



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:42 AM UTC

PDB ID : 4X2T / pdb_00004x2t
Title : X-ray crystal structure of the orally available aminopeptidase inhibitor, Tosedostat, bound to the M17 Leucyl Aminopeptidase from *P. falciparum*
Authors : Drinkwater, N.; McGowan, S.
Deposited on : 2014-11-27
Resolution : 2.73 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

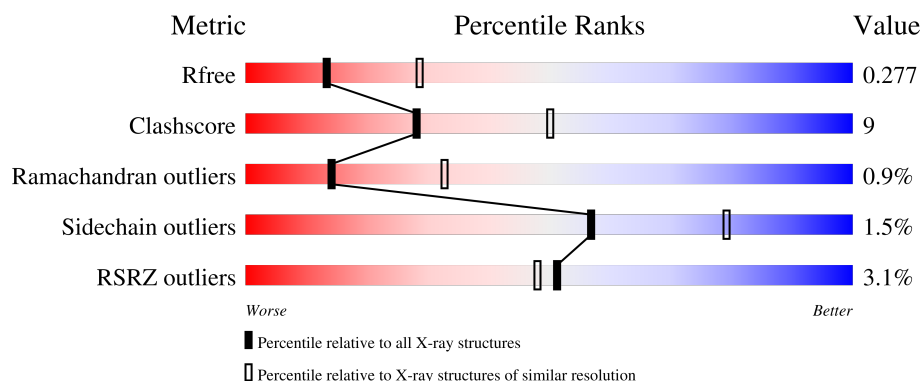
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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.



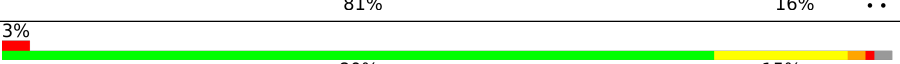
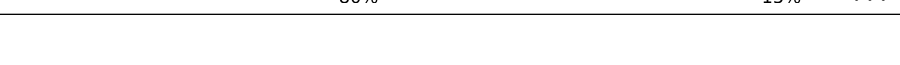
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	519	3% 86% 13% ..
1	B	519	5% 80% 15% ...
1	C	519	2% 82% 15% .
1	D	519	3% 82% 16% ..
1	E	519	2% 82% 15% ..

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Mol	Chain	Length	Quality of chain
1	F	519	
1	G	519	
1	H	519	
1	I	519	
1	J	519	
1	K	519	
1	L	519	

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
4	CO3	A	704	-	-	X	-
4	CO3	G	704	-	-	X	-
4	CO3	J	704	-	-	X	-
4	CO3	K	704	-	-	X	-
6	1PE	C	706	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 48055 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	1	0
			3928	2527	628	754	19			
1	B	510	Total	C	N	O	S	0	0	0
			3837	2475	619	724	19			
1	C	517	Total	C	N	O	S	0	0	0
			3942	2537	636	750	19			
1	D	511	Total	C	N	O	S	0	0	0
			3899	2511	628	741	19			
1	E	509	Total	C	N	O	S	0	0	0
			3884	2500	622	743	19			
1	F	509	Total	C	N	O	S	0	0	0
			3762	2421	606	716	19			
1	G	519	Total	C	N	O	S	0	0	0
			3979	2554	637	768	20			
1	H	510	Total	C	N	O	S	0	0	0
			3855	2480	621	735	19			
1	I	515	Total	C	N	O	S	0	0	0
			3912	2520	631	742	19			
1	J	511	Total	C	N	O	S	0	0	0
			3875	2499	624	733	19			
1	K	509	Total	C	N	O	S	0	0	0
			3878	2496	621	742	19			
1	L	508	Total	C	N	O	S	0	0	0
			3806	2447	612	728	19			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11

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

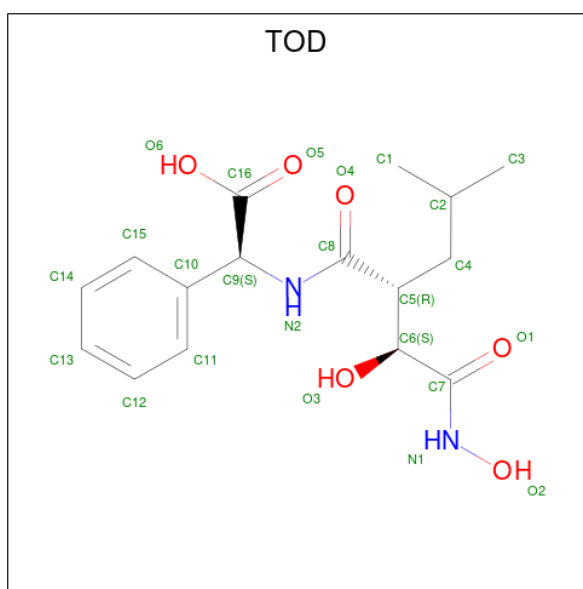
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

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

- Molecule 3 is (2S)-({(2R)-2-[(1S)-1-hydroxy-2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}amino)(phenyl)ethanoic acid (CCD ID: TOD) (formula: C₁₆H₂₂N₂O₆).



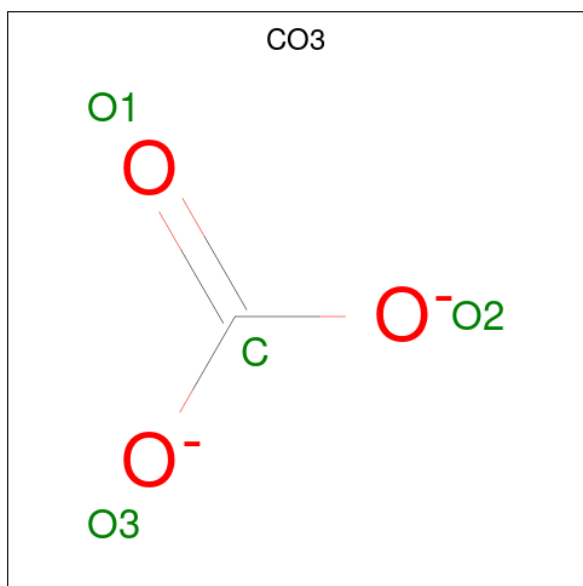
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	16	2	6		
3	B	1	Total	C	N	O	0	0
			24	16	2	6		
3	C	1	Total	C	N	O	0	0
			17	11	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			15	9	2	4		
3	F	1	Total	C	N	O	0	0
			24	16	2	6		
3	G	1	Total	C	N	O	0	0
			22	16	2	4		
3	H	1	Total	C	N	O	0	0
			14	8	2	4		
3	I	1	Total	C	N	O	0	0
			24	16	2	6		
3	J	1	Total	C	N	O	0	0
			22	16	2	4		
3	K	1	Total	C	N	O	0	0
			22	16	2	4		
3	L	1	Total	C	N	O	0	0
			24	16	2	6		

- Molecule 4 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



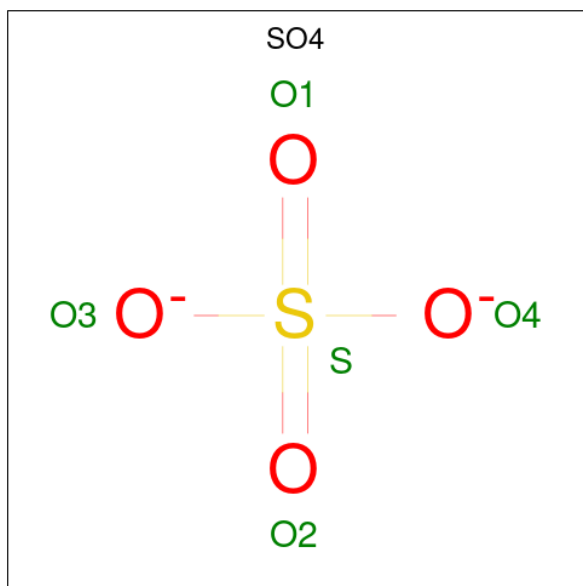
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	1	3		
4	B	1	Total	C	O	0	0
			4	1	3		
4	C	1	Total	C	O	0	0
			4	1	3		

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



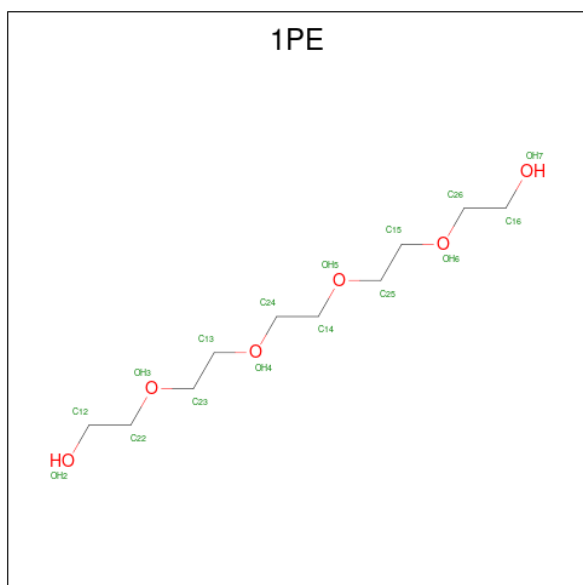
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 6 3	0	0
6	B	1	Total C O 7 5 2	0	0
6	C	1	Total C O 13 9 4	0	0
6	C	1	Total C O 9 6 3	0	0
6	D	1	Total C O 10 7 3	0	0
6	D	1	Total C O 10 7 3	0	0
6	E	1	Total C O 12 8 4	0	0
6	G	1	Total C O 9 6 3	0	0
6	G	1	Total C O 9 6 3	0	0
6	H	1	Total C O 10 7 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	102	Total O 102 102	0	0
7	B	74	Total O 74 74	0	0
7	C	70	Total O 70 70	0	0
7	D	80	Total O 80 80	0	0
7	E	113	Total O 113 113	0	0
7	F	88	Total O 88 88	0	0
7	G	93	Total O 93 93	0	0
7	H	74	Total O 74 74	0	0
7	I	91	Total O 91 91	0	0
7	J	86	Total O 86 86	0	0

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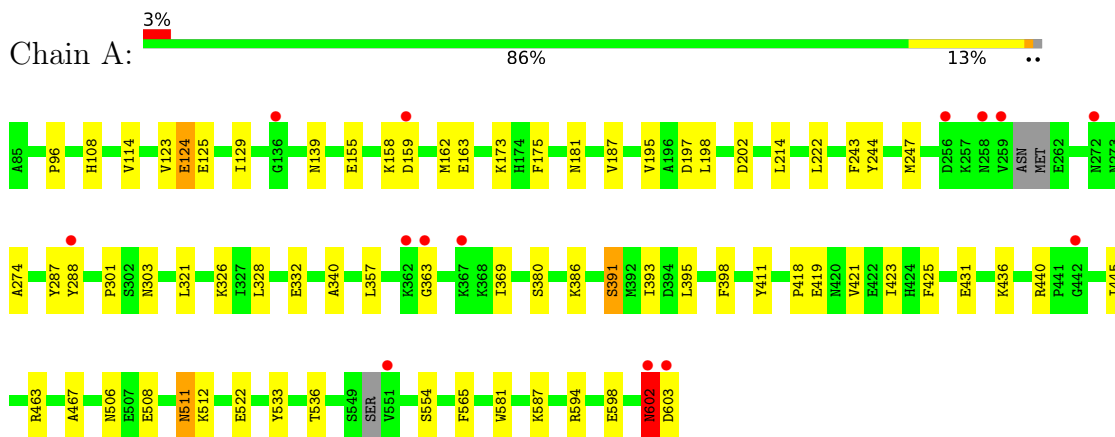
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	91	Total 91	O 91	0	0
7	L	69	Total 69	O 69	0	0

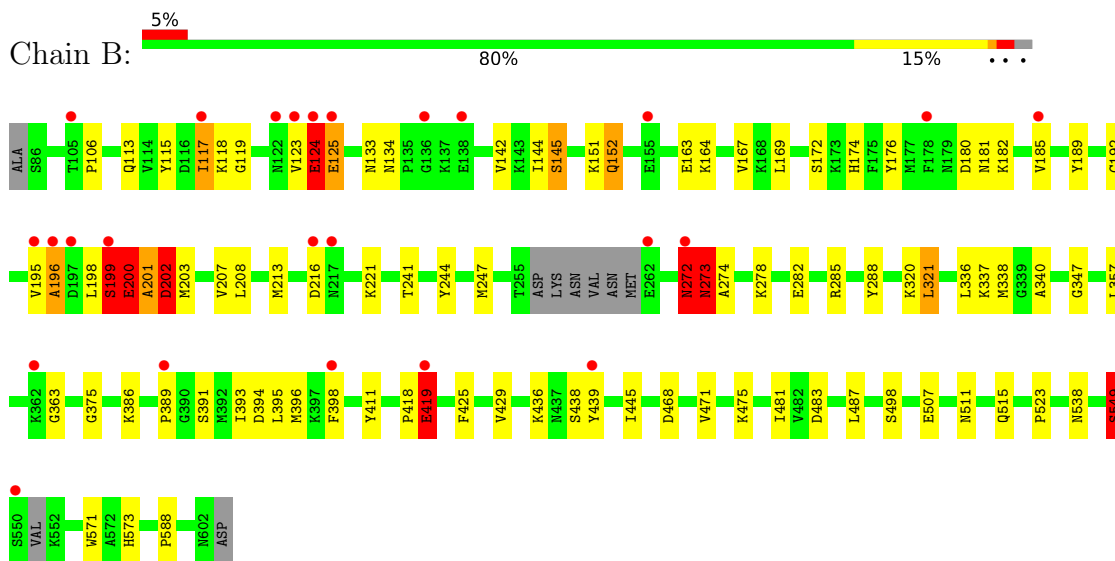
3 Residue-property plots

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

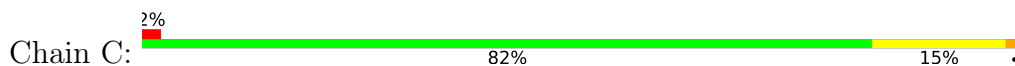
- Molecule 1: M17 leucyl aminopeptidase

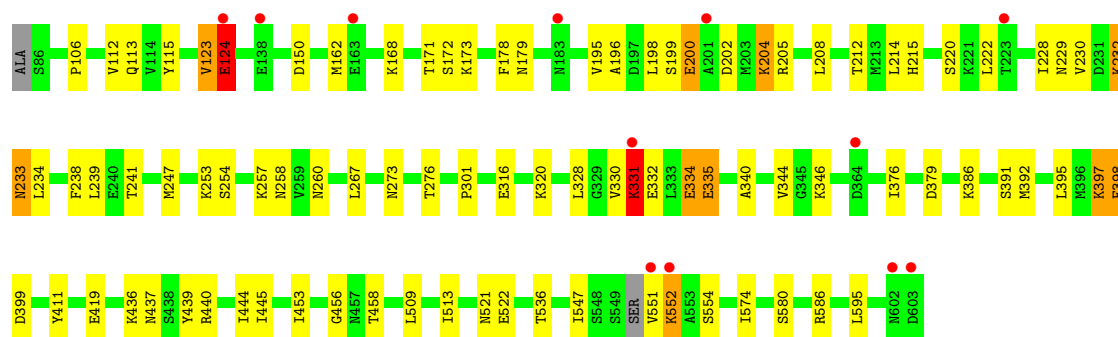


- Molecule 1: M17 leucyl aminopeptidase

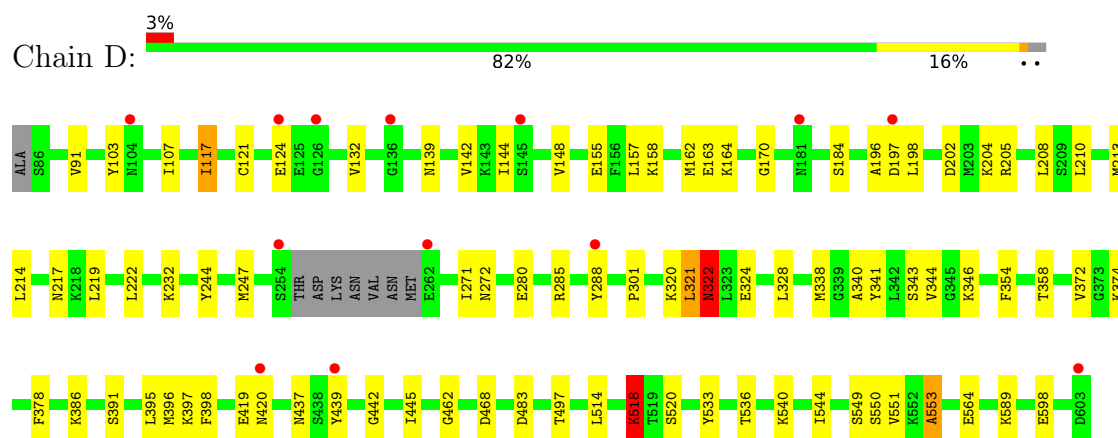


- Molecule 1: M17 leucyl aminopeptidase

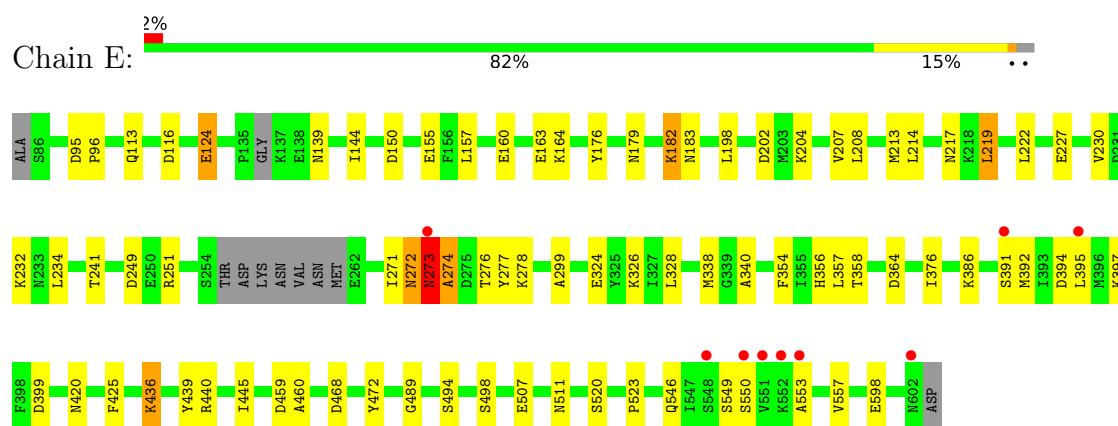




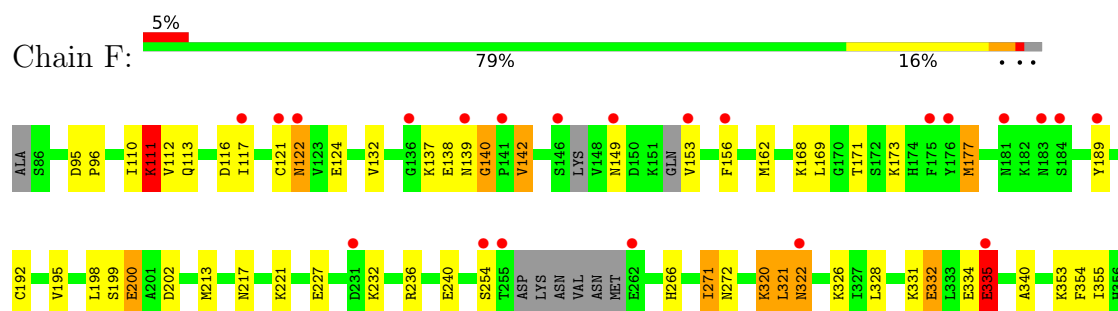
• Molecule 1: M17 leucyl aminopeptidase

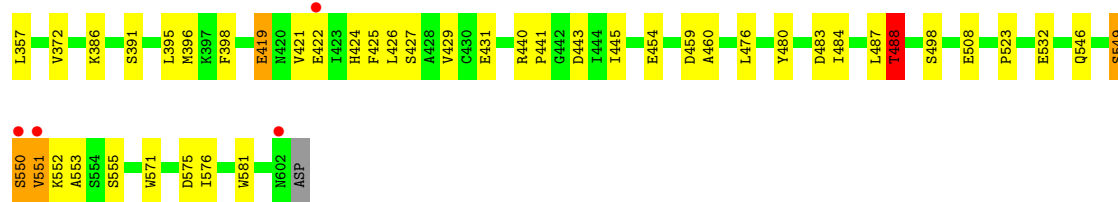


• Molecule 1: M17 leucyl aminopeptidase

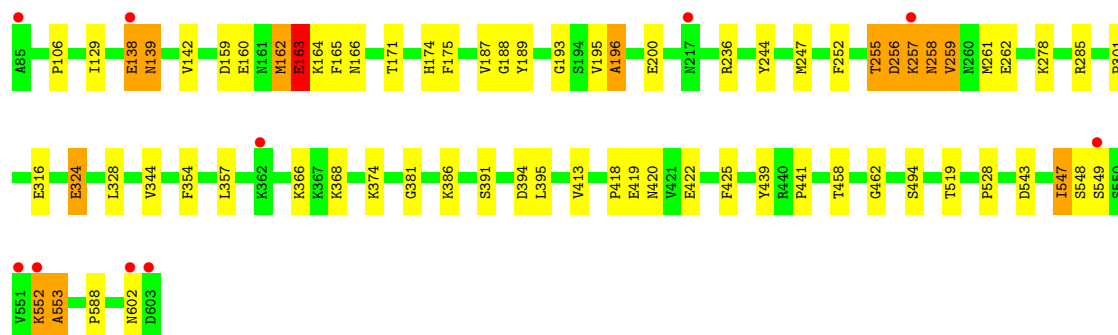
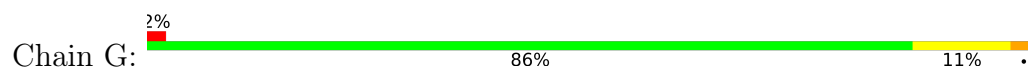


• Molecule 1: M17 leucyl aminopeptidase

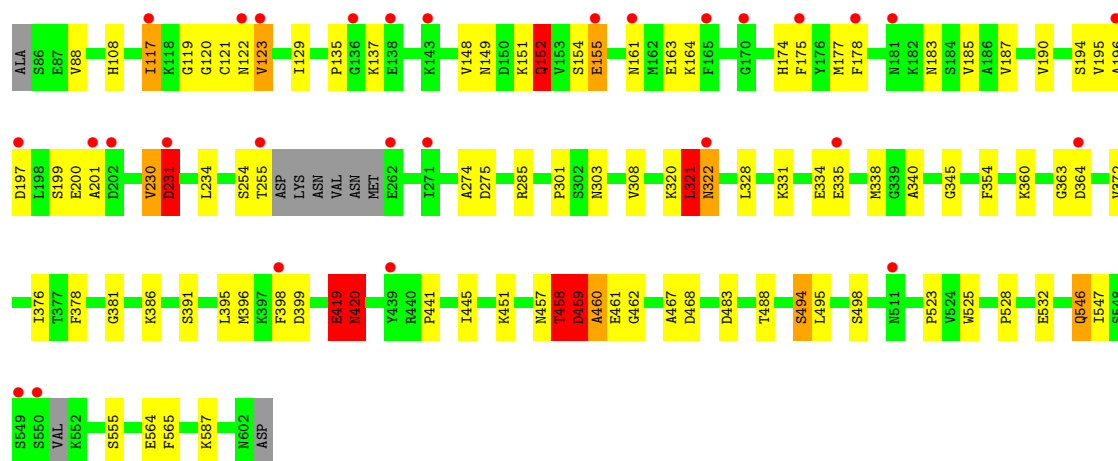
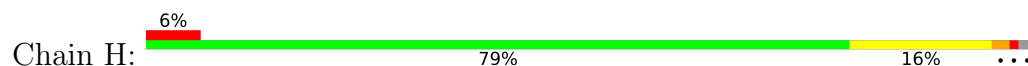




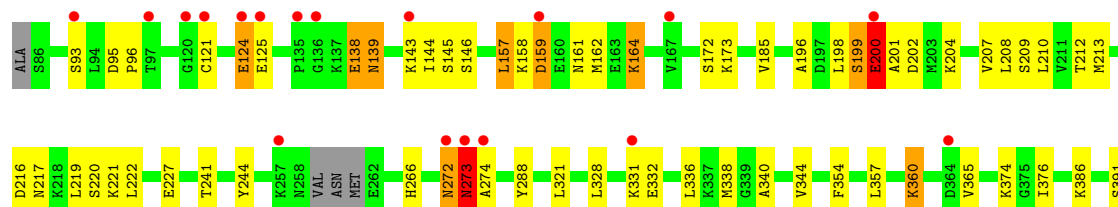
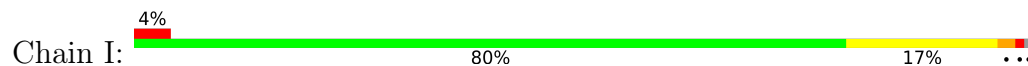
● Molecule 1: M17 leucyl aminopeptidase



● Molecule 1: M17 leucyl aminopeptidase

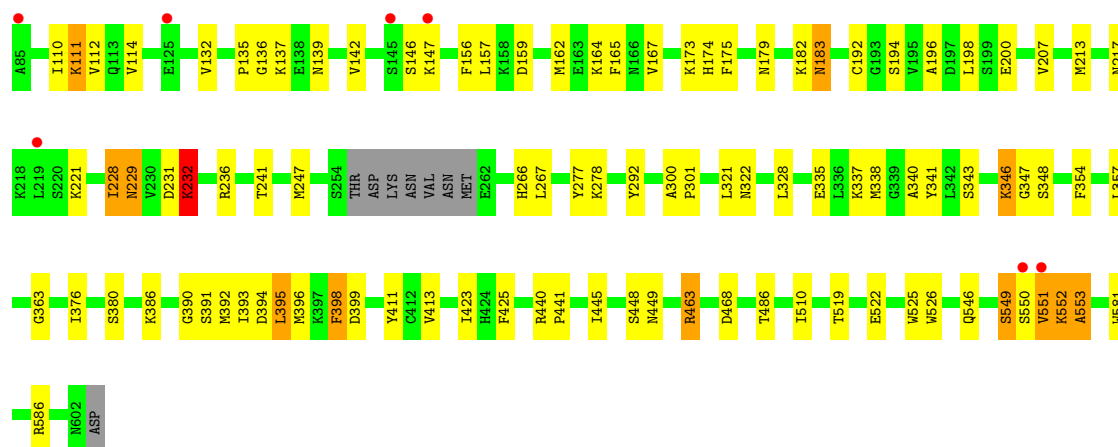
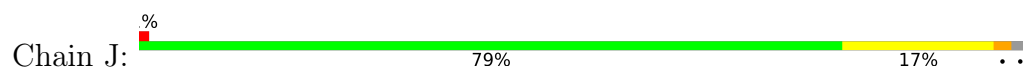


● Molecule 1: M17 leucyl aminopeptidase

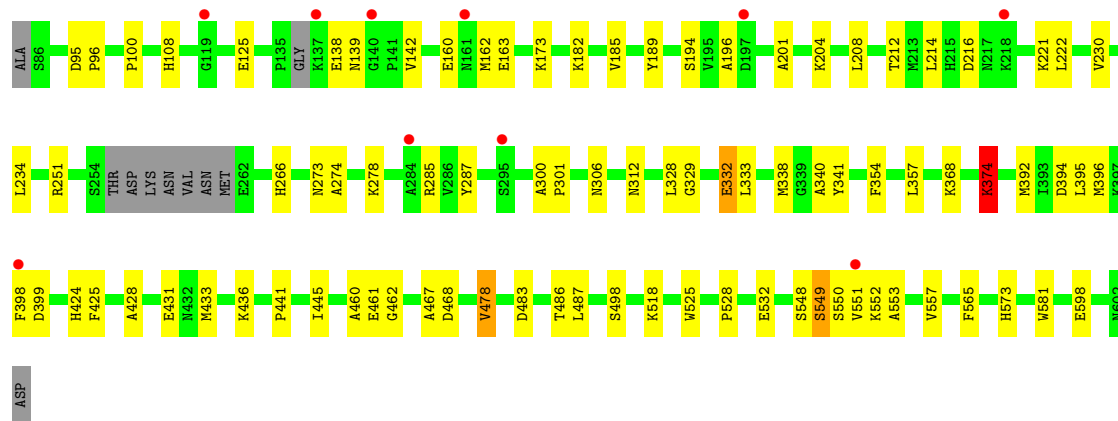
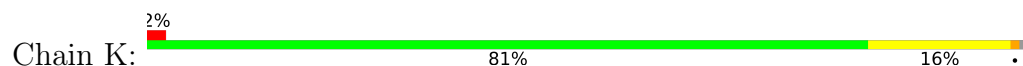




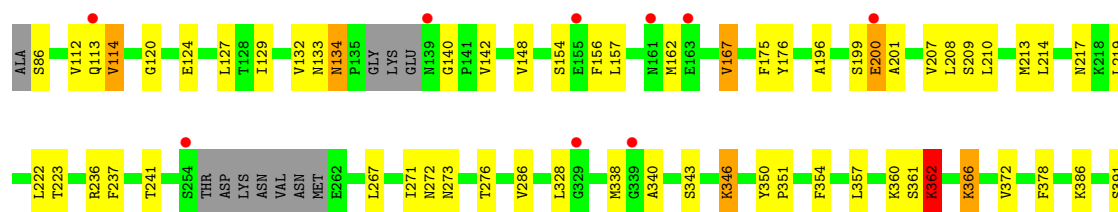
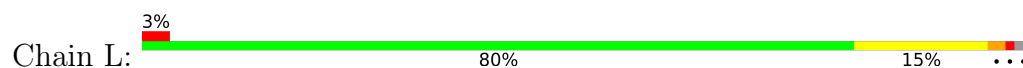
• Molecule 1: M17 leucyl aminopeptidase

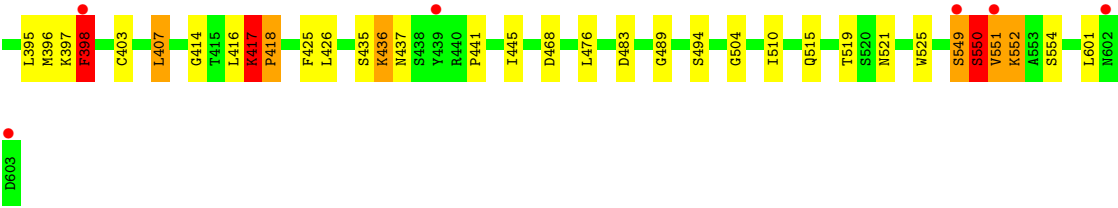


• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.72Å 176.70Å 223.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.73 48.75 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.75-2.73) 94.0 (48.75-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.220 , 0.274 0.224 , 0.277	Depositor DCC
R_{free} test set	9021 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48055	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2380e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CO3, ZN, 1PE, SO4, TOD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	3/4007 (0.1%)	0.89	11/5440 (0.2%)
1	B	0.60	8/3913 (0.2%)	1.13	34/5316 (0.6%)
1	C	0.52	8/4019 (0.2%)	1.10	19/5453 (0.3%)
1	D	0.40	1/3976 (0.0%)	0.91	11/5395 (0.2%)
1	E	0.43	3/3960 (0.1%)	0.92	13/5375 (0.2%)
1	F	0.57	6/3835 (0.2%)	1.00	24/5222 (0.5%)
1	G	0.40	0/4057	0.96	16/5505 (0.3%)
1	H	0.48	2/3931 (0.1%)	0.99	26/5340 (0.5%)
1	I	0.48	2/3989 (0.1%)	0.99	26/5414 (0.5%)
1	J	0.51	3/3952 (0.1%)	0.98	21/5366 (0.4%)
1	K	0.49	2/3954 (0.1%)	0.87	4/5367 (0.1%)
1	L	0.52	2/3881 (0.1%)	1.00	25/5282 (0.5%)
All	All	0.49	40/47474 (0.1%)	0.98	230/64475 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	9
1	C	0	5
1	D	0	2
1	E	0	2
1	F	0	6
1	G	0	3
1	H	0	3
1	I	0	4
1	J	0	3
1	K	0	1
1	L	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	43

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	488	THR	C-O	-18.61	1.02	1.24
1	B	549	SER	C-O	-15.62	1.10	1.23
1	C	398	PHE	C-O	-15.29	1.04	1.24
1	L	418	PRO	N-CD	11.46	1.63	1.47
1	F	488	THR	N-CA	-9.61	1.34	1.46
1	B	439	TYR	C-O	-8.70	1.13	1.23
1	I	159	ASP	N-CA	-8.45	1.35	1.46
1	B	439	TYR	CG-CD1	-8.31	1.21	1.39
1	B	549	SER	CA-CB	-7.93	1.43	1.53
1	F	487	LEU	C-N	-7.59	1.23	1.33
1	A	587	LYS	C-N	7.32	1.42	1.33
1	B	439	TYR	CE2-CZ	-7.30	1.20	1.38
1	A	587	LYS	C-O	-7.14	1.17	1.24
1	I	158	LYS	C-N	-7.11	1.24	1.33
1	B	549	SER	CB-OG	-7.08	1.27	1.42
1	C	397	LYS	C-N	-6.91	1.24	1.33
1	E	183	ASN	N-CA	-6.85	1.37	1.45
1	J	217	ASN	CA-C	-6.84	1.44	1.52
1	K	424	HIS	C-O	-6.42	1.16	1.24
1	E	182	LYS	CA-C	-6.38	1.44	1.52
1	A	418	PRO	N-CD	6.37	1.56	1.47
1	C	398	PHE	N-CA	-6.20	1.37	1.46
1	F	488	THR	CB-CG2	-6.03	1.32	1.52
1	B	439	TYR	N-CA	-5.92	1.38	1.46
1	L	398	PHE	C-O	-5.87	1.16	1.24
1	F	321	LEU	CA-C	-5.82	1.45	1.52
1	D	117	ILE	CG1-CD1	-5.77	1.29	1.51
1	C	215	HIS	ND1-CE1	5.77	1.38	1.32
1	C	398	PHE	C-N	-5.76	1.24	1.33
1	B	549	SER	CA-C	-5.68	1.47	1.53
1	C	215	HIS	CG-ND1	-5.66	1.32	1.38
1	J	398	PHE	C-O	-5.56	1.16	1.24
1	J	217	ASN	C-O	-5.47	1.17	1.24
1	F	320	LYS	CA-C	-5.44	1.45	1.52
1	H	494	SER	C-O	-5.38	1.18	1.24
1	H	459	ASP	CA-C	5.32	1.59	1.52
1	C	398	PHE	CG-CD1	-5.27	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	182	LYS	C-N	-5.18	1.25	1.33
1	K	374	LYS	C-O	-5.09	1.17	1.24
1	C	398	PHE	CG-CD2	-5.02	1.28	1.38

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	GLU	O-C-N	-33.18	81.06	122.21
1	B	151	LYS	CA-C-N	-19.54	91.81	122.49
1	B	151	LYS	C-N-CA	-19.54	91.81	122.49
1	C	123	VAL	CA-C-N	-18.77	85.40	121.81
1	C	123	VAL	C-N-CA	-18.77	85.40	121.81
1	C	334	GLU	CA-C-N	-14.02	100.22	122.65
1	C	334	GLU	C-N-CA	-14.02	100.22	122.65
1	E	549	SER	CA-C-N	12.41	138.33	120.71
1	E	549	SER	C-N-CA	12.41	138.33	120.71
1	B	418	PRO	CA-C-N	11.35	137.65	121.42
1	B	418	PRO	C-N-CA	11.35	137.65	121.42
1	G	164	LYS	N-CA-C	-11.05	99.61	112.87
1	E	272	ASN	N-CA-C	-11.04	94.18	110.52
1	I	273	ASN	O-C-N	-11.01	107.95	122.59
1	F	254	SER	N-CA-C	-10.83	98.86	112.72
1	F	111	LYS	O-C-N	-10.81	108.21	122.59
1	G	418	PRO	CA-C-N	-10.47	104.37	123.01
1	G	418	PRO	C-N-CA	-10.47	104.37	123.01
1	B	163	GLU	CA-C-N	10.22	141.06	121.54
1	B	163	GLU	C-N-CA	10.22	141.06	121.54
1	G	258	ASN	N-CA-C	-10.18	94.08	107.73
1	B	180	ASP	CA-C-N	10.12	136.78	120.60
1	B	180	ASP	C-N-CA	10.12	136.78	120.60
1	B	152	GLN	O-C-N	-10.02	109.19	122.22
1	F	422	GLU	O-C-N	-9.92	110.63	123.13
1	I	159	ASP	N-CA-CB	-9.87	95.25	110.06
1	A	125	GLU	N-CA-C	-9.77	95.78	110.14
1	I	159	ASP	N-CA-C	9.75	123.13	111.33
1	L	201	ALA	N-CA-C	-9.73	100.66	111.07
1	B	202	ASP	O-C-N	-9.71	108.61	122.41
1	H	587	LYS	N-CA-C	9.47	116.74	108.22
1	L	199	SER	CA-C-N	9.43	133.27	120.54
1	L	199	SER	C-N-CA	9.43	133.27	120.54
1	J	159	ASP	N-CA-C	9.16	121.26	111.28
1	F	334	GLU	CA-C-N	9.16	135.75	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	334	GLU	C-N-CA	9.16	135.75	121.19
1	B	321	LEU	N-CA-C	-9.06	96.14	109.63
1	B	180	ASP	N-CA-C	9.03	121.13	111.28
1	G	162	MET	N-CA-C	8.88	123.42	112.23
1	E	163	GLU	CA-C-N	8.85	132.50	120.38
1	E	163	GLU	C-N-CA	8.85	132.50	120.38
1	B	272	ASN	CA-C-N	8.78	138.32	121.54
1	B	272	ASN	C-N-CA	8.78	138.32	121.54
1	C	330	VAL	CA-C-N	-8.77	105.75	122.06
1	C	330	VAL	C-N-CA	-8.77	105.75	122.06
1	C	397	LYS	CA-C-N	8.67	137.12	120.99
1	C	397	LYS	C-N-CA	8.67	137.12	120.99
1	E	394	ASP	CA-C-N	8.60	135.30	120.68
1	E	394	ASP	C-N-CA	8.60	135.30	120.68
1	G	255	THR	N-CA-C	-8.57	97.15	109.31
1	L	549	SER	N-CA-C	8.50	123.85	112.88
1	J	146	SER	CA-C-N	-8.43	109.61	122.09
1	J	146	SER	C-N-CA	-8.43	109.61	122.09
1	K	549	SER	N-CA-C	8.42	123.18	111.56
1	B	201	ALA	CA-C-N	-8.38	106.47	122.06
1	B	201	ALA	C-N-CA	-8.38	106.47	122.06
1	H	460	ALA	N-CA-C	-8.34	99.80	111.81
1	J	232	LYS	O-C-N	-8.30	110.62	122.41
1	L	417	LYS	O-C-N	8.19	130.73	121.32
1	G	138	GLU	N-CA-C	-8.15	97.73	110.36
1	D	322	ASN	O-C-N	-8.12	111.80	122.59
1	I	518	LYS	CA-C-N	8.10	131.14	120.28
1	I	518	LYS	C-N-CA	8.10	131.14	120.28
1	H	419	GLU	CA-C-N	-8.10	112.23	126.32
1	H	419	GLU	C-N-CA	-8.10	112.23	126.32
1	E	272	ASN	CA-C-N	8.05	136.91	121.54
1	E	272	ASN	C-N-CA	8.05	136.91	121.54
1	L	435	SER	CA-C-N	7.96	131.29	120.38
1	L	435	SER	C-N-CA	7.96	131.29	120.38
1	J	231	ASP	CA-C-N	-7.89	107.39	122.06
1	J	231	ASP	C-N-CA	-7.89	107.39	122.06
1	E	550	SER	O-C-N	-7.88	113.18	122.87
1	F	121	CYS	CA-C-N	-7.67	110.76	122.81
1	F	121	CYS	C-N-CA	-7.67	110.76	122.81
1	I	272	ASN	CA-C-N	-7.61	107.01	121.54
1	I	272	ASN	C-N-CA	-7.61	107.01	121.54
1	H	151	LYS	CA-C-N	7.59	131.35	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	151	LYS	C-N-CA	7.59	131.35	120.79
1	I	199	SER	CA-C-N	7.51	133.14	121.19
1	I	199	SER	C-N-CA	7.51	133.14	121.19
1	F	488	THR	N-CA-C	7.36	121.20	108.76
1	F	488	THR	N-CA-CB	-7.36	98.08	110.80
1	H	163	GLU	CA-C-N	-7.34	109.94	122.56
1	H	163	GLU	C-N-CA	-7.34	109.94	122.56
1	B	419	GLU	O-C-N	-7.29	114.40	123.01
1	L	418	PRO	N-CA-CB	7.22	110.05	103.33
1	F	110	ILE	CA-C-N	7.11	135.11	121.54
1	F	110	ILE	C-N-CA	7.11	135.11	121.54
1	C	232	LYS	CA-C-N	-7.01	108.88	121.14
1	C	232	LYS	C-N-CA	-7.01	108.88	121.14
1	J	229	ASN	N-CA-C	6.94	120.25	109.07
1	D	163	GLU	N-CA-C	-6.92	104.71	113.01
1	A	123	VAL	CA-C-N	6.91	134.75	121.54
1	A	123	VAL	C-N-CA	6.91	134.75	121.54
1	J	182	LYS	CA-C-N	-6.91	111.20	122.81
1	J	182	LYS	C-N-CA	-6.91	111.20	122.81
1	G	162	MET	CA-C-N	6.88	134.68	121.54
1	G	162	MET	C-N-CA	6.88	134.68	121.54
1	G	549	SER	O-C-N	-6.84	113.50	121.99
1	A	124	GLU	N-CA-C	6.83	125.35	110.80
1	J	552	LYS	N-CA-C	6.78	118.03	108.00
1	B	144	ILE	CA-C-N	6.78	132.81	122.37
1	B	144	ILE	C-N-CA	6.78	132.81	122.37
1	E	273	ASN	O-C-N	6.70	131.50	122.59
1	F	550	SER	O-C-N	6.68	131.48	122.59
1	G	138	GLU	CA-C-N	-6.68	108.77	121.54
1	G	138	GLU	C-N-CA	-6.68	108.77	121.54
1	K	461	GLU	N-CA-C	6.67	121.16	112.89
1	H	230	VAL	CA-C-N	6.55	134.06	121.54
1	H	230	VAL	C-N-CA	6.55	134.06	121.54
1	L	120	GLY	N-CA-C	-6.55	104.96	112.29
1	I	549	SER	N-CA-C	-6.52	105.63	113.97
1	C	233	ASN	O-C-N	-6.52	113.47	122.46
1	B	145	SER	O-C-N	-6.51	114.31	122.19
1	L	549	SER	CA-C-N	6.51	133.41	121.70
1	L	549	SER	C-N-CA	6.51	133.41	121.70
1	A	391	SER	N-CA-C	6.47	119.32	111.82
1	D	117	ILE	CB-CG1-CD1	-6.46	100.22	113.80
1	H	322	ASN	CA-C-O	6.43	128.24	120.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	366	LYS	N-CA-C	6.43	120.10	110.14
1	B	134	ASN	CA-C-N	6.41	127.42	119.98
1	B	134	ASN	C-N-CA	6.41	127.42	119.98
1	E	274	ALA	N-CA-CB	6.41	119.36	110.07
1	H	321	LEU	CA-C-N	-6.41	111.85	121.72
1	H	321	LEU	C-N-CA	-6.41	111.85	121.72
1	G	324	GLU	O-C-N	-6.37	115.05	122.95
1	C	162	MET	N-CA-C	6.35	120.77	112.89
1	F	140	GLY	CA-C-N	6.27	126.19	119.85
1	F	140	GLY	C-N-CA	6.27	126.19	119.85
1	I	124	GLU	CA-C-N	6.27	134.48	121.32
1	I	124	GLU	C-N-CA	6.27	134.48	121.32
1	I	158	LYS	CA-C-O	6.26	128.19	121.55
1	A	587	LYS	N-CA-C	6.26	115.34	108.14
1	L	114	VAL	CB-CA-C	-6.20	102.57	111.19
1	F	421	VAL	CA-C-N	6.16	131.85	123.11
1	F	421	VAL	C-N-CA	6.16	131.85	123.11
1	B	124	GLU	CA-C-N	6.13	131.56	121.39
1	B	124	GLU	C-N-CA	6.13	131.56	121.39
1	L	551	VAL	CA-C-N	-6.13	110.11	122.55
1	L	551	VAL	C-N-CA	-6.13	110.11	122.55
1	H	321	LEU	N-CA-C	-6.11	97.79	110.80
1	I	551	VAL	O-C-N	-6.10	114.94	122.57
1	L	397	LYS	CA-C-N	6.09	132.32	120.99
1	L	397	LYS	C-N-CA	6.09	132.32	120.99
1	I	272	ASN	N-CA-C	6.08	119.80	110.20
1	L	418	PRO	CA-N-CD	-6.07	103.50	112.00
1	H	152	GLN	O-C-N	6.05	128.56	122.08
1	L	362	LYS	N-CA-C	6.05	118.15	108.41
1	C	554	SER	N-CA-C	6.05	117.87	111.28
1	B	200	GLU	N-CA-C	-5.99	105.63	113.12
1	J	549	SER	N-CA-C	-5.99	105.95	113.20
1	C	331	LYS	O-C-N	-5.99	113.91	122.41
1	L	271	ILE	CA-C-N	-5.96	112.50	122.64
1	L	271	ILE	C-N-CA	-5.96	112.50	122.64
1	F	232	LYS	N-CA-C	-5.96	104.87	111.36
1	D	321	LEU	CA-C-N	-5.93	110.21	121.54
1	D	321	LEU	C-N-CA	-5.93	110.21	121.54
1	C	330	VAL	N-CA-C	5.92	116.11	110.42
1	I	550	SER	N-CA-C	5.85	113.58	108.78
1	I	550	SER	CA-C-O	5.84	121.33	117.94
1	C	398	PHE	N-CA-C	5.82	119.86	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	110	ILE	CA-C-N	-5.80	114.02	122.19
1	J	110	ILE	C-N-CA	-5.80	114.02	122.19
1	I	552	LYS	N-CA-C	5.79	120.09	113.19
1	G	261	MET	N-CA-C	5.78	117.71	108.41
1	D	550	SER	O-C-N	5.76	130.25	122.59
1	H	274	ALA	N-CA-C	5.76	117.56	111.28
1	K	196	ALA	CA-C-N	-5.72	115.40	122.84
1	K	196	ALA	C-N-CA	-5.72	115.40	122.84
1	D	518	LYS	O-C-N	-5.71	114.67	122.33
1	H	322	ASN	N-CA-C	5.69	116.73	107.23
1	H	420	ASN	O-C-N	-5.64	116.25	122.00
1	B	182	LYS	N-CA-CB	-5.62	103.63	112.46
1	I	438	SER	CA-C-N	5.61	130.71	121.39
1	I	438	SER	C-N-CA	5.61	130.71	121.39
1	F	335	GLU	O-C-N	5.61	128.99	122.20
1	I	274	ALA	N-CA-C	5.59	118.91	111.75
1	C	228	ILE	CA-C-N	-5.59	115.28	123.00
1	C	228	ILE	C-N-CA	-5.59	115.28	123.00
1	L	199	SER	N-CA-C	-5.58	102.50	110.59
1	B	439	TYR	CA-CB-CG	5.55	123.89	113.90
1	F	112	VAL	CA-C-N	-5.52	114.00	122.62
1	F	112	VAL	C-N-CA	-5.52	114.00	122.62
1	J	147	LYS	O-C-N	5.50	129.54	123.16
1	I	397	LYS	N-CA-C	-5.47	105.87	112.54
1	J	228	ILE	CA-C-N	-5.46	115.47	123.00
1	J	228	ILE	C-N-CA	-5.46	115.47	123.00
1	A	511	ASN	O-C-N	-5.46	115.56	122.27
1	D	553	ALA	N-CA-C	-5.44	99.21	110.80
1	E	219	LEU	N-CA-C	5.40	117.65	110.53
1	B	117	ILE	CB-CG1-CD1	-5.39	102.49	113.80
1	I	519	THR	N-CA-C	5.38	117.15	111.28
1	I	200	GLU	O-C-N	5.38	128.71	122.20
1	J	552	LYS	CB-CA-C	-5.38	108.81	116.34
1	D	549	SER	CA-C-N	5.35	131.76	121.54
1	D	549	SER	C-N-CA	5.35	131.76	121.54
1	B	163	GLU	N-CA-C	5.30	118.85	112.38
1	B	202	ASP	N-CA-C	-5.30	106.81	113.28
1	J	157	LEU	N-CA-C	5.29	119.72	113.16
1	H	119	GLY	N-CA-C	-5.29	100.65	113.18
1	J	111	LYS	O-C-N	5.29	129.25	123.22
1	I	274	ALA	N-CA-CB	-5.28	101.80	110.14
1	A	554	SER	N-CA-C	5.26	117.02	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	ASN	CA-C-N	-5.26	112.24	121.70
1	A	602	ASN	C-N-CA	-5.26	112.24	121.70
1	L	551	VAL	N-CA-C	-5.25	101.90	108.84
1	B	272	ASN	N-CA-C	-5.22	102.02	110.32
1	H	199	SER	CA-C-N	5.21	127.57	120.54
1	H	199	SER	C-N-CA	5.21	127.57	120.54
1	J	522	GLU	CA-C-N	5.20	125.45	119.83
1	J	522	GLU	C-N-CA	5.20	125.45	119.83
1	B	199	SER	CA-CB-OG	-5.19	100.71	111.10
1	D	91	VAL	N-CA-C	-5.18	106.63	111.45
1	B	273	ASN	O-C-N	5.17	129.47	122.59
1	G	602	ASN	N-CA-C	5.17	119.28	112.25
1	H	458	THR	O-C-N	-5.14	115.75	122.59
1	H	177	MET	N-CA-C	5.14	116.10	108.60
1	B	182	LYS	N-CA-C	5.14	118.80	111.92
1	F	271	ILE	CA-C-N	-5.12	113.31	122.07
1	F	271	ILE	C-N-CA	-5.12	113.31	122.07
1	H	458	THR	N-CA-C	-5.09	99.95	110.80
1	H	121	CYS	CA-C-N	-5.08	115.99	123.00
1	H	121	CYS	C-N-CA	-5.08	115.99	123.00
1	F	549	SER	CA-C-N	5.06	131.20	121.54
1	F	549	SER	C-N-CA	5.06	131.20	121.54
1	L	552	LYS	N-CA-C	5.05	119.02	113.21
1	G	549	SER	N-CA-C	5.04	116.91	110.61
1	L	550	SER	O-C-N	-5.02	114.97	123.00
1	A	129	ILE	N-CA-C	5.01	115.12	108.11
1	I	138	GLU	N-CA-C	-5.00	104.08	110.53

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	SER	Mainchain
1	B	152	GLN	Mainchain
1	B	164	LYS	Mainchain
1	B	181	ASN	Mainchain
1	B	199	SER	Peptide
1	B	202	ASP	Mainchain
1	B	272	ASN	Peptide
1	B	273	ASN	Mainchain
1	B	549	SER	Peptide
1	C	124	GLU	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	C	233	ASN	Mainchain
1	C	331	LYS	Mainchain
1	C	335	GLU	Mainchain
1	D	322	ASN	Mainchain
1	D	518	LYS	Mainchain
1	E	164	LYS	Mainchain
1	E	273	ASN	Mainchain
1	F	111	LYS	Mainchain
1	F	335	GLU	Mainchain
1	F	488	THR	Mainchain
1	F	549	SER	Peptide
1	F	550	SER	Peptide,Mainchain
1	G	138	GLU	Peptide
1	G	139	ASN	Mainchain
1	G	163	GLU	Mainchain
1	H	164	LYS	Mainchain
1	H	321	LEU	Peptide
1	H	420	ASN	Mainchain
1	I	145	SER	Mainchain
1	I	200	GLU	Mainchain
1	I	273	ASN	Mainchain
1	I	550	SER	Peptide
1	J	183	ASN	Sidechain
1	J	232	LYS	Mainchain
1	J	549	SER	Peptide
1	K	163	GLU	Mainchain
1	L	398	PHE	Mainchain
1	L	417	LYS	Mainchain
1	L	436	LYS	Mainchain
1	L	550	SER	Peptide
1	L	552	LYS	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	3928	0	3824	48	1
1	B	3837	0	3716	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3942	0	3865	92	0
1	D	3899	0	3817	67	0
1	E	3884	0	3789	66	0
1	F	3762	0	3570	76	0
1	G	3979	0	3890	49	1
1	H	3855	0	3732	74	0
1	I	3912	0	3831	89	0
1	J	3875	0	3773	70	1
1	K	3878	0	3776	69	1
1	L	3806	0	3638	83	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	24	0	20	0	0
3	B	24	0	21	4	0
3	C	17	0	15	0	0
3	E	15	0	14	3	0
3	F	24	0	20	1	0
3	G	22	0	20	0	0
3	H	14	0	13	0	0
3	I	24	0	21	2	0
3	J	22	0	20	2	0
3	K	22	0	20	3	0
3	L	24	0	20	1	0
4	A	4	0	0	3	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	1	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	2	0
4	H	4	0	0	1	0
4	I	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	4	0	0	3	0
4	K	4	0	0	3	0
4	L	4	0	0	0	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	1	0
5	E	10	0	0	0	0
5	G	10	0	0	1	0
5	I	5	0	0	0	0
5	L	10	0	0	1	0
6	A	9	0	10	1	0
6	B	7	0	6	0	0
6	C	22	0	24	12	0
6	D	20	0	20	5	0
6	E	12	0	14	0	0
6	G	18	0	18	4	0
6	H	10	0	10	1	0
7	A	102	0	0	5	0
7	B	74	0	0	4	0
7	C	70	0	0	5	0
7	D	80	0	0	7	0
7	E	113	0	0	6	0
7	F	88	0	0	11	0
7	G	93	0	0	6	0
7	H	74	0	0	5	0
7	I	91	0	0	6	0
7	J	86	0	0	16	0
7	K	91	0	0	4	0
7	L	69	0	0	4	0
All	All	48055	0	45527	827	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (827) 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)
7:G:885:HOH:O	1:L:551:VAL:HG22	1.25	1.35
1:C:331:LYS:CG	1:C:334:GLU:OE1	1.75	1.34
1:C:331:LYS:HG3	1:C:334:GLU:OE1	1.16	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:278:LYS:HG3	7:J:865:HOH:O	1.29	1.27
1:D:320:LYS:NZ	6:D:706:1PE:H142	1.48	1.25
1:I:143:LYS:HD3	1:I:159:ASP:OD1	1.29	1.22
1:C:320:LYS:NZ	6:C:706:1PE:OH3	1.75	1.18
1:L:200:GLU:OE2	1:L:521:ASN:HB3	1.40	1.18
1:D:344:VAL:HA	1:D:439:TYR:CE2	1.79	1.17
1:I:396:MET:SD	1:I:398:PHE:HE2	1.69	1.15
1:B:142:VAL:HG12	1:B:167:VAL:HG12	1.25	1.12
1:I:272:ASN:O	1:I:273:ASN:HB2	1.32	1.12
1:C:320:LYS:HZ2	6:C:706:1PE:C12	1.62	1.12
1:L:396:MET:SD	1:L:398:PHE:HE2	1.71	1.11
1:I:144:ILE:HG13	1:I:157:LEU:HG	1.18	1.11
1:B:124:GLU:CB	1:B:125:GLU:OE1	2.00	1.09
1:J:278:LYS:CG	7:J:865:HOH:O	1.88	1.08
1:L:148:VAL:CG2	1:L:154:SER:HB2	1.83	1.08
1:L:200:GLU:OE2	1:L:521:ASN:CB	2.00	1.08
1:A:598:GLU:O	1:A:602:ASN:ND2	1.87	1.07
1:C:331:LYS:HG3	1:C:334:GLU:CD	1.78	1.07
1:C:436:LYS:NZ	7:C:826:HOH:O	1.67	1.07
1:B:125:GLU:OE1	1:B:125:GLU:N	1.87	1.07
1:K:462:GLY:N	4:K:704:CO3:O2	1.87	1.07
1:I:519:THR:CG2	1:I:598:GLU:OE1	2.03	1.06
1:F:198:LEU:HD11	1:F:202:ASP:CB	1.86	1.05
1:F:320:LYS:NZ	7:F:877:HOH:O	1.88	1.05
1:D:320:LYS:HZ1	6:D:706:1PE:H142	0.90	1.04
1:E:124:GLU:OE1	7:E:801:HOH:O	1.75	1.03
1:I:272:ASN:O	1:I:273:ASN:CB	2.04	1.03
1:B:199:SER:CB	1:B:202:ASP:H	1.71	1.02
1:D:540:LYS:NZ	7:D:877:HOH:O	1.92	1.02
1:G:462:GLY:N	4:G:704:CO3:O2	1.91	1.02
1:C:172:SER:O	1:C:173:LYS:HD2	1.59	1.01
1:L:200:GLU:OE2	1:L:521:ASN:C	2.05	0.99
1:B:125:GLU:CD	1:B:125:GLU:H	1.70	0.99
1:L:200:GLU:OE2	1:L:521:ASN:CA	2.11	0.99
1:L:272:ASN:OD1	1:L:273:ASN:N	1.96	0.99
1:B:142:VAL:HG12	1:B:167:VAL:CG1	1.93	0.98
1:K:374:LYS:HE2	1:K:462:GLY:HA3	1.46	0.98
1:G:494:SER:OG	1:L:494:SER:HB3	1.65	0.97
1:F:198:LEU:HD11	1:F:202:ASP:HB3	1.47	0.97
1:L:414:GLY:O	7:L:864:HOH:O	1.79	0.97
1:I:519:THR:HG21	1:I:598:GLU:OE1	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:TYR:HA	1:A:288:TYR:HE1	1.27	0.96
1:I:396:MET:CE	1:I:398:PHE:CE2	2.47	0.96
1:B:386:LYS:HB2	1:B:393:ILE:HD13	1.44	0.96
1:C:398:PHE:HE1	1:C:580:SER:HB3	1.30	0.95
1:D:320:LYS:HZ1	6:D:706:1PE:C14	1.79	0.95
1:I:396:MET:SD	1:I:398:PHE:CE2	2.60	0.95
1:H:532:GLU:OE1	1:K:498:SER:OG	1.84	0.95
1:A:386:LYS:HB2	1:A:393:ILE:HD13	1.46	0.94
1:A:173:LYS:NZ	7:A:857:HOH:O	1.99	0.94
1:C:320:LYS:NZ	6:C:706:1PE:C12	2.29	0.94
1:I:396:MET:CE	1:I:398:PHE:HE2	1.81	0.94
1:I:144:ILE:HG13	1:I:157:LEU:CG	1.96	0.93
1:L:200:GLU:OE2	1:L:521:ASN:O	1.85	0.93
1:D:321:LEU:O	1:D:322:ASN:CB	2.15	0.93
1:C:316:GLU:CD	6:C:706:1PE:H231	1.95	0.92
1:F:419:GLU:HA	1:F:419:GLU:OE1	1.69	0.92
1:B:199:SER:OG	1:B:201:ALA:N	2.03	0.91
1:G:494:SER:OG	1:L:494:SER:CB	2.19	0.91
1:G:258:ASN:OD1	1:G:259:VAL:N	2.05	0.90
1:I:519:THR:HG22	1:I:598:GLU:OE1	1.70	0.90
1:I:144:ILE:CG1	1:I:157:LEU:HG	2.02	0.89
1:L:200:GLU:CD	1:L:521:ASN:HB3	1.97	0.89
1:J:114:VAL:H	1:J:278:LYS:NZ	1.71	0.89
1:J:278:LYS:CD	7:J:865:HOH:O	2.10	0.89
1:F:173:LYS:N	1:F:189:TYR:CE2	2.42	0.87
1:L:148:VAL:HG21	1:L:154:SER:HB2	1.54	0.87
1:L:396:MET:SD	1:L:398:PHE:CE2	2.64	0.87
1:D:344:VAL:HA	1:D:439:TYR:HE2	1.36	0.87
1:F:480:TYR:OH	1:F:508:GLU:OE2	1.92	0.87
1:J:200:GLU:CG	7:J:863:HOH:O	2.22	0.86
1:F:322:ASN:ND2	1:K:160:GLU:OE2	2.09	0.86
1:H:419:GLU:O	1:H:420:ASN:HB2	1.75	0.86
1:J:463:ARG:HG3	4:J:704:CO3:O1	1.74	0.86
1:L:357:LEU:HB2	1:L:425:PHE:HB2	1.58	0.86
1:H:345:GLY:O	7:H:861:HOH:O	1.93	0.86
1:A:155:GLU:O	1:A:158:LYS:HG2	1.76	0.85
1:I:143:LYS:CD	1:I:159:ASP:OD1	2.22	0.85
1:L:396:MET:HA	1:L:398:PHE:HD2	1.41	0.85
1:I:172:SER:HB2	1:I:213:MET:HE3	1.56	0.85
1:B:199:SER:OG	1:B:200:GLU:C	2.19	0.85
1:J:278:LYS:CE	7:J:865:HOH:O	2.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ASN:OD1	1:F:149:ASN:CB	2.25	0.85
1:A:244:TYR:CA	1:A:288:TYR:HE1	1.91	0.83
1:J:463:ARG:NH1	1:J:546:GLN:O	2.10	0.83
1:H:458:THR:O	1:H:460:ALA:N	2.10	0.83
1:C:331:LYS:HG2	1:C:334:GLU:OE1	1.78	0.83
1:J:200:GLU:HG2	7:J:863:HOH:O	1.78	0.83
1:A:506:ASN:OD1	7:A:886:HOH:O	1.96	0.82
1:I:396:MET:HA	1:I:398:PHE:CD2	2.14	0.82
1:C:316:GLU:OE2	6:C:706:1PE:OH4	1.96	0.82
1:G:193:GLY:HA3	7:G:863:HOH:O	1.79	0.81
1:H:195:VAL:HG23	1:H:195:VAL:O	1.81	0.81
1:E:392:MET:HE3	1:E:395:LEU:CD2	2.11	0.81
1:C:171:THR:HG23	1:C:173:LYS:NZ	1.96	0.81
1:L:396:MET:HA	1:L:398:PHE:CD2	2.16	0.81
1:F:142:VAL:HG23	1:F:162:MET:HB3	1.63	0.80
1:C:172:SER:C	1:C:173:LYS:HD2	2.04	0.80
1:B:282:GLU:OE1	1:B:285:ARG:NH2	2.13	0.80
1:C:123:VAL:C	1:C:124:GLU:HG3	2.05	0.80
1:C:398:PHE:CE1	1:C:580:SER:HB3	2.16	0.80
1:L:200:GLU:CD	1:L:521:ASN:O	2.24	0.80
1:B:199:SER:HB2	1:B:202:ASP:H	1.44	0.80
1:J:390:GLY:O	1:J:392:MET:N	2.12	0.80
1:I:418:PRO:HB3	1:I:601:LEU:HD11	1.64	0.79
1:J:396:MET:SD	1:J:398:PHE:HE2	2.06	0.79
1:H:152:GLN:HG2	1:H:178:PHE:O	1.83	0.79
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.64	0.78
1:I:344:VAL:HA	1:I:439:TYR:CE2	2.18	0.78
1:J:386:LYS:HB2	1:J:393:ILE:HD13	1.63	0.78
1:G:543:ASP:OD2	1:H:254:SER:OG	2.00	0.78
1:K:182:LYS:O	7:K:801:HOH:O	2.01	0.78
1:B:386:LYS:NZ	3:B:1004:TOD:O3	2.16	0.78
1:I:396:MET:HA	1:I:398:PHE:HD2	1.47	0.78
1:C:316:GLU:OE2	6:C:706:1PE:C23	2.32	0.77
1:L:148:VAL:HG23	1:L:154:SER:HB2	1.65	0.77
1:J:278:LYS:HE2	7:J:865:HOH:O	1.84	0.77
1:C:232:LYS:HD3	1:C:276:THR:O	1.85	0.76
1:B:199:SER:OG	1:B:200:GLU:N	2.08	0.76
1:C:320:LYS:NZ	6:C:706:1PE:C22	2.47	0.76
1:F:488:THR:HG22	1:F:575:ASP:OD2	1.85	0.76
1:L:200:GLU:HG2	1:L:237:PHE:CZ	2.19	0.76
1:A:244:TYR:HA	1:A:288:TYR:CE1	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:GLU:O	1:A:421:VAL:HG23	1.85	0.76
1:F:443:ASP:OD2	7:F:849:HOH:O	2.04	0.75
1:F:153:VAL:HB	1:F:177:MET:HE1	1.69	0.75
1:B:199:SER:CB	1:B:202:ASP:N	2.46	0.75
1:I:338:MET:HE3	1:I:468:ASP:HB3	1.68	0.75
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.67	0.75
1:K:332:GLU:CD	1:K:332:GLU:H	1.93	0.74
1:J:586:ARG:NH2	7:J:884:HOH:O	2.19	0.74
1:C:113:GLN:OE1	1:C:115:TYR:OH	2.06	0.74
1:J:114:VAL:HB	1:J:278:LYS:HD3	1.67	0.74
7:G:885:HOH:O	1:L:551:VAL:CG2	2.01	0.74
1:D:321:LEU:O	1:D:322:ASN:HB2	1.87	0.74
1:D:320:LYS:HZ2	6:D:706:1PE:H142	1.52	0.74
1:E:392:MET:O	1:E:395:LEU:HB3	1.87	0.73
1:I:216:ASP:CB	7:I:871:HOH:O	2.35	0.73
1:L:148:VAL:HG21	1:L:154:SER:CB	2.18	0.73
1:F:198:LEU:CD1	1:F:202:ASP:HB2	2.18	0.73
1:D:338:MET:HE3	1:D:468:ASP:HB3	1.70	0.73
1:C:253:LYS:O	1:C:257:LYS:NZ	2.18	0.73
1:C:316:GLU:OE2	6:C:706:1PE:H231	1.88	0.73
1:F:427:SER:O	7:F:812:HOH:O	2.07	0.73
1:B:320:LYS:NZ	7:B:1174:HOH:O	2.11	0.72
1:B:471:VAL:HG12	1:B:475:LYS:HE3	1.72	0.72
1:J:386:LYS:HD2	1:J:393:ILE:HD12	1.70	0.72
1:F:198:LEU:HD11	1:F:202:ASP:HB2	1.70	0.72
1:F:137:LYS:CB	1:F:140:GLY:H	2.03	0.72
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.71	0.72
1:L:148:VAL:CG2	1:L:154:SER:CB	2.67	0.72
1:J:114:VAL:H	1:J:278:LYS:HZ3	1.36	0.71
1:K:483:ASP:OD1	1:K:573:HIS:ND1	2.20	0.71
1:H:122:ASN:ND2	1:H:149:ASN:HB2	2.05	0.71
1:I:396:MET:HE2	1:I:398:PHE:CE2	2.25	0.71
1:B:169:LEU:HD21	1:B:202:ASP:CB	2.20	0.71
1:G:163:GLU:C	1:G:165:PHE:N	2.47	0.71
1:K:338:MET:HE3	1:K:468:ASP:HB3	1.71	0.71
1:F:198:LEU:CD1	1:F:202:ASP:CB	2.66	0.71
1:E:392:MET:O	1:E:395:LEU:CB	2.39	0.71
1:I:125:GLU:OE2	1:I:220:SER:OG	2.08	0.71
1:F:173:LYS:N	1:F:189:TYR:HE2	1.87	0.70
1:E:326:LYS:HE3	1:E:328:LEU:HD11	1.73	0.70
1:J:357:LEU:HB2	1:J:425:PHE:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:463:ARG:CG	4:J:704:CO3:O1	2.40	0.70
1:D:117:ILE:HD11	1:D:271:ILE:HA	1.74	0.70
1:H:381:GLY:O	1:H:458:THR:OG1	2.05	0.70
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.74	0.70
1:D:321:LEU:O	1:D:322:ASN:HB3	1.92	0.69
1:D:155:GLU:OE1	1:D:155:GLU:HA	1.89	0.69
1:C:254:SER:HA	1:C:257:LYS:NZ	2.08	0.69
1:H:419:GLU:O	1:H:420:ASN:CB	2.40	0.69
1:H:462:GLY:N	4:H:704:CO3:O2	2.25	0.69
1:L:133:ASN:HA	1:L:167:VAL:HG11	1.74	0.69
1:I:161:ASN:O	1:I:164:LYS:HE2	1.93	0.69
1:L:361:SER:OG	1:L:366:LYS:NZ	2.26	0.69
1:I:418:PRO:HB3	1:I:601:LEU:CD1	2.23	0.69
1:C:195:VAL:HG23	1:C:195:VAL:O	1.93	0.68
1:C:301:PRO:HA	1:C:397:LYS:HD2	1.76	0.68
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.74	0.68
3:E:703:TOD:H5	3:E:703:TOD:O1	1.93	0.68
1:J:247:MET:CE	7:J:849:HOH:O	2.40	0.68
1:C:123:VAL:O	1:C:124:GLU:CG	2.42	0.68
1:E:436:LYS:NZ	7:E:827:HOH:O	2.26	0.68
1:F:221:LYS:HG3	1:F:266:HIS:HB2	1.74	0.68
1:I:551:VAL:HG12	1:I:551:VAL:O	1.94	0.68
1:C:398:PHE:HE1	1:C:580:SER:CB	2.04	0.67
1:C:522:GLU:OE2	7:C:848:HOH:O	2.13	0.67
1:D:396:MET:SD	1:D:398:PHE:HE2	2.17	0.67
1:H:331:LYS:O	1:H:335:GLU:HG3	1.95	0.67
1:E:326:LYS:CE	1:E:328:LEU:HD11	2.24	0.67
1:G:344:VAL:HA	1:G:439:TYR:CE2	2.29	0.67
1:I:146:SER:OG	1:I:227:GLU:OE2	2.06	0.67
1:C:171:THR:HG23	1:C:173:LYS:HZ2	1.58	0.67
1:C:328:LEU:HG	1:C:332:GLU:CD	2.20	0.67
3:J:703:TOD:O2	4:J:704:CO3:O2	2.13	0.67
1:J:449:ASN:O	7:J:874:HOH:O	2.13	0.66
1:B:123:VAL:O	1:B:125:GLU:CD	2.38	0.66
1:B:199:SER:OG	1:B:202:ASP:N	2.28	0.66
1:L:129:ILE:HD11	1:L:213:MET:HE1	1.77	0.66
1:C:395:LEU:O	1:C:398:PHE:HB3	1.95	0.66
1:D:144:ILE:HD13	1:D:157:LEU:HD22	1.76	0.66
1:D:217:ASN:HD21	1:D:219:LEU:HD12	1.61	0.66
1:D:232:LYS:NZ	1:D:280:GLU:OE2	2.29	0.66
1:B:176:TYR:HB3	1:F:177:MET:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.76	0.66
1:D:442:GLY:O	7:D:824:HOH:O	2.12	0.66
1:F:353:LYS:O	7:F:812:HOH:O	2.14	0.66
1:L:112:VAL:HG22	1:L:267:LEU:HB3	1.76	0.66
1:E:324:GLU:CG	1:E:358:THR:HB	2.26	0.66
1:J:200:GLU:HG3	7:J:863:HOH:O	1.86	0.65
1:H:175:PHE:N	1:H:187:VAL:O	2.25	0.65
1:E:324:GLU:OE2	1:E:358:THR:HB	1.96	0.65
1:G:163:GLU:C	1:G:165:PHE:H	2.04	0.65
1:A:533:TYR:O	1:A:536:THR:HG22	1.96	0.65
1:B:199:SER:HG	1:B:200:GLU:C	2.05	0.65
1:I:208:LEU:O	7:I:867:HOH:O	2.14	0.65
1:G:374:LYS:HE3	1:G:462:GLY:HA3	1.79	0.65
1:L:200:GLU:CG	1:L:521:ASN:HB3	2.27	0.65
1:E:324:GLU:CD	1:E:358:THR:HB	2.21	0.65
1:K:357:LEU:HB2	1:K:425:PHE:HB2	1.77	0.65
7:D:847:HOH:O	1:F:454:GLU:OE2	2.14	0.65
1:B:389:PRO:O	7:B:1143:HOH:O	2.15	0.65
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.77	0.65
1:G:262:GLU:O	7:G:867:HOH:O	2.15	0.64
1:B:338:MET:HE3	1:B:468:ASP:HB3	1.79	0.64
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.80	0.64
1:E:392:MET:HE3	1:E:395:LEU:HD23	1.80	0.64
1:L:129:ILE:CD1	1:L:213:MET:HE1	2.28	0.64
1:H:460:ALA:HB3	1:H:546:GLN:NE2	2.13	0.64
1:I:143:LYS:NZ	1:I:159:ASP:HB3	2.12	0.64
1:I:374:LYS:HE3	1:I:462:GLY:HA3	1.79	0.64
1:D:184:SER:OG	5:D:704:SO4:O3	2.15	0.64
1:F:331:LYS:O	1:F:335:GLU:HG3	1.97	0.64
1:D:205:ARG:NH1	7:D:836:HOH:O	2.30	0.64
1:L:338:MET:HE3	1:L:468:ASP:HB3	1.79	0.63
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.79	0.63
1:C:439:TYR:CE1	1:C:458:THR:HG22	2.34	0.63
1:I:221:LYS:HD2	1:I:266:HIS:HB2	1.80	0.63
1:C:220:SER:OG	5:C:705:SO4:O2	2.16	0.63
1:G:547:ILE:HG12	1:G:548:SER:H	1.63	0.63
1:L:208:LEU:CD2	7:L:856:HOH:O	2.46	0.63
1:D:247:MET:HB2	1:D:288:TYR:OH	1.99	0.63
1:E:232:LYS:NZ	1:E:276:THR:O	2.32	0.63
1:F:326:LYS:HE3	1:F:328:LEU:HD21	1.79	0.63
1:J:114:VAL:H	1:J:278:LYS:HZ2	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:VAL:HG22	1:F:162:MET:O	1.99	0.63
1:K:431:GLU:HG2	1:K:433:MET:HG2	1.79	0.63
1:K:551:VAL:O	1:K:553:ALA:N	2.32	0.63
1:I:418:PRO:CB	1:I:601:LEU:HD11	2.28	0.62
1:F:142:VAL:CG2	1:F:162:MET:HB3	2.29	0.62
1:F:322:ASN:HB2	1:K:160:GLU:OE2	1.99	0.62
1:H:122:ASN:HD21	1:H:149:ASN:HB2	1.64	0.62
1:H:338:MET:HE3	1:H:468:ASP:HB3	1.81	0.62
1:I:125:GLU:OE1	1:I:221:LYS:HD3	1.98	0.62
1:D:244:TYR:HA	1:D:288:TYR:HE1	1.64	0.62
1:I:199:SER:HG	1:I:200:GLU:CD	2.06	0.62
1:F:332:GLU:HA	1:F:335:GLU:CD	2.25	0.62
1:J:343:SER:HA	1:J:346:LYS:HD3	1.82	0.62
1:F:117:ILE:CB	1:F:272:ASN:ND2	2.63	0.61
1:H:148:VAL:HG23	1:H:154:SER:OG	1.99	0.61
1:F:459:ASP:OD2	7:F:822:HOH:O	2.16	0.61
1:J:114:VAL:HB	1:J:278:LYS:CD	2.30	0.61
1:F:396:MET:SD	1:F:398:PHE:HE2	2.22	0.61
1:G:236:ARG:NH2	1:G:519:THR:O	2.32	0.61
1:K:329:GLY:O	1:K:332:GLU:OE1	2.17	0.61
1:I:551:VAL:O	1:I:551:VAL:CG1	2.47	0.61
1:J:156:PHE:O	1:J:162:MET:HE3	2.00	0.61
1:B:347:GLY:HA3	1:B:438:SER:OG	2.00	0.61
1:L:386:LYS:HB3	1:L:391:SER:HB3	1.82	0.61
1:L:208:LEU:HD22	7:L:856:HOH:O	2.00	0.60
1:C:258:ASN:OD1	1:C:260:ASN:N	2.29	0.60
1:C:316:GLU:OE2	6:C:706:1PE:C13	2.50	0.60
1:E:230:VAL:HG12	1:E:234:LEU:HD23	1.82	0.60
1:E:273:ASN:O	1:E:276:THR:OG1	2.16	0.60
1:E:364:ASP:O	1:E:420:ASN:HA	2.02	0.60
1:L:436:LYS:HE3	5:L:705:SO4:O2	2.02	0.60
1:A:108:HIS:CD2	6:A:708:1PE:H221	2.36	0.60
1:L:362:LYS:HD3	1:L:362:LYS:N	2.16	0.60
3:I:703:TOD:O2	4:I:704:CO3:O2	2.19	0.60
1:C:328:LEU:HG	1:C:332:GLU:OE1	2.02	0.60
1:K:396:MET:CE	1:K:398:PHE:HE2	2.14	0.60
1:D:514:LEU:O	1:D:518:LYS:HG3	2.02	0.60
1:I:336:LEU:HD23	7:I:883:HOH:O	2.00	0.60
1:C:123:VAL:O	1:C:124:GLU:HG3	2.01	0.59
1:H:135:PRO:HA	1:H:194:SER:O	2.01	0.59
1:B:386:LYS:HB3	1:B:391:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:532:GLU:OE1	7:F:847:HOH:O	2.15	0.59
1:H:200:GLU:OE1	1:H:523:PRO:HD3	2.02	0.59
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.85	0.59
1:A:244:TYR:CA	1:A:288:TYR:CE1	2.80	0.59
1:G:160:GLU:O	1:G:163:GLU:OE1	2.20	0.59
1:H:360:LYS:HD2	7:H:858:HOH:O	2.02	0.59
1:C:316:GLU:CD	6:C:706:1PE:C23	2.69	0.59
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.85	0.59
1:E:249:ASP:OD2	1:E:251:ARG:NH2	2.31	0.59
1:G:175:PHE:N	1:G:187:VAL:O	2.35	0.58
1:L:395:LEU:O	1:L:398:PHE:HB3	2.03	0.58
1:C:411:TYR:HE1	6:C:707:1PE:H232	1.66	0.58
1:B:123:VAL:HG23	1:B:124:GLU:H	1.67	0.58
1:K:221:LYS:HG3	1:K:266:HIS:HB2	1.84	0.58
1:G:494:SER:HG	1:L:494:SER:HB3	1.65	0.58
1:C:331:LYS:HE3	1:C:334:GLU:OE2	2.04	0.58
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.86	0.58
3:B:1004:TOD:H5	3:B:1004:TOD:N1	2.16	0.58
1:E:338:MET:HE3	1:E:468:ASP:HB3	1.85	0.58
1:K:549:SER:N	1:K:550:SER:HA	2.18	0.58
1:F:440:ARG:NH2	7:F:849:HOH:O	2.36	0.58
1:G:381:GLY:O	1:G:458:THR:OG1	2.21	0.58
1:I:418:PRO:HG3	1:I:601:LEU:CD1	2.33	0.57
1:H:396:MET:SD	1:H:398:PHE:HE2	2.26	0.57
1:G:494:SER:OG	1:L:494:SER:CA	2.53	0.57
1:C:238:PHE:HD2	1:C:239:LEU:HD12	1.69	0.57
1:E:160:GLU:OE1	1:E:160:GLU:N	2.35	0.57
1:G:106:PRO:HD2	1:G:247:MET:HE1	1.86	0.57
1:C:171:THR:HG23	1:C:173:LYS:HZ3	1.70	0.57
1:H:457:ASN:C	1:H:458:THR:O	2.46	0.57
1:I:144:ILE:HG13	1:I:157:LEU:CD2	2.34	0.57
1:D:419:GLU:HG2	1:D:420:ASN:CG	2.29	0.57
1:E:273:ASN:O	1:E:277:TYR:CD2	2.58	0.57
1:D:324:GLU:HB2	1:D:358:THR:HB	1.87	0.57
1:K:312:ASN:CB	7:K:845:HOH:O	2.52	0.57
1:K:396:MET:SD	1:K:398:PHE:HE2	2.27	0.57
1:I:550:SER:OG	1:I:551:VAL:N	2.38	0.56
1:L:148:VAL:HG11	1:L:157:LEU:HD12	1.87	0.56
1:B:118:LYS:HE3	1:B:272:ASN:OD1	2.05	0.56
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.86	0.56
1:F:138:GLU:N	1:F:139:ASN:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:LYS:HD3	1:I:159:ASP:CG	2.24	0.56
1:J:337:LYS:HB3	1:J:448:SER:HA	1.87	0.56
1:C:171:THR:CG2	1:C:173:LYS:NZ	2.67	0.56
1:E:392:MET:HB3	1:E:395:LEU:HD22	1.87	0.56
1:I:143:LYS:CE	1:I:159:ASP:HB3	2.35	0.56
1:I:143:LYS:HZ1	1:I:159:ASP:HB3	1.71	0.56
1:C:254:SER:HA	1:C:257:LYS:HZ1	1.71	0.56
1:J:348:SER:N	7:J:873:HOH:O	2.39	0.56
1:D:462:GLY:N	4:D:703:CO3:O2	2.35	0.56
1:I:418:PRO:CG	1:I:601:LEU:HD11	2.36	0.56
1:A:214:LEU:HD21	1:A:222:LEU:HD22	1.87	0.56
1:C:536:THR:HG21	1:C:551:VAL:CG2	2.36	0.56
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.87	0.56
1:I:418:PRO:HG3	1:I:601:LEU:HD11	1.87	0.56
1:K:332:GLU:CD	1:K:332:GLU:N	2.63	0.56
1:L:148:VAL:HG23	1:L:148:VAL:O	2.05	0.56
1:C:411:TYR:OH	7:C:834:HOH:O	2.15	0.55
1:E:176:TYR:OH	1:E:217:ASN:OD1	2.16	0.55
1:C:376:ILE:HB	1:C:399:ASP:HB3	1.88	0.55
1:E:440:ARG:NH2	1:F:431:GLU:OE2	2.39	0.55
1:H:152:GLN:CG	1:H:178:PHE:O	2.52	0.55
1:H:395:LEU:O	1:H:398:PHE:CD2	2.59	0.55
1:I:396:MET:HE1	1:I:398:PHE:CE2	2.39	0.55
1:F:173:LYS:CB	1:F:189:TYR:HE2	2.19	0.55
1:L:127:LEU:HD11	1:L:129:ILE:HD11	1.89	0.55
1:L:360:LYS:O	1:L:362:LYS:NZ	2.31	0.55
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.89	0.55
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.88	0.55
1:K:329:GLY:C	1:K:332:GLU:OE1	2.50	0.55
1:E:227:GLU:OE1	7:E:850:HOH:O	2.18	0.54
1:E:392:MET:CB	1:E:395:LEU:HD22	2.37	0.54
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.89	0.54
1:I:244:TYR:HA	1:I:288:TYR:HE1	1.72	0.54
1:L:200:GLU:HG3	1:L:521:ASN:HB3	1.88	0.54
1:F:198:LEU:HD12	1:F:199:SER:H	1.73	0.54
1:J:192:CYS:HB3	1:J:198:LEU:HD11	1.90	0.54
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.35	0.54
1:C:331:LYS:CD	1:C:334:GLU:OE1	2.52	0.54
1:C:456:GLY:HA3	1:C:547:ILE:HD11	1.89	0.54
5:G:706:SO4:O2	1:J:164:LYS:HE3	2.07	0.54
1:H:458:THR:C	1:H:460:ALA:H	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:395:LEU:O	1:H:398:PHE:HD2	1.91	0.54
1:L:129:ILE:HG21	1:L:210:LEU:HD21	1.88	0.54
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.88	0.54
1:D:343:SER:O	1:D:439:TYR:HD2	1.90	0.54
1:K:395:LEU:O	1:K:398:PHE:CD2	2.61	0.54
1:F:498:SER:O	1:F:523:PRO:HG2	2.08	0.54
1:L:140:GLY:O	1:L:167:VAL:HG23	2.08	0.54
1:A:522:GLU:OE2	7:A:858:HOH:O	2.19	0.54
1:B:538:ASN:O	1:C:586:ARG:NH2	2.41	0.54
1:F:132:VAL:HG22	1:F:227:GLU:OE1	2.07	0.54
1:K:306:ASN:ND2	7:K:848:HOH:O	2.24	0.54
1:B:207:VAL:HG11	1:B:241:THR:HG22	1.89	0.53
1:C:273:ASN:O	1:C:276:THR:HG22	2.09	0.53
1:C:316:GLU:HG3	6:C:706:1PE:OH3	2.07	0.53
1:E:392:MET:O	1:E:395:LEU:HB2	2.07	0.53
1:L:148:VAL:HG21	1:L:154:SER:CA	2.39	0.53
1:G:494:SER:OG	1:L:494:SER:HA	2.09	0.53
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.89	0.53
1:J:386:LYS:HB2	1:J:393:ILE:CD1	2.36	0.53
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.90	0.53
1:F:386:LYS:HB3	1:F:391:SER:HB3	1.90	0.53
1:I:594:ARG:NH2	7:I:803:HOH:O	2.42	0.53
1:E:489:GLY:N	3:E:703:TOD:O4	2.30	0.53
1:K:395:LEU:O	1:K:398:PHE:HD2	1.92	0.53
1:F:117:ILE:CB	1:F:272:ASN:HD21	2.22	0.53
1:C:331:LYS:CE	1:C:334:GLU:OE1	2.56	0.53
1:K:138:GLU:HA	1:K:194:SER:OG	2.09	0.52
1:B:336:LEU:O	1:B:337:LYS:HB2	2.08	0.52
1:C:199:SER:HG	1:C:202:ASP:CG	2.17	0.52
1:I:210:LEU:HD21	1:I:222:LEU:HD21	1.91	0.52
1:I:217:ASN:OD1	1:I:219:LEU:HG	2.09	0.52
3:K:703:TOD:N1	4:K:704:CO3:O3	2.43	0.52
1:E:214:LEU:HD11	1:E:222:LEU:HD22	1.90	0.52
1:B:244:TYR:OH	1:B:588:PRO:O	2.28	0.52
1:C:199:SER:OG	1:C:202:ASP:CG	2.52	0.52
1:H:200:GLU:OE1	7:H:848:HOH:O	2.19	0.52
1:I:221:LYS:HD2	1:I:266:HIS:CB	2.40	0.52
1:A:463:ARG:NE	4:A:704:CO3:O1	2.29	0.52
1:C:171:THR:CG2	1:C:173:LYS:HZ3	2.21	0.52
1:L:200:GLU:HG2	1:L:237:PHE:CE2	2.44	0.52
1:A:244:TYR:N	1:A:288:TYR:CE1	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:LYS:HB3	1:E:391:SER:HB3	1.92	0.52
1:J:292:TYR:OH	7:J:850:HOH:O	2.10	0.52
1:D:117:ILE:HD12	1:D:271:ILE:C	2.35	0.52
1:B:198:LEU:O	1:B:199:SER:O	2.28	0.52
1:C:536:THR:HG21	1:C:551:VAL:HG21	1.91	0.52
1:D:144:ILE:HD11	1:D:162:MET:HE2	1.92	0.52
1:D:343:SER:O	1:D:439:TYR:CD2	2.63	0.52
1:J:399:ASP:OD1	1:J:486:THR:OG1	2.28	0.52
1:L:217:ASN:HB3	1:L:219:LEU:HG	1.91	0.52
1:C:112:VAL:HG22	1:C:267:LEU:HB3	1.92	0.52
1:A:155:GLU:CD	1:A:158:LYS:HD3	2.35	0.51
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.92	0.51
1:H:451:LYS:NZ	1:H:564:GLU:O	2.36	0.51
1:I:336:LEU:CD2	7:I:883:HOH:O	2.54	0.51
1:F:326:LYS:CE	1:F:328:LEU:HD21	2.39	0.51
1:I:198:LEU:HD22	1:I:202:ASP:HB3	1.92	0.51
1:A:431:GLU:OE2	1:C:440:ARG:NE	2.43	0.51
1:I:418:PRO:CB	1:I:601:LEU:CD1	2.86	0.51
1:I:512:LYS:HD3	1:I:603:ASP:C	2.36	0.51
1:K:100:PRO:O	1:K:251:ARG:NH1	2.36	0.51
1:C:150:ASP:OD1	1:C:179:ASN:HB2	2.10	0.51
1:G:368:LYS:HD3	1:G:422:GLU:HB3	1.92	0.51
1:H:195:VAL:O	1:H:195:VAL:CG2	2.54	0.51
1:H:321:LEU:O	1:H:322:ASN:HB3	2.09	0.51
1:I:439:TYR:CE1	1:I:458:THR:HB	2.46	0.51
1:L:134:ASN:OD1	1:L:134:ASN:C	2.53	0.51
1:H:459:ASP:C	1:H:461:GLU:H	2.17	0.51
1:A:440:ARG:NH1	7:A:824:HOH:O	2.43	0.51
1:B:199:SER:OG	1:B:200:GLU:CA	2.59	0.51
1:E:356:HIS:ND1	1:E:472:TYR:OH	2.39	0.51
1:J:135:PRO:HA	1:J:194:SER:O	2.10	0.51
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.93	0.51
1:K:374:LYS:HE3	1:K:487:LEU:HD12	1.92	0.51
1:E:338:MET:HE1	1:E:354:PHE:CE2	2.46	0.51
1:F:488:THR:HG21	1:F:555:SER:OG	2.10	0.50
1:H:532:GLU:CD	1:K:498:SER:HG	2.03	0.50
1:J:174:HIS:ND1	1:J:213:MET:HE2	2.26	0.50
1:L:213:MET:O	1:L:217:ASN:ND2	2.41	0.50
1:D:386:LYS:HB3	1:D:391:SER:HB3	1.92	0.50
1:D:397:LYS:NZ	7:D:847:HOH:O	2.03	0.50
1:E:507:GLU:O	1:E:511:ASN:ND2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:551:VAL:O	1:F:553:ALA:N	2.44	0.50
1:I:199:SER:OG	1:I:200:GLU:OE1	2.26	0.50
1:D:117:ILE:HD12	1:D:272:ASN:N	2.27	0.50
1:E:324:GLU:OE2	1:E:358:THR:CG2	2.59	0.50
1:L:554:SER:HA	7:L:839:HOH:O	2.11	0.50
1:I:360:LYS:HD3	1:I:422:GLU:OE1	2.12	0.50
1:K:460:ALA:HA	3:K:703:TOD:H2	1.92	0.50
1:C:376:ILE:O	1:C:399:ASP:HB3	2.12	0.50
1:F:200:GLU:OE1	7:F:860:HOH:O	2.19	0.50
1:H:148:VAL:CG2	1:H:154:SER:OG	2.59	0.50
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.93	0.50
1:H:320:LYS:HB3	6:H:705:1PE:H141	1.94	0.50
1:G:386:LYS:HB3	1:G:391:SER:HB3	1.94	0.49
1:H:376:ILE:HB	1:H:399:ASP:HB3	1.92	0.49
1:J:440:ARG:NH1	7:J:812:HOH:O	2.41	0.49
1:B:113:GLN:OE1	1:B:115:TYR:OH	2.26	0.49
1:H:108:HIS:HA	1:H:285:ARG:HH11	1.77	0.49
1:H:386:LYS:HB3	1:H:391:SER:HB3	1.94	0.49
1:I:510:ILE:HD13	1:I:526:TRP:NE1	2.27	0.49
1:B:216:ASP:HA	7:B:1148:HOH:O	2.11	0.49
1:B:419:GLU:CD	1:B:419:GLU:H	2.20	0.49
1:D:155:GLU:OE2	1:D:158:LYS:HD3	2.12	0.49
1:E:213:MET:O	1:E:217:ASN:ND2	2.39	0.49
1:H:532:GLU:HG3	1:K:201:ALA:HB1	1.93	0.49
1:F:395:LEU:HD11	1:F:581:TRP:CE2	2.46	0.49
1:I:200:GLU:HG2	1:I:201:ALA:H	1.77	0.49
1:J:198:LEU:HD12	1:J:228:ILE:HD12	1.95	0.49
1:C:198:LEU:HD22	1:C:202:ASP:HB3	1.93	0.49
1:C:379:ASP:HB2	1:C:399:ASP:OD1	2.11	0.49
1:I:376:ILE:HB	1:I:399:ASP:HB3	1.94	0.49
1:A:332:GLU:HG3	7:A:874:HOH:O	2.13	0.49
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.95	0.49
1:L:549:SER:N	1:L:550:SER:HA	2.27	0.49
1:F:221:LYS:HG3	1:F:266:HIS:CB	2.41	0.49
1:F:156:PHE:O	1:F:162:MET:HE3	2.12	0.49
1:F:332:GLU:O	1:F:335:GLU:HB2	2.13	0.49
1:G:316:GLU:HG3	6:G:708:1PE:C13	2.42	0.49
3:B:1004:TOD:N1	3:B:1004:TOD:C4	2.74	0.49
1:E:326:LYS:HE2	1:E:328:LEU:HD11	1.95	0.48
1:G:255:THR:O	1:G:256:ASP:C	2.56	0.48
1:H:396:MET:HA	1:H:398:PHE:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:413:VAL:HG11	1:J:423:ILE:HD12	1.95	0.48
1:I:396:MET:HE1	1:I:398:PHE:CZ	2.48	0.48
1:J:221:LYS:HG3	1:J:266:HIS:HB2	1.94	0.48
1:A:214:LEU:HD11	1:A:222:LEU:HD22	1.96	0.48
1:A:247:MET:HB2	1:A:288:TYR:OH	2.14	0.48
1:E:116:ASP:HA	1:E:271:ILE:O	2.13	0.48
1:L:176:TYR:OH	1:L:217:ASN:OD1	2.17	0.48
1:L:357:LEU:HD11	1:L:407:LEU:HD12	1.94	0.48
1:A:395:LEU:O	1:A:398:PHE:HD2	1.97	0.48
1:B:202:ASP:O	1:B:203:MET:C	2.50	0.48
1:C:230:VAL:HG12	1:C:234:LEU:HD23	1.96	0.48
1:H:88:VAL:HG22	1:H:308:VAL:HB	1.95	0.48
1:A:328:LEU:HD22	1:A:332:GLU:OE1	2.14	0.48
1:K:332:GLU:OE1	1:K:332:GLU:N	2.38	0.48
1:A:195:VAL:O	1:A:197:ASP:N	2.44	0.48
1:D:204:LYS:O	1:D:208:LEU:HD13	2.14	0.48
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.96	0.48
1:I:173:LYS:NZ	1:K:216:ASP:O	2.42	0.48
1:E:439:TYR:HD1	7:E:891:HOH:O	1.97	0.48
1:K:312:ASN:HB2	7:K:845:HOH:O	2.12	0.48
1:L:504:GLY:HA3	1:L:510:ILE:HD11	1.95	0.48
1:A:243:PHE:C	1:A:288:TYR:CE1	2.92	0.48
1:F:169:LEU:HD23	1:F:192:CYS:HA	1.95	0.48
1:F:355:ILE:N	7:F:812:HOH:O	2.45	0.48
1:I:396:MET:HA	1:I:398:PHE:CE2	2.49	0.48
1:F:213:MET:O	1:F:217:ASN:ND2	2.44	0.47
1:F:357:LEU:HB2	1:F:425:PHE:HB2	1.95	0.47
1:G:547:ILE:HG12	1:G:548:SER:N	2.26	0.47
1:C:124:GLU:HB3	1:C:179:ASN:ND2	2.29	0.47
1:E:392:MET:CE	1:E:395:LEU:CD2	2.89	0.47
1:H:178:PHE:HA	1:H:183:ASN:O	2.14	0.47
1:H:488:THR:HG21	1:H:555:SER:HA	1.95	0.47
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.96	0.47
1:I:209:SER:O	1:I:212:THR:OG1	2.31	0.47
1:J:395:LEU:HD21	1:J:581:TRP:CE2	2.50	0.47
1:K:214:LEU:HD11	1:K:222:LEU:HD22	1.95	0.47
1:E:392:MET:HB2	1:E:395:LEU:HD23	1.97	0.47
1:H:459:ASP:C	1:H:461:GLU:N	2.73	0.47
1:H:458:THR:C	1:H:460:ALA:N	2.73	0.47
1:J:395:LEU:O	1:J:398:PHE:CD2	2.67	0.47
1:K:462:GLY:CA	4:K:704:CO3:O2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:396:MET:HA	1:H:398:PHE:CD2	2.49	0.47
1:E:274:ALA:O	1:E:278:LYS:HG3	2.14	0.47
1:E:392:MET:CB	1:E:395:LEU:CD2	2.93	0.47
1:B:172:SER:HB2	1:B:213:MET:HE3	1.97	0.47
1:H:254:SER:OG	1:H:255:THR:N	2.31	0.47
1:L:214:LEU:HD11	1:L:222:LEU:HD22	1.96	0.47
1:E:271:ILE:HG12	1:E:272:ASN:O	2.16	0.46
1:K:341:TYR:CE1	1:K:428:ALA:HB1	2.50	0.46
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.97	0.46
1:C:123:VAL:O	1:C:124:GLU:CB	2.47	0.46
1:D:170:GLY:HA3	1:D:205:ARG:NH1	2.29	0.46
1:B:396:MET:SD	1:B:398:PHE:HE2	2.39	0.46
1:G:139:ASN:HB2	1:G:166:ASN:HB2	1.98	0.46
1:C:331:LYS:CE	1:C:334:GLU:OE2	2.63	0.46
1:D:497:THR:O	1:D:589:LYS:NZ	2.48	0.46
1:E:324:GLU:HG3	1:E:358:THR:HB	1.98	0.46
1:F:321:LEU:O	1:F:322:ASN:CB	2.63	0.46
1:J:179:ASN:OD1	1:J:183:ASN:N	2.29	0.46
1:E:459:ASP:O	3:E:703:TOD:O1	2.33	0.46
1:G:413:VAL:HG21	1:G:425:PHE:HZ	1.79	0.46
1:I:161:ASN:HA	1:I:164:LYS:NZ	2.30	0.46
1:C:205:ARG:HG2	7:C:839:HOH:O	2.14	0.46
1:C:205:ARG:O	7:C:839:HOH:O	2.21	0.46
1:D:533:TYR:O	1:D:536:THR:HG22	2.15	0.46
1:E:324:GLU:OE2	1:E:358:THR:CB	2.63	0.46
1:B:142:VAL:HG11	1:B:189:TYR:CE2	2.51	0.46
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.97	0.46
1:I:395:LEU:O	1:I:398:PHE:CD2	2.69	0.46
1:J:132:VAL:HG11	1:J:142:VAL:HG13	1.98	0.46
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.97	0.46
1:I:207:VAL:HG11	1:I:241:THR:HG22	1.96	0.46
1:K:173:LYS:HB2	1:K:189:TYR:HE1	1.80	0.46
1:J:247:MET:HE1	7:J:849:HOH:O	2.10	0.46
1:A:467:ALA:HB1	1:A:565:PHE:CE2	2.51	0.45
1:B:498:SER:O	1:B:523:PRO:HG2	2.16	0.45
1:J:338:MET:HE3	1:J:468:ASP:HB3	1.97	0.45
1:K:274:ALA:O	1:K:278:LYS:HG3	2.16	0.45
1:A:287:TYR:CD2	1:A:594:ARG:HG2	2.52	0.45
1:B:487:LEU:O	3:B:1004:TOD:N1	2.49	0.45
1:D:396:MET:HA	1:D:398:PHE:HD2	1.79	0.45
1:F:429:VAL:HG23	7:F:812:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:552:LYS:HB3	1:J:553:ALA:H	1.40	0.45
1:L:286:VAL:HG11	1:L:416:LEU:HG	1.98	0.45
1:A:287:TYR:OH	1:A:598:GLU:OE2	2.33	0.45
1:J:338:MET:HE2	1:J:341:TYR:CD2	2.52	0.45
1:H:525:TRP:CZ3	1:K:528:PRO:HB3	2.51	0.45
1:K:95:ASP:HA	1:K:96:PRO:HD3	1.73	0.45
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.99	0.45
1:C:344:VAL:HA	1:C:439:TYR:CE2	2.51	0.45
1:J:510:ILE:HD13	1:J:526:TRP:NE1	2.32	0.45
1:L:112:VAL:O	1:L:113:GLN:HG3	2.17	0.45
1:L:436:LYS:HG3	1:L:437:ASN:N	2.32	0.45
1:B:125:GLU:CG	1:B:221:LYS:HD3	2.47	0.45
1:K:204:LYS:O	1:K:208:LEU:HD13	2.17	0.45
1:A:467:ALA:HB1	1:A:565:PHE:CD2	2.51	0.45
1:D:301:PRO:HA	1:D:397:LYS:HD2	1.98	0.45
1:B:124:GLU:C	1:B:125:GLU:OE1	2.58	0.45
1:E:217:ASN:HB3	1:E:219:LEU:HG	1.99	0.45
1:J:550:SER:CB	1:J:551:VAL:HA	2.47	0.45
1:D:144:ILE:HD12	1:D:162:MET:HG3	1.98	0.44
1:F:236:ARG:NE	1:F:240:GLU:OE2	2.39	0.44
1:H:460:ALA:O	1:H:546:GLN:NE2	2.50	0.44
1:K:230:VAL:HG12	1:K:234:LEU:HD23	1.99	0.44
1:A:512:LYS:HD3	1:A:603:ASP:OD2	2.18	0.44
1:F:460:ALA:HB3	1:F:546:GLN:NE2	2.32	0.44
1:H:364:ASP:OD1	1:H:364:ASP:O	2.35	0.44
1:K:396:MET:HA	1:K:398:PHE:HD2	1.81	0.44
1:E:494:SER:HB3	7:E:903:HOH:O	2.18	0.44
1:E:498:SER:O	1:E:523:PRO:HG2	2.18	0.44
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.53	0.44
1:I:395:LEU:O	1:I:398:PHE:HD2	2.01	0.44
1:A:463:ARG:HE	4:A:704:CO3:C	2.25	0.44
1:G:244:TYR:OH	1:G:588:PRO:O	2.35	0.44
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.98	0.44
1:I:440:ARG:NH2	7:I:816:HOH:O	2.50	0.44
1:D:374:LYS:HB3	7:D:811:HOH:O	2.17	0.44
1:F:328:LEU:HA	1:F:328:LEU:HD23	1.83	0.44
1:I:519:THR:HG22	1:I:519:THR:O	2.17	0.44
1:J:165:PHE:CD2	1:J:173:LYS:HG3	2.53	0.44
1:A:380:SER:HA	1:A:393:ILE:HD11	1.99	0.44
1:E:150:ASP:OD1	1:E:179:ASN:HB2	2.17	0.44
1:F:138:GLU:N	1:F:139:ASN:CA	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:MET:O	1:G:165:PHE:CD2	2.71	0.44
1:H:129:ILE:HG21	1:H:190:VAL:HG23	2.00	0.44
1:I:157:LEU:HD12	1:I:162:MET:SD	2.58	0.44
1:K:108:HIS:HA	1:K:285:ARG:HH11	1.82	0.44
3:K:703:TOD:H4	3:K:703:TOD:C7	2.48	0.44
1:L:207:VAL:HG11	1:L:241:THR:HG22	2.00	0.44
1:G:255:THR:O	1:G:257:LYS:N	2.50	0.44
1:F:111:LYS:HA	1:F:111:LYS:HD3	1.74	0.44
1:G:316:GLU:HG3	6:G:708:1PE:H132	2.00	0.44
1:D:247:MET:CB	1:D:288:TYR:OH	2.66	0.44
1:I:199:SER:OG	1:I:200:GLU:CD	2.61	0.44
1:I:200:GLU:OE1	1:I:200:GLU:N	2.31	0.44
1:J:396:MET:SD	1:J:398:PHE:CE2	2.98	0.44
1:K:551:VAL:C	1:K:553:ALA:H	2.24	0.44
1:A:175:PHE:N	1:A:187:VAL:O	2.47	0.43
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.99	0.43
1:B:274:ALA:O	1:B:278:LYS:HG3	2.18	0.43
1:C:386:LYS:HB3	1:C:391:SER:HB2	2.00	0.43
1:F:326:LYS:HE3	1:F:328:LEU:CD2	2.46	0.43
1:G:328:LEU:HB2	1:G:354:PHE:HB3	2.00	0.43
1:E:376:ILE:HB	1:E:399:ASP:HB3	2.00	0.43
1:G:552:LYS:O	1:G:553:ALA:C	2.60	0.43
1:H:155:GLU:O	1:H:161:ASN:ND2	2.51	0.43
1:J:142:VAL:HG22	1:J:167:VAL:HG12	2.00	0.43
1:D:144:ILE:CD1	1:D:157:LEU:HD22	2.45	0.43
1:D:372:VAL:O	1:D:483:ASP:HA	2.18	0.43
7:H:874:HOH:O	1:K:532:GLU:CB	2.65	0.43
1:I:138:GLU:O	1:I:139:ASN:C	2.61	0.43
1:I:396:MET:CA	1:I:398:PHE:HD2	2.26	0.43
1:K:287:TYR:OH	1:K:598:GLU:OE2	2.33	0.43
1:B:142:VAL:CG1	1:B:167:VAL:CG1	2.81	0.43
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.84	0.43
1:D:396:MET:HA	1:D:398:PHE:CD2	2.53	0.43
1:E:204:LYS:O	1:E:208:LEU:HD13	2.18	0.43
1:G:462:GLY:CA	4:G:704:CO3:O2	2.64	0.43
1:I:161:ASN:O	1:I:164:LYS:CE	2.63	0.43
1:I:480:TYR:CD1	1:I:509:LEU:HD13	2.53	0.43
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.99	0.43
1:J:347:GLY:C	7:J:873:HOH:O	2.60	0.43
1:K:368:LYS:C	1:K:478:VAL:HG22	2.43	0.43
1:E:207:VAL:HG11	1:E:241:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:451:LYS:NZ	1:H:564:GLU:HB3	2.33	0.43
3:I:703:TOD:H9	3:I:703:TOD:H4	2.00	0.43
1:L:236:ARG:NH2	1:L:519:THR:O	2.51	0.43
1:L:343:SER:HA	1:L:346:LYS:HD3	1.99	0.43
1:A:321:LEU:HD11	1:A:411:TYR:HA	2.00	0.43
1:B:199:SER:HG	1:B:203:MET:H	1.67	0.43
1:B:471:VAL:CG1	1:B:475:LYS:HE3	2.46	0.43
1:F:321:LEU:O	1:F:322:ASN:HB3	2.18	0.43
1:G:316:GLU:OE1	6:G:708:1PE:H241	2.19	0.43
1:H:498:SER:O	1:H:523:PRO:HG2	2.17	0.43
1:C:509:LEU:O	1:C:513:ILE:HG12	2.19	0.43
1:D:107:ILE:HG21	1:D:288:TYR:CE2	2.53	0.43
1:E:198:LEU:HD22	1:E:202:ASP:HB3	2.00	0.43
1:G:366:LYS:HG2	1:G:420:ASN:HB3	2.00	0.43
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.99	0.43
1:B:117:ILE:CD1	1:B:272:ASN:N	2.82	0.43
1:B:481:ILE:O	1:B:571:TRP:HA	2.19	0.43
1:D:395:LEU:HD12	7:D:821:HOH:O	2.18	0.43
1:K:300:ALA:HA	1:K:301:PRO:HD3	1.93	0.43
1:L:209:SER:O	1:L:213:MET:HG3	2.19	0.43
1:B:549:SER:O	7:B:1167:HOH:O	2.21	0.43
1:C:253:LYS:HB2	1:C:257:LYS:HG2	2.01	0.43
1:C:574:ILE:HD13	1:C:595:LEU:HD21	2.00	0.43
1:D:117:ILE:HD11	1:D:271:ILE:CA	2.47	0.43
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.99	0.43
1:J:236:ARG:NH2	1:J:519:THR:O	2.46	0.43
1:C:204:LYS:HG2	1:C:241:THR:HG21	2.00	0.43
1:D:544:ILE:HD12	1:D:564:GLU:HG3	2.01	0.43
1:G:285:ARG:HD3	7:G:858:HOH:O	2.18	0.43
1:I:95:ASP:HA	1:I:96:PRO:HD3	1.86	0.43
1:K:441:PRO:HD2	1:L:378:PHE:CZ	2.54	0.43
1:B:195:VAL:O	1:B:196:ALA:C	2.62	0.42
1:B:507:GLU:O	1:B:511:ASN:ND2	2.48	0.42
1:C:124:GLU:HB3	1:C:179:ASN:HD22	1.84	0.42
1:D:338:MET:HE2	1:D:341:TYR:HD2	1.84	0.42
1:F:171:THR:HG22	1:F:189:TYR:OH	2.19	0.42
1:H:372:VAL:O	1:H:483:ASP:HA	2.19	0.42
1:J:232:LYS:HA	1:J:277:TYR:HE1	1.84	0.42
1:F:322:ASN:CB	1:K:160:GLU:OE2	2.67	0.42
1:J:441:PRO:HB2	1:K:394:ASP:HA	2.01	0.42
1:K:173:LYS:HB2	1:K:189:TYR:CE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:329:GLY:O	1:K:333:LEU:HG	2.19	0.42
1:G:195:VAL:O	1:G:196:ALA:C	2.62	0.42
1:G:252:PHE:CZ	1:G:301:PRO:HD2	2.54	0.42
7:G:891:HOH:O	1:J:164:LYS:HD3	2.19	0.42
1:K:329:GLY:N	1:K:332:GLU:OE1	2.52	0.42
1:A:463:ARG:HB3	4:A:704:CO3:O1	2.20	0.42
1:K:395:LEU:HD11	1:K:581:TRP:NE1	2.34	0.42
1:K:467:ALA:HB1	1:K:565:PHE:CE2	2.54	0.42
1:E:553:ALA:O	1:E:557:VAL:HG23	2.18	0.42
1:F:321:LEU:HA	1:F:321:LEU:HD23	1.77	0.42
1:K:142:VAL:HG11	1:K:162:MET:HE3	2.02	0.42
1:L:272:ASN:OD1	1:L:272:ASN:C	2.57	0.42
1:B:133:ASN:HB3	1:B:192:CYS:HB2	2.02	0.42
1:D:214:LEU:HD11	1:D:222:LEU:HD22	2.02	0.42
1:J:380:SER:HA	1:J:393:ILE:HD11	2.00	0.42
1:L:112:VAL:C	1:L:113:GLN:HG3	2.44	0.42
1:L:426:LEU:HD11	1:L:476:LEU:HD11	2.01	0.42
1:A:395:LEU:HD11	1:A:581:TRP:CD1	2.55	0.42
1:B:125:GLU:HG2	1:B:221:LYS:HD3	2.02	0.42
1:B:244:TYR:HA	1:B:288:TYR:HE1	1.85	0.42
1:C:200:GLU:HG3	1:C:521:ASN:O	2.20	0.42
1:C:208:LEU:O	1:C:212:THR:HG23	2.20	0.42
1:D:419:GLU:HG2	1:D:420:ASN:ND2	2.35	0.42
1:E:95:ASP:HA	1:E:96:PRO:HD3	1.93	0.42
1:H:117:ILE:HD13	1:H:117:ILE:HG21	1.74	0.42
1:H:137:LYS:O	1:H:194:SER:OG	2.34	0.42
1:C:331:LYS:CE	1:C:334:GLU:CD	2.92	0.42
1:E:273:ASN:O	1:E:277:TYR:HD2	2.01	0.42
1:J:300:ALA:HA	1:J:301:PRO:HD3	1.83	0.42
1:J:395:LEU:O	1:J:398:PHE:HD2	2.02	0.42
1:C:124:GLU:HG2	1:C:179:ASN:HD22	1.85	0.42
1:E:299:ALA:O	1:E:397:LYS:NZ	2.50	0.42
1:K:125:GLU:HA	1:K:185:VAL:HG12	2.01	0.42
1:L:418:PRO:HB3	1:L:601:LEU:HD12	2.02	0.42
1:A:326:LYS:HG3	1:A:328:LEU:HD23	2.02	0.42
1:B:124:GLU:O	1:B:185:VAL:HG12	2.19	0.42
1:D:198:LEU:HD12	1:D:202:ASP:HB3	2.01	0.42
1:L:129:ILE:HD13	1:L:129:ILE:HA	1.78	0.42
1:A:96:PRO:HG2	1:A:303:ASN:O	2.20	0.41
1:A:301:PRO:HB2	1:A:303:ASN:OD1	2.19	0.41
1:D:170:GLY:HA3	1:D:205:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:703:TOD:C8	3:F:703:TOD:H19	2.50	0.41
1:H:123:VAL:HG11	1:H:185:VAL:HG21	2.02	0.41
1:H:334:GLU:CD	1:I:93:SER:HB3	2.45	0.41
1:H:441:PRO:HB2	1:I:394:ASP:HA	2.02	0.41
1:K:399:ASP:OD1	1:K:486:THR:OG1	2.32	0.41
1:A:386:LYS:HB3	1:A:391:SER:HB3	2.01	0.41
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.55	0.41
1:H:255:THR:O	1:H:255:THR:OG1	2.35	0.41
1:L:328:LEU:HB2	1:L:354:PHE:HB3	2.02	0.41
1:C:331:LYS:HE2	1:C:334:GLU:OE1	2.20	0.41
1:F:168:LYS:HB3	1:F:171:THR:OG1	2.21	0.41
1:G:316:GLU:HG3	6:G:708:1PE:H131	2.02	0.41
1:G:528:PRO:HB3	1:L:525:TRP:CZ3	2.55	0.41
1:H:200:GLU:CG	1:H:201:ALA:N	2.83	0.41
1:H:494:SER:OG	1:H:495:LEU:N	2.52	0.41
1:J:207:VAL:HG11	1:J:241:THR:HG22	2.01	0.41
3:J:703:TOD:C8	3:J:703:TOD:H19	2.49	0.41
1:L:489:GLY:N	3:L:703:TOD:O4	2.33	0.41
1:B:106:PRO:HD2	1:B:247:MET:SD	2.61	0.41
1:F:95:ASP:HA	1:F:96:PRO:HD3	1.91	0.41
1:F:484:ILE:HD11	1:F:576:ILE:HG21	2.02	0.41
1:H:467:ALA:HB1	1:H:565:PHE:CD2	2.54	0.41
1:J:376:ILE:HB	1:J:399:ASP:HB3	2.02	0.41
1:K:212:THR:HG22	1:K:216:ASP:OD2	2.21	0.41
1:L:403:CYS:O	1:L:407:LEU:HD22	2.20	0.41
1:C:346:LYS:HB3	1:C:437:ASN:O	2.20	0.41
1:D:210:LEU:HD12	1:D:213:MET:HE3	2.02	0.41
1:F:355:ILE:HG13	7:F:812:HOH:O	2.20	0.41
1:H:546:GLN:HG3	1:H:547:ILE:HG23	2.01	0.41
1:K:548:SER:HB2	1:K:557:VAL:HG11	2.02	0.41
1:L:156:PHE:O	1:L:162:MET:HE3	2.21	0.41
1:A:195:VAL:O	1:A:195:VAL:HG12	2.21	0.41
1:A:369:ILE:HB	1:A:423:ILE:HD13	2.02	0.41
1:C:106:PRO:HD2	1:C:247:MET:HE1	2.02	0.41
1:C:168:LYS:HB3	1:C:171:THR:OG1	2.20	0.41
1:C:444:ILE:HA	1:C:453:ILE:O	2.20	0.41
1:G:142:VAL:HG21	1:G:189:TYR:CE2	2.56	0.41
1:G:395:LEU:HD23	1:G:395:LEU:HA	1.85	0.41
1:C:392:MET:HE3	1:C:392:MET:HB2	1.86	0.41
1:E:460:ALA:O	1:E:546:GLN:NE2	2.53	0.41
1:H:301:PRO:HB2	1:H:303:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:VAL:HG22	1:J:267:LEU:HB3	2.03	0.41
1:K:396:MET:HA	1:K:398:PHE:CD2	2.55	0.41
1:B:375:GLY:O	1:B:429:VAL:HA	2.20	0.41
1:D:121:CYS:HB2	1:D:148:VAL:HG12	2.02	0.41
1:D:285:ARG:O	1:D:288:TYR:HB3	2.21	0.41
1:D:346:LYS:HB3	1:D:437:ASN:O	2.21	0.41
1:H:230:VAL:C	1:H:231:ASP:O	2.64	0.41
1:B:394:ASP:OD1	1:B:395:LEU:HG	2.21	0.41
1:C:419:GLU:OE1	1:C:419:GLU:N	2.52	0.41
1:F:372:VAL:HG22	1:F:426:LEU:HD12	2.03	0.41
1:H:195:VAL:O	1:H:197:ASP:N	2.54	0.41
1:H:528:PRO:HD3	1:K:525:TRP:CE2	2.55	0.41
7:H:866:HOH:O	1:K:551:VAL:CB	2.68	0.41
1:I:418:PRO:CG	1:I:601:LEU:CD1	2.98	0.41
1:L:350:TYR:HA	1:L:351:PRO:HD3	1.93	0.41
1:A:159:ASP:HA	1:A:162:MET:HB2	2.03	0.41
1:E:392:MET:SD	1:E:395:LEU:HD22	2.60	0.41
1:I:328:LEU:HA	1:I:332:GLU:OE1	2.21	0.41
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.56	0.41
1:D:103:TYR:HB3	6:D:705:1PE:H241	2.03	0.40
1:D:244:TYR:HA	1:D:288:TYR:CE1	2.49	0.40
1:E:494:SER:CB	7:E:903:HOH:O	2.70	0.40
1:F:424:HIS:CG	1:F:476:LEU:HD13	2.56	0.40
1:L:372:VAL:O	1:L:483:ASP:HA	2.21	0.40
1:C:229:ASN:OD1	1:C:230:VAL:N	2.53	0.40
1:E:520:SER:HB3	1:E:598:GLU:HG3	2.03	0.40
1:F:116:ASP:HA	1:F:271:ILE:O	2.21	0.40
1:C:536:THR:HG21	1:C:551:VAL:HG23	2.04	0.40
1:D:162:MET:C	1:D:164:LYS:N	2.80	0.40
1:D:378:PHE:CZ	1:F:441:PRO:HD2	2.57	0.40
1:G:129:ILE:HA	1:G:188:GLY:O	2.21	0.40
1:G:159:ASP:O	1:G:163:GLU:HG3	2.21	0.40
1:K:392:MET:HE3	1:K:392:MET:HB2	1.94	0.40
1:B:174:HIS:CE1	1:B:213:MET:HG2	2.57	0.40
1:F:483:ASP:OD2	1:F:571:TRP:NE1	2.48	0.40
1:G:441:PRO:HD2	1:H:378:PHE:CZ	2.57	0.40
1:H:120:GLY:HA3	1:H:149:ASN:OD1	2.22	0.40
1:I:386:LYS:HB3	1:I:391:SER:HB3	2.03	0.40
1:L:112:VAL:HA	1:L:267:LEU:O	2.22	0.40
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.96	0.40
1:E:392:MET:HB2	1:E:395:LEU:CD2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:321:LEU:HD11	1:I:411:TYR:HA	2.03	0.40
1:J:321:LEU:O	1:J:322:ASN:HB2	2.21	0.40
1:K:396:MET:CE	1:K:398:PHE:CE2	3.01	0.40
1:K:431:GLU:HG2	1:K:433:MET:CG	2.48	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:OD1	1:G:278:LYS:NZ[2_564]	1.65	0.55
1:J:229:ASN:ND2	1:K:273:ASN:ND2[4_456]	2.12	0.08

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	511/519 (98%)	492 (96%)	16 (3%)	3 (1%)	21	42
1	B	504/519 (97%)	479 (95%)	19 (4%)	6 (1%)	10	25
1	C	513/519 (99%)	499 (97%)	12 (2%)	2 (0%)	30	52
1	D	507/519 (98%)	490 (97%)	11 (2%)	6 (1%)	10	25
1	E	503/519 (97%)	489 (97%)	10 (2%)	4 (1%)	16	35
1	F	501/519 (96%)	478 (95%)	19 (4%)	4 (1%)	16	35
1	G	517/519 (100%)	491 (95%)	19 (4%)	7 (1%)	9	22
1	H	504/519 (97%)	480 (95%)	18 (4%)	6 (1%)	10	25
1	I	511/519 (98%)	489 (96%)	17 (3%)	5 (1%)	12	30
1	J	507/519 (98%)	486 (96%)	13 (3%)	8 (2%)	7	18
1	K	503/519 (97%)	486 (97%)	15 (3%)	2 (0%)	30	52
1	L	502/519 (97%)	484 (96%)	15 (3%)	3 (1%)	21	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6083/6228 (98%)	5843 (96%)	184 (3%)	56 (1%)	14	33

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	GLU
1	A	139	ASN
1	B	196	ALA
1	B	199	SER
1	C	196	ALA
1	D	322	ASN
1	D	553	ALA
1	E	139	ASN
1	F	124	GLU
1	F	322	ASN
1	F	552	LYS
1	G	163	GLU
1	G	196	ALA
1	G	256	ASP
1	G	257	LYS
1	H	196	ALA
1	H	231	ASP
1	I	124	GLU
1	I	139	ASN
1	I	196	ALA
1	I	551	VAL
1	J	137	LYS
1	J	139	ASN
1	J	196	ALA
1	J	391	SER
1	K	139	ASN
1	K	552	LYS
1	L	196	ALA
1	B	273	ASN
1	C	552	LYS
1	D	124	GLU
1	D	139	ASN
1	E	124	GLU
1	E	273	ASN
1	G	259	VAL
1	H	363	GLY
1	I	602	ASN

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Mol	Chain	Res	Type
1	L	124	GLU
1	B	124	GLU
1	D	196	ALA
1	G	552	LYS
1	G	553	ALA
1	H	458	THR
1	H	459	ASP
1	E	182	LYS
1	H	123	VAL
1	J	553	ALA
1	B	119	GLY
1	F	551	VAL
1	J	551	VAL
1	L	417	LYS
1	B	363	GLY
1	D	551	VAL
1	J	136	GLY
1	J	363	GLY
1	A	363	GLY

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	414/447 (93%)	409 (99%)	5 (1%)	63	82
1	B	396/447 (89%)	391 (99%)	5 (1%)	61	81
1	C	417/447 (93%)	412 (99%)	5 (1%)	63	82
1	D	411/447 (92%)	410 (100%)	1 (0%)	87	95
1	E	411/447 (92%)	409 (100%)	2 (0%)	81	91
1	F	379/447 (85%)	370 (98%)	9 (2%)	43	70
1	G	424/447 (95%)	419 (99%)	5 (1%)	63	82
1	H	402/447 (90%)	395 (98%)	7 (2%)	53	77
1	I	412/447 (92%)	402 (98%)	10 (2%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	402/447 (90%)	396 (98%)	6 (2%)	57	79
1	K	409/447 (92%)	404 (99%)	5 (1%)	63	82
1	L	391/447 (88%)	380 (97%)	11 (3%)	38	67
All	All	4868/5364 (91%)	4797 (98%)	71 (2%)	57	79

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
1	A	436	LYS
1	A	508	GLU
1	A	511	ASN
1	A	602	ASN
1	B	125	GLU
1	B	200	GLU
1	B	419	GLU
1	B	436	LYS
1	B	515	GLN
1	C	200	GLU
1	C	204	LYS
1	C	331	LYS
1	C	335	GLU
1	C	552	LYS
1	D	197	ASP
1	E	113	GLN
1	E	436	LYS
1	F	111	LYS
1	F	113	GLN
1	F	122	ASN
1	F	142	VAL
1	F	177	MET
1	F	195	VAL
1	F	200	GLU
1	F	332	GLU
1	F	419	GLU
1	G	171	THR
1	G	200	GLU
1	G	324	GLU
1	G	419	GLU
1	G	547	ILE
1	H	117	ILE

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Mol	Chain	Res	Type
1	H	152	GLN
1	H	155	GLU
1	H	231	ASP
1	H	275	ASP
1	H	419	GLU
1	H	546	GLN
1	I	121	CYS
1	I	157	LEU
1	I	164	LYS
1	I	185	VAL
1	I	204	LYS
1	I	331	LYS
1	I	360	LYS
1	I	365	VAL
1	I	478	VAL
1	I	551	VAL
1	J	111	LYS
1	J	232	LYS
1	J	335	GLU
1	J	346	LYS
1	J	395	LEU
1	J	463	ARG
1	K	332	GLU
1	K	374	LYS
1	K	436	LYS
1	K	478	VAL
1	K	518	LYS
1	L	86	SER
1	L	114	VAL
1	L	134	ASN
1	L	167	VAL
1	L	200	GLU
1	L	223	THR
1	L	276	THR
1	L	346	LYS
1	L	362	LYS
1	L	407	LEU
1	L	515	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	ASN
1	A	531	ASN
1	B	104	ASN
1	B	122	ASN
1	B	420	ASN
1	D	122	ASN
1	D	166	ASN
1	D	181	ASN
1	D	183	ASN
1	D	229	ASN
1	D	266	HIS
1	D	322	ASN
1	D	420	ASN
1	D	521	ASN
1	E	602	ASN
1	F	108	HIS
1	F	215	HIS
1	F	272	ASN
1	G	174	HIS
1	G	424	HIS
1	G	437	ASN
1	H	122	ASN
1	I	420	ASN
1	J	181	ASN
1	J	266	HIS
1	J	437	ASN
1	J	521	ASN
1	K	174	HIS
1	K	567	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 70 ligands modelled in this entry, 24 are monoatomic - leaving 46 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
6	1PE	G	707	-	8,8,15	0.57	0	7,7,14	0.38	0
5	SO4	C	705	-	4,4,4	0.24	0	6,6,6	0.07	0
6	1PE	D	705	-	9,9,15	0.46	0	8,8,14	0.30	0
4	CO3	J	704	-	3,3,3	0.48	0	2,3,3	1.42	0
3	TOD	A	703	2	23,24,24	2.05	2 (8%)	27,32,32	1.02	2 (7%)
3	TOD	F	703	2	23,24,24	2.04	4 (17%)	27,32,32	1.72	4 (14%)
5	SO4	B	1005	-	4,4,4	0.22	0	6,6,6	0.13	0
6	1PE	E	707	-	11,11,15	0.39	0	10,10,14	0.52	0
6	1PE	G	708	-	8,8,15	0.71	0	7,7,14	0.65	0
4	CO3	I	704	-	3,3,3	0.48	0	2,3,3	1.39	0
5	SO4	E	706	-	4,4,4	1.04	0	6,6,6	1.39	1 (16%)
4	CO3	L	704	-	3,3,3	0.50	0	2,3,3	1.39	0
4	CO3	C	704	-	3,3,3	0.47	0	2,3,3	1.40	0
4	CO3	B	1001	-	3,3,3	0.50	0	2,3,3	2.25	2 (100%)
6	1PE	B	1006	-	6,6,15	0.44	0	5,5,14	0.66	0
3	TOD	I	703	2	23,24,24	1.97	2 (8%)	27,32,32	1.19	6 (22%)
6	1PE	C	706	-	12,12,15	0.56	0	11,11,14	0.49	0
5	SO4	G	706	-	4,4,4	0.20	0	6,6,6	0.23	0
3	TOD	H	703	2	12,13,24	1.02	1 (8%)	13,17,32	0.99	1 (7%)
5	SO4	G	705	-	4,4,4	0.25	0	6,6,6	0.11	0
6	1PE	H	705	-	9,9,15	0.53	0	8,8,14	0.55	0
3	TOD	L	703	2	23,24,24	1.96	2 (8%)	27,32,32	1.41	5 (18%)
6	1PE	A	708	-	8,8,15	0.52	0	7,7,14	0.24	0
5	SO4	L	706	-	4,4,4	0.24	0	6,6,6	0.07	0
4	CO3	G	704	-	3,3,3	0.49	0	2,3,3	1.40	0
5	SO4	E	705	-	4,4,4	0.22	0	6,6,6	0.10	0
5	SO4	D	704	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	I	705	-	4,4,4	0.23	0	6,6,6	0.16	0
5	SO4	L	705	-	4,4,4	0.29	0	6,6,6	0.13	0
6	1PE	C	707	-	8,8,15	0.53	0	7,7,14	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CO3	H	704	-	3,3,3	0.49	0	2,3,3	1.40	0
3	TOD	E	703	2	13,14,24	0.97	1 (7%)	14,18,32	1.18	1 (7%)
4	CO3	D	703	-	3,3,3	0.51	0	2,3,3	1.40	0
4	CO3	A	704	-	3,3,3	0.48	0	2,3,3	1.40	0
3	TOD	J	703	2	21,22,24	1.39	2 (9%)	25,29,32	1.62	4 (16%)
3	TOD	B	1004	2	23,24,24	2.21	5 (21%)	27,32,32	1.84	8 (29%)
4	CO3	E	704	-	3,3,3	0.48	0	2,3,3	1.40	0
5	SO4	A	706	-	4,4,4	0.23	0	6,6,6	0.08	0
3	TOD	C	703	2	15,16,24	1.73	2 (13%)	17,21,32	2.22	4 (23%)
3	TOD	G	703	2	21,22,24	1.16	1 (4%)	25,29,32	1.65	7 (28%)
5	SO4	A	705	-	4,4,4	0.26	0	6,6,6	0.09	0
4	CO3	K	704	-	3,3,3	0.49	0	2,3,3	1.41	0
6	1PE	D	706	-	9,9,15	0.74	0	8,8,14	0.80	0
3	TOD	K	703	2	21,22,24	1.21	1 (4%)	25,29,32	2.13	5 (20%)
4	CO3	F	704	-	3,3,3	0.49	0	2,3,3	1.40	0
5	SO4	A	707	-	4,4,4	0.25	0	6,6,6	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	D	705	-	-	6/7/7/13	-
3	TOD	A	703	2	-	4/30/30/30	0/1/1/1
3	TOD	F	703	2	-	5/30/30/30	0/1/1/1
6	1PE	E	707	-	-	0/9/9/13	-
6	1PE	G	708	-	-	4/6/6/13	-
6	1PE	B	1006	-	-	2/4/4/13	-
3	TOD	I	703	2	-	6/30/30/30	0/1/1/1
6	1PE	C	706	-	-	2/10/10/13	-
3	TOD	H	703	2	-	4/18/18/30	-
6	1PE	H	705	-	-	2/7/7/13	-
3	TOD	L	703	2	-	4/30/30/30	0/1/1/1
6	1PE	A	708	-	-	2/6/6/13	-
6	1PE	C	707	-	-	4/6/6/13	-
3	TOD	E	703	2	-	2/20/20/30	-
3	TOD	J	703	2	-	5/26/26/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TOD	B	1004	2	-	7/30/30/30	0/1/1/1
3	TOD	C	703	2	-	4/22/22/30	-
3	TOD	G	703	2	-	6/26/26/30	0/1/1/1
6	1PE	D	706	-	-	3/7/7/13	-
3	TOD	K	703	2	-	7/26/26/30	0/1/1/1
6	1PE	G	707	-	-	6/6/6/13	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	TOD	C10-C9	-8.62	1.39	1.52
3	L	703	TOD	C10-C9	-8.38	1.39	1.52
3	B	1004	TOD	C10-C9	-7.63	1.41	1.52
3	F	703	TOD	C10-C9	-7.60	1.41	1.52
3	I	703	TOD	C10-C9	-7.50	1.41	1.52
3	B	1004	TOD	O2-N1	5.63	1.53	1.40
3	C	703	TOD	O2-N1	5.17	1.52	1.40
3	K	703	TOD	C10-C9	-4.90	1.39	1.52
3	J	703	TOD	C10-C9	-4.60	1.40	1.52
3	G	703	TOD	C10-C9	-4.58	1.40	1.52
3	I	703	TOD	O2-N1	4.33	1.50	1.40
3	C	703	TOD	C10-C9	-3.87	1.39	1.51
3	F	703	TOD	O2-N1	3.74	1.49	1.40
3	J	703	TOD	O2-N1	3.70	1.48	1.40
3	E	703	TOD	O2-N1	2.68	1.46	1.40
3	L	703	TOD	C5-C6	-2.66	1.51	1.54
3	F	703	TOD	C5-C8	2.62	1.56	1.51
3	B	1004	TOD	C9-N2	2.43	1.50	1.46
3	F	703	TOD	C9-N2	2.34	1.50	1.46
3	H	703	TOD	C5-C8	2.15	1.54	1.51
3	B	1004	TOD	O6-C16	2.08	1.37	1.30
3	A	703	TOD	C5-C8	2.03	1.55	1.51
3	B	1004	TOD	C5-C8	2.03	1.55	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	703	TOD	C4-C5-C8	-5.99	92.44	110.98
3	K	703	TOD	C5-C8-N2	-5.65	109.17	116.01
3	C	703	TOD	C4-C5-C8	-5.58	93.69	110.98
3	J	703	TOD	C5-C8-N2	-5.03	109.91	116.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	703	TOD	C9-N2-C8	4.64	130.69	121.18
3	C	703	TOD	C5-C8-N2	-4.37	110.72	116.01
3	F	703	TOD	C5-C8-N2	-4.15	110.99	116.01
3	G	703	TOD	C5-C4-C2	-4.03	109.35	115.82
3	K	703	TOD	C6-C5-C8	-4.00	98.81	108.17
3	E	703	TOD	C5-C4-C2	-3.93	109.51	115.82
3	B	1004	TOD	O3-C6-C7	-3.92	102.44	110.63
3	C	703	TOD	C6-C5-C8	-3.73	99.43	108.17
3	B	1004	TOD	C5-C4-C2	3.63	121.65	115.82
3	B	1004	TOD	O4-C8-C5	-3.51	117.47	121.67
3	B	1004	TOD	C6-C5-C8	3.27	115.84	108.17
3	G	703	TOD	C10-C9-N2	3.26	119.13	111.38
3	K	703	TOD	C5-C4-C2	3.12	120.84	115.82
5	E	706	SO4	O4-S-O3	3.06	125.39	108.54
3	K	703	TOD	O4-C8-N2	3.05	128.43	122.96
3	F	703	TOD	C10-C9-N2	2.88	120.02	112.75
3	L	703	TOD	C10-C9-C16	2.85	114.90	109.44
3	F	703	TOD	C6-C5-C8	2.83	114.81	108.17
3	J	703	TOD	C10-C9-N2	2.75	117.92	111.38
3	L	703	TOD	O4-C8-C5	-2.69	118.45	121.67
3	I	703	TOD	C3-C2-C4	2.66	120.65	111.08
3	A	703	TOD	O4-C8-C5	-2.61	118.55	121.67
3	L	703	TOD	C5-C8-N2	2.57	119.12	116.01
3	B	1004	TOD	C9-N2-C8	2.56	126.43	121.18
3	G	703	TOD	C6-C7-N1	2.49	119.22	116.11
3	J	703	TOD	O4-C8-N2	2.48	127.40	122.96
3	H	703	TOD	C6-C5-C8	2.45	113.92	108.17
3	C	703	TOD	C5-C4-C2	2.42	119.71	115.82
3	B	1004	TOD	C15-C10-C9	-2.41	116.91	120.78
4	B	1001	CO3	O3-C-O1	-2.40	113.53	119.68
3	A	703	TOD	C3-C2-C4	2.37	119.61	111.08
3	J	703	TOD	C4-C5-C8	2.32	118.17	110.98
3	L	703	TOD	C3-C2-C4	2.32	119.42	111.08
3	L	703	TOD	C10-C9-N2	-2.32	106.91	112.75
3	I	703	TOD	C9-N2-C8	2.27	125.83	121.18
3	G	703	TOD	C5-C8-N2	-2.27	113.26	116.01
3	B	1004	TOD	O3-C6-C5	-2.24	105.58	110.63
3	B	1004	TOD	C4-C5-C8	2.23	117.88	110.98
3	I	703	TOD	C6-C7-N1	2.21	118.87	116.11
3	G	703	TOD	C9-N2-C8	2.19	125.94	122.91
3	I	703	TOD	C4-C5-C8	-2.18	104.22	110.98
3	I	703	TOD	O4-C8-C5	-2.14	119.11	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	703	TOD	C6-C5-C8	-2.13	103.18	108.17
3	G	703	TOD	C16-C9-C10	-2.13	107.23	112.22
3	I	703	TOD	C6-C5-C8	2.10	113.08	108.17
4	B	1001	CO3	O2-C-O1	2.08	124.99	119.68

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1004	TOD	C4-C5-C6-C7
3	B	1004	TOD	C4-C5-C6-O3
3	B	1004	TOD	C10-C9-N2-C8
3	C	703	TOD	C4-C5-C6-O3
3	C	703	TOD	O3-C6-C7-O1
3	C	703	TOD	O3-C6-C7-N1
3	F	703	TOD	C10-C9-N2-C8
3	H	703	TOD	O3-C6-C7-O1
3	I	703	TOD	C10-C9-N2-C8
3	K	703	TOD	C4-C5-C6-O3
3	L	703	TOD	C3-C2-C4-C5
3	I	703	TOD	C3-C2-C4-C5
6	D	706	1PE	OH5-C14-C24-OH4
6	G	707	1PE	OH5-C14-C24-OH4
6	G	708	1PE	OH4-C13-C23-OH3
6	C	707	1PE	OH4-C13-C23-OH3
6	D	705	1PE	OH5-C14-C24-OH4
6	B	1006	1PE	OH5-C14-C24-OH4
3	A	703	TOD	C3-C2-C4-C5
3	J	703	TOD	C10-C9-N2-C8
6	A	708	1PE	OH4-C13-C23-OH3
6	G	707	1PE	OH4-C13-C23-OH3
3	K	703	TOD	C16-C9-N2-C8
3	L	703	TOD	C1-C2-C4-C5
6	D	705	1PE	OH4-C13-C23-OH3
3	A	703	TOD	C16-C9-N2-C8
3	A	703	TOD	O3-C6-C7-O1
3	A	703	TOD	O3-C6-C7-N1
3	H	703	TOD	O3-C6-C7-N1
3	J	703	TOD	O3-C6-C7-N1
3	K	703	TOD	O3-C6-C7-O1
3	K	703	TOD	O3-C6-C7-N1
3	L	703	TOD	O3-C6-C7-N1

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Mol	Chain	Res	Type	Atoms
6	G	708	1PE	OH5-C14-C24-OH4
3	G	703	TOD	C10-C9-N2-C8
3	F	703	TOD	O6-C16-C9-N2
3	F	703	TOD	O3-C6-C7-O1
3	F	703	TOD	O3-C6-C7-N1
3	J	703	TOD	O3-C6-C7-O1
3	L	703	TOD	O3-C6-C7-O1
6	C	706	1PE	C12-C22-OH3-C23
6	G	707	1PE	C24-C14-OH5-C25
6	C	707	1PE	C12-C22-OH3-C23
3	I	703	TOD	C11-C10-C9-C16
6	G	707	1PE	C13-C23-OH3-C22
6	D	705	1PE	C23-C13-OH4-C24
3	I	703	TOD	C15-C10-C9-C16
6	G	708	1PE	C14-C24-OH4-C13
6	C	707	1PE	OH5-C14-C24-OH4
6	C	706	1PE	C13-C23-OH3-C22
6	D	706	1PE	C13-C23-OH3-C22
3	G	703	TOD	O3-C6-C7-O1
3	G	703	TOD	O3-C6-C7-N1
3	I	703	TOD	O3-C6-C7-O1
3	I	703	TOD	O3-C6-C7-N1
3	E	703	TOD	C5-C6-C7-O1
6	A	708	1PE	C13-C23-OH3-C22
3	C	703	TOD	C4-C5-C6-C7
3	K	703	TOD	C4-C5-C6-C7
3	H	703	TOD	C6-C5-C8-N2
6	G	707	1PE	C23-C13-OH4-C24
6	D	705	1PE	C13-C23-OH3-C22
3	G	703	TOD	C16-C9-N2-C8
3	F	703	TOD	O5-C16-C9-N2
6	D	706	1PE	C12-C22-OH3-C23
6	D	705	1PE	C12-C22-OH3-C23
3	K	703	TOD	C11-C10-C9-C16
3	E	703	TOD	C5-C6-C7-N1
6	H	705	1PE	C12-C22-OH3-C23
3	K	703	TOD	C15-C10-C9-C16
6	H	705	1PE	OH5-C14-C24-OH4
3	B	1004	TOD	C8-C5-C6-O3
3	J	703	TOD	C15-C10-C9-C16
6	B	1006	1PE	C24-C14-OH5-C25
3	B	1004	TOD	O3-C6-C7-O1

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Mol	Chain	Res	Type	Atoms
3	J	703	TOD	C11-C10-C9-C16
6	D	705	1PE	C24-C14-OH5-C25
6	G	707	1PE	C14-C24-OH4-C13
3	B	1004	TOD	C11-C10-C9-C16
6	C	707	1PE	C23-C13-OH4-C24
3	G	703	TOD	C15-C10-C9-C16
3	B	1004	TOD	C3-C2-C4-C5
3	G	703	TOD	C11-C10-C9-C16
3	H	703	TOD	C6-C5-C8-O4
6	G	708	1PE	C12-C22-OH3-C23

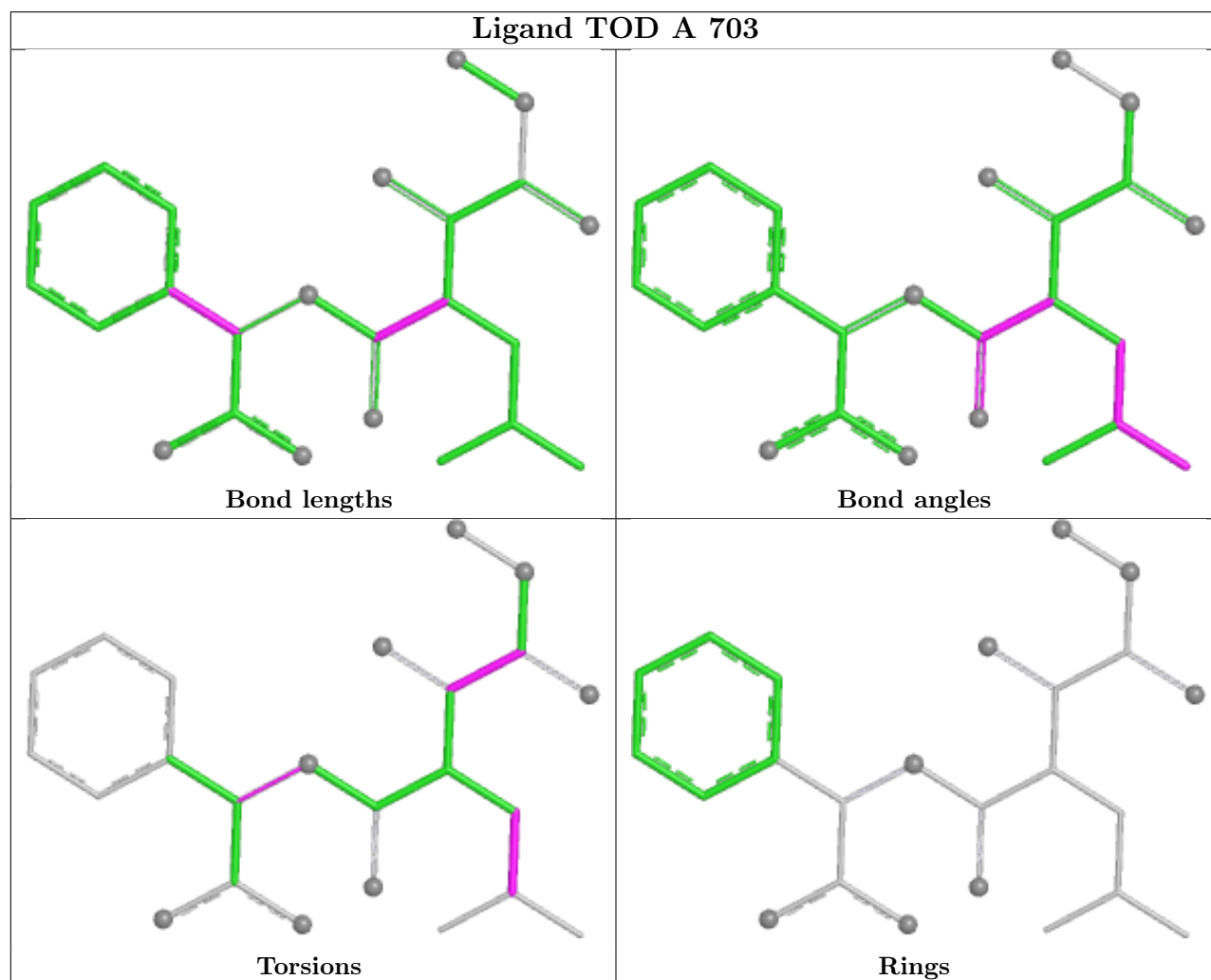
There are no ring outliers.

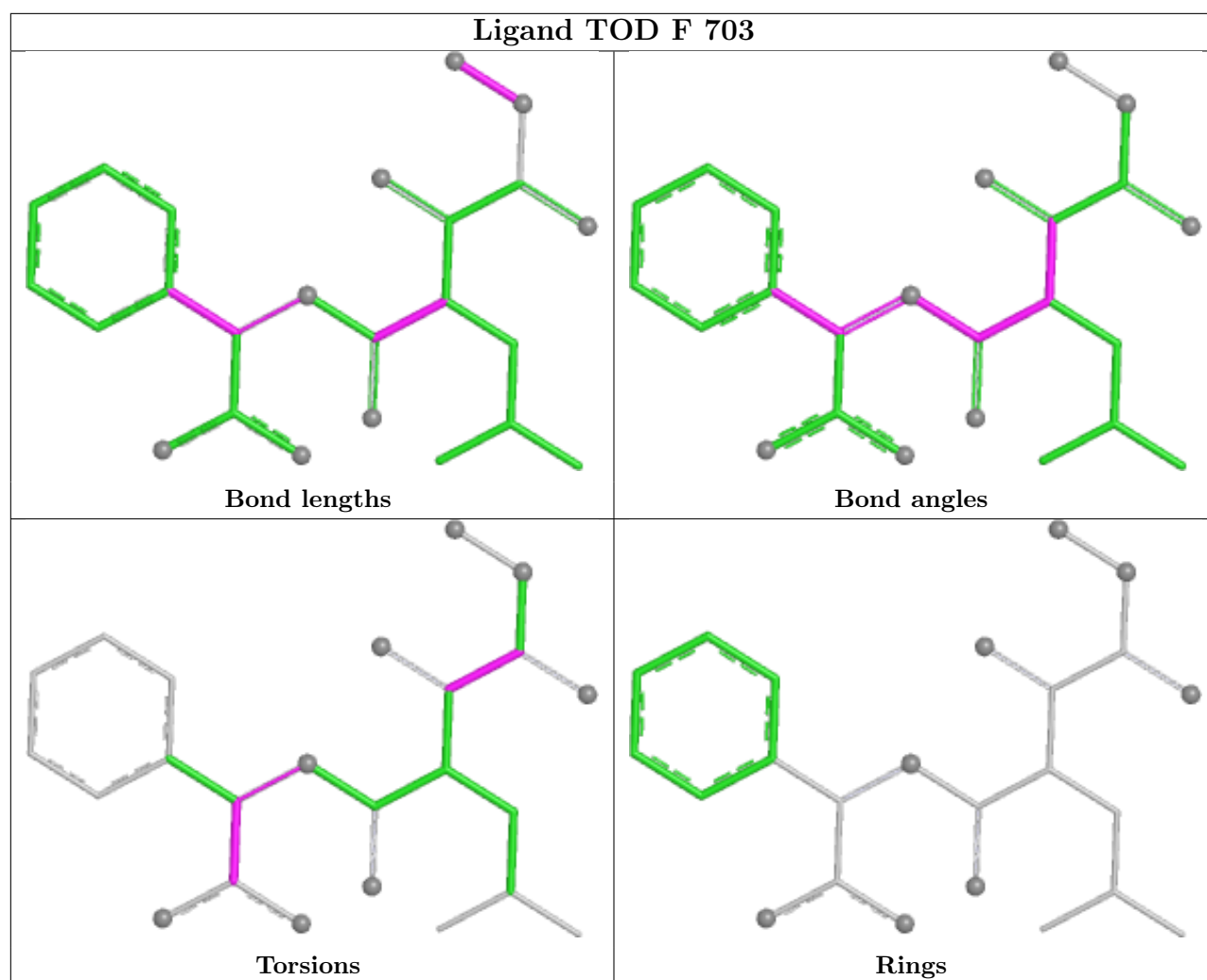
25 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	705	SO4	1	0
6	D	705	1PE	1	0
4	J	704	CO3	3	0
3	F	703	TOD	1	0
6	G	708	1PE	4	0
4	I	704	CO3	1	0
3	I	703	TOD	2	0
6	C	706	1PE	11	0
5	G	706	SO4	1	0
6	H	705	1PE	1	0
3	L	703	TOD	1	0
6	A	708	1PE	1	0
4	G	704	CO3	2	0
5	D	704	SO4	1	0
5	L	705	SO4	1	0
6	C	707	1PE	1	0
4	H	704	CO3	1	0
3	E	703	TOD	3	0
4	D	703	CO3	1	0
4	A	704	CO3	3	0
3	J	703	TOD	2	0
3	B	1004	TOD	4	0
4	K	704	CO3	3	0
6	D	706	1PE	4	0
3	K	703	TOD	3	0

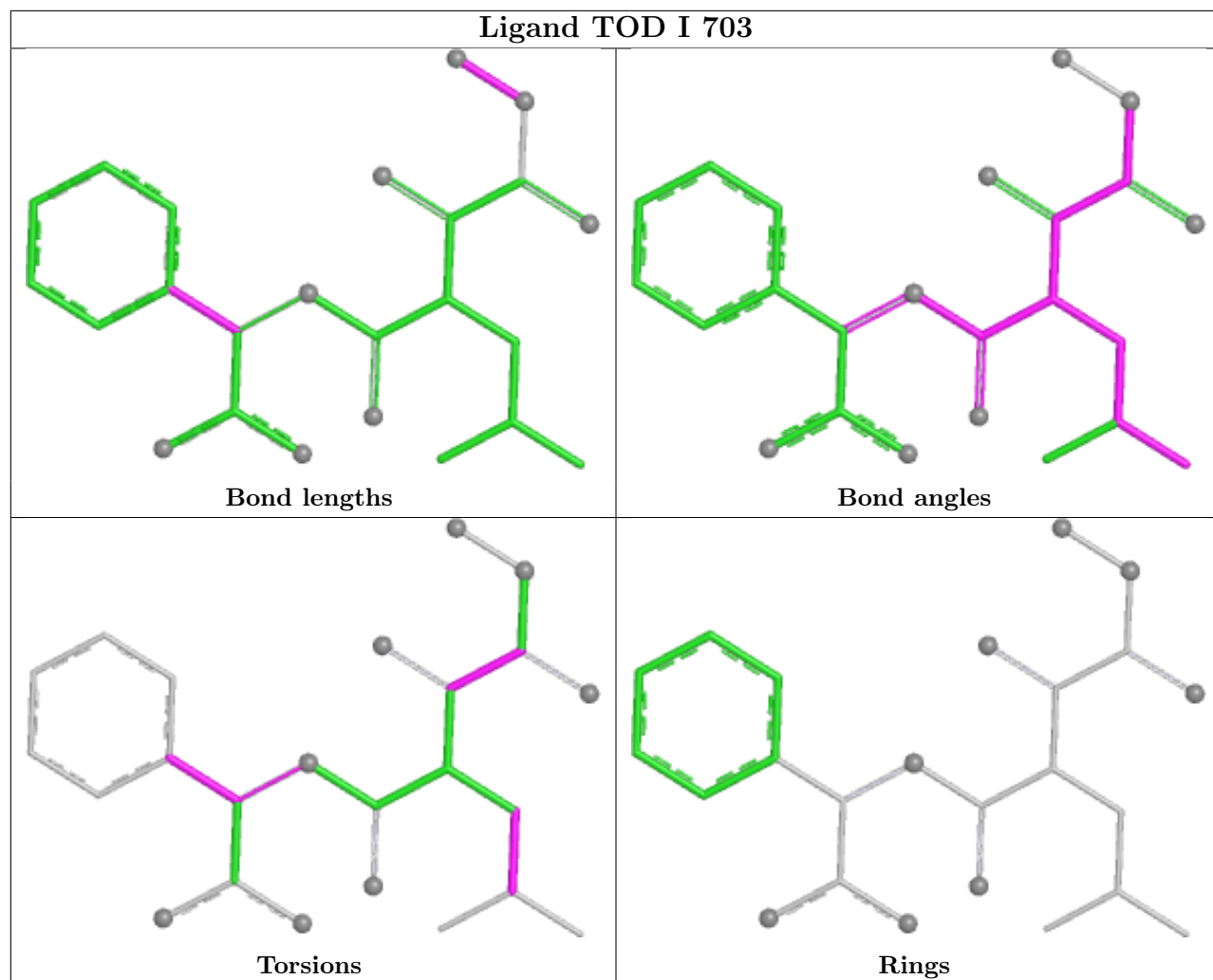
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

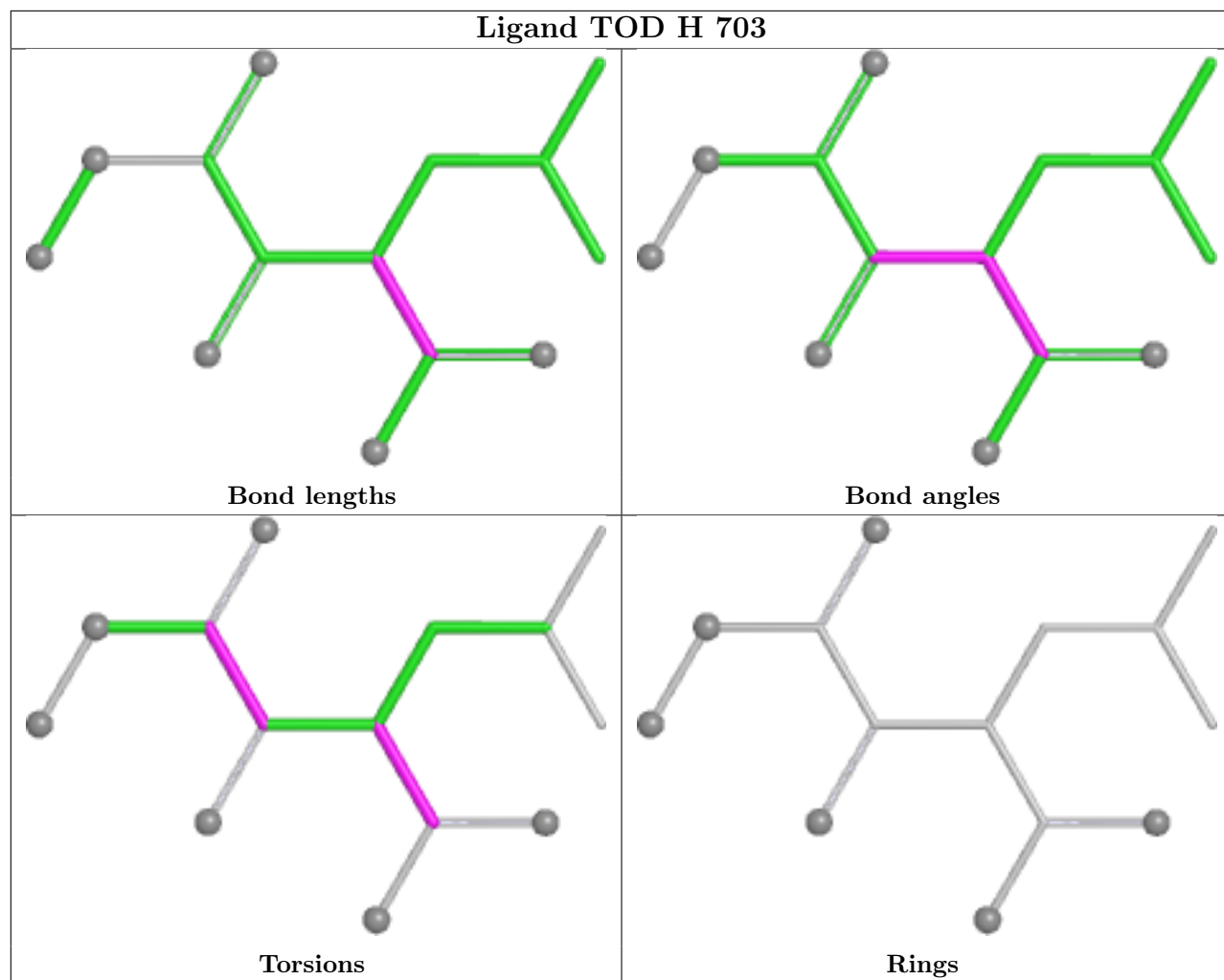
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

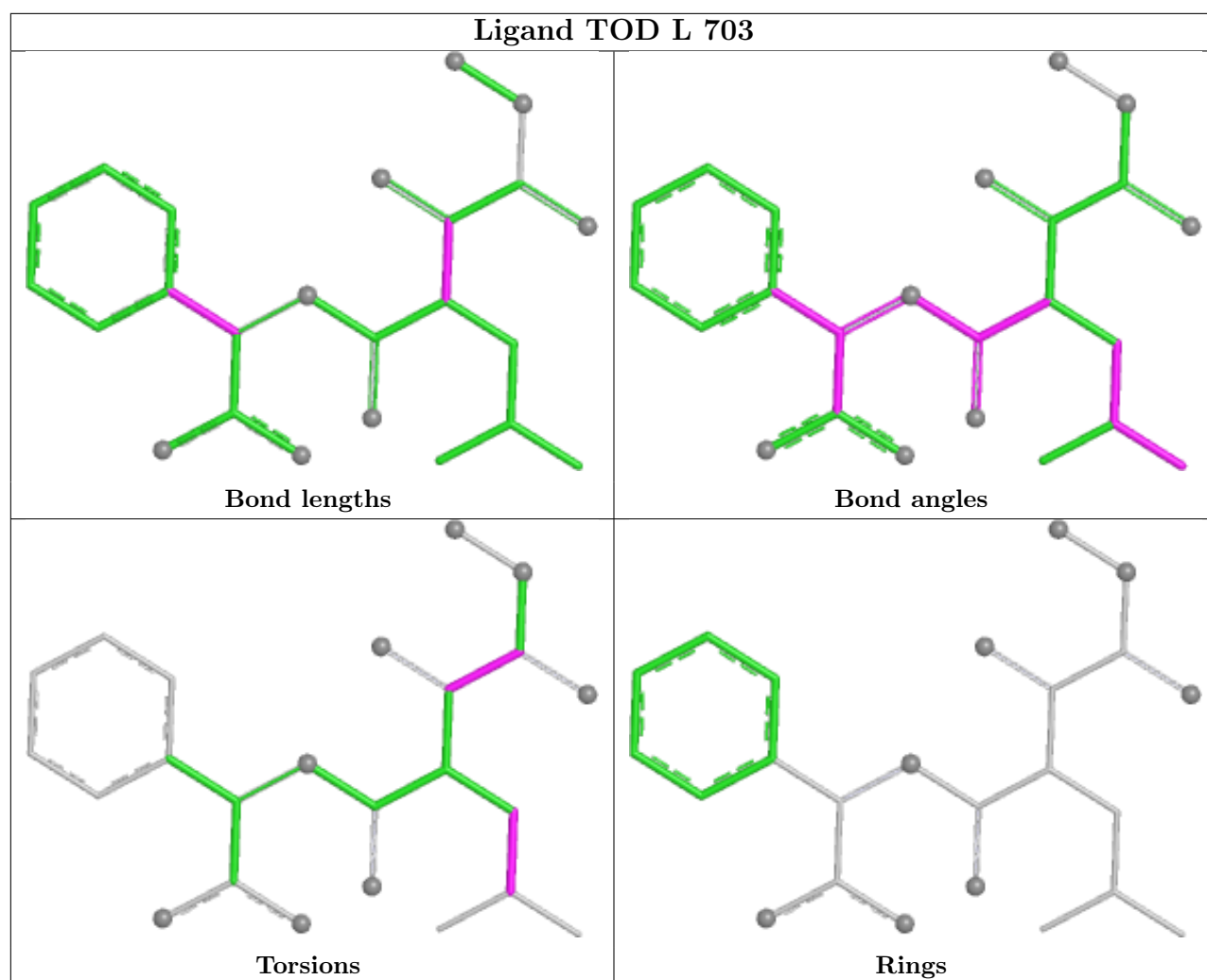


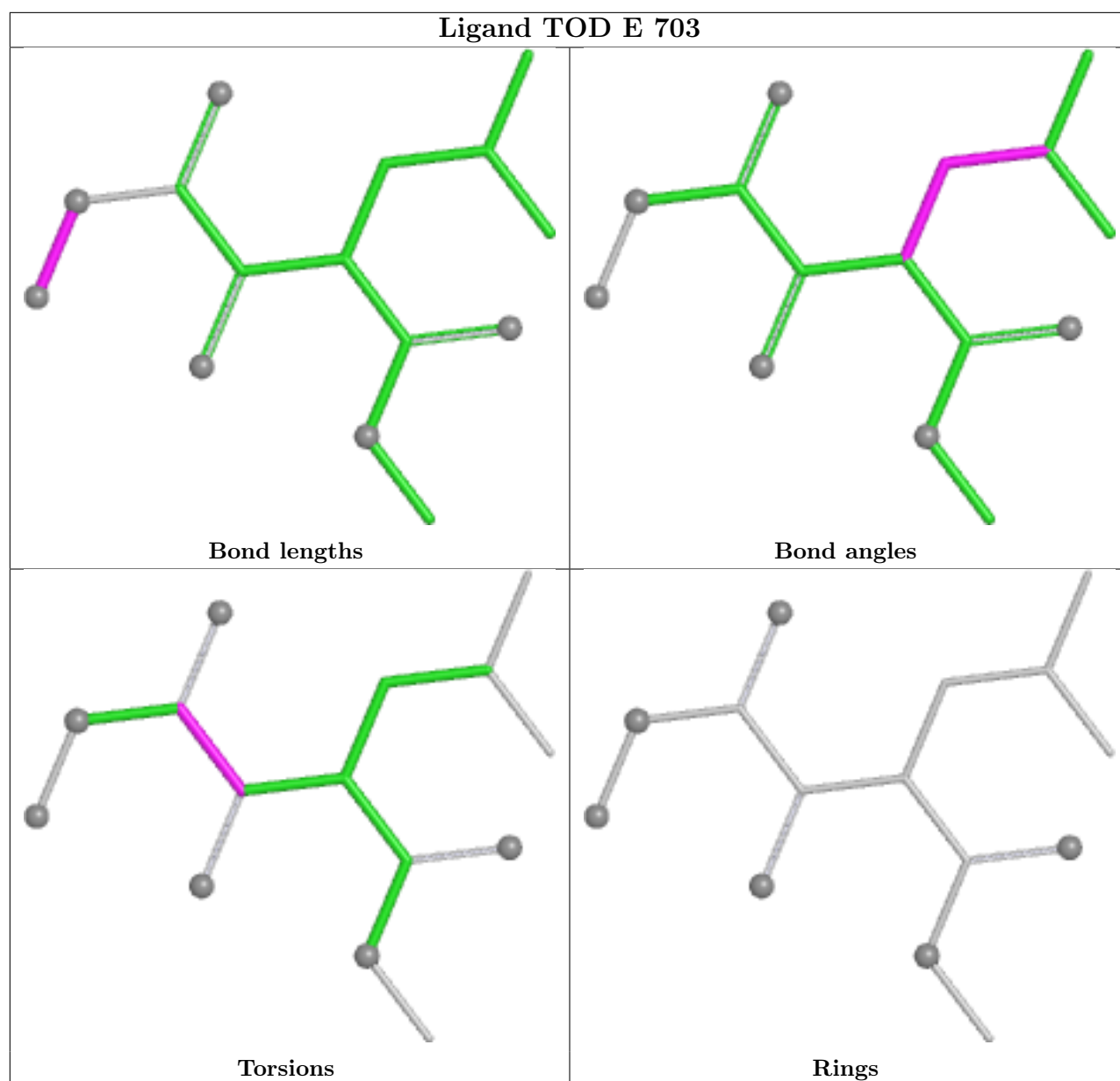


Ligand TOD I 703

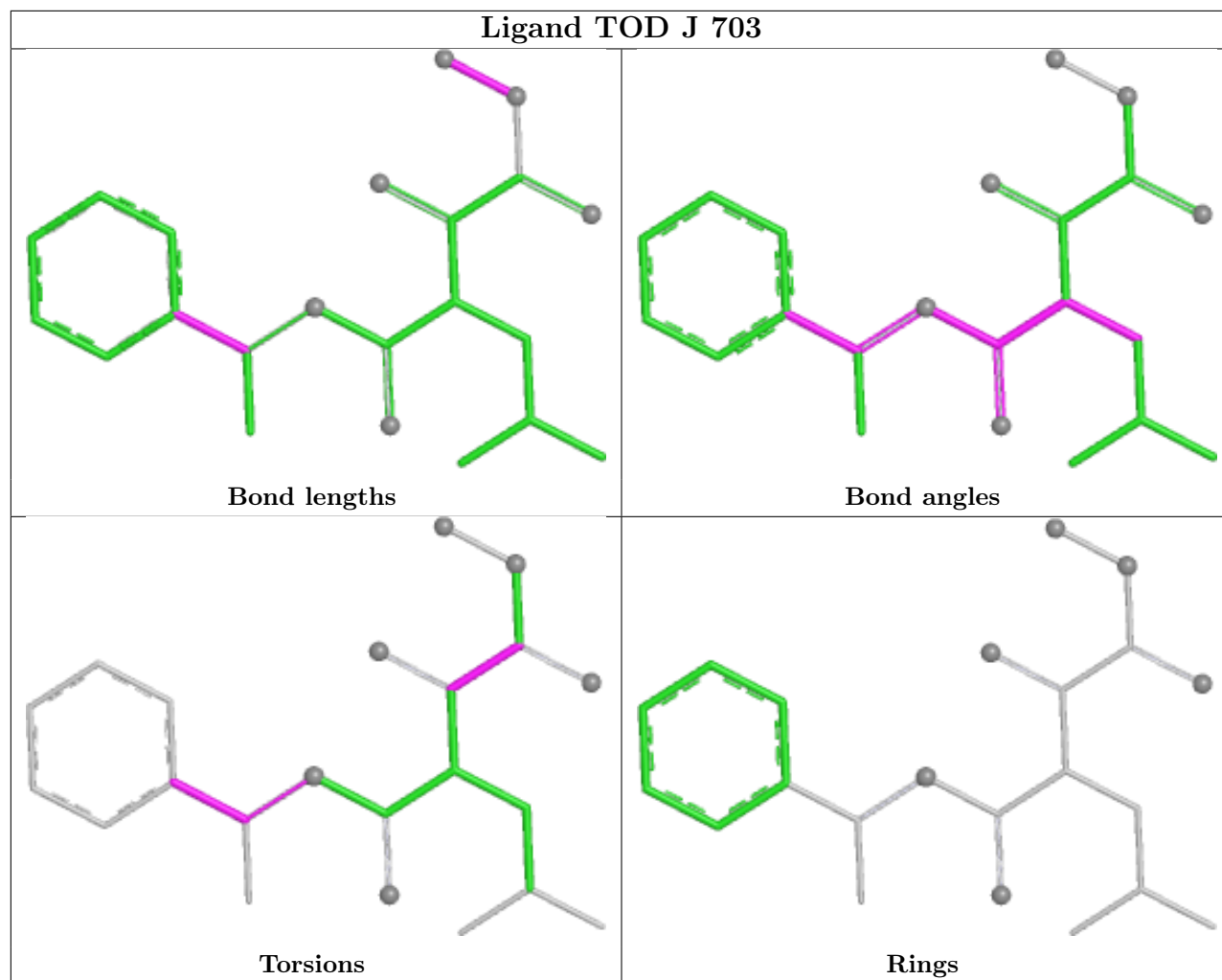


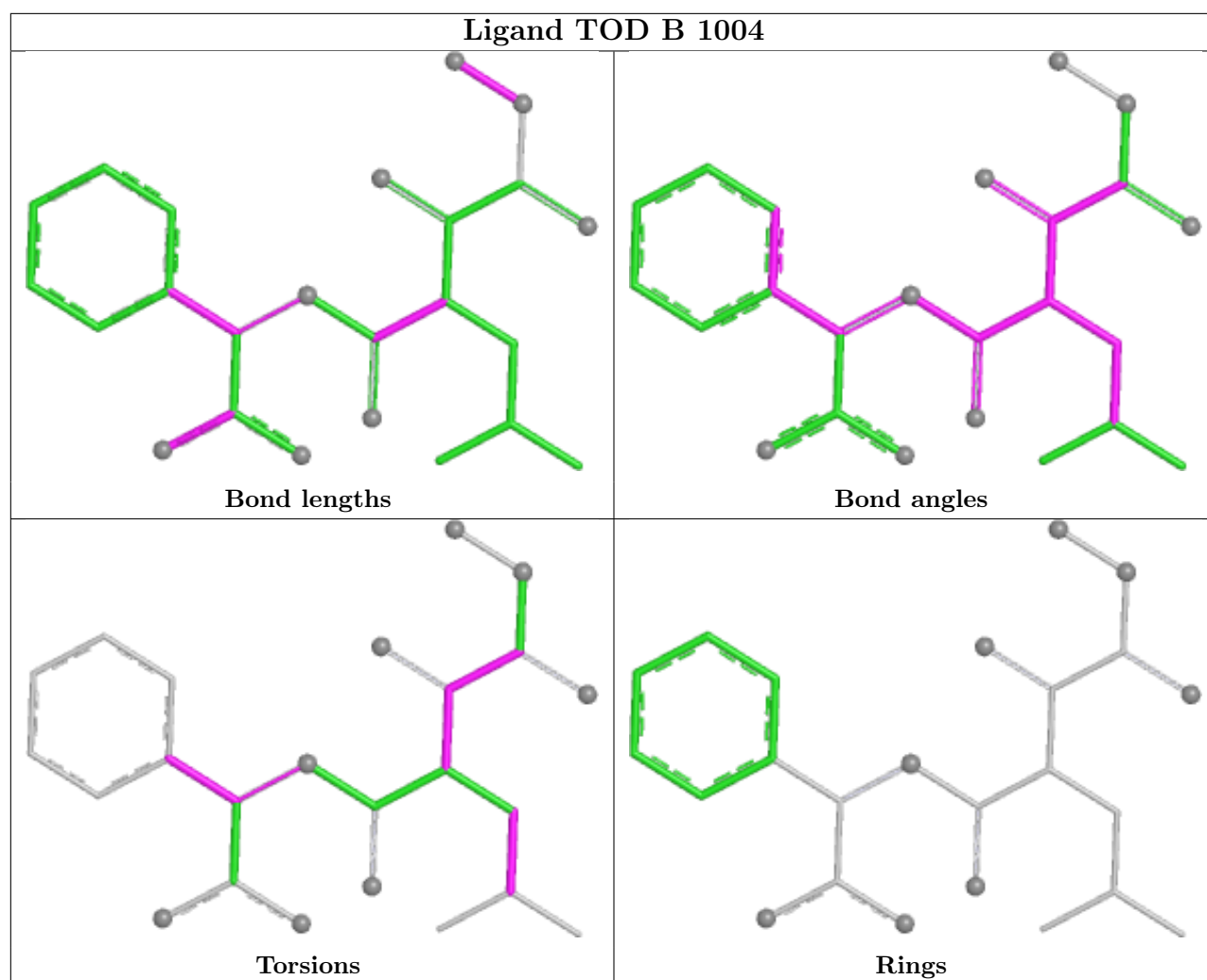


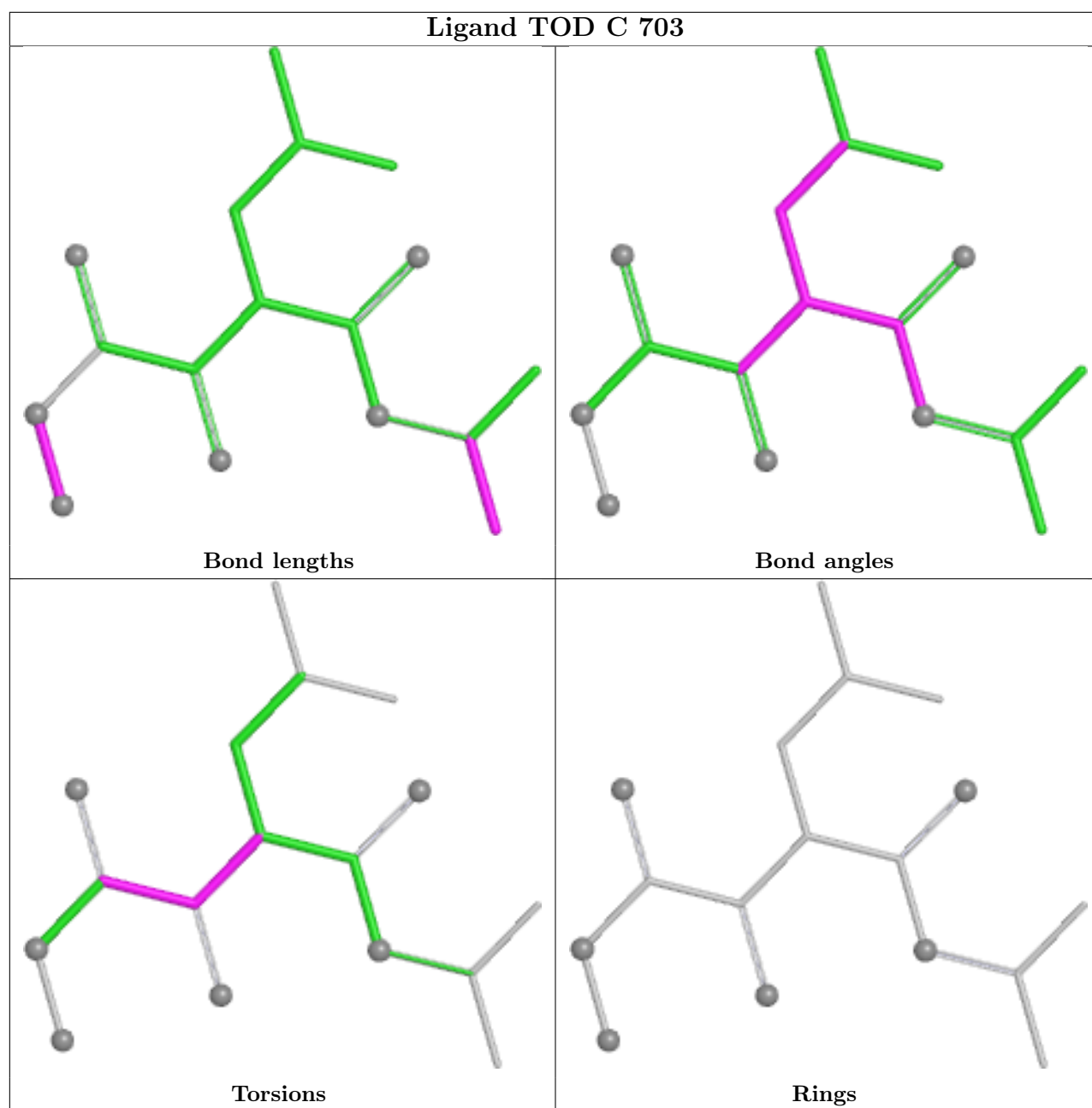


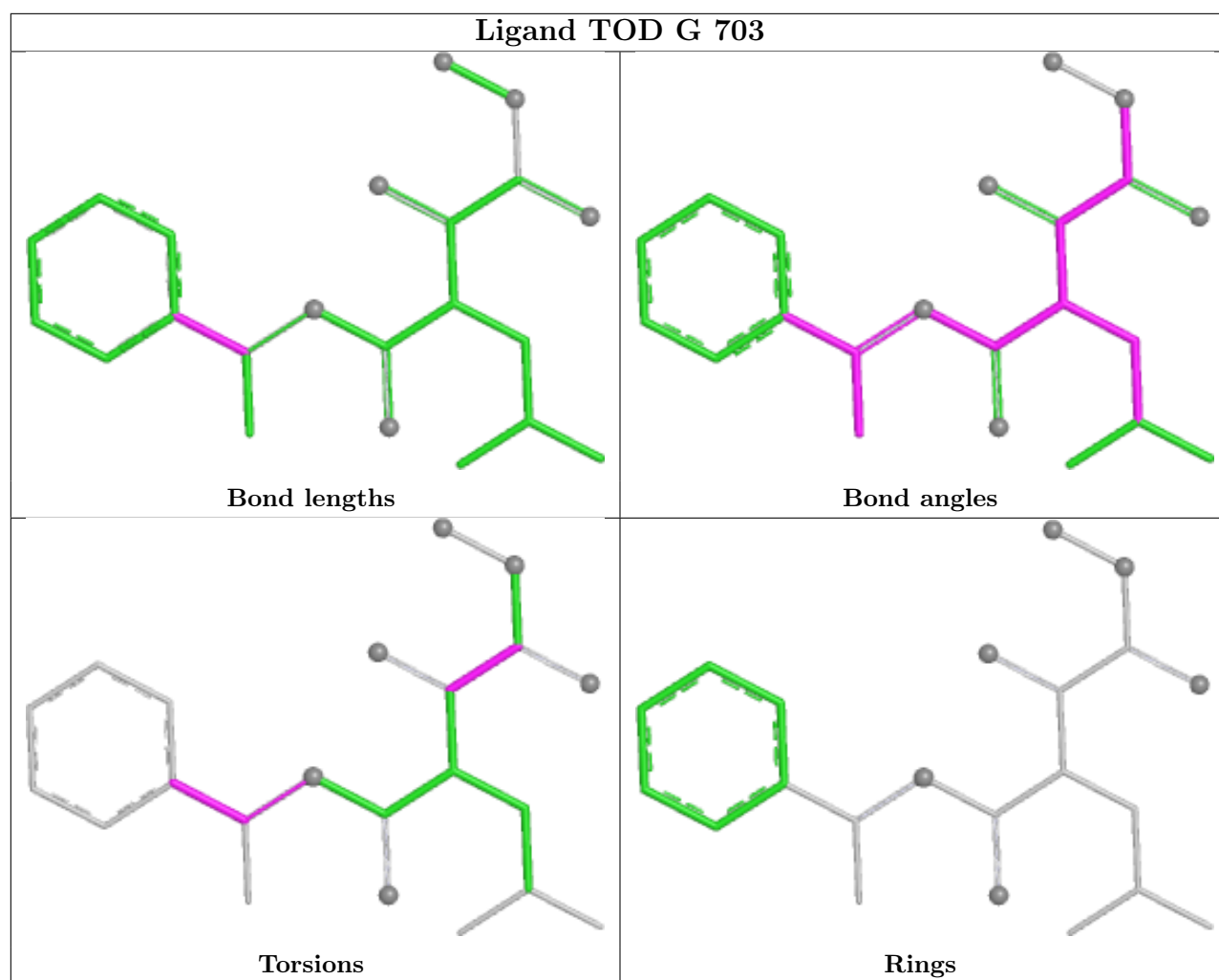


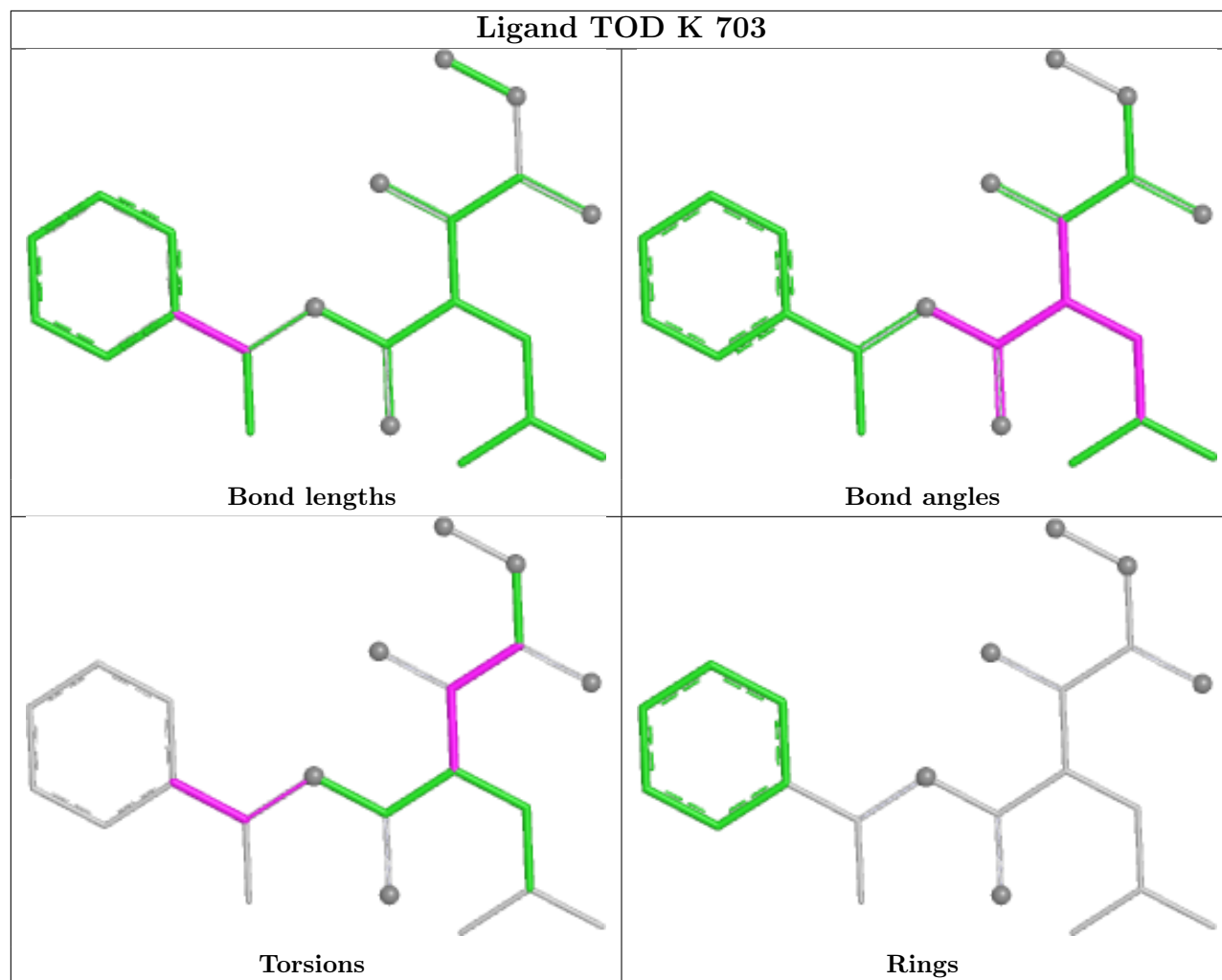
Ligand TOD J 703











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	516/519 (99%)	0.25	14 (2%)	56	53	20, 28, 50, 96	1 (0%)
1	B	510/519 (98%)	0.39	25 (4%)	35	32	19, 29, 61, 79	0
1	C	517/519 (99%)	0.21	12 (2%)	61	58	18, 27, 50, 82	0
1	D	511/519 (98%)	0.18	13 (2%)	58	55	15, 24, 46, 70	0
1	E	509/519 (98%)	0.12	9 (1%)	67	65	14, 25, 42, 63	0
1	F	509/519 (98%)	0.47	26 (5%)	33	30	15, 31, 59, 73	0
1	G	519/519 (100%)	0.35	10 (1%)	66	63	22, 30, 53, 94	0
1	H	510/519 (98%)	0.46	29 (5%)	29	26	20, 32, 63, 78	1 (0%)
1	I	515/519 (99%)	0.40	23 (4%)	38	35	18, 28, 53, 80	0
1	J	511/519 (98%)	0.22	7 (1%)	73	71	15, 27, 46, 65	0
1	K	509/519 (98%)	0.19	10 (1%)	65	62	15, 26, 44, 78	5 (0%)
1	L	508/519 (97%)	0.37	15 (2%)	52	49	18, 31, 54, 70	2 (0%)
All	All	6144/6228 (98%)	0.30	193 (3%)	51	48	14, 28, 54, 96	9 (0%)

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	GLU	6.6
1	A	551	VAL	6.2
1	I	439	TYR	5.9
1	K	137	LYS	5.6
1	D	439	TYR	5.3
1	B	136	GLY	5.0
1	G	551	VAL	4.5
1	I	121	CYS	4.2
1	A	136	GLY	4.2
1	E	550	SER	4.1
1	D	288	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	603	ASP	4.0
1	E	273	ASN	3.9
1	G	552	LYS	3.9
1	B	125	GLU	3.8
1	F	551	VAL	3.8
1	D	262	GLU	3.8
1	L	603	ASP	3.8
1	F	189	TYR	3.7
1	A	288	TYR	3.6
1	A	603	ASP	3.6
1	J	550	SER	3.6
1	B	199	SER	3.5
1	F	550	SER	3.5
1	H	549	SER	3.5
1	B	124	GLU	3.5
1	H	550	SER	3.4
1	J	145	SER	3.4
1	G	362	LYS	3.3
1	I	274	ALA	3.3
1	E	553	ALA	3.3
1	B	197	ASP	3.3
1	I	120	GLY	3.3
1	H	262	GLU	3.3
1	C	552	LYS	3.3
1	K	197	ASP	3.3
1	A	159	ASP	3.2
1	A	362	LYS	3.2
1	A	259	VAL	3.2
1	A	272	ASN	3.2
1	H	181	ASN	3.2
1	D	124	GLU	3.2
1	H	138	GLU	3.2
1	I	124	GLU	3.2
1	L	551	VAL	3.1
1	A	258	ASN	3.1
1	A	363	GLY	3.1
1	B	196	ALA	3.0
1	I	398	PHE	3.0
1	F	121	CYS	3.0
1	A	602	ASN	3.0
1	H	117	ILE	2.9
1	F	184	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	254	SER	2.9
1	G	217	ASN	2.9
1	I	200	GLU	2.9
1	E	551	VAL	2.9
1	F	122	ASN	2.8
1	H	122	ASN	2.8
1	K	551	VAL	2.8
1	F	602	ASN	2.8
1	D	136	GLY	2.8
1	J	85	ALA	2.8
1	F	153	VAL	2.8
1	H	170	GLY	2.8
1	C	551	VAL	2.7
1	E	552	LYS	2.7
1	C	223	THR	2.7
1	H	197	ASP	2.7
1	K	398	PHE	2.7
1	L	439	TYR	2.7
1	B	419	GLU	2.7
1	F	422	GLU	2.6
1	C	602	ASN	2.6
1	H	143	LYS	2.6
1	H	136	GLY	2.6
1	D	254	SER	2.6
1	H	123	VAL	2.6
1	L	398	PHE	2.6
1	D	603	ASP	2.6
1	G	602	ASN	2.6
1	C	138	GLU	2.6
1	D	104	ASN	2.6
1	F	117	ILE	2.5
1	F	136	GLY	2.5
1	H	178	PHE	2.5
1	H	201	ALA	2.5
1	L	139	ASN	2.5
1	B	362	LYS	2.5
1	B	389	PRO	2.5
1	H	398	PHE	2.5
1	F	181	ASN	2.5
1	L	163	GLU	2.5
1	J	551	VAL	2.5
1	G	257	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	181	ASN	2.4
1	H	161	ASN	2.4
1	L	161	ASN	2.4
1	D	145	SER	2.4
1	F	335	GLU	2.4
1	C	331	LYS	2.4
1	L	155	GLU	2.4
1	F	176	TYR	2.4
1	D	420	ASN	2.4
1	I	273	ASN	2.4
1	I	125	GLU	2.4
1	I	507	GLU	2.4
1	I	257	LYS	2.4
1	L	329	GLY	2.4
1	H	439	TYR	2.4
1	J	219	LEU	2.4
1	H	255	THR	2.4
1	B	272	ASN	2.4
1	B	155	GLU	2.4
1	F	146	SER	2.4
1	D	126	GLY	2.4
1	B	123	VAL	2.4
1	G	85	ALA	2.4
1	H	196	ALA	2.4
1	E	391	SER	2.3
1	H	202	ASP	2.3
1	I	93	SER	2.3
1	B	117	ILE	2.3
1	F	149	ASN	2.3
1	K	218	LYS	2.3
1	B	216	ASP	2.3
1	F	156	PHE	2.3
1	A	442	GLY	2.3
1	A	367	LYS	2.3
1	F	255	THR	2.3
1	I	143	LYS	2.3
1	B	138	GLU	2.3
1	E	602	ASN	2.3
1	F	322	ASN	2.3
1	A	256	ASP	2.3
1	C	603	ASP	2.3
1	G	549	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	159	ASP	2.3
1	I	603	ASP	2.3
1	C	163	GLU	2.2
1	I	364	ASP	2.2
1	H	175	PHE	2.2
1	C	201	ALA	2.2
1	K	284	ALA	2.2
1	L	602	ASN	2.2
1	J	147	LYS	2.2
1	B	185	VAL	2.2
1	B	178	PHE	2.2
1	B	398	PHE	2.2
1	H	155	GLU	2.2
1	E	395	LEU	2.2
1	L	339	GLY	2.2
1	D	197	ASP	2.2
1	F	175	PHE	2.2
1	C	124	GLU	2.1
1	F	183	ASN	2.1
1	I	395	LEU	2.1
1	F	231	ASP	2.1
1	L	549	SER	2.1
1	H	165	PHE	2.1
1	I	331	LYS	2.1
1	F	139	ASN	2.1
1	K	140	GLY	2.1
1	H	231	ASP	2.1
1	I	167	VAL	2.1
1	K	295	SER	2.1
1	H	271	ILE	2.1
1	H	364	ASP	2.1
1	F	262	GLU	2.1
1	B	105	THR	2.1
1	F	141	PRO	2.1
1	B	217	ASN	2.1
1	C	183	ASN	2.1
1	I	272	ASN	2.1
1	I	136	GLY	2.1
1	B	439	TYR	2.1
1	B	195	VAL	2.1
1	G	138	GLU	2.0
1	H	335	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	125	GLU	2.0
1	L	200	GLU	2.0
1	B	550	SER	2.0
1	L	254	SER	2.0
1	B	122	ASN	2.0
1	H	511	ASN	2.0
1	K	119	GLY	2.0
1	C	364	ASP	2.0
1	E	548	SER	2.0
1	I	97	THR	2.0
1	I	135	PRO	2.0
1	L	113	GLN	2.0
1	H	322	ASN	2.0
1	K	161	ASN	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($\text{\AA}^2$)	Q<0.9
6	1PE	G	708	9/16	0.72	0.19	39,48,57,57	0
5	SO4	A	705	5/5	0.73	0.12	57,59,65,65	0
6	1PE	D	706	10/16	0.74	0.20	40,49,56,56	0
6	1PE	C	706	13/16	0.74	0.20	35,48,54,58	0
6	1PE	B	1006	7/16	0.76	0.24	44,48,55,58	0
6	1PE	A	708	9/16	0.76	0.20	38,43,54,58	0
6	1PE	D	705	10/16	0.78	0.20	34,46,52,52	0
6	1PE	H	705	10/16	0.78	0.20	47,52,55,56	0
6	1PE	G	707	9/16	0.79	0.18	31,35,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CO3	I	704	4/4	0.80	0.21	28,34,37,41	0
5	SO4	C	705	5/5	0.82	0.16	79,80,81,82	0
5	SO4	G	705	5/5	0.83	0.11	61,63,66,68	0
4	CO3	E	704	4/4	0.83	0.19	30,31,33,38	0
3	TOD	B	1004	24/24	0.83	0.16	27,37,52,63	0
5	SO4	A	707	5/5	0.84	0.28	65,66,72,77	0
5	SO4	L	706	5/5	0.85	0.10	53,60,63,65	0
3	TOD	C	703	17/24	0.85	0.14	20,29,39,46	0
5	SO4	G	706	5/5	0.85	0.15	52,57,66,70	0
4	CO3	J	704	4/4	0.86	0.17	33,38,42,43	0
3	TOD	K	703	22/24	0.87	0.15	32,44,54,58	0
3	TOD	E	703	15/24	0.88	0.14	26,41,51,51	0
3	TOD	J	703	22/24	0.89	0.13	27,35,42,51	0
3	TOD	L	703	24/24	0.89	0.12	19,38,46,48	0
6	1PE	E	707	12/16	0.89	0.14	30,40,51,53	0
3	TOD	I	703	24/24	0.90	0.12	23,35,43,55	0
4	CO3	G	704	4/4	0.90	0.20	35,36,38,40	0
3	TOD	A	703	24/24	0.90	0.14	25,49,58,61	0
5	SO4	E	706	5/5	0.90	0.28	71,72,77,78	0
4	CO3	A	704	4/4	0.90	0.10	19,20,20,20	0
6	1PE	C	707	9/16	0.90	0.13	29,34,42,51	0
4	CO3	L	704	4/4	0.91	0.11	27,35,37,37	0
4	CO3	K	704	4/4	0.91	0.09	17,22,23,30	0
3	TOD	F	703	24/24	0.92	0.14	33,46,59,64	0
3	TOD	G	703	22/24	0.93	0.10	21,28,36,40	0
5	SO4	A	706	5/5	0.94	0.18	37,44,49,62	0
3	TOD	H	703	14/24	0.95	0.10	20,33,39,43	0
5	SO4	D	704	5/5	0.95	0.18	44,50,51,62	0
4	CO3	B	1001	4/4	0.95	0.09	18,19,20,29	0
4	CO3	C	704	4/4	0.95	0.08	25,27,27,30	0
4	CO3	H	704	4/4	0.96	0.08	20,20,20,27	0
4	CO3	F	704	4/4	0.96	0.08	15,16,24,29	0
5	SO4	L	705	5/5	0.97	0.07	21,26,32,36	0
4	CO3	D	703	4/4	0.97	0.05	15,19,20,23	0
2	ZN	J	702	1/1	0.98	0.12	51,51,51,51	0
5	SO4	B	1005	5/5	0.98	0.06	21,21,21,25	0
5	SO4	E	705	5/5	0.98	0.07	12,22,26,33	0
2	ZN	A	702	1/1	0.99	0.02	27,27,27,27	0
2	ZN	B	1002	1/1	0.99	0.02	19,19,19,19	0
2	ZN	B	1003	1/1	0.99	0.05	29,29,29,29	0
5	SO4	I	705	5/5	0.99	0.05	23,23,23,28	0
2	ZN	C	702	1/1	0.99	0.02	27,27,27,27	0

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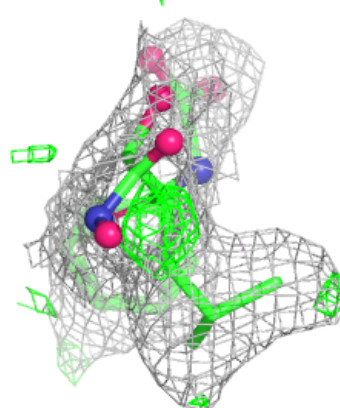
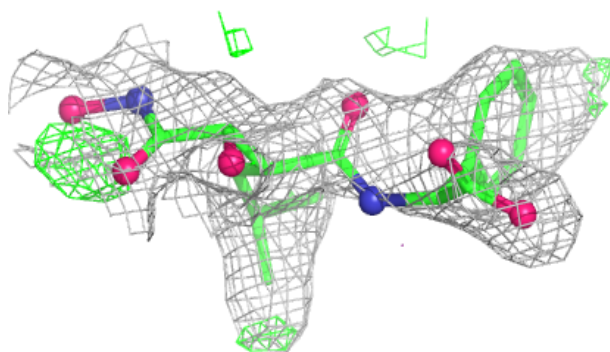
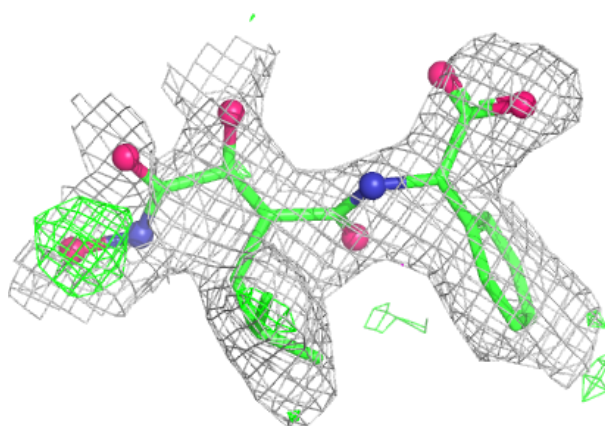
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	D	701	1/1	0.99	0.07	26,26,26,26	0
2	ZN	D	702	1/1	0.99	0.02	23,23,23,23	0
2	ZN	E	701	1/1	0.99	0.04	30,30,30,30	0
2	ZN	E	702	1/1	0.99	0.03	30,30,30,30	0
2	ZN	H	702	1/1	0.99	0.03	21,21,21,21	0
2	ZN	I	702	1/1	0.99	0.03	27,27,27,27	0
2	ZN	J	701	1/1	0.99	0.04	30,30,30,30	0
2	ZN	A	701	1/1	0.99	0.03	19,19,19,19	0
2	ZN	K	702	1/1	0.99	0.04	32,32,32,32	0
2	ZN	L	701	1/1	0.99	0.02	21,21,21,21	0
2	ZN	L	702	1/1	0.99	0.02	24,24,24,24	0
2	ZN	H	701	1/1	1.00	0.02	27,27,27,27	0
2	ZN	C	701	1/1	1.00	0.03	23,23,23,23	0
2	ZN	I	701	1/1	1.00	0.01	19,19,19,19	0
2	ZN	F	701	1/1	1.00	0.02	14,14,14,14	0
2	ZN	F	702	1/1	1.00	0.02	32,32,32,32	0
2	ZN	G	701	1/1	1.00	0.01	23,23,23,23	0
2	ZN	K	701	1/1	1.00	0.01	19,19,19,19	0
2	ZN	G	702	1/1	1.00	0.03	23,23,23,23	0

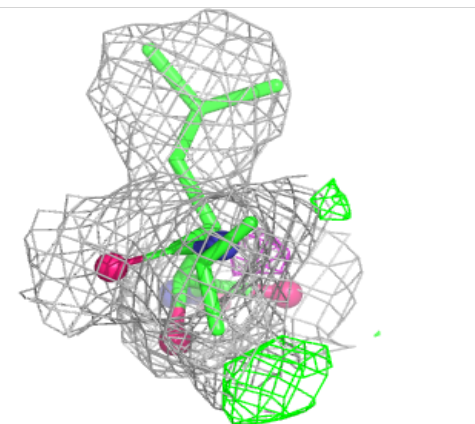
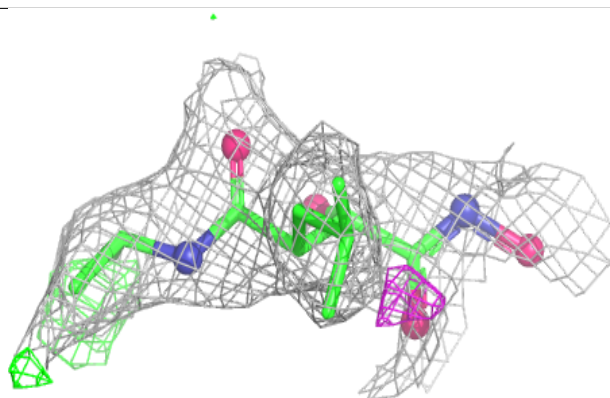
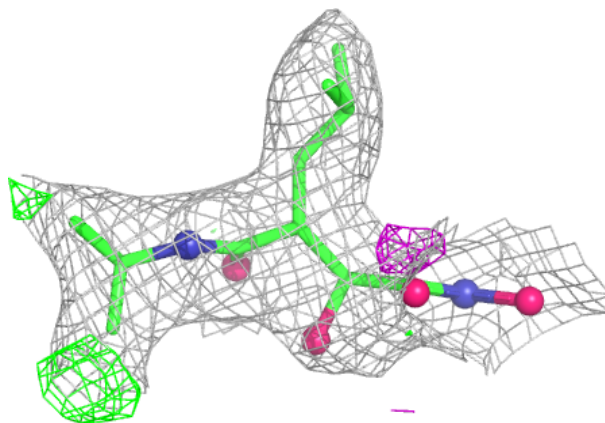
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TOD B 1004:

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

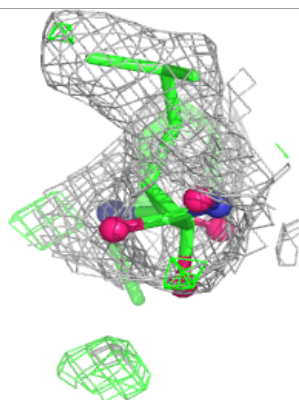
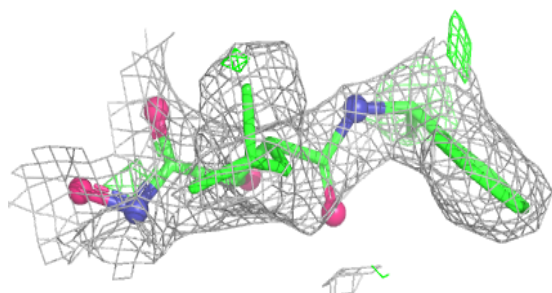
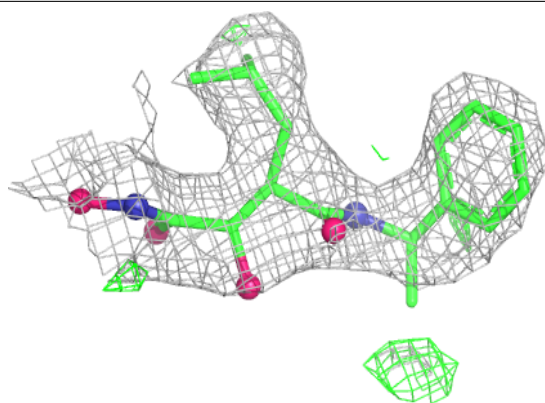
**Electron density around TOD C 703:**

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

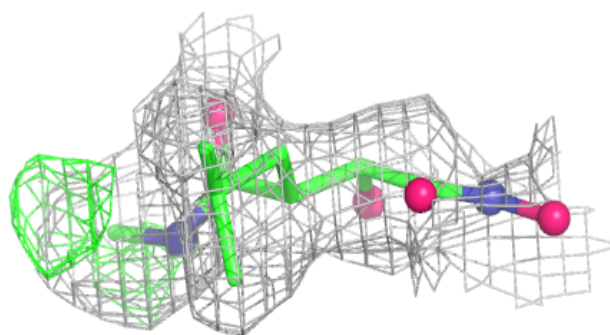
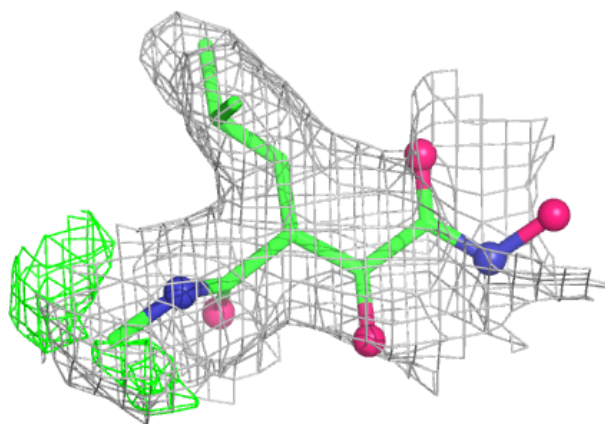


Electron density around TOD K 703:

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

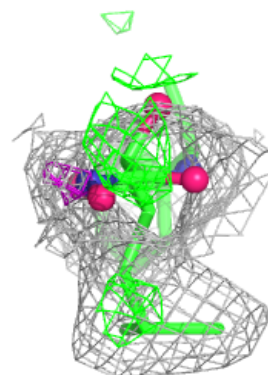
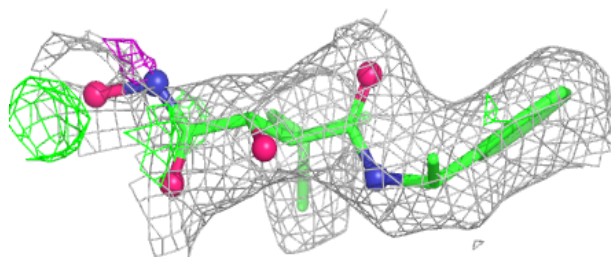
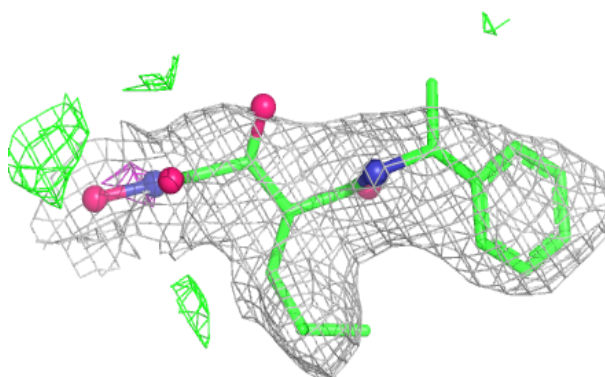
**Electron density around TOD E 703:**

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

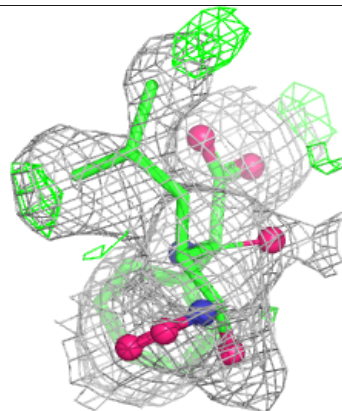
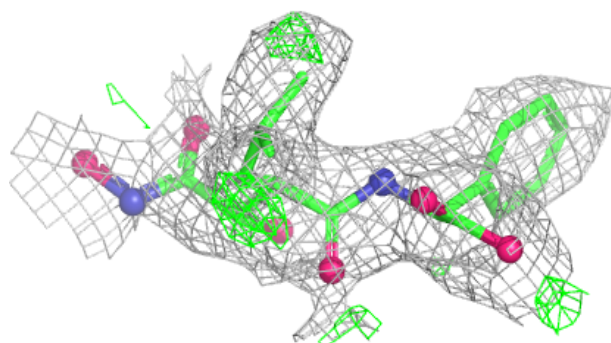
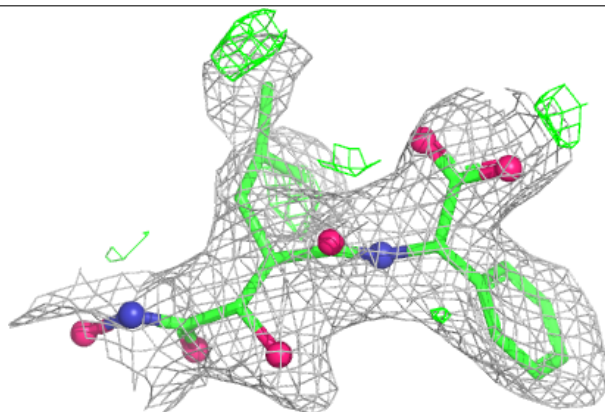


Electron density around TOD J 703:

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

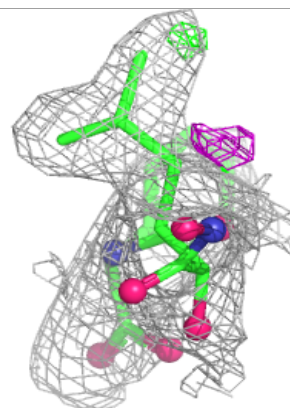
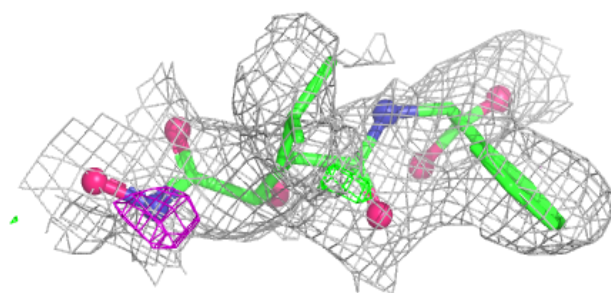
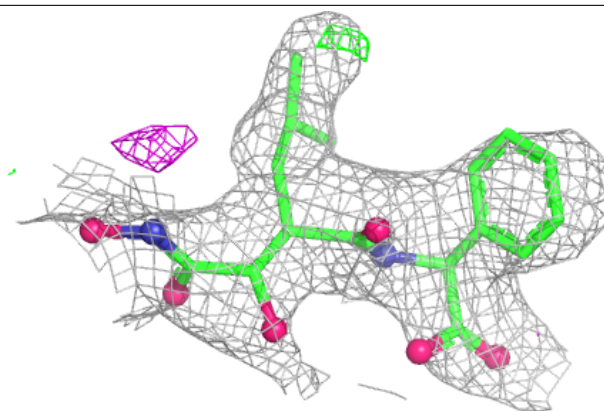
**Electron density around TOD L 703:**

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

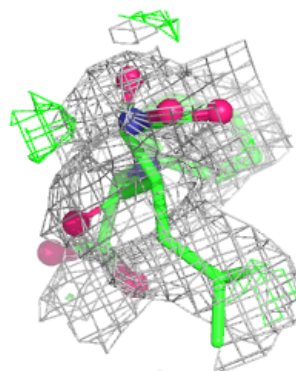
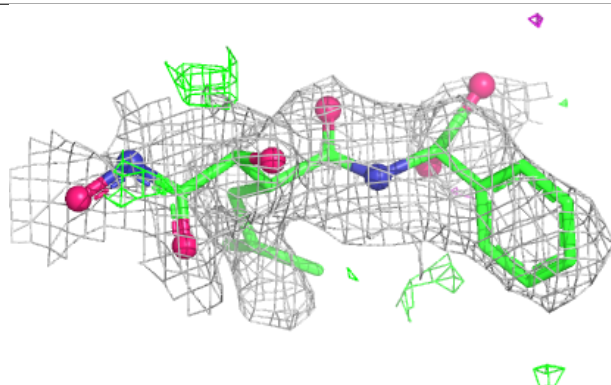
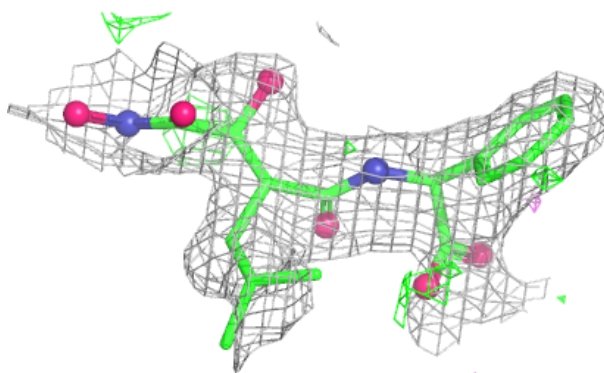


Electron density around TOD I 703:

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

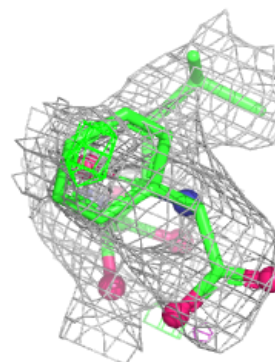
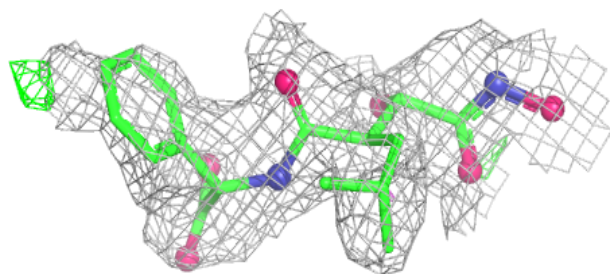
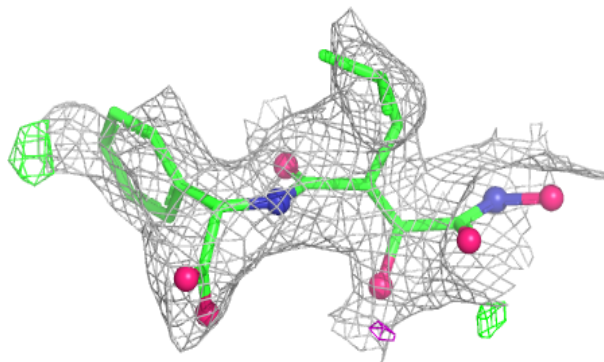
**Electron density around TOD A 703:**

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

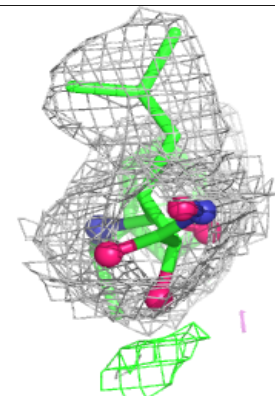
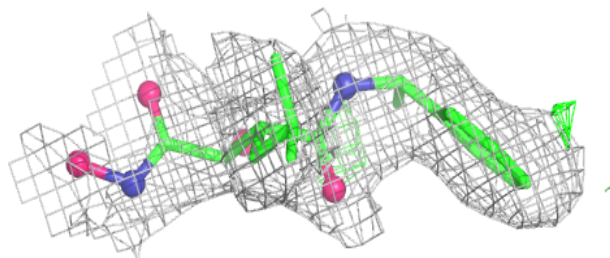
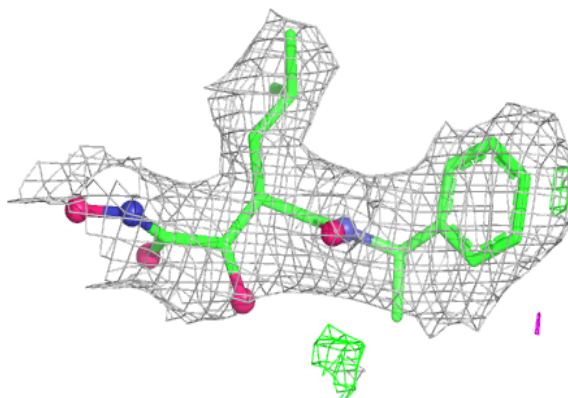


Electron density around TOD F 703:

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

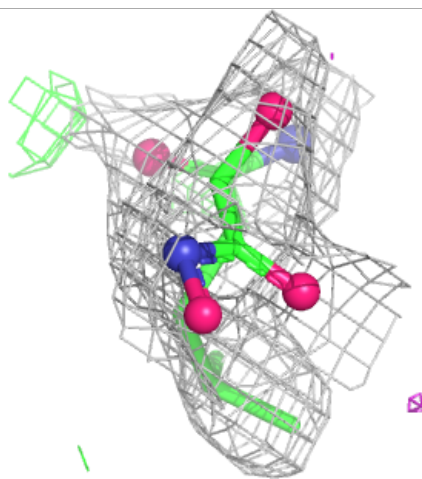
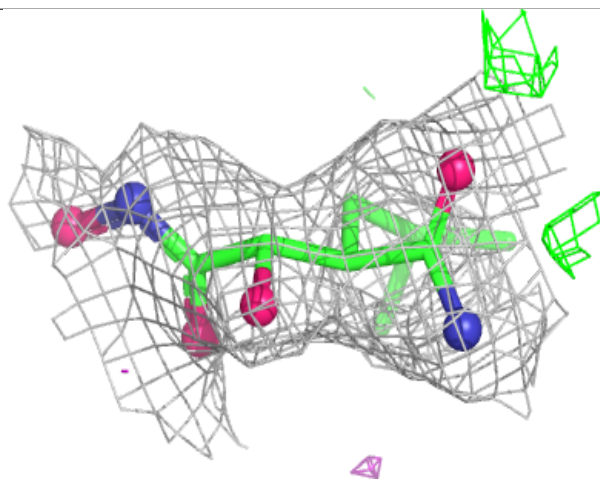
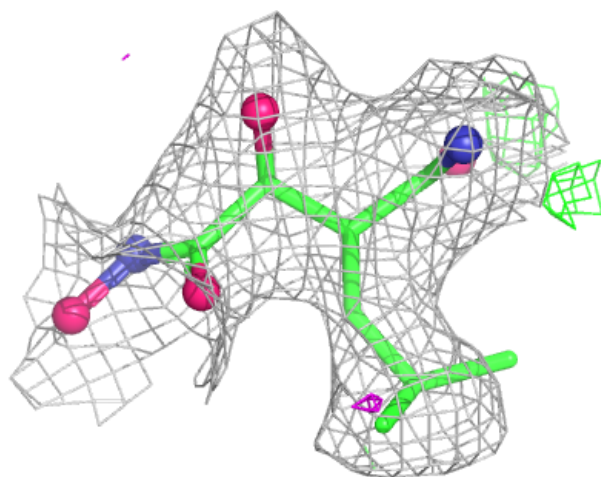
**Electron density around TOD G 703:**

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



Electron density around TOD H 703:

$2mF_o-DF_c$ (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.