



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:36 AM UTC

PDB ID : 8XGY / pdb_00008xgy
Title : Crystal structure of human Golgi resident glutaminyl cyclase in complex with (R,Z)-3-((1H-benzo[d]imidazol-5-yl)methylene)-4-((1-acetylpyrrolidin-3-yl)oxy)indolin-2-one
Authors : Li, G.-B.; Wang, X.-Y.
Deposited on : 2023-12-16
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:

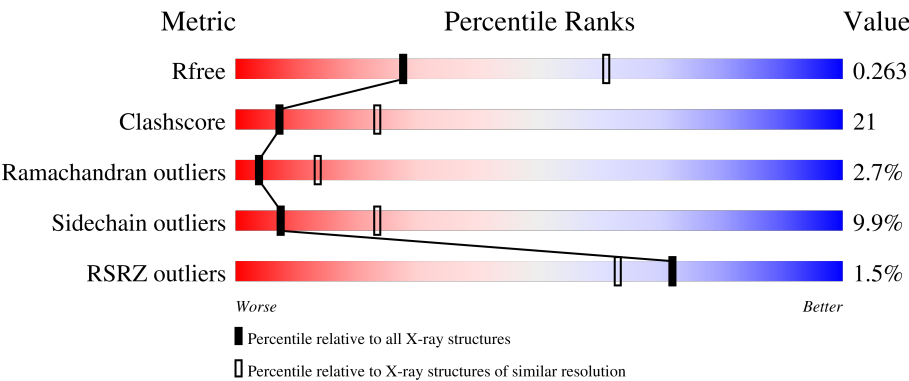
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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	2% 56% 36% 5%
1	B	329	2% 50% 39% 8%
1	C	329	% 59% 32% 6%
1	D	329	% 60% 33% 5%

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Mol	Chain	Length	Quality of chain
1	E	329	
1	F	329	
1	G	329	
1	H	329	
1	I	329	
1	J	329	
1	K	329	
1	L	329	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	L	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31701 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).

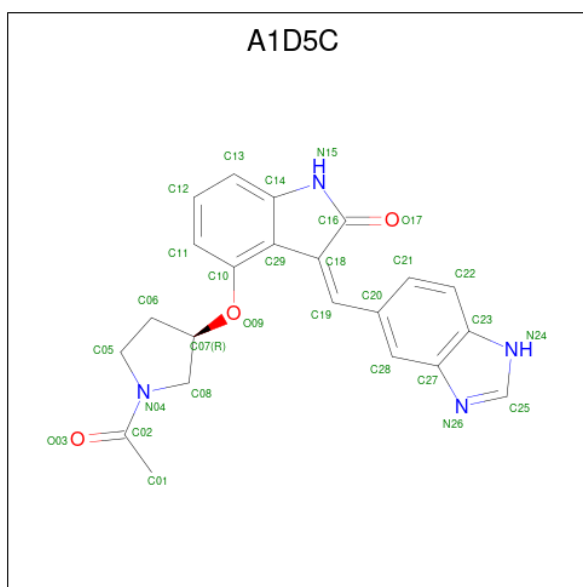
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

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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-[(3 {R})-1-ethanoylpyrrolidin-3-yl]oxy-1 {H}-indol-2-one (CCD ID: A1D5C) (formula: C₂₂H₂₀N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 29 22 4 3	0	0
3	A	1	Total C N O 29 22 4 3	0	0
3	C	1	Total C N O 29 22 4 3	0	0
3	D	1	Total C N O 29 22 4 3	0	0
3	E	1	Total C N O 29 22 4 3	0	0
3	F	1	Total C N O 29 22 4 3	0	0
3	G	1	Total C N O 29 22 4 3	0	0
3	H	1	Total C N O 29 22 4 3	0	0
3	I	1	Total C N O 29 22 4 3	0	0
3	J	1	Total C N O 29 22 4 3	0	0
3	K	1	Total C N O 29 22 4 3	0	0
3	L	1	Total C N O 29 22 4 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total O 5 5	0	0
4	A	1	Total O 1 1	0	0
4	C	3	Total O 3 3	0	0
4	D	1	Total O 1 1	0	0
4	E	2	Total O 2 2	0	0
4	F	3	Total O 3 3	0	0
4	G	1	Total O 1 1	0	0
4	H	1	Total O 1 1	0	0

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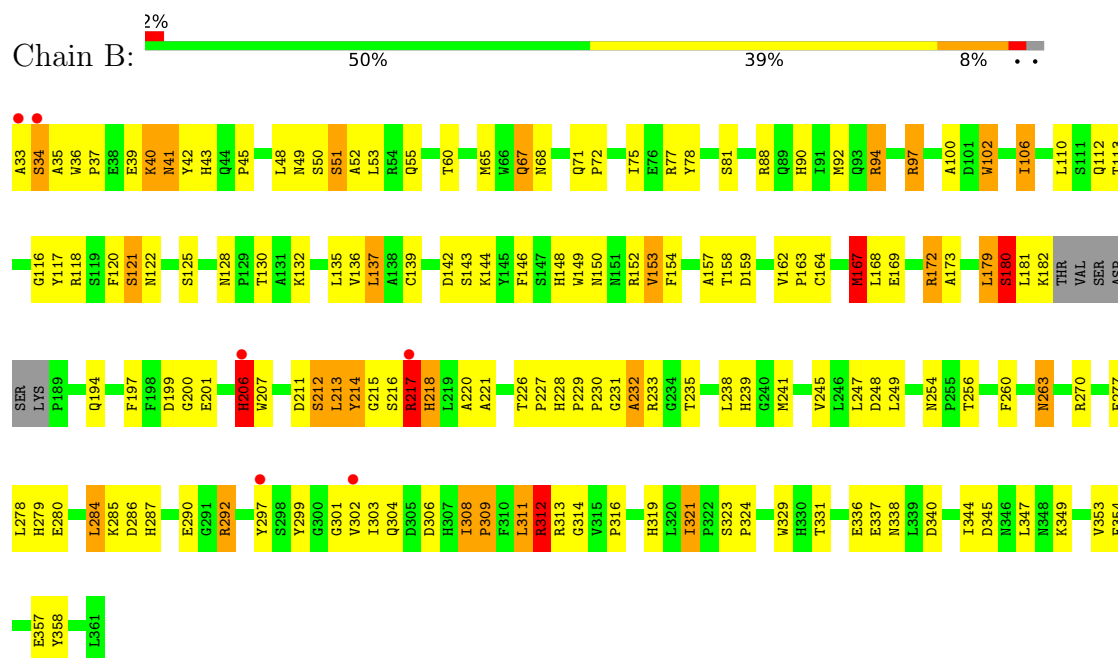
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	3	Total	O	0	0
			3	3		
4	L	1	Total	O	0	0
			1	1		

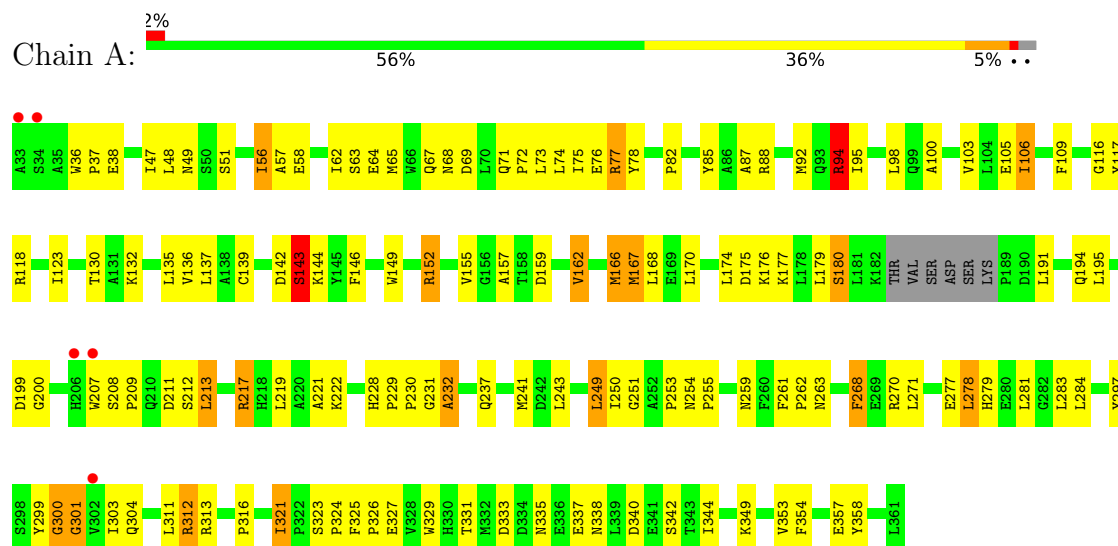
3 Residue-property plots

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.

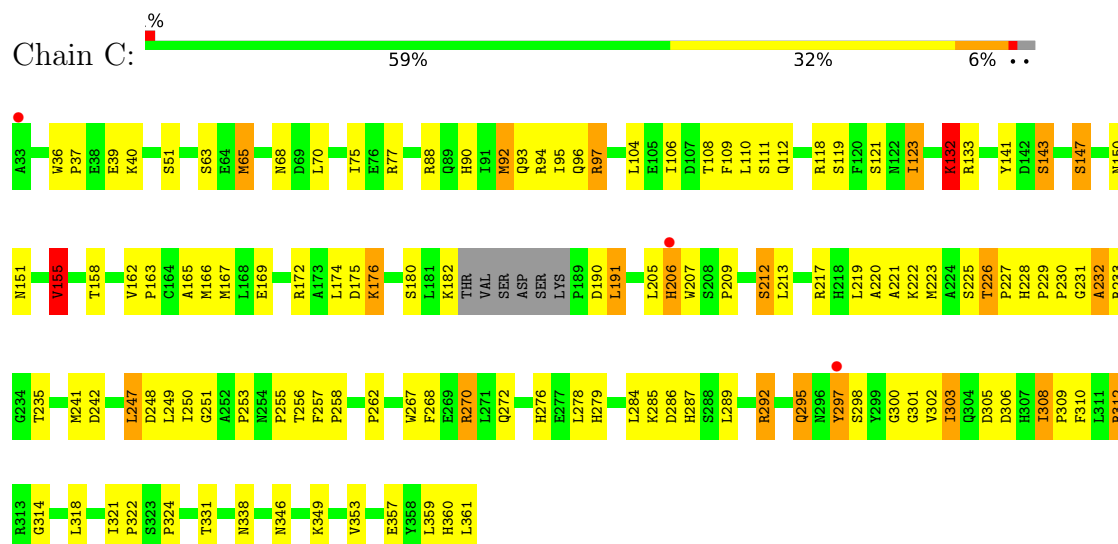
• Molecule 1: Glutaminyl-peptide cyclotransferase



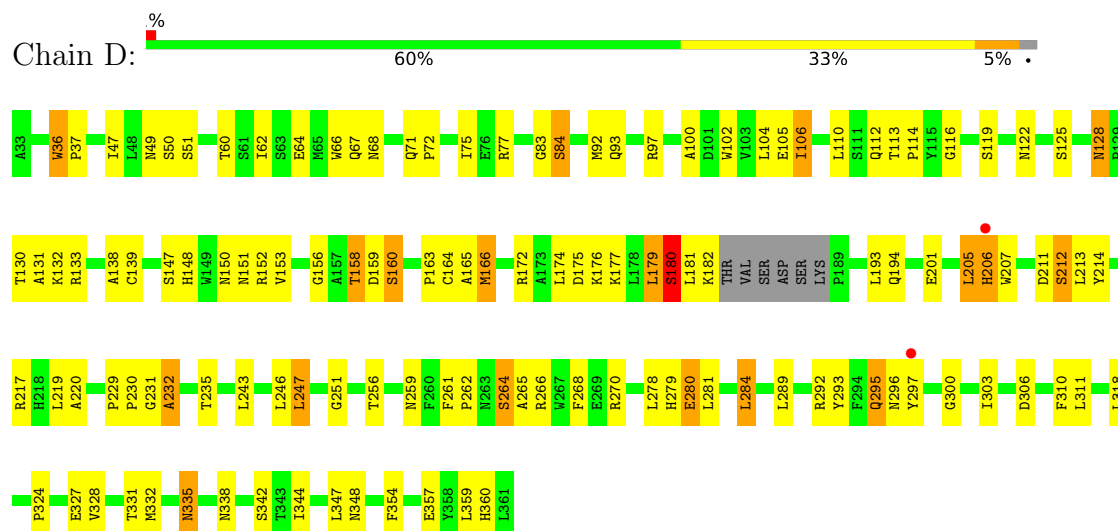
• Molecule 1: Glutaminyl-peptide cyclotransferase



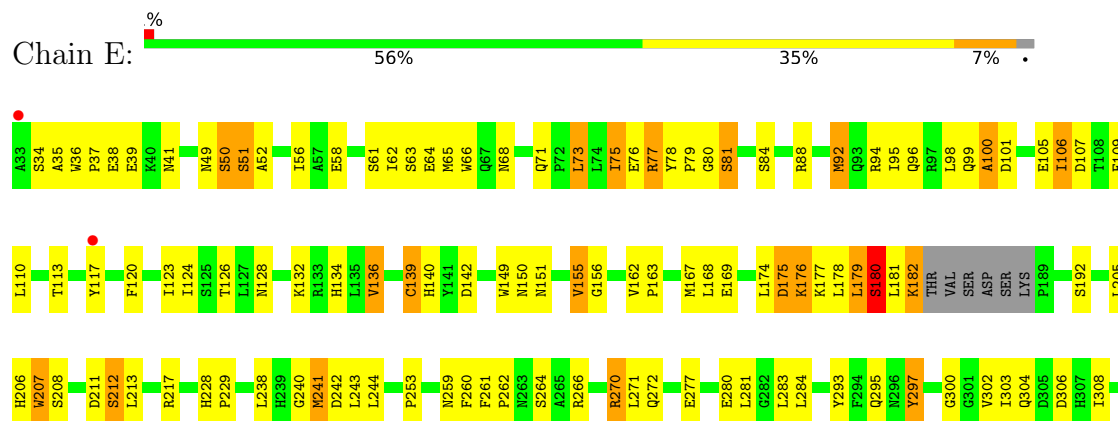
• Molecule 1: Glutaminyl-peptide cyclotransferase



• Molecule 1: Glutaminyl-peptide cyclotransferase

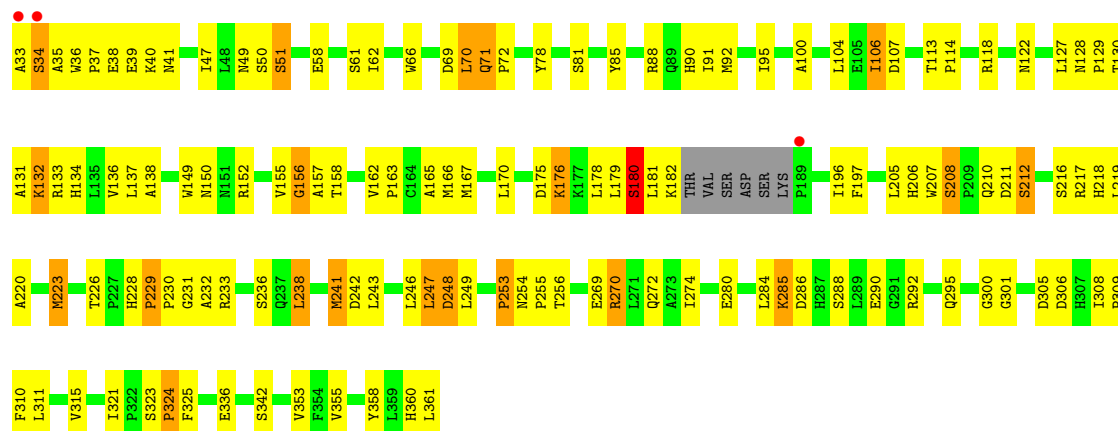


• Molecule 1: Glutaminyl-peptide cyclotransferase

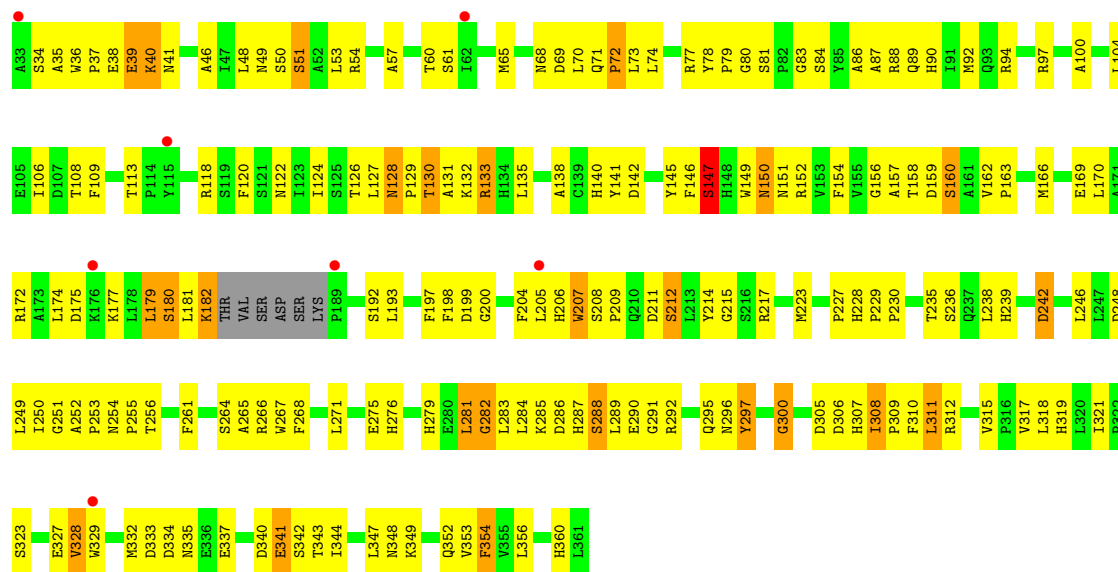
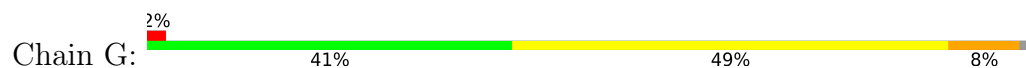




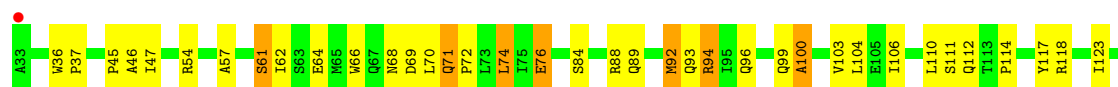
• Molecule 1: Glutaminyl-peptide cyclotransferase

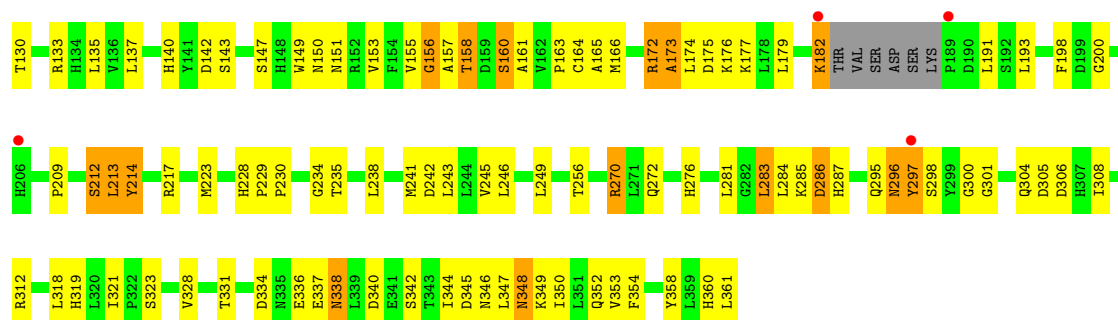


• Molecule 1: Glutaminyl-peptide cyclotransferase

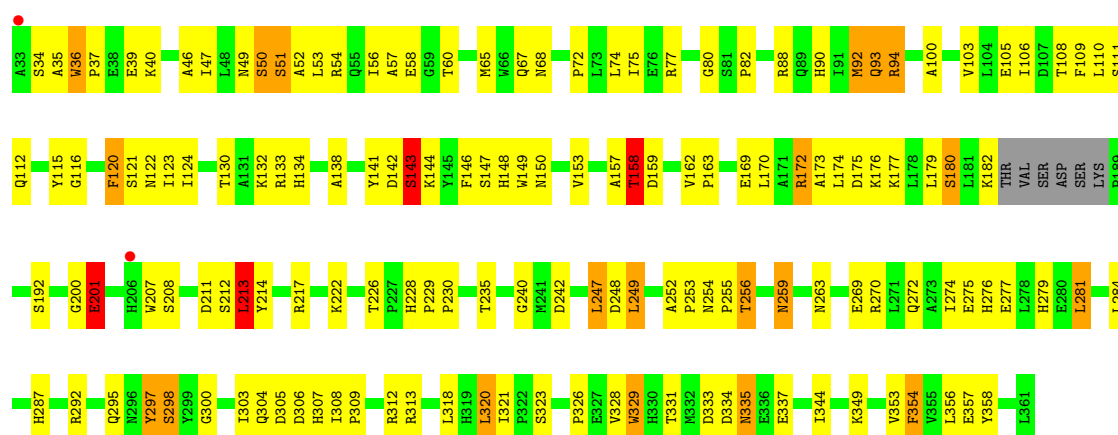


• Molecule 1: Glutaminyl-peptide cyclotransferase

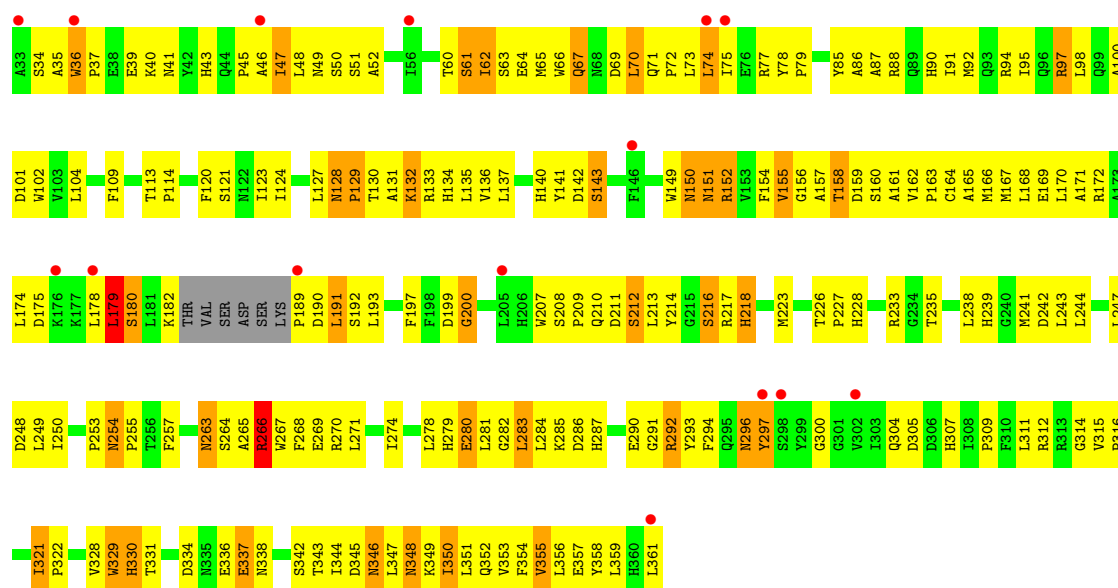




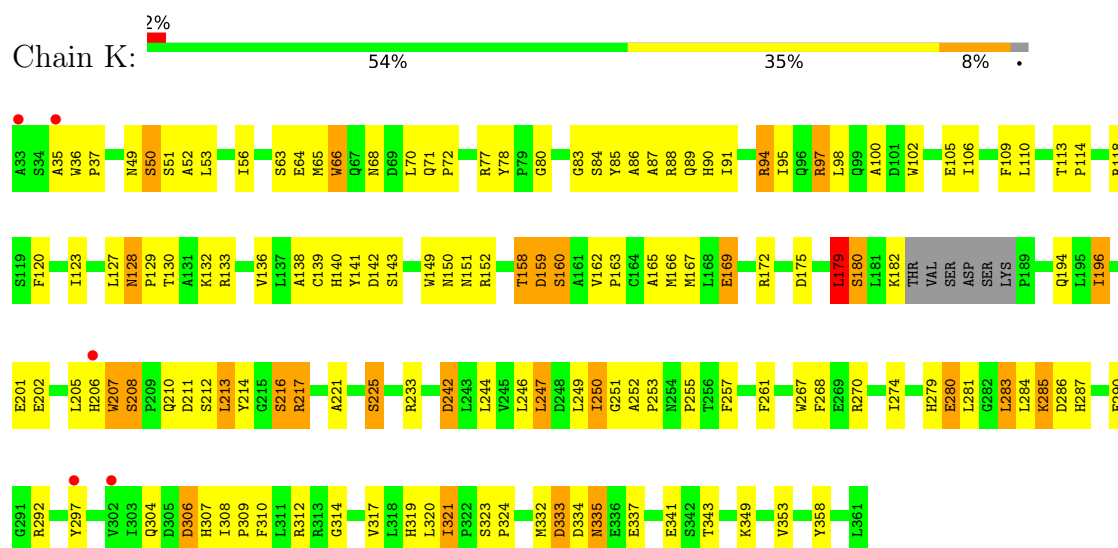
• Molecule 1: Glutaminyl-peptide cyclotransferase



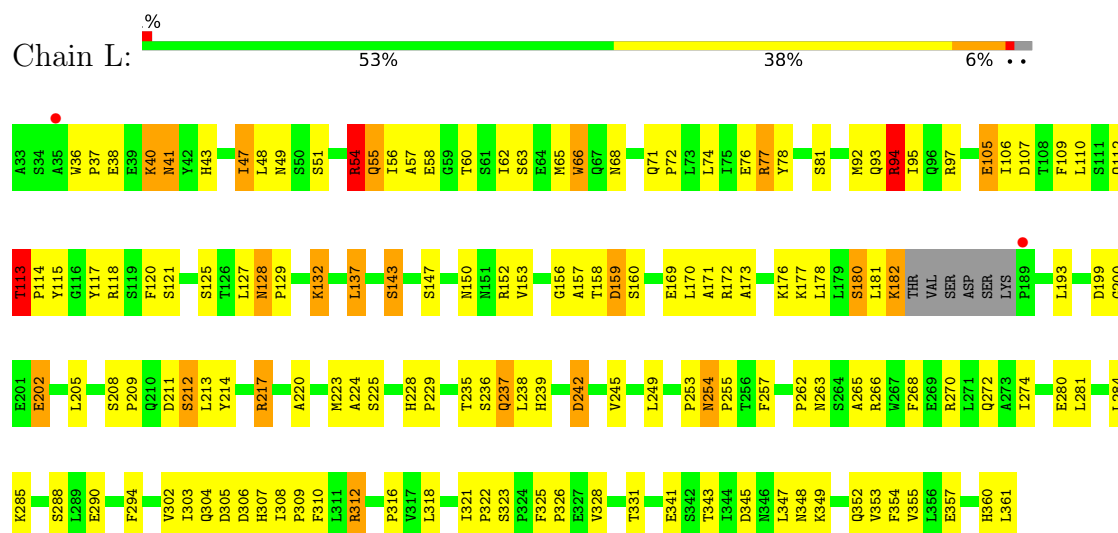
• Molecule 1: Glutaminyl-peptide cyclotransferase



• 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	83.72Å 217.25Å 242.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.12 – 2.81 78.12 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.12-2.81) 99.8 (78.12-2.81)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.188 , 0.258 0.200 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.7	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	31701	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: ZN, A1D5C

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	2.18	58/2687 (2.2%)	1.27	3/3656 (0.1%)
1	B	2.20	61/2687 (2.3%)	1.32	10/3656 (0.3%)
1	C	2.09	42/2687 (1.6%)	1.28	6/3656 (0.2%)
1	D	2.06	39/2687 (1.5%)	1.21	8/3656 (0.2%)
1	E	1.98	39/2687 (1.5%)	1.22	3/3656 (0.1%)
1	F	1.87	18/2687 (0.7%)	1.17	2/3656 (0.1%)
1	G	1.27	2/2687 (0.1%)	0.96	0/3656
1	H	1.49	5/2687 (0.2%)	1.08	0/3656
1	I	1.63	14/2687 (0.5%)	1.15	4/3656 (0.1%)
1	J	1.17	0/2687	1.01	0/3656
1	K	1.90	27/2687 (1.0%)	1.20	1/3656 (0.0%)
1	L	1.79	14/2687 (0.5%)	1.25	5/3656 (0.1%)
All	All	1.83	319/32244 (1.0%)	1.18	42/43872 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (319) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	323	SER	CA-C	-11.80	1.42	1.52
1	B	312	ARG	C-O	-11.62	1.09	1.24
1	K	333	ASP	C-O	-10.39	1.10	1.24
1	L	323	SER	CA-C	-9.55	1.44	1.52
1	B	216	SER	CA-C	-9.44	1.41	1.52
1	K	332	MET	C-N	-9.42	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	THR	CB-CG2	-9.04	1.22	1.52
1	K	335	ASN	CB-CG	-8.20	1.31	1.52
1	C	270	ARG	CZ-NH1	-8.08	1.21	1.32
1	K	159	ASP	N-CA	-7.99	1.35	1.46
1	C	256	THR	CB-CG2	-7.99	1.26	1.52
1	A	94	ARG	CZ-NH1	-7.86	1.21	1.32
1	E	323	SER	C-O	-7.82	1.16	1.24
1	B	214	TYR	C-N	-7.52	1.25	1.34
1	K	323	SER	C-O	-7.47	1.15	1.25
1	A	123	ILE	CG1-CD1	-7.39	1.23	1.51
1	A	324	PRO	CB-CG	-7.34	1.22	1.51
1	A	217	ARG	CZ-NH2	-7.27	1.24	1.33
1	C	255	PRO	CB-CG	-7.27	1.13	1.49
1	B	323	SER	C-O	-7.24	1.16	1.25
1	B	139	CYS	CB-SG	-7.24	1.57	1.81
1	B	323	SER	CA-C	-7.20	1.46	1.52
1	L	77	ARG	CZ-NH1	-7.18	1.22	1.32
1	C	324	PRO	CG-CD	-7.15	1.32	1.51
1	D	259	ASN	CG-ND2	-7.14	1.18	1.33
1	A	331	THR	CB-CG2	-7.12	1.29	1.52
1	B	311	LEU	C-N	-7.10	1.23	1.33
1	A	261	PHE	CE1-CZ	-7.05	1.17	1.38
1	E	142	ASP	CB-CG	-7.05	1.34	1.52
1	K	324	PRO	CB-CG	-6.95	1.24	1.51
1	D	139	CYS	CB-SG	-6.94	1.58	1.81
1	B	254	ASN	CA-C	-6.93	1.49	1.53
1	B	329	TRP	CD1-NE1	-6.92	1.23	1.37
1	F	106	ILE	CB-CG2	-6.88	1.29	1.52
1	D	106	ILE	CG1-CD1	-6.84	1.25	1.51
1	D	62	ILE	CB-CG2	-6.84	1.29	1.52
1	C	331	THR	CB-CG2	-6.81	1.30	1.52
1	B	164	CYS	CB-SG	-6.74	1.59	1.81
1	B	256	THR	CB-CG2	-6.73	1.30	1.52
1	F	229	PRO	CG-CD	-6.73	1.33	1.51
1	A	69	ASP	CG-OD1	-6.71	1.12	1.25
1	D	256	THR	CB-CG2	-6.66	1.30	1.52
1	C	247	LEU	CG-CD1	-6.62	1.30	1.52
1	A	167	MET	SD-CE	-6.51	1.63	1.79
1	D	324	PRO	CG-CD	-6.50	1.34	1.51
1	B	270	ARG	CG-CD	-6.48	1.32	1.52
1	A	338	ASN	CB-CG	-6.47	1.35	1.52
1	A	166	MET	CG-SD	-6.47	1.64	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	268	PHE	CD2-CE2	-6.47	1.19	1.38
1	B	347	LEU	CG-CD2	-6.46	1.31	1.52
1	I	335	ASN	CB-CG	-6.45	1.35	1.52
1	F	305	ASP	CB-CG	-6.43	1.35	1.52
1	B	142	ASP	CG-OD1	-6.43	1.13	1.25
1	C	338	ASN	CG-ND2	-6.42	1.19	1.33
1	C	292	ARG	CB-CG	-6.42	1.33	1.52
1	A	337	GLU	CG-CD	6.39	1.68	1.52
1	B	120	PHE	CE2-CZ	-6.39	1.19	1.38
1	E	126	THR	CA-CB	-6.38	1.38	1.53
1	B	106	ILE	CG1-CD1	-6.37	1.26	1.51
1	B	121	SER	CB-OG	-6.37	1.29	1.42
1	F	122	ASN	CB-CG	-6.28	1.36	1.52
1	A	76	GLU	CB-CG	-6.28	1.33	1.52
1	A	323	SER	CA-CB	-6.27	1.43	1.53
1	F	69	ASP	CB-CG	-6.24	1.36	1.52
1	K	324	PRO	CG-CD	-6.24	1.34	1.51
1	E	124	ILE	CG1-CD1	-6.24	1.27	1.51
1	A	329	TRP	CE3-CZ3	-6.22	1.20	1.38
1	C	257	PHE	CE2-CZ	-6.22	1.20	1.38
1	B	292	ARG	CB-CG	-6.21	1.33	1.52
1	E	272	GLN	CB-CG	-6.21	1.33	1.52
1	E	241	MET	SD-CE	-6.21	1.64	1.79
1	C	155	VAL	CB-CG2	-6.20	1.32	1.52
1	F	324	PRO	C-N	-6.19	1.20	1.33
1	D	251	GLY	C-N	-6.18	1.24	1.33
1	B	172	ARG	CZ-NH2	-6.16	1.25	1.33
1	A	136	VAL	CB-CG2	-6.13	1.32	1.52
1	B	260	PHE	CD2-CE2	-6.13	1.20	1.38
1	L	212	SER	CA-CB	-6.13	1.41	1.53
1	E	260	PHE	CG-CD2	-6.11	1.26	1.38
1	A	78	TYR	CE1-CZ	-6.10	1.23	1.38
1	A	263	ASN	CB-CG	-6.10	1.36	1.52
1	A	243	LEU	CG-CD1	-6.09	1.32	1.52
1	K	211	ASP	CB-CG	-6.07	1.36	1.52
1	L	77	ARG	CZ-NH2	-6.07	1.25	1.33
1	B	214	TYR	CE2-CZ	-6.05	1.23	1.38
1	A	73	LEU	CA-CB	-6.03	1.43	1.53
1	D	36	TRP	C-N	-6.02	1.26	1.33
1	E	261	PHE	CD1-CE1	-6.00	1.20	1.38
1	D	158	THR	CB-CG2	-5.99	1.32	1.52
1	A	168	LEU	CG-CD1	-5.98	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	324	PRO	CB-CG	-5.98	1.27	1.51
1	B	139	CYS	CA-C	-5.97	1.45	1.52
1	D	335	ASN	CB-CG	-5.96	1.37	1.52
1	A	241	MET	CB-CG	-5.95	1.34	1.52
1	K	66	TRP	CB-CG	-5.92	1.31	1.50
1	L	343	THR	CB-CG2	-5.92	1.33	1.52
1	C	301	GLY	C-N	-5.92	1.23	1.33
1	C	166	MET	SD-CE	-5.91	1.64	1.79
1	B	324	PRO	CA-C	-5.90	1.41	1.52
1	B	338	ASN	CB-CG	-5.87	1.37	1.52
1	C	324	PRO	C-O	-5.87	1.11	1.23
1	A	324	PRO	CG-CD	-5.87	1.35	1.51
1	E	316	PRO	CG-CD	-5.87	1.30	1.50
1	A	316	PRO	CG-CD	-5.85	1.30	1.50
1	A	321	ILE	CG1-CD1	-5.85	1.28	1.51
1	C	318	LEU	C-N	-5.85	1.24	1.33
1	F	241	MET	SD-CE	-5.84	1.65	1.79
1	D	122	ASN	CG-ND2	-5.84	1.21	1.33
1	D	357	GLU	CG-CD	-5.81	1.37	1.52
1	D	327	GLU	C-N	-5.81	1.27	1.33
1	B	331	THR	CB-CG2	-5.81	1.33	1.52
1	A	262	PRO	CB-CG	-5.81	1.20	1.49
1	C	253	PRO	CG-CD	-5.81	1.31	1.50
1	C	359	LEU	CG-CD2	-5.80	1.33	1.52
1	B	157	ALA	CA-C	-5.80	1.45	1.52
1	C	123	ILE	CB-CG2	-5.78	1.33	1.52
1	C	318	LEU	C-O	-5.78	1.17	1.24
1	I	320	LEU	CG-CD2	-5.77	1.33	1.52
1	A	194	GLN	CD-NE2	-5.77	1.21	1.33
1	E	260	PHE	CD2-CE2	-5.77	1.21	1.38
1	G	323	SER	CA-C	-5.75	1.45	1.52
1	I	120	PHE	CE1-CZ	-5.75	1.21	1.38
1	F	253	PRO	C-N	-5.75	1.21	1.33
1	A	135	LEU	CG-CD1	-5.74	1.33	1.52
1	E	311	LEU	CG-CD1	-5.74	1.33	1.52
1	C	174	LEU	CG-CD2	-5.73	1.33	1.52
1	A	312	ARG	CZ-NH2	5.73	1.40	1.33
1	D	293	TYR	CE2-CZ	-5.73	1.24	1.38
1	D	293	TYR	CE1-CZ	-5.73	1.24	1.38
1	E	270	ARG	C-N	-5.73	1.26	1.34
1	K	169	GLU	C-N	-5.72	1.26	1.34
1	F	255	PRO	CG-CD	-5.71	1.31	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	241	MET	SD-CE	-5.71	1.65	1.79
1	B	139	CYS	C-N	-5.71	1.25	1.33
1	F	248	ASP	CB-CG	-5.71	1.37	1.52
1	B	60	THR	CB-CG2	-5.71	1.33	1.52
1	C	278	LEU	CG-CD2	-5.70	1.33	1.52
1	A	283	LEU	CG-CD2	-5.70	1.33	1.52
1	A	261	PHE	CD2-CE2	-5.69	1.21	1.38
1	A	253	PRO	CG-CD	-5.68	1.31	1.50
1	I	82	PRO	CG-CD	-5.67	1.31	1.50
1	B	270	ARG	CZ-NH1	-5.67	1.24	1.32
1	K	250	ILE	CB-CG1	-5.67	1.42	1.53
1	D	268	PHE	CD1-CE1	-5.66	1.21	1.38
1	E	261	PHE	CE1-CZ	-5.64	1.21	1.38
1	K	244	LEU	CG-CD2	-5.63	1.33	1.52
1	E	264	SER	CA-CB	-5.62	1.45	1.53
1	H	241	MET	SD-CE	-5.62	1.65	1.79
1	L	113	THR	C-N	-5.61	1.20	1.33
1	C	172	ARG	C-N	-5.61	1.26	1.33
1	C	268	PHE	CD1-CE1	-5.60	1.21	1.38
1	L	323	SER	C-O	-5.60	1.18	1.25
1	C	324	PRO	CB-CG	-5.59	1.29	1.51
1	K	180	SER	CA-C	-5.59	1.45	1.52
1	K	257	PHE	CD2-CE2	-5.59	1.21	1.38
1	C	165	ALA	C-O	-5.58	1.16	1.24
1	D	354	PHE	CE1-CZ	-5.57	1.22	1.38
1	D	166	MET	SD-CE	-5.57	1.65	1.79
1	D	133	ARG	CB-CG	-5.57	1.35	1.52
1	F	216	SER	CB-OG	-5.57	1.31	1.42
1	E	344	ILE	CB-CG2	-5.56	1.34	1.52
1	A	268	PHE	CE1-CZ	-5.56	1.22	1.38
1	D	235	THR	CB-CG2	-5.56	1.34	1.52
1	D	194	GLN	CG-CD	-5.55	1.38	1.52
1	D	243	LEU	CG-CD1	-5.55	1.34	1.52
1	F	246	LEU	CG-CD2	-5.55	1.34	1.52
1	G	160	SER	CA-C	-5.55	1.41	1.52
1	C	65	MET	CB-CG	-5.54	1.35	1.52
1	B	102	TRP	CE3-CZ3	-5.54	1.22	1.38
1	A	281	LEU	CG-CD2	-5.54	1.34	1.52
1	E	355	VAL	CB-CG1	-5.53	1.34	1.52
1	H	318	LEU	CG-CD1	-5.53	1.34	1.52
1	B	312	ARG	N-CA	-5.52	1.39	1.46
1	K	310	PHE	CE1-CZ	-5.51	1.22	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	218	HIS	CA-CB	-5.50	1.44	1.53
1	K	324	PRO	C-O	-5.50	1.12	1.23
1	A	155	VAL	CB-CG2	-5.50	1.34	1.52
1	E	243	LEU	CG-CD2	-5.50	1.34	1.52
1	A	358	TYR	CE2-CZ	-5.49	1.25	1.38
1	A	82	PRO	CG-CD	-5.49	1.32	1.50
1	A	326	PRO	CB-CG	-5.49	1.22	1.49
1	E	322	PRO	CG-CD	-5.47	1.32	1.50
1	C	257	PHE	CE1-CZ	-5.47	1.22	1.38
1	F	270	ARG	C-N	-5.46	1.26	1.33
1	B	167	MET	CA-C	-5.46	1.45	1.52
1	A	94	ARG	CZ-NH2	-5.46	1.26	1.33
1	A	123	ILE	CB-CG2	-5.45	1.34	1.52
1	E	355	VAL	CB-CG2	-5.44	1.34	1.52
1	B	120	PHE	CG-CD1	-5.44	1.27	1.38
1	I	354	PHE	CG-CD1	-5.44	1.27	1.38
1	B	323	SER	CA-CB	-5.44	1.45	1.53
1	A	56	ILE	C-N	-5.44	1.26	1.33
1	E	139	CYS	CB-SG	-5.43	1.63	1.81
1	E	243	LEU	N-CA	-5.43	1.40	1.46
1	D	266	ARG	CZ-NH1	-5.43	1.25	1.32
1	I	138	ALA	C-O	-5.43	1.17	1.23
1	K	77	ARG	CZ-NH1	-5.42	1.25	1.32
1	B	135	LEU	CG-CD1	-5.41	1.34	1.52
1	E	77	ARG	CZ-NH1	-5.40	1.25	1.32
1	D	122	ASN	CG-OD1	-5.40	1.13	1.23
1	A	271	LEU	CG-CD1	-5.39	1.34	1.52
1	A	249	LEU	CG-CD2	-5.39	1.34	1.52
1	L	94	ARG	CZ-NH1	-5.39	1.25	1.32
1	D	344	ILE	CB-CG2	-5.39	1.34	1.52
1	A	219	LEU	CG-CD2	-5.38	1.34	1.52
1	D	164	CYS	CB-SG	-5.38	1.63	1.81
1	F	134	HIS	CA-CB	-5.37	1.42	1.54
1	L	214	TYR	C-N	-5.37	1.25	1.33
1	I	256	THR	C-N	-5.35	1.25	1.33
1	C	268	PHE	CE1-CZ	-5.35	1.22	1.38
1	E	73	LEU	CG-CD2	-5.34	1.34	1.52
1	K	317	VAL	CB-CG1	-5.34	1.34	1.52
1	B	194	GLN	CB-CG	-5.33	1.36	1.52
1	B	154	PHE	CE2-CZ	-5.33	1.22	1.38
1	B	324	PRO	CB-CG	-5.33	1.30	1.51
1	D	193	LEU	CG-CD2	-5.32	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	VAL	C-N	-5.31	1.21	1.33
1	D	318	LEU	CG-CD1	-5.31	1.35	1.52
1	K	268	PHE	CE1-CZ	-5.31	1.22	1.38
1	B	249	LEU	CG-CD2	-5.31	1.35	1.52
1	K	306	ASP	C-O	-5.31	1.17	1.24
1	C	251	GLY	CA-C	-5.30	1.44	1.51
1	C	167	MET	CB-CG	-5.30	1.36	1.52
1	C	258	PRO	CB-CG	-5.30	1.23	1.49
1	H	245	VAL	CB-CG1	-5.30	1.35	1.52
1	B	214	TYR	CG-CD2	-5.29	1.28	1.39
1	K	283	LEU	CG-CD2	-5.29	1.35	1.52
1	A	195	LEU	CA-CB	-5.29	1.41	1.53
1	B	122	ASN	CG-ND2	-5.29	1.22	1.33
1	E	259	ASN	CB-CG	-5.29	1.38	1.52
1	B	45	PRO	CB-CG	-5.29	1.23	1.49
1	B	41	ASN	CB-CG	-5.28	1.38	1.52
1	D	165	ALA	CA-CB	-5.28	1.44	1.53
1	I	143	SER	C-N	-5.28	1.25	1.33
1	I	120	PHE	CG-CD1	-5.27	1.27	1.38
1	K	321	ILE	CG1-CD1	-5.26	1.31	1.51
1	A	162	VAL	CB-CG1	-5.25	1.35	1.52
1	C	257	PHE	CG-CD1	-5.24	1.27	1.38
1	A	137	LEU	CG-CD1	-5.23	1.35	1.52
1	C	262	PRO	C-N	-5.23	1.26	1.33
1	L	285	LYS	C-N	-5.22	1.26	1.33
1	E	136	VAL	CB-CG2	-5.22	1.35	1.52
1	B	321	ILE	CG1-CD1	-5.22	1.31	1.51
1	F	228	HIS	CA-C	-5.22	1.47	1.53
1	H	214	TYR	C-N	-5.22	1.25	1.33
1	B	102	TRP	CE2-CZ2	-5.22	1.28	1.39
1	E	41	ASN	CG-OD1	-5.20	1.13	1.23
1	K	343	THR	CB-CG2	-5.20	1.35	1.52
1	B	173	ALA	C-N	-5.20	1.24	1.33
1	D	77	ARG	CB-CG	-5.20	1.36	1.52
1	A	344	ILE	CG1-CD1	-5.19	1.31	1.51
1	A	152	ARG	CA-CB	-5.19	1.44	1.53
1	A	358	TYR	CD2-CE2	-5.19	1.23	1.38
1	B	213	LEU	C-N	-5.19	1.26	1.34
1	E	264	SER	CB-OG	-5.19	1.31	1.42
1	A	325	PHE	CE2-CZ	-5.18	1.23	1.38
1	D	214	TYR	CE1-CZ	-5.18	1.25	1.38
1	E	319	HIS	C-O	-5.18	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	LEU	CG-CD2	-5.18	1.35	1.52
1	I	103	VAL	CB-CG2	-5.17	1.35	1.52
1	D	331	THR	CB-CG2	-5.17	1.35	1.52
1	A	103	VAL	CB-CG1	-5.17	1.35	1.52
1	A	213	LEU	CG-CD1	-5.17	1.35	1.52
1	B	309	PRO	CB-CG	-5.16	1.23	1.49
1	A	243	LEU	CG-CD2	-5.16	1.35	1.52
1	I	249	LEU	CG-CD2	-5.16	1.35	1.52
1	B	358	TYR	CE1-CZ	-5.16	1.25	1.38
1	L	217	ARG	C-N	-5.16	1.26	1.33
1	C	359	LEU	CG-CD1	-5.15	1.35	1.52
1	B	212	SER	C-N	-5.14	1.26	1.33
1	C	310	PHE	CE2-CZ	-5.14	1.23	1.38
1	K	261	PHE	CE2-CZ	-5.14	1.23	1.38
1	A	143	SER	C-N	-5.13	1.26	1.33
1	C	226	THR	CB-CG2	-5.13	1.35	1.52
1	B	340	ASP	C-O	-5.12	1.18	1.23
1	D	266	ARG	CZ-NH2	-5.12	1.26	1.33
1	E	325	PHE	CE2-CZ	-5.12	1.23	1.38
1	B	354	PHE	CG-CD2	-5.11	1.28	1.38
1	H	198	PHE	CD1-CE1	-5.11	1.23	1.38
1	C	346	ASN	CG-ND2	-5.11	1.22	1.33
1	D	172	ARG	CZ-NH2	-5.11	1.26	1.33
1	E	271	LEU	CG-CD1	-5.10	1.35	1.52
1	E	329	TRP	CD2-CE2	-5.10	1.32	1.41
1	I	344	ILE	CG1-CD1	-5.10	1.31	1.51
1	L	214	TYR	CE2-CZ	-5.09	1.26	1.38
1	L	157	ALA	CA-CB	-5.09	1.45	1.53
1	C	287	HIS	C-O	-5.09	1.17	1.23
1	D	77	ARG	CA-CB	-5.08	1.49	1.53
1	E	266	ARG	CZ-NH1	-5.08	1.25	1.32
1	B	347	LEU	CG-CD1	-5.08	1.35	1.52
1	B	316	PRO	CG-CD	-5.08	1.33	1.50
1	A	139	CYS	C-O	-5.08	1.19	1.24
1	C	250	ILE	CG1-CD1	-5.08	1.31	1.51
1	K	139	CYS	C-O	-5.08	1.19	1.24
1	L	66	TRP	CE2-CZ2	-5.07	1.29	1.39
1	B	142	ASP	CB-CG	-5.07	1.39	1.52
1	K	196	ILE	C-N	-5.07	1.24	1.33
1	C	322	PRO	CB-CG	-5.07	1.24	1.49
1	A	142	ASP	CG-OD1	-5.06	1.15	1.25
1	A	95	ILE	CG1-CD1	-5.06	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	LEU	C-N	-5.06	1.26	1.33
1	I	275	GLU	CG-CD	-5.06	1.39	1.52
1	D	261	PHE	CE1-CZ	-5.06	1.23	1.38
1	E	244	LEU	CG-CD1	-5.05	1.35	1.52
1	E	350	ILE	CB-CG2	-5.05	1.35	1.52
1	C	268	PHE	CE2-CZ	-5.05	1.23	1.38
1	F	223	MET	CG-SD	-5.03	1.68	1.80
1	F	315	VAL	CB-CG1	-5.03	1.35	1.52
1	D	264	SER	CB-OG	-5.03	1.32	1.42
1	B	357	GLU	CA-C	-5.02	1.46	1.52
1	I	122	ASN	CG-ND2	-5.02	1.22	1.33
1	E	41	ASN	CB-CG	-5.02	1.39	1.52
1	D	270	ARG	CZ-NH1	-5.02	1.25	1.32
1	B	48	LEU	CG-CD2	-5.01	1.36	1.52
1	B	163	PRO	N-CA	-5.01	1.41	1.47
1	E	316	PRO	N-CA	-5.01	1.41	1.47
1	C	267	TRP	CZ2-CH2	-5.01	1.27	1.37
1	E	253	PRO	CG-CD	-5.00	1.33	1.50
1	E	293	TYR	CE1-CZ	-5.00	1.26	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	333	ASP	O-C-N	-8.34	111.49	122.59
1	L	159	ASP	CB-CG-OD1	-7.49	101.19	118.40
1	B	218	HIS	N-CA-C	7.17	131.07	111.00
1	B	216	SER	N-CA-C	-7.07	97.68	109.07
1	L	159	ASP	CB-CG-OD2	6.57	133.51	118.40
1	A	94	ARG	NE-CZ-NH2	6.53	125.08	119.20
1	L	202	GLU	CG-CD-OE1	-6.51	103.42	118.40
1	B	312	ARG	O-C-N	-6.28	114.24	122.59
1	L	54	ARG	CB-CG-CD	-6.08	97.32	111.30
1	C	92	MET	CG-SD-CE	-6.00	87.69	100.90
1	I	142	ASP	CA-CB-CG	6.00	118.60	112.60
1	I	158	THR	CA-C-N	5.99	130.86	122.41
1	I	158	THR	C-N-CA	5.99	130.86	122.41
1	D	335	ASN	N-CA-C	5.91	117.57	109.18
1	B	217	ARG	CA-C-N	5.77	132.08	121.70
1	B	217	ARG	C-N-CA	5.77	132.08	121.70
1	C	132	LYS	CB-CA-C	-5.43	101.45	110.68
1	E	329	TRP	CA-C-N	5.36	129.96	122.36
1	E	329	TRP	C-N-CA	5.36	129.96	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	THR	CA-C-N	5.35	130.59	123.20
1	D	158	THR	C-N-CA	5.35	130.59	123.20
1	B	311	LEU	CA-C-N	-5.32	111.39	121.54
1	B	311	LEU	C-N-CA	-5.32	111.39	121.54
1	A	324	PRO	CB-CG-CD	5.28	117.55	105.40
1	F	33	ALA	CA-C-N	-5.22	113.49	121.74
1	F	33	ALA	C-N-CA	-5.22	113.49	121.74
1	D	328	VAL	N-CA-C	-5.19	107.41	112.29
1	B	206	HIS	CA-C-N	5.15	131.37	121.54
1	B	206	HIS	C-N-CA	5.15	131.37	121.54
1	C	141	TYR	CA-CB-CG	5.11	123.10	113.90
1	I	115	TYR	CA-CB-CG	5.10	123.08	113.90
1	C	270	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	D	131	ALA	CA-C-N	5.08	127.39	120.54
1	D	131	ALA	C-N-CA	5.08	127.39	120.54
1	C	272	GLN	CA-C-N	5.07	127.84	120.79
1	C	272	GLN	C-N-CA	5.07	127.84	120.79
1	B	153	VAL	N-CA-C	5.06	115.77	108.48
1	D	206	HIS	CA-C-N	5.04	131.17	121.54
1	D	206	HIS	C-N-CA	5.04	131.17	121.54
1	A	159	ASP	O-C-N	-5.03	117.31	122.64
1	E	80	GLY	N-CA-C	-5.01	107.60	114.67
1	L	54	ARG	NE-CZ-NH2	-5.00	114.69	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	215	GLY	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2610	0	2529	68	0
1	B	2610	0	2529	98	0
1	C	2610	0	2529	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2610	0	2529	63	0
1	E	2610	0	2529	78	0
1	F	2610	0	2529	113	0
1	G	2610	0	2529	157	0
1	H	2610	0	2529	105	0
1	I	2610	0	2529	106	0
1	J	2610	0	2529	238	0
1	K	2610	0	2529	92	0
1	L	2610	0	2529	130	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
2	D	1	0	0	1	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	2	0
3	A	29	0	0	2	0
3	B	29	0	0	3	0
3	C	29	0	0	1	0
3	D	29	0	0	2	0
3	E	29	0	0	0	0
3	F	29	0	0	0	0
3	G	29	0	0	4	0
3	H	29	0	0	1	0
3	I	29	0	0	2	0
3	J	29	0	0	2	0
3	K	29	0	0	5	0
3	L	29	0	0	5	0
4	A	1	0	0	2	0
4	B	5	0	0	1	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	1	0
4	G	1	0	0	1	0
4	H	1	0	0	0	0
4	K	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
All	All	31701	0	30348	1279	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 21.

All (1279) 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)
3:B:402:A1D5C:C07	3:B:402:A1D5C:C08	1.77	1.51
3:D:402:A1D5C:C07	3:D:402:A1D5C:C08	1.77	1.49
3:C:402:A1D5C:C08	3:C:402:A1D5C:C07	1.74	1.38
3:A:402:A1D5C:C07	3:A:402:A1D5C:C08	1.74	1.34
1:B:217:ARG:HB2	1:B:220:ALA:CB	1.67	1.24
1:B:217:ARG:CB	1:B:220:ALA:HB3	1.77	1.13
1:F:34:SER:OG	1:L:280:GLU:OE1	1.67	1.10
1:B:217:ARG:HB3	1:B:309:PRO:HB3	1.36	1.06
1:J:66:TRP:NE1	1:J:336:GLU:OE2	1.88	1.05
1:F:130:THR:O	1:F:132:LYS:N	1.93	1.02
1:L:212:SER:O	1:L:217:ARG:NH1	1.96	0.97
1:B:217:ARG:O	1:B:217:ARG:NE	1.97	0.97
1:F:232:ALA:O	1:L:54:ARG:NH2	1.96	0.97
1:B:217:ARG:HB2	1:B:220:ALA:HB3	0.98	0.96
1:B:217:ARG:CB	1:B:309:PRO:HB3	1.97	0.95
1:J:130:THR:O	1:J:132:LYS:N	2.00	0.95
1:L:202:GLU:OE2	3:L:402:A1D5C:N26	2.01	0.94
1:C:132:LYS:HZ2	1:C:132:LYS:HB2	1.31	0.93
1:H:347:LEU:O	1:H:349:LYS:N	2.01	0.93
1:J:265:ALA:O	1:J:268:PHE:N	2.01	0.92
1:K:212:SER:O	1:K:217:ARG:NH1	2.03	0.92
1:L:159:ASP:OD2	3:L:402:A1D5C:C25	2.19	0.90
1:I:212:SER:O	1:I:217:ARG:NH1	2.06	0.88
1:F:34:SER:OG	1:L:280:GLU:CD	2.16	0.88
1:G:49:ASN:OD1	1:G:51:SER:N	2.07	0.87
1:G:69:ASP:OD1	1:G:94:ARG:NH1	2.07	0.87
1:F:232:ALA:C	1:L:54:ARG:HH22	1.84	0.85
1:K:216:SER:OG	1:K:306:ASP:OD1	1.93	0.85
1:B:217:ARG:HG3	1:B:313:ARG:HH12	1.40	0.85
1:B:68:ASN:HB3	1:B:94:ARG:NH1	1.93	0.84
1:A:68:ASN:HB3	1:A:94:ARG:NH1	1.93	0.84
1:B:228:HIS:O	1:B:235:THR:OG1	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:HB3	1:B:309:PRO:CB	2.07	0.83
1:L:159:ASP:OD2	1:L:202:GLU:OE2	1.96	0.83
1:I:68:ASN:HB3	1:I:94:ARG:HH12	1.44	0.83
1:E:179:LEU:O	1:E:181:LEU:N	2.12	0.83
1:C:132:LYS:HZ3	1:C:190:ASP:HB3	1.42	0.83
1:G:68:ASN:O	1:G:94:ARG:NH1	2.12	0.82
1:J:249:LEU:HD12	1:J:321:ILE:HD11	1.62	0.82
1:A:68:ASN:HB3	1:A:94:ARG:HH12	1.42	0.82
1:H:228:HIS:O	1:H:235:THR:OG1	1.99	0.81
1:L:92:MET:HE2	1:L:106:ILE:HD11	1.62	0.81
1:F:285:LYS:HZ1	1:F:286:ASP:CG	1.88	0.81
1:G:158:THR:O	1:G:249:LEU:HA	1.81	0.81
1:J:73:LEU:O	1:J:75:ILE:N	2.14	0.81
1:I:169:GLU:OE1	1:I:172:ARG:NH2	2.15	0.80
1:L:159:ASP:OD2	3:L:402:A1D5C:N26	2.15	0.80
1:G:199:ASP:OD1	1:G:200:GLY:N	2.15	0.80
1:J:69:ASP:CG	1:J:94:ARG:HH22	1.88	0.79
1:H:172:ARG:O	1:H:174:LEU:N	2.16	0.79
1:J:228:HIS:O	1:J:235:THR:OG1	2.01	0.79
1:K:91:ILE:O	1:K:95:ILE:HD12	1.82	0.78
1:C:40:LYS:HB3	1:C:242:ASP:OD1	1.82	0.78
1:A:212:SER:O	1:A:217:ARG:NH1	2.16	0.77
1:L:236:SER:O	1:L:238:LEU:N	2.17	0.77
1:G:212:SER:O	1:G:217:ARG:NH1	2.18	0.77
1:G:157:ALA:O	1:G:162:VAL:HG23	1.85	0.76
1:H:295:GLN:O	1:H:297:TYR:N	2.18	0.76
1:I:328:VAL:O	1:I:331:THR:OG1	2.01	0.76
1:J:355:VAL:O	1:J:358:TYR:N	2.17	0.76
1:J:88:ARG:HG3	1:J:123:ILE:HD11	1.67	0.76
1:G:157:ALA:N	1:G:334:ASP:OD1	2.19	0.75
1:G:335:ASN:ND2	1:G:337:GLU:OE2	2.18	0.75
1:B:217:ARG:H	1:B:220:ALA:H	1.31	0.74
1:C:132:LYS:NZ	1:C:190:ASP:HB3	2.01	0.74
1:H:69:ASP:OD1	1:H:94:ARG:NH1	2.21	0.73
1:K:128:ASN:O	1:K:130:THR:N	2.21	0.73
1:C:111:SER:OG	1:C:112:GLN:N	2.16	0.73
1:J:151:ASN:O	1:J:151:ASN:ND2	2.20	0.73
1:C:132:LYS:HZ2	1:C:132:LYS:CB	2.01	0.73
1:A:47:ILE:HD12	1:A:357:GLU:OE2	1.89	0.73
1:C:92:MET:HE1	1:C:106:ILE:CG1	2.18	0.73
1:H:177:LYS:NZ	1:H:361:LEU:O	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:177:LYS:O	1:G:180:SER:OG	2.07	0.72
1:L:47:ILE:HG13	1:L:270:ARG:NH2	2.03	0.72
1:G:228:HIS:O	1:G:235:THR:OG1	2.07	0.72
1:J:35:ALA:C	1:J:37:PRO:HD2	2.14	0.72
1:D:212:SER:O	1:D:217:ARG:NH1	2.22	0.72
1:H:158:THR:OG1	1:H:334:ASP:OD2	2.07	0.72
1:J:69:ASP:OD2	1:J:94:ARG:NH2	2.19	0.72
1:H:283:LEU:HD12	1:H:283:LEU:H	1.55	0.71
1:D:205:LEU:O	1:D:206:HIS:ND1	2.22	0.71
1:G:264:SER:O	1:G:267:TRP:N	2.22	0.71
1:A:38:GLU:OE2	1:C:147:SER:OG	2.08	0.71
1:I:36:TRP:CD1	1:I:37:PRO:HD3	2.26	0.71
1:F:233:ARG:NH2	1:L:58:GLU:OE1	2.24	0.71
1:G:279:HIS:O	1:G:282:GLY:N	2.19	0.71
1:L:106:ILE:HD13	1:L:106:ILE:N	2.04	0.70
1:C:92:MET:HE1	1:C:106:ILE:HD11	1.70	0.70
1:C:229:PRO:O	1:C:230:PRO:C	2.31	0.70
1:H:140:HIS:ND1	1:H:142:ASP:OD1	2.24	0.70
1:J:40:LYS:HB3	1:J:242:ASP:OD1	1.92	0.70
1:E:92:MET:CE	1:E:106:ILE:HD11	2.23	0.69
1:A:68:ASN:CB	1:A:94:ARG:HH12	2.04	0.69
1:D:179:LEU:O	1:D:181:LEU:N	2.25	0.69
1:A:149:TRP:O	1:A:152:ARG:N	2.23	0.69
1:I:277:GLU:O	1:I:281:LEU:HD12	1.93	0.69
1:H:285:LYS:O	1:H:287:HIS:N	2.26	0.68
1:I:252:ALA:HB1	1:I:253:PRO:HD2	1.76	0.68
1:B:68:ASN:HB3	1:B:94:ARG:HH12	1.57	0.68
1:F:285:LYS:HE3	1:F:286:ASP:CG	2.19	0.68
1:H:155:VAL:O	1:H:156:GLY:C	2.33	0.68
1:F:212:SER:O	1:F:217:ARG:NH1	2.27	0.68
1:K:279:HIS:O	1:K:281:LEU:N	2.27	0.67
1:J:109:PHE:CE1	1:J:120:PHE:HB2	2.29	0.67
1:K:133:ARG:NH2	1:K:242:ASP:OD2	2.26	0.67
1:J:71:GLN:HA	1:J:74:LEU:HD12	1.76	0.67
1:L:159:ASP:OD2	2:L:401:ZN:ZN	1.42	0.67
1:B:34:SER:OG	1:B:35:ALA:N	2.28	0.67
1:G:130:THR:O	1:G:132:LYS:N	2.28	0.67
1:I:284:LEU:HD23	1:I:287:HIS:CG	2.30	0.67
1:J:133:ARG:O	1:J:134:HIS:ND1	2.27	0.67
1:B:136:VAL:HG21	1:B:241:MET:HE3	1.76	0.66
1:D:66:TRP:O	1:D:71:GLN:HG3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:222:LYS:O	1:I:226:THR:OG1	2.13	0.66
1:E:175:ASP:O	1:E:177:LYS:N	2.28	0.66
1:I:349:LYS:O	1:I:353:VAL:HG23	1.96	0.66
1:F:232:ALA:C	1:L:54:ARG:NH2	2.50	0.66
1:J:69:ASP:CG	1:J:94:ARG:HH12	2.03	0.66
1:J:274:ILE:O	1:J:278:LEU:HD12	1.95	0.66
1:L:263:ASN:ND2	1:L:316:PRO:HA	2.10	0.66
1:J:328:VAL:O	1:J:331:THR:OG1	2.10	0.66
1:C:92:MET:HE1	1:C:106:ILE:CD1	2.25	0.66
1:H:347:LEU:O	1:H:348:ASN:C	2.38	0.65
1:F:285:LYS:HE3	1:F:286:ASP:OD2	1.96	0.65
1:J:100:ALA:HA	1:J:179:LEU:HD12	1.79	0.65
1:B:248:ASP:OD2	3:B:402:A1D5C:N24	2.30	0.65
1:G:92:MET:HG2	1:G:104:LEU:HD13	1.77	0.65
1:I:133:ARG:NH2	1:I:242:ASP:OD2	2.28	0.65
1:G:140:HIS:O	1:G:140:HIS:ND1	2.29	0.65
1:I:169:GLU:CD	1:I:172:ARG:NH2	2.54	0.65
1:L:305:ASP:O	1:L:307:HIS:N	2.29	0.65
1:L:328:VAL:O	1:L:331:THR:OG1	2.15	0.65
1:B:49:ASN:OD1	1:B:52:ALA:N	2.25	0.65
1:J:271:LEU:HB3	1:J:294:PHE:CD2	2.32	0.65
1:L:236:SER:O	1:L:237:GLN:C	2.36	0.65
1:E:211:ASP:O	1:E:212:SER:HB3	1.96	0.64
1:E:206:HIS:ND1	1:K:314:GLY:O	2.30	0.64
1:H:61:SER:O	1:H:61:SER:OG	2.10	0.64
1:J:43:HIS:NE2	1:J:358:TYR:O	2.29	0.64
1:H:347:LEU:C	1:H:349:LYS:N	2.56	0.64
1:G:307:HIS:O	1:G:308:ILE:C	2.38	0.64
1:I:177:LYS:O	1:I:180:SER:OG	2.14	0.64
1:K:158:THR:OG1	1:K:334:ASP:OD1	2.15	0.64
1:G:261:PHE:O	1:G:264:SER:OG	2.16	0.63
1:I:169:GLU:OE2	1:I:172:ARG:NH2	2.31	0.63
1:E:92:MET:HE2	1:E:106:ILE:HD11	1.80	0.63
1:G:158:THR:N	1:G:334:ASP:OD1	2.30	0.63
1:J:348:ASN:O	1:J:352:GLN:HG3	1.99	0.63
1:B:217:ARG:HG3	1:B:313:ARG:NH1	2.13	0.63
1:K:349:LYS:O	1:K:353:VAL:HG23	1.99	0.63
1:J:66:TRP:CE2	1:J:336:GLU:OE2	2.52	0.63
1:E:136:VAL:HG21	1:E:241:MET:HE3	1.80	0.63
1:K:98:LEU:HB3	1:K:175:ASP:OD2	1.99	0.63
1:G:300:GLY:HA3	1:J:300:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:202:GLU:OE2	2:L:401:ZN:ZN	1.45	0.63
1:E:212:SER:O	1:E:217:ARG:NH1	2.31	0.62
1:I:256:THR:OG1	1:I:323:SER:O	2.17	0.62
1:G:281:LEU:HD12	1:G:281:LEU:N	2.14	0.62
1:A:207:TRP:HZ2	1:A:304:GLN:HB2	1.65	0.62
1:E:333:ASP:O	1:E:338:ASN:ND2	2.33	0.62
1:F:231:GLY:C	1:L:54:ARG:NH1	2.57	0.62
1:I:333:ASP:O	1:I:335:ASN:N	2.33	0.62
1:J:36:TRP:CZ3	1:J:132:LYS:CB	2.81	0.62
1:J:61:SER:OG	1:J:61:SER:O	2.12	0.62
1:L:66:TRP:O	1:L:71:GLN:HG3	1.99	0.62
1:E:328:VAL:O	1:E:329:TRP:C	2.42	0.62
1:H:62:ILE:HB	1:H:345:ASP:CG	2.25	0.62
1:C:68:ASN:O	1:C:94:ARG:NH1	2.31	0.62
1:F:233:ARG:HA	1:L:54:ARG:HH22	1.63	0.62
1:I:77:ARG:HG3	1:I:143:SER:HB3	1.82	0.62
1:I:111:SER:OG	1:I:112:GLN:N	2.31	0.62
1:J:248:ASP:OD2	3:J:402:A1D5C:N24	2.33	0.61
1:G:211:ASP:O	1:G:212:SER:HB3	2.00	0.61
1:I:124:ILE:HD12	1:I:124:ILE:N	2.15	0.61
1:J:274:ILE:HG22	1:J:350:ILE:HG23	1.80	0.61
1:J:279:HIS:NE2	1:J:287:HIS:O	2.33	0.61
1:B:159:ASP:OD2	2:B:401:ZN:ZN	1.47	0.61
1:B:217:ARG:CA	1:B:220:ALA:HB3	2.30	0.61
1:F:285:LYS:NZ	1:F:286:ASP:CG	2.59	0.61
1:J:61:SER:O	1:J:63:SER:N	2.33	0.61
1:J:192:SER:OG	1:J:193:LEU:N	2.31	0.61
1:I:88:ARG:O	1:I:92:MET:HG3	1.99	0.61
1:I:158:THR:OG1	1:I:334:ASP:OD1	2.17	0.61
1:I:284:LEU:CD2	1:I:287:HIS:ND1	2.63	0.61
1:I:354:PHE:C	1:I:354:PHE:CD1	2.76	0.61
1:B:217:ARG:N	1:B:220:ALA:H	1.97	0.61
1:B:65:MET:HG3	1:B:169:GLU:HB2	1.83	0.61
1:G:333:ASP:O	1:G:335:ASN:OD1	2.19	0.61
1:H:212:SER:O	1:H:214:TYR:N	2.33	0.61
1:L:236:SER:O	1:L:239:HIS:N	2.32	0.61
3:G:402:A1D5C:O17	3:G:402:A1D5C:C28	2.48	0.61
1:G:353:VAL:O	1:G:356:LEU:N	2.33	0.60
1:J:336:GLU:O	1:J:337:GLU:C	2.44	0.60
1:D:159:ASP:OD2	2:D:401:ZN:ZN	1.50	0.60
1:G:288:SER:OG	1:G:291:GLY:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:SER:OG	1:E:35:ALA:N	2.35	0.60
1:L:345:ASP:O	1:L:349:LYS:HG3	2.01	0.60
1:J:40:LYS:CB	1:J:242:ASP:OD1	2.48	0.60
1:L:348:ASN:O	1:L:352:GLN:HG3	2.00	0.60
1:F:155:VAL:O	1:F:156:GLY:C	2.44	0.60
1:H:229:PRO:O	1:H:230:PRO:C	2.44	0.60
1:B:199:ASP:OD1	1:B:200:GLY:N	2.33	0.60
1:J:254:ASN:N	1:J:255:PRO:HD3	2.16	0.60
1:E:106:ILE:HG22	1:E:107:ASP:N	2.16	0.60
1:G:65:MET:HG3	1:G:169:GLU:HB2	1.83	0.59
1:J:36:TRP:CZ3	1:J:132:LYS:HB3	2.37	0.59
1:A:92:MET:SD	1:A:106:ILE:HD11	2.42	0.59
1:C:95:ILE:HG21	1:C:104:LEU:HD21	1.84	0.59
1:G:340:ASP:O	1:G:342:SER:N	2.35	0.59
1:L:105:GLU:C	1:L:106:ILE:HD13	2.27	0.59
1:H:345:ASP:O	1:H:349:LYS:HG3	2.01	0.59
1:J:284:LEU:HG	1:J:346:ASN:OD1	2.01	0.59
1:J:311:LEU:O	1:J:314:GLY:N	2.30	0.59
1:F:39:GLU:HB2	1:F:133:ARG:NH1	2.17	0.59
1:K:212:SER:O	1:K:213:LEU:C	2.45	0.59
1:D:71:GLN:N	1:D:72:PRO:CD	2.65	0.59
1:G:122:ASN:ND2	1:G:215:GLY:O	2.23	0.59
1:H:328:VAL:O	1:H:331:THR:OG1	2.18	0.59
1:K:68:ASN:HB3	1:K:94:ARG:NH1	2.18	0.59
1:A:211:ASP:O	1:A:212:SER:HB3	2.00	0.59
1:F:70:LEU:O	1:F:70:LEU:HG	2.02	0.59
1:H:348:ASN:O	1:H:352:GLN:HG3	2.03	0.59
1:E:175:ASP:O	1:E:178:LEU:N	2.33	0.59
1:G:166:MET:SD	1:G:250:ILE:HG21	2.43	0.59
1:H:348:ASN:O	1:H:352:GLN:NE2	2.36	0.59
1:L:36:TRP:CG	1:L:37:PRO:HD3	2.38	0.59
1:F:175:ASP:O	1:F:178:LEU:N	2.29	0.59
1:J:40:LYS:HG3	1:J:41:ASN:OD1	2.03	0.59
1:H:61:SER:HG	1:H:64:GLU:H	1.50	0.58
1:H:272:GLN:CD	1:H:296:ASN:OD1	2.45	0.58
1:I:92:MET:CE	1:I:106:ILE:HD11	2.32	0.58
1:F:232:ALA:CA	1:L:54:ARG:NH1	2.66	0.58
1:B:285:LYS:O	1:B:286:ASP:C	2.46	0.58
1:G:285:LYS:NZ	1:G:286:ASP:OD1	2.28	0.58
1:A:116:GLY:HA2	1:H:114:PRO:O	2.03	0.58
1:E:179:LEU:C	1:E:181:LEU:H	2.08	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:TRP:CG	1:F:37:PRO:HD3	2.38	0.58
1:F:231:GLY:C	1:L:54:ARG:CZ	2.76	0.58
1:J:65:MET:HG3	1:J:169:GLU:HB2	1.85	0.58
1:J:70:LEU:C	1:J:70:LEU:HD12	2.27	0.58
1:G:149:TRP:CE3	1:G:150:ASN:HB2	2.38	0.58
1:J:94:ARG:NH2	1:J:168:LEU:HB3	2.18	0.58
1:D:177:LYS:O	1:D:180:SER:OG	2.21	0.58
1:G:169:GLU:O	1:G:172:ARG:N	2.36	0.58
3:B:402:A1D5C:C08	1:E:262:PRO:HG3	2.33	0.58
1:C:92:MET:HE1	1:C:106:ILE:HG12	1.84	0.58
1:C:205:LEU:O	1:C:206:HIS:ND1	2.36	0.58
1:I:92:MET:O	1:I:93:GLN:C	2.47	0.58
1:K:201:GLU:OE1	1:K:202:GLU:HG2	2.04	0.58
1:B:306:ASP:OD1	4:B:501:HOH:O	2.17	0.58
1:C:295:GLN:O	1:C:297:TYR:N	2.37	0.58
1:L:228:HIS:O	1:L:235:THR:OG1	2.17	0.58
1:J:223:MET:HB2	1:J:238:LEU:HD21	1.86	0.57
1:J:278:LEU:HB3	1:J:284:LEU:HD11	1.86	0.57
1:B:308:ILE:O	1:B:312:ARG:HG3	2.04	0.57
1:K:149:TRP:O	1:K:152:ARG:N	2.32	0.57
1:B:231:GLY:O	1:B:232:ALA:C	2.45	0.57
1:E:308:ILE:O	1:E:312:ARG:HG3	2.03	0.57
1:G:36:TRP:CG	1:G:37:PRO:HD3	2.40	0.57
1:G:354:PHE:CD1	1:G:354:PHE:C	2.82	0.57
1:H:344:ILE:O	1:H:348:ASN:HB2	2.04	0.57
1:B:217:ARG:CB	1:B:220:ALA:CB	2.57	0.57
1:H:281:LEU:HB3	1:H:283:LEU:HD11	1.87	0.57
1:I:170:LEU:C	1:I:170:LEU:HD23	2.30	0.57
1:J:69:ASP:CG	1:J:94:ARG:NH2	2.61	0.57
1:B:36:TRP:CD2	1:B:37:PRO:HD3	2.40	0.57
1:E:174:LEU:O	1:E:178:LEU:HG	2.05	0.57
1:J:132:LYS:CE	1:J:190:ASP:HB3	2.35	0.57
1:J:278:LEU:O	1:J:284:LEU:HD13	2.05	0.57
1:K:221:ALA:O	1:K:225:SER:OG	2.18	0.57
1:L:158:THR:O	1:L:160:SER:HA	2.04	0.57
1:K:49:ASN:OD1	1:K:49:ASN:C	2.47	0.57
1:L:253:PRO:O	1:L:254:ASN:HB2	2.05	0.57
1:L:36:TRP:CD2	1:L:37:PRO:HD3	2.39	0.56
1:A:231:GLY:O	1:A:232:ALA:O	2.24	0.56
1:A:303:ILE:N	1:A:303:ILE:HD13	2.19	0.56
1:F:138:ALA:HA	1:F:196:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:LYS:CE	1:F:286:ASP:CG	2.78	0.56
1:I:308:ILE:O	1:I:309:PRO:C	2.43	0.56
1:J:213:LEU:O	1:J:214:TYR:C	2.44	0.56
1:K:36:TRP:N	1:K:37:PRO:CD	2.68	0.56
1:K:90:HIS:O	1:K:91:ILE:C	2.48	0.56
1:K:208:SER:O	1:K:210:GLN:N	2.38	0.56
1:G:39:GLU:C	1:G:133:ARG:NH2	2.63	0.56
1:I:36:TRP:HA	1:I:39:GLU:HG3	1.87	0.56
1:I:212:SER:O	1:I:213:LEU:C	2.45	0.56
1:B:49:ASN:OD1	1:B:49:ASN:C	2.49	0.56
1:B:49:ASN:OD1	1:B:51:SER:N	2.38	0.56
1:G:169:GLU:OE2	1:G:172:ARG:NH2	2.32	0.56
1:B:211:ASP:O	1:B:212:SER:HB3	2.05	0.56
1:J:265:ALA:O	1:J:267:TRP:N	2.38	0.56
1:C:228:HIS:O	1:C:235:THR:OG1	2.22	0.56
1:D:180:SER:O	1:D:181:LEU:HD23	2.06	0.56
1:F:128:ASN:O	1:F:129:PRO:C	2.49	0.56
1:F:128:ASN:O	1:F:130:THR:N	2.38	0.56
1:F:231:GLY:O	1:L:281:LEU:HD22	2.05	0.56
1:L:68:ASN:HB3	1:L:94:ARG:NH1	2.21	0.56
1:C:219:LEU:O	1:C:220:ALA:C	2.44	0.56
1:L:121:SER:O	1:L:199:ASP:HB2	2.05	0.56
1:F:66:TRP:O	1:F:71:GLN:HB2	2.05	0.56
1:H:347:LEU:C	1:H:349:LYS:H	2.14	0.56
1:K:94:ARG:NH2	1:K:97:ARG:NH1	2.54	0.56
1:K:335:ASN:C	1:K:335:ASN:OD1	2.46	0.56
1:G:86:ALA:O	1:G:89:GLN:HB2	2.06	0.56
1:G:343:THR:O	1:G:347:LEU:HD12	2.06	0.56
1:J:133:ARG:O	1:J:134:HIS:CG	2.59	0.56
1:J:163:PRO:HB3	1:J:247:LEU:HB2	1.88	0.55
1:J:346:ASN:O	1:J:350:ILE:HG13	2.07	0.55
1:G:138:ALA:O	1:G:246:LEU:HD12	2.05	0.55
1:H:99:GLN:O	1:H:100:ALA:O	2.25	0.55
1:A:199:ASP:OD1	1:A:200:GLY:N	2.38	0.55
1:F:232:ALA:CA	1:L:54:ARG:HH12	2.19	0.55
1:J:149:TRP:C	1:J:151:ASN:H	2.15	0.55
1:L:92:MET:HE2	1:L:106:ILE:CD1	2.35	0.55
1:A:231:GLY:O	1:A:232:ALA:C	2.49	0.55
1:D:289:LEU:O	1:D:292:ARG:HG3	2.06	0.55
1:K:49:ASN:OD1	1:K:49:ASN:O	2.25	0.55
1:J:36:TRP:CD1	1:J:37:PRO:HD3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:PHE:CZ	1:L:120:PHE:HB2	2.42	0.55
1:G:128:ASN:OD1	1:G:128:ASN:N	2.37	0.55
1:G:162:VAL:HB	1:G:163:PRO:HD3	1.89	0.55
1:C:104:LEU:N	1:C:104:LEU:HD23	2.21	0.55
1:F:158:THR:O	1:F:249:LEU:HA	2.07	0.55
1:K:165:ALA:O	1:K:166:MET:C	2.43	0.55
1:D:310:PHE:O	1:D:311:LEU:C	2.48	0.55
1:G:70:LEU:O	1:G:74:LEU:HD12	2.07	0.55
1:H:285:LYS:HG3	1:H:286:ASP:N	2.21	0.55
1:L:109:PHE:CE1	1:L:120:PHE:HB2	2.41	0.55
1:B:39:GLU:O	1:B:40:LYS:C	2.49	0.54
1:F:167:MET:HE2	1:F:197:PHE:CE2	2.42	0.54
1:F:360:HIS:O	1:F:361:LEU:HD23	2.07	0.54
1:H:92:MET:HG2	1:H:104:LEU:HD13	1.88	0.54
1:J:36:TRP:CZ3	1:J:133:ARG:HG3	2.42	0.54
1:J:359:LEU:HB2	1:J:361:LEU:HG	1.89	0.54
1:L:41:ASN:OD1	1:L:41:ASN:N	2.40	0.54
1:B:314:GLY:HA3	1:K:206:HIS:HB3	1.88	0.54
1:D:219:LEU:O	1:D:220:ALA:C	2.47	0.54
1:E:175:ASP:O	1:E:176:LYS:C	2.47	0.54
1:H:103:VAL:HG12	1:H:103:VAL:O	2.07	0.54
1:H:165:ALA:O	1:H:166:MET:C	2.50	0.54
1:J:149:TRP:O	1:J:152:ARG:HG3	2.08	0.54
1:J:278:LEU:C	1:J:284:LEU:HD13	2.32	0.54
1:J:347:LEU:C	1:J:349:LYS:N	2.64	0.54
1:K:252:ALA:HB1	1:K:253:PRO:HD2	1.88	0.54
1:L:77:ARG:HG2	1:L:143:SER:HB3	1.88	0.54
1:L:354:PHE:O	1:L:355:VAL:C	2.50	0.54
1:A:47:ILE:HD13	1:A:270:ARG:NH2	2.23	0.54
1:C:292:ARG:O	1:C:295:GLN:NE2	2.40	0.54
1:J:69:ASP:OD1	1:J:94:ARG:NH1	2.37	0.54
1:E:302:VAL:HG22	1:E:303:ILE:O	2.07	0.54
1:D:179:LEU:C	1:D:181:LEU:H	2.15	0.54
1:F:35:ALA:O	1:F:36:TRP:C	2.43	0.54
1:J:141:TYR:HD2	1:J:197:PHE:O	1.91	0.54
1:J:178:LEU:O	1:J:180:SER:N	2.41	0.54
1:J:280:GLU:O	1:J:280:GLU:HG3	2.07	0.54
1:K:109:PHE:CZ	1:K:120:PHE:HB2	2.43	0.54
1:H:57:ALA:HB3	1:H:283:LEU:HD23	1.90	0.54
1:J:191:LEU:HD12	1:J:242:ASP:OD2	2.08	0.54
1:J:49:ASN:C	1:J:49:ASN:OD1	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:GLN:N	1:L:72:PRO:CD	2.71	0.54
1:L:159:ASP:CG	3:L:402:A1D5C:C25	2.81	0.54
1:I:277:GLU:HG3	1:I:281:LEU:HD12	1.89	0.54
1:J:36:TRP:HZ3	1:J:133:ARG:N	2.06	0.54
1:J:158:THR:HG22	1:J:250:ILE:O	2.07	0.54
1:J:160:SER:C	1:J:163:PRO:HD2	2.32	0.54
1:H:172:ARG:O	1:H:173:ALA:C	2.51	0.54
1:I:54:ARG:O	1:I:58:GLU:HG3	2.07	0.54
1:I:249:LEU:HD12	1:I:321:ILE:HD11	1.90	0.54
1:B:217:ARG:CB	1:B:309:PRO:CB	2.77	0.53
1:C:308:ILE:O	1:C:312:ARG:HG3	2.07	0.53
1:E:88:ARG:HG3	1:E:123:ILE:HD11	1.90	0.53
1:F:256:THR:O	1:F:256:THR:OG1	2.24	0.53
1:L:181:LEU:O	1:L:182:LYS:C	2.50	0.53
1:B:92:MET:SD	1:B:106:ILE:HD11	2.47	0.53
1:A:217:ARG:HD2	4:A:501:HOH:O	2.07	0.53
1:C:77:ARG:HG2	1:C:143:SER:HB3	1.90	0.53
1:J:351:LEU:O	1:J:354:PHE:N	2.42	0.53
1:E:353:VAL:O	1:E:357:GLU:HG3	2.08	0.53
1:K:49:ASN:O	1:K:50:SER:C	2.50	0.53
1:K:72:PRO:HB2	1:K:90:HIS:CD2	2.44	0.53
1:L:43:HIS:O	1:L:266:ARG:NH2	2.36	0.53
1:F:210:GLN:HG3	4:F:501:HOH:O	2.08	0.53
1:I:121:SER:O	1:I:141:TYR:OH	2.23	0.53
1:D:201:GLU:HG3	1:D:306:ASP:OD2	2.09	0.53
1:F:231:GLY:HA2	1:L:54:ARG:NE	2.23	0.53
1:I:228:HIS:O	1:I:235:THR:OG1	2.25	0.53
1:B:40:LYS:HG3	1:B:41:ASN:OD1	2.09	0.53
1:A:207:TRP:CZ2	1:A:304:GLN:HB2	2.43	0.53
1:J:102:TRP:CZ3	1:J:127:LEU:HG	2.44	0.53
1:K:172:ARG:HH11	1:K:172:ARG:HG2	1.73	0.53
1:L:49:ASN:OD1	1:L:49:ASN:C	2.52	0.53
1:G:335:ASN:OD1	1:G:335:ASN:N	2.41	0.53
1:J:268:PHE:O	1:J:271:LEU:N	2.34	0.53
1:B:78:TYR:CE1	1:B:81:SER:HB3	2.44	0.53
1:B:207:TRP:HZ2	1:B:304:GLN:HB2	1.74	0.53
1:F:49:ASN:OD1	1:F:49:ASN:C	2.52	0.53
1:H:36:TRP:N	1:H:37:PRO:CD	2.72	0.53
1:K:128:ASN:O	1:K:129:PRO:C	2.51	0.53
1:F:206:HIS:ND1	1:I:313:ARG:O	2.34	0.53
1:H:212:SER:O	1:H:213:LEU:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:ASN:O	1:I:50:SER:C	2.50	0.53
1:J:61:SER:O	1:J:64:GLU:N	2.42	0.53
1:J:69:ASP:CA	1:J:94:ARG:HH12	2.22	0.53
1:C:226:THR:O	1:C:227:PRO:C	2.48	0.53
1:J:71:GLN:N	1:J:72:PRO:CD	2.72	0.53
1:K:149:TRP:O	1:K:150:ASN:C	2.52	0.52
1:D:159:ASP:OD2	3:D:402:A1D5C:N26	2.42	0.52
1:K:52:ALA:O	1:K:56:ILE:HG12	2.08	0.52
1:K:102:TRP:CZ3	1:K:127:LEU:HG	2.44	0.52
1:K:138:ALA:HA	1:K:167:MET:HE1	1.89	0.52
1:H:117:TYR:O	1:H:118:ARG:HG2	2.08	0.52
1:L:172:ARG:O	1:L:173:ALA:C	2.51	0.52
1:H:45:PRO:HG3	1:H:270:ARG:HD3	1.90	0.52
1:D:211:ASP:O	1:D:212:SER:HB3	2.08	0.52
1:G:92:MET:SD	1:G:106:ILE:HD11	2.50	0.52
1:J:170:LEU:HD11	1:J:355:VAL:HG21	1.90	0.52
1:K:127:LEU:O	1:K:128:ASN:HB2	2.09	0.52
1:D:347:LEU:O	1:D:348:ASN:C	2.50	0.52
1:G:152:ARG:O	1:G:332:MET:HE3	2.10	0.52
1:G:321:ILE:HG23	1:G:321:ILE:O	2.10	0.52
1:H:246:LEU:HD23	1:H:319:HIS:CD2	2.44	0.52
1:A:62:ILE:HG13	1:A:62:ILE:O	2.10	0.52
1:A:228:HIS:HB2	1:A:237:GLN:HG2	1.91	0.52
1:H:157:ALA:HA	1:H:161:ALA:HB3	1.90	0.52
1:J:135:LEU:O	1:J:193:LEU:HD12	2.09	0.52
1:L:181:LEU:HD23	1:L:181:LEU:N	2.24	0.52
1:L:305:ASP:C	1:L:307:HIS:H	2.18	0.52
1:B:299:TYR:HD2	1:B:301:GLY:O	1.93	0.52
1:C:132:LYS:HE3	1:C:190:ASP:OD2	2.09	0.52
1:E:206:HIS:HB3	1:K:314:GLY:HA3	1.91	0.52
1:G:206:HIS:O	1:G:207:TRP:C	2.52	0.52
1:G:264:SER:O	1:G:265:ALA:C	2.53	0.52
1:I:305:ASP:C	1:I:307:HIS:H	2.18	0.52
1:J:140:HIS:O	1:J:160:SER:HB2	2.10	0.52
1:B:217:ARG:HB2	1:B:220:ALA:HB2	1.81	0.52
1:E:99:GLN:HB3	1:E:179:LEU:HD11	1.92	0.52
1:A:92:MET:CE	1:A:106:ILE:HD11	2.40	0.52
1:D:49:ASN:O	1:D:50:SER:C	2.53	0.52
1:G:223:MET:HB3	1:G:238:LEU:HD23	1.92	0.52
1:J:293:TYR:CZ	1:J:343:THR:HG23	2.44	0.52
1:E:106:ILE:CG2	1:E:107:ASP:N	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:LEU:HD23	1:H:193:LEU:CD1	2.39	0.51
1:J:97:ARG:O	1:J:97:ARG:HG3	2.09	0.51
1:J:257:PHE:CD2	1:J:294:PHE:HE1	2.29	0.51
1:J:268:PHE:O	1:J:271:LEU:HB2	2.10	0.51
1:L:211:ASP:O	1:L:212:SER:HB3	2.09	0.51
1:B:72:PRO:HG2	1:B:90:HIS:CE1	2.46	0.51
1:A:71:GLN:N	1:A:72:PRO:CD	2.72	0.51
1:E:155:VAL:O	1:E:155:VAL:HG23	2.10	0.51
1:J:281:LEU:HB2	1:J:283:LEU:HD11	1.91	0.51
1:J:345:ASP:O	1:J:349:LYS:HG3	2.10	0.51
1:K:100:ALA:HA	1:K:179:LEU:HD12	1.91	0.51
1:G:349:LYS:O	1:G:353:VAL:HG23	2.10	0.51
1:A:47:ILE:HD13	1:A:270:ARG:HH22	1.75	0.51
1:G:38:GLU:O	1:G:40:LYS:N	2.43	0.51
1:J:69:ASP:HA	1:J:94:ARG:NH1	2.26	0.51
1:C:132:LYS:CE	1:C:190:ASP:OD2	2.58	0.51
1:E:36:TRP:N	1:E:37:PRO:CD	2.74	0.51
1:F:170:LEU:C	1:F:170:LEU:HD23	2.36	0.51
1:G:94:ARG:HH21	1:G:97:ARG:NH1	2.09	0.51
1:L:150:ASN:HB3	1:L:152:ARG:HG3	1.92	0.51
1:D:112:GLN:OE1	1:D:116:GLY:HA2	2.11	0.51
1:D:231:GLY:O	1:D:232:ALA:C	2.52	0.51
1:E:139:CYS:SG	1:E:140:HIS:N	2.80	0.51
1:F:127:LEU:O	1:F:128:ASN:HB2	2.11	0.51
1:F:206:HIS:O	1:F:207:TRP:C	2.54	0.51
1:J:253:PRO:C	1:J:255:PRO:HD3	2.36	0.51
1:J:279:HIS:O	1:J:282:GLY:N	2.27	0.51
1:C:36:TRP:CD1	1:C:37:PRO:HD3	2.46	0.51
1:F:355:VAL:O	1:F:358:TYR:N	2.43	0.51
1:G:248:ASP:OD2	1:G:305:ASP:OD2	2.28	0.51
1:G:285:LYS:HD2	1:G:286:ASP:H	1.75	0.51
1:I:51:SER:O	1:I:54:ARG:N	2.40	0.51
1:F:248:ASP:O	1:F:249:LEU:HB2	2.11	0.51
1:G:57:ALA:O	1:G:349:LYS:HE2	2.10	0.51
1:G:207:TRP:CE3	3:G:402:A1D5C:C16	2.94	0.51
1:I:49:ASN:O	1:I:49:ASN:OD1	2.29	0.51
1:C:221:ALA:O	1:C:222:LYS:C	2.52	0.51
1:F:179:LEU:C	1:F:181:LEU:H	2.19	0.51
1:I:49:ASN:O	1:I:51:SER:N	2.44	0.51
1:J:77:ARG:HG3	1:J:143:SER:HB3	1.93	0.51
1:J:137:LEU:O	1:J:167:MET:HE3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:O	1:B:181:LEU:N	2.44	0.50
1:B:233:ARG:NH2	1:G:80:GLY:O	2.44	0.50
1:E:206:HIS:CE1	1:K:314:GLY:O	2.64	0.50
1:I:65:MET:O	1:I:65:MET:HG2	2.11	0.50
1:B:36:TRP:CG	1:B:37:PRO:HD3	2.47	0.50
1:D:160:SER:C	1:D:163:PRO:HD2	2.36	0.50
1:J:109:PHE:CZ	1:J:120:PHE:HB2	2.46	0.50
1:J:279:HIS:C	1:J:281:LEU:H	2.18	0.50
3:K:402:A1D5C:C01	4:K:503:HOH:O	2.59	0.50
1:L:304:GLN:O	1:L:305:ASP:HB2	2.10	0.50
1:C:191:LEU:HD13	1:C:242:ASP:OD2	2.12	0.50
1:D:102:TRP:CE3	1:D:125:SER:OG	2.64	0.50
1:D:279:HIS:O	1:D:281:LEU:N	2.44	0.50
1:J:128:ASN:N	1:J:129:PRO:CD	2.74	0.50
1:J:168:LEU:O	1:J:171:ALA:HB3	2.11	0.50
1:B:148:HIS:N	1:B:148:HIS:CD2	2.79	0.50
1:I:247:LEU:HD22	1:I:320:LEU:HD12	1.94	0.50
1:I:305:ASP:O	1:I:307:HIS:N	2.44	0.50
1:J:88:ARG:O	1:J:92:MET:HG3	2.11	0.50
1:J:291:GLY:O	1:J:292:ARG:O	2.29	0.50
1:L:263:ASN:HD22	1:L:316:PRO:HA	1.73	0.50
1:C:158:THR:O	1:C:249:LEU:HA	2.12	0.50
1:I:207:TRP:CD1	1:I:207:TRP:C	2.89	0.50
1:J:257:PHE:CD2	1:J:294:PHE:CE1	2.99	0.50
1:B:180:SER:C	1:B:181:LEU:HD23	2.37	0.50
1:D:247:LEU:HD23	1:D:247:LEU:N	2.26	0.50
1:G:157:ALA:HB3	1:G:334:ASP:OD1	2.11	0.50
1:H:71:GLN:N	1:H:72:PRO:CD	2.74	0.50
1:H:133:ARG:NH2	1:H:242:ASP:OD2	2.45	0.50
1:J:39:GLU:HB3	1:J:133:ARG:NH1	2.27	0.50
1:J:347:LEU:O	1:J:349:LYS:N	2.44	0.50
1:B:206:HIS:CG	1:E:314:GLY:HA3	2.46	0.50
1:B:279:HIS:HE1	1:B:287:HIS:O	1.95	0.50
1:A:87:ALA:O	1:A:88:ARG:C	2.53	0.50
1:E:180:SER:O	1:E:181:LEU:HD23	2.12	0.50
1:I:57:ALA:HB1	1:I:349:LYS:HD3	1.94	0.50
1:I:308:ILE:HB	1:I:309:PRO:HD3	1.93	0.50
1:J:135:LEU:HD23	1:J:193:LEU:HD13	1.94	0.50
1:K:87:ALA:O	1:K:91:ILE:HG13	2.12	0.50
1:K:105:GLU:C	1:K:106:ILE:HD13	2.37	0.50
1:K:159:ASP:OD1	3:K:402:A1D5C:C25	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:202:GLU:OE2	3:L:402:A1D5C:C25	2.57	0.50
1:B:33:ALA:O	1:B:34:SER:O	2.29	0.50
1:H:70:LEU:O	1:H:74:LEU:HD12	2.12	0.50
1:J:102:TRP:CD2	1:J:127:LEU:HD21	2.46	0.50
1:C:108:THR:HG22	1:C:109:PHE:N	2.24	0.50
1:D:36:TRP:N	1:D:37:PRO:CD	2.75	0.50
1:D:92:MET:HE2	1:D:106:ILE:CD1	2.42	0.50
1:B:226:THR:O	1:B:227:PRO:C	2.54	0.49
1:C:212:SER:O	1:C:217:ARG:NH1	2.40	0.49
1:E:68:ASN:HB3	1:E:94:ARG:NH1	2.27	0.49
1:K:250:ILE:HG22	1:K:251:GLY:N	2.26	0.49
1:L:37:PRO:O	1:L:40:LYS:HE3	2.12	0.49
1:L:325:PHE:O	1:L:326:PRO:C	2.53	0.49
1:F:229:PRO:O	1:F:230:PRO:C	2.53	0.49
1:H:256:THR:OG1	1:H:323:SER:O	2.30	0.49
1:J:271:LEU:HB3	1:J:294:PHE:CE2	2.47	0.49
1:J:296:ASN:OD1	1:J:296:ASN:N	2.38	0.49
1:B:299:TYR:CD2	1:B:301:GLY:O	2.66	0.49
1:A:212:SER:O	1:A:213:LEU:C	2.55	0.49
1:I:157:ALA:O	1:I:162:VAL:HG23	2.11	0.49
1:I:229:PRO:O	1:I:230:PRO:C	2.55	0.49
1:J:347:LEU:C	1:J:349:LYS:H	2.20	0.49
1:G:279:HIS:CE1	1:G:289:LEU:HG	2.48	0.49
1:J:329:TRP:O	1:J:330:HIS:C	2.55	0.49
1:L:77:ARG:CG	1:L:143:SER:HB3	2.42	0.49
1:C:231:GLY:O	1:C:232:ALA:C	2.54	0.49
1:E:99:GLN:O	1:E:100:ALA:C	2.53	0.49
1:E:120:PHE:CD1	1:E:120:PHE:N	2.79	0.49
1:F:211:ASP:CG	1:F:211:ASP:O	2.50	0.49
1:F:232:ALA:HA	1:L:54:ARG:HH12	1.75	0.49
1:J:265:ALA:O	1:J:266:ARG:C	2.54	0.49
1:L:308:ILE:HB	1:L:309:PRO:HD3	1.94	0.49
1:B:201:GLU:HG3	1:B:306:ASP:OD2	2.12	0.49
1:A:250:ILE:HG22	1:A:251:GLY:N	2.27	0.49
1:G:305:ASP:OD1	1:G:306:ASP:N	2.46	0.49
1:H:89:GLN:O	1:H:93:GLN:HG3	2.12	0.49
1:J:274:ILE:O	1:J:274:ILE:HG22	2.12	0.49
1:L:137:LEU:HD12	1:L:245:VAL:HB	1.93	0.49
1:A:249:LEU:HD12	1:A:321:ILE:HD11	1.95	0.49
1:F:232:ALA:C	1:L:54:ARG:HH12	2.21	0.49
1:G:236:SER:O	1:G:239:HIS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:279:HIS:C	1:K:281:LEU:H	2.19	0.49
1:L:360:HIS:O	1:L:361:LEU:HD23	2.13	0.49
1:A:311:LEU:O	1:A:313:ARG:N	2.46	0.49
1:D:36:TRP:CG	1:D:37:PRO:HD3	2.48	0.49
1:E:56:ILE:O	1:E:56:ILE:HG22	2.11	0.49
1:E:349:LYS:O	1:E:353:VAL:HG23	2.13	0.49
1:F:39:GLU:CB	1:F:133:ARG:NH1	2.76	0.49
1:G:78:TYR:CE1	1:G:81:SER:HB3	2.48	0.49
1:I:276:HIS:O	1:I:279:HIS:N	2.45	0.49
1:J:36:TRP:CZ3	1:J:132:LYS:HB2	2.48	0.49
1:J:216:SER:HB2	1:J:309:PRO:HG2	1.95	0.49
1:L:228:HIS:HA	1:L:229:PRO:C	2.37	0.49
1:B:211:ASP:HA	1:B:214:TYR:OH	2.13	0.49
1:F:34:SER:HB2	1:L:280:GLU:HA	1.94	0.49
1:F:100:ALA:HA	1:F:179:LEU:CD1	2.43	0.49
1:J:174:LEU:HD22	1:J:356:LEU:HD11	1.95	0.49
1:L:71:GLN:N	1:L:72:PRO:HD2	2.28	0.49
1:D:229:PRO:O	1:D:230:PRO:C	2.55	0.49
1:G:207:TRP:CZ3	3:G:402:A1D5C:O17	2.66	0.49
1:I:74:LEU:C	1:I:75:ILE:HG23	2.38	0.48
1:K:279:HIS:C	1:K:281:LEU:N	2.71	0.48
1:A:333:ASP:O	1:A:335:ASN:N	2.44	0.48
1:H:305:ASP:CG	1:H:306:ASP:H	2.21	0.48
1:I:292:ARG:NH2	1:I:295:GLN:HG2	2.28	0.48
1:J:102:TRP:HA	1:J:127:LEU:CD2	2.43	0.48
1:J:169:GLU:OE2	1:J:172:ARG:NH2	2.43	0.48
1:D:104:LEU:HD23	1:D:125:SER:HB2	1.94	0.48
1:B:238:LEU:O	1:B:239:HIS:C	2.53	0.48
1:D:279:HIS:C	1:D:281:LEU:H	2.22	0.48
1:E:162:VAL:HB	1:E:163:PRO:HD3	1.95	0.48
1:F:180:SER:C	1:F:181:LEU:HD23	2.38	0.48
1:H:285:LYS:HG3	1:H:286:ASP:H	1.78	0.48
1:J:278:LEU:HB3	1:J:284:LEU:CD1	2.44	0.48
1:K:212:SER:O	1:K:214:TYR:N	2.46	0.48
1:A:231:GLY:C	1:A:232:ALA:O	2.57	0.48
1:E:75:ILE:HG13	1:E:76:GLU:O	2.13	0.48
1:E:295:GLN:O	1:E:297:TYR:N	2.46	0.48
1:G:135:LEU:O	1:G:193:LEU:HD12	2.14	0.48
1:G:206:HIS:HB3	1:J:314:GLY:HA3	1.94	0.48
1:J:132:LYS:HE3	1:J:190:ASP:HB3	1.96	0.48
1:J:168:LEU:O	1:J:171:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:162:VAL:O	1:K:166:MET:HG3	2.14	0.48
1:L:78:TYR:CE1	1:L:81:SER:HB3	2.48	0.48
1:C:175:ASP:O	1:C:176:LYS:C	2.56	0.48
1:E:56:ILE:HD12	1:E:356:LEU:CD1	2.43	0.48
1:G:78:TYR:CE2	1:G:145:TYR:HD2	2.31	0.48
3:J:402:A1D5C:C28	3:J:402:A1D5C:O17	2.61	0.48
1:K:250:ILE:CG2	1:K:251:GLY:N	2.76	0.48
1:L:170:LEU:O	1:L:171:ALA:C	2.55	0.48
1:A:229:PRO:O	1:A:230:PRO:C	2.53	0.48
1:G:162:VAL:HB	1:G:163:PRO:CD	2.44	0.48
1:H:111:SER:OG	1:H:112:GLN:N	2.45	0.48
1:J:69:ASP:N	1:J:94:ARG:HH12	2.11	0.48
1:J:154:PHE:O	1:J:155:VAL:CG1	2.62	0.48
1:L:199:ASP:OD1	1:L:200:GLY:N	2.45	0.48
1:A:77:ARG:HG3	1:A:143:SER:HB3	1.96	0.48
1:G:39:GLU:O	1:G:133:ARG:NH2	2.47	0.48
1:I:212:SER:O	1:I:214:TYR:N	2.47	0.48
1:J:263:ASN:N	1:J:263:ASN:HD22	2.11	0.48
1:H:249:LEU:HD12	1:H:321:ILE:HD11	1.95	0.48
1:I:52:ALA:O	1:I:53:LEU:C	2.56	0.48
1:L:223:MET:O	1:L:225:SER:N	2.47	0.48
1:B:137:LEU:HD12	1:B:245:VAL:HB	1.96	0.48
1:D:292:ARG:HG3	1:D:292:ARG:HH11	1.77	0.48
1:G:70:LEU:O	1:G:74:LEU:CD1	2.61	0.48
1:G:288:SER:OG	1:G:289:LEU:N	2.42	0.48
1:H:305:ASP:OD1	1:H:306:ASP:N	2.43	0.48
1:K:128:ASN:OD1	1:K:128:ASN:N	2.47	0.48
1:K:205:LEU:O	1:K:206:HIS:ND1	2.47	0.48
1:L:268:PHE:C	1:L:268:PHE:CD1	2.92	0.48
1:D:112:GLN:HG3	1:D:113:THR:N	2.28	0.47
1:H:321:ILE:HG23	1:H:321:ILE:O	2.13	0.47
1:I:123:ILE:C	1:I:124:ILE:HD12	2.39	0.47
1:I:248:ASP:OD2	3:I:402:A1D5C:N24	2.48	0.47
1:J:149:TRP:O	1:J:152:ARG:N	2.46	0.47
1:B:228:HIS:HA	1:B:229:PRO:C	2.38	0.47
1:F:274:ILE:HD13	1:F:353:VAL:HG12	1.96	0.47
1:H:340:ASP:OD1	1:H:342:SER:N	2.46	0.47
1:J:160:SER:O	1:J:163:PRO:HD2	2.14	0.47
1:J:278:LEU:O	1:J:283:LEU:HD12	2.15	0.47
1:K:78:TYR:O	1:K:84:SER:HB2	2.15	0.47
1:L:38:GLU:O	1:L:41:ASN:OD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:HG22	1:B:303:ILE:O	2.15	0.47
1:A:100:ALA:HA	1:A:179:LEU:CD1	2.45	0.47
1:F:175:ASP:O	1:F:176:LYS:C	2.54	0.47
1:G:169:GLU:O	1:G:170:LEU:C	2.56	0.47
1:H:347:LEU:O	1:H:350:ILE:N	2.48	0.47
1:I:144:LYS:HG2	1:I:146:PHE:CE2	2.49	0.47
1:G:192:SER:OG	1:G:193:LEU:N	2.46	0.47
1:G:285:LYS:C	1:G:287:HIS:N	2.71	0.47
1:H:174:LEU:O	1:H:175:ASP:C	2.57	0.47
1:B:36:TRP:N	1:B:37:PRO:HD2	2.29	0.47
1:C:289:LEU:O	1:C:292:ARG:HG3	2.15	0.47
1:E:73:LEU:O	1:E:77:ARG:NH1	2.47	0.47
1:G:73:LEU:O	1:G:77:ARG:NH1	2.48	0.47
1:G:252:ALA:HB1	1:G:253:PRO:HD2	1.96	0.47
1:H:285:LYS:O	1:H:287:HIS:HB2	2.14	0.47
1:K:65:MET:O	1:K:66:TRP:C	2.56	0.47
1:K:128:ASN:C	1:K:130:THR:N	2.71	0.47
1:B:77:ARG:HG2	1:B:143:SER:HB3	1.97	0.47
1:B:231:GLY:C	1:B:232:ALA:O	2.57	0.47
1:C:155:VAL:O	1:C:155:VAL:HG23	2.10	0.47
1:C:285:LYS:NZ	1:C:286:ASP:OD1	2.45	0.47
1:H:89:GLN:O	1:H:93:GLN:CG	2.62	0.47
1:B:292:ARG:HG3	1:B:292:ARG:HH11	1.78	0.47
1:A:47:ILE:HG13	1:A:48:LEU:N	2.29	0.47
1:A:56:ILE:O	1:A:57:ALA:C	2.55	0.47
1:F:178:LEU:O	1:F:181:LEU:HG	2.15	0.47
1:F:285:LYS:O	1:F:286:ASP:HB2	2.14	0.47
1:G:265:ALA:O	1:G:266:ARG:C	2.54	0.47
1:H:92:MET:O	1:H:93:GLN:C	2.58	0.47
1:H:99:GLN:O	1:H:100:ALA:C	2.56	0.47
1:H:99:GLN:HB2	1:H:175:ASP:OD2	2.15	0.47
1:K:88:ARG:HG3	1:K:123:ILE:HD11	1.96	0.47
1:B:277:GLU:O	1:B:278:LEU:C	2.53	0.47
1:E:78:TYR:O	1:E:81:SER:HB3	2.15	0.47
1:F:78:TYR:O	1:F:81:SER:OG	2.17	0.47
1:F:223:MET:HB3	1:F:238:LEU:HD23	1.96	0.47
1:H:360:HIS:O	1:H:361:LEU:HD23	2.14	0.47
1:I:211:ASP:O	1:I:212:SER:HB3	2.14	0.47
1:I:353:VAL:O	1:I:354:PHE:C	2.56	0.47
1:J:136:VAL:HG21	1:J:241:MET:HE3	1.97	0.47
1:J:161:ALA:O	1:J:162:VAL:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:VAL:O	1:A:354:PHE:C	2.57	0.47
1:D:64:GLU:O	1:D:68:ASN:HB2	2.15	0.47
1:G:70:LEU:HG	1:G:74:LEU:HD11	1.97	0.47
3:G:402:A1D5C:C28	3:G:402:A1D5C:C16	2.93	0.47
1:I:100:ALA:HB2	1:I:175:ASP:OD1	2.15	0.47
1:J:164:CYS:O	1:J:165:ALA:C	2.57	0.47
1:J:279:HIS:C	1:J:281:LEU:N	2.72	0.47
1:E:110:LEU:HD21	1:E:117:TYR:CD2	2.50	0.47
1:G:333:ASP:C	1:G:335:ASN:OD1	2.58	0.47
3:H:402:A1D5C:O17	3:H:402:A1D5C:C28	2.62	0.47
1:J:98:LEU:HB3	1:J:175:ASP:OD2	2.15	0.47
1:J:149:TRP:C	1:J:151:ASN:N	2.73	0.47
1:K:285:LYS:HE3	1:K:286:ASP:OD1	2.15	0.47
1:D:128:ASN:OD1	1:D:128:ASN:N	2.47	0.46
1:D:174:LEU:O	1:D:175:ASP:C	2.57	0.46
1:E:181:LEU:C	1:E:182:LYS:HG2	2.40	0.46
1:G:140:HIS:O	1:G:140:HIS:CG	2.67	0.46
1:J:69:ASP:CG	1:J:94:ARG:NH1	2.72	0.46
1:K:85:TYR:O	1:K:86:ALA:C	2.55	0.46
1:K:110:LEU:HD12	1:K:118:ARG:O	2.15	0.46
1:K:270:ARG:O	1:K:274:ILE:HG13	2.15	0.46
1:K:308:ILE:HB	1:K:309:PRO:HD3	1.97	0.46
1:B:172:ARG:O	1:B:172:ARG:HG2	2.14	0.46
1:F:49:ASN:OD1	1:F:51:SER:N	2.49	0.46
1:G:68:ASN:OD1	1:G:68:ASN:N	2.49	0.46
1:K:281:LEU:HB2	1:K:283:LEU:HD12	1.97	0.46
1:A:299:TYR:CD2	1:A:300:GLY:O	2.68	0.46
1:D:36:TRP:CD1	1:D:37:PRO:HD3	2.51	0.46
1:D:92:MET:O	1:D:93:GLN:C	2.56	0.46
1:F:71:GLN:N	1:F:72:PRO:CD	2.78	0.46
1:G:246:LEU:HD23	1:G:319:HIS:CE1	2.50	0.46
1:G:310:PHE:O	1:G:311:LEU:C	2.58	0.46
1:G:328:VAL:O	1:G:334:ASP:HB2	2.15	0.46
1:H:182:LYS:HD3	1:H:182:LYS:N	2.31	0.46
1:L:308:ILE:O	1:L:312:ARG:HG3	2.15	0.46
1:C:132:LYS:HZ1	1:C:190:ASP:CG	2.24	0.46
1:D:359:LEU:O	1:D:360:HIS:C	2.58	0.46
1:E:64:GLU:O	1:E:65:MET:C	2.55	0.46
1:F:90:HIS:O	1:F:91:ILE:C	2.58	0.46
1:F:249:LEU:HD12	1:F:321:ILE:HD11	1.98	0.46
1:G:308:ILE:HB	1:G:309:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:LEU:HD23	1:H:287:HIS:CG	2.51	0.46
1:J:72:PRO:HG2	1:J:90:HIS:CE1	2.50	0.46
1:J:92:MET:HE2	1:J:104:LEU:HD12	1.97	0.46
1:J:157:ALA:O	1:J:162:VAL:HG23	2.15	0.46
1:K:249:LEU:HD12	1:K:321:ILE:HD11	1.97	0.46
1:C:108:THR:CG2	1:C:109:PHE:N	2.78	0.46
1:C:360:HIS:C	1:C:361:LEU:HD23	2.41	0.46
1:F:39:GLU:OE1	1:F:133:ARG:NH1	2.48	0.46
1:G:46:ALA:HB3	1:G:360:HIS:HA	1.96	0.46
1:H:54:ARG:HA	1:H:283:LEU:CD2	2.44	0.46
1:I:148:HIS:CE1	1:I:153:VAL:HG22	2.50	0.46
1:J:62:ILE:O	1:J:66:TRP:HB2	2.16	0.46
1:J:165:ALA:O	1:J:166:MET:C	2.55	0.46
1:J:283:LEU:HD12	1:J:283:LEU:H	1.81	0.46
1:L:249:LEU:HD12	1:L:321:ILE:HD11	1.97	0.46
1:B:92:MET:CE	1:B:106:ILE:HD11	2.45	0.46
1:B:181:LEU:N	1:B:181:LEU:HD23	2.30	0.46
1:E:50:SER:O	1:E:51:SER:C	2.55	0.46
1:F:226:THR:O	1:F:236:SER:HA	2.15	0.46
1:H:281:LEU:HB3	1:H:283:LEU:CD1	2.46	0.46
1:I:72:PRO:HG2	1:I:90:HIS:CE1	2.50	0.46
1:I:77:ARG:CG	1:I:143:SER:HB3	2.44	0.46
1:J:191:LEU:CD1	1:J:242:ASP:OD2	2.64	0.46
1:D:295:GLN:O	1:D:297:TYR:N	2.41	0.46
1:E:212:SER:O	1:E:213:LEU:HB2	2.16	0.46
1:F:92:MET:SD	1:F:106:ILE:HD11	2.56	0.46
1:G:141:TYR:O	1:G:141:TYR:CD1	2.68	0.46
1:H:66:TRP:O	1:H:66:TRP:CD1	2.69	0.46
1:I:108:THR:HG22	1:I:109:PHE:N	2.29	0.46
1:I:284:LEU:HD22	1:I:287:HIS:ND1	2.29	0.46
1:J:329:TRP:O	1:J:331:THR:HG23	2.15	0.46
1:K:158:THR:O	1:K:160:SER:HA	2.16	0.46
1:A:217:ARG:CD	4:A:501:HOH:O	2.61	0.46
1:K:201:GLU:HB2	1:K:306:ASP:OD2	2.15	0.46
1:K:307:HIS:O	1:K:308:ILE:C	2.58	0.46
1:L:177:LYS:O	1:L:180:SER:OG	2.15	0.46
1:L:274:ILE:HD13	1:L:353:VAL:HG12	1.97	0.46
1:L:354:PHE:CD1	1:L:354:PHE:C	2.94	0.46
1:B:217:ARG:CA	1:B:220:ALA:H	2.29	0.46
1:E:95:ILE:O	1:E:96:GLN:C	2.58	0.46
1:F:34:SER:CB	1:L:280:GLU:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:LEU:HB2	1:G:53:LEU:HD21	1.96	0.46
1:H:46:ALA:O	1:H:47:ILE:C	2.58	0.46
1:H:99:GLN:C	1:H:100:ALA:O	2.59	0.46
1:L:268:PHE:CD1	1:L:268:PHE:O	2.69	0.46
1:A:277:GLU:O	1:A:278:LEU:C	2.54	0.46
1:H:336:GLU:O	1:H:337:GLU:C	2.58	0.46
1:J:155:VAL:O	1:J:156:GLY:C	2.56	0.46
1:A:221:ALA:O	1:A:222:LYS:C	2.57	0.45
1:D:148:HIS:NE2	1:D:153:VAL:HG22	2.31	0.45
1:E:150:ASN:O	1:E:151:ASN:CB	2.64	0.45
1:F:100:ALA:N	1:F:179:LEU:HD11	2.31	0.45
1:I:134:HIS:HA	1:I:192:SER:O	2.16	0.45
1:J:248:ASP:O	1:J:249:LEU:HB2	2.15	0.45
1:K:127:LEU:O	1:K:128:ASN:CB	2.64	0.45
1:B:319:HIS:CE1	1:B:321:ILE:HG21	2.51	0.45
1:C:302:VAL:HG22	1:C:303:ILE:N	2.31	0.45
1:H:163:PRO:O	1:H:164:CYS:C	2.57	0.45
1:I:304:GLN:OE1	1:I:308:ILE:HG13	2.16	0.45
1:J:226:THR:O	1:J:227:PRO:C	2.58	0.45
1:J:266:ARG:NH1	1:J:267:TRP:CE2	2.84	0.45
1:K:90:HIS:ND1	1:K:90:HIS:C	2.75	0.45
1:F:70:LEU:HB2	1:F:165:ALA:HB2	1.98	0.45
1:G:321:ILE:O	1:G:321:ILE:CG2	2.64	0.45
1:G:327:GLU:C	1:G:329:TRP:H	2.24	0.45
1:H:64:GLU:O	1:H:68:ASN:HB2	2.17	0.45
1:H:172:ARG:C	1:H:174:LEU:N	2.75	0.45
1:J:69:ASP:CA	1:J:94:ARG:NH1	2.79	0.45
1:K:252:ALA:O	1:K:255:PRO:HD3	2.17	0.45
1:B:217:ARG:HA	1:B:221:ALA:H	1.81	0.45
1:C:349:LYS:O	1:C:353:VAL:HG23	2.15	0.45
1:F:162:VAL:HB	1:F:163:PRO:HD3	1.99	0.45
1:G:154:PHE:N	1:G:332:MET:SD	2.89	0.45
1:I:57:ALA:CB	1:I:349:LYS:HD3	2.46	0.45
1:J:36:TRP:CH2	1:J:132:LYS:C	2.94	0.45
1:J:109:PHE:CB	1:J:218:HIS:CE1	3.00	0.45
1:J:199:ASP:OD1	1:J:200:GLY:N	2.45	0.45
1:J:264:SER:O	1:J:265:ALA:C	2.57	0.45
1:K:35:ALA:C	1:K:37:PRO:HD2	2.41	0.45
1:L:236:SER:C	1:L:238:LEU:N	2.73	0.45
1:L:302:VAL:HG22	1:L:303:ILE:N	2.31	0.45
1:A:300:GLY:O	1:A:301:GLY:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:SER:O	1:D:265:ALA:C	2.58	0.45
1:E:62:ILE:O	1:E:66:TRP:HB2	2.16	0.45
1:G:100:ALA:HB1	1:G:127:LEU:HD21	1.98	0.45
1:H:304:GLN:HA	1:H:304:GLN:OE1	2.17	0.45
1:K:140:HIS:ND1	1:K:142:ASP:OD1	2.49	0.45
1:B:132:LYS:HA	1:B:228:HIS:NE2	2.32	0.45
1:C:308:ILE:N	1:C:309:PRO:CD	2.79	0.45
1:C:314:GLY:HA3	1:D:206:HIS:HB3	1.99	0.45
1:F:100:ALA:HA	1:F:179:LEU:HD12	1.98	0.45
1:F:308:ILE:HB	1:F:309:PRO:HD3	1.99	0.45
1:G:38:GLU:C	1:G:40:LYS:H	2.25	0.45
1:G:229:PRO:O	1:G:230:PRO:C	2.58	0.45
1:G:288:SER:HG	1:G:291:GLY:N	2.14	0.45
1:L:40:LYS:HB3	1:L:242:ASP:OD1	2.16	0.45
1:L:112:GLN:NE2	1:L:117:TYR:CZ	2.85	0.45
1:A:311:LEU:O	1:A:312:ARG:C	2.57	0.45
1:E:238:LEU:C	1:E:240:GLY:N	2.70	0.45
1:F:167:MET:HE2	1:F:197:PHE:CZ	2.51	0.45
1:F:219:LEU:O	1:F:220:ALA:C	2.54	0.45
1:G:39:GLU:C	1:G:133:ARG:HH21	2.25	0.45
1:G:79:PRO:HG2	1:G:204:PHE:CZ	2.52	0.45
1:H:158:THR:OG1	1:H:334:ASP:CG	2.60	0.45
1:I:163:PRO:HB3	1:I:247:LEU:HB2	1.99	0.45
1:J:48:LEU:N	1:J:357:GLU:OE2	2.44	0.45
1:J:158:THR:OG1	1:J:334:ASP:OD1	2.31	0.45
1:J:199:ASP:O	1:J:200:GLY:C	2.60	0.45
1:J:268:PHE:O	1:J:269:GLU:C	2.60	0.45
1:K:133:ARG:HE	1:K:242:ASP:CG	2.25	0.45
1:C:229:PRO:O	1:C:230:PRO:O	2.34	0.45
1:F:36:TRP:HD1	1:L:280:GLU:HG3	1.81	0.45
1:G:40:LYS:HA	1:G:133:ARG:NH2	2.32	0.45
1:G:87:ALA:O	1:G:88:ARG:C	2.59	0.45
1:G:227:PRO:HA	1:G:235:THR:O	2.17	0.45
1:G:281:LEU:HB2	1:G:283:LEU:CD1	2.47	0.45
1:G:329:TRP:HZ3	1:J:263:ASN:HA	1.82	0.45
1:I:284:LEU:HD23	1:I:287:HIS:CB	2.46	0.45
1:J:36:TRP:HD1	1:J:37:PRO:HD3	1.80	0.45
1:J:170:LEU:HD23	1:J:170:LEU:C	2.41	0.45
1:J:344:ILE:O	1:J:348:ASN:HB2	2.16	0.45
1:K:105:GLU:O	1:K:106:ILE:HD13	2.16	0.45
1:L:254:ASN:N	1:L:255:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:270:ARG:HA	1:L:270:ARG:HD2	1.85	0.45
1:A:208:SER:OG	1:A:211:ASP:HB3	2.17	0.45
1:D:71:GLN:N	1:D:72:PRO:HD2	2.31	0.45
1:E:277:GLU:O	1:E:277:GLU:HG3	2.17	0.45
1:E:348:ASN:O	1:E:349:LYS:C	2.57	0.45
1:F:91:ILE:O	1:F:95:ILE:HG13	2.17	0.45
1:G:140:HIS:ND1	1:G:140:HIS:C	2.74	0.45
1:J:64:GLU:O	1:J:67:GLN:HB2	2.16	0.45
1:J:159:ASP:HB2	1:J:249:LEU:CD2	2.47	0.45
1:J:266:ARG:CG	1:J:266:ARG:HH11	2.30	0.45
1:J:281:LEU:HB2	1:J:283:LEU:CD1	2.46	0.45
1:K:72:PRO:HG2	1:K:90:HIS:NE2	2.31	0.45
1:K:279:HIS:O	1:K:280:GLU:C	2.60	0.45
1:A:64:GLU:O	1:A:65:MET:C	2.60	0.45
1:F:92:MET:HG2	1:F:104:LEU:HD13	1.98	0.45
1:G:146:PHE:C	1:G:147:SER:O	2.58	0.45
1:J:43:HIS:CD2	1:J:358:TYR:CE1	3.05	0.45
1:A:36:TRP:N	1:A:37:PRO:CD	2.80	0.44
1:I:170:LEU:HD23	1:I:170:LEU:O	2.17	0.44
1:B:149:TRP:O	1:B:150:ASN:C	2.59	0.44
1:E:208:SER:OG	1:E:211:ASP:HB3	2.17	0.44
1:F:253:PRO:O	1:F:254:ASN:C	2.58	0.44
1:J:128:ASN:N	1:J:128:ASN:ND2	2.65	0.44
1:J:208:SER:O	1:J:210:GLN:N	2.50	0.44
1:B:230:PRO:C	1:B:232:ALA:H	2.25	0.44
1:F:285:LYS:CE	1:F:286:ASP:OD2	2.65	0.44
1:G:113:THR:HG22	1:G:214:TYR:CE2	2.52	0.44
1:I:207:TRP:CD1	1:I:208:SER:N	2.86	0.44
1:I:279:HIS:C	1:I:279:HIS:CD2	2.95	0.44
1:I:297:TYR:O	1:I:297:TYR:CG	2.70	0.44
1:C:95:ILE:CG2	1:C:104:LEU:HD21	2.45	0.44
1:D:104:LEU:CD2	1:D:125:SER:HB2	2.47	0.44
1:F:71:GLN:OE1	1:F:336:GLU:OE2	2.35	0.44
1:G:162:VAL:O	1:G:163:PRO:C	2.60	0.44
1:I:270:ARG:O	1:I:274:ILE:HG13	2.17	0.44
1:J:87:ALA:O	1:J:91:ILE:HG13	2.18	0.44
1:J:133:ARG:HB3	1:J:191:LEU:HD12	1.99	0.44
1:L:76:GLU:HB2	1:L:153:VAL:CG1	2.48	0.44
1:B:212:SER:O	1:B:213:LEU:C	2.58	0.44
1:B:231:GLY:O	1:B:232:ALA:O	2.36	0.44
3:A:402:A1D5C:C08	1:D:262:PRO:HG3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:HB3	1:C:133:ARG:NH1	2.32	0.44
1:D:201:GLU:HG2	1:D:213:LEU:HD23	1.98	0.44
1:H:300:GLY:HA3	1:I:300:GLY:HA3	1.98	0.44
1:J:133:ARG:HE	1:J:242:ASP:CG	2.25	0.44
1:K:207:TRP:HZ2	1:K:304:GLN:HB2	1.82	0.44
1:C:95:ILE:O	1:C:96:GLN:C	2.59	0.44
1:G:208:SER:O	1:G:209:PRO:C	2.60	0.44
1:G:297:TYR:O	1:G:297:TYR:CG	2.71	0.44
1:H:61:SER:O	1:H:62:ILE:C	2.61	0.44
1:H:76:GLU:HG3	1:H:153:VAL:HG13	1.99	0.44
1:H:172:ARG:O	1:H:175:ASP:N	2.36	0.44
1:J:49:ASN:OD1	1:J:52:ALA:N	2.35	0.44
1:J:189:PRO:HD2	1:J:189:PRO:O	2.17	0.44
1:J:243:LEU:HG	1:J:244:LEU:N	2.33	0.44
1:L:223:MET:C	1:L:225:SER:H	2.25	0.44
1:L:288:SER:C	1:L:290:GLU:N	2.73	0.44
1:B:52:ALA:O	1:B:55:GLN:N	2.51	0.44
1:C:297:TYR:CE1	1:C:298:SER:O	2.71	0.44
1:D:83:GLY:O	1:D:84:SER:C	2.59	0.44
1:I:92:MET:HE1	1:I:106:ILE:HD11	1.99	0.44
1:I:357:GLU:O	1:I:358:TYR:C	2.60	0.44
1:A:174:LEU:O	1:A:175:ASP:C	2.61	0.44
1:E:134:HIS:O	1:E:242:ASP:HB2	2.18	0.44
1:G:152:ARG:O	1:G:332:MET:CE	2.66	0.44
1:H:285:LYS:CG	1:H:286:ASP:H	2.31	0.44
1:I:335:ASN:C	1:I:335:ASN:OD1	2.53	0.44
1:J:132:LYS:NZ	1:J:190:ASP:HB3	2.32	0.44
1:B:68:ASN:CB	1:B:94:ARG:HH12	2.29	0.44
1:B:88:ARG:HG2	1:B:92:MET:HE2	2.00	0.44
1:C:162:VAL:HB	1:C:163:PRO:HD3	2.00	0.44
1:E:345:ASP:O	1:E:349:LYS:HG3	2.18	0.44
1:F:206:HIS:O	1:F:208:SER:HB3	2.17	0.44
1:G:340:ASP:O	1:G:341:GLU:C	2.61	0.44
1:H:345:ASP:O	1:H:346:ASN:C	2.60	0.44
1:J:36:TRP:CZ3	1:J:132:LYS:C	2.96	0.44
1:J:85:TYR:O	1:J:86:ALA:C	2.61	0.44
1:J:113:THR:HG22	1:J:214:TYR:CE1	2.53	0.44
1:J:217:ARG:O	1:J:218:HIS:C	2.61	0.44
1:J:269:GLU:O	1:J:270:ARG:C	2.61	0.44
1:J:315:VAL:HG12	1:J:316:PRO:N	2.32	0.44
1:J:354:PHE:O	1:J:355:VAL:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:MET:HG3	1:K:169:GLU:HB2	2.00	0.44
1:B:278:LEU:HB3	1:B:284:LEU:HD13	2.00	0.43
1:A:268:PHE:CD1	1:A:268:PHE:C	2.95	0.43
1:C:132:LYS:NZ	1:C:190:ASP:CB	2.76	0.43
1:C:297:TYR:CD1	1:C:298:SER:O	2.71	0.43
1:E:344:ILE:O	1:E:345:ASP:C	2.57	0.43
1:G:109:PHE:CZ	1:G:215:GLY:HA2	2.53	0.43
1:G:205:LEU:HD21	1:J:239:HIS:NE2	2.33	0.43
1:J:35:ALA:O	1:J:36:TRP:C	2.60	0.43
3:K:402:A1D5C:C11	3:K:402:A1D5C:C06	2.94	0.43
1:L:71:GLN:HA	1:L:74:LEU:HD12	2.00	0.43
1:L:307:HIS:O	1:L:310:PHE:N	2.46	0.43
1:A:349:LYS:O	1:A:353:VAL:HG23	2.19	0.43
1:C:248:ASP:OD2	1:C:305:ASP:OD2	2.36	0.43
1:E:98:LEU:HB3	1:E:175:ASP:OD2	2.17	0.43
1:G:109:PHE:HZ	1:G:215:GLY:HA2	1.83	0.43
1:J:124:ILE:N	1:J:124:ILE:HD12	2.33	0.43
1:J:189:PRO:O	1:J:189:PRO:CD	2.65	0.43
1:J:233:ARG:NH2	1:K:80:GLY:O	2.51	0.43
1:A:170:LEU:C	1:A:170:LEU:HD23	2.43	0.43
1:C:249:LEU:HD12	1:C:321:ILE:HD11	1.99	0.43
1:D:100:ALA:HA	1:D:179:LEU:CD1	2.49	0.43
1:F:36:TRP:CD1	1:F:37:PRO:HD3	2.53	0.43
1:F:128:ASN:C	1:F:130:THR:N	2.74	0.43
1:F:157:ALA:O	1:F:162:VAL:HG23	2.19	0.43
1:F:181:LEU:C	1:F:182:LYS:HG2	2.43	0.43
1:G:146:PHE:O	1:G:147:SER:O	2.36	0.43
1:G:254:ASN:N	1:G:255:PRO:CD	2.81	0.43
1:H:283:LEU:HD12	1:H:283:LEU:N	2.29	0.43
1:J:149:TRP:O	1:J:151:ASN:N	2.50	0.43
1:B:336:GLU:O	1:B:337:GLU:C	2.55	0.43
1:F:233:ARG:HG2	1:L:54:ARG:NH2	2.33	0.43
1:F:270:ARG:O	1:F:274:ILE:HG13	2.18	0.43
1:G:57:ALA:HB1	1:G:349:LYS:HE2	2.00	0.43
1:J:46:ALA:O	1:J:47:ILE:C	2.61	0.43
1:B:112:GLN:OE1	1:B:117:TYR:CE1	2.71	0.43
1:C:276:HIS:O	1:C:279:HIS:HB3	2.19	0.43
1:G:159:ASP:OD1	1:G:159:ASP:C	2.61	0.43
1:G:174:LEU:O	1:G:175:ASP:C	2.60	0.43
1:H:88:ARG:HG3	1:H:123:ILE:HD11	2.01	0.43
1:I:68:ASN:CB	1:I:94:ARG:HH12	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:158:THR:OG1	1:I:334:ASP:CG	2.61	0.43
1:L:223:MET:C	1:L:225:SER:N	2.77	0.43
1:B:34:SER:HG	1:B:35:ALA:H	1.61	0.43
1:B:100:ALA:HA	1:B:179:LEU:HD12	2.01	0.43
1:A:177:LYS:O	1:A:180:SER:OG	2.29	0.43
1:E:167:MET:O	1:E:168:LEU:C	2.62	0.43
1:F:85:TYR:HD1	1:F:88:ARG:HH12	1.66	0.43
1:F:301:GLY:H	1:I:300:GLY:C	2.27	0.43
1:G:49:ASN:OD1	1:G:51:SER:CA	2.66	0.43
1:H:272:GLN:OE1	1:H:296:ASN:OD1	2.36	0.43
1:I:35:ALA:O	1:I:37:PRO:HD2	2.19	0.43
1:K:83:GLY:O	1:K:84:SER:C	2.61	0.43
1:L:257:PHE:HE1	1:L:322:PRO:HD3	1.84	0.43
1:A:85:TYR:OH	1:L:55:GLN:CG	2.67	0.43
1:C:231:GLY:O	1:C:232:ALA:O	2.36	0.43
1:E:38:GLU:O	1:E:39:GLU:C	2.55	0.43
1:F:324:PRO:O	1:F:325:PHE:C	2.61	0.43
1:G:40:LYS:HB3	1:G:242:ASP:OD1	2.18	0.43
1:I:132:LYS:O	1:I:240:GLY:HA3	2.19	0.43
1:J:45:PRO:HB2	1:J:357:GLU:HB3	2.00	0.43
1:J:130:THR:O	1:J:132:LYS:CA	2.67	0.43
1:J:269:GLU:C	1:J:271:LEU:N	2.76	0.43
1:B:42:TYR:O	1:B:43:HIS:C	2.60	0.43
1:G:211:ASP:O	1:G:212:SER:CB	2.67	0.43
1:H:36:TRP:CD1	1:H:37:PRO:HD3	2.52	0.43
1:J:101:ASP:O	1:J:127:LEU:HD22	2.19	0.43
1:J:102:TRP:HA	1:J:127:LEU:HD23	2.00	0.43
1:J:270:ARG:O	1:J:274:ILE:HG13	2.19	0.43
1:K:36:TRP:CD2	1:K:132:LYS:HD2	2.53	0.43
1:B:349:LYS:O	1:B:353:VAL:HG23	2.18	0.43
1:C:90:HIS:O	1:C:94:ARG:HG2	2.18	0.43
1:D:114:PRO:O	1:I:116:GLY:HA2	2.19	0.43
1:E:75:ILE:O	1:E:75:ILE:HG12	2.19	0.43
1:E:207:TRP:HZ2	1:E:304:GLN:HB2	1.84	0.43
1:F:78:TYR:CE1	1:F:81:SER:HB3	2.54	0.43
1:F:181:LEU:O	1:F:182:LYS:HG2	2.19	0.43
1:F:232:ALA:HA	1:L:54:ARG:NH1	2.31	0.43
1:F:300:GLY:CA	1:H:301:GLY:H	2.32	0.43
1:G:149:TRP:CZ3	1:G:150:ASN:HB2	2.53	0.43
1:G:281:LEU:HB2	1:G:283:LEU:HD12	2.01	0.43
1:I:51:SER:O	1:I:52:ALA:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:305:ASP:O	1:J:307:HIS:N	2.52	0.43
1:A:74:LEU:C	1:A:75:ILE:HG23	2.43	0.43
1:A:75:ILE:O	1:A:77:ARG:HG2	2.19	0.43
1:D:100:ALA:HA	1:D:179:LEU:HD12	2.01	0.43
1:D:152:ARG:O	1:D:332:MET:HE3	2.19	0.43
1:D:166:MET:HG2	1:D:348:ASN:OD1	2.18	0.43
1:E:281:LEU:HB2	1:E:283:LEU:HD12	2.01	0.43
1:G:36:TRP:CD1	1:G:37:PRO:HD3	2.54	0.43
1:G:86:ALA:O	1:G:90:HIS:N	2.45	0.43
1:I:56:ILE:HD12	1:I:356:LEU:CD1	2.49	0.43
1:I:252:ALA:HB1	1:I:253:PRO:CD	2.47	0.43
1:I:307:HIS:O	1:I:308:ILE:C	2.62	0.43
1:J:100:ALA:HA	1:J:179:LEU:CD1	2.47	0.43
1:J:154:PHE:C	1:J:155:VAL:CG1	2.92	0.43
1:L:128:ASN:N	1:L:129:PRO:CD	2.81	0.43
1:L:265:ALA:O	1:L:266:ARG:C	2.60	0.43
1:B:344:ILE:O	1:B:345:ASP:C	2.60	0.42
1:C:97:ARG:O	1:C:97:ARG:HG2	2.17	0.42
1:D:49:ASN:O	1:D:49:ASN:OD1	2.36	0.42
1:E:169:GLU:O	1:E:169:GLU:HG3	2.16	0.42
1:F:36:TRP:N	1:F:37:PRO:CD	2.82	0.42
1:G:344:ILE:O	1:G:348:ASN:HB2	2.18	0.42
1:H:92:MET:HE3	1:H:106:ILE:HD11	2.01	0.42
1:H:191:LEU:HD21	1:H:358:TYR:CD1	2.53	0.42
1:I:259:ASN:C	1:I:259:ASN:HD22	2.26	0.42
1:J:35:ALA:C	1:J:37:PRO:CD	2.87	0.42
1:J:269:GLU:O	1:J:271:LEU:N	2.52	0.42
3:K:402:A1D5C:O17	3:K:402:A1D5C:C28	2.67	0.42
1:E:106:ILE:CG2	1:E:107:ASP:H	2.33	0.42
1:J:154:PHE:C	1:J:155:VAL:HG13	2.45	0.42
1:G:128:ASN:O	1:G:129:PRO:C	2.61	0.42
1:J:128:ASN:O	1:J:129:PRO:C	2.62	0.42
1:J:267:TRP:CZ2	1:J:358:TYR:CE2	3.06	0.42
1:J:292:ARG:HG3	1:J:292:ARG:HH11	1.83	0.42
1:L:62:ILE:HG12	1:L:341:GLU:HG2	2.01	0.42
1:L:68:ASN:HB3	1:L:94:ARG:HH12	1.85	0.42
1:L:178:LEU:C	1:L:180:SER:H	2.28	0.42
1:L:180:SER:O	1:L:182:LYS:HE3	2.20	0.42
1:L:212:SER:O	1:L:213:LEU:C	2.62	0.42
1:A:117:TYR:C	1:A:118:ARG:HG2	2.44	0.42
1:A:144:LYS:HG2	1:A:146:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:GLY:O	1:D:232:ALA:O	2.37	0.42
1:G:71:GLN:HA	1:G:74:LEU:CD1	2.48	0.42
1:G:159:ASP:N	1:G:160:SER:HA	2.34	0.42
1:G:348:ASN:O	1:G:352:GLN:HG3	2.19	0.42
1:J:141:TYR:CD1	1:J:141:TYR:O	2.73	0.42
1:J:353:VAL:O	1:J:354:PHE:C	2.61	0.42
1:E:149:TRP:CE3	1:E:150:ASN:HB2	2.55	0.42
1:G:40:LYS:N	1:G:133:ARG:HH21	2.18	0.42
1:J:191:LEU:HG	1:J:192:SER:N	2.33	0.42
1:F:232:ALA:C	1:L:54:ARG:NH1	2.77	0.42
1:I:149:TRP:CE3	1:I:150:ASN:HB2	2.55	0.42
1:J:135:LEU:HD13	1:J:358:TYR:CG	2.55	0.42
1:J:140:HIS:ND1	1:J:142:ASP:OD1	2.52	0.42
1:L:132:LYS:HA	1:L:228:HIS:NE2	2.35	0.42
1:A:175:ASP:O	1:A:176:LYS:C	2.58	0.42
1:D:279:HIS:C	1:D:281:LEU:N	2.77	0.42
1:E:128:ASN:OD1	1:E:128:ASN:N	2.52	0.42
1:G:118:ARG:NH2	4:G:501:HOH:O	2.53	0.42
1:G:229:PRO:HB2	1:G:230:PRO:HD2	2.01	0.42
1:H:71:GLN:OE1	1:H:336:GLU:OE2	2.37	0.42
1:J:154:PHE:O	1:J:155:VAL:HG12	2.19	0.42
1:J:321:ILE:HG13	1:J:322:PRO:HD2	2.02	0.42
1:K:52:ALA:O	1:K:53:LEU:C	2.60	0.42
1:L:127:LEU:O	1:L:128:ASN:C	2.60	0.42
1:E:92:MET:HE1	1:E:106:ILE:HD11	1.99	0.42
1:E:174:LEU:HD22	1:E:356:LEU:HD11	2.01	0.42
1:F:149:TRP:CE3	1:F:150:ASN:HB2	2.55	0.42
1:G:49:ASN:OD1	1:G:49:ASN:C	2.63	0.42
1:G:179:LEU:C	1:G:181:LEU:N	2.76	0.42
1:I:297:TYR:C	1:I:298:SER:O	2.61	0.42
1:J:94:ARG:HE	1:J:94:ARG:HB3	1.62	0.42
1:K:128:ASN:N	1:K:129:PRO:HD3	2.33	0.42
1:L:65:MET:HG3	1:L:169:GLU:HB2	2.01	0.42
1:A:109:PHE:CD1	1:A:109:PHE:C	2.98	0.42
1:A:157:ALA:O	1:A:162:VAL:HG23	2.20	0.42
1:A:259:ASN:OD1	1:A:259:ASN:C	2.62	0.42
1:F:136:VAL:HG21	1:F:241:MET:HE3	2.02	0.42
1:F:163:PRO:HB3	1:F:247:LEU:HB2	2.02	0.42
1:F:308:ILE:N	1:F:309:PRO:HD2	2.34	0.42
1:G:140:HIS:NE2	1:G:159:ASP:OD1	2.52	0.42
1:G:305:ASP:CG	1:G:306:ASP:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:304:GLN:OE1	1:H:308:ILE:HG13	2.19	0.42
1:I:247:LEU:CD2	1:I:320:LEU:HD12	2.49	0.42
1:I:254:ASN:N	1:I:255:PRO:CD	2.83	0.42
1:J:254:ASN:N	1:J:255:PRO:CD	2.83	0.42
1:J:263:ASN:HD22	1:J:263:ASN:H	1.68	0.42
1:J:279:HIS:CD2	1:J:287:HIS:O	2.73	0.42
1:L:274:ILE:HD11	1:L:357:GLU:OE1	2.19	0.42
1:B:49:ASN:O	1:B:53:LEU:HG	2.20	0.42
1:A:49:ASN:OD1	1:A:49:ASN:C	2.62	0.42
1:A:340:ASP:OD1	1:K:286:ASP:OD2	2.37	0.42
1:E:49:ASN:O	1:E:52:ALA:HB3	2.20	0.42
1:E:79:PRO:C	1:E:81:SER:H	2.28	0.42
1:G:142:ASP:OD1	1:G:142:ASP:N	2.40	0.42
1:G:288:SER:OG	1:G:290:GLU:N	2.53	0.42
1:J:91:ILE:O	1:J:95:ILE:HG13	2.19	0.42
1:J:113:THR:HB	1:J:114:PRO:HD2	2.01	0.42
1:B:167:MET:HE2	1:B:197:PHE:CE2	2.55	0.41
1:D:150:ASN:O	1:D:151:ASN:HB2	2.20	0.41
1:F:38:GLU:O	1:F:41:ASN:HB2	2.20	0.41
1:F:113:THR:O	1:F:114:PRO:C	2.62	0.41
1:F:323:SER:HA	1:F:324:PRO:HA	1.76	0.41
1:G:340:ASP:C	1:G:342:SER:N	2.79	0.41
1:H:223:MET:HB3	1:H:238:LEU:HD23	2.02	0.41
1:I:34:SER:OG	1:I:35:ALA:N	2.50	0.41
1:I:263:ASN:OD1	1:I:263:ASN:N	2.46	0.41
1:J:49:ASN:OD1	1:J:49:ASN:O	2.38	0.41
1:J:168:LEU:O	1:J:169:GLU:C	2.62	0.41
1:L:47:ILE:HG13	1:L:270:ARG:HH22	1.80	0.41
1:L:178:LEU:C	1:L:180:SER:N	2.78	0.41
1:B:110:LEU:CD2	1:B:117:TYR:HD2	2.32	0.41
1:C:223:MET:C	1:C:225:SER:H	2.28	0.41
1:G:70:LEU:O	1:G:70:LEU:HG	2.18	0.41
1:G:108:THR:HG23	1:G:120:PHE:O	2.20	0.41
1:G:181:LEU:O	1:G:182:LYS:C	2.63	0.41
1:H:96:GLN:HG3	1:H:104:LEU:HD11	2.02	0.41
1:I:159:ASP:CG	3:I:402:A1D5C:C25	2.92	0.41
1:I:328:VAL:O	1:I:329:TRP:C	2.63	0.41
1:J:78:TYR:O	1:J:79:PRO:C	2.63	0.41
1:L:272:GLN:HG2	1:L:294:PHE:O	2.20	0.41
1:B:292:ARG:HG3	1:B:292:ARG:NH1	2.35	0.41
1:C:223:MET:C	1:C:225:SER:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASN:OD1	1:D:49:ASN:C	2.62	0.41
1:H:54:ARG:HA	1:H:283:LEU:HD21	2.02	0.41
1:H:160:SER:OG	1:H:163:PRO:HG2	2.21	0.41
1:H:212:SER:O	1:H:217:ARG:NH1	2.53	0.41
1:H:285:LYS:CG	1:H:286:ASP:N	2.83	0.41
1:J:208:SER:O	1:J:209:PRO:C	2.57	0.41
1:J:355:VAL:O	1:J:357:GLU:N	2.53	0.41
1:K:68:ASN:HB3	1:K:94:ARG:HH12	1.83	0.41
1:K:113:THR:HB	1:K:114:PRO:HD2	2.03	0.41
1:B:67:GLN:HG3	1:B:68:ASN:N	2.34	0.41
1:B:68:ASN:HB3	1:B:94:ARG:HH11	1.77	0.41
1:C:88:ARG:HG3	1:C:123:ILE:HD11	2.02	0.41
1:E:109:PHE:CE1	1:E:120:PHE:HB2	2.55	0.41
1:E:228:HIS:HA	1:E:229:PRO:C	2.45	0.41
1:F:310:PHE:O	1:F:311:LEU:C	2.61	0.41
1:G:141:TYR:CD2	1:G:198:PHE:O	2.74	0.41
1:H:149:TRP:O	1:H:150:ASN:C	2.62	0.41
1:J:36:TRP:CZ3	1:J:133:ARG:N	2.86	0.41
1:J:150:ASN:O	1:J:151:ASN:CB	2.69	0.41
1:J:150:ASN:O	1:J:151:ASN:HB3	2.21	0.41
1:J:170:LEU:HD23	1:J:170:LEU:O	2.20	0.41
1:J:270:ARG:O	1:J:274:ILE:HD12	2.21	0.41
1:K:246:LEU:HD23	1:K:319:HIS:CD2	2.55	0.41
1:K:279:HIS:HE1	1:K:287:HIS:O	2.03	0.41
1:L:128:ASN:N	1:L:128:ASN:OD1	2.53	0.41
1:L:182:LYS:HD3	1:L:182:LYS:H	1.85	0.41
1:B:144:LYS:HD3	1:B:146:PHE:CE2	2.56	0.41
1:F:39:GLU:HB2	1:F:133:ARG:HH11	1.81	0.41
1:G:34:SER:OG	1:G:35:ALA:N	2.51	0.41
1:H:117:TYR:O	1:H:118:ARG:CG	2.69	0.41
1:I:46:ALA:O	1:I:47:ILE:C	2.63	0.41
1:J:61:SER:C	1:J:63:SER:N	2.78	0.41
1:A:68:ASN:CB	1:A:94:ARG:NH1	2.70	0.41
1:F:61:SER:O	1:F:62:ILE:C	2.61	0.41
1:F:300:GLY:HA3	1:H:301:GLY:H	1.85	0.41
1:I:109:PHE:CZ	1:I:120:PHE:HB2	2.56	0.41
1:J:70:LEU:CD1	1:J:74:LEU:HD11	2.50	0.41
1:J:285:LYS:H	1:J:346:ASN:HD21	1.68	0.41
1:J:336:GLU:O	1:J:338:ASN:N	2.53	0.41
1:K:136:VAL:HG22	1:K:194:GLN:HB3	2.03	0.41
1:L:95:ILE:O	1:L:95:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:178:LEU:O	1:L:180:SER:N	2.53	0.41
1:L:305:ASP:C	1:L:307:HIS:N	2.77	0.41
1:B:94:ARG:HH21	1:B:97:ARG:NH1	2.19	0.41
1:B:311:LEU:C	1:B:313:ARG:N	2.78	0.41
1:C:231:GLY:C	1:C:232:ALA:O	2.63	0.41
1:C:233:ARG:NH2	1:I:80:GLY:O	2.54	0.41
1:D:92:MET:CE	1:D:106:ILE:HD11	2.51	0.41
1:F:232:ALA:N	1:L:54:ARG:CZ	2.84	0.41
1:F:253:PRO:O	1:F:254:ASN:HB2	2.21	0.41
1:G:83:GLY:O	1:G:84:SER:C	2.63	0.41
1:H:69:ASP:OD1	1:H:94:ARG:HD3	2.21	0.41
1:H:150:ASN:O	1:H:151:ASN:HB2	2.20	0.41
1:H:353:VAL:O	1:H:354:PHE:C	2.63	0.41
1:J:65:MET:HA	1:J:69:ASP:CG	2.45	0.41
1:J:297:TYR:O	1:J:297:TYR:CG	2.74	0.41
1:K:100:ALA:HA	1:K:179:LEU:CD1	2.50	0.41
1:K:163:PRO:HB3	1:K:247:LEU:HB2	2.03	0.41
1:K:165:ALA:C	1:K:167:MET:N	2.77	0.41
1:L:94:ARG:HH21	1:L:97:ARG:HH11	1.68	0.41
1:L:347:LEU:HD23	1:L:347:LEU:HA	1.84	0.41
1:B:102:TRP:CE3	1:B:125:SER:OG	2.72	0.41
1:B:263:ASN:OD1	3:K:402:A1D5C:C12	2.68	0.41
1:F:285:LYS:NZ	1:F:286:ASP:OD1	2.25	0.41
1:I:170:LEU:HD21	1:I:174:LEU:HD12	2.02	0.41
1:I:229:PRO:C	1:I:230:PRO:O	2.64	0.41
1:J:354:PHE:O	1:J:355:VAL:O	2.38	0.41
1:K:90:HIS:CE1	1:K:94:ARG:HG3	2.55	0.41
1:K:172:ARG:HG2	1:K:172:ARG:NH1	2.34	0.41
1:C:92:MET:O	1:C:93:GLN:C	2.62	0.41
1:D:92:MET:CE	1:D:106:ILE:CD1	2.98	0.41
1:E:175:ASP:C	1:E:177:LYS:N	2.79	0.41
1:F:165:ALA:O	1:F:166:MET:C	2.62	0.41
1:F:179:LEU:C	1:F:181:LEU:N	2.77	0.41
1:G:71:GLN:N	1:G:72:PRO:HD2	2.35	0.41
1:G:197:PHE:CD1	1:G:197:PHE:N	2.88	0.41
1:H:276:HIS:O	1:H:276:HIS:ND1	2.54	0.41
1:I:247:LEU:N	1:I:247:LEU:HD23	2.36	0.41
1:J:328:VAL:O	1:J:329:TRP:C	2.63	0.41
1:K:247:LEU:HD22	1:K:320:LEU:HD12	2.03	0.41
1:L:56:ILE:O	1:L:57:ALA:C	2.63	0.41
1:L:158:THR:C	1:L:160:SER:HA	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TYR:CZ	1:L:55:GLN:HG2	2.56	0.41
1:F:233:ARG:NH2	1:L:58:GLU:CD	2.78	0.41
1:G:223:MET:HB3	1:G:238:LEU:CD2	2.51	0.41
1:I:213:LEU:O	1:I:217:ARG:HG3	2.20	0.41
1:J:47:ILE:HG12	1:J:48:LEU:N	2.36	0.41
1:J:211:ASP:O	1:J:212:SER:HB3	2.21	0.41
1:K:267:TRP:CZ2	1:K:358:TYR:CE2	3.09	0.41
1:B:116:GLY:O	1:B:118:ARG:HG2	2.19	0.40
1:B:179:LEU:C	1:B:181:LEU:N	2.79	0.40
1:C:150:ASN:O	1:C:151:ASN:HB2	2.21	0.40
1:D:335:ASN:OD1	1:D:338:ASN:ND2	2.54	0.40
1:G:253:PRO:HB3	1:G:340:ASP:OD2	2.21	0.40
1:G:279:HIS:C	1:G:281:LEU:N	2.78	0.40
1:J:137:LEU:O	1:J:167:MET:CE	2.70	0.40
1:J:178:LEU:C	1:J:180:SER:N	2.79	0.40
1:L:208:SER:O	1:L:209:PRO:C	2.61	0.40
1:A:279:HIS:CD2	1:A:279:HIS:C	2.98	0.40
1:D:177:LYS:HE2	1:D:177:LYS:HB3	1.93	0.40
1:E:337:GLU:CD	1:E:337:GLU:H	2.29	0.40
1:F:232:ALA:C	1:L:54:ARG:CZ	2.94	0.40
1:H:338:ASN:N	1:H:338:ASN:HD22	2.19	0.40
1:I:172:ARG:O	1:I:173:ALA:C	2.64	0.40
1:J:207:TRP:HZ2	1:J:304:GLN:HB2	1.86	0.40
1:J:285:LYS:HG3	1:J:286:ASP:N	2.36	0.40
1:A:277:GLU:C	1:A:279:HIS:N	2.77	0.40
1:D:205:LEU:O	1:D:206:HIS:CG	2.74	0.40
1:E:302:VAL:HG22	1:E:303:ILE:N	2.36	0.40
1:G:46:ALA:CB	1:G:360:HIS:HA	2.51	0.40
1:G:268:PHE:O	1:G:271:LEU:HB2	2.22	0.40
1:H:133:ARG:O	1:H:191:LEU:HA	2.21	0.40
1:H:295:GLN:O	1:H:296:ASN:C	2.65	0.40
1:I:200:GLY:O	1:I:201:GLU:C	2.64	0.40
1:J:135:LEU:HD23	1:J:193:LEU:CD1	2.50	0.40
1:J:158:THR:O	1:J:249:LEU:HA	2.21	0.40
1:J:266:ARG:NH1	1:J:266:ARG:HG3	2.37	0.40
1:B:247:LEU:N	1:B:247:LEU:HD23	2.35	0.40
1:A:299:TYR:O	1:A:300:GLY:O	2.40	0.40
1:D:278:LEU:HB3	1:D:284:LEU:HD13	2.02	0.40
1:E:181:LEU:O	1:E:182:LYS:CB	2.67	0.40
1:E:181:LEU:O	1:E:182:LYS:HB2	2.22	0.40
1:G:157:ALA:CA	1:G:334:ASP:OD1	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:SER:O	1:G:238:LEU:N	2.54	0.40
1:G:311:LEU:HD12	1:G:317:VAL:HG23	2.02	0.40
1:J:41:ASN:OD1	1:J:41:ASN:N	2.53	0.40
1:A:47:ILE:CD1	1:A:357:GLU:OE2	2.66	0.40
1:A:254:ASN:N	1:A:255:PRO:CD	2.84	0.40
1:C:65:MET:HG3	1:C:169:GLU:HB2	2.02	0.40
1:C:213:LEU:HB2	1:C:217:ARG:HD3	2.04	0.40
1:C:270:ARG:HH11	1:C:270:ARG:HD2	1.61	0.40
1:C:353:VAL:O	1:C:357:GLU:HG3	2.22	0.40
1:D:138:ALA:O	1:D:246:LEU:HD12	2.22	0.40
1:E:100:ALA:HA	1:E:179:LEU:HD12	2.02	0.40
1:F:39:GLU:O	1:F:40:LYS:C	2.62	0.40
1:G:206:HIS:O	1:G:207:TRP:O	2.39	0.40
1:G:275:GLU:O	1:G:276:HIS:C	2.63	0.40
1:J:50:SER:O	1:J:51:SER:C	2.64	0.40
1:J:342:SER:O	1:J:346:ASN:HB2	2.22	0.40
1:L:113:THR:O	1:L:115:TYR:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/329 (97%)	286 (90%)	30 (9%)	3 (1%)	14	38
1	B	319/329 (97%)	288 (90%)	26 (8%)	5 (2%)	7	24
1	C	319/329 (97%)	290 (91%)	24 (8%)	5 (2%)	7	24
1	D	319/329 (97%)	288 (90%)	24 (8%)	7 (2%)	5	17
1	E	319/329 (97%)	282 (88%)	28 (9%)	9 (3%)	4	13
1	F	319/329 (97%)	277 (87%)	36 (11%)	6 (2%)	6	20
1	G	319/329 (97%)	260 (82%)	45 (14%)	14 (4%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	319/329 (97%)	273 (86%)	35 (11%)	11 (3%)	3	10
1	I	319/329 (97%)	270 (85%)	42 (13%)	7 (2%)	5	17
1	J	319/329 (97%)	252 (79%)	47 (15%)	20 (6%)	1	3
1	K	319/329 (97%)	282 (88%)	29 (9%)	8 (2%)	4	15
1	L	319/329 (97%)	274 (86%)	38 (12%)	7 (2%)	5	17
All	All	3828/3948 (97%)	3322 (87%)	404 (11%)	102 (3%)	4	13

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	SER
1	B	218	HIS
1	B	232	ALA
1	A	232	ALA
1	A	301	GLY
1	D	180	SER
1	D	207	TRP
1	D	212	SER
1	E	175	ASP
1	E	180	SER
1	F	131	ALA
1	F	132	LYS
1	G	147	SER
1	G	207	TRP
1	G	212	SER
1	G	341	GLU
1	H	100	ALA
1	H	173	ALA
1	H	213	LEU
1	H	286	ASP
1	H	296	ASN
1	H	348	ASN
1	I	298	SER
1	J	74	LEU
1	J	131	ALA
1	J	151	ASN
1	J	179	LEU
1	J	297	TYR
1	J	355	VAL
1	K	179	LEU

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Mol	Chain	Res	Type
1	L	224	ALA
1	L	237	GLN
1	A	300	GLY
1	C	207	TRP
1	C	306	ASP
1	E	156	GLY
1	E	176	LYS
1	E	300	GLY
1	F	180	SER
1	G	131	ALA
1	G	156	GLY
1	G	282	GLY
1	H	156	GLY
1	I	50	SER
1	I	213	LEU
1	J	62	ILE
1	J	155	VAL
1	J	266	ARG
1	J	292	ARG
1	J	330	HIS
1	J	337	GLU
1	J	348	ASN
1	K	292	ARG
1	L	306	ASP
1	B	180	SER
1	C	232	ALA
1	D	156	GLY
1	E	212	SER
1	G	296	ASN
1	G	300	GLY
1	G	354	PHE
1	H	172	ARG
1	H	200	GLY
1	I	201	GLU
1	J	212	SER
1	K	207	TRP
1	C	212	SER
1	D	232	ALA
1	G	39	GLU
1	H	212	SER
1	I	306	ASP
1	I	329	TRP

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Mol	Chain	Res	Type
1	J	280	GLU
1	J	329	TRP
1	K	213	LEU
1	K	280	GLU
1	K	333	ASP
1	L	114	PRO
1	L	220	ALA
1	B	217	ARG
1	D	280	GLU
1	E	100	ALA
1	E	207	TRP
1	E	306	ASP
1	F	306	ASP
1	I	36	TRP
1	J	218	HIS
1	K	128	ASN
1	F	212	SER
1	J	200	GLY
1	J	129	PRO
1	L	156	GLY
1	F	156	GLY
1	G	72	PRO
1	G	328	VAL
1	H	234	GLY
1	C	300	GLY
1	L	254	ASN
1	G	251	GLY
1	K	208	SER
1	D	300	GLY
1	J	254	ASN

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%)	263 (93%)	21 (7%)	13 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	284/290 (98%)	256 (90%)	28 (10%)	7	23
1	C	284/290 (98%)	258 (91%)	26 (9%)	8	26
1	D	284/290 (98%)	256 (90%)	28 (10%)	7	23
1	E	284/290 (98%)	258 (91%)	26 (9%)	8	26
1	F	284/290 (98%)	255 (90%)	29 (10%)	7	22
1	G	284/290 (98%)	253 (89%)	31 (11%)	6	19
1	H	284/290 (98%)	259 (91%)	25 (9%)	9	28
1	I	284/290 (98%)	253 (89%)	31 (11%)	6	19
1	J	284/290 (98%)	255 (90%)	29 (10%)	7	22
1	K	284/290 (98%)	253 (89%)	31 (11%)	6	19
1	L	284/290 (98%)	252 (89%)	32 (11%)	5	18
All	All	3408/3480 (98%)	3071 (90%)	337 (10%)	7	23

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	B	50	SER
1	B	51	SER
1	B	67	GLN
1	B	71	GLN
1	B	75	ILE
1	B	94	ARG
1	B	97	ARG
1	B	113	THR
1	B	121	SER
1	B	128	ASN
1	B	130	THR
1	B	137	LEU
1	B	152	ARG
1	B	153	VAL
1	B	167	MET
1	B	179	LEU
1	B	180	SER
1	B	182	LYS
1	B	206	HIS
1	B	217	ARG
1	B	263	ASN

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Mol	Chain	Res	Type
1	B	280	GLU
1	B	284	LEU
1	B	290	GLU
1	B	297	TYR
1	B	308	ILE
1	B	312	ARG
1	A	51	SER
1	A	58	GLU
1	A	63	SER
1	A	67	GLN
1	A	77	ARG
1	A	94	ARG
1	A	98	LEU
1	A	105	GLU
1	A	106	ILE
1	A	130	THR
1	A	132	LYS
1	A	143	SER
1	A	166	MET
1	A	167	MET
1	A	180	SER
1	A	191	LEU
1	A	209	PRO
1	A	284	LEU
1	A	297	TYR
1	A	327	GLU
1	A	342	SER
1	C	51	SER
1	C	63	SER
1	C	70	LEU
1	C	75	ILE
1	C	97	ARG
1	C	110	LEU
1	C	118	ARG
1	C	119	SER
1	C	121	SER
1	C	132	LYS
1	C	143	SER
1	C	147	SER
1	C	155	VAL
1	C	176	LYS
1	C	180	SER

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Mol	Chain	Res	Type
1	C	182	LYS
1	C	191	LEU
1	C	206	HIS
1	C	209	PRO
1	C	247	LEU
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	D	47	ILE
1	D	51	SER
1	D	60	THR
1	D	67	GLN
1	D	75	ILE
1	D	84	SER
1	D	97	ARG
1	D	105	GLU
1	D	110	LEU
1	D	119	SER
1	D	128	ASN
1	D	130	THR
1	D	132	LYS
1	D	147	SER
1	D	158	THR
1	D	160	SER
1	D	176	LYS
1	D	179	LEU
1	D	180	SER
1	D	182	LYS
1	D	205	LEU
1	D	247	LEU
1	D	280	GLU
1	D	284	LEU
1	D	295	GLN
1	D	296	ASN
1	D	303	ILE
1	D	342	SER
1	E	50	SER
1	E	51	SER
1	E	58	GLU

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Mol	Chain	Res	Type
1	E	61	SER
1	E	63	SER
1	E	71	GLN
1	E	75	ILE
1	E	81	SER
1	E	84	SER
1	E	92	MET
1	E	101	ASP
1	E	105	GLU
1	E	106	ILE
1	E	113	THR
1	E	132	LYS
1	E	155	VAL
1	E	179	LEU
1	E	180	SER
1	E	182	LYS
1	E	192	SER
1	E	205	LEU
1	E	270	ARG
1	E	280	GLU
1	E	284	LEU
1	E	297	TYR
1	E	312	ARG
1	F	34	SER
1	F	47	ILE
1	F	50	SER
1	F	51	SER
1	F	58	GLU
1	F	70	LEU
1	F	71	GLN
1	F	107	ASP
1	F	118	ARG
1	F	137	LEU
1	F	152	ARG
1	F	176	LYS
1	F	180	SER
1	F	205	LEU
1	F	208	SER
1	F	238	LEU
1	F	242	ASP
1	F	243	LEU
1	F	247	LEU

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Mol	Chain	Res	Type
1	F	269	GLU
1	F	272	GLN
1	F	280	GLU
1	F	284	LEU
1	F	285	LYS
1	F	288	SER
1	F	290	GLU
1	F	292	ARG
1	F	295	GLN
1	F	342	SER
1	G	40	LYS
1	G	41	ASN
1	G	50	SER
1	G	51	SER
1	G	54	ARG
1	G	60	THR
1	G	61	SER
1	G	124	ILE
1	G	126	THR
1	G	128	ASN
1	G	130	THR
1	G	133	ARG
1	G	147	SER
1	G	150	ASN
1	G	151	ASN
1	G	179	LEU
1	G	180	SER
1	G	182	LYS
1	G	242	ASP
1	G	256	THR
1	G	281	LEU
1	G	284	LEU
1	G	288	SER
1	G	292	ARG
1	G	295	GLN
1	G	297	TYR
1	G	308	ILE
1	G	311	LEU
1	G	312	ARG
1	G	315	VAL
1	G	318	LEU
1	H	61	SER

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Mol	Chain	Res	Type
1	H	71	GLN
1	H	74	LEU
1	H	76	GLU
1	H	84	SER
1	H	92	MET
1	H	94	ARG
1	H	110	LEU
1	H	130	THR
1	H	137	LEU
1	H	143	SER
1	H	147	SER
1	H	158	THR
1	H	160	SER
1	H	176	LYS
1	H	179	LEU
1	H	182	LYS
1	H	209	PRO
1	H	243	LEU
1	H	270	ARG
1	H	283	LEU
1	H	297	TYR
1	H	298	SER
1	H	312	ARG
1	H	338	ASN
1	I	40	LYS
1	I	51	SER
1	I	60	THR
1	I	67	GLN
1	I	92	MET
1	I	93	GLN
1	I	94	ARG
1	I	105	GLU
1	I	110	LEU
1	I	130	THR
1	I	143	SER
1	I	147	SER
1	I	158	THR
1	I	172	ARG
1	I	176	LYS
1	I	179	LEU
1	I	180	SER
1	I	182	LYS

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Mol	Chain	Res	Type
1	I	201	GLU
1	I	213	LEU
1	I	247	LEU
1	I	259	ASN
1	I	269	GLU
1	I	272	GLN
1	I	281	LEU
1	I	297	TYR
1	I	303	ILE
1	I	312	ARG
1	I	318	LEU
1	I	326	PRO
1	I	337	GLU
1	J	34	SER
1	J	36	TRP
1	J	47	ILE
1	J	60	THR
1	J	61	SER
1	J	67	GLN
1	J	70	LEU
1	J	97	ARG
1	J	121	SER
1	J	128	ASN
1	J	132	LYS
1	J	143	SER
1	J	150	ASN
1	J	152	ARG
1	J	158	THR
1	J	179	LEU
1	J	180	SER
1	J	182	LYS
1	J	191	LEU
1	J	216	SER
1	J	263	ASN
1	J	266	ARG
1	J	283	LEU
1	J	290	GLU
1	J	296	ASN
1	J	312	ARG
1	J	321	ILE
1	J	346	ASN
1	J	350	ILE

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Mol	Chain	Res	Type
1	K	50	SER
1	K	51	SER
1	K	63	SER
1	K	64	GLU
1	K	70	LEU
1	K	71	GLN
1	K	89	GLN
1	K	94	ARG
1	K	97	ARG
1	K	141	TYR
1	K	143	SER
1	K	151	ASN
1	K	158	THR
1	K	160	SER
1	K	179	LEU
1	K	180	SER
1	K	182	LYS
1	K	196	ILE
1	K	216	SER
1	K	217	ARG
1	K	225	SER
1	K	233	ARG
1	K	242	ASP
1	K	247	LEU
1	K	284	LEU
1	K	285	LYS
1	K	290	GLU
1	K	297	TYR
1	K	312	ARG
1	K	337	GLU
1	K	341	GLU
1	L	40	LYS
1	L	41	ASN
1	L	47	ILE
1	L	48	LEU
1	L	51	SER
1	L	54	ARG
1	L	55	GLN
1	L	60	THR
1	L	63	SER
1	L	93	GLN
1	L	94	ARG

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Mol	Chain	Res	Type
1	L	105	GLU
1	L	107	ASP
1	L	110	LEU
1	L	113	THR
1	L	118	ARG
1	L	125	SER
1	L	128	ASN
1	L	132	LYS
1	L	137	LEU
1	L	143	SER
1	L	147	SER
1	L	176	LYS
1	L	180	SER
1	L	182	LYS
1	L	193	LEU
1	L	205	LEU
1	L	242	ASP
1	L	262	PRO
1	L	284	LEU
1	L	312	ARG
1	L	318	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	218	HIS
1	B	296	ASN
1	B	319	HIS
1	A	44	GLN
1	A	90	HIS
1	A	237	GLN
1	A	254	ASN
1	A	272	GLN
1	A	296	ASN
1	C	55	GLN
1	C	68	ASN
1	C	112	GLN
1	C	194	GLN
1	C	304	GLN
1	C	319	HIS
1	D	41	ASN
1	D	44	GLN

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Mol	Chain	Res	Type
1	D	194	GLN
1	E	71	GLN
1	E	90	HIS
1	E	96	GLN
1	E	254	ASN
1	E	276	HIS
1	F	93	GLN
1	F	112	GLN
1	F	128	ASN
1	F	134	HIS
1	F	307	HIS
1	G	93	GLN
1	G	99	GLN
1	G	319	HIS
1	H	41	ASN
1	H	134	HIS
1	H	272	GLN
1	H	338	ASN
1	I	41	ASN
1	I	44	GLN
1	I	128	ASN
1	J	90	HIS
1	J	112	GLN
1	J	151	ASN
1	J	206	HIS
1	K	43	HIS
1	K	44	GLN
1	K	67	GLN
1	K	295	GLN
1	L	112	GLN
1	L	194	GLN
1	L	304	GLN
1	L	352	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	A1D5C	E	402	2	33,33,33	3.73	14 (42%)	44,48,48	2.84	16 (36%)
3	A1D5C	H	402	-	33,33,33	3.82	16 (48%)	44,48,48	3.15	16 (36%)
3	A1D5C	I	402	2	33,33,33	4.02	16 (48%)	44,48,48	3.45	14 (31%)
3	A1D5C	F	402	2	33,33,33	3.84	16 (48%)	44,48,48	3.38	20 (45%)
3	A1D5C	A	402	2	33,33,33	4.20	18 (54%)	44,48,48	3.87	20 (45%)
3	A1D5C	D	402	2	33,33,33	4.21	17 (51%)	44,48,48	4.30	25 (56%)
3	A1D5C	L	402	-	33,33,33	3.86	16 (48%)	44,48,48	2.99	17 (38%)
3	A1D5C	B	402	2	33,33,33	4.27	17 (51%)	44,48,48	3.54	19 (43%)
3	A1D5C	G	402	2	33,33,33	3.97	17 (51%)	44,48,48	2.80	20 (45%)
3	A1D5C	K	402	-	33,33,33	3.63	18 (54%)	44,48,48	3.77	22 (50%)
3	A1D5C	C	402	-	33,33,33	4.40	18 (54%)	44,48,48	4.30	22 (50%)
3	A1D5C	J	402	-	33,33,33	3.77	15 (45%)	44,48,48	2.81	14 (31%)

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	A1D5C	E	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	H	402	-	-	4/12/39/39	0/5/5/5
3	A1D5C	I	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	F	402	2	-	4/12/39/39	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1D5C	A	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	D	402	2	-	6/12/39/39	0/5/5/5
3	A1D5C	L	402	-	-	2/12/39/39	0/5/5/5
3	A1D5C	B	402	2	-	4/12/39/39	0/5/5/5
3	A1D5C	G	402	2	-	1/12/39/39	0/5/5/5
3	A1D5C	K	402	-	-	3/12/39/39	0/5/5/5
3	A1D5C	C	402	-	-	4/12/39/39	0/5/5/5
3	A1D5C	J	402	-	-	2/12/39/39	0/5/5/5

All (198) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	A1D5C	C08-C07	15.88	1.77	1.52
3	B	402	A1D5C	C08-C07	15.75	1.77	1.52
3	C	402	A1D5C	C08-C07	13.96	1.74	1.52
3	A	402	A1D5C	C08-C07	13.91	1.74	1.52
3	I	402	A1D5C	C08-C07	13.57	1.74	1.52
3	E	402	A1D5C	C08-C07	12.98	1.73	1.52
3	F	402	A1D5C	C08-C07	12.63	1.72	1.52
3	H	402	A1D5C	C08-C07	12.08	1.71	1.52
3	L	402	A1D5C	C08-C07	11.89	1.71	1.52
3	K	402	A1D5C	C08-C07	11.55	1.71	1.52
3	J	402	A1D5C	C08-C07	11.00	1.70	1.52
3	G	402	A1D5C	C16-N15	10.66	1.47	1.36
3	C	402	A1D5C	C16-N15	9.92	1.46	1.36
3	J	402	A1D5C	C16-N15	9.78	1.46	1.36
3	G	402	A1D5C	C08-C07	9.46	1.67	1.52
3	A	402	A1D5C	C05-N04	8.95	1.65	1.47
3	L	402	A1D5C	C16-N15	8.73	1.45	1.36
3	D	402	A1D5C	C05-N04	8.17	1.64	1.47
3	B	402	A1D5C	C05-N04	8.10	1.63	1.47
3	B	402	A1D5C	C02-N04	8.04	1.57	1.35
3	I	402	A1D5C	C05-N04	7.92	1.63	1.47
3	E	402	A1D5C	C16-N15	7.78	1.44	1.36
3	A	402	A1D5C	C02-N04	7.59	1.56	1.35
3	C	402	A1D5C	C05-N04	7.58	1.62	1.47
3	I	402	A1D5C	C16-N15	7.34	1.43	1.36
3	H	402	A1D5C	C16-N15	7.23	1.43	1.36
3	F	402	A1D5C	C16-N15	7.11	1.43	1.36
3	F	402	A1D5C	C05-N04	7.09	1.61	1.47
3	C	402	A1D5C	C02-N04	7.05	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	402	A1D5C	C05-N04	6.95	1.61	1.47
3	A	402	A1D5C	C06-C05	6.82	1.65	1.52
3	H	402	A1D5C	C05-N04	6.81	1.61	1.47
3	B	402	A1D5C	C06-C05	6.78	1.65	1.52
3	G	402	A1D5C	C08-N04	-6.66	1.33	1.46
3	D	402	A1D5C	C02-N04	6.63	1.53	1.35
3	C	402	A1D5C	C06-C05	6.60	1.65	1.52
3	E	402	A1D5C	C05-N04	6.58	1.60	1.47
3	B	402	A1D5C	C16-N15	6.48	1.42	1.36
3	J	402	A1D5C	C05-N04	6.44	1.60	1.47
3	D	402	A1D5C	C06-C05	6.43	1.64	1.52
3	I	402	A1D5C	C02-N04	6.35	1.53	1.35
3	H	402	A1D5C	C14-N15	6.26	1.50	1.38
3	A	402	A1D5C	C16-N15	6.18	1.42	1.36
3	L	402	A1D5C	C08-N04	-6.11	1.34	1.46
3	J	402	A1D5C	C08-N04	-6.10	1.34	1.46
3	G	402	A1D5C	C14-N15	6.05	1.49	1.38
3	I	402	A1D5C	C06-C05	6.02	1.63	1.52
3	H	402	A1D5C	C06-C05	5.99	1.63	1.52
3	K	402	A1D5C	C05-N04	5.91	1.59	1.47
3	K	402	A1D5C	C14-N15	5.89	1.49	1.38
3	F	402	A1D5C	C02-N04	5.81	1.51	1.35
3	L	402	A1D5C	C05-N04	5.79	1.59	1.47
3	H	402	A1D5C	C02-N04	5.71	1.51	1.35
3	K	402	A1D5C	C23-N24	-5.67	1.28	1.37
3	K	402	A1D5C	C06-C05	5.55	1.63	1.52
3	E	402	A1D5C	C02-N04	5.51	1.50	1.35
3	C	402	A1D5C	C14-N15	5.49	1.48	1.38
3	F	402	A1D5C	O09-C10	5.42	1.46	1.37
3	K	402	A1D5C	C16-N15	5.34	1.41	1.36
3	E	402	A1D5C	C14-N15	5.30	1.48	1.38
3	E	402	A1D5C	C06-C05	5.29	1.62	1.52
3	J	402	A1D5C	C02-N04	5.29	1.50	1.35
3	L	402	A1D5C	C22-C23	5.25	1.48	1.39
3	F	402	A1D5C	C14-N15	5.25	1.48	1.38
3	F	402	A1D5C	C06-C05	5.25	1.62	1.52
3	A	402	A1D5C	C22-C23	5.24	1.48	1.39
3	L	402	A1D5C	C06-C05	5.23	1.62	1.52
3	G	402	A1D5C	C23-C27	-5.13	1.32	1.40
3	D	402	A1D5C	C20-C19	5.10	1.56	1.46
3	E	402	A1D5C	C08-N04	-5.05	1.36	1.46
3	K	402	A1D5C	C08-N04	-4.95	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	402	A1D5C	C22-C23	4.93	1.47	1.39
3	L	402	A1D5C	C14-N15	4.92	1.47	1.38
3	C	402	A1D5C	O09-C10	4.87	1.45	1.37
3	F	402	A1D5C	C08-N04	-4.87	1.37	1.46
3	G	402	A1D5C	C23-N24	-4.84	1.30	1.37
3	J	402	A1D5C	C14-N15	4.78	1.47	1.38
3	L	402	A1D5C	C02-N04	4.78	1.48	1.35
3	I	402	A1D5C	C18-C16	-4.77	1.43	1.50
3	F	402	A1D5C	C23-N24	-4.77	1.30	1.37
3	J	402	A1D5C	C22-C23	4.74	1.47	1.39
3	B	402	A1D5C	C23-C27	-4.66	1.33	1.40
3	K	402	A1D5C	C02-N04	4.58	1.48	1.35
3	G	402	A1D5C	C12-C11	4.53	1.46	1.38
3	I	402	A1D5C	C08-N04	-4.49	1.38	1.46
3	H	402	A1D5C	C08-N04	-4.40	1.38	1.46
3	I	402	A1D5C	C14-N15	4.40	1.46	1.38
3	C	402	A1D5C	C22-C23	4.40	1.46	1.39
3	I	402	A1D5C	C20-C19	4.32	1.54	1.46
3	C	402	A1D5C	C29-C10	4.30	1.48	1.40
3	A	402	A1D5C	C14-N15	4.29	1.46	1.38
3	A	402	A1D5C	C23-N24	-4.27	1.30	1.37
3	J	402	A1D5C	C20-C19	4.18	1.54	1.46
3	G	402	A1D5C	C02-N04	4.17	1.47	1.35
3	H	402	A1D5C	C23-N24	-4.16	1.31	1.37
3	D	402	A1D5C	C19-C18	4.15	1.40	1.34
3	A	402	A1D5C	C08-N04	-4.07	1.38	1.46
3	K	402	A1D5C	C22-C21	-4.05	1.32	1.38
3	D	402	A1D5C	C14-N15	4.04	1.46	1.38
3	J	402	A1D5C	C06-C07	-4.04	1.31	1.52
3	D	402	A1D5C	C23-N24	-3.99	1.31	1.37
3	B	402	A1D5C	C23-N24	-3.88	1.31	1.37
3	J	402	A1D5C	C12-C11	3.88	1.45	1.38
3	D	402	A1D5C	C16-N15	3.84	1.40	1.36
3	C	402	A1D5C	C08-N04	-3.84	1.39	1.46
3	G	402	A1D5C	C06-C07	-3.81	1.32	1.52
3	C	402	A1D5C	C22-C21	-3.81	1.32	1.38
3	G	402	A1D5C	C06-C05	3.76	1.59	1.52
3	A	402	A1D5C	O09-C10	3.74	1.43	1.37
3	K	402	A1D5C	C22-C23	3.67	1.45	1.39
3	L	402	A1D5C	O09-C10	3.66	1.43	1.37
3	J	402	A1D5C	C06-C05	3.63	1.59	1.52
3	L	402	A1D5C	C23-N24	-3.54	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	402	A1D5C	C20-C19	3.53	1.53	1.46
3	I	402	A1D5C	O09-C10	3.49	1.43	1.37
3	A	402	A1D5C	C22-C21	-3.47	1.33	1.38
3	B	402	A1D5C	C14-N15	3.46	1.45	1.38
3	L	402	A1D5C	C20-C19	3.43	1.53	1.46
3	E	402	A1D5C	C06-C07	-3.43	1.34	1.52
3	G	402	A1D5C	C28-C27	-3.39	1.34	1.40
3	C	402	A1D5C	C20-C19	3.38	1.53	1.46
3	C	402	A1D5C	C12-C11	3.33	1.44	1.38
3	H	402	A1D5C	O09-C10	3.32	1.43	1.37
3	H	402	A1D5C	C18-C16	-3.32	1.46	1.50
3	G	402	A1D5C	C22-C23	3.31	1.45	1.39
3	L	402	A1D5C	C06-C07	-3.30	1.35	1.52
3	D	402	A1D5C	C22-C21	-3.29	1.33	1.38
3	E	402	A1D5C	C18-C16	-3.28	1.46	1.50
3	K	402	A1D5C	C20-C19	3.26	1.52	1.46
3	B	402	A1D5C	C22-C21	-3.24	1.33	1.38
3	B	402	A1D5C	C06-C07	-3.20	1.36	1.52
3	L	402	A1D5C	C27-N26	3.19	1.45	1.39
3	F	402	A1D5C	C22-C23	3.19	1.44	1.39
3	D	402	A1D5C	C22-C23	3.17	1.44	1.39
3	I	402	A1D5C	O17-C16	-3.16	1.17	1.23
3	D	402	A1D5C	C13-C14	-3.16	1.34	1.39
3	L	402	A1D5C	C12-C11	3.15	1.44	1.38
3	L	402	A1D5C	C19-C18	3.13	1.39	1.34
3	E	402	A1D5C	C22-C23	3.08	1.44	1.39
3	F	402	A1D5C	C12-C11	3.07	1.44	1.38
3	E	402	A1D5C	O09-C10	3.07	1.42	1.37
3	C	402	A1D5C	C06-C07	-3.07	1.36	1.52
3	I	402	A1D5C	C22-C21	-3.05	1.33	1.38
3	D	402	A1D5C	C08-N04	-3.03	1.40	1.46
3	C	402	A1D5C	C19-C18	3.02	1.39	1.34
3	C	402	A1D5C	C29-C18	3.02	1.52	1.45
3	D	402	A1D5C	O09-C10	3.01	1.42	1.37
3	I	402	A1D5C	C06-C07	-2.99	1.37	1.52
3	G	402	A1D5C	C19-C18	2.98	1.39	1.34
3	A	402	A1D5C	C06-C07	-2.98	1.37	1.52
3	H	402	A1D5C	C06-C07	-2.94	1.37	1.52
3	F	402	A1D5C	C22-C21	-2.90	1.34	1.38
3	D	402	A1D5C	C29-C18	2.85	1.52	1.45
3	F	402	A1D5C	C06-C07	-2.85	1.37	1.52
3	K	402	A1D5C	C06-C07	-2.83	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1D5C	C08-N04	-2.81	1.41	1.46
3	D	402	A1D5C	C06-C07	-2.80	1.38	1.52
3	K	402	A1D5C	C23-C27	-2.79	1.36	1.40
3	A	402	A1D5C	C20-C19	2.73	1.51	1.46
3	K	402	A1D5C	C18-C16	-2.70	1.46	1.50
3	E	402	A1D5C	C22-C21	-2.63	1.34	1.38
3	A	402	A1D5C	C12-C11	2.59	1.43	1.38
3	B	402	A1D5C	C22-C23	2.58	1.43	1.39
3	J	402	A1D5C	C22-C21	-2.56	1.34	1.38
3	J	402	A1D5C	O09-C10	2.55	1.41	1.37
3	C	402	A1D5C	C28-C27	2.54	1.43	1.40
3	B	402	A1D5C	C28-C20	-2.54	1.35	1.39
3	A	402	A1D5C	C23-C27	-2.53	1.36	1.40
3	B	402	A1D5C	C12-C11	2.48	1.43	1.38
3	H	402	A1D5C	C22-C21	-2.47	1.34	1.38
3	H	402	A1D5C	C20-C19	2.47	1.51	1.46
3	H	402	A1D5C	C12-C11	2.47	1.43	1.38
3	B	402	A1D5C	C19-C18	2.46	1.38	1.34
3	A	402	A1D5C	C18-C16	-2.46	1.47	1.50
3	K	402	A1D5C	O17-C16	-2.45	1.18	1.23
3	B	402	A1D5C	O09-C10	2.41	1.41	1.37
3	A	402	A1D5C	C29-C10	2.41	1.45	1.40
3	I	402	A1D5C	C23-N24	-2.40	1.34	1.37
3	F	402	A1D5C	C23-C27	-2.38	1.36	1.40
3	J	402	A1D5C	C18-C16	-2.35	1.47	1.50
3	C	402	A1D5C	C29-C14	2.34	1.45	1.41
3	I	402	A1D5C	C12-C11	2.29	1.42	1.38
3	J	402	A1D5C	C19-C18	2.28	1.38	1.34
3	E	402	A1D5C	C23-N24	-2.27	1.34	1.37
3	G	402	A1D5C	C22-C21	-2.27	1.35	1.38
3	K	402	A1D5C	C12-C11	2.20	1.42	1.38
3	F	402	A1D5C	C20-C19	2.16	1.50	1.46
3	E	402	A1D5C	C12-C11	2.15	1.42	1.38
3	B	402	A1D5C	C27-N26	-2.12	1.35	1.39
3	F	402	A1D5C	C18-C16	-2.11	1.47	1.50
3	D	402	A1D5C	C28-C27	-2.10	1.36	1.40
3	A	402	A1D5C	O17-C16	-2.09	1.19	1.23
3	K	402	A1D5C	C25-N26	-2.09	1.28	1.32
3	L	402	A1D5C	C28-C27	2.09	1.43	1.40
3	H	402	A1D5C	C23-C27	-2.08	1.37	1.40
3	G	402	A1D5C	C27-N26	-2.07	1.35	1.39
3	K	402	A1D5C	O09-C10	2.06	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	402	A1D5C	C23-C27	-2.01	1.37	1.40

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	A1D5C	C05-N04-C08	-17.59	91.83	112.38
3	B	402	A1D5C	C05-N04-C08	-16.11	93.56	112.38
3	D	402	A1D5C	C05-N04-C08	-13.94	96.10	112.38
3	A	402	A1D5C	C05-N04-C08	-13.57	96.53	112.38
3	K	402	A1D5C	C14-N15-C16	-12.80	103.45	111.35
3	A	402	A1D5C	C01-C02-N04	12.21	133.68	118.24
3	I	402	A1D5C	C05-N04-C08	-11.43	99.03	112.38
3	F	402	A1D5C	C05-N04-C08	-11.06	99.46	112.38
3	E	402	A1D5C	C05-N04-C08	-10.87	99.68	112.38
3	I	402	A1D5C	C14-N15-C16	-10.47	104.89	111.35
3	H	402	A1D5C	C05-N04-C08	-10.32	100.32	112.38
3	L	402	A1D5C	C05-N04-C08	-10.28	100.37	112.38
3	J	402	A1D5C	C05-N04-C08	-10.26	100.40	112.38
3	C	402	A1D5C	O03-C02-N04	10.15	132.95	120.98
3	I	402	A1D5C	C18-C16-N15	9.76	112.26	106.91
3	K	402	A1D5C	C05-N04-C08	-9.62	101.14	112.38
3	F	402	A1D5C	C29-C18-C16	8.97	110.22	105.31
3	C	402	A1D5C	C29-C18-C16	8.86	110.16	105.31
3	D	402	A1D5C	O17-C16-N15	-8.79	112.29	126.30
3	H	402	A1D5C	C14-N15-C16	-8.71	105.97	111.35
3	G	402	A1D5C	C14-N15-C16	-8.39	106.17	111.35
3	D	402	A1D5C	O17-C16-C18	7.77	137.43	127.70
3	K	402	A1D5C	C18-C16-N15	7.68	111.11	106.91
3	D	402	A1D5C	O09-C10-C11	-7.45	106.59	123.91
3	J	402	A1D5C	C14-N15-C16	-7.34	106.82	111.35
3	D	402	A1D5C	O09-C10-C29	7.23	133.25	117.51
3	K	402	A1D5C	C28-C27-C23	-7.15	110.52	120.50
3	D	402	A1D5C	C14-N15-C16	-6.97	107.05	111.35
3	F	402	A1D5C	C01-C02-N04	6.93	127.01	118.24
3	L	402	A1D5C	C20-C28-C27	6.90	126.70	120.27
3	L	402	A1D5C	C28-C27-C23	-6.90	110.88	120.50
3	G	402	A1D5C	C18-C16-N15	6.85	110.67	106.91
3	C	402	A1D5C	O09-C10-C29	6.67	132.02	117.51
3	D	402	A1D5C	O03-C02-N04	6.49	128.63	120.98
3	E	402	A1D5C	C14-N15-C16	-6.41	107.39	111.35
3	H	402	A1D5C	C01-C02-N04	6.41	126.34	118.24
3	E	402	A1D5C	C01-C02-N04	6.24	126.13	118.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	A1D5C	C14-C29-C10	6.19	123.36	117.69
3	D	402	A1D5C	C18-C16-N15	6.15	110.28	106.91
3	A	402	A1D5C	C14-N15-C16	-6.12	107.57	111.35
3	D	402	A1D5C	C20-C28-C27	6.11	125.96	120.27
3	G	402	A1D5C	C05-N04-C08	-6.08	105.28	112.38
3	B	402	A1D5C	C06-C05-N04	5.96	110.59	102.93
3	B	402	A1D5C	O03-C02-N04	5.91	127.94	120.98
3	C	402	A1D5C	C14-N15-C16	-5.85	107.74	111.35
3	I	402	A1D5C	C20-C28-C27	5.82	125.69	120.27
3	C	402	A1D5C	O09-C10-C11	-5.80	110.43	123.91
3	G	402	A1D5C	C20-C28-C27	5.73	125.61	120.27
3	I	402	A1D5C	C01-C02-N04	5.69	125.44	118.24
3	K	402	A1D5C	C20-C28-C27	5.68	125.56	120.27
3	J	402	A1D5C	C20-C28-C27	5.63	125.51	120.27
3	B	402	A1D5C	C01-C02-N04	5.62	125.34	118.24
3	A	402	A1D5C	O09-C10-C29	5.59	129.66	117.51
3	D	402	A1D5C	C10-O09-C07	5.54	137.94	120.14
3	A	402	A1D5C	O09-C10-C11	-5.39	111.39	123.91
3	H	402	A1D5C	C20-C28-C27	5.31	125.22	120.27
3	B	402	A1D5C	C14-N15-C16	-5.31	108.08	111.35
3	H	402	A1D5C	C28-C27-C23	-5.30	113.11	120.50
3	F	402	A1D5C	C14-N15-C16	-5.29	108.09	111.35
3	H	402	A1D5C	C18-C16-N15	5.29	109.81	106.91
3	G	402	A1D5C	C20-C19-C18	-5.20	119.42	129.68
3	A	402	A1D5C	O03-C02-C01	-5.15	101.81	122.03
3	D	402	A1D5C	C06-C05-N04	5.14	109.53	102.93
3	C	402	A1D5C	C28-C27-C23	-5.01	113.52	120.50
3	I	402	A1D5C	O17-C16-C18	-4.89	121.56	127.70
3	L	402	A1D5C	C27-N26-C25	-4.89	95.69	105.18
3	F	402	A1D5C	C28-C27-C23	-4.86	113.72	120.50
3	J	402	A1D5C	C28-C27-C23	-4.82	113.78	120.50
3	D	402	A1D5C	C27-N26-C25	-4.72	96.01	105.18
3	J	402	A1D5C	C01-C02-N04	4.68	124.16	118.24
3	A	402	A1D5C	C20-C28-C27	4.64	124.59	120.27
3	K	402	A1D5C	C14-C29-C10	4.58	121.89	117.69
3	C	402	A1D5C	O03-C02-C01	-4.53	104.26	122.03
3	A	402	A1D5C	C10-O09-C07	4.53	134.69	120.14
3	E	402	A1D5C	C28-C27-C23	-4.53	114.19	120.50
3	A	402	A1D5C	C29-C18-C16	4.51	107.78	105.31
3	L	402	A1D5C	C14-N15-C16	-4.49	108.58	111.35
3	C	402	A1D5C	C20-C28-C27	4.44	124.41	120.27
3	B	402	A1D5C	O09-C10-C29	4.44	127.16	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	402	A1D5C	C18-C16-N15	4.41	109.32	106.91
3	K	402	A1D5C	C06-C05-N04	-4.39	97.29	102.93
3	A	402	A1D5C	C06-C05-N04	4.35	108.53	102.93
3	C	402	A1D5C	C10-O09-C07	4.32	134.01	120.14
3	B	402	A1D5C	O09-C10-C11	-4.28	113.97	123.91
3	A	402	A1D5C	O17-C16-N15	-4.17	119.66	126.30
3	K	402	A1D5C	O09-C07-C06	4.17	123.05	108.71
3	A	402	A1D5C	C28-C27-C23	-4.11	114.77	120.50
3	E	402	A1D5C	C20-C28-C27	4.08	124.07	120.27
3	K	402	A1D5C	C01-C02-N04	4.02	123.32	118.24
3	K	402	A1D5C	C27-N26-C25	-4.01	97.39	105.18
3	F	402	A1D5C	C20-C28-C27	4.01	124.01	120.27
3	K	402	A1D5C	C20-C19-C18	-3.97	121.85	129.68
3	E	402	A1D5C	C14-C29-C10	3.96	121.32	117.69
3	D	402	A1D5C	C28-C27-C23	-3.93	115.01	120.50
3	B	402	A1D5C	O03-C02-C01	-3.91	106.70	122.03
3	C	402	A1D5C	C05-N04-C02	3.89	136.41	124.18
3	H	402	A1D5C	C27-N26-C25	-3.83	97.74	105.18
3	I	402	A1D5C	C06-C05-N04	3.82	107.84	102.93
3	K	402	A1D5C	C22-C23-C27	3.74	126.21	122.10
3	D	402	A1D5C	N24-C25-N26	3.74	119.58	113.87
3	H	402	A1D5C	C14-C29-C10	3.73	121.11	117.69
3	B	402	A1D5C	O17-C16-N15	-3.71	120.38	126.30
3	F	402	A1D5C	C27-N26-C25	-3.70	97.99	105.18
3	D	402	A1D5C	C23-N24-C25	-3.70	102.49	106.73
3	L	402	A1D5C	O17-C16-C18	3.70	132.33	127.70
3	F	402	A1D5C	O09-C07-C06	3.66	121.31	108.71
3	I	402	A1D5C	C28-C27-C23	-3.66	115.40	120.50
3	K	402	A1D5C	C22-C21-C20	-3.64	116.52	121.22
3	H	402	A1D5C	C20-C19-C18	-3.63	122.53	129.68
3	F	402	A1D5C	C29-C18-C19	-3.63	116.08	130.26
3	L	402	A1D5C	C19-C18-C16	3.60	133.77	119.87
3	C	402	A1D5C	C01-C02-N04	3.60	122.79	118.24
3	K	402	A1D5C	C29-C18-C16	3.59	107.28	105.31
3	B	402	A1D5C	C10-O09-C07	3.59	131.67	120.14
3	G	402	A1D5C	C28-C27-C23	-3.58	115.50	120.50
3	F	402	A1D5C	C19-C18-C16	3.58	133.69	119.87
3	C	402	A1D5C	C06-C05-N04	3.57	107.52	102.93
3	K	402	A1D5C	O17-C16-N15	-3.57	120.61	126.30
3	A	402	A1D5C	O17-C16-C18	3.54	132.13	127.70
3	L	402	A1D5C	C22-C21-C20	-3.50	116.70	121.22
3	J	402	A1D5C	C06-C05-N04	-3.45	98.50	102.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	A1D5C	C10-O09-C07	3.44	131.19	120.14
3	L	402	A1D5C	C14-C29-C10	3.37	120.78	117.69
3	L	402	A1D5C	O17-C16-N15	-3.36	120.94	126.30
3	E	402	A1D5C	O09-C07-C06	3.35	120.26	108.71
3	B	402	A1D5C	C19-C18-C16	3.25	132.42	119.87
3	D	402	A1D5C	C19-C18-C16	3.25	132.41	119.87
3	A	402	A1D5C	C19-C18-C16	3.21	132.27	119.87
3	A	402	A1D5C	C05-N04-C02	3.19	134.20	124.18
3	L	402	A1D5C	N24-C25-N26	3.13	118.64	113.87
3	F	402	A1D5C	C22-C21-C20	-3.13	117.19	121.22
3	L	402	A1D5C	C29-C18-C16	3.12	107.02	105.31
3	K	402	A1D5C	C29-C14-N15	3.12	112.58	108.05
3	I	402	A1D5C	O09-C10-C11	-3.11	116.69	123.91
3	D	402	A1D5C	C13-C14-N15	-3.09	124.57	130.83
3	G	402	A1D5C	C23-C27-N26	3.09	115.05	108.39
3	K	402	A1D5C	C23-C27-N26	3.08	115.04	108.39
3	C	402	A1D5C	C14-C29-C10	3.08	120.51	117.69
3	H	402	A1D5C	C23-C27-N26	3.07	115.02	108.39
3	G	402	A1D5C	C14-C29-C18	3.07	111.33	106.51
3	G	402	A1D5C	C22-C21-C20	-3.06	117.27	121.22
3	J	402	A1D5C	C22-C21-C20	-3.05	117.29	121.22
3	E	402	A1D5C	C19-C18-C16	3.05	131.63	119.87
3	H	402	A1D5C	C22-C21-C20	-3.03	117.31	121.22
3	H	402	A1D5C	O09-C07-C06	3.02	119.09	108.71
3	F	402	A1D5C	O17-C16-C18	3.01	131.47	127.70
3	E	402	A1D5C	C29-C18-C16	3.00	106.95	105.31
3	B	402	A1D5C	C18-C16-N15	2.99	108.55	106.91
3	A	402	A1D5C	O03-C02-N04	2.99	124.50	120.98
3	G	402	A1D5C	C14-C29-C10	2.98	120.42	117.69
3	G	402	A1D5C	C23-N24-C25	2.98	110.14	106.73
3	J	402	A1D5C	O09-C07-C06	-2.95	98.55	108.71
3	D	402	A1D5C	O03-C02-C01	-2.94	110.49	122.03
3	L	402	A1D5C	O09-C07-C06	2.91	118.74	108.71
3	D	402	A1D5C	C23-C27-N26	2.90	114.64	108.39
3	C	402	A1D5C	C27-N26-C25	-2.89	99.57	105.18
3	I	402	A1D5C	C21-C20-C28	-2.89	115.08	118.72
3	L	402	A1D5C	C28-C27-N26	2.86	135.33	130.51
3	A	402	A1D5C	C27-N26-C25	-2.86	99.63	105.18
3	J	402	A1D5C	C19-C18-C16	2.86	130.89	119.87
3	B	402	A1D5C	C05-N04-C02	2.85	133.13	124.18
3	E	402	A1D5C	C20-C19-C18	-2.84	124.09	129.68
3	L	402	A1D5C	C29-C18-C19	-2.83	119.20	130.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	A1D5C	C18-C16-N15	2.78	108.43	106.91
3	J	402	A1D5C	C14-C29-C10	2.77	120.23	117.69
3	F	402	A1D5C	C11-C10-C29	-2.74	114.57	120.14
3	H	402	A1D5C	C29-C18-C16	2.72	106.80	105.31
3	E	402	A1D5C	C10-O09-C07	2.72	128.86	120.14
3	I	402	A1D5C	O09-C10-C29	2.71	123.41	117.51
3	G	402	A1D5C	C19-C18-C16	2.70	130.30	119.87
3	B	402	A1D5C	O17-C16-C18	2.68	131.06	127.70
3	D	402	A1D5C	C14-C29-C10	-2.68	115.23	117.69
3	A	402	A1D5C	C29-C18-C19	-2.68	119.78	130.26
3	K	402	A1D5C	C19-C18-C16	2.67	130.18	119.87
3	H	402	A1D5C	O03-C02-C01	-2.66	111.58	122.03
3	H	402	A1D5C	C19-C18-C16	2.64	130.05	119.87
3	C	402	A1D5C	C21-C20-C19	-2.61	112.24	121.22
3	D	402	A1D5C	C29-C14-N15	2.60	111.84	108.05
3	G	402	A1D5C	C06-C05-N04	2.58	106.25	102.93
3	F	402	A1D5C	C23-C27-N26	2.54	113.87	108.39
3	L	402	A1D5C	C23-C27-N26	2.50	113.79	108.39
3	B	402	A1D5C	C20-C28-C27	2.50	122.59	120.27
3	G	402	A1D5C	C10-C29-C18	-2.49	128.24	135.25
3	G	402	A1D5C	O09-C10-C29	-2.48	112.12	117.51
3	I	402	A1D5C	C27-N26-C25	-2.47	100.38	105.18
3	F	402	A1D5C	O03-C02-N04	-2.45	118.09	120.98
3	H	402	A1D5C	C22-C23-C27	2.42	124.76	122.10
3	C	402	A1D5C	O17-C16-C18	-2.41	124.67	127.70
3	B	402	A1D5C	C29-C18-C19	-2.37	120.99	130.26
3	A	402	A1D5C	C18-C16-N15	2.37	108.20	106.91
3	G	402	A1D5C	C27-N26-C25	-2.35	100.61	105.18
3	C	402	A1D5C	C06-C07-C08	-2.34	98.76	104.39
3	K	402	A1D5C	C28-C27-N26	2.33	134.44	130.51
3	K	402	A1D5C	C27-C23-N24	-2.32	102.31	106.15
3	B	402	A1D5C	C14-C29-C10	2.31	119.81	117.69
3	I	402	A1D5C	O03-C02-C01	-2.30	113.00	122.03
3	C	402	A1D5C	C28-C27-N26	2.29	134.37	130.51
3	D	402	A1D5C	C06-C07-C08	-2.29	98.89	104.39
3	J	402	A1D5C	C27-N26-C25	-2.28	100.76	105.18
3	L	402	A1D5C	C20-C19-C18	-2.28	125.19	129.68
3	C	402	A1D5C	C29-C14-N15	2.27	111.36	108.05
3	E	402	A1D5C	C29-C18-C19	-2.27	121.40	130.26
3	E	402	A1D5C	O03-C02-C01	-2.26	113.15	122.03
3	F	402	A1D5C	C06-C05-N04	2.24	105.82	102.93
3	E	402	A1D5C	C27-N26-C25	-2.22	100.87	105.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	402	A1D5C	C22-C23-N24	2.20	134.27	130.74
3	D	402	A1D5C	C05-N04-C02	2.20	131.09	124.18
3	G	402	A1D5C	C10-O09-C07	-2.20	113.08	120.14
3	F	402	A1D5C	O17-C16-N15	-2.19	122.81	126.30
3	I	402	A1D5C	C10-O09-C07	2.19	127.16	120.14
3	F	402	A1D5C	C18-C16-N15	-2.16	105.72	106.91
3	J	402	A1D5C	C20-C19-C18	-2.15	125.45	129.68
3	G	402	A1D5C	C27-C23-N24	-2.14	102.62	106.15
3	A	402	A1D5C	C23-C27-N26	2.12	112.96	108.39
3	B	402	A1D5C	C29-C18-C16	2.10	106.46	105.31
3	C	402	A1D5C	C28-C20-C19	2.09	128.45	120.79
3	D	402	A1D5C	C01-C02-N04	2.08	120.88	118.24
3	G	402	A1D5C	C29-C18-C16	-2.07	104.18	105.31
3	K	402	A1D5C	C23-N24-C25	2.06	109.09	106.73
3	J	402	A1D5C	C14-C29-C18	2.04	109.72	106.51
3	C	402	A1D5C	N24-C25-N26	2.04	116.98	113.87
3	K	402	A1D5C	O03-C02-N04	-2.04	118.57	120.98
3	B	402	A1D5C	C22-C23-C27	-2.04	119.87	122.10
3	E	402	A1D5C	C10-C29-C18	-2.01	129.62	135.25
3	D	402	A1D5C	C29-C18-C19	-2.00	122.42	130.26

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1D5C	C16-C18-C19-C20
3	C	402	A1D5C	C29-C18-C19-C20
3	C	402	A1D5C	C16-C18-C19-C20
3	D	402	A1D5C	C06-C07-O09-C10
3	D	402	A1D5C	C08-C07-O09-C10
3	E	402	A1D5C	C06-C07-O09-C10
3	F	402	A1D5C	C06-C07-O09-C10
3	F	402	A1D5C	C08-C07-O09-C10
3	F	402	A1D5C	C16-C18-C19-C20
3	I	402	A1D5C	C29-C18-C19-C20
3	I	402	A1D5C	C16-C18-C19-C20
3	J	402	A1D5C	C06-C07-O09-C10
3	J	402	A1D5C	C08-C07-O09-C10
3	K	402	A1D5C	C16-C18-C19-C20
3	L	402	A1D5C	C06-C07-O09-C10
3	L	402	A1D5C	C08-C07-O09-C10
3	A	402	A1D5C	C29-C10-O09-C07

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Mol	Chain	Res	Type	Atoms
3	C	402	A1D5C	C29-C10-O09-C07
3	E	402	A1D5C	C29-C18-C19-C20
3	F	402	A1D5C	C29-C18-C19-C20
3	K	402	A1D5C	C29-C18-C19-C20
3	B	402	A1D5C	C16-C18-C19-C20
3	D	402	A1D5C	C16-C18-C19-C20
3	E	402	A1D5C	C16-C18-C19-C20
3	H	402	A1D5C	C16-C18-C19-C20
3	I	402	A1D5C	C29-C10-O09-C07
3	I	402	A1D5C	C11-C10-O09-C07
3	A	402	A1D5C	C11-C10-O09-C07
3	D	402	A1D5C	C11-C10-O09-C07
3	K	402	A1D5C	C06-C07-O09-C10
3	D	402	A1D5C	C29-C10-O09-C07
3	B	402	A1D5C	C29-C18-C19-C20
3	A	402	A1D5C	C29-C18-C19-C20
3	C	402	A1D5C	C11-C10-O09-C07
3	B	402	A1D5C	C29-C10-O09-C07
3	B	402	A1D5C	C11-C10-O09-C07
3	D	402	A1D5C	C29-C18-C19-C20
3	H	402	A1D5C	C29-C18-C19-C20
3	E	402	A1D5C	C08-C07-O09-C10
3	H	402	A1D5C	C11-C10-O09-C07
3	H	402	A1D5C	C06-C07-O09-C10
3	G	402	A1D5C	C11-C10-O09-C07

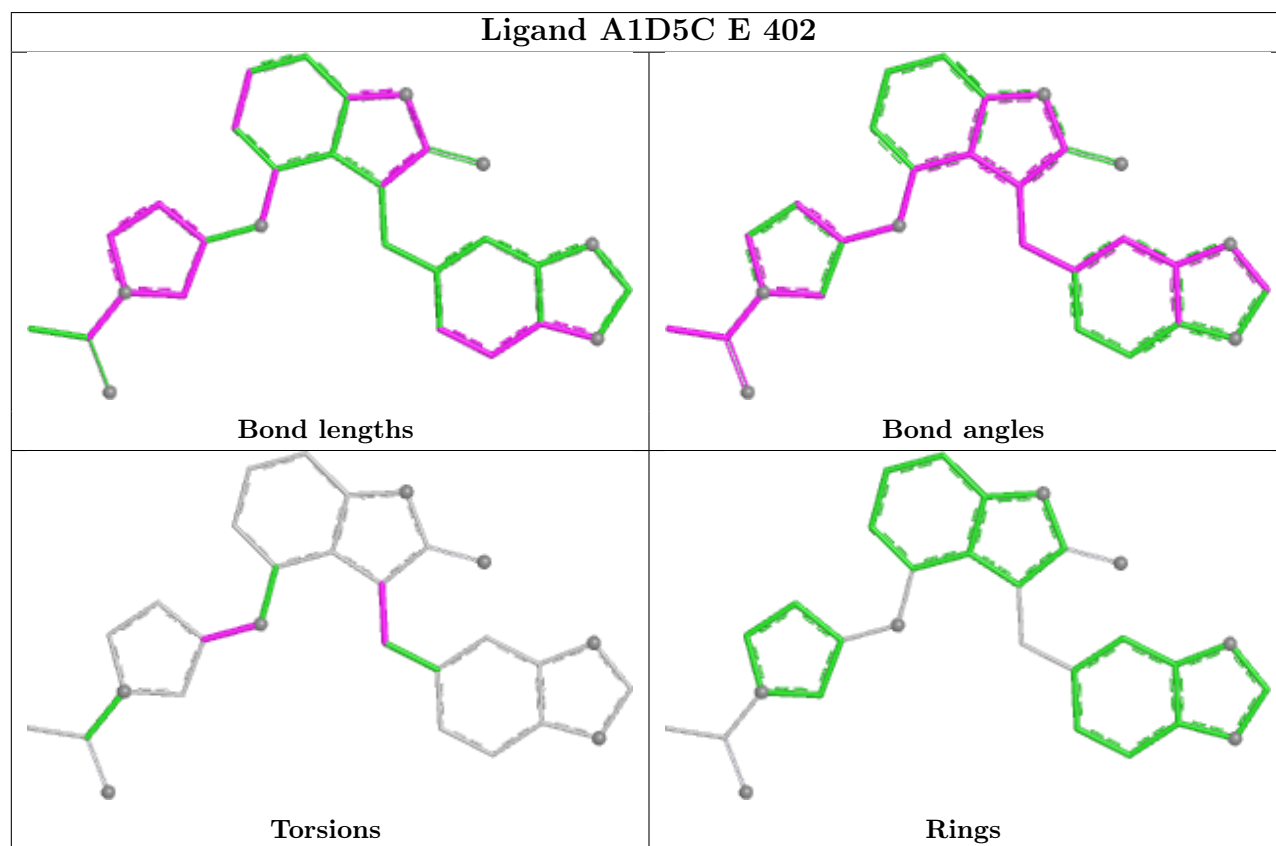
There are no ring outliers.

10 monomers are involved in 27 short contacts:

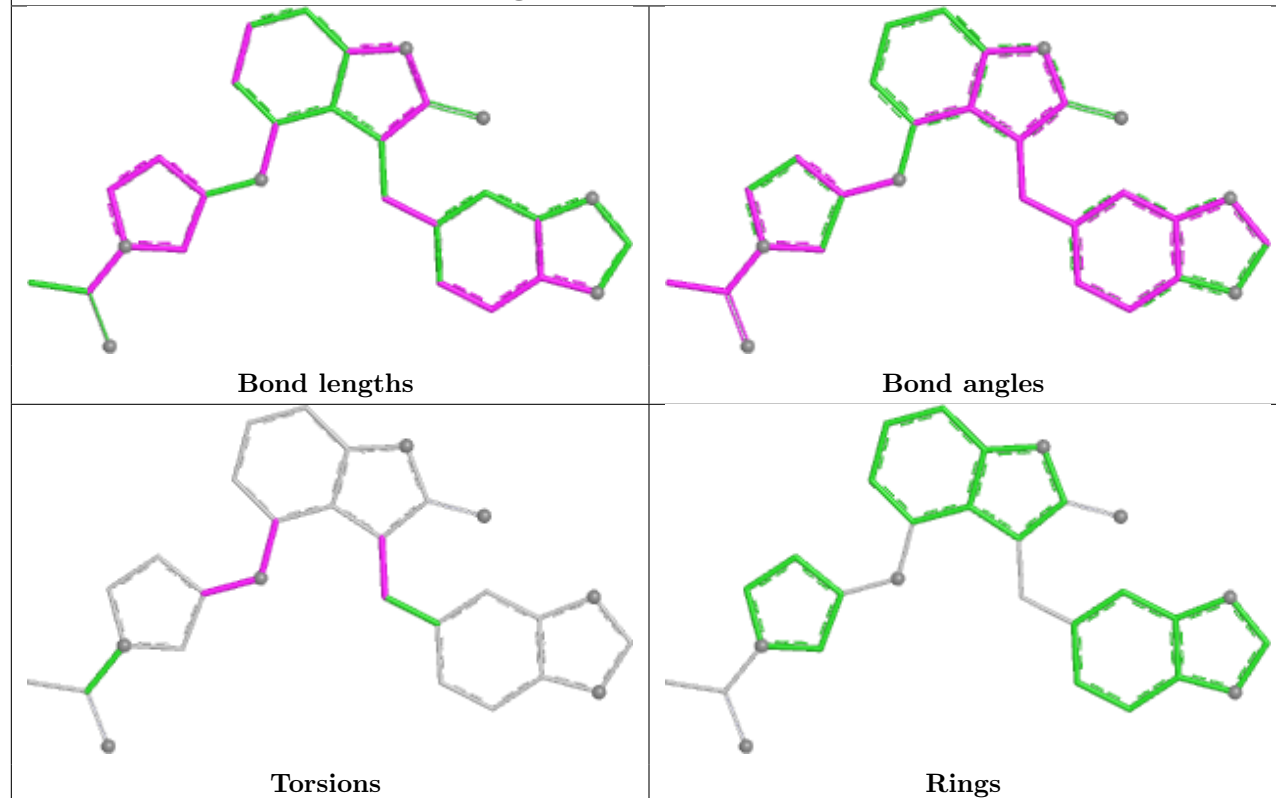
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	402	A1D5C	1	0
3	I	402	A1D5C	2	0
3	A	402	A1D5C	2	0
3	D	402	A1D5C	2	0
3	L	402	A1D5C	5	0
3	B	402	A1D5C	3	0
3	G	402	A1D5C	4	0
3	K	402	A1D5C	5	0
3	C	402	A1D5C	1	0
3	J	402	A1D5C	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

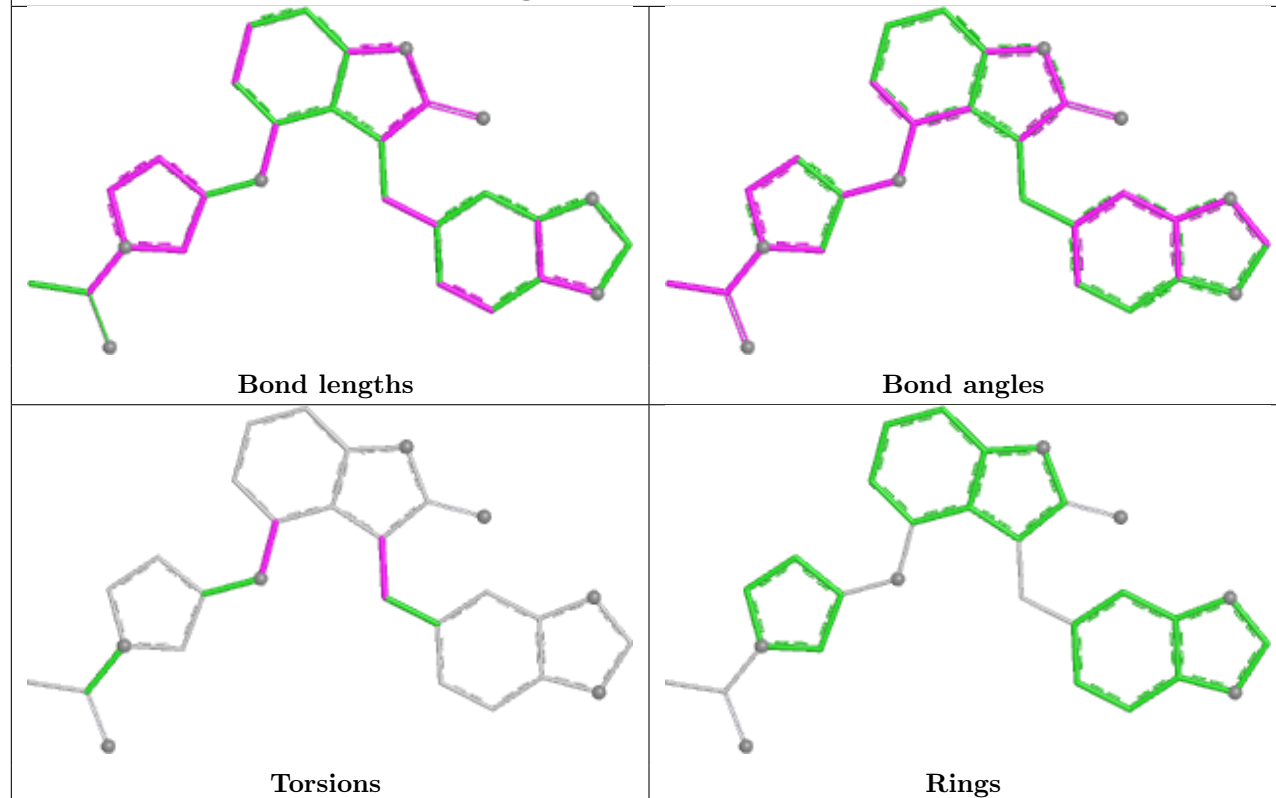
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



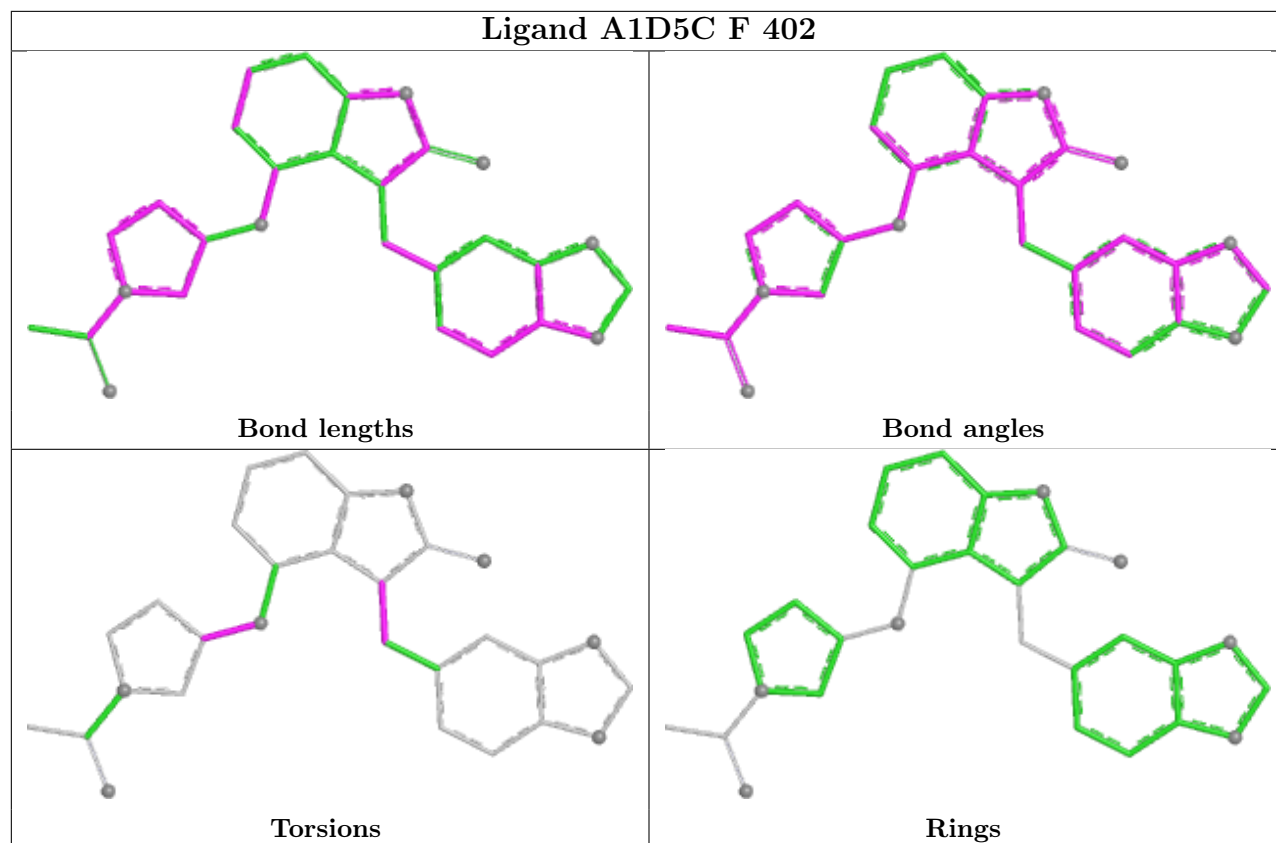
Ligand A1D5C H 402



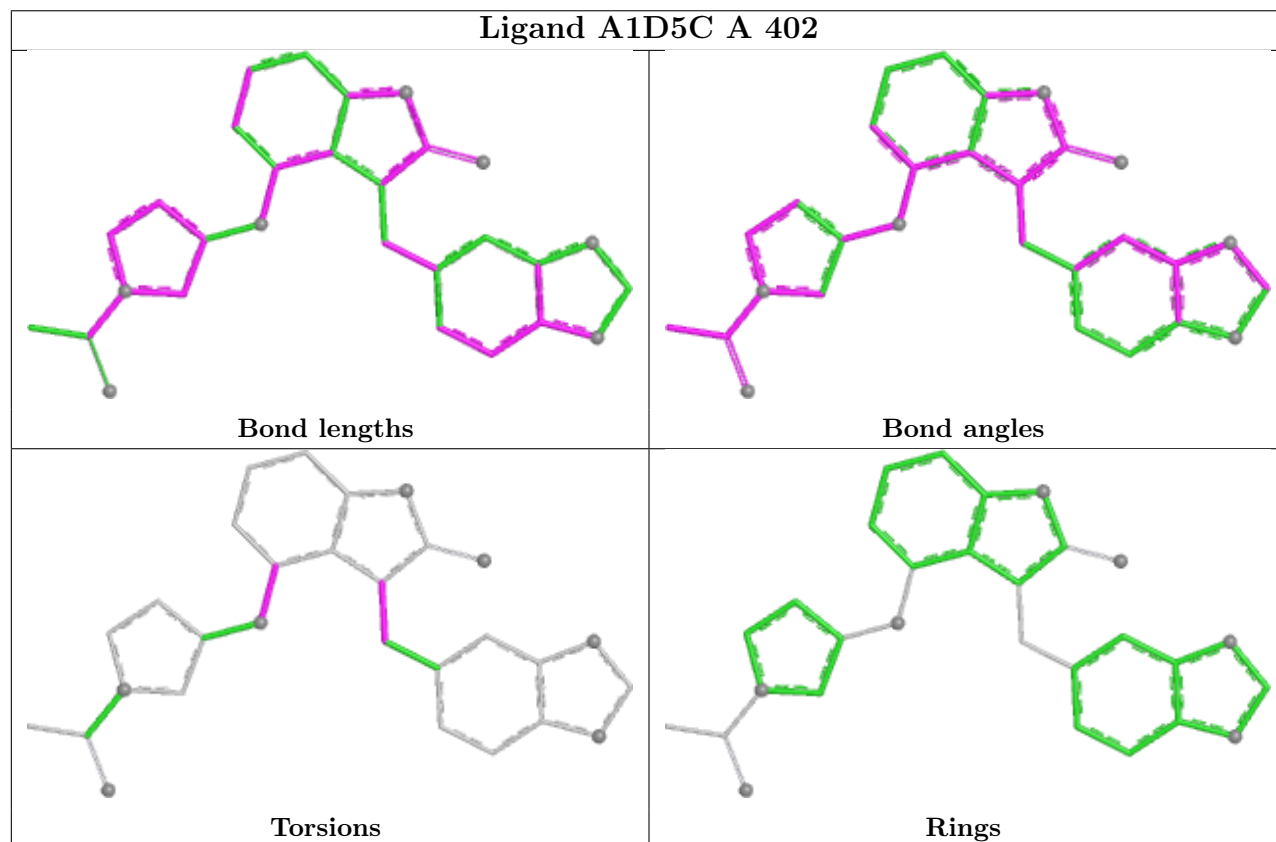
Ligand A1D5C I 402



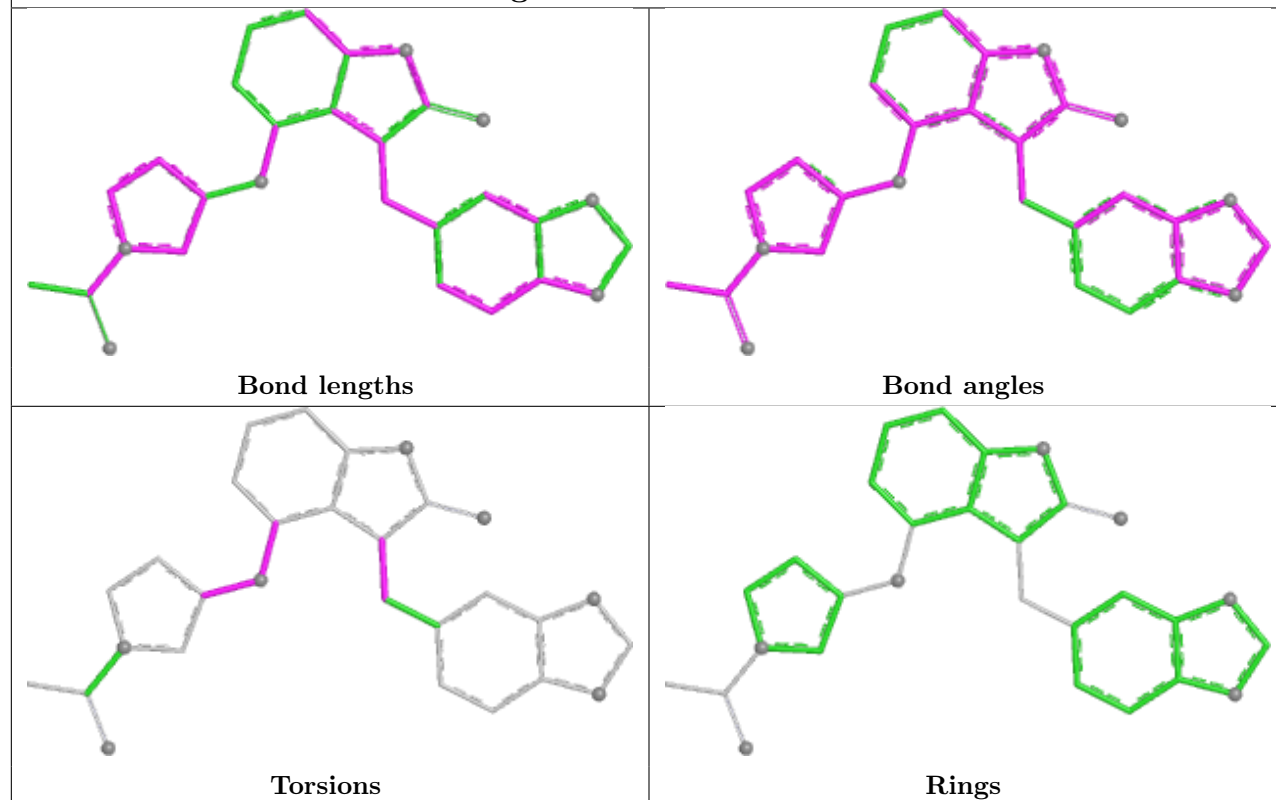
Ligand A1D5C F 402



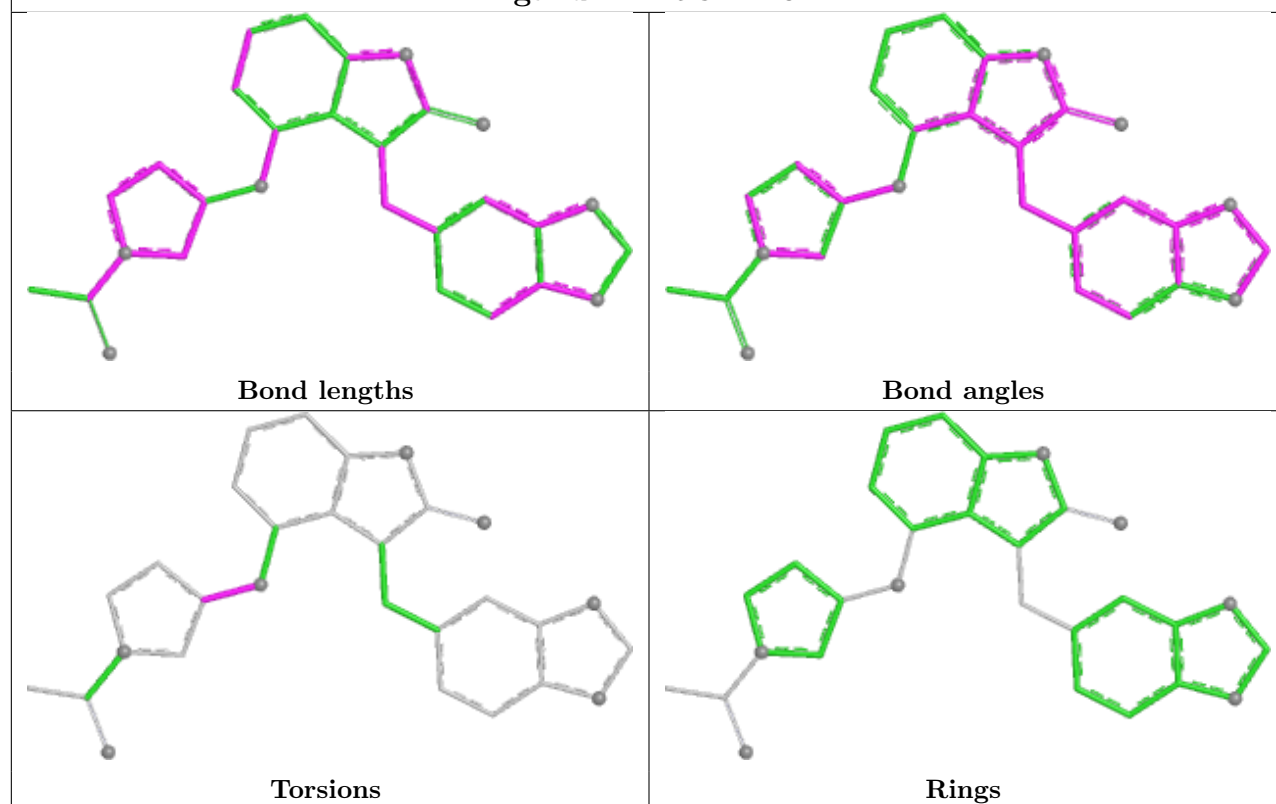
Ligand A1D5C A 402



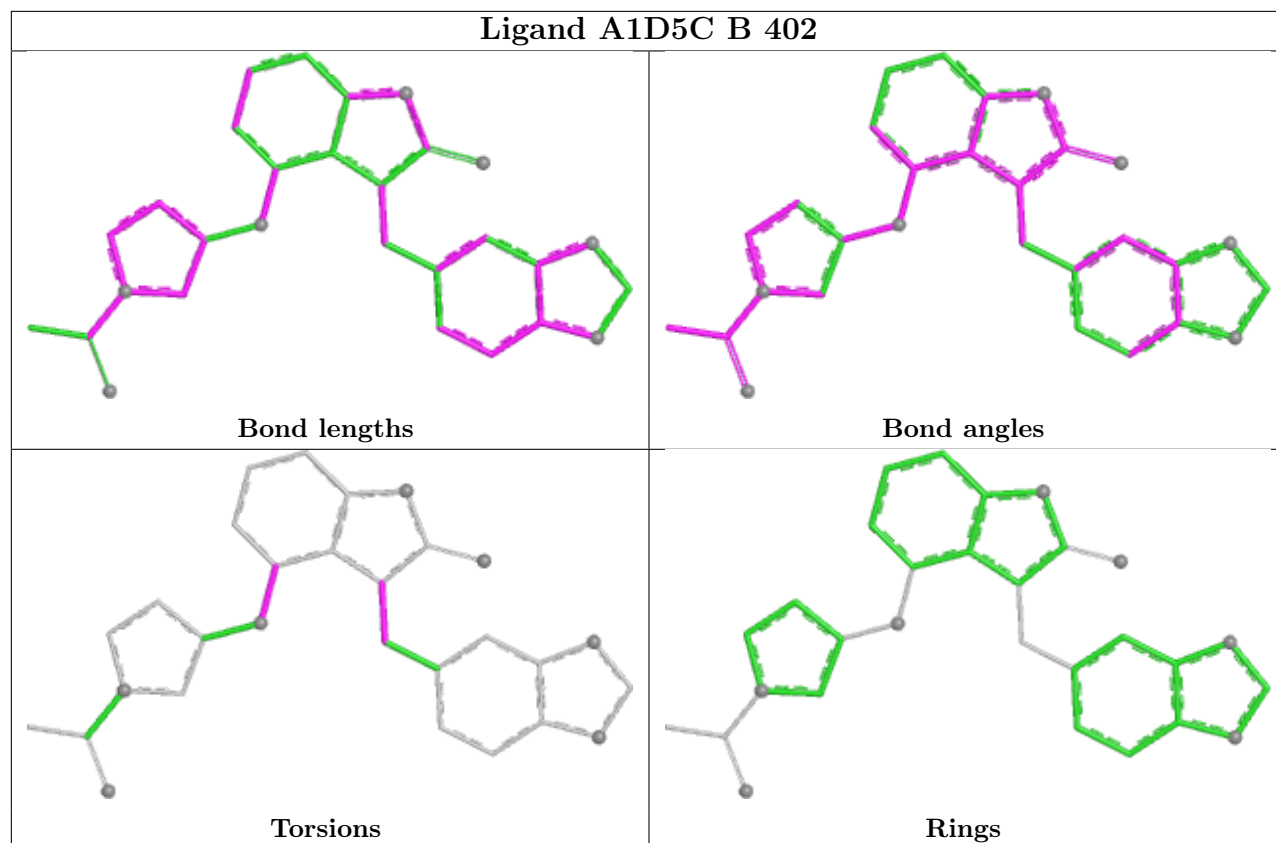
Ligand A1D5C D 402



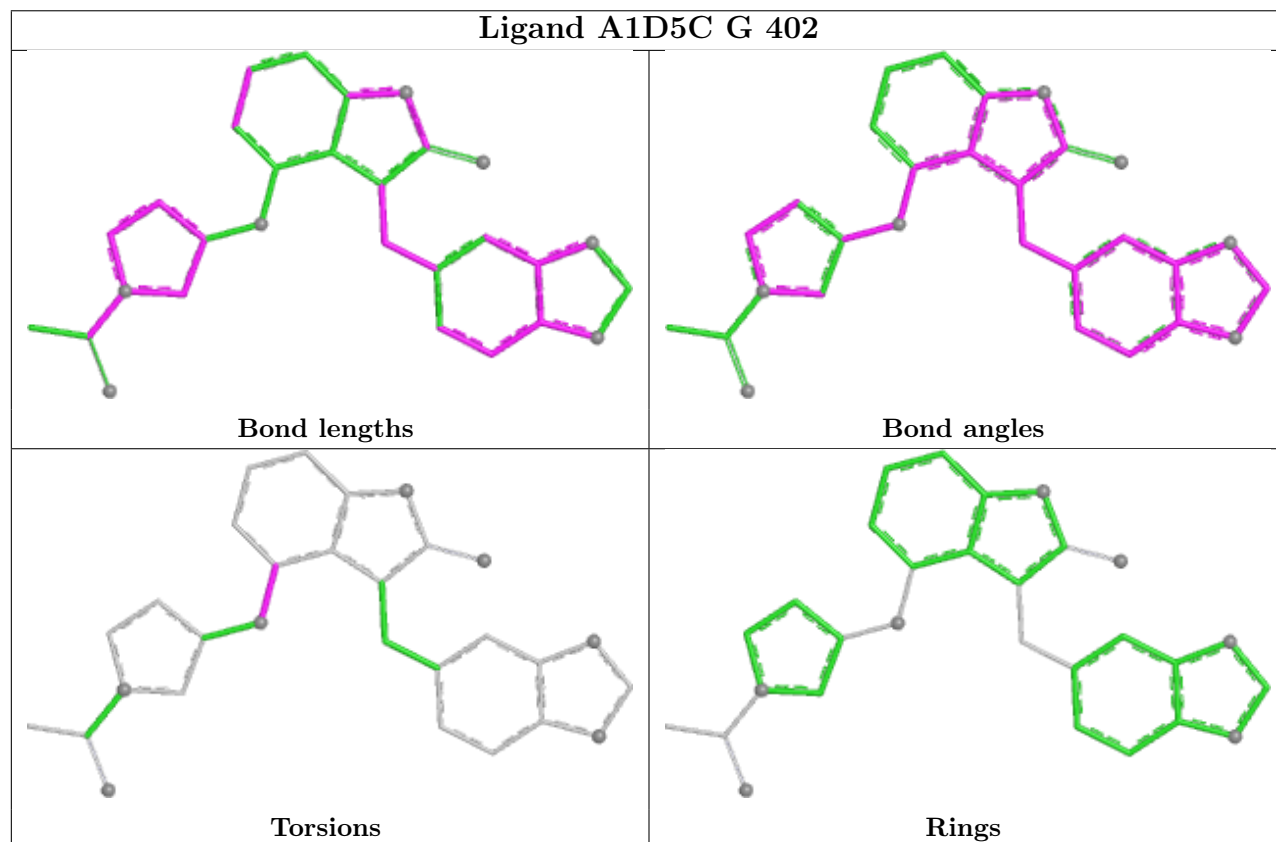
Ligand A1D5C L 402



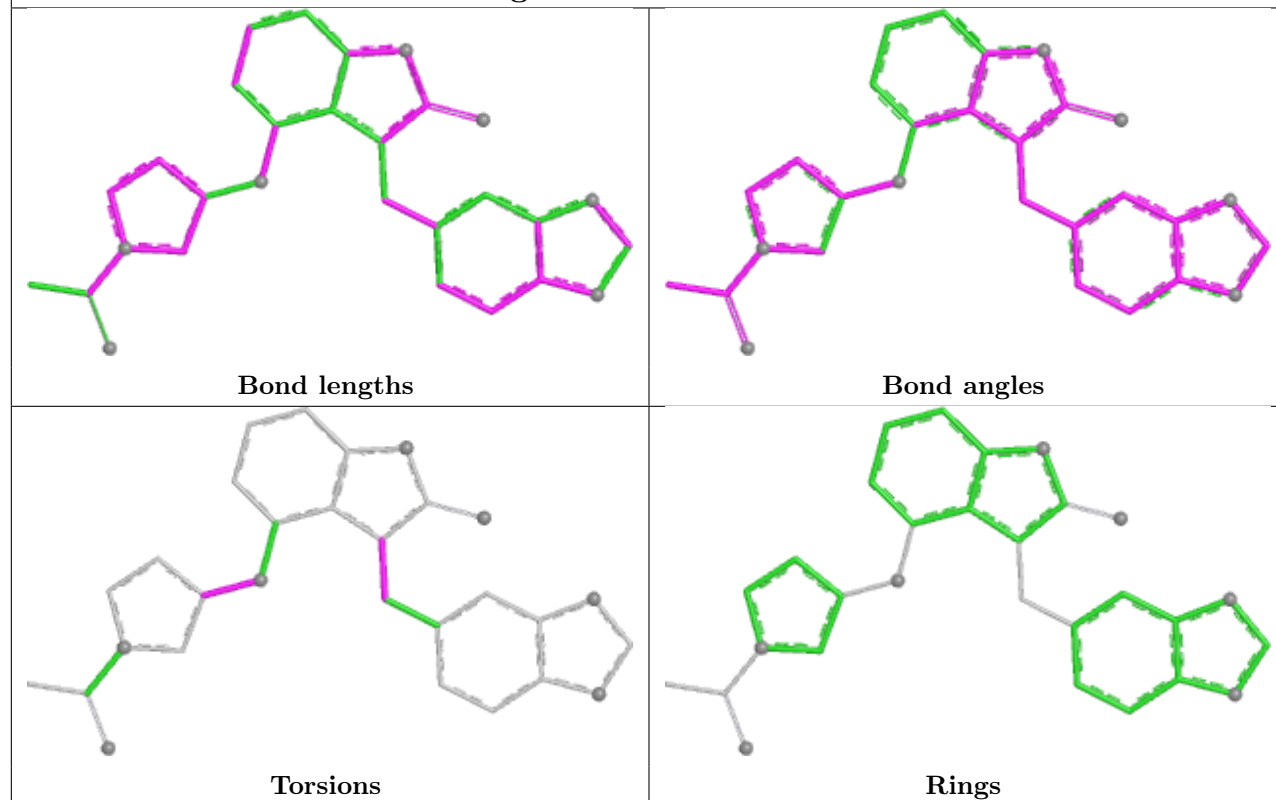
Ligand A1D5C B 402



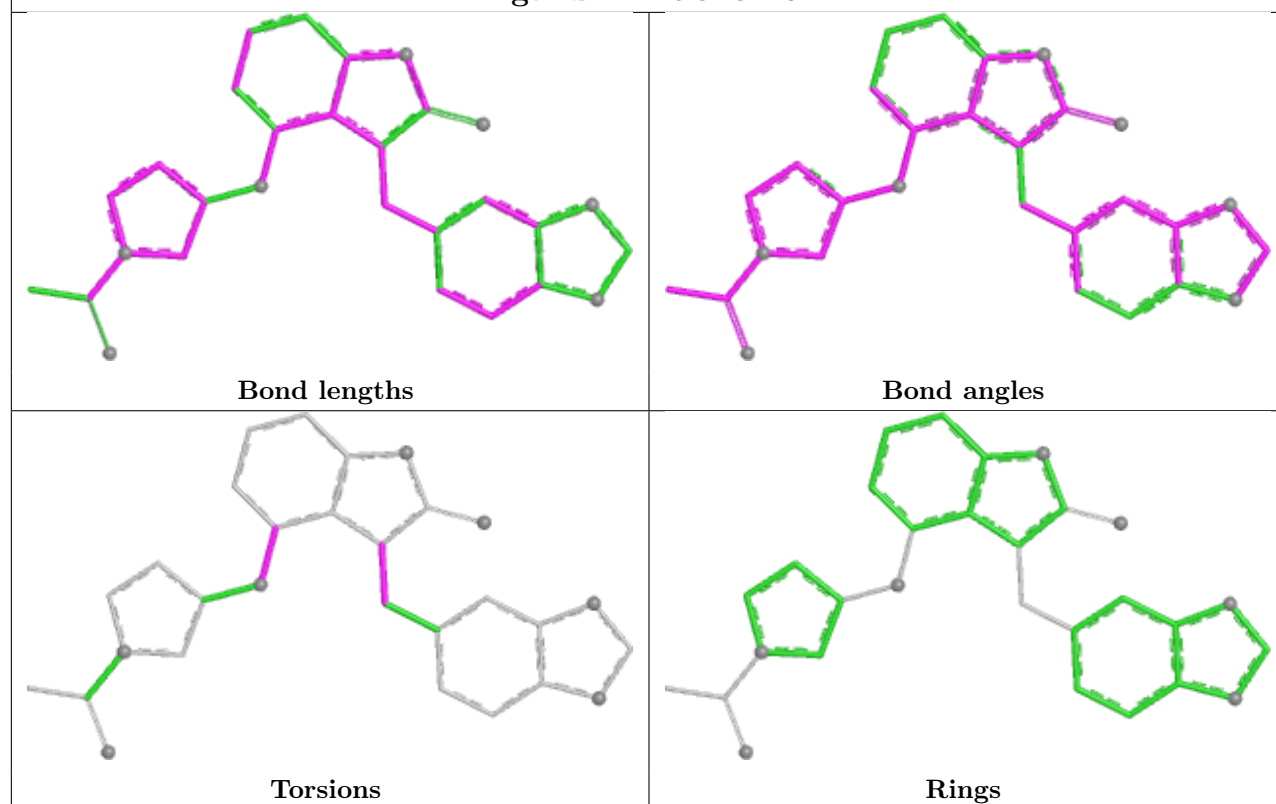
Ligand A1D5C G 402

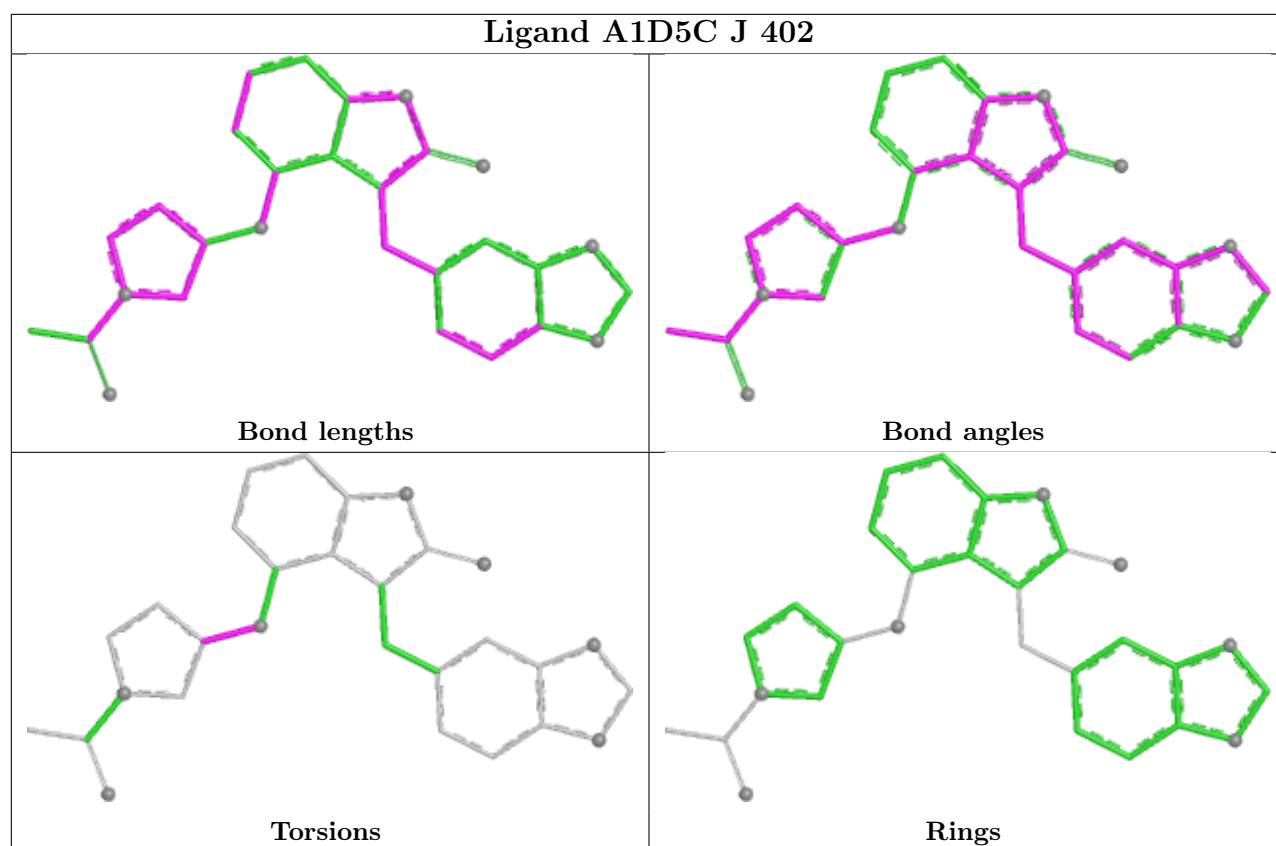


Ligand A1D5C K 402



Ligand A1D5C C 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%)	-0.47	5 (1%) 70 61	19, 35, 70, 125	0
1	B	322/329 (97%)	-0.46	6 (1%) 66 57	16, 36, 66, 105	0
1	C	322/329 (97%)	-0.40	3 (0%) 81 74	18, 39, 72, 136	0
1	D	322/329 (97%)	-0.44	2 (0%) 85 80	22, 39, 69, 122	0
1	E	322/329 (97%)	-0.33	2 (0%) 85 80	19, 42, 73, 110	0
1	F	322/329 (97%)	-0.32	3 (0%) 81 74	25, 45, 75, 98	0
1	G	322/329 (97%)	0.44	7 (2%) 62 52	40, 75, 110, 135	0
1	H	322/329 (97%)	0.07	5 (1%) 70 61	34, 61, 94, 135	0
1	I	322/329 (97%)	-0.06	2 (0%) 85 80	29, 54, 90, 116	0
1	J	322/329 (97%)	0.76	15 (4%) 36 28	48, 87, 116, 150	0
1	K	322/329 (97%)	-0.23	5 (1%) 70 61	24, 47, 74, 136	0
1	L	322/329 (97%)	-0.23	2 (0%) 85 80	27, 45, 84, 130	0
All	All	3864/3948 (97%)	-0.14	57 (1%) 72 63	16, 48, 97, 150	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	ARG	4.5
1	L	35	ALA	3.3
1	A	33	ALA	3.1
1	F	33	ALA	3.0
1	G	33	ALA	3.0
1	B	206	HIS	3.0
1	K	33	ALA	2.9
1	J	302	VAL	2.9
1	L	189	PRO	2.9
1	A	206	HIS	2.9
1	E	117	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	297	TYR	2.8
1	K	302	VAL	2.8
1	E	33	ALA	2.7
1	G	115	TYR	2.7
1	I	206	HIS	2.7
1	H	206	HIS	2.6
1	J	75	ILE	2.6
1	H	182	LYS	2.5
1	B	297	TYR	2.5
1	J	74	LEU	2.5
1	C	297	TYR	2.5
1	F	34	SER	2.5
1	J	298	SER	2.4
1	D	206	HIS	2.4
1	J	189	PRO	2.4
1	G	205	LEU	2.3
1	K	206	HIS	2.3
1	J	56	ILE	2.3
1	J	297	TYR	2.3
1	J	36	TRP	2.3
1	J	33	ALA	2.3
1	J	361	LEU	2.3
1	G	176	LYS	2.3
1	J	176	LYS	2.2
1	G	189	PRO	2.2
1	J	146	PHE	2.2
1	J	46	ALA	2.2
1	K	297	TYR	2.2
1	B	302	VAL	2.2
1	F	189	PRO	2.2
1	H	189	PRO	2.2
1	A	302	VAL	2.2
1	G	62	ILE	2.1
1	A	207	TRP	2.1
1	J	205	LEU	2.1
1	C	33	ALA	2.1
1	A	34	SER	2.1
1	B	33	ALA	2.1
1	K	35	ALA	2.1
1	J	178	LEU	2.1
1	H	297	TYR	2.1
1	B	34	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	329	TRP	2.0
1	C	206	HIS	2.0
1	H	33	ALA	2.0
1	I	33	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	A1D5C	A	402	29/29	0.82	0.15	32,59,85,89	0
3	A1D5C	H	402	29/29	0.82	0.14	54,67,94,100	0
3	A1D5C	J	402	29/29	0.82	0.15	64,81,113,115	0
3	A1D5C	E	402	29/29	0.84	0.14	36,63,93,96	0
3	A1D5C	F	402	29/29	0.84	0.15	42,70,101,111	0
3	A1D5C	L	402	29/29	0.84	0.16	43,79,115,120	0
3	A1D5C	G	402	29/29	0.85	0.16	50,98,120,128	0
3	A1D5C	I	402	29/29	0.85	0.17	43,71,107,119	0
3	A1D5C	B	402	29/29	0.88	0.12	30,44,78,88	0
3	A1D5C	D	402	29/29	0.91	0.12	32,51,89,98	0
3	A1D5C	K	402	29/29	0.91	0.11	38,53,84,93	0
3	A1D5C	C	402	29/29	0.91	0.12	33,59,93,96	0
2	ZN	G	401	1/1	0.99	0.04	52,52,52,52	0
2	ZN	J	401	1/1	0.99	0.04	53,53,53,53	0
2	ZN	L	401	1/1	0.99	0.04	78,78,78,78	0
2	ZN	B	401	1/1	1.00	0.03	31,31,31,31	0
2	ZN	H	401	1/1	1.00	0.01	52,52,52,52	0
2	ZN	I	401	1/1	1.00	0.02	40,40,40,40	0
2	ZN	A	401	1/1	1.00	0.04	28,28,28,28	0

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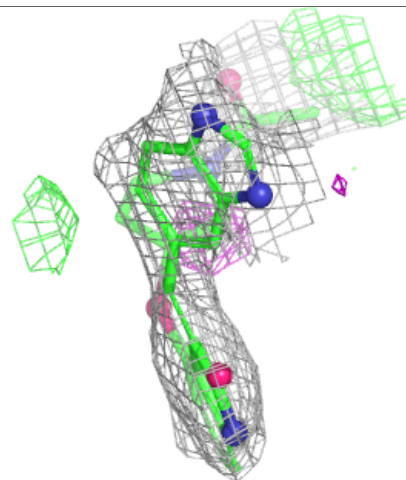
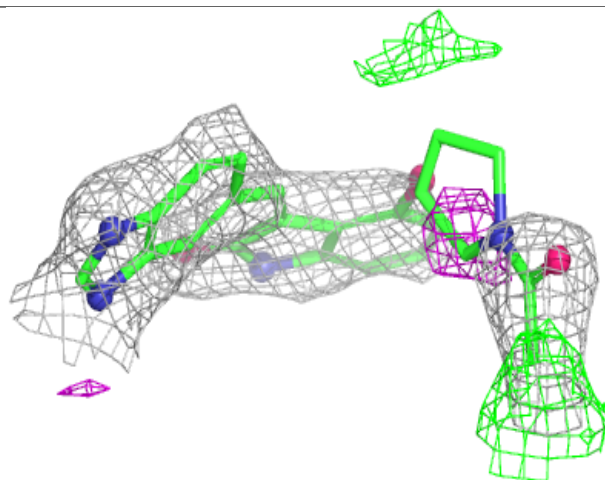
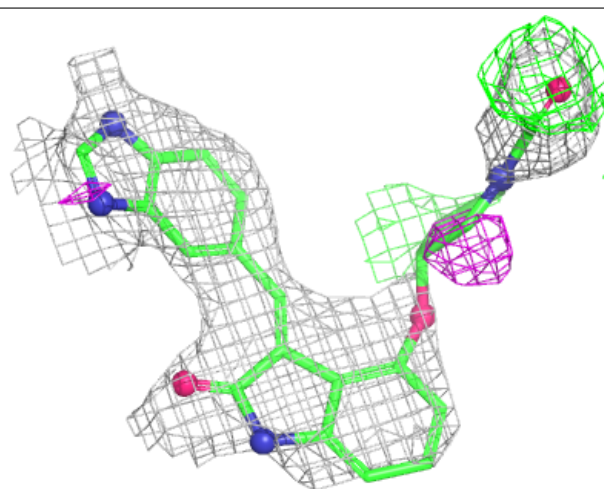
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	K	401	1/1	1.00	0.03	34,34,34,34	0
2	ZN	C	401	1/1	1.00	0.03	29,29,29,29	0
2	ZN	D	401	1/1	1.00	0.01	36,36,36,36	0
2	ZN	E	401	1/1	1.00	0.03	33,33,33,33	0
2	ZN	F	401	1/1	1.00	0.03	35,35,35,35	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.

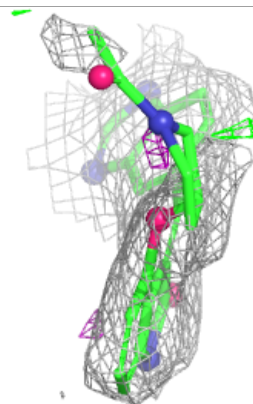
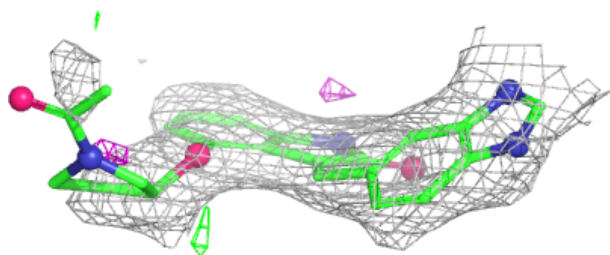
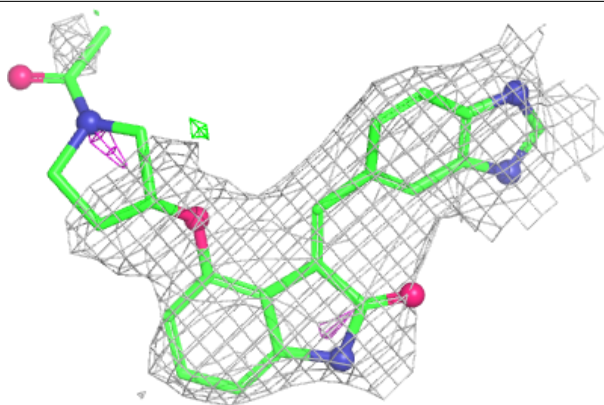
Electron density around A1D5C A 402:

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

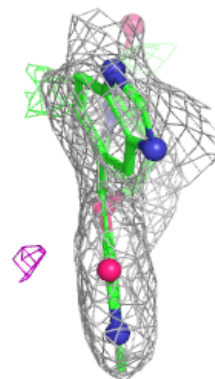
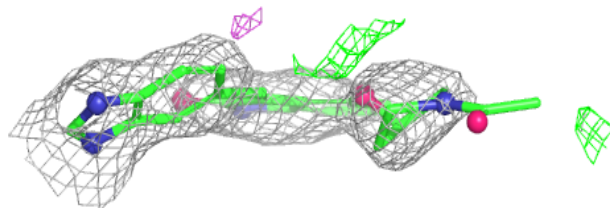
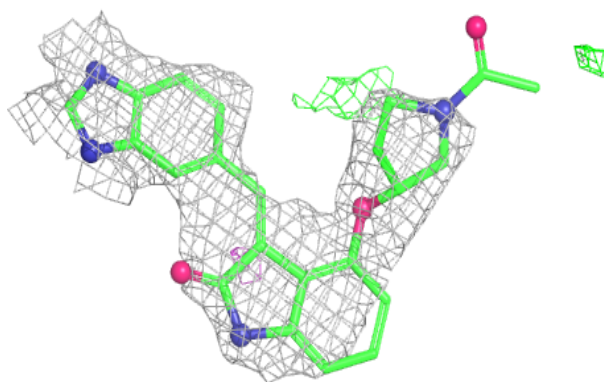


Electron density around A1D5C H 402:

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

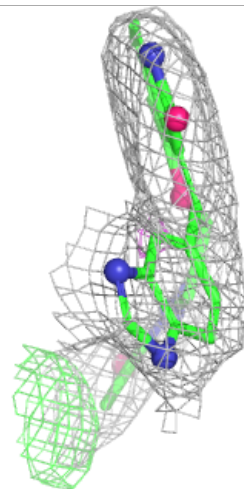
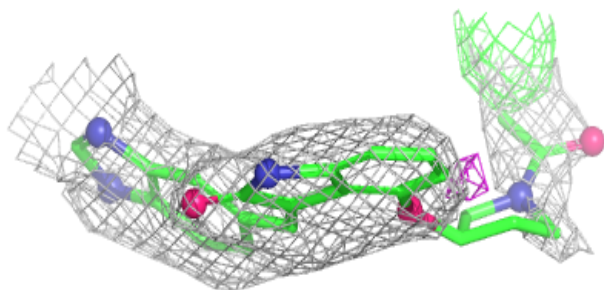
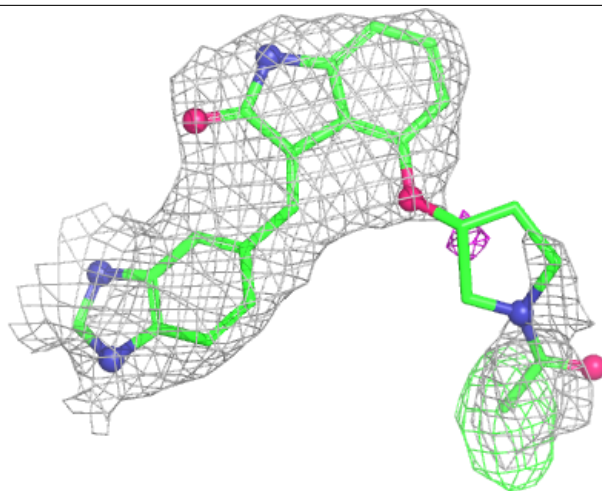
**Electron density around A1D5C J 402:**

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



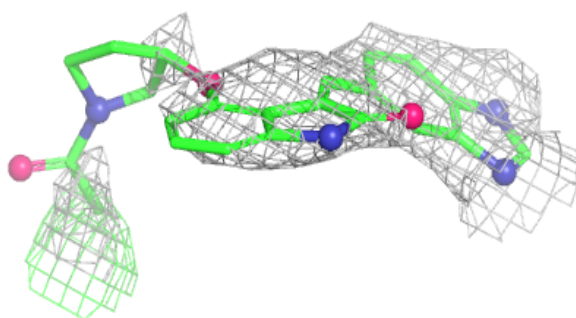
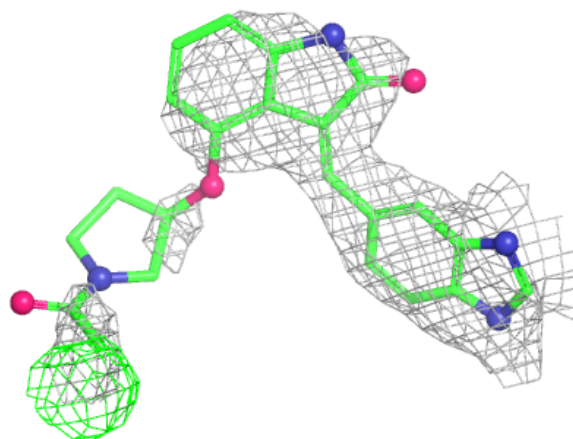
Electron density around A1D5C E 402:

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and green (positive)

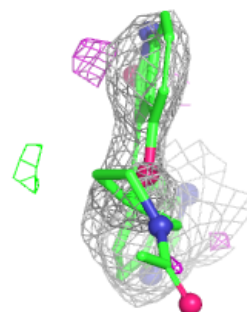
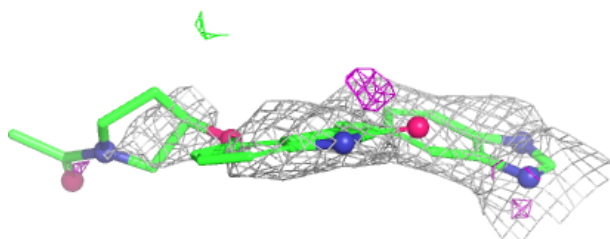
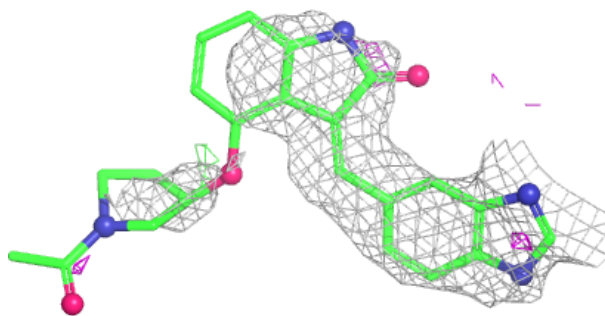


Electron density around A1D5C F 402:

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and green (positive)

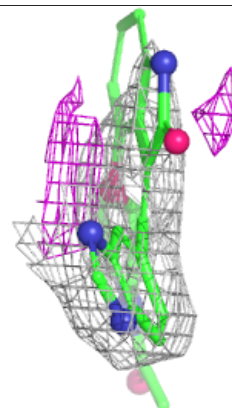
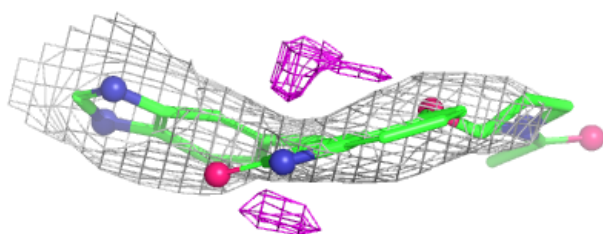
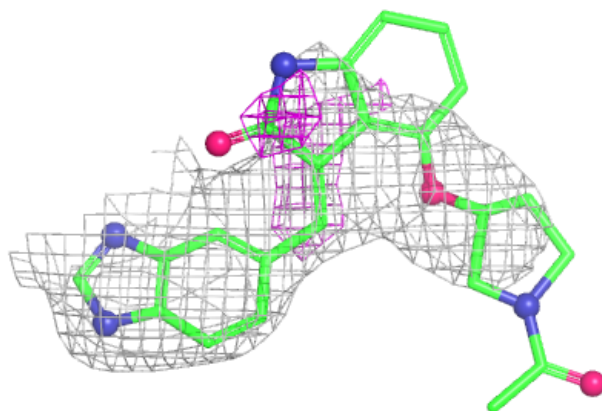
**Electron density around A1D5C L 402:**

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



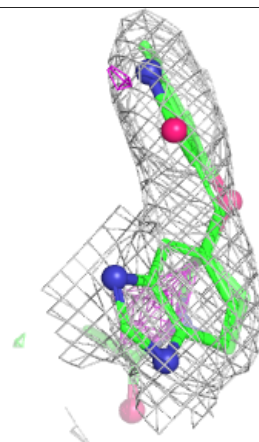
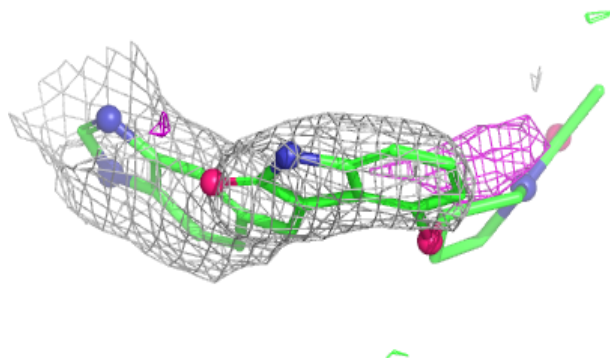
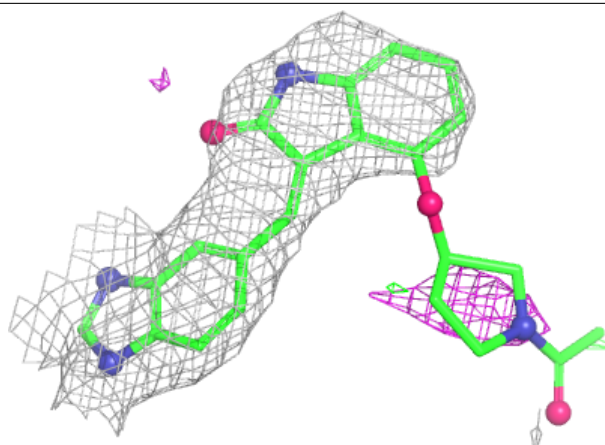
Electron density around A1D5C G 402:

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



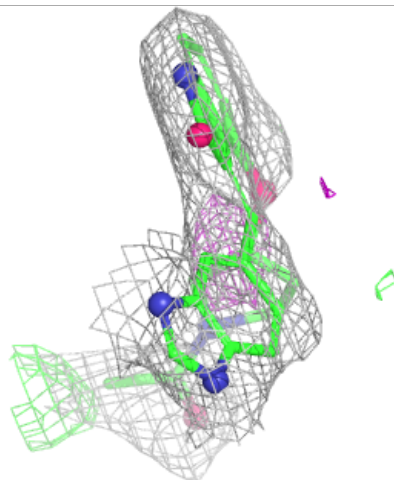
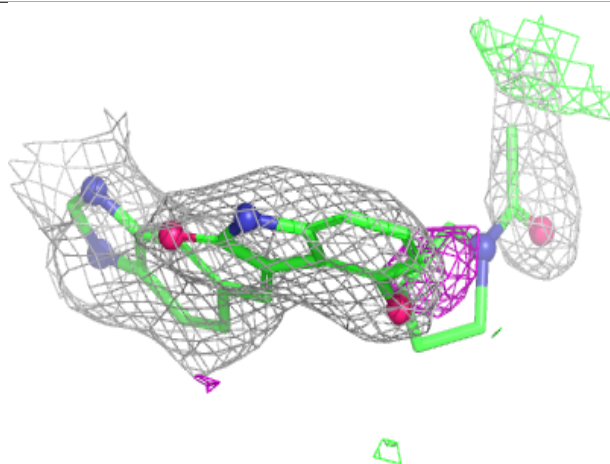
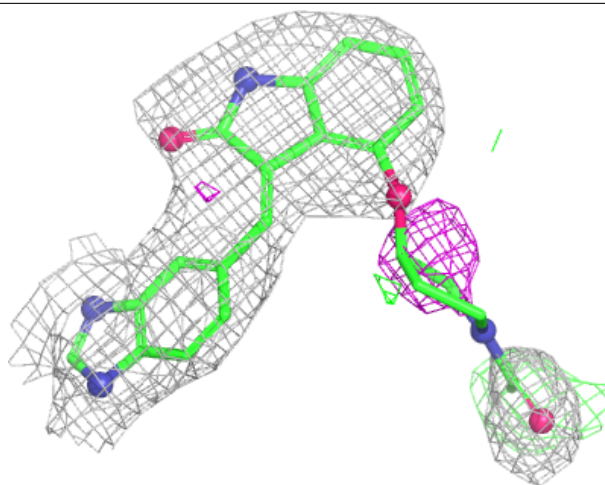
Electron density around A1D5C I 402:

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and green (positive)



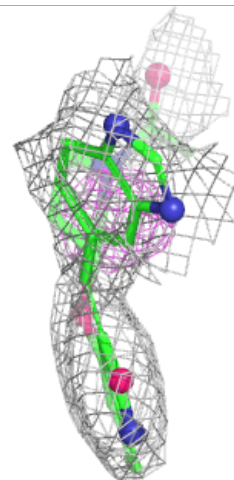
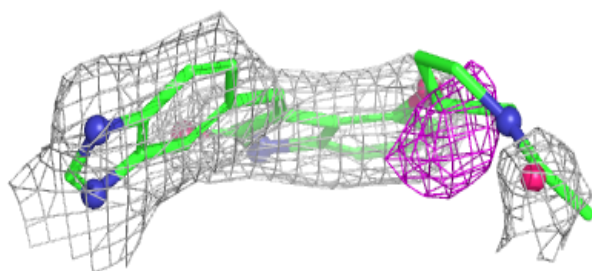
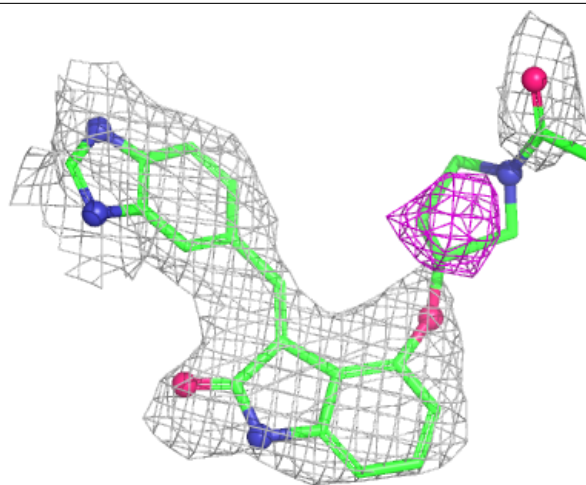
Electron density around A1D5C B 402:

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and green (positive)



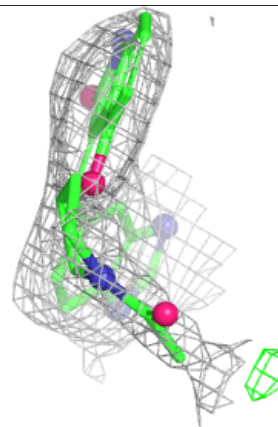
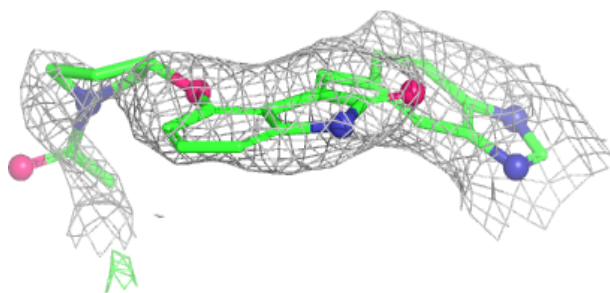
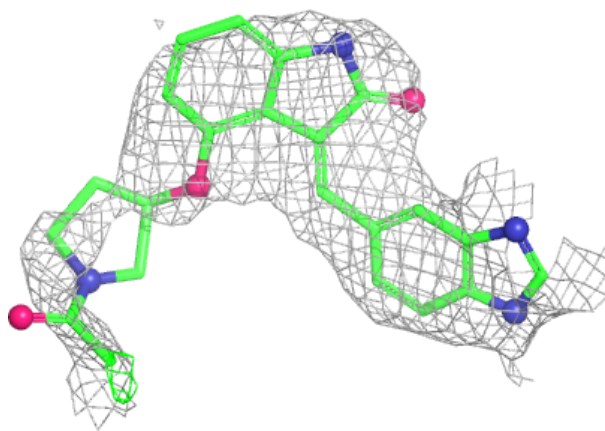
Electron density around A1D5C D 402:

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



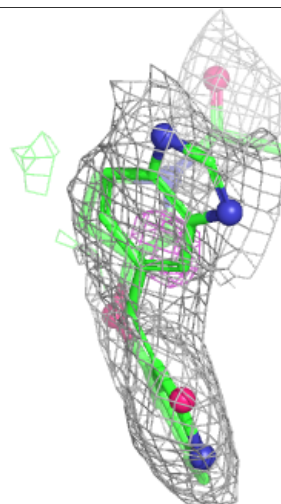
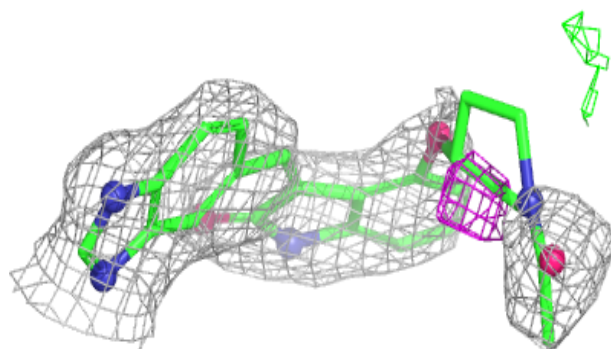
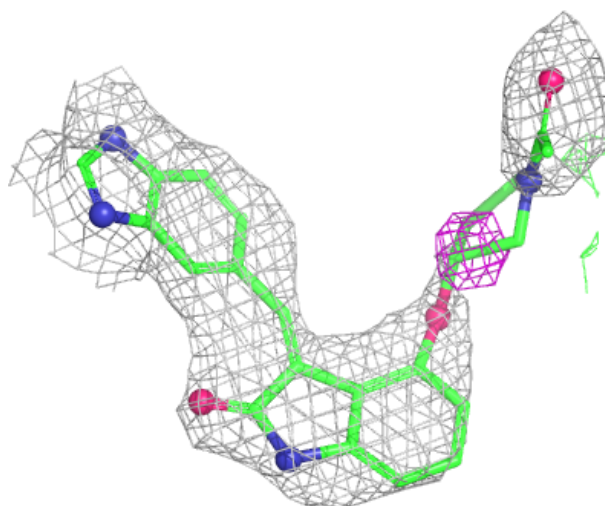
Electron density around A1D5C K 402:

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



Electron density around A1D5C 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.