



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:15 AM UTC

PDB ID : 1KIF / pdb_00001kif
Title : D-AMINO ACID OXIDASE FROM PIG KIDNEY
Authors : Todone, F.; Mattevi, A.
Deposited on : 1996-01-19
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

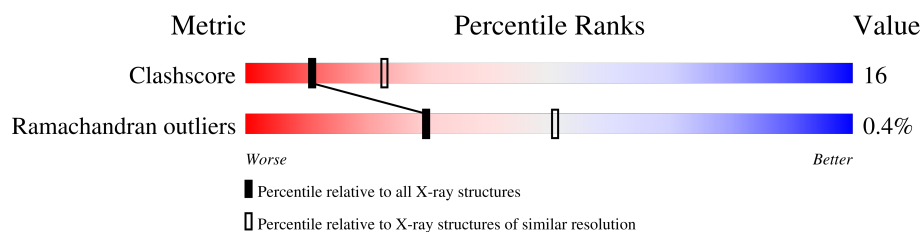
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)

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	347	63% 30% 5% .
1	B	347	62% 29% 7% .
1	C	347	61% 32% 5% .
1	D	347	62% 31% 5% .
1	E	347	61% 32% 5% .
1	F	347	63% 29% 5% .
1	G	347	64% 29% . .
1	H	347	61% 32% 5% .

2 Entry composition

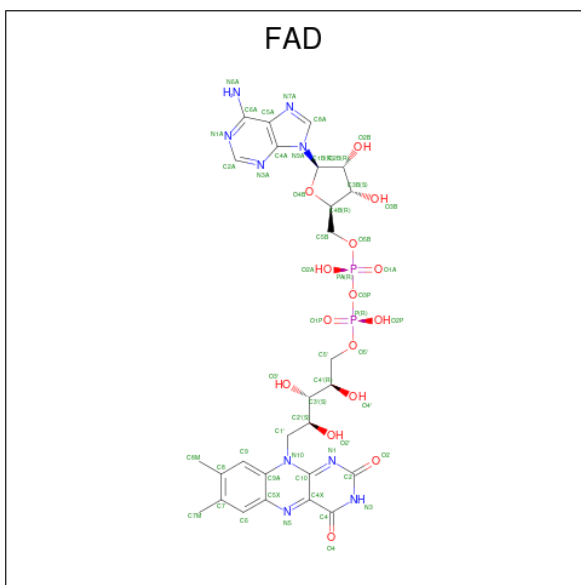
There are 4 unique types of molecules in this entry. The entry contains 22550 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-AMINO ACID OXIDASE.

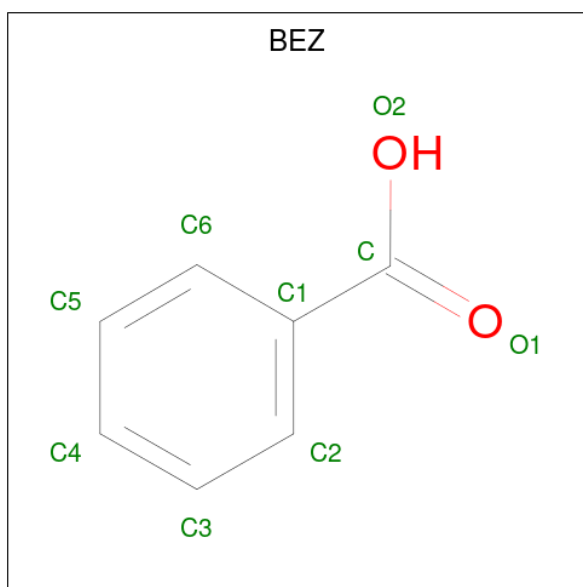
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	56	0	0
			2720	1749	473	489	9			
1	B	339	Total	C	N	O	S	58	0	0
			2720	1749	473	489	9			
1	C	339	Total	C	N	O	S	57	0	0
			2720	1749	473	489	9			
1	D	339	Total	C	N	O	S	45	0	0
			2720	1749	473	489	9			
1	E	339	Total	C	N	O	S	55	0	0
			2720	1749	473	489	9			
1	F	339	Total	C	N	O	S	63	0	0
			2720	1749	473	489	9			
1	G	339	Total	C	N	O	S	69	0	0
			2720	1749	473	489	9			
1	H	339	Total	C	N	O	S	40	0	0
			2720	1749	473	489	9			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	7	2		
3	B	1	Total	C	O	0	0
			9	7	2		
3	C	1	Total	C	O	0	0
			9	7	2		
3	D	1	Total	C	O	0	0
			9	7	2		
3	E	1	Total	C	O	0	0
			9	7	2		
3	F	1	Total	C	O	0	0
			9	7	2		
3	G	1	Total	C	O	0	0
			9	7	2		
3	H	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	31	Total	O	0	0
			31	31		
4	C	25	Total	O	0	0
			25	25		
4	D	53	Total	O	0	0
			53	53		

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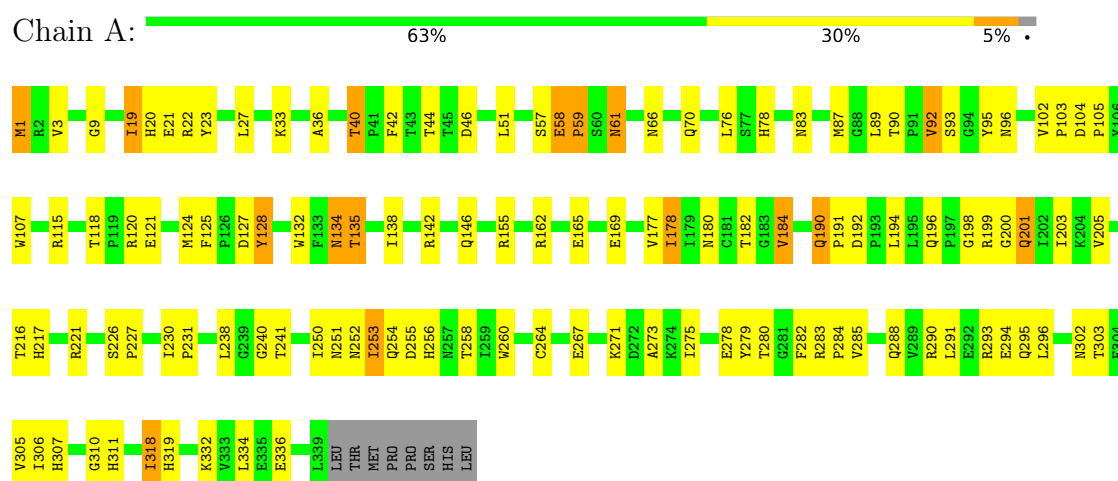
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	35	Total 35	O 35	0	0
4	F	42	Total 42	O 42	0	0
4	G	22	Total 22	O 22	0	0
4	H	35	Total 35	O 35	0	0

3 Residue-property plots

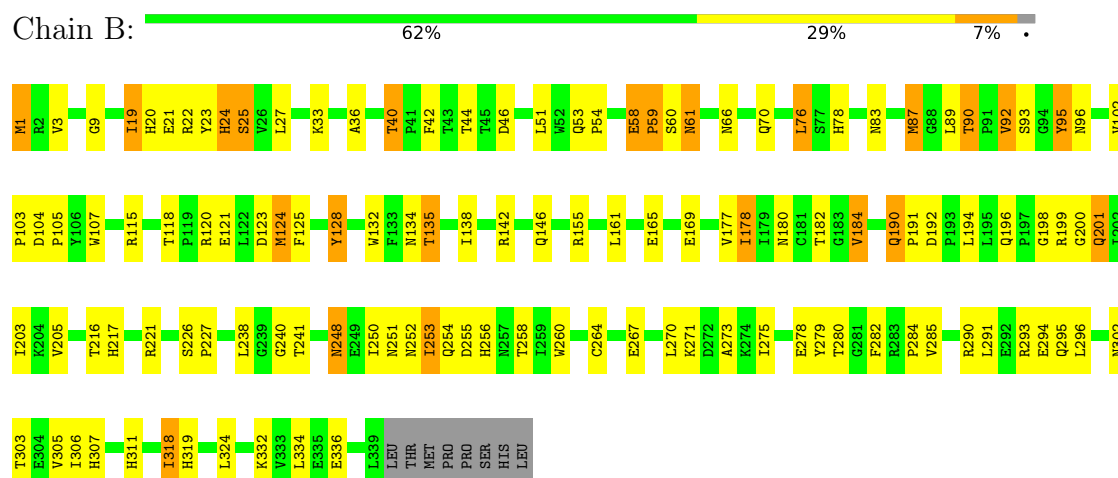
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

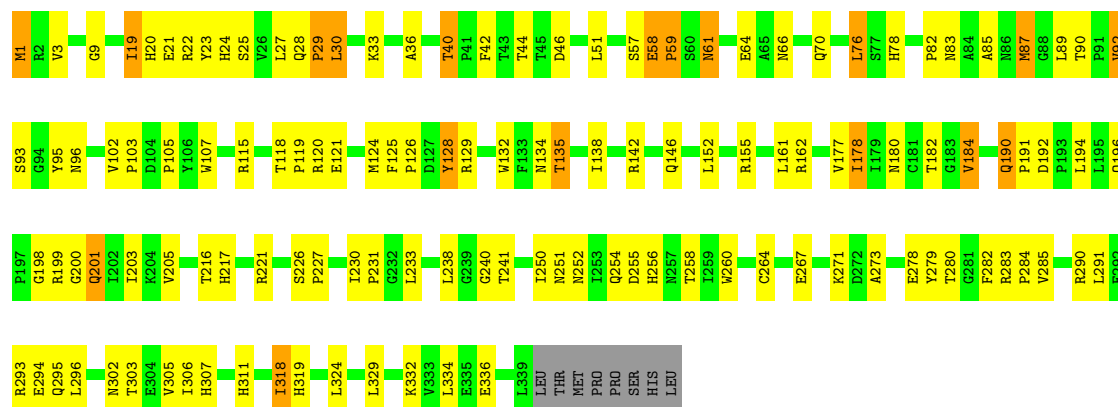


• Molecule 1: D-AMINO ACID OXIDASE



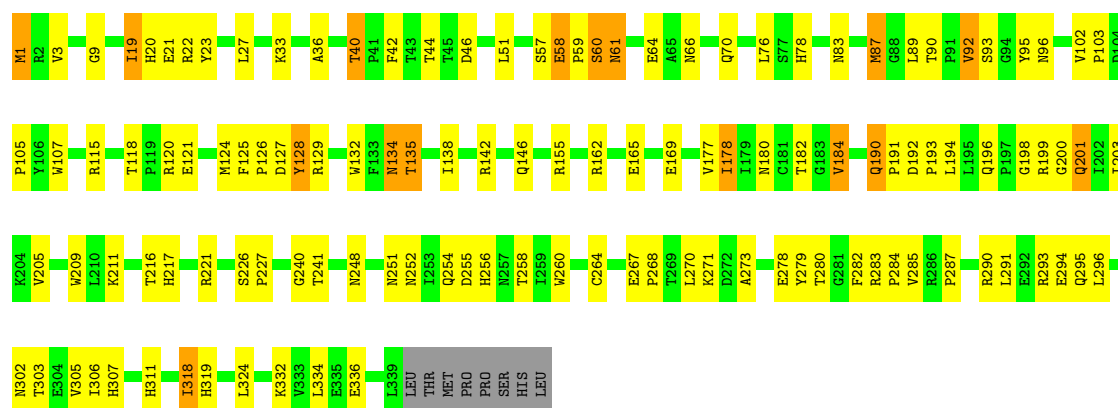
• Molecule 1: D-AMINO ACID OXIDASE





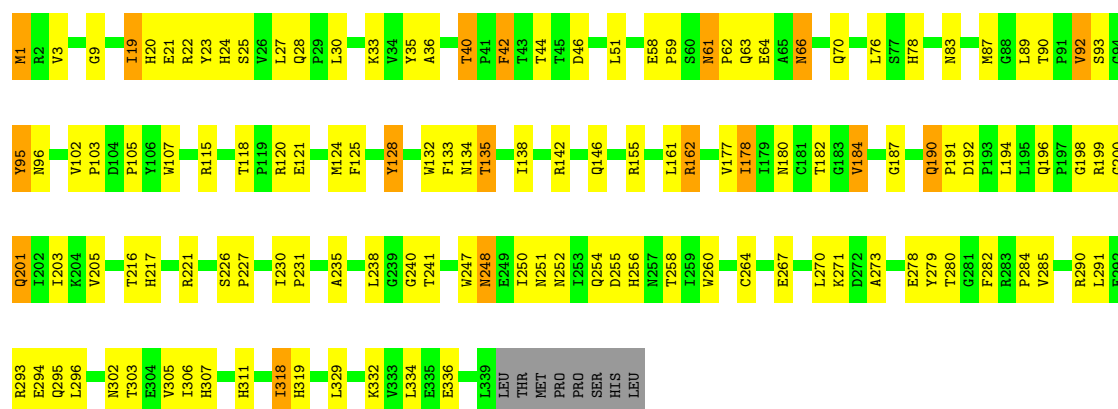
• Molecule 1: D-AMINO ACID OXIDASE

Chain D: 62% 31% 5% .



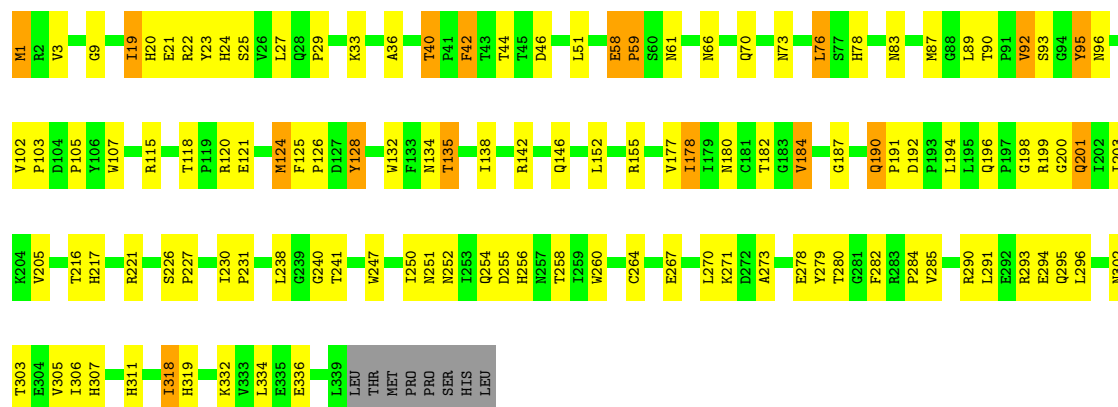
• Molecule 1: D-AMINO ACID OXIDASE

Chain E: 61% 32% 5% .



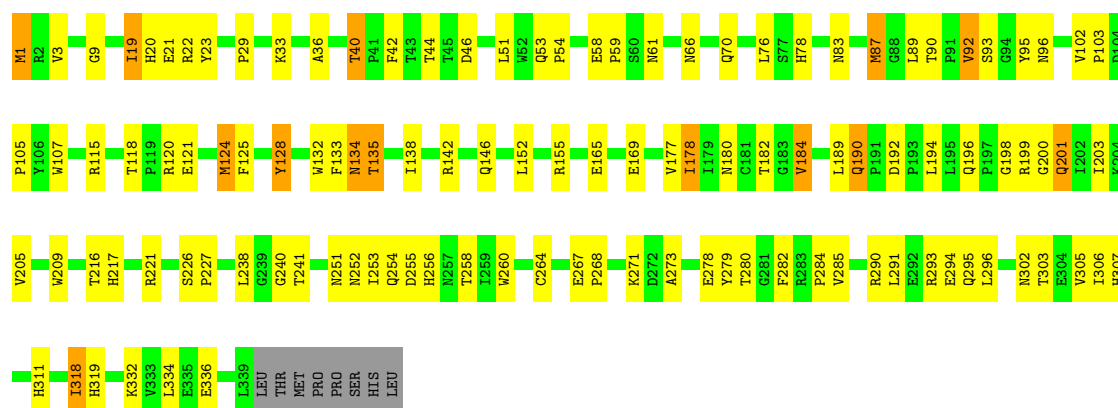
• Molecule 1: D-AMINO ACID OXIDASE

Chain F: 63% 29% 5% .



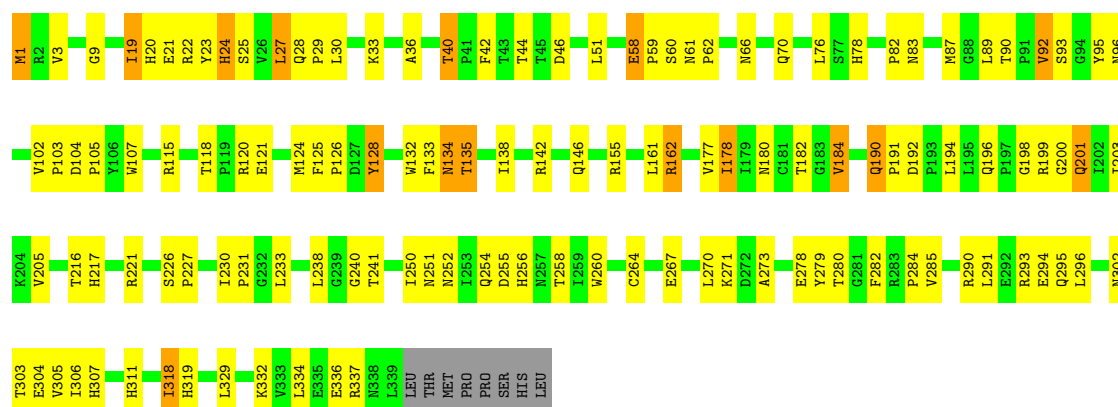
• Molecule 1: D-AMINO ACID OXIDASE

Chain G: 64% 29% . .



• Molecule 1: D-AMINO ACID OXIDASE

Chain H: 61% 32% 5% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	326.48Å 138.10Å 200.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22550	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: FAD, BEZ

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	0.80	1/2796 (0.0%)	1.69	64/3808 (1.7%)
1	B	0.80	1/2796 (0.0%)	1.68	67/3808 (1.8%)
1	C	0.79	1/2796 (0.0%)	1.69	66/3808 (1.7%)
1	D	0.82	2/2796 (0.1%)	1.74	72/3808 (1.9%)
1	E	0.81	1/2796 (0.0%)	1.67	60/3808 (1.6%)
1	F	0.80	1/2796 (0.0%)	1.67	60/3808 (1.6%)
1	G	0.79	1/2796 (0.0%)	1.67	63/3808 (1.7%)
1	H	0.82	1/2796 (0.0%)	1.71	70/3808 (1.8%)
All	All	0.80	9/22368 (0.0%)	1.69	522/30464 (1.7%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	MET	SD-CE	-7.04	1.61	1.79
1	F	124	MET	SD-CE	-7.01	1.62	1.79
1	D	124	MET	SD-CE	-7.01	1.62	1.79
1	G	124	MET	SD-CE	-7.01	1.62	1.79
1	C	124	MET	SD-CE	-7.01	1.62	1.79
1	B	124	MET	SD-CE	-7.00	1.62	1.79
1	H	124	MET	SD-CE	-7.00	1.62	1.79
1	E	124	MET	SD-CE	-6.97	1.62	1.79
1	D	127	ASP	N-CA	-5.82	1.38	1.46

All (522) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	PRO	CA-C-N	-12.50	101.30	120.31
1	D	126	PRO	C-N-CA	-12.50	101.30	120.31
1	A	61	ASN	CA-C-N	10.24	130.00	119.56
1	A	61	ASN	C-N-CA	10.24	130.00	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	ASN	CA-C-N	-9.84	109.62	119.56
1	D	61	ASN	C-N-CA	-9.84	109.62	119.56
1	H	318	ILE	CB-CA-C	-9.36	101.43	110.70
1	E	318	ILE	CB-CA-C	-9.36	101.44	110.70
1	A	318	ILE	CB-CA-C	-9.35	101.44	110.70
1	G	318	ILE	CB-CA-C	-9.34	101.46	110.70
1	B	318	ILE	CB-CA-C	-9.33	101.46	110.70
1	F	318	ILE	CB-CA-C	-9.33	101.46	110.70
1	D	318	ILE	CB-CA-C	-9.31	101.48	110.70
1	C	318	ILE	CB-CA-C	-9.30	101.49	110.70
1	D	302	ASN	N-CA-C	-9.22	94.46	109.96
1	A	302	ASN	N-CA-C	-9.20	94.50	109.96
1	B	302	ASN	N-CA-C	-9.20	94.51	109.96
1	E	302	ASN	N-CA-C	-9.19	94.51	109.96
1	H	302	ASN	N-CA-C	-9.19	94.52	109.96
1	C	302	ASN	N-CA-C	-9.19	94.52	109.96
1	G	302	ASN	N-CA-C	-9.19	94.52	109.96
1	F	302	ASN	N-CA-C	-9.18	94.53	109.96
1	F	1	MET	CB-CA-C	-9.12	92.77	110.10
1	H	1	MET	CB-CA-C	-9.11	92.79	110.10
1	C	1	MET	CB-CA-C	-9.11	92.79	110.10
1	G	1	MET	CB-CA-C	-9.11	92.79	110.10
1	D	1	MET	CB-CA-C	-9.11	92.79	110.10
1	B	1	MET	CB-CA-C	-9.10	92.80	110.10
1	E	1	MET	CB-CA-C	-9.10	92.81	110.10
1	A	1	MET	CB-CA-C	-9.10	92.82	110.10
1	B	61	ASN	N-CA-C	-8.86	98.94	109.93
1	H	42	PHE	N-CA-C	8.70	123.72	113.20
1	D	42	PHE	N-CA-C	8.67	123.69	113.20
1	G	42	PHE	N-CA-C	8.67	123.69	113.20
1	B	42	PHE	N-CA-C	8.67	123.69	113.20
1	C	42	PHE	N-CA-C	8.65	123.67	113.20
1	F	42	PHE	N-CA-C	8.65	123.67	113.20
1	E	42	PHE	N-CA-C	8.64	123.66	113.20
1	A	42	PHE	N-CA-C	8.64	123.65	113.20
1	C	303	THR	N-CA-C	-8.54	93.58	108.69
1	E	303	THR	N-CA-C	-8.53	93.58	108.69
1	A	23	TYR	N-CA-C	8.53	123.88	113.38
1	A	303	THR	N-CA-C	-8.53	93.59	108.69
1	E	23	TYR	N-CA-C	8.53	123.86	113.38
1	F	303	THR	N-CA-C	-8.52	93.61	108.69
1	H	303	THR	N-CA-C	-8.52	93.61	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	303	THR	N-CA-C	-8.52	93.62	108.69
1	B	303	THR	N-CA-C	-8.51	93.64	108.69
1	F	23	TYR	N-CA-C	8.51	123.84	113.38
1	G	303	THR	N-CA-C	-8.50	93.64	108.69
1	D	23	TYR	N-CA-C	8.49	123.83	113.38
1	D	248	ASN	CB-CA-C	-8.49	96.30	109.89
1	B	23	TYR	N-CA-C	8.49	123.82	113.38
1	H	23	TYR	N-CA-C	8.47	123.80	113.38
1	G	23	TYR	N-CA-C	8.44	123.88	113.50
1	C	23	TYR	N-CA-C	8.42	123.85	113.50
1	F	89	LEU	N-CA-C	8.38	123.66	110.17
1	B	89	LEU	N-CA-C	8.37	123.65	110.17
1	H	89	LEU	N-CA-C	8.37	123.64	110.17
1	D	89	LEU	N-CA-C	8.36	123.63	110.17
1	C	89	LEU	N-CA-C	8.36	123.62	110.17
1	G	89	LEU	N-CA-C	8.36	123.62	110.17
1	A	89	LEU	N-CA-C	8.35	123.62	110.17
1	E	89	LEU	N-CA-C	8.35	123.62	110.17
1	C	59	PRO	N-CA-C	8.28	123.84	111.41
1	G	311	HIS	N-CA-C	8.26	123.19	113.20
1	C	311	HIS	N-CA-C	8.26	123.19	113.20
1	D	311	HIS	N-CA-C	8.25	123.19	113.20
1	E	311	HIS	N-CA-C	8.25	123.18	113.20
1	A	311	HIS	N-CA-C	8.24	123.18	113.20
1	H	311	HIS	N-CA-C	8.23	123.16	113.20
1	F	311	HIS	N-CA-C	8.23	123.16	113.20
1	B	311	HIS	N-CA-C	8.22	123.15	113.20
1	H	58	GLU	CB-CA-C	8.18	122.27	109.42
1	F	59	PRO	N-CA-C	7.97	124.06	111.38
1	D	267	GLU	CB-CA-C	-7.91	100.76	110.81
1	E	267	GLU	CB-CA-C	-7.90	100.78	110.81
1	F	267	GLU	CB-CA-C	-7.90	100.78	110.81
1	G	267	GLU	CB-CA-C	-7.89	100.79	110.81
1	A	267	GLU	CB-CA-C	-7.89	100.79	110.81
1	B	267	GLU	CB-CA-C	-7.88	100.80	110.81
1	C	267	GLU	CB-CA-C	-7.88	100.80	110.81
1	H	267	GLU	CB-CA-C	-7.88	100.80	110.81
1	D	58	GLU	CA-C-N	7.75	127.81	119.90
1	D	58	GLU	C-N-CA	7.75	127.81	119.90
1	G	61	ASN	N-CA-C	-7.73	100.06	109.72
1	F	90	THR	N-CA-CB	7.68	124.05	110.37
1	B	90	THR	N-CA-CB	7.68	124.04	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	THR	N-CA-CB	7.67	124.03	110.37
1	E	90	THR	N-CA-CB	7.67	124.03	110.37
1	G	90	THR	N-CA-CB	7.67	124.02	110.37
1	A	90	THR	N-CA-CB	7.66	124.01	110.37
1	A	58	GLU	N-CA-C	7.66	119.56	109.83
1	H	90	THR	N-CA-CB	7.66	124.00	110.37
1	C	58	GLU	CA-C-N	7.66	127.61	120.03
1	C	58	GLU	C-N-CA	7.66	127.61	120.03
1	C	90	THR	N-CA-CB	7.66	124.00	110.37
1	E	162	ARG	CB-CA-C	-7.58	96.22	109.86
1	F	1	MET	CB-CG-SD	-7.56	90.03	112.70
1	F	22	ARG	N-CA-C	7.55	120.97	111.69
1	G	1	MET	CB-CG-SD	-7.55	90.06	112.70
1	C	1	MET	CB-CG-SD	-7.55	90.06	112.70
1	B	1	MET	CB-CG-SD	-7.54	90.06	112.70
1	A	1	MET	CB-CG-SD	-7.54	90.07	112.70
1	E	1	MET	CB-CG-SD	-7.54	90.08	112.70
1	H	1	MET	CB-CG-SD	-7.54	90.08	112.70
1	D	1	MET	CB-CG-SD	-7.53	90.11	112.70
1	E	22	ARG	N-CA-C	7.52	120.94	111.69
1	H	22	ARG	N-CA-C	7.52	120.94	111.69
1	D	22	ARG	N-CA-C	7.51	120.93	111.69
1	B	22	ARG	N-CA-C	7.50	120.91	111.69
1	G	22	ARG	N-CA-C	7.50	120.91	111.69
1	A	22	ARG	N-CA-C	7.50	120.91	111.69
1	C	22	ARG	N-CA-C	7.48	120.89	111.69
1	E	61	ASN	N-CA-C	-7.45	100.41	109.72
1	H	162	ARG	CB-CG-CD	-7.38	94.33	111.30
1	H	92	VAL	N-CA-C	-7.33	97.94	108.42
1	A	92	VAL	N-CA-C	-7.32	97.95	108.42
1	E	92	VAL	N-CA-C	-7.32	97.95	108.42
1	C	92	VAL	N-CA-C	-7.32	97.96	108.42
1	F	92	VAL	N-CA-C	-7.31	97.96	108.42
1	D	92	VAL	N-CA-C	-7.31	97.97	108.42
1	B	92	VAL	N-CA-C	-7.30	97.97	108.42
1	G	92	VAL	N-CA-C	-7.28	98.00	108.42
1	H	61	ASN	N-CA-C	-7.27	100.60	109.83
1	H	28	GLN	N-CA-CB	7.20	118.92	110.42
1	C	29	PRO	N-CA-C	-7.16	98.28	111.03
1	G	44	THR	N-CA-C	-7.16	103.51	111.82
1	D	44	THR	N-CA-C	-7.16	103.51	111.82
1	E	44	THR	N-CA-C	-7.16	103.52	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	THR	N-CA-C	-7.14	103.54	111.82
1	F	44	THR	N-CA-C	-7.13	103.54	111.82
1	H	44	THR	N-CA-C	-7.13	103.54	111.82
1	B	44	THR	N-CA-C	-7.13	103.55	111.82
1	C	83	ASN	N-CA-C	7.13	121.98	113.28
1	A	44	THR	N-CA-C	-7.13	103.55	111.82
1	A	83	ASN	N-CA-C	7.12	121.97	113.28
1	F	83	ASN	N-CA-C	7.12	121.96	113.28
1	G	83	ASN	N-CA-C	7.10	121.95	113.28
1	E	83	ASN	N-CA-C	7.10	121.95	113.28
1	B	83	ASN	N-CA-C	7.09	121.94	113.28
1	H	83	ASN	N-CA-C	7.09	121.93	113.28
1	D	83	ASN	N-CA-C	7.09	121.93	113.28
1	C	51	LEU	N-CA-C	7.06	120.93	110.48
1	C	58	GLU	CB-CA-C	7.06	121.31	109.67
1	F	51	LEU	N-CA-C	7.04	120.90	110.48
1	G	51	LEU	N-CA-C	7.04	120.90	110.48
1	A	51	LEU	N-CA-C	7.04	120.89	110.48
1	H	51	LEU	N-CA-C	7.02	120.88	110.48
1	E	51	LEU	N-CA-C	7.01	120.86	110.48
1	E	19	ILE	CB-CA-C	-7.01	102.84	112.02
1	B	51	LEU	N-CA-C	7.00	120.84	110.48
1	D	51	LEU	N-CA-C	6.99	120.83	110.48
1	F	19	ILE	CB-CA-C	-6.98	102.88	112.02
1	B	19	ILE	CB-CA-C	-6.97	102.88	112.02
1	H	19	ILE	CB-CA-C	-6.97	102.89	112.02
1	A	19	ILE	CB-CA-C	-6.97	102.89	112.02
1	G	19	ILE	CB-CA-C	-6.97	102.89	112.02
1	A	95	TYR	N-CA-C	6.96	121.02	109.95
1	C	19	ILE	CB-CA-C	-6.95	102.92	112.02
1	F	95	TYR	N-CA-C	6.95	120.99	109.95
1	H	95	TYR	N-CA-C	6.94	120.99	109.95
1	D	19	ILE	CB-CA-C	-6.94	102.93	112.02
1	G	95	TYR	N-CA-C	6.94	120.98	109.95
1	D	95	TYR	N-CA-C	6.93	120.97	109.95
1	E	221	ARG	N-CA-C	6.93	121.32	113.01
1	C	95	TYR	N-CA-C	6.91	120.94	109.95
1	A	221	ARG	N-CA-C	6.91	121.30	113.01
1	B	221	ARG	N-CA-C	6.91	121.30	113.01
1	F	221	ARG	N-CA-C	6.91	121.30	113.01
1	E	95	TYR	N-CA-C	6.90	120.93	109.95
1	D	57	SER	O-C-N	6.90	130.76	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	TYR	N-CA-C	6.90	120.92	109.95
1	G	221	ARG	N-CA-C	6.90	121.29	113.01
1	C	221	ARG	N-CA-C	6.88	121.27	113.01
1	D	221	ARG	N-CA-C	6.88	121.27	113.01
1	H	221	ARG	N-CA-C	6.88	121.27	113.01
1	D	248	ASN	N-CA-CB	6.85	120.05	109.85
1	C	89	LEU	CB-CA-C	-6.84	97.94	109.50
1	F	89	LEU	CB-CA-C	-6.84	97.94	109.50
1	E	89	LEU	CB-CA-C	-6.83	97.96	109.50
1	G	89	LEU	CB-CA-C	-6.83	97.96	109.50
1	B	89	LEU	CB-CA-C	-6.83	97.97	109.50
1	D	89	LEU	CB-CA-C	-6.83	97.97	109.50
1	H	89	LEU	CB-CA-C	-6.82	97.97	109.50
1	E	66	ASN	CB-CA-C	-6.82	100.12	110.90
1	A	89	LEU	CB-CA-C	-6.81	97.99	109.50
1	A	57	SER	O-C-N	-6.79	115.29	122.96
1	H	28	GLN	CB-CA-C	6.78	124.09	113.04
1	D	61	ASN	N-CA-C	-6.74	99.77	109.48
1	D	9	GLY	N-CA-C	-6.72	102.33	112.41
1	H	9	GLY	N-CA-C	-6.72	102.33	112.41
1	A	9	GLY	N-CA-C	-6.72	102.34	112.41
1	F	9	GLY	N-CA-C	-6.71	102.34	112.41
1	B	9	GLY	N-CA-C	-6.70	102.36	112.41
1	E	9	GLY	N-CA-C	-6.70	102.36	112.41
1	C	9	GLY	N-CA-C	-6.70	102.36	112.41
1	D	126	PRO	O-C-N	6.69	129.94	122.24
1	G	9	GLY	N-CA-C	-6.69	102.37	112.41
1	H	58	GLU	CA-C-N	6.67	126.59	119.85
1	H	58	GLU	C-N-CA	6.67	126.59	119.85
1	F	61	ASN	N-CA-C	-6.60	99.00	109.04
1	F	58	GLU	N-CA-C	6.57	118.17	109.83
1	E	92	VAL	CB-CA-C	-6.56	99.38	111.18
1	H	92	VAL	CB-CA-C	-6.56	99.38	111.18
1	B	92	VAL	CB-CA-C	-6.55	99.38	111.18
1	D	92	VAL	CB-CA-C	-6.55	99.39	111.18
1	C	92	VAL	CB-CA-C	-6.54	99.41	111.18
1	G	92	VAL	CB-CA-C	-6.53	99.42	111.18
1	A	92	VAL	CB-CA-C	-6.53	99.43	111.18
1	F	92	VAL	CB-CA-C	-6.53	99.43	111.18
1	F	306	ILE	N-CA-C	-6.46	98.21	107.77
1	A	306	ILE	N-CA-C	-6.45	98.22	107.77
1	G	306	ILE	N-CA-C	-6.45	98.22	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	306	ILE	N-CA-C	-6.44	98.24	107.77
1	C	306	ILE	N-CA-C	-6.43	98.25	107.77
1	D	306	ILE	N-CA-C	-6.43	98.25	107.77
1	H	24	HIS	N-CA-C	6.43	120.23	112.38
1	B	306	ILE	N-CA-C	-6.43	98.25	107.77
1	E	306	ILE	N-CA-C	-6.42	98.26	107.77
1	C	129	ARG	CB-CA-C	-6.42	98.70	109.75
1	A	61	ASN	N-CA-C	-6.38	99.35	109.04
1	A	162	ARG	CB-CA-C	-6.33	99.04	109.80
1	C	162	ARG	NE-CZ-NH2	6.33	124.89	119.20
1	H	282	PHE	N-CA-C	6.28	119.11	107.99
1	D	127	ASP	CB-CA-C	6.27	122.71	110.67
1	A	282	PHE	N-CA-C	6.27	119.09	107.99
1	C	282	PHE	N-CA-C	6.27	119.09	107.99
1	F	61	ASN	CA-C-N	6.27	125.89	119.56
1	F	61	ASN	C-N-CA	6.27	125.89	119.56
1	D	282	PHE	N-CA-C	6.26	119.06	107.99
1	B	282	PHE	N-CA-C	6.25	119.05	107.99
1	F	282	PHE	N-CA-C	6.25	119.05	107.99
1	E	282	PHE	N-CA-C	6.24	119.03	107.99
1	G	282	PHE	N-CA-C	6.24	119.03	107.99
1	B	24	HIS	CB-CA-C	-6.19	100.15	110.68
1	B	59	PRO	N-CA-C	6.11	121.89	111.68
1	G	59	PRO	N-CA-C	6.11	125.06	112.47
1	C	271	LYS	N-CA-CB	-6.10	100.19	110.49
1	E	271	LYS	N-CA-CB	-6.09	100.20	110.49
1	B	271	LYS	N-CA-CB	-6.09	100.20	110.49
1	A	271	LYS	N-CA-CB	-6.08	100.21	110.49
1	G	271	LYS	N-CA-CB	-6.08	100.21	110.49
1	H	271	LYS	N-CA-CB	-6.08	100.22	110.49
1	D	271	LYS	N-CA-CB	-6.08	100.22	110.49
1	F	271	LYS	N-CA-CB	-6.08	100.22	110.49
1	D	162	ARG	CB-CA-C	-6.03	99.70	109.89
1	D	58	GLU	O-C-N	5.92	127.02	121.27
1	G	201	GLN	CB-CA-C	-5.91	100.04	109.80
1	F	178	ILE	CB-CA-C	-5.91	100.95	110.28
1	C	178	ILE	CB-CA-C	-5.90	100.96	110.28
1	H	201	GLN	CB-CA-C	-5.90	100.06	109.80
1	F	198	GLY	N-CA-C	-5.90	99.21	113.18
1	F	201	GLN	CB-CA-C	-5.90	100.07	109.80
1	A	198	GLY	N-CA-C	-5.89	99.21	113.18
1	E	198	GLY	N-CA-C	-5.89	99.21	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	GLY	N-CA-C	-5.89	99.22	113.18
1	G	198	GLY	N-CA-C	-5.89	99.23	113.18
1	H	198	GLY	N-CA-C	-5.88	99.24	113.18
1	H	178	ILE	CB-CA-C	-5.88	100.99	110.28
1	B	253	ILE	CB-CA-C	-5.88	103.05	112.16
1	D	198	GLY	N-CA-C	-5.88	99.25	113.18
1	B	178	ILE	CB-CA-C	-5.88	101.00	110.28
1	B	198	GLY	N-CA-C	-5.88	99.25	113.18
1	G	178	ILE	CB-CA-C	-5.88	101.00	110.28
1	A	178	ILE	CB-CA-C	-5.88	101.00	110.28
1	C	201	GLN	CB-CA-C	-5.87	100.11	109.80
1	D	178	ILE	CB-CA-C	-5.87	101.00	110.28
1	D	201	GLN	CB-CA-C	-5.87	100.11	109.80
1	B	201	GLN	CB-CA-C	-5.87	100.12	109.80
1	A	253	ILE	CA-C-N	-5.86	111.97	120.29
1	A	253	ILE	C-N-CA	-5.86	111.97	120.29
1	E	178	ILE	CB-CA-C	-5.86	101.02	110.28
1	E	201	GLN	CB-CA-C	-5.86	100.14	109.80
1	A	201	GLN	CB-CA-C	-5.84	100.16	109.80
1	G	305	VAL	N-CA-C	-5.82	99.83	108.45
1	E	118	THR	N-CA-C	-5.81	103.33	110.31
1	D	118	THR	N-CA-C	-5.81	103.34	110.31
1	D	305	VAL	N-CA-C	-5.81	99.85	108.45
1	E	305	VAL	N-CA-C	-5.80	99.86	108.45
1	F	118	THR	N-CA-C	-5.80	103.35	110.31
1	B	118	THR	N-CA-C	-5.80	103.35	110.31
1	H	305	VAL	N-CA-C	-5.80	99.86	108.45
1	C	305	VAL	N-CA-C	-5.80	99.87	108.45
1	C	118	THR	N-CA-C	-5.80	103.35	110.31
1	H	118	THR	N-CA-C	-5.79	103.36	110.31
1	B	305	VAL	N-CA-C	-5.79	99.89	108.45
1	G	118	THR	N-CA-C	-5.79	103.37	110.31
1	A	118	THR	N-CA-C	-5.78	103.37	110.31
1	A	182	THR	N-CA-C	5.78	120.19	113.20
1	A	305	VAL	N-CA-C	-5.77	99.91	108.45
1	A	319	HIS	N-CA-C	5.77	118.32	111.33
1	B	182	THR	N-CA-C	5.77	120.19	113.20
1	H	319	HIS	N-CA-C	5.77	118.31	111.33
1	F	319	HIS	N-CA-C	5.76	118.30	111.33
1	G	319	HIS	N-CA-C	5.76	118.30	111.33
1	C	319	HIS	N-CA-C	5.76	118.29	111.33
1	D	319	HIS	N-CA-C	5.76	118.30	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	182	THR	N-CA-C	5.75	120.16	113.20
1	D	182	THR	N-CA-C	5.75	120.16	113.20
1	F	182	THR	N-CA-C	5.75	120.16	113.20
1	C	182	THR	N-CA-C	5.74	120.15	113.20
1	F	305	VAL	N-CA-C	-5.74	99.95	108.45
1	G	182	THR	N-CA-C	5.74	120.15	113.20
1	E	319	HIS	N-CA-C	5.73	118.26	111.33
1	H	3	VAL	N-CA-C	-5.72	99.94	108.46
1	A	3	VAL	N-CA-C	-5.72	99.94	108.46
1	E	3	VAL	N-CA-C	-5.72	99.94	108.46
1	C	3	VAL	N-CA-C	-5.72	99.94	108.46
1	B	319	HIS	N-CA-C	5.71	118.24	111.33
1	D	3	VAL	N-CA-C	-5.71	99.94	108.46
1	B	3	VAL	N-CA-C	-5.71	99.95	108.46
1	H	182	THR	N-CA-C	5.71	120.11	113.20
1	C	184	VAL	CB-CA-C	-5.70	101.94	111.29
1	G	3	VAL	N-CA-C	-5.70	99.97	108.46
1	E	184	VAL	CB-CA-C	-5.68	101.97	111.29
1	F	190	GLN	CA-C-N	5.68	125.70	119.90
1	F	190	GLN	C-N-CA	5.68	125.70	119.90
1	F	3	VAL	N-CA-C	-5.68	99.99	108.46
1	H	24	HIS	CB-CA-C	5.68	122.30	110.32
1	C	190	GLN	CA-C-N	5.67	125.69	119.90
1	C	190	GLN	C-N-CA	5.67	125.69	119.90
1	G	120	ARG	N-CA-C	-5.67	105.24	111.82
1	B	120	ARG	N-CA-C	-5.66	105.25	111.82
1	B	184	VAL	CB-CA-C	-5.66	102.00	111.29
1	C	120	ARG	N-CA-C	-5.66	105.25	111.82
1	C	135	THR	N-CA-C	-5.66	100.95	109.95
1	D	184	VAL	CB-CA-C	-5.66	102.01	111.29
1	F	184	VAL	CB-CA-C	-5.66	102.02	111.29
1	G	184	VAL	CB-CA-C	-5.65	102.02	111.29
1	E	120	ARG	N-CA-C	-5.65	105.26	111.82
1	A	184	VAL	CB-CA-C	-5.65	102.02	111.29
1	B	135	THR	N-CA-C	-5.65	100.97	109.95
1	E	135	THR	N-CA-C	-5.65	100.97	109.95
1	E	248	ASN	N-CA-CB	-5.65	100.58	109.51
1	D	120	ARG	N-CA-C	-5.65	105.27	111.82
1	H	184	VAL	CB-CA-C	-5.65	102.03	111.29
1	A	135	THR	N-CA-C	-5.65	100.97	109.95
1	B	190	GLN	CA-C-N	5.65	125.66	119.90
1	B	190	GLN	C-N-CA	5.65	125.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	120	ARG	N-CA-C	-5.64	105.28	111.82
1	H	135	THR	N-CA-C	-5.64	100.98	109.95
1	A	120	ARG	N-CA-C	-5.64	105.28	111.82
1	D	135	THR	N-CA-C	-5.64	100.99	109.95
1	G	135	THR	N-CA-C	-5.63	100.99	109.95
1	G	190	GLN	CA-C-N	5.63	125.64	119.90
1	G	190	GLN	C-N-CA	5.63	125.64	119.90
1	F	135	THR	N-CA-C	-5.63	101.00	109.95
1	G	318	ILE	N-CA-CB	-5.63	104.06	112.67
1	B	318	ILE	N-CA-CB	-5.62	104.06	112.67
1	H	190	GLN	CA-C-N	5.62	125.64	119.90
1	H	190	GLN	C-N-CA	5.62	125.64	119.90
1	F	318	ILE	N-CA-CB	-5.62	104.07	112.67
1	E	318	ILE	N-CA-CB	-5.62	104.07	112.67
1	F	120	ARG	N-CA-C	-5.62	105.31	111.82
1	D	318	ILE	N-CA-CB	-5.61	104.09	112.67
1	A	190	GLN	CA-C-N	5.60	125.61	119.90
1	A	190	GLN	C-N-CA	5.60	125.61	119.90
1	E	190	GLN	CA-C-N	5.60	125.61	119.90
1	E	190	GLN	C-N-CA	5.60	125.61	119.90
1	C	318	ILE	N-CA-CB	-5.59	104.11	112.67
1	D	190	GLN	CA-C-N	5.59	125.60	119.90
1	D	190	GLN	C-N-CA	5.59	125.60	119.90
1	A	318	ILE	N-CA-CB	-5.59	104.12	112.67
1	H	318	ILE	N-CA-CB	-5.58	104.13	112.67
1	G	29	PRO	N-CA-C	-5.58	100.71	111.69
1	A	192	ASP	CA-C-N	5.57	125.19	119.56
1	A	192	ASP	C-N-CA	5.57	125.19	119.56
1	D	267	GLU	CA-C-N	5.57	125.24	119.56
1	D	267	GLU	C-N-CA	5.57	125.24	119.56
1	F	76	LEU	CB-CA-C	-5.57	99.65	110.46
1	C	61	ASN	N-CA-CB	-5.57	101.21	109.90
1	G	76	LEU	CB-CA-C	-5.57	99.66	110.46
1	A	267	GLU	CA-C-N	5.57	125.24	119.56
1	A	267	GLU	C-N-CA	5.57	125.24	119.56
1	B	76	LEU	CB-CA-C	-5.57	99.66	110.46
1	H	162	ARG	CD-NE-CZ	-5.56	116.61	124.40
1	C	192	ASP	CA-C-N	5.56	125.17	119.56
1	C	192	ASP	C-N-CA	5.56	125.17	119.56
1	H	76	LEU	CB-CA-C	-5.56	99.67	110.46
1	A	76	LEU	CB-CA-C	-5.56	99.68	110.46
1	H	192	ASP	CA-C-N	5.56	125.17	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	192	ASP	C-N-CA	5.56	125.17	119.56
1	F	192	ASP	CA-C-N	5.55	125.17	119.56
1	F	192	ASP	C-N-CA	5.55	125.17	119.56
1	D	76	LEU	CB-CA-C	-5.54	99.71	110.46
1	E	76	LEU	CB-CA-C	-5.54	99.71	110.46
1	C	76	LEU	CB-CA-C	-5.54	99.72	110.46
1	E	192	ASP	CA-C-N	5.53	125.15	119.56
1	E	192	ASP	C-N-CA	5.53	125.15	119.56
1	G	192	ASP	CA-C-N	5.53	125.14	119.56
1	G	192	ASP	C-N-CA	5.53	125.14	119.56
1	D	192	ASP	CA-C-N	5.53	125.14	119.56
1	D	192	ASP	C-N-CA	5.53	125.14	119.56
1	F	267	GLU	CA-C-N	5.52	125.19	119.56
1	F	267	GLU	C-N-CA	5.52	125.19	119.56
1	C	267	GLU	CA-C-N	5.51	125.18	119.56
1	C	267	GLU	C-N-CA	5.51	125.18	119.56
1	B	58	GLU	CB-CA-C	5.50	119.41	109.61
1	G	125	PHE	CB-CA-C	-5.50	102.07	111.15
1	C	125	PHE	CB-CA-C	-5.50	102.08	111.15
1	A	125	PHE	CB-CA-C	-5.50	102.08	111.15
1	B	192	ASP	CA-C-N	5.50	125.11	119.56
1	B	192	ASP	C-N-CA	5.50	125.11	119.56
1	E	267	GLU	CA-C-N	5.50	125.17	119.56
1	E	267	GLU	C-N-CA	5.50	125.17	119.56
1	B	267	GLU	CA-C-N	5.50	125.17	119.56
1	B	267	GLU	C-N-CA	5.50	125.17	119.56
1	H	267	GLU	CA-C-N	5.50	125.17	119.56
1	H	267	GLU	C-N-CA	5.50	125.17	119.56
1	G	267	GLU	CA-C-N	5.49	125.16	119.56
1	G	267	GLU	C-N-CA	5.49	125.16	119.56
1	H	125	PHE	CB-CA-C	-5.49	102.08	111.15
1	F	125	PHE	CB-CA-C	-5.49	102.09	111.15
1	E	125	PHE	CB-CA-C	-5.49	102.10	111.15
1	A	59	PRO	N-CA-C	5.48	119.64	111.41
1	B	125	PHE	CB-CA-C	-5.48	102.11	111.15
1	D	125	PHE	CB-CA-C	-5.48	102.11	111.15
1	C	58	GLU	N-CA-C	-5.46	101.47	109.50
1	G	87	MET	CB-CA-C	-5.44	100.22	110.01
1	D	87	MET	CB-CA-C	-5.43	100.23	110.01
1	H	27	LEU	CA-C-N	-5.43	113.04	119.78
1	H	27	LEU	C-N-CA	-5.43	113.04	119.78
1	D	201	GLN	N-CA-CB	5.43	119.03	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	201	GLN	N-CA-CB	5.42	119.02	110.56
1	B	87	MET	CB-CA-C	-5.42	100.26	110.01
1	H	201	GLN	N-CA-CB	5.42	119.01	110.56
1	G	134	ASN	CA-C-N	-5.41	114.15	122.87
1	G	134	ASN	C-N-CA	-5.41	114.15	122.87
1	B	201	GLN	N-CA-CB	5.41	119.00	110.56
1	H	29	PRO	N-CA-C	-5.41	101.33	112.47
1	A	201	GLN	N-CA-CB	5.40	118.99	110.56
1	C	201	GLN	N-CA-CB	5.40	118.99	110.56
1	B	134	ASN	CA-C-N	-5.40	114.18	122.87
1	B	134	ASN	C-N-CA	-5.40	114.18	122.87
1	C	87	MET	CB-CA-C	-5.40	100.29	110.01
1	E	134	ASN	CA-C-N	-5.40	114.18	122.87
1	E	134	ASN	C-N-CA	-5.40	114.18	122.87
1	D	134	ASN	CA-C-N	-5.39	114.19	122.87
1	D	134	ASN	C-N-CA	-5.39	114.19	122.87
1	A	134	ASN	CA-C-N	-5.39	114.19	122.87
1	A	134	ASN	C-N-CA	-5.39	114.19	122.87
1	G	201	GLN	N-CA-CB	5.39	118.97	110.56
1	C	134	ASN	CA-C-N	-5.38	114.20	122.87
1	C	134	ASN	C-N-CA	-5.38	114.20	122.87
1	E	201	GLN	N-CA-CB	5.38	118.95	110.56
1	F	134	ASN	CA-C-N	-5.38	114.21	122.87
1	F	134	ASN	C-N-CA	-5.38	114.21	122.87
1	H	134	ASN	CA-C-N	-5.37	114.22	122.87
1	H	134	ASN	C-N-CA	-5.37	114.22	122.87
1	F	203	ILE	CB-CA-C	-5.36	102.51	110.33
1	B	253	ILE	CA-C-N	-5.35	112.70	120.29
1	B	253	ILE	C-N-CA	-5.35	112.70	120.29
1	H	203	ILE	CB-CA-C	-5.35	102.53	110.33
1	A	203	ILE	CB-CA-C	-5.34	102.53	110.33
1	A	203	ILE	N-CA-C	-5.33	100.45	108.12
1	D	203	ILE	N-CA-C	-5.32	100.45	108.12
1	F	203	ILE	N-CA-C	-5.32	100.45	108.12
1	G	203	ILE	CB-CA-C	-5.32	102.56	110.33
1	B	203	ILE	CB-CA-C	-5.32	102.56	110.33
1	C	203	ILE	CB-CA-C	-5.32	102.56	110.33
1	E	203	ILE	CB-CA-C	-5.32	102.56	110.33
1	E	203	ILE	N-CA-C	-5.32	100.46	108.12
1	B	203	ILE	N-CA-C	-5.32	100.47	108.12
1	C	203	ILE	N-CA-C	-5.31	100.47	108.12
1	C	33	LYS	N-CA-C	-5.31	101.00	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	ILE	CB-CA-C	-5.30	102.59	110.33
1	G	203	ILE	N-CA-C	-5.29	100.50	108.12
1	H	203	ILE	N-CA-C	-5.29	100.50	108.12
1	C	107	TRP	N-CA-C	5.29	119.72	113.16
1	B	33	LYS	N-CA-C	-5.29	101.03	109.23
1	E	33	LYS	N-CA-C	-5.29	101.03	109.23
1	E	107	TRP	N-CA-C	5.29	119.72	113.16
1	F	107	TRP	N-CA-C	5.28	119.71	113.16
1	D	33	LYS	N-CA-C	-5.28	101.05	109.23
1	H	33	LYS	N-CA-C	-5.28	101.05	109.23
1	G	33	LYS	N-CA-C	-5.27	101.06	109.23
1	F	33	LYS	N-CA-C	-5.27	101.06	109.23
1	A	33	LYS	N-CA-C	-5.27	101.07	109.23
1	B	60	SER	N-CA-C	-5.24	105.21	111.03
1	H	107	TRP	N-CA-C	5.24	119.66	113.16
1	G	253	ILE	CA-C-N	-5.23	112.87	120.29
1	G	253	ILE	C-N-CA	-5.23	112.87	120.29
1	A	107	TRP	N-CA-C	5.22	119.64	113.16
1	B	107	TRP	N-CA-C	5.22	119.64	113.16
1	G	107	TRP	N-CA-C	5.21	119.63	113.16
1	D	107	TRP	N-CA-C	5.21	119.62	113.16
1	C	57	SER	O-C-N	5.20	128.84	122.96
1	G	58	GLU	CA-C-N	5.19	126.33	119.84
1	G	58	GLU	C-N-CA	5.19	126.33	119.84
1	B	40	THR	N-CA-C	-5.14	102.70	109.84
1	C	40	THR	N-CA-C	-5.13	102.71	109.84
1	F	40	THR	N-CA-C	-5.12	102.72	109.84
1	B	248	ASN	CB-CA-C	-5.12	101.50	109.84
1	D	40	THR	N-CA-C	-5.11	102.74	109.84
1	E	28	GLN	O-C-N	5.11	123.79	120.27
1	A	128	TYR	CA-CB-CG	-5.11	104.71	113.90
1	H	128	TYR	CA-CB-CG	-5.11	104.71	113.90
1	D	128	TYR	CA-CB-CG	-5.10	104.72	113.90
1	G	40	THR	N-CA-C	-5.10	102.75	109.84
1	B	128	TYR	CA-CB-CG	-5.10	104.72	113.90
1	C	128	TYR	CA-CB-CG	-5.10	104.72	113.90
1	E	128	TYR	CA-CB-CG	-5.10	104.73	113.90
1	H	40	THR	N-CA-C	-5.09	102.77	109.84
1	A	40	THR	N-CA-C	-5.09	102.77	109.84
1	D	61	ASN	CA-C-O	5.09	124.53	119.75
1	E	40	THR	N-CA-C	-5.08	102.77	109.84
1	G	128	TYR	CA-CB-CG	-5.08	104.75	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	128	TYR	CA-CB-CG	-5.07	104.77	113.90
1	H	192	ASP	N-CA-C	-5.06	98.63	109.81
1	F	192	ASP	N-CA-C	-5.05	98.64	109.81
1	E	192	ASP	N-CA-C	-5.04	98.66	109.81
1	D	192	ASP	N-CA-C	-5.04	98.67	109.81
1	B	192	ASP	N-CA-C	-5.04	98.67	109.81
1	A	192	ASP	N-CA-C	-5.04	98.67	109.81
1	C	192	ASP	N-CA-C	-5.03	98.68	109.81
1	G	192	ASP	N-CA-C	-5.03	98.70	109.81
1	B	25	SER	CA-C-N	5.01	126.83	120.72
1	B	25	SER	C-N-CA	5.01	126.83	120.72
1	D	127	ASP	N-CA-C	5.00	117.62	111.82
1	H	25	SER	CA-C-N	5.00	126.82	120.72
1	H	25	SER	C-N-CA	5.00	126.82	120.72

There are no chirality outliers.

There are no planarity outliers.

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	2720	0	2675	91	0
1	B	2720	0	2675	101	0
1	C	2720	0	2675	92	1
1	D	2720	0	2675	86	0
1	E	2720	0	2675	99	1
1	F	2720	0	2675	94	1
1	G	2720	0	2675	77	0
1	H	2720	0	2675	90	1
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
2	E	53	0	31	1	0
2	F	53	0	31	1	0
2	G	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	53	0	31	1	0
3	A	9	0	5	0	0
3	B	9	0	5	0	0
3	C	9	0	5	0	0
3	D	9	0	5	0	0
3	E	9	0	5	0	0
3	F	9	0	5	0	0
3	G	9	0	5	0	0
3	H	9	0	5	0	0
4	A	51	0	0	4	0
4	B	31	0	0	2	0
4	C	25	0	0	2	0
4	D	53	0	0	4	0
4	E	35	0	0	5	0
4	F	42	0	0	3	0
4	G	22	0	0	4	0
4	H	35	0	0	3	0
All	All	22550	0	21688	706	2

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 16.

All (706) 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:C:201:GLN:NE2	1:C:252:ASN:H	1.47	1.13
1:A:201:GLN:NE2	1:A:252:ASN:H	1.47	1.12
1:H:201:GLN:NE2	1:H:252:ASN:H	1.47	1.12
1:B:201:GLN:NE2	1:B:252:ASN:H	1.47	1.11
1:E:201:GLN:NE2	1:E:252:ASN:H	1.47	1.11
1:F:201:GLN:NE2	1:F:252:ASN:H	1.47	1.10
1:D:201:GLN:NE2	1:D:252:ASN:H	1.47	1.10
1:G:201:GLN:NE2	1:G:252:ASN:H	1.47	1.09
1:B:24:HIS:ND1	1:B:25:SER:N	2.12	0.98
1:H:92:VAL:HG21	1:H:138:ILE:HG13	1.48	0.95
1:D:180:ASN:HD22	1:D:307:HIS:HD2	1.14	0.95
1:F:92:VAL:HG21	1:F:138:ILE:HG13	1.48	0.95
1:G:180:ASN:HD22	1:G:307:HIS:HD2	1.14	0.95
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.14	0.95
1:A:92:VAL:HG21	1:A:138:ILE:HG13	1.48	0.95
1:E:180:ASN:HD22	1:E:307:HIS:HD2	1.14	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:VAL:HG21	1:C:138:ILE:HG13	1.49	0.94
1:H:180:ASN:HD22	1:H:307:HIS:HD2	1.15	0.94
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.14	0.94
1:D:92:VAL:HG21	1:D:138:ILE:HG13	1.49	0.94
1:C:180:ASN:HD22	1:C:307:HIS:HD2	1.14	0.94
1:E:92:VAL:HG21	1:E:138:ILE:HG13	1.48	0.92
1:G:92:VAL:HG21	1:G:138:ILE:HG13	1.48	0.92
1:F:180:ASN:HD22	1:F:307:HIS:HD2	1.14	0.92
1:H:21:GLU:HA	1:H:155:ARG:HH12	1.36	0.92
1:C:21:GLU:HA	1:C:155:ARG:HH12	1.35	0.91
1:F:21:GLU:HA	1:F:155:ARG:HH12	1.35	0.91
1:B:92:VAL:HG21	1:B:138:ILE:HG13	1.49	0.91
1:G:21:GLU:HA	1:G:155:ARG:HH12	1.36	0.91
1:A:21:GLU:HA	1:A:155:ARG:HH12	1.36	0.90
1:B:21:GLU:HA	1:B:155:ARG:HH12	1.35	0.90
1:D:21:GLU:HA	1:D:155:ARG:HH12	1.36	0.90
1:E:21:GLU:HA	1:E:155:ARG:HH12	1.36	0.89
1:C:61:ASN:HB3	1:C:64:GLU:HG3	1.55	0.88
1:E:78:HIS:CD2	1:E:87:MET:HE1	2.09	0.88
1:B:78:HIS:CD2	1:B:87:MET:HE1	2.09	0.87
1:C:78:HIS:CD2	1:C:87:MET:HE1	2.09	0.87
1:F:78:HIS:CD2	1:F:87:MET:HE1	2.09	0.87
1:D:78:HIS:CD2	1:D:87:MET:HE1	2.09	0.87
1:A:78:HIS:CD2	1:A:87:MET:HE1	2.09	0.87
1:H:78:HIS:CD2	1:H:87:MET:HE1	2.09	0.87
1:G:78:HIS:CD2	1:G:87:MET:HE1	2.09	0.86
1:E:21:GLU:HG3	1:E:155:ARG:HH22	1.41	0.86
1:F:21:GLU:HG3	1:F:155:ARG:HH22	1.41	0.85
1:G:201:GLN:HG2	1:G:280:THR:HG22	1.58	0.85
1:D:201:GLN:HG2	1:D:280:THR:HG22	1.58	0.85
1:A:21:GLU:HG3	1:A:155:ARG:HH22	1.41	0.85
1:H:201:GLN:HG2	1:H:280:THR:HG22	1.58	0.85
1:D:21:GLU:HG3	1:D:155:ARG:HH22	1.41	0.85
1:H:21:GLU:HG3	1:H:155:ARG:HH22	1.41	0.85
1:B:92:VAL:CG2	1:B:138:ILE:HG13	2.07	0.84
1:C:21:GLU:HG3	1:C:155:ARG:HH22	1.41	0.84
1:E:201:GLN:HG2	1:E:280:THR:HG22	1.58	0.84
1:G:21:GLU:HG3	1:G:155:ARG:HH22	1.41	0.84
1:A:92:VAL:CG2	1:A:138:ILE:HG13	2.07	0.84
1:A:165:GLU:HB3	1:A:169:GLU:OE1	1.78	0.84
1:B:21:GLU:HG3	1:B:155:ARG:HH22	1.41	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:VAL:CG2	1:D:138:ILE:HG13	2.08	0.83
1:G:201:GLN:NE2	1:G:252:ASN:N	2.27	0.83
1:H:92:VAL:CG2	1:H:138:ILE:HG13	2.07	0.83
1:C:92:VAL:CG2	1:C:138:ILE:HG13	2.07	0.83
1:B:201:GLN:HG2	1:B:280:THR:HG22	1.58	0.83
1:G:92:VAL:CG2	1:G:138:ILE:HG13	2.07	0.83
1:F:92:VAL:CG2	1:F:138:ILE:HG13	2.07	0.83
1:A:201:GLN:HG2	1:A:280:THR:HG22	1.58	0.83
1:E:92:VAL:CG2	1:E:138:ILE:HG13	2.07	0.83
1:F:201:GLN:HG2	1:F:280:THR:HG22	1.58	0.83
1:A:201:GLN:NE2	1:A:252:ASN:N	2.27	0.82
1:C:201:GLN:HG2	1:C:280:THR:HG22	1.58	0.82
1:B:201:GLN:NE2	1:B:252:ASN:N	2.27	0.82
1:C:201:GLN:NE2	1:C:252:ASN:N	2.27	0.82
1:F:201:GLN:NE2	1:F:252:ASN:N	2.27	0.82
1:C:256:HIS:ND1	1:C:278:GLU:OE2	2.13	0.82
1:A:256:HIS:ND1	1:A:278:GLU:OE2	2.13	0.82
1:D:201:GLN:NE2	1:D:252:ASN:N	2.27	0.82
1:G:256:HIS:ND1	1:G:278:GLU:OE2	2.13	0.81
1:B:102:VAL:HG13	1:B:103:PRO:HD2	1.63	0.81
1:E:256:HIS:ND1	1:E:278:GLU:OE2	2.13	0.81
1:H:256:HIS:ND1	1:H:278:GLU:OE2	2.13	0.81
1:C:102:VAL:HG13	1:C:103:PRO:HD2	1.63	0.81
1:E:201:GLN:NE2	1:E:252:ASN:N	2.27	0.81
1:G:102:VAL:HG13	1:G:103:PRO:HD2	1.63	0.81
1:F:102:VAL:HG13	1:F:103:PRO:HD2	1.63	0.80
1:F:256:HIS:ND1	1:F:278:GLU:OE2	2.13	0.80
1:B:256:HIS:ND1	1:B:278:GLU:OE2	2.13	0.80
1:C:21:GLU:HG3	1:C:155:ARG:NH2	1.97	0.80
1:E:21:GLU:HG3	1:E:155:ARG:NH2	1.97	0.80
1:D:256:HIS:ND1	1:D:278:GLU:OE2	2.13	0.80
1:B:21:GLU:HG3	1:B:155:ARG:NH2	1.97	0.80
1:H:201:GLN:NE2	1:H:252:ASN:N	2.27	0.80
1:H:21:GLU:HG3	1:H:155:ARG:NH2	1.97	0.79
1:H:102:VAL:HG13	1:H:103:PRO:HD2	1.63	0.79
1:B:201:GLN:HE22	1:B:252:ASN:H	1.31	0.79
1:E:102:VAL:HG13	1:E:103:PRO:HD2	1.63	0.79
1:D:102:VAL:HG13	1:D:103:PRO:HD2	1.63	0.79
1:G:54:PRO:O	4:G:371:HOH:O	1.99	0.79
1:D:21:GLU:HG3	1:D:155:ARG:NH2	1.96	0.79
1:A:102:VAL:HG13	1:A:103:PRO:HD2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:GLN:HE22	1:F:252:ASN:H	1.31	0.79
1:G:21:GLU:HG3	1:G:155:ARG:NH2	1.97	0.79
1:D:201:GLN:HE22	1:D:252:ASN:H	1.31	0.79
1:A:21:GLU:HG3	1:A:155:ARG:NH2	1.97	0.78
1:E:201:GLN:HE22	1:E:252:ASN:H	1.30	0.78
1:F:21:GLU:HG3	1:F:155:ARG:NH2	1.97	0.78
1:G:201:GLN:HE22	1:G:252:ASN:H	1.30	0.78
1:G:180:ASN:HD22	1:G:307:HIS:CD2	2.01	0.78
1:A:201:GLN:HE22	1:A:252:ASN:H	1.30	0.77
1:B:180:ASN:HD22	1:B:307:HIS:CD2	2.01	0.77
1:H:21:GLU:HA	1:H:155:ARG:NH1	2.00	0.77
1:C:21:GLU:HA	1:C:155:ARG:NH1	2.00	0.77
1:F:21:GLU:HA	1:F:155:ARG:NH1	2.00	0.77
1:D:21:GLU:HA	1:D:155:ARG:NH1	2.00	0.77
1:A:180:ASN:HD22	1:A:307:HIS:CD2	2.01	0.77
1:F:180:ASN:HD22	1:F:307:HIS:CD2	2.01	0.77
1:F:1:MET:HE3	1:F:334:LEU:HD21	1.68	0.76
1:H:180:ASN:HD22	1:H:307:HIS:CD2	2.02	0.76
1:A:1:MET:HE3	1:A:334:LEU:HD21	1.68	0.76
1:E:180:ASN:HD22	1:E:307:HIS:CD2	2.01	0.76
1:C:180:ASN:HD22	1:C:307:HIS:CD2	2.01	0.76
1:E:1:MET:HE3	1:E:334:LEU:HD21	1.68	0.76
1:G:1:MET:HE3	1:G:334:LEU:HD21	1.68	0.76
1:H:201:GLN:HE22	1:H:252:ASN:H	1.31	0.76
1:B:21:GLU:HA	1:B:155:ARG:NH1	2.00	0.76
1:E:21:GLU:HA	1:E:155:ARG:NH1	2.00	0.76
1:G:21:GLU:HA	1:G:155:ARG:NH1	2.00	0.76
1:A:21:GLU:HA	1:A:155:ARG:NH1	2.00	0.76
1:B:1:MET:HE3	1:B:334:LEU:HD21	1.68	0.75
1:D:193:PRO:HG2	1:F:73:ASN:HB2	1.68	0.75
1:D:1:MET:HE3	1:D:334:LEU:HD21	1.68	0.75
1:F:58:GLU:HG3	1:F:59:PRO:HD2	1.70	0.74
1:C:1:MET:HE3	1:C:334:LEU:HD21	1.68	0.74
1:H:1:MET:HE3	1:H:334:LEU:HD21	1.68	0.74
1:E:61:ASN:HD22	1:E:62:PRO:N	1.85	0.74
1:C:201:GLN:HE22	1:C:252:ASN:H	1.31	0.74
1:H:278:GLU:HG3	4:H:374:HOH:O	1.87	0.74
1:A:1:MET:HE3	1:A:334:LEU:CD2	2.19	0.73
1:G:1:MET:HE3	1:G:334:LEU:CD2	2.19	0.73
1:D:61:ASN:HB2	1:D:64:GLU:HG3	1.70	0.73
1:D:180:ASN:HD22	1:D:307:HIS:CD2	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE3	1:C:334:LEU:CD2	2.19	0.73
1:D:1:MET:HE3	1:D:334:LEU:CD2	2.19	0.73
1:B:1:MET:HE3	1:B:334:LEU:CD2	2.19	0.72
1:E:1:MET:HE3	1:E:334:LEU:CD2	2.19	0.72
1:H:1:MET:HE3	1:H:334:LEU:CD2	2.19	0.72
1:D:58:GLU:HB3	1:D:59:PRO:HD2	1.71	0.72
1:F:1:MET:HE3	1:F:334:LEU:CD2	2.19	0.72
1:B:58:GLU:CG	1:B:59:PRO:HD2	2.21	0.71
1:A:61:ASN:ND2	1:A:288:GLN:OE1	2.24	0.71
1:A:201:GLN:HE22	1:A:252:ASN:N	1.89	0.71
1:B:295:GLN:O	1:B:296:LEU:HD23	1.92	0.70
1:D:295:GLN:O	1:D:296:LEU:HD23	1.92	0.69
1:D:134:ASN:ND2	4:D:381:HOH:O	2.24	0.69
1:G:201:GLN:HE22	1:G:252:ASN:N	1.89	0.69
1:B:123:ASP:OD2	1:D:287:PRO:HB3	1.93	0.69
1:G:66:ASN:O	1:G:70:GLN:HG3	1.93	0.69
1:F:295:GLN:O	1:F:296:LEU:HD23	1.92	0.69
1:G:295:GLN:O	1:G:296:LEU:HD23	1.92	0.69
1:C:201:GLN:HE22	1:C:252:ASN:N	1.89	0.69
1:D:201:GLN:HE22	1:D:252:ASN:N	1.89	0.68
1:E:295:GLN:O	1:E:296:LEU:HD23	1.92	0.68
1:B:201:GLN:HE22	1:B:252:ASN:N	1.89	0.68
1:C:295:GLN:O	1:C:296:LEU:HD23	1.92	0.68
1:A:295:GLN:O	1:A:296:LEU:HD23	1.92	0.68
1:F:278:GLU:HG3	4:F:364:HOH:O	1.93	0.68
1:H:295:GLN:O	1:H:296:LEU:HD23	1.92	0.68
1:A:58:GLU:CG	1:A:59:PRO:HD2	2.24	0.67
1:F:58:GLU:CG	1:F:59:PRO:HD2	2.27	0.65
1:D:66:ASN:O	1:D:70:GLN:HG3	1.95	0.65
1:F:201:GLN:HE21	1:F:252:ASN:H	1.44	0.65
1:A:253:ILE:HA	1:F:42:PHE:CE2	2.32	0.65
1:H:134:ASN:ND2	4:H:355:HOH:O	2.29	0.65
1:F:201:GLN:HE22	1:F:252:ASN:N	1.89	0.64
1:B:254:GLN:O	1:B:258:THR:HG23	1.98	0.64
1:C:201:GLN:HE21	1:C:252:ASN:H	1.44	0.64
1:F:254:GLN:O	1:F:258:THR:HG23	1.98	0.64
1:A:58:GLU:HG3	1:A:59:PRO:HD2	1.77	0.64
1:E:254:GLN:O	1:E:258:THR:HG23	1.98	0.64
1:B:58:GLU:HG3	1:B:59:PRO:HD2	1.80	0.64
1:D:254:GLN:O	1:D:258:THR:HG23	1.98	0.64
1:E:93:SER:OG	1:E:135:THR:HB	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:GLN:HE22	1:H:252:ASN:N	1.89	0.64
1:A:254:GLN:O	1:A:258:THR:HG23	1.98	0.64
1:D:93:SER:OG	1:D:135:THR:HB	1.98	0.64
1:G:165:GLU:HB3	1:G:169:GLU:OE1	1.98	0.64
1:C:254:GLN:O	1:C:258:THR:HG23	1.98	0.63
1:G:93:SER:OG	1:G:135:THR:HB	1.98	0.63
1:C:216:THR:HB	1:C:227:PRO:O	1.99	0.63
1:G:254:GLN:O	1:G:258:THR:HG23	1.98	0.63
1:F:93:SER:OG	1:F:135:THR:HB	1.98	0.63
1:B:93:SER:OG	1:B:135:THR:HB	1.98	0.63
1:B:250:ILE:HD11	1:E:250:ILE:HD13	1.80	0.63
1:H:201:GLN:HE21	1:H:252:ASN:H	1.44	0.63
1:B:216:THR:HB	1:B:227:PRO:O	1.99	0.63
1:A:93:SER:OG	1:A:135:THR:HB	1.98	0.62
1:E:216:THR:HB	1:E:227:PRO:O	1.99	0.62
1:G:216:THR:HB	1:G:227:PRO:O	1.99	0.62
1:A:201:GLN:HE21	1:A:252:ASN:H	1.44	0.62
1:B:250:ILE:HD11	1:E:250:ILE:CD1	2.29	0.62
1:C:93:SER:OG	1:C:135:THR:HB	1.98	0.62
1:F:216:THR:HB	1:F:227:PRO:O	1.99	0.62
1:H:93:SER:OG	1:H:135:THR:HB	1.98	0.62
1:H:254:GLN:O	1:H:258:THR:HG23	1.98	0.62
1:H:216:THR:HB	1:H:227:PRO:O	1.99	0.62
1:D:216:THR:HB	1:D:227:PRO:O	1.99	0.62
1:E:201:GLN:HE22	1:E:252:ASN:N	1.89	0.62
1:D:201:GLN:HE21	1:D:252:ASN:H	1.44	0.61
1:A:216:THR:HB	1:A:227:PRO:O	1.99	0.61
1:C:28:GLN:N	1:C:29:PRO:HD2	2.14	0.61
1:D:278:GLU:HG3	4:D:361:HOH:O	2.01	0.61
1:H:126:PRO:HD2	4:H:358:HOH:O	2.01	0.61
1:H:304:GLU:HG2	1:H:337:ARG:NH2	2.15	0.61
1:G:19:ILE:HG22	1:G:20:HIS:N	2.16	0.60
1:H:58:GLU:CG	1:H:59:PRO:HD2	2.31	0.60
1:C:105:PRO:HG3	1:C:132:TRP:CH2	2.37	0.60
1:G:189:LEU:HB2	4:G:368:HOH:O	2.00	0.60
1:G:105:PRO:HG3	1:G:132:TRP:CH2	2.37	0.60
1:B:19:ILE:HG22	1:B:20:HIS:N	2.16	0.60
1:H:105:PRO:HG3	1:H:132:TRP:CH2	2.37	0.60
1:B:105:PRO:HG3	1:B:132:TRP:CH2	2.37	0.60
1:D:105:PRO:HG3	1:D:132:TRP:CH2	2.37	0.60
1:F:105:PRO:HG3	1:F:132:TRP:CH2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:ILE:HG22	1:F:20:HIS:N	2.16	0.59
1:H:19:ILE:HG22	1:H:20:HIS:N	2.16	0.59
1:A:250:ILE:HD11	1:F:250:ILE:HD13	1.84	0.59
1:G:201:GLN:HE21	1:G:252:ASN:H	1.44	0.59
1:A:291:LEU:HA	1:A:307:HIS:O	2.03	0.59
1:G:291:LEU:HA	1:G:307:HIS:O	2.03	0.59
1:A:105:PRO:HG3	1:A:132:TRP:CH2	2.37	0.59
1:C:19:ILE:HG22	1:C:20:HIS:N	2.16	0.59
1:D:19:ILE:HG22	1:D:20:HIS:N	2.16	0.59
1:A:19:ILE:HG22	1:A:20:HIS:N	2.16	0.59
1:G:142:ARG:O	1:G:146:GLN:HG3	2.03	0.59
1:C:205:VAL:HG13	1:C:273:ALA:HB1	1.85	0.59
1:D:205:VAL:HG13	1:D:273:ALA:HB1	1.85	0.59
1:E:142:ARG:O	1:E:146:GLN:HG3	2.03	0.59
1:C:291:LEU:HA	1:C:307:HIS:O	2.03	0.59
1:D:291:LEU:HA	1:D:307:HIS:O	2.03	0.59
1:E:105:PRO:HG3	1:E:132:TRP:CH2	2.37	0.59
1:E:205:VAL:HG13	1:E:273:ALA:HB1	1.85	0.59
1:H:291:LEU:HA	1:H:307:HIS:O	2.03	0.59
1:B:291:LEU:HA	1:B:307:HIS:O	2.03	0.58
1:D:142:ARG:O	1:D:146:GLN:HG3	2.03	0.58
1:E:184:VAL:HG13	1:E:284:PRO:HA	1.86	0.58
1:F:291:LEU:HA	1:F:307:HIS:O	2.03	0.58
1:H:184:VAL:HG13	1:H:284:PRO:HA	1.85	0.58
1:A:142:ARG:O	1:A:146:GLN:HG3	2.03	0.58
1:C:142:ARG:O	1:C:146:GLN:HG3	2.03	0.58
1:C:184:VAL:HG13	1:C:284:PRO:HA	1.86	0.58
1:B:24:HIS:CE1	1:B:25:SER:HB3	2.38	0.58
1:B:205:VAL:HG13	1:B:273:ALA:HB1	1.85	0.58
1:C:126:PRO:HD2	4:C:360:HOH:O	2.02	0.58
1:D:184:VAL:HG13	1:D:284:PRO:HA	1.86	0.58
1:F:205:VAL:HG13	1:F:273:ALA:HB1	1.85	0.58
1:E:61:ASN:ND2	1:E:63:GLN:H	2.01	0.58
1:G:184:VAL:HG13	1:G:284:PRO:HA	1.86	0.58
1:H:205:VAL:HG13	1:H:273:ALA:HB1	1.85	0.58
1:B:184:VAL:HG13	1:B:284:PRO:HA	1.86	0.58
1:H:142:ARG:O	1:H:146:GLN:HG3	2.03	0.58
1:B:201:GLN:HE21	1:B:252:ASN:H	1.44	0.58
1:A:205:VAL:HG13	1:A:273:ALA:HB1	1.85	0.58
1:E:19:ILE:HG22	1:E:20:HIS:N	2.16	0.58
1:E:201:GLN:HE21	1:E:252:ASN:H	1.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:LEU:HA	1:E:307:HIS:O	2.03	0.57
1:G:205:VAL:HG13	1:G:273:ALA:HB1	1.85	0.57
1:F:142:ARG:O	1:F:146:GLN:HG3	2.03	0.57
1:F:184:VAL:HG13	1:F:284:PRO:HA	1.85	0.57
1:A:184:VAL:HG13	1:A:284:PRO:HA	1.85	0.57
1:E:58:GLU:HG2	1:E:59:PRO:HD2	1.86	0.57
1:B:58:GLU:HG2	1:B:59:PRO:HD2	1.86	0.57
1:C:105:PRO:HG3	1:C:132:TRP:CZ3	2.40	0.57
1:A:105:PRO:HG3	1:A:132:TRP:CZ3	2.40	0.57
1:F:190:GLN:NE2	1:F:290:ARG:HH12	2.03	0.57
1:H:105:PRO:HG3	1:H:132:TRP:CZ3	2.40	0.57
1:H:190:GLN:NE2	1:H:290:ARG:HH12	2.03	0.57
1:A:190:GLN:NE2	1:A:290:ARG:HH12	2.03	0.57
1:B:190:GLN:NE2	1:B:290:ARG:HH12	2.03	0.57
1:D:105:PRO:HG3	1:D:132:TRP:CZ3	2.40	0.57
1:B:105:PRO:HG3	1:B:132:TRP:CZ3	2.40	0.57
1:D:190:GLN:NE2	1:D:290:ARG:HH12	2.03	0.57
1:E:190:GLN:NE2	1:E:290:ARG:HH12	2.03	0.57
1:B:142:ARG:O	1:B:146:GLN:HG3	2.03	0.56
1:G:105:PRO:HG3	1:G:132:TRP:CZ3	2.40	0.56
1:B:256:HIS:HD1	1:B:278:GLU:CD	2.14	0.56
1:E:105:PRO:HG3	1:E:132:TRP:CZ3	2.40	0.56
1:A:134:ASN:ND2	4:A:386:HOH:O	2.38	0.56
1:A:275:ILE:HD12	1:F:142:ARG:HH21	1.70	0.56
1:A:293:ARG:NH2	1:A:336:GLU:OE1	2.39	0.56
1:G:190:GLN:NE2	1:G:290:ARG:HH12	2.03	0.56
1:E:293:ARG:NH2	1:E:336:GLU:OE1	2.39	0.56
1:G:293:ARG:NH2	1:G:336:GLU:OE1	2.39	0.56
1:F:105:PRO:HG3	1:F:132:TRP:CZ3	2.40	0.56
1:D:293:ARG:NH2	1:D:336:GLU:OE1	2.39	0.56
1:E:61:ASN:HD22	1:E:61:ASN:C	2.14	0.56
1:F:293:ARG:NH2	1:F:336:GLU:OE1	2.39	0.56
1:A:250:ILE:HD11	1:F:250:ILE:CD1	2.36	0.55
1:C:190:GLN:NE2	1:C:290:ARG:HH12	2.03	0.55
1:B:293:ARG:NH2	1:B:336:GLU:OE1	2.39	0.55
1:B:20:HIS:CE1	1:B:155:ARG:HD3	2.42	0.55
1:B:248:ASN:OD1	1:B:248:ASN:N	2.37	0.55
1:H:293:ARG:NH2	1:H:336:GLU:OE1	2.39	0.55
1:H:332:LYS:O	1:H:336:GLU:HG3	2.07	0.55
1:C:293:ARG:NH2	1:C:336:GLU:OE1	2.39	0.55
1:D:332:LYS:O	1:D:336:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:HIS:CE1	1:F:155:ARG:HD3	2.42	0.55
1:H:20:HIS:CE1	1:H:155:ARG:HD3	2.42	0.55
1:C:20:HIS:CE1	1:C:155:ARG:HD3	2.42	0.55
1:E:20:HIS:CE1	1:E:155:ARG:HD3	2.42	0.55
1:B:250:ILE:CD1	1:E:250:ILE:HD13	2.37	0.55
1:D:20:HIS:CE1	1:D:155:ARG:HD3	2.42	0.55
1:F:58:GLU:HG3	1:F:59:PRO:CD	2.37	0.55
1:G:332:LYS:O	1:G:336:GLU:HG3	2.07	0.55
1:G:256:HIS:HD1	1:G:278:GLU:CD	2.14	0.55
1:B:96:ASN:OD1	1:B:217:HIS:HE1	1.90	0.54
1:C:332:LYS:O	1:C:336:GLU:HG3	2.07	0.54
1:D:96:ASN:OD1	1:D:217:HIS:HE1	1.91	0.54
1:F:96:ASN:OD1	1:F:217:HIS:HE1	1.91	0.54
1:B:332:LYS:O	1:B:336:GLU:HG3	2.07	0.54
1:F:115:ARG:HH22	1:F:121:GLU:CD	2.15	0.54
1:G:20:HIS:CE1	1:G:155:ARG:HD3	2.42	0.54
1:A:20:HIS:CE1	1:A:155:ARG:HD3	2.42	0.54
1:A:66:ASN:O	1:A:70:GLN:HG3	2.07	0.54
1:B:196:GLN:HG2	4:B:373:HOH:O	2.06	0.54
1:F:200:GLY:HA2	1:F:241:THR:OG1	2.08	0.54
1:C:200:GLY:HA2	1:C:241:THR:OG1	2.08	0.54
1:E:58:GLU:HG2	1:E:59:PRO:CD	2.37	0.54
1:E:96:ASN:OD1	1:E:217:HIS:HE1	1.91	0.54
1:E:332:LYS:O	1:E:336:GLU:HG3	2.07	0.54
1:H:96:ASN:OD1	1:H:217:HIS:HE1	1.91	0.54
1:C:256:HIS:HD1	1:C:278:GLU:CD	2.14	0.54
1:E:115:ARG:HH22	1:E:121:GLU:CD	2.15	0.54
1:E:200:GLY:HA2	1:E:241:THR:OG1	2.08	0.54
1:B:115:ARG:HH22	1:B:121:GLU:CD	2.15	0.54
1:C:96:ASN:OD1	1:C:217:HIS:HE1	1.91	0.54
1:E:256:HIS:HD1	1:E:278:GLU:CD	2.14	0.54
1:F:1:MET:N	1:F:29:PRO:O	2.41	0.54
1:F:93:SER:HA	1:F:135:THR:HA	1.89	0.54
1:G:102:VAL:CG1	1:G:103:PRO:HD2	2.37	0.54
1:H:93:SER:HA	1:H:135:THR:HA	1.89	0.54
1:H:304:GLU:HG2	1:H:337:ARG:HH21	1.70	0.54
1:A:93:SER:HA	1:A:135:THR:HA	1.89	0.54
1:B:200:GLY:HA2	1:B:241:THR:OG1	2.08	0.54
1:F:332:LYS:O	1:F:336:GLU:HG3	2.07	0.54
1:A:332:LYS:O	1:A:336:GLU:HG3	2.07	0.54
1:D:200:GLY:HA2	1:D:241:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:SER:HA	1:G:135:THR:HA	1.89	0.54
1:D:256:HIS:HD1	1:D:278:GLU:CD	2.14	0.54
1:G:96:ASN:OD1	1:G:217:HIS:HE1	1.90	0.54
1:B:93:SER:HA	1:B:135:THR:HA	1.89	0.53
1:H:115:ARG:HH22	1:H:121:GLU:CD	2.15	0.53
1:H:200:GLY:HA2	1:H:241:THR:OG1	2.08	0.53
1:B:165:GLU:HB3	1:B:169:GLU:OE1	2.08	0.53
1:B:275:ILE:HD12	1:E:142:ARG:HH21	1.72	0.53
1:G:115:ARG:HH22	1:G:121:GLU:CD	2.15	0.53
1:G:200:GLY:HA2	1:G:241:THR:OG1	2.08	0.53
1:A:135:THR:HG21	4:E:363:HOH:O	2.08	0.53
1:C:93:SER:HA	1:C:135:THR:HA	1.89	0.53
1:C:102:VAL:CG1	1:C:103:PRO:HD2	2.37	0.53
1:C:115:ARG:HH22	1:C:121:GLU:CD	2.15	0.53
1:E:93:SER:HA	1:E:135:THR:HA	1.89	0.53
1:A:96:ASN:OD1	1:A:217:HIS:HE1	1.91	0.53
1:B:253:ILE:HA	1:E:42:PHE:CE2	2.43	0.53
1:D:115:ARG:HH22	1:D:121:GLU:CD	2.15	0.53
1:F:126:PRO:HD2	4:F:368:HOH:O	2.07	0.53
1:A:200:GLY:HA2	1:A:241:THR:OG1	2.08	0.53
1:H:24:HIS:HB2	1:H:30:LEU:HD23	1.89	0.53
1:A:128:TYR:CD1	1:A:128:TYR:N	2.77	0.53
1:D:93:SER:HA	1:D:135:THR:HA	1.89	0.53
1:E:184:VAL:CG1	1:E:284:PRO:HA	2.39	0.53
1:G:128:TYR:CD1	1:G:128:TYR:N	2.77	0.53
1:A:184:VAL:CG1	1:A:284:PRO:HA	2.39	0.53
1:F:184:VAL:CG1	1:F:284:PRO:HA	2.39	0.53
1:H:184:VAL:CG1	1:H:284:PRO:HA	2.39	0.53
1:H:102:VAL:CG1	1:H:103:PRO:HD2	2.37	0.53
1:A:115:ARG:HH22	1:A:121:GLU:CD	2.15	0.52
1:C:184:VAL:CG1	1:C:284:PRO:HA	2.39	0.52
1:D:128:TYR:N	1:D:128:TYR:CD1	2.77	0.52
1:D:184:VAL:CG1	1:D:284:PRO:HA	2.39	0.52
1:F:66:ASN:O	1:F:70:GLN:HG3	2.09	0.52
1:B:59:PRO:HB2	1:B:61:ASN:O	2.10	0.52
1:A:201:GLN:HG2	1:A:280:THR:CG2	2.36	0.52
1:C:128:TYR:N	1:C:128:TYR:CD1	2.77	0.52
1:F:102:VAL:CG1	1:F:103:PRO:HD2	2.37	0.52
1:C:29:PRO:O	1:C:30:LEU:HB2	2.08	0.52
1:B:58:GLU:HG3	1:B:59:PRO:CD	2.37	0.52
1:F:256:HIS:HD1	1:F:278:GLU:CD	2.14	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:TYR:CD1	1:F:128:TYR:N	2.77	0.52
1:G:184:VAL:CG1	1:G:284:PRO:HA	2.39	0.52
1:A:256:HIS:HD1	1:A:278:GLU:CD	2.14	0.51
1:H:58:GLU:HG2	1:H:59:PRO:HD2	1.92	0.51
1:E:128:TYR:N	1:E:128:TYR:CD1	2.77	0.51
1:H:128:TYR:CD1	1:H:128:TYR:N	2.77	0.51
1:B:201:GLN:HG2	1:B:280:THR:CG2	2.36	0.51
1:G:201:GLN:HG2	1:G:280:THR:CG2	2.36	0.51
1:B:102:VAL:CG1	1:B:103:PRO:HD2	2.37	0.51
1:B:184:VAL:CG1	1:B:284:PRO:HA	2.39	0.51
1:C:201:GLN:HG2	1:C:280:THR:CG2	2.36	0.51
1:D:201:GLN:HG2	1:D:280:THR:CG2	2.36	0.51
1:E:102:VAL:CG1	1:E:103:PRO:HD2	2.37	0.51
1:E:66:ASN:O	1:E:70:GLN:HG3	2.10	0.51
1:C:58:GLU:HG3	1:C:59:PRO:CD	2.41	0.51
1:H:201:GLN:HG2	1:H:280:THR:CG2	2.36	0.51
1:D:251:ASN:OD1	1:D:280:THR:HG23	2.11	0.51
1:B:128:TYR:N	1:B:128:TYR:CD1	2.77	0.51
1:B:251:ASN:OD1	1:B:280:THR:HG23	2.11	0.50
1:D:128:TYR:C	1:D:129:ARG:HG2	2.35	0.50
1:F:251:ASN:OD1	1:F:280:THR:HG23	2.11	0.50
1:C:82:PRO:HA	1:G:268:PRO:HB2	1.93	0.50
1:E:24:HIS:CG	1:E:25:SER:N	2.80	0.50
1:B:205:VAL:CG1	1:B:273:ALA:HB1	2.42	0.50
1:B:250:ILE:CD1	1:E:250:ILE:CD1	2.89	0.50
1:H:251:ASN:OD1	1:H:280:THR:HG23	2.11	0.50
1:B:58:GLU:CG	1:B:59:PRO:CD	2.90	0.50
1:B:275:ILE:HD12	1:E:142:ARG:NH2	2.27	0.50
1:E:248:ASN:ND2	4:E:384:HOH:O	2.34	0.50
1:G:205:VAL:CG1	1:G:273:ALA:HB1	2.42	0.50
1:E:251:ASN:OD1	1:E:280:THR:HG23	2.11	0.50
1:H:256:HIS:HD1	1:H:278:GLU:CD	2.14	0.50
1:D:268:PRO:HB2	1:H:82:PRO:HA	1.93	0.49
1:E:205:VAL:CG1	1:E:273:ALA:HB1	2.42	0.49
1:A:251:ASN:OD1	1:A:280:THR:HG23	2.11	0.49
1:C:251:ASN:OD1	1:C:280:THR:HG23	2.11	0.49
1:D:102:VAL:CG1	1:D:103:PRO:HD2	2.37	0.49
1:G:251:ASN:OD1	1:G:280:THR:HG23	2.11	0.49
1:H:205:VAL:CG1	1:H:273:ALA:HB1	2.42	0.49
1:E:201:GLN:HG2	1:E:280:THR:CG2	2.36	0.49
1:F:201:GLN:HG2	1:F:280:THR:CG2	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:134:ASN:ND2	4:G:358:HOH:O	2.46	0.49
1:F:205:VAL:CG1	1:F:273:ALA:HB1	2.42	0.49
1:C:205:VAL:CG1	1:C:273:ALA:HB1	2.42	0.49
1:E:250:ILE:HD12	1:E:250:ILE:HG23	1.55	0.49
1:B:216:THR:HG22	1:B:226:SER:OG	2.14	0.48
1:H:161:LEU:O	1:H:162:ARG:HG3	2.13	0.48
1:A:205:VAL:CG1	1:A:273:ALA:HB1	2.42	0.48
1:C:216:THR:HG22	1:C:226:SER:OG	2.13	0.48
1:D:205:VAL:CG1	1:D:273:ALA:HB1	2.42	0.48
1:B:260:TRP:O	1:B:264:CYS:HB2	2.14	0.48
1:C:28:GLN:N	1:C:29:PRO:CD	2.77	0.48
1:C:260:TRP:O	1:C:264:CYS:HB2	2.14	0.48
1:A:58:GLU:HG2	1:A:59:PRO:HD2	1.93	0.48
1:A:102:VAL:CG1	1:A:103:PRO:HD2	2.37	0.48
1:G:216:THR:HG22	1:G:226:SER:OG	2.14	0.48
1:F:24:HIS:CG	1:F:25:SER:N	2.80	0.48
1:A:260:TRP:O	1:A:264:CYS:HB2	2.14	0.48
1:E:216:THR:HG22	1:E:226:SER:OG	2.14	0.48
1:G:199:ARG:HH22	1:G:201:GLN:HE21	1.62	0.47
1:G:260:TRP:O	1:G:264:CYS:HB2	2.14	0.47
1:A:36:ALA:HA	2:A:348:FAD:N3A	2.30	0.47
1:D:199:ARG:HH22	1:D:201:GLN:HE21	1.62	0.47
1:E:61:ASN:HB3	1:E:64:GLU:HG3	1.96	0.47
1:F:36:ALA:HA	2:F:348:FAD:N3A	2.30	0.47
1:F:199:ARG:HH22	1:F:201:GLN:HE21	1.62	0.47
1:B:250:ILE:HD12	1:B:250:ILE:HG23	1.55	0.47
1:D:260:TRP:O	1:D:264:CYS:HB2	2.14	0.47
1:H:216:THR:HG22	1:H:226:SER:OG	2.13	0.47
1:B:36:ALA:HA	2:B:348:FAD:N3A	2.30	0.47
1:D:216:THR:HG22	1:D:226:SER:OG	2.14	0.47
1:F:216:THR:HG22	1:F:226:SER:OG	2.14	0.47
1:F:260:TRP:O	1:F:264:CYS:HB2	2.14	0.47
1:H:36:ALA:HA	2:H:348:FAD:N3A	2.30	0.47
1:H:260:TRP:O	1:H:264:CYS:HB2	2.14	0.47
1:C:250:ILE:HG23	1:C:250:ILE:HD12	1.55	0.47
1:B:27:LEU:HA	1:B:27:LEU:HD23	1.38	0.47
1:B:199:ARG:HH22	1:B:201:GLN:HE21	1.62	0.47
1:C:194:LEU:HA	1:C:194:LEU:HD23	1.67	0.47
1:E:260:TRP:O	1:E:264:CYS:HB2	2.14	0.47
1:C:66:ASN:O	1:C:70:GLN:HG3	2.15	0.47
1:D:36:ALA:HA	2:D:348:FAD:N3A	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:ILE:HD12	1:H:250:ILE:HG23	1.55	0.47
1:C:177:VAL:HG12	1:C:178:ILE:N	2.30	0.46
1:G:36:ALA:HA	2:G:348:FAD:N3A	2.30	0.46
1:G:177:VAL:HG12	1:G:178:ILE:N	2.30	0.46
1:A:217:HIS:HA	4:A:395:HOH:O	2.15	0.46
1:C:58:GLU:CG	1:C:59:PRO:HD2	2.46	0.46
1:C:199:ARG:HH22	1:C:201:GLN:HE21	1.62	0.46
1:E:27:LEU:HA	1:E:27:LEU:HD23	1.38	0.46
1:E:177:VAL:HG12	1:E:178:ILE:N	2.31	0.46
1:H:199:ARG:HH22	1:H:201:GLN:HE21	1.62	0.46
1:F:92:VAL:HG21	1:F:138:ILE:CG1	2.35	0.46
1:B:177:VAL:HG12	1:B:178:ILE:N	2.30	0.46
1:E:36:ALA:HA	2:E:348:FAD:N3A	2.30	0.46
1:A:216:THR:HG22	1:A:226:SER:OG	2.14	0.46
1:B:252:ASN:HD21	1:B:255:ASP:CG	2.24	0.46
1:H:24:HIS:HD2	1:H:30:LEU:HB3	1.81	0.46
1:A:199:ARG:HH22	1:A:201:GLN:HE21	1.62	0.46
1:C:76:LEU:CD2	1:G:124:MET:HE2	2.45	0.46
1:B:24:HIS:CG	1:B:25:SER:N	2.81	0.46
1:C:24:HIS:CG	1:C:25:SER:N	2.84	0.46
1:C:216:THR:HG22	1:C:217:HIS:N	2.31	0.46
1:E:58:GLU:CG	1:E:59:PRO:CD	2.94	0.46
1:E:190:GLN:HA	1:E:191:PRO:HD3	1.61	0.46
1:E:293:ARG:HH22	1:E:336:GLU:CD	2.24	0.46
1:F:187:GLY:HA3	4:F:378:HOH:O	2.15	0.46
1:H:216:THR:HG22	1:H:217:HIS:N	2.31	0.46
1:C:36:ALA:HA	2:C:348:FAD:N3A	2.30	0.46
1:A:293:ARG:HH22	1:A:336:GLU:CD	2.24	0.46
1:C:58:GLU:HG3	1:C:59:PRO:HD3	1.98	0.46
1:D:216:THR:HG22	1:D:217:HIS:N	2.31	0.46
1:D:252:ASN:HD21	1:D:255:ASP:CG	2.24	0.46
1:D:318:ILE:HG12	1:D:318:ILE:O	2.16	0.46
1:G:252:ASN:HD21	1:G:255:ASP:CG	2.24	0.46
1:G:318:ILE:O	1:G:318:ILE:HG12	2.16	0.46
1:H:58:GLU:HA	1:H:59:PRO:HD3	1.66	0.46
1:A:61:ASN:HD22	1:A:61:ASN:N	2.14	0.45
1:D:177:VAL:HG12	1:D:178:ILE:N	2.31	0.45
1:H:318:ILE:HG12	1:H:318:ILE:O	2.16	0.45
1:D:211:LYS:O	4:D:367:HOH:O	2.21	0.45
1:D:258:THR:HG22	4:D:390:HOH:O	2.16	0.45
1:A:177:VAL:HG12	1:A:178:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASN:HD21	1:C:255:ASP:CG	2.24	0.45
1:E:252:ASN:HD21	1:E:255:ASP:CG	2.24	0.45
1:F:190:GLN:HA	1:F:191:PRO:HD3	1.61	0.45
1:F:252:ASN:HD21	1:F:255:ASP:CG	2.24	0.45
1:F:318:ILE:HG12	1:F:318:ILE:O	2.16	0.45
1:A:250:ILE:CD1	1:F:250:ILE:HD13	2.46	0.45
1:A:318:ILE:HG12	1:A:318:ILE:O	2.16	0.45
1:B:92:VAL:HG21	1:B:138:ILE:CG1	2.35	0.45
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.67	0.45
1:H:293:ARG:HH22	1:H:336:GLU:CD	2.24	0.45
1:A:216:THR:HG22	1:A:217:HIS:N	2.31	0.45
1:C:27:LEU:HA	1:C:27:LEU:HD23	1.38	0.45
1:E:199:ARG:HH22	1:E:201:GLN:HE21	1.62	0.45
1:F:177:VAL:HG12	1:F:178:ILE:N	2.30	0.45
1:H:177:VAL:HG12	1:H:178:ILE:N	2.30	0.45
1:C:58:GLU:HA	1:C:59:PRO:HD3	1.63	0.45
1:C:115:ARG:NH2	1:C:121:GLU:OE2	2.42	0.45
1:H:115:ARG:NH2	1:H:121:GLU:OE2	2.42	0.45
1:H:230:ILE:HA	1:H:231:PRO:HD3	1.70	0.45
1:A:252:ASN:HD21	1:A:255:ASP:CG	2.24	0.45
1:C:293:ARG:HH22	1:C:336:GLU:CD	2.24	0.45
1:D:293:ARG:HH22	1:D:336:GLU:CD	2.24	0.45
1:H:60:SER:O	1:H:62:PRO:HD3	2.15	0.45
1:B:66:ASN:O	1:B:70:GLN:HG3	2.17	0.45
1:C:318:ILE:HG12	1:C:318:ILE:O	2.16	0.45
1:E:230:ILE:HA	1:E:231:PRO:HD3	1.70	0.45
1:E:318:ILE:HG12	1:E:318:ILE:O	2.16	0.45
1:H:252:ASN:HD21	1:H:255:ASP:CG	2.24	0.45
1:C:40:THR:HA	1:C:46:ASP:OD2	2.17	0.44
1:C:152:LEU:HA	1:C:152:LEU:HD23	1.78	0.44
1:A:40:THR:HA	1:A:46:ASP:OD2	2.17	0.44
1:B:293:ARG:HH22	1:B:336:GLU:CD	2.24	0.44
1:F:293:ARG:HH22	1:F:336:GLU:CD	2.24	0.44
1:B:40:THR:HA	1:B:46:ASP:OD2	2.17	0.44
1:G:216:THR:HG22	1:G:217:HIS:N	2.31	0.44
1:A:275:ILE:HD12	1:F:142:ARG:NH2	2.31	0.44
1:C:233:LEU:HD22	1:G:209:TRP:HB2	1.98	0.44
1:D:58:GLU:HA	1:D:59:PRO:HD3	1.78	0.44
1:E:40:THR:HA	1:E:46:ASP:OD2	2.17	0.44
1:D:40:THR:HA	1:D:46:ASP:OD2	2.17	0.44
1:G:40:THR:HA	1:G:46:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:ARG:HH22	1:G:336:GLU:CD	2.24	0.44
1:D:209:TRP:HB2	1:H:233:LEU:HD22	1.99	0.44
1:H:40:THR:HA	1:H:46:ASP:OD2	2.17	0.44
1:D:92:VAL:HG21	1:D:138:ILE:CG1	2.35	0.44
1:F:40:THR:HA	1:F:46:ASP:OD2	2.17	0.44
1:F:250:ILE:HD12	1:F:250:ILE:HG23	1.55	0.44
1:H:92:VAL:HG21	1:H:138:ILE:CG1	2.35	0.44
1:H:294:GLU:OE1	1:H:307:HIS:HE1	2.01	0.44
1:E:294:GLU:OE1	1:E:307:HIS:HE1	2.01	0.44
1:G:294:GLU:OE1	1:G:307:HIS:HE1	2.01	0.44
1:A:190:GLN:HA	1:A:191:PRO:HD3	1.61	0.44
1:B:216:THR:CG2	1:B:217:HIS:N	2.80	0.44
1:B:318:ILE:O	1:B:318:ILE:HG12	2.16	0.44
1:C:230:ILE:HA	1:C:231:PRO:HD3	1.70	0.44
1:D:294:GLU:OE1	1:D:307:HIS:HE1	2.01	0.44
1:F:294:GLU:OE1	1:F:307:HIS:HE1	2.01	0.44
1:E:235:ALA:HA	4:E:365:HOH:O	2.17	0.43
1:G:216:THR:CG2	1:G:217:HIS:N	2.80	0.43
1:B:190:GLN:HA	1:B:191:PRO:HD3	1.61	0.43
1:H:190:GLN:HA	1:H:191:PRO:HD3	1.61	0.43
1:B:294:GLU:OE1	1:B:307:HIS:HE1	2.01	0.43
1:D:216:THR:CG2	1:D:217:HIS:N	2.80	0.43
1:F:216:THR:HG22	1:F:217:HIS:N	2.31	0.43
1:C:85:ALA:N	4:C:365:HOH:O	2.50	0.43
1:C:190:GLN:HA	1:C:191:PRO:HD3	1.61	0.43
1:E:35:TYR:CZ	1:E:162:ARG:NH1	2.84	0.43
1:G:238:LEU:HA	1:G:238:LEU:HD12	1.75	0.43
1:G:334:LEU:HA	1:G:334:LEU:HD23	1.80	0.43
1:H:196:GLN:O	1:H:285:VAL:HB	2.19	0.43
1:H:216:THR:CG2	1:H:217:HIS:N	2.80	0.43
1:A:196:GLN:O	1:A:285:VAL:HB	2.19	0.43
1:A:294:GLU:OE1	1:A:307:HIS:HE1	2.01	0.43
1:C:196:GLN:O	1:C:285:VAL:HB	2.19	0.43
1:D:60:SER:HB2	1:D:61:ASN:H	1.35	0.43
1:E:115:ARG:NH2	1:E:121:GLU:OE2	2.42	0.43
1:E:196:GLN:O	1:E:285:VAL:HB	2.19	0.43
1:F:196:GLN:O	1:F:285:VAL:HB	2.19	0.43
1:G:194:LEU:HA	1:G:194:LEU:HD23	1.67	0.43
1:B:196:GLN:O	1:B:285:VAL:HB	2.19	0.43
1:C:293:ARG:NH2	1:C:336:GLU:CD	2.77	0.43
1:G:53:GLN:HG2	4:G:371:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:GLN:O	1:G:285:VAL:HB	2.19	0.43
1:A:196:GLN:HG2	4:A:373:HOH:O	2.19	0.43
1:C:294:GLU:OE1	1:C:307:HIS:HE1	2.01	0.43
1:C:329:LEU:HD23	1:C:329:LEU:HA	1.73	0.43
1:F:293:ARG:NH2	1:F:336:GLU:CD	2.77	0.43
1:H:24:HIS:CD2	1:H:30:LEU:HB3	2.54	0.43
1:B:76:LEU:CD2	1:F:124:MET:HE2	2.49	0.43
1:B:216:THR:HG22	1:B:217:HIS:N	2.31	0.43
1:D:293:ARG:NH2	1:D:336:GLU:CD	2.77	0.43
1:A:238:LEU:HA	1:A:238:LEU:HD12	1.75	0.42
1:F:27:LEU:HD23	1:F:27:LEU:HA	1.38	0.42
1:H:293:ARG:NH2	1:H:336:GLU:CD	2.77	0.42
1:A:216:THR:CG2	1:A:217:HIS:N	2.80	0.42
1:A:250:ILE:HD12	1:A:250:ILE:HG23	1.55	0.42
1:B:90:THR:HG22	4:B:376:HOH:O	2.19	0.42
1:C:216:THR:CG2	1:C:217:HIS:N	2.80	0.42
1:E:293:ARG:NH2	1:E:336:GLU:CD	2.77	0.42
1:F:115:ARG:NH2	1:F:121:GLU:OE2	2.42	0.42
1:H:329:LEU:HD23	1:H:329:LEU:HA	1.73	0.42
1:A:250:ILE:HA	1:A:250:ILE:HD13	1.82	0.42
1:A:293:ARG:NH2	1:A:336:GLU:CD	2.77	0.42
1:C:238:LEU:HA	1:C:238:LEU:HD12	1.75	0.42
1:D:27:LEU:HD23	1:D:27:LEU:HA	1.38	0.42
1:D:270:LEU:HD23	1:D:270:LEU:HA	1.89	0.42
1:G:152:LEU:HA	1:G:152:LEU:HD23	1.78	0.42
1:H:334:LEU:HD23	1:H:334:LEU:HA	1.80	0.42
1:A:256:HIS:CE1	1:A:278:GLU:OE2	2.73	0.42
1:D:196:GLN:O	1:D:285:VAL:HB	2.19	0.42
1:E:61:ASN:HD22	1:E:62:PRO:CD	2.32	0.42
1:H:278:GLU:C	1:H:279:TYR:CG	2.98	0.42
1:A:127:ASP:HB2	1:A:128:TYR:CE1	2.54	0.42
1:B:53:GLN:HA	1:B:54:PRO:HD3	1.85	0.42
1:D:165:GLU:HB2	1:D:169:GLU:OE1	2.18	0.42
1:F:152:LEU:HD23	1:F:152:LEU:HA	1.78	0.42
1:D:194:LEU:HD23	1:D:194:LEU:HA	1.67	0.42
1:E:216:THR:HG22	1:E:217:HIS:N	2.31	0.42
1:E:252:ASN:HB3	4:E:384:HOH:O	2.19	0.42
1:H:66:ASN:O	1:H:70:GLN:HG3	2.20	0.42
1:B:293:ARG:NH2	1:B:336:GLU:CD	2.77	0.42
1:E:256:HIS:CE1	1:E:278:GLU:OE2	2.73	0.42
1:G:293:ARG:NH2	1:G:336:GLU:CD	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HA	1:A:231:PRO:HD3	1.70	0.42
1:B:318:ILE:HG21	1:B:318:ILE:HD13	1.86	0.42
1:F:270:LEU:HA	1:F:270:LEU:HD23	1.89	0.42
1:H:238:LEU:HA	1:H:238:LEU:HD12	1.75	0.42
1:E:329:LEU:HD23	1:E:329:LEU:HA	1.73	0.42
1:G:278:GLU:C	1:G:279:TYR:CG	2.98	0.42
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.89	0.41
1:E:187:GLY:HA3	4:E:374:HOH:O	2.19	0.41
1:E:270:LEU:HD23	1:E:270:LEU:HA	1.89	0.41
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.67	0.41
1:C:278:GLU:C	1:C:279:TYR:CG	2.98	0.41
1:F:334:LEU:HA	1:F:334:LEU:HD23	1.80	0.41
1:H:27:LEU:HD23	1:H:27:LEU:HA	1.38	0.41
1:H:194:LEU:HA	1:H:194:LEU:HD23	1.67	0.41
1:D:58:GLU:CB	1:D:59:PRO:HD2	2.34	0.41
1:D:278:GLU:C	1:D:279:TYR:CG	2.98	0.41
1:E:238:LEU:HA	1:E:238:LEU:HD12	1.75	0.41
1:E:278:GLU:C	1:E:279:TYR:CG	2.98	0.41
1:F:58:GLU:CG	1:F:59:PRO:CD	2.98	0.41
1:F:216:THR:CG2	1:F:217:HIS:N	2.80	0.41
1:B:124:MET:HE2	1:F:76:LEU:CD2	2.50	0.41
1:D:190:GLN:HA	1:D:191:PRO:HD3	1.61	0.41
1:F:278:GLU:C	1:F:279:TYR:CG	2.98	0.41
1:A:278:GLU:C	1:A:279:TYR:CG	2.98	0.41
1:B:278:GLU:C	1:B:279:TYR:CG	2.98	0.41
1:E:161:LEU:HD12	1:E:161:LEU:HA	1.90	0.41
1:H:104:ASP:HA	1:H:105:PRO:HD3	1.86	0.41
1:A:283:ARG:HH11	1:A:283:ARG:HD2	1.70	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD12	1.75	0.41
1:F:230:ILE:HA	1:F:231:PRO:HD3	1.70	0.41
1:G:256:HIS:CE1	1:G:278:GLU:OE2	2.73	0.41
1:A:58:GLU:HG3	1:A:59:PRO:CD	2.48	0.41
1:B:20:HIS:CE1	1:B:155:ARG:HB3	2.56	0.41
1:B:104:ASP:HA	1:B:105:PRO:HD3	1.86	0.41
1:C:324:LEU:HA	1:C:324:LEU:HD23	1.83	0.41
1:D:256:HIS:CE1	1:D:278:GLU:OE2	2.73	0.41
1:E:92:VAL:HG21	1:E:138:ILE:CG1	2.35	0.41
1:E:95:TYR:CD1	1:E:95:TYR:N	2.89	0.41
1:E:194:LEU:HD23	1:E:194:LEU:HA	1.67	0.41
1:E:318:ILE:HD13	1:E:318:ILE:HG21	1.86	0.41
1:F:20:HIS:CE1	1:F:155:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:GLU:HG2	1:F:59:PRO:HD2	2.03	0.41
1:F:256:HIS:CE1	1:F:278:GLU:OE2	2.73	0.41
1:G:318:ILE:HD13	1:G:318:ILE:HG21	1.86	0.41
1:B:123:ASP:OD2	1:D:287:PRO:CB	2.65	0.41
1:B:250:ILE:HD13	1:B:250:ILE:HA	1.82	0.41
1:B:324:LEU:HA	1:B:324:LEU:HD23	1.83	0.41
1:C:256:HIS:CE1	1:C:278:GLU:OE2	2.73	0.41
1:C:58:GLU:HG3	1:C:59:PRO:HD2	2.02	0.40
1:D:20:HIS:CE1	1:D:155:ARG:HB3	2.56	0.40
1:D:324:LEU:HD23	1:D:324:LEU:HA	1.83	0.40
1:A:104:ASP:HA	1:A:105:PRO:HD3	1.86	0.40
1:A:310:GLY:O	4:A:374:HOH:O	2.22	0.40
1:B:95:TYR:CD1	1:B:95:TYR:N	2.89	0.40
1:C:20:HIS:CE1	1:C:155:ARG:HB3	2.56	0.40
1:C:250:ILE:HD13	1:C:250:ILE:HA	1.82	0.40
1:D:283:ARG:HH11	1:D:283:ARG:HD2	1.70	0.40
1:A:20:HIS:CE1	1:A:155:ARG:HB3	2.56	0.40
1:C:161:LEU:HD12	1:C:161:LEU:HA	1.90	0.40
1:E:133:PHE:CD1	1:E:133:PHE:C	3.00	0.40
1:E:216:THR:CG2	1:E:217:HIS:N	2.80	0.40
1:F:194:LEU:HA	1:F:194:LEU:HD23	1.67	0.40
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.38	0.40
1:B:115:ARG:NH2	1:B:121:GLU:OE2	2.42	0.40
1:C:76:LEU:HD21	1:G:124:MET:HE2	2.04	0.40
1:E:20:HIS:CE1	1:E:155:ARG:HB3	2.56	0.40
1:G:133:PHE:CD1	1:G:133:PHE:C	3.00	0.40
1:H:20:HIS:CE1	1:H:155:ARG:HB3	2.56	0.40
1:H:270:LEU:HD23	1:H:270:LEU:HA	1.89	0.40
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.89	0.40
1:C:283:ARG:HH11	1:C:283:ARG:HD2	1.70	0.40
1:E:30:LEU:HD12	1:E:30:LEU:HA	1.92	0.40
1:F:95:TYR:CD1	1:F:95:TYR:N	2.89	0.40
1:F:238:LEU:HD12	1:F:238:LEU:HA	1.75	0.40
1:H:133:PHE:CD1	1:H:133:PHE:C	3.00	0.40

All (2) 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:E:247:TRP:NE1	1:F:247:TRP:NE1[7_555]	2.02	0.18
1:C:119:PRO:O	1:H:162:ARG:NH2[4_565]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	337/347 (97%)	321 (95%)	15 (4%)	1 (0%)	36	58
1	B	337/347 (97%)	322 (96%)	14 (4%)	1 (0%)	36	58
1	C	337/347 (97%)	323 (96%)	12 (4%)	2 (1%)	21	42
1	D	337/347 (97%)	320 (95%)	15 (4%)	2 (1%)	21	42
1	E	337/347 (97%)	323 (96%)	13 (4%)	1 (0%)	36	58
1	F	337/347 (97%)	322 (96%)	14 (4%)	1 (0%)	36	58
1	G	337/347 (97%)	320 (95%)	16 (5%)	1 (0%)	36	58
1	H	337/347 (97%)	322 (96%)	14 (4%)	1 (0%)	36	58
All	All	2696/2776 (97%)	2573 (95%)	113 (4%)	10 (0%)	30	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	30	LEU
1	D	60	SER
1	A	240	GLY
1	B	240	GLY
1	C	240	GLY
1	D	240	GLY
1	E	240	GLY
1	F	240	GLY
1	G	240	GLY
1	H	240	GLY

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	BEZ	H	349	-	9,9,9	1.85	2 (22%)	11,11,11	1.30	1 (9%)
2	FAD	G	348	-	58,58,58	0.90	4 (6%)	85,89,89	1.20	6 (7%)
2	FAD	H	348	-	58,58,58	0.89	4 (6%)	85,89,89	1.21	6 (7%)
3	BEZ	B	349	-	9,9,9	1.85	2 (22%)	11,11,11	1.30	1 (9%)
3	BEZ	F	349	-	9,9,9	1.84	2 (22%)	11,11,11	1.30	1 (9%)
2	FAD	F	348	-	58,58,58	0.91	4 (6%)	85,89,89	1.21	6 (7%)
2	FAD	C	348	-	58,58,58	0.90	4 (6%)	85,89,89	1.21	6 (7%)
3	BEZ	G	349	-	9,9,9	1.85	2 (22%)	11,11,11	1.30	1 (9%)
3	BEZ	A	349	-	9,9,9	1.85	2 (22%)	11,11,11	1.30	1 (9%)
3	BEZ	C	349	-	9,9,9	1.85	2 (22%)	11,11,11	1.30	1 (9%)
2	FAD	A	348	-	58,58,58	0.90	4 (6%)	85,89,89	1.21	6 (7%)
3	BEZ	D	349	-	9,9,9	1.85	2 (22%)	11,11,11	1.28	1 (9%)
3	BEZ	E	349	-	9,9,9	1.84	2 (22%)	11,11,11	1.32	1 (9%)
2	FAD	D	348	-	58,58,58	0.89	4 (6%)	85,89,89	1.21	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	E	348	-	58,58,58	0.90	4 (6%)	85,89,89	1.21	6 (7%)
2	FAD	B	348	-	58,58,58	0.90	4 (6%)	85,89,89	1.21	6 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEZ	H	349	-	-	0/4/4/4	0/1/1/1
2	FAD	G	348	-	-	2/34/50/50	0/6/6/6
2	FAD	H	348	-	-	2/34/50/50	0/6/6/6
3	BEZ	B	349	-	-	0/4/4/4	0/1/1/1
3	BEZ	F	349	-	-	0/4/4/4	0/1/1/1
2	FAD	F	348	-	-	2/34/50/50	0/6/6/6
2	FAD	C	348	-	-	2/34/50/50	0/6/6/6
3	BEZ	G	349	-	-	0/4/4/4	0/1/1/1
3	BEZ	A	349	-	-	0/4/4/4	0/1/1/1
3	BEZ	C	349	-	-	0/4/4/4	0/1/1/1
2	FAD	A	348	-	-	2/34/50/50	0/6/6/6
3	BEZ	D	349	-	-	0/4/4/4	0/1/1/1
3	BEZ	E	349	-	-	0/4/4/4	0/1/1/1
2	FAD	D	348	-	-	2/34/50/50	0/6/6/6
2	FAD	E	348	-	-	2/34/50/50	0/6/6/6
2	FAD	B	348	-	-	2/34/50/50	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	349	BEZ	C1-C	-4.91	1.39	1.49
3	D	349	BEZ	C1-C	-4.91	1.39	1.49
3	F	349	BEZ	C1-C	-4.89	1.39	1.49
3	H	349	BEZ	C1-C	-4.89	1.39	1.49
3	G	349	BEZ	C1-C	-4.89	1.39	1.49
3	A	349	BEZ	C1-C	-4.88	1.39	1.49
3	C	349	BEZ	C1-C	-4.87	1.39	1.49
3	E	349	BEZ	C1-C	-4.86	1.39	1.49
2	F	348	FAD	C5X-N5	-2.88	1.34	1.39
2	G	348	FAD	C5X-N5	-2.87	1.34	1.39
2	B	348	FAD	C5X-N5	-2.86	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	348	FAD	C5X-N5	-2.86	1.34	1.39
2	E	348	FAD	C5X-N5	-2.85	1.34	1.39
2	A	348	FAD	C5X-N5	-2.85	1.34	1.39
2	D	348	FAD	C5X-N5	-2.85	1.34	1.39
2	H	348	FAD	C5X-N5	-2.83	1.34	1.39
2	A	348	FAD	C9A-N10	-2.61	1.36	1.41
2	F	348	FAD	C9A-N10	-2.57	1.36	1.41
2	B	348	FAD	C9A-N10	-2.56	1.36	1.41
2	C	348	FAD	C9A-N10	-2.56	1.36	1.41
2	E	348	FAD	C9A-N10	-2.52	1.36	1.41
2	H	348	FAD	C9A-N10	-2.52	1.36	1.41
2	G	348	FAD	C9A-N10	-2.51	1.36	1.41
2	D	348	FAD	C9A-N10	-2.50	1.36	1.41
3	G	349	BEZ	O2-C	-2.50	1.23	1.30
3	C	349	BEZ	O2-C	-2.49	1.23	1.30
3	E	349	BEZ	O2-C	-2.48	1.23	1.30
3	D	349	BEZ	O2-C	-2.48	1.23	1.30
3	A	349	BEZ	O2-C	-2.48	1.23	1.30
3	H	349	BEZ	O2-C	-2.48	1.23	1.30
3	B	349	BEZ	O2-C	-2.48	1.23	1.30
3	F	349	BEZ	O2-C	-2.47	1.23	1.30
2	E	348	FAD	P-O3P	2.12	1.61	1.59
2	C	348	FAD	P-O3P	2.12	1.61	1.59
2	B	348	FAD	P-O3P	2.10	1.61	1.59
2	G	348	FAD	P-O3P	2.09	1.61	1.59
2	A	348	FAD	P-O3P	2.09	1.61	1.59
2	D	348	FAD	P-O3P	2.07	1.61	1.59
2	A	348	FAD	C2-N1	-2.06	1.32	1.36
2	H	348	FAD	C2-N1	-2.06	1.32	1.36
2	F	348	FAD	P-O3P	2.06	1.61	1.59
2	G	348	FAD	C2-N1	-2.06	1.32	1.36
2	H	348	FAD	P-O3P	2.05	1.61	1.59
2	F	348	FAD	C2-N1	-2.05	1.32	1.36
2	E	348	FAD	C2-N1	-2.04	1.32	1.36
2	D	348	FAD	C2-N1	-2.04	1.32	1.36
2	B	348	FAD	C2-N1	-2.03	1.32	1.36
2	C	348	FAD	C2-N1	-2.02	1.32	1.36

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	348	FAD	C4'-C3'-C2'	-4.77	105.63	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	348	FAD	C4'-C3'-C2'	-4.76	105.65	113.57
2	A	348	FAD	C4'-C3'-C2'	-4.76	105.66	113.57
2	H	348	FAD	C4'-C3'-C2'	-4.75	105.66	113.57
2	E	348	FAD	C4'-C3'-C2'	-4.74	105.69	113.57
2	G	348	FAD	C4'-C3'-C2'	-4.74	105.69	113.57
2	B	348	FAD	C4'-C3'-C2'	-4.74	105.69	113.57
2	C	348	FAD	C4'-C3'-C2'	-4.73	105.70	113.57
2	A	348	FAD	C6-C5X-C9A	3.18	123.41	119.05
2	C	348	FAD	C6-C5X-C9A	3.17	123.40	119.05
2	D	348	FAD	C6-C5X-C9A	3.17	123.40	119.05
2	B	348	FAD	C6-C5X-C9A	3.16	123.39	119.05
2	H	348	FAD	C6-C5X-C9A	3.15	123.38	119.05
2	E	348	FAD	C6-C5X-C9A	3.15	123.38	119.05
2	F	348	FAD	C6-C5X-C9A	3.13	123.35	119.05
2	G	348	FAD	C6-C5X-C9A	3.12	123.33	119.05
2	C	348	FAD	C5X-C9A-N10	2.82	120.52	117.97
2	E	348	FAD	C5X-C9A-N10	2.78	120.48	117.97
2	A	348	FAD	C5X-C9A-N10	2.76	120.46	117.97
2	B	348	FAD	C5X-C9A-N10	2.75	120.46	117.97
2	D	348	FAD	C5X-C9A-N10	2.73	120.44	117.97
2	F	348	FAD	C5X-C9A-N10	2.73	120.44	117.97
2	G	348	FAD	C5X-C9A-N10	2.73	120.43	117.97
2	H	348	FAD	C5X-C9A-N10	2.73	120.43	117.97
3	E	349	BEZ	C3-C2-C1	-2.40	118.00	120.36
3	F	349	BEZ	C3-C2-C1	-2.36	118.04	120.36
3	G	349	BEZ	C3-C2-C1	-2.36	118.05	120.36
2	A	348	FAD	O3B-C3B-C2B	-2.34	104.31	111.82
2	G	348	FAD	O3B-C3B-C2B	-2.34	104.33	111.82
2	E	348	FAD	O3B-C3B-C2B	-2.33	104.33	111.82
2	F	348	FAD	O3B-C3B-C2B	-2.33	104.33	111.82
2	D	348	FAD	O3B-C3B-C2B	-2.33	104.34	111.82
2	H	348	FAD	O3B-C3B-C2B	-2.33	104.34	111.82
2	C	348	FAD	O3B-C3B-C2B	-2.33	104.35	111.82
3	A	349	BEZ	C3-C2-C1	-2.33	118.08	120.36
3	H	349	BEZ	C3-C2-C1	-2.32	118.08	120.36
2	B	348	FAD	O3B-C3B-C2B	-2.32	104.38	111.82
3	C	349	BEZ	C3-C2-C1	-2.31	118.09	120.36
3	B	349	BEZ	C3-C2-C1	-2.30	118.10	120.36
3	D	349	BEZ	C3-C2-C1	-2.27	118.13	120.36
2	B	348	FAD	O3'-C3'-C4'	-2.26	103.80	108.93
2	D	348	FAD	O3'-C3'-C4'	-2.26	103.80	108.93
2	C	348	FAD	O3'-C3'-C4'	-2.25	103.82	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	348	FAD	O3'-C3'-C4'	-2.25	103.82	108.93
2	G	348	FAD	O3'-C3'-C4'	-2.24	103.83	108.93
2	E	348	FAD	O3'-C3'-C4'	-2.23	103.85	108.93
2	A	348	FAD	O3'-C3'-C4'	-2.23	103.87	108.93
2	F	348	FAD	O3'-C3'-C4'	-2.22	103.88	108.93
2	F	348	FAD	C3B-C2B-C1B	-2.09	97.51	101.46
2	H	348	FAD	C3B-C2B-C1B	-2.09	97.52	101.46
2	E	348	FAD	C3B-C2B-C1B	-2.08	97.53	101.46
2	B	348	FAD	C3B-C2B-C1B	-2.08	97.53	101.46
2	G	348	FAD	C3B-C2B-C1B	-2.07	97.54	101.46
2	C	348	FAD	C3B-C2B-C1B	-2.07	97.55	101.46
2	D	348	FAD	C3B-C2B-C1B	-2.07	97.55	101.46
2	A	348	FAD	C3B-C2B-C1B	-2.06	97.57	101.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	348	FAD	O4B-C4B-C5B-O5B
2	B	348	FAD	O4B-C4B-C5B-O5B
2	C	348	FAD	O4B-C4B-C5B-O5B
2	D	348	FAD	O4B-C4B-C5B-O5B
2	E	348	FAD	O4B-C4B-C5B-O5B
2	F	348	FAD	O4B-C4B-C5B-O5B
2	G	348	FAD	O4B-C4B-C5B-O5B
2	H	348	FAD	O4B-C4B-C5B-O5B
2	B	348	FAD	O2'-C2'-C3'-C4'
2	D	348	FAD	O2'-C2'-C3'-C4'
2	H	348	FAD	O2'-C2'-C3'-C4'
2	A	348	FAD	O2'-C2'-C3'-C4'
2	C	348	FAD	O2'-C2'-C3'-C4'
2	E	348	FAD	O2'-C2'-C3'-C4'
2	F	348	FAD	O2'-C2'-C3'-C4'
2	G	348	FAD	O2'-C2'-C3'-C4'

There are no ring outliers.

8 monomers are involved in 8 short contacts:

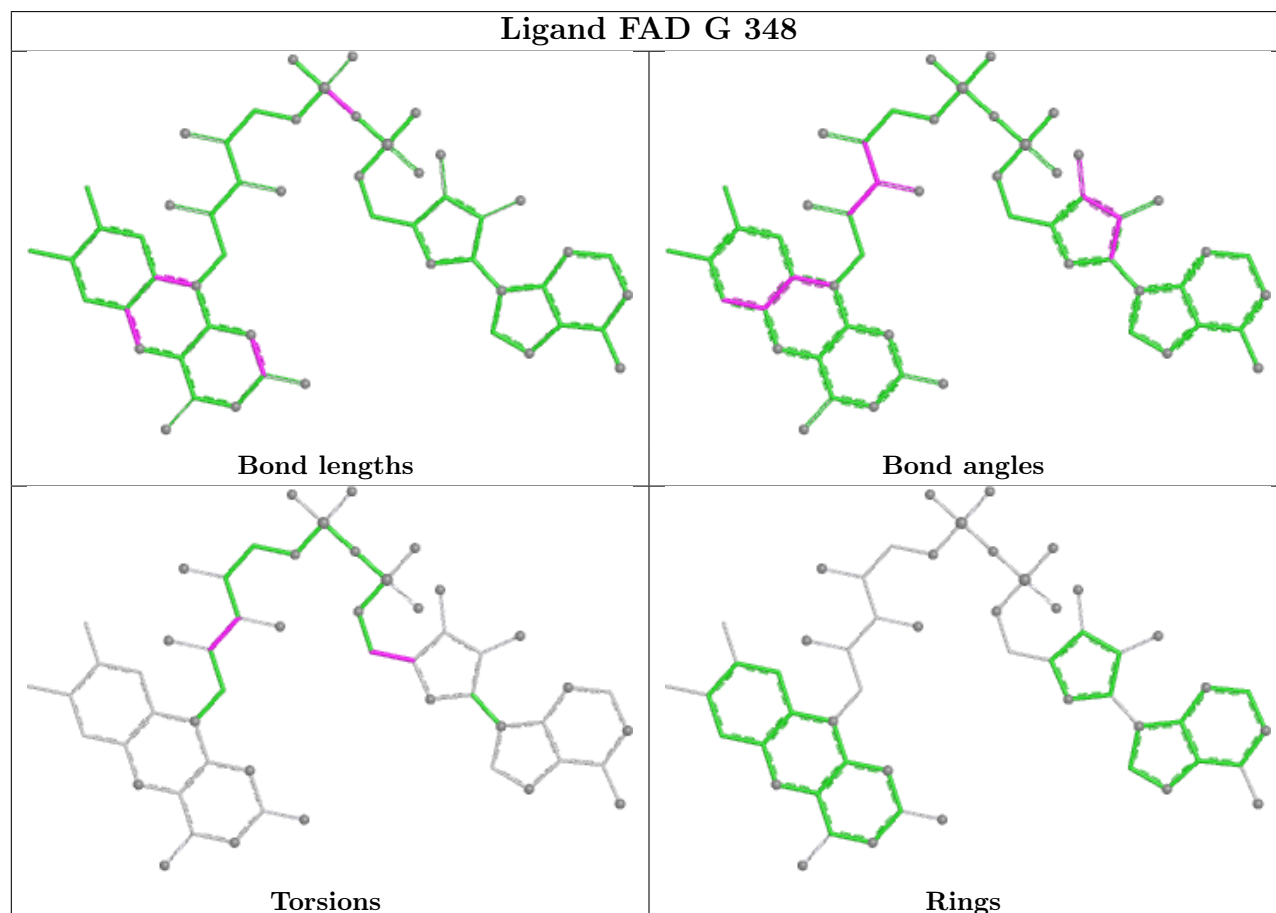
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	348	FAD	1	0
2	H	348	FAD	1	0

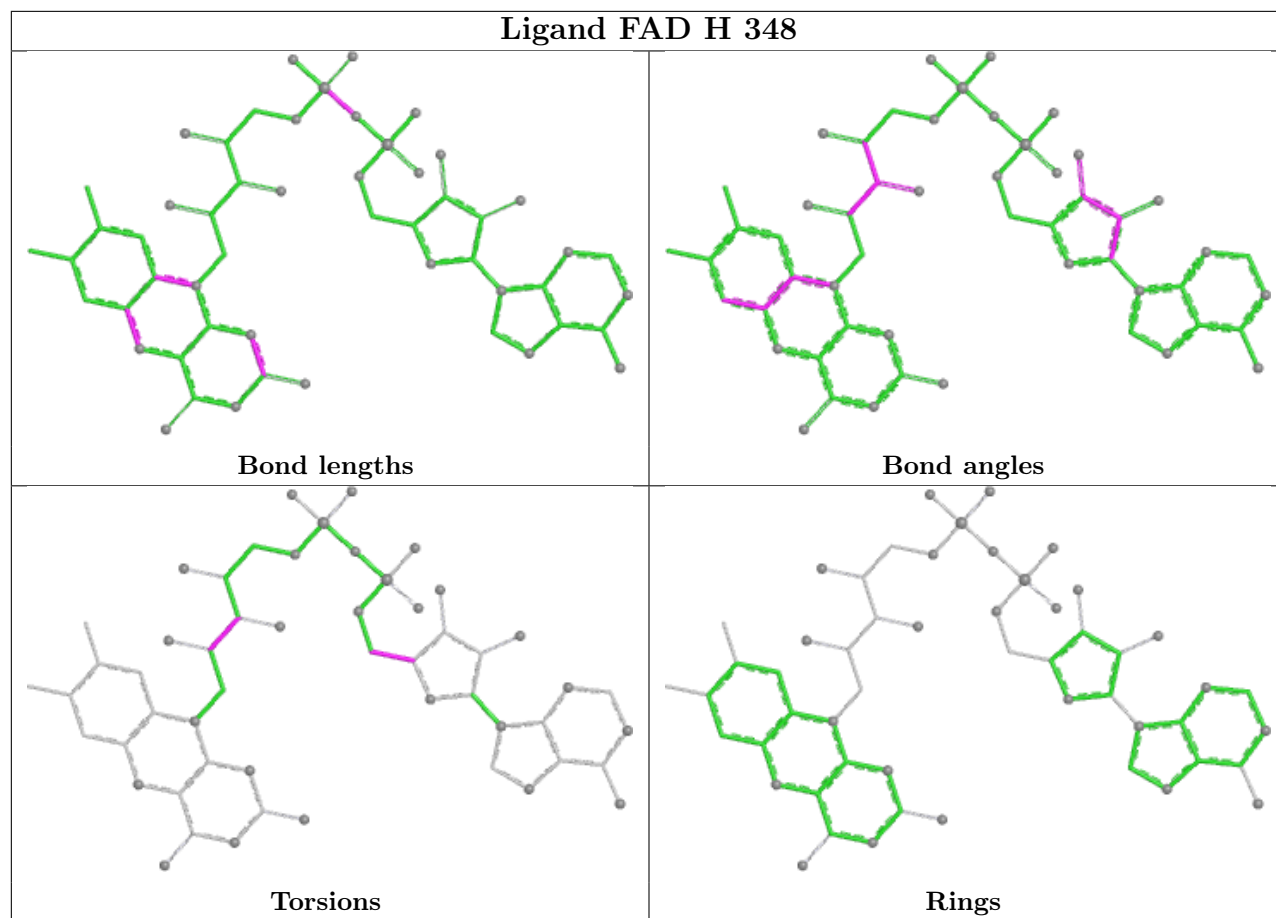
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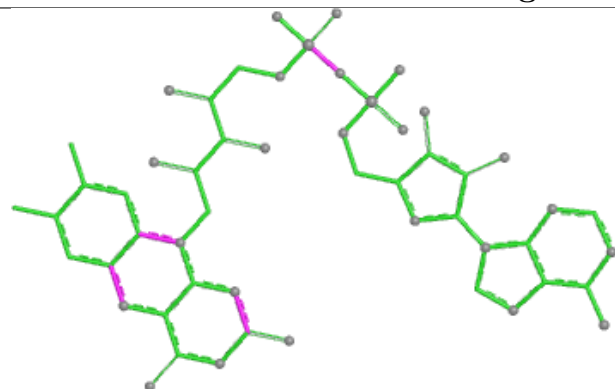
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	348	FAD	1	0
2	C	348	FAD	1	0
2	A	348	FAD	1	0
2	D	348	FAD	1	0
2	E	348	FAD	1	0
2	B	348	FAD	1	0

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

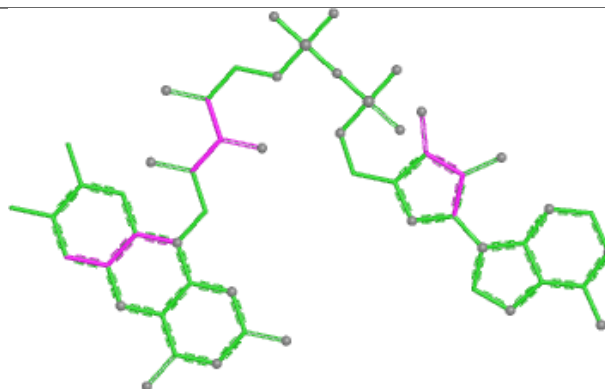




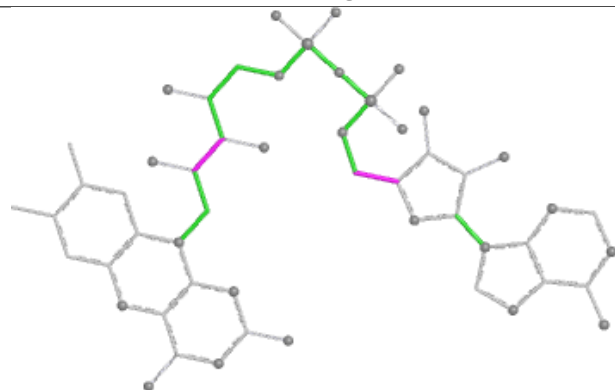
Ligand FAD F 348



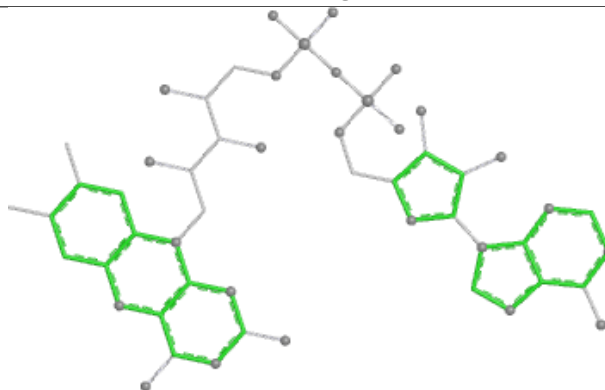
Bond lengths



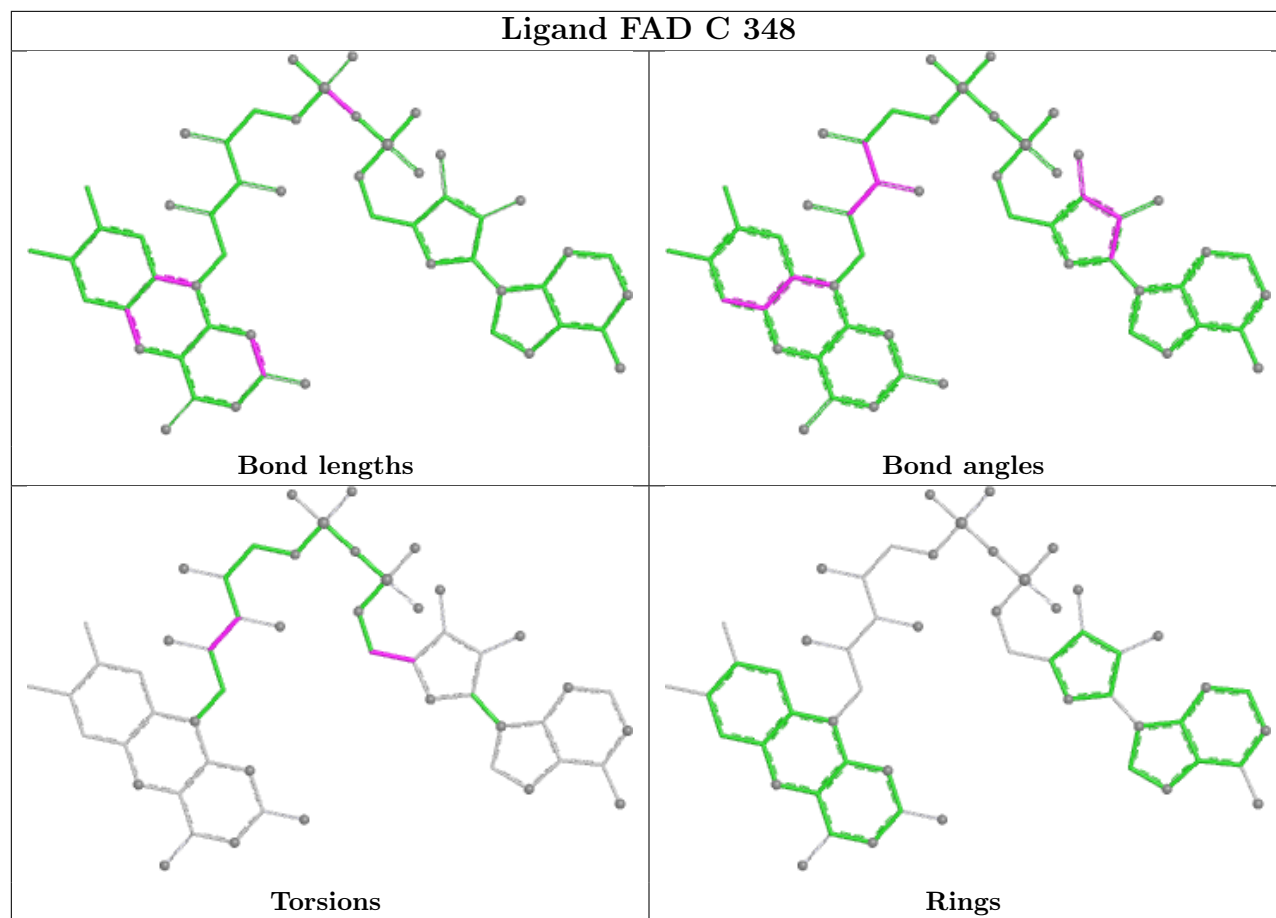
Bond angles

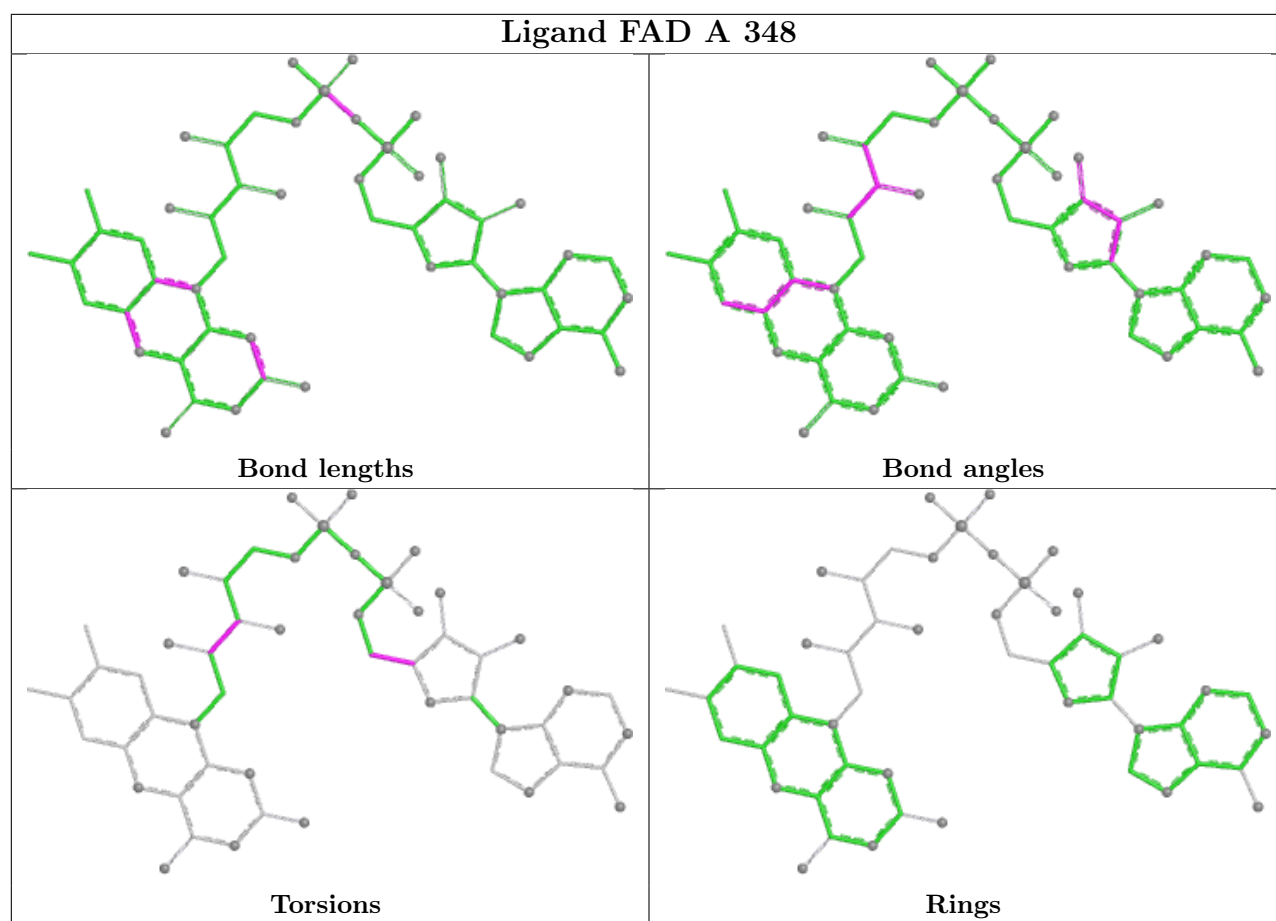


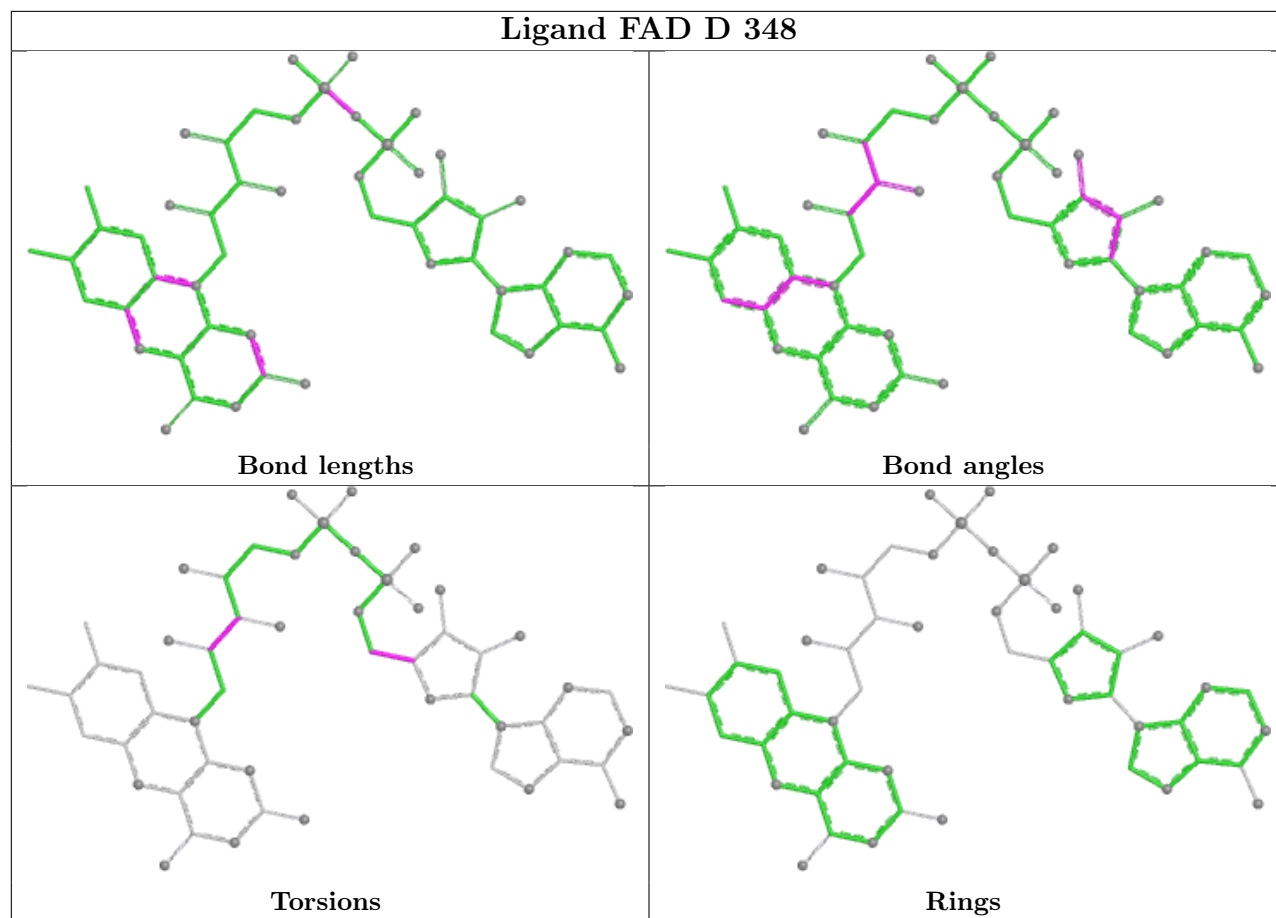
Torsions



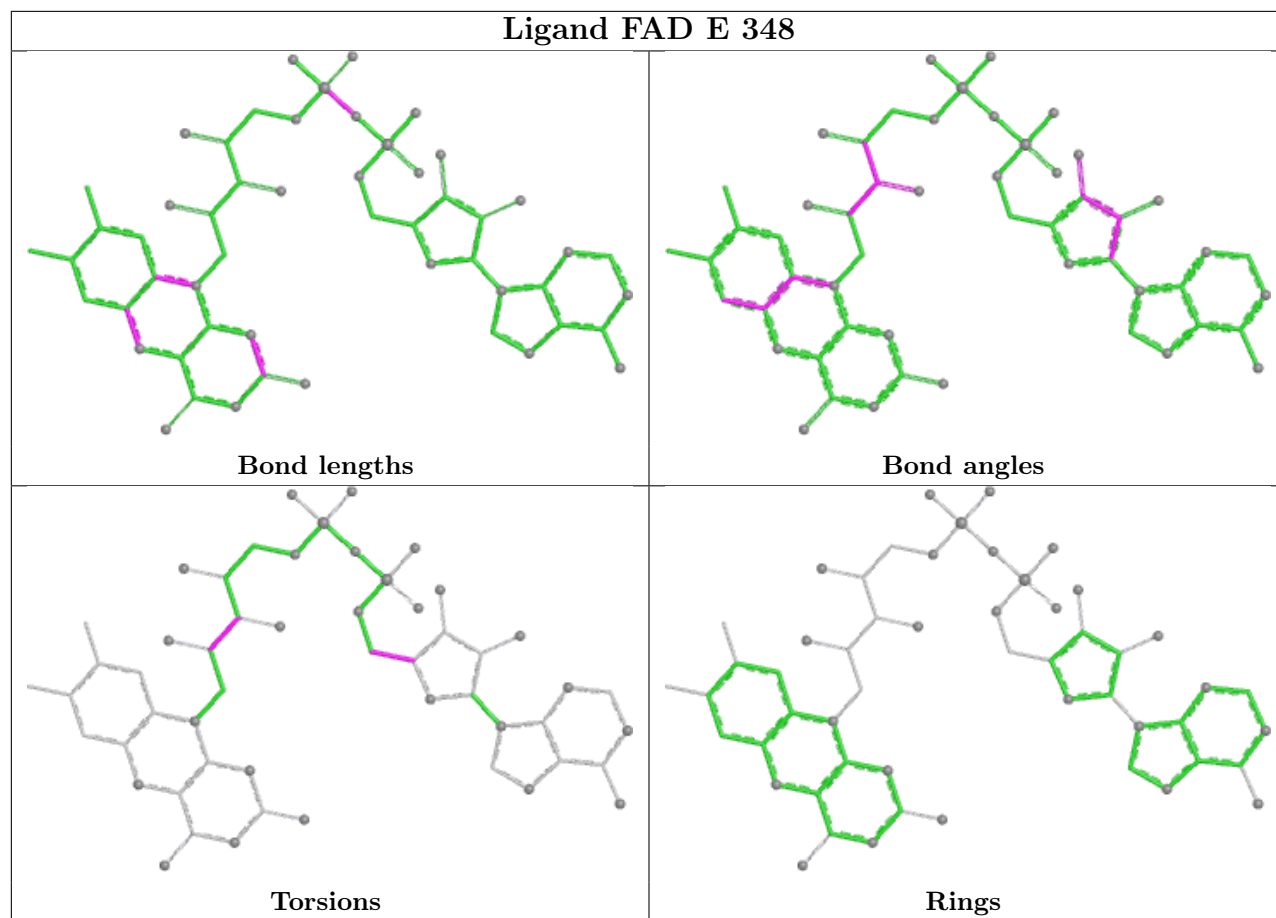
Rings

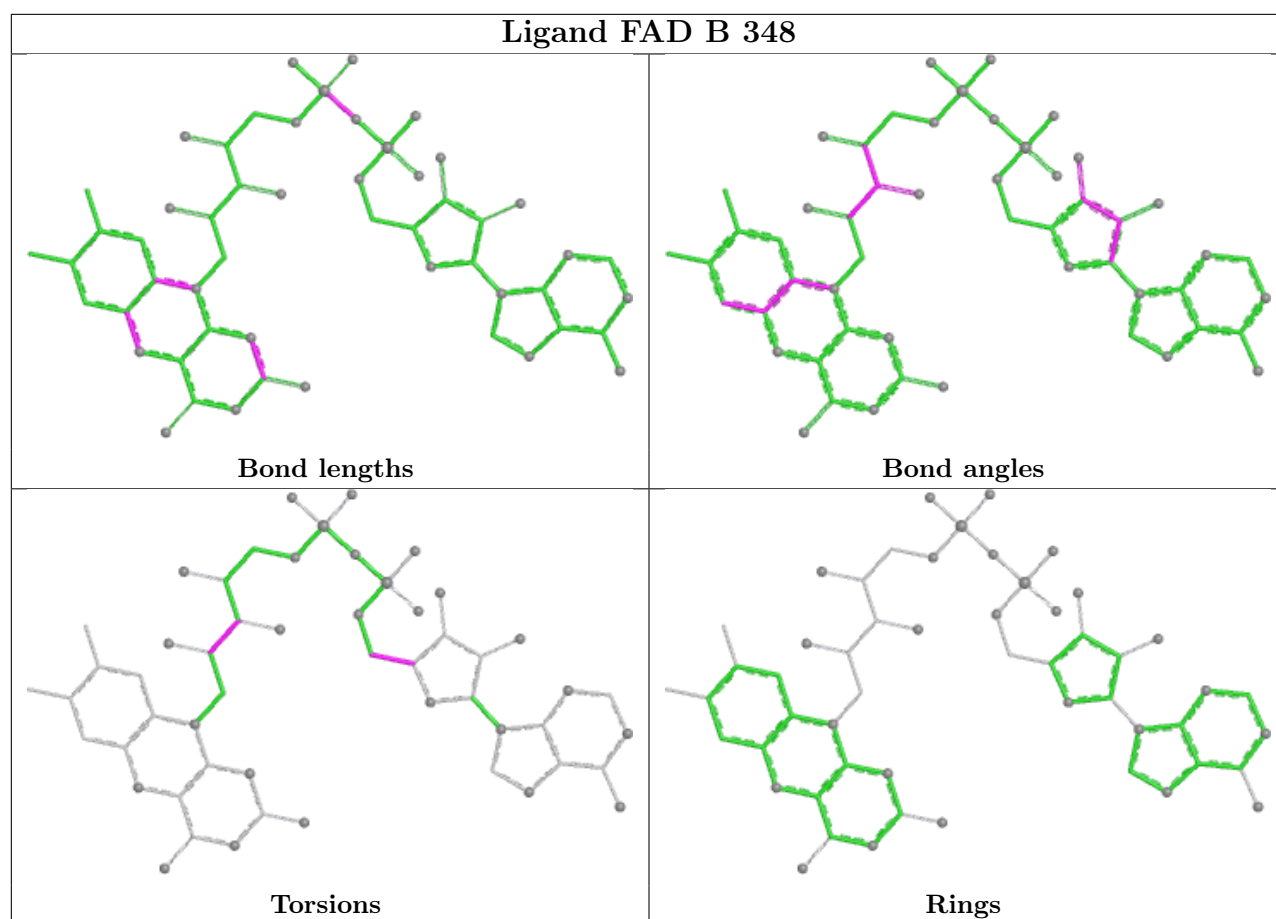






Ligand FAD E 348





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.