1.75	0.84
1:C:244:LYS:HD3	1:C:246:ALA:O	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLN:CA	1:B:183:GLN:HE21	1.85	0.84
1:A:169:ARG:HG2	1:C:67:HIS:HD2	1.37	0.84
1:D:183:GLN:HE21	1:D:183:GLN:CA	1.85	0.84
1:B:15:MET:HE1	1:B:18:ASN:HB3	1.60	0.83
1:A:183:GLN:HE21	1:A:183:GLN:HA	1.44	0.83
1:D:183:GLN:HE21	1:D:183:GLN:HA	1.44	0.83
1:B:178:PHE:O	1:B:179:SER:HB2	1.80	0.82
1:A:178:PHE:O	1:A:179:SER:HB2	1.79	0.82
1:D:178:PHE:O	1:D:179:SER:HB2	1.80	0.82
1:B:183:GLN:HE21	1:B:183:GLN:HA	1.44	0.81
1:C:178:PHE:O	1:C:179:SER:HB2	1.80	0.80
1:D:240:ILE:HG21	1:D:247:THR:CG2	2.11	0.80
1:A:240:ILE:HG21	1:A:247:THR:CG2	2.11	0.80
1:C:183:GLN:HE21	1:C:183:GLN:HA	1.44	0.80
1:C:240:ILE:HG21	1:C:247:THR:CG2	2.11	0.80
1:C:240:ILE:HG21	1:C:247:THR:HG23	1.64	0.80
1:A:208:VAL:O	1:A:210:PRO:HD3	1.82	0.80
1:B:208:VAL:O	1:B:210:PRO:HD3	1.82	0.80
1:D:208:VAL:O	1:D:210:PRO:HD3	1.82	0.79
1:A:240:ILE:HG21	1:A:247:THR:HG23	1.64	0.79
1:B:240:ILE:HG21	1:B:247:THR:CG2	2.11	0.79
1:D:240:ILE:HG21	1:D:247:THR:HG23	1.64	0.79
1:C:208:VAL:O	1:C:210:PRO:HD3	1.82	0.79
1:D:32:GLY:O	1:D:36:VAL:HG23	1.83	0.79
1:B:32:GLY:O	1:B:36:VAL:HG23	1.83	0.79
1:C:32:GLY:O	1:C:36:VAL:HG23	1.83	0.78
1:B:240:ILE:HG21	1:B:247:THR:HG23	1.64	0.78
1:A:32:GLY:O	1:A:36:VAL:HG23	1.83	0.78
1:A:136:ALA:HB1	1:A:251:ILE:HD11	1.67	0.77
1:D:15:MET:HE1	1:D:18:ASN:HB3	1.66	0.77
1:C:199:PRO:O	1:C:199:PRO:HG2	1.85	0.77
1:A:189:ILE:CD1	1:A:233:VAL:HG11	2.15	0.77
1:D:136:ALA:HB1	1:D:251:ILE:HD11	1.67	0.77
1:B:136:ALA:HB1	1:B:251:ILE:HD11	1.67	0.77
1:A:279:LEU:HD12	1:A:303:GLU:OE1	1.85	0.76
1:B:279:LEU:HD12	1:B:303:GLU:OE1	1.85	0.76
1:B:313:ARG:HG2	1:B:313:ARG:NH1	2.00	0.76
1:C:183:GLN:HE22	4:C:6:FBP:C3	1.98	0.76
1:D:313:ARG:HG2	1:D:313:ARG:NH1	2.00	0.76
1:C:74:LYS:HE2	1:D:266:GLU:CD	2.06	0.76
1:D:183:GLN:HE22	4:D:2:FBP:C3	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ILE:CD1	1:B:233:VAL:HG11	2.15	0.76
1:C:214:LEU:CD1	1:C:215:VAL:N	2.45	0.76
1:D:189:ILE:CD1	1:D:233:VAL:HG11	2.15	0.76
1:A:160:GLY:HA3	1:A:273:SER:CB	2.16	0.76
1:A:199:PRO:HG2	1:A:199:PRO:O	1.85	0.76
1:C:189:ILE:CD1	1:C:233:VAL:HG11	2.15	0.76
1:C:313:ARG:HG2	1:C:313:ARG:NH1	2.00	0.76
1:C:160:GLY:HA3	1:C:273:SER:CB	2.16	0.76
1:C:240:ILE:CG2	1:C:247:THR:HG23	2.16	0.76
1:C:266:GLU:CD	1:D:74:LYS:HE2	2.06	0.76
1:D:240:ILE:CG2	1:D:247:THR:HG23	2.16	0.76
1:C:279:LEU:HD12	1:C:303:GLU:OE1	1.85	0.76
1:B:160:GLY:HA3	1:B:273:SER:CB	2.16	0.75
1:D:199:PRO:O	1:D:199:PRO:HG2	1.85	0.75
1:A:313:ARG:HG2	1:A:313:ARG:NH1	2.00	0.75
1:B:214:LEU:CD1	1:B:215:VAL:N	2.45	0.75
1:B:240:ILE:CG2	1:B:247:THR:HG23	2.16	0.75
1:D:113:ASN:O	1:D:117:PHE:HB2	1.87	0.75
1:A:74:LYS:HE2	1:B:266:GLU:CD	2.06	0.75
1:A:240:ILE:CG2	1:A:247:THR:HG23	2.16	0.75
1:B:199:PRO:O	1:B:199:PRO:HG2	1.85	0.75
1:A:15:MET:HE1	1:A:18:ASN:HB3	1.68	0.75
1:B:243:LYS:NZ	1:B:243:LYS:HB3	2.02	0.75
1:D:160:GLY:HA3	1:D:273:SER:CB	2.16	0.75
1:A:113:ASN:O	1:A:117:PHE:HB2	1.87	0.74
1:A:214:LEU:CD1	1:A:215:VAL:N	2.45	0.74
1:A:215:VAL:O	1:A:216:GLU:HG2	1.87	0.74
1:A:266:GLU:CD	1:B:74:LYS:HE2	2.06	0.74
1:B:215:VAL:O	1:B:216:GLU:HG2	1.87	0.74
1:B:113:ASN:O	1:B:117:PHE:HB2	1.87	0.74
1:D:279:LEU:HD12	1:D:303:GLU:OE1	1.85	0.74
1:C:136:ALA:HB1	1:C:251:ILE:HD11	1.67	0.74
1:C:295:ARG:HG2	1:C:295:ARG:NH1	2.03	0.74
1:C:215:VAL:O	1:C:216:GLU:HG2	1.87	0.74
1:C:113:ASN:O	1:C:117:PHE:HB2	1.87	0.74
1:B:87:ARG:HG3	1:B:127:SER:O	1.88	0.74
1:D:243:LYS:HB3	1:D:243:LYS:NZ	2.02	0.74
1:D:215:VAL:O	1:D:216:GLU:HG2	1.87	0.74
1:A:87:ARG:HG3	1:A:127:SER:O	1.88	0.73
1:C:87:ARG:HG3	1:C:127:SER:O	1.88	0.73
1:D:295:ARG:HG2	1:D:295:ARG:NH1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LYS:NZ	1:C:243:LYS:HB3	2.02	0.73
1:C:183:GLN:NE2	1:C:183:GLN:HA	2.03	0.73
1:D:83:TYR:HD2	1:D:124:VAL:HG12	1.54	0.73
1:A:83:TYR:HD2	1:A:124:VAL:HG12	1.53	0.73
1:B:183:GLN:HA	1:B:183:GLN:NE2	2.03	0.73
1:C:83:TYR:HD2	1:C:124:VAL:HG12	1.54	0.73
1:D:214:LEU:CD1	1:D:215:VAL:N	2.45	0.72
1:B:295:ARG:HG2	1:B:295:ARG:NH1	2.03	0.72
1:D:183:GLN:NE2	1:D:183:GLN:HA	2.03	0.72
1:A:243:LYS:NZ	1:A:243:LYS:HB3	2.02	0.72
1:B:83:TYR:HD2	1:B:124:VAL:HG12	1.54	0.72
1:B:59:ILE:HG22	1:D:243:LYS:HD3	1.72	0.72
1:A:295:ARG:HG2	1:A:295:ARG:NH1	2.03	0.72
1:C:170:PHE:HA	1:C:233:VAL:CG2	2.20	0.72
1:A:170:PHE:HA	1:A:233:VAL:CG2	2.20	0.71
1:A:183:GLN:HA	1:A:183:GLN:NE2	2.03	0.71
1:D:190:ILE:HD11	1:D:306:LEU:HD11	1.72	0.71
1:A:59:ILE:HG22	1:C:243:LYS:HD3	1.72	0.71
1:C:216:GLU:CG	1:C:217:SER:H	2.00	0.71
1:B:110:VAL:HG22	1:B:139:PRO:HG3	1.72	0.71
1:C:15:MET:HE1	1:C:18:ASN:HB3	1.70	0.71
1:C:147:THR:O	1:C:151:SER:HB3	1.90	0.71
1:D:87:ARG:HG3	1:D:127:SER:O	1.88	0.71
1:B:170:PHE:HA	1:B:233:VAL:CG2	2.20	0.71
1:D:147:THR:O	1:D:151:SER:HB3	1.90	0.71
1:D:170:PHE:HA	1:D:233:VAL:CG2	2.20	0.71
1:A:190:ILE:HD11	1:A:306:LEU:HD11	1.73	0.71
1:B:147:THR:O	1:B:151:SER:HB3	1.91	0.71
1:B:243:LYS:HD3	1:D:59:ILE:HG22	1.72	0.71
1:A:110:VAL:HG22	1:A:139:PRO:HG3	1.72	0.70
1:B:226:LEU:C	1:B:228:ARG:H	1.95	0.70
1:D:110:VAL:HG22	1:D:139:PRO:HG3	1.72	0.70
1:A:59:ILE:CG2	1:C:243:LYS:HD3	2.21	0.70
1:A:147:THR:O	1:A:151:SER:HB3	1.91	0.70
1:A:243:LYS:HD3	1:C:59:ILE:HG22	1.72	0.70
1:A:243:LYS:HD3	1:C:59:ILE:CG2	2.21	0.70
1:B:73:PRO:O	1:B:74:LYS:HB2	1.92	0.70
1:B:243:LYS:HD3	1:D:59:ILE:CG2	2.21	0.70
1:C:226:LEU:C	1:C:228:ARG:H	1.95	0.70
1:A:73:PRO:O	1:A:74:LYS:HB2	1.92	0.70
1:A:226:LEU:C	1:A:228:ARG:H	1.95	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:CG2	1:D:243:LYS:HD3	2.21	0.70
1:B:190:ILE:HD11	1:B:306:LEU:HD11	1.72	0.69
1:C:190:ILE:HD11	1:C:306:LEU:HD11	1.72	0.69
1:B:279:LEU:C	1:B:281:GLY:H	1.96	0.69
1:D:73:PRO:O	1:D:74:LYS:HB2	1.91	0.69
1:A:214:LEU:CD1	1:A:215:VAL:H	1.90	0.69
1:C:110:VAL:HG22	1:C:139:PRO:HG3	1.72	0.69
1:C:279:LEU:C	1:C:281:GLY:H	1.96	0.69
1:C:73:PRO:O	1:C:74:LYS:HB2	1.92	0.69
1:A:279:LEU:C	1:A:281:GLY:H	1.96	0.68
1:D:226:LEU:C	1:D:228:ARG:H	1.95	0.68
1:A:132:LEU:CD1	1:A:262:ILE:HD13	2.24	0.68
1:B:283:ARG:N	1:B:322:LYS:HZ2	1.92	0.68
1:C:132:LEU:CD1	1:C:262:ILE:HD13	2.24	0.68
1:D:132:LEU:CD1	1:D:262:ILE:HD13	2.24	0.68
1:B:132:LEU:CD1	1:B:262:ILE:HD13	2.24	0.67
1:A:170:PHE:HA	1:A:233:VAL:HG21	1.77	0.67
1:B:183:GLN:CA	1:B:183:GLN:NE2	2.58	0.67
1:C:170:PHE:HA	1:C:233:VAL:HG21	1.77	0.67
1:D:170:PHE:HA	1:D:233:VAL:HG21	1.77	0.67
1:A:176:GLU:OE1	5:A:348:HOH:O	2.12	0.66
1:A:183:GLN:CA	1:A:183:GLN:NE2	2.58	0.66
1:D:183:GLN:NE2	1:D:183:GLN:CA	2.58	0.66
1:B:170:PHE:HA	1:B:233:VAL:HG21	1.77	0.66
1:D:279:LEU:C	1:D:281:GLY:H	1.96	0.66
1:A:61:ASP:OD1	1:C:244:LYS:HE3	1.96	0.66
1:B:61:ASP:OD1	1:D:244:LYS:HE3	1.96	0.65
1:A:244:LYS:HE3	1:C:61:ASP:OD1	1.96	0.65
1:D:214:LEU:CD1	1:D:215:VAL:H	1.91	0.65
1:A:189:ILE:HD11	1:A:233:VAL:HG11	1.79	0.65
1:C:294:ASN:C	1:C:294:ASN:HD22	1.99	0.65
1:D:294:ASN:C	1:D:294:ASN:HD22	1.99	0.65
1:B:313:ARG:HH11	1:B:313:ARG:CG	2.05	0.65
1:D:283:ARG:N	1:D:322:LYS:HZ2	1.92	0.65
1:D:189:ILE:HD11	1:D:233:VAL:HG11	1.79	0.65
1:A:294:ASN:C	1:A:294:ASN:HD22	1.99	0.65
1:B:294:ASN:C	1:B:294:ASN:HD22	1.99	0.65
1:B:244:LYS:HE3	1:D:61:ASP:OD1	1.96	0.64
1:A:272:VAL:O	1:A:288:GLY:HA2	1.97	0.64
1:C:272:VAL:O	1:C:288:GLY:HA2	1.96	0.64
1:A:107:LEU:CD1	1:A:328:ALA:HB2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ILE:HD11	1:B:233:VAL:HG11	1.79	0.64
1:B:206:ILE:HB	1:B:213:LYS:HE3	1.80	0.64
1:D:148:TRP:CH2	1:D:275:TYR:CE2	2.86	0.64
1:D:272:VAL:O	1:D:288:GLY:HA2	1.96	0.64
1:B:272:VAL:O	1:B:288:GLY:HA2	1.97	0.64
1:C:148:TRP:CH2	1:C:275:TYR:CE2	2.86	0.64
1:C:206:ILE:HB	1:C:213:LYS:HE3	1.80	0.64
1:A:148:TRP:CH2	1:A:275:TYR:CE2	2.86	0.64
1:C:189:ILE:HD11	1:C:233:VAL:HG11	1.79	0.64
1:B:107:LEU:CD1	1:B:328:ALA:HB2	2.28	0.63
1:D:107:LEU:CD1	1:D:328:ALA:HB2	2.28	0.63
1:A:313:ARG:NH1	1:A:313:ARG:CG	2.61	0.63
1:C:209:MET:HB3	1:C:213:LYS:HE2	1.81	0.63
1:D:87:ARG:O	1:D:88:ASP:CB	2.44	0.63
1:B:214:LEU:CD1	1:B:215:VAL:H	1.91	0.63
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.64	0.63
1:A:206:ILE:HB	1:A:213:LYS:HE3	1.80	0.63
1:A:215:VAL:C	1:A:216:GLU:CG	2.67	0.63
1:B:148:TRP:CH2	1:B:275:TYR:CE2	2.86	0.63
1:A:157:ARG:HG2	1:A:157:ARG:HH11	1.64	0.63
1:A:283:ARG:N	1:A:322:LYS:HZ2	1.93	0.63
1:A:296:ASN:OD1	1:B:15:MET:HG3	1.99	0.63
1:C:107:LEU:CD1	1:C:328:ALA:HB2	2.28	0.63
1:D:206:ILE:HB	1:D:213:LYS:HE3	1.80	0.63
1:D:215:VAL:C	1:D:216:GLU:HG2	2.20	0.63
1:D:216:GLU:CG	1:D:217:SER:H	2.00	0.63
1:C:296:ASN:OD1	1:D:15:MET:HG3	1.99	0.62
1:A:215:VAL:C	1:A:216:GLU:HG2	2.19	0.62
1:D:157:ARG:HG2	1:D:157:ARG:HH11	1.64	0.62
1:C:15:MET:HG3	1:D:296:ASN:OD1	1.99	0.62
1:B:209:MET:HB3	1:B:213:LYS:HE2	1.80	0.62
1:D:313:ARG:NH1	1:D:313:ARG:CG	2.61	0.62
1:B:313:ARG:NH1	1:B:313:ARG:CG	2.61	0.62
1:A:15:MET:HG3	1:B:296:ASN:OD1	1.99	0.62
1:C:215:VAL:C	1:C:216:GLU:CG	2.67	0.62
1:A:59:ILE:HG22	1:C:243:LYS:CD	2.30	0.62
1:B:215:VAL:C	1:B:216:GLU:HG2	2.19	0.62
1:B:289:VAL:HG11	1:B:301:VAL:HG13	1.82	0.62
1:B:59:ILE:HG22	1:D:243:LYS:CD	2.30	0.62
1:B:157:ARG:HH11	1:B:157:ARG:HG2	1.64	0.62
1:A:251:ILE:HD12	3:A:1:NAD:C3N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:HG11	1:A:301:VAL:HG13	1.82	0.62
1:B:251:ILE:HD12	3:B:5:NAD:C3N	2.30	0.62
1:C:289:VAL:HG11	1:C:301:VAL:HG13	1.82	0.61
1:A:98:ALA:HB2	1:A:112:LYS:HG2	1.83	0.61
1:C:251:ILE:HD12	3:C:9:NAD:C3N	2.30	0.61
1:A:29:GLY:HA3	3:A:1:NAD:H52A	1.83	0.61
1:B:243:LYS:CD	1:D:59:ILE:HG22	2.30	0.61
1:D:29:GLY:HA3	3:D:13:NAD:H52A	1.83	0.61
1:A:209:MET:HB3	1:A:213:LYS:HE2	1.81	0.61
1:A:243:LYS:CD	1:C:59:ILE:HG22	2.30	0.61
1:D:251:ILE:HD12	3:D:13:NAD:C3N	2.30	0.61
1:C:215:VAL:C	1:C:216:GLU:HG2	2.20	0.61
1:D:209:MET:HB3	1:D:213:LYS:HE2	1.81	0.61
1:A:107:LEU:HB2	1:A:327:ARG:NH2	2.12	0.61
1:D:174:LEU:O	1:D:177:TYR:HB3	2.01	0.61
1:D:289:VAL:HG11	1:D:301:VAL:HG13	1.82	0.60
1:B:98:ALA:HB2	1:B:112:LYS:HG2	1.83	0.60
1:C:29:GLY:HA3	3:C:9:NAD:H52A	1.83	0.60
1:C:214:LEU:CD1	1:C:215:VAL:H	1.91	0.60
1:D:98:ALA:HB2	1:D:112:LYS:HG2	1.83	0.60
1:D:215:VAL:C	1:D:216:GLU:CG	2.67	0.60
1:A:174:LEU:O	1:A:177:TYR:HB3	2.02	0.60
1:B:279:LEU:HD12	1:B:303:GLU:CD	2.22	0.60
1:C:279:LEU:HD12	1:C:303:GLU:CD	2.22	0.60
1:B:174:LEU:O	1:B:177:TYR:HB3	2.01	0.60
1:D:15:MET:HE3	1:D:18:ASN:CB	2.28	0.60
1:B:215:VAL:C	1:B:216:GLU:CG	2.67	0.60
1:C:243:LYS:HB3	1:C:243:LYS:HZ3	1.64	0.60
1:C:15:MET:HE3	1:C:18:ASN:CB	2.24	0.60
1:C:174:LEU:O	1:C:177:TYR:HB3	2.01	0.60
1:B:29:GLY:HA3	3:B:5:NAD:H52A	1.83	0.59
1:C:53:ALA:H	3:C:9:NAD:C2A	2.16	0.59
1:B:107:LEU:HB2	1:B:327:ARG:NH2	2.12	0.59
1:D:136:ALA:O	3:D:13:NAD:H2N	2.03	0.59
1:A:320:THR:O	1:A:324:VAL:HG23	2.03	0.59
1:C:98:ALA:HB2	1:C:112:LYS:HG2	1.83	0.59
1:C:319:ALA:O	1:C:323:SER:OG	2.20	0.59
1:D:107:LEU:HB2	1:D:327:ARG:NH2	2.12	0.59
1:A:279:LEU:HD12	1:A:303:GLU:CD	2.22	0.59
1:A:136:ALA:O	3:A:1:NAD:H2N	2.03	0.59
1:D:53:ALA:H	3:D:13:NAD:C2A	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:H	3:A:1:NAD:C2A	2.15	0.59
1:D:279:LEU:HD12	1:D:303:GLU:CD	2.22	0.59
1:B:35:TYR:O	1:B:38:ALA:HB3	2.03	0.58
1:C:136:ALA:O	3:C:9:NAD:H2N	2.03	0.58
1:A:125:MET:CE	1:A:129:PHE:HB3	2.33	0.58
1:A:132:LEU:HD12	1:A:262:ILE:HG21	1.85	0.58
1:B:53:ALA:H	3:B:5:NAD:C2A	2.15	0.58
1:B:129:PHE:CE2	1:B:133:PHE:CE1	2.92	0.58
1:C:283:ARG:N	1:C:322:LYS:HZ2	1.94	0.58
1:A:87:ARG:O	1:A:88:ASP:CB	2.44	0.58
1:A:132:LEU:HD12	1:A:262:ILE:HD13	1.86	0.58
1:C:125:MET:CE	1:C:129:PHE:HB3	2.33	0.58
1:B:132:LEU:HD12	1:B:262:ILE:HG21	1.85	0.58
1:C:279:LEU:C	1:C:281:GLY:N	2.57	0.58
1:D:279:LEU:C	1:D:281:GLY:N	2.57	0.58
1:D:320:THR:O	1:D:324:VAL:HG23	2.03	0.58
1:A:129:PHE:CE2	1:A:133:PHE:CE1	2.92	0.58
1:B:151:SER:HB2	1:B:153:LEU:HD12	1.85	0.58
1:B:320:THR:O	1:B:324:VAL:HG23	2.03	0.58
1:C:129:PHE:CE2	1:C:133:PHE:CE1	2.91	0.58
1:C:35:TYR:O	1:C:38:ALA:HB3	2.03	0.58
1:C:240:ILE:HG21	1:C:247:THR:HG22	1.85	0.58
1:C:320:THR:O	1:C:324:VAL:HG23	2.03	0.58
1:D:125:MET:CE	1:D:129:PHE:HB3	2.33	0.58
1:C:245:GLY:O	1:C:246:ALA:HB2	2.04	0.58
1:D:240:ILE:HG21	1:D:247:THR:HG22	1.86	0.58
1:B:136:ALA:O	3:B:5:NAD:H2N	2.03	0.58
1:D:129:PHE:CE2	1:D:133:PHE:CE1	2.92	0.58
1:D:132:LEU:HD12	1:D:262:ILE:HG21	1.85	0.58
1:B:132:LEU:HD12	1:B:262:ILE:HD13	1.86	0.58
1:B:169:ARG:HG2	1:D:67:HIS:CG	2.32	0.58
1:D:35:TYR:O	1:D:38:ALA:HB3	2.03	0.58
1:D:151:SER:HB2	1:D:153:LEU:HD12	1.85	0.58
1:A:35:TYR:O	1:A:38:ALA:HB3	2.03	0.57
1:B:216:GLU:CG	1:B:217:SER:H	2.00	0.57
1:B:125:MET:CE	1:B:129:PHE:HB3	2.33	0.57
1:B:279:LEU:C	1:B:281:GLY:N	2.57	0.57
1:B:245:GLY:O	1:B:246:ALA:HB2	2.04	0.57
1:C:15:MET:SD	1:C:16:LYS:N	2.73	0.57
1:C:151:SER:HB2	1:C:153:LEU:HD12	1.85	0.57
1:C:313:ARG:NH1	1:C:313:ARG:CG	2.61	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ALA:O	1:A:323:SER:OG	2.20	0.57
1:D:132:LEU:HD12	1:D:262:ILE:HD13	1.86	0.57
1:A:15:MET:HE3	1:A:18:ASN:CB	2.27	0.57
1:A:125:MET:HE3	1:A:129:PHE:HB3	1.87	0.57
2:B:7:SO4:O3	3:B:5:NAD:C4N	2.53	0.57
1:C:132:LEU:HD12	1:C:262:ILE:HG21	1.85	0.57
2:C:11:SO4:O3	3:C:9:NAD:C4N	2.53	0.57
1:A:151:SER:HB2	1:A:153:LEU:HD12	1.85	0.57
1:A:279:LEU:C	1:A:281:GLY:N	2.57	0.57
1:C:125:MET:CE	1:C:125:MET:HA	2.35	0.57
1:A:240:ILE:HG21	1:A:247:THR:HG22	1.86	0.57
1:B:125:MET:CE	1:B:125:MET:HA	2.35	0.57
1:D:200:VAL:HG21	1:D:304:ILE:HD11	1.87	0.56
1:B:319:ALA:O	1:B:323:SER:OG	2.20	0.56
1:C:117:PHE:HE1	1:C:137:THR:HG21	1.70	0.56
1:D:245:GLY:O	1:D:246:ALA:HB2	2.04	0.56
1:B:166:ASP:OD1	1:B:193:HIS:ND1	2.34	0.56
1:B:200:VAL:HG21	1:B:304:ILE:HD11	1.87	0.56
1:C:132:LEU:HD12	1:C:262:ILE:HD13	1.86	0.56
1:D:117:PHE:HE1	1:D:137:THR:HG21	1.70	0.56
2:D:332:SO4:O3	3:D:13:NAD:C4N	2.53	0.56
1:D:166:ASP:OD1	1:D:193:HIS:ND1	2.34	0.56
1:A:42:GLN:OE1	1:A:44:ILE:HD11	2.06	0.56
1:A:215:VAL:O	1:A:216:GLU:CG	2.53	0.56
1:D:35:TYR:HA	1:D:252:ALA:HB1	1.87	0.56
1:A:216:GLU:CG	1:A:217:SER:H	2.00	0.56
1:A:245:GLY:O	1:A:246:ALA:HB2	2.04	0.56
1:B:240:ILE:HG21	1:B:247:THR:HG22	1.86	0.56
1:A:125:MET:CE	1:A:125:MET:HA	2.35	0.56
1:B:117:PHE:HE1	1:B:137:THR:HG21	1.70	0.56
1:A:199:PRO:O	1:A:199:PRO:CG	2.54	0.56
1:D:15:MET:SD	1:D:16:LYS:N	2.73	0.56
1:A:117:PHE:HE1	1:A:137:THR:HG21	1.70	0.56
1:A:267:ASN:ND2	1:A:299:ARG:NH2	2.54	0.56
1:B:190:ILE:HG12	1:B:200:VAL:CG2	2.36	0.56
1:C:125:MET:HE3	1:C:129:PHE:HB3	1.88	0.56
1:A:200:VAL:HG21	1:A:304:ILE:HD11	1.87	0.55
1:B:125:MET:HE3	1:B:129:PHE:HB3	1.88	0.55
1:B:329:PHE:O	1:B:330:THR:C	2.44	0.55
1:C:42:GLN:OE1	1:C:44:ILE:HD11	2.06	0.55
1:C:98:ALA:HB3	1:C:113:ASN:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LEU:HB2	1:C:327:ARG:NH2	2.12	0.55
1:D:125:MET:CE	1:D:125:MET:HA	2.35	0.55
1:A:190:ILE:HG12	1:A:200:VAL:CG2	2.36	0.55
2:A:3:SO4:O3	3:A:1:NAD:C4N	2.53	0.55
1:B:35:TYR:HA	1:B:252:ALA:HB1	1.87	0.55
1:C:54:ASN:C	1:C:54:ASN:HD22	2.09	0.55
1:A:35:TYR:HA	1:A:252:ALA:HB1	1.88	0.55
1:C:190:ILE:HG12	1:C:200:VAL:CG2	2.37	0.55
1:C:200:VAL:HG21	1:C:304:ILE:HD11	1.87	0.55
1:C:266:GLU:CG	1:D:74:LYS:HE2	2.36	0.55
1:D:160:GLY:CA	1:D:273:SER:HB3	2.32	0.55
1:D:215:VAL:O	1:D:216:GLU:CG	2.54	0.55
1:A:74:LYS:HE2	1:B:266:GLU:CG	2.36	0.55
1:B:15:MET:SD	1:B:16:LYS:N	2.73	0.55
1:B:42:GLN:OE1	1:B:44:ILE:HD11	2.06	0.55
1:B:54:ASN:HD22	1:B:54:ASN:C	2.09	0.55
1:B:98:ALA:HB1	1:B:112:LYS:HE3	1.89	0.55
1:B:295:ARG:NH1	1:B:295:ARG:CG	2.65	0.55
1:C:267:ASN:ND2	1:C:299:ARG:NH2	2.55	0.55
1:D:98:ALA:HB3	1:D:113:ASN:OD1	2.06	0.55
1:A:98:ALA:HB3	1:A:113:ASN:OD1	2.06	0.55
1:B:199:PRO:O	1:B:199:PRO:CG	2.54	0.55
1:D:42:GLN:OE1	1:D:44:ILE:HD11	2.06	0.55
1:D:125:MET:HE3	1:D:129:PHE:HB3	1.89	0.55
1:A:67:HIS:CG	1:C:169:ARG:HG2	2.32	0.55
1:B:267:ASN:ND2	1:B:299:ARG:NH2	2.54	0.55
1:C:160:GLY:CA	1:C:273:SER:HB3	2.33	0.55
1:A:54:ASN:C	1:A:54:ASN:HD22	2.09	0.55
1:B:173:LEU:O	1:B:176:GLU:HB3	2.07	0.55
1:A:266:GLU:CG	1:B:74:LYS:HE2	2.36	0.55
1:A:329:PHE:O	1:A:330:THR:C	2.44	0.55
1:B:98:ALA:HB3	1:B:113:ASN:OD1	2.06	0.55
1:A:198:LEU:N	1:A:198:LEU:HD23	2.22	0.55
1:B:110:VAL:O	1:B:114:ILE:HD12	2.07	0.55
1:C:98:ALA:HB1	1:C:112:LYS:HE3	1.89	0.55
1:D:190:ILE:HG12	1:D:200:VAL:CG2	2.36	0.55
1:A:111:ASP:O	1:A:115:ALA:HB2	2.07	0.55
1:C:35:TYR:HA	1:C:252:ALA:HB1	1.87	0.55
1:B:21:ALA:HB3	1:B:46:ASP:HB2	1.89	0.54
1:B:87:ARG:O	1:B:88:ASP:CB	2.44	0.54
1:B:111:ASP:O	1:B:115:ALA:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:O	1:B:216:GLU:CG	2.53	0.54
1:C:74:LYS:HE2	1:D:266:GLU:CG	2.36	0.54
1:C:173:LEU:O	1:C:176:GLU:HB3	2.07	0.54
1:D:111:ASP:O	1:D:115:ALA:HB2	2.07	0.54
1:A:110:VAL:O	1:A:114:ILE:HD12	2.07	0.54
1:C:199:PRO:O	1:C:199:PRO:CG	2.54	0.54
1:D:173:LEU:O	1:D:176:GLU:HB3	2.07	0.54
1:C:111:ASP:O	1:C:115:ALA:HB2	2.07	0.54
1:C:132:LEU:HD23	1:C:157:ARG:HB3	1.90	0.54
1:D:267:ASN:ND2	1:D:299:ARG:NH2	2.55	0.54
1:D:329:PHE:O	1:D:330:THR:C	2.44	0.54
1:B:283:ARG:HG2	1:B:283:ARG:O	2.08	0.54
1:C:329:PHE:O	1:C:330:THR:C	2.44	0.54
1:D:21:ALA:HB3	1:D:46:ASP:HB2	1.90	0.54
1:B:167:THR:O	1:B:171:ARG:HG3	2.08	0.54
1:C:110:VAL:O	1:C:114:ILE:HD12	2.07	0.54
1:A:167:THR:O	1:A:171:ARG:HG3	2.08	0.54
1:D:319:ALA:O	1:D:323:SER:OG	2.20	0.54
1:C:166:ASP:OD1	1:C:193:HIS:ND1	2.34	0.54
1:D:98:ALA:HB1	1:D:112:LYS:HE3	1.89	0.54
1:A:173:LEU:O	1:A:176:GLU:HB3	2.07	0.54
1:C:215:VAL:O	1:C:216:GLU:CG	2.54	0.54
1:B:198:LEU:HD23	1:B:198:LEU:N	2.22	0.54
1:C:283:ARG:O	1:C:283:ARG:HG2	2.08	0.54
1:D:198:LEU:N	1:D:198:LEU:HD23	2.22	0.54
1:A:98:ALA:HB1	1:A:112:LYS:HE3	1.89	0.54
1:D:167:THR:O	1:D:171:ARG:HG3	2.08	0.54
1:C:21:ALA:HB3	1:C:46:ASP:HB2	1.89	0.53
1:C:83:TYR:CD2	1:C:124:VAL:HG12	2.41	0.53
1:C:132:LEU:HD13	1:C:262:ILE:HD13	1.90	0.53
1:A:21:ALA:HB3	1:A:46:ASP:HB2	1.89	0.53
1:A:132:LEU:HD13	1:A:262:ILE:HD13	1.90	0.53
1:A:204:ALA:O	1:A:211:ILE:HG13	2.09	0.53
1:D:54:ASN:C	1:D:54:ASN:HD22	2.09	0.53
1:D:83:TYR:CD2	1:D:124:VAL:HG12	2.41	0.53
1:C:167:THR:O	1:C:171:ARG:HG3	2.08	0.53
1:C:215:VAL:O	1:C:216:GLU:CB	2.57	0.53
1:D:110:VAL:O	1:D:114:ILE:HD12	2.07	0.53
1:D:132:LEU:HD23	1:D:157:ARG:HB3	1.90	0.53
1:D:132:LEU:HD13	1:D:262:ILE:HD13	1.90	0.53
1:D:178:PHE:O	1:D:179:SER:CB	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLY:O	1:C:71:PHE:HB2	2.09	0.53
1:D:154:PRO:HD2	1:D:157:ARG:HD3	1.91	0.53
1:D:199:PRO:O	1:D:199:PRO:CG	2.54	0.53
1:A:278:GLY:HA2	1:A:282:GLU:O	2.09	0.53
1:B:154:PRO:HD2	1:B:157:ARG:HD3	1.91	0.53
1:B:204:ALA:O	1:B:211:ILE:HG13	2.09	0.53
1:C:198:LEU:N	1:C:198:LEU:HD23	2.22	0.53
1:A:67:HIS:HB3	1:C:169:ARG:HG3	1.91	0.53
1:B:73:PRO:O	1:B:74:LYS:CB	2.57	0.53
1:C:204:ALA:O	1:C:211:ILE:HG13	2.09	0.53
1:C:73:PRO:O	1:C:74:LYS:CB	2.57	0.53
1:D:137:THR:HG22	1:D:143:LEU:CD1	2.39	0.53
1:D:283:ARG:O	1:D:283:ARG:HG2	2.08	0.53
1:A:132:LEU:HD23	1:A:157:ARG:HB3	1.89	0.53
1:A:169:ARG:HG3	1:C:67:HIS:HB3	1.91	0.53
1:A:283:ARG:O	1:A:283:ARG:HG2	2.08	0.53
1:B:132:LEU:HD13	1:B:262:ILE:HD13	1.90	0.53
1:C:154:PRO:HD2	1:C:157:ARG:HD3	1.91	0.53
1:D:202:SER:HA	1:D:218:LYS:HE2	1.91	0.53
1:A:68:GLY:O	1:A:71:PHE:HB2	2.09	0.53
1:A:295:ARG:NH1	1:A:295:ARG:CG	2.65	0.53
1:B:68:GLY:O	1:B:71:PHE:HB2	2.09	0.53
1:D:215:VAL:O	1:D:216:GLU:CB	2.57	0.53
1:A:166:ASP:OD1	1:A:193:HIS:ND1	2.34	0.52
1:A:15:MET:SD	1:A:16:LYS:N	2.73	0.52
1:B:137:THR:HG22	1:B:143:LEU:CD1	2.39	0.52
1:C:137:THR:HG22	1:C:143:LEU:CD1	2.39	0.52
1:D:68:GLY:O	1:D:71:PHE:HB2	2.09	0.52
1:D:278:GLY:HA2	1:D:282:GLU:O	2.09	0.52
1:C:295:ARG:HH11	1:C:295:ARG:CG	2.04	0.52
1:A:73:PRO:O	1:A:74:LYS:CB	2.57	0.52
1:B:132:LEU:HD23	1:B:157:ARG:HB3	1.90	0.52
1:D:204:ALA:O	1:D:211:ILE:HG13	2.09	0.52
1:A:148:TRP:CD1	1:A:153:LEU:O	2.63	0.52
1:C:202:SER:HA	1:C:218:LYS:HE2	1.92	0.52
1:A:154:PRO:HD2	1:A:157:ARG:HD3	1.91	0.52
1:B:278:GLY:HA2	1:B:282:GLU:O	2.09	0.52
1:D:148:TRP:CD1	1:D:153:LEU:O	2.63	0.52
1:A:215:VAL:O	1:A:216:GLU:CB	2.57	0.52
1:B:160:GLY:CA	1:B:273:SER:HB3	2.32	0.52
1:B:202:SER:HA	1:B:218:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:TRP:CD1	1:C:153:LEU:O	2.63	0.52
1:A:289:VAL:CG1	1:A:301:VAL:HG13	2.40	0.52
2:B:7:SO4:O3	3:B:5:NAD:O7N	2.28	0.52
1:A:94:ILE:HD11	1:A:133:PHE:CE2	2.45	0.51
1:A:137:THR:HG22	1:A:143:LEU:CD1	2.39	0.51
1:B:15:MET:HE1	1:B:18:ASN:CB	2.38	0.51
1:B:67:HIS:HB3	1:D:169:ARG:HG3	1.91	0.51
1:B:215:VAL:O	1:B:216:GLU:CB	2.57	0.51
1:C:278:GLY:HA2	1:C:282:GLU:O	2.09	0.51
1:A:125:MET:HE1	1:A:129:PHE:HD2	1.74	0.51
1:C:110:VAL:CG2	1:C:139:PRO:HG3	2.40	0.51
1:D:110:VAL:CG2	1:D:139:PRO:HG3	2.40	0.51
1:D:321:LEU:O	1:D:323:SER:N	2.44	0.51
1:A:160:GLY:CA	1:A:273:SER:HB3	2.32	0.51
1:B:94:ILE:HD11	1:B:133:PHE:CE2	2.45	0.51
1:B:289:VAL:CG1	1:B:301:VAL:HG13	2.40	0.51
1:C:289:VAL:CG1	1:C:301:VAL:HG13	2.40	0.51
1:D:295:ARG:NH1	1:D:295:ARG:CG	2.65	0.51
1:A:216:GLU:CG	1:A:217:SER:N	2.61	0.51
1:B:142:ILE:HD11	1:B:324:VAL:HG11	1.93	0.51
1:C:94:ILE:HD11	1:C:133:PHE:CE2	2.45	0.51
1:C:189:ILE:HD13	1:C:233:VAL:HG11	1.93	0.51
1:C:265:ASN:HD22	1:C:295:ARG:H	1.58	0.51
1:C:321:LEU:O	1:C:323:SER:N	2.44	0.51
1:D:73:PRO:O	1:D:74:LYS:CB	2.57	0.51
1:D:265:ASN:HD22	1:D:295:ARG:H	1.58	0.51
1:A:189:ILE:HD13	1:A:233:VAL:HG11	1.92	0.51
1:D:189:ILE:HD13	1:D:233:VAL:HG11	1.93	0.51
1:A:202:SER:HA	1:A:218:LYS:HE2	1.91	0.51
2:A:3:SO4:O3	3:A:1:NAD:O7N	2.29	0.51
1:B:148:TRP:CD1	1:B:153:LEU:O	2.63	0.51
1:B:169:ARG:HG3	1:D:67:HIS:HB3	1.91	0.51
1:D:94:ILE:HD11	1:D:133:PHE:CE2	2.45	0.51
1:D:243:LYS:HB3	1:D:243:LYS:HZ2	1.75	0.51
1:A:321:LEU:O	1:A:323:SER:N	2.44	0.51
1:B:279:LEU:CD1	1:B:303:GLU:HG3	2.41	0.51
1:B:321:LEU:C	1:B:323:SER:N	2.64	0.51
1:B:321:LEU:O	1:B:323:SER:N	2.44	0.51
1:C:295:ARG:NH1	1:C:295:ARG:CG	2.65	0.51
1:A:125:MET:CE	1:A:129:PHE:HD2	2.24	0.51
1:A:157:ARG:HG2	1:A:157:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:HG2	1:C:67:HIS:CG	2.32	0.51
1:A:169:ARG:CG	1:C:67:HIS:HD2	2.12	0.51
1:A:313:ARG:HH11	1:A:313:ARG:CG	2.05	0.51
1:B:265:ASN:HD22	1:B:295:ARG:H	1.58	0.51
1:D:94:ILE:HD11	1:D:133:PHE:CD2	2.45	0.51
1:D:157:ARG:HG2	1:D:157:ARG:NH1	2.25	0.51
1:B:107:LEU:HD13	1:B:328:ALA:HB2	1.93	0.51
1:B:169:ARG:O	1:B:173:LEU:HG	2.11	0.51
1:C:94:ILE:HD11	1:C:133:PHE:CD2	2.46	0.51
1:B:110:VAL:CG2	1:B:139:PRO:HG3	2.40	0.50
1:B:125:MET:CE	1:B:129:PHE:HD2	2.24	0.50
1:C:169:ARG:O	1:C:173:LEU:HG	2.11	0.50
1:C:226:LEU:C	1:C:228:ARG:N	2.64	0.50
2:C:11:SO4:O3	3:C:9:NAD:O7N	2.28	0.50
1:D:279:LEU:CD1	1:D:303:GLU:HG3	2.41	0.50
1:D:289:VAL:CG1	1:D:301:VAL:HG13	2.40	0.50
1:D:169:ARG:O	1:D:173:LEU:HG	2.11	0.50
1:A:169:ARG:O	1:A:173:LEU:HG	2.11	0.50
1:A:178:PHE:O	1:A:179:SER:CB	2.54	0.50
1:A:265:ASN:HD22	1:A:295:ARG:H	1.58	0.50
1:B:189:ILE:HD13	1:B:233:VAL:HG11	1.92	0.50
1:B:284:ASP:H	1:B:322:LYS:HE3	1.77	0.50
1:C:279:LEU:CD1	1:C:303:GLU:HG3	2.41	0.50
1:B:94:ILE:HD11	1:B:133:PHE:CD2	2.45	0.50
1:A:94:ILE:HD11	1:A:133:PHE:CD2	2.45	0.50
1:A:259:THR:HG22	1:A:263:LEU:HD12	1.94	0.50
1:A:279:LEU:CD1	1:A:303:GLU:HG3	2.41	0.50
1:B:169:ARG:CG	1:D:67:HIS:HD2	2.12	0.50
1:C:142:ILE:HD11	1:C:324:VAL:HG11	1.93	0.50
1:C:259:THR:HG22	1:C:263:LEU:HD12	1.94	0.50
1:C:316:HIS:C	1:C:316:HIS:CD2	2.85	0.50
1:D:125:MET:CE	1:D:129:PHE:HD2	2.24	0.50
1:B:226:LEU:C	1:B:228:ARG:N	2.63	0.50
1:A:214:LEU:HD12	1:A:214:LEU:C	2.18	0.50
1:A:329:PHE:O	1:A:331:ARG:N	2.45	0.50
1:C:284:ASP:H	1:C:322:LYS:HE3	1.76	0.50
1:A:107:LEU:HD13	1:A:328:ALA:HB2	1.93	0.50
1:A:316:HIS:CD2	1:A:316:HIS:C	2.85	0.50
1:B:157:ARG:HG2	1:B:157:ARG:NH1	2.26	0.50
1:B:67:HIS:CG	1:D:169:ARG:HG2	2.32	0.50
1:B:169:ARG:NH1	2:B:7:SO4:O2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:MET:CE	1:C:129:PHE:HD2	2.24	0.50
1:D:259:THR:HG22	1:D:263:LEU:HD12	1.94	0.50
1:A:142:ILE:HD11	1:A:324:VAL:HG11	1.93	0.49
1:B:316:HIS:CD2	1:B:316:HIS:C	2.85	0.49
1:C:329:PHE:O	1:C:331:ARG:N	2.45	0.49
1:D:284:ASP:H	1:D:322:LYS:HE3	1.76	0.49
1:B:329:PHE:O	1:B:331:ARG:N	2.45	0.49
1:C:107:LEU:HD13	1:C:328:ALA:HB2	1.93	0.49
1:D:329:PHE:O	1:D:331:ARG:N	2.45	0.49
2:D:332:SO4:O3	3:D:13:NAD:O7N	2.28	0.49
1:A:110:VAL:CG2	1:A:139:PRO:HG3	2.40	0.49
1:B:83:TYR:CD2	1:B:124:VAL:HG12	2.41	0.49
1:B:83:TYR:C	1:B:85:ASP:N	2.66	0.49
1:D:316:HIS:C	1:D:316:HIS:CD2	2.85	0.49
1:A:32:GLY:O	1:A:35:TYR:HB3	2.13	0.49
1:D:142:ILE:HD11	1:D:324:VAL:HG11	1.93	0.49
1:C:83:TYR:C	1:C:85:ASP:H	2.16	0.49
1:C:234:ARG:HG2	1:C:234:ARG:O	2.13	0.49
1:C:244:LYS:O	1:C:244:LYS:CG	2.55	0.49
1:D:83:TYR:C	1:D:85:ASP:N	2.66	0.49
1:D:107:LEU:HD13	1:D:328:ALA:HB2	1.93	0.49
1:B:259:THR:HG22	1:B:263:LEU:HD12	1.94	0.49
1:D:196:THR:HG21	1:D:320:THR:HG21	1.95	0.49
1:B:15:MET:CE	1:B:18:ASN:CB	2.79	0.49
1:D:125:MET:HA	1:D:125:MET:HE2	1.94	0.49
1:A:321:LEU:C	1:A:323:SER:N	2.64	0.49
1:B:32:GLY:O	1:B:35:TYR:HB3	2.13	0.49
1:B:234:ARG:O	1:B:234:ARG:HG2	2.13	0.49
1:D:321:LEU:C	1:D:323:SER:N	2.64	0.49
1:A:174:LEU:HD23	1:A:229:ILE:HD12	1.95	0.49
1:A:205:TYR:HD2	1:A:210:PRO:HA	1.78	0.49
1:B:205:TYR:HD2	1:B:210:PRO:HA	1.78	0.49
1:C:321:LEU:C	1:C:323:SER:N	2.64	0.49
1:D:205:TYR:HD2	1:D:210:PRO:HA	1.78	0.49
1:A:164:ILE:HG21	1:A:164:ILE:HD13	1.48	0.48
1:C:32:GLY:O	1:C:35:TYR:HB3	2.13	0.48
1:C:169:ARG:NH1	2:C:11:SO4:O2	2.38	0.48
1:C:157:ARG:HG2	1:C:157:ARG:NH1	2.25	0.48
1:D:32:GLY:O	1:D:35:TYR:HB3	2.13	0.48
1:A:200:VAL:HG21	1:A:304:ILE:CD1	2.44	0.48
1:D:174:LEU:HD23	1:D:229:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:O	1:A:234:ARG:HG2	2.13	0.48
1:A:284:ASP:H	1:A:322:LYS:HE3	1.77	0.48
1:B:294:ASN:C	1:B:294:ASN:ND2	2.67	0.48
1:C:83:TYR:C	1:C:85:ASP:N	2.66	0.48
1:D:145:TYR:O	1:D:148:TRP:HB3	2.13	0.48
1:D:328:ALA:O	1:D:329:PHE:CB	2.62	0.48
1:A:145:TYR:O	1:A:148:TRP:HB3	2.14	0.48
1:B:145:TYR:O	1:B:148:TRP:HB3	2.14	0.48
1:C:145:TYR:O	1:C:148:TRP:HB3	2.13	0.48
1:C:174:LEU:HD23	1:C:229:ILE:HD12	1.95	0.48
1:C:200:VAL:HG21	1:C:304:ILE:CD1	2.44	0.48
1:D:321:LEU:C	1:D:323:SER:H	2.16	0.48
1:D:200:VAL:HG21	1:D:304:ILE:CD1	2.44	0.48
1:D:234:ARG:O	1:D:234:ARG:HG2	2.13	0.48
1:A:83:TYR:C	1:A:85:ASP:H	2.16	0.48
1:B:196:THR:HG21	1:B:320:THR:HG21	1.95	0.48
1:B:321:LEU:C	1:B:323:SER:H	2.16	0.48
1:C:239:GLN:O	1:C:242:GLU:HG2	2.14	0.48
1:D:244:LYS:O	1:D:244:LYS:CG	2.55	0.48
1:D:294:ASN:C	1:D:294:ASN:ND2	2.67	0.48
1:A:83:TYR:C	1:A:85:ASP:N	2.66	0.48
1:A:321:LEU:C	1:A:323:SER:H	2.16	0.48
1:B:83:TYR:C	1:B:85:ASP:H	2.16	0.48
1:B:174:LEU:HD23	1:B:229:ILE:HD12	1.95	0.47
1:A:196:THR:HG21	1:A:320:THR:HG21	1.95	0.47
1:A:228:ARG:HH11	1:A:228:ARG:HD2	1.47	0.47
1:B:200:VAL:HG21	1:B:304:ILE:CD1	2.43	0.47
1:B:203:GLN:HE22	1:B:305:GLU:H	1.62	0.47
1:D:239:GLN:O	1:D:242:GLU:HG2	2.14	0.47
1:B:125:MET:HE1	1:B:129:PHE:HD2	1.79	0.47
1:B:328:ALA:O	1:B:329:PHE:CB	2.62	0.47
1:C:74:LYS:HE2	1:D:266:GLU:OE2	2.15	0.47
1:C:205:TYR:HD2	1:C:210:PRO:HA	1.78	0.47
1:C:279:LEU:HD12	1:C:303:GLU:HG3	1.97	0.47
1:A:294:ASN:C	1:A:294:ASN:ND2	2.67	0.47
1:C:178:PHE:O	1:C:179:SER:CB	2.54	0.47
1:D:83:TYR:C	1:D:85:ASP:H	2.16	0.47
1:D:226:LEU:C	1:D:228:ARG:N	2.64	0.47
1:B:164:ILE:HG21	1:B:164:ILE:HD13	1.48	0.47
1:A:279:LEU:HD12	1:A:303:GLU:HG3	1.97	0.47
1:B:279:LEU:HD12	1:B:303:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ALA:O	1:C:329:PHE:CB	2.62	0.47
1:D:155:HIS:CD2	1:D:275:TYR:HB3	2.50	0.47
1:B:239:GLN:O	1:B:242:GLU:HG2	2.14	0.47
1:C:321:LEU:C	1:C:323:SER:H	2.16	0.47
1:A:155:HIS:CD2	1:A:275:TYR:HB3	2.50	0.47
1:A:328:ALA:O	1:A:329:PHE:CB	2.62	0.47
1:C:111:ASP:HB3	1:C:331:ARG:O	2.15	0.47
1:D:15:MET:CE	1:D:18:ASN:CB	2.78	0.47
1:D:203:GLN:HE22	1:D:305:GLU:H	1.62	0.47
1:A:132:LEU:HD12	1:A:262:ILE:CG2	2.45	0.47
1:C:155:HIS:CD2	1:C:275:TYR:HB3	2.50	0.47
1:C:226:LEU:HA	1:C:229:ILE:HG13	1.97	0.47
1:C:190:ILE:CD1	1:C:306:LEU:HD11	2.44	0.47
1:A:226:LEU:HA	1:A:229:ILE:HG13	1.97	0.46
1:B:67:HIS:HD2	1:D:169:ARG:CG	2.12	0.46
1:C:87:ARG:O	1:C:88:ASP:CB	2.44	0.46
1:C:294:ASN:C	1:C:294:ASN:ND2	2.67	0.46
1:C:196:THR:HG21	1:C:320:THR:HG21	1.95	0.46
1:A:239:GLN:O	1:A:242:GLU:HG2	2.14	0.46
1:A:266:GLU:OE2	1:B:74:LYS:HE2	2.15	0.46
1:B:18:ASN:OD1	1:B:18:ASN:N	2.47	0.46
1:B:214:LEU:HD12	1:B:214:LEU:C	2.17	0.46
1:C:18:ASN:OD1	1:C:18:ASN:N	2.47	0.46
1:D:18:ASN:OD1	1:D:18:ASN:N	2.47	0.46
1:D:279:LEU:HD12	1:D:303:GLU:HG3	1.97	0.46
1:A:142:ILE:CD1	1:A:324:VAL:HG11	2.46	0.46
1:B:262:ILE:HD13	1:B:262:ILE:HG21	1.56	0.46
1:C:15:MET:CE	1:C:18:ASN:CB	2.78	0.46
1:A:198:LEU:HD23	1:A:198:LEU:H	1.81	0.46
1:B:142:ILE:CD1	1:B:324:VAL:HG11	2.46	0.46
1:B:155:HIS:CD2	1:B:275:TYR:HB3	2.50	0.46
1:C:203:GLN:HE22	1:C:305:GLU:H	1.62	0.46
1:D:153:LEU:HA	1:D:154:PRO:HD3	1.81	0.46
1:D:198:LEU:HD23	1:D:198:LEU:H	1.81	0.46
1:A:86:CYS:HA	1:A:89:ALA:CB	2.46	0.46
1:A:169:ARG:NH1	2:A:3:SO4:O2	2.38	0.46
1:A:203:GLN:HE21	1:A:304:ILE:HB	1.81	0.46
1:B:203:GLN:HE21	1:B:304:ILE:HB	1.81	0.46
1:B:226:LEU:HA	1:B:229:ILE:HG13	1.97	0.46
1:C:63:MET:O	1:C:64:ASP:C	2.54	0.46
1:C:142:ILE:CD1	1:C:324:VAL:HG11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:GLN:HE21	1:C:304:ILE:HB	1.81	0.46
1:C:266:GLU:OE2	1:D:74:LYS:HE2	2.15	0.46
1:D:111:ASP:HB3	1:D:331:ARG:O	2.15	0.46
1:D:142:ILE:CD1	1:D:324:VAL:HG11	2.46	0.46
1:B:198:LEU:HD23	1:B:198:LEU:H	1.81	0.46
1:B:203:GLN:NE2	1:B:304:ILE:HB	2.31	0.46
1:C:132:LEU:HD12	1:C:262:ILE:CG2	2.45	0.46
1:D:63:MET:O	1:D:64:ASP:C	2.54	0.46
1:D:160:GLY:CA	1:D:273:SER:CB	2.93	0.46
1:D:203:GLN:HE21	1:D:304:ILE:HB	1.81	0.46
1:A:82:ASP:HB3	1:A:83:TYR:H	1.34	0.46
1:A:83:TYR:CD2	1:A:124:VAL:HG12	2.40	0.46
1:A:262:ILE:HD13	1:A:262:ILE:HG21	1.57	0.46
1:B:59:ILE:HG13	1:B:79:TRP:CE2	2.51	0.46
1:B:190:ILE:CD1	1:B:306:LEU:HD11	2.44	0.46
1:C:203:GLN:NE2	1:C:304:ILE:HB	2.31	0.46
1:C:216:GLU:CG	1:C:217:SER:N	2.61	0.46
1:D:169:ARG:NH1	2:D:332:SO4:O2	2.38	0.46
1:A:63:MET:O	1:A:64:ASP:C	2.54	0.46
1:B:153:LEU:HA	1:B:154:PRO:HD3	1.81	0.46
1:B:209:MET:HB3	1:B:213:LYS:CE	2.46	0.46
1:B:269:ILE:HD13	1:B:269:ILE:HG21	1.70	0.46
1:D:86:CYS:HA	1:D:89:ALA:CB	2.46	0.46
1:A:74:LYS:HE2	1:B:266:GLU:OE2	2.15	0.45
1:B:111:ASP:HB3	1:B:331:ARG:O	2.15	0.45
1:B:132:LEU:HD12	1:B:262:ILE:CG2	2.45	0.45
1:B:178:PHE:O	1:B:179:SER:CB	2.54	0.45
1:D:132:LEU:HD12	1:D:262:ILE:CG2	2.45	0.45
1:D:226:LEU:HA	1:D:229:ILE:HG13	1.97	0.45
1:A:18:ASN:OD1	1:A:18:ASN:N	2.47	0.45
1:A:59:ILE:HG13	1:A:79:TRP:CE2	2.51	0.45
1:A:203:GLN:HE22	1:A:305:GLU:H	1.62	0.45
1:C:86:CYS:HA	1:C:89:ALA:CB	2.46	0.45
1:C:107:LEU:C	1:C:109:LEU:H	2.19	0.45
1:A:293:ILE:O	1:A:294:ASN:HB3	2.17	0.45
1:C:59:ILE:HG13	1:C:79:TRP:CE2	2.51	0.45
1:A:111:ASP:HB3	1:A:331:ARG:O	2.15	0.45
1:A:243:LYS:HB3	1:A:243:LYS:HZ3	1.79	0.45
1:B:63:MET:O	1:B:64:ASP:C	2.54	0.45
1:B:86:CYS:HA	1:B:89:ALA:CB	2.46	0.45
1:B:107:LEU:C	1:B:109:LEU:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ILE:O	1:B:295:ARG:HA	2.17	0.45
1:B:269:ILE:HD13	1:B:302:ILE:HD13	1.99	0.45
1:D:262:ILE:O	1:D:295:ARG:HA	2.17	0.45
1:A:107:LEU:C	1:A:109:LEU:H	2.19	0.45
1:A:203:GLN:NE2	1:A:304:ILE:HB	2.31	0.45
1:A:243:LYS:HB2	1:C:56:SER:O	2.17	0.45
1:B:37:PHE:HE2	1:D:34:SER:O	2.00	0.45
1:B:113:ASN:OD1	1:B:116:ILE:HD12	2.17	0.45
1:C:262:ILE:O	1:C:295:ARG:HA	2.17	0.45
1:D:59:ILE:HG13	1:D:79:TRP:CE2	2.51	0.45
1:D:262:ILE:HD13	1:D:262:ILE:HG21	1.56	0.45
1:D:269:ILE:HD13	1:D:302:ILE:HD13	1.99	0.45
1:A:190:ILE:CD1	1:A:306:LEU:HD11	2.45	0.45
1:A:262:ILE:O	1:A:295:ARG:HA	2.17	0.45
1:B:243:LYS:HB2	1:D:56:SER:O	2.17	0.45
1:C:113:ASN:OD1	1:C:116:ILE:HD12	2.17	0.45
1:C:244:LYS:HE2	1:C:248:TYR:CZ	2.52	0.45
1:C:284:ASP:N	1:C:322:LYS:NZ	2.65	0.45
1:D:203:GLN:NE2	1:D:304:ILE:HB	2.31	0.45
1:A:284:ASP:N	1:A:322:LYS:NZ	2.65	0.45
1:B:56:SER:O	1:D:243:LYS:HB2	2.17	0.45
1:C:241:ILE:O	1:C:245:GLY:N	2.49	0.45
1:D:209:MET:HB3	1:D:213:LYS:CE	2.46	0.45
1:D:216:GLU:CG	1:D:217:SER:N	2.61	0.45
1:D:293:ILE:O	1:D:294:ASN:HB3	2.17	0.45
1:A:37:PHE:HE2	1:C:34:SER:O	2.00	0.45
1:B:244:LYS:O	1:B:244:LYS:CG	2.55	0.45
1:B:283:ARG:H	1:B:322:LYS:NZ	2.03	0.45
1:C:209:MET:HB3	1:C:213:LYS:CE	2.46	0.45
1:A:269:ILE:HD13	1:A:302:ILE:HD13	1.99	0.45
1:C:198:LEU:HD23	1:C:198:LEU:H	1.81	0.45
1:C:293:ILE:O	1:C:294:ASN:HB3	2.17	0.45
1:D:39:LEU:HD22	1:D:44:ILE:HB	1.99	0.45
1:A:244:LYS:HE2	1:A:248:TYR:CZ	2.52	0.44
1:D:107:LEU:C	1:D:109:LEU:H	2.19	0.44
1:B:34:SER:O	1:D:37:PHE:HE2	2.00	0.44
1:B:244:LYS:HE2	1:B:248:TYR:CZ	2.52	0.44
1:D:113:ASN:OD1	1:D:116:ILE:HD12	2.17	0.44
1:A:39:LEU:HD22	1:A:44:ILE:HB	1.99	0.44
1:A:170:PHE:HD1	1:A:233:VAL:HG21	1.83	0.44
1:A:226:LEU:C	1:A:228:ARG:N	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LEU:HD22	1:C:44:ILE:HB	1.99	0.44
1:D:244:LYS:HE2	1:D:248:TYR:CZ	2.52	0.44
1:A:56:SER:O	1:C:243:LYS:HB2	2.17	0.44
1:C:153:LEU:HA	1:C:154:PRO:HD3	1.81	0.44
1:C:269:ILE:HD13	1:C:302:ILE:HD13	1.99	0.44
1:C:294:ASN:HD22	1:C:295:ARG:N	2.15	0.44
1:D:164:ILE:HD13	1:D:164:ILE:HG21	1.48	0.44
1:A:113:ASN:OD1	1:A:116:ILE:HD12	2.17	0.44
1:B:39:LEU:HD22	1:B:44:ILE:HB	1.99	0.44
1:B:82:ASP:HB3	1:B:83:TYR:H	1.34	0.44
1:C:125:MET:HA	1:C:125:MET:HE2	1.97	0.44
1:C:249:TYR:OH	5:C:385:HOH:O	2.16	0.44
1:A:15:MET:CE	1:A:18:ASN:CB	2.79	0.44
1:A:63:MET:O	1:A:66:ASN:N	2.51	0.44
1:A:209:MET:HB3	1:A:213:LYS:CE	2.46	0.44
1:B:283:ARG:O	1:B:284:ASP:HB2	2.18	0.44
1:B:294:ASN:HD22	1:B:295:ARG:N	2.15	0.44
1:C:39:LEU:HD23	1:C:39:LEU:HA	1.72	0.44
1:C:214:LEU:HD12	1:C:214:LEU:C	2.17	0.44
1:C:254:GLY:O	1:C:258:VAL:HG23	2.18	0.44
1:D:284:ASP:N	1:D:322:LYS:NZ	2.65	0.44
1:B:63:MET:O	1:B:66:ASN:N	2.51	0.44
1:B:170:PHE:HD1	1:B:233:VAL:HG21	1.83	0.44
1:D:170:PHE:HD1	1:D:233:VAL:HG21	1.83	0.44
1:D:269:ILE:HD13	1:D:269:ILE:HG21	1.70	0.44
1:A:34:SER:O	1:C:37:PHE:HE2	2.00	0.44
1:B:70:VAL:H	1:B:70:VAL:HG23	1.42	0.44
1:C:295:ARG:HG3	1:D:18:ASN:HD21	1.83	0.44
1:D:254:GLY:O	1:D:258:VAL:HG23	2.18	0.44
1:A:170:PHE:CD1	1:A:233:VAL:HG21	2.53	0.43
1:C:63:MET:O	1:C:66:ASN:N	2.51	0.43
1:C:283:ARG:O	1:C:284:ASP:HB2	2.18	0.43
1:D:63:MET:O	1:D:66:ASN:N	2.51	0.43
1:A:171:ARG:HH11	1:A:171:ARG:HD3	1.56	0.43
1:A:244:LYS:O	1:A:244:LYS:CG	2.55	0.43
1:B:170:PHE:CD1	1:B:233:VAL:HG21	2.53	0.43
1:B:241:ILE:O	1:B:245:GLY:N	2.49	0.43
1:B:284:ASP:N	1:B:322:LYS:NZ	2.65	0.43
1:C:262:ILE:HD13	1:C:262:ILE:HG21	1.56	0.43
1:D:190:ILE:CD1	1:D:306:LEU:HD11	2.44	0.43
1:B:293:ILE:O	1:B:294:ASN:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:TRP:NE1	1:C:227:GLU:OE1	2.51	0.43
1:D:170:PHE:CD1	1:D:233:VAL:HG21	2.54	0.43
1:D:322:LYS:HA	1:D:325:LEU:HD12	2.01	0.43
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.59	0.43
1:A:241:ILE:O	1:A:245:GLY:N	2.49	0.43
1:A:283:ARG:O	1:A:284:ASP:HB2	2.18	0.43
1:A:295:ARG:HG3	1:B:18:ASN:HD21	1.83	0.43
1:D:171:ARG:HH11	1:D:171:ARG:HD3	1.56	0.43
1:A:18:ASN:HD21	1:B:295:ARG:HG3	1.83	0.43
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.73	0.43
1:A:107:LEU:HD22	1:A:327:ARG:CG	2.49	0.43
1:A:294:ASN:HD22	1:A:295:ARG:N	2.15	0.43
1:A:307:ASN:HB3	1:A:310:GLU:CD	2.39	0.43
1:B:107:LEU:HD22	1:B:327:ARG:CG	2.49	0.43
1:B:329:PHE:HB3	1:B:330:THR:H	1.58	0.43
1:C:109:LEU:HA	1:C:109:LEU:HD12	1.59	0.43
1:D:198:LEU:O	1:D:198:LEU:HG	2.18	0.43
1:D:294:ASN:HD22	1:D:295:ARG:N	2.15	0.43
1:A:31:VAL:HG22	1:A:251:ILE:CG2	2.48	0.43
1:A:196:THR:CG2	1:A:320:THR:HG21	2.49	0.43
1:D:283:ARG:O	1:D:284:ASP:HB2	2.18	0.43
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.60	0.43
1:B:15:MET:HE3	1:B:18:ASN:CB	2.35	0.43
1:B:196:THR:CG2	1:B:320:THR:HG21	2.49	0.43
1:C:125:MET:HE1	1:C:129:PHE:HD2	1.83	0.43
1:C:160:GLY:CA	1:C:273:SER:CB	2.93	0.43
1:C:170:PHE:CD1	1:C:233:VAL:HG21	2.53	0.43
1:D:241:ILE:O	1:D:245:GLY:N	2.49	0.43
1:D:307:ASN:HB3	1:D:310:GLU:CD	2.39	0.43
1:B:254:GLY:O	1:B:258:VAL:HG23	2.18	0.43
1:C:121:VAL:O	1:C:124:VAL:HG22	2.19	0.43
1:C:170:PHE:HD1	1:C:233:VAL:HG21	1.83	0.43
1:C:183:GLN:NE2	4:C:6:FBP:H4	2.33	0.43
1:C:307:ASN:HB3	1:C:310:GLU:CD	2.39	0.43
1:A:322:LYS:HA	1:A:325:LEU:HD12	2.01	0.43
1:A:329:PHE:HB3	1:A:330:THR:H	1.58	0.43
1:B:39:LEU:HD23	1:B:39:LEU:HA	1.73	0.43
1:B:307:ASN:HB3	1:B:310:GLU:CD	2.39	0.43
1:D:109:LEU:HD12	1:D:109:LEU:HA	1.59	0.43
1:A:260:ARG:HH11	1:A:260:ARG:HD2	1.15	0.42
1:B:121:VAL:O	1:B:124:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASN:OD1	3:C:9:NAD:C2N	2.67	0.42
1:C:196:THR:CG2	1:C:320:THR:HG21	2.49	0.42
1:D:31:VAL:HG22	1:D:251:ILE:CG2	2.49	0.42
1:A:138:ASN:OD1	3:A:1:NAD:C2N	2.68	0.42
1:A:198:LEU:HG	1:A:198:LEU:O	2.18	0.42
1:D:183:GLN:NE2	4:D:2:FBP:H4	2.33	0.42
1:A:254:GLY:O	1:A:258:VAL:HG23	2.18	0.42
1:B:243:LYS:HB3	1:B:243:LYS:HZ3	1.80	0.42
1:C:31:VAL:HG22	1:C:251:ILE:CG2	2.49	0.42
1:D:260:ARG:HH11	1:D:260:ARG:HD2	1.15	0.42
1:B:125:MET:HA	1:B:125:MET:HE2	2.02	0.42
1:B:322:LYS:HA	1:B:325:LEU:HD12	2.01	0.42
1:B:31:VAL:HG22	1:B:251:ILE:CG2	2.49	0.42
1:B:201:TRP:NE1	1:B:227:GLU:OE1	2.51	0.42
1:C:322:LYS:HA	1:C:325:LEU:HD12	2.01	0.42
1:B:129:PHE:HE2	1:B:133:PHE:CE1	2.37	0.42
1:B:267:ASN:H	1:B:294:ASN:HB3	1.85	0.42
1:C:328:ALA:O	1:C:329:PHE:HB2	2.20	0.42
1:B:198:LEU:O	1:B:198:LEU:HG	2.18	0.42
1:C:156:GLU:O	1:C:298:ILE:N	2.50	0.42
1:C:198:LEU:HG	1:C:198:LEU:O	2.18	0.42
1:D:138:ASN:OD1	3:D:13:NAD:C2N	2.67	0.42
1:D:143:LEU:HD23	1:D:143:LEU:HA	1.93	0.42
1:A:124:VAL:CG2	1:A:133:PHE:HZ	2.32	0.42
1:B:328:ALA:O	1:B:329:PHE:HB2	2.20	0.42
1:B:138:ASN:OD1	3:B:5:NAD:C2N	2.68	0.42
1:C:18:ASN:HD21	1:D:295:ARG:HG3	1.83	0.42
1:C:192:GLU:HB3	1:C:196:THR:OG1	2.20	0.42
1:C:276:LEU:HG	1:C:287:ILE:HG22	2.02	0.42
1:D:121:VAL:O	1:D:124:VAL:HG22	2.19	0.42
1:A:121:VAL:O	1:A:124:VAL:HG22	2.19	0.42
1:A:267:ASN:H	1:A:294:ASN:HB3	1.85	0.42
1:B:253:MET:CE	1:D:72:ALA:HB2	2.50	0.42
1:C:124:VAL:CG2	1:C:133:PHE:HZ	2.33	0.42
1:C:165:LEU:HD21	1:C:169:ARG:NH2	2.35	0.42
1:D:201:TRP:NE1	1:D:227:GLU:OE1	2.52	0.42
1:A:253:MET:CE	1:C:72:ALA:HB2	2.50	0.41
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.92	0.41
1:C:267:ASN:H	1:C:294:ASN:HB3	1.85	0.41
1:D:107:LEU:HD22	1:D:327:ARG:CG	2.49	0.41
1:D:124:VAL:CG2	1:D:133:PHE:HZ	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LEU:HD21	1:D:169:ARG:NH2	2.35	0.41
1:A:201:TRP:NE1	1:A:227:GLU:OE1	2.52	0.41
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.93	0.41
1:A:328:ALA:O	1:A:329:PHE:HB2	2.20	0.41
1:B:228:ARG:HH11	1:B:228:ARG:HD2	1.47	0.41
1:C:276:LEU:HD21	1:C:289:VAL:HG21	2.03	0.41
1:D:173:LEU:HA	1:D:173:LEU:HD23	1.61	0.41
1:D:196:THR:CG2	1:D:320:THR:HG21	2.49	0.41
1:A:72:ALA:HB2	1:C:253:MET:CE	2.50	0.41
1:A:156:GLU:O	1:A:298:ILE:N	2.50	0.41
1:C:227:GLU:OE1	1:C:227:GLU:HA	2.20	0.41
1:D:148:TRP:HD1	1:D:153:LEU:O	2.04	0.41
1:A:124:VAL:HG21	1:A:133:PHE:HZ	1.86	0.41
1:B:72:ALA:HB2	1:D:253:MET:CE	2.50	0.41
1:B:160:GLY:CA	1:B:273:SER:CB	2.93	0.41
1:B:165:LEU:HD21	1:B:169:ARG:NH2	2.35	0.41
1:C:276:LEU:HD23	1:C:276:LEU:HA	1.92	0.41
1:A:15:MET:HE1	1:A:18:ASN:CB	2.46	0.41
1:A:83:TYR:CD2	1:A:124:VAL:CG1	3.04	0.41
1:B:134:LEU:HD21	1:B:255:LEU:HD12	2.03	0.41
1:B:276:LEU:HG	1:B:287:ILE:HG22	2.02	0.41
1:D:192:GLU:HB3	1:D:196:THR:OG1	2.20	0.41
1:D:276:LEU:HG	1:D:287:ILE:HG22	2.02	0.41
1:D:276:LEU:HD21	1:D:289:VAL:HG21	2.03	0.41
1:A:227:GLU:OE1	1:A:227:GLU:HA	2.20	0.41
1:D:267:ASN:H	1:D:294:ASN:HB3	1.85	0.41
1:D:328:ALA:O	1:D:329:PHE:HB2	2.20	0.41
2:D:332:SO4:O3	3:D:13:NAD:C7N	2.69	0.41
2:A:3:SO4:O3	3:A:1:NAD:C7N	2.69	0.41
1:B:124:VAL:CG2	1:B:133:PHE:HZ	2.32	0.41
2:B:7:SO4:O3	3:B:5:NAD:C7N	2.69	0.41
1:C:129:PHE:HE2	1:C:133:PHE:CE1	2.37	0.41
2:C:11:SO4:O3	3:C:9:NAD:C7N	2.69	0.41
1:D:39:LEU:HA	1:D:39:LEU:HD23	1.73	0.41
1:D:83:TYR:CD2	1:D:124:VAL:CG1	3.04	0.41
1:D:125:MET:HE1	1:D:129:PHE:HD2	1.86	0.41
1:A:194:GLY:O	1:A:197:GLU:OE2	2.39	0.41
1:B:26:ILE:HG21	1:B:120:ILE:CG2	2.52	0.40
1:B:124:VAL:HG21	1:B:133:PHE:HZ	1.86	0.40
1:B:227:GLU:OE1	1:B:227:GLU:HA	2.20	0.40
1:B:279:LEU:HD12	1:B:303:GLU:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:CD2	1:C:124:VAL:CG1	3.04	0.40
1:A:192:GLU:HB3	1:A:196:THR:OG1	2.20	0.40
1:B:194:GLY:O	1:B:197:GLU:OE2	2.39	0.40
1:B:276:LEU:HD21	1:B:289:VAL:HG21	2.03	0.40
1:C:267:ASN:HA	1:C:293:ILE:O	2.21	0.40
1:C:279:LEU:HD12	1:C:303:GLU:CG	2.51	0.40
1:D:24:VAL:HG22	1:D:49:VAL:CG2	2.52	0.40
1:B:98:ALA:CB	1:B:113:ASN:OD1	2.70	0.40
1:B:169:ARG:CG	1:D:67:HIS:CG	3.01	0.40
1:C:173:LEU:HA	1:C:173:LEU:HD23	1.60	0.40
1:C:228:ARG:HH11	1:C:228:ARG:HD2	1.47	0.40
1:D:276:LEU:HD23	1:D:276:LEU:HA	1.92	0.40
1:A:24:VAL:HG22	1:A:49:VAL:CG2	2.52	0.40
1:A:67:HIS:HD2	1:C:169:ARG:CG	2.12	0.40
1:A:165:LEU:HD21	1:A:169:ARG:NH2	2.36	0.40
1:A:269:ILE:HD13	1:A:269:ILE:HG21	1.70	0.40
1:C:26:ILE:HG21	1:C:120:ILE:CG2	2.52	0.40
1:C:329:PHE:HB3	1:C:330:THR:H	1.59	0.40
1:D:134:LEU:HD21	1:D:255:LEU:HD12	2.03	0.40
1:A:267:ASN:HA	1:A:293:ILE:O	2.21	0.40
1:B:24:VAL:HG22	1:B:49:VAL:CG2	2.52	0.40
1:D:279:LEU:HD12	1:D:303:GLU:CG	2.52	0.40

All (63) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:C	1:D:331:ARG:CB[6_665]	0.13	2.07
1:A:327:ARG:CB	1:D:330:THR:O[6_665]	0.27	1.93
1:A:324:VAL:N	1:D:330:THR:CG2[6_665]	0.54	1.66
1:A:325:LEU:C	1:D:331:ARG:NE[6_665]	0.77	1.43
1:B:107:LEU:CG	5:A:378:HOH:O[5_554]	0.77	1.43
1:C:316:HIS:CE1	1:D:316:HIS:NE2[6_655]	0.93	1.27
1:A:327:ARG:CB	1:D:330:THR:C[6_665]	1.03	1.17
1:A:327:ARG:N	1:D:331:ARG:CA[6_665]	1.05	1.15
1:A:323:SER:C	1:D:330:THR:CB[6_665]	1.06	1.14
1:A:325:LEU:O	1:D:331:ARG:NE[6_665]	1.10	1.10
1:A:325:LEU:C	1:D:331:ARG:CD[6_665]	1.17	1.03
1:C:316:HIS:NE2	1:D:316:HIS:CE1[6_655]	1.20	1.00
1:A:327:ARG:N	1:D:331:ARG:N[6_665]	1.21	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:O	1:D:330:THR:CB[6_665]	1.24	0.96
1:A:325:LEU:O	1:D:331:ARG:CD[6_665]	1.24	0.96
1:A:326:ALA:O	1:D:331:ARG:CB[6_665]	1.31	0.89
1:A:326:ALA:N	1:D:331:ARG:CD[6_665]	1.33	0.87
1:A:326:ALA:N	1:D:331:ARG:CG[6_665]	1.34	0.86
1:A:327:ARG:CG	1:D:330:THR:O[6_665]	1.39	0.81
1:C:316:HIS:CE1	1:D:316:HIS:CE1[6_655]	1.39	0.81
1:C:316:HIS:NE2	1:D:316:HIS:NE2[6_655]	1.39	0.81
1:A:326:ALA:CA	1:D:331:ARG:CB[6_665]	1.40	0.80
1:A:327:ARG:N	1:D:331:ARG:CB[6_665]	1.40	0.80
1:A:111:ASP:OD2	1:D:118:ARG:NH2[6_665]	1.44	0.76
1:A:326:ALA:C	1:D:331:ARG:CA[6_665]	1.46	0.74
1:A:327:ARG:CA	1:D:330:THR:O[6_665]	1.48	0.72
1:A:323:SER:C	1:D:330:THR:CG2[6_665]	1.49	0.71
1:A:325:LEU:CB	1:D:331:ARG:NH2[6_665]	1.53	0.67
1:A:326:ALA:CA	1:D:331:ARG:CG[6_665]	1.53	0.67
1:C:235:ASP:OD2	1:D:235:ASP:OD2[6_655]	1.53	0.67
1:A:327:ARG:CA	1:D:331:ARG:CA[6_665]	1.55	0.65
1:A:326:ALA:C	1:D:331:ARG:CG[6_665]	1.57	0.63
1:A:325:LEU:CA	1:D:331:ARG:NE[6_665]	1.59	0.61
1:A:326:ALA:CA	1:D:331:ARG:CD[6_665]	1.61	0.59
1:A:324:VAL:N	1:D:330:THR:CB[6_665]	1.64	0.56
1:A:327:ARG:CA	1:D:331:ARG:N[6_665]	1.67	0.53
1:A:327:ARG:CA	1:D:330:THR:C[6_665]	1.68	0.52
1:A:324:VAL:CA	1:D:330:THR:CG2[6_665]	1.69	0.51
1:B:107:LEU:CD1	5:A:378:HOH:O[5_554]	1.69	0.51
1:A:325:LEU:C	1:D:331:ARG:CG[6_665]	1.77	0.43
1:A:327:ARG:N	1:D:331:ARG:CG[6_665]	1.78	0.42
1:A:323:SER:C	1:D:330:THR:OG1[6_665]	1.88	0.32
1:A:326:ALA:N	1:D:331:ARG:NE[6_665]	1.88	0.32
1:A:323:SER:CA	1:D:330:THR:OG1[6_665]	1.89	0.31
1:A:323:SER:CB	1:D:330:THR:OG1[6_665]	1.94	0.26
1:A:323:SER:O	1:D:331:ARG:N[6_665]	1.95	0.25
1:B:107:LEU:CB	5:A:378:HOH:O[5_554]	1.95	0.25
1:A:325:LEU:CG	1:D:331:ARG:NH2[6_665]	1.96	0.24
1:A:325:LEU:CB	1:D:331:ARG:CZ[6_665]	1.98	0.22
1:A:326:ALA:O	1:D:331:ARG:CA[6_665]	2.01	0.19
1:A:325:LEU:CD2	1:D:331:ARG:NH2[6_665]	2.04	0.16
1:C:316:HIS:CD2	1:D:316:HIS:CE1[6_655]	2.04	0.16
1:C:320:THR:OG1	1:D:316:HIS:ND1[6_655]	2.04	0.16
1:A:325:LEU:O	1:D:331:ARG:CZ[6_665]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:HIS:CE1	1:D:316:HIS:CD2[6_655]	2.05	0.15
1:A:323:SER:O	1:D:330:THR:OG1[6_665]	2.07	0.13
1:B:107:LEU:CD2	5:A:378:HOH:O[5_554]	2.07	0.13
1:A:325:LEU:C	1:D:331:ARG:CZ[6_665]	2.08	0.12
1:A:327:ARG:N	1:D:330:THR:C[6_665]	2.12	0.08
1:A:327:ARG:CB	1:D:331:ARG:N[6_665]	2.13	0.07
1:C:316:HIS:ND1	1:D:316:HIS:CE1[6_655]	2.13	0.07
1:C:316:HIS:ND1	1:D:320:THR:OG1[6_655]	2.16	0.04
1:A:323:SER:O	1:D:330:THR:CA[6_665]	2.17	0.03

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	293/317 (92%)	235 (80%)	40 (14%)	18 (6%)	1	7
1	B	293/317 (92%)	235 (80%)	40 (14%)	18 (6%)	1	7
1	C	293/317 (92%)	235 (80%)	40 (14%)	18 (6%)	1	7
1	D	293/317 (92%)	235 (80%)	40 (14%)	18 (6%)	1	7
All	All	1172/1268 (92%)	940 (80%)	160 (14%)	72 (6%)	1	7

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	88	ASP
1	A	217	SER
1	A	328	ALA
1	A	329	PHE
1	B	74	LYS
1	B	88	ASP
1	B	217	SER

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Mol	Chain	Res	Type
1	B	328	ALA
1	B	329	PHE
1	C	74	LYS
1	C	88	ASP
1	C	217	SER
1	C	328	ALA
1	C	329	PHE
1	D	74	LYS
1	D	88	ASP
1	D	217	SER
1	D	328	ALA
1	D	329	PHE
1	A	69	LYS
1	A	75	PRO
1	A	216	GLU
1	A	330	THR
1	B	69	LYS
1	B	75	PRO
1	B	216	GLU
1	B	330	THR
1	C	69	LYS
1	C	75	PRO
1	C	216	GLU
1	C	330	THR
1	D	69	LYS
1	D	75	PRO
1	D	216	GLU
1	D	330	THR
1	A	18	ASN
1	A	87	ARG
1	B	18	ASN
1	B	87	ARG
1	C	18	ASN
1	C	87	ARG
1	D	18	ASN
1	D	87	ARG
1	A	73	PRO
1	B	73	PRO
1	C	73	PRO
1	D	73	PRO
1	A	70	VAL
1	A	172	PHE

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Mol	Chain	Res	Type
1	A	246	ALA
1	A	284	ASP
1	B	70	VAL
1	B	172	PHE
1	B	246	ALA
1	B	284	ASP
1	C	70	VAL
1	C	172	PHE
1	C	246	ALA
1	C	284	ASP
1	D	70	VAL
1	D	172	PHE
1	D	246	ALA
1	D	284	ASP
1	A	19	GLY
1	A	180	VAL
1	B	19	GLY
1	B	180	VAL
1	C	19	GLY
1	C	180	VAL
1	D	19	GLY
1	D	180	VAL

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	243/255 (95%)	212 (87%)	31 (13%)	3	16
1	B	243/255 (95%)	212 (87%)	31 (13%)	3	16
1	C	243/255 (95%)	212 (87%)	31 (13%)	3	16
1	D	243/255 (95%)	212 (87%)	31 (13%)	3	16
All	All	972/1020 (95%)	848 (87%)	124 (13%)	3	16

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	26	ILE
1	A	54	ASN
1	A	56	SER
1	A	79	TRP
1	A	87	ARG
1	A	88	ASP
1	A	91	LEU
1	A	111	ASP
1	A	119	SER
1	A	125	MET
1	A	147	THR
1	A	161	SER
1	A	183	GLN
1	A	198	LEU
1	A	199	PRO
1	A	202	SER
1	A	210	PRO
1	A	214	LEU
1	A	227	GLU
1	A	243	LYS
1	A	247	THR
1	A	257	ARG
1	A	271	THR
1	A	273	SER
1	A	289	VAL
1	A	293	ILE
1	A	294	ASN
1	A	296	ASN
1	A	320	THR
1	A	330	THR
1	B	15	MET
1	B	26	ILE
1	B	54	ASN
1	B	56	SER
1	B	79	TRP
1	B	87	ARG
1	B	88	ASP
1	B	91	LEU
1	B	111	ASP
1	B	119	SER
1	B	125	MET
1	B	147	THR

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Mol	Chain	Res	Type
1	B	161	SER
1	B	183	GLN
1	B	198	LEU
1	B	199	PRO
1	B	202	SER
1	B	210	PRO
1	B	214	LEU
1	B	227	GLU
1	B	243	LYS
1	B	247	THR
1	B	257	ARG
1	B	271	THR
1	B	273	SER
1	B	289	VAL
1	B	293	ILE
1	B	294	ASN
1	B	296	ASN
1	B	320	THR
1	B	330	THR
1	C	15	MET
1	C	26	ILE
1	C	54	ASN
1	C	56	SER
1	C	79	TRP
1	C	87	ARG
1	C	88	ASP
1	C	91	LEU
1	C	111	ASP
1	C	119	SER
1	C	125	MET
1	C	147	THR
1	C	161	SER
1	C	183	GLN
1	C	198	LEU
1	C	199	PRO
1	C	202	SER
1	C	210	PRO
1	C	214	LEU
1	C	227	GLU
1	C	243	LYS
1	C	247	THR
1	C	257	ARG

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Mol	Chain	Res	Type
1	C	271	THR
1	C	273	SER
1	C	289	VAL
1	C	293	ILE
1	C	294	ASN
1	C	296	ASN
1	C	320	THR
1	C	330	THR
1	D	15	MET
1	D	26	ILE
1	D	54	ASN
1	D	56	SER
1	D	79	TRP
1	D	87	ARG
1	D	88	ASP
1	D	91	LEU
1	D	111	ASP
1	D	119	SER
1	D	125	MET
1	D	147	THR
1	D	161	SER
1	D	183	GLN
1	D	198	LEU
1	D	199	PRO
1	D	202	SER
1	D	210	PRO
1	D	214	LEU
1	D	227	GLU
1	D	243	LYS
1	D	247	THR
1	D	257	ARG
1	D	271	THR
1	D	273	SER
1	D	289	VAL
1	D	293	ILE
1	D	294	ASN
1	D	296	ASN
1	D	320	THR
1	D	330	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	67	HIS
1	A	155	HIS
1	A	183	GLN
1	A	232	ASN
1	A	239	GLN
1	A	264	HIS
1	A	265	ASN
1	A	267	ASN
1	A	294	ASN
1	A	316	HIS
1	B	54	ASN
1	B	67	HIS
1	B	155	HIS
1	B	183	GLN
1	B	203	GLN
1	B	232	ASN
1	B	239	GLN
1	B	264	HIS
1	B	265	ASN
1	B	267	ASN
1	B	294	ASN
1	B	316	HIS
1	C	54	ASN
1	C	67	HIS
1	C	155	HIS
1	C	183	GLN
1	C	203	GLN
1	C	232	ASN
1	C	239	GLN
1	C	264	HIS
1	C	265	ASN
1	C	267	ASN
1	C	294	ASN
1	C	316	HIS
1	D	54	ASN
1	D	67	HIS
1	D	155	HIS
1	D	183	GLN
1	D	203	GLN
1	D	232	ASN
1	D	239	GLN
1	D	264	HIS

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Mol	Chain	Res	Type
1	D	265	ASN
1	D	267	ASN
1	D	294	ASN
1	D	316	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FBP	D	2	-	18,20,20	0.78	0	21,32,32	0.95	1 (4%)
2	SO4	B	7	-	4,4,4	0.81	0	6,6,6	0.57	0
3	NAD	D	13	-	42,48,48	1.50	6 (14%)	50,73,73	2.73	13 (26%)
2	SO4	D	333	-	4,4,4	0.98	0	6,6,6	0.22	0
4	FBP	C	6	-	18,20,20	0.79	0	21,32,32	0.95	1 (4%)
2	SO4	C	12	-	4,4,4	0.97	0	6,6,6	0.22	0
2	SO4	D	332	-	4,4,4	0.82	0	6,6,6	0.57	0
3	NAD	C	9	-	42,48,48	1.50	6 (14%)	50,73,73	2.73	13 (26%)
3	NAD	A	1	-	42,48,48	1.49	7 (16%)	50,73,73	2.73	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	B	5	-	42,48,48	1.49	6 (14%)	50,73,73	2.73	13 (26%)
2	SO4	C	11	-	4,4,4	0.82	0	6,6,6	0.57	0
2	SO4	A	4	-	4,4,4	0.97	0	6,6,6	0.21	0
2	SO4	A	3	-	4,4,4	0.81	0	6,6,6	0.57	0
2	SO4	B	8	-	4,4,4	0.98	0	6,6,6	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FBP	D	2	-	-	6/13/32/32	0/1/1/1
4	FBP	C	6	-	-	6/13/32/32	0/1/1/1
3	NAD	C	9	-	-	10/26/62/62	0/5/5/5
3	NAD	A	1	-	-	10/26/62/62	0/5/5/5
3	NAD	B	5	-	-	10/26/62/62	0/5/5/5
3	NAD	D	13	-	-	10/26/62/62	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	9	NAD	O4B-C1B	3.85	1.45	1.40
3	D	13	NAD	O4B-C1B	3.84	1.45	1.40
3	B	5	NAD	O4B-C1B	3.84	1.45	1.40
3	A	1	NAD	O4B-C1B	3.79	1.45	1.40
3	D	13	NAD	C3N-C7N	3.59	1.55	1.50
3	C	9	NAD	C3N-C7N	3.56	1.55	1.50
3	A	1	NAD	C3N-C7N	3.49	1.55	1.50
3	B	5	NAD	C3N-C7N	3.48	1.55	1.50
3	B	5	NAD	C2A-N1A	3.46	1.40	1.33
3	A	1	NAD	C2A-N1A	3.44	1.40	1.33
3	D	13	NAD	O4D-C4D	3.44	1.52	1.45
3	D	13	NAD	C2A-N1A	3.43	1.40	1.33
3	C	9	NAD	O4D-C4D	3.42	1.52	1.45
3	B	5	NAD	O4D-C4D	3.41	1.52	1.45
3	A	1	NAD	O4D-C4D	3.40	1.52	1.45
3	C	9	NAD	C2A-N1A	3.39	1.39	1.33
3	A	1	NAD	C6N-N1N	2.90	1.41	1.35
3	B	5	NAD	C6N-N1N	2.89	1.41	1.35
3	C	9	NAD	C6N-N1N	2.89	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	13	NAD	C6N-N1N	2.87	1.41	1.35
3	A	1	NAD	PN-O3	-2.46	1.56	1.59
3	D	13	NAD	PN-O3	-2.34	1.57	1.59
3	B	5	NAD	PN-O3	-2.32	1.57	1.59
3	C	9	NAD	PN-O3	-2.32	1.57	1.59
3	A	1	NAD	C2N-C3N	-2.00	1.35	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	NAD	C4D-O4D-C1D	-8.68	101.97	109.92
3	D	13	NAD	C4B-O4B-C1B	-8.67	101.99	109.92
3	B	5	NAD	C4D-O4D-C1D	-8.62	102.03	109.92
3	D	13	NAD	C4D-O4D-C1D	-8.60	102.05	109.92
3	B	5	NAD	C4B-O4B-C1B	-8.59	102.06	109.92
3	C	9	NAD	C4B-O4B-C1B	-8.59	102.06	109.92
3	C	9	NAD	C4D-O4D-C1D	-8.58	102.06	109.92
3	A	1	NAD	C4B-O4B-C1B	-8.57	102.08	109.92
3	C	9	NAD	C5N-C4N-C3N	-7.31	113.18	120.36
3	D	13	NAD	C5N-C4N-C3N	-7.29	113.20	120.36
3	B	5	NAD	C5N-C4N-C3N	-7.28	113.21	120.36
3	A	1	NAD	C5N-C4N-C3N	-7.27	113.22	120.36
3	C	9	NAD	C6N-C5N-C4N	6.30	128.53	119.45
3	D	13	NAD	C6N-C5N-C4N	6.29	128.51	119.45
3	B	5	NAD	C6N-C5N-C4N	6.28	128.49	119.45
3	A	1	NAD	C6N-C5N-C4N	6.25	128.46	119.45
3	D	13	NAD	C5N-C6N-N1N	-5.41	113.00	120.38
3	C	9	NAD	C5N-C6N-N1N	-5.40	113.02	120.38
3	B	5	NAD	C5N-C6N-N1N	-5.39	113.04	120.38
3	A	1	NAD	C5N-C6N-N1N	-5.36	113.07	120.38
3	A	1	NAD	O4B-C1B-N9A	-4.48	102.81	108.75
3	D	13	NAD	O4B-C1B-N9A	-4.46	102.83	108.75
3	B	5	NAD	O4B-C1B-N9A	-4.45	102.84	108.75
3	C	9	NAD	O4B-C1B-N9A	-4.44	102.85	108.75
3	C	9	NAD	C4N-C3N-C7N	-3.54	111.41	121.06
3	D	13	NAD	C4N-C3N-C7N	-3.54	111.41	121.06
3	A	1	NAD	C4N-C3N-C7N	-3.54	111.43	121.06
3	B	5	NAD	C4N-C3N-C7N	-3.53	111.45	121.06
3	C	9	NAD	C2N-C3N-C4N	3.30	122.10	118.26
3	B	5	NAD	C2N-C3N-C4N	3.27	122.07	118.26
3	D	13	NAD	C2N-C3N-C4N	3.27	122.06	118.26
3	A	1	NAD	C2N-C3N-C4N	3.27	122.06	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5	NAD	O2A-PA-O3	3.06	115.55	107.27
3	D	13	NAD	O2A-PA-O3	3.06	115.55	107.27
3	A	1	NAD	O2A-PA-O3	3.05	115.53	107.27
3	C	9	NAD	O2A-PA-O3	3.05	115.53	107.27
3	A	1	NAD	O4D-C4D-C5D	-2.49	101.34	109.33
3	B	5	NAD	O4D-C4D-C5D	-2.49	101.37	109.33
3	D	13	NAD	O4D-C4D-C5D	-2.48	101.40	109.33
3	C	9	NAD	O4D-C4D-C5D	-2.47	101.41	109.33
3	B	5	NAD	O2D-C2D-C3D	2.44	119.63	111.82
3	C	9	NAD	O2D-C2D-C3D	2.43	119.62	111.82
3	D	13	NAD	O2D-C2D-C3D	2.43	119.59	111.82
3	A	1	NAD	O2D-C2D-C3D	2.42	119.58	111.82
3	D	13	NAD	C2N-C3N-C7N	2.34	126.22	119.46
3	A	1	NAD	C2N-C3N-C7N	2.34	126.22	119.46
3	C	9	NAD	C2N-C3N-C7N	2.33	126.19	119.46
3	B	5	NAD	C2N-C3N-C7N	2.33	126.19	119.46
3	C	9	NAD	C5B-C4B-C3B	2.10	122.76	115.21
3	A	1	NAD	C5B-C4B-C3B	2.09	122.73	115.21
3	D	13	NAD	C5B-C4B-C3B	2.09	122.72	115.21
3	B	5	NAD	C5B-C4B-C3B	2.08	122.70	115.21
4	D	2	FBP	O2P-P1-O1P	2.05	118.81	110.83
4	C	6	FBP	O2P-P1-O1P	2.04	118.80	110.83

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAD	C5D-O5D-PN-O3
3	A	1	NAD	C5D-O5D-PN-O1N
3	A	1	NAD	C5D-O5D-PN-O2N
3	A	1	NAD	O4D-C1D-N1N-C6N
3	B	5	NAD	C5D-O5D-PN-O3
3	B	5	NAD	C5D-O5D-PN-O1N
3	B	5	NAD	C5D-O5D-PN-O2N
3	B	5	NAD	O4D-C1D-N1N-C6N
3	C	9	NAD	C5D-O5D-PN-O3
3	C	9	NAD	C5D-O5D-PN-O1N
3	C	9	NAD	C5D-O5D-PN-O2N
3	C	9	NAD	O4D-C1D-N1N-C6N
3	D	13	NAD	C5D-O5D-PN-O3
3	D	13	NAD	C5D-O5D-PN-O1N
3	D	13	NAD	C5D-O5D-PN-O2N

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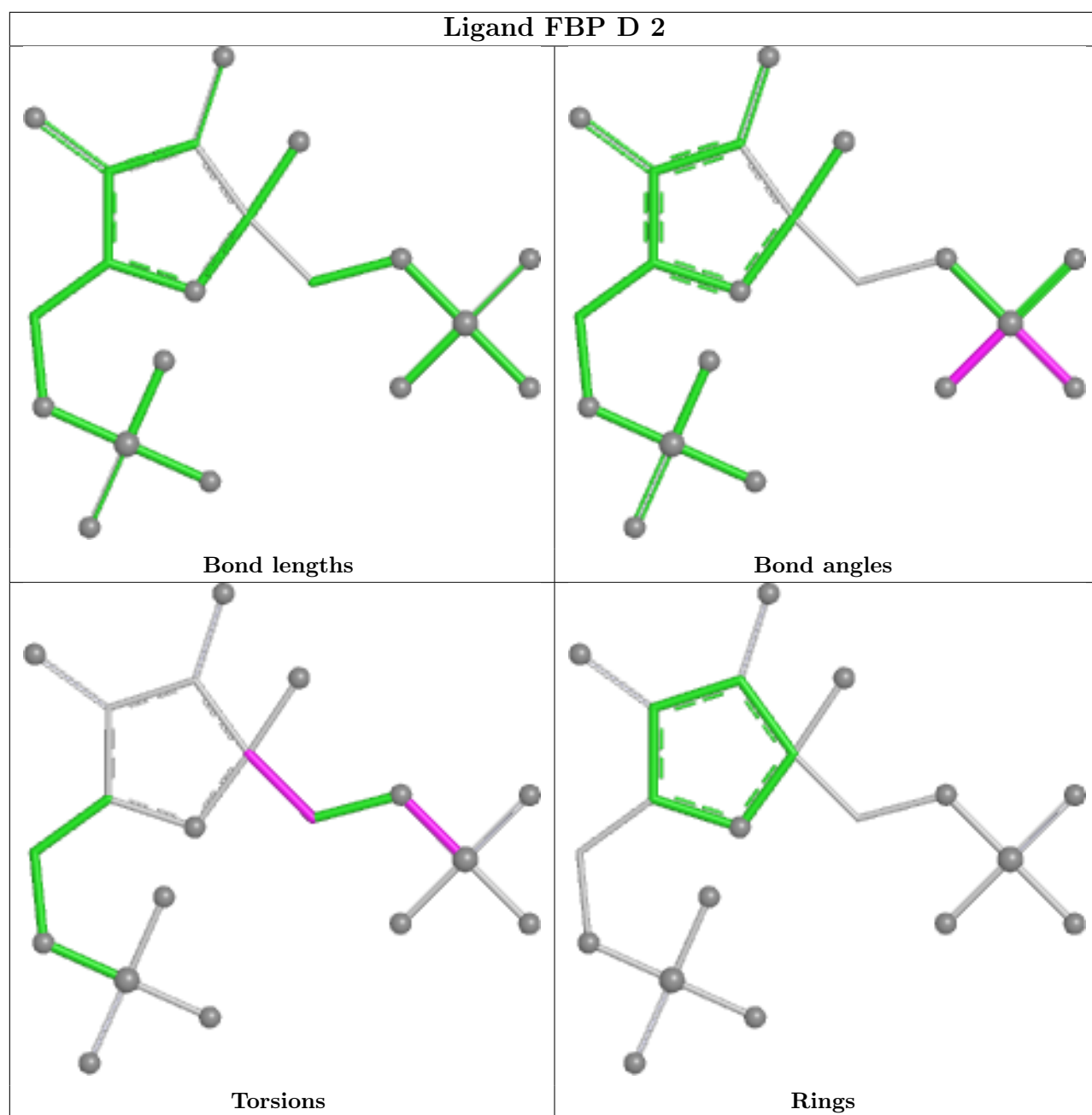
Mol	Chain	Res	Type	Atoms
3	D	13	NAD	O4D-C1D-N1N-C6N
4	C	6	FBP	C1-O1-P1-O2P
4	C	6	FBP	C1-O1-P1-O3P
4	C	6	FBP	O1-C1-C2-C3
4	C	6	FBP	O1-C1-C2-O5
4	D	2	FBP	C1-O1-P1-O2P
4	D	2	FBP	C1-O1-P1-O3P
4	D	2	FBP	O1-C1-C2-C3
4	D	2	FBP	O1-C1-C2-O5
3	A	1	NAD	O4D-C4D-C5D-O5D
3	B	5	NAD	O4D-C4D-C5D-O5D
3	C	9	NAD	O4D-C4D-C5D-O5D
3	D	13	NAD	O4D-C4D-C5D-O5D
3	A	1	NAD	C3D-C4D-C5D-O5D
3	B	5	NAD	C3D-C4D-C5D-O5D
3	A	1	NAD	O4B-C4B-C5B-O5B
3	B	5	NAD	O4B-C4B-C5B-O5B
3	C	9	NAD	O4B-C4B-C5B-O5B
3	C	9	NAD	C3D-C4D-C5D-O5D
3	D	13	NAD	O4B-C4B-C5B-O5B
3	D	13	NAD	C3D-C4D-C5D-O5D
4	C	6	FBP	C1-O1-P1-O1P
4	D	2	FBP	C1-O1-P1-O1P
4	C	6	FBP	O1-C1-C2-O2
4	D	2	FBP	O1-C1-C2-O2
3	A	1	NAD	PN-O3-PA-O2A
3	B	5	NAD	PN-O3-PA-O2A
3	C	9	NAD	PN-O3-PA-O2A
3	D	13	NAD	PN-O3-PA-O2A
3	A	1	NAD	O4D-C1D-N1N-C2N
3	B	5	NAD	O4D-C1D-N1N-C2N
3	C	9	NAD	O4D-C1D-N1N-C2N
3	D	13	NAD	O4D-C1D-N1N-C2N
3	A	1	NAD	PN-O3-PA-O1A
3	B	5	NAD	PN-O3-PA-O1A
3	C	9	NAD	PN-O3-PA-O1A
3	D	13	NAD	PN-O3-PA-O1A

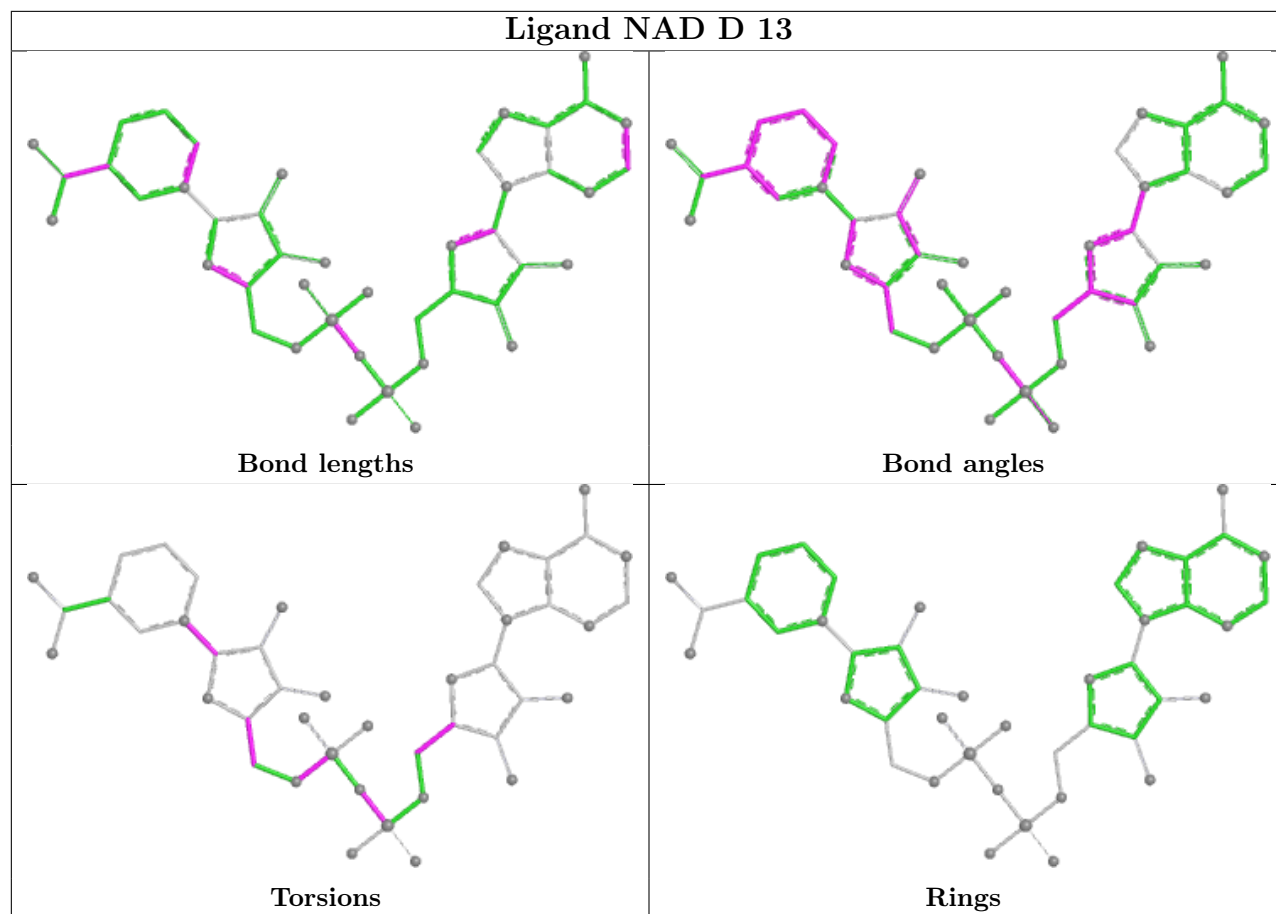
There are no ring outliers.

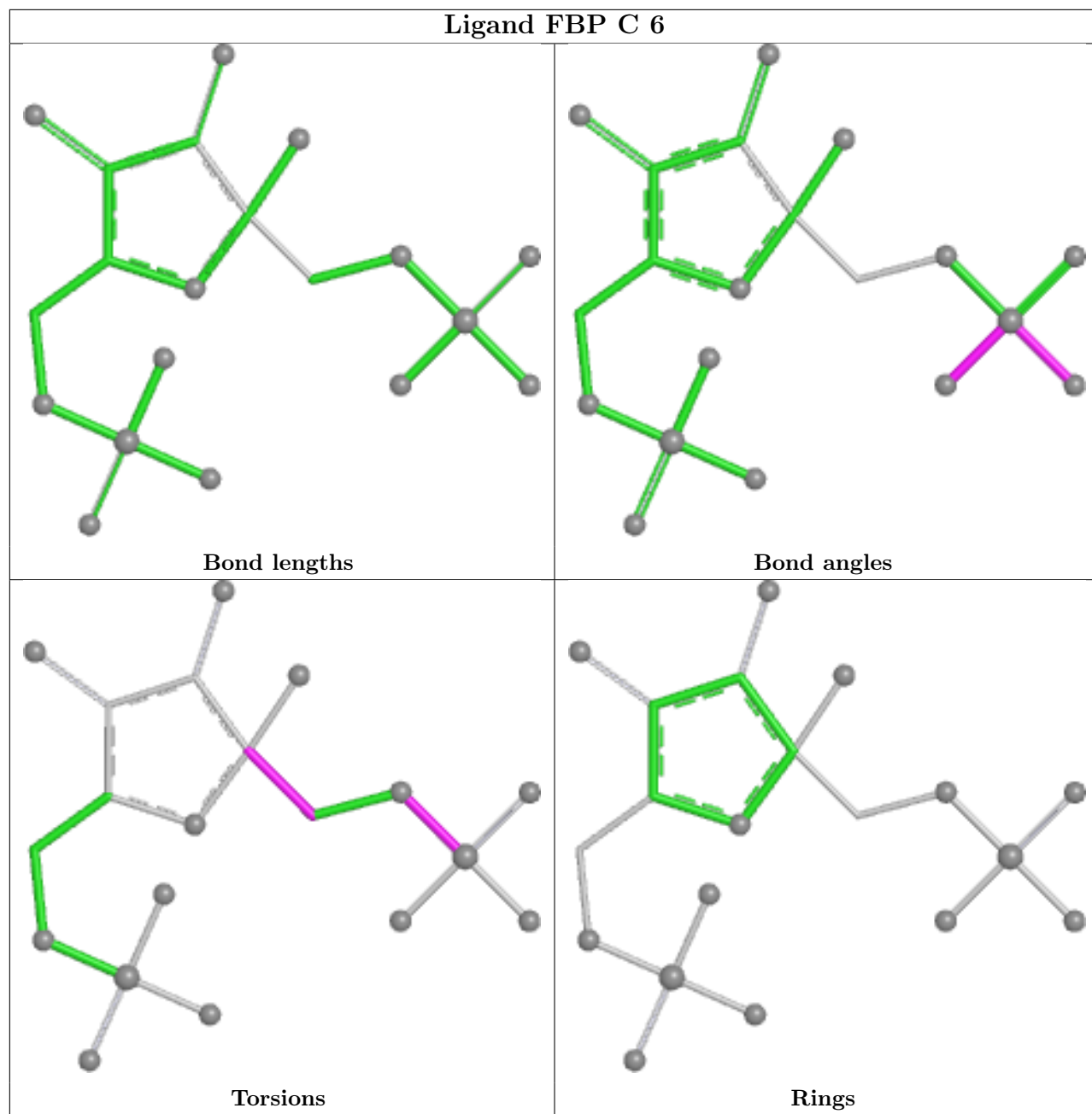
10 monomers are involved in 42 short contacts:

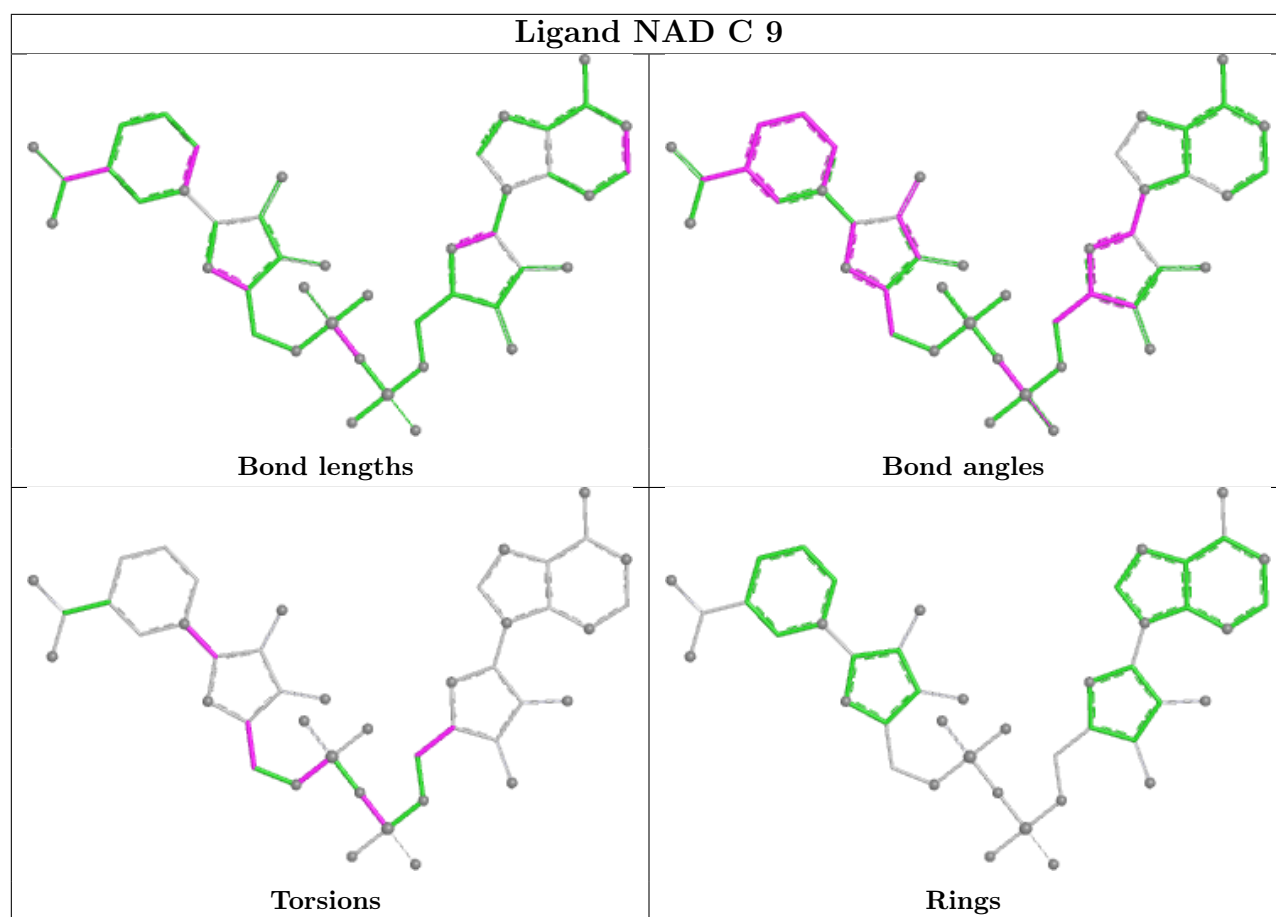
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	FBP	3	0
2	B	7	SO4	4	0
3	D	13	NAD	8	0
4	C	6	FBP	3	0
2	D	332	SO4	4	0
3	C	9	NAD	8	0
3	A	1	NAD	8	0
3	B	5	NAD	8	0
2	C	11	SO4	4	0
2	A	3	SO4	4	0

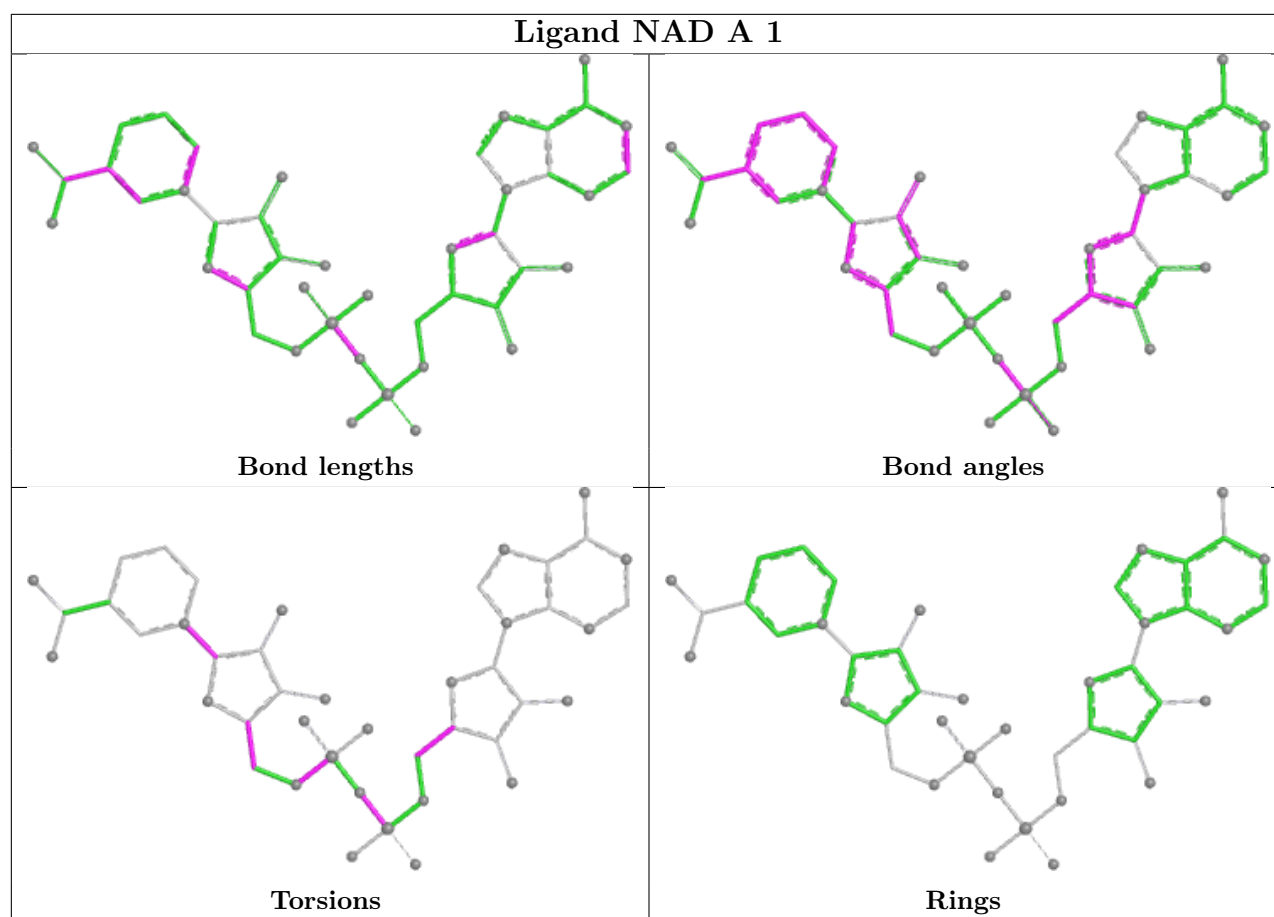
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

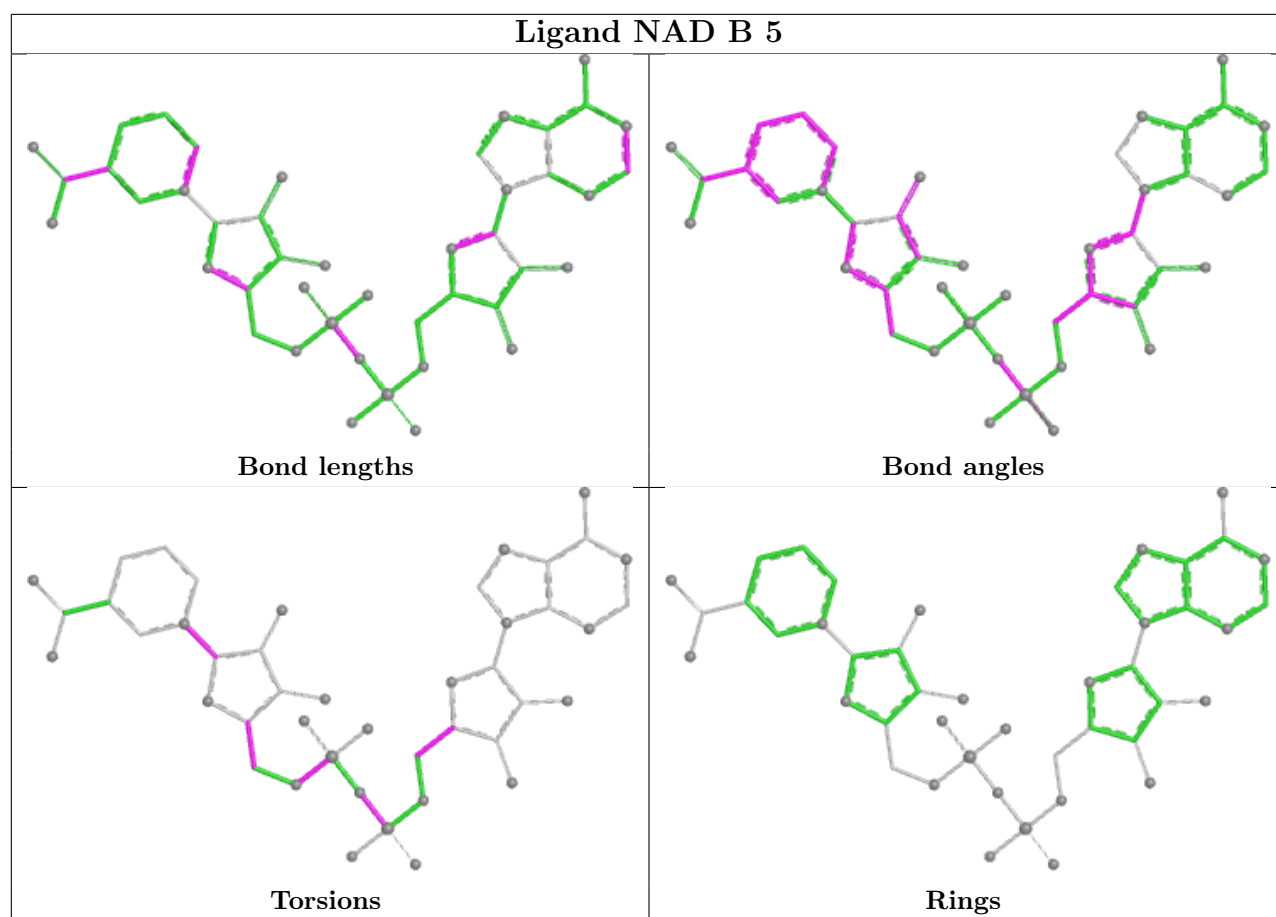












5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.