



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 PM UTC

PDB ID : 1MX5 / pdb_00001mx5
Title : Crystal Structure of Human Liver Carboxylesterase in complexed with homatropine, a cocaine analogue
Authors : Bencharit, S.; Morton, C.L.; Xue, Y.; Potter, P.M.; Redinbo, M.R.
Deposited on : 2002-10-01
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

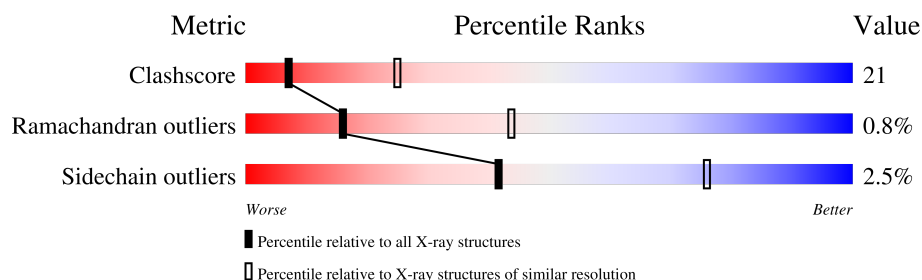
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	279	X	-	-	-
2	NAG	D	479	X	-	-	-
2	NAG	F	679	X	-	-	-
3	SIA	B	282	-	-	X	-
4	CL	A	11	-	-	X	-
4	CL	E	15	-	-	X	-
5	HTQ	A	111	-	-	X	-
5	HTQ	B	212	-	-	X	-
5	HTQ	E	515	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26960 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.

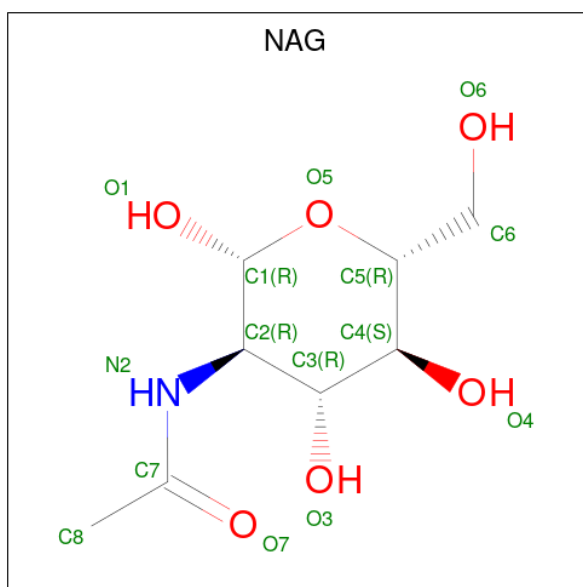
- Molecule 1 is a protein called liver Carboxylesterase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	C	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	D	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	E	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	F	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			

There are 6 discrepancies between the modelled and reference sequences:

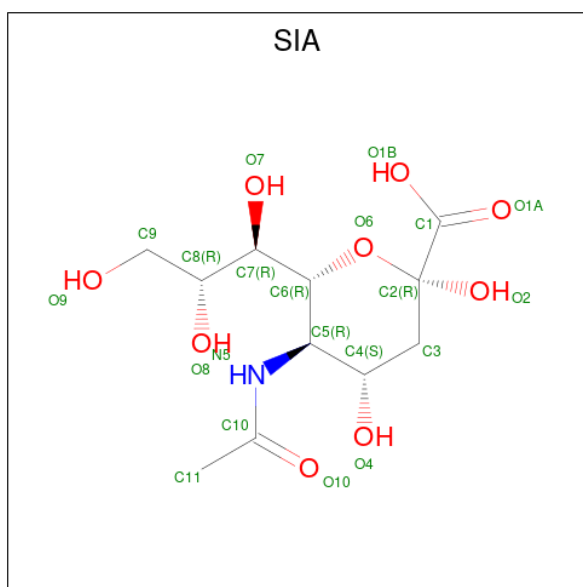
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141
D	?	-	GLN	deletion	UNP P23141
E	?	-	GLN	deletion	UNP P23141
F	?	-	GLN	deletion	UNP P23141

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).

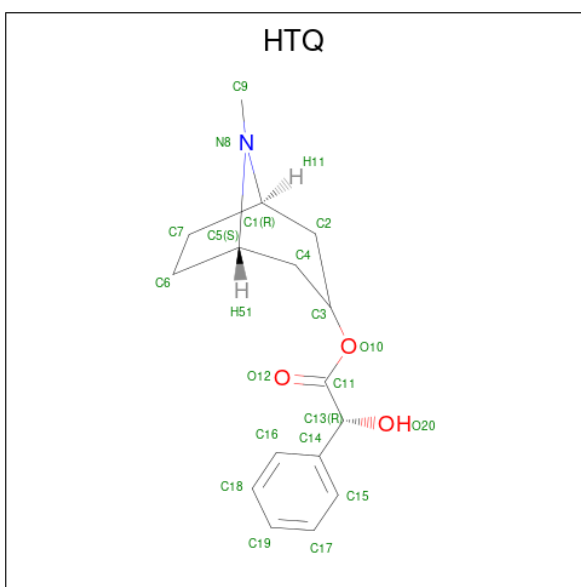


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	F	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is HOMOTROPINE (CCD ID: HTQ) (formula: C₁₆H₂₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	16	1	3		
5	A	1	Total	C	N	O	0	1
			40	32	2	6		
5	B	1	Total	C	N	O	0	0
			20	16	1	3		
5	B	1	Total	C	N	O	0	1
			40	32	2	6		
5	C	1	Total	C	N	O	0	0
			20	16	1	3		
5	C	1	Total	C	N	O	0	1
			40	32	2	6		
5	D	1	Total	C	N	O	0	0
			20	16	1	3		
5	D	1	Total	C	N	O	0	1
			40	32	2	6		
5	E	1	Total	C	N	O	0	0
			20	16	1	3		
5	E	1	Total	C	N	O	0	1
			40	32	2	6		
5	F	1	Total	C	N	O	0	0
			20	16	1	3		
5	F	1	Total	C	N	O	0	1
			40	32	2	6		

- Molecule 6 is water.

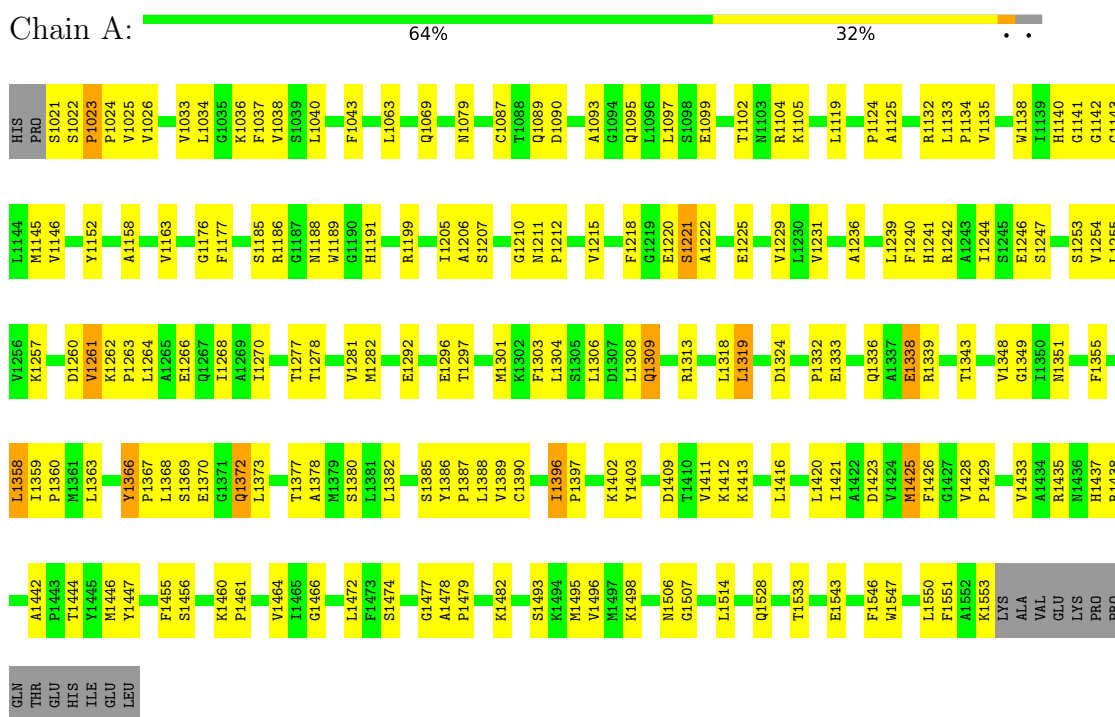
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	249	Total 249	O 249	0	0
6	B	303	Total 303	O 303	0	0
6	C	289	Total 289	O 289	0	0
6	D	291	Total 291	O 291	0	0
6	E	295	Total 295	O 295	0	0
6	F	254	Total 254	O 254	0	0

3 Residue-property plots

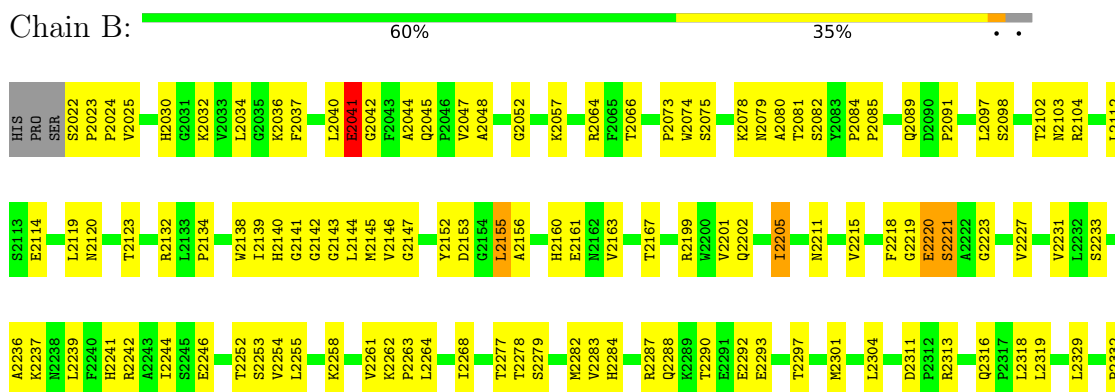
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

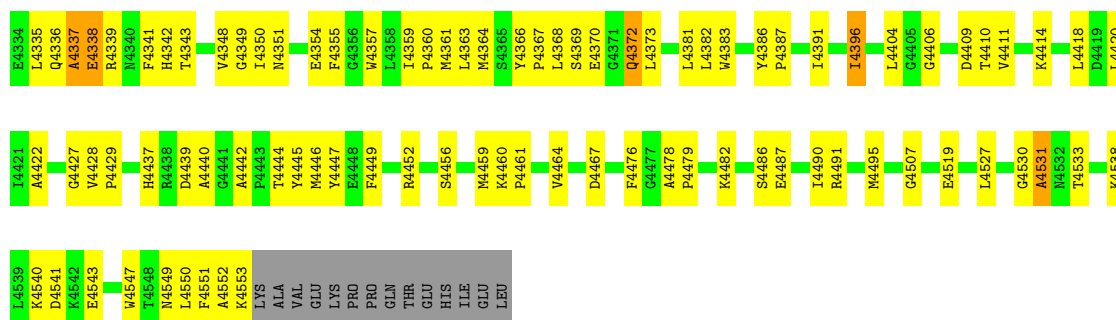
• Molecule 1: liver Carboxylesterase I



• Molecule 1: liver Carboxylesterase I

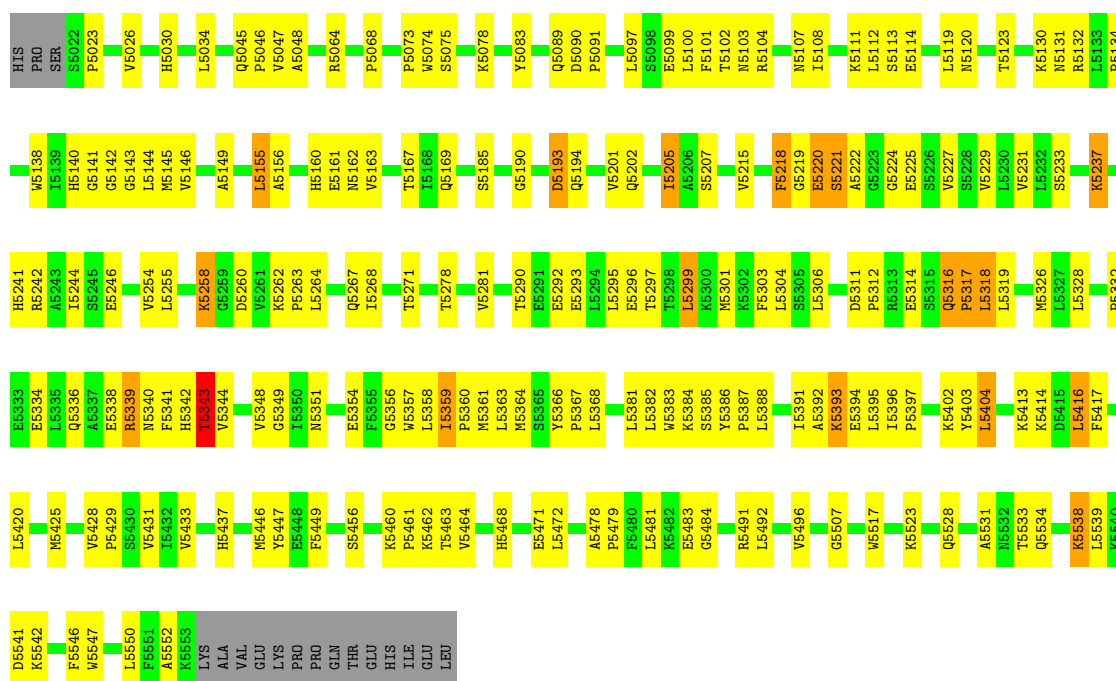






• Molecule 1: liver Carboxylesterase I

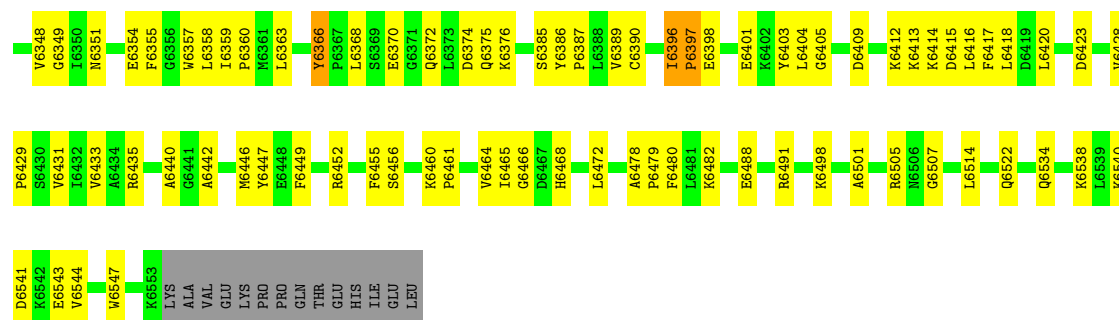
Chain E: 60% 33%



• Molecule 1: liver Carboxylesterase I

Chain F: 64% 32%





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.40Å 178.80Å 199.60Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	19.96 – 2.80	Depositor
% Data completeness (in resolution range)	92.3 (19.96-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.158 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26960	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, HTQ, CL, NAG

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	0.40	0/4236	0.90	9/5754 (0.2%)
1	B	0.40	0/4230	0.90	4/5746 (0.1%)
1	C	0.40	0/4230	0.91	5/5746 (0.1%)
1	D	0.40	0/4236	0.92	11/5754 (0.2%)
1	E	0.40	0/4230	0.93	13/5746 (0.2%)
1	F	0.40	0/4230	0.91	5/5746 (0.1%)
All	All	0.40	0/25392	0.91	47/34492 (0.1%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3303	PHE	N-CA-C	8.62	120.76	111.36
1	F	6075	SER	N-CA-C	8.48	121.75	111.40
1	D	4552	ALA	N-CA-C	-8.13	103.36	113.20
1	B	2114	GLU	N-CA-C	-8.02	102.94	112.89
1	B	2075	SER	N-CA-C	7.80	119.69	111.03
1	C	3075	SER	N-CA-C	7.68	122.41	112.89
1	E	5075	SER	N-CA-C	7.56	121.76	112.23
1	E	5343	THR	N-CA-C	7.20	121.30	110.14
1	C	3507	GLY	N-CA-C	-6.81	106.31	115.36
1	D	4114	GLU	N-CA-C	-6.76	104.51	112.89
1	E	5339	ARG	N-CA-C	-6.72	103.03	111.90
1	D	4507	GLY	N-CA-C	-6.66	105.46	115.32
1	E	5318	LEU	N-CA-C	6.59	119.89	109.81
1	E	5507	GLY	N-CA-C	-5.99	106.99	115.43
1	B	2507	GLY	N-CA-C	-5.97	105.71	114.90
1	D	4311	ASP	CA-C-N	5.96	125.67	119.05
1	D	4311	ASP	C-N-CA	5.96	125.67	119.05
1	D	4177	PHE	N-CA-C	5.96	120.41	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4531	ALA	N-CA-C	-5.93	103.99	111.11
1	D	4337	ALA	N-CA-C	-5.92	106.06	113.28
1	F	6507	GLY	N-CA-C	-5.69	106.32	115.08
1	C	3114	GLU	N-CA-C	-5.62	105.92	112.89
1	E	5233	SER	N-CA-C	5.59	116.71	109.72
1	B	2160	HIS	N-CA-C	5.58	117.05	111.07
1	E	5222	ALA	N-CA-C	-5.56	104.60	111.33
1	A	1022	SER	CA-C-N	5.53	126.08	120.38
1	A	1022	SER	C-N-CA	5.53	126.08	120.38
1	D	4324	ASP	N-CA-C	5.48	117.33	111.36
1	E	5359	ILE	CB-CA-C	-5.46	108.51	113.70
1	A	1507	GLY	N-CA-C	-5.45	107.73	115.30
1	A	1023	PRO	CA-C-N	5.40	125.57	119.90
1	A	1023	PRO	C-N-CA	5.40	125.57	119.90
1	E	5531	ALA	N-CA-C	-5.35	105.55	111.71
1	D	4318	LEU	N-CA-C	5.33	115.40	107.88
1	F	6396	ILE	CB-CA-C	-5.29	108.68	113.70
1	E	5416	LEU	N-CA-C	-5.27	105.70	111.82
1	A	1396	ILE	CB-CA-C	-5.27	108.70	113.70
1	D	4396	ILE	CB-CA-C	-5.21	108.75	113.70
1	C	3233	SER	N-CA-C	5.17	116.18	109.72
1	A	1425	MET	N-CA-C	5.16	116.72	111.14
1	E	5193	ASP	N-CA-C	-5.14	105.75	111.36
1	F	6319	LEU	N-CA-C	-5.11	102.19	110.32
1	F	6114	GLU	N-CA-C	-5.07	106.61	112.89
1	E	5090	ASP	CA-C-N	5.06	126.16	119.84
1	E	5090	ASP	C-N-CA	5.06	126.16	119.84
1	A	1319	LEU	N-CA-C	-5.05	101.00	109.24
1	A	1506	ASN	N-CA-C	5.05	120.29	113.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4131	174	0
1	B	4124	0	4126	190	0
1	C	4124	0	4126	187	0
1	D	4130	0	4131	152	0
1	E	4124	0	4126	186	0
1	F	4124	0	4126	159	0
2	A	14	0	13	0	0
2	B	14	0	13	3	0
2	C	14	0	13	0	0
2	D	14	0	13	2	0
2	E	28	0	26	2	0
2	F	14	0	13	2	0
3	A	21	0	18	5	0
3	B	21	0	18	17	0
3	F	21	0	18	5	0
4	A	1	0	0	5	0
4	E	1	0	0	2	0
5	A	60	0	63	21	0
5	B	60	0	63	15	0
5	C	60	0	63	13	0
5	D	60	0	63	13	0
5	E	60	0	63	15	0
5	F	60	0	63	13	0
6	A	249	0	0	13	0
6	B	303	0	0	26	0
6	C	289	0	0	27	0
6	D	291	0	0	16	0
6	E	295	0	0	22	0
6	F	254	0	0	25	0
All	All	26960	0	25289	1056	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1056) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5221:SER:HB3	4:E:15:CL:CL	1.58	1.39
1:F:6258:LYS:H	1:F:6258:LYS:HE2	1.17	1.08
1:C:3258:LYS:H	1:C:3258:LYS:HE2	1.19	1.02
1:B:2304:LEU:HD13	5:B:212:HTQ:H171	1.39	1.01
1:B:2079:ASN:HB3	3:B:282:SIA:H113	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.43	1.00
1:E:5221:SER:CB	4:E:15:CL:CL	2.48	0.98
1:C:3339:ARG:HD2	1:C:3440:ALA:HA	1.48	0.96
1:F:6215:VAL:H	1:F:6241:HIS:HD2	1.06	0.96
3:B:282:SIA:H92	1:C:3278:THR:HA	1.48	0.94
1:E:5215:VAL:H	1:E:5241:HIS:HD2	0.95	0.94
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.51	0.92
1:E:5317:PRO:HG2	1:E:5387:PRO:HB3	1.52	0.92
1:A:1215:VAL:H	1:A:1241:HIS:HD2	1.18	0.92
1:C:3215:VAL:H	1:C:3241:HIS:HD2	1.00	0.91
1:E:5317:PRO:CG	1:E:5387:PRO:HB3	2.00	0.91
1:B:2395:LEU:HB3	1:B:2550:LEU:HD11	1.51	0.91
1:E:5091:PRO:HG3	1:E:5112:LEU:HD11	1.51	0.90
6:D:7908:HOH:O	3:F:682:SIA:H91	1.72	0.90
1:E:5215:VAL:H	1:E:5241:HIS:CD2	1.87	0.90
1:C:3215:VAL:H	1:C:3241:HIS:CD2	1.88	0.89
2:B:279:NAG:H2	6:B:7845:HOH:O	1.72	0.88
1:A:1304:LEU:HD13	5:A:111:HTQ:H171	1.55	0.87
1:D:4242:ARG:HG2	1:D:4242:ARG:HH11	1.40	0.87
1:B:2237:LYS:HA	1:B:2342:HIS:CE1	2.10	0.86
1:B:2290:THR:OG1	1:B:2293:GLU:HG3	1.75	0.86
1:C:3296:GLU:HB3	6:C:7587:HOH:O	1.74	0.85
1:A:1368:LEU:HB2	5:A:1[Z]:HTQ:H151	1.57	0.85
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.22	0.85
1:F:6258:LYS:HE2	1:F:6258:LYS:N	1.90	0.85
2:E:579:NAG:O4	2:E:580:NAG:H5	1.78	0.83
1:A:1423:ASP:OD2	1:A:1543:GLU:HG2	1.78	0.83
3:B:282:SIA:H92	1:C:3278:THR:CA	2.08	0.83
1:F:6498:LYS:HB3	1:F:6514:LEU:HD11	1.62	0.81
1:C:3268:ILE:HG12	1:C:3301:MET:HE2	1.61	0.81
1:D:4215:VAL:H	1:D:4241:HIS:HD2	1.27	0.81
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.62	0.80
1:A:1363:LEU:HD22	5:A:111:HTQ:H181	1.63	0.80
1:E:5343:THR:HG21	1:E:5437:HIS:HE1	1.45	0.80
1:E:5104:ARG:HD3	6:E:7408:HOH:O	1.82	0.79
1:B:2132:ARG:HB3	1:B:2211:ASN:HB2	1.64	0.79
1:D:4290:THR:OG1	1:D:4293:GLU:HG3	1.83	0.79
1:E:5311:ASP:HB3	1:E:5314:GLU:HG2	1.65	0.78
1:F:6255:LEU:HD11	5:F:616:HTQ:H91	1.64	0.78
1:F:6343:THR:HA	6:F:7102:HOH:O	1.82	0.78
1:C:3392:ALA:HB3	1:C:3395:LEU:HG	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4132:ARG:HB3	1:D:4211:ASN:HB2	1.66	0.78
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.65	0.78
1:C:3318:LEU:HB2	6:C:7622:HOH:O	1.83	0.77
1:D:4145:MET:HB2	1:D:4304:LEU:HD11	1.67	0.77
1:E:5202:GLN:HE22	1:E:5215:VAL:HG21	1.47	0.77
1:F:6409:ASP:HB3	1:F:6412:LYS:HB3	1.67	0.77
1:A:1132:ARG:HB3	1:A:1211:ASN:HB2	1.65	0.77
1:F:6105:LYS:HG3	1:F:6106:GLU:H	1.48	0.76
1:F:6134:PRO:HG2	1:F:6163:VAL:HG12	1.67	0.76
1:E:5343:THR:HG21	1:E:5437:HIS:CE1	2.21	0.76
1:E:5130:LYS:HE3	1:E:5132:ARG:NH1	2.01	0.76
1:F:6275:LYS:HD2	6:F:8229:HOH:O	1.85	0.75
1:A:1261:VAL:HB	6:A:7809:HOH:O	1.85	0.75
3:A:182:SIA:H92	1:B:2279:SER:H	1.50	0.75
1:F:6339:ARG:HD2	1:F:6440:ALA:HA	1.68	0.75
1:B:2366:TYR:HB3	1:B:2368:LEU:HD13	1.69	0.75
1:A:1215:VAL:H	1:A:1241:HIS:CD2	2.05	0.75
1:A:1355:PHE:CE1	1:A:1360:PRO:HG3	2.21	0.75
1:E:5396:ILE:HB	1:E:5397:PRO:HD3	1.69	0.75
1:B:2142:GLY:HA2	5:B:212:HTQ:H131	1.68	0.75
1:F:6220:GLU:HG2	1:F:6472:LEU:HD21	1.69	0.75
1:D:4343:THR:HB	1:D:4442:ALA:HB2	1.69	0.74
1:E:5220:GLU:HG2	1:E:5472:LEU:HD21	1.68	0.74
1:F:6023:PRO:HB2	1:F:6034:LEU:HD21	1.67	0.74
1:D:4370:GLU:HG3	6:D:7641:HOH:O	1.87	0.74
1:A:1079:ASN:HB2	3:A:182:SIA:H113	1.69	0.74
1:F:6215:VAL:H	1:F:6241:HIS:CD2	1.98	0.74
1:B:2220:GLU:OE2	1:B:2221:SER:HB2	1.86	0.74
1:C:3105:LYS:HG3	1:C:3106:GLU:H	1.53	0.74
1:F:6258:LYS:H	1:F:6258:LYS:CE	1.98	0.74
1:B:2390:CYS:HB3	6:B:8305:HOH:O	1.87	0.74
1:B:2254:VAL:HG11	5:B:212:HTQ:H61	1.68	0.73
1:F:6095:GLN:O	1:F:6099:GLU:HG3	1.88	0.73
1:C:3258:LYS:H	1:C:3258:LYS:CE	1.98	0.73
1:E:5237:LYS:HG3	6:E:7151:HOH:O	1.88	0.73
1:E:5317:PRO:HB2	6:E:8626:HOH:O	1.88	0.73
1:B:2084:PRO:HA	3:B:282:SIA:O1B	1.89	0.73
1:C:3242:ARG:HG2	1:C:3242:ARG:HH11	1.52	0.72
1:B:2414:LYS:HZ2	5:B:2[Y]:HTQ:H181	1.53	0.72
1:E:5290:THR:OG1	1:E:5293:GLU:HG3	1.89	0.72
1:B:2023:PRO:HB3	1:B:2034:LEU:HD21	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3290:THR:OG1	1:C:3293:GLU:HG3	1.90	0.72
1:F:6288:GLN:HG3	6:F:8386:HOH:O	1.89	0.72
1:B:2376:LYS:HA	1:B:2379:MET:HE3	1.72	0.71
1:E:5388:LEU:HD22	1:E:5425:MET:HE1	1.71	0.71
1:D:4357:TRP:O	1:D:4360:PRO:HD2	1.90	0.71
1:E:5268:ILE:HD11	1:E:5319:LEU:HD21	1.72	0.71
1:E:5268:ILE:HG12	1:E:5301:MET:HE2	1.73	0.71
1:F:6370:GLU:HG2	6:F:7775:HOH:O	1.90	0.71
1:C:3215:VAL:N	1:C:3241:HIS:HD2	1.83	0.71
1:E:5215:VAL:N	1:E:5241:HIS:HD2	1.79	0.71
1:A:1105:LYS:HD2	6:A:8564:HOH:O	1.88	0.70
1:B:2264:LEU:HD13	1:B:2316:GLN:HG3	1.72	0.70
1:F:6190:GLY:O	1:F:6194:GLN:HG3	1.91	0.70
1:E:5343:THR:CG2	1:E:5437:HIS:HE1	2.03	0.70
1:A:1421:ILE:CG2	1:A:1425:MET:HE2	2.21	0.70
1:C:3339:ARG:HD2	1:C:3440:ALA:CA	2.20	0.70
1:C:3355:PHE:CE1	1:C:3360:PRO:HG3	2.27	0.70
1:E:5318:LEU:HB2	6:E:8626:HOH:O	1.92	0.70
1:A:1236:ALA:HA	1:A:1239:LEU:HD12	1.74	0.70
1:D:4268:ILE:HD11	1:D:4319:LEU:HD21	1.72	0.69
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.73	0.69
1:A:1498:LYS:HB3	1:A:1514:LEU:HD11	1.74	0.69
1:C:3316:GLN:HA	1:C:3316:GLN:HE21	1.56	0.69
1:E:5363:LEU:HB3	5:E:515:HTQ:H181	1.74	0.69
1:B:2082:SER:O	3:B:282:SIA:H32	1.93	0.69
1:E:5134:PRO:HG2	1:E:5163:VAL:HG12	1.75	0.69
3:A:182:SIA:C9	1:B:2279:SER:H	2.06	0.68
1:C:3417:PHE:O	1:C:3420:LEU:HB3	1.93	0.68
1:B:2252:THR:HG22	1:B:2254:VAL:HG12	1.74	0.68
1:E:5241:HIS:O	1:E:5344:VAL:HB	1.94	0.68
1:A:1255:LEU:HD11	5:A:111:HTQ:H91	1.74	0.68
1:F:6423:ASP:OD2	1:F:6543:GLU:HG2	1.94	0.68
1:F:6452:ARG:HB2	1:F:6465:ILE:HG12	1.76	0.68
1:C:3105:LYS:HG3	1:C:3106:GLU:N	2.07	0.68
1:C:3316:GLN:HE21	1:C:3316:GLN:CA	2.06	0.68
1:D:4456:SER:HB3	1:D:4460:LYS:HD3	1.75	0.68
1:E:5404:LEU:HB3	1:E:5413:LYS:HG2	1.76	0.67
1:F:6102:THR:OG1	1:F:6104:ARG:HG2	1.94	0.67
1:B:2215:VAL:H	1:B:2241:HIS:CD2	2.09	0.67
1:F:6260:ASP:OD2	1:F:6263:PRO:HD3	1.95	0.67
1:B:2237:LYS:HA	1:B:2342:HIS:HE1	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2367:PRO:C	1:B:2368:LEU:HD12	2.19	0.67
1:F:6024:PRO:HG3	1:F:6037:PHE:CZ	2.30	0.67
1:B:2352:LYS:HG2	1:B:2450:GLN:HE21	1.59	0.67
1:F:6105:LYS:HG3	1:F:6106:GLU:N	2.09	0.67
1:C:3225:GLU:O	1:C:3229:VAL:HG23	1.95	0.67
1:A:1262:LYS:HE2	1:A:1282:MET:HE1	1.75	0.67
1:B:2264:LEU:HD21	1:B:2319:LEU:HD23	1.78	0.66
1:D:4134:PRO:HG2	1:D:4163:VAL:HG12	1.75	0.66
1:E:5278:THR:OG1	1:E:5281:VAL:HG23	1.95	0.66
1:F:6398:GLU:HG3	6:F:7627:HOH:O	1.94	0.66
1:C:3278:THR:OG1	1:C:3281:VAL:HG23	1.95	0.66
1:C:3316:GLN:HA	1:C:3316:GLN:NE2	2.10	0.66
1:C:3254:VAL:HG11	5:C:313:HTQ:H61	1.76	0.66
1:C:3297:THR:O	1:C:3301:MET:HG2	1.94	0.66
1:E:5227:VAL:O	1:E:5231:VAL:HG23	1.95	0.66
1:B:2279:SER:O	1:B:2283:VAL:HG23	1.95	0.66
1:C:3292:GLU:O	1:C:3296:GLU:HG3	1.96	0.66
1:F:6355:PHE:CE1	1:F:6360:PRO:HG3	2.30	0.66
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.78	0.66
1:B:2091:PRO:HG3	1:B:2112:LEU:HD11	1.76	0.66
1:C:3258:LYS:HE2	1:C:3258:LYS:N	2.03	0.66
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.77	0.66
1:B:2097:LEU:HD13	5:B:212:HTQ:H161	1.78	0.65
1:D:4242:ARG:HG2	1:D:4242:ARG:NH1	2.12	0.65
1:D:4428:VAL:HB	1:D:4429:PRO:HD3	1.79	0.65
1:E:5317:PRO:HG3	1:E:5387:PRO:HB3	1.78	0.65
1:E:5395:LEU:HB3	1:E:5550:LEU:HD11	1.79	0.65
1:B:2084:PRO:HA	3:B:282:SIA:C1	2.26	0.65
1:F:6202:GLN:HG3	6:F:7812:HOH:O	1.97	0.65
1:F:6428:VAL:HB	1:F:6429:PRO:HD3	1.77	0.65
1:B:2084:PRO:HB3	3:B:282:SIA:O1A	1.97	0.65
1:A:1242:ARG:HG2	1:A:1242:ARG:HH11	1.62	0.65
1:B:2462:LYS:HG2	6:B:8127:HOH:O	1.96	0.65
1:F:6461:PRO:HB2	1:F:6464:VAL:HG23	1.79	0.65
1:C:3067:PRO:HB3	1:C:3192:LEU:HD13	1.79	0.64
1:E:5417:PHE:O	1:E:5420:LEU:HB3	1.98	0.64
1:B:2398:GLU:HG3	6:B:7416:HOH:O	1.97	0.64
1:E:5349:GLY:HA3	1:E:5447:TYR:CE1	2.32	0.64
1:C:3342:HIS:HB2	6:C:8259:HOH:O	1.98	0.64
1:D:4317:PRO:HD3	1:D:4387:PRO:HB2	1.80	0.64
1:E:5260:ASP:OD2	1:E:5263:PRO:HD3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6501:ALA:O	1:F:6505:ARG:HG2	1.98	0.64
1:D:4024:PRO:HG3	1:D:4037:PHE:CE1	2.33	0.64
1:C:3330:LYS:HB2	6:C:8029:HOH:O	1.97	0.64
1:A:1254:VAL:HG11	5:A:111:HTQ:H61	1.80	0.63
1:C:3364:MET:HE1	1:C:3388:LEU:HD11	1.80	0.63
1:E:5326:MET:HE2	6:E:8169:HOH:O	1.97	0.63
1:B:2052:GLY:HA3	3:B:282:SIA:H31	1.79	0.63
1:F:6420:LEU:HD12	1:F:6547:TRP:HZ2	1.63	0.63
1:A:1373:LEU:HD23	6:A:7567:HOH:O	1.97	0.63
1:C:3411:VAL:O	1:C:3414:LYS:HG2	1.99	0.63
1:C:3464:VAL:HG22	5:C:3[Y]:HTQ:H191	1.80	0.63
1:E:5341:PHE:HD1	1:E:5343:THR:HG23	1.64	0.63
1:A:1221:SER:HB3	4:A:11:CL:CL	2.34	0.63
1:C:3336:GLN:HE22	1:C:3433:VAL:HG13	1.62	0.63
1:C:3024:PRO:HG3	1:C:3037:PHE:CZ	2.33	0.63
1:D:4372:GLN:HG2	1:D:4410:THR:HB	1.79	0.63
1:A:1460:LYS:HE2	6:A:7357:HOH:O	1.99	0.62
1:B:2420:LEU:HD13	1:B:2547:TRP:CZ2	2.35	0.62
1:F:6368:LEU:HD12	5:F:6[Z]:HTQ:H151	1.81	0.62
1:A:1140:HIS:HD2	1:A:1141:GLY:O	1.83	0.62
1:A:1338:GLU:O	1:A:1339:ARG:HD2	2.00	0.62
1:C:3336:GLN:NE2	1:C:3433:VAL:HG13	2.14	0.62
1:D:4355:PHE:CE1	1:D:4360:PRO:HG3	2.33	0.62
1:A:1372:GLN:HE21	1:A:1372:GLN:N	1.96	0.62
3:B:282:SIA:C9	1:C:3278:THR:HA	2.24	0.62
1:D:4338:GLU:HG2	1:D:4341:PHE:HB2	1.82	0.62
1:E:5264:LEU:HD22	1:E:5316:GLN:HE21	1.65	0.62
1:A:1277:THR:HG22	1:A:1278:THR:HG23	1.81	0.62
1:E:5102:THR:OG1	1:E:5104:ARG:HG2	1.99	0.62
1:F:6083:TYR:CE2	1:F:6108:ILE:HD13	2.35	0.62
1:E:5403:TYR:CD1	1:E:5420:LEU:HD13	2.34	0.62
1:D:4370:GLU:HB3	1:D:4372:GLN:NE2	2.15	0.62
1:B:2202:GLN:HE22	1:B:2215:VAL:HG21	1.63	0.62
1:B:2352:LYS:HG2	1:B:2450:GLN:NE2	2.14	0.62
1:C:3145:MET:HG3	1:C:3304:LEU:HD11	1.82	0.62
1:F:6089:GLN:HB2	1:F:6146:VAL:HG12	1.81	0.62
1:E:5312:PRO:HG3	1:E:5384:LYS:HD3	1.82	0.62
1:D:4261:VAL:HA	6:D:7290:HOH:O	2.00	0.61
1:F:6262:LYS:HE2	1:F:6282:MET:HE1	1.82	0.61
1:B:2236:ALA:HA	1:B:2239:LEU:HD12	1.82	0.61
1:C:3095:GLN:O	1:C:3099:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4143:GLY:CA	5:D:414:HTQ:H42	2.30	0.61
1:D:4459:MET:HE2	6:D:8676:HOH:O	1.99	0.61
1:F:6538:LYS:HB3	1:F:6541:ASP:HB2	1.81	0.61
1:F:6538:LYS:HE2	6:F:8409:HOH:O	1.99	0.61
1:D:4487:GLU:HG3	1:D:4491:ARG:NH1	2.15	0.61
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.36	0.61
1:B:2215:VAL:N	1:B:2241:HIS:HD2	1.96	0.61
1:F:6417:PHE:O	1:F:6420:LEU:HB3	2.00	0.61
1:A:1370:GLU:HB3	1:A:1372:GLN:HE22	1.66	0.60
1:B:2079:ASN:HB2	6:B:8690:HOH:O	2.01	0.60
1:B:2428:VAL:HB	1:B:2429:PRO:HD3	1.83	0.60
1:E:5140:HIS:HD2	1:E:5141:GLY:O	1.84	0.60
1:B:2085:PRO:HD3	3:B:282:SIA:O1B	2.00	0.60
1:C:3260:ASP:OD2	1:C:3263:PRO:HD3	2.01	0.60
1:E:5296:GLU:HG2	6:E:8471:HOH:O	2.01	0.60
1:E:5366:TYR:HB3	1:E:5368:LEU:HD13	1.82	0.60
1:E:5538:LYS:HE2	6:E:8549:HOH:O	2.00	0.60
1:E:5264:LEU:HD22	1:E:5316:GLN:NE2	2.15	0.60
1:A:1143:GLY:N	4:A:11:CL:CL	2.68	0.60
1:E:5429:PRO:O	1:E:5433:VAL:HG23	2.01	0.60
1:F:6252:THR:HG22	1:F:6254:VAL:HG12	1.82	0.60
1:E:5403:TYR:O	1:E:5416:LEU:HD13	2.00	0.60
1:E:5089:GLN:OE1	1:E:5146:VAL:HB	2.02	0.60
1:E:5089:GLN:HB2	1:E:5146:VAL:HG12	1.83	0.60
1:A:1145:MET:HB2	1:A:1304:LEU:HD11	1.83	0.59
1:D:4237:LYS:HE3	1:D:4342:HIS:HB2	1.84	0.59
1:D:4105:LYS:HA	1:D:4482:LYS:HG2	1.84	0.59
1:D:4292:GLU:CD	1:D:4292:GLU:H	2.10	0.59
1:C:3242:ARG:HD3	1:C:3503:PHE:O	2.02	0.59
1:C:3414:LYS:HG3	1:C:3415:ASP:N	2.16	0.59
1:F:6370:GLU:HB3	1:F:6372:GLN:HG2	1.84	0.59
1:F:6429:PRO:O	1:F:6433:VAL:HG23	2.02	0.59
1:A:1308:LEU:HD11	1:A:1367:PRO:HG3	1.83	0.59
1:D:4238:ASN:HB2	6:D:7053:HOH:O	2.01	0.59
1:E:5292:GLU:CD	1:E:5292:GLU:H	2.09	0.59
1:C:3315:SER:HA	6:C:8252:HOH:O	2.03	0.59
1:B:2363:LEU:HD13	5:B:212:HTQ:C16	2.31	0.59
1:C:3349:GLY:HA3	1:C:3447:TYR:CE1	2.38	0.59
1:F:6342:HIS:HB2	6:F:7674:HOH:O	2.03	0.59
1:A:1456:SER:HB3	1:A:1460:LYS:HD3	1.84	0.58
1:B:2363:LEU:HD22	5:B:212:HTQ:H181	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2414:LYS:NZ	5:B:2[Y]:HTQ:H181	2.17	0.58
1:E:5363:LEU:HD13	5:E:515:HTQ:H161	1.85	0.58
1:F:6332:PRO:O	1:F:6336:GLN:HG3	2.02	0.58
1:B:2375:GLN:HG3	1:B:2379:MET:HE2	1.86	0.58
1:B:2420:LEU:HD13	1:B:2547:TRP:HZ2	1.68	0.58
1:E:5190:GLY:O	1:E:5194:GLN:HG3	2.03	0.58
1:D:4445:TYR:CE1	1:D:4519:GLU:HA	2.38	0.58
1:C:3400:THR:HG23	1:C:3404:LEU:HD12	1.85	0.58
1:A:1297:THR:O	1:A:1301:MET:HG2	2.03	0.58
1:D:4199:ARG:HG2	1:D:4199:ARG:HH11	1.68	0.58
1:E:5428:VAL:HB	1:E:5429:PRO:HD3	1.85	0.58
1:B:2255:LEU:HD11	5:B:212:HTQ:H91	1.85	0.58
1:C:3357:TRP:HB2	5:C:3[Z]:HTQ:H171	1.84	0.58
1:D:4081:THR:OG1	2:D:479:NAG:H82	2.04	0.58
1:A:1024:PRO:HG3	1:A:1037:PHE:CZ	2.39	0.58
1:B:2145:MET:HB2	1:B:2304:LEU:HD11	1.86	0.58
1:A:1021:SER:HB2	6:A:8675:HOH:O	2.04	0.57
1:A:1097:LEU:HD13	5:A:111:HTQ:H161	1.87	0.57
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.19	0.57
1:A:1023:PRO:CB	1:A:1034:LEU:HD21	2.34	0.57
1:A:1377:THR:O	1:A:1380:SER:HB3	2.05	0.57
1:F:6522:GLN:HB2	6:F:8312:HOH:O	2.04	0.57
1:A:1343:THR:HB	1:A:1442:ALA:HB2	1.86	0.57
1:A:1351:ASN:HB3	1:A:1466:GLY:O	2.05	0.57
1:B:2461:PRO:HG2	1:B:2464:VAL:HG23	1.87	0.57
1:C:3149:ALA:HB2	1:C:3169:GLN:HG3	1.86	0.57
1:A:1215:VAL:N	1:A:1241:HIS:HD2	1.96	0.57
1:E:5023:PRO:HB2	1:E:5034:LEU:HD21	1.87	0.57
1:F:6176:GLY:HA2	1:F:6189:TRP:HB2	1.87	0.57
1:F:6339:ARG:HD2	1:F:6440:ALA:CA	2.35	0.57
1:B:2547:TRP:CZ3	1:B:2550:LEU:HD23	2.40	0.57
1:D:4251:LEU:HD22	1:D:4333:GLU:OE2	2.05	0.57
1:F:6268:ILE:HD11	1:F:6319:LEU:HD21	1.86	0.56
1:A:1292:GLU:CD	1:A:1292:GLU:H	2.13	0.56
1:A:1474:SER:HB3	1:A:1496:VAL:HG21	1.87	0.56
1:C:3104:ARG:HD3	6:C:8237:HOH:O	2.04	0.56
1:F:6255:LEU:HD23	1:F:6318:LEU:HD11	1.87	0.56
1:B:2353:GLN:NE2	1:B:2465:ILE:H	2.03	0.56
1:C:3045:GLN:NE2	1:C:3046:PRO:HD2	2.20	0.56
1:E:5332:PRO:O	1:E:5336:GLN:HG3	2.06	0.56
1:F:6156:ALA:HB3	6:F:7194:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6357:TRP:HA	5:F:6[Y]:HTQ:H181	1.88	0.56
1:F:6386:TYR:N	1:F:6387:PRO:HD2	2.20	0.56
1:B:2220:GLU:HG3	6:B:7802:HOH:O	2.06	0.56
1:C:3414:LYS:NZ	5:C:3[Z]:HTQ:H161	2.20	0.56
1:E:5538:LYS:HD2	1:E:5541:ASP:OD2	2.05	0.56
1:F:6258:LYS:HD3	6:F:8619:HOH:O	2.05	0.56
1:B:2461:PRO:HG2	1:B:2464:VAL:CG2	2.35	0.56
1:E:5149:ALA:HB2	1:E:5169:GLN:HG3	1.88	0.56
1:E:5237:LYS:HZ3	1:E:5342:HIS:CB	2.19	0.56
1:E:5303:PHE:HD2	1:E:5317:PRO:O	1.88	0.56
1:A:1370:GLU:HB3	1:A:1372:GLN:NE2	2.21	0.56
1:B:2254:VAL:HG22	1:B:2318:LEU:HD12	1.88	0.56
1:D:4199:ARG:HG2	1:D:4199:ARG:NH1	2.19	0.56
1:D:4275:LYS:HG3	6:F:8666:HOH:O	2.05	0.56
1:E:5202:GLN:NE2	1:E:5215:VAL:HG21	2.19	0.56
1:A:1135:VAL:HG21	1:A:1205:ILE:HG12	1.88	0.56
1:B:2246:GLU:HG2	1:B:2447:TYR:OH	2.06	0.56
1:C:3338:GLU:OE1	1:C:3340:ASN:HB3	2.05	0.56
1:F:6455:PHE:CD2	1:F:6482:LYS:HD3	2.40	0.56
1:D:4338:GLU:CG	1:D:4341:PHE:HB2	2.36	0.55
1:B:2074:TRP:CD2	1:B:2078:LYS:HE2	2.41	0.55
1:E:5342:HIS:HD2	6:E:8426:HOH:O	1.89	0.55
1:A:1363:LEU:HD13	5:A:111:HTQ:C16	2.37	0.55
1:D:4089:GLN:HB2	1:D:4146:VAL:HG12	1.88	0.55
1:F:6315:SER:HB2	6:F:8469:HOH:O	2.06	0.55
1:A:1043:PHE:HA	6:A:7064:HOH:O	2.07	0.55
1:A:1403:TYR:O	1:A:1416:LEU:HD13	2.06	0.55
1:D:4215:VAL:H	1:D:4241:HIS:CD2	2.17	0.55
1:E:5258:LYS:HD2	1:E:5258:LYS:O	2.06	0.55
1:E:5262:LYS:HB3	1:E:5263:PRO:HD3	1.88	0.55
1:A:1403:TYR:CD1	1:A:1420:LEU:HD23	2.42	0.55
1:D:4105:LYS:HG2	6:D:7281:HOH:O	2.06	0.55
1:E:5140:HIS:HE1	6:E:7090:HOH:O	1.90	0.55
1:F:6255:LEU:HD11	5:F:616:HTQ:C9	2.36	0.55
1:A:1368:LEU:O	5:A:1[Y]:HTQ:H22	2.06	0.55
1:B:2024:PRO:HG3	1:B:2037:PHE:CZ	2.42	0.55
1:D:4236:ALA:HA	1:D:4239:LEU:HD12	1.89	0.55
1:D:4461:PRO:HG2	1:D:4464:VAL:HG23	1.89	0.55
1:F:6414:LYS:HG3	1:F:6415:ASP:N	2.21	0.55
1:F:6242:ARG:HG2	1:F:6242:ARG:HH11	1.71	0.55
1:F:6431:VAL:HG21	1:F:6540:LYS:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4262:LYS:O	1:D:4266:GLU:HG3	2.07	0.55
1:E:5131:ASN:HB2	6:E:7188:HOH:O	2.06	0.55
1:E:5357:TRP:HA	5:E:5[Y]:HTQ:H171	1.88	0.55
1:C:3262:LYS:HB3	1:C:3263:PRO:HD3	1.89	0.55
1:D:4103:ASN:ND2	1:D:4476:PHE:HB3	2.22	0.55
1:E:5461:PRO:HG2	1:E:5464:VAL:CG2	2.37	0.55
1:D:4140:HIS:HD2	1:D:4141:GLY:O	1.90	0.54
1:B:2338:GLU:O	1:B:2339:ARG:C	2.49	0.54
1:C:3145:MET:HG3	1:C:3318:LEU:HD21	1.89	0.54
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.22	0.54
1:D:4297:THR:O	1:D:4301:MET:HG2	2.07	0.54
1:A:1199:ARG:HG2	1:A:1199:ARG:HH11	1.71	0.54
1:B:2047:VAL:HG21	1:B:2155:LEU:HD23	1.89	0.54
1:C:3348:VAL:O	1:C:3446:MET:HA	2.07	0.54
1:F:6403:TYR:O	1:F:6416:LEU:HD13	2.08	0.54
1:B:2436:ASN:HB3	6:B:7545:HOH:O	2.06	0.54
1:A:1343:THR:HA	6:A:7195:HOH:O	2.07	0.54
1:D:4086:MET:HE3	1:D:4112:LEU:HD21	1.90	0.54
1:A:1428:VAL:HB	1:A:1429:PRO:HD3	1.89	0.54
1:A:1138:TRP:HH2	1:A:1220:GLU:HB2	1.71	0.54
1:D:4404:LEU:C	1:D:4406:GLY:H	2.16	0.54
1:A:1461:PRO:HG2	1:A:1464:VAL:HG23	1.90	0.54
1:F:6241:HIS:O	1:F:6242:ARG:HG2	2.08	0.54
1:F:6304:LEU:HD23	5:F:616:HTQ:C17	2.38	0.54
1:A:1369:SER:O	5:A:1[Z]:HTQ:H91	2.08	0.54
1:B:2486:SER:O	1:B:2490:ILE:HG13	2.08	0.54
1:E:5364:MET:HE1	1:E:5388:LEU:HD21	1.89	0.54
1:A:1025:VAL:HG22	1:A:1034:LEU:HD23	1.90	0.53
1:D:4254:VAL:HG11	5:D:414:HTQ:H72	1.90	0.53
1:D:4461:PRO:HG2	1:D:4464:VAL:CG2	2.38	0.53
1:E:5388:LEU:HD22	1:E:5425:MET:CE	2.38	0.53
1:B:2264:LEU:HD21	1:B:2319:LEU:CD2	2.38	0.53
1:B:2495:MET:HE1	1:B:2533:THR:OG1	2.09	0.53
1:C:3437:HIS:HE1	6:C:7026:HOH:O	1.90	0.53
1:E:5268:ILE:CD1	1:E:5319:LEU:HD21	2.37	0.53
1:A:1221:SER:CB	4:A:11:CL:CL	2.93	0.53
1:B:2292:GLU:CD	1:B:2292:GLU:H	2.16	0.53
1:B:2403:TYR:O	1:B:2416:LEU:HD13	2.07	0.53
1:E:5241:HIS:C	1:E:5242:ARG:HD2	2.34	0.53
1:E:5255:LEU:HD11	5:E:515:HTQ:H91	1.90	0.53
1:B:2220:GLU:HA	1:B:2246:GLU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2242:ARG:HG3	1:B:2242:ARG:HH11	1.74	0.53
1:E:5220:GLU:O	1:E:5221:SER:HB2	2.08	0.53
1:E:5491:ARG:HG2	1:E:5491:ARG:HH11	1.74	0.53
1:F:6284:HIS:O	1:F:6288:GLN:HG2	2.08	0.53
1:F:6456:SER:HB3	1:F:6460:LYS:HD3	1.91	0.53
1:A:1254:VAL:HG12	6:A:7530:HOH:O	2.09	0.53
1:B:2024:PRO:HG3	1:B:2037:PHE:CE1	2.43	0.53
1:F:6119:LEU:HD12	1:F:6119:LEU:C	2.34	0.53
1:A:1221:SER:HA	1:A:1247:SER:O	2.09	0.53
1:B:2452:ARG:NE	1:B:2462:LYS:HA	2.23	0.53
1:C:3138:TRP:CZ3	1:C:3219:GLY:HA2	2.44	0.53
1:C:3429:PRO:O	1:C:3433:VAL:HG23	2.09	0.53
1:D:4227:VAL:O	1:D:4231:VAL:HG23	2.09	0.53
1:E:5402:LYS:NZ	1:E:5546:PHE:CD1	2.75	0.53
1:F:6090:ASP:HB3	1:F:6093:ALA:HB3	1.91	0.53
1:A:1132:ARG:HG2	6:A:8191:HOH:O	2.09	0.52
1:C:3023:PRO:HB2	1:C:3034:LEU:HD21	1.91	0.52
1:F:6040:LEU:HG	6:F:8070:HOH:O	2.09	0.52
1:F:6119:LEU:HD12	1:F:6119:LEU:O	2.09	0.52
1:A:1102:THR:OG1	1:A:1104:ARG:HG2	2.08	0.52
1:B:2081:THR:OG1	2:B:279:NAG:H82	2.10	0.52
1:B:2372:GLN:O	1:B:2373:LEU:HB2	2.08	0.52
1:D:4357:TRP:CH2	1:D:4361:MET:HE2	2.44	0.52
1:D:4486:SER:O	1:D:4490:ILE:HG13	2.08	0.52
1:D:4553:LYS:HB3	6:D:7920:HOH:O	2.08	0.52
1:E:5030:HIS:HD2	6:E:7229:HOH:O	1.92	0.52
1:C:3139:ILE:HG12	1:C:3168:ILE:HD11	1.91	0.52
1:C:3398:GLU:HG3	6:C:7478:HOH:O	2.09	0.52
1:C:3456:SER:HA	6:C:7789:HOH:O	2.10	0.52
1:B:2292:GLU:HG3	6:C:8454:HOH:O	2.10	0.52
1:C:3464:VAL:HG22	5:C:3[Z]:HTQ:H191	1.92	0.52
1:F:6351:ASN:ND2	1:F:6449:PHE:HB3	2.25	0.52
1:A:1366:TYR:O	5:A:1[Z]:HTQ:H171	2.09	0.52
1:B:2104:ARG:CZ	1:B:2153:ASP:HB2	2.39	0.52
1:B:2389:VAL:HB	1:B:2424:VAL:HG11	1.90	0.52
1:D:4383:TRP:O	1:D:4386:TYR:HB2	2.10	0.52
1:E:5354:GLU:O	1:E:5468:HIS:HB2	2.09	0.52
1:F:6030:HIS:HD2	6:F:8639:HOH:O	1.91	0.52
1:B:2351:ASN:ND2	1:B:2449:PHE:HB3	2.24	0.52
1:C:3388:LEU:HD22	1:C:3425:MET:HE1	1.92	0.52
1:D:4262:LYS:HE3	1:D:4279:SER:OG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:LEU:HD12	5:A:1[Y]:HTQ:H151	1.92	0.52
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.25	0.52
1:A:1421:ILE:HG22	1:A:1425:MET:HE2	1.92	0.52
1:B:2084:PRO:CB	3:B:282:SIA:O1A	2.58	0.52
1:D:4339:ARG:HG3	1:D:4440:ALA:HA	1.91	0.52
1:F:6220:GLU:HA	1:F:6246:GLU:O	2.10	0.52
1:A:1402:LYS:HG2	1:A:1546:PHE:CE1	2.45	0.52
1:B:2052:GLY:HA3	3:B:282:SIA:O1A	2.09	0.52
1:B:2261:VAL:HA	6:B:7763:HOH:O	2.10	0.52
1:D:4491:ARG:HG3	1:D:4491:ARG:HH11	1.75	0.52
1:D:4495:MET:HE1	1:D:4533:THR:OG1	2.09	0.52
1:A:1241:HIS:O	1:A:1242:ARG:HG2	2.10	0.52
1:E:5358:LEU:HG	1:E:5363:LEU:HD12	1.92	0.52
1:A:1034:LEU:HD13	1:A:1034:LEU:C	2.35	0.51
1:B:2231:VAL:HA	1:B:2342:HIS:HD2	1.73	0.51
1:C:3334:GLU:HG2	6:C:8402:HOH:O	2.10	0.51
1:C:3382:LEU:HD23	1:C:3396:ILE:HG23	1.90	0.51
1:E:5382:LEU:HD11	1:E:5391:ILE:HD12	1.92	0.51
1:F:6135:VAL:HB	1:F:6215:VAL:HG22	1.92	0.51
1:F:6480:PHE:HB3	6:F:8202:HOH:O	2.10	0.51
1:B:2227:VAL:O	1:B:2231:VAL:HG23	2.10	0.51
1:B:2352:LYS:HE2	1:B:2450:GLN:NE2	2.24	0.51
1:D:4201:VAL:HG13	1:D:4205:ILE:HB	1.92	0.51
1:D:4332:PRO:O	1:D:4336:GLN:HG2	2.11	0.51
1:E:5304:LEU:HD13	5:E:515:HTQ:C19	2.41	0.51
1:F:6292:GLU:CD	1:F:6292:GLU:H	2.18	0.51
1:C:3512:GLU:HB3	6:C:7617:HOH:O	2.10	0.51
1:D:4369:SER:O	5:D:4[Z]:HTQ:H51	2.10	0.51
1:F:6358:LEU:HD23	1:F:6468:HIS:HD2	1.75	0.51
1:F:6478:ALA:N	1:F:6479:PRO:CD	2.74	0.51
1:A:1308:LEU:HD11	1:A:1367:PRO:CG	2.40	0.51
1:E:5242:ARG:HG3	1:E:5242:ARG:HH11	1.74	0.51
1:B:2040:LEU:HD22	1:B:2156:ALA:HA	1.92	0.51
1:A:1079:ASN:CB	3:A:182:SIA:H113	2.40	0.51
1:A:1551:PHE:C	1:A:1553:LYS:H	2.18	0.51
1:C:3364:MET:CE	1:C:3388:LEU:HD11	2.41	0.51
1:C:3407:THR:HG21	6:C:7543:HOH:O	2.09	0.51
1:D:4386:TYR:N	1:D:4387:PRO:HD2	2.26	0.51
1:F:6396:ILE:HB	1:F:6397:PRO:HD3	1.91	0.51
1:A:1385:SER:O	1:A:1389:VAL:HG22	2.11	0.51
1:B:2534:GLN:HG2	6:B:7715:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3102:THR:OG1	1:C:3104:ARG:HG2	2.11	0.51
1:D:4024:PRO:HG3	1:D:4037:PHE:CZ	2.45	0.51
1:D:4349:GLY:HA3	1:D:4447:TYR:CE1	2.46	0.51
1:F:6237:LYS:HG3	1:F:6238:ASN:ND2	2.26	0.51
1:B:2025:VAL:HG22	1:B:2034:LEU:HD23	1.92	0.51
1:B:2268:ILE:HD11	1:B:2319:LEU:HD21	1.92	0.51
1:B:2352:LYS:HE2	1:B:2450:GLN:HE22	1.75	0.51
1:B:2541:ASP:HB3	6:B:8152:HOH:O	2.11	0.51
2:B:279:NAG:H4	6:B:8352:HOH:O	2.11	0.51
1:D:4206:ALA:HB3	6:D:7552:HOH:O	2.10	0.51
1:B:2341:PHE:HA	6:B:7548:HOH:O	2.10	0.51
1:D:4304:LEU:HD13	5:D:414:HTQ:C17	2.40	0.51
1:F:6152:TYR:CD1	1:F:6152:TYR:N	2.79	0.51
1:A:1254:VAL:HG21	1:A:1388:LEU:HD23	1.93	0.50
1:A:1313:ARG:HA	1:A:1386:TYR:CD2	2.46	0.50
1:C:3522:GLN:HB2	6:C:7554:HOH:O	2.12	0.50
1:B:2119:LEU:HD12	1:B:2119:LEU:O	2.11	0.50
1:D:4237:LYS:HG3	1:D:4342:HIS:ND1	2.25	0.50
2:D:479:NAG:H3	6:D:8543:HOH:O	2.11	0.50
1:F:6363:LEU:HB3	5:F:616:HTQ:C18	2.41	0.50
1:F:6368:LEU:HB2	5:F:6[Z]:HTQ:H151	1.93	0.50
1:C:3268:ILE:HD11	1:C:3319:LEU:HD21	1.93	0.50
1:C:3355:PHE:CD1	1:C:3360:PRO:HG3	2.46	0.50
1:C:3364:MET:SD	1:C:3388:LEU:HD11	2.52	0.50
1:B:2084:PRO:CA	3:B:282:SIA:O1A	2.60	0.50
1:B:2338:GLU:HB2	1:B:2340:ASN:HB3	1.91	0.50
1:C:3140:HIS:HD2	1:C:3141:GLY:O	1.95	0.50
1:C:3339:ARG:HB3	6:C:7469:HOH:O	2.10	0.50
1:E:5241:HIS:HA	1:E:5344:VAL:HG11	1.93	0.50
1:B:2138:TRP:CZ3	1:B:2219:GLY:HA2	2.46	0.50
1:B:2357:TRP:CE3	1:B:2460:LYS:HB2	2.47	0.50
1:D:4279:SER:HA	1:D:4282:MET:HE3	1.93	0.50
1:E:5478:ALA:HB3	1:E:5479:PRO:HD3	1.92	0.50
1:B:2032:LYS:HG3	6:B:7916:HOH:O	2.10	0.50
1:E:5394:GLU:O	1:E:5397:PRO:HD2	2.10	0.50
1:F:6357:TRP:HA	5:F:6[Y]:HTQ:C18	2.41	0.50
1:C:3375:GLN:O	1:C:3379:MET:HG3	2.12	0.50
1:F:6306:LEU:HD22	1:F:6366:TYR:CE1	2.46	0.50
1:A:1063:LEU:HD21	1:A:1069:GLN:NE2	2.27	0.50
5:B:2[Z]:HTQ:H51	6:B:8669:HOH:O	2.12	0.50
1:C:3304:LEU:HG	5:C:313:HTQ:C19	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4040:LEU:O	1:D:4041:GLU:C	2.54	0.50
1:D:4225:GLU:O	1:D:4229:VAL:HG23	2.11	0.50
1:E:5099:GLU:HG3	1:E:5107:ASN:OD1	2.12	0.50
1:E:5237:LYS:HZ3	1:E:5342:HIS:HB2	1.77	0.50
1:B:2437:HIS:HD2	1:B:2444:THR:OG1	1.95	0.50
1:C:3376:LYS:HE3	6:C:8551:HOH:O	2.11	0.50
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.94	0.50
1:F:6036:LYS:NZ	6:F:7752:HOH:O	2.44	0.50
1:B:2284:HIS:O	1:B:2288:GLN:HG2	2.12	0.49
1:C:3242:ARG:HG2	1:C:3242:ARG:NH1	2.25	0.49
1:E:5364:MET:SD	1:E:5388:LEU:HD11	2.52	0.49
1:C:3456:SER:HB3	1:C:3460:LYS:HD3	1.94	0.49
2:F:679:NAG:H81	3:F:682:SIA:O9	2.11	0.49
1:A:1447:TYR:C	1:A:1447:TYR:CD2	2.89	0.49
1:E:5220:GLU:HA	1:E:5246:GLU:O	2.12	0.49
1:A:1143:GLY:O	1:A:1318:LEU:HD22	2.13	0.49
1:A:1358:LEU:HG	1:A:1363:LEU:HD11	1.94	0.49
1:D:4547:TRP:CZ3	1:D:4550:LEU:HD23	2.46	0.49
1:C:3383:TRP:HB2	6:C:7716:HOH:O	2.13	0.49
1:C:3528:GLN:O	1:C:3533:THR:HA	2.13	0.49
1:D:4308:LEU:HD11	1:D:4367:PRO:HG3	1.95	0.49
1:B:2023:PRO:CB	1:B:2034:LEU:HD21	2.39	0.49
1:B:2080:ALA:HA	3:B:282:SIA:O4	2.12	0.49
1:D:4263:PRO:HD2	6:D:7290:HOH:O	2.12	0.49
1:B:2145:MET:CB	1:B:2304:LEU:HD11	2.43	0.49
1:C:3220:GLU:HG2	1:C:3472:LEU:HD21	1.94	0.49
1:E:5254:VAL:HG11	5:E:515:HTQ:H61	1.94	0.49
1:E:5356:GLY:O	5:E:5[Y]:HTQ:H171	2.13	0.49
1:F:6404:LEU:O	1:F:6413:LYS:HE2	2.11	0.49
1:A:1551:PHE:C	1:A:1553:LYS:N	2.69	0.49
1:C:3461:PRO:HB2	1:C:3464:VAL:HG23	1.95	0.49
1:B:2143:GLY:O	1:B:2144:LEU:HB2	2.12	0.49
1:C:3352:LYS:HG2	6:C:8697:HOH:O	2.13	0.49
1:E:5145:MET:HG2	1:E:5318:LEU:HD21	1.95	0.49
1:E:5386:TYR:N	1:E:5387:PRO:CD	2.75	0.49
1:F:6079:ASN:O	3:F:682:SIA:H6	2.12	0.49
1:C:3375:GLN:NE2	1:C:3400:THR:HG22	2.28	0.49
1:D:4437:HIS:HD2	1:D:4444:THR:OG1	1.96	0.49
1:E:5237:LYS:NZ	1:E:5342:HIS:HB2	2.28	0.49
1:E:5296:GLU:HG3	6:E:7989:HOH:O	2.13	0.49
1:E:5348:VAL:O	1:E:5446:MET:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6231:VAL:HG13	6:F:7815:HOH:O	2.12	0.49
1:A:1095:GLN:O	1:A:1099:GLU:HG3	2.13	0.48
1:B:2025:VAL:CG2	1:B:2034:LEU:HD23	2.43	0.48
3:B:282:SIA:H92	1:C:3279:SER:H	1.78	0.48
1:D:4040:LEU:HD22	1:D:4156:ALA:HA	1.94	0.48
1:F:6368:LEU:HB2	5:F:6[Y]:HTQ:H151	1.95	0.48
1:A:1372:GLN:N	1:A:1372:GLN:NE2	2.62	0.48
1:B:2119:LEU:HD12	1:B:2119:LEU:C	2.37	0.48
1:D:4339:ARG:HH21	1:D:4439:ASP:HB2	1.78	0.48
1:E:5271:THR:CG2	1:E:5297:THR:HG23	2.43	0.48
1:E:5292:GLU:CD	1:E:5292:GLU:N	2.71	0.48
1:A:1403:TYR:CG	1:A:1420:LEU:HD23	2.48	0.48
1:E:5045:GLN:NE2	1:E:5046:PRO:HD2	2.28	0.48
1:E:5338:GLU:C	1:E:5340:ASN:N	2.67	0.48
1:A:1097:LEU:HD13	5:A:111:HTQ:C16	2.42	0.48
1:A:1186:ARG:HB3	1:A:1324:ASP:HB2	1.95	0.48
1:A:1373:LEU:HD11	6:A:8101:HOH:O	2.13	0.48
1:B:2337:ALA:C	1:B:2339:ARG:H	2.22	0.48
1:C:3308:LEU:HD11	1:C:3367:PRO:HG3	1.95	0.48
1:E:5552:ALA:HB3	6:E:8130:HOH:O	2.13	0.48
1:F:6140:HIS:HD2	1:F:6141:GLY:O	1.97	0.48
1:F:6254:VAL:HG11	5:F:616:HTQ:H61	1.96	0.48
1:F:6264:LEU:HD11	1:F:6316:GLN:HG2	1.94	0.48
1:A:1348:VAL:O	1:A:1446:MET:HA	2.14	0.48
1:B:2478:ALA:HB3	1:B:2479:PRO:HD3	1.96	0.48
1:D:4105:LYS:HG3	1:D:4106:GLU:N	2.28	0.48
1:B:2048:ALA:HB3	1:B:2123:THR:CG2	2.44	0.48
1:E:5074:TRP:CD2	1:E:5078:LYS:HE2	2.48	0.48
1:E:5351:ASN:ND2	1:E:5449:PHE:HB3	2.28	0.48
1:A:1420:LEU:HD22	1:A:1547:TRP:HZ2	1.78	0.48
1:B:2103:ASN:HB3	6:B:8481:HOH:O	2.14	0.48
1:B:2140:HIS:CD2	1:B:2147:GLY:HA3	2.49	0.48
1:B:2366:TYR:HB3	1:B:2368:LEU:CD1	2.41	0.48
1:D:4355:PHE:CD1	1:D:4360:PRO:HG3	2.49	0.48
1:D:4369:SER:HA	5:D:4[Y]:HTQ:H21	1.95	0.48
1:E:5026:VAL:CG1	1:E:5207:SER:HB3	2.44	0.48
1:E:5048:ALA:HB3	1:E:5123:THR:HG23	1.95	0.48
1:E:5138:TRP:CZ3	1:E:5219:GLY:HA2	2.49	0.48
1:F:6414:LYS:O	1:F:6418:LEU:HG	2.14	0.48
1:A:1221:SER:OG	4:A:11:CL:CL	2.68	0.48
1:A:1304:LEU:CD1	5:A:111:HTQ:H171	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1435:ARG:O	1:A:1438:ARG:HB3	2.14	0.48
1:B:2044:ALA:O	1:F:6491:ARG:HD2	2.13	0.48
1:B:2425:MET:CE	5:B:212:HTQ:H72	2.44	0.48
1:C:3254:VAL:HG13	1:C:3255:LEU:HG	1.95	0.48
1:F:6146:VAL:HG21	5:F:616:HTQ:H171	1.95	0.48
1:B:2369:SER:O	5:B:2[Y]:HTQ:H51	2.14	0.48
1:D:4382:LEU:HD23	1:D:4396:ILE:HG23	1.95	0.48
1:F:6351:ASN:HB3	1:F:6466:GLY:O	2.13	0.48
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.96	0.48
1:B:2023:PRO:HA	1:B:2024:PRO:HD3	1.83	0.48
1:D:4211:ASN:C	1:D:4213:GLY:H	2.22	0.48
1:D:4452:ARG:HG2	6:D:8033:HOH:O	2.14	0.48
1:F:6225:GLU:O	1:F:6229:VAL:HG23	2.13	0.48
1:F:6447:TYR:C	1:F:6447:TYR:CD2	2.92	0.48
1:B:2334:GLU:O	1:B:2338:GLU:HG3	2.14	0.47
2:E:579:NAG:HO4	2:E:580:NAG:H5	1.75	0.47
1:F:6237:LYS:HG2	6:F:8213:HOH:O	2.14	0.47
1:A:1124:PRO:HD3	1:A:1158:ALA:HB1	1.96	0.47
1:A:1138:TRP:CH2	1:A:1220:GLU:HB2	2.49	0.47
1:A:1222:ALA:N	4:A:11:CL:CL	2.83	0.47
1:A:1260:ASP:OD2	1:A:1263:PRO:HD3	2.14	0.47
1:A:1372:GLN:NE2	1:A:1372:GLN:H	2.12	0.47
1:B:2022:SER:HB3	6:B:8445:HOH:O	2.14	0.47
1:B:2368:LEU:HD12	1:B:2368:LEU:N	2.29	0.47
1:B:2498:LYS:HG2	1:B:2514:LEU:HD11	1.95	0.47
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.44	0.47
1:E:5542:LYS:HB2	6:E:8311:HOH:O	2.14	0.47
1:A:1338:GLU:C	1:A:1339:ARG:HD2	2.40	0.47
1:C:3257:LYS:HB3	6:C:7331:HOH:O	2.13	0.47
1:D:4354:GLU:HB2	1:D:4422:ALA:HB1	1.96	0.47
1:E:5221:SER:O	1:E:5224:GLY:N	2.47	0.47
1:C:3425:MET:CE	5:C:313:HTQ:H72	2.45	0.47
1:A:1089:GLN:OE1	1:A:1146:VAL:HB	2.14	0.47
1:D:4242:ARG:NH1	1:D:4242:ARG:CG	2.77	0.47
1:E:5030:HIS:HB3	1:E:5073:PRO:HA	1.96	0.47
1:E:5523:LYS:HD2	6:E:8003:HOH:O	2.13	0.47
1:B:2152:TYR:CD1	1:B:2152:TYR:N	2.82	0.47
1:A:1242:ARG:HG2	1:A:1242:ARG:NH1	2.29	0.47
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.77	0.47
1:B:2348:VAL:O	1:B:2446:MET:HA	2.15	0.47
1:C:3236:ALA:O	1:C:3238:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3268:ILE:HG12	1:C:3301:MET:CE	2.37	0.47
1:E:5100:LEU:HD13	1:E:5358:LEU:HD11	1.96	0.47
1:E:5383:TRP:CH2	1:E:5393:LYS:HB2	2.50	0.47
1:E:5431:VAL:HG21	1:E:5539:LEU:O	2.15	0.47
1:F:6349:GLY:HA3	1:F:6447:TYR:CE1	2.48	0.47
1:F:6359:ILE:HB	1:F:6360:PRO:HD3	1.97	0.47
1:F:6370:GLU:C	1:F:6372:GLN:H	2.21	0.47
1:D:4038:VAL:HG21	1:D:4049:ILE:HD12	1.97	0.47
1:D:4336:GLN:O	1:D:4339:ARG:NH1	2.48	0.47
1:A:1199:ARG:NH1	1:A:1239:LEU:HD21	2.30	0.47
1:D:4025:VAL:HG22	1:D:4034:LEU:HD23	1.96	0.47
1:D:4306:LEU:HD23	1:D:4308:LEU:HD21	1.96	0.47
1:D:4478:ALA:N	1:D:4479:PRO:CD	2.78	0.47
1:E:5267:GLN:HB2	6:E:8396:HOH:O	2.15	0.47
1:F:6385:SER:O	1:F:6389:VAL:HG22	2.15	0.47
1:A:1220:GLU:HG3	1:A:1472:LEU:HD21	1.97	0.47
1:B:2139:ILE:O	1:B:2223:GLY:HA3	2.15	0.47
1:C:3371:GLY:HA2	5:C:3[Y]:HTQ:O12	2.15	0.47
1:C:3538:LYS:HB3	1:C:3541:ASP:HB2	1.96	0.47
1:D:4418:LEU:HD11	5:D:4[Z]:HTQ:C18	2.45	0.47
1:E:5297:THR:O	1:E:5301:MET:HG2	2.15	0.47
1:E:5425:MET:CE	5:E:515:HTQ:H72	2.45	0.47
1:A:1349:GLY:HA3	1:A:1447:TYR:CZ	2.49	0.46
1:C:3380:SER:O	1:C:3384:LYS:HG2	2.15	0.46
1:E:5271:THR:HG22	1:E:5297:THR:HG23	1.97	0.46
1:A:1355:PHE:CD1	1:A:1360:PRO:HG3	2.49	0.46
1:A:1455:PHE:HB3	1:A:1482:LYS:NZ	2.30	0.46
1:A:1461:PRO:HG2	1:A:1464:VAL:CG2	2.44	0.46
1:C:3308:LEU:HD21	1:C:3367:PRO:HG2	1.96	0.46
1:C:3414:LYS:HZ2	5:C:3[Z]:HTQ:H161	1.79	0.46
1:C:3533:THR:C	1:C:3534:GLN:HG3	2.40	0.46
1:D:4278:THR:OG1	1:D:4281:VAL:HG23	2.16	0.46
1:F:6186:ARG:HB3	1:F:6324:ASP:HB2	1.96	0.46
1:A:1119:LEU:HD12	1:A:1119:LEU:O	2.14	0.46
1:A:1176:GLY:HA2	1:A:1189:TRP:HB2	1.97	0.46
1:A:1403:TYR:CE2	1:A:1420:LEU:HA	2.50	0.46
1:A:1426:PHE:HZ	5:A:111:HTQ:H11	1.81	0.46
1:C:3217:ILE:HG13	1:C:3217:ILE:O	2.14	0.46
1:C:3254:VAL:HG13	1:C:3255:LEU:N	2.30	0.46
1:E:5492:LEU:O	1:E:5496:VAL:HG23	2.16	0.46
1:F:6143:GLY:O	1:F:6318:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6246:GLU:HG2	1:F:6447:TYR:OH	2.15	0.46
1:F:6332:PRO:HD2	1:F:6333:GLU:OE1	2.16	0.46
1:F:6357:TRP:O	1:F:6360:PRO:HD2	2.15	0.46
1:F:6358:LEU:HD23	1:F:6468:HIS:CD2	2.51	0.46
1:A:1262:LYS:O	1:A:1266:GLU:HG3	2.16	0.46
1:B:2329:LEU:HD21	6:B:7603:HOH:O	2.15	0.46
1:C:3161:GLU:O	1:C:3163:VAL:HG13	2.14	0.46
1:C:3220:GLU:HA	1:C:3246:GLU:O	2.15	0.46
1:C:3242:ARG:HD2	1:C:3504:ALA:HA	1.97	0.46
1:D:4089:GLN:OE1	1:D:4146:VAL:HB	2.16	0.46
1:E:5393:LYS:HA	1:E:5396:ILE:HG12	1.97	0.46
1:A:1140:HIS:CD2	1:A:1141:GLY:O	2.67	0.46
1:A:1254:VAL:CG1	5:A:111:HTQ:H61	2.44	0.46
1:A:1409:ASP:O	1:A:1413:LYS:HG3	2.16	0.46
1:A:1024:PRO:HG3	1:A:1037:PHE:CE1	2.51	0.46
1:A:1036:LYS:HE3	1:A:1038:VAL:CG2	2.46	0.46
1:A:1333:GLU:H	1:A:1333:GLU:CD	2.23	0.46
1:C:3161:GLU:HB3	1:C:3501:ALA:CB	2.45	0.46
1:D:4540:LYS:HA	1:D:4543:GLU:OE2	2.16	0.46
1:E:5414:LYS:HD3	1:E:5414:LYS:C	2.40	0.46
1:A:1429:PRO:O	1:A:1433:VAL:HG23	2.16	0.46
1:B:2104:ARG:NH1	1:B:2153:ASP:HB2	2.31	0.46
1:B:2357:TRP:HB3	1:B:2467:ASP:OD2	2.15	0.46
1:B:2396:ILE:HB	1:B:2397:PRO:HD3	1.98	0.46
1:C:3140:HIS:HE1	6:C:7059:HOH:O	1.99	0.46
1:C:3498:LYS:HE2	6:C:7202:HOH:O	2.15	0.46
1:E:5363:LEU:HD13	5:E:515:HTQ:C16	2.45	0.46
1:E:5402:LYS:O	1:E:5402:LYS:HD3	2.16	0.46
1:B:2264:LEU:HD22	1:B:2316:GLN:HE21	1.81	0.46
1:C:3477:GLY:HA2	1:C:3493:SER:OG	2.16	0.46
1:D:4139:ILE:O	1:D:4223:GLY:HA3	2.16	0.46
1:F:6264:LEU:HD22	1:F:6268:ILE:HD11	1.97	0.46
1:A:1025:VAL:CG2	1:A:1034:LEU:HD23	2.46	0.46
1:B:2455:PHE:CD2	1:B:2482:LYS:HD3	2.51	0.46
1:B:2532:ASN:ND2	1:B:2534:GLN:NE2	2.64	0.46
1:D:4022:SER:O	1:D:4023:PRO:C	2.59	0.46
1:D:4530:GLY:O	1:D:4531:ALA:C	2.59	0.46
1:E:5383:TRP:CZ3	1:E:5393:LYS:HB2	2.51	0.46
1:F:6366:TYR:O	5:F:6[Z]:HTQ:H171	2.16	0.46
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.51	0.45
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5461:PRO:HB3	6:E:8667:HOH:O	2.16	0.45
1:B:2064:ARG:O	1:B:2066:THR:HG23	2.17	0.45
1:B:2120:ASN:HB2	1:B:2167:THR:OG1	2.16	0.45
1:B:2233:SER:O	1:B:2342:HIS:NE2	2.48	0.45
1:C:3251:LEU:CD2	1:C:3333:GLU:HG3	2.46	0.45
1:D:4190:GLY:O	1:D:4194:GLN:HG3	2.17	0.45
1:F:6082:SER:OG	3:F:682:SIA:N5	2.49	0.45
1:A:1152:TYR:N	1:A:1152:TYR:CD1	2.84	0.45
3:B:282:SIA:H92	1:C:3279:SER:N	2.30	0.45
1:B:2084:PRO:CA	3:B:282:SIA:C1	2.95	0.45
1:B:2262:LYS:HE3	1:B:2279:SER:OG	2.17	0.45
1:B:2420:LEU:HD12	1:B:2420:LEU:C	2.42	0.45
1:C:3074:TRP:CD2	1:C:3078:LYS:HE2	2.52	0.45
1:C:3205:ILE:HD12	1:C:3205:ILE:HA	1.78	0.45
1:E:5316:GLN:HA	1:E:5316:GLN:OE1	2.16	0.45
1:E:5368:LEU:HD12	1:E:5368:LEU:N	2.31	0.45
1:F:6220:GLU:CB	1:F:6246:GLU:HB2	2.47	0.45
1:F:6341:PHE:O	1:F:6342:HIS:C	2.59	0.45
1:C:3067:PRO:HB3	1:C:3192:LEU:CD1	2.44	0.45
1:C:3024:PRO:HG3	1:C:3037:PHE:CE2	2.52	0.45
1:C:3284:HIS:O	1:C:3288:GLN:HG2	2.17	0.45
1:C:3353:GLN:O	1:C:3467:ASP:HA	2.16	0.45
1:C:3425:MET:HE1	5:C:313:HTQ:H72	1.99	0.45
1:C:3428:VAL:HG21	1:C:3547:TRP:CD1	2.52	0.45
1:E:5461:PRO:HG2	1:E:5464:VAL:HG23	1.97	0.45
1:F:6311:ASP:OD1	1:F:6313:ARG:HB2	2.16	0.45
1:B:2279:SER:HA	1:B:2282:MET:HE3	1.98	0.45
1:C:3097:LEU:HD11	1:C:3101:PHE:CE2	2.52	0.45
1:C:3272:ALA:O	1:C:3289:LYS:NZ	2.49	0.45
5:A:1[Z]:HTQ:H191	6:A:8638:HOH:O	2.17	0.45
1:B:2040:LEU:O	1:B:2041:GLU:C	2.60	0.45
1:B:2045:GLN:N	1:F:6488:GLU:HG3	2.32	0.45
1:B:2140:HIS:HD2	1:B:2141:GLY:O	2.00	0.45
1:B:2338:GLU:C	1:B:2340:ASN:N	2.74	0.45
1:C:3527:LEU:HD11	1:C:3533:THR:HG22	1.98	0.45
1:A:1199:ARG:HG2	1:A:1199:ARG:NH1	2.30	0.45
1:A:1292:GLU:O	1:A:1296:GLU:HG3	2.16	0.45
1:D:4551:PHE:C	1:D:4553:LYS:H	2.25	0.45
1:E:5047:VAL:HG21	1:E:5155:LEU:HD23	1.99	0.45
1:A:1355:PHE:CZ	1:A:1360:PRO:HG3	2.52	0.45
1:B:2452:ARG:CZ	1:B:2462:LYS:HA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4104:ARG:CZ	1:D:4153:ASP:HB2	2.47	0.45
1:D:4391:ILE:CG2	1:D:4396:ILE:HD13	2.47	0.45
1:E:5420:LEU:HD12	1:E:5547:TRP:HZ2	1.82	0.45
1:F:6343:THR:HB	1:F:6442:ALA:HB2	1.99	0.45
1:B:2104:ARG:NH1	1:B:2104:ARG:HB3	2.30	0.44
1:C:3304:LEU:HD22	1:C:3304:LEU:N	2.32	0.44
1:C:3366:TYR:HA	1:C:3367:PRO:HD3	1.83	0.44
1:C:3383:TRP:CZ3	1:C:3393:LYS:HB2	2.52	0.44
1:D:4414:LYS:HZ1	5:D:4[Y]:HTQ:H181	1.82	0.44
1:D:4527:LEU:HD11	1:D:4533:THR:CG2	2.48	0.44
1:B:2355:PHE:HD1	1:B:2418:LEU:HD22	1.82	0.44
1:D:4143:GLY:N	5:D:414:HTQ:H42	2.32	0.44
1:D:4351:ASN:ND2	1:D:4449:PHE:HB3	2.31	0.44
1:E:5097:LEU:HD11	1:E:5101:PHE:CE2	2.52	0.44
1:E:5359:ILE:N	1:E:5360:PRO:HD2	2.32	0.44
1:F:6072:GLU:HG3	6:F:8439:HOH:O	2.17	0.44
1:B:2132:ARG:HA	1:B:2132:ARG:HD3	1.83	0.44
1:D:4221:SER:HA	1:D:4247:SER:O	2.18	0.44
1:D:4246:GLU:HG2	1:D:4447:TYR:OH	2.17	0.44
1:B:2201:VAL:O	1:B:2205:ILE:HB	2.17	0.44
1:C:3198:LEU:HB3	1:C:3239:LEU:HB3	1.99	0.44
1:D:4206:ALA:HA	1:D:4210:GLY:O	2.17	0.44
1:F:6370:GLU:C	1:F:6372:GLN:N	2.74	0.44
1:F:6389:VAL:O	1:F:6390:CYS:HB2	2.16	0.44
1:D:4074:TRP:CD2	1:D:4078:LYS:HE2	2.52	0.44
1:D:4119:LEU:HD12	1:D:4119:LEU:O	2.17	0.44
1:E:5254:VAL:HG13	1:E:5255:LEU:N	2.31	0.44
1:E:5304:LEU:HD13	5:E:515:HTQ:H191	2.00	0.44
1:E:5334:GLU:O	1:E:5338:GLU:HG3	2.18	0.44
1:F:6201:VAL:HG13	1:F:6205:ILE:HB	1.99	0.44
1:B:2425:MET:HE1	5:B:212:HTQ:H72	1.98	0.44
1:C:3492:LEU:O	1:C:3496:VAL:HG23	2.17	0.44
1:D:4111:LYS:HG2	6:D:7506:HOH:O	2.18	0.44
1:D:4119:LEU:HD12	1:D:4119:LEU:C	2.42	0.44
1:E:5068:PRO:HB3	1:E:5193:ASP:OD1	2.18	0.44
1:E:5156:ALA:O	1:E:5160:HIS:HB2	2.17	0.44
1:E:5456:SER:HB3	1:E:5460:LYS:HD3	2.00	0.44
1:A:1278:THR:OG1	1:A:1281:VAL:HG23	2.18	0.44
1:A:1389:VAL:O	1:A:1390:CYS:HB2	2.18	0.44
1:B:2311:ASP:OD1	1:B:2313:ARG:HB2	2.17	0.44
1:C:3414:LYS:O	1:C:3418:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4464:VAL:HG12	1:D:4467:ASP:HB2	2.00	0.44
1:E:5205:ILE:HD12	1:E:5205:ILE:HA	1.80	0.44
1:A:1318:LEU:HD12	1:A:1318:LEU:C	2.42	0.44
1:B:2304:LEU:CD2	1:B:2318:LEU:HD21	2.48	0.44
1:C:3191:HIS:HA	1:C:3194:GLN:OE1	2.17	0.44
1:D:4087:CYS:O	1:D:4088:THR:C	2.61	0.44
1:E:5064:ARG:NH2	1:E:5114:GLU:OE2	2.50	0.44
1:F:6348:VAL:O	1:F:6446:MET:HA	2.18	0.44
1:A:1382:LEU:HD23	1:A:1396:ILE:HG23	2.00	0.44
1:B:2524:GLU:OE2	1:B:2538:LYS:HD3	2.18	0.44
1:C:3242:ARG:NH1	1:C:3242:ARG:CG	2.81	0.44
1:D:4292:GLU:CD	1:D:4292:GLU:N	2.74	0.44
1:E:5461:PRO:O	1:E:5464:VAL:HG23	2.18	0.44
1:F:6039:SER:HA	6:F:8282:HOH:O	2.17	0.44
1:A:1026:VAL:CG1	1:A:1207:SER:HB3	2.48	0.43
1:B:2349:GLY:HA3	1:B:2447:TYR:CE1	2.53	0.43
1:C:3149:ALA:CB	1:C:3169:GLN:HG3	2.48	0.43
1:C:3182:ASP:OD2	1:C:3182:ASP:C	2.61	0.43
1:C:3308:LEU:HB2	1:C:3309:GLN:NE2	2.33	0.43
1:C:3420:LEU:HD12	1:C:3547:TRP:HZ2	1.83	0.43
1:D:4312:PRO:HG2	1:D:4383:TRP:CD1	2.53	0.43
1:E:5143:GLY:O	1:E:5144:LEU:HB2	2.17	0.43
1:E:5258:LYS:HE2	6:E:7744:HOH:O	2.18	0.43
1:E:5306:LEU:HD22	1:E:5366:TYR:CE1	2.53	0.43
1:E:5366:TYR:HD2	1:E:5368:LEU:HD11	1.83	0.43
1:E:5447:TYR:HB3	1:E:5517:TRP:CZ2	2.53	0.43
1:F:6052:GLY:O	3:F:682:SIA:O1A	2.36	0.43
1:F:6257:LYS:NZ	1:F:6316:GLN:NE2	2.66	0.43
1:A:1268:ILE:HD11	1:A:1319:LEU:HD21	2.00	0.43
1:B:2098:SER:O	1:B:2102:THR:HB	2.19	0.43
1:B:2199:ARG:HD2	6:B:7112:HOH:O	2.18	0.43
1:B:2255:LEU:HD21	5:B:212:HTQ:H91	2.00	0.43
1:C:3357:TRP:HB2	5:C:3[Y]:HTQ:H171	1.99	0.43
1:D:4409:ASP:OD1	1:D:4411:VAL:N	2.51	0.43
1:E:5142:GLY:HA2	5:E:515:HTQ:H151	1.99	0.43
1:A:1495:MET:HE1	1:A:1533:THR:OG1	2.18	0.43
1:B:2283:VAL:HG12	1:B:2287:ARG:NH1	2.33	0.43
1:D:4357:TRP:C	1:D:4360:PRO:HD2	2.43	0.43
1:F:6215:VAL:N	1:F:6241:HIS:HD2	1.91	0.43
1:A:1125:ALA:HB2	1:A:1133:LEU:CD1	2.49	0.43
1:A:1218:PHE:HB2	1:A:1244:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1402:LYS:HG2	1:A:1546:PHE:CZ	2.54	0.43
1:C:3350:ILE:O	1:C:3448:GLU:HA	2.18	0.43
1:D:4335:LEU:C	1:D:4337:ALA:H	2.26	0.43
1:A:1119:LEU:HD12	1:A:1119:LEU:C	2.43	0.43
1:A:1409:ASP:HB3	1:A:1412:LYS:HB2	2.01	0.43
1:B:2332:PRO:O	1:B:2336:GLN:HG3	2.17	0.43
1:B:2540:LYS:O	1:B:2544:VAL:HG23	2.18	0.43
1:D:4359:ILE:HB	1:D:4360:PRO:HD3	2.01	0.43
1:E:5221:SER:OG	1:E:5468:HIS:NE2	2.50	0.43
1:F:6058:PRO:HA	6:F:7119:HOH:O	2.18	0.43
1:F:6374:ASP:CG	1:F:6376:LYS:HB3	2.43	0.43
1:A:1366:TYR:O	5:A:1[Y]:HTQ:H171	2.19	0.43
1:B:2089:GLN:HB2	1:B:2146:VAL:HG12	2.00	0.43
1:C:3414:LYS:O	1:C:3417:PHE:HB3	2.19	0.43
1:C:3464:VAL:CG2	5:C:3[Y]:HTQ:H191	2.48	0.43
1:D:4369:SER:HA	5:D:4[Z]:HTQ:H42	1.99	0.43
1:D:4372:GLN:HG2	1:D:4373:LEU:N	2.34	0.43
1:F:6435:ARG:NH1	1:F:6544:VAL:HG11	2.33	0.43
1:A:1177:PHE:HE1	1:A:1191:HIS:CD2	2.36	0.43
1:A:1225:GLU:O	1:A:1229:VAL:HG23	2.18	0.43
1:A:1266:GLU:O	1:A:1270:ILE:HG13	2.18	0.43
1:F:6310:GLY:HA3	6:F:7283:HOH:O	2.18	0.43
1:B:2218:PHE:CB	1:B:2244:ILE:HB	2.49	0.43
1:B:2547:TRP:CE3	1:B:2550:LEU:HD23	2.53	0.43
1:C:3341:PHE:O	1:C:3342:HIS:C	2.62	0.43
1:D:4063:LEU:HD21	1:D:4069:GLN:NE2	2.34	0.43
1:E:5461:PRO:O	1:E:5463:THR:N	2.51	0.43
1:A:1409:ASP:OD1	1:A:1411:VAL:N	2.50	0.43
1:B:2102:THR:OG1	1:B:2104:ARG:HG2	2.19	0.43
1:B:2404:LEU:C	1:B:2406:GLY:H	2.27	0.43
1:C:3038:VAL:CG2	1:C:3049:ILE:HD12	2.48	0.43
1:C:3369:SER:HA	5:C:3[Z]:HTQ:H11	2.01	0.43
1:C:3452:ARG:HD2	1:C:3464:VAL:O	2.19	0.43
1:D:4264:LEU:HD11	1:D:4319:LEU:HD23	1.99	0.43
1:D:4370:GLU:HB2	6:D:7875:HOH:O	2.19	0.43
1:E:5145:MET:CG	1:E:5318:LEU:HD21	2.48	0.43
1:E:5149:ALA:CB	1:E:5169:GLN:HG3	2.48	0.43
1:A:1079:ASN:O	3:A:182:SIA:C4	2.67	0.43
1:B:2030:HIS:HB3	1:B:2073:PRO:HA	2.00	0.43
1:B:2199:ARG:CD	6:B:7112:HOH:O	2.67	0.43
1:B:2262:LYS:N	1:B:2263:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2553:LYS:HD3	6:B:8382:HOH:O	2.19	0.43
1:E:5255:LEU:HD21	5:E:515:HTQ:H51	2.01	0.43
1:E:5264:LEU:HD21	1:E:5319:LEU:HD23	2.01	0.43
1:E:5394:GLU:HG3	1:E:5395:LEU:CD2	2.49	0.43
1:F:6420:LEU:CD1	1:F:6547:TRP:HZ2	2.30	0.43
1:B:2268:ILE:HG12	1:B:2301:MET:HE2	2.01	0.42
1:B:2375:GLN:O	1:B:2378:ALA:HB3	2.18	0.42
1:C:3140:HIS:HB2	6:C:7490:HOH:O	2.18	0.42
1:C:3143:GLY:O	1:C:3144:LEU:HB2	2.19	0.42
1:D:4211:ASN:C	1:D:4213:GLY:N	2.77	0.42
1:D:4311:ASP:OD1	1:D:4313:ARG:HB2	2.19	0.42
1:D:4404:LEU:C	1:D:4406:GLY:N	2.77	0.42
1:E:5026:VAL:HG13	1:E:5207:SER:HB3	2.01	0.42
1:E:5460:LYS:HA	1:E:5461:PRO:HD2	1.79	0.42
1:F:6359:ILE:CD1	5:F:616:HTQ:H22	2.49	0.42
1:A:1477:GLY:HA2	1:A:1493:SER:OG	2.19	0.42
1:B:2407:THR:O	1:B:2413:LYS:HE2	2.19	0.42
1:C:3045:GLN:HA	1:C:3046:PRO:HD3	1.91	0.42
1:C:3304:LEU:O	1:C:3364:MET:HG2	2.19	0.42
1:E:5464:VAL:HB	6:E:7870:HOH:O	2.19	0.42
1:F:6375:GLN:HE21	1:F:6375:GLN:HB3	1.60	0.42
1:F:6409:ASP:OD2	1:F:6412:LYS:HB2	2.19	0.42
1:A:1378:ALA:HA	6:A:8101:HOH:O	2.19	0.42
1:C:3119:LEU:HD12	1:C:3119:LEU:O	2.18	0.42
1:C:3268:ILE:CD1	1:C:3319:LEU:HD21	2.49	0.42
1:C:3501:ALA:O	1:C:3505:ARG:HG2	2.19	0.42
1:F:6188:ASN:HD22	1:F:6324:ASP:CG	2.27	0.42
1:F:6268:ILE:HD11	1:F:6319:LEU:CD2	2.50	0.42
1:A:1257:LYS:NZ	1:A:1318:LEU:O	2.51	0.42
1:A:1420:LEU:C	1:A:1420:LEU:HD13	2.44	0.42
1:A:1437:HIS:HD2	1:A:1444:THR:OG1	2.02	0.42
1:B:2268:ILE:HD11	1:B:2319:LEU:CD2	2.49	0.42
1:B:2414:LYS:HB3	1:B:2414:LYS:HE3	1.74	0.42
1:C:3357:TRP:C	1:C:3360:PRO:HD2	2.44	0.42
1:C:3373:LEU:HD12	1:C:3377:THR:HB	2.01	0.42
1:A:1306:LEU:HD22	1:A:1366:TYR:CE1	2.55	0.42
1:B:2464:VAL:HA	6:B:8607:HOH:O	2.18	0.42
1:C:3090:ASP:OD1	1:C:3090:ASP:C	2.62	0.42
1:C:3251:LEU:HD21	1:C:3333:GLU:HG3	2.00	0.42
1:C:3357:TRP:O	1:C:3360:PRO:HD2	2.19	0.42
1:D:4277:THR:HG22	1:D:4278:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4324:ASP:OD2	1:D:4327:LEU:HB3	2.19	0.42
1:D:4326:MET:HE2	6:D:8398:HOH:O	2.20	0.42
1:B:2036:LYS:HG2	6:B:8453:HOH:O	2.20	0.42
1:C:3100:LEU:HD13	1:C:3358:LEU:HD11	2.02	0.42
1:C:3361:MET:SD	1:C:3361:MET:C	3.03	0.42
1:D:4030:HIS:HB3	1:D:4073:PRO:HA	2.02	0.42
1:D:4125:ALA:HB2	1:D:4133:LEU:HD12	2.02	0.42
1:E:5146:VAL:HG22	5:E:515:HTQ:H171	2.01	0.42
1:F:6266:GLU:O	1:F:6270:ILE:HG13	2.20	0.42
1:A:1385:SER:C	1:A:1387:PRO:HD2	2.45	0.42
1:B:2079:ASN:CB	6:B:8690:HOH:O	2.61	0.42
1:B:2346:TYR:HB3	1:B:2437:HIS:CD2	2.54	0.42
1:C:3139:ILE:O	1:C:3223:GLY:HA3	2.20	0.42
1:F:6262:LYS:HE2	1:F:6282:MET:CE	2.49	0.42
1:B:2205:ILE:HD12	1:B:2205:ILE:HA	1.81	0.42
1:C:3100:LEU:HD13	1:C:3358:LEU:CD1	2.49	0.42
1:C:3405:GLY:O	1:C:3406:GLY:C	2.63	0.42
1:D:4447:TYR:CD2	1:D:4447:TYR:C	2.98	0.42
1:E:5316:GLN:C	6:E:8686:HOH:O	2.63	0.42
1:E:5478:ALA:N	1:E:5479:PRO:CD	2.82	0.42
1:A:1304:LEU:HD13	5:A:111:HTQ:C17	2.39	0.42
1:B:2373:LEU:HA	6:B:7705:HOH:O	2.19	0.42
1:C:3218:PHE:HB2	1:C:3244:ILE:HB	2.02	0.42
1:E:5391:ILE:HB	6:E:7649:HOH:O	2.20	0.42
1:A:1090:ASP:HB3	1:A:1093:ALA:HB3	2.02	0.42
1:A:1306:LEU:HD23	1:A:1367:PRO:HD3	2.02	0.42
1:C:3153:ASP:OD2	1:C:3155:LEU:HB2	2.19	0.42
1:C:3237:LYS:HG2	6:C:7248:HOH:O	2.20	0.42
1:D:4079:ASN:HB2	6:D:8164:HOH:O	2.18	0.42
1:E:5528:GLN:O	1:E:5533:THR:HA	2.20	0.42
1:F:6083:TYR:CZ	1:F:6108:ILE:HD13	2.55	0.42
1:F:6292:GLU:CD	1:F:6292:GLU:N	2.77	0.42
1:F:6354:GLU:O	1:F:6468:HIS:HB2	2.19	0.42
1:A:1087:CYS:O	1:A:1089:GLN:HG2	2.20	0.41
1:B:2364:MET:HE2	1:B:2364:MET:HB3	1.96	0.41
1:C:3251:LEU:HD23	1:C:3251:LEU:HA	1.87	0.41
1:F:6241:HIS:C	1:F:6242:ARG:CG	2.93	0.41
1:A:1205:ILE:HD12	1:A:1205:ILE:HA	1.91	0.41
1:A:1241:HIS:C	1:A:1242:ARG:CG	2.93	0.41
1:A:1292:GLU:CD	1:A:1292:GLU:N	2.78	0.41
1:C:3249:VAL:HG23	1:C:3251:LEU:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3329:LEU:HG	6:C:8361:HOH:O	2.20	0.41
1:C:3495:MET:HE1	1:C:3533:THR:OG1	2.20	0.41
1:D:4205:ILE:HD12	1:D:4205:ILE:HA	1.86	0.41
1:D:4361:MET:CE	1:D:4363:LEU:HG	2.50	0.41
1:D:4366:TYR:HA	1:D:4367:PRO:HD3	1.86	0.41
1:E:5083:TYR:CE2	1:E:5108:ILE:HD12	2.55	0.41
1:E:5338:GLU:O	1:E:5339:ARG:C	2.63	0.41
1:E:5425:MET:HE1	5:E:515:HTQ:H72	2.01	0.41
1:A:1040:LEU:HG	6:A:8379:HOH:O	2.19	0.41
1:B:2140:HIS:HE1	6:B:7338:HOH:O	2.02	0.41
1:C:3119:LEU:HD12	1:C:3119:LEU:C	2.45	0.41
1:D:4343:THR:HB	1:D:4442:ALA:CB	2.44	0.41
1:E:5311:ASP:HA	1:E:5312:PRO:HD3	1.88	0.41
1:E:5491:ARG:HG2	1:E:5491:ARG:NH1	2.35	0.41
1:F:6104:ARG:O	1:F:6482:LYS:NZ	2.52	0.41
1:A:1206:ALA:HA	1:A:1210:GLY:O	2.21	0.41
1:B:2218:PHE:HA	1:B:2244:ILE:O	2.21	0.41
1:B:2262:LYS:HE2	1:B:2282:MET:HE1	2.02	0.41
1:B:2297:THR:O	1:B:2301:MET:HG2	2.21	0.41
1:B:2464:VAL:HG22	5:B:2[Y]:HTQ:H171	2.01	0.41
1:C:3375:GLN:HG3	1:C:3413:LYS:NZ	2.35	0.41
1:C:3460:LYS:HD2	6:C:7823:HOH:O	2.20	0.41
1:D:4364:MET:HG3	5:D:414:HTQ:H181	2.02	0.41
1:E:5023:PRO:HB2	1:E:5034:LEU:CD2	2.51	0.41
1:F:6086:MET:HE2	1:F:6110:LEU:HB2	2.02	0.41
1:A:1528:GLN:O	1:A:1533:THR:HA	2.21	0.41
1:C:3173:GLY:HA3	6:C:7272:HOH:O	2.19	0.41
1:C:3340:ASN:O	1:C:3341:PHE:HB3	2.20	0.41
1:D:4218:PHE:CB	1:D:4244:ILE:HB	2.50	0.41
1:D:4538:LYS:HB3	1:D:4541:ASP:HB2	2.03	0.41
1:E:5229:VAL:HG13	1:E:5328:LEU:HD21	2.03	0.41
1:F:6218:PHE:CB	1:F:6244:ILE:HB	2.49	0.41
1:A:1309:GLN:O	1:A:1309:GLN:NE2	2.54	0.41
1:D:4023:PRO:CB	1:D:4034:LEU:HD21	2.50	0.41
1:D:4262:LYS:N	1:D:4263:PRO:CD	2.84	0.41
1:E:5119:LEU:C	1:E:5119:LEU:HD12	2.46	0.41
1:E:5420:LEU:CD1	1:E:5547:TRP:HZ2	2.33	0.41
1:E:5483:GLU:CG	1:E:5484:GLY:N	2.84	0.41
1:A:1188:ASN:HD22	1:A:1324:ASP:CG	2.29	0.41
1:B:2533:THR:C	1:B:2534:GLN:HG3	2.46	0.41
1:C:3145:MET:CG	1:C:3318:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4304:LEU:HB3	5:D:414:HTQ:C19	2.50	0.41
1:D:4348:VAL:O	1:D:4446:MET:HA	2.20	0.41
1:D:4368:LEU:HB3	5:D:4[Y]:HTQ:O20	2.21	0.41
1:E:5130:LYS:HE3	1:E:5132:ARG:HH12	1.81	0.41
1:F:6048:ALA:HB3	1:F:6123:THR:HG23	2.03	0.41
1:F:6151:THR:HB	1:F:6152:TYR:CE1	2.55	0.41
1:F:6257:LYS:NZ	1:F:6318:LEU:O	2.42	0.41
1:F:6337:ALA:C	1:F:6339:ARG:N	2.77	0.41
1:F:6401:GLU:OE2	1:F:6405:GLY:HA3	2.20	0.41
1:A:1332:PRO:O	1:A:1336:GLN:HG2	2.20	0.41
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.83	0.41
1:D:4249:VAL:HG23	1:D:4251:LEU:H	1.86	0.41
1:E:5428:VAL:HG21	1:E:5547:TRP:CD1	2.56	0.41
1:F:6336:GLN:HE22	1:F:6433:VAL:HG22	1.86	0.41
1:A:1211:ASN:HA	1:A:1212:PRO:HD2	1.92	0.41
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.50	0.41
1:A:1220:GLU:HA	1:A:1246:GLU:O	2.21	0.41
1:A:1231:VAL:HA	1:A:1240:PHE:HZ	1.84	0.41
1:B:2057:LYS:HE2	6:B:8660:HOH:O	2.20	0.41
1:B:2161:GLU:HB3	1:B:2501:ALA:CB	2.50	0.41
1:C:3238:ASN:N	6:C:8682:HOH:O	2.53	0.41
1:D:4350:ILE:HD13	1:D:4427:GLY:HA2	2.03	0.41
5:D:414:HTQ:H41	6:D:14:HOH:O	2.20	0.41
1:E:5112:LEU:O	1:E:5113:SER:HB2	2.20	0.41
1:E:5218:PHE:CB	1:E:5244:ILE:HB	2.50	0.41
1:E:5367:PRO:HA	6:E:8558:HOH:O	2.21	0.41
1:F:6025:VAL:CG2	1:F:6034:LEU:HD23	2.51	0.41
1:B:2277:THR:HG22	1:B:2278:THR:HG23	2.03	0.41
1:D:4135:VAL:HG21	1:D:4205:ILE:HG12	2.03	0.41
1:D:4551:PHE:C	1:D:4553:LYS:N	2.78	0.41
1:E:5161:GLU:O	1:E:5163:VAL:HG13	2.21	0.41
1:E:5201:VAL:HG13	1:E:5205:ILE:HB	2.03	0.41
1:F:6057:LYS:HE3	6:F:8439:HOH:O	2.21	0.41
1:F:6143:GLY:O	1:F:6144:LEU:HB2	2.21	0.41
1:F:6336:GLN:NE2	1:F:6433:VAL:HG13	2.36	0.41
1:A:1547:TRP:CZ3	1:A:1550:LEU:HD23	2.56	0.40
1:C:3252:THR:HG22	1:C:3254:VAL:HG12	2.03	0.40
1:D:4143:GLY:O	1:D:4144:LEU:HB2	2.21	0.40
1:F:6089:GLN:OE1	1:F:6146:VAL:HB	2.20	0.40
1:F:6140:HIS:HE1	6:F:7206:HOH:O	2.04	0.40
1:A:1142:GLY:HA2	5:A:111:HTQ:H131	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:LEU:HB2	5:A:1[Y]:HTQ:H151	2.04	0.40
1:C:3317:PRO:O	1:C:3318:LEU:C	2.64	0.40
1:D:4527:LEU:HD11	1:D:4533:THR:HG22	2.03	0.40
1:E:5361:MET:HB2	5:E:5[Z]:HTQ:H181	2.02	0.40
1:F:6264:LEU:O	1:F:6268:ILE:HG13	2.21	0.40
1:B:2048:ALA:HB3	1:B:2123:THR:HG23	2.03	0.40
1:B:2353:GLN:O	1:B:2467:ASP:HA	2.22	0.40
1:C:3368:LEU:C	1:C:3370:GLU:N	2.78	0.40
1:D:4125:ALA:HB2	1:D:4133:LEU:CD1	2.51	0.40
1:E:5103:ASN:ND2	1:E:5481:LEU:HD12	2.36	0.40
1:E:5246:GLU:OE1	1:E:5471:GLU:OE1	2.40	0.40
1:F:6034:LEU:HD13	1:F:6034:LEU:C	2.46	0.40
1:A:1241:HIS:C	1:A:1242:ARG:HG2	2.46	0.40
1:C:3188:ASN:HD22	1:C:3324:ASP:CG	2.29	0.40
1:C:3241:HIS:C	1:C:3242:ARG:HG3	2.46	0.40
1:E:5120:ASN:HB2	1:E:5167:THR:OG1	2.21	0.40
1:E:5385:SER:C	1:E:5387:PRO:HD2	2.46	0.40
1:F:6079:ASN:HB2	2:F:679:NAG:H83	2.02	0.40
1:A:1301:MET:HB2	1:A:1303:PHE:CE1	2.57	0.40
1:A:1363:LEU:HD13	5:A:111:HTQ:C18	2.51	0.40
1:C:3089:GLN:OE1	1:C:3146:VAL:HB	2.22	0.40
1:C:3402:LYS:HE2	1:C:3546:PHE:CD1	2.57	0.40
1:D:4051:LEU:HD13	1:D:4083:TYR:CD1	2.57	0.40
1:E:5295:LEU:O	1:E:5299:LEU:HD22	2.22	0.40
1:E:5340:ASN:O	1:E:5340:ASN:CG	2.64	0.40
1:E:5392:ALA:O	1:E:5394:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/548 (97%)	495 (93%)	33 (6%)	2 (0%)	30	60
1	B	529/548 (96%)	496 (94%)	28 (5%)	5 (1%)	14	41
1	C	529/548 (96%)	488 (92%)	38 (7%)	3 (1%)	21	51
1	D	530/548 (97%)	503 (95%)	23 (4%)	4 (1%)	16	44
1	E	529/548 (96%)	495 (94%)	27 (5%)	7 (1%)	9	31
1	F	529/548 (96%)	493 (93%)	32 (6%)	4 (1%)	16	44
All	All	3176/3288 (97%)	2970 (94%)	181 (6%)	25 (1%)	16	44

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2253	SER
1	C	3237	LYS
1	E	5393	LYS
1	E	5462	LYS
1	F	6341	PHE
1	A	1185	SER
1	B	2041	GLU
1	C	3185	SER
1	D	4253	SER
1	E	5237	LYS
1	F	6185	SER
1	B	2373	LEU
1	C	3341	PHE
1	D	4041	GLU
1	E	5538	LYS
1	A	1253	SER
1	B	2042	GLY
1	B	2540	LYS
1	D	4023	PRO
1	E	5185	SER
1	F	6127	LEU
1	E	5221	SER
1	E	5317	PRO
1	D	4205	ILE
1	F	6397	PRO

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	448/463 (97%)	439 (98%)	9 (2%)	48	80
1	B	447/463 (96%)	436 (98%)	11 (2%)	42	76
1	C	447/463 (96%)	433 (97%)	14 (3%)	35	70
1	D	448/463 (97%)	437 (98%)	11 (2%)	42	76
1	E	447/463 (96%)	433 (97%)	14 (3%)	35	70
1	F	447/463 (96%)	439 (98%)	8 (2%)	51	82
All	All	2684/2778 (97%)	2617 (98%)	67 (2%)	42	76

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1033	VAL
1	A	1221	SER
1	A	1261	VAL
1	A	1264	LEU
1	A	1309	GLN
1	A	1338	GLU
1	A	1358	LEU
1	A	1366	TYR
1	A	1372	GLN
1	B	2041	GLU
1	B	2155	LEU
1	B	2205	ILE
1	B	2220	GLU
1	B	2221	SER
1	B	2258	LYS
1	B	2340	ASN
1	B	2343	THR
1	B	2358	LEU
1	B	2420	LEU
1	B	2534	GLN
1	C	3034	LEU
1	C	3132	ARG

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Mol	Chain	Res	Type
1	C	3155	LEU
1	C	3218	PHE
1	C	3258	LYS
1	C	3264	LEU
1	C	3299	LEU
1	C	3304	LEU
1	C	3316	GLN
1	C	3318	LEU
1	C	3366	TYR
1	C	3375	GLN
1	C	3381	LEU
1	C	3534	GLN
1	D	4023	PRO
1	D	4079	ASN
1	D	4095	GLN
1	D	4218	PHE
1	D	4264	LEU
1	D	4309	GLN
1	D	4338	GLU
1	D	4372	GLN
1	D	4381	LEU
1	D	4420	LEU
1	D	4549	ASN
1	E	5111	LYS
1	E	5155	LEU
1	E	5162	ASN
1	E	5205	ILE
1	E	5218	PHE
1	E	5220	GLU
1	E	5225	GLU
1	E	5258	LYS
1	E	5299	LEU
1	E	5316	GLN
1	E	5343	THR
1	E	5381	LEU
1	E	5404	LEU
1	E	5534	GLN
1	F	6155	LEU
1	F	6218	PHE
1	F	6258	LYS
1	F	6264	LEU
1	F	6299	LEU

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Mol	Chain	Res	Type
1	F	6318	LEU
1	F	6366	TYR
1	F	6534	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	A	1069	GLN
1	A	1131	ASN
1	A	1140	HIS
1	A	1162	ASN
1	A	1241	HIS
1	A	1309	GLN
1	A	1316	GLN
1	A	1336	GLN
1	A	1351	ASN
1	A	1372	GLN
1	A	1375	GLN
1	A	1437	HIS
1	A	1506	ASN
1	A	1516	HIS
1	A	1528	GLN
1	A	1537	GLN
1	B	2140	HIS
1	B	2202	GLN
1	B	2241	HIS
1	B	2267	GLN
1	B	2342	HIS
1	B	2351	ASN
1	B	2353	GLN
1	B	2372	GLN
1	B	2436	ASN
1	B	2450	GLN
1	B	2532	ASN
1	B	2534	GLN
1	B	2537	GLN
1	C	3030	HIS
1	C	3045	GLN
1	C	3095	GLN
1	C	3131	ASN
1	C	3140	HIS

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Mol	Chain	Res	Type
1	C	3162	ASN
1	C	3241	HIS
1	C	3309	GLN
1	C	3336	GLN
1	C	3340	ASN
1	C	3351	ASN
1	C	3372	GLN
1	C	3375	GLN
1	C	3436	ASN
1	C	3437	HIS
1	C	3450	GLN
1	C	3516	HIS
1	C	3532	ASN
1	C	3537	GLN
1	D	4069	GLN
1	D	4140	HIS
1	D	4162	ASN
1	D	4241	HIS
1	D	4267	GLN
1	D	4309	GLN
1	D	4351	ASN
1	D	4372	GLN
1	D	4537	GLN
1	E	5030	HIS
1	E	5045	GLN
1	E	5140	HIS
1	E	5162	ASN
1	E	5202	GLN
1	E	5238	ASN
1	E	5241	HIS
1	E	5284	HIS
1	E	5288	GLN
1	E	5351	ASN
1	E	5353	GLN
1	E	5372	GLN
1	E	5436	ASN
1	E	5437	HIS
1	E	5506	ASN
1	E	5532	ASN
1	E	5537	GLN
1	F	6069	GLN
1	F	6131	ASN

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Mol	Chain	Res	Type
1	F	6140	HIS
1	F	6238	ASN
1	F	6241	HIS
1	F	6316	GLN
1	F	6336	GLN
1	F	6351	ASN
1	F	6353	GLN
1	F	6372	GLN
1	F	6375	GLN
1	F	6516	HIS
1	F	6532	ASN
1	F	6537	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\# Z > 2$
5	HTQ	D	414	-	22,22,22	2.15	11 (50%)	30,31,31	1.95	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SIA	F	682	-	21,21,21	1.27	2 (9%)	24,31,31	1.11	2 (8%)
5	HTQ	E	5[Y]	-	22,22,22	2.16	8 (36%)	30,31,31	1.20	3 (10%)
2	NAG	A	179	1	14,14,15	0.64	0	17,19,21	0.72	1 (5%)
5	HTQ	A	111	-	22,22,22	2.03	8 (36%)	30,31,31	1.64	5 (16%)
5	HTQ	B	212	-	22,22,22	2.01	9 (40%)	30,31,31	1.58	4 (13%)
5	HTQ	C	313	-	22,22,22	2.14	10 (45%)	30,31,31	1.35	3 (10%)
5	HTQ	E	5[Z]	-	22,22,22	2.15	9 (40%)	30,31,31	1.40	2 (6%)
2	NAG	E	580	-	14,14,15	0.56	0	17,19,21	0.66	1 (5%)
5	HTQ	D	4[Y]	-	22,22,22	2.13	8 (36%)	30,31,31	1.31	3 (10%)
2	NAG	B	279	1	14,14,15	0.53	0	17,19,21	0.77	1 (5%)
3	SIA	A	182	-	21,21,21	1.11	2 (9%)	24,31,31	1.33	5 (20%)
5	HTQ	E	515	-	22,22,22	2.11	10 (45%)	30,31,31	1.39	2 (6%)
5	HTQ	C	3[Y]	-	22,22,22	2.15	8 (36%)	30,31,31	1.41	3 (10%)
5	HTQ	B	2[Y]	-	22,22,22	2.09	9 (40%)	30,31,31	1.10	2 (6%)
5	HTQ	F	6[Y]	-	22,22,22	2.17	8 (36%)	30,31,31	1.28	2 (6%)
5	HTQ	A	1[Y]	-	22,22,22	2.21	11 (50%)	30,31,31	1.41	3 (10%)
5	HTQ	D	4[Z]	-	22,22,22	2.06	8 (36%)	30,31,31	1.15	2 (6%)
2	NAG	E	579	1	14,14,15	0.57	0	17,19,21	0.70	1 (5%)
2	NAG	F	679	1	14,14,15	0.63	0	17,19,21	0.67	0
5	HTQ	C	3[Z]	-	22,22,22	2.20	9 (40%)	30,31,31	1.34	4 (13%)
5	HTQ	B	2[Z]	-	22,22,22	2.13	9 (40%)	30,31,31	1.28	3 (10%)
5	HTQ	F	616	-	22,22,22	2.01	10 (45%)	30,31,31	1.29	2 (6%)
5	HTQ	F	6[Z]	-	22,22,22	2.18	9 (40%)	30,31,31	1.42	3 (10%)
5	HTQ	A	1[Z]	-	22,22,22	2.23	9 (40%)	30,31,31	1.71	4 (13%)
2	NAG	C	379	1	14,14,15	0.58	0	17,19,21	0.69	0
2	NAG	D	479	1	14,14,15	0.54	0	17,19,21	0.65	0
3	SIA	B	282	-	21,21,21	1.32	2 (9%)	24,31,31	1.40	3 (12%)

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
5	HTQ	D	414	-	-	5/12/33/33	0/4/3/3
3	SIA	F	682	-	-	1/20/38/38	0/1/1/1
5	HTQ	E	5[Y]	-	-	4/12/33/33	0/4/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	179	1	-	4/6/23/26	0/1/1/1
5	HTQ	A	111	-	-	1/12/33/33	0/4/3/3
5	HTQ	B	212	-	-	1/12/33/33	0/4/3/3
5	HTQ	C	313	-	-	5/12/33/33	0/4/3/3
5	HTQ	E	5[Z]	-	-	5/12/33/33	0/4/3/3
2	NAG	E	580	-	-	4/6/23/26	0/1/1/1
5	HTQ	D	4[Y]	-	-	5/12/33/33	0/4/3/3
2	NAG	B	279	1	1/1/5/7	2/6/23/26	0/1/1/1
3	SIA	A	182	-	-	2/20/38/38	0/1/1/1
5	HTQ	E	515	-	-	5/12/33/33	0/4/3/3
5	HTQ	C	3[Y]	-	-	1/12/33/33	0/4/3/3
5	HTQ	B	2[Y]	-	-	4/12/33/33	0/4/3/3
5	HTQ	F	6[Y]	-	-	5/12/33/33	0/4/3/3
5	HTQ	A	1[Y]	-	-	4/12/33/33	0/4/3/3
5	HTQ	D	4[Z]	-	-	3/12/33/33	0/4/3/3
2	NAG	E	579	1	-	2/6/23/26	0/1/1/1
2	NAG	F	679	1	1/1/5/7	4/6/23/26	0/1/1/1
5	HTQ	C	3[Z]	-	-	5/12/33/33	0/4/3/3
5	HTQ	B	2[Z]	-	-	6/12/33/33	0/4/3/3
5	HTQ	F	616	-	-	4/12/33/33	0/4/3/3
5	HTQ	F	6[Z]	-	-	4/12/33/33	0/4/3/3
5	HTQ	A	1[Z]	-	-	5/12/33/33	0/4/3/3
2	NAG	C	379	1	-	4/6/23/26	0/1/1/1
2	NAG	D	479	1	1/1/5/7	2/6/23/26	0/1/1/1
3	SIA	B	282	-	-	1/20/38/38	0/1/1/1

All (169) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	682	SIA	C4-C5	3.84	1.56	1.53
5	B	2[Z]	HTQ	C4-C3	3.78	1.61	1.52
5	D	4[Y]	HTQ	C4-C3	3.75	1.61	1.52
5	E	5[Y]	HTQ	C4-C3	3.74	1.61	1.52
5	C	3[Z]	HTQ	C4-C3	3.68	1.60	1.52
5	C	3[Y]	HTQ	C4-C3	3.60	1.60	1.52
5	C	3[Z]	HTQ	O10-C11	3.57	1.42	1.34
5	C	3[Y]	HTQ	C4-C5	3.54	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1[Z]	HTQ	O10-C11	3.54	1.42	1.34
5	A	1[Y]	HTQ	C4-C3	3.54	1.60	1.52
5	D	414	HTQ	C16-C14	3.53	1.44	1.39
5	E	515	HTQ	C9-N8	3.52	1.52	1.47
5	D	4[Y]	HTQ	O10-C11	3.48	1.42	1.34
5	F	6[Z]	HTQ	C4-C3	3.48	1.60	1.52
5	F	6[Y]	HTQ	C4-C3	3.47	1.60	1.52
5	C	3[Z]	HTQ	C4-C5	3.46	1.59	1.53
5	B	2[Z]	HTQ	O10-C11	3.42	1.42	1.34
5	C	313	HTQ	C9-N8	3.42	1.52	1.47
5	B	212	HTQ	C4-C3	3.41	1.60	1.52
5	D	4[Z]	HTQ	C9-N8	3.41	1.52	1.47
5	E	5[Z]	HTQ	C9-N8	3.40	1.52	1.47
5	A	111	HTQ	C4-C5	3.40	1.59	1.53
5	C	3[Z]	HTQ	C2-C3	3.39	1.60	1.52
5	F	6[Z]	HTQ	C9-N8	3.39	1.52	1.47
5	F	6[Y]	HTQ	C2-C3	3.39	1.60	1.52
5	F	6[Y]	HTQ	O10-C11	3.39	1.42	1.34
5	E	5[Y]	HTQ	O10-C11	3.38	1.42	1.34
5	A	1[Y]	HTQ	C9-N8	3.38	1.52	1.47
5	A	1[Y]	HTQ	C4-C5	3.38	1.59	1.53
5	E	5[Y]	HTQ	C9-N8	3.37	1.52	1.47
5	E	515	HTQ	C2-C3	3.37	1.60	1.52
5	C	3[Y]	HTQ	C9-N8	3.36	1.52	1.47
5	B	2[Y]	HTQ	C9-N8	3.35	1.52	1.47
5	F	6[Y]	HTQ	C9-N8	3.34	1.52	1.47
5	B	212	HTQ	C4-C5	3.34	1.59	1.53
5	D	4[Y]	HTQ	C9-N8	3.32	1.52	1.47
5	D	4[Z]	HTQ	C4-C3	3.32	1.60	1.52
5	E	515	HTQ	O10-C11	3.32	1.41	1.34
5	D	414	HTQ	O10-C11	3.31	1.41	1.34
5	B	212	HTQ	C2-C3	3.31	1.60	1.52
5	E	5[Y]	HTQ	C2-C3	3.30	1.60	1.52
5	F	6[Z]	HTQ	C4-C5	3.29	1.59	1.53
5	C	3[Y]	HTQ	C2-C3	3.29	1.59	1.52
5	A	111	HTQ	C4-C3	3.28	1.59	1.52
5	B	2[Z]	HTQ	C4-C5	3.28	1.59	1.53
5	D	4[Y]	HTQ	C4-C5	3.27	1.59	1.53
5	C	3[Z]	HTQ	C9-N8	3.27	1.52	1.47
5	F	6[Z]	HTQ	C2-C3	3.27	1.59	1.52
5	B	2[Z]	HTQ	C9-N8	3.26	1.52	1.47
5	A	1[Y]	HTQ	C2-C3	3.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2[Z]	HTQ	C2-C3	3.26	1.59	1.52
5	C	313	HTQ	O10-C11	3.25	1.41	1.34
5	A	1[Y]	HTQ	C16-C14	3.25	1.44	1.39
5	D	4[Z]	HTQ	C2-C3	3.24	1.59	1.52
5	E	5[Y]	HTQ	C4-C5	3.24	1.59	1.53
5	A	1[Z]	HTQ	C9-N8	3.23	1.52	1.47
5	C	313	HTQ	C2-C3	3.23	1.59	1.52
5	E	5[Z]	HTQ	O10-C11	3.22	1.41	1.34
5	B	2[Y]	HTQ	C2-C3	3.21	1.59	1.52
5	D	4[Y]	HTQ	C2-C3	3.20	1.59	1.52
5	A	1[Z]	HTQ	C2-C1	3.20	1.59	1.53
5	A	1[Z]	HTQ	C2-C3	3.20	1.59	1.52
5	E	515	HTQ	C4-C3	3.20	1.59	1.52
3	B	282	SIA	C4-C5	3.18	1.56	1.53
5	A	111	HTQ	C2-C3	3.17	1.59	1.52
5	C	313	HTQ	C4-C3	3.16	1.59	1.52
5	D	414	HTQ	C9-N8	3.13	1.51	1.47
5	F	616	HTQ	C4-C5	3.12	1.59	1.53
5	D	414	HTQ	C2-C1	3.12	1.59	1.53
5	A	1[Z]	HTQ	C4-C5	3.10	1.59	1.53
5	A	1[Z]	HTQ	C4-C3	3.10	1.59	1.52
5	F	616	HTQ	O10-C11	3.10	1.41	1.34
5	A	1[Z]	HTQ	C16-C14	3.09	1.44	1.39
5	F	616	HTQ	C4-C3	3.08	1.59	1.52
5	F	6[Y]	HTQ	C4-C5	3.08	1.59	1.53
5	B	2[Y]	HTQ	C4-C3	3.07	1.59	1.52
5	F	6[Y]	HTQ	C2-C1	3.06	1.59	1.53
5	F	6[Z]	HTQ	C16-C14	3.05	1.43	1.39
5	E	5[Z]	HTQ	C2-C3	3.04	1.59	1.52
5	E	5[Z]	HTQ	C2-C1	3.03	1.59	1.53
5	E	5[Z]	HTQ	C16-C14	3.02	1.43	1.39
5	D	4[Z]	HTQ	O10-C11	3.01	1.41	1.34
5	B	2[Y]	HTQ	C4-C5	3.00	1.58	1.53
5	E	5[Y]	HTQ	C16-C14	2.99	1.43	1.39
5	F	616	HTQ	C2-C3	2.99	1.59	1.52
5	E	515	HTQ	C4-C5	2.98	1.58	1.53
5	C	313	HTQ	C4-C5	2.97	1.58	1.53
5	B	212	HTQ	C9-N8	2.96	1.51	1.47
5	E	5[Z]	HTQ	C4-C3	2.96	1.59	1.52
5	B	2[Y]	HTQ	C2-C1	2.94	1.58	1.53
5	A	111	HTQ	C9-N8	2.93	1.51	1.47
5	D	4[Z]	HTQ	C2-C1	2.93	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	4[Y]	HTQ	C16-C14	2.93	1.43	1.39
5	E	5[Z]	HTQ	C4-C5	2.92	1.58	1.53
5	C	313	HTQ	C2-C1	2.91	1.58	1.53
5	E	515	HTQ	C16-C14	2.90	1.43	1.39
5	F	616	HTQ	C9-N8	2.90	1.51	1.47
5	F	6[Z]	HTQ	O10-C11	2.90	1.40	1.34
5	C	3[Y]	HTQ	C16-C14	2.89	1.43	1.39
5	C	313	HTQ	C16-C14	2.89	1.43	1.39
5	B	2[Y]	HTQ	C16-C14	2.85	1.43	1.39
5	A	111	HTQ	O10-C11	2.84	1.40	1.34
5	C	3[Z]	HTQ	C16-C14	2.83	1.43	1.39
5	B	2[Z]	HTQ	C16-C14	2.82	1.43	1.39
5	A	1[Y]	HTQ	C15-C14	2.79	1.43	1.39
5	D	4[Z]	HTQ	C15-C14	2.79	1.43	1.39
5	F	6[Y]	HTQ	C16-C14	2.79	1.43	1.39
5	D	414	HTQ	C2-C3	2.78	1.58	1.52
5	B	2[Y]	HTQ	O10-C11	2.78	1.40	1.34
5	C	3[Y]	HTQ	C15-C14	2.76	1.43	1.39
5	F	6[Z]	HTQ	C2-C1	2.75	1.58	1.53
5	F	616	HTQ	C16-C14	2.72	1.43	1.39
5	B	2[Y]	HTQ	C15-C14	2.71	1.43	1.39
5	A	111	HTQ	C16-C14	2.71	1.43	1.39
5	A	1[Z]	HTQ	C15-C14	2.71	1.43	1.39
5	D	414	HTQ	C4-C5	2.70	1.58	1.53
5	E	5[Z]	HTQ	C15-C14	2.70	1.43	1.39
5	F	6[Z]	HTQ	C15-C14	2.70	1.43	1.39
5	F	6[Y]	HTQ	C15-C14	2.68	1.43	1.39
5	D	414	HTQ	C15-C14	2.68	1.43	1.39
3	B	282	SIA	O6-C2	2.67	1.45	1.43
5	D	4[Y]	HTQ	C2-C1	2.67	1.58	1.53
5	A	1[Y]	HTQ	O10-C11	2.67	1.40	1.34
5	E	5[Y]	HTQ	C2-C1	2.66	1.58	1.53
5	B	212	HTQ	C15-C14	2.65	1.43	1.39
5	B	212	HTQ	C16-C14	2.65	1.43	1.39
5	D	4[Z]	HTQ	C4-C5	2.64	1.58	1.53
5	C	313	HTQ	C15-C14	2.64	1.43	1.39
5	C	3[Z]	HTQ	C2-C1	2.62	1.58	1.53
5	A	1[Y]	HTQ	C2-C1	2.61	1.58	1.53
5	C	3[Y]	HTQ	O10-C11	2.61	1.40	1.34
5	F	616	HTQ	C2-C1	2.59	1.58	1.53
5	E	515	HTQ	C2-C1	2.59	1.58	1.53
5	B	212	HTQ	O10-C11	2.59	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3[Z]	HTQ	C15-C14	2.55	1.43	1.39
5	A	111	HTQ	C15-C14	2.55	1.43	1.39
5	C	3[Y]	HTQ	C2-C1	2.54	1.58	1.53
3	A	182	SIA	C4-C5	2.54	1.55	1.53
5	D	4[Z]	HTQ	C16-C14	2.52	1.43	1.39
5	B	2[Z]	HTQ	C2-C1	2.52	1.58	1.53
5	E	515	HTQ	C15-C14	2.49	1.43	1.39
5	F	616	HTQ	C15-C14	2.48	1.43	1.39
5	B	2[Z]	HTQ	C15-C14	2.48	1.43	1.39
5	E	5[Y]	HTQ	C15-C14	2.44	1.43	1.39
5	D	4[Y]	HTQ	C15-C14	2.37	1.42	1.39
5	F	616	HTQ	C17-C15	2.24	1.42	1.38
5	D	414	HTQ	C4-C3	2.24	1.57	1.52
5	A	1[Z]	HTQ	C13-C11	2.18	1.55	1.53
5	E	5[Z]	HTQ	C13-C11	2.16	1.55	1.53
5	A	111	HTQ	C2-C1	2.15	1.57	1.53
5	C	313	HTQ	C17-C15	2.15	1.42	1.38
5	A	1[Y]	HTQ	C17-C15	2.15	1.42	1.38
3	A	182	SIA	O6-C2	2.15	1.45	1.43
5	B	2[Y]	HTQ	C17-C15	2.14	1.42	1.38
5	D	414	HTQ	C17-C15	2.13	1.42	1.38
5	E	515	HTQ	C18-C16	2.09	1.42	1.38
5	D	414	HTQ	C18-C16	2.08	1.42	1.38
5	B	212	HTQ	C18-C16	2.08	1.42	1.38
5	D	414	HTQ	C13-C11	2.08	1.55	1.53
5	F	6[Z]	HTQ	C13-C11	2.07	1.55	1.53
5	A	1[Y]	HTQ	C13-C11	2.06	1.55	1.53
3	F	682	SIA	O6-C2	2.06	1.45	1.43
5	F	616	HTQ	C18-C16	2.04	1.42	1.38
5	B	2[Z]	HTQ	C17-C15	2.04	1.42	1.38
5	B	212	HTQ	C17-C15	2.04	1.42	1.38
5	C	3[Z]	HTQ	C17-C15	2.04	1.42	1.38
5	A	1[Y]	HTQ	C18-C16	2.02	1.42	1.38
5	C	313	HTQ	C18-C16	2.00	1.42	1.38
5	E	515	HTQ	C17-C15	2.00	1.42	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	414	HTQ	C3-O10-C11	9.43	132.54	117.72
5	A	1[Z]	HTQ	C3-O10-C11	8.08	130.41	117.72
5	A	111	HTQ	C3-O10-C11	6.62	128.12	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	5[Z]	HTQ	C3-O10-C11	6.42	127.81	117.72
5	B	212	HTQ	C3-O10-C11	6.25	127.54	117.72
5	F	6[Z]	HTQ	C3-O10-C11	6.04	127.21	117.72
5	A	1[Y]	HTQ	C3-O10-C11	5.99	127.13	117.72
5	E	515	HTQ	C3-O10-C11	5.93	127.03	117.72
5	C	313	HTQ	C3-O10-C11	5.83	126.88	117.72
5	F	616	HTQ	C3-O10-C11	5.52	126.40	117.72
5	F	6[Y]	HTQ	C3-O10-C11	5.29	126.03	117.72
5	C	3[Y]	HTQ	C3-O10-C11	5.23	125.94	117.72
5	D	4[Z]	HTQ	C3-O10-C11	4.82	125.29	117.72
5	B	2[Z]	HTQ	C3-O10-C11	4.62	124.98	117.72
5	C	3[Z]	HTQ	C3-O10-C11	4.54	124.85	117.72
5	D	4[Y]	HTQ	C3-O10-C11	4.49	124.78	117.72
5	B	2[Y]	HTQ	C3-O10-C11	4.36	124.57	117.72
5	E	5[Y]	HTQ	C3-O10-C11	4.07	124.12	117.72
3	B	282	SIA	O6-C6-C7	3.49	112.10	106.65
3	B	282	SIA	O1A-C1-C2	-3.19	118.53	123.85
3	A	182	SIA	O1A-C1-C2	-3.09	118.70	123.85
5	A	1[Z]	HTQ	O10-C3-C2	3.00	114.83	107.77
5	D	414	HTQ	O10-C3-C4	2.81	114.37	107.77
3	A	182	SIA	O6-C6-C7	2.78	110.99	106.65
3	F	682	SIA	O1A-C1-C2	-2.76	119.24	123.85
5	A	111	HTQ	C3-C4-C5	2.74	116.64	112.73
5	C	3[Y]	HTQ	C3-C4-C5	2.73	116.62	112.73
5	D	4[Y]	HTQ	C3-C4-C5	2.70	116.58	112.73
3	B	282	SIA	C3-C2-C1	-2.69	107.84	112.84
5	C	3[Z]	HTQ	C3-C4-C5	2.69	116.57	112.73
5	B	212	HTQ	C3-C4-C5	2.64	116.50	112.73
5	D	414	HTQ	O10-C11-O12	2.63	128.69	123.95
5	B	2[Z]	HTQ	C3-C4-C5	2.45	116.23	112.73
5	F	616	HTQ	C5-N8-C1	2.44	103.66	100.79
5	A	111	HTQ	C5-N8-C1	2.39	103.61	100.79
5	E	5[Z]	HTQ	C5-N8-C1	2.39	103.60	100.79
5	B	212	HTQ	C5-N8-C1	2.38	103.60	100.79
5	D	414	HTQ	C5-N8-C1	2.38	103.59	100.79
5	E	5[Y]	HTQ	C3-C4-C5	2.38	116.12	112.73
5	E	5[Y]	HTQ	C5-N8-C1	2.35	103.56	100.79
3	A	182	SIA	O6-C6-C5	2.34	111.99	109.84
5	E	515	HTQ	C5-N8-C1	2.34	103.54	100.79
5	C	313	HTQ	C5-N8-C1	2.33	103.54	100.79
5	C	3[Z]	HTQ	C5-N8-C1	2.33	103.53	100.79
5	A	1[Z]	HTQ	C5-N8-C1	2.32	103.52	100.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6[Z]	HTQ	C3-C4-C5	2.31	116.03	112.73
5	F	6[Y]	HTQ	C5-N8-C1	2.31	103.51	100.79
3	F	682	SIA	O6-C6-C5	2.31	111.96	109.84
5	D	4[Z]	HTQ	C5-N8-C1	2.31	103.51	100.79
5	B	2[Z]	HTQ	C5-N8-C1	2.31	103.51	100.79
5	B	2[Y]	HTQ	C5-N8-C1	2.30	103.50	100.79
5	A	1[Y]	HTQ	C3-C4-C5	2.28	115.98	112.73
5	A	1[Y]	HTQ	C5-N8-C1	2.28	103.47	100.79
5	F	6[Z]	HTQ	C5-N8-C1	2.27	103.46	100.79
5	D	4[Y]	HTQ	C5-N8-C1	2.23	103.42	100.79
3	A	182	SIA	C3-C2-C1	-2.22	108.71	112.84
5	C	3[Y]	HTQ	C5-N8-C1	2.22	103.40	100.79
2	A	179	NAG	C2-N2-C7	-2.21	119.94	122.90
5	B	212	HTQ	O10-C11-O12	2.20	127.93	123.95
3	A	182	SIA	C3-C4-C5	2.11	112.99	109.72
2	E	579	NAG	C2-N2-C7	-2.09	120.10	122.90
5	A	111	HTQ	C2-C1-N8	-2.07	104.71	107.54
5	C	313	HTQ	O10-C3-C2	2.05	112.58	107.77
5	A	111	HTQ	O10-C3-C2	2.04	112.57	107.77
2	B	279	NAG	C2-N2-C7	-2.02	120.20	122.90
5	C	3[Z]	HTQ	C2-C1-N8	-2.01	104.80	107.54
5	A	1[Z]	HTQ	O10-C11-O12	2.01	127.57	123.95
2	E	580	NAG	C2-N2-C7	-2.00	120.22	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	279	NAG	C1
2	D	479	NAG	C1
2	F	679	NAG	C1

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	179	NAG	C8-C7-N2-C2
2	A	179	NAG	O7-C7-N2-C2
2	B	279	NAG	O7-C7-N2-C2
2	E	580	NAG	C8-C7-N2-C2
2	E	580	NAG	O7-C7-N2-C2
2	F	679	NAG	C8-C7-N2-C2
2	F	679	NAG	O7-C7-N2-C2
5	A	111	HTQ	C2-C3-O10-C11

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Mol	Chain	Res	Type	Atoms
5	A	1[Y]	HTQ	O10-C11-C13-O20
5	A	1[Y]	HTQ	O12-C11-C13-O20
5	A	1[Z]	HTQ	C2-C3-O10-C11
5	A	1[Z]	HTQ	O10-C11-C13-C14
5	A	1[Z]	HTQ	O10-C11-C13-O20
5	A	1[Z]	HTQ	O12-C11-C13-C14
5	A	1[Z]	HTQ	O12-C11-C13-O20
5	B	2[Y]	HTQ	O10-C11-C13-O20
5	B	2[Y]	HTQ	O12-C11-C13-C14
5	B	2[Y]	HTQ	O12-C11-C13-O20
5	B	2[Z]	HTQ	O10-C11-C13-O20
5	B	2[Z]	HTQ	O12-C11-C13-O20
5	C	313	HTQ	O10-C11-C13-C14
5	C	313	HTQ	O10-C11-C13-O20
5	C	313	HTQ	O12-C11-C13-C14
5	C	313	HTQ	O12-C11-C13-O20
5	C	3[Z]	HTQ	O10-C11-C13-O20
5	C	3[Z]	HTQ	O12-C11-C13-O20
5	D	414	HTQ	C4-C3-O10-C11
5	D	414	HTQ	O10-C11-C13-O20
5	D	414	HTQ	O12-C11-C13-C14
5	D	414	HTQ	O12-C11-C13-O20
5	D	4[Y]	HTQ	O10-C11-C13-O20
5	D	4[Y]	HTQ	O12-C11-C13-O20
5	E	515	HTQ	O10-C11-C13-O20
5	E	515	HTQ	O12-C11-C13-C14
5	E	515	HTQ	O12-C11-C13-O20
5	E	5[Y]	HTQ	O10-C11-C13-O20
5	E	5[Y]	HTQ	O12-C11-C13-O20
5	E	5[Z]	HTQ	O10-C11-C13-O20
5	E	5[Z]	HTQ	O12-C11-C13-C14
5	E	5[Z]	HTQ	O12-C11-C13-O20
5	F	616	HTQ	O12-C11-C13-O20
5	F	6[Y]	HTQ	O10-C11-C13-O20
5	F	6[Y]	HTQ	O12-C11-C13-O20
5	F	6[Z]	HTQ	O10-C11-C13-O20
5	F	6[Z]	HTQ	O12-C11-C13-C14
5	F	6[Z]	HTQ	O12-C11-C13-O20
5	B	212	HTQ	C2-C3-O10-C11
5	C	313	HTQ	C2-C3-O10-C11
5	C	3[Z]	HTQ	C2-C3-O10-C11
5	D	4[Y]	HTQ	C2-C3-O10-C11

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Mol	Chain	Res	Type	Atoms
5	E	515	HTQ	C2-C3-O10-C11
5	F	6[Y]	HTQ	C2-C3-O10-C11
2	B	279	NAG	C8-C7-N2-C2
2	C	379	NAG	C8-C7-N2-C2
2	C	379	NAG	O7-C7-N2-C2
2	A	179	NAG	O5-C5-C6-O6
2	A	179	NAG	C4-C5-C6-O6
2	E	579	NAG	C8-C7-N2-C2
2	E	580	NAG	C4-C5-C6-O6
5	E	5[Z]	HTQ	C2-C3-O10-C11
2	E	579	NAG	O7-C7-N2-C2
5	E	5[Y]	HTQ	C2-C3-O10-C11
5	B	2[Z]	HTQ	C2-C3-O10-C11
5	A	1[Y]	HTQ	O10-C11-C13-C14
5	B	2[Y]	HTQ	O10-C11-C13-C14
5	D	414	HTQ	O10-C11-C13-C14
5	D	4[Y]	HTQ	O10-C11-C13-C14
5	E	515	HTQ	O10-C11-C13-C14
5	E	5[Z]	HTQ	O10-C11-C13-C14
5	F	6[Y]	HTQ	O10-C11-C13-C14
5	F	6[Z]	HTQ	O10-C11-C13-C14
2	E	580	NAG	O5-C5-C6-O6
2	C	379	NAG	O5-C5-C6-O6
2	C	379	NAG	C4-C5-C6-O6
5	F	616	HTQ	C4-C3-O10-C11
5	C	3[Z]	HTQ	O10-C11-C13-C14
2	F	679	NAG	C4-C5-C6-O6
5	A	1[Y]	HTQ	O12-C11-C13-C14
5	B	2[Z]	HTQ	O12-C11-C13-C14
5	C	3[Z]	HTQ	O12-C11-C13-C14
5	D	4[Y]	HTQ	O12-C11-C13-C14
5	D	4[Z]	HTQ	O12-C11-C13-C14
5	F	6[Y]	HTQ	O12-C11-C13-C14
2	F	679	NAG	O5-C5-C6-O6
5	F	616	HTQ	O10-C11-C13-O20
5	D	4[Z]	HTQ	C4-C3-O10-C11
3	A	182	SIA	O1A-C1-C2-O2
3	A	182	SIA	O1A-C1-C2-O6
5	F	616	HTQ	C2-C3-O10-C11
2	D	479	NAG	C8-C7-N2-C2
5	B	2[Z]	HTQ	O10-C11-C13-C14
5	D	4[Z]	HTQ	O10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
5	E	5[Y]	HTQ	C4-C3-O10-C11
2	D	479	NAG	O7-C7-N2-C2
5	B	2[Z]	HTQ	C4-C3-O10-C11
3	B	282	SIA	O1B-C1-C2-O2
3	F	682	SIA	O1B-C1-C2-C3
5	C	3[Y]	HTQ	C2-C3-O10-C11

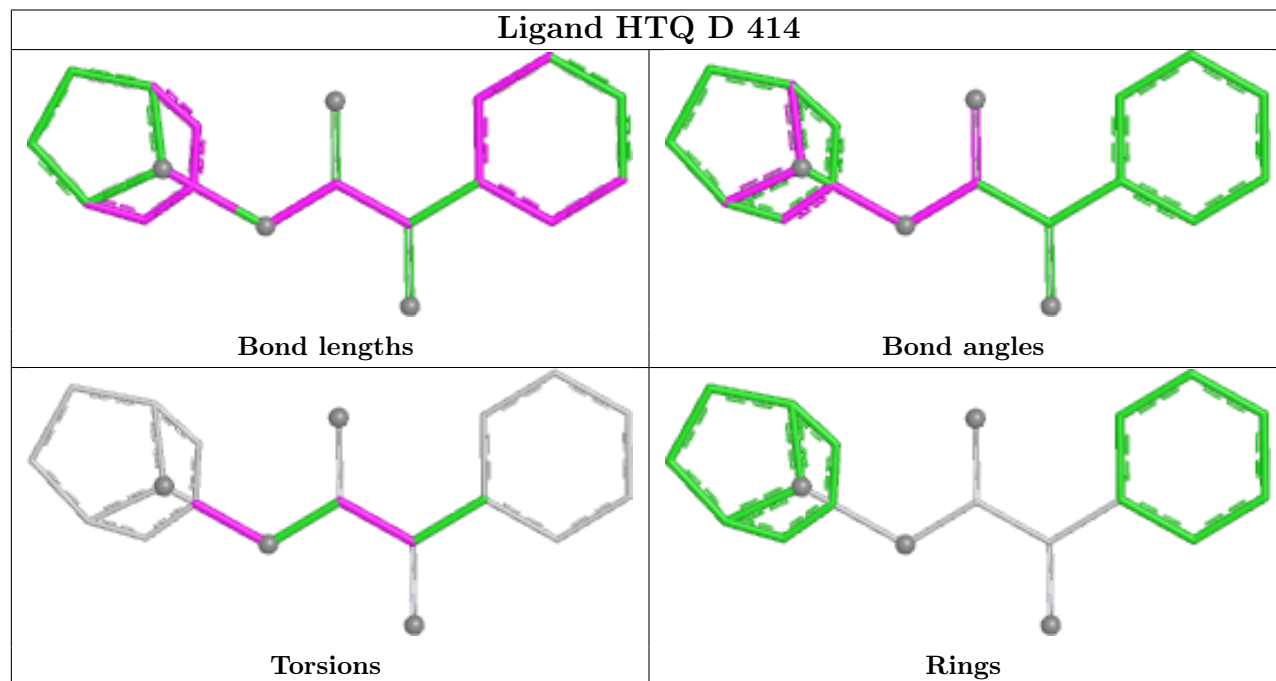
There are no ring outliers.

26 monomers are involved in 125 short contacts:

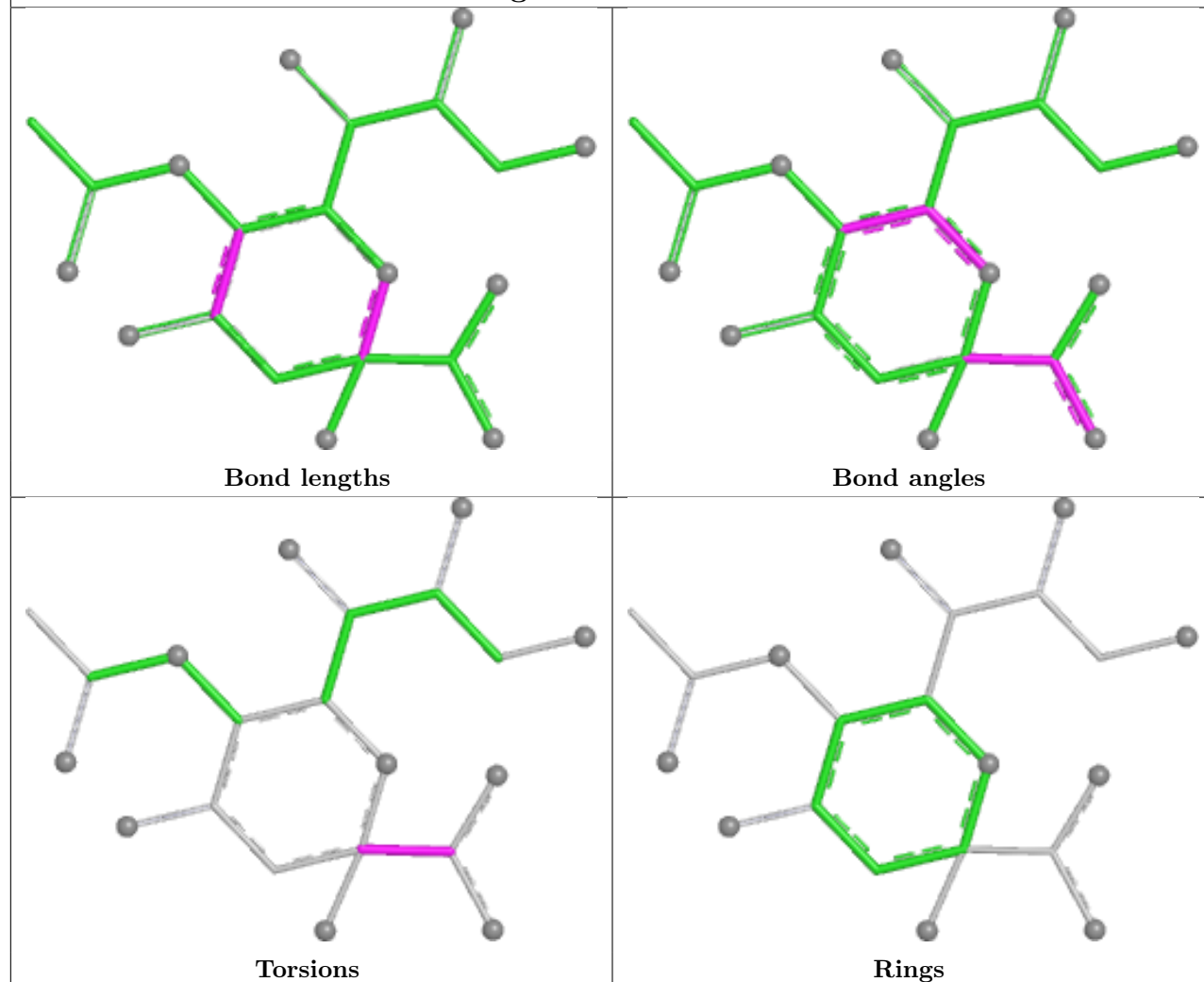
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	414	HTQ	7	0
3	F	682	SIA	5	0
5	E	5[Y]	HTQ	2	0
5	A	111	HTQ	13	0
5	B	212	HTQ	10	0
5	C	313	HTQ	4	0
5	E	5[Z]	HTQ	1	0
2	E	580	NAG	2	0
5	D	4[Y]	HTQ	3	0
2	B	279	NAG	3	0
3	A	182	SIA	5	0
5	E	515	HTQ	12	0
5	C	3[Y]	HTQ	4	0
5	B	2[Y]	HTQ	4	0
5	F	6[Y]	HTQ	3	0
5	A	1[Y]	HTQ	4	0
5	D	4[Z]	HTQ	3	0
2	E	579	NAG	2	0
2	F	679	NAG	2	0
5	C	3[Z]	HTQ	5	0
5	B	2[Z]	HTQ	1	0
5	F	616	HTQ	7	0
5	F	6[Z]	HTQ	3	0
5	A	1[Z]	HTQ	4	0
2	D	479	NAG	2	0
3	B	282	SIA	17	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

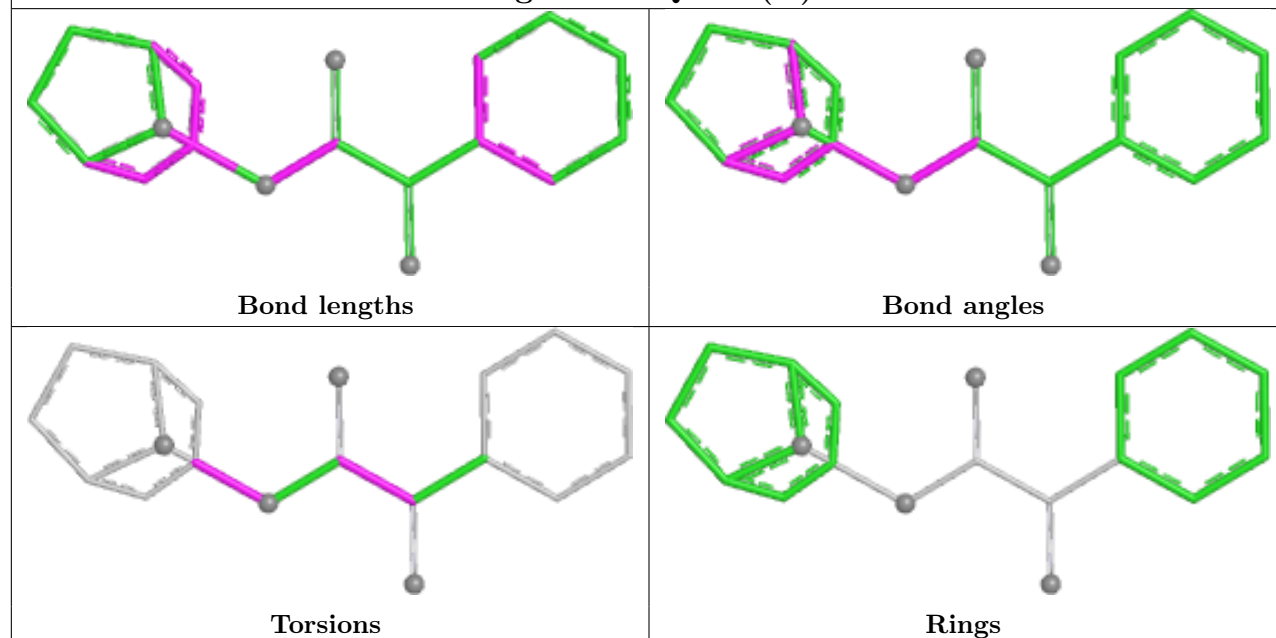
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

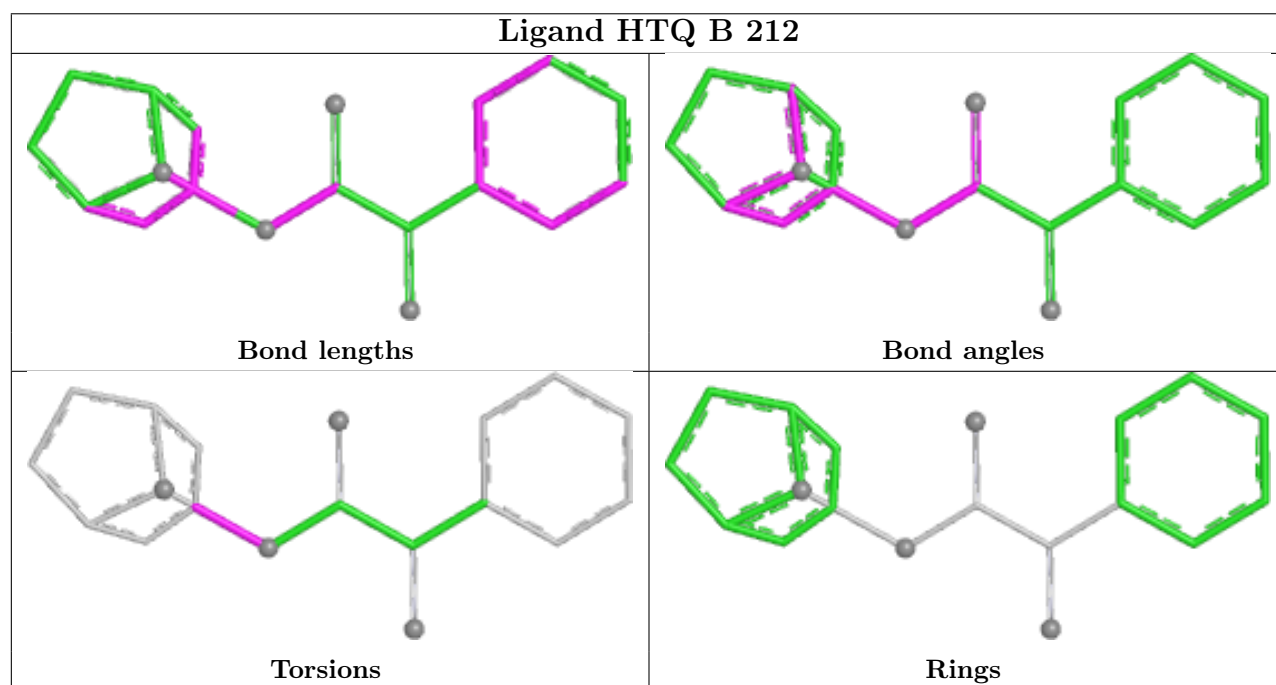
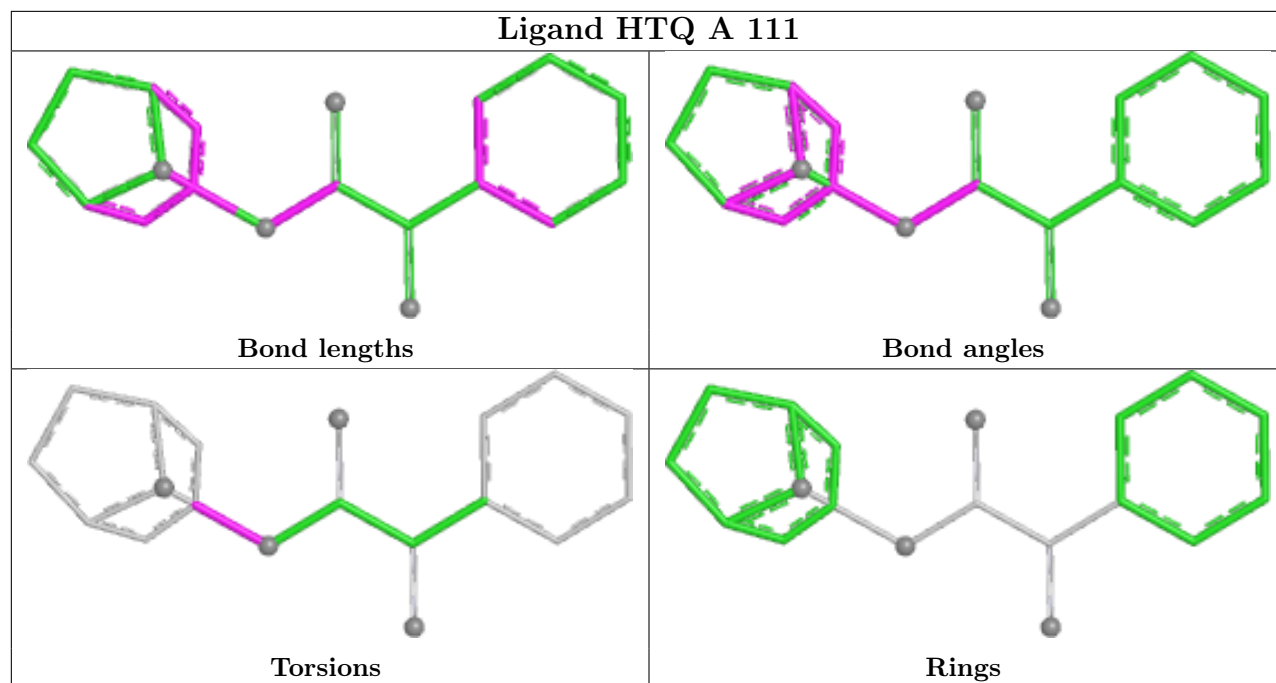


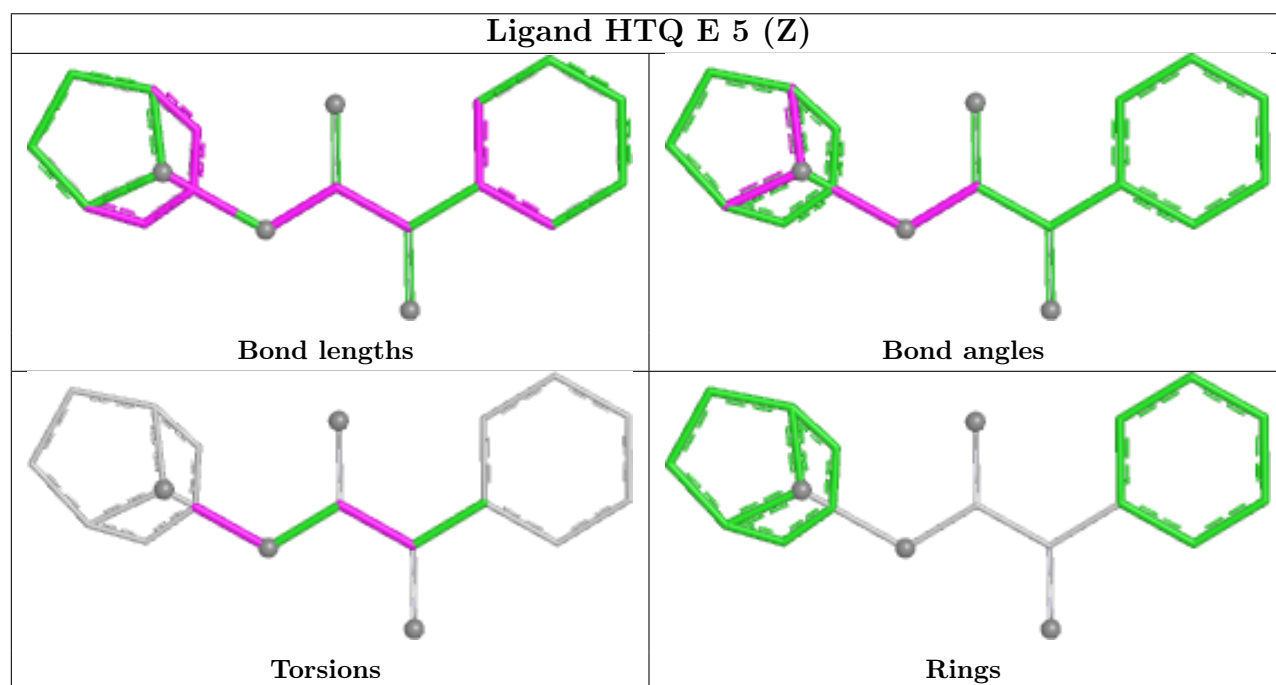
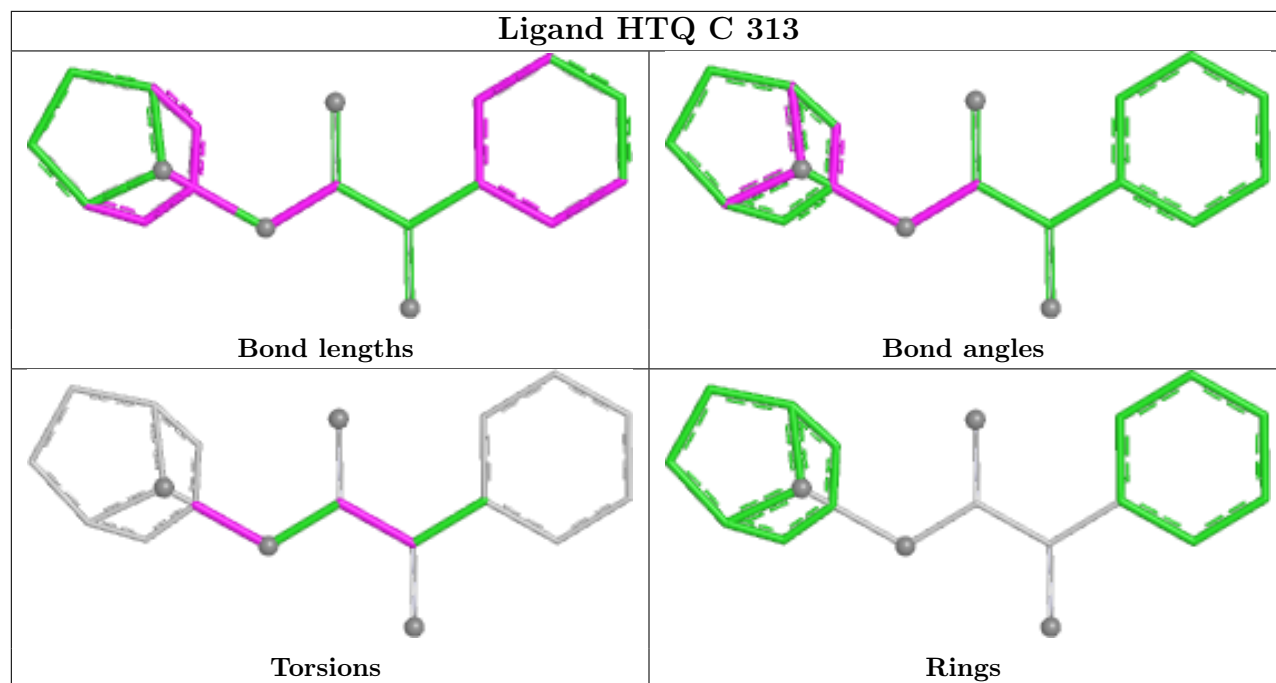
Ligand SIA F 682



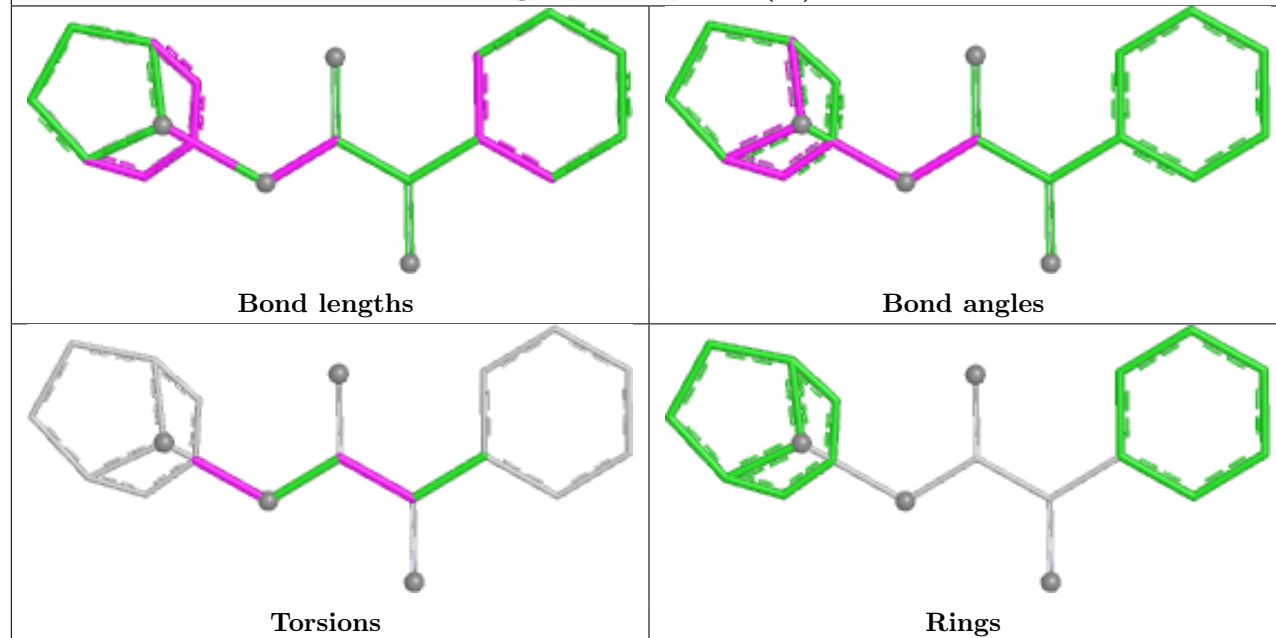
Ligand HTQ E 5 (Y)



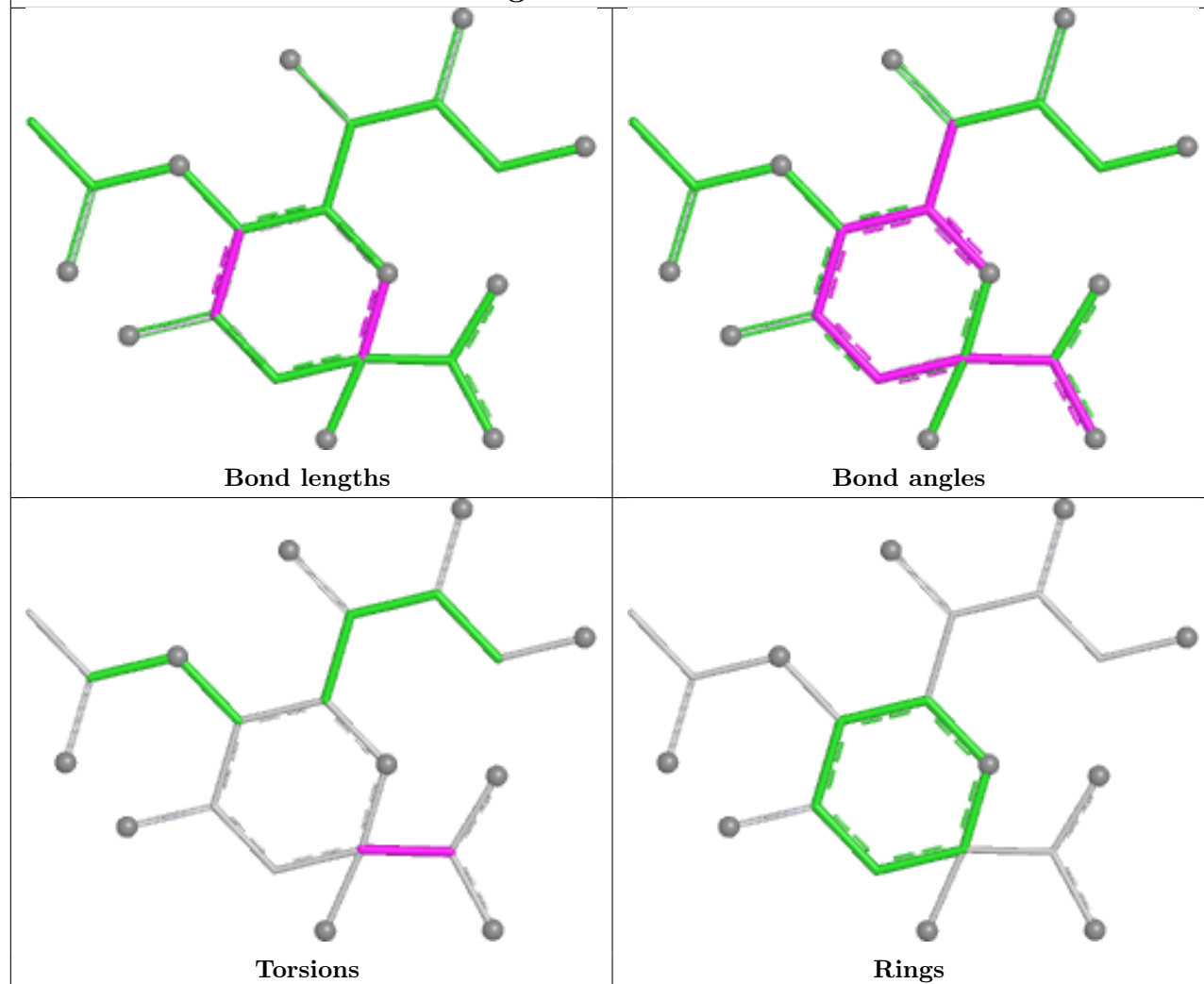




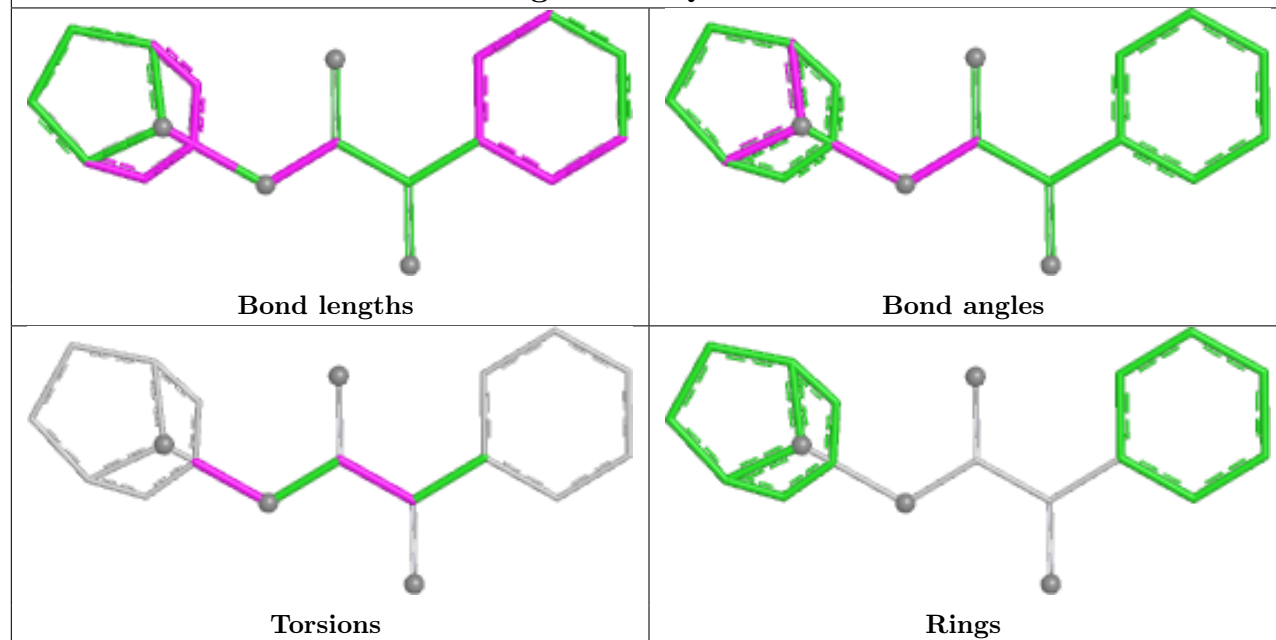
Ligand HTQ D 4 (Y)



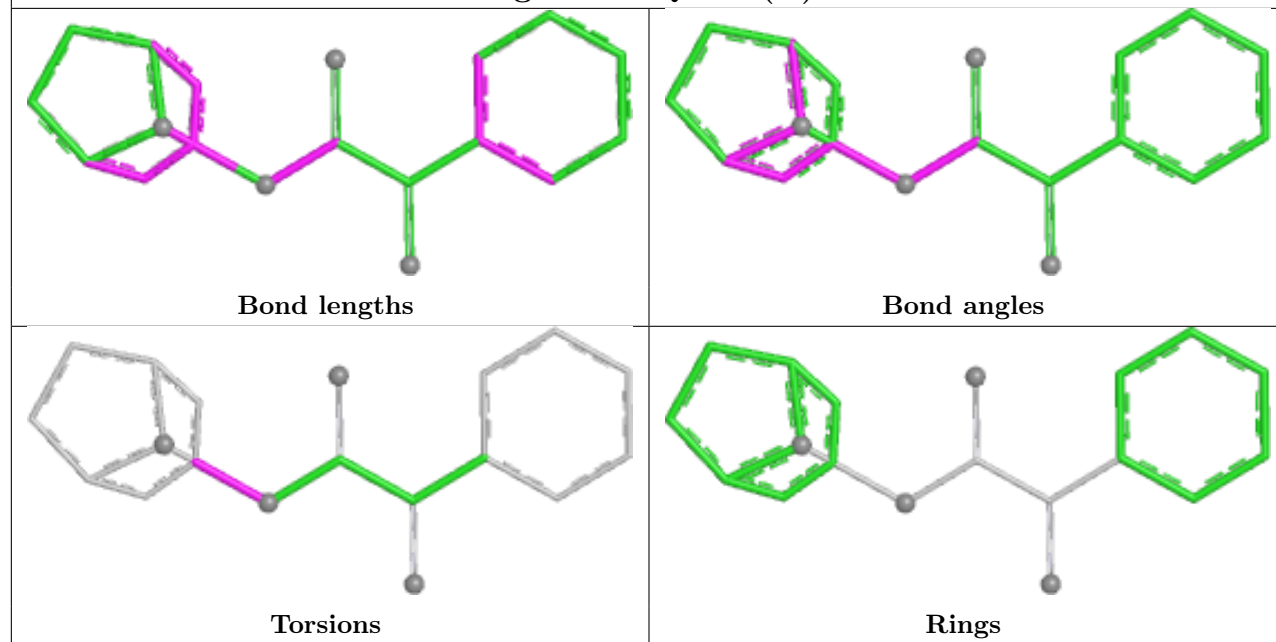
Ligand SIA A 182



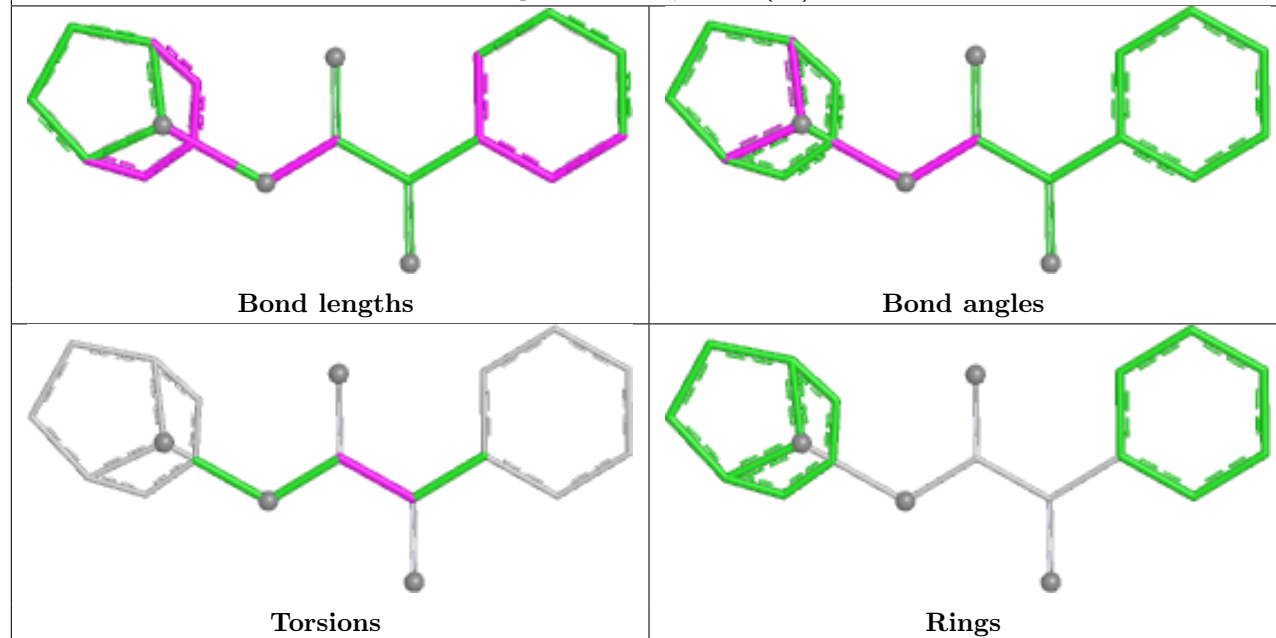
Ligand HTQ E 515



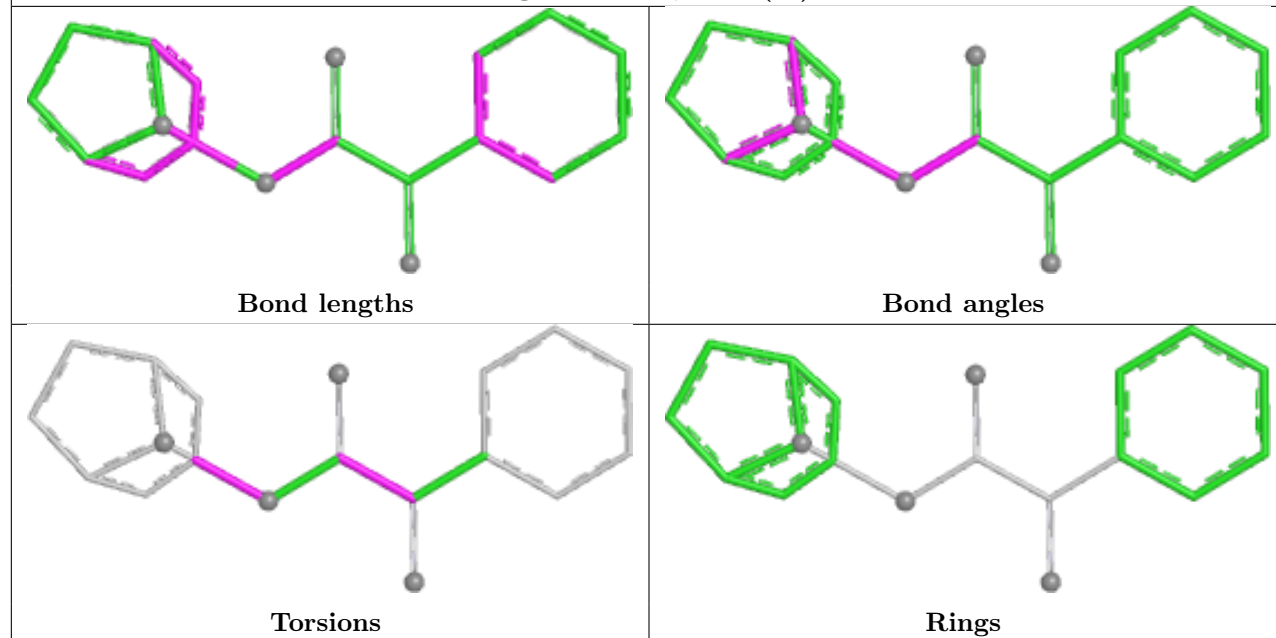
Ligand HTQ C 3 (Y)



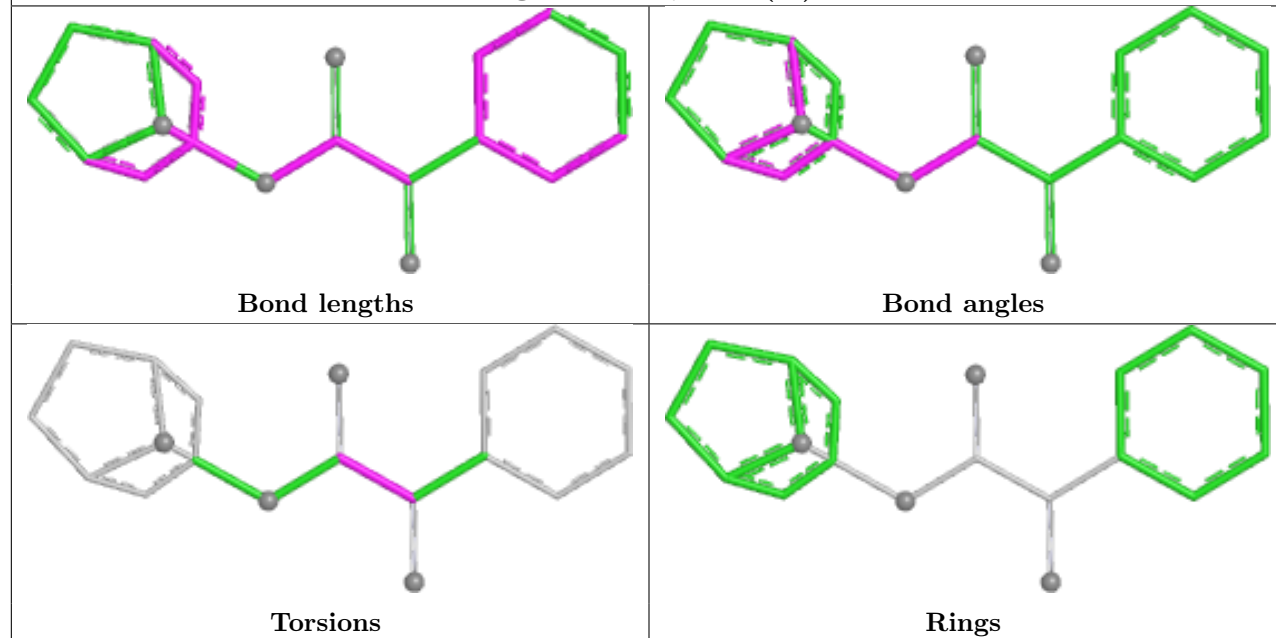
Ligand HTQ B 2 (Y)



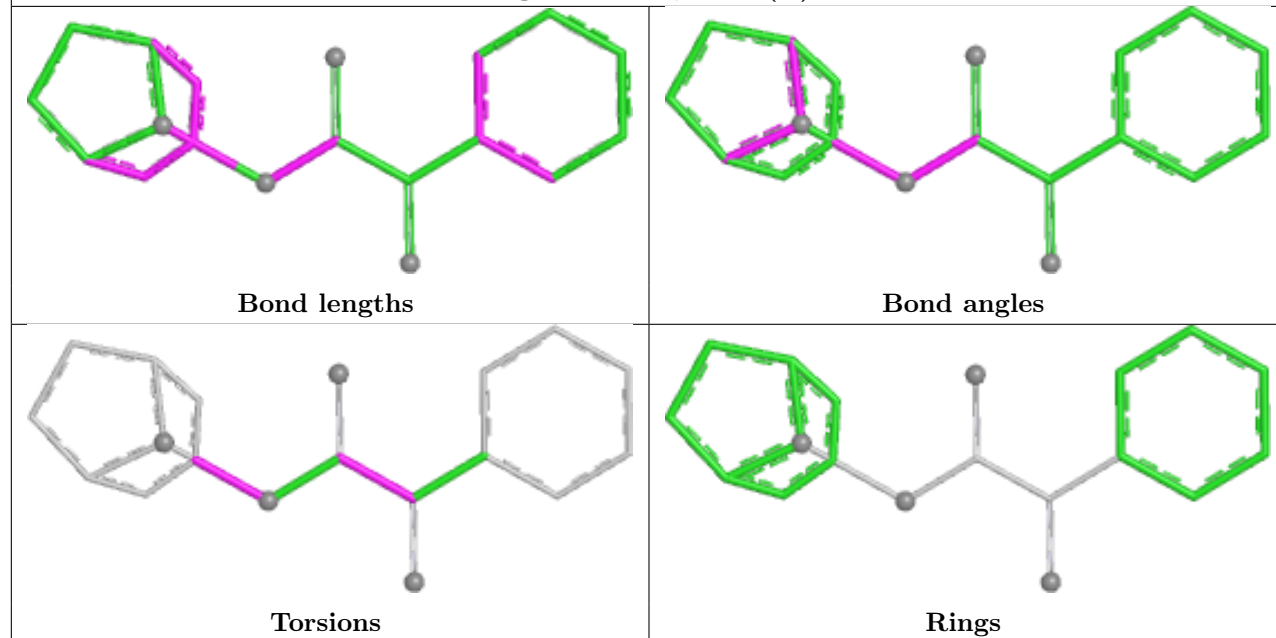
Ligand HTQ F 6 (Y)



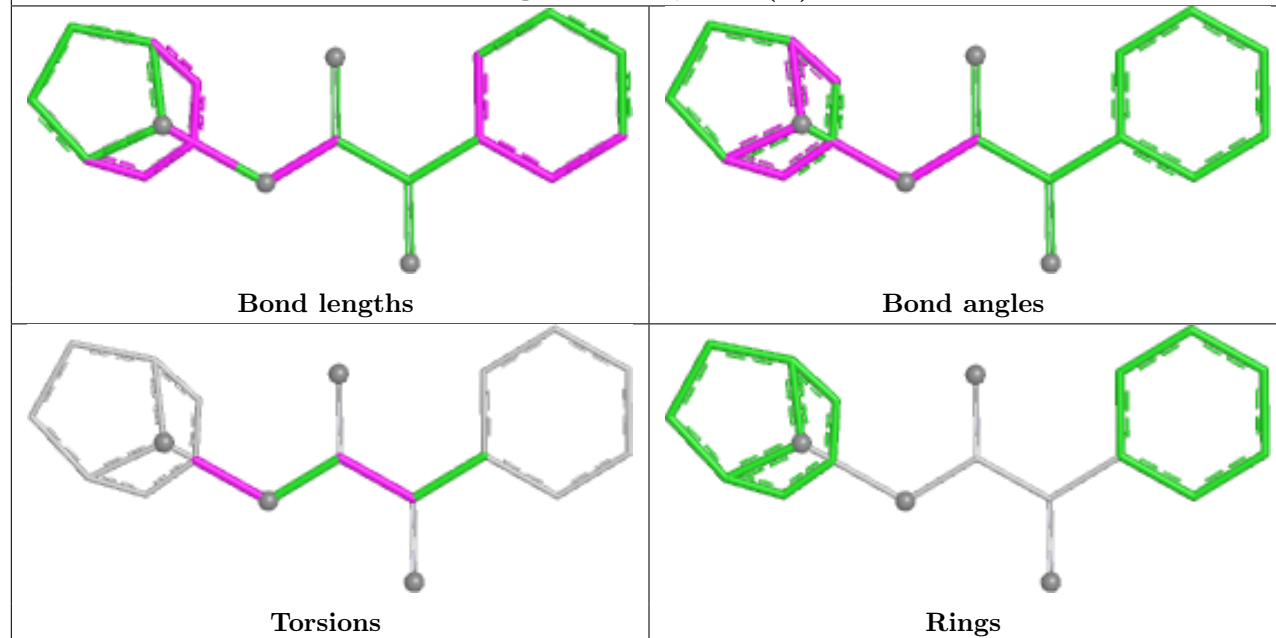
Ligand HTQ A 1 (Y)



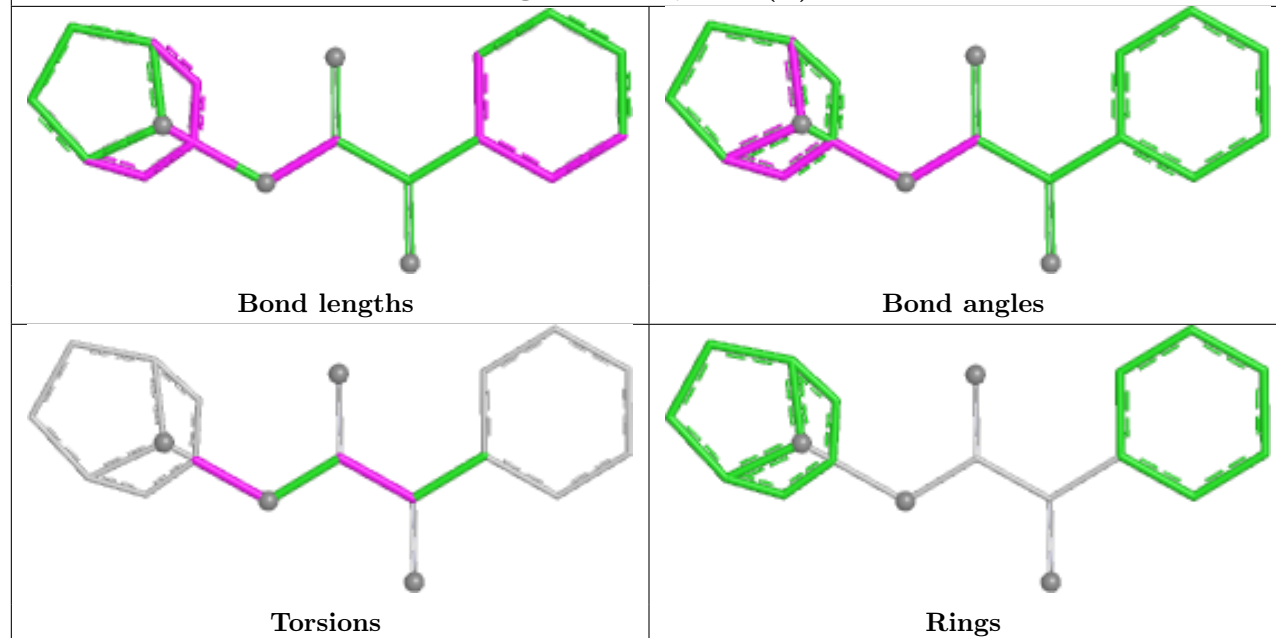
Ligand HTQ D 4 (Z)



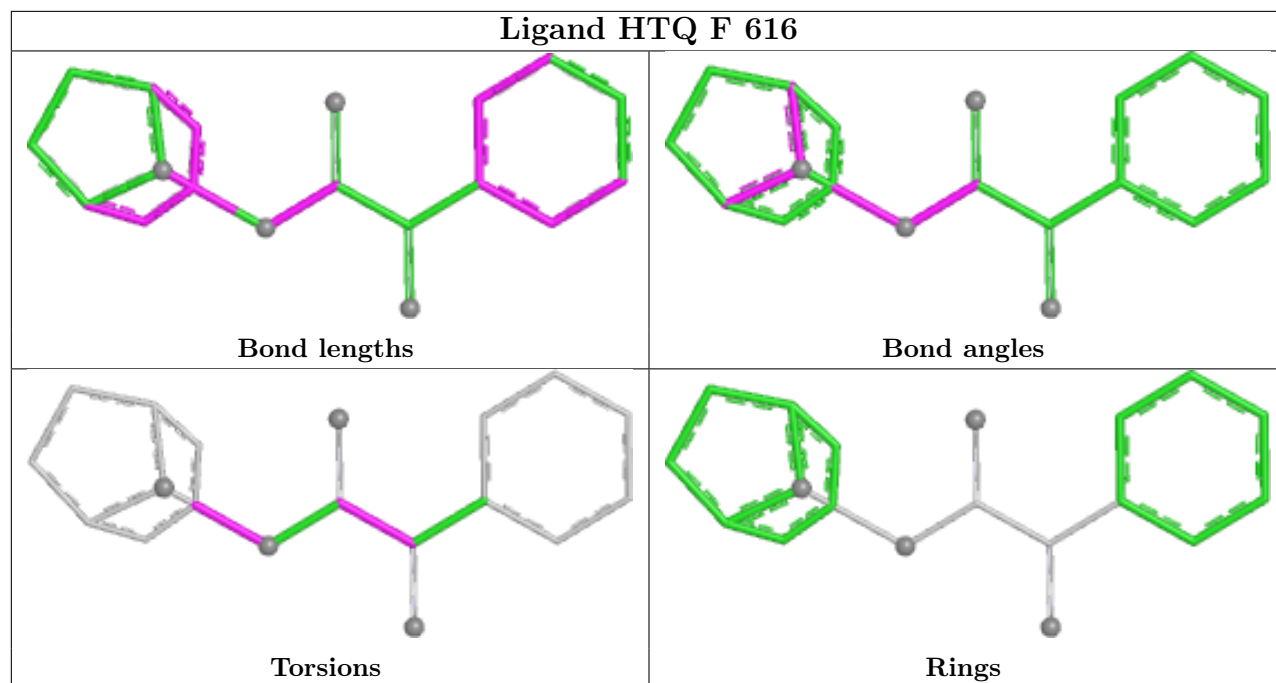
Ligand HTQ C 3 (Z)



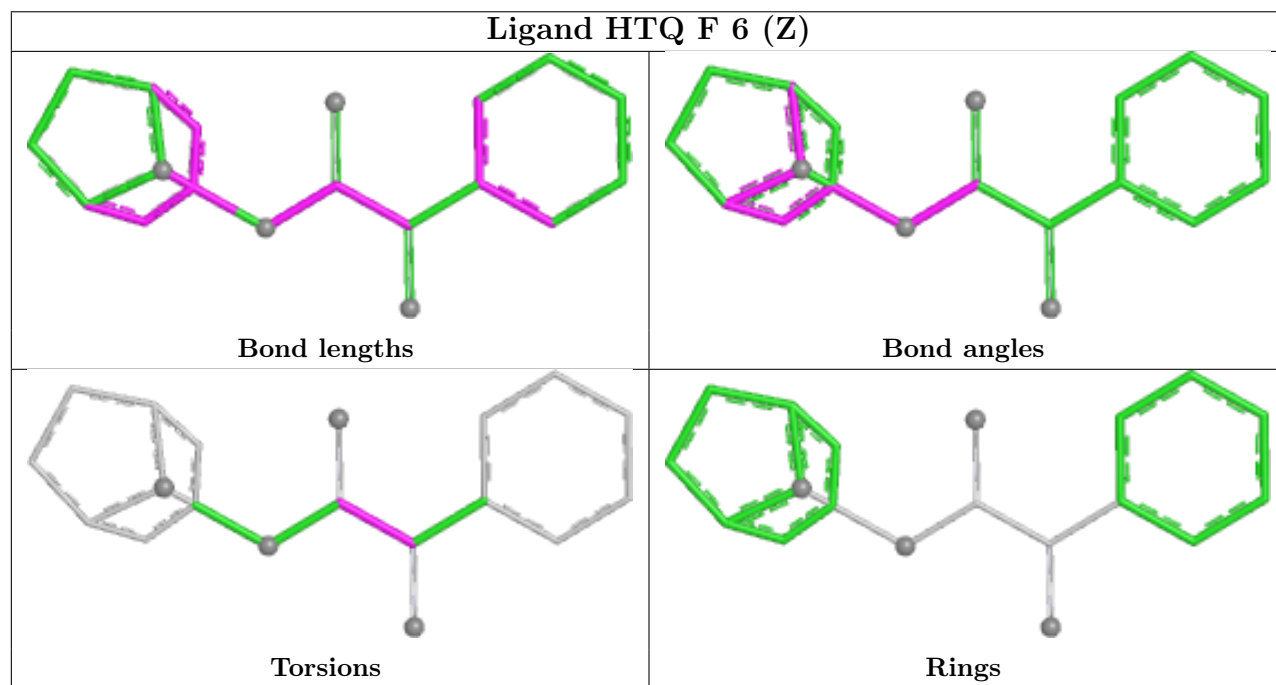
Ligand HTQ B 2 (Z)



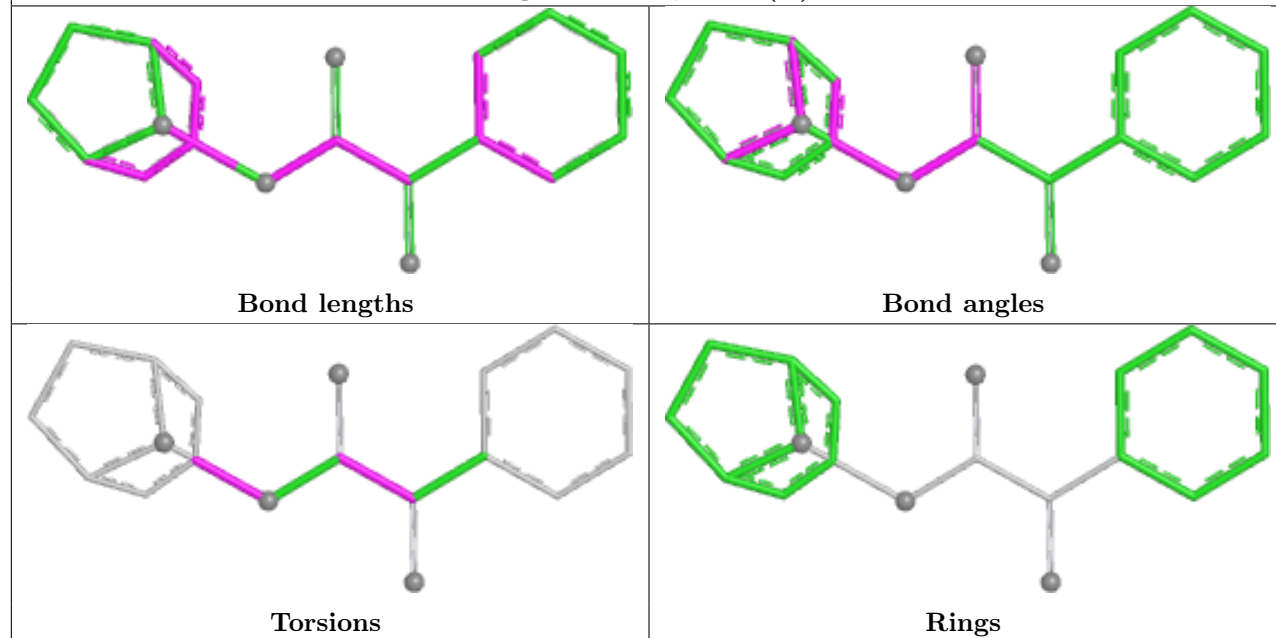
Ligand HTQ F 616



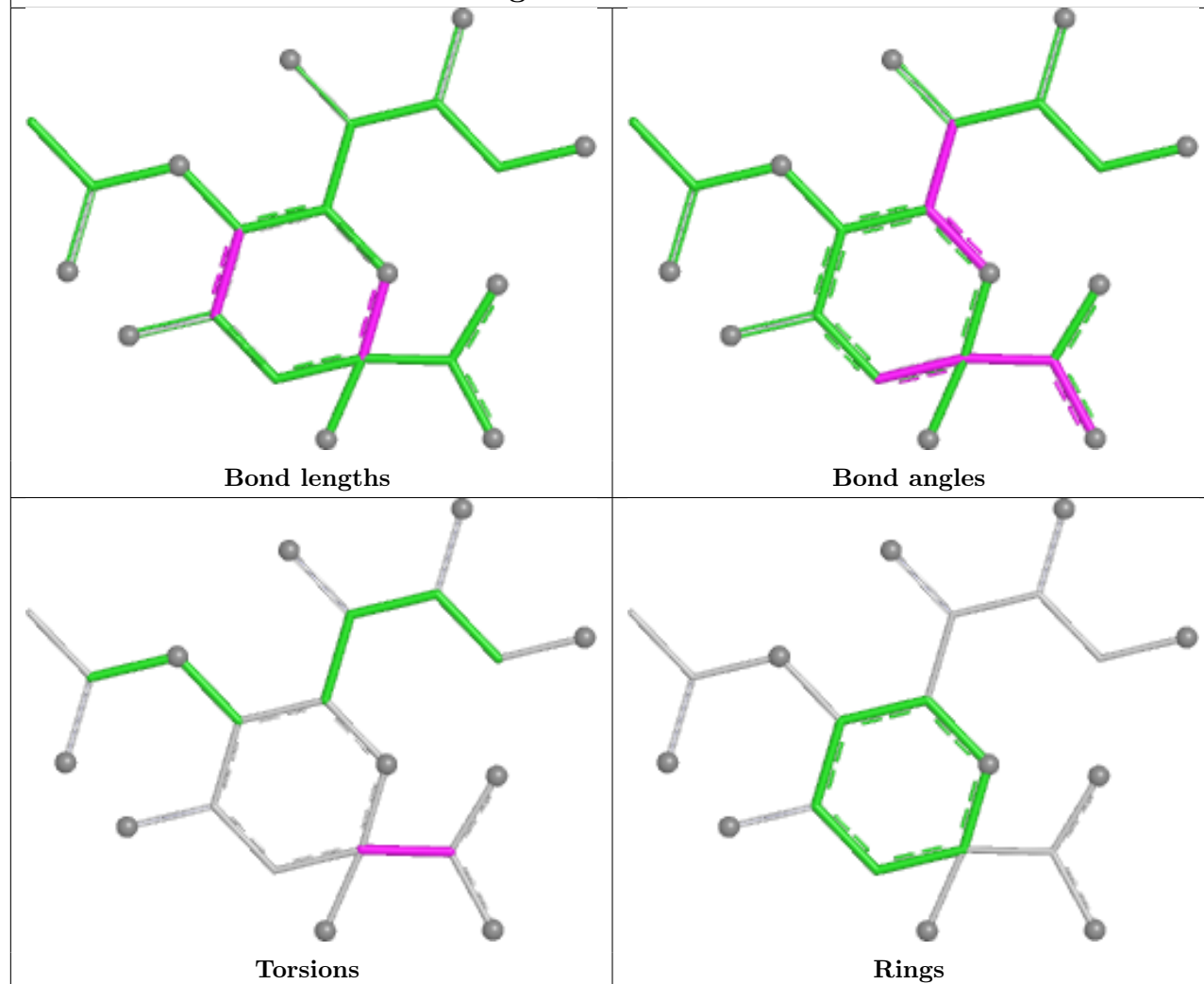
Ligand HTQ F 6 (Z)



Ligand HTQ A 1 (Z)



Ligand SIA B 282



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.