



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:37 AM UTC

PDB ID : 8XGT / pdb_00008xgt
Title : Crystal structure of human secretory glutaminyl cyclase in complex with (Z)-3-((1H-benzo[d]imidazol-5-yl)methylene)-4-hydroxyindolin-2-one
Authors : Li, G.-B.; Wang, X.-Y.
Deposited on : 2023-12-15
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

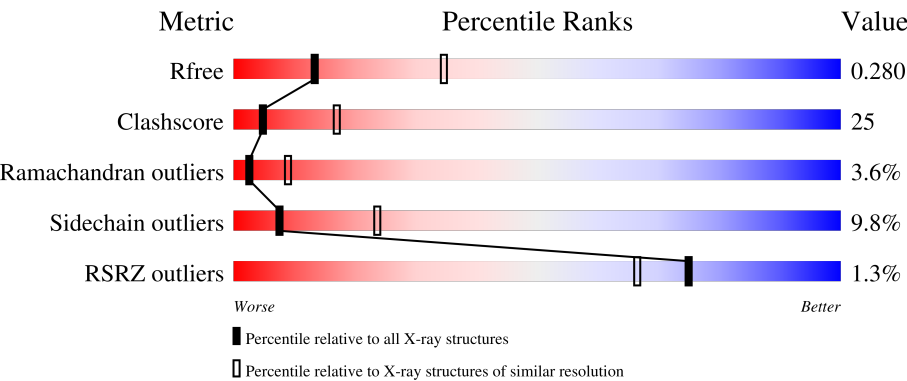
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	329	% 56%36%6%..
1	B	329	% 50%40%8%. .
1	C	329	59%33%6%. .
1	D	329	62%31%5%..
1	E	329	% 57%34%7%. .

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Mol	Chain	Length	Quality of chain
1	F	329	%57%36%5%.
1	G	329	2%40%47%11%..
1	H	329	%51%39%7%..
1	I	329	%47%43%8%..
1	J	329	4%30%54%12%..
1	K	329	%54%35%9%..
1	L	329	2%48%40%9%.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31587 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	A	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	C	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	D	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	E	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	F	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	G	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	H	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	I	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	J	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	K	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	L	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

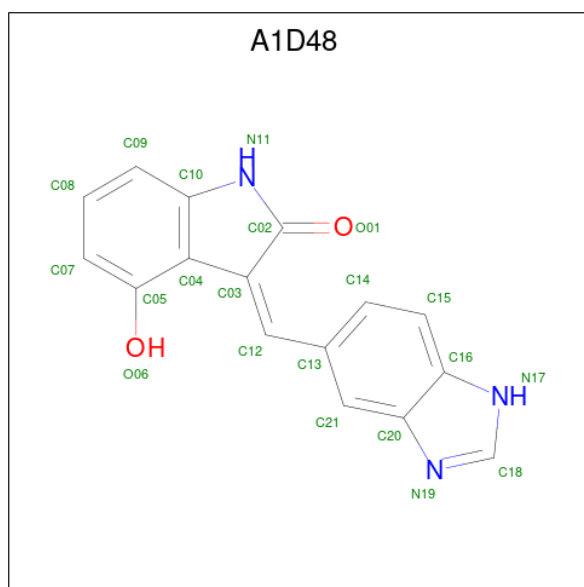
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		
2	G	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	I	1	Total	Zn	0	0
			1	1		
2	J	1	Total	Zn	0	0
			1	1		
2	K	1	Total	Zn	0	0
			1	1		
2	L	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (3 {Z})-3-(1 {H}-benzimidazol-5-ylmethylidene)-4-oxidanyl-1 {H}-indol-2-one (CCD ID: A1D48) (formula: C₁₆H₁₁N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			21	16	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	16	3	2		
3	C	1	Total	C	N	O	0	0
			21	16	3	2		
3	D	1	Total	C	N	O	0	0
			21	16	3	2		
3	E	1	Total	C	N	O	0	0
			21	16	3	2		
3	F	1	Total	C	N	O	0	0
			21	16	3	2		
3	G	1	Total	C	N	O	0	0
			21	16	3	2		
3	H	1	Total	C	N	O	0	0
			21	16	3	2		
3	I	1	Total	C	N	O	0	0
			21	16	3	2		
3	J	1	Total	C	N	O	0	0
			21	16	3	2		
3	K	1	Total	C	N	O	0	0
			21	16	3	2		
3	L	1	Total	C	N	O	0	0
			21	16	3	2		

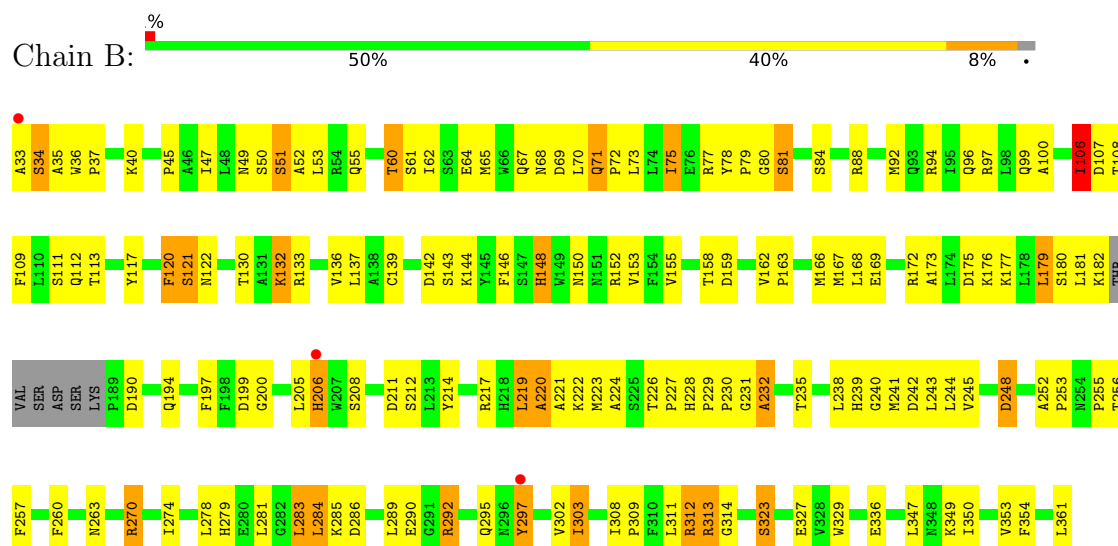
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	O	0	0
			2	2		
4	J	1	Total	O	0	0
			1	1		

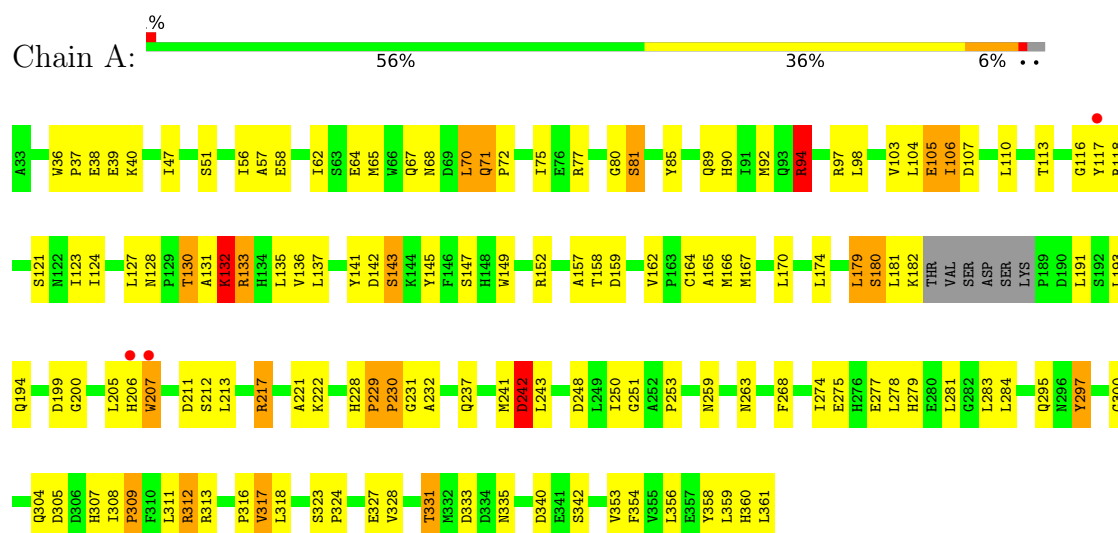
3 Residue-property plots

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

• Molecule 1: Glutaminyl-peptide cyclotransferase

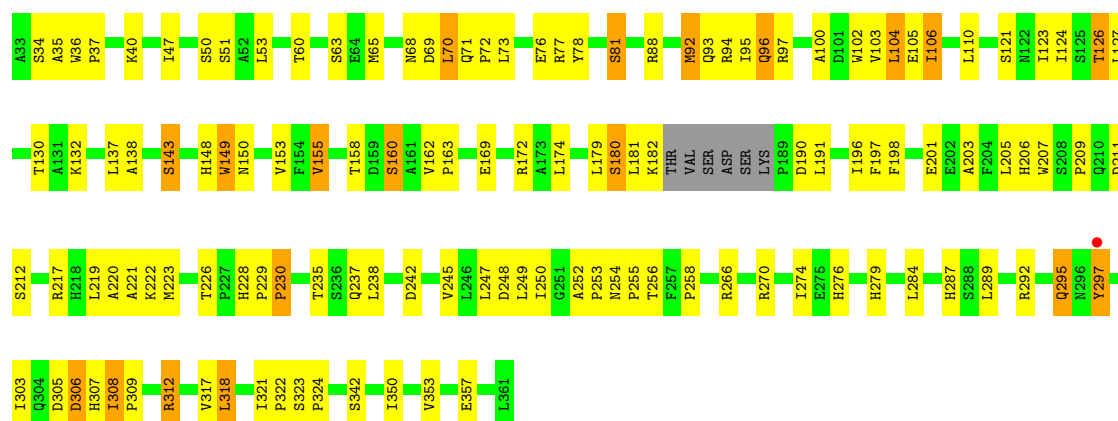


• Molecule 1: Glutaminyl-peptide cyclotransferase



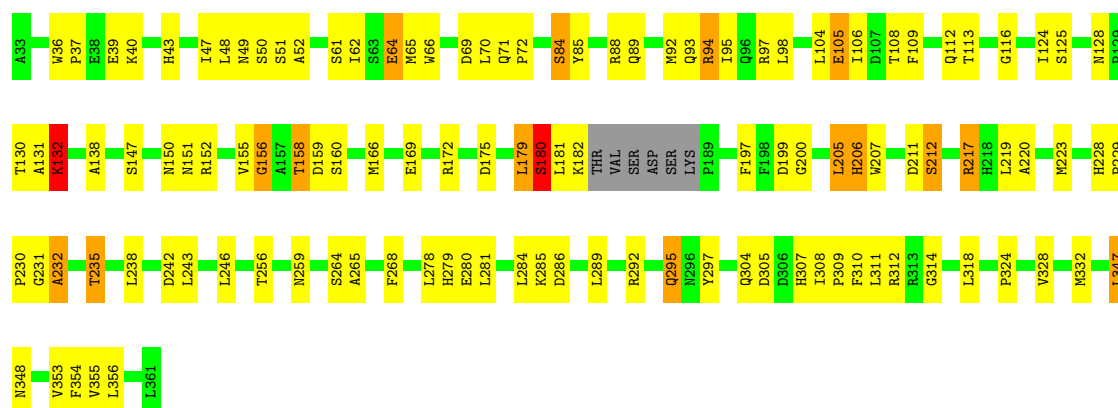
• Molecule 1: Glutaminyl-peptide cyclotransferase





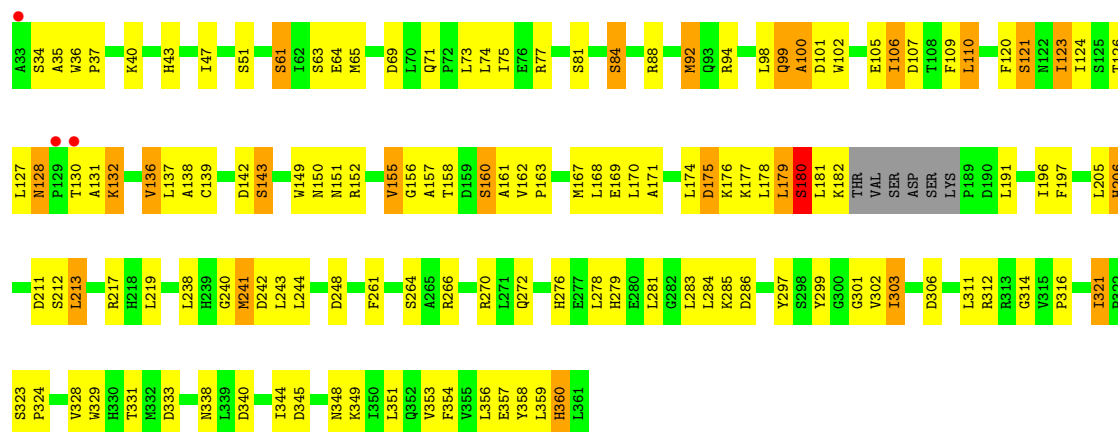
• Molecule 1: Glutaminyl-peptide cyclotransferase

Chain D: 62% 31% 5% ..



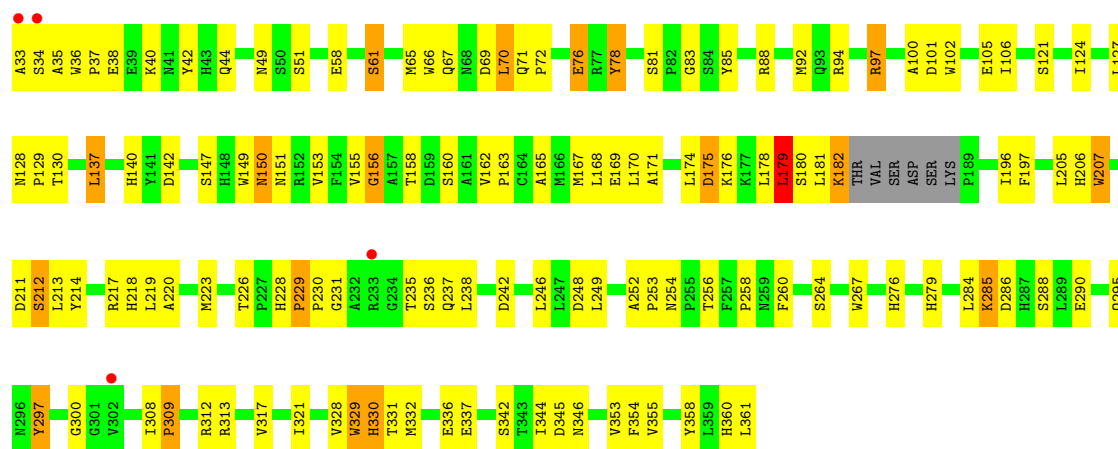
• Molecule 1: Glutaminyl-peptide cyclotransferase

Chain E: 57% 34% 7% .

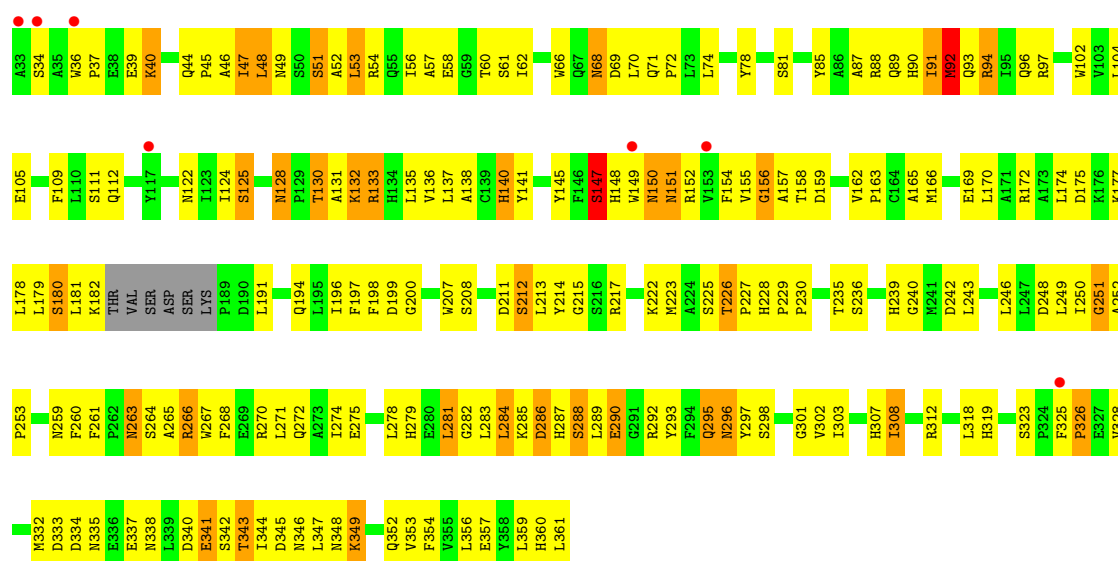


• Molecule 1: Glutaminyl-peptide cyclotransferase

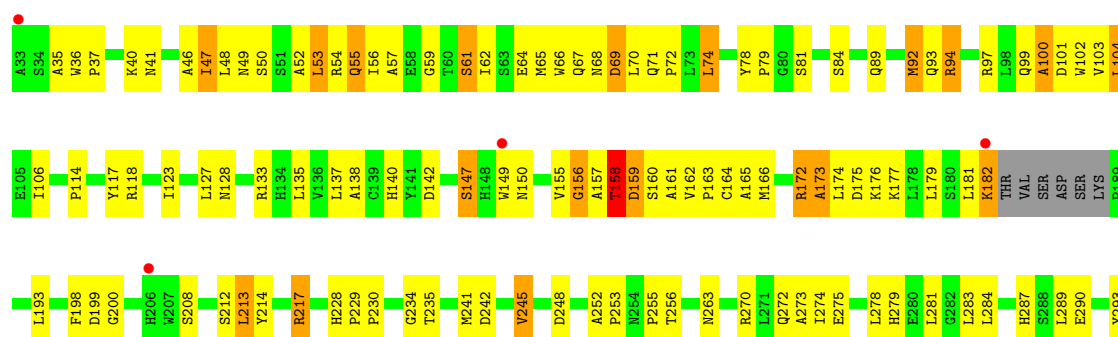
Chain F: 57% 36% 5% .



• Molecule 1: Glutaminyl-peptide cyclotransferase

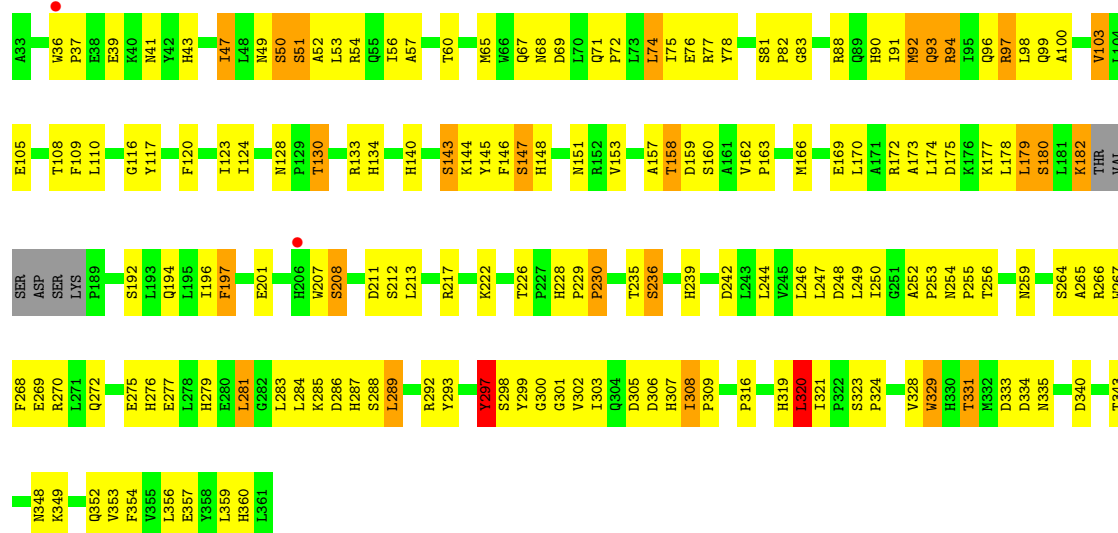


• Molecule 1: Glutaminyl-peptide cyclotransferase

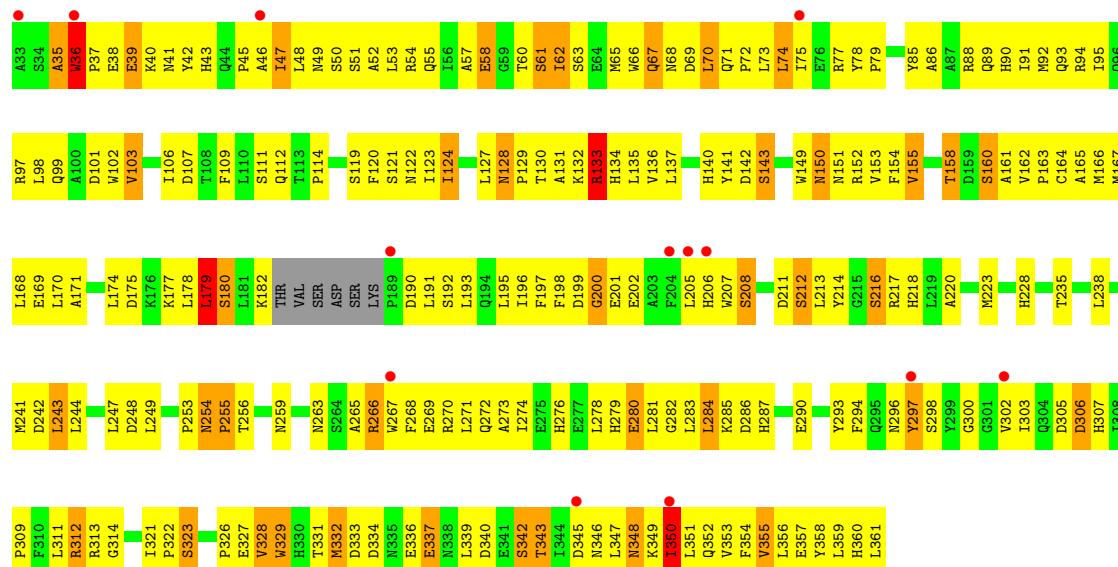




• Molecule 1: Glutaminyl-peptide cyclotransferase

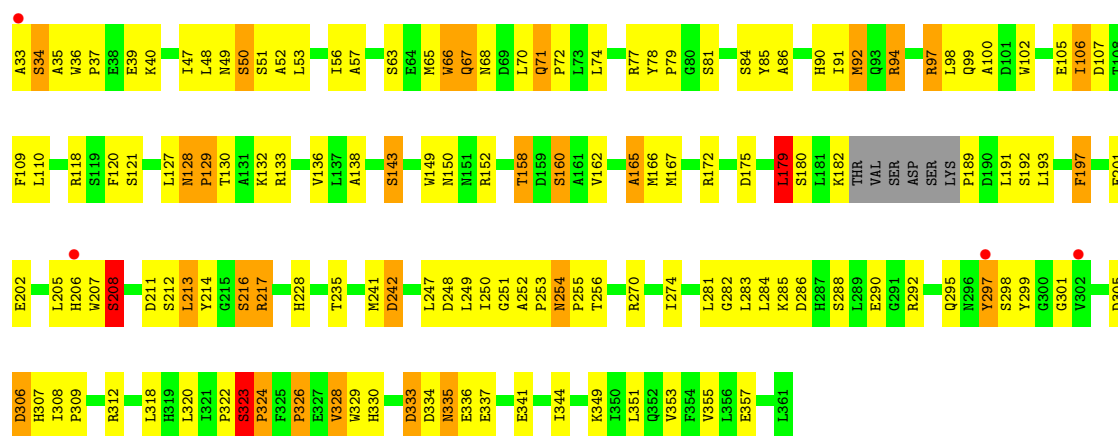


• Molecule 1: Glutaminyl-peptide cyclotransferase

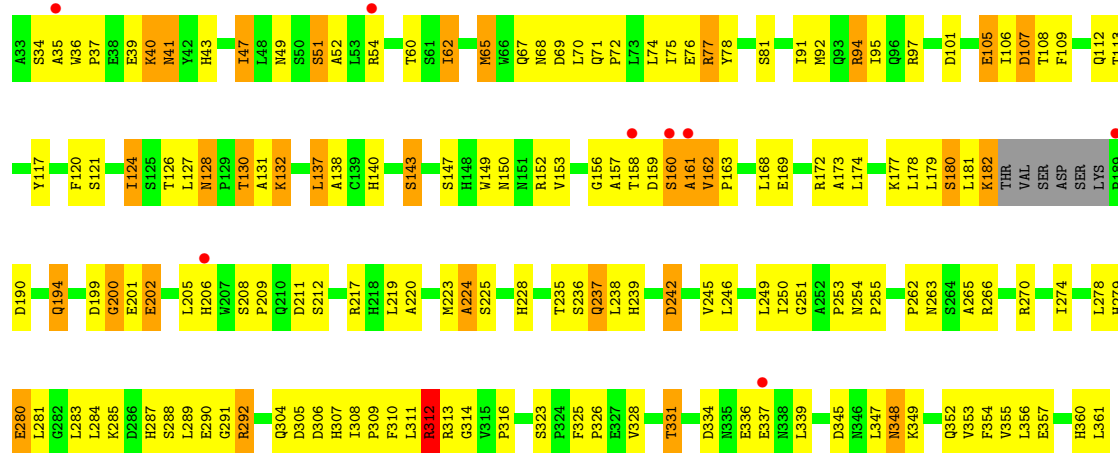


• Molecule 1: Glutaminyl-peptide cyclotransferase





● Molecule 1: Glutaminyl-peptide cyclotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.96Å 217.39Å 242.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.86 – 2.81 54.86 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (54.86-2.81) 99.2 (54.86-2.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.194 , 0.282 0.203 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31587	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1D48, ZN

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	1.95	27/2687 (1.0%)	1.26	9/3656 (0.2%)
1	B	1.95	30/2687 (1.1%)	1.17	2/3656 (0.1%)
1	C	1.90	22/2687 (0.8%)	1.20	5/3656 (0.1%)
1	D	1.85	17/2687 (0.6%)	1.12	1/3656 (0.0%)
1	E	1.82	18/2687 (0.7%)	1.13	0/3656
1	F	1.66	4/2687 (0.1%)	1.12	6/3656 (0.2%)
1	G	1.12	0/2687	0.88	0/3656
1	H	1.34	6/2687 (0.2%)	1.00	2/3656 (0.1%)
1	I	1.48	5/2687 (0.2%)	1.06	0/3656
1	J	1.07	1/2687 (0.0%)	0.92	1/3656 (0.0%)
1	K	1.62	8/2687 (0.3%)	1.12	4/3656 (0.1%)
1	L	1.60	9/2687 (0.3%)	1.14	3/3656 (0.1%)
All	All	1.64	147/32244 (0.5%)	1.10	33/43872 (0.1%)

All (147) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	250	ILE	CG1-CD1	-7.75	1.21	1.51
1	E	323	SER	C-O	-7.66	1.15	1.25
1	C	256	THR	CB-CG2	-7.58	1.27	1.52
1	F	246	LEU	CG-CD2	-7.24	1.28	1.52
1	D	324	PRO	CG-CD	-7.18	1.32	1.51
1	A	123	ILE	CG1-CD1	-6.93	1.24	1.51
1	K	323	SER	CA-C	-6.93	1.44	1.52
1	D	158	THR	CB-CG2	-6.91	1.29	1.52
1	L	62	ILE	CB-CG2	-6.87	1.29	1.52
1	C	318	LEU	C-N	-6.76	1.22	1.33
1	D	256	THR	CB-CG2	-6.74	1.30	1.52
1	A	323	SER	C-O	-6.69	1.15	1.24
1	D	62	ILE	CB-CG2	-6.67	1.30	1.52
1	H	245	VAL	CB-CG1	-6.66	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	247	LEU	CG-CD2	-6.60	1.30	1.52
1	F	309	PRO	CB-CG	-6.59	1.16	1.49
1	K	288	SER	CA-CB	-6.50	1.42	1.53
1	A	253	PRO	CG-CD	-6.45	1.28	1.50
1	E	106	ILE	CG1-CD1	-6.45	1.26	1.51
1	A	243	LEU	CG-CD2	-6.43	1.31	1.52
1	B	347	LEU	CG-CD2	-6.36	1.31	1.52
1	E	243	LEU	CG-CD2	-6.35	1.31	1.52
1	K	335	ASN	CB-CG	-6.33	1.36	1.52
1	B	329	TRP	CD1-NE1	-6.33	1.24	1.37
1	A	241	MET	SD-CE	-6.30	1.63	1.79
1	E	272	GLN	CB-CG	-6.29	1.33	1.52
1	A	159	ASP	CG-OD1	-6.26	1.13	1.25
1	A	137	LEU	CG-CD1	-6.17	1.32	1.52
1	E	123	ILE	CB-CG2	-6.17	1.32	1.52
1	B	323	SER	CA-C	-6.15	1.45	1.52
1	E	264	SER	CB-OG	-6.14	1.29	1.42
1	B	245	VAL	CB-CG1	-6.12	1.32	1.52
1	D	324	PRO	CB-CG	-6.11	1.27	1.51
1	C	53	LEU	CG-CD2	-6.11	1.32	1.52
1	A	217	ARG	CZ-NH2	-6.10	1.25	1.33
1	B	70	LEU	CG-CD1	-6.09	1.32	1.52
1	B	167	MET	CG-SD	-6.06	1.65	1.80
1	D	309	PRO	CB-CG	-6.04	1.19	1.49
1	L	77	ARG	CZ-NH2	-6.04	1.25	1.33
1	A	164	CYS	CB-SG	-6.03	1.61	1.81
1	B	303	ILE	CB-CG2	-6.00	1.32	1.52
1	B	142	ASP	CG-OD1	-5.99	1.14	1.25
1	L	323	SER	CA-C	-5.98	1.45	1.52
1	E	219	LEU	CG-CD1	-5.95	1.32	1.52
1	A	103	VAL	CB-CG1	-5.90	1.33	1.52
1	A	316	PRO	CG-CD	-5.90	1.30	1.50
1	A	166	MET	SD-CE	-5.89	1.64	1.79
1	A	229	PRO	CB-CG	-5.86	1.28	1.51
1	A	135	LEU	CG-CD1	-5.85	1.33	1.52
1	D	328	VAL	CB-CG1	-5.82	1.33	1.52
1	E	126	THR	CA-CB	-5.80	1.40	1.53
1	K	66	TRP	CB-CG	-5.79	1.32	1.50
1	C	324	PRO	C-O	-5.78	1.11	1.23
1	C	123	ILE	CB-CG2	-5.76	1.33	1.52
1	E	311	LEU	CG-CD1	-5.74	1.33	1.52
1	A	166	MET	CG-SD	-5.61	1.66	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	LEU	CG-CD1	-5.61	1.34	1.52
1	E	124	ILE	CG1-CD1	-5.60	1.29	1.51
1	C	350	ILE	CG1-CD1	-5.59	1.29	1.51
1	B	166	MET	CG-SD	-5.58	1.66	1.80
1	K	326	PRO	C-O	-5.58	1.17	1.23
1	E	316	PRO	CG-CD	-5.57	1.31	1.50
1	B	219	LEU	CG-CD1	-5.56	1.34	1.52
1	E	324	PRO	CB-CG	-5.55	1.29	1.51
1	E	65	MET	SD-CE	-5.53	1.65	1.79
1	B	168	LEU	CG-CD2	-5.52	1.34	1.52
1	C	322	PRO	CB-CG	-5.51	1.22	1.49
1	A	324	PRO	CB-CG	-5.51	1.29	1.51
1	D	243	LEU	CG-CD1	-5.47	1.34	1.52
1	B	260	PHE	CD2-CE2	-5.47	1.22	1.38
1	E	241	MET	SD-CE	-5.46	1.65	1.79
1	B	45	PRO	CB-CG	-5.46	1.22	1.49
1	K	323	SER	C-O	-5.45	1.17	1.24
1	B	158	THR	CB-CG2	-5.45	1.34	1.52
1	A	317	VAL	CB-CG2	-5.44	1.34	1.52
1	H	308	ILE	C-N	-5.43	1.21	1.33
1	J	133	ARG	CZ-NH2	-5.41	1.26	1.33
1	A	323	SER	CA-C	-5.40	1.46	1.52
1	C	287	HIS	C-O	-5.40	1.17	1.23
1	B	244	LEU	CG-CD1	-5.40	1.34	1.52
1	D	235	THR	CB-CG2	-5.36	1.34	1.52
1	A	323	SER	CA-CB	-5.35	1.45	1.53
1	A	324	PRO	CG-CD	-5.35	1.37	1.51
1	D	43	HIS	CA-CB	-5.34	1.44	1.53
1	B	255	PRO	CG-CD	-5.33	1.32	1.50
1	F	229	PRO	CG-CD	-5.32	1.37	1.51
1	K	324	PRO	CB-CG	-5.32	1.30	1.51
1	L	77	ARG	CZ-NH1	-5.30	1.25	1.32
1	B	257	PHE	CB-CG	-5.28	1.38	1.50
1	E	278	LEU	CG-CD1	-5.28	1.35	1.52
1	H	198	PHE	CD1-CE1	-5.28	1.22	1.38
1	L	65	MET	SD-CE	-5.28	1.66	1.79
1	C	255	PRO	CB-CG	-5.25	1.23	1.49
1	E	244	LEU	CG-CD1	-5.25	1.35	1.52
1	B	350	ILE	CG1-CD1	-5.24	1.31	1.51
1	C	266	ARG	CA-CB	-5.23	1.45	1.53
1	B	106	ILE	CG1-CD1	-5.23	1.31	1.51
1	B	139	CYS	CB-SG	-5.23	1.64	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	ARG	CG-CD	-5.22	1.36	1.52
1	K	344	ILE	CG1-CD1	-5.22	1.31	1.51
1	C	174	LEU	CG-CD2	-5.22	1.35	1.52
1	B	347	LEU	CA-CB	-5.21	1.44	1.53
1	H	123	ILE	CG1-CD1	-5.19	1.31	1.51
1	C	198	PHE	CB-CG	-5.19	1.38	1.50
1	C	324	PRO	CB-CG	-5.19	1.30	1.51
1	I	103	VAL	CB-CG1	-5.17	1.35	1.52
1	D	94	ARG	CB-CG	-5.17	1.36	1.52
1	D	259	ASN	CG-ND2	-5.17	1.22	1.33
1	A	309	PRO	CB-CG	-5.16	1.23	1.49
1	C	318	LEU	C-O	-5.15	1.18	1.24
1	A	263	ASN	CB-CG	-5.15	1.39	1.52
1	A	331	THR	CB-CG2	-5.15	1.35	1.52
1	D	318	LEU	CG-CD1	-5.15	1.35	1.52
1	E	136	VAL	CB-CG2	-5.15	1.35	1.52
1	L	91	ILE	CG1-CD1	-5.14	1.31	1.51
1	C	172	ARG	C-N	-5.14	1.27	1.34
1	L	168	LEU	CG-CD2	-5.14	1.35	1.52
1	A	259	ASN	CB-CG	-5.13	1.39	1.52
1	B	120	PHE	CD1-CE1	-5.13	1.23	1.38
1	B	60	THR	CB-CG2	-5.13	1.35	1.52
1	I	82	PRO	CG-CD	-5.12	1.33	1.50
1	I	320	LEU	CG-CD2	-5.12	1.35	1.52
1	B	120	PHE	CE2-CZ	-5.11	1.23	1.38
1	B	121	SER	CB-OG	-5.11	1.31	1.42
1	D	166	MET	CG-SD	-5.11	1.68	1.80
1	D	268	PHE	CD2-CE2	-5.11	1.23	1.38
1	H	241	MET	SD-CE	-5.11	1.66	1.79
1	D	347	LEU	CA-CB	-5.10	1.45	1.53
1	I	120	PHE	CE1-CZ	-5.09	1.23	1.38
1	L	348	ASN	CB-CG	-5.08	1.39	1.52
1	H	348	ASN	CB-CG	-5.08	1.39	1.52
1	A	136	VAL	CB-CG2	-5.08	1.35	1.52
1	C	258	PRO	CB-CG	-5.08	1.24	1.49
1	B	309	PRO	CB-CG	-5.07	1.24	1.49
1	C	209	PRO	CA-C	-5.07	1.45	1.52
1	I	308	ILE	CB-CG2	-5.07	1.35	1.52
1	C	350	ILE	CA-C	-5.06	1.46	1.52
1	C	226	THR	CB-CG2	-5.04	1.35	1.52
1	B	248	ASP	C-O	-5.04	1.17	1.23
1	B	263	ASN	CA-C	-5.04	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	124	ILE	CG1-CD1	-5.04	1.32	1.51
1	C	73	LEU	CG-CD2	-5.02	1.35	1.52
1	B	327	GLU	CA-C	-5.02	1.45	1.52
1	E	261	PHE	CD1-CE1	-5.02	1.23	1.38
1	A	193	LEU	CA-CB	-5.01	1.44	1.53
1	A	124	ILE	CG1-CD1	-5.00	1.32	1.51
1	F	218	HIS	CA-CB	-5.00	1.45	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ARG	NE-CZ-NH2	-9.86	110.33	119.20
1	A	133	ARG	CG-CD-NE	-7.84	94.75	112.00
1	H	158	THR	CB-CA-C	-5.80	101.73	110.90
1	A	158	THR	CA-C-N	5.75	130.50	122.79
1	A	158	THR	C-N-CA	5.75	130.50	122.79
1	B	159	ASP	CA-C-N	5.75	132.04	121.70
1	B	159	ASP	C-N-CA	5.75	132.04	121.70
1	C	256	THR	OG1-CB-CG2	-5.67	97.97	109.30
1	A	159	ASP	OD1-CG-OD2	-5.60	109.46	122.90
1	A	159	ASP	CA-CB-CG	5.53	118.13	112.60
1	F	76	GLU	N-CA-C	-5.48	100.86	109.25
1	C	323	SER	CA-C-N	5.48	140.16	127.00
1	C	323	SER	C-N-CA	5.48	140.16	127.00
1	A	94	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	C	323	SER	C-N-CD	-5.42	108.69	120.60
1	C	34	SER	N-CA-C	-5.40	103.35	110.43
1	J	133	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	D	159	ASP	OD1-CG-OD2	-5.39	109.97	122.90
1	A	159	ASP	CB-CG-OD1	5.38	130.78	118.40
1	A	133	ARG	CA-CB-CG	5.26	124.62	114.10
1	K	288	SER	CA-CB-OG	-5.18	100.73	111.10
1	L	202	GLU	CB-CG-CD	5.14	121.33	112.60
1	K	165	ALA	CA-C-N	-5.12	112.91	120.28
1	K	165	ALA	C-N-CA	-5.12	112.91	120.28
1	L	62	ILE	CA-C-N	-5.11	113.73	122.11
1	L	62	ILE	C-N-CA	-5.11	113.73	122.11
1	F	137	LEU	CA-C-N	-5.10	112.82	121.85
1	F	137	LEU	C-N-CA	-5.10	112.82	121.85
1	F	78	TYR	N-CA-C	-5.10	103.25	110.29
1	K	208	SER	CA-CB-OG	-5.08	100.93	111.10
1	H	159	ASP	N-CA-C	5.06	117.62	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	33	ALA	CA-C-N	-5.02	113.58	121.86
1	F	33	ALA	C-N-CA	-5.02	113.58	121.86

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	2610	0	2529	94	0
1	B	2610	0	2529	107	0
1	C	2610	0	2529	80	0
1	D	2610	0	2529	79	0
1	E	2610	0	2529	83	0
1	F	2610	0	2529	98	0
1	G	2610	0	2529	185	0
1	H	2610	0	2529	135	0
1	I	2610	0	2528	148	0
1	J	2610	0	2529	277	0
1	K	2610	0	2529	120	0
1	L	2610	0	2529	174	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	21	0	0	1	0
3	B	21	0	0	1	0
3	C	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	21	0	0	0	0
3	E	21	0	0	1	0
3	F	21	0	0	0	0
3	G	21	0	0	2	0
3	H	21	0	0	2	0
3	I	21	0	0	3	0
3	J	21	0	0	1	0
3	K	21	0	0	2	0
3	L	21	0	0	2	0
4	C	2	0	0	0	0
4	J	1	0	0	1	0
All	All	31587	0	30347	1569	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1569) 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:L:160:SER:HB2	1:L:163:PRO:CD	1.37	1.49
1:L:160:SER:CB	1:L:163:PRO:HD2	1.50	1.41
1:L:160:SER:CB	1:L:163:PRO:HG2	1.49	1.39
1:L:160:SER:CB	1:L:163:PRO:CD	2.02	1.38
1:L:160:SER:HB2	1:L:163:PRO:CG	1.55	1.36
1:L:160:SER:CB	1:L:163:PRO:CG	2.06	1.32
1:L:157:ALA:CA	1:L:161:ALA:HB3	1.64	1.27
1:L:157:ALA:HA	1:L:161:ALA:CB	1.68	1.22
1:I:328:VAL:O	1:I:331:THR:OG1	1.55	1.21
1:I:158:THR:OG1	1:I:334:ASP:OD1	1.60	1.19
1:L:160:SER:O	1:L:162:VAL:N	1.76	1.18
1:L:130:THR:O	1:L:132:LYS:N	1.85	1.08
1:G:147:SER:OG	1:J:38:GLU:OE1	1.72	1.08
1:L:159:ASP:N	1:L:160:SER:HA	1.69	1.08
1:F:34:SER:OG	1:L:280:GLU:OE1	1.71	1.07
1:J:328:VAL:O	1:J:331:THR:OG1	1.72	1.06
1:K:133:ARG:NH2	1:K:242:ASP:OD2	1.87	1.06
1:L:160:SER:C	1:L:162:VAL:H	1.56	1.05
1:G:212:SER:O	1:G:217:ARG:NH1	1.90	1.05
1:J:66:TRP:NE1	1:J:336:GLU:OE2	1.91	1.03
1:L:328:VAL:O	1:L:331:THR:OG1	1.78	1.02
1:L:158:THR:O	1:L:249:LEU:HA	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:THR:O	1:D:132:LYS:N	1.93	1.02
1:L:160:SER:O	1:L:163:PRO:HD2	1.60	1.00
1:B:212:SER:O	1:B:217:ARG:NH1	1.94	0.99
1:J:69:ASP:OD1	1:J:94:ARG:NH1	1.96	0.98
1:E:130:THR:O	1:E:132:LYS:N	1.97	0.98
1:J:130:THR:O	1:J:132:LYS:N	1.98	0.97
1:L:160:SER:HB3	1:L:163:PRO:CG	1.95	0.97
1:L:156:GLY:O	1:L:161:ALA:HB2	1.64	0.95
1:J:228:HIS:O	1:J:235:THR:OG1	1.85	0.95
1:L:160:SER:C	1:L:163:PRO:HD2	1.92	0.94
1:K:158:THR:OG1	1:K:334:ASP:OD1	1.84	0.94
1:J:36:TRP:O	1:J:133:ARG:NH1	2.00	0.94
1:L:70:LEU:CD1	1:L:161:ALA:O	2.16	0.94
1:L:212:SER:O	1:L:217:ARG:NH1	2.01	0.93
1:L:160:SER:HB3	1:L:163:PRO:CD	1.98	0.93
1:L:160:SER:CA	1:L:163:PRO:HD2	1.98	0.93
1:L:160:SER:HB3	1:L:163:PRO:HG2	1.47	0.93
1:G:68:ASN:O	1:G:94:ARG:NH1	2.01	0.92
1:A:133:ARG:HH22	1:A:242:ASP:CG	1.77	0.92
1:L:69:ASP:OD1	1:L:94:ARG:NH1	2.02	0.92
1:F:329:TRP:O	1:F:331:THR:N	2.03	0.91
1:G:140:HIS:O	1:G:140:HIS:ND1	2.05	0.90
1:H:133:ARG:NH2	1:H:242:ASP:OD2	2.04	0.89
1:C:92:MET:HE2	1:C:106:ILE:HD11	1.51	0.89
1:I:158:THR:OG1	1:I:334:ASP:CG	2.16	0.89
1:A:212:SER:O	1:A:217:ARG:NH1	2.06	0.88
1:I:159:ASP:HB2	1:I:249:LEU:CD2	2.04	0.88
1:L:157:ALA:HB1	1:L:339:LEU:HD21	1.56	0.88
1:L:92:MET:HE2	1:L:106:ILE:HD11	1.53	0.88
1:L:236:SER:O	1:L:238:LEU:N	2.07	0.87
1:E:179:LEU:O	1:E:181:LEU:N	2.08	0.86
1:I:159:ASP:HB2	1:I:249:LEU:HD23	1.57	0.86
1:L:70:LEU:HD11	1:L:161:ALA:O	1.73	0.86
1:B:285:LYS:NZ	1:B:286:ASP:OD1	2.07	0.86
1:G:69:ASP:OD1	1:G:94:ARG:NH1	2.08	0.86
1:B:228:HIS:O	1:B:235:THR:OG1	1.92	0.86
1:H:158:THR:OG1	1:H:334:ASP:OD2	1.92	0.86
1:L:158:THR:C	1:L:160:SER:HA	2.00	0.86
1:G:335:ASN:ND2	1:G:337:GLU:OE2	2.08	0.85
1:H:295:GLN:O	1:H:297:TYR:N	2.10	0.85
1:D:205:LEU:O	1:D:206:HIS:ND1	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:SER:OG	1:L:163:PRO:HG2	1.75	0.84
1:K:128:ASN:O	1:K:130:THR:N	2.10	0.84
1:J:216:SER:OG	1:J:306:ASP:OD1	1.95	0.84
1:L:177:LYS:O	1:L:180:SER:OG	1.96	0.84
1:L:160:SER:HB2	1:L:163:PRO:HD2	0.98	0.83
1:G:340:ASP:O	1:G:342:SER:N	2.11	0.83
1:J:265:ALA:O	1:J:268:PHE:N	2.11	0.83
1:G:199:ASP:OD1	1:G:200:GLY:N	2.12	0.82
1:H:328:VAL:O	1:H:331:THR:OG1	1.96	0.82
1:G:130:THR:O	1:G:132:LYS:N	2.13	0.81
1:L:236:SER:O	1:L:239:HIS:N	2.13	0.81
1:H:158:THR:OG1	1:H:334:ASP:CG	2.22	0.81
1:L:205:LEU:O	1:L:206:HIS:ND1	2.14	0.81
1:A:130:THR:O	1:A:132:LYS:N	2.14	0.80
1:H:228:HIS:O	1:H:235:THR:OG1	1.99	0.80
1:C:40:LYS:HB3	1:C:242:ASP:OD1	1.82	0.79
1:G:49:ASN:OD1	1:G:52:ALA:N	2.15	0.79
1:G:328:VAL:HG11	1:G:334:ASP:N	1.98	0.79
1:J:40:LYS:N	1:J:133:ARG:HH22	1.81	0.79
1:J:279:HIS:NE2	1:J:287:HIS:O	2.16	0.79
1:E:175:ASP:O	1:E:178:LEU:N	2.17	0.78
1:L:47:ILE:HD11	1:L:270:ARG:CZ	2.14	0.78
1:L:160:SER:O	1:L:163:PRO:CD	2.30	0.78
1:G:122:ASN:ND2	1:G:215:GLY:O	2.14	0.78
1:I:279:HIS:CG	1:I:289:LEU:HD21	2.19	0.78
1:K:212:SER:O	1:K:217:ARG:NH1	2.17	0.78
1:J:279:HIS:O	1:J:282:GLY:N	2.12	0.77
1:J:248:ASP:OD2	3:J:402:A1D48:N17	2.17	0.77
1:L:156:GLY:O	1:L:161:ALA:CB	2.32	0.77
1:G:228:HIS:O	1:G:235:THR:OG1	2.02	0.77
1:E:69:ASP:OD1	1:E:94:ARG:NH1	2.18	0.77
1:J:88:ARG:HG3	1:J:123:ILE:HD11	1.68	0.76
1:I:212:SER:O	1:I:217:ARG:NH1	2.18	0.75
1:H:117:TYR:O	1:H:118:ARG:HG2	1.87	0.75
1:J:249:LEU:HD12	1:J:321:ILE:HD11	1.67	0.75
1:B:205:LEU:O	1:B:206:HIS:ND1	2.20	0.75
1:J:61:SER:OG	1:J:61:SER:O	1.93	0.74
1:A:133:ARG:NH2	1:A:242:ASP:OD1	2.20	0.74
1:C:212:SER:O	1:C:217:ARG:NH1	2.19	0.74
1:B:36:TRP:CG	1:B:37:PRO:HD3	2.23	0.74
1:C:132:LYS:NZ	1:C:190:ASP:OD2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:337:GLU:N	1:K:337:GLU:OE1	2.20	0.74
1:B:281:LEU:HB2	1:B:283:LEU:HD11	1.68	0.74
1:A:68:ASN:HB3	1:A:94:ARG:NH1	2.03	0.74
1:L:159:ASP:N	1:L:160:SER:CA	2.49	0.74
1:B:36:TRP:N	1:B:37:PRO:HD2	2.03	0.73
1:J:311:LEU:O	1:J:314:GLY:N	2.18	0.73
1:A:248:ASP:OD2	3:A:402:A1D48:N17	2.21	0.73
1:L:228:HIS:O	1:L:235:THR:OG1	2.06	0.73
1:B:49:ASN:OD1	1:B:52:ALA:N	2.20	0.73
1:I:228:HIS:O	1:I:235:THR:OG1	2.07	0.73
1:I:284:LEU:HD23	1:I:287:HIS:ND1	2.04	0.72
1:F:100:ALA:HA	1:F:179:LEU:HD12	1.70	0.72
1:A:133:ARG:HH22	1:A:242:ASP:CB	2.03	0.72
1:C:105:GLU:C	1:C:106:ILE:HD13	2.13	0.72
1:I:169:GLU:OE2	1:I:172:ARG:NH2	2.20	0.72
1:F:69:ASP:OD1	1:F:94:ARG:NH1	2.23	0.72
1:I:177:LYS:O	1:I:180:SER:OG	2.08	0.72
1:C:78:TYR:O	1:C:81:SER:OG	2.08	0.72
1:G:285:LYS:NZ	1:G:286:ASP:OD1	2.19	0.71
1:G:328:VAL:HG11	1:G:334:ASP:CA	2.21	0.71
1:F:228:HIS:O	1:F:235:THR:OG1	2.09	0.71
1:F:34:SER:OG	1:L:280:GLU:CD	2.33	0.71
1:H:172:ARG:O	1:H:174:LEU:N	2.24	0.71
1:H:177:LYS:NZ	1:H:361:LEU:O	2.22	0.71
1:H:61:SER:O	1:H:61:SER:OG	2.07	0.70
1:A:133:ARG:NH2	1:A:242:ASP:CG	2.49	0.70
1:J:70:LEU:HD11	1:J:74:LEU:HD11	1.73	0.70
1:H:155:VAL:O	1:H:156:GLY:C	2.34	0.70
1:L:236:SER:O	1:L:237:GLN:C	2.33	0.70
1:I:222:LYS:O	1:I:226:THR:OG1	2.10	0.70
1:J:328:VAL:HG12	1:J:331:THR:OG1	1.91	0.70
1:E:136:VAL:HG21	1:E:241:MET:HE3	1.74	0.70
1:G:259:ASN:OD1	1:G:268:PHE:CG	2.45	0.70
1:H:347:LEU:O	1:H:349:LYS:N	2.25	0.70
1:G:57:ALA:HA	1:G:349:LYS:CE	2.22	0.69
1:B:33:ALA:O	1:B:34:SER:O	2.11	0.69
1:J:158:THR:OG1	1:J:334:ASP:OD2	2.09	0.69
1:L:305:ASP:O	1:L:307:HIS:N	2.24	0.69
1:C:92:MET:CE	1:C:106:ILE:HD11	2.23	0.69
1:C:228:HIS:O	1:C:235:THR:OG1	2.10	0.69
1:B:36:TRP:CD2	1:B:37:PRO:HD3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:GLU:O	1:G:172:ARG:N	2.26	0.68
1:H:162:VAL:HB	1:H:163:PRO:HD3	1.75	0.68
1:L:92:MET:CE	1:L:106:ILE:HD11	2.22	0.68
1:I:77:ARG:HG3	1:I:143:SER:HB3	1.75	0.68
1:G:56:ILE:O	1:G:349:LYS:NZ	2.26	0.68
1:F:175:ASP:O	1:F:178:LEU:N	2.23	0.68
1:A:133:ARG:HH12	1:A:242:ASP:CG	2.02	0.67
1:D:212:SER:O	1:D:217:ARG:NH1	2.27	0.67
1:H:92:MET:CE	1:H:106:ILE:HD11	2.24	0.67
1:J:50:SER:O	1:J:53:LEU:N	2.27	0.67
1:I:47:ILE:HD12	1:I:270:ARG:HH22	1.60	0.67
1:K:216:SER:OG	1:K:306:ASP:OD1	2.12	0.67
1:H:160:SER:OG	1:H:163:PRO:HG2	1.94	0.67
1:I:123:ILE:C	1:I:124:ILE:HD12	2.19	0.67
1:J:40:LYS:N	1:J:133:ARG:NH2	2.43	0.67
1:J:124:ILE:N	1:J:124:ILE:HD12	2.10	0.66
1:C:106:ILE:HD13	1:C:106:ILE:N	2.08	0.66
1:F:40:LYS:HB3	1:F:242:ASP:OD1	1.96	0.66
1:G:56:ILE:C	1:G:349:LYS:HZ1	2.03	0.66
1:B:36:TRP:CD1	1:B:37:PRO:HD3	2.30	0.66
1:L:74:LEU:CD2	1:L:161:ALA:HB1	2.26	0.66
1:G:279:HIS:O	1:G:282:GLY:N	2.23	0.66
1:G:157:ALA:N	1:G:334:ASP:OD1	2.28	0.66
1:E:73:LEU:O	1:E:77:ARG:NH1	2.29	0.65
1:L:106:ILE:HD13	1:L:106:ILE:N	2.09	0.65
1:L:157:ALA:O	1:L:161:ALA:N	2.30	0.65
1:L:158:THR:HG22	1:L:250:ILE:O	1.97	0.65
1:H:133:ARG:HH21	1:H:242:ASP:CG	2.05	0.65
1:K:349:LYS:O	1:K:353:VAL:HG23	1.97	0.65
1:H:157:ALA:O	1:H:162:VAL:HG23	1.97	0.65
1:J:133:ARG:O	1:J:134:HIS:ND1	2.30	0.65
1:E:179:LEU:C	1:E:181:LEU:H	2.05	0.65
1:J:337:GLU:OE2	1:J:337:GLU:N	2.24	0.65
1:G:261:PHE:O	1:G:264:SER:OG	2.14	0.65
1:H:158:THR:OG1	1:H:334:ASP:OD1	2.13	0.65
1:J:350:ILE:HD12	1:J:351:LEU:N	2.12	0.65
1:L:278:LEU:HB3	1:L:284:LEU:HD13	1.79	0.65
1:A:205:LEU:O	1:A:206:HIS:ND1	2.29	0.65
1:G:279:HIS:CE1	1:G:289:LEU:HG	2.32	0.65
1:J:62:ILE:HB	1:J:345:ASP:OD2	1.98	0.65
1:G:39:GLU:C	1:G:133:ARG:HH21	2.05	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ILE:O	1:C:312:ARG:HG3	1.97	0.64
1:E:92:MET:CE	1:E:106:ILE:HD11	2.27	0.64
1:J:49:ASN:O	1:J:53:LEU:HG	1.97	0.64
1:J:329:TRP:O	1:J:331:THR:HG23	1.97	0.64
1:G:57:ALA:HA	1:G:349:LYS:HD2	1.78	0.64
1:B:314:GLY:HA3	1:K:206:HIS:HB3	1.79	0.64
1:A:149:TRP:O	1:A:152:ARG:N	2.28	0.64
1:L:157:ALA:CB	1:L:339:LEU:HD21	2.26	0.64
1:D:279:HIS:O	1:D:281:LEU:N	2.31	0.64
1:K:36:TRP:CG	1:K:37:PRO:HD3	2.32	0.64
1:B:285:LYS:O	1:B:286:ASP:C	2.41	0.63
1:A:133:ARG:HB3	1:A:133:ARG:CZ	2.26	0.63
1:G:169:GLU:OE2	1:G:172:ARG:NH2	2.31	0.63
1:H:281:LEU:HB3	1:H:283:LEU:HD11	1.80	0.63
1:L:157:ALA:HA	1:L:161:ALA:HB3	0.76	0.63
1:J:66:TRP:CE2	1:J:336:GLU:OE2	2.51	0.63
1:J:347:LEU:HA	1:J:350:ILE:HD11	1.80	0.63
1:G:328:VAL:HG12	1:G:328:VAL:O	1.97	0.63
1:J:71:GLN:HA	1:J:74:LEU:HD12	1.79	0.63
1:J:340:ASP:OD2	1:J:343:THR:OG1	2.16	0.63
1:A:40:LYS:HB2	1:A:242:ASP:OD1	1.98	0.63
1:I:68:ASN:HB3	1:I:94:ARG:HH12	1.61	0.63
1:J:336:GLU:O	1:J:337:GLU:C	2.41	0.63
1:L:69:ASP:OD1	1:L:94:ARG:HD3	1.98	0.63
1:J:65:MET:HG3	1:J:169:GLU:HB2	1.80	0.63
1:J:102:TRP:CZ3	1:J:127:LEU:HB2	2.34	0.63
1:J:36:TRP:CZ3	1:J:132:LYS:HB3	2.33	0.63
1:J:40:LYS:CB	1:J:242:ASP:OD1	2.47	0.63
1:K:35:ALA:C	1:K:37:PRO:HD2	2.23	0.62
1:K:47:ILE:HG13	1:K:357:GLU:OE2	1.99	0.62
1:A:77:ARG:HG2	1:A:143:SER:HB3	1.80	0.62
1:D:71:GLN:N	1:D:72:PRO:CD	2.62	0.62
1:G:157:ALA:O	1:G:162:VAL:HG23	1.99	0.62
1:K:78:TYR:O	1:K:84:SER:HB2	2.00	0.62
1:G:328:VAL:CG1	1:G:334:ASP:N	2.61	0.62
1:E:175:ASP:O	1:E:176:LYS:C	2.43	0.62
1:F:355:VAL:O	1:F:358:TYR:N	2.30	0.62
1:J:39:GLU:C	1:J:133:ARG:HH22	2.06	0.62
1:L:43:HIS:O	1:L:266:ARG:NH2	2.27	0.62
1:L:74:LEU:HD23	1:L:161:ALA:HB1	1.80	0.62
1:J:199:ASP:OD1	1:J:200:GLY:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HH22	1:A:242:ASP:CA	2.13	0.62
1:J:355:VAL:O	1:J:358:TYR:N	2.30	0.62
1:B:34:SER:OG	1:B:35:ALA:N	2.29	0.62
1:H:56:ILE:O	1:H:59:GLY:N	2.33	0.62
1:H:283:LEU:HD12	1:H:283:LEU:H	1.65	0.62
1:K:252:ALA:HB1	1:K:253:PRO:HD2	1.81	0.62
1:E:212:SER:O	1:E:217:ARG:NH1	2.33	0.61
1:G:353:VAL:O	1:G:356:LEU:N	2.33	0.61
1:J:70:LEU:C	1:J:70:LEU:HD12	2.25	0.61
1:J:73:LEU:O	1:J:75:ILE:N	2.33	0.61
1:G:328:VAL:HG11	1:G:333:ASP:C	2.26	0.61
1:J:158:THR:O	1:J:249:LEU:HA	2.00	0.61
1:H:272:GLN:CD	1:H:296:ASN:OD1	2.44	0.61
1:L:311:LEU:O	1:L:314:GLY:N	2.32	0.61
1:J:43:HIS:NE2	1:J:358:TYR:O	2.30	0.61
1:B:206:HIS:CG	1:E:314:GLY:HA3	2.36	0.61
1:E:34:SER:OG	1:E:35:ALA:N	2.33	0.61
1:G:268:PHE:O	1:G:271:LEU:N	2.28	0.61
1:G:333:ASP:O	1:G:335:ASN:N	2.32	0.61
1:H:53:LEU:HD12	1:H:278:LEU:HD21	1.82	0.61
1:J:61:SER:O	1:J:63:SER:N	2.34	0.61
1:I:92:MET:O	1:I:93:GLN:C	2.44	0.61
1:I:158:THR:OG1	1:I:334:ASP:OD2	2.18	0.61
1:K:133:ARG:NE	1:K:242:ASP:OD1	2.33	0.61
1:G:281:LEU:HB3	1:G:283:LEU:HD11	1.82	0.60
1:J:133:ARG:HG2	1:J:242:ASP:OD2	2.01	0.60
1:D:61:SER:HB3	1:D:64:GLU:HG3	1.82	0.60
1:K:133:ARG:HH21	1:K:242:ASP:CG	2.09	0.60
1:L:121:SER:O	1:L:199:ASP:HB2	2.00	0.60
1:B:65:MET:HG3	1:B:169:GLU:HB2	1.84	0.60
1:E:212:SER:O	1:E:213:LEU:HB2	2.01	0.60
1:I:57:ALA:HB1	1:I:349:LYS:HE2	1.84	0.60
1:I:252:ALA:HB1	1:I:253:PRO:HD2	1.83	0.60
1:A:38:GLU:O	1:A:40:LYS:N	2.34	0.60
1:A:228:HIS:HB2	1:A:237:GLN:HG2	1.84	0.60
1:B:229:PRO:HB2	1:B:230:PRO:HD2	1.83	0.60
1:K:109:PHE:CZ	1:K:120:PHE:HB2	2.36	0.60
1:K:201:GLU:OE1	1:K:202:GLU:HG2	2.02	0.60
1:F:61:SER:O	1:F:61:SER:OG	2.14	0.60
1:H:62:ILE:HB	1:H:345:ASP:CG	2.27	0.60
1:J:99:GLN:O	1:J:179:LEU:HD11	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:LYS:NZ	1:E:286:ASP:OD1	2.26	0.60
1:F:36:TRP:CG	1:F:37:PRO:HD3	2.36	0.60
1:K:172:ARG:HH11	1:K:172:ARG:HG2	1.66	0.60
1:B:144:LYS:HD3	1:B:146:PHE:CE2	2.36	0.60
1:G:208:SER:O	1:G:212:SER:OG	2.18	0.59
1:J:102:TRP:CE3	1:J:127:LEU:HD12	2.37	0.59
1:J:199:ASP:O	1:J:200:GLY:C	2.45	0.59
1:D:179:LEU:O	1:D:181:LEU:N	2.36	0.59
1:G:166:MET:SD	1:G:250:ILE:HG21	2.43	0.59
1:J:106:ILE:HG22	1:J:107:ASP:N	2.18	0.59
1:J:285:LYS:NZ	1:J:286:ASP:OD1	2.32	0.59
1:B:78:TYR:CE1	1:B:81:SER:HB3	2.36	0.59
1:B:211:ASP:O	1:B:212:SER:HB3	2.00	0.59
1:J:205:LEU:O	1:J:206:HIS:ND1	2.36	0.59
1:J:39:GLU:CG	1:J:133:ARG:NH2	2.65	0.59
1:A:80:GLY:O	1:A:81:SER:O	2.20	0.59
1:I:279:HIS:CD2	1:I:289:LEU:CD2	2.86	0.59
1:I:323:SER:N	1:I:324:PRO:O	2.35	0.59
1:L:308:ILE:HB	1:L:309:PRO:HD3	1.85	0.59
1:G:91:ILE:O	1:G:94:ARG:N	2.36	0.59
1:G:177:LYS:O	1:G:180:SER:OG	2.18	0.59
1:L:160:SER:HB2	1:L:163:PRO:CB	2.28	0.59
1:B:36:TRP:CG	1:B:37:PRO:CD	2.85	0.59
1:G:275:GLU:OE2	1:G:293:TYR:N	2.33	0.59
1:I:133:ARG:NH2	1:I:242:ASP:OD2	2.24	0.59
1:C:305:ASP:O	1:C:307:HIS:N	2.36	0.58
1:G:49:ASN:OD1	1:G:51:SER:N	2.37	0.58
1:F:229:PRO:O	1:F:230:PRO:C	2.43	0.58
1:H:69:ASP:OD1	1:H:94:ARG:NH1	2.36	0.58
1:A:211:ASP:O	1:A:212:SER:HB3	2.03	0.58
1:G:264:SER:O	1:G:267:TRP:N	2.33	0.58
1:H:158:THR:O	1:H:160:SER:HA	2.04	0.58
1:K:128:ASN:O	1:K:129:PRO:C	2.46	0.58
1:B:36:TRP:N	1:B:37:PRO:CD	2.67	0.58
1:H:212:SER:O	1:H:214:TYR:N	2.35	0.58
1:I:281:LEU:HB3	1:I:283:LEU:HD11	1.84	0.58
1:K:33:ALA:O	1:K:34:SER:HB3	2.03	0.58
1:C:229:PRO:O	1:C:230:PRO:C	2.47	0.58
1:E:170:LEU:HD23	1:E:170:LEU:C	2.28	0.58
1:I:36:TRP:CG	1:I:37:PRO:HD3	2.38	0.58
1:J:70:LEU:HD12	1:J:70:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:ILE:O	1:F:312:ARG:HG2	2.04	0.58
1:K:100:ALA:HA	1:K:179:LEU:HD12	1.84	0.58
1:J:77:ARG:HG3	1:J:143:SER:HB3	1.86	0.58
1:J:293:TYR:OH	1:J:343:THR:HG23	2.03	0.58
1:B:92:MET:HE1	1:B:106:ILE:HD11	1.86	0.58
1:E:155:VAL:HG23	1:E:155:VAL:O	2.02	0.58
1:F:34:SER:HB2	1:L:280:GLU:HA	1.86	0.58
1:J:85:TYR:O	1:J:88:ARG:N	2.37	0.57
1:L:325:PHE:O	1:L:326:PRO:C	2.41	0.57
1:D:132:LYS:HA	1:D:228:HIS:NE2	2.19	0.57
1:F:155:VAL:O	1:F:156:GLY:C	2.46	0.57
1:I:43:HIS:O	1:I:266:ARG:NH1	2.32	0.57
1:J:213:LEU:O	1:J:214:TYR:C	2.45	0.57
1:J:296:ASN:O	1:J:298:SER:N	2.37	0.57
1:B:112:GLN:OE1	1:B:117:TYR:CE1	2.57	0.57
1:E:333:ASP:O	1:E:338:ASN:ND2	2.37	0.57
1:F:329:TRP:O	1:F:330:HIS:C	2.46	0.57
1:L:288:SER:O	1:L:291:GLY:N	2.37	0.57
1:G:328:VAL:HG11	1:G:334:ASP:HA	1.85	0.57
1:B:49:ASN:OD1	1:B:49:ASN:C	2.48	0.57
1:G:284:LEU:HD23	1:G:287:HIS:ND1	2.19	0.57
1:F:35:ALA:O	1:F:38:GLU:N	2.37	0.57
1:F:66:TRP:NE1	1:F:336:GLU:OE2	2.36	0.57
1:J:305:ASP:O	1:J:307:HIS:N	2.38	0.57
1:G:272:GLN:NE2	1:G:296:ASN:OD1	2.29	0.57
1:I:328:VAL:C	1:I:331:THR:OG1	2.41	0.57
1:G:56:ILE:C	1:G:349:LYS:NZ	2.61	0.57
1:H:161:ALA:O	1:H:162:VAL:C	2.46	0.57
1:L:140:HIS:NE2	1:L:159:ASP:OD1	2.32	0.57
1:L:160:SER:C	1:L:162:VAL:N	2.30	0.57
1:B:36:TRP:CE2	1:B:37:PRO:HD3	2.39	0.57
1:G:307:HIS:O	1:G:308:ILE:C	2.48	0.57
1:J:55:GLN:O	1:J:58:GLU:N	2.38	0.57
1:L:201:GLU:OE1	1:L:202:GLU:HG2	2.05	0.57
1:L:94:ARG:HH21	1:L:97:ARG:NH1	2.02	0.56
1:C:92:MET:O	1:C:93:GLN:C	2.48	0.56
1:C:205:LEU:O	1:C:206:HIS:ND1	2.38	0.56
1:G:60:THR:HG22	1:G:349:LYS:HZ3	1.70	0.56
1:L:36:TRP:CD2	1:L:37:PRO:HD3	2.40	0.56
1:A:133:ARG:NH1	1:A:242:ASP:OD2	2.29	0.56
1:F:158:THR:O	1:F:249:LEU:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:GLN:O	1:H:93:GLN:HG3	2.05	0.56
1:I:279:HIS:CD2	1:I:289:LEU:HD21	2.40	0.56
1:I:354:PHE:C	1:I:354:PHE:CD1	2.83	0.56
1:J:95:ILE:HG23	1:J:102:TRP:CD1	2.40	0.56
1:J:347:LEU:O	1:J:349:LYS:N	2.38	0.56
1:B:248:ASP:OD2	3:B:402:A1D48:N17	2.38	0.56
1:A:65:MET:O	1:A:65:MET:HG2	2.05	0.56
1:I:170:LEU:HG	1:I:352:GLN:HG2	1.88	0.56
1:A:333:ASP:O	1:A:335:ASN:N	2.37	0.56
1:D:347:LEU:O	1:D:348:ASN:C	2.47	0.56
1:A:68:ASN:CB	1:A:94:ARG:NH1	2.69	0.56
1:G:53:LEU:N	1:G:53:LEU:HD23	2.20	0.56
1:G:57:ALA:HA	1:G:349:LYS:CD	2.34	0.56
1:I:319:HIS:O	1:I:321:ILE:N	2.36	0.56
1:J:323:SER:O	1:J:323:SER:OG	2.19	0.56
1:H:140:HIS:ND1	1:H:142:ASP:OD1	2.37	0.56
1:H:182:LYS:HD3	1:H:182:LYS:N	2.21	0.56
1:J:331:THR:O	1:J:333:ASP:N	2.39	0.56
1:B:132:LYS:HA	1:B:228:HIS:NE2	2.21	0.56
1:F:36:TRP:CD2	1:F:37:PRO:HD3	2.41	0.56
1:I:248:ASP:OD2	3:I:402:A1D48:N17	2.39	0.56
1:L:140:HIS:CE1	1:L:159:ASP:O	2.58	0.56
1:H:128:ASN:ND2	1:H:181:LEU:O	2.36	0.55
1:K:36:TRP:N	1:K:37:PRO:CD	2.68	0.55
1:L:77:ARG:HG3	1:L:143:SER:HB3	1.87	0.55
1:E:328:VAL:O	1:E:329:TRP:C	2.47	0.55
1:J:212:SER:O	1:J:212:SER:OG	2.24	0.55
1:F:127:LEU:O	1:F:128:ASN:HB2	2.06	0.55
1:G:91:ILE:HG22	1:G:92:MET:N	2.20	0.55
3:G:402:A1D48:C21	3:G:402:A1D48:O01	2.55	0.55
1:J:348:ASN:O	1:J:352:GLN:HG3	2.07	0.55
1:L:158:THR:HG22	1:L:251:GLY:HA3	1.88	0.55
1:E:281:LEU:HB2	1:E:283:LEU:HD12	1.87	0.55
1:E:351:LEU:O	1:E:354:PHE:N	2.39	0.55
1:F:168:LEU:O	1:F:171:ALA:N	2.40	0.55
1:F:248:ASP:O	1:F:249:LEU:HB2	2.06	0.55
1:J:133:ARG:O	1:J:134:HIS:CG	2.60	0.55
1:K:133:ARG:CZ	1:K:242:ASP:OD2	2.51	0.55
1:L:37:PRO:O	1:L:40:LYS:HE3	2.06	0.55
1:L:157:ALA:C	1:L:161:ALA:HB3	2.29	0.55
1:L:236:SER:C	1:L:238:LEU:N	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:C	1:A:118:ARG:HG2	2.31	0.55
1:E:142:ASP:OD1	1:E:142:ASP:N	2.33	0.55
1:D:61:SER:CB	1:D:64:GLU:HG3	2.36	0.55
1:I:49:ASN:OD1	1:I:49:ASN:O	2.25	0.55
1:I:88:ARG:O	1:I:92:MET:HG3	2.07	0.55
1:K:36:TRP:N	1:K:37:PRO:HD2	2.22	0.55
1:K:128:ASN:C	1:K:130:THR:N	2.62	0.55
1:L:47:ILE:HD11	1:L:270:ARG:NH1	2.22	0.55
1:L:65:MET:HG3	1:L:169:GLU:HB2	1.87	0.55
1:E:77:ARG:HG2	1:E:143:SER:HB3	1.89	0.55
1:F:92:MET:CE	1:F:106:ILE:HD11	2.36	0.55
1:J:141:TYR:HD2	1:J:197:PHE:O	1.89	0.55
1:J:331:THR:O	1:J:334:ASP:N	2.38	0.55
1:G:140:HIS:ND1	1:G:140:HIS:C	2.64	0.55
1:J:70:LEU:C	1:J:72:PRO:CD	2.80	0.55
1:J:216:SER:HB2	1:J:309:PRO:HG2	1.88	0.55
1:J:349:LYS:O	1:J:350:ILE:C	2.49	0.55
1:I:328:VAL:O	1:I:329:TRP:C	2.50	0.55
1:K:52:ALA:O	1:K:56:ILE:HG12	2.07	0.55
1:B:283:LEU:HD12	1:B:283:LEU:H	1.72	0.55
1:L:328:VAL:C	1:L:331:THR:OG1	2.47	0.55
1:H:35:ALA:C	1:H:37:PRO:HD2	2.32	0.54
1:K:106:ILE:O	1:K:106:ILE:HG22	2.08	0.54
1:L:51:SER:O	1:L:54:ARG:N	2.38	0.54
1:L:78:TYR:CE1	1:L:81:SER:HB3	2.42	0.54
1:G:46:ALA:HB3	1:G:360:HIS:HA	1.89	0.54
1:H:212:SER:O	1:H:213:LEU:C	2.50	0.54
1:K:133:ARG:HE	1:K:242:ASP:CG	2.15	0.54
1:K:205:LEU:O	1:K:206:HIS:ND1	2.40	0.54
1:L:137:LEU:HD12	1:L:245:VAL:HB	1.89	0.54
1:D:40:LYS:HB3	1:D:242:ASP:OD1	2.07	0.54
1:G:158:THR:N	1:G:334:ASP:OD1	2.34	0.54
1:H:348:ASN:O	1:H:352:GLN:HG3	2.06	0.54
1:I:124:ILE:HD12	1:I:124:ILE:N	2.22	0.54
1:A:133:ARG:CZ	1:A:242:ASP:OD1	2.56	0.54
1:H:272:GLN:NE2	1:H:296:ASN:OD1	2.40	0.54
1:J:57:ALA:HA	1:J:349:LYS:HD3	1.89	0.54
1:E:158:THR:O	1:E:160:SER:HA	2.07	0.54
1:H:321:ILE:HG23	1:H:321:ILE:O	2.07	0.54
1:J:158:THR:OG1	1:J:334:ASP:CG	2.51	0.54
1:J:253:PRO:O	1:J:254:ASN:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LYS:HB3	1:E:242:ASP:OD1	2.07	0.54
1:F:124:ILE:N	1:F:124:ILE:HD12	2.23	0.54
1:G:40:LYS:N	1:G:133:ARG:HH21	2.04	0.54
1:G:68:ASN:OD1	1:G:68:ASN:N	2.40	0.54
1:G:263:ASN:HD22	1:G:263:ASN:H	1.54	0.54
1:H:281:LEU:HB3	1:H:283:LEU:CD1	2.36	0.54
1:I:99:GLN:N	1:I:175:ASP:OD2	2.41	0.54
1:J:283:LEU:HD12	1:J:283:LEU:H	1.73	0.54
1:C:229:PRO:O	1:C:230:PRO:O	2.26	0.54
1:H:78:TYR:CE1	1:H:81:SER:HB3	2.43	0.54
1:I:335:ASN:C	1:I:335:ASN:OD1	2.50	0.54
1:L:68:ASN:HB3	1:L:94:ARG:NH1	2.23	0.54
1:J:65:MET:O	1:J:65:MET:HG2	2.08	0.54
1:B:52:ALA:O	1:B:55:GLN:N	2.41	0.54
1:F:94:ARG:HH21	1:F:97:ARG:CZ	2.19	0.54
1:F:167:MET:HE2	1:F:197:PHE:CE2	2.43	0.54
1:G:248:ASP:OD2	3:G:402:A1D48:N17	2.41	0.54
1:H:235:THR:OG1	1:H:235:THR:O	2.26	0.54
1:D:211:ASP:O	1:D:212:SER:HB3	2.07	0.54
1:F:102:TRP:CE3	1:F:127:LEU:HG	2.43	0.54
1:J:49:ASN:C	1:J:49:ASN:OD1	2.50	0.54
1:J:68:ASN:HB3	1:J:94:ARG:NH1	2.23	0.54
1:D:279:HIS:C	1:D:281:LEU:H	2.16	0.53
1:H:57:ALA:HB3	1:H:283:LEU:HD23	1.90	0.53
1:J:274:ILE:O	1:J:278:LEU:HD12	2.09	0.53
1:K:66:TRP:NE1	1:K:336:GLU:OE2	2.29	0.53
1:B:281:LEU:CB	1:B:283:LEU:HD11	2.38	0.53
1:E:92:MET:HE2	1:E:106:ILE:HD11	1.89	0.53
1:H:347:LEU:O	1:H:348:ASN:C	2.47	0.53
1:I:98:LEU:HB3	1:I:175:ASP:OD2	2.07	0.53
1:I:128:ASN:O	1:I:130:THR:N	2.41	0.53
1:I:211:ASP:O	1:I:212:SER:HB3	2.08	0.53
1:F:328:VAL:O	1:F:331:THR:OG1	2.26	0.53
1:K:34:SER:OG	1:K:35:ALA:N	2.34	0.53
1:G:354:PHE:CD1	1:G:354:PHE:C	2.86	0.53
1:H:160:SER:O	1:H:163:PRO:HD2	2.09	0.53
1:L:348:ASN:O	1:L:352:GLN:HG3	2.08	0.53
1:B:229:PRO:HB2	1:B:230:PRO:CD	2.38	0.53
1:A:36:TRP:N	1:A:37:PRO:CD	2.71	0.53
1:A:133:ARG:NH1	1:A:242:ASP:CG	2.66	0.53
1:E:61:SER:HG	1:E:64:GLU:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ILE:O	1:G:92:MET:C	2.51	0.53
1:G:253:PRO:HB3	1:G:340:ASP:OD2	2.08	0.53
1:A:92:MET:CE	1:A:106:ILE:HD11	2.38	0.53
1:E:43:HIS:O	1:E:266:ARG:NH1	2.35	0.53
1:H:347:LEU:C	1:H:349:LYS:N	2.66	0.53
1:K:85:TYR:O	1:K:86:ALA:C	2.50	0.53
1:B:224:ALA:HA	1:B:238:LEU:HG	1.90	0.53
1:A:340:ASP:OD1	1:K:286:ASP:OD2	2.27	0.53
1:I:259:ASN:HD21	1:I:265:ALA:HA	1.73	0.53
1:J:49:ASN:OD1	1:J:52:ALA:N	2.29	0.53
1:J:191:LEU:CD1	1:J:242:ASP:OD2	2.56	0.53
1:A:181:LEU:HD21	1:A:361:LEU:HD21	1.90	0.53
1:F:78:TYR:CE1	1:F:81:SER:HB3	2.44	0.53
1:G:140:HIS:C	1:G:140:HIS:HD1	2.16	0.53
1:H:149:TRP:O	1:H:150:ASN:C	2.52	0.53
1:J:174:LEU:O	1:J:175:ASP:C	2.51	0.53
1:I:229:PRO:O	1:I:230:PRO:C	2.51	0.53
1:L:219:LEU:O	1:L:220:ALA:C	2.52	0.53
1:B:49:ASN:OD1	1:B:51:SER:N	2.42	0.52
1:E:92:MET:HE1	1:E:106:ILE:HD11	1.90	0.52
1:J:92:MET:O	1:J:95:ILE:N	2.38	0.52
1:J:279:HIS:O	1:J:281:LEU:N	2.42	0.52
1:J:328:VAL:HG11	1:J:333:ASP:O	2.09	0.52
1:B:281:LEU:HB2	1:B:283:LEU:CD1	2.38	0.52
1:F:212:SER:O	1:F:217:ARG:NH1	2.39	0.52
1:H:256:THR:OG1	1:H:323:SER:O	2.27	0.52
1:J:347:LEU:HA	1:J:350:ILE:CG1	2.39	0.52
1:J:347:LEU:C	1:J:349:LYS:N	2.64	0.52
1:L:174:LEU:HD22	1:L:356:LEU:HD11	1.91	0.52
1:B:34:SER:HB3	1:B:36:TRP:HD1	1.73	0.52
1:B:295:GLN:O	1:B:297:TYR:N	2.42	0.52
1:G:138:ALA:O	1:G:246:LEU:HD12	2.09	0.52
1:H:92:MET:HE1	1:H:106:ILE:HD11	1.92	0.52
1:I:197:PHE:N	1:I:197:PHE:CD1	2.73	0.52
1:K:128:ASN:C	1:K:130:THR:H	2.17	0.52
1:C:289:LEU:O	1:C:292:ARG:HG3	2.10	0.52
1:F:167:MET:HE2	1:F:197:PHE:CZ	2.44	0.52
1:F:181:LEU:O	1:F:182:LYS:CB	2.57	0.52
1:G:252:ALA:HB1	1:G:253:PRO:HD2	1.91	0.52
1:G:265:ALA:O	1:G:266:ARG:C	2.50	0.52
1:J:98:LEU:HB3	1:J:175:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:140:HIS:ND1	1:J:142:ASP:OD1	2.39	0.52
1:D:152:ARG:O	1:D:332:MET:HE3	2.09	0.52
1:E:88:ARG:HG3	1:E:123:ILE:HD11	1.91	0.52
1:E:281:LEU:CB	1:E:283:LEU:HD12	2.39	0.52
1:H:65:MET:HA	1:H:69:ASP:OD2	2.10	0.52
1:H:300:GLY:HA3	1:I:300:GLY:HA3	1.91	0.52
1:I:157:ALA:O	1:I:162:VAL:HG23	2.10	0.52
1:J:331:THR:C	1:J:333:ASP:N	2.67	0.52
1:E:127:LEU:O	1:E:128:ASN:HB2	2.08	0.52
1:G:88:ARG:O	1:G:92:MET:HG3	2.09	0.52
1:G:158:THR:O	1:G:249:LEU:HA	2.09	0.52
1:A:231:GLY:O	1:A:232:ALA:C	2.53	0.52
1:F:35:ALA:O	1:F:36:TRP:C	2.51	0.52
1:G:70:LEU:O	1:G:74:LEU:HD12	2.09	0.52
1:I:49:ASN:OD1	1:I:51:SER:N	2.43	0.52
1:I:140:HIS:HE2	1:I:160:SER:HG	1.58	0.52
1:J:153:VAL:O	1:J:155:VAL:HG13	2.09	0.52
1:G:295:GLN:O	1:G:297:TYR:N	2.43	0.52
1:J:40:LYS:HB2	1:J:242:ASP:OD1	2.09	0.52
1:J:128:ASN:H	1:J:129:PRO:CD	2.23	0.52
1:L:47:ILE:HD11	1:L:270:ARG:NH2	2.25	0.52
1:B:136:VAL:HG21	1:B:241:MET:HE3	1.91	0.52
1:D:112:GLN:HG3	1:D:113:THR:N	2.25	0.52
1:F:181:LEU:O	1:F:182:LYS:CG	2.58	0.52
1:B:169:GLU:HA	1:B:169:GLU:OE1	2.10	0.52
1:B:199:ASP:OD1	1:B:200:GLY:N	2.42	0.52
1:G:340:ASP:O	1:G:341:GLU:C	2.53	0.52
1:H:71:GLN:N	1:H:72:PRO:CD	2.73	0.52
1:H:283:LEU:HD12	1:H:283:LEU:N	2.24	0.52
1:J:102:TRP:CE3	1:J:127:LEU:HG	2.44	0.52
1:K:249:LEU:HB2	1:K:322:PRO:HD2	1.91	0.52
1:L:132:LYS:HG3	1:L:190:ASP:OD2	2.10	0.52
1:B:256:THR:OG1	1:B:323:SER:O	2.28	0.51
1:F:206:HIS:O	1:F:207:TRP:C	2.53	0.51
1:G:92:MET:O	1:G:93:GLN:C	2.51	0.51
1:K:248:ASP:OD2	3:K:402:A1D48:N17	2.42	0.51
1:G:140:HIS:O	1:G:140:HIS:CG	2.61	0.51
1:G:227:PRO:HA	1:G:235:THR:O	2.10	0.51
1:I:247:LEU:CD2	1:I:320:LEU:HD12	2.41	0.51
1:K:77:ARG:O	1:K:77:ARG:HG3	2.10	0.51
1:A:229:PRO:O	1:A:230:PRO:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:O	1:A:331:THR:OG1	2.26	0.51
1:D:47:ILE:HG12	1:D:48:LEU:N	2.24	0.51
1:D:231:GLY:O	1:D:232:ALA:C	2.53	0.51
1:G:57:ALA:HA	1:G:349:LYS:HZ3	1.75	0.51
1:G:78:TYR:O	1:G:81:SER:OG	2.22	0.51
1:J:102:TRP:CZ3	1:J:127:LEU:HD12	2.46	0.51
1:D:95:ILE:O	1:D:97:ARG:N	2.44	0.51
1:H:305:ASP:CG	1:H:306:ASP:H	2.19	0.51
1:J:342:SER:O	1:J:346:ASN:HB2	2.10	0.51
1:G:47:ILE:HB	1:G:357:GLU:OE2	2.10	0.51
1:G:57:ALA:N	1:G:349:LYS:HE2	2.26	0.51
1:H:212:SER:O	1:H:217:ARG:NH1	2.44	0.51
1:J:62:ILE:O	1:J:66:TRP:HB2	2.10	0.51
1:J:223:MET:HB2	1:J:238:LEU:HD21	1.93	0.51
1:J:255:PRO:HD2	1:J:293:TYR:CD1	2.45	0.51
1:I:146:PHE:C	1:I:147:SER:O	2.53	0.51
1:I:359:LEU:O	1:I:360:HIS:HB2	2.09	0.51
1:J:109:PHE:CE1	1:J:120:PHE:HB2	2.46	0.51
1:L:253:PRO:O	1:L:254:ASN:HB2	2.10	0.51
1:H:36:TRP:CG	1:H:37:PRO:HD3	2.46	0.51
1:L:291:GLY:O	1:L:292:ARG:C	2.54	0.51
1:B:68:ASN:HB2	1:B:94:ARG:NH1	2.26	0.51
1:I:308:ILE:O	1:I:309:PRO:C	2.53	0.51
1:J:36:TRP:HH2	1:J:132:LYS:O	1.94	0.51
1:J:48:LEU:HD13	1:J:52:ALA:HB1	1.93	0.51
1:A:68:ASN:CB	1:A:94:ARG:HH12	2.24	0.51
1:I:276:HIS:O	1:I:279:HIS:N	2.44	0.51
1:J:69:ASP:OD2	1:J:168:LEU:HB3	2.10	0.51
1:J:92:MET:O	1:J:93:GLN:C	2.53	0.51
1:L:181:LEU:HD23	1:L:181:LEU:N	2.25	0.51
1:E:120:PHE:O	1:E:121:SER:OG	2.23	0.50
1:G:57:ALA:HA	1:G:349:LYS:NZ	2.26	0.50
1:H:94:ARG:HH21	1:H:97:ARG:NH1	2.09	0.50
1:I:170:LEU:HD21	1:I:174:LEU:HD12	1.93	0.50
1:J:268:PHE:O	1:J:269:GLU:C	2.54	0.50
1:K:149:TRP:O	1:K:152:ARG:N	2.32	0.50
1:E:120:PHE:C	1:E:121:SER:HG	2.15	0.50
1:F:70:LEU:HG	1:F:70:LEU:O	2.11	0.50
1:H:174:LEU:O	1:H:175:ASP:C	2.52	0.50
1:K:201:GLU:HG3	1:K:306:ASP:OD2	2.11	0.50
1:C:93:GLN:O	1:C:96:GLN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:GLN:O	1:D:305:ASP:HB2	2.10	0.50
1:F:40:LYS:CB	1:F:242:ASP:OD1	2.58	0.50
1:F:328:VAL:O	1:F:329:TRP:O	2.29	0.50
1:G:152:ARG:O	1:G:332:MET:HE3	2.12	0.50
1:G:348:ASN:O	1:G:352:GLN:HG3	2.10	0.50
1:H:172:ARG:O	1:H:173:ALA:C	2.54	0.50
1:I:49:ASN:OD1	1:I:49:ASN:C	2.53	0.50
1:K:49:ASN:O	1:K:50:SER:C	2.55	0.50
1:B:353:VAL:O	1:B:354:PHE:C	2.52	0.50
1:C:92:MET:HE2	1:C:106:ILE:CD1	2.32	0.50
1:C:353:VAL:O	1:C:357:GLU:HG3	2.12	0.50
1:G:229:PRO:HB2	1:G:230:PRO:HD2	1.94	0.50
1:I:36:TRP:CD1	1:I:37:PRO:HD3	2.46	0.50
1:J:132:LYS:NZ	1:J:190:ASP:HB3	2.27	0.50
1:L:105:GLU:C	1:L:106:ILE:HD13	2.37	0.50
1:C:219:LEU:O	1:C:220:ALA:C	2.53	0.50
1:F:76:GLU:O	1:F:83:GLY:HA3	2.12	0.50
1:G:141:TYR:O	1:G:141:TYR:CD1	2.65	0.50
1:K:138:ALA:HA	1:K:167:MET:HE1	1.93	0.50
1:C:155:VAL:O	1:C:155:VAL:HG23	2.10	0.50
1:D:295:GLN:O	1:D:297:TYR:N	2.40	0.50
1:I:348:ASN:O	1:I:352:GLN:HG3	2.11	0.50
1:J:41:ASN:O	1:J:42:TYR:CD1	2.64	0.50
1:J:127:LEU:O	1:J:128:ASN:HB2	2.12	0.50
1:J:268:PHE:O	1:J:271:LEU:N	2.37	0.50
1:K:254:ASN:N	1:K:255:PRO:CD	2.75	0.50
1:L:305:ASP:C	1:L:307:HIS:H	2.17	0.50
1:B:80:GLY:O	1:B:81:SER:O	2.30	0.50
1:B:278:LEU:O	1:B:283:LEU:HD12	2.12	0.50
1:G:263:ASN:H	1:G:263:ASN:ND2	2.09	0.50
1:J:160:SER:O	1:J:163:PRO:HD2	2.11	0.50
1:C:35:ALA:C	1:C:37:PRO:CD	2.85	0.50
1:C:40:LYS:CB	1:C:242:ASP:OD1	2.55	0.50
1:E:299:TYR:CD2	1:E:301:GLY:O	2.64	0.50
1:F:337:GLU:CD	1:F:337:GLU:H	2.18	0.50
1:G:128:ASN:OD1	1:G:128:ASN:N	2.45	0.50
1:I:331:THR:HB	1:I:333:ASP:H	1.77	0.50
1:K:212:SER:O	1:K:214:TYR:N	2.45	0.50
1:L:140:HIS:O	1:L:140:HIS:CG	2.65	0.50
1:B:78:TYR:HB2	1:B:79:PRO:CD	2.42	0.50
1:C:221:ALA:O	1:C:222:LYS:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:GLN:O	1:C:297:TYR:N	2.45	0.50
1:F:85:TYR:HD1	1:F:88:ARG:HH12	1.59	0.50
1:J:85:TYR:O	1:J:86:ALA:C	2.54	0.50
1:J:274:ILE:HG22	1:J:350:ILE:HG22	1.93	0.50
1:D:47:ILE:CG1	1:D:48:LEU:N	2.74	0.49
1:F:252:ALA:HB1	1:F:253:PRO:HD2	1.94	0.49
1:K:90:HIS:CE1	1:K:94:ARG:HG3	2.47	0.49
1:C:169:GLU:HG3	1:C:169:GLU:O	2.13	0.49
1:D:278:LEU:HB3	1:D:284:LEU:HD13	1.92	0.49
1:H:252:ALA:HB1	1:H:253:PRO:HD2	1.95	0.49
1:I:65:MET:O	1:I:65:MET:HG2	2.11	0.49
1:K:71:GLN:HA	1:K:74:LEU:HD13	1.94	0.49
1:A:199:ASP:OD1	1:A:200:GLY:N	2.45	0.49
1:C:35:ALA:C	1:C:37:PRO:HD2	2.37	0.49
1:F:329:TRP:CG	1:F:330:HIS:H	2.31	0.49
1:L:47:ILE:CD1	1:L:270:ARG:CZ	2.88	0.49
1:F:71:GLN:N	1:F:72:PRO:CD	2.76	0.49
1:J:135:LEU:HD23	1:J:359:LEU:HD21	1.95	0.49
1:J:347:LEU:CA	1:J:350:ILE:HD11	2.43	0.49
1:L:71:GLN:N	1:L:72:PRO:HD2	2.28	0.49
1:L:159:ASP:OD1	3:L:402:A1D48:C18	2.61	0.49
1:A:309:PRO:O	1:A:313:ARG:HD2	2.12	0.49
1:C:71:GLN:N	1:C:72:PRO:HD2	2.28	0.49
1:E:175:ASP:O	1:E:177:LYS:N	2.46	0.49
1:F:140:HIS:CE1	1:F:142:ASP:O	2.65	0.49
1:F:181:LEU:O	1:F:182:LYS:HG2	2.13	0.49
1:G:47:ILE:HG13	1:G:48:LEU:N	2.23	0.49
1:G:169:GLU:O	1:G:170:LEU:C	2.56	0.49
1:H:49:ASN:OD1	1:H:52:ALA:N	2.41	0.49
1:H:162:VAL:O	1:H:165:ALA:HB3	2.13	0.49
1:I:228:HIS:HB3	1:I:236:SER:O	2.13	0.49
1:J:154:PHE:C	1:J:155:VAL:HG13	2.38	0.49
1:K:57:ALA:CB	1:K:283:LEU:HD22	2.43	0.49
1:K:192:SER:OG	1:K:193:LEU:N	2.46	0.49
1:D:310:PHE:O	1:D:311:LEU:C	2.53	0.49
1:G:39:GLU:C	1:G:133:ARG:NH2	2.70	0.49
1:J:328:VAL:HG11	1:J:333:ASP:C	2.38	0.49
1:A:38:GLU:C	1:A:40:LYS:H	2.21	0.49
1:E:99:GLN:HB3	1:E:179:LEU:HD11	1.95	0.49
1:E:149:TRP:O	1:E:152:ARG:N	2.30	0.49
1:J:72:PRO:HG2	1:J:90:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:36:TRP:CD1	1:K:37:PRO:HD3	2.47	0.49
1:B:68:ASN:CB	1:B:94:ARG:NH1	2.75	0.49
1:A:71:GLN:N	1:A:72:PRO:CD	2.75	0.49
1:A:174:LEU:HD22	1:A:356:LEU:HD11	1.94	0.49
1:A:212:SER:O	1:A:213:LEU:C	2.55	0.49
1:D:179:LEU:C	1:D:181:LEU:H	2.21	0.49
1:E:106:ILE:HG22	1:E:107:ASP:N	2.28	0.49
1:E:348:ASN:O	1:E:349:LYS:C	2.56	0.49
1:G:328:VAL:HG13	1:G:333:ASP:HB2	1.95	0.49
1:H:160:SER:C	1:H:163:PRO:HD2	2.38	0.49
1:J:50:SER:O	1:J:51:SER:C	2.54	0.49
1:L:36:TRP:CG	1:L:37:PRO:HD3	2.48	0.49
1:L:126:THR:HG23	1:L:194:GLN:HB2	1.95	0.49
1:B:283:LEU:HD12	1:B:283:LEU:N	2.28	0.49
1:J:321:ILE:HG13	1:J:322:PRO:HD2	1.95	0.49
1:B:112:GLN:HG3	1:B:113:THR:N	2.27	0.49
1:C:36:TRP:CD1	1:C:37:PRO:HD3	2.47	0.49
1:E:344:ILE:O	1:E:345:ASP:C	2.54	0.49
1:F:308:ILE:HB	1:F:309:PRO:HD3	1.94	0.49
1:G:36:TRP:CG	1:G:37:PRO:HD3	2.48	0.49
1:G:71:GLN:N	1:G:72:PRO:CD	2.75	0.49
1:B:100:ALA:HA	1:B:179:LEU:HD12	1.95	0.48
1:A:90:HIS:CE1	1:A:94:ARG:HG3	2.48	0.48
1:A:268:PHE:O	1:A:268:PHE:CD1	2.66	0.48
1:C:203:ALA:HA	1:C:211:ASP:O	2.13	0.48
1:H:346:ASN:O	1:H:347:LEU:C	2.56	0.48
1:K:335:ASN:C	1:K:335:ASN:OD1	2.55	0.48
1:B:52:ALA:O	1:B:53:LEU:C	2.55	0.48
1:B:148:HIS:ND1	1:B:148:HIS:N	2.60	0.48
1:C:60:THR:OG1	1:C:169:GLU:OE2	2.29	0.48
1:D:112:GLN:OE1	1:D:116:GLY:HA2	2.13	0.48
1:D:286:ASP:OD2	1:E:340:ASP:OD1	2.31	0.48
1:E:302:VAL:HG22	1:E:303:ILE:O	2.13	0.48
1:G:174:LEU:O	1:G:175:ASP:C	2.54	0.48
1:G:236:SER:O	1:G:239:HIS:N	2.44	0.48
1:G:325:PHE:O	1:G:326:PRO:O	2.30	0.48
1:I:144:LYS:HG2	1:I:146:PHE:CE2	2.48	0.48
1:J:39:GLU:HG2	1:J:133:ARG:NH2	2.28	0.48
1:J:71:GLN:N	1:J:72:PRO:CD	2.75	0.48
1:J:127:LEU:O	1:J:192:SER:OG	2.09	0.48
1:J:274:ILE:HD11	1:J:357:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:353:VAL:O	1:K:357:GLU:HG3	2.12	0.48
1:L:181:LEU:O	1:L:182:LYS:C	2.56	0.48
1:C:88:ARG:HG2	1:C:92:MET:HE3	1.95	0.48
1:I:246:LEU:HD21	1:I:305:ASP:OD2	2.13	0.48
1:J:272:GLN:HG2	1:J:294:PHE:O	2.13	0.48
1:L:160:SER:O	1:L:163:PRO:N	2.45	0.48
1:B:176:LYS:HA	1:B:179:LEU:HD22	1.94	0.48
1:G:78:TYR:CE1	1:G:81:SER:HB3	2.47	0.48
1:G:136:VAL:HG22	1:G:194:GLN:HB3	1.95	0.48
1:G:178:LEU:O	1:G:181:LEU:HG	2.13	0.48
1:J:154:PHE:O	1:J:155:VAL:CG1	2.61	0.48
1:L:127:LEU:O	1:L:128:ASN:C	2.56	0.48
1:A:283:LEU:N	1:A:283:LEU:HD12	2.28	0.48
1:G:265:ALA:O	1:G:268:PHE:N	2.47	0.48
1:L:149:TRP:CE3	1:L:150:ASN:HB2	2.48	0.48
1:L:157:ALA:O	1:L:161:ALA:C	2.56	0.48
1:D:231:GLY:O	1:D:232:ALA:O	2.31	0.48
1:G:102:TRP:CE3	1:G:125:SER:OG	2.65	0.48
1:G:155:VAL:O	1:G:156:GLY:O	2.32	0.48
1:I:259:ASN:ND2	1:I:268:PHE:HB3	2.29	0.48
1:D:84:SER:O	1:D:88:ARG:HB2	2.13	0.48
1:D:124:ILE:N	1:D:124:ILE:HD12	2.28	0.48
1:F:49:ASN:OD1	1:F:49:ASN:C	2.57	0.48
1:F:285:LYS:O	1:F:286:ASP:HB2	2.14	0.48
1:G:157:ALA:HB2	1:G:334:ASP:O	2.14	0.48
1:H:103:VAL:HG12	1:H:103:VAL:O	2.13	0.48
1:J:152:ARG:HB2	1:J:332:MET:HE3	1.93	0.48
1:J:347:LEU:O	1:J:348:ASN:C	2.57	0.48
1:B:88:ARG:HG2	1:B:92:MET:HE2	1.96	0.48
1:A:62:ILE:O	1:A:62:ILE:HG13	2.12	0.48
1:H:53:LEU:HD12	1:H:278:LEU:CD2	2.42	0.48
1:J:305:ASP:C	1:J:307:HIS:H	2.22	0.48
1:J:331:THR:C	1:J:333:ASP:H	2.21	0.48
1:K:212:SER:O	1:K:213:LEU:C	2.56	0.48
1:B:197:PHE:N	1:B:197:PHE:CD1	2.81	0.48
1:A:64:GLU:O	1:A:67:GLN:N	2.47	0.48
1:C:88:ARG:O	1:C:92:MET:HG3	2.14	0.48
1:C:158:THR:C	1:C:160:SER:HA	2.39	0.48
1:F:76:GLU:HG3	1:F:153:VAL:CG1	2.43	0.48
1:I:94:ARG:HH21	1:I:97:ARG:NH1	2.12	0.48
1:J:65:MET:SD	1:J:348:ASN:ND2	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:VAL:O	1:D:156:GLY:C	2.53	0.48
1:L:39:GLU:O	1:L:41:ASN:N	2.47	0.48
1:C:223:MET:HE2	1:C:238:LEU:HD23	1.96	0.47
1:D:36:TRP:CG	1:D:37:PRO:HD3	2.49	0.47
1:G:54:ARG:HH21	1:G:281:LEU:HD21	1.79	0.47
1:G:283:LEU:C	1:G:284:LEU:HD13	2.39	0.47
1:H:46:ALA:O	1:H:47:ILE:O	2.31	0.47
1:H:49:ASN:O	1:H:52:ALA:N	2.46	0.47
1:H:99:GLN:O	1:H:100:ALA:O	2.32	0.47
1:I:292:ARG:HG3	1:I:292:ARG:HH11	1.79	0.47
1:J:168:LEU:O	1:J:171:ALA:HB3	2.14	0.47
1:J:279:HIS:CD2	1:J:287:HIS:O	2.65	0.47
1:J:347:LEU:HA	1:J:350:ILE:CD1	2.44	0.47
1:B:133:ARG:HB2	1:B:190:ASP:O	2.13	0.47
1:I:170:LEU:C	1:I:170:LEU:HD23	2.38	0.47
1:J:35:ALA:C	1:J:37:PRO:CD	2.87	0.47
1:J:39:GLU:CB	1:J:133:ARG:NH2	2.77	0.47
1:J:61:SER:O	1:J:62:ILE:C	2.56	0.47
1:J:170:LEU:HD11	1:J:355:VAL:HG21	1.96	0.47
1:J:248:ASP:O	1:J:249:LEU:HB2	2.14	0.47
1:K:77:ARG:HG2	1:K:143:SER:HB3	1.96	0.47
1:L:281:LEU:HB2	1:L:283:LEU:HD11	1.95	0.47
1:G:60:THR:HG22	1:G:349:LYS:NZ	2.29	0.47
1:G:71:GLN:N	1:G:72:PRO:HD2	2.30	0.47
1:G:340:ASP:C	1:G:342:SER:N	2.72	0.47
1:H:92:MET:HB3	1:H:104:LEU:HD13	1.96	0.47
1:I:201:GLU:HG3	1:I:306:ASP:OD2	2.14	0.47
1:L:172:ARG:O	1:L:173:ALA:C	2.54	0.47
1:B:169:GLU:OE1	1:B:169:GLU:CA	2.63	0.47
1:A:277:GLU:C	1:A:279:HIS:N	2.71	0.47
1:I:51:SER:O	1:I:54:ARG:N	2.46	0.47
1:J:47:ILE:HA	1:J:357:GLU:OE2	2.14	0.47
1:K:49:ASN:OD1	1:K:49:ASN:C	2.56	0.47
1:B:68:ASN:HB2	1:B:94:ARG:HH12	1.79	0.47
1:D:36:TRP:CD1	1:D:37:PRO:HD3	2.50	0.47
1:E:102:TRP:CZ3	1:E:127:LEU:HG	2.49	0.47
1:G:359:LEU:O	1:G:360:HIS:C	2.57	0.47
1:H:50:SER:HB2	1:H:281:LEU:HD11	1.97	0.47
1:H:71:GLN:N	1:H:72:PRO:HD2	2.29	0.47
1:H:336:GLU:O	1:H:337:GLU:C	2.58	0.47
1:I:103:VAL:O	1:I:103:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:141:TYR:CD2	1:J:197:PHE:O	2.66	0.47
1:J:161:ALA:O	1:J:162:VAL:C	2.55	0.47
1:L:74:LEU:HD21	1:L:161:ALA:HB1	1.95	0.47
1:L:132:LYS:HA	1:L:228:HIS:NE2	2.30	0.47
1:L:360:HIS:O	1:L:361:LEU:HD23	2.14	0.47
1:B:211:ASP:OD1	1:B:214:TYR:OH	2.25	0.47
1:C:158:THR:O	1:C:160:SER:HA	2.15	0.47
1:F:71:GLN:NE2	1:F:336:GLU:OE2	2.47	0.47
1:F:128:ASN:N	1:F:129:PRO:CD	2.77	0.47
1:I:305:ASP:C	1:I:307:HIS:H	2.22	0.47
1:B:60:THR:HG23	1:B:60:THR:O	2.14	0.47
1:B:77:ARG:HG3	1:B:143:SER:HB3	1.96	0.47
1:A:77:ARG:CG	1:A:143:SER:HB3	2.45	0.47
1:A:268:PHE:CD1	1:A:268:PHE:C	2.92	0.47
1:A:311:LEU:O	1:A:313:ARG:N	2.48	0.47
1:D:108:THR:HG22	1:D:109:PHE:N	2.29	0.47
1:D:112:GLN:HG3	1:D:113:THR:H	1.79	0.47
1:D:228:HIS:O	1:D:235:THR:OG1	2.31	0.47
1:D:289:LEU:O	1:D:292:ARG:HG3	2.15	0.47
1:E:160:SER:O	1:E:163:PRO:HD2	2.15	0.47
1:E:276:HIS:O	1:E:279:HIS:HB3	2.15	0.47
1:H:62:ILE:HB	1:H:345:ASP:CB	2.45	0.47
1:H:345:ASP:O	1:H:348:ASN:HB2	2.14	0.47
1:I:148:HIS:NE2	1:I:153:VAL:HG22	2.30	0.47
1:I:323:SER:CA	1:I:324:PRO:O	2.63	0.47
1:J:35:ALA:O	1:J:37:PRO:N	2.47	0.47
1:J:39:GLU:CA	1:J:133:ARG:HH22	2.28	0.47
1:J:78:TYR:O	1:J:79:PRO:C	2.58	0.47
1:C:229:PRO:C	1:C:230:PRO:O	2.58	0.47
1:D:180:SER:O	1:D:181:LEU:HD23	2.14	0.47
1:G:111:SER:OG	1:G:112:GLN:N	2.46	0.47
1:H:54:ARG:HA	1:H:283:LEU:CD2	2.45	0.47
1:H:92:MET:HE3	1:H:106:ILE:HD11	1.97	0.47
1:H:278:LEU:HB3	1:H:284:LEU:HD13	1.97	0.47
1:I:134:HIS:HA	1:I:192:SER:O	2.14	0.47
1:I:275:GLU:OE2	1:I:293:TYR:N	2.33	0.47
1:K:162:VAL:O	1:K:166:MET:HG3	2.14	0.47
1:K:205:LEU:O	1:K:206:HIS:CG	2.68	0.47
1:L:265:ALA:O	1:L:266:ARG:C	2.54	0.47
1:E:205:LEU:HG	1:E:206:HIS:HB2	1.97	0.47
1:I:178:LEU:C	1:I:180:SER:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:LEU:C	1:I:180:SER:N	2.73	0.47
1:I:284:LEU:HD23	1:I:287:HIS:CE1	2.49	0.47
1:J:265:ALA:O	1:J:267:TRP:N	2.48	0.47
1:K:127:LEU:O	1:K:128:ASN:HB2	2.15	0.47
1:K:308:ILE:HB	1:K:309:PRO:HD3	1.95	0.47
1:C:100:ALA:HA	1:C:179:LEU:CD1	2.45	0.47
1:D:205:LEU:C	1:D:205:LEU:HD12	2.40	0.47
1:G:283:LEU:HD12	1:G:283:LEU:H	1.80	0.47
1:J:101:ASP:C	1:J:127:LEU:HD21	2.40	0.47
1:J:280:GLU:O	1:J:280:GLU:HG3	2.15	0.47
1:J:345:ASP:O	1:J:349:LYS:HG3	2.15	0.47
1:B:219:LEU:O	1:B:220:ALA:C	2.57	0.46
1:D:219:LEU:O	1:D:220:ALA:C	2.54	0.46
1:F:38:GLU:OE2	1:H:147:SER:OG	2.33	0.46
1:J:48:LEU:HD13	1:J:52:ALA:CB	2.45	0.46
1:J:164:CYS:O	1:J:165:ALA:C	2.57	0.46
1:J:279:HIS:C	1:J:281:LEU:N	2.71	0.46
1:J:328:VAL:O	1:J:329:TRP:C	2.57	0.46
1:B:226:THR:O	1:B:227:PRO:C	2.56	0.46
1:A:56:ILE:C	1:A:58:GLU:N	2.72	0.46
1:G:181:LEU:HD23	1:G:181:LEU:N	2.29	0.46
1:I:178:LEU:O	1:I:180:SER:N	2.49	0.46
1:J:89:GLN:O	1:J:90:HIS:C	2.58	0.46
1:J:106:ILE:CG2	1:J:107:ASP:N	2.77	0.46
1:J:201:GLU:OE1	1:J:202:GLU:HG2	2.15	0.46
1:K:128:ASN:H	1:K:129:PRO:HD3	1.80	0.46
1:K:211:ASP:O	1:K:212:SER:HB3	2.13	0.46
1:L:71:GLN:N	1:L:72:PRO:CD	2.77	0.46
1:L:278:LEU:HB3	1:L:284:LEU:CD1	2.44	0.46
1:D:169:GLU:OE2	1:D:172:ARG:NH2	2.46	0.46
1:F:36:TRP:CD1	1:F:37:PRO:HD3	2.51	0.46
1:J:70:LEU:C	1:J:72:PRO:HD2	2.41	0.46
1:L:49:ASN:OD1	1:L:49:ASN:C	2.58	0.46
1:L:107:ASP:OD1	1:L:107:ASP:C	2.56	0.46
1:L:199:ASP:OD1	1:L:200:GLY:N	2.41	0.46
1:L:199:ASP:O	1:L:200:GLY:C	2.57	0.46
1:C:191:LEU:HD13	1:C:242:ASP:OD2	2.15	0.46
1:D:199:ASP:OD1	1:D:200:GLY:N	2.49	0.46
1:G:66:TRP:O	1:G:71:GLN:HG3	2.16	0.46
1:H:70:LEU:O	1:H:74:LEU:HD12	2.15	0.46
1:H:78:TYR:HB2	1:H:79:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:256:THR:OG1	1:I:323:SER:O	2.24	0.46
1:J:37:PRO:O	1:J:133:ARG:NH1	2.48	0.46
1:K:67:GLN:HG2	1:K:68:ASN:OD1	2.16	0.46
1:L:281:LEU:CB	1:L:283:LEU:HD11	2.45	0.46
1:B:211:ASP:HA	1:B:214:TYR:OH	2.15	0.46
1:B:252:ALA:HB1	1:B:253:PRO:HD2	1.97	0.46
1:B:270:ARG:O	1:B:274:ILE:HG13	2.15	0.46
1:D:182:LYS:HD3	1:D:182:LYS:N	2.30	0.46
1:F:256:THR:O	1:F:256:THR:OG1	2.26	0.46
1:I:201:GLU:HG3	1:I:306:ASP:CG	2.41	0.46
1:J:40:LYS:HB3	1:J:242:ASP:OD1	2.16	0.46
1:J:54:ARG:O	1:J:55:GLN:C	2.57	0.46
1:L:149:TRP:O	1:L:152:ARG:HG3	2.16	0.46
1:A:250:ILE:HG22	1:A:251:GLY:N	2.30	0.46
1:D:223:MET:HB3	1:D:238:LEU:HD23	1.97	0.46
1:F:36:TRP:HD1	1:L:280:GLU:HG3	1.80	0.46
1:G:213:LEU:O	1:G:214:TYR:C	2.55	0.46
1:G:281:LEU:CB	1:G:283:LEU:HD11	2.44	0.46
1:J:70:LEU:O	1:J:71:GLN:C	2.57	0.46
1:J:152:ARG:O	1:J:332:MET:HE1	2.15	0.46
1:J:284:LEU:HG	1:J:346:ASN:OD1	2.15	0.46
1:K:127:LEU:O	1:K:128:ASN:CB	2.63	0.46
1:L:274:ILE:HD13	1:L:353:VAL:HG12	1.98	0.46
1:C:305:ASP:C	1:C:307:HIS:H	2.23	0.46
1:F:249:LEU:HD12	1:F:321:ILE:HD11	1.97	0.46
1:G:85:TYR:O	1:G:89:GLN:HB2	2.15	0.46
1:G:149:TRP:HZ3	1:G:152:ARG:CD	2.28	0.46
1:G:191:LEU:HD13	1:G:242:ASP:OD2	2.15	0.46
1:I:248:ASP:OD1	1:I:249:LEU:N	2.49	0.46
1:I:277:GLU:O	1:I:277:GLU:HG3	2.15	0.46
1:J:70:LEU:HB2	1:J:165:ALA:HB2	1.96	0.46
1:K:78:TYR:HB2	1:K:79:PRO:CD	2.46	0.46
1:L:68:ASN:HB3	1:L:94:ARG:HH12	1.80	0.46
1:A:133:ARG:CZ	1:A:242:ASP:CG	2.89	0.46
1:D:49:ASN:O	1:D:50:SER:C	2.57	0.46
1:G:285:LYS:C	1:G:287:HIS:N	2.70	0.46
1:H:62:ILE:HB	1:H:345:ASP:HB2	1.97	0.46
1:I:71:GLN:HA	1:I:74:LEU:HD12	1.98	0.46
1:J:136:VAL:HG21	1:J:241:MET:HE3	1.98	0.46
1:J:177:LYS:O	1:J:361:LEU:HD13	2.16	0.46
1:J:178:LEU:O	1:J:179:LEU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:279:HIS:C	1:J:281:LEU:H	2.24	0.46
1:C:35:ALA:O	1:C:36:TRP:C	2.57	0.46
1:F:85:TYR:HD1	1:F:88:ARG:NH1	2.14	0.46
1:F:128:ASN:O	1:F:129:PRO:C	2.58	0.46
1:G:48:LEU:HB2	1:G:53:LEU:CD2	2.46	0.46
1:H:162:VAL:HB	1:H:163:PRO:CD	2.43	0.46
1:I:108:THR:HG22	1:I:109:PHE:N	2.31	0.46
1:I:159:ASP:HA	1:I:160:SER:OG	2.16	0.46
1:I:162:VAL:O	1:I:166:MET:HG3	2.16	0.46
1:J:163:PRO:HB3	1:J:247:LEU:HB2	1.97	0.46
1:L:334:ASP:C	1:L:334:ASP:OD1	2.57	0.46
1:A:105:GLU:C	1:A:106:ILE:HG12	2.40	0.46
1:C:137:LEU:HD12	1:C:245:VAL:HB	1.98	0.46
1:E:120:PHE:C	1:E:121:SER:OG	2.57	0.46
1:H:102:TRP:CE3	1:H:127:LEU:HG	2.51	0.46
1:H:304:GLN:HA	1:H:304:GLN:OE1	2.16	0.46
1:I:49:ASN:O	1:I:50:SER:C	2.59	0.46
1:I:302:VAL:HG22	1:I:303:ILE:N	2.31	0.46
1:J:283:LEU:O	1:J:349:LYS:NZ	2.49	0.46
1:J:336:GLU:HA	1:J:339:LEU:CD1	2.46	0.46
1:K:172:ARG:HG2	1:K:172:ARG:NH1	2.31	0.46
1:L:223:MET:C	1:L:225:SER:H	2.24	0.46
1:A:127:LEU:O	1:A:128:ASN:HB2	2.16	0.45
1:D:49:ASN:O	1:D:52:ALA:N	2.45	0.45
1:E:149:TRP:O	1:E:151:ASN:N	2.49	0.45
1:G:94:ARG:HH21	1:G:97:ARG:NH1	2.14	0.45
1:G:149:TRP:O	1:G:152:ARG:N	2.40	0.45
1:H:66:TRP:O	1:H:66:TRP:CD1	2.70	0.45
1:J:151:ASN:O	1:J:151:ASN:CG	2.56	0.45
1:K:299:TYR:HD2	1:K:301:GLY:O	1.99	0.45
1:L:304:GLN:O	1:L:305:ASP:HB2	2.15	0.45
1:D:95:ILE:C	1:D:97:ARG:N	2.72	0.45
1:E:157:ALA:O	1:E:162:VAL:HG23	2.17	0.45
1:F:223:MET:HG2	1:F:237:GLN:OE1	2.15	0.45
1:G:165:ALA:O	1:G:166:MET:C	2.60	0.45
1:G:229:PRO:O	1:G:230:PRO:C	2.57	0.45
1:H:272:GLN:O	1:H:275:GLU:N	2.49	0.45
1:H:303:ILE:O	1:H:307:HIS:HE1	1.99	0.45
1:I:254:ASN:N	1:I:255:PRO:HD3	2.32	0.45
1:J:101:ASP:O	1:J:127:LEU:CD2	2.63	0.45
1:B:279:HIS:CD2	1:B:289:LEU:HG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:C	1:A:170:LEU:HD23	2.41	0.45
1:G:90:HIS:O	1:G:91:ILE:C	2.58	0.45
1:G:92:MET:O	1:G:96:GLN:N	2.47	0.45
1:G:109:PHE:HZ	1:G:215:GLY:HA2	1.81	0.45
1:G:166:MET:HG2	1:G:348:ASN:OD1	2.17	0.45
1:H:36:TRP:N	1:H:37:PRO:CD	2.79	0.45
1:K:133:ARG:NH2	1:K:242:ASP:CG	2.67	0.45
1:G:259:ASN:OD1	1:G:268:PHE:CB	2.65	0.45
1:G:359:LEU:O	1:G:361:LEU:HG	2.17	0.45
1:H:78:TYR:CD1	1:H:78:TYR:C	2.95	0.45
1:H:138:ALA:N	1:H:245:VAL:O	2.49	0.45
1:J:201:GLU:HG3	1:J:306:ASP:OD2	2.17	0.45
1:K:158:THR:O	1:K:160:SER:HA	2.15	0.45
1:L:40:LYS:HB3	1:L:242:ASP:OD1	2.16	0.45
1:L:68:ASN:CB	1:L:94:ARG:HH12	2.29	0.45
1:L:149:TRP:O	1:L:152:ARG:HB2	2.17	0.45
1:L:254:ASN:N	1:L:255:PRO:CD	2.80	0.45
1:B:36:TRP:H	1:B:37:PRO:HD2	1.81	0.45
1:B:228:HIS:HA	1:B:229:PRO:C	2.40	0.45
1:D:65:MET:O	1:D:66:TRP:C	2.59	0.45
1:F:66:TRP:O	1:F:71:GLN:HB2	2.16	0.45
1:F:105:GLU:O	1:F:106:ILE:HD13	2.17	0.45
1:F:175:ASP:O	1:F:176:LYS:C	2.60	0.45
1:I:76:GLU:O	1:I:83:GLY:HA3	2.17	0.45
1:I:207:TRP:CD1	1:I:207:TRP:C	2.94	0.45
1:I:249:LEU:HD12	1:I:321:ILE:HD11	1.97	0.45
1:K:40:LYS:HB3	1:K:242:ASP:CG	2.42	0.45
1:L:178:LEU:O	1:L:180:SER:N	2.50	0.45
1:L:263:ASN:OD1	1:L:263:ASN:N	2.50	0.45
1:B:71:GLN:NE2	1:B:336:GLU:OE2	2.49	0.45
1:B:175:ASP:O	1:B:176:LYS:C	2.57	0.45
1:B:302:VAL:HG22	1:B:303:ILE:O	2.17	0.45
1:A:307:HIS:HB2	1:A:317:VAL:HG11	1.99	0.45
1:C:92:MET:O	1:C:96:GLN:N	2.37	0.45
1:E:162:VAL:HB	1:E:163:PRO:HD3	1.98	0.45
1:E:174:LEU:HD22	1:E:356:LEU:HD11	1.97	0.45
1:G:152:ARG:O	1:G:332:MET:CE	2.65	0.45
1:H:92:MET:O	1:H:93:GLN:C	2.58	0.45
1:I:71:GLN:N	1:I:72:PRO:HD2	2.32	0.45
1:J:168:LEU:O	1:J:169:GLU:C	2.59	0.45
1:J:169:GLU:O	1:J:170:LEU:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:279:HIS:HA	4:J:501:HOH:O	2.16	0.45
1:J:355:VAL:HG12	1:J:356:LEU:N	2.31	0.45
1:L:211:ASP:O	1:L:212:SER:HB3	2.14	0.45
1:C:292:ARG:O	1:C:295:GLN:NE2	2.46	0.45
1:F:328:VAL:C	1:F:329:TRP:O	2.59	0.45
1:G:78:TYR:CE2	1:G:145:TYR:HD1	2.35	0.45
1:J:149:TRP:CE3	1:J:150:ASN:HB2	2.52	0.45
1:J:212:SER:O	1:J:213:LEU:HB2	2.17	0.45
1:B:36:TRP:HZ3	1:B:240:GLY:HA2	1.81	0.45
1:A:92:MET:SD	1:A:106:ILE:HD11	2.57	0.45
1:A:205:LEU:C	1:A:206:HIS:ND1	2.75	0.45
1:G:36:TRP:CD1	1:G:37:PRO:HD3	2.51	0.45
1:I:78:TYR:CE1	1:I:81:SER:HB3	2.51	0.45
1:I:259:ASN:ND2	1:I:268:PHE:CB	2.80	0.45
1:J:69:ASP:OD2	1:J:168:LEU:CB	2.64	0.45
1:J:114:PRO:HG2	1:J:211:ASP:OD2	2.17	0.45
1:J:127:LEU:O	1:J:128:ASN:CB	2.64	0.45
1:J:160:SER:C	1:J:163:PRO:HD2	2.41	0.45
1:J:191:LEU:HD12	1:J:242:ASP:OD2	2.17	0.45
1:J:349:LYS:O	1:J:351:LEU:N	2.50	0.45
1:J:355:VAL:O	1:J:357:GLU:N	2.50	0.45
1:K:323:SER:HA	1:K:324:PRO:C	2.41	0.45
1:D:71:GLN:N	1:D:72:PRO:HD2	2.32	0.45
1:E:211:ASP:O	1:E:212:SER:HB3	2.17	0.45
1:H:272:GLN:O	1:H:273:ALA:C	2.59	0.45
1:J:134:HIS:O	1:J:242:ASP:HB2	2.16	0.45
1:L:178:LEU:C	1:L:180:SER:N	2.72	0.45
1:L:307:HIS:O	1:L:310:PHE:N	2.42	0.45
1:A:308:ILE:O	1:A:312:ARG:HG3	2.17	0.45
1:C:276:HIS:O	1:C:279:HIS:HB3	2.17	0.45
1:F:70:LEU:HB2	1:F:165:ALA:CB	2.47	0.45
1:F:264:SER:OG	1:F:317:VAL:O	2.35	0.45
1:H:135:LEU:HD23	1:H:193:LEU:CD1	2.47	0.45
1:H:347:LEU:C	1:H:349:LYS:H	2.24	0.45
1:I:305:ASP:O	1:I:307:HIS:N	2.49	0.45
1:J:102:TRP:CE3	1:J:127:LEU:CG	3.00	0.45
1:J:296:ASN:OD1	1:J:296:ASN:N	2.49	0.45
1:K:35:ALA:C	1:K:37:PRO:CD	2.90	0.45
1:K:189:PRO:O	1:K:191:LEU:N	2.49	0.45
1:B:223:MET:HB2	1:B:238:LEU:HD21	1.99	0.44
1:B:238:LEU:O	1:B:239:HIS:C	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ILE:O	1:B:312:ARG:HG3	2.17	0.44
1:B:349:LYS:O	1:B:353:VAL:HG23	2.17	0.44
1:A:56:ILE:O	1:A:57:ALA:C	2.58	0.44
1:A:179:LEU:O	1:A:181:LEU:N	2.50	0.44
1:D:92:MET:O	1:D:93:GLN:C	2.57	0.44
1:F:128:ASN:O	1:F:130:THR:N	2.49	0.44
1:F:253:PRO:O	1:F:254:ASN:C	2.58	0.44
1:H:165:ALA:O	1:H:166:MET:C	2.59	0.44
1:I:36:TRP:HA	1:I:39:GLU:HG3	2.00	0.44
1:J:154:PHE:C	1:J:155:VAL:CG1	2.90	0.44
1:J:349:LYS:O	1:J:352:GLN:N	2.50	0.44
1:J:353:VAL:O	1:J:354:PHE:C	2.60	0.44
1:A:38:GLU:C	1:A:40:LYS:N	2.75	0.44
1:A:304:GLN:O	1:A:305:ASP:HB2	2.16	0.44
1:C:149:TRP:CE3	1:C:150:ASN:HB2	2.53	0.44
1:C:308:ILE:N	1:C:309:PRO:CD	2.80	0.44
1:D:158:THR:O	1:D:160:SER:HA	2.17	0.44
1:G:281:LEU:HB3	1:G:283:LEU:CD1	2.47	0.44
1:I:68:ASN:HB3	1:I:94:ARG:NH1	2.30	0.44
1:I:77:ARG:CG	1:I:143:SER:HB3	2.45	0.44
1:I:249:LEU:CD1	1:I:321:ILE:HD11	2.48	0.44
1:I:289:LEU:CD2	1:I:289:LEU:N	2.80	0.44
1:I:349:LYS:O	1:I:353:VAL:HG23	2.18	0.44
1:J:278:LEU:HB3	1:J:284:LEU:HD13	1.98	0.44
1:J:347:LEU:C	1:J:349:LYS:H	2.26	0.44
1:J:349:LYS:C	1:J:351:LEU:N	2.72	0.44
1:K:49:ASN:O	1:K:49:ASN:OD1	2.34	0.44
1:L:280:GLU:OE1	1:L:280:GLU:HA	2.17	0.44
1:L:345:ASP:O	1:L:349:LYS:HG3	2.17	0.44
1:C:95:ILE:CG2	1:C:104:LEU:HD21	2.47	0.44
1:E:77:ARG:CG	1:E:143:SER:HB3	2.47	0.44
1:G:301:GLY:H	1:J:300:GLY:HA3	1.82	0.44
1:I:123:ILE:HG22	1:I:124:ILE:N	2.31	0.44
1:I:159:ASP:HB2	1:I:249:LEU:HD22	1.93	0.44
1:I:255:PRO:HD2	1:I:293:TYR:CD1	2.51	0.44
1:J:35:ALA:O	1:J:37:PRO:CD	2.66	0.44
1:J:135:LEU:HD22	1:J:358:TYR:CG	2.53	0.44
1:J:297:TYR:CG	1:J:297:TYR:O	2.69	0.44
1:K:102:TRP:CE2	1:K:127:LEU:HD21	2.52	0.44
1:K:149:TRP:O	1:K:150:ASN:C	2.59	0.44
1:K:207:TRP:CZ3	1:K:212:SER:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:253:PRO:O	1:K:254:ASN:HB2	2.16	0.44
1:A:107:ASP:O	1:A:121:SER:HA	2.17	0.44
1:F:65:MET:HE1	1:F:344:ILE:HG21	1.99	0.44
1:G:36:TRP:N	1:G:37:PRO:CD	2.80	0.44
1:I:212:SER:O	1:I:213:LEU:C	2.61	0.44
1:I:308:ILE:HB	1:I:309:PRO:HD3	1.98	0.44
1:K:102:TRP:CD2	1:K:127:LEU:HD21	2.51	0.44
1:B:108:THR:HG22	1:B:109:PHE:N	2.32	0.44
1:B:162:VAL:HB	1:B:163:PRO:HD3	1.98	0.44
1:A:141:TYR:CE2	1:A:199:ASP:HB2	2.52	0.44
1:C:100:ALA:HA	1:C:179:LEU:HD12	1.98	0.44
1:C:223:MET:HG2	1:C:237:GLN:OE1	2.17	0.44
1:D:264:SER:O	1:D:265:ALA:C	2.60	0.44
1:E:36:TRP:CD1	1:E:37:PRO:HD3	2.52	0.44
1:E:238:LEU:C	1:E:240:GLY:N	2.73	0.44
1:H:340:ASP:O	1:H:342:SER:N	2.50	0.44
1:I:207:TRP:CD1	1:I:208:SER:N	2.85	0.44
1:J:69:ASP:OD2	1:J:169:GLU:N	2.51	0.44
1:J:137:LEU:HD13	1:J:193:LEU:HD11	2.00	0.44
1:J:151:ASN:O	1:J:151:ASN:OD1	2.35	0.44
1:J:267:TRP:HB3	1:J:354:PHE:CZ	2.53	0.44
1:A:277:GLU:O	1:A:278:LEU:C	2.59	0.44
1:C:36:TRP:N	1:C:37:PRO:CD	2.81	0.44
1:G:62:ILE:HB	1:G:345:ASP:OD1	2.18	0.44
1:G:260:PHE:CD2	1:G:319:HIS:HB3	2.52	0.44
1:G:302:VAL:HG22	1:G:303:ILE:O	2.17	0.44
1:G:342:SER:O	1:G:343:THR:C	2.60	0.44
1:I:252:ALA:HB1	1:I:253:PRO:CD	2.48	0.44
1:I:268:PHE:CD1	1:I:268:PHE:C	2.95	0.44
1:J:137:LEU:O	1:J:167:MET:CE	2.65	0.44
1:J:217:ARG:O	1:J:218:HIS:C	2.61	0.44
1:K:39:GLU:O	1:K:40:LYS:C	2.59	0.44
1:K:197:PHE:N	1:K:197:PHE:CD1	2.85	0.44
1:K:281:LEU:O	1:K:282:GLY:C	2.58	0.44
1:A:142:ASP:OD1	1:A:142:ASP:N	2.38	0.44
1:A:157:ALA:O	1:A:162:VAL:HG23	2.18	0.44
1:F:78:TYR:O	1:F:81:SER:OG	2.20	0.44
1:G:265:ALA:C	1:G:267:TRP:N	2.74	0.44
1:H:135:LEU:HD23	1:H:193:LEU:HD13	1.99	0.44
1:H:308:ILE:O	1:H:309:PRO:C	2.54	0.44
1:I:71:GLN:N	1:I:72:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:158:THR:HG22	1:L:250:ILE:C	2.41	0.44
1:L:336:GLU:O	1:L:337:GLU:C	2.59	0.44
1:B:71:GLN:N	1:B:72:PRO:HD2	2.33	0.44
1:A:106:ILE:O	1:A:106:ILE:HG22	2.18	0.44
1:A:242:ASP:CG	1:A:358:TYR:HH	2.25	0.44
1:E:353:VAL:O	1:E:357:GLU:HG3	2.17	0.44
1:F:295:GLN:O	1:F:297:TYR:N	2.48	0.44
1:G:222:LYS:O	1:G:226:THR:OG1	2.34	0.44
1:H:40:LYS:O	1:H:41:ASN:C	2.61	0.44
1:H:172:ARG:O	1:H:175:ASP:N	2.44	0.44
1:H:229:PRO:O	1:H:230:PRO:C	2.60	0.44
1:I:39:GLU:O	1:I:41:ASN:N	2.51	0.44
1:J:61:SER:C	1:J:63:SER:N	2.75	0.44
1:B:78:TYR:CD1	1:B:78:TYR:C	2.96	0.44
1:B:311:LEU:C	1:B:313:ARG:H	2.25	0.44
1:A:274:ILE:O	1:A:275:GLU:C	2.59	0.44
1:E:359:LEU:O	1:E:360:HIS:C	2.60	0.44
1:J:165:ALA:O	1:J:166:MET:C	2.58	0.44
1:J:228:HIS:N	1:J:235:THR:O	2.41	0.44
1:K:136:VAL:HG21	1:K:241:MET:HG2	1.99	0.44
1:K:297:TYR:CD1	1:K:298:SER:O	2.71	0.44
1:E:81:SER:O	1:E:84:SER:HB2	2.18	0.43
1:F:231:GLY:HA2	1:L:54:ARG:CZ	2.48	0.43
1:J:66:TRP:CZ2	1:J:336:GLU:OE2	2.71	0.43
1:J:350:ILE:HD12	1:J:351:LEU:H	1.82	0.43
1:A:221:ALA:O	1:A:222:LYS:C	2.61	0.43
1:F:360:HIS:O	1:F:361:LEU:HD23	2.18	0.43
1:G:94:ARG:O	1:G:97:ARG:HG2	2.18	0.43
1:G:328:VAL:CG1	1:G:334:ASP:CA	2.95	0.43
1:J:158:THR:O	1:J:249:LEU:CA	2.66	0.43
1:K:33:ALA:HA	1:K:235:THR:CG2	2.48	0.43
1:K:133:ARG:NE	1:K:242:ASP:CG	2.76	0.43
1:K:297:TYR:CD1	1:K:297:TYR:C	2.96	0.43
1:A:110:LEU:HD23	1:A:117:TYR:CD1	2.53	0.43
1:A:359:LEU:O	1:A:360:HIS:HB2	2.18	0.43
1:C:124:ILE:N	1:C:124:ILE:HD12	2.33	0.43
1:D:36:TRP:N	1:D:37:PRO:CD	2.81	0.43
1:G:147:SER:O	1:G:148:HIS:ND1	2.52	0.43
1:H:340:ASP:O	1:H:340:ASP:OD1	2.37	0.43
1:I:170:LEU:CD2	1:I:174:LEU:HD12	2.48	0.43
1:I:180:SER:C	1:I:182:LYS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:LEU:N	1:I:316:PRO:O	2.50	0.43
1:J:37:PRO:C	1:J:133:ARG:HH12	2.26	0.43
1:L:101:ASP:O	1:L:101:ASP:CG	2.60	0.43
1:L:128:ASN:OD1	1:L:128:ASN:N	2.49	0.43
1:L:354:PHE:CD1	1:L:354:PHE:C	2.96	0.43
1:B:34:SER:HB3	1:B:36:TRP:CD1	2.53	0.43
1:C:71:GLN:N	1:C:72:PRO:CD	2.81	0.43
1:E:36:TRP:N	1:E:37:PRO:CD	2.81	0.43
1:F:169:GLU:O	1:F:169:GLU:HG3	2.18	0.43
1:I:90:HIS:O	1:I:91:ILE:C	2.60	0.43
1:K:68:ASN:HB3	1:K:94:ARG:NH1	2.32	0.43
1:L:51:SER:O	1:L:52:ALA:C	2.60	0.43
1:B:62:ILE:O	1:B:62:ILE:HG13	2.19	0.43
1:C:248:ASP:O	1:C:249:LEU:HB2	2.18	0.43
1:F:170:LEU:C	1:F:170:LEU:HD23	2.43	0.43
1:G:147:SER:C	1:G:148:HIS:ND1	2.77	0.43
1:G:228:HIS:HA	1:G:229:PRO:C	2.43	0.43
1:H:35:ALA:O	1:H:36:TRP:C	2.58	0.43
1:H:335:ASN:N	1:H:335:ASN:OD1	2.48	0.43
1:J:39:GLU:CB	1:J:133:ARG:HH22	2.32	0.43
1:L:112:GLN:NE2	1:L:117:TYR:CZ	2.86	0.43
1:L:150:ASN:CB	1:L:152:ARG:HG3	2.48	0.43
1:L:308:ILE:O	1:L:309:PRO:C	2.60	0.43
1:L:311:LEU:O	1:L:312:ARG:C	2.61	0.43
1:B:67:GLN:HG3	1:B:68:ASN:OD1	2.19	0.43
1:E:120:PHE:CD1	1:E:120:PHE:N	2.87	0.43
1:H:263:ASN:OD1	3:I:402:A1D48:C08	2.66	0.43
1:I:49:ASN:O	1:I:51:SER:N	2.52	0.43
1:I:116:GLY:O	1:I:117:TYR:C	2.59	0.43
1:J:347:LEU:O	1:J:350:ILE:CD1	2.67	0.43
1:K:47:ILE:HG12	1:K:48:LEU:N	2.33	0.43
1:K:128:ASN:N	1:K:129:PRO:HD3	2.34	0.43
1:L:109:PHE:CZ	1:L:120:PHE:HB2	2.53	0.43
1:L:311:LEU:O	1:L:313:ARG:N	2.51	0.43
1:C:70:LEU:O	1:C:70:LEU:HG	2.19	0.43
1:G:303:ILE:O	1:G:307:HIS:HE1	2.01	0.43
1:J:101:ASP:O	1:J:127:LEU:HD21	2.19	0.43
1:J:128:ASN:N	1:J:129:PRO:CD	2.82	0.43
1:J:293:TYR:CZ	1:J:343:THR:CG2	3.01	0.43
1:J:302:VAL:HG22	1:J:303:ILE:O	2.19	0.43
1:K:90:HIS:O	1:K:91:ILE:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:MET:HG3	1:C:169:GLU:HB2	2.00	0.43
1:D:229:PRO:O	1:D:230:PRO:C	2.59	0.43
1:D:285:LYS:NZ	1:D:286:ASP:OD1	2.49	0.43
1:E:99:GLN:O	1:E:100:ALA:C	2.61	0.43
1:G:44:GLN:HB3	1:G:45:PRO:HD2	2.01	0.43
1:G:278:LEU:O	1:G:283:LEU:HD12	2.18	0.43
1:H:156:GLY:HA3	1:H:159:ASP:O	2.18	0.43
1:I:247:LEU:O	1:I:248:ASP:HB2	2.18	0.43
1:J:285:LYS:N	1:J:346:ASN:HD21	2.16	0.43
1:A:318:LEU:HD12	1:A:318:LEU:HA	1.83	0.43
1:C:65:MET:O	1:C:69:ASP:HB2	2.19	0.43
1:C:201:GLU:HG3	1:C:306:ASP:OD2	2.19	0.43
1:D:138:ALA:O	1:D:246:LEU:HD12	2.18	0.43
1:E:138:ALA:HA	1:E:196:ILE:O	2.19	0.43
1:G:45:PRO:HB2	1:G:357:GLU:HB3	2.00	0.43
1:G:284:LEU:O	1:G:285:LYS:HB2	2.18	0.43
1:H:175:ASP:O	1:H:176:LYS:C	2.60	0.43
1:H:199:ASP:O	1:H:200:GLY:C	2.59	0.43
1:H:255:PRO:HD2	1:H:293:TYR:CD1	2.53	0.43
1:H:353:VAL:O	1:H:354:PHE:C	2.62	0.43
1:J:253:PRO:O	1:J:254:ASN:C	2.61	0.43
1:J:270:ARG:O	1:J:274:ILE:HD12	2.19	0.43
1:J:278:LEU:HD12	1:J:350:ILE:HG22	2.00	0.43
1:K:270:ARG:O	1:K:274:ILE:HG13	2.18	0.43
1:B:92:MET:O	1:B:96:GLN:N	2.44	0.43
1:C:68:ASN:HB2	1:C:94:ARG:HH12	1.83	0.43
1:H:52:ALA:O	1:H:53:LEU:C	2.62	0.43
1:I:88:ARG:HG3	1:I:123:ILE:HD11	2.01	0.43
1:I:297:TYR:O	1:I:297:TYR:CG	2.71	0.43
1:K:165:ALA:O	1:K:166:MET:C	2.60	0.43
1:L:208:SER:O	1:L:209:PRO:C	2.61	0.43
1:L:263:ASN:HD22	1:L:316:PRO:HB3	1.84	0.43
1:L:347:LEU:HD23	1:L:347:LEU:HA	1.77	0.43
1:F:42:TYR:O	1:F:44:GLN:HG2	2.19	0.42
1:H:133:ARG:CZ	1:H:242:ASP:OD2	2.64	0.42
1:I:74:LEU:C	1:I:75:ILE:HG23	2.43	0.42
1:I:201:GLU:HG2	1:I:306:ASP:OD1	2.19	0.42
1:K:132:LYS:HA	1:K:228:HIS:NE2	2.34	0.42
1:K:328:VAL:HG12	1:K:333:ASP:HB2	2.02	0.42
1:B:172:ARG:O	1:B:173:ALA:C	2.60	0.42
1:D:94:ARG:NH2	1:D:97:ARG:CZ	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LEU:O	1:D:205:LEU:HD12	2.20	0.42
1:D:279:HIS:C	1:D:281:LEU:N	2.77	0.42
1:F:149:TRP:CE3	1:F:150:ASN:HB2	2.54	0.42
1:F:174:LEU:O	1:F:178:LEU:HG	2.19	0.42
1:H:64:GLU:O	1:H:65:MET:C	2.61	0.42
1:H:304:GLN:O	1:H:305:ASP:HB2	2.19	0.42
1:J:36:TRP:CD1	1:J:37:PRO:HD3	2.54	0.42
1:J:273:ALA:O	1:J:276:HIS:N	2.48	0.42
1:K:78:TYR:CE1	1:K:81:SER:HB3	2.54	0.42
1:K:307:HIS:O	1:K:308:ILE:C	2.63	0.42
1:B:77:ARG:NH1	1:B:155:VAL:O	2.50	0.42
1:A:70:LEU:HB2	1:A:165:ALA:CB	2.49	0.42
1:C:92:MET:HB3	1:C:104:LEU:HD13	2.01	0.42
1:D:104:LEU:HD23	1:D:125:SER:HB2	2.00	0.42
1:E:174:LEU:O	1:E:178:LEU:HG	2.19	0.42
1:F:101:ASP:O	1:F:127:LEU:HD23	2.19	0.42
1:G:92:MET:SD	1:G:104:LEU:HD13	2.59	0.42
1:I:279:HIS:ND1	1:I:289:LEU:HD21	2.34	0.42
1:J:259:ASN:OD1	1:J:265:ALA:HA	2.19	0.42
1:J:328:VAL:CG1	1:J:333:ASP:HB2	2.49	0.42
1:L:223:MET:C	1:L:225:SER:N	2.77	0.42
1:A:116:GLY:HA2	1:H:114:PRO:O	2.19	0.42
1:E:167:MET:O	1:E:168:LEU:C	2.58	0.42
1:I:47:ILE:HA	1:I:357:GLU:OE2	2.19	0.42
1:J:109:PHE:CZ	1:J:120:PHE:HB2	2.53	0.42
1:J:195:LEU:C	1:J:196:ILE:HG13	2.45	0.42
1:J:211:ASP:O	1:J:212:SER:HB3	2.20	0.42
1:J:235:THR:OG1	1:J:235:THR:O	2.37	0.42
1:J:305:ASP:C	1:J:307:HIS:N	2.74	0.42
1:K:94:ARG:NH2	1:K:97:ARG:NH1	2.67	0.42
1:K:110:LEU:HD12	1:K:118:ARG:O	2.19	0.42
1:K:299:TYR:CD2	1:K:301:GLY:O	2.73	0.42
1:L:71:GLN:HA	1:L:74:LEU:HD12	2.01	0.42
1:L:76:GLU:HB2	1:L:153:VAL:CG1	2.49	0.42
1:L:150:ASN:HB3	1:L:152:ARG:HG3	2.01	0.42
1:A:113:THR:OG1	1:A:116:GLY:O	2.31	0.42
1:C:76:GLU:HB2	1:C:153:VAL:HG11	2.02	0.42
1:C:179:LEU:O	1:C:181:LEU:N	2.52	0.42
1:D:105:GLU:O	1:D:106:ILE:HD13	2.20	0.42
1:E:77:ARG:NH2	1:E:161:ALA:HB2	2.34	0.42
1:F:353:VAL:O	1:F:354:PHE:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:ALA:O	1:G:88:ARG:C	2.61	0.42
1:G:288:SER:OG	1:G:290:GLU:N	2.52	0.42
1:H:46:ALA:O	1:H:47:ILE:C	2.62	0.42
1:J:53:LEU:O	1:J:54:ARG:C	2.62	0.42
1:J:102:TRP:CD2	1:J:127:LEU:HD12	2.54	0.42
1:J:103:VAL:O	1:J:103:VAL:HG12	2.18	0.42
1:C:317:VAL:CG1	1:C:318:LEU:N	2.82	0.42
1:E:61:SER:OG	1:E:64:GLU:N	2.42	0.42
1:F:229:PRO:C	1:F:230:PRO:O	2.61	0.42
1:H:279:HIS:NE2	1:H:287:HIS:O	2.53	0.42
1:H:347:LEU:O	1:H:350:ILE:N	2.51	0.42
1:J:36:TRP:CD1	1:J:37:PRO:CD	3.01	0.42
1:J:168:LEU:O	1:J:171:ALA:N	2.49	0.42
1:K:71:GLN:N	1:K:72:PRO:CD	2.82	0.42
1:K:305:ASP:O	1:K:307:HIS:N	2.53	0.42
1:B:69:ASP:OD1	1:B:94:ARG:NH1	2.52	0.42
1:E:99:GLN:O	1:E:100:ALA:O	2.38	0.42
1:G:211:ASP:O	1:G:212:SER:HB3	2.19	0.42
1:J:359:LEU:O	1:J:360:HIS:C	2.62	0.42
1:L:34:SER:OG	1:L:35:ALA:N	2.52	0.42
1:B:278:LEU:HB3	1:B:284:LEU:HD13	2.00	0.42
1:A:64:GLU:O	1:A:65:MET:C	2.61	0.42
1:C:317:VAL:HG12	1:C:318:LEU:N	2.33	0.42
1:E:43:HIS:CD2	1:E:358:TYR:CE1	3.08	0.42
1:F:226:THR:O	1:F:236:SER:HA	2.19	0.42
1:G:162:VAL:O	1:G:163:PRO:C	2.63	0.42
1:G:259:ASN:HD21	1:G:265:ALA:CB	2.32	0.42
1:H:64:GLU:O	1:H:68:ASN:HB2	2.19	0.42
1:H:293:TYR:O	1:H:295:GLN:N	2.53	0.42
1:I:285:LYS:O	1:I:286:ASP:HB2	2.18	0.42
1:J:71:GLN:N	1:J:72:PRO:HD3	2.35	0.42
1:J:137:LEU:O	1:J:167:MET:HE3	2.20	0.42
1:K:247:LEU:CD2	1:K:320:LEU:HD12	2.50	0.42
1:K:250:ILE:HG22	1:K:251:GLY:N	2.34	0.42
1:K:252:ALA:O	1:K:255:PRO:HD3	2.19	0.42
1:K:337:GLU:H	1:K:337:GLU:CD	2.26	0.42
1:L:305:ASP:C	1:L:307:HIS:N	2.77	0.42
1:B:107:ASP:HB3	1:B:122:ASN:HB2	2.02	0.42
1:B:220:ALA:O	1:B:221:ALA:C	2.62	0.42
1:C:305:ASP:C	1:C:307:HIS:N	2.77	0.42
1:E:180:SER:O	1:E:181:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:ASP:HB3	1:E:321:ILE:HG13	2.01	0.42
1:G:213:LEU:HB2	1:G:217:ARG:HD3	2.00	0.42
1:I:128:ASN:C	1:I:130:THR:N	2.78	0.42
1:I:144:LYS:HG3	1:I:145:TYR:N	2.34	0.42
1:J:150:ASN:O	1:J:151:ASN:C	2.62	0.42
1:L:157:ALA:O	1:L:161:ALA:CA	2.68	0.42
1:L:279:HIS:HE1	1:L:287:HIS:O	2.03	0.42
1:B:99:GLN:O	1:B:100:ALA:C	2.60	0.42
1:B:181:LEU:HD21	1:B:361:LEU:HD21	2.02	0.42
1:B:221:ALA:O	1:B:222:LYS:C	2.59	0.42
1:C:77:ARG:HG2	1:C:143:SER:HB3	2.02	0.42
1:C:102:TRP:CE3	1:C:127:LEU:HG	2.54	0.42
1:C:252:ALA:HB1	1:C:253:PRO:HD2	2.02	0.42
1:D:95:ILE:C	1:D:97:ARG:H	2.28	0.42
1:D:104:LEU:CD2	1:D:125:SER:HB2	2.50	0.42
1:E:106:ILE:CG2	1:E:107:ASP:N	2.81	0.42
1:G:92:MET:O	1:G:96:GLN:HB2	2.20	0.42
1:J:102:TRP:CE3	1:J:127:LEU:CD1	3.03	0.42
1:J:359:LEU:HB2	1:J:361:LEU:HG	2.01	0.42
1:K:74:LEU:N	1:K:74:LEU:HD12	2.35	0.42
1:K:105:GLU:O	1:K:106:ILE:HG12	2.19	0.42
1:A:281:LEU:CB	1:A:283:LEU:HD11	2.50	0.41
1:C:105:GLU:O	1:C:106:ILE:HD13	2.20	0.41
1:C:197:PHE:CD1	1:C:197:PHE:N	2.88	0.41
1:E:168:LEU:O	1:E:171:ALA:HB3	2.20	0.41
1:G:208:SER:OG	1:G:211:ASP:HB3	2.19	0.41
1:G:301:GLY:H	1:J:300:GLY:CA	2.32	0.41
1:H:321:ILE:O	1:H:321:ILE:CG2	2.67	0.41
1:I:248:ASP:OD1	1:I:249:LEU:HG	2.20	0.41
1:J:91:ILE:O	1:J:95:ILE:HG13	2.19	0.41
1:J:158:THR:OG1	1:J:334:ASP:OD1	2.37	0.41
1:J:243:LEU:HG	1:J:244:LEU:N	2.35	0.41
1:K:92:MET:CE	1:K:106:ILE:HD11	2.50	0.41
1:K:323:SER:HA	1:K:324:PRO:O	2.20	0.41
1:L:281:LEU:HB2	1:L:283:LEU:CD1	2.50	0.41
3:L:402:A1D48:O01	3:L:402:A1D48:C21	2.68	0.41
1:A:128:ASN:O	1:A:130:THR:N	2.53	0.41
1:C:103:VAL:N	1:C:126:THR:O	2.43	0.41
1:D:197:PHE:CD1	1:D:197:PHE:N	2.89	0.41
1:D:305:ASP:HB3	1:D:307:HIS:ND1	2.36	0.41
1:D:355:VAL:HG12	1:D:356:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:TRP:O	1:G:150:ASN:C	2.63	0.41
1:G:154:PHE:N	1:G:332:MET:SD	2.93	0.41
1:G:343:THR:O	1:G:347:LEU:HD12	2.20	0.41
1:H:272:GLN:OE1	1:H:296:ASN:OD1	2.38	0.41
1:I:52:ALA:O	1:I:53:LEU:C	2.60	0.41
1:I:194:GLN:OE1	1:I:196:ILE:HD11	2.20	0.41
1:L:36:TRP:CE3	1:L:36:TRP:C	2.98	0.41
1:L:71:GLN:H	1:L:72:PRO:HD2	1.84	0.41
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.85	0.41
1:B:292:ARG:HG3	1:B:292:ARG:NH1	2.35	0.41
1:A:311:LEU:C	1:A:313:ARG:N	2.77	0.41
1:D:69:ASP:OD1	1:D:94:ARG:NH1	2.41	0.41
1:D:128:ASN:OD1	1:D:128:ASN:N	2.52	0.41
1:E:77:ARG:HG3	1:E:77:ARG:O	2.20	0.41
1:G:78:TYR:CD1	1:G:78:TYR:C	2.98	0.41
1:G:346:ASN:O	1:G:349:LYS:HB2	2.21	0.41
1:I:248:ASP:O	1:I:250:ILE:HG13	2.20	0.41
1:J:160:SER:O	1:J:163:PRO:CD	2.69	0.41
1:J:220:ALA:HB2	1:J:309:PRO:HB2	2.02	0.41
1:J:297:TYR:O	1:J:297:TYR:CD2	2.73	0.41
1:J:355:VAL:C	1:J:357:GLU:N	2.78	0.41
1:K:48:LEU:HD12	1:K:53:LEU:HD23	2.02	0.41
1:K:65:MET:O	1:K:66:TRP:C	2.62	0.41
1:B:34:SER:HG	1:B:35:ALA:H	1.61	0.41
1:A:311:LEU:C	1:A:313:ARG:H	2.28	0.41
1:C:162:VAL:HB	1:C:163:PRO:HD3	2.03	0.41
1:E:168:LEU:O	1:E:169:GLU:C	2.61	0.41
1:E:212:SER:O	1:E:213:LEU:CB	2.68	0.41
1:G:135:LEU:HG	1:G:136:VAL:N	2.35	0.41
1:G:211:ASP:O	1:G:212:SER:CB	2.68	0.41
1:I:162:VAL:O	1:I:163:PRO:C	2.61	0.41
1:J:36:TRP:CZ3	1:J:132:LYS:C	2.98	0.41
1:J:178:LEU:O	1:J:180:SER:N	2.53	0.41
1:C:95:ILE:O	1:C:96:GLN:C	2.64	0.41
1:C:138:ALA:HA	1:C:196:ILE:O	2.20	0.41
1:C:205:LEU:HG	1:C:206:HIS:CG	2.56	0.41
1:E:149:TRP:C	1:E:151:ASN:N	2.76	0.41
1:I:264:SER:O	1:I:267:TRP:N	2.54	0.41
1:I:307:HIS:O	1:I:308:ILE:C	2.64	0.41
1:J:191:LEU:HD11	1:J:242:ASP:OD2	2.21	0.41
1:L:283:LEU:H	1:L:283:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:O	1:A:118:ARG:HG2	2.21	0.41
1:D:48:LEU:N	1:D:48:LEU:HD23	2.35	0.41
1:E:174:LEU:CD2	1:E:356:LEU:HD11	2.51	0.41
1:F:219:LEU:O	1:F:220:ALA:C	2.61	0.41
1:F:223:MET:HB3	1:F:238:LEU:HD23	2.02	0.41
1:F:267:TRP:CZ2	1:F:358:TYR:CE2	3.08	0.41
1:F:345:ASP:O	1:F:346:ASN:C	2.63	0.41
1:G:56:ILE:HG22	1:G:349:LYS:HZ1	1.86	0.41
1:H:163:PRO:O	1:H:164:CYS:C	2.63	0.41
1:I:51:SER:HA	1:I:54:ARG:NH1	2.36	0.41
1:J:45:PRO:HA	1:J:357:GLU:O	2.19	0.41
1:L:219:LEU:O	1:L:220:ALA:O	2.38	0.41
1:B:177:LYS:O	1:B:361:LEU:HD13	2.20	0.41
1:B:231:GLY:O	1:B:232:ALA:C	2.61	0.41
1:A:85:TYR:O	1:A:89:GLN:HB2	2.20	0.41
1:C:94:ARG:HH21	1:C:97:ARG:NH1	2.17	0.41
1:E:74:LEU:HD23	1:E:74:LEU:HA	1.91	0.41
1:F:285:LYS:O	1:F:285:LYS:CG	2.68	0.41
1:H:295:GLN:O	1:H:296:ASN:C	2.55	0.41
1:J:35:ALA:O	1:J:37:PRO:HD2	2.21	0.41
1:J:46:ALA:O	1:J:47:ILE:C	2.63	0.41
1:L:288:SER:C	1:L:290:GLU:N	2.78	0.41
1:A:231:GLY:C	1:A:232:ALA:O	2.64	0.41
1:D:92:MET:CE	1:D:106:ILE:HD11	2.50	0.41
1:E:98:LEU:HB3	1:E:175:ASP:OD2	2.21	0.41
1:E:331:THR:C	1:E:333:ASP:N	2.76	0.41
3:E:402:A1D48:C21	3:E:402:A1D48:O01	2.69	0.41
1:G:325:PHE:O	1:G:326:PRO:C	2.63	0.41
1:H:199:ASP:OD1	1:H:200:GLY:N	2.48	0.41
1:I:285:LYS:HE3	1:I:286:ASP:OD2	2.20	0.41
1:I:299:TYR:CD2	1:I:301:GLY:O	2.74	0.41
1:J:36:TRP:CD1	1:J:37:PRO:HG3	2.55	0.41
1:K:94:ARG:HH21	1:K:97:ARG:NH1	2.18	0.41
1:K:99:GLN:N	1:K:175:ASP:OD2	2.46	0.41
1:K:247:LEU:N	1:K:247:LEU:HD23	2.36	0.41
1:B:73:LEU:O	1:B:75:ILE:N	2.51	0.41
1:B:120:PHE:C	1:B:121:SER:OG	2.62	0.41
1:B:120:PHE:C	1:B:121:SER:HG	2.28	0.41
1:A:133:ARG:NH1	1:A:242:ASP:OD1	2.54	0.41
1:D:109:PHE:CD1	1:D:109:PHE:C	2.99	0.41
1:D:205:LEU:O	1:D:206:HIS:CG	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ILE:O	1:D:312:ARG:HG2	2.21	0.41
1:E:299:TYR:HD2	1:E:301:GLY:O	2.02	0.41
1:F:258:PRO:HG2	1:F:260:PHE:CZ	2.56	0.41
1:F:276:HIS:O	1:F:279:HIS:HB3	2.21	0.41
1:G:87:ALA:O	1:G:90:HIS:N	2.54	0.41
1:G:264:SER:O	1:G:265:ALA:C	2.63	0.41
1:H:48:LEU:HD12	1:H:353:VAL:HG13	2.03	0.41
1:H:279:HIS:CE1	1:H:289:LEU:HG	2.56	0.41
1:I:51:SER:O	1:I:52:ALA:C	2.63	0.41
1:I:56:ILE:HD12	1:I:356:LEU:CD1	2.50	0.41
1:I:78:TYR:CD1	1:I:81:SER:HB3	2.56	0.41
1:J:67:GLN:HG2	1:J:68:ASN:OD1	2.21	0.41
1:J:88:ARG:O	1:J:92:MET:HG3	2.20	0.41
1:J:111:SER:OG	1:J:112:GLN:N	2.53	0.41
1:J:170:LEU:C	1:J:170:LEU:HD23	2.46	0.41
1:J:249:LEU:HA	1:J:249:LEU:HD23	1.87	0.41
1:J:350:ILE:H	1:J:350:ILE:HG13	1.76	0.41
1:L:223:MET:O	1:L:225:SER:N	2.54	0.41
1:L:354:PHE:O	1:L:355:VAL:C	2.59	0.41
1:A:145:TYR:CD2	1:A:145:TYR:C	2.99	0.41
1:A:279:HIS:CD2	1:A:279:HIS:C	2.98	0.41
1:A:353:VAL:O	1:A:354:PHE:C	2.62	0.41
1:D:150:ASN:O	1:D:151:ASN:HB2	2.21	0.41
1:E:167:MET:HE2	1:E:197:PHE:CZ	2.56	0.41
1:G:197:PHE:CD1	1:G:197:PHE:N	2.88	0.41
1:G:340:ASP:C	1:G:342:SER:H	2.28	0.41
1:H:349:LYS:O	1:H:353:VAL:HG23	2.20	0.41
1:I:172:ARG:O	1:I:173:ALA:C	2.61	0.41
1:I:236:SER:N	1:I:239:HIS:ND1	2.69	0.41
1:I:279:HIS:ND1	1:I:279:HIS:C	2.79	0.41
3:I:402:A1D48:O01	3:I:402:A1D48:C21	2.69	0.41
1:J:149:TRP:O	1:J:152:ARG:N	2.49	0.41
1:K:81:SER:O	1:K:84:SER:HB3	2.21	0.41
1:L:47:ILE:HA	1:L:357:GLU:HG2	2.02	0.41
1:A:295:GLN:O	1:A:297:TYR:N	2.52	0.40
1:D:353:VAL:O	1:D:354:PHE:C	2.62	0.40
1:F:162:VAL:HB	1:F:163:PRO:HD3	2.04	0.40
1:G:196:ILE:HG21	1:G:198:PHE:CE1	2.56	0.40
1:H:308:ILE:HB	1:H:309:PRO:HD3	2.02	0.40
1:H:343:THR:O	1:H:346:ASN:HB2	2.21	0.40
1:I:340:ASP:OD2	1:I:343:THR:OG1	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:318:LEU:HD12	1:K:318:LEU:HA	1.93	0.40
1:L:205:LEU:O	1:L:205:LEU:HD12	2.21	0.40
1:L:325:PHE:O	1:L:326:PRO:O	2.39	0.40
1:A:68:ASN:HB3	1:A:94:ARG:HH12	1.81	0.40
1:A:206:HIS:HB3	1:D:314:GLY:HA3	2.03	0.40
1:D:85:TYR:CZ	1:D:89:GLN:HG3	2.56	0.40
1:D:98:LEU:HB3	1:D:175:ASP:OD2	2.20	0.40
1:D:223:MET:HB3	1:D:238:LEU:CD2	2.51	0.40
1:E:109:PHE:CD2	1:E:110:LEU:N	2.89	0.40
1:F:178:LEU:O	1:F:181:LEU:HG	2.21	0.40
1:F:196:ILE:HD13	1:F:196:ILE:HG21	1.89	0.40
1:F:300:GLY:CA	1:H:301:GLY:H	2.34	0.40
1:F:354:PHE:C	1:F:354:PHE:CD1	2.99	0.40
1:G:57:ALA:CA	1:G:349:LYS:CE	2.97	0.40
1:G:149:TRP:C	1:G:151:ASN:N	2.79	0.40
1:G:159:ASP:CG	1:G:159:ASP:O	2.63	0.40
1:G:223:MET:C	1:G:225:SER:N	2.78	0.40
1:G:229:PRO:C	1:G:230:PRO:O	2.63	0.40
1:H:248:ASP:OD2	3:H:402:A1D48:N17	2.55	0.40
1:H:270:ARG:O	1:H:274:ILE:HD12	2.20	0.40
1:J:39:GLU:C	1:J:41:ASN:H	2.27	0.40
1:J:90:HIS:O	1:J:91:ILE:C	2.63	0.40
1:J:265:ALA:O	1:J:266:ARG:C	2.64	0.40
1:K:158:THR:OG1	1:K:334:ASP:CG	2.57	0.40
1:K:351:LEU:O	1:K:355:VAL:HG23	2.21	0.40
3:K:402:A1D48:O01	3:K:402:A1D48:C21	2.69	0.40
1:L:224:ALA:N	1:L:238:LEU:HG	2.37	0.40
1:L:289:LEU:O	1:L:292:ARG:HG3	2.21	0.40
1:B:136:VAL:HA	1:B:194:GLN:O	2.21	0.40
1:C:148:HIS:CD2	1:C:153:VAL:HG22	2.57	0.40
1:D:36:TRP:HA	1:D:39:GLU:HG3	2.04	0.40
1:G:49:ASN:CG	1:G:51:SER:HG	2.28	0.40
1:G:157:ALA:CB	1:G:334:ASP:O	2.68	0.40
1:G:251:GLY:HA2	1:G:344:ILE:HD11	2.03	0.40
1:G:261:PHE:HB2	1:G:264:SER:OG	2.21	0.40
1:G:270:ARG:O	1:G:274:ILE:HD12	2.21	0.40
1:H:54:ARG:O	1:H:55:GLN:C	2.64	0.40
3:H:402:A1D48:C21	3:H:402:A1D48:O01	2.69	0.40
1:J:41:ASN:OD1	1:J:41:ASN:N	2.54	0.40
1:J:69:ASP:CG	1:J:168:LEU:HB3	2.47	0.40
1:J:88:ARG:CG	1:J:123:ILE:HD11	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:312:ARG:NH1	1:J:313:ARG:NH1	2.70	0.40
1:K:150:ASN:C	1:K:152:ARG:N	2.79	0.40
1:K:328:VAL:O	1:K:329:TRP:C	2.63	0.40
1:B:84:SER:O	1:B:88:ARG:HB2	2.22	0.40
1:A:242:ASP:OD2	1:A:358:TYR:OH	2.37	0.40
1:C:270:ARG:O	1:C:274:ILE:HG13	2.21	0.40
1:F:100:ALA:HA	1:F:179:LEU:CD1	2.47	0.40
1:H:69:ASP:O	1:H:72:PRO:HD2	2.21	0.40
1:H:279:HIS:CD2	1:H:287:HIS:O	2.75	0.40
1:I:36:TRP:CE2	1:I:37:PRO:HG3	2.56	0.40
1:J:36:TRP:CH2	1:J:132:LYS:O	2.74	0.40
1:J:197:PHE:CD1	1:J:197:PHE:N	2.89	0.40
1:K:74:LEU:CD2	1:K:336:GLU:HB2	2.51	0.40
1:K:250:ILE:CG2	1:K:251:GLY:N	2.84	0.40
1:L:62:ILE:O	1:L:62:ILE:HG13	2.20	0.40
1:B:61:SER:OG	1:B:64:GLU:HG2	2.22	0.40
1:B:106:ILE:HG22	1:B:107:ASP:N	2.36	0.40
1:C:158:THR:O	1:C:249:LEU:HA	2.22	0.40
1:C:169:GLU:O	1:C:169:GLU:CG	2.70	0.40
1:F:162:VAL:O	1:F:163:PRO:C	2.63	0.40
1:F:211:ASP:HA	1:F:214:TYR:OH	2.21	0.40
1:G:70:LEU:O	1:G:70:LEU:HD12	2.22	0.40
1:G:297:TYR:CD1	1:G:297:TYR:C	2.99	0.40
1:I:100:ALA:HB2	1:I:175:ASP:OD1	2.21	0.40
1:I:201:GLU:CG	1:I:306:ASP:OD1	2.69	0.40
1:J:47:ILE:C	1:J:47:ILE:HD13	2.46	0.40
1:L:95:ILE:O	1:L:95:ILE:HG22	2.20	0.40
1:L:138:ALA:O	1:L:246:LEU:HD12	2.21	0.40
1:L:149:TRP:O	1:L:152:ARG:CB	2.69	0.40
1:L:174:LEU:CD2	1:L:356:LEU:HD11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/329 (97%)	276 (86%)	33 (10%)	10 (3%)	3	11
1	B	319/329 (97%)	288 (90%)	27 (8%)	4 (1%)	9	29
1	C	319/329 (97%)	283 (89%)	30 (9%)	6 (2%)	6	20
1	D	319/329 (97%)	285 (89%)	26 (8%)	8 (2%)	4	15
1	E	319/329 (97%)	271 (85%)	36 (11%)	12 (4%)	2	8
1	F	319/329 (97%)	282 (88%)	28 (9%)	9 (3%)	4	13
1	G	319/329 (97%)	253 (79%)	50 (16%)	16 (5%)	1	5
1	H	319/329 (97%)	269 (84%)	37 (12%)	13 (4%)	2	7
1	I	319/329 (97%)	268 (84%)	43 (14%)	8 (2%)	4	15
1	J	319/329 (97%)	236 (74%)	56 (18%)	27 (8%)	0	1
1	K	319/329 (97%)	275 (86%)	32 (10%)	12 (4%)	2	8
1	L	319/329 (97%)	262 (82%)	44 (14%)	13 (4%)	2	7
All	All	3828/3948 (97%)	3248 (85%)	442 (12%)	138 (4%)	2	9

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	SER
1	A	81	SER
1	A	131	ALA
1	A	132	LYS
1	A	147	SER
1	A	180	SER
1	D	131	ALA
1	D	132	LYS
1	D	180	SER
1	D	207	TRP
1	D	212	SER
1	D	232	ALA
1	E	100	ALA
1	E	131	ALA
1	E	180	SER
1	F	329	TRP
1	F	330	HIS
1	G	91	ILE
1	G	131	ALA

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Mol	Chain	Res	Type
1	G	147	SER
1	G	150	ASN
1	G	207	TRP
1	G	212	SER
1	G	326	PRO
1	G	341	GLU
1	H	100	ALA
1	H	213	LEU
1	H	296	ASN
1	H	341	GLU
1	I	297	TYR
1	I	298	SER
1	J	35	ALA
1	J	128	ASN
1	J	131	ALA
1	J	179	LEU
1	J	297	TYR
1	J	355	VAL
1	K	34	SER
1	K	213	LEU
1	L	131	ALA
1	L	132	LYS
1	L	161	ALA
1	L	237	GLN
1	C	180	SER
1	C	306	ASP
1	D	156	GLY
1	D	280	GLU
1	E	150	ASN
1	E	175	ASP
1	F	156	GLY
1	F	179	LEU
1	F	212	SER
1	G	92	MET
1	G	132	LYS
1	G	156	GLY
1	G	296	ASN
1	H	47	ILE
1	H	156	GLY
1	H	173	ALA
1	H	294	PHE
1	H	348	ASN

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Mol	Chain	Res	Type
1	I	50	SER
1	I	179	LEU
1	I	320	LEU
1	J	74	LEU
1	J	155	VAL
1	J	198	PHE
1	J	212	SER
1	J	332	MET
1	J	348	ASN
1	K	179	LEU
1	K	292	ARG
1	L	40	LYS
1	L	162	VAL
1	L	200	GLY
1	L	224	ALA
1	L	292	ARG
1	A	39	GLU
1	A	242	ASP
1	C	230	PRO
1	C	254	ASN
1	E	213	LEU
1	E	306	ASP
1	F	207	TRP
1	H	172	ARG
1	H	234	GLY
1	H	329	TRP
1	J	122	ASN
1	J	200	GLY
1	J	255	PRO
1	J	280	GLU
1	J	306	ASP
1	J	329	TRP
1	K	106	ILE
1	K	128	ASN
1	K	254	ASN
1	L	306	ASP
1	L	312	ARG
1	B	81	SER
1	B	220	ALA
1	A	207	TRP
1	A	300	GLY
1	C	81	SER

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Mol	Chain	Res	Type
1	E	99	GLN
1	E	128	ASN
1	E	132	LYS
1	E	156	GLY
1	F	332	MET
1	G	286	ASP
1	H	346	ASN
1	I	236	SER
1	J	36	TRP
1	J	337	GLU
1	K	129	PRO
1	K	306	ASP
1	B	232	ALA
1	C	207	TRP
1	E	360	HIS
1	F	175	ASP
1	G	343	THR
1	I	230	PRO
1	I	329	TRP
1	J	208	SER
1	J	254	ASN
1	J	266	ARG
1	K	330	HIS
1	K	333	ASP
1	L	179	LEU
1	F	213	LEU
1	J	207	TRP
1	L	262	PRO
1	A	230	PRO
1	G	240	GLY
1	J	62	ILE
1	G	251	GLY
1	J	326	PRO
1	K	208	SER
1	J	350	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/290 (98%)	257 (90%)	27 (10%)	8	25
1	B	284/290 (98%)	254 (89%)	30 (11%)	6	20
1	C	284/290 (98%)	257 (90%)	27 (10%)	8	25
1	D	284/290 (98%)	272 (96%)	12 (4%)	26	59
1	E	284/290 (98%)	256 (90%)	28 (10%)	7	23
1	F	284/290 (98%)	261 (92%)	23 (8%)	11	32
1	G	284/290 (98%)	243 (86%)	41 (14%)	3	10
1	H	284/290 (98%)	262 (92%)	22 (8%)	12	34
1	I	284/290 (98%)	254 (89%)	30 (11%)	6	20
1	J	284/290 (98%)	249 (88%)	35 (12%)	4	15
1	K	284/290 (98%)	250 (88%)	34 (12%)	5	16
1	L	284/290 (98%)	258 (91%)	26 (9%)	8	26
All	All	3408/3480 (98%)	3073 (90%)	335 (10%)	7	24

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	B	47	ILE
1	B	50	SER
1	B	51	SER
1	B	71	GLN
1	B	75	ILE
1	B	97	ARG
1	B	106	ILE
1	B	111	SER
1	B	130	THR
1	B	132	LYS
1	B	137	LEU
1	B	148	HIS
1	B	150	ASN
1	B	152	ARG
1	B	153	VAL
1	B	179	LEU
1	B	180	SER
1	B	182	LYS
1	B	206	HIS

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Mol	Chain	Res	Type
1	B	208	SER
1	B	242	ASP
1	B	243	LEU
1	B	283	LEU
1	B	284	LEU
1	B	290	GLU
1	B	292	ARG
1	B	297	TYR
1	B	312	ARG
1	B	313	ARG
1	A	47	ILE
1	A	51	SER
1	A	70	LEU
1	A	71	GLN
1	A	75	ILE
1	A	94	ARG
1	A	97	ARG
1	A	98	LEU
1	A	104	LEU
1	A	105	GLU
1	A	106	ILE
1	A	130	THR
1	A	132	LYS
1	A	143	SER
1	A	167	MET
1	A	179	LEU
1	A	180	SER
1	A	182	LYS
1	A	191	LEU
1	A	194	GLN
1	A	207	TRP
1	A	242	ASP
1	A	284	LEU
1	A	297	TYR
1	A	312	ARG
1	A	327	GLU
1	A	342	SER
1	C	47	ILE
1	C	50	SER
1	C	51	SER
1	C	63	SER
1	C	70	LEU

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Mol	Chain	Res	Type
1	C	92	MET
1	C	96	GLN
1	C	104	LEU
1	C	106	ILE
1	C	110	LEU
1	C	121	SER
1	C	126	THR
1	C	130	THR
1	C	143	SER
1	C	149	TRP
1	C	155	VAL
1	C	160	SER
1	C	180	SER
1	C	182	LYS
1	C	284	LEU
1	C	295	GLN
1	C	297	TYR
1	C	303	ILE
1	C	308	ILE
1	C	312	ARG
1	C	321	ILE
1	C	342	SER
1	D	51	SER
1	D	64	GLU
1	D	84	SER
1	D	105	GLU
1	D	132	LYS
1	D	147	SER
1	D	179	LEU
1	D	180	SER
1	D	205	LEU
1	D	206	HIS
1	D	217	ARG
1	D	295	GLN
1	E	47	ILE
1	E	51	SER
1	E	61	SER
1	E	63	SER
1	E	71	GLN
1	E	75	ILE
1	E	84	SER
1	E	92	MET

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Mol	Chain	Res	Type
1	E	101	ASP
1	E	105	GLU
1	E	110	LEU
1	E	121	SER
1	E	137	LEU
1	E	139	CYS
1	E	143	SER
1	E	155	VAL
1	E	160	SER
1	E	179	LEU
1	E	180	SER
1	E	182	LYS
1	E	191	LEU
1	E	206	HIS
1	E	270	ARG
1	E	284	LEU
1	E	297	TYR
1	E	303	ILE
1	E	312	ARG
1	E	321	ILE
1	F	51	SER
1	F	58	GLU
1	F	61	SER
1	F	67	GLN
1	F	70	LEU
1	F	97	ARG
1	F	121	SER
1	F	137	LEU
1	F	147	SER
1	F	150	ASN
1	F	151	ASN
1	F	160	SER
1	F	179	LEU
1	F	180	SER
1	F	182	LYS
1	F	205	LEU
1	F	284	LEU
1	F	285	LYS
1	F	288	SER
1	F	290	GLU
1	F	297	TYR
1	F	313	ARG

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Mol	Chain	Res	Type
1	F	342	SER
1	G	34	SER
1	G	40	LYS
1	G	47	ILE
1	G	48	LEU
1	G	51	SER
1	G	53	LEU
1	G	58	GLU
1	G	61	SER
1	G	68	ASN
1	G	92	MET
1	G	94	ARG
1	G	105	GLU
1	G	124	ILE
1	G	125	SER
1	G	128	ASN
1	G	130	THR
1	G	133	ARG
1	G	137	LEU
1	G	140	HIS
1	G	147	SER
1	G	151	ASN
1	G	179	LEU
1	G	180	SER
1	G	182	LYS
1	G	226	THR
1	G	243	LEU
1	G	263	ASN
1	G	266	ARG
1	G	281	LEU
1	G	284	LEU
1	G	288	SER
1	G	290	GLU
1	G	292	ARG
1	G	295	GLN
1	G	298	SER
1	G	308	ILE
1	G	312	ARG
1	G	318	LEU
1	G	323	SER
1	G	338	ASN
1	G	349	LYS

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Mol	Chain	Res	Type
1	H	53	LEU
1	H	55	GLN
1	H	61	SER
1	H	67	GLN
1	H	69	ASP
1	H	74	LEU
1	H	84	SER
1	H	92	MET
1	H	94	ARG
1	H	101	ASP
1	H	104	LEU
1	H	137	LEU
1	H	147	SER
1	H	158	THR
1	H	179	LEU
1	H	182	LYS
1	H	208	SER
1	H	217	ARG
1	H	290	GLU
1	H	297	TYR
1	H	312	ARG
1	H	328	VAL
1	I	47	ILE
1	I	51	SER
1	I	60	THR
1	I	67	GLN
1	I	69	ASP
1	I	74	LEU
1	I	92	MET
1	I	93	GLN
1	I	94	ARG
1	I	96	GLN
1	I	97	ARG
1	I	105	GLU
1	I	110	LEU
1	I	130	THR
1	I	143	SER
1	I	147	SER
1	I	151	ASN
1	I	158	THR
1	I	179	LEU
1	I	180	SER

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Mol	Chain	Res	Type
1	I	182	LYS
1	I	197	PHE
1	I	208	SER
1	I	269	GLU
1	I	272	GLN
1	I	281	LEU
1	I	288	SER
1	I	289	LEU
1	I	297	TYR
1	I	331	THR
1	J	36	TRP
1	J	39	GLU
1	J	47	ILE
1	J	58	GLU
1	J	60	THR
1	J	61	SER
1	J	67	GLN
1	J	70	LEU
1	J	97	ARG
1	J	103	VAL
1	J	119	SER
1	J	121	SER
1	J	124	ILE
1	J	133	ARG
1	J	143	SER
1	J	150	ASN
1	J	158	THR
1	J	160	SER
1	J	179	LEU
1	J	180	SER
1	J	182	LYS
1	J	208	SER
1	J	216	SER
1	J	243	LEU
1	J	256	THR
1	J	263	ASN
1	J	284	LEU
1	J	290	GLU
1	J	312	ARG
1	J	323	SER
1	J	327	GLU
1	J	328	VAL

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Mol	Chain	Res	Type
1	J	342	SER
1	J	343	THR
1	J	350	ILE
1	K	50	SER
1	K	51	SER
1	K	63	SER
1	K	67	GLN
1	K	70	LEU
1	K	71	GLN
1	K	92	MET
1	K	94	ARG
1	K	97	ARG
1	K	98	LEU
1	K	107	ASP
1	K	121	SER
1	K	143	SER
1	K	158	THR
1	K	160	SER
1	K	179	LEU
1	K	180	SER
1	K	182	LYS
1	K	197	PHE
1	K	208	SER
1	K	216	SER
1	K	217	ARG
1	K	242	ASP
1	K	256	THR
1	K	284	LEU
1	K	285	LYS
1	K	290	GLU
1	K	295	GLN
1	K	297	TYR
1	K	312	ARG
1	K	323	SER
1	K	326	PRO
1	K	328	VAL
1	K	341	GLU
1	L	41	ASN
1	L	47	ILE
1	L	51	SER
1	L	60	THR
1	L	67	GLN

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Mol	Chain	Res	Type
1	L	75	ILE
1	L	94	ARG
1	L	105	GLU
1	L	107	ASP
1	L	108	THR
1	L	113	THR
1	L	124	ILE
1	L	128	ASN
1	L	130	THR
1	L	137	LEU
1	L	143	SER
1	L	147	SER
1	L	160	SER
1	L	180	SER
1	L	182	LYS
1	L	194	GLN
1	L	242	ASP
1	L	280	GLU
1	L	285	LYS
1	L	312	ARG
1	L	331	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	HIS
1	A	134	HIS
1	A	218	HIS
1	A	237	GLN
1	C	68	ASN
1	C	93	GLN
1	C	194	GLN
1	C	263	ASN
1	D	44	GLN
1	E	41	ASN
1	F	68	ASN
1	F	112	GLN
1	F	272	GLN
1	F	279	HIS
1	G	41	ASN
1	G	93	GLN
1	G	218	HIS

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Mol	Chain	Res	Type
1	H	194	GLN
1	H	352	GLN
1	I	41	ASN
1	I	44	GLN
1	I	237	GLN
1	I	259	ASN
1	I	276	HIS
1	I	352	GLN
1	J	112	GLN
1	J	194	GLN
1	J	218	HIS
1	K	41	ASN
1	K	44	GLN
1	K	90	HIS
1	K	112	GLN
1	L	112	GLN
1	L	194	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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	A1D48	I	402	2	24,24,24	2.85	9 (37%)	34,35,35	1.94	6 (17%)
3	A1D48	E	402	2	24,24,24	2.87	11 (45%)	34,35,35	2.06	10 (29%)
3	A1D48	J	402	2	24,24,24	2.74	8 (33%)	34,35,35	2.20	10 (29%)
3	A1D48	K	402	2	24,24,24	2.85	10 (41%)	34,35,35	2.26	10 (29%)
3	A1D48	B	402	2	24,24,24	2.78	12 (50%)	34,35,35	1.92	8 (23%)
3	A1D48	C	402	2	24,24,24	2.95	11 (45%)	34,35,35	1.97	9 (26%)
3	A1D48	D	402	2	24,24,24	2.77	13 (54%)	34,35,35	2.44	11 (32%)
3	A1D48	A	402	2	24,24,24	2.84	9 (37%)	34,35,35	2.32	10 (29%)
3	A1D48	F	402	2	24,24,24	2.97	10 (41%)	34,35,35	2.22	10 (29%)
3	A1D48	L	402	2	24,24,24	2.73	10 (41%)	34,35,35	2.05	8 (23%)
3	A1D48	G	402	2	24,24,24	3.10	9 (37%)	34,35,35	2.01	7 (20%)
3	A1D48	H	402	2	24,24,24	2.92	11 (45%)	34,35,35	2.12	11 (32%)

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	A1D48	I	402	2	-	2/4/16/16	0/4/4/4
3	A1D48	E	402	2	-	2/4/16/16	0/4/4/4
3	A1D48	J	402	2	-	0/4/16/16	0/4/4/4
3	A1D48	K	402	2	-	2/4/16/16	0/4/4/4
3	A1D48	B	402	2	-	1/4/16/16	0/4/4/4
3	A1D48	C	402	2	-	2/4/16/16	0/4/4/4
3	A1D48	D	402	2	-	2/4/16/16	0/4/4/4
3	A1D48	A	402	2	-	2/4/16/16	0/4/4/4
3	A1D48	F	402	2	-	2/4/16/16	0/4/4/4
3	A1D48	L	402	2	-	2/4/16/16	0/4/4/4
3	A1D48	G	402	2	-	0/4/16/16	0/4/4/4
3	A1D48	H	402	2	-	2/4/16/16	0/4/4/4

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	402	A1D48	C02-N11	8.11	1.44	1.36
3	J	402	A1D48	C02-N11	7.97	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	A1D48	C02-N11	7.46	1.43	1.36
3	F	402	A1D48	C02-N11	7.30	1.43	1.36
3	G	402	A1D48	C10-N11	7.25	1.51	1.38
3	I	402	A1D48	C02-N11	7.03	1.43	1.36
3	H	402	A1D48	C02-N11	6.98	1.43	1.36
3	F	402	A1D48	C10-N11	6.64	1.50	1.38
3	A	402	A1D48	C02-N11	6.56	1.43	1.36
3	J	402	A1D48	C10-N11	6.53	1.50	1.38
3	K	402	A1D48	C10-N11	6.45	1.50	1.38
3	L	402	A1D48	C02-N11	6.42	1.42	1.36
3	A	402	A1D48	C10-N11	6.42	1.50	1.38
3	H	402	A1D48	C10-N11	6.35	1.50	1.38
3	C	402	A1D48	C02-N11	6.35	1.42	1.36
3	C	402	A1D48	C10-N11	6.29	1.50	1.38
3	K	402	A1D48	C16-C20	-6.16	1.31	1.40
3	I	402	A1D48	C10-N11	6.13	1.49	1.38
3	E	402	A1D48	C10-N11	6.07	1.49	1.38
3	B	402	A1D48	C02-N11	6.01	1.42	1.36
3	L	402	A1D48	C16-C20	-5.85	1.32	1.40
3	K	402	A1D48	C02-N11	5.84	1.42	1.36
3	L	402	A1D48	C10-N11	5.78	1.49	1.38
3	D	402	A1D48	C10-N11	5.71	1.49	1.38
3	G	402	A1D48	C16-C20	-5.58	1.32	1.40
3	B	402	A1D48	C10-N11	5.53	1.48	1.38
3	H	402	A1D48	C16-C20	-5.48	1.32	1.40
3	E	402	A1D48	C16-C20	-5.47	1.32	1.40
3	D	402	A1D48	C16-N17	-5.46	1.29	1.37
3	B	402	A1D48	C16-C20	-5.36	1.32	1.40
3	C	402	A1D48	C16-C20	-5.36	1.32	1.40
3	F	402	A1D48	C16-C20	-5.23	1.32	1.40
3	I	402	A1D48	C16-C20	-5.23	1.32	1.40
3	H	402	A1D48	C20-N19	-5.15	1.30	1.39
3	A	402	A1D48	C16-C20	-4.94	1.33	1.40
3	D	402	A1D48	C02-N11	4.75	1.41	1.36
3	C	402	A1D48	C03-C02	-4.61	1.44	1.50
3	G	402	A1D48	C16-N17	-4.28	1.30	1.37
3	A	402	A1D48	C20-N19	-4.21	1.31	1.39
3	F	402	A1D48	C20-N19	-4.19	1.32	1.39
3	B	402	A1D48	O01-C02	-4.13	1.15	1.23
3	A	402	A1D48	O01-C02	-4.09	1.15	1.23
3	E	402	A1D48	O01-C02	-4.07	1.15	1.23
3	I	402	A1D48	O01-C02	-3.93	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	A1D48	O01-C02	-3.90	1.16	1.23
3	C	402	A1D48	C20-N19	-3.87	1.32	1.39
3	I	402	A1D48	C13-C12	3.87	1.54	1.46
3	D	402	A1D48	C16-C20	-3.86	1.34	1.40
3	J	402	A1D48	C16-C20	-3.79	1.34	1.40
3	K	402	A1D48	O01-C02	-3.76	1.16	1.23
3	I	402	A1D48	C03-C02	-3.63	1.45	1.50
3	L	402	A1D48	C20-N19	-3.60	1.33	1.39
3	B	402	A1D48	C03-C02	-3.59	1.45	1.50
3	H	402	A1D48	O01-C02	-3.58	1.16	1.23
3	D	402	A1D48	C13-C12	3.57	1.53	1.46
3	D	402	A1D48	O01-C02	-3.51	1.16	1.23
3	G	402	A1D48	C03-C02	-3.51	1.45	1.50
3	K	402	A1D48	C20-N19	-3.49	1.33	1.39
3	F	402	A1D48	C16-N17	-3.47	1.32	1.37
3	B	402	A1D48	C20-N19	-3.44	1.33	1.39
3	G	402	A1D48	C12-C03	-3.29	1.29	1.34
3	F	402	A1D48	C12-C03	-3.29	1.29	1.34
3	L	402	A1D48	O01-C02	-3.29	1.17	1.23
3	K	402	A1D48	C03-C02	-3.24	1.46	1.50
3	E	402	A1D48	C03-C02	-3.21	1.46	1.50
3	B	402	A1D48	C16-N17	-3.16	1.32	1.37
3	J	402	A1D48	C16-N17	-3.15	1.32	1.37
3	G	402	A1D48	C20-N19	-3.11	1.34	1.39
3	L	402	A1D48	C13-C12	3.09	1.52	1.46
3	F	402	A1D48	O01-C02	-3.08	1.17	1.23
3	C	402	A1D48	C12-C03	-3.03	1.30	1.34
3	B	402	A1D48	C04-C05	-3.03	1.36	1.41
3	A	402	A1D48	C03-C02	-3.00	1.46	1.50
3	D	402	A1D48	C09-C10	-2.95	1.35	1.39
3	F	402	A1D48	C04-C05	-2.94	1.36	1.41
3	C	402	A1D48	C16-N17	-2.89	1.33	1.37
3	A	402	A1D48	C16-N17	-2.87	1.33	1.37
3	H	402	A1D48	C21-C13	-2.87	1.34	1.39
3	J	402	A1D48	O01-C02	-2.84	1.18	1.23
3	E	402	A1D48	C16-N17	-2.84	1.33	1.37
3	D	402	A1D48	C21-C20	-2.84	1.35	1.40
3	K	402	A1D48	C12-C03	-2.84	1.30	1.34
3	I	402	A1D48	C04-C03	2.83	1.52	1.45
3	D	402	A1D48	C20-N19	-2.76	1.34	1.39
3	E	402	A1D48	C04-C05	-2.69	1.37	1.41
3	D	402	A1D48	C14-C15	-2.69	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	A1D48	C20-N19	-2.67	1.34	1.39
3	G	402	A1D48	O01-C02	-2.66	1.18	1.23
3	K	402	A1D48	C16-N17	-2.64	1.33	1.37
3	H	402	A1D48	C03-C02	-2.62	1.46	1.50
3	B	402	A1D48	C13-C12	2.59	1.51	1.46
3	F	402	A1D48	C03-C02	-2.58	1.47	1.50
3	L	402	A1D48	C03-C02	-2.56	1.47	1.50
3	E	402	A1D48	C12-C03	-2.54	1.30	1.34
3	G	402	A1D48	C13-C12	2.51	1.51	1.46
3	D	402	A1D48	C04-C05	-2.49	1.37	1.41
3	L	402	A1D48	C16-N17	-2.48	1.33	1.37
3	J	402	A1D48	C12-C03	-2.45	1.31	1.34
3	J	402	A1D48	C08-C07	2.41	1.43	1.38
3	K	402	A1D48	C13-C12	2.40	1.51	1.46
3	E	402	A1D48	C21-C13	-2.37	1.35	1.39
3	A	402	A1D48	C12-C03	-2.36	1.31	1.34
3	C	402	A1D48	C13-C12	2.33	1.51	1.46
3	B	402	A1D48	C21-C13	-2.32	1.35	1.39
3	F	402	A1D48	C21-C13	-2.30	1.35	1.39
3	H	402	A1D48	C16-N17	-2.30	1.34	1.37
3	C	402	A1D48	C21-C13	-2.29	1.35	1.39
3	A	402	A1D48	C21-C13	-2.23	1.36	1.39
3	D	402	A1D48	C04-C10	-2.23	1.38	1.41
3	L	402	A1D48	C12-C03	-2.19	1.31	1.34
3	H	402	A1D48	C13-C12	2.18	1.50	1.46
3	H	402	A1D48	C12-C03	-2.17	1.31	1.34
3	I	402	A1D48	C16-N17	-2.16	1.34	1.37
3	L	402	A1D48	O06-C05	2.15	1.40	1.36
3	E	402	A1D48	C13-C12	2.12	1.50	1.46
3	J	402	A1D48	O06-C05	2.11	1.40	1.36
3	C	402	A1D48	C04-C03	2.10	1.50	1.45
3	D	402	A1D48	C21-C13	-2.08	1.36	1.39
3	K	402	A1D48	C21-C13	-2.07	1.36	1.39
3	I	402	A1D48	C20-N19	-2.07	1.35	1.39
3	B	402	A1D48	C18-N17	-2.06	1.30	1.35
3	H	402	A1D48	O06-C05	2.04	1.40	1.36
3	B	402	A1D48	C12-C03	-2.03	1.31	1.34

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	A1D48	C10-N11-C02	-8.09	106.36	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1D48	C10-N11-C02	-7.87	106.50	111.35
3	G	402	A1D48	C04-C03-C02	6.92	109.10	105.31
3	K	402	A1D48	C10-N11-C02	-6.87	107.11	111.35
3	I	402	A1D48	C10-N11-C02	-6.82	107.14	111.35
3	F	402	A1D48	C10-N11-C02	-6.58	107.29	111.35
3	E	402	A1D48	C10-N11-C02	-6.40	107.40	111.35
3	L	402	A1D48	C10-N11-C02	-6.35	107.43	111.35
3	J	402	A1D48	C10-N11-C02	-6.16	107.55	111.35
3	B	402	A1D48	C10-N11-C02	-6.09	107.59	111.35
3	H	402	A1D48	C10-N11-C02	-5.82	107.76	111.35
3	C	402	A1D48	C10-N11-C02	-5.32	108.07	111.35
3	I	402	A1D48	C03-C02-N11	5.24	109.78	106.91
3	K	402	A1D48	N17-C18-N19	-5.21	105.93	113.87
3	F	402	A1D48	C04-C03-C02	5.11	108.11	105.31
3	G	402	A1D48	C10-N11-C02	-5.07	108.22	111.35
3	H	402	A1D48	N17-C18-N19	-5.06	106.16	113.87
3	A	402	A1D48	C10-C04-C05	4.98	122.34	117.81
3	K	402	A1D48	C04-C03-C02	4.93	108.01	105.31
3	C	402	A1D48	C04-C03-C02	4.92	108.00	105.31
3	D	402	A1D48	O01-C02-N11	-4.88	118.52	126.30
3	J	402	A1D48	C04-C03-C02	4.87	107.98	105.31
3	L	402	A1D48	N17-C18-N19	-4.66	106.77	113.87
3	F	402	A1D48	C10-C04-C05	4.56	121.95	117.81
3	C	402	A1D48	N17-C18-N19	-4.49	107.03	113.87
3	B	402	A1D48	C03-C02-N11	4.46	109.35	106.91
3	J	402	A1D48	C10-C04-C05	4.38	121.79	117.81
3	A	402	A1D48	C03-C02-N11	4.27	109.25	106.91
3	E	402	A1D48	N17-C18-N19	-3.98	107.81	113.87
3	E	402	A1D48	C03-C02-N11	3.87	109.03	106.91
3	F	402	A1D48	N17-C18-N19	-3.86	108.00	113.87
3	D	402	A1D48	C03-C02-N11	3.84	109.01	106.91
3	D	402	A1D48	O01-C02-C03	3.80	132.45	127.70
3	B	402	A1D48	C10-C04-C05	3.79	121.25	117.81
3	A	402	A1D48	C12-C03-C02	3.74	134.32	119.87
3	E	402	A1D48	C10-C04-C05	3.62	121.10	117.81
3	F	402	A1D48	C12-C03-C02	3.58	133.70	119.87
3	L	402	A1D48	C03-C02-N11	3.57	108.86	106.91
3	H	402	A1D48	C10-C04-C05	3.49	120.98	117.81
3	J	402	A1D48	C21-C20-C16	-3.46	115.67	120.50
3	D	402	A1D48	C12-C03-C02	3.45	133.18	119.87
3	H	402	A1D48	C20-N19-C18	3.42	111.82	105.18
3	J	402	A1D48	C15-C14-C13	-3.41	116.81	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	402	A1D48	C20-N19-C18	3.37	111.72	105.18
3	E	402	A1D48	C12-C03-C02	3.37	132.87	119.87
3	D	402	A1D48	C20-N19-C18	-3.37	98.64	105.18
3	G	402	A1D48	C13-C12-C03	-3.31	123.15	129.68
3	H	402	A1D48	C04-C03-C02	3.26	107.09	105.31
3	D	402	A1D48	C21-C20-C16	-3.25	115.96	120.50
3	J	402	A1D48	C12-C03-C02	3.24	132.37	119.87
3	B	402	A1D48	C12-C03-C02	3.21	132.25	119.87
3	C	402	A1D48	C20-N19-C18	3.20	111.39	105.18
3	H	402	A1D48	C15-C16-C20	-3.12	118.68	122.10
3	J	402	A1D48	C14-C13-C21	3.10	122.62	118.72
3	F	402	A1D48	C04-C03-C12	-3.09	118.19	130.26
3	G	402	A1D48	N17-C18-N19	-3.03	109.25	113.87
3	H	402	A1D48	C13-C12-C03	-3.01	123.74	129.68
3	H	402	A1D48	C12-C03-C02	2.99	131.40	119.87
3	A	402	A1D48	N17-C18-N19	-2.98	109.33	113.87
3	A	402	A1D48	C04-C03-C12	-2.92	118.84	130.26
3	K	402	A1D48	C03-C02-N11	2.90	108.50	106.91
3	L	402	A1D48	C15-C16-C20	-2.87	118.95	122.10
3	L	402	A1D48	O01-C02-N11	-2.84	121.77	126.30
3	I	402	A1D48	C21-C20-N19	2.82	135.25	130.51
3	F	402	A1D48	C13-C21-C20	-2.80	117.66	120.27
3	B	402	A1D48	N17-C18-N19	-2.77	109.66	113.87
3	A	402	A1D48	C04-C03-C02	2.76	106.82	105.31
3	J	402	A1D48	C04-C03-C12	-2.72	119.64	130.26
3	L	402	A1D48	C12-C03-C02	2.70	130.29	119.87
3	C	402	A1D48	C03-C02-N11	2.69	108.38	106.91
3	L	402	A1D48	C20-N19-C18	2.68	110.39	105.18
3	G	402	A1D48	C10-C04-C05	2.66	120.23	117.81
3	L	402	A1D48	C04-C03-C02	2.61	106.74	105.31
3	I	402	A1D48	C13-C21-C20	2.59	122.68	120.27
3	I	402	A1D48	N17-C18-N19	-2.58	109.94	113.87
3	K	402	A1D48	C15-C16-C20	-2.52	119.34	122.10
3	E	402	A1D48	C13-C12-C03	-2.50	124.75	129.68
3	K	402	A1D48	C13-C12-C03	-2.48	124.78	129.68
3	K	402	A1D48	C12-C03-C02	2.48	129.43	119.87
3	H	402	A1D48	C03-C02-N11	2.48	108.26	106.91
3	D	402	A1D48	C04-C03-C12	-2.47	120.60	130.26
3	E	402	A1D48	C04-C03-C12	-2.39	120.91	130.26
3	C	402	A1D48	C10-C04-C05	2.39	119.98	117.81
3	K	402	A1D48	C10-C04-C05	2.37	119.96	117.81
3	F	402	A1D48	C14-C13-C21	2.37	121.70	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	A1D48	C13-C21-C20	-2.35	118.08	120.27
3	J	402	A1D48	C13-C12-C03	-2.33	125.08	129.68
3	A	402	A1D48	C15-C16-C20	-2.31	119.57	122.10
3	B	402	A1D48	C15-C16-C20	-2.27	119.61	122.10
3	H	402	A1D48	C04-C03-C12	-2.25	121.48	130.26
3	E	402	A1D48	C15-C16-C20	-2.22	119.66	122.10
3	D	402	A1D48	C16-C20-N19	2.22	113.19	108.39
3	D	402	A1D48	C15-C16-C20	2.20	124.52	122.10
3	C	402	A1D48	O01-C02-C03	-2.19	124.95	127.70
3	C	402	A1D48	C15-C16-C20	-2.19	119.70	122.10
3	K	402	A1D48	C21-C20-N19	2.15	134.13	130.51
3	F	402	A1D48	C20-N19-C18	2.14	109.34	105.18
3	B	402	A1D48	C10-C04-C03	2.14	109.87	106.51
3	I	402	A1D48	C20-C16-N17	2.13	109.67	106.15
3	B	402	A1D48	C04-C03-C12	-2.12	121.99	130.26
3	A	402	A1D48	C13-C21-C20	-2.11	118.31	120.27
3	F	402	A1D48	C13-C12-C03	-2.08	125.57	129.68
3	E	402	A1D48	C20-N19-C18	2.07	109.20	105.18
3	D	402	A1D48	C15-C16-N17	-2.06	127.44	130.74
3	J	402	A1D48	O01-C02-N11	-2.06	123.02	126.30
3	E	402	A1D48	C10-C04-C03	2.03	109.70	106.51
3	G	402	A1D48	C15-C14-C13	-2.03	118.60	121.22
3	H	402	A1D48	O01-C02-N11	-2.03	123.07	126.30
3	G	402	A1D48	C12-C03-C02	2.01	127.63	119.87
3	A	402	A1D48	C20-C16-N17	2.00	109.46	106.15

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	402	A1D48	C02-C03-C12-C13
3	C	402	A1D48	C04-C03-C12-C13
3	F	402	A1D48	C04-C03-C12-C13
3	K	402	A1D48	C04-C03-C12-C13
3	A	402	A1D48	C02-C03-C12-C13
3	C	402	A1D48	C02-C03-C12-C13
3	E	402	A1D48	C02-C03-C12-C13
3	F	402	A1D48	C02-C03-C12-C13
3	H	402	A1D48	C02-C03-C12-C13
3	I	402	A1D48	C02-C03-C12-C13
3	A	402	A1D48	C04-C03-C12-C13
3	H	402	A1D48	C04-C03-C12-C13

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Mol	Chain	Res	Type	Atoms
3	B	402	A1D48	C02-C03-C12-C13
3	D	402	A1D48	C02-C03-C12-C13
3	L	402	A1D48	C02-C03-C12-C13
3	D	402	A1D48	C04-C03-C12-C13
3	E	402	A1D48	C04-C03-C12-C13
3	I	402	A1D48	C04-C03-C12-C13
3	L	402	A1D48	C04-C03-C12-C13

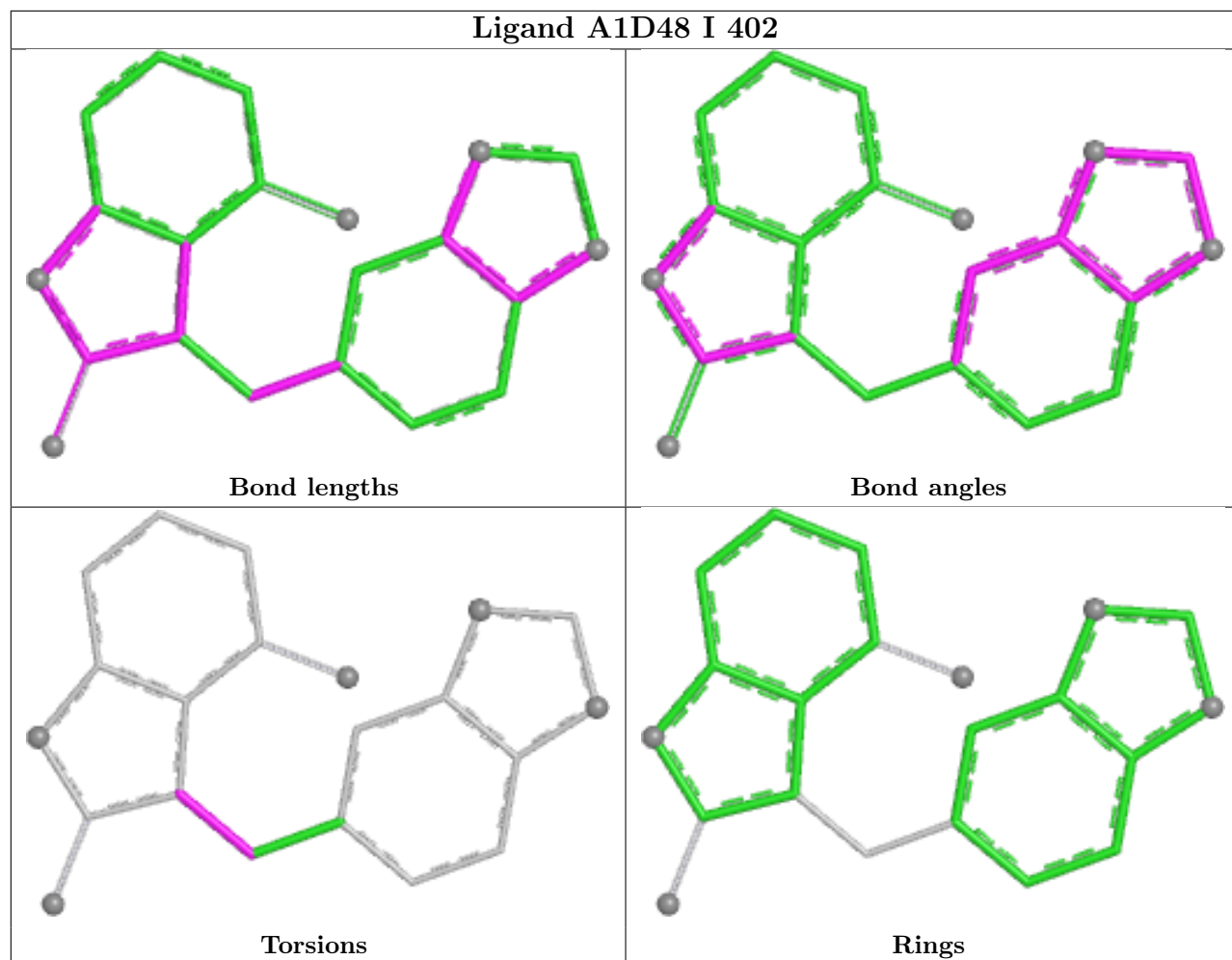
There are no ring outliers.

9 monomers are involved in 15 short contacts:

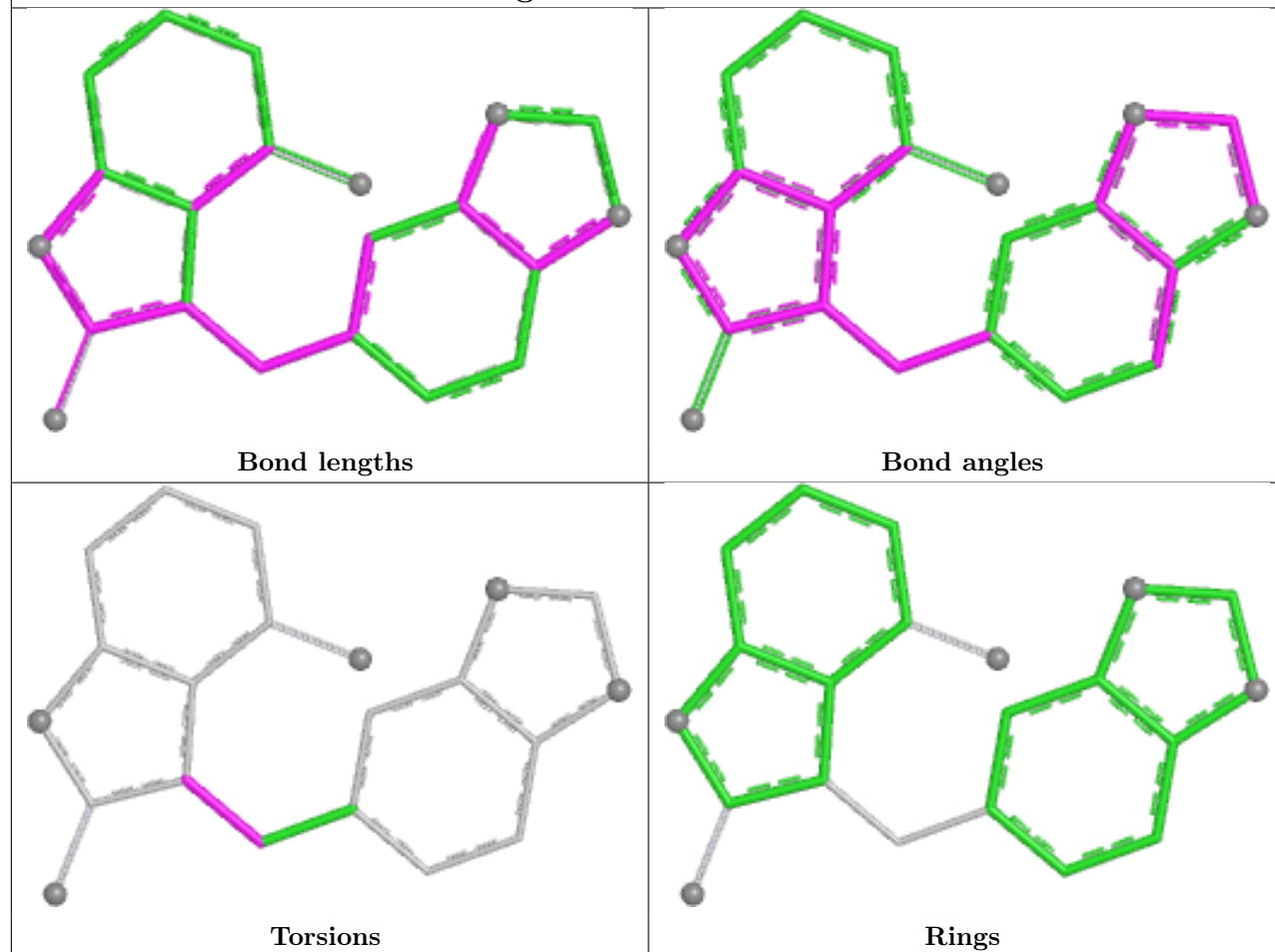
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	402	A1D48	3	0
3	E	402	A1D48	1	0
3	J	402	A1D48	1	0
3	K	402	A1D48	2	0
3	B	402	A1D48	1	0
3	A	402	A1D48	1	0
3	L	402	A1D48	2	0
3	G	402	A1D48	2	0
3	H	402	A1D48	2	0

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.

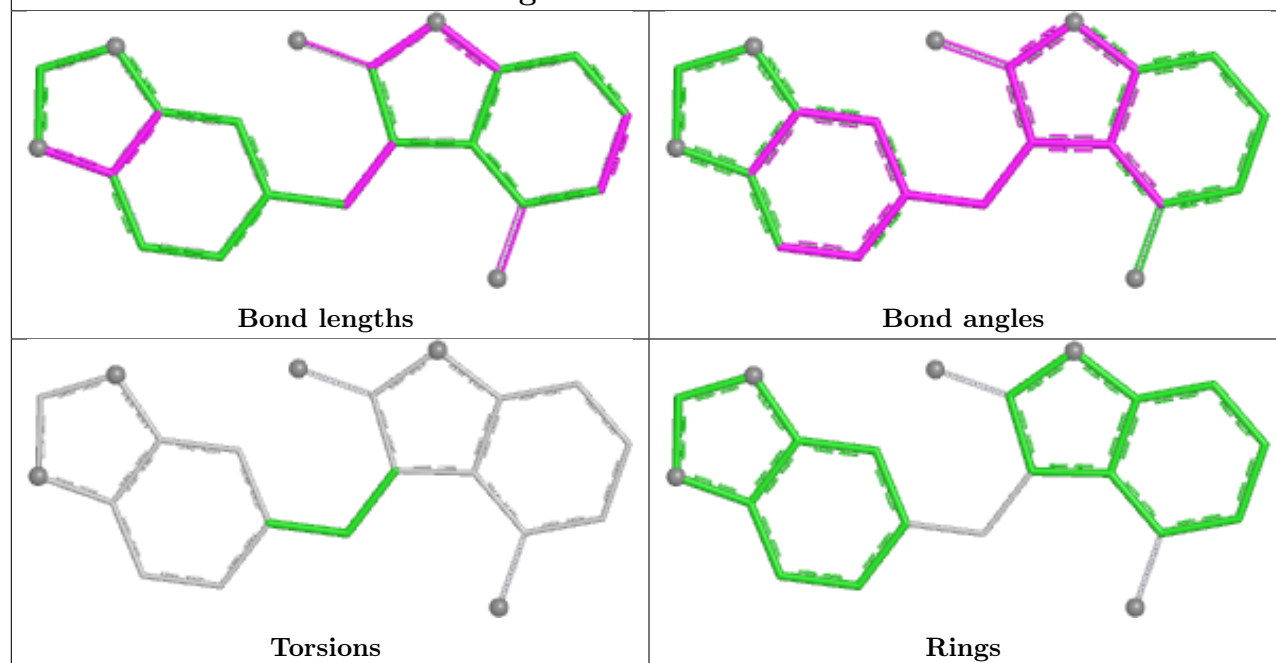
Ligand A1D48 I 402



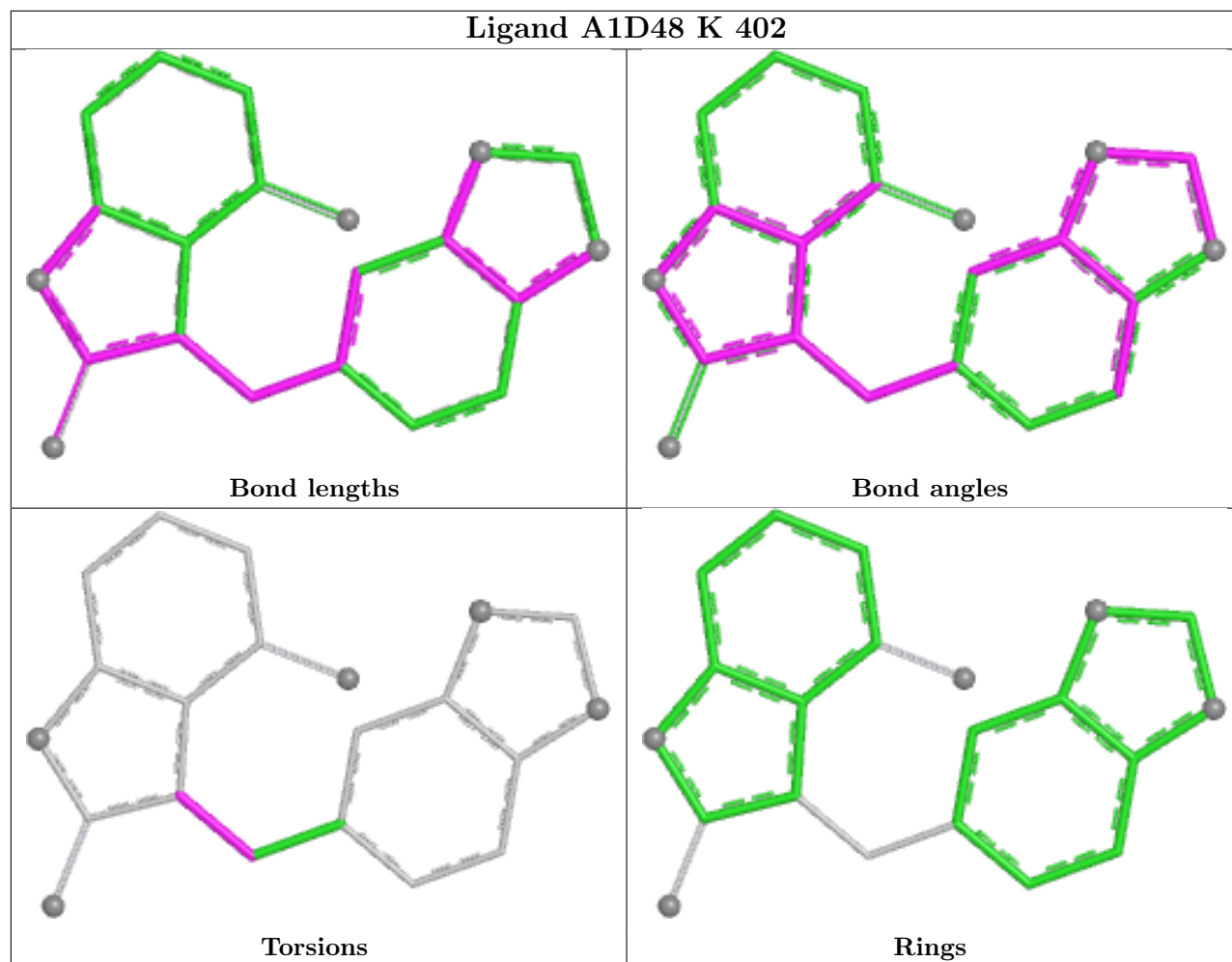
Ligand A1D48 E 402



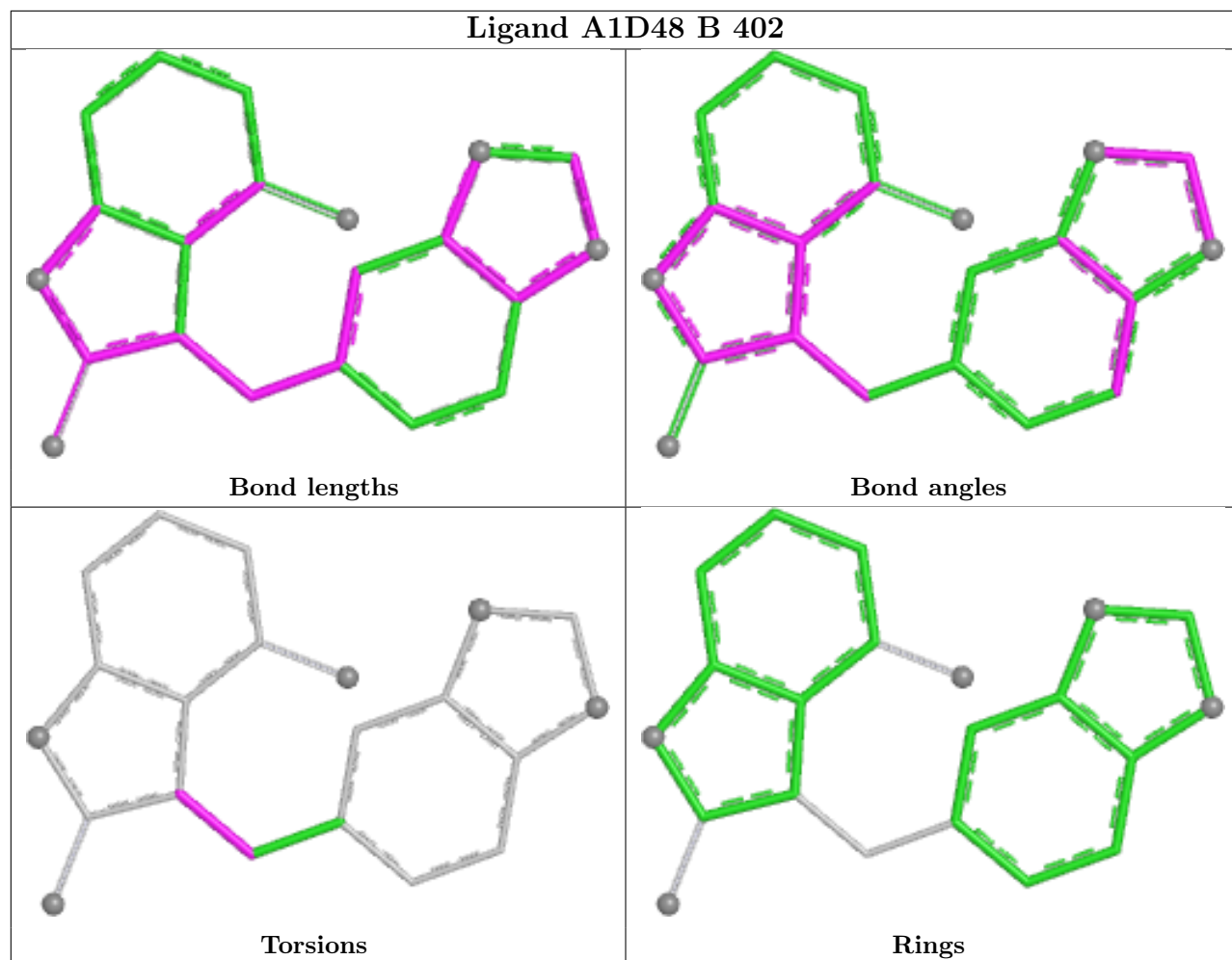
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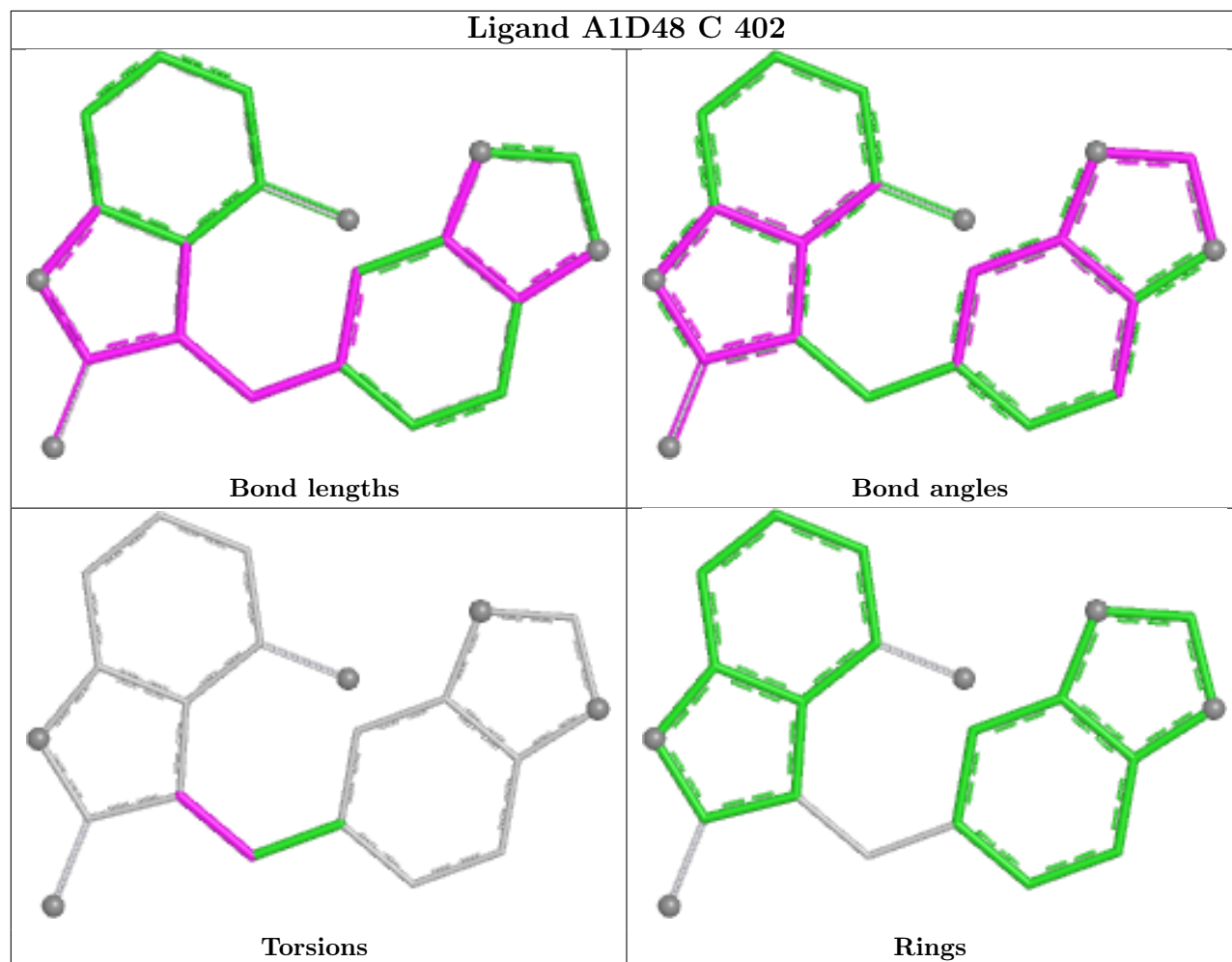
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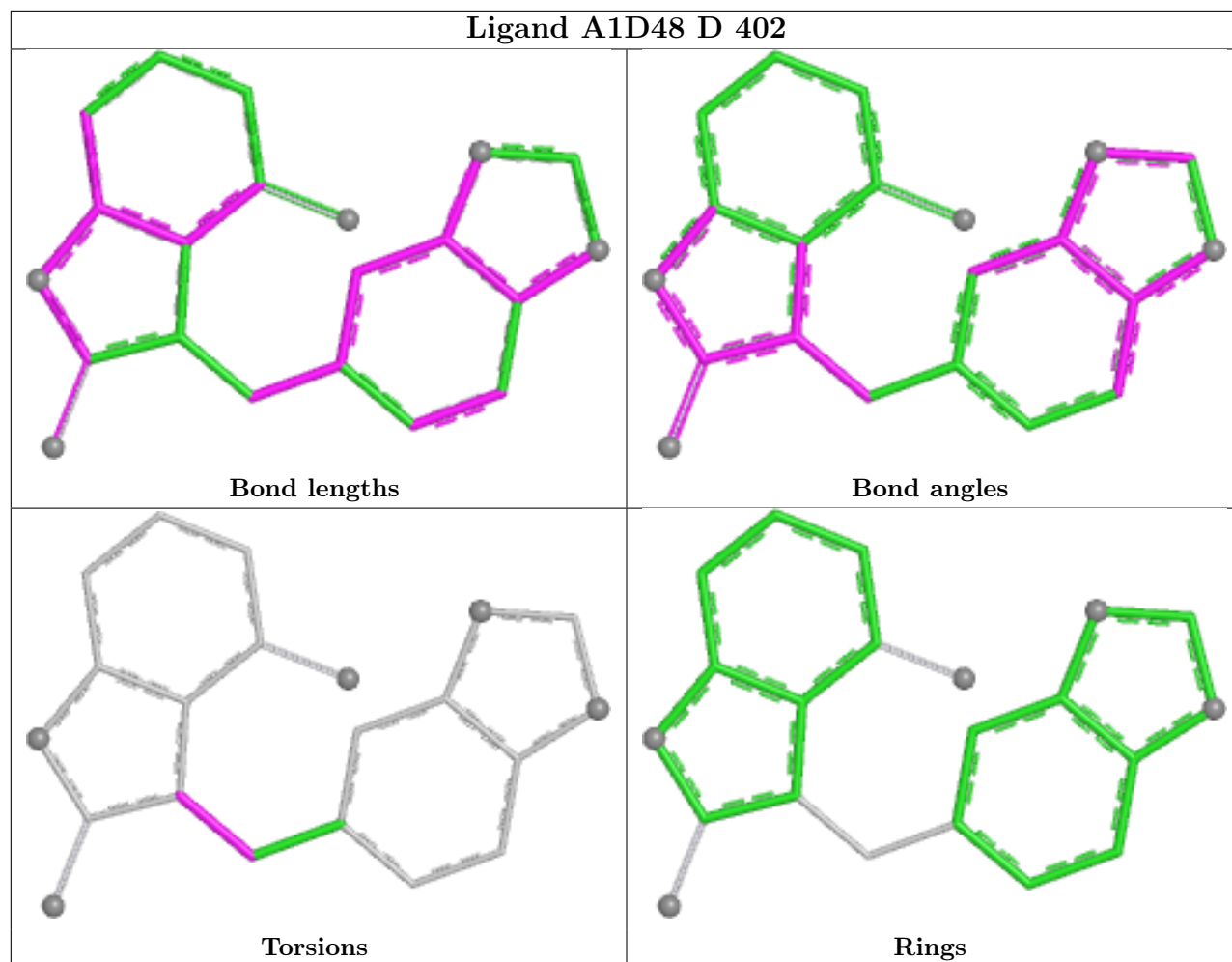
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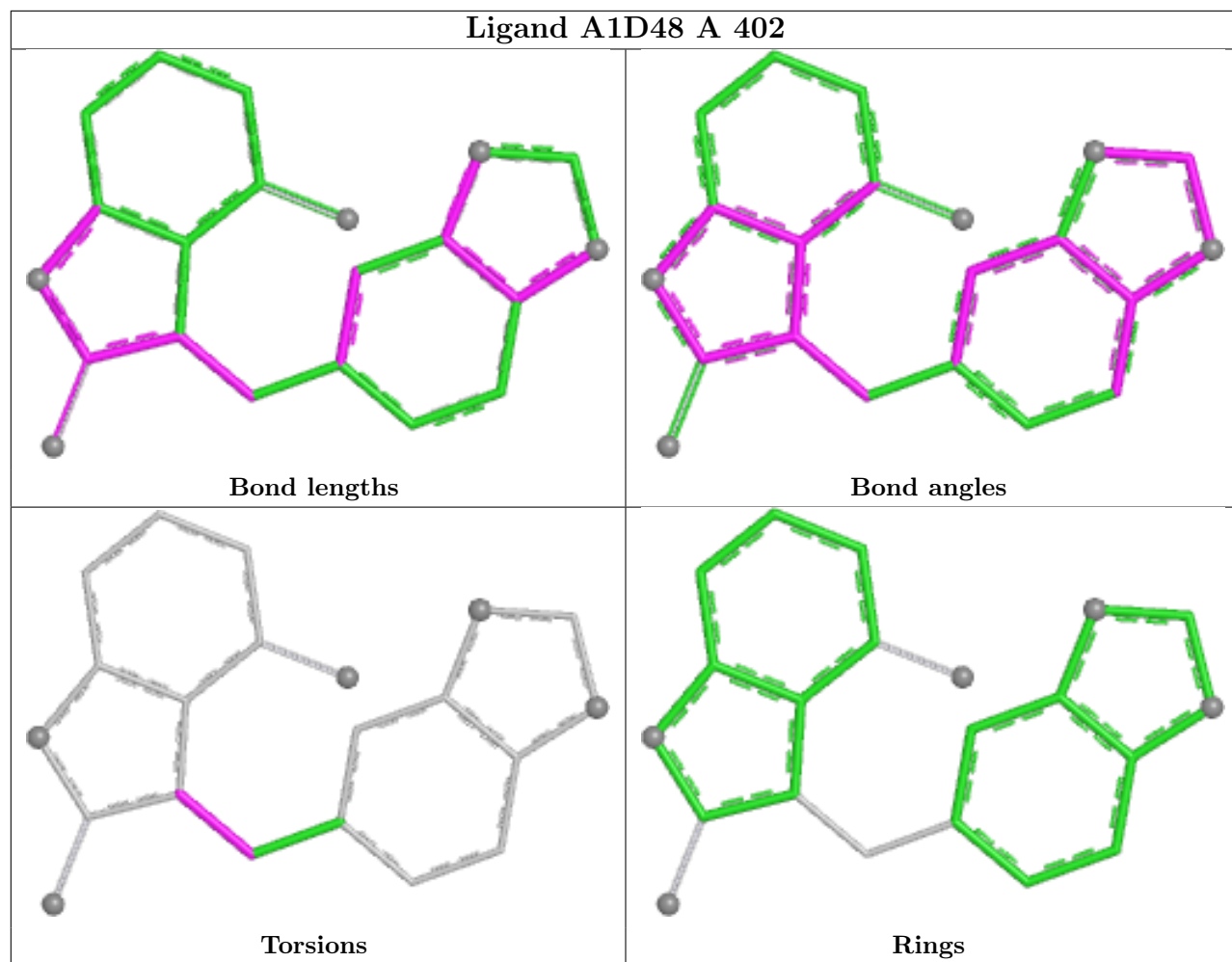
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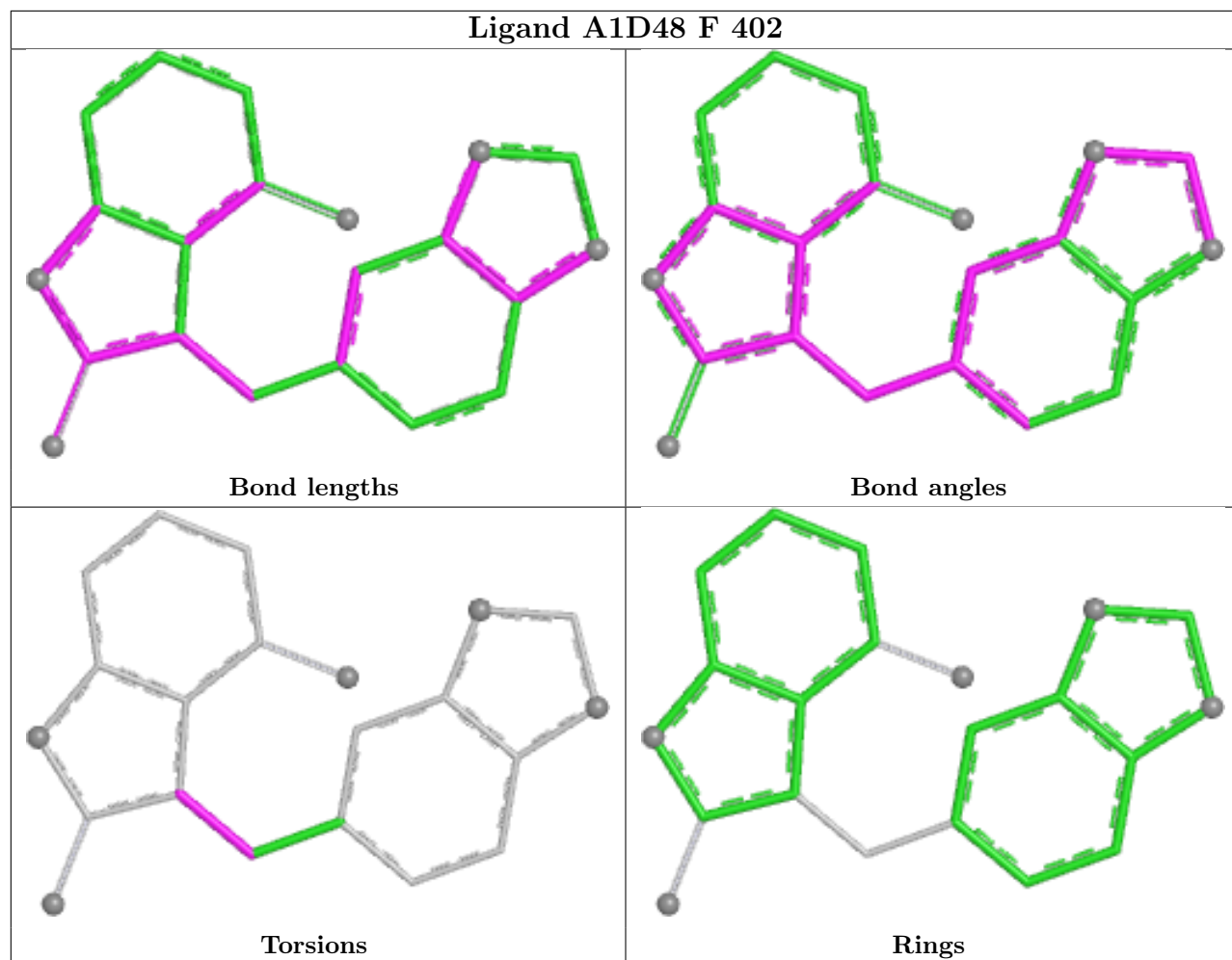
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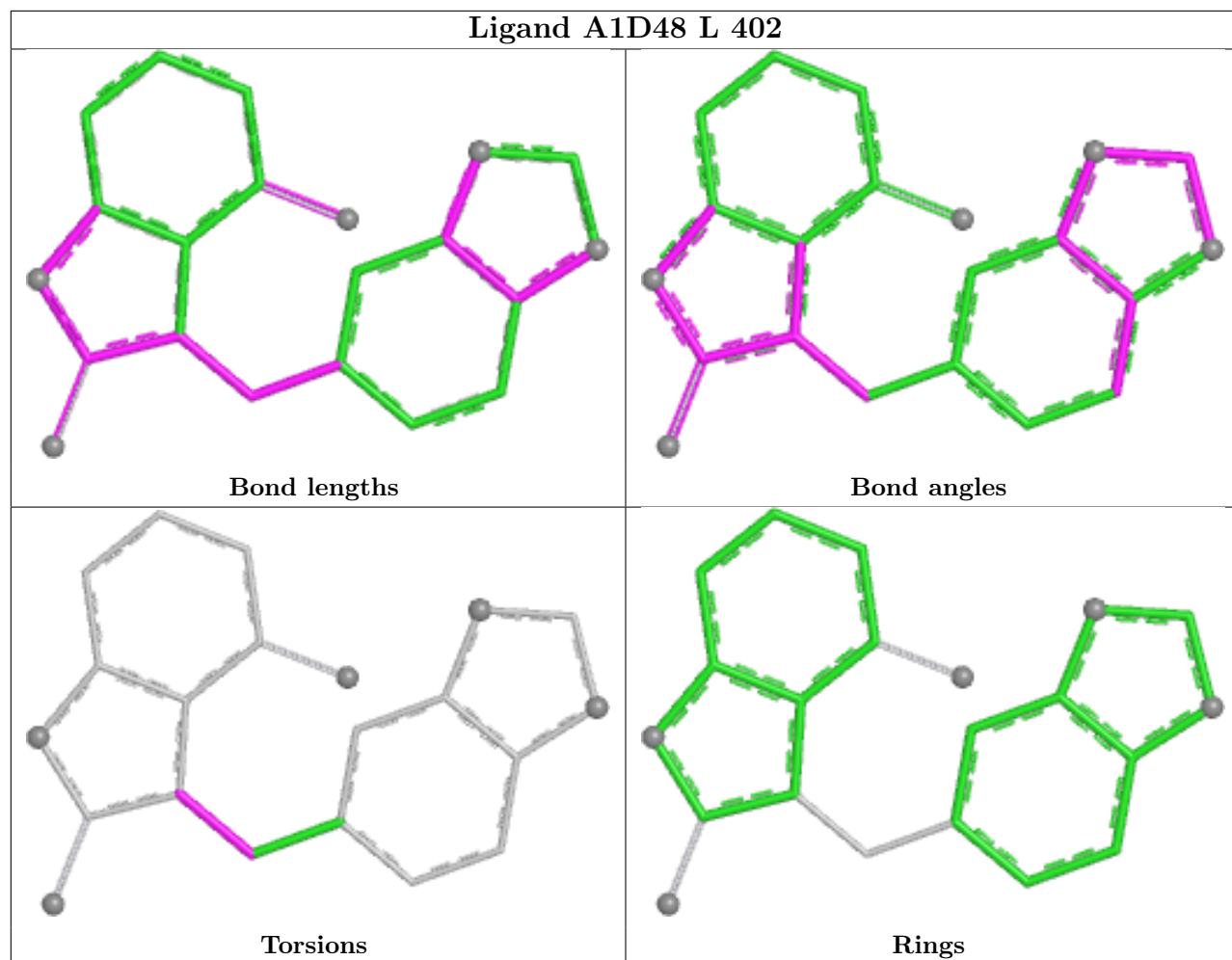
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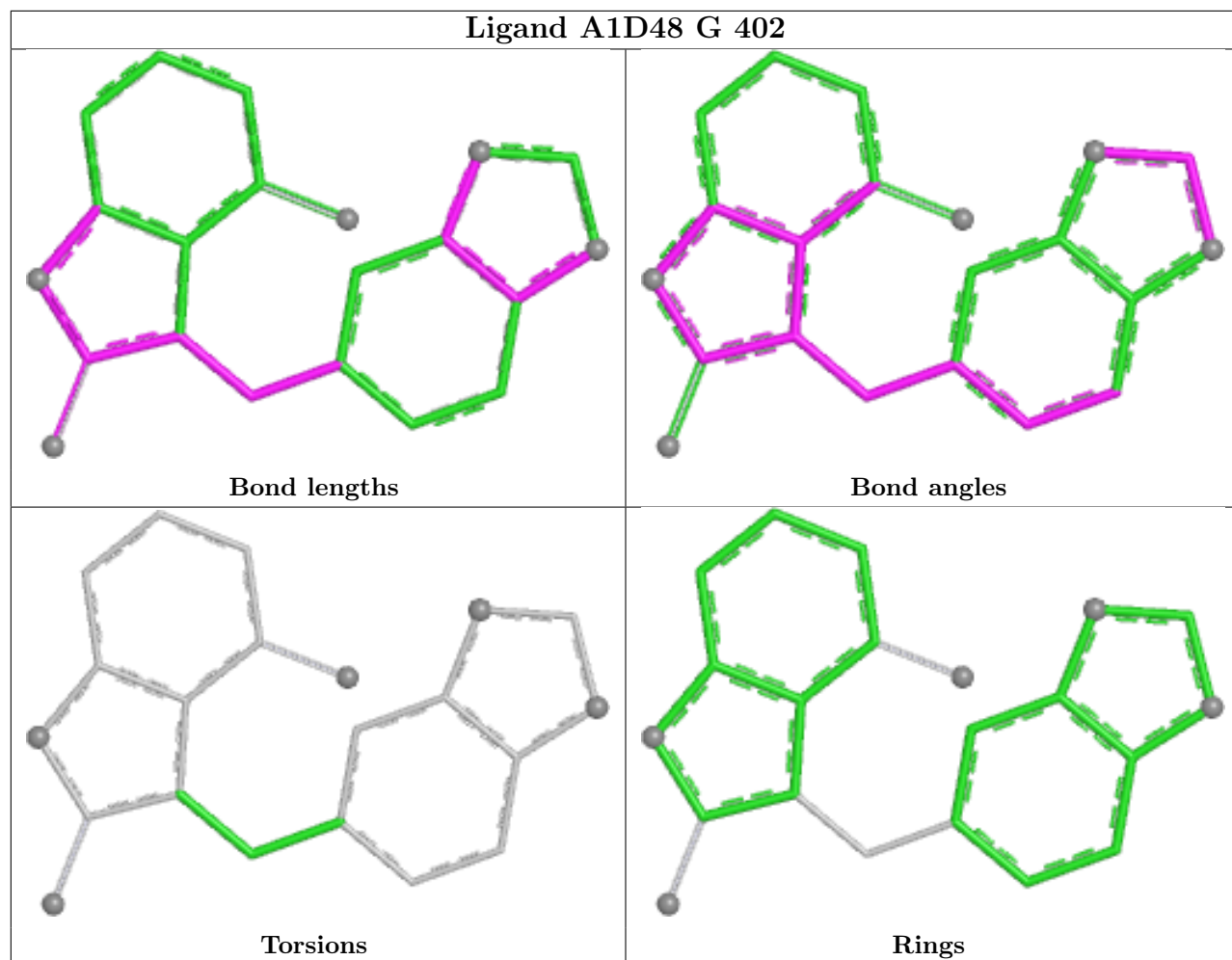
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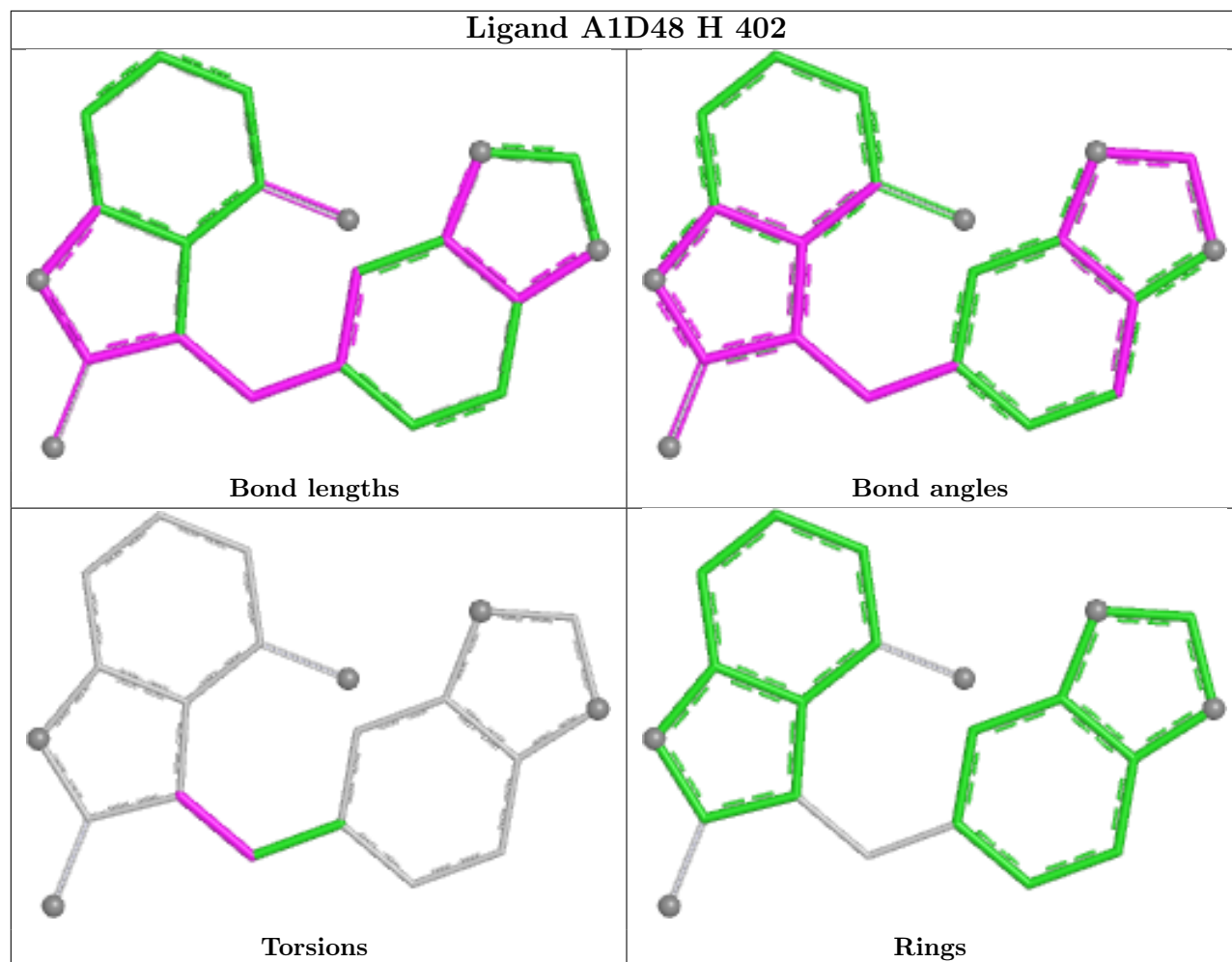


Ligand A1D48 L 402



Ligand A1D48 G 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/329 (97%)	-0.48	3 (0%) 81 74	19, 39, 76, 105	0
1	B	322/329 (97%)	-0.41	3 (0%) 81 74	16, 40, 71, 109	0
1	C	322/329 (97%)	-0.38	1 (0%) 90 86	14, 41, 77, 139	0
1	D	322/329 (97%)	-0.40	0 100 100	23, 42, 76, 119	0
1	E	322/329 (97%)	-0.29	3 (0%) 81 74	20, 44, 80, 114	0
1	F	322/329 (97%)	-0.24	4 (1%) 76 68	30, 49, 82, 111	0
1	G	322/329 (97%)	0.46	7 (2%) 62 52	45, 83, 115, 143	0
1	H	322/329 (97%)	0.16	4 (1%) 76 68	41, 71, 100, 126	0
1	I	322/329 (97%)	-0.05	2 (0%) 85 80	28, 57, 92, 122	0
1	J	322/329 (97%)	0.77	13 (4%) 42 33	54, 93, 122, 148	0
1	K	322/329 (97%)	-0.19	4 (1%) 76 68	24, 51, 81, 123	0
1	L	322/329 (97%)	-0.08	8 (2%) 58 48	28, 50, 89, 133	0
All	All	3864/3948 (97%)	-0.10	52 (1%) 75 66	14, 53, 104, 148	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	161	ALA	11.6
1	L	160	SER	5.8
1	E	129	PRO	4.6
1	E	130	THR	3.4
1	F	33	ALA	3.2
1	L	158	THR	3.2
1	H	206	HIS	3.0
1	H	182	LYS	2.9
1	B	206	HIS	2.9
1	I	206	HIS	2.9
1	E	33	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	33	ALA	2.7
1	L	189	PRO	2.7
1	L	206	HIS	2.6
1	J	75	ILE	2.6
1	G	33	ALA	2.6
1	A	206	HIS	2.6
1	A	207	TRP	2.6
1	K	302	VAL	2.5
1	B	33	ALA	2.5
1	C	297	TYR	2.5
1	K	206	HIS	2.4
1	J	267	TRP	2.4
1	L	35	ALA	2.4
1	J	46	ALA	2.4
1	B	297	TYR	2.4
1	G	117	TYR	2.3
1	J	297	TYR	2.3
1	J	350	ILE	2.3
1	K	297	TYR	2.3
1	G	36	TRP	2.3
1	J	36	TRP	2.3
1	L	337	GLU	2.2
1	I	36	TRP	2.2
1	F	233	ARG	2.2
1	G	149	TRP	2.2
1	L	54	ARG	2.1
1	G	153	VAL	2.1
1	J	189	PRO	2.1
1	H	33	ALA	2.1
1	J	206	HIS	2.1
1	F	34	SER	2.1
1	G	34	SER	2.1
1	J	205	LEU	2.1
1	G	325	PHE	2.1
1	J	204	PHE	2.1
1	J	33	ALA	2.1
1	F	302	VAL	2.1
1	J	345	ASP	2.1
1	H	149	TRP	2.0
1	A	117	TYR	2.0
1	J	302	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

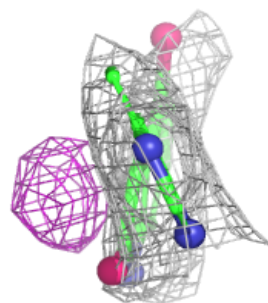
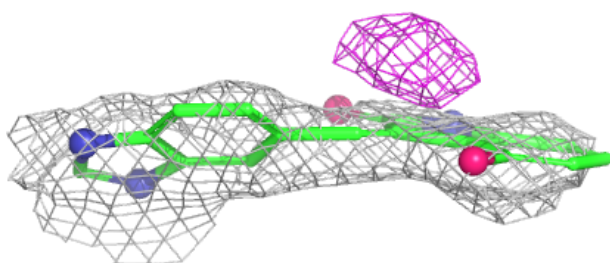
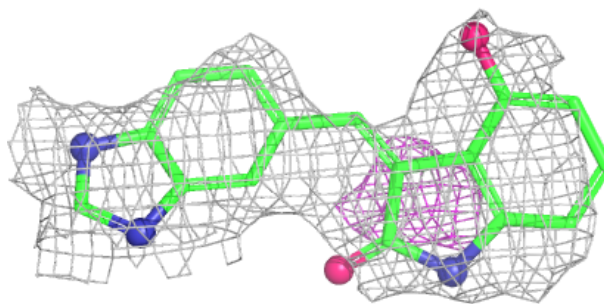
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1D48	J	402	21/21	0.82	0.14	64,78,87,90	0
3	A1D48	G	402	21/21	0.87	0.12	59,81,97,105	0
3	A1D48	H	402	21/21	0.88	0.12	58,69,83,87	0
3	A1D48	E	402	21/21	0.90	0.10	36,48,65,66	0
3	A1D48	I	402	21/21	0.91	0.11	44,57,74,75	0
3	A1D48	L	402	21/21	0.92	0.12	43,67,100,103	0
3	A1D48	F	402	21/21	0.93	0.09	39,60,73,76	0
3	A1D48	A	402	21/21	0.93	0.11	30,57,84,91	0
3	A1D48	K	402	21/21	0.93	0.08	39,49,59,70	0
3	A1D48	B	402	21/21	0.93	0.08	35,39,51,68	0
2	ZN	B	401	1/1	0.95	0.07	25,25,25,25	0
3	A1D48	D	402	21/21	0.95	0.08	33,42,52,60	0
3	A1D48	C	402	21/21	0.96	0.07	30,50,67,76	0
2	ZN	A	401	1/1	0.97	0.07	21,21,21,21	0
2	ZN	H	401	1/1	0.99	0.03	49,49,49,49	0
2	ZN	I	401	1/1	0.99	0.04	34,34,34,34	0
2	ZN	J	401	1/1	0.99	0.03	54,54,54,54	0
2	ZN	K	401	1/1	0.99	0.02	32,32,32,32	0
2	ZN	C	401	1/1	0.99	0.02	31,31,31,31	0
2	ZN	E	401	1/1	0.99	0.04	30,30,30,30	0
2	ZN	F	401	1/1	0.99	0.04	35,35,35,35	0
2	ZN	G	401	1/1	0.99	0.06	55,55,55,55	0
2	ZN	D	401	1/1	1.00	0.05	28,28,28,28	0
2	ZN	L	401	1/1	1.00	0.05	31,31,31,31	0

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

orientation to approximate a three-dimensional view.

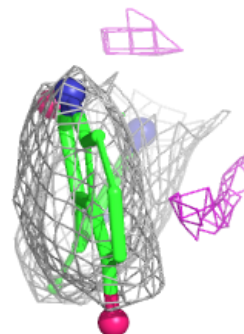
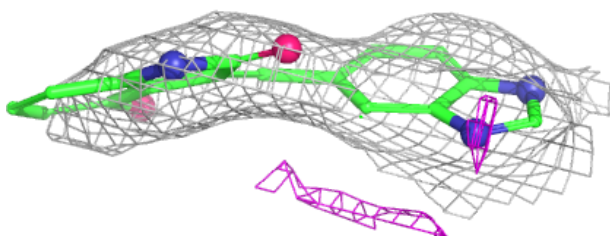
Electron density around A1D48 J 402:

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



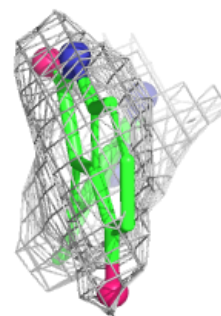
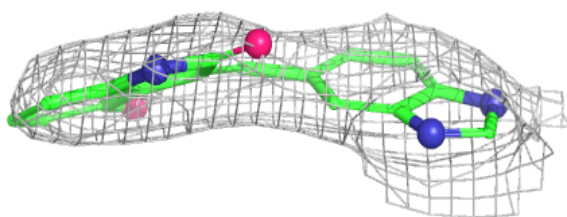
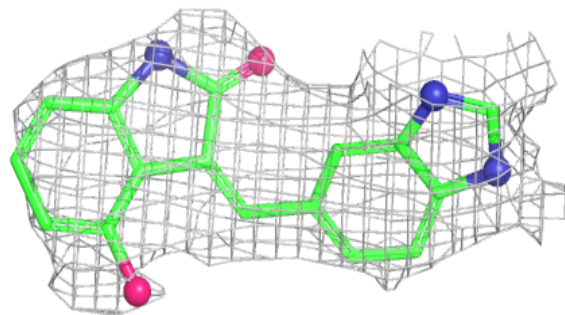
Electron density around A1D48 G 402:

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

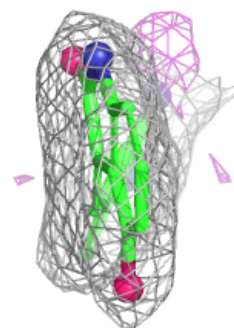
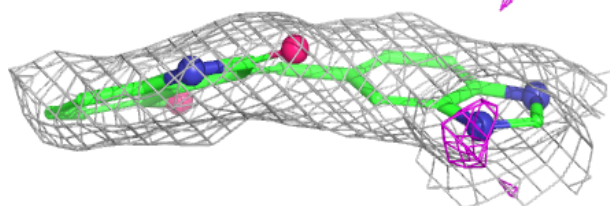
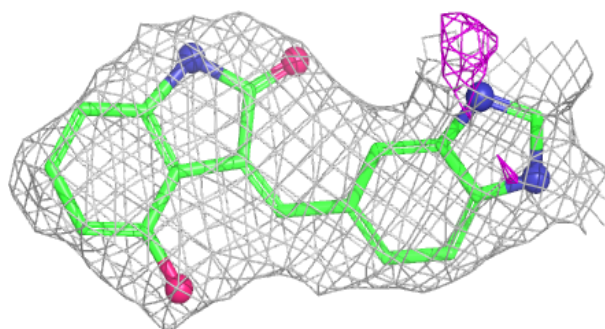


Electron density around A1D48 H 402:

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

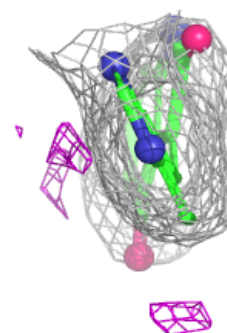
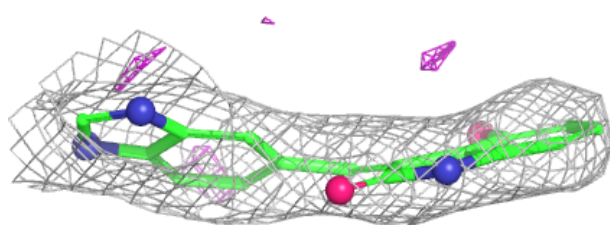
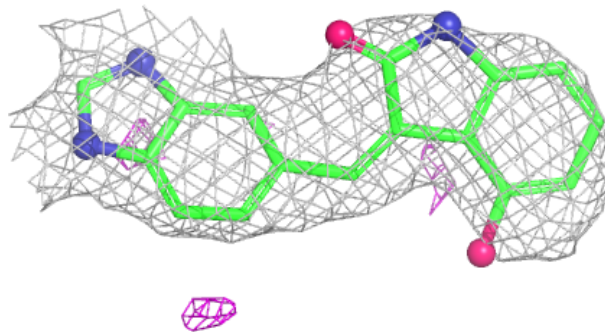
**Electron density around A1D48 E 402:**

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

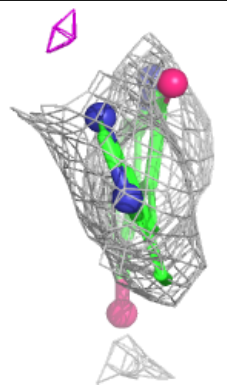
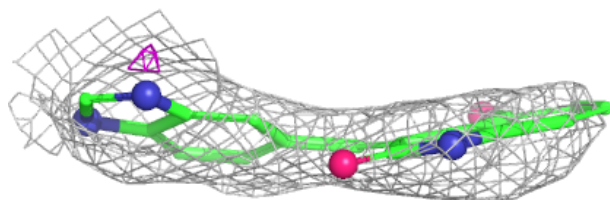
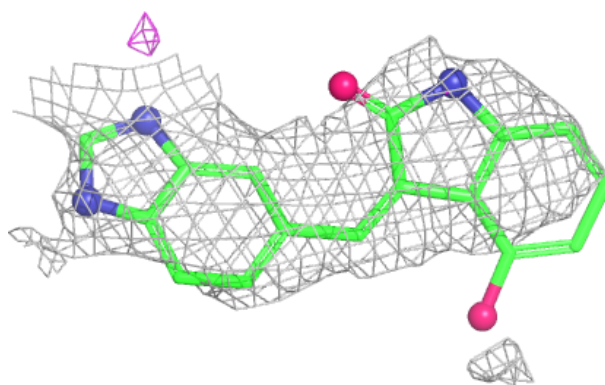


Electron density around A1D48 I 402:

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

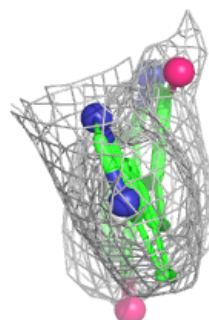
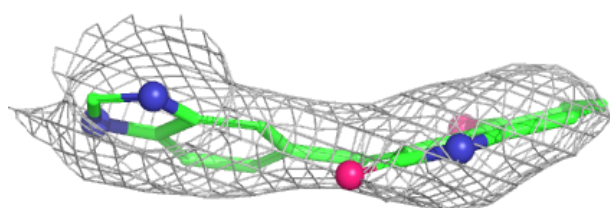
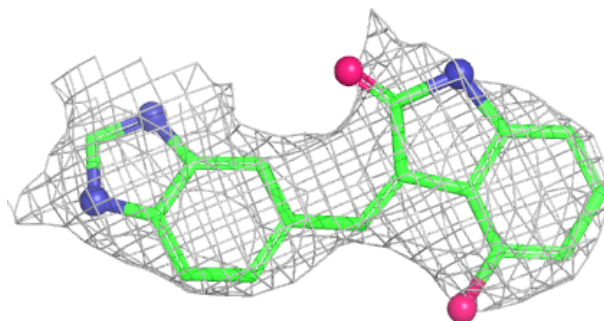
**Electron density around A1D48 L 402:**

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

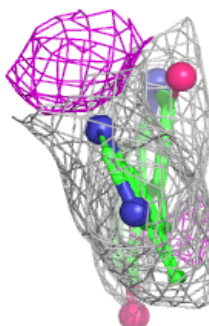
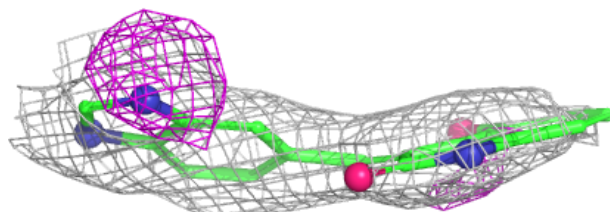
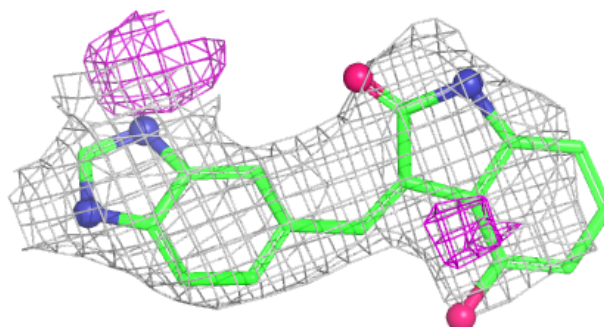


Electron density around A1D48 F 402:

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

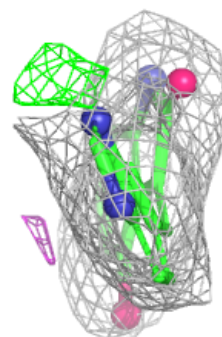
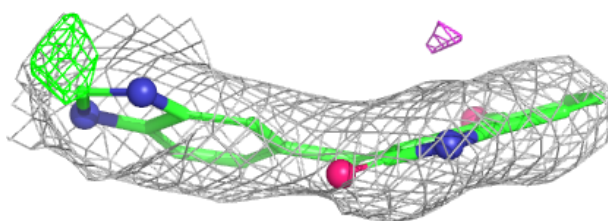
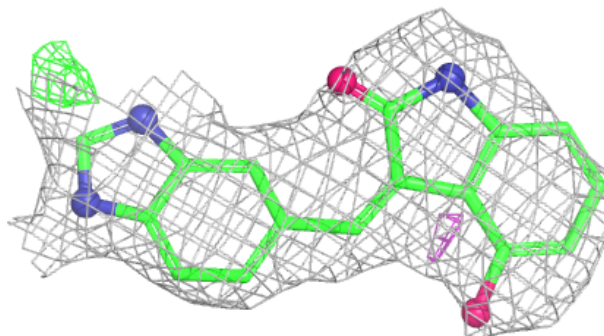
**Electron density around A1D48 A 402:**

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

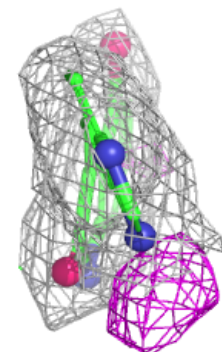
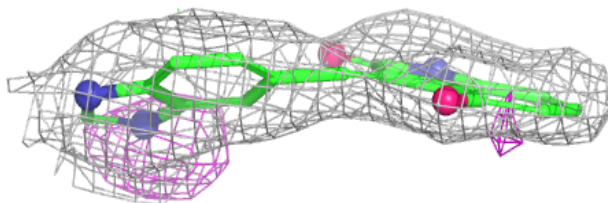
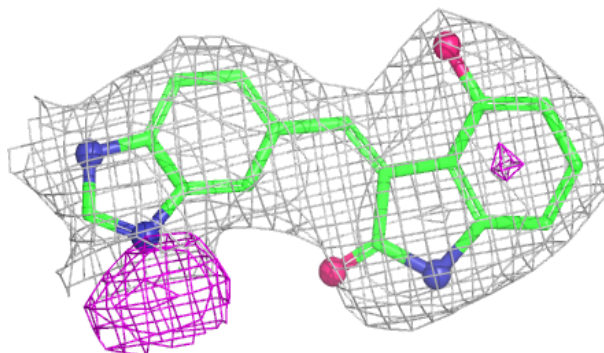


Electron density around A1D48 K 402:

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

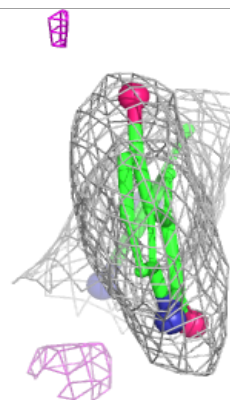
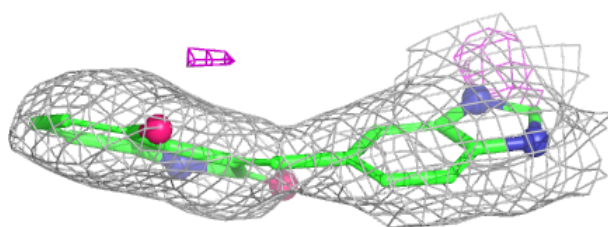
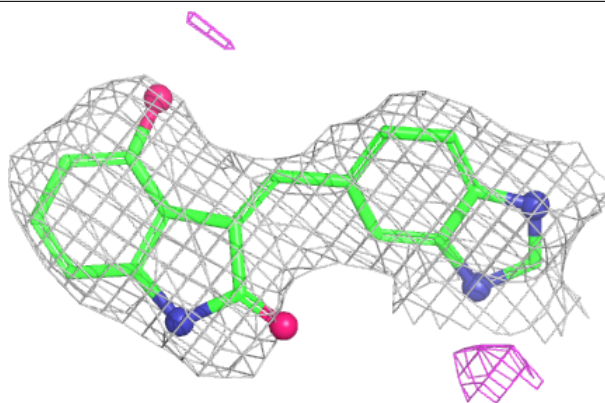
**Electron density around A1D48 B 402:**

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

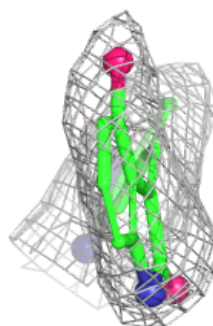
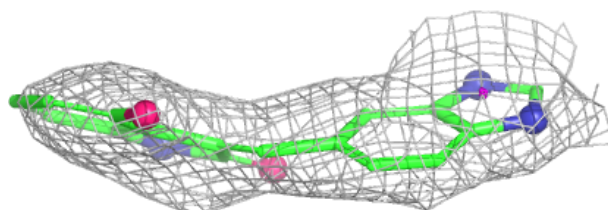
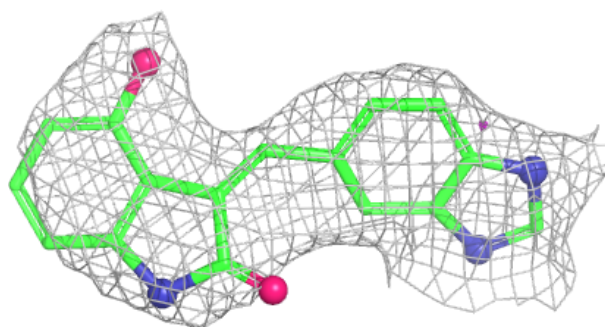


Electron density around A1D48 D 402:

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

**Electron density around A1D48 C 402:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.