Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:32 AM BST

PDB ID	:	1MX5
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 following versions of software and data (see references ⓘ) were used in the production of this report:

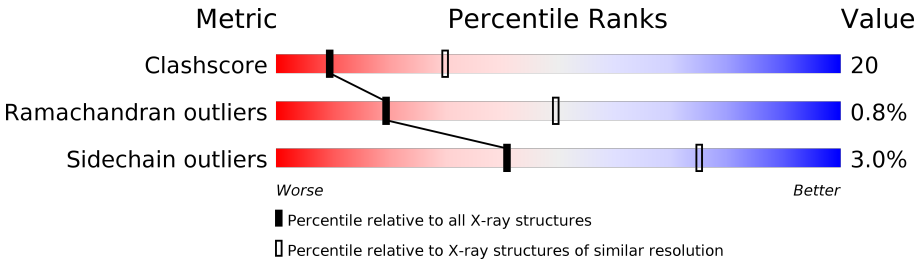
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	65% 31%
1	B	548	61% 33%
1	C	548	62% 32%
1	D	548	64% 32%
1	E	548	62% 32%
1	F	548	65% 30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	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.

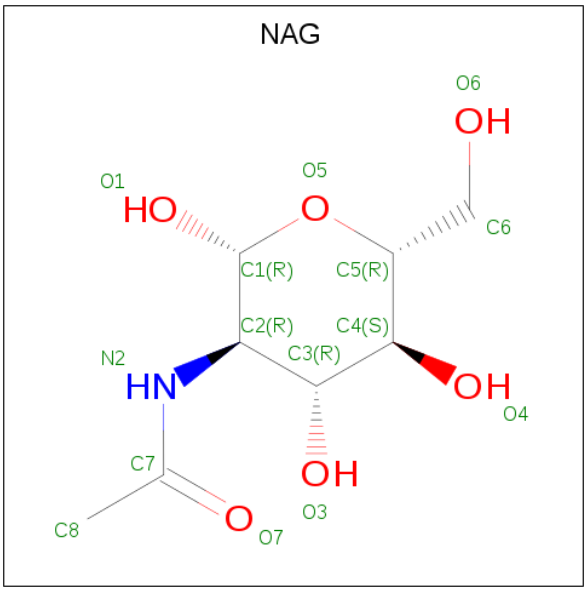
- Molecule 1 is a protein called liver Carboxylesterase I.

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:

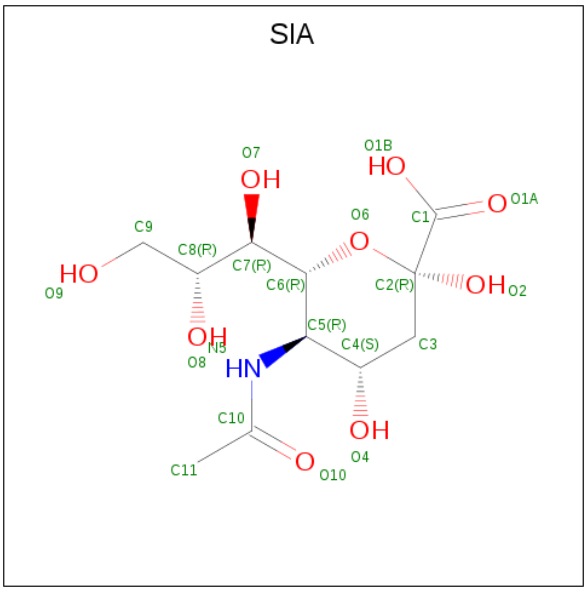
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141
D	?	-	GLN	deletion	UNP P23141
E	?	-	GLN	deletion	UNP P23141
F	?	-	GLN	deletion	UNP P23141

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

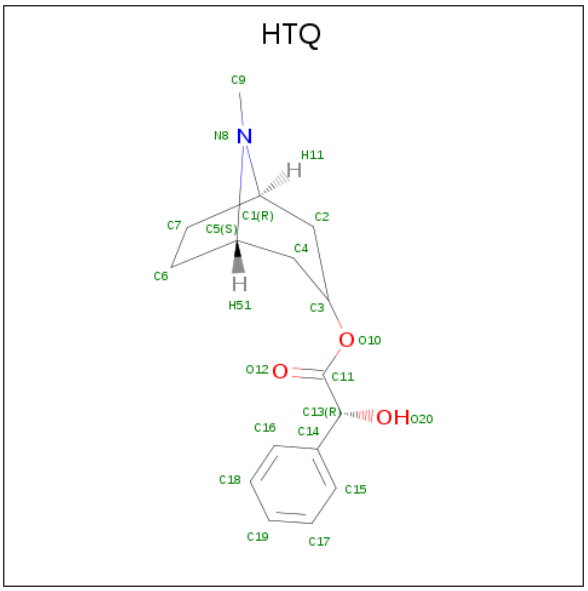


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 21 11 1 9	0	0
3	B	1	Total C N O 21 11 1 9	0	0
3	F	1	Total C N O 21 11 1 9	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is HOMOTROPINE (three-letter code: HTQ) (formula: $C_{16}H_{21}NO_3$).



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 O 249 249	0	0
6	B	303	Total O 303 303	0	0
6	C	289	Total O 289 289	0	0
6	D	291	Total O 291 291	0	0
6	E	295	Total O 295 295	0	0
6	F	254	Total O 254 254	0	0

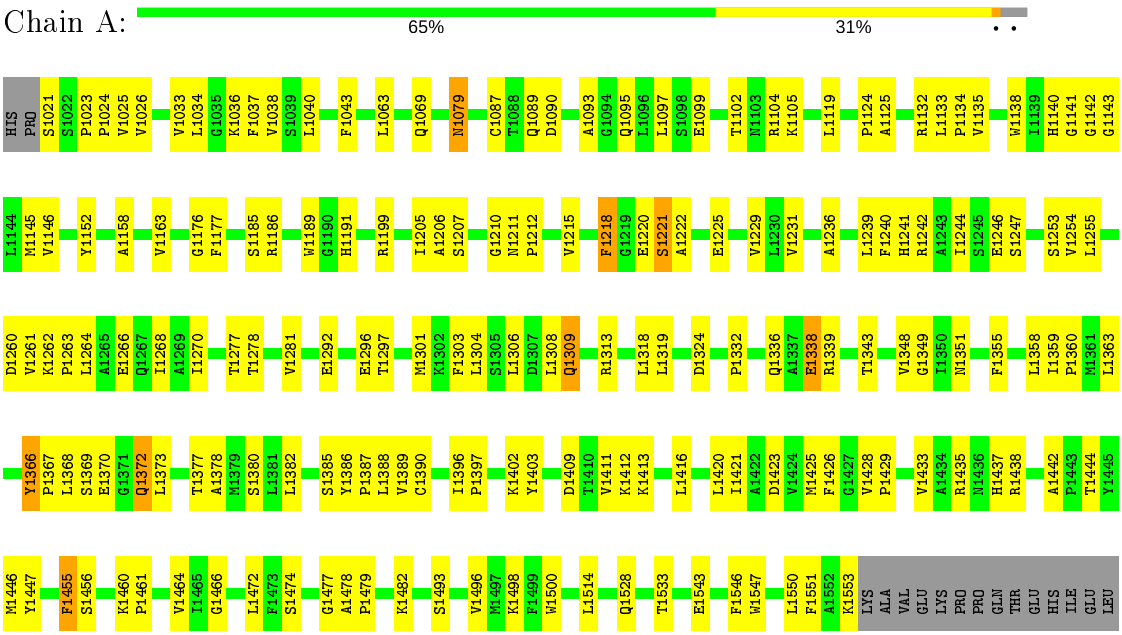
3 Residue-property plots (i)

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.

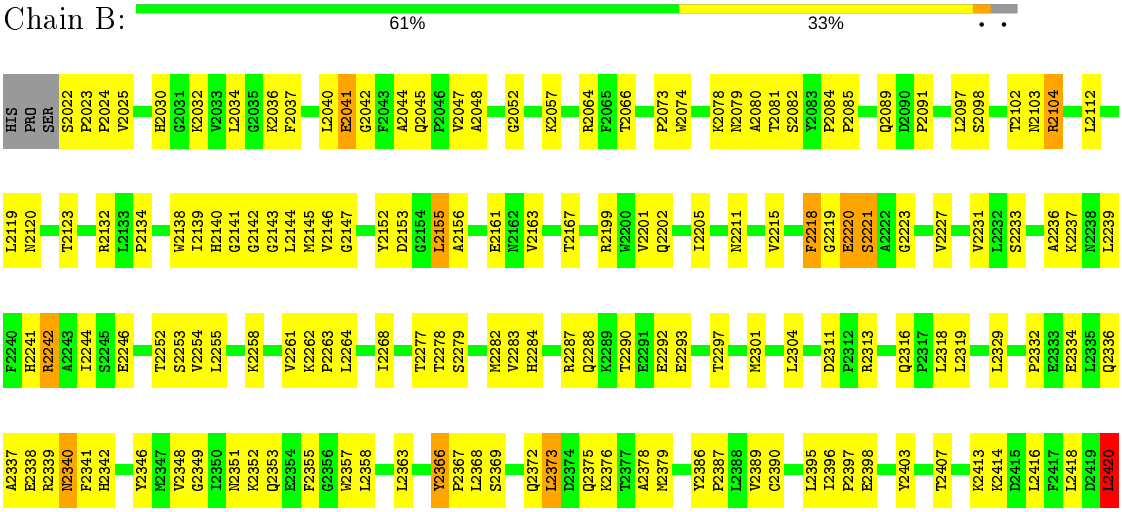
- Molecule 1: liver Carboxylesterase I

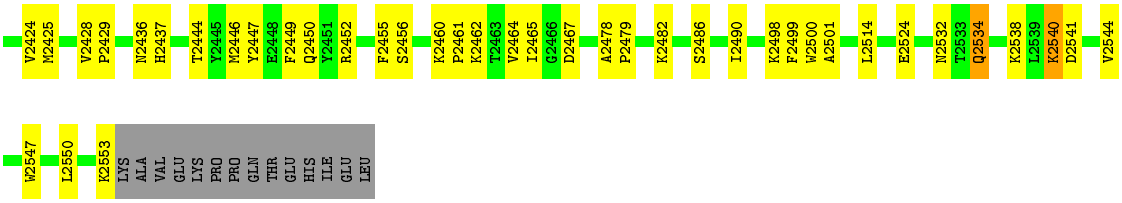
Chain A:



- Molecule 1: liver Carboxylesterase I

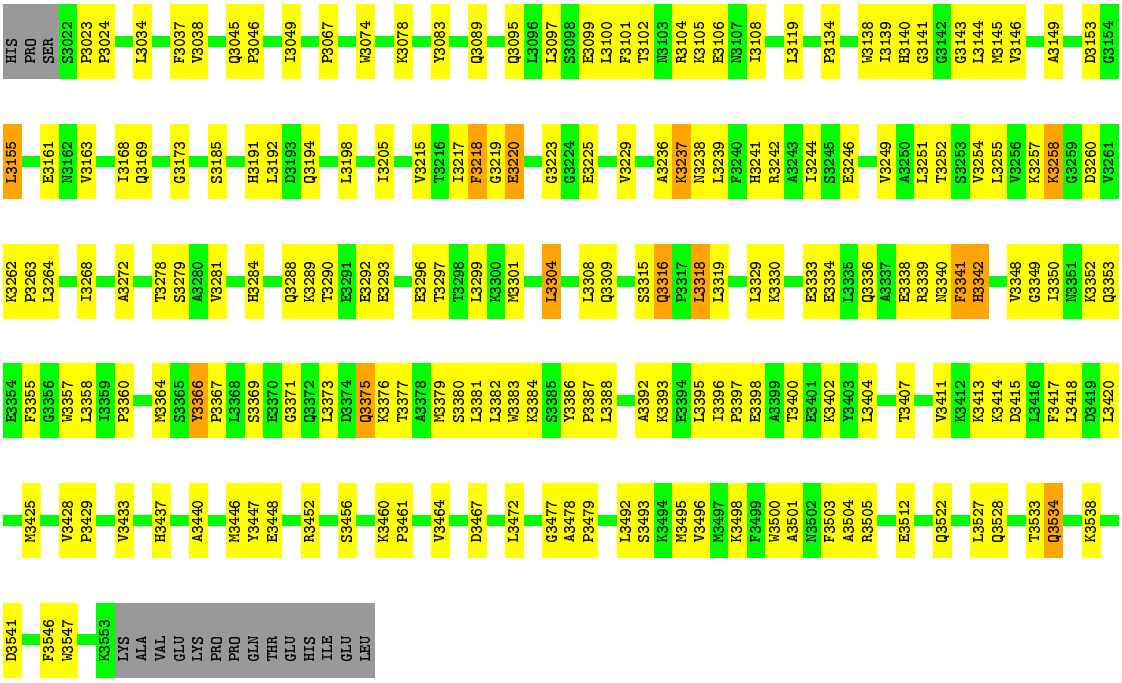
Chain B:





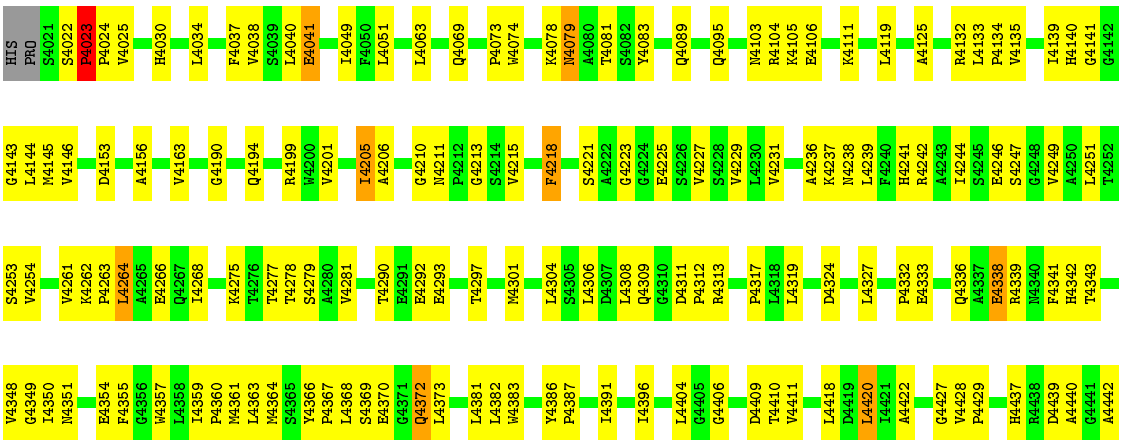
• Molecule 1: liver Carboxylesterase I

Chain C:



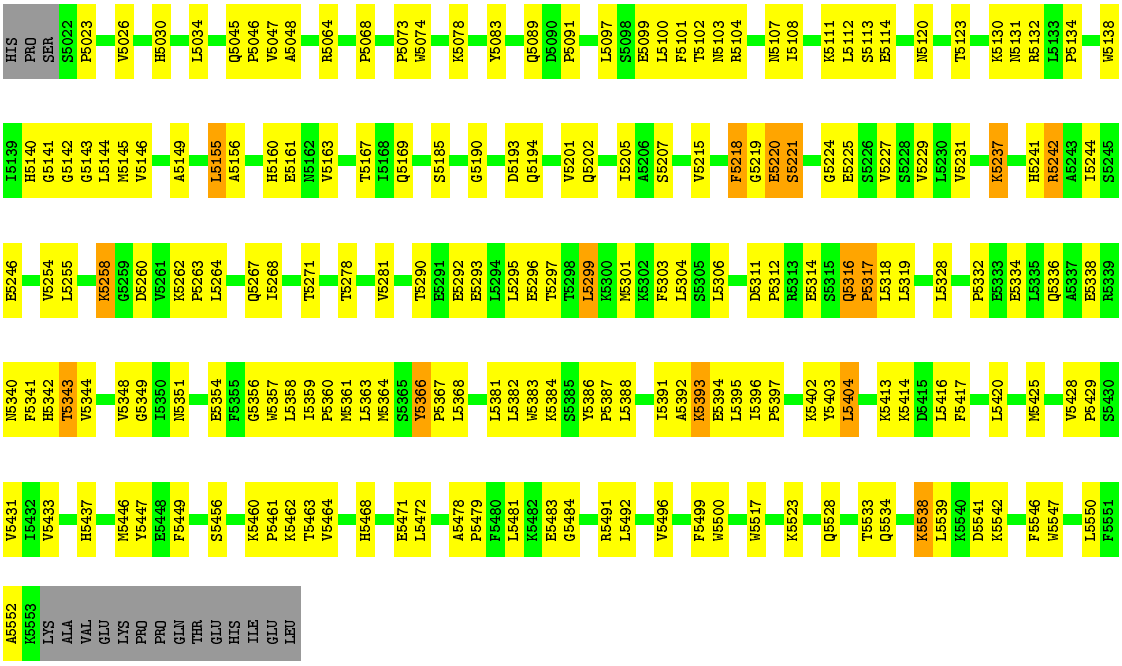
• Molecule 1: liver Carboxylesterase I

Chain D:



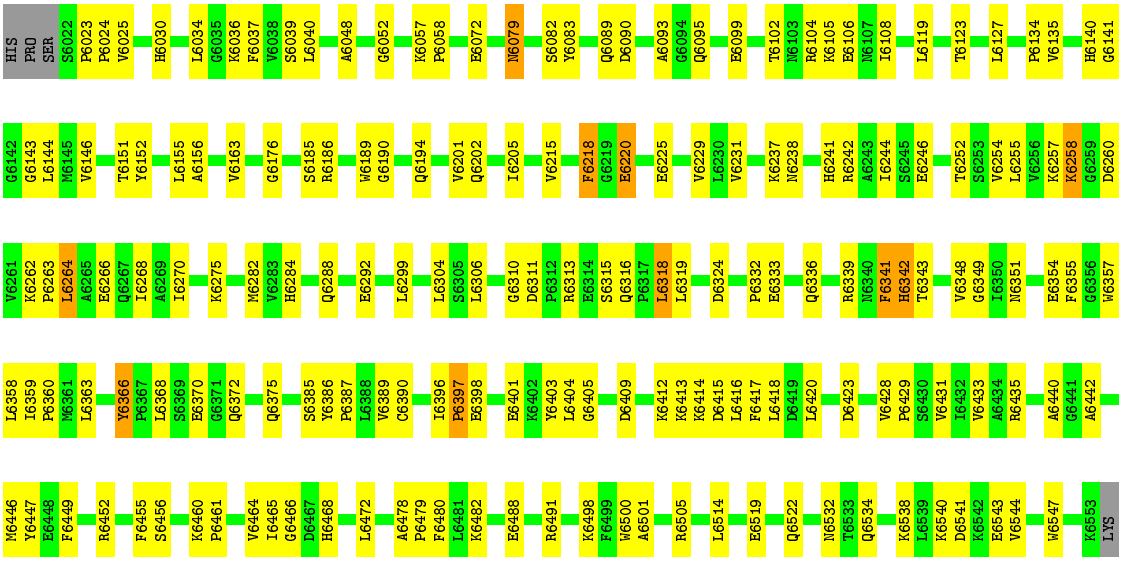
• Molecule 1: liver Carboxylesterase I

Chain E:



• Molecule 1: liver Carboxylesterase I

Chain F:




ALA
VAL
GLU
LYS
PRO
PRO
GLN
THR
GLU
HIS
ILE
GLU
LEU

4 Data and refinement statistics (i)

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, NAG, HTQ, CL

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	0.33	0/4236	0.57	0/5754
1	B	0.34	0/4230	0.59	1/5746 (0.0%)
1	C	0.34	0/4230	0.58	0/5746
1	D	0.34	0/4236	0.59	1/5754 (0.0%)
1	E	0.33	0/4230	0.60	0/5746
1	F	0.33	0/4230	0.58	0/5746
All	All	0.34	0/25392	0.58	2/34492 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2420	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	4420	LEU	CA-CB-CG	5.05	126.91	115.30

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	161	0
1	B	4124	0	4126	181	0
1	C	4124	0	4126	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4130	0	4131	137	0
1	E	4124	0	4126	178	0
1	F	4124	0	4126	151	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	14	0
5	C	60	0	63	11	0
5	D	60	0	63	12	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	15	0
6	E	295	0	0	20	0
6	F	254	0	0	25	0
All	All	26960	0	25289	990	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 20.

All (990) 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:2134:PRO:HG2	1:B:2163:VAL:HG12	1.43	1.00
1:B:2079:ASN:HB3	3:B:282:SIA:H113	1.41	1.00
1:E:5221:SER:CB	4:E:15:CL:CL	2.48	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:F:6258:LYS:HE2	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:3268:ILE:HG12	1:C:3301:MET:HE2	1.65	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:CE	1:F:6258:LYS:H	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:CE	1:C:3258:LYS:H	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:HH11	1:C:3242:ARG:HG2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:3105:LYS:HG3	1:C:3106:GLU:N	2.07	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:5388:LEU:HD22	1:E:5425:MET:HE1	1.72	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:6452:ARG:HB2	1:F:6465:ILE:HG12	1.76	0.68
1:F:6423:ASP:OD2	1:F:6543:GLU:HG2	1.94	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
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:B:2264:LEU:HD21	1:B:2319:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:A:1242:ARG:HG2	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2367:PRO:C	1:B:2368:LEU:HD12	2.19	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:N	1:A:1372:GLN:HE21	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: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
1:D:4143:GLY:CA	5:D:414:HTQ:H42	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:3414:LYS:HG3	1:C:3415:ASP:N	2.16	0.59
1:C:3242:ARG:HD3	1:C:3503:PHE:O	2.02	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:3388:LEU:HD22	1:C:3425:MET:HE1	1.87	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: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:F:6156:ALA:HB3	6:F:7194:HOH:O	2.04	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:579:NAG:HO4	2:E:580:NAG:H5	1.69	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:D:4459:MET:HE2	6:D:8676:HOH:O	2.07	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:HH11	1:F:6242:ARG:HG2	1.71	0.55
1:F:6431:VAL:HG21	1:F:6540:LYS:HB2	1.88	0.55
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:D:4292:GLU:CD	1:D:4292:GLU:H	2.10	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: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:E:5292:GLU:CD	1:E:5292:GLU:H	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:ARG:HH11	1:A:1199:ARG:HG2	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: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: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:A:1025:VAL:HG22	1:A:1034:LEU:HD23	1.90	0.53
1:C:3268:ILE:HG12	1:C:3301:MET:CE	2.37	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: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:2403:TYR:O	1:B:2416:LEU:HD13	2.07	0.53
1:E:5255:LEU:HD11	5:E:515:HTQ:H91	1.90	0.53
1:B:2242:ARG:HH11	1:B:2242:ARG:HG3	1.74	0.53
1:B:2220:GLU:HA	1:B:2246:GLU:O	2.09	0.53
1:E:5220:GLU:O	1:E:5221:SER:HB2	2.08	0.53
1:E:5491:ARG:HH11	1:E:5491:ARG:HG2	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:D:4361:MET:HE1	1:D:4363:LEU:HG	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1421:ILE:HG22	1:A:1425:MET:HE3	1.91	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:O	1:F:6119:LEU:HD12	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: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:D:4262:LYS:HE3	1:D:4279:SER:OG	2.10	0.52
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: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:1292:GLU:H	1:A:1292:GLU:CD	2.13	0.52
1:A:1402:LYS:HG2	1:A:1546:PHE:CE1	2.45	0.52
1:B:2261:VAL:HA	6:B:7763:HOH:O	2.10	0.52
1:B:2052:GLY:HA3	3:B:282:SIA:O1A	2.09	0.52
1:D:4491:ARG:HH11	1:D:4491:ARG:HG3	1.75	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HH11	1:E:5242:ARG:HG3	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: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
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:N	1:F:6152:TYR:CD1	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:F:6262:LYS:HE2	1:F:6282:MET:HE1	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2338:GLU:HB2	1:B:2340:ASN:HB3	1.91	0.50
1:B:2084:PRO:CA	3:B:282:SIA:O1A	2.60	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: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
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:B:2338:GLU:O	1:B:2339:ARG:C	2.49	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: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:D:4404:LEU:C	1:D:4406:GLY:H	2.16	0.49
1:B:2023:PRO:CB	1:B:2034:LEU:HD21	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:2292:GLU:H	1:B:2292:GLU:CD	2.16	0.48
1:D:4339:ARG:HH21	1:D:4439:ASP:HB2	1.78	0.48
1:E:5241:HIS:C	1:E:5242:ARG:HD2	2.34	0.48
1:E:5271:THR:CG2	1:E:5297:THR:HG23	2.43	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4105:LYS:HG3	1:D:4106:GLU:N	2.28	0.48
1:F:6119:LEU:C	1:F:6119:LEU:HD12	2.34	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:1304:LEU:CD1	5:A:111:HTQ:H171	2.36	0.48
1:A:1435:ARG:O	1:A:1438:ARG:HB3	2.14	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:2044:ALA:O	1:F:6491:ARG:HD2	2.13	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: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:B:2334:GLU:O	1:B:2338:GLU:HG3	2.14	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:1222:ALA:N	4:A:11:CL:CL	2.83	0.47
1:A:1138:TRP:CH2	1:A:1220:GLU:HB2	2.49	0.47
1:A:1260:ASP:OD2	1:A:1263:PRO:HD3	2.14	0.47
1:A:1372:GLN:H	1:A:1372:GLN:NE2	2.12	0.47
1:B:2022:SER:HB3	6:B:8445:HOH:O	2.14	0.47
1:B:2368:LEU:N	1:B:2368:LEU:HD12	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:C:3257:LYS:HB3	6:C:7331:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:D:4242:ARG:NH1	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:1478:ALA:N	1:A:1479:PRO:CD	2.77	0.47
1:E:5100:LEU:HD13	1:E:5358:LEU:HD11	1.96	0.47
1:E:5338:GLU:C	1:E:5340:ASN:N	2.67	0.47
1:A:1242:ARG:NH1	1:A:1242:ARG:HG2	2.29	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
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:6359:ILE:HB	1:F:6360:PRO:HD3	1.97	0.47
1:F:6349:GLY:HA3	1:F:6447:TYR:CE1	2.48	0.47
1:A:1034:LEU:C	1:A:1034:LEU:HD13	2.35	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:B:2376:LYS:HA	1:B:2379:MET:HE2	1.97	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:3538:LYS:HB3	1:C:3541:ASP:HB2	1.96	0.47
1:C:3371:GLY:HA2	5:C:3[Y]:HTQ:O12	2.15	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:F:6292:GLU:H	1:F:6292:GLU:CD	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	1:A:1119:LEU:HD12	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:A:1551:PHE:C	1:A:1553:LYS:H	2.18	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:6246:GLU:HG2	1:F:6447:TYR:OH	2.15	0.46
1:F:6143:GLY:O	1:F:6318:LEU:HD13	2.16	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:3242:ARG:HD2	1:C:3504:ALA:HA	1.97	0.46
1:C:3220:GLU:HA	1:C:3246:GLU:O	2.15	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: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: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:5237:LYS:HZ3	1:E:5342:HIS:H	1.63	0.46
1:E:5402:LYS:HD3	1:E:5402:LYS:O	2.16	0.46
1:B:2264:LEU:HD22	1:B:2316:GLN:HE21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:E:5461:PRO:HB3	6:E:8667:HOH:O	2.16	0.45
1:A:1551:PHE:C	1:A:1553:LYS:N	2.69	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:CD1	1:A:1152:TYR:N	2.84	0.45
3:B:282:SIA:H92	1:C:3279:SER:N	2.30	0.45
1:B:2262:LYS:HE3	1:B:2279:SER:OG	2.17	0.45
1:B:2084:PRO:CA	3:B:282:SIA:C1	2.95	0.45
1:C:3074:TRP:CD2	1:C:3078:LYS:HE2	2.52	0.45
1:C:3205:ILE:HA	1:C:3205:ILE:HD12	1.78	0.45
1:E:5316:GLN:OE1	1:E:5316:GLN:HA	2.16	0.45
1:E:5368:LEU:N	1:E:5368:LEU:HD12	2.31	0.45
1:F:6220:GLU:CB	1:F:6246:GLU:HB2	2.47	0.45
1:C:3067:PRO:HB3	1:C:3192:LEU:CD1	2.44	0.45
1:D:4040:LEU:O	1:D:4041:GLU:C	2.54	0.45
1:B:2119:LEU:HD12	1:B:2119:LEU:C	2.37	0.45
1:B:2262:LYS:HE2	1:B:2282:MET:HE1	1.99	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: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: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
1:F:6389:VAL:O	1:F:6390:CYS:HB2	2.16	0.45
5:A:1[Z]:HTQ:H191	6:A:8638:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1447:TYR:C	1:A:1447:TYR:CD2	2.89	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
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:HB3	1:B:2104:ARG:NH1	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: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:HD3	1:B:2132:ARG:HA	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:A:1221:SER:OG	4:A:11:CL:CL	2.68	0.44
1:D:4074:TRP:CD2	1:D:4078:LYS:HE2	2.52	0.44
1:D:4119:LEU:O	1:D:4119:LEU:HD12	2.17	0.44
1:E:5304:LEU:HD13	5:E:515:HTQ:H191	2.00	0.44
1:E:5254:VAL:HG13	1:E:5255:LEU:N	2.31	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: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:E:5156:ALA:O	1:E:5160:HIS:HB2	2.17	0.44
1:E:5068:PRO:HB3	1:E:5193:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:4464:VAL:HG12	1:D:4467:ASP:HB2	2.00	0.44
1:E:5205:ILE:HA	1:E:5205:ILE:HD12	1.80	0.44
1:E:5292:GLU:CD	1:E:5292:GLU:N	2.71	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: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:CG	1:C:3242:ARG:NH1	2.81	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:2337:ALA:C	1:B:2339:ARG:H	2.22	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: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:B:2283:VAL:HG12	1:B:2287:ARG:NH1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:PHE:HB2	1:A:1244:ILE:HB	2.00	0.43
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: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: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:D:4211:ASN:C	1:D:4213:GLY:H	2.22	0.43
1:F:6310:GLY:HA3	6:F:7283:HOH:O	2.18	0.43
1:F:6447:TYR:CD2	1:F:6447:TYR:C	2.92	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:D:4063:LEU:HD21	1:D:4069:GLN:NE2	2.34	0.43
1:E:5425:MET:HE1	5:E:515:HTQ:H72	1.99	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: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:A:1338:GLU:C	1:A:1339:ARG:HD2	2.40	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: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:4311:ASP:OD1	1:D:4313:ARG:HB2	2.19	0.42
1:E:5026:VAL:HG13	1:E:5207:SER:HB3	2.01	0.42
1:E:5237:LYS:HZ3	1:E:5342:HIS:CB	2.31	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:O	1:C:3119:LEU:HD12	2.18	0.42
1:C:3268:ILE:CD1	1:C:3319:LEU:HD21	2.49	0.42
1:C:3495:MET:HE3	1:C:3533:THR:HG21	2.01	0.42
1:C:3501:ALA:O	1:C:3505:ARG:HG2	2.19	0.42
1:F:6268:ILE:HD11	1:F:6319:LEU:CD2	2.50	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:3373:LEU:HD12	1:C:3377:THR:HB	2.01	0.42
1:F:6370:GLU:C	1:F:6372:GLN:H	2.21	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: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
1:D:4324:ASP:OD2	1:D:4327:LEU:HB3	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:3251:LEU:HD23	1:C:3251:LEU:HA	1.87	0.41
1:A:1205:ILE:HA	1:A:1205:ILE:HD12	1.91	0.41
1:C:3249:VAL:HG23	1:C:3251:LEU:H	1.84	0.41
1:C:3329:LEU:HG	6:C:8361:HOH:O	2.20	0.41
1:C:3533:THR:C	1:C:3534:GLN:HG3	2.40	0.41
1:D:4205:ILE:HD12	1:D:4205:ILE:HA	1.86	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: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:D:4343:THR:HB	1:D:4442:ALA:CB	2.44	0.41
1:E:5112:LEU:O	1:E:5113:SER:HB2	2.20	0.41
1:E:5311:ASP:HA	1:E:5312:PRO:HD3	1.88	0.41
1:E:5491:ARG:NH1	1:E:5491:ARG:HG2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:5414:LYS:HD3	1:E:5414:LYS:C	2.40	0.41
1:F:6218:PHE:CB	1:F:6244:ILE:HB	2.49	0.41
1:A:1309:GLN:NE2	1:A:1309:GLN:O	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: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:C:3145:MET:CG	1:C:3318:LEU:HD21	2.50	0.41
1:C:3257:LYS:NZ	1:C:3318:LEU:O	2.53	0.41
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: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:4022:SER:O	1:D:4023:PRO:C	2.59	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:1231:VAL:HA	1:A:1240:PHE:HZ	1.84	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:B:2057:LYS:HE2	6:B:8660:HOH:O	2.20	0.41
1:D:4350:ILE:HD13	1:D:4427:GLY:HA2	2.03	0.41
1:D:4530:GLY:O	1:D:4531:ALA:C	2.59	0.41
1:E:5218:PHE:CB	1:E:5244:ILE:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
5:D:414:HTQ:H41	6:D:14:HOH:O	2.20	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: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:B:2420:LEU:C	1:B:2420:LEU:HD12	2.42	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
1:A:1368:LEU:HB2	5:A:1[Y]:HTQ:H151	2.04	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:F:6341:PHE:O	1:F:6342:HIS:C	2.59	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:D:4125:ALA:HB2	1:D:4133:LEU:CD1	2.51	0.40
1:D:4361:MET:CE	1:D:4363:LEU:HG	2.50	0.40
1:E:5246:GLU:OE1	1:E:5471:GLU:OE1	2.40	0.40
1:E:5103:ASN:ND2	1:E:5481:LEU:HD12	2.36	0.40
1:E:5120:ASN:HB2	1:E:5167:THR:OG1	2.21	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:B:2040:LEU:O	1:B:2041:GLU:C	2.60	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:5392:ALA:O	1:E:5394:GLU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/548 (97%)	495 (93%)	33 (6%)	2 (0%)	34	66
1	B	529/548 (96%)	496 (94%)	28 (5%)	5 (1%)	17	46
1	C	529/548 (96%)	488 (92%)	38 (7%)	3 (1%)	25	56
1	D	530/548 (97%)	503 (95%)	23 (4%)	4 (1%)	19	49
1	E	529/548 (96%)	495 (94%)	27 (5%)	7 (1%)	12	36
1	F	529/548 (96%)	493 (93%)	32 (6%)	4 (1%)	19	49
All	All	3176/3288 (97%)	2970 (94%)	181 (6%)	25 (1%)	19	49

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

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Mol	Chain	Res	Type
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 (i)

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%)	437 (98%)	11 (2%)	47	80
1	B	447/463 (96%)	433 (97%)	14 (3%)	40	74
1	C	447/463 (96%)	432 (97%)	15 (3%)	37	71
1	D	448/463 (97%)	437 (98%)	11 (2%)	47	80
1	E	447/463 (96%)	431 (96%)	16 (4%)	35	69
1	F	447/463 (96%)	433 (97%)	14 (3%)	40	74
All	All	2684/2778 (97%)	2603 (97%)	81 (3%)	41	75

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1033	VAL
1	A	1079	ASN
1	A	1218	PHE
1	A	1221	SER
1	A	1264	LEU
1	A	1309	GLN
1	A	1338	GLU
1	A	1366	TYR
1	A	1372	GLN
1	A	1455	PHE
1	A	1500	TRP
1	B	2104	ARG
1	B	2155	LEU

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Mol	Chain	Res	Type
1	B	2218	PHE
1	B	2220	GLU
1	B	2221	SER
1	B	2242	ARG
1	B	2258	LYS
1	B	2340	ASN
1	B	2358	LEU
1	B	2366	TYR
1	B	2420	LEU
1	B	2499	PHE
1	B	2500	TRP
1	B	2534	GLN
1	C	3155	LEU
1	C	3218	PHE
1	C	3220	GLU
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	3342	HIS
1	C	3366	TYR
1	C	3375	GLN
1	C	3381	LEU
1	C	3500	TRP
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	5218	PHE
1	E	5220	GLU

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Mol	Chain	Res	Type
1	E	5225	GLU
1	E	5242	ARG
1	E	5258	LYS
1	E	5299	LEU
1	E	5316	GLN
1	E	5343	THR
1	E	5366	TYR
1	E	5381	LEU
1	E	5404	LEU
1	E	5499	PHE
1	E	5500	TRP
1	E	5534	GLN
1	F	6079	ASN
1	F	6155	LEU
1	F	6218	PHE
1	F	6220	GLU
1	F	6258	LYS
1	F	6264	LEU
1	F	6299	LEU
1	F	6318	LEU
1	F	6342	HIS
1	F	6366	TYR
1	F	6500	TRP
1	F	6519	GLU
1	F	6532	ASN
1	F	6534	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1069	GLN
1	A	1131	ASN
1	A	1140	HIS
1	A	1162	ASN
1	A	1241	HIS
1	A	1284	HIS
1	A	1309	GLN
1	A	1336	GLN
1	A	1351	ASN
1	A	1372	GLN
1	A	1436	ASN
1	A	1437	HIS

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Mol	Chain	Res	Type
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	2437	HIS
1	B	2450	GLN
1	B	2528	GLN
1	B	2532	ASN
1	B	2537	GLN
1	C	3107	ASN
1	C	3131	ASN
1	C	3140	HIS
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	3528	GLN
1	C	3532	ASN
1	C	3537	GLN
1	D	4045	GLN
1	D	4069	GLN
1	D	4107	ASN
1	D	4140	HIS
1	D	4162	ASN
1	D	4241	HIS
1	D	4309	GLN
1	D	4351	ASN
1	D	4372	GLN
1	D	4375	GLN
1	D	4436	ASN
1	D	4437	HIS

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Mol	Chain	Res	Type
1	D	4537	GLN
1	E	5030	HIS
1	E	5095	GLN
1	E	5131	ASN
1	E	5140	HIS
1	E	5162	ASN
1	E	5202	GLN
1	E	5241	HIS
1	E	5288	GLN
1	E	5336	GLN
1	E	5351	ASN
1	E	5372	GLN
1	E	5436	ASN
1	E	5437	HIS
1	E	5534	GLN
1	E	5537	GLN
1	F	6069	GLN
1	F	6095	GLN
1	F	6140	HIS
1	F	6162	ASN
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	6450	GLN
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 monosaccharides 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	E	515	-	22,22,22	2.02	8 (36%)	30,31,31	1.35	2 (6%)
5	HTQ	F	6[Y]	-	22,22,22	2.09	9 (40%)	30,31,31	1.24	2 (6%)
3	SIA	A	182	-	18,21,21	1.12	2 (11%)	21,31,31	1.10	2 (9%)
5	HTQ	D	4[Y]	-	22,22,22	2.04	8 (36%)	30,31,31	1.27	3 (10%)
5	HTQ	F	616	-	22,22,22	1.91	8 (36%)	30,31,31	1.25	2 (6%)
5	HTQ	E	5[Y]	-	22,22,22	2.06	8 (36%)	30,31,31	1.17	3 (10%)
3	SIA	F	682	-	18,21,21	1.33	2 (11%)	21,31,31	0.92	1 (4%)
5	HTQ	E	5[Z]	-	22,22,22	2.07	9 (40%)	30,31,31	1.35	2 (6%)
5	HTQ	C	3[Y]	-	22,22,22	2.05	8 (36%)	30,31,31	1.36	3 (10%)
2	NAG	E	579	1	14,14,15	0.55	0	17,19,21	0.67	0
5	HTQ	C	3[Z]	-	22,22,22	2.10	8 (36%)	30,31,31	1.30	3 (10%)
2	NAG	C	379	1	14,14,15	0.56	0	17,19,21	0.67	0
5	HTQ	B	212	-	22,22,22	1.90	7 (31%)	30,31,31	1.52	4 (13%)
2	NAG	F	679	1	14,14,15	0.61	0	17,19,21	0.64	0
2	NAG	A	179	1	14,14,15	0.61	0	17,19,21	0.70	1 (5%)
5	HTQ	A	1[Z]	-	22,22,22	2.14	9 (40%)	30,31,31	1.65	3 (10%)
2	NAG	B	279	1	14,14,15	0.53	0	17,19,21	0.74	0
5	HTQ	A	1[Y]	-	22,22,22	2.12	9 (40%)	30,31,31	1.36	3 (10%)
5	HTQ	F	6[Z]	-	22,22,22	2.09	9 (40%)	30,31,31	1.37	3 (10%)
5	HTQ	A	111	-	22,22,22	1.94	8 (36%)	30,31,31	1.58	3 (10%)
5	HTQ	B	2[Y]	-	22,22,22	2.00	8 (36%)	30,31,31	1.07	2 (6%)
5	HTQ	B	2[Z]	-	22,22,22	2.03	8 (36%)	30,31,31	1.24	3 (10%)
2	NAG	E	580	-	14,14,15	0.54	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	479	1	14,14,15	0.53	0	17,19,21	0.62	0
5	HTQ	D	414	-	22,22,22	2.06	9 (40%)	30,31,31	1.88	4 (13%)
5	HTQ	C	313	-	22,22,22	2.04	8 (36%)	30,31,31	1.32	2 (6%)
3	SIA	B	282	-	18,21,21	1.33	2 (11%)	21,31,31	1.13	1 (4%)
5	HTQ	D	4[Z]	-	22,22,22	1.97	8 (36%)	30,31,31	1.11	2 (6%)

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	E	515	-	-	5/12/33/33	0/4/3/3
5	HTQ	F	6[Y]	-	-	5/12/33/33	0/4/3/3
3	SIA	A	182	-	-	0/14/38/38	0/1/1/1
5	HTQ	D	4[Y]	-	-	5/12/33/33	0/4/3/3
5	HTQ	F	616	-	-	4/12/33/33	0/4/3/3
5	HTQ	E	5[Y]	-	-	4/12/33/33	0/4/3/3
3	SIA	F	682	-	-	0/14/38/38	0/1/1/1
5	HTQ	E	5[Z]	-	-	5/12/33/33	0/4/3/3
5	HTQ	C	3[Y]	-	-	0/12/33/33	0/4/3/3
2	NAG	E	579	1	-	2/6/23/26	0/1/1/1
5	HTQ	C	3[Z]	-	-	5/12/33/33	0/4/3/3
2	NAG	C	379	1	-	4/6/23/26	0/1/1/1
5	HTQ	B	212	-	-	1/12/33/33	0/4/3/3
2	NAG	F	679	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	A	179	1	-	4/6/23/26	0/1/1/1
5	HTQ	A	1[Z]	-	-	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
5	HTQ	A	1[Y]	-	-	4/12/33/33	0/4/3/3
5	HTQ	F	6[Z]	-	-	4/12/33/33	0/4/3/3
5	HTQ	A	111	-	-	1/12/33/33	0/4/3/3
5	HTQ	B	2[Y]	-	-	4/12/33/33	0/4/3/3
5	HTQ	B	2[Z]	-	-	6/12/33/33	0/4/3/3
2	NAG	E	580	-	-	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
5	HTQ	D	414	-	-	5/12/33/33	0/4/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HTQ	C	313	-	-	5/12/33/33	0/4/3/3
3	SIA	B	282	-	-	0/14/38/38	0/1/1/1
5	HTQ	D	4[Z]	-	-	3/12/33/33	0/4/3/3

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	682	SIA	C4-C5	3.99	1.56	1.53
5	B	2[Z]	HTQ	C4-C3	3.52	1.61	1.52
5	D	4[Y]	HTQ	C4-C3	3.50	1.61	1.52
5	C	3[Z]	HTQ	O10-C11	3.50	1.42	1.34
5	D	414	HTQ	C16-C14	3.49	1.44	1.39
5	E	5[Y]	HTQ	C4-C3	3.49	1.61	1.52
5	E	515	HTQ	C9-N8	3.48	1.52	1.47
5	A	1[Z]	HTQ	O10-C11	3.47	1.42	1.34
5	C	3[Y]	HTQ	C4-C5	3.44	1.60	1.53
5	C	3[Z]	HTQ	C4-C3	3.44	1.60	1.52
5	D	4[Y]	HTQ	O10-C11	3.41	1.42	1.34
5	C	313	HTQ	C9-N8	3.38	1.52	1.47
5	D	4[Z]	HTQ	C9-N8	3.37	1.52	1.47
5	E	5[Z]	HTQ	C9-N8	3.36	1.52	1.47
5	B	2[Z]	HTQ	O10-C11	3.36	1.42	1.34
5	C	3[Y]	HTQ	C4-C3	3.35	1.60	1.52
5	C	3[Z]	HTQ	C4-C5	3.35	1.59	1.53
5	F	6[Z]	HTQ	C9-N8	3.35	1.52	1.47
5	A	1[Y]	HTQ	C9-N8	3.34	1.52	1.47
5	E	5[Y]	HTQ	C9-N8	3.33	1.52	1.47
3	B	282	SIA	C4-C5	3.33	1.56	1.53
5	F	6[Y]	HTQ	O10-C11	3.32	1.42	1.34
5	C	3[Y]	HTQ	C9-N8	3.32	1.52	1.47
5	E	5[Y]	HTQ	O10-C11	3.32	1.42	1.34
5	B	2[Y]	HTQ	C9-N8	3.31	1.52	1.47
5	A	1[Y]	HTQ	C4-C3	3.30	1.60	1.52
5	F	6[Y]	HTQ	C9-N8	3.30	1.52	1.47
5	A	111	HTQ	C4-C5	3.30	1.59	1.53
5	D	4[Y]	HTQ	C9-N8	3.28	1.52	1.47
5	A	1[Y]	HTQ	C4-C5	3.28	1.59	1.53
5	E	515	HTQ	O10-C11	3.26	1.41	1.34
5	D	414	HTQ	O10-C11	3.25	1.41	1.34
5	F	6[Z]	HTQ	C4-C3	3.24	1.60	1.52
5	B	212	HTQ	C4-C5	3.24	1.59	1.53
5	C	3[Z]	HTQ	C9-N8	3.24	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	6[Y]	HTQ	C4-C3	3.23	1.60	1.52
5	B	2[Z]	HTQ	C9-N8	3.22	1.52	1.47
5	A	1[Y]	HTQ	C16-C14	3.22	1.44	1.39
5	F	6[Z]	HTQ	C4-C5	3.19	1.59	1.53
5	A	1[Z]	HTQ	C9-N8	3.19	1.52	1.47
5	C	313	HTQ	O10-C11	3.19	1.41	1.34
5	B	212	HTQ	C4-C3	3.18	1.60	1.52
5	B	2[Z]	HTQ	C4-C5	3.18	1.59	1.53
5	D	4[Y]	HTQ	C4-C5	3.18	1.59	1.53
5	C	3[Z]	HTQ	C2-C3	3.16	1.60	1.52
5	F	6[Y]	HTQ	C2-C3	3.16	1.60	1.52
5	E	5[Z]	HTQ	O10-C11	3.15	1.41	1.34
5	E	515	HTQ	C2-C3	3.15	1.60	1.52
5	E	5[Y]	HTQ	C4-C5	3.14	1.59	1.53
5	A	1[Z]	HTQ	C2-C1	3.11	1.59	1.53
5	D	414	HTQ	C9-N8	3.10	1.51	1.47
5	D	4[Z]	HTQ	C4-C3	3.10	1.60	1.52
5	B	212	HTQ	C2-C3	3.08	1.60	1.52
5	E	5[Y]	HTQ	C2-C3	3.08	1.60	1.52
5	A	1[Z]	HTQ	C16-C14	3.07	1.44	1.39
5	C	3[Y]	HTQ	C2-C3	3.06	1.59	1.52
5	A	111	HTQ	C4-C3	3.06	1.59	1.52
5	F	6[Z]	HTQ	C2-C3	3.05	1.59	1.52
5	F	616	HTQ	O10-C11	3.04	1.41	1.34
5	A	1[Y]	HTQ	C2-C3	3.04	1.59	1.52
5	B	2[Z]	HTQ	C2-C3	3.04	1.59	1.52
5	F	616	HTQ	C4-C5	3.03	1.59	1.53
5	D	414	HTQ	C2-C1	3.02	1.59	1.53
5	D	4[Z]	HTQ	C2-C3	3.02	1.59	1.52
5	F	6[Z]	HTQ	C16-C14	3.02	1.43	1.39
5	A	1[Z]	HTQ	C4-C5	3.01	1.59	1.53
5	C	313	HTQ	C2-C3	3.01	1.59	1.52
5	B	2[Y]	HTQ	C2-C3	3.00	1.59	1.52
5	E	5[Z]	HTQ	C16-C14	2.99	1.43	1.39
5	D	4[Y]	HTQ	C2-C3	2.99	1.59	1.52
5	A	1[Z]	HTQ	C2-C3	2.99	1.59	1.52
5	F	6[Y]	HTQ	C4-C5	2.99	1.59	1.53
5	E	515	HTQ	C4-C3	2.99	1.59	1.52
5	E	5[Y]	HTQ	C16-C14	2.97	1.43	1.39
5	F	6[Y]	HTQ	C2-C1	2.97	1.59	1.53
5	A	111	HTQ	C2-C3	2.96	1.59	1.52
5	D	4[Z]	HTQ	O10-C11	2.95	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	313	HTQ	C4-C3	2.94	1.59	1.52
5	E	5[Z]	HTQ	C2-C1	2.94	1.59	1.53
5	B	212	HTQ	C9-N8	2.93	1.51	1.47
5	B	2[Y]	HTQ	C4-C5	2.91	1.58	1.53
5	D	4[Y]	HTQ	C16-C14	2.91	1.43	1.39
5	A	111	HTQ	C9-N8	2.90	1.51	1.47
5	A	1[Z]	HTQ	C4-C3	2.89	1.59	1.52
5	E	515	HTQ	C4-C5	2.89	1.58	1.53
5	E	515	HTQ	C16-C14	2.88	1.43	1.39
5	C	313	HTQ	C4-C5	2.88	1.58	1.53
5	C	3[Y]	HTQ	C16-C14	2.88	1.43	1.39
5	F	616	HTQ	C4-C3	2.87	1.59	1.52
5	C	313	HTQ	C16-C14	2.87	1.43	1.39
5	F	616	HTQ	C9-N8	2.86	1.51	1.47
5	B	2[Y]	HTQ	C4-C3	2.86	1.59	1.52
5	B	2[Y]	HTQ	C2-C1	2.85	1.58	1.53
3	B	282	SIA	O6-C2	2.85	1.45	1.43
5	D	4[Z]	HTQ	C2-C1	2.84	1.58	1.53
5	F	6[Z]	HTQ	O10-C11	2.84	1.40	1.34
5	B	2[Y]	HTQ	C16-C14	2.83	1.43	1.39
5	E	5[Z]	HTQ	C2-C3	2.83	1.59	1.52
5	E	5[Z]	HTQ	C4-C5	2.83	1.58	1.53
5	C	313	HTQ	C2-C1	2.82	1.58	1.53
5	C	3[Z]	HTQ	C16-C14	2.81	1.43	1.39
5	B	2[Z]	HTQ	C16-C14	2.80	1.43	1.39
5	F	616	HTQ	C2-C3	2.78	1.59	1.52
5	A	111	HTQ	O10-C11	2.78	1.40	1.34
5	A	1[Y]	HTQ	C15-C14	2.78	1.43	1.39
5	D	4[Z]	HTQ	C15-C14	2.78	1.43	1.39
5	F	6[Y]	HTQ	C16-C14	2.78	1.43	1.39
5	E	5[Z]	HTQ	C4-C3	2.76	1.59	1.52
5	C	3[Y]	HTQ	C15-C14	2.74	1.43	1.39
5	B	2[Y]	HTQ	O10-C11	2.73	1.40	1.34
5	F	616	HTQ	C16-C14	2.71	1.43	1.39
5	B	2[Y]	HTQ	C15-C14	2.70	1.43	1.39
5	A	111	HTQ	C16-C14	2.70	1.43	1.39
5	A	1[Z]	HTQ	C15-C14	2.70	1.43	1.39
5	E	5[Z]	HTQ	C15-C14	2.69	1.43	1.39
5	F	6[Z]	HTQ	C15-C14	2.69	1.43	1.39
5	F	6[Y]	HTQ	C15-C14	2.67	1.43	1.39
5	F	6[Z]	HTQ	C2-C1	2.67	1.58	1.53
3	A	182	SIA	C4-C5	2.66	1.55	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	414	HTQ	C15-C14	2.66	1.43	1.39
5	B	212	HTQ	C15-C14	2.64	1.43	1.39
5	B	212	HTQ	C16-C14	2.63	1.43	1.39
5	C	313	HTQ	C15-C14	2.63	1.43	1.39
5	D	414	HTQ	C4-C5	2.62	1.58	1.53
5	A	1[Y]	HTQ	O10-C11	2.61	1.40	1.34
5	D	414	HTQ	C2-C3	2.59	1.58	1.52
5	D	4[Y]	HTQ	C2-C1	2.59	1.58	1.53
5	E	5[Y]	HTQ	C2-C1	2.58	1.58	1.53
5	D	4[Z]	HTQ	C4-C5	2.56	1.58	1.53
5	C	3[Y]	HTQ	O10-C11	2.56	1.40	1.34
5	C	3[Z]	HTQ	C15-C14	2.54	1.43	1.39
5	C	3[Z]	HTQ	C2-C1	2.54	1.58	1.53
5	A	111	HTQ	C15-C14	2.54	1.43	1.39
5	B	212	HTQ	O10-C11	2.54	1.40	1.34
5	A	1[Y]	HTQ	C2-C1	2.53	1.58	1.53
5	F	616	HTQ	C2-C1	2.52	1.58	1.53
5	D	4[Z]	HTQ	C16-C14	2.52	1.43	1.39
5	E	515	HTQ	C2-C1	2.51	1.58	1.53
5	E	515	HTQ	C15-C14	2.48	1.43	1.39
5	F	616	HTQ	C15-C14	2.48	1.43	1.39
5	B	2[Z]	HTQ	C15-C14	2.47	1.43	1.39
5	C	3[Y]	HTQ	C2-C1	2.46	1.58	1.53
5	B	2[Z]	HTQ	C2-C1	2.44	1.58	1.53
5	E	5[Y]	HTQ	C15-C14	2.43	1.43	1.39
5	A	1[Z]	HTQ	C13-C11	2.40	1.55	1.52
5	E	5[Z]	HTQ	C13-C11	2.38	1.55	1.52
5	D	4[Y]	HTQ	C15-C14	2.36	1.42	1.39
3	A	182	SIA	O6-C2	2.32	1.45	1.43
5	D	414	HTQ	C13-C11	2.30	1.55	1.52
5	F	6[Z]	HTQ	C13-C11	2.29	1.55	1.52
5	A	1[Y]	HTQ	C13-C11	2.28	1.55	1.52
3	F	682	SIA	O6-C2	2.23	1.45	1.43
5	A	111	HTQ	C2-C1	2.09	1.57	1.53
5	D	414	HTQ	C4-C3	2.08	1.57	1.52
5	F	6[Y]	HTQ	C13-C11	2.00	1.55	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	414	HTQ	C3-O10-C11	9.06	132.54	117.69
5	A	1[Z]	HTQ	C3-O10-C11	7.76	130.41	117.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	111	HTQ	C3-O10-C11	6.36	128.12	117.69
5	E	5[Z]	HTQ	C3-O10-C11	6.17	127.81	117.69
5	B	212	HTQ	C3-O10-C11	6.00	127.54	117.69
5	F	6[Z]	HTQ	C3-O10-C11	5.80	127.21	117.69
5	A	1[Y]	HTQ	C3-O10-C11	5.76	127.13	117.69
5	E	515	HTQ	C3-O10-C11	5.70	127.03	117.69
5	C	313	HTQ	C3-O10-C11	5.60	126.88	117.69
5	F	616	HTQ	C3-O10-C11	5.31	126.40	117.69
5	F	6[Y]	HTQ	C3-O10-C11	5.08	126.03	117.69
5	C	3[Y]	HTQ	C3-O10-C11	5.03	125.94	117.69
5	D	4[Z]	HTQ	C3-O10-C11	4.63	125.29	117.69
5	B	2[Z]	HTQ	C3-O10-C11	4.45	124.98	117.69
5	C	3[Z]	HTQ	C3-O10-C11	4.37	124.85	117.69
5	D	4[Y]	HTQ	C3-O10-C11	4.32	124.78	117.69
5	B	2[Y]	HTQ	C3-O10-C11	4.20	124.57	117.69
5	E	5[Y]	HTQ	C3-O10-C11	3.92	124.12	117.69
3	B	282	SIA	O6-C6-C7	3.12	112.10	107.29
5	A	1[Z]	HTQ	O10-C3-C2	2.93	114.83	107.79
5	D	414	HTQ	O10-C3-C4	2.74	114.37	107.79
5	A	111	HTQ	C3-C4-C5	2.62	116.64	112.69
5	C	3[Y]	HTQ	C3-C4-C5	2.61	116.62	112.69
5	D	4[Y]	HTQ	C3-C4-C5	2.59	116.58	112.69
5	C	3[Z]	HTQ	C3-C4-C5	2.58	116.57	112.69
5	D	414	HTQ	O10-C11-O12	2.55	128.69	123.94
5	B	212	HTQ	C3-C4-C5	2.53	116.50	112.69
3	A	182	SIA	O6-C6-C7	2.40	110.99	107.29
5	F	616	HTQ	C5-N8-C1	2.36	103.66	100.80
5	B	2[Z]	HTQ	C3-C4-C5	2.36	116.23	112.69
5	A	111	HTQ	C5-N8-C1	2.32	103.61	100.80
5	E	5[Z]	HTQ	C5-N8-C1	2.32	103.60	100.80
5	B	212	HTQ	C5-N8-C1	2.31	103.60	100.80
5	D	414	HTQ	C5-N8-C1	2.31	103.59	100.80
5	E	5[Y]	HTQ	C3-C4-C5	2.28	116.12	112.69
5	E	5[Y]	HTQ	C5-N8-C1	2.28	103.56	100.80
5	E	515	HTQ	C5-N8-C1	2.27	103.54	100.80
5	C	313	HTQ	C5-N8-C1	2.26	103.54	100.80
3	A	182	SIA	O6-C6-C5	2.26	111.99	109.78
5	C	3[Z]	HTQ	C5-N8-C1	2.25	103.53	100.80
5	A	1[Z]	HTQ	C5-N8-C1	2.25	103.52	100.80
5	F	6[Y]	HTQ	C5-N8-C1	2.24	103.51	100.80
5	D	4[Z]	HTQ	C5-N8-C1	2.24	103.51	100.80
3	F	682	SIA	O6-C6-C5	2.24	111.96	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2[Z]	HTQ	C5-N8-C1	2.24	103.51	100.80
5	B	2[Y]	HTQ	C5-N8-C1	2.23	103.50	100.80
5	F	6[Z]	HTQ	C3-C4-C5	2.22	116.03	112.69
5	A	1[Y]	HTQ	C5-N8-C1	2.21	103.47	100.80
5	F	6[Z]	HTQ	C5-N8-C1	2.20	103.46	100.80
5	A	1[Y]	HTQ	C3-C4-C5	2.19	115.98	112.69
5	D	4[Y]	HTQ	C5-N8-C1	2.16	103.42	100.80
5	C	3[Y]	HTQ	C5-N8-C1	2.15	103.40	100.80
5	B	212	HTQ	O10-C11-O12	2.14	127.93	123.94
2	A	179	NAG	C2-N2-C7	-2.08	119.94	122.90

All (3) chirality outliers are listed below:

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

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	515	HTQ	C2-C3-O10-C11
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	F	616	HTQ	O12-C11-C13-O20
5	F	6[Y]	HTQ	C2-C3-O10-C11
5	F	6[Y]	HTQ	O10-C11-C13-O20
5	F	6[Y]	HTQ	O12-C11-C13-O20
5	D	4[Y]	HTQ	C2-C3-O10-C11
5	D	4[Y]	HTQ	O10-C11-C13-O20
5	D	4[Y]	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	C	3[Z]	HTQ	C2-C3-O10-C11
5	C	3[Z]	HTQ	O10-C11-C13-O20
5	C	3[Z]	HTQ	O12-C11-C13-O20
5	B	212	HTQ	C2-C3-O10-C11
2	F	679	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	F	679	NAG	O7-C7-N2-C2
2	A	179	NAG	C8-C7-N2-C2
2	A	179	NAG	O7-C7-N2-C2
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
2	B	279	NAG	O7-C7-N2-C2
5	A	1[Y]	HTQ	O10-C11-C13-O20
5	A	1[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	A	111	HTQ	C2-C3-O10-C11
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
2	E	580	NAG	C8-C7-N2-C2
2	E	580	NAG	O7-C7-N2-C2
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	C	313	HTQ	C2-C3-O10-C11
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
2	C	379	NAG	C8-C7-N2-C2
2	B	279	NAG	C8-C7-N2-C2
2	C	379	NAG	O7-C7-N2-C2
2	A	179	NAG	O5-C5-C6-O6
2	E	579	NAG	C8-C7-N2-C2
2	A	179	NAG	C4-C5-C6-O6
2	E	580	NAG	C4-C5-C6-O6
2	E	579	NAG	O7-C7-N2-C2
5	E	5[Z]	HTQ	C2-C3-O10-C11
5	E	5[Y]	HTQ	C2-C3-O10-C11
2	C	379	NAG	O5-C5-C6-O6

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

There are no ring outliers.

26 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	515	HTQ	12	0
5	F	6[Y]	HTQ	3	0
3	A	182	SIA	5	0
5	D	4[Y]	HTQ	2	0
5	F	616	HTQ	7	0
5	E	5[Y]	HTQ	2	0
3	F	682	SIA	5	0

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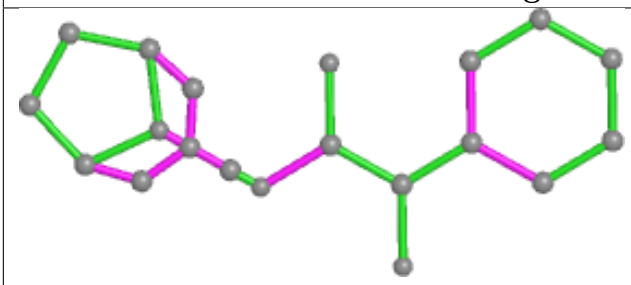
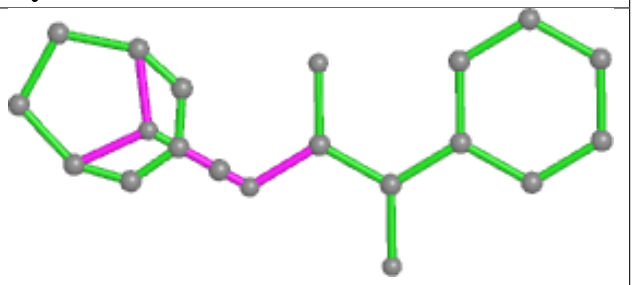
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	5[Z]	HTQ	1	0
5	C	3[Y]	HTQ	4	0
2	E	579	NAG	2	0
5	C	3[Z]	HTQ	4	0
5	B	212	HTQ	9	0
2	F	679	NAG	2	0
5	A	1[Z]	HTQ	4	0
2	B	279	NAG	3	0
5	A	1[Y]	HTQ	4	0
5	F	6[Z]	HTQ	3	0
5	A	111	HTQ	13	0
5	B	2[Y]	HTQ	4	0
5	B	2[Z]	HTQ	1	0
2	E	580	NAG	2	0
2	D	479	NAG	2	0
5	D	414	HTQ	7	0
5	C	313	HTQ	3	0
3	B	282	SIA	17	0
5	D	4[Z]	HTQ	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 then 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.

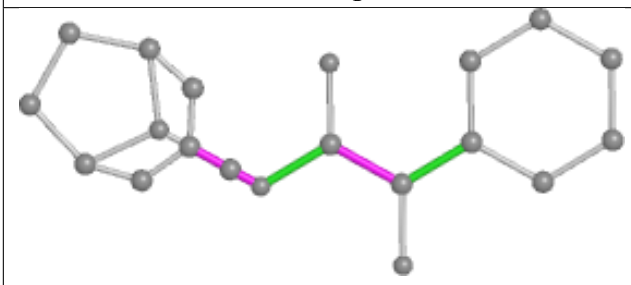
Ligand HTQ E 515



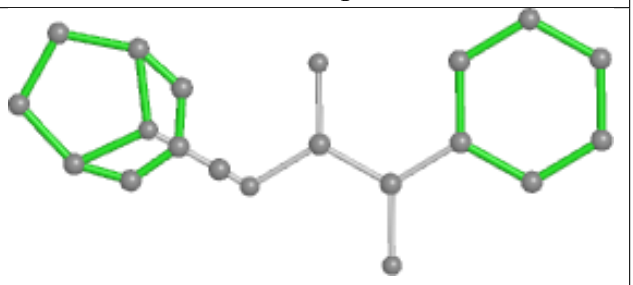
Bond lengths



Bond angles

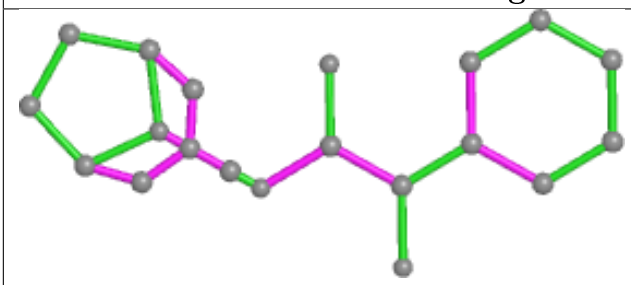


Torsions

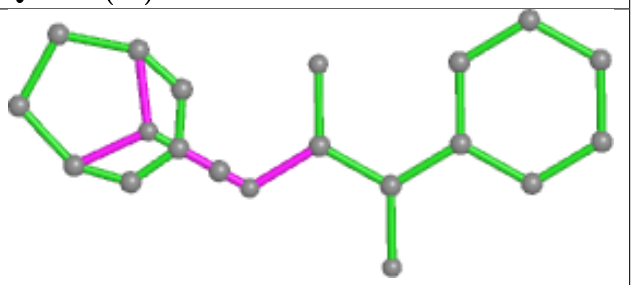


Rings

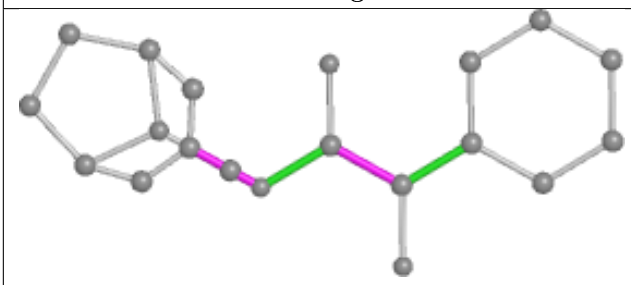
Ligand HTQ F 6 (Y)



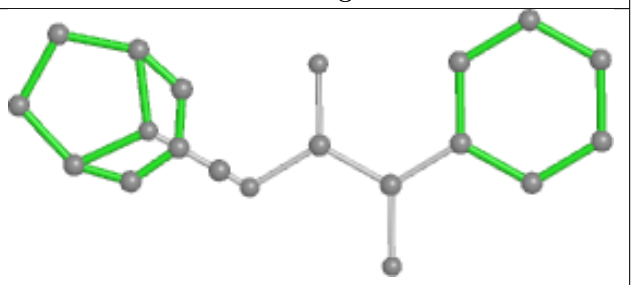
Bond lengths



Bond angles

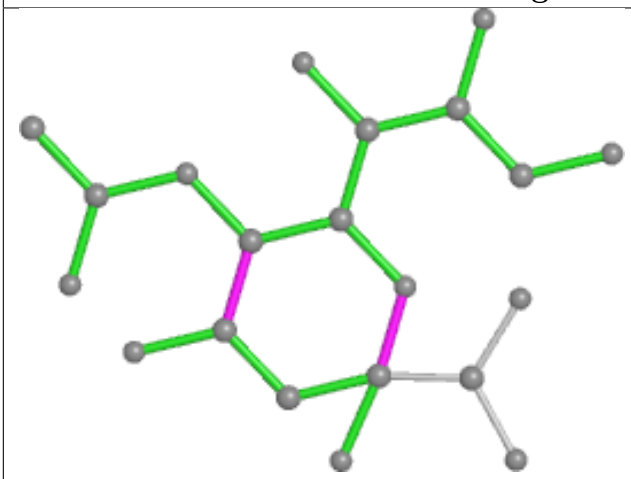


Torsions

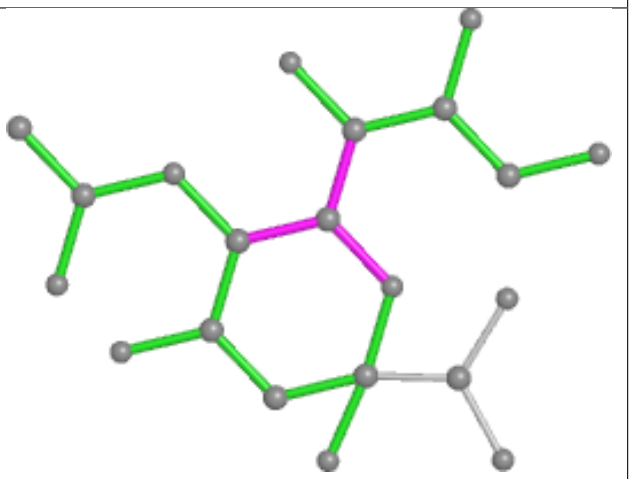


Rings

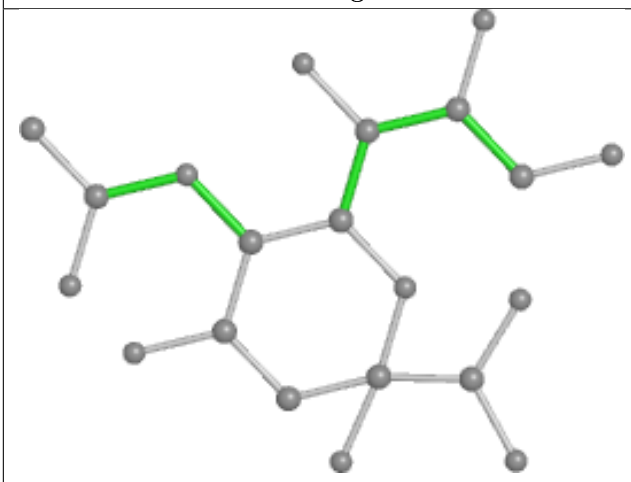
Ligand SIA A 182



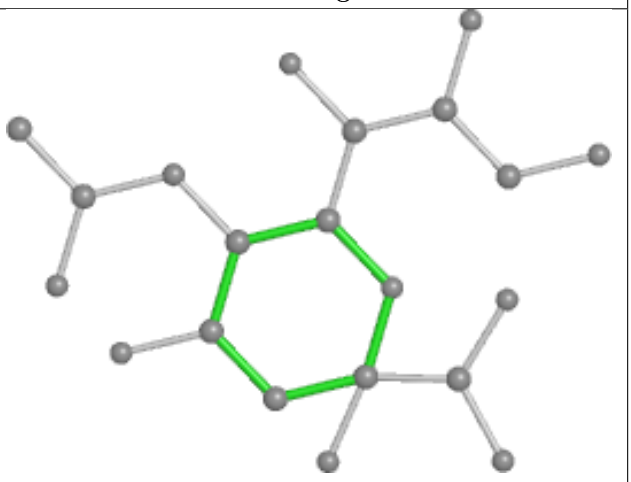
Bond lengths



Bond angles

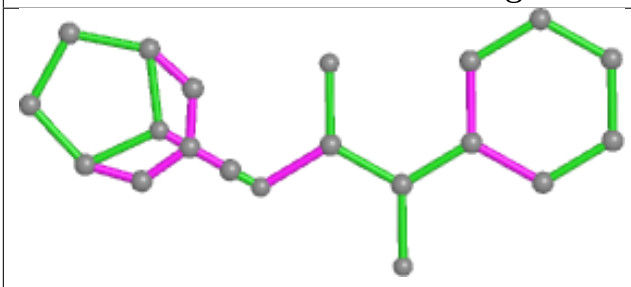


Torsions

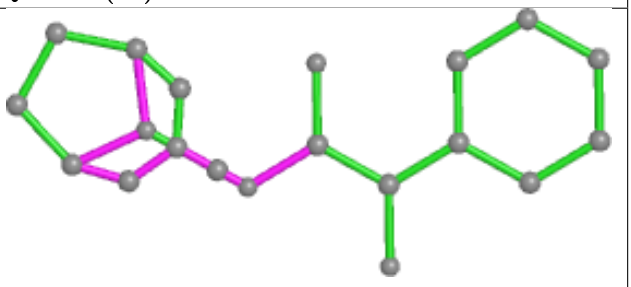


Rings

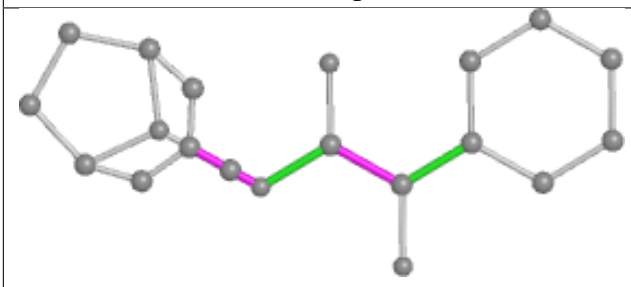
Ligand HTQ D 4 (Y)



Bond lengths



Bond angles



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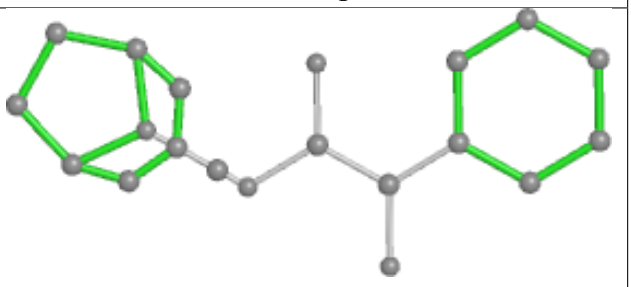
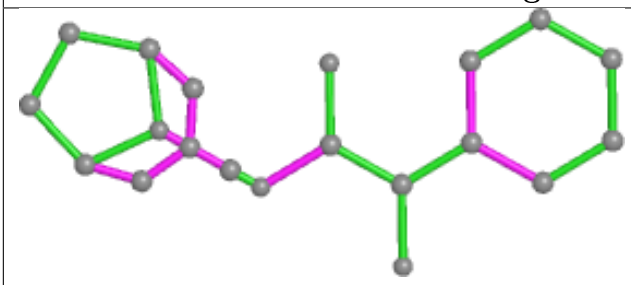


Rings

Ligand HTQ F 616



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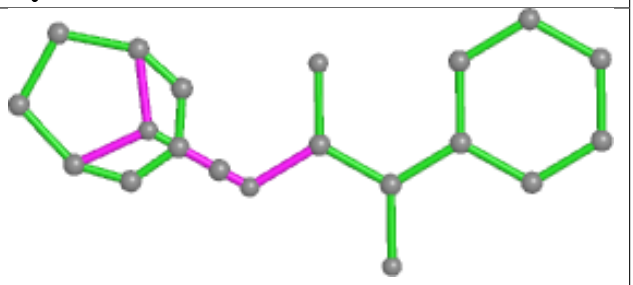
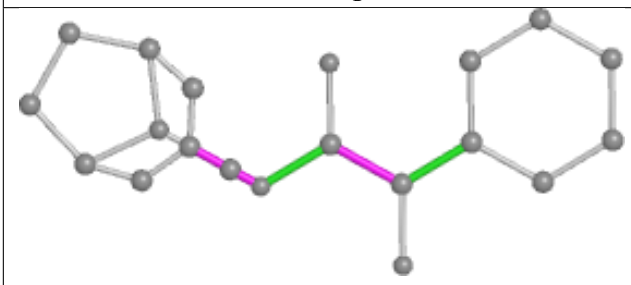


Bond angles



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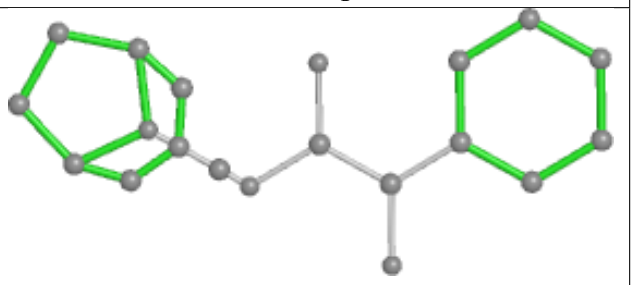
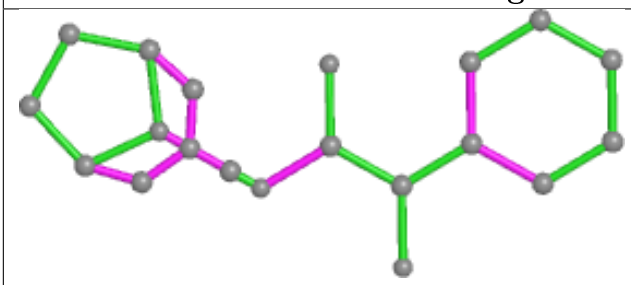


Rings

Ligand HTQ E 5 (Y)



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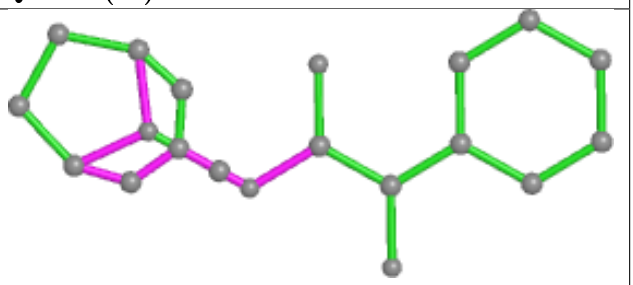
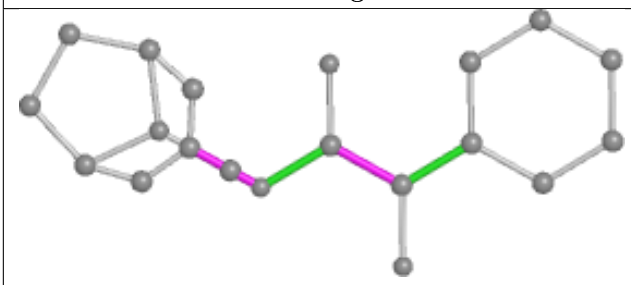
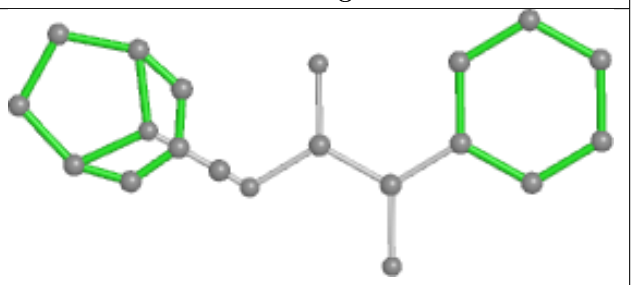


Bond angles

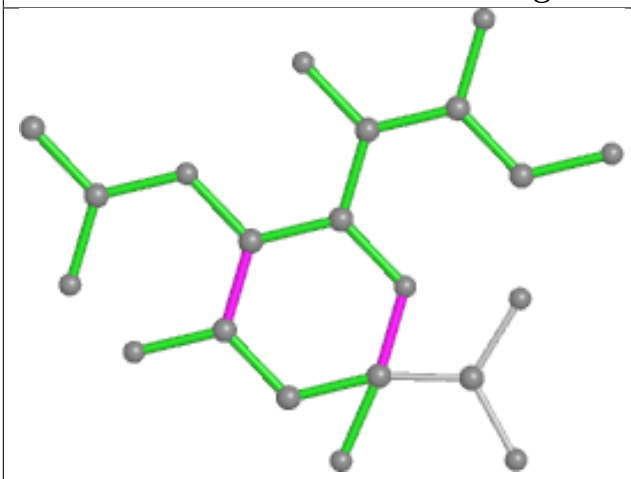


Torsions



Rings

Ligand SIA F 682



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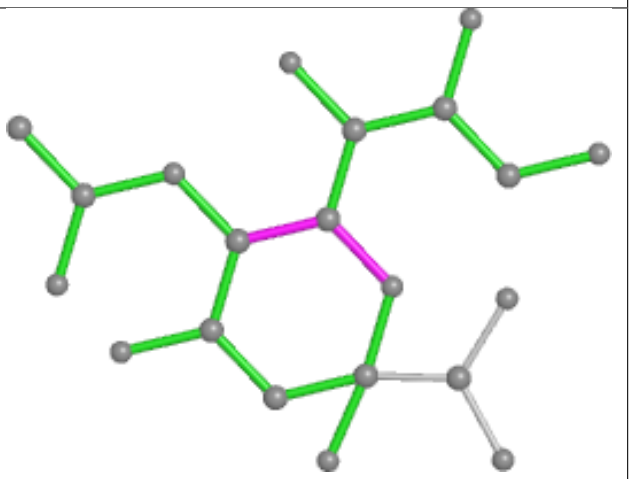
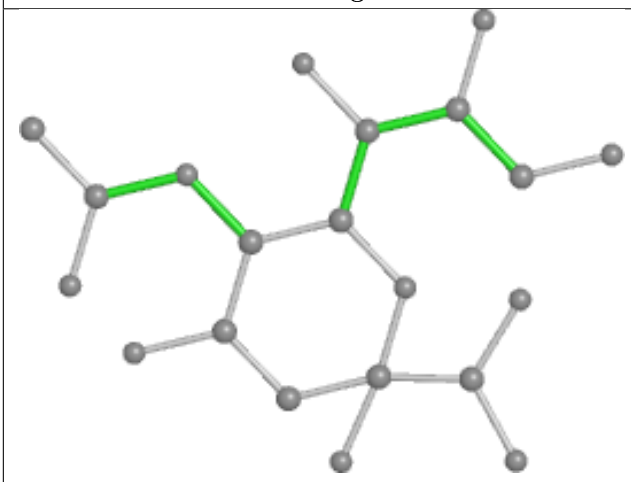
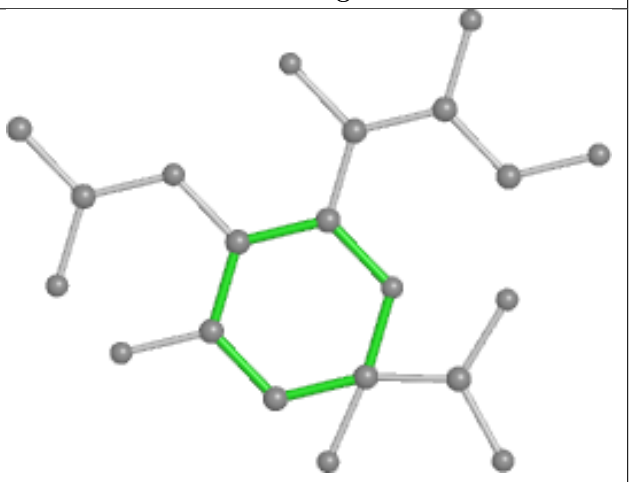


Bond angles

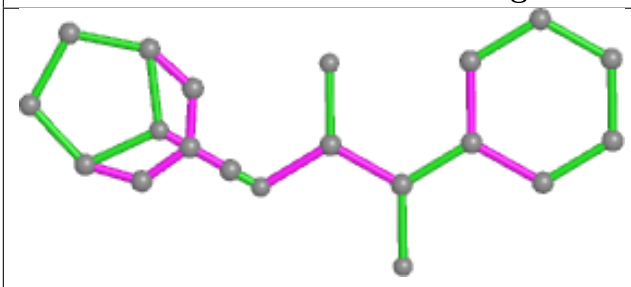


Torsions



Rings

Ligand HTQ E 5 (Z)



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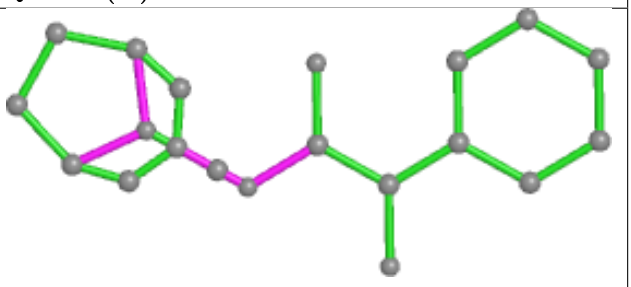
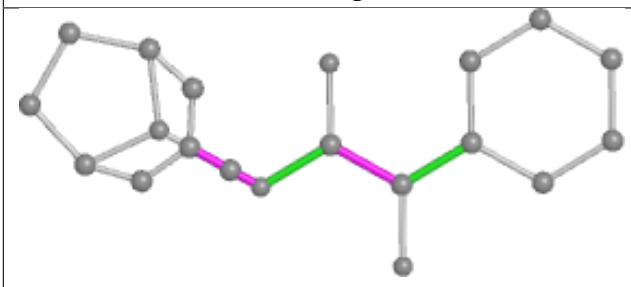


Bond angles



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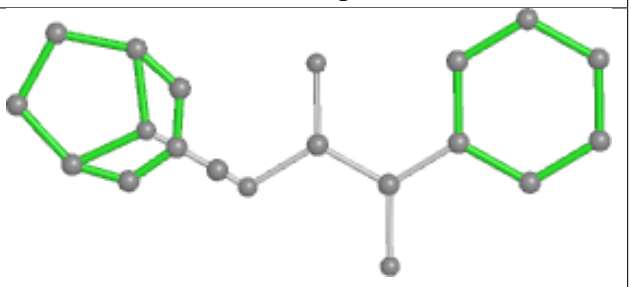
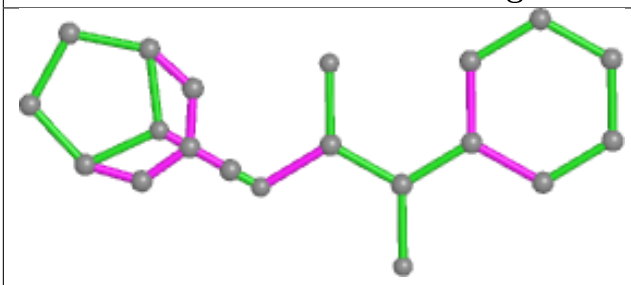


Rings

Ligand HTQ C 3 (Y)



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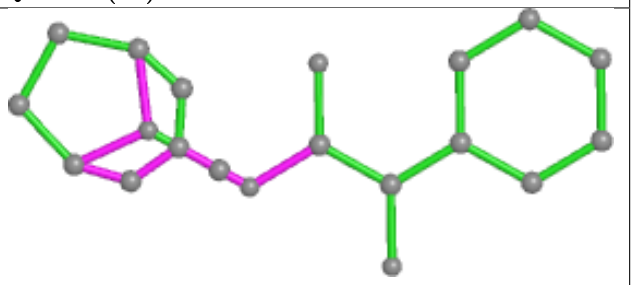
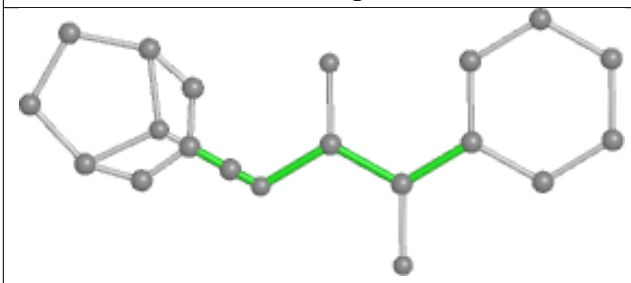


Bond angles



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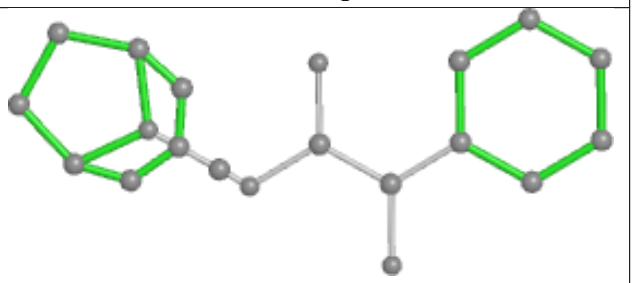
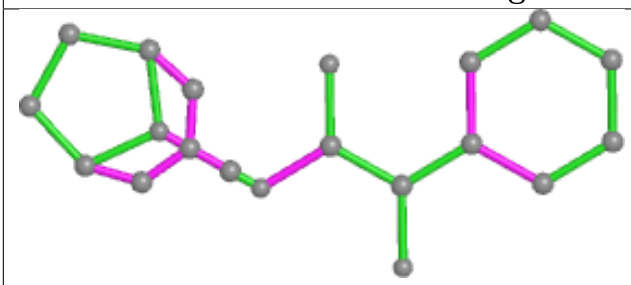


Rings

Ligand HTQ C 3 (Z)



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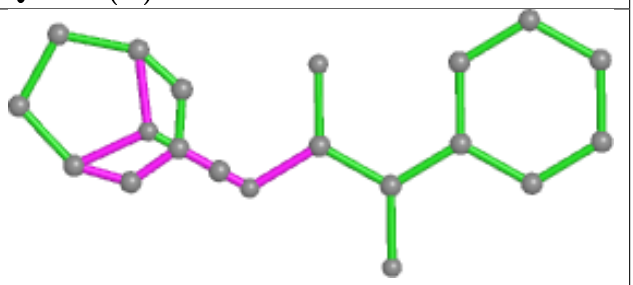
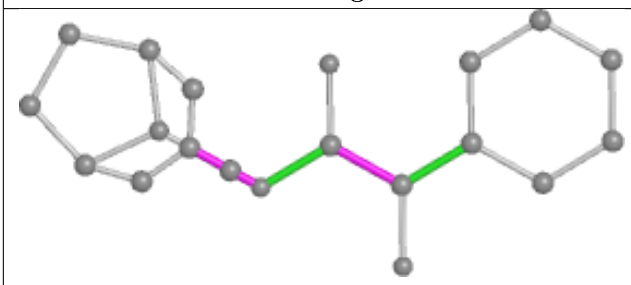
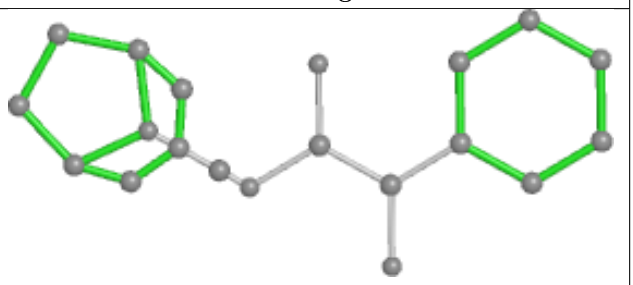


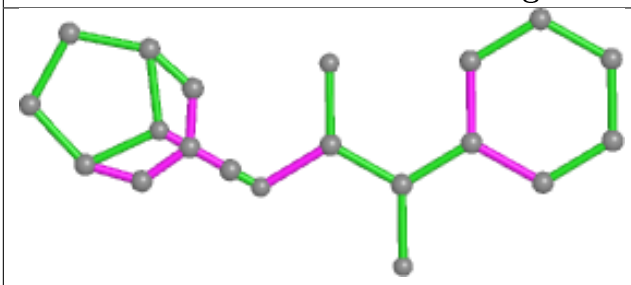
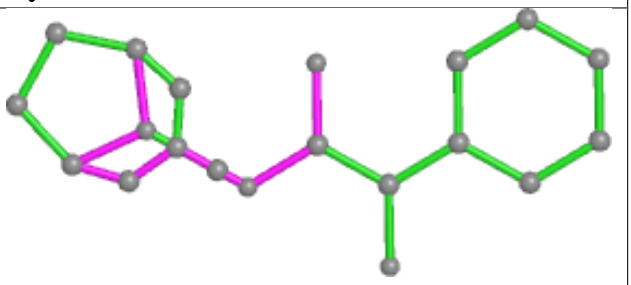
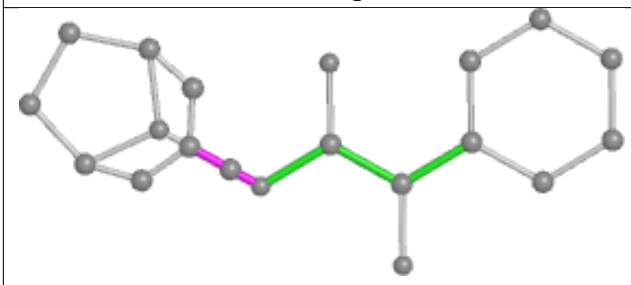
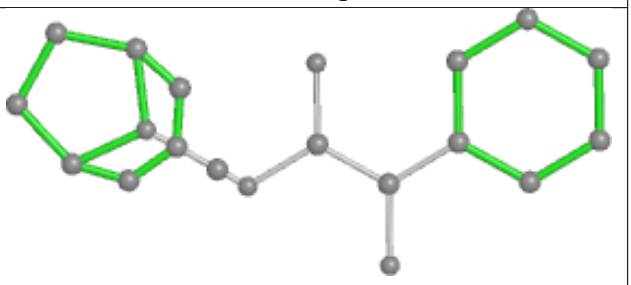
Bond angles

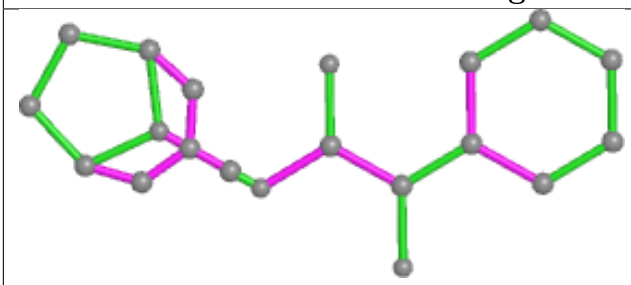
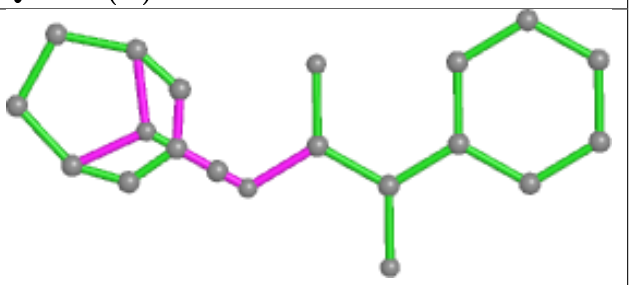
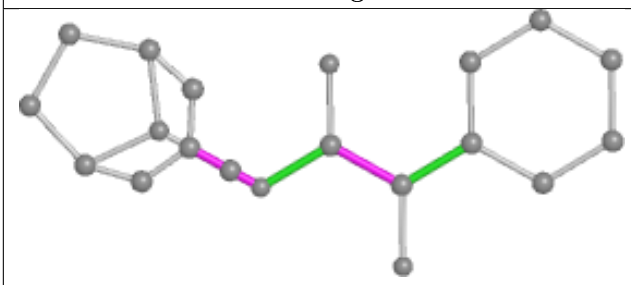
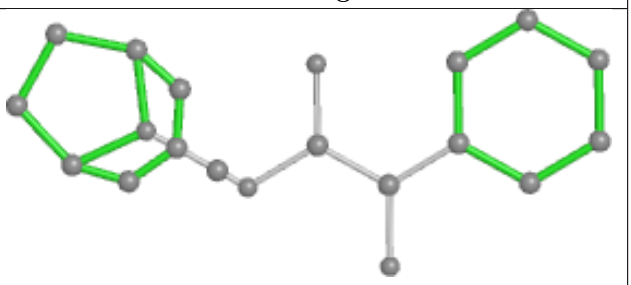


Torsions

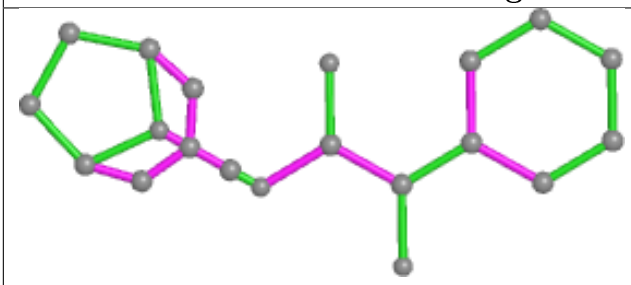


Rings

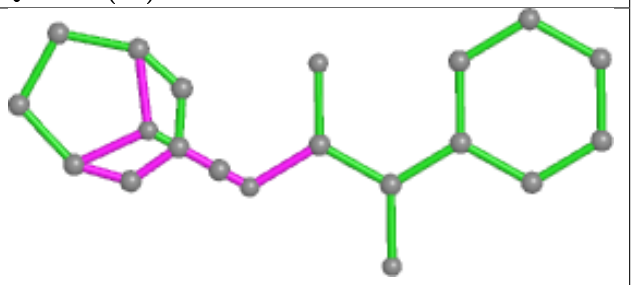
Ligand HTQ B 212	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTQ A 1 (Z)	
 Bond lengths	 Bond angles
 Torsions	 Rings

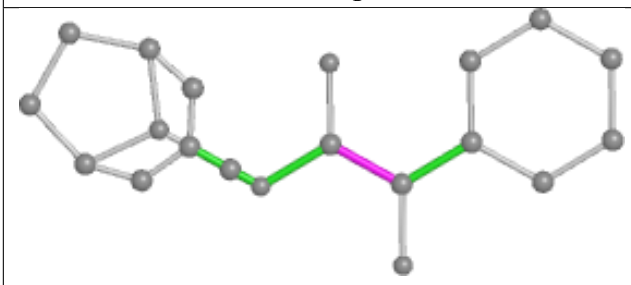
Ligand HTQ A 1 (Y)



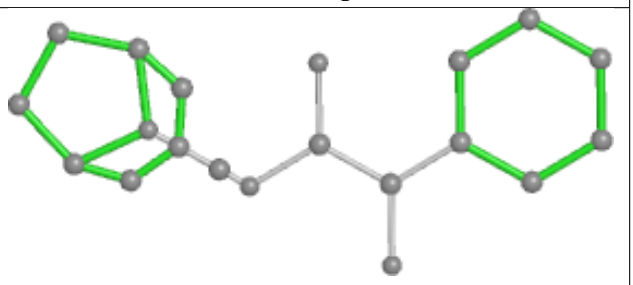
Bond lengths



Bond angles

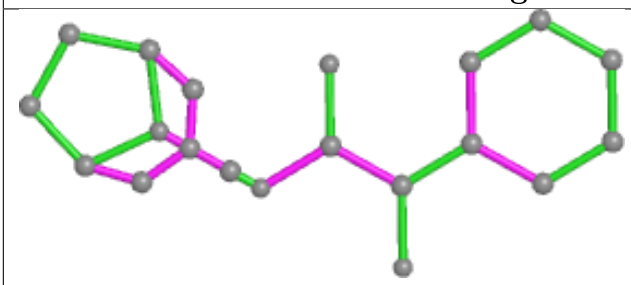


Torsions

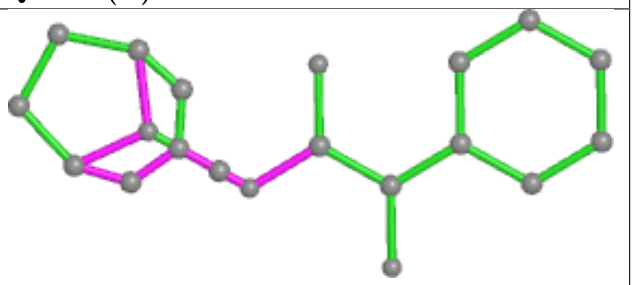


Rings

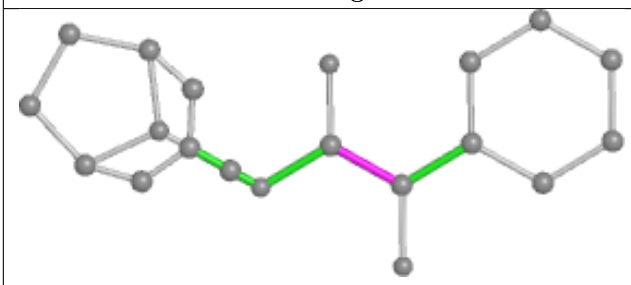
Ligand HTQ F 6 (Z)



Bond lengths



Bond angles



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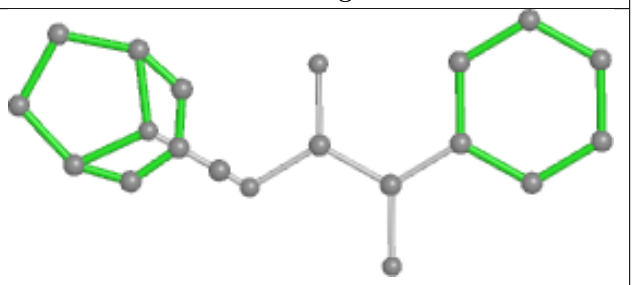
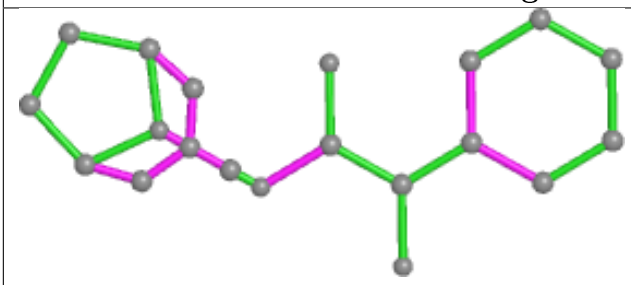


Rings

Ligand HTQ A 111



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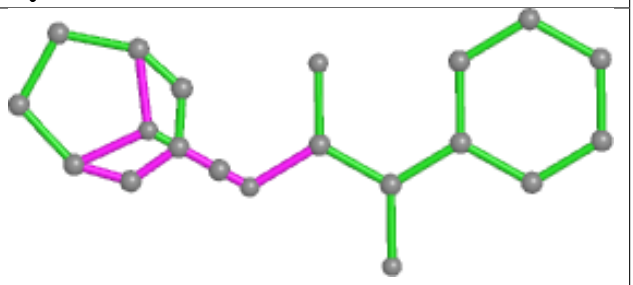
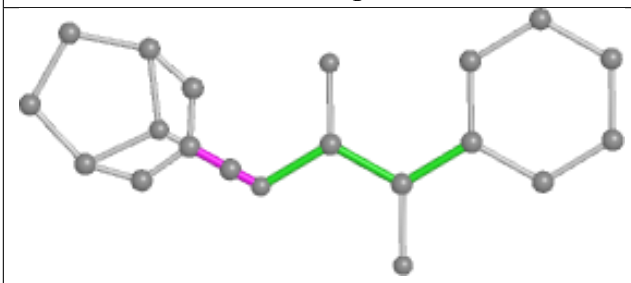


Bond angles



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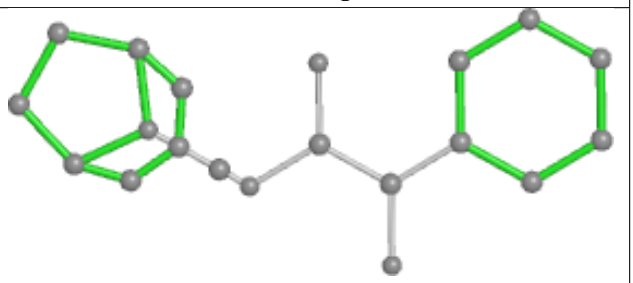
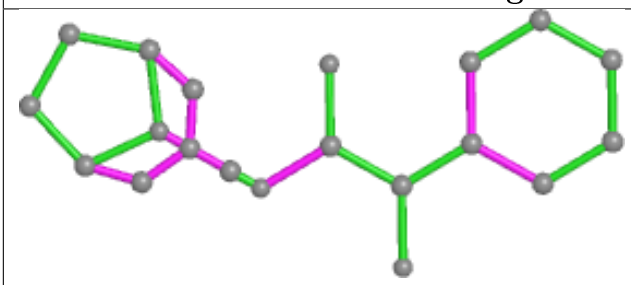
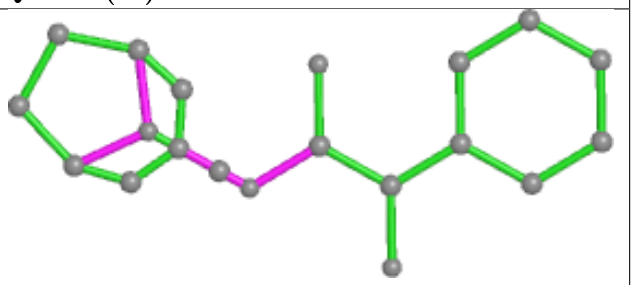


Rings

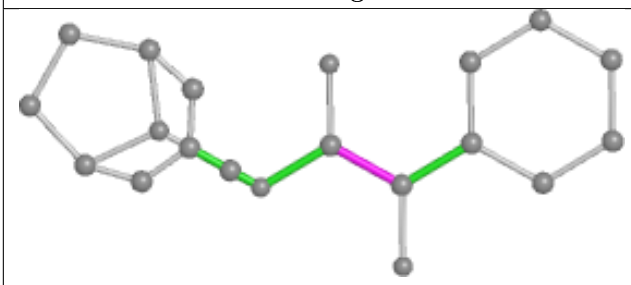
Ligand HTQ B 2 (Y)



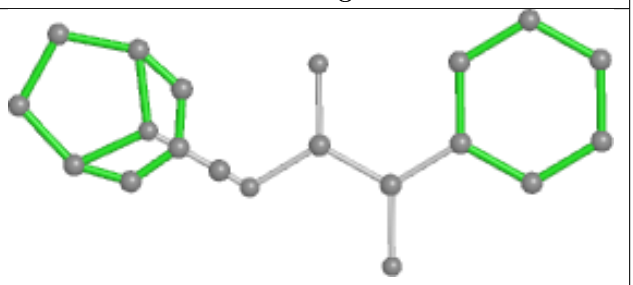
Bond lengths



Bond angles

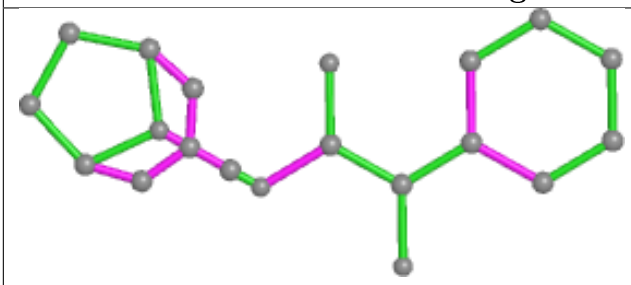


Torsions

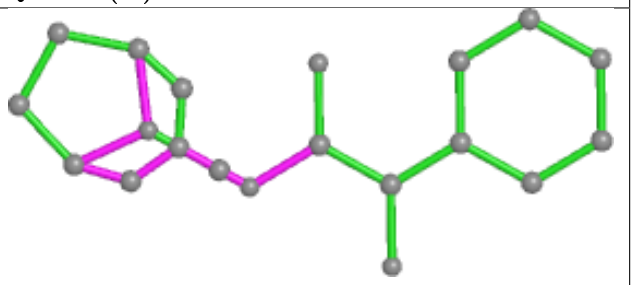


Rings

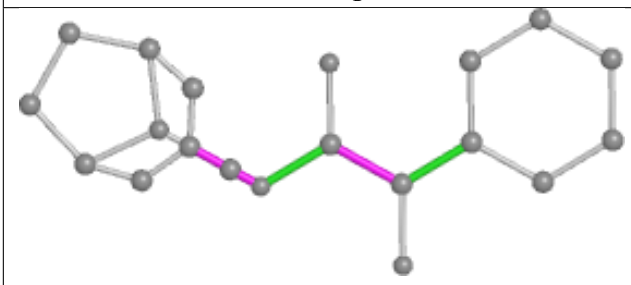
Ligand HTQ B 2 (Z)



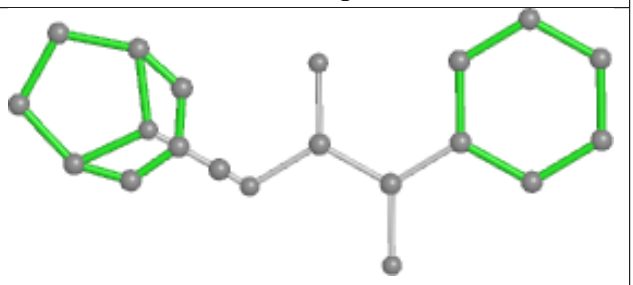
Bond lengths



Bond angles

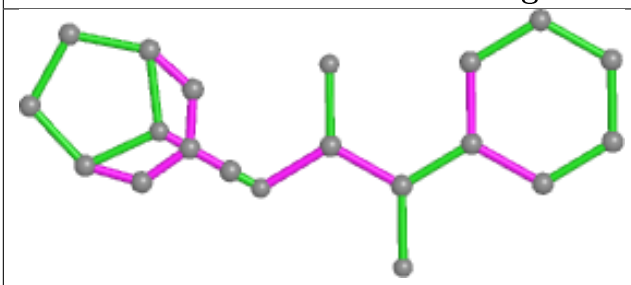


Torsions

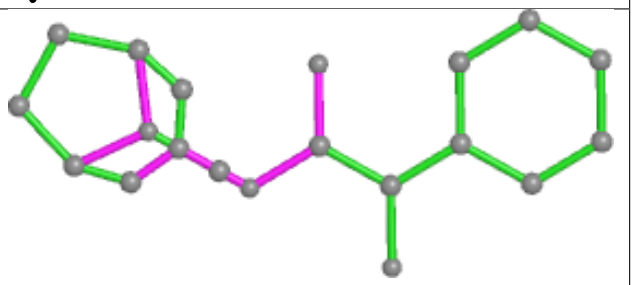


Rings

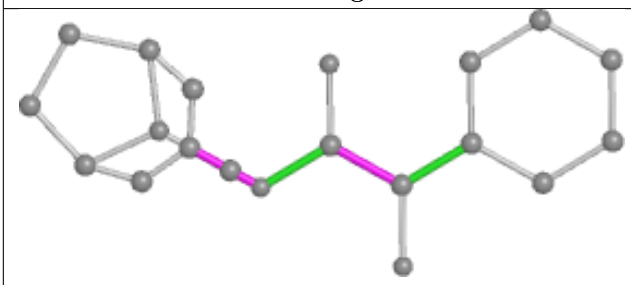
Ligand HTQ D 414



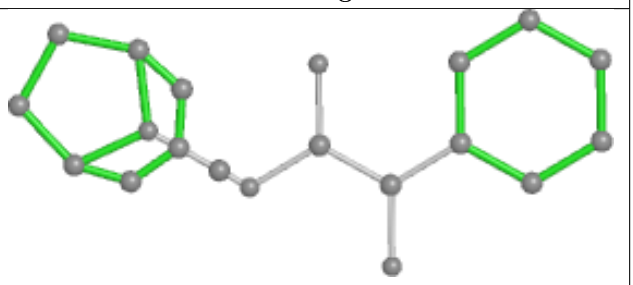
Bond lengths



Bond angles

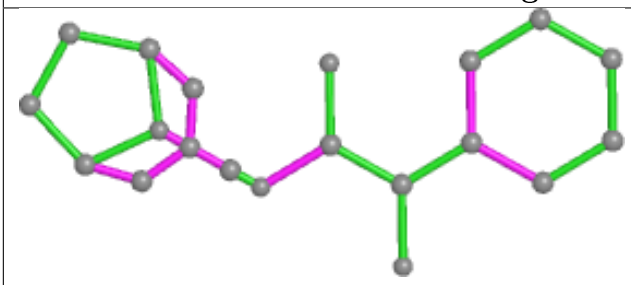


Torsions

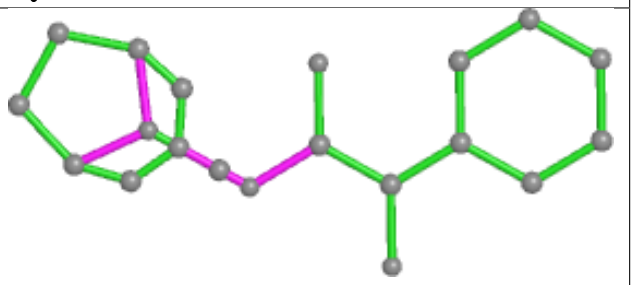


Rings

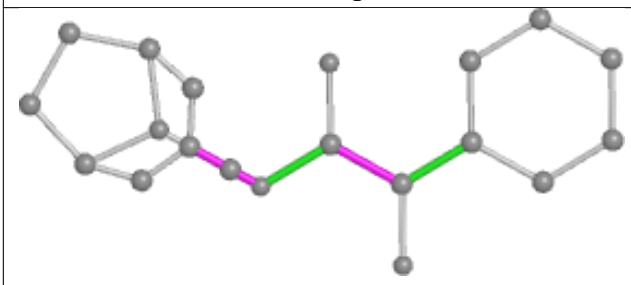
Ligand HTQ C 313



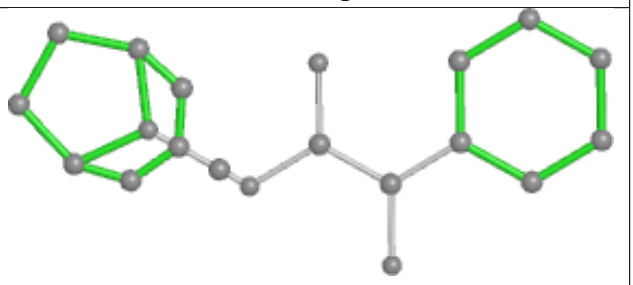
Bond lengths



Bond angles

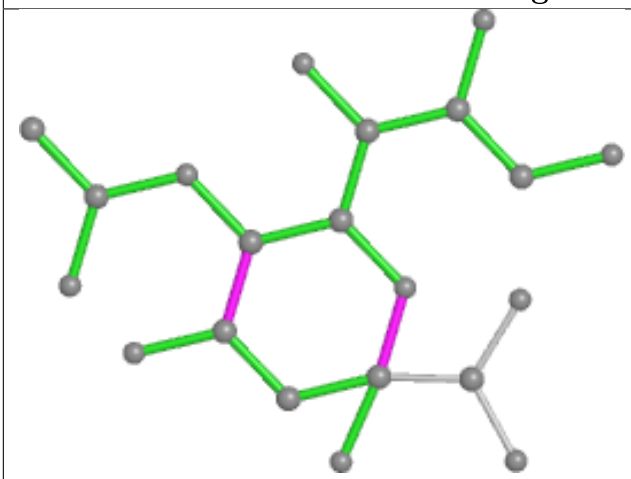


Torsions

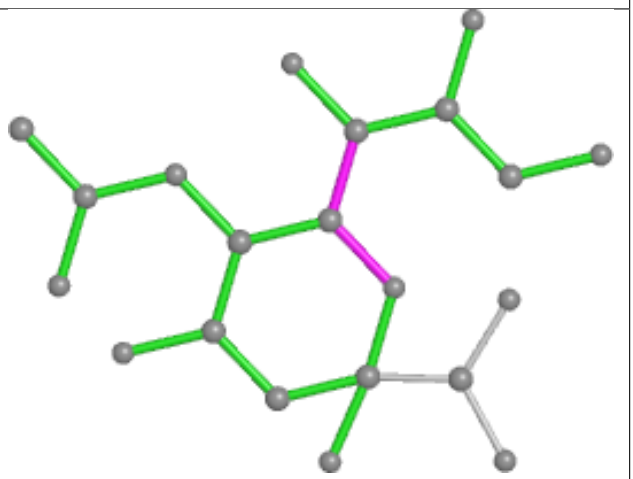


Rings

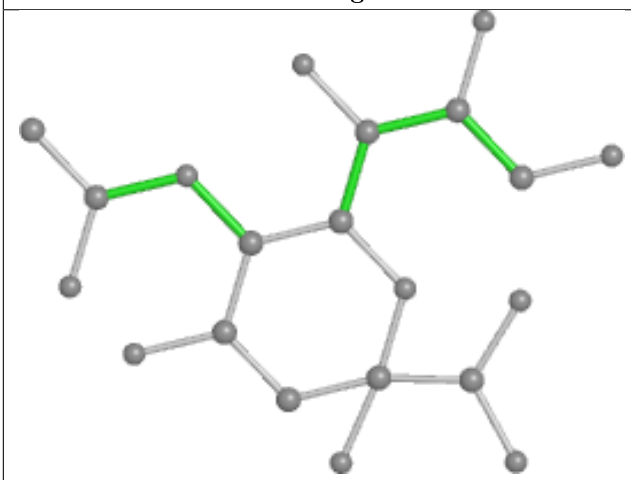
Ligand SIA B 282



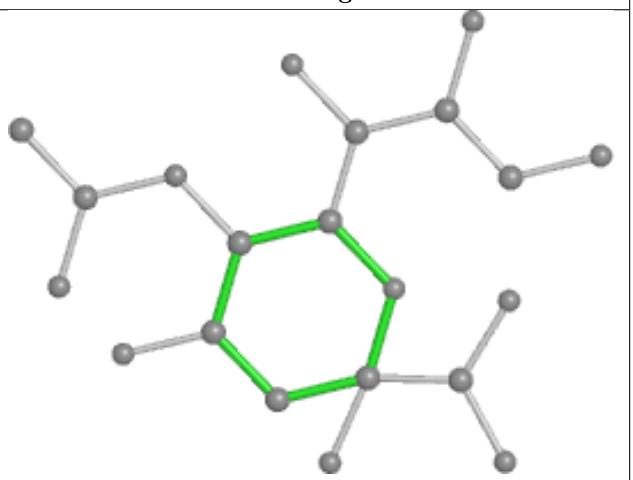
Bond lengths



Bond angles

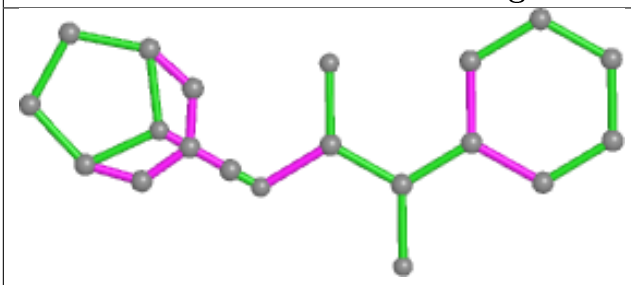


Torsions

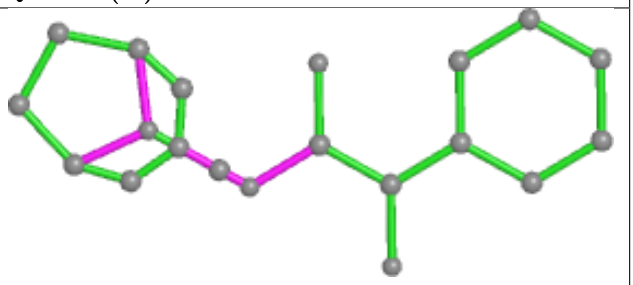


Rings

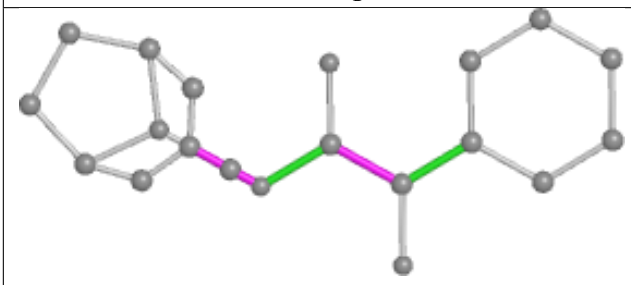
Ligand HTQ D 4 (Z)



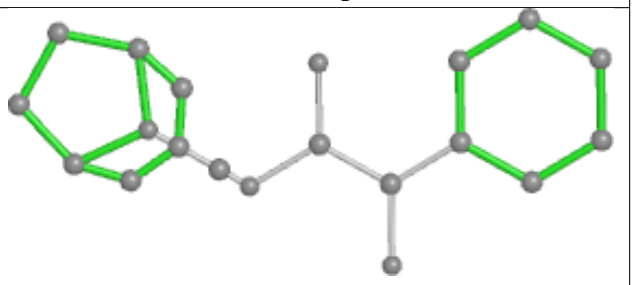
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.