



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 06:16 AM BST

PDB ID : 2DQZ
Title : Crystal structure of human carboxylesterase in complex with homatropine, coenzyme A, and palmitate
Authors : Bencharit, S.; Redinbo, M.R.
Deposited on : 2006-06-02
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

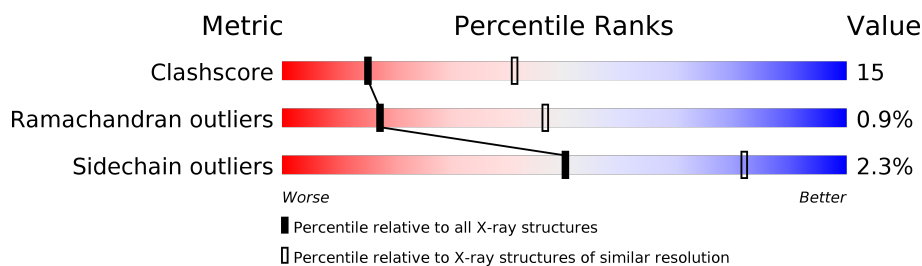
1 Overall quality at a glance

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	542	
1	B	542	
1	C	542	

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	C	379	X	-	-	-
8	COA	C	1	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13161 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.

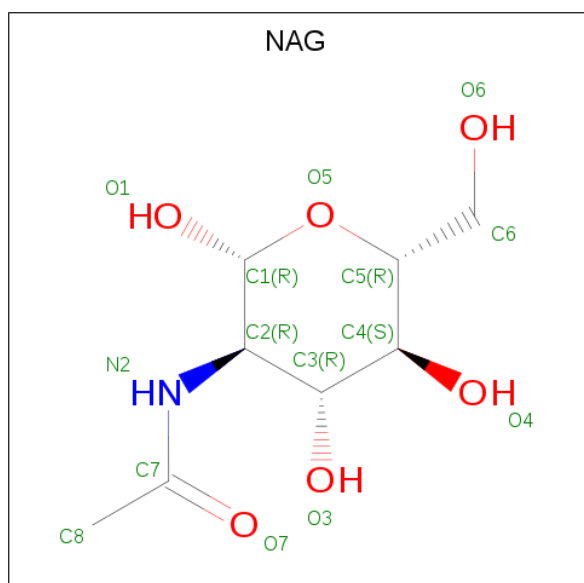
- Molecule 1 is a protein called Liver carboxylesterase 1.

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	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	C	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			

There are 3 discrepancies between the modelled and reference sequences:

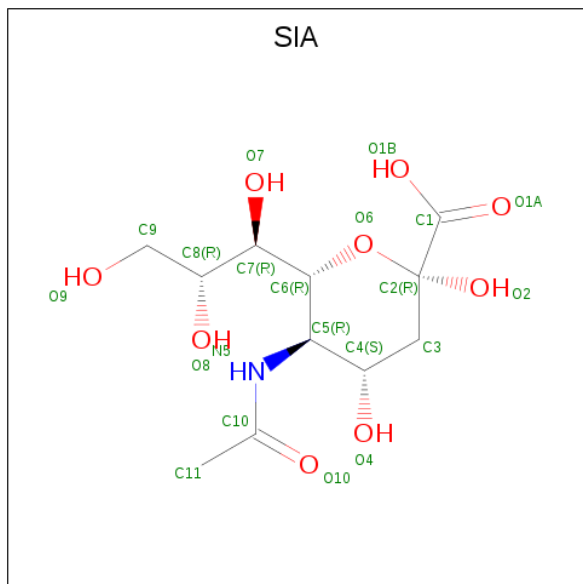
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141

- 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	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	C	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

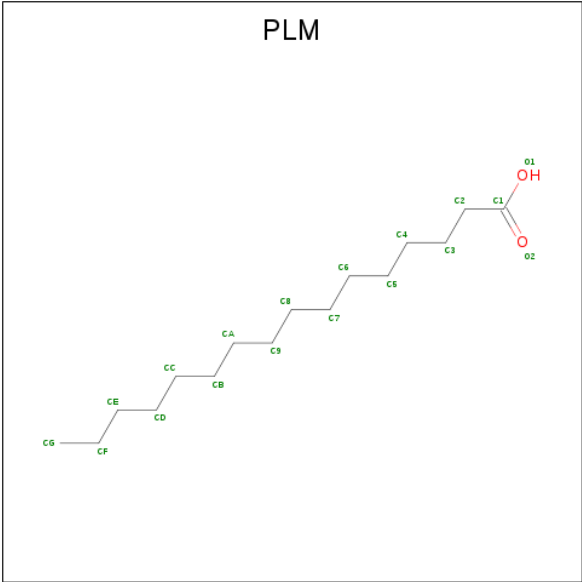


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is FLUORIDE ION (three-letter code: F) (formula: F).

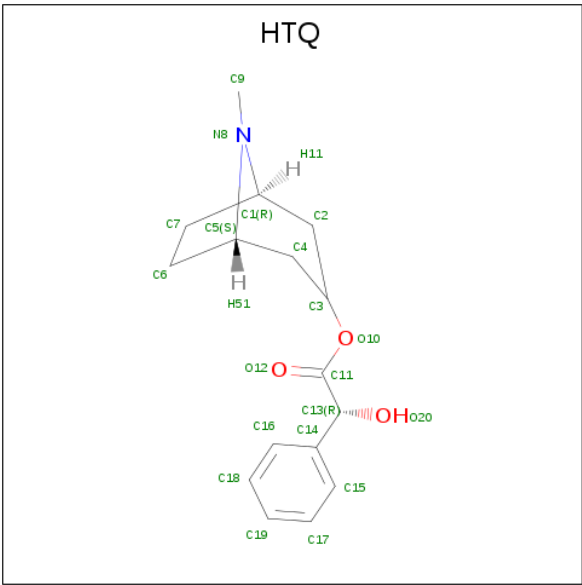
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	F	0	0
			1	1		
5	A	1	Total	F	0	0
			1	1		
5	C	1	Total	F	0	0
			1	1		

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	9	2		
6	B	1	Total	C	O	0	0
			11	9	2		
6	C	1	Total	C	O	0	0
			11	9	2		

- Molecule 7 is HOMOTROPINE (three-letter code: HTQ) (formula: C₁₆H₂₁NO₃).



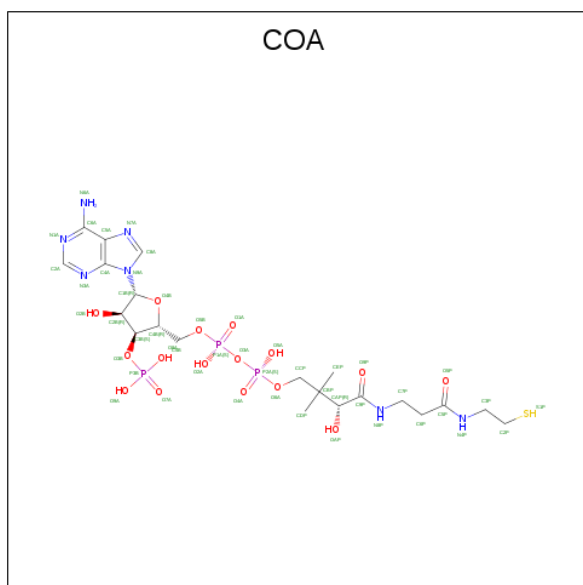
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			20	16	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			20	16	1	3		
7	C	1	Total	C	N	O	0	1
			40	32	2	6		

- Molecule 8 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).

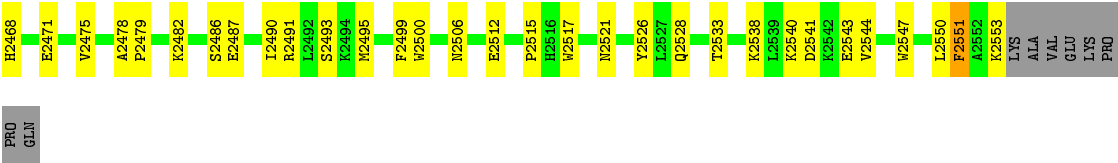


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	S	0	0
			7	4	1	1	1		

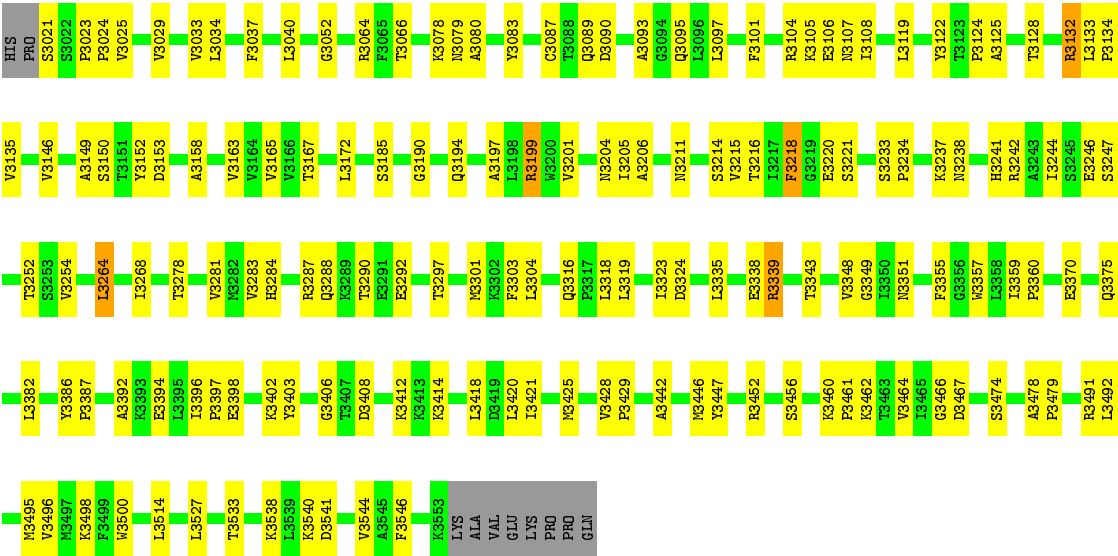
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	179	Total	O	0	0
			179	179		
9	B	135	Total	O	0	0
			135	135		
9	C	194	Total	O	0	0
			194	194		





● Molecule 1: Liver carboxylesterase 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.56 Å 181.02 Å 202.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.60 – 2.80	Depositor
% Data completeness (in resolution range)	97.9 (22.60-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13161	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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: NAG, F, COA, SIA, SO4, HTQ, PLM

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	0.39	0/4236	0.58	0/5754
1	B	0.38	0/4236	0.56	0/5754
1	C	0.39	0/4236	0.58	0/5754
All	All	0.39	0/12708	0.57	0/17262

There are no bond length outliers.

There are no bond angle outliers.

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	125	0
1	B	4130	0	4131	132	0
1	C	4130	0	4130	111	0
2	A	14	0	13	1	0
2	B	14	0	13	2	0
2	C	14	0	13	1	0
3	A	21	0	18	5	0
3	B	21	0	18	6	0
3	C	21	0	18	4	0
4	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	0	0	0
4	C	10	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	11	0	14	0	0
6	B	11	0	14	2	0
6	C	11	0	14	0	0
7	A	20	0	21	2	0
7	B	20	0	21	0	0
7	C	40	0	42	0	0
8	C	7	0	6	0	0
9	A	179	0	0	17	0
9	B	135	0	0	15	0
9	C	194	0	0	23	0
All	All	13161	0	12617	379	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 15.

All (379) 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:C:3292:GLU:HB2	9:C:7340:HOH:O	1.52	1.10
1:A:1199:ARG:HH11	1:A:1199:ARG:HB3	1.22	1.02
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.45	0.96
1:C:3199:ARG:HB3	1:C:3199:ARG:HH11	1.33	0.93
1:A:1237:LYS:HE2	1:A:1342:HIS:HB2	1.55	0.87
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.57	0.85
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.59	0.84
3:C:382:SIA:H8	9:C:7032:HOH:O	1.77	0.83
1:C:3242:ARG:HH11	1:C:3242:ARG:HG2	1.46	0.80
3:A:182:SIA:H91	9:A:7095:HOH:O	1.82	0.80
1:B:2343:THR:HB	1:B:2442:ALA:HB2	1.65	0.78
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.66	0.77
1:A:1495:MET:HE3	1:A:1533:THR:HG21	1.65	0.75
1:C:3023:PRO:HB2	1:C:3034:LEU:HD21	1.67	0.75
1:C:3297:THR:O	1:C:3301:MET:HG2	1.87	0.74
1:B:2024:PRO:HG3	1:B:2037:PHE:CZ	2.24	0.73
1:A:1252:THR:HG22	1:A:1254:VAL:HG12	1.73	0.71
1:A:1041:GLU:HG2	9:A:7502:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3343:THR:HB	1:C:3442:ALA:HB2	1.74	0.69
1:B:2487:GLU:O	1:B:2491:ARG:HG3	1.93	0.69
1:A:1339:ARG:HG3	1:A:1440:ALA:HA	1.75	0.68
1:B:2086:MET:HE2	1:B:2110:LEU:HD12	1.75	0.67
1:C:3370:GLU:HG3	9:C:7261:HOH:O	1.93	0.67
1:C:3024:PRO:HG3	1:C:3037:PHE:CZ	2.31	0.66
1:B:2396:ILE:HB	1:B:2397:PRO:HD3	1.76	0.66
1:B:2382:LEU:HD23	1:B:2396:ILE:HG23	1.77	0.66
1:B:2538:LYS:HB3	1:B:2541:ASP:HB2	1.77	0.65
1:A:1025:VAL:HG22	1:A:1034:LEU:HD23	1.78	0.65
1:A:1199:ARG:HB3	1:A:1199:ARG:NH1	2.04	0.65
1:A:1335:LEU:O	1:A:1338:GLU:HG2	1.96	0.65
1:B:2370:GLU:HB3	1:B:2372:GLN:NE2	2.11	0.65
1:B:2132:ARG:HB3	1:B:2211:ASN:HB2	1.78	0.65
1:C:3456:SER:HB3	1:C:3460:LYS:HE2	1.79	0.65
1:C:3498:LYS:HB3	1:C:3514:LEU:HD11	1.78	0.65
1:B:2023:PRO:HB2	1:B:2034:LEU:HD21	1.79	0.64
1:B:2355:PHE:CE1	1:B:2360:PRO:HG3	2.32	0.64
1:B:2095:GLN:O	1:B:2099:GLU:HG3	1.96	0.64
1:B:2177:PHE:HB3	1:B:2319:LEU:O	1.98	0.64
1:B:2104:ARG:O	1:B:2482:LYS:HE2	1.98	0.64
1:A:1330:LYS:HG3	1:A:1335:LEU:HG	1.80	0.64
1:B:2398:GLU:HG2	9:B:7215:HOH:O	1.98	0.63
1:A:1260:ASP:OD2	2:C:379:NAG:H83	1.97	0.63
1:A:1368:LEU:HB2	7:A:11:HTQ:H151	1.80	0.63
1:B:2039:SER:OG	1:B:2046:PRO:HB3	1.99	0.63
1:C:3132:ARG:HB3	1:C:3211:ASN:HB2	1.81	0.62
1:B:2375:GLN:HE22	1:B:2404:LEU:HB2	1.64	0.62
1:C:3357:TRP:O	1:C:3360:PRO:HD2	1.98	0.62
1:B:2359:ILE:HB	1:B:2360:PRO:HD3	1.82	0.62
1:A:1290:THR:OG1	1:A:1293:GLU:HG3	2.00	0.62
2:B:279:NAG:H83	3:B:282:SIA:H32	1.82	0.62
1:A:1198:LEU:O	1:A:1202:GLN:HG2	2.00	0.61
1:A:1429:PRO:O	1:A:1433:VAL:HG23	2.00	0.61
1:B:2241:HIS:C	1:B:2242:ARG:HG3	2.20	0.61
1:A:1102:THR:OG1	1:A:1104:ARG:HG2	2.01	0.61
1:A:1242:ARG:HH11	1:A:1242:ARG:HG2	1.65	0.61
1:B:2343:THR:HA	9:B:7381:HOH:O	2.00	0.61
1:A:1026:VAL:CG1	1:A:1207:SER:HB3	2.31	0.61
1:B:2486:SER:O	1:B:2490:ILE:HG13	2.01	0.61
1:A:1423:ASP:OD2	1:A:1543:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1339:ARG:CG	1:A:1440:ALA:HA	2.31	0.60
1:A:1199:ARG:HH11	1:A:1199:ARG:CB	2.07	0.60
1:A:1177:PHE:HB3	1:A:1319:LEU:O	2.01	0.59
1:B:2323:ILE:HG12	9:B:7369:HOH:O	2.02	0.59
1:B:2526:TYR:HA	9:B:7102:HOH:O	2.02	0.59
1:A:1316:GLN:HG3	9:A:7342:HOH:O	2.03	0.59
1:A:1296:GLU:HG2	9:A:7429:HOH:O	2.03	0.59
1:C:3040:LEU:HG	9:C:7232:HOH:O	2.02	0.59
1:C:3283:VAL:HG12	1:C:3287:ARG:NH1	2.17	0.59
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.18	0.58
1:B:2242:ARG:HH11	1:B:2242:ARG:HG2	1.68	0.58
2:A:179:NAG:H2	9:A:7409:HOH:O	2.04	0.58
1:B:2095:GLN:HG2	9:B:7175:HOH:O	2.03	0.58
1:B:2493:SER:HB2	9:B:7364:HOH:O	2.04	0.58
1:C:3025:VAL:HG22	1:C:3034:LEU:HD23	1.84	0.58
1:C:3343:THR:HA	9:C:7127:HOH:O	2.04	0.58
1:B:2227:VAL:O	1:B:2231:VAL:HG23	2.03	0.57
1:A:1491:ARG:HB2	1:A:1491:ARG:NH1	2.20	0.57
1:B:2104:ARG:HD2	1:B:2108:ILE:HG12	1.86	0.57
1:C:3064:ARG:CZ	9:C:7150:HOH:O	2.52	0.57
1:A:1241:HIS:O	1:A:1242:ARG:HG3	2.05	0.57
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.20	0.57
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.85	0.57
1:B:2086:MET:HG3	1:B:2112:LEU:HD23	1.86	0.57
1:C:3461:PRO:HG2	1:C:3464:VAL:HG23	1.87	0.57
1:B:2447:TYR:HB3	1:B:2517:TRP:CZ2	2.39	0.57
1:B:2461:PRO:HG2	1:B:2464:VAL:HG23	1.86	0.57
1:B:2236:ALA:HA	1:B:2239:LEU:HD12	1.87	0.56
1:B:2264:LEU:HD22	1:B:2268:ILE:HD11	1.87	0.56
1:C:3242:ARG:NH1	1:C:3242:ARG:HG2	2.16	0.56
1:A:1403:TYR:O	1:A:1416:LEU:HD13	2.05	0.56
1:B:2403:TYR:CD1	1:B:2420:LEU:HD23	2.40	0.56
1:C:3398:GLU:HB2	9:C:7501:HOH:O	2.05	0.56
1:C:3021:SER:HB2	9:C:7270:HOH:O	2.05	0.56
1:B:2423:ASP:OD2	1:B:2543:GLU:HG2	2.06	0.56
1:C:3304:LEU:HD21	1:C:3318:LEU:HD23	1.87	0.56
1:B:2428:VAL:HB	1:B:2429:PRO:HD3	1.88	0.55
3:C:382:SIA:O7	9:C:7034:HOH:O	2.18	0.55
3:A:182:SIA:H7	9:A:7498:HOH:O	2.06	0.55
1:B:2403:TYR:CG	1:B:2420:LEU:HD23	2.42	0.55
1:B:2521:ASN:HB2	9:B:7023:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1538:LYS:HB3	1:A:1541:ASP:HB2	1.88	0.55
1:C:3197:ALA:O	1:C:3201:VAL:HG23	2.06	0.55
1:A:1143:GLY:O	1:A:1318:LEU:HD22	2.07	0.55
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.88	0.55
1:A:1331:THR:HB	1:A:1333:GLU:OE1	2.07	0.55
1:C:3268:ILE:HD11	1:C:3319:LEU:HD21	1.87	0.54
1:A:1024:PRO:HG3	1:A:1037:PHE:CZ	2.43	0.54
1:A:1393:LYS:HA	1:A:1396:ILE:HG12	1.90	0.54
1:A:1343:THR:HB	1:A:1442:ALA:HB2	1.88	0.54
1:A:1262:LYS:HB3	1:A:1263:PRO:HD3	1.90	0.54
1:A:1060:LEU:O	1:A:1063:LEU:HB2	2.08	0.54
1:C:3024:PRO:HG3	1:C:3037:PHE:CE1	2.43	0.54
1:B:2343:THR:HB	1:B:2442:ALA:CB	2.34	0.53
1:C:3132:ARG:HH22	1:C:3206:ALA:HB1	1.73	0.53
1:C:3335:LEU:O	1:C:3338:GLU:HG2	2.07	0.53
1:A:1139:ILE:HG12	1:A:1168:ILE:HD11	1.91	0.53
1:A:1241:HIS:C	1:A:1242:ARG:HG3	2.29	0.53
1:C:3462:LYS:HD3	9:C:7401:HOH:O	2.09	0.53
1:B:2038:VAL:HG21	1:B:2049:ILE:HD12	1.90	0.53
1:B:2348:VAL:O	1:B:2446:MET:HA	2.08	0.53
1:C:3349:GLY:HA3	1:C:3447:TYR:CE1	2.44	0.53
1:A:1409:ASP:OD2	1:A:1412:LYS:HG3	2.08	0.53
1:B:2176:GLY:HA2	1:B:2189:TRP:HB2	1.91	0.53
1:B:2409:ASP:HB3	1:B:2412:LYS:HB2	1.91	0.53
3:B:282:SIA:H112	9:B:7170:HOH:O	2.07	0.53
1:B:2423:ASP:O	1:B:2428:VAL:HG23	2.08	0.52
1:C:3264:LEU:HB2	9:C:7153:HOH:O	2.09	0.52
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.91	0.52
1:C:3491:ARG:NH1	9:C:7248:HOH:O	2.42	0.52
1:A:1297:THR:O	1:A:1301:MET:HG2	2.10	0.52
1:A:1553:LYS:C	1:A:1553:LYS:HD3	2.29	0.52
1:B:2349:GLY:HA3	1:B:2447:TYR:CE1	2.44	0.52
1:B:2220:GLU:HG3	1:B:2471:GLU:OE1	2.10	0.52
1:C:3119:LEU:O	1:C:3119:LEU:HD12	2.09	0.52
1:C:3351:ASN:HB3	1:C:3466:GLY:O	2.09	0.52
1:A:1292:GLU:O	1:A:1296:GLU:HG3	2.09	0.52
1:B:2024:PRO:HG3	1:B:2037:PHE:CE2	2.44	0.52
1:C:3237:LYS:O	1:C:3238:ASN:HB2	2.08	0.52
1:C:3199:ARG:CB	1:C:3199:ARG:HH11	2.13	0.52
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.25	0.52
1:C:3392:ALA:HB1	1:C:3394:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:ARG:HH11	1:A:1242:ARG:CG	2.22	0.52
1:A:1528:GLN:O	1:A:1533:THR:HA	2.09	0.52
1:B:2284:HIS:O	1:B:2288:GLN:HG2	2.09	0.52
1:C:3403:TYR:CG	1:C:3420:LEU:HD23	2.45	0.52
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.45	0.51
1:B:2452:ARG:NE	9:B:7045:HOH:O	2.42	0.51
1:B:2471:GLU:O	1:B:2475:VAL:HG23	2.10	0.51
1:A:1487:GLU:HG3	1:A:1491:ARG:HH12	1.75	0.51
1:A:1103:ASN:ND2	1:A:1481:LEU:HD12	2.25	0.51
1:B:2386:TYR:HA	9:B:7472:HOH:O	2.09	0.51
1:B:2495:MET:HE3	1:B:2533:THR:HG21	1.93	0.51
1:B:2241:HIS:O	1:B:2242:ARG:HG3	2.10	0.51
1:B:2279:SER:O	1:B:2283:VAL:HG23	2.10	0.51
1:C:3349:GLY:HA3	1:C:3447:TYR:CZ	2.46	0.51
1:A:1046:PRO:HA	9:A:7348:HOH:O	2.10	0.51
1:A:1086:MET:CE	1:A:1110:LEU:HB2	2.40	0.51
1:B:2338:GLU:HG2	1:B:2339:ARG:N	2.26	0.51
1:A:1420:LEU:HD22	1:A:1547:TRP:HZ2	1.77	0.50
1:A:1540:LYS:O	1:A:1544:VAL:HG23	2.11	0.50
1:C:3323:ILE:HG12	9:C:7053:HOH:O	2.11	0.50
1:A:1316:GLN:HB3	9:A:7317:HOH:O	2.11	0.50
1:A:1317:PRO:HG2	1:A:1318:LEU:H	1.76	0.50
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.94	0.50
1:C:3052:GLY:HA3	9:C:7347:HOH:O	2.11	0.50
1:C:3104:ARG:NH1	1:C:3153:ASP:HB2	2.26	0.50
1:B:2186:ARG:HB3	1:B:2324:ASP:HB2	1.92	0.50
1:C:3421:ILE:O	1:C:3425:MET:HG3	2.10	0.50
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.75	0.49
1:A:1095:GLN:O	1:A:1099:GLU:HG3	2.11	0.49
1:A:1149:ALA:HB2	1:A:1169:GLN:HG3	1.93	0.49
1:B:2029:VAL:HG23	1:B:2204:ASN:OD1	2.13	0.49
1:B:2393:LYS:HA	1:B:2396:ILE:HG12	1.94	0.49
1:B:2417:PHE:O	1:B:2420:LEU:HB3	2.13	0.49
1:C:3125:ALA:HB2	1:C:3133:LEU:HD12	1.95	0.49
1:C:3216:THR:OG1	1:C:3242:ARG:HB2	2.13	0.49
1:B:2455:PHE:CD2	1:B:2482:LYS:HD2	2.47	0.49
1:C:3492:LEU:O	1:C:3496:VAL:HG23	2.12	0.49
1:C:3135:VAL:HB	1:C:3215:VAL:HG22	1.93	0.49
2:B:279:NAG:C8	3:B:282:SIA:H32	2.43	0.49
1:A:1149:ALA:HB1	1:A:1167:THR:HB	1.95	0.49
1:C:3538:LYS:HB3	1:C:3541:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.94	0.48
1:C:3408:ASP:HB3	9:C:7144:HOH:O	2.13	0.48
1:A:1120:ASN:HB2	1:A:1167:THR:OG1	2.13	0.48
1:B:2130:LYS:C	1:B:2131:ASN:HD22	2.16	0.48
1:B:2319:LEU:O	1:B:2320:GLY:O	2.32	0.48
1:A:1330:LYS:HD3	1:A:1334:GLU:HB3	1.96	0.48
1:A:1420:LEU:O	1:A:1424:VAL:HG23	2.13	0.48
1:B:2149:ALA:HB1	1:B:2167:THR:HB	1.96	0.48
1:B:2283:VAL:HG12	1:B:2287:ARG:NH1	2.29	0.48
1:C:3252:THR:HG22	1:C:3254:VAL:HG12	1.94	0.48
1:C:3079:ASN:HB2	3:C:382:SIA:C1	2.43	0.48
1:B:2048:ALA:HB3	1:B:2123:THR:HG23	1.96	0.48
1:C:3241:HIS:O	1:C:3242:ARG:HG2	2.14	0.48
1:C:3382:LEU:HD23	1:C:3396:ILE:HG23	1.96	0.48
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.77	0.48
1:C:3104:ARG:CZ	1:C:3153:ASP:HB2	2.43	0.48
1:B:2217:ILE:HG13	1:B:2217:ILE:O	2.14	0.48
1:B:2343:THR:CB	1:B:2442:ALA:HB2	2.40	0.48
1:C:3089:GLN:HB2	1:C:3146:VAL:HG12	1.96	0.48
1:A:1375:GLN:O	1:A:1379:MET:HG3	2.14	0.47
1:B:2304:LEU:HD13	6:B:112:PLM:H82	1.96	0.47
1:C:3278:THR:OG1	1:C:3281:VAL:HG23	2.14	0.47
1:A:1235:LEU:HD12	1:A:1327:LEU:HA	1.96	0.47
1:B:2292:GLU:O	1:B:2296:GLU:HG3	2.14	0.47
1:B:2044:ALA:N	9:B:7280:HOH:O	2.47	0.47
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.44	0.47
1:A:1355:PHE:CE1	1:A:1360:PRO:HG3	2.50	0.47
1:A:1403:TYR:CG	1:A:1420:LEU:HD23	2.49	0.47
1:C:3095:GLN:HB2	9:C:7254:HOH:O	2.15	0.47
1:A:1023:PRO:HA	1:A:1024:PRO:HD3	1.76	0.47
1:A:1371:GLY:C	1:A:1414:LYS:HD3	2.34	0.47
1:A:1461:PRO:HG2	1:A:1464:VAL:CG2	2.45	0.47
1:B:2034:LEU:HB3	1:B:2079:ASN:HA	1.95	0.47
3:C:382:SIA:H32	9:C:7432:HOH:O	2.15	0.47
3:A:182:SIA:C8	9:A:7008:HOH:O	2.62	0.47
1:B:2370:GLU:HB3	1:B:2372:GLN:HE21	1.76	0.47
1:C:3403:TYR:CD1	1:C:3420:LEU:HD23	2.49	0.47
1:A:1452:ARG:CZ	1:A:1462:LYS:HA	2.45	0.47
1:B:2262:LYS:HB3	1:B:2263:PRO:HD3	1.97	0.47
1:B:2538:LYS:HB3	1:B:2541:ASP:CB	2.44	0.47
1:C:3412:LYS:HE3	9:C:7417:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3495:MET:HG3	1:C:3514:LEU:HD22	1.97	0.47
1:A:1296:GLU:O	1:A:1300:LYS:HG3	2.15	0.47
1:B:2333:GLU:CD	1:B:2333:GLU:H	2.18	0.47
1:B:2461:PRO:HG2	1:B:2464:VAL:CG2	2.45	0.47
1:A:1104:ARG:HD2	9:A:7464:HOH:O	2.14	0.46
1:B:2279:SER:HA	1:B:2282:MET:HE2	1.97	0.46
1:A:1246:GLU:HG2	1:A:1447:TYR:OH	2.16	0.46
1:A:1242:ARG:NH1	1:A:1242:ARG:CG	2.78	0.46
1:A:1316:GLN:HA	1:A:1316:GLN:OE1	2.16	0.46
1:B:2420:LEU:HD22	1:B:2547:TRP:HZ2	1.80	0.46
1:C:3090:ASP:HB3	1:C:3093:ALA:HB3	1.98	0.46
1:B:2237:LYS:O	1:B:2238:ASN:HB2	2.16	0.46
1:B:2254:VAL:HG21	1:B:2388:LEU:HD23	1.97	0.46
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.46	0.46
1:A:1492:LEU:O	1:A:1496:VAL:HG23	2.15	0.46
1:B:2205:ILE:HD12	1:B:2205:ILE:HA	1.78	0.46
1:B:2457:SER:N	9:B:7206:HOH:O	2.49	0.46
1:C:3087:CYS:HB2	1:C:3172:LEU:HD12	1.98	0.46
1:A:1180:THR:OG1	1:A:1182:ASP:OD2	2.26	0.46
1:B:2452:ARG:HE	1:B:2462:LYS:HA	1.81	0.46
1:A:1257:LYS:HE3	1:A:1318:LEU:O	2.16	0.46
1:B:2201:VAL:HG13	1:B:2205:ILE:HB	1.98	0.46
1:A:1267:GLN:CG	9:A:7226:HOH:O	2.64	0.46
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.79	0.46
1:A:1339:ARG:HD2	1:A:1339:ARG:N	2.31	0.45
3:A:182:SIA:H8	9:A:7008:HOH:O	2.16	0.45
1:C:3246:GLU:HG2	1:C:3447:TYR:OH	2.15	0.45
1:C:3284:HIS:O	1:C:3288:GLN:HG2	2.16	0.45
1:B:2551:PHE:C	1:B:2553:LYS:H	2.19	0.45
1:B:2079:ASN:HB2	3:B:282:SIA:C1	2.46	0.45
1:C:3324:ASP:OD2	1:C:3324:ASP:N	2.50	0.45
1:B:2383:TRP:CH2	1:B:2393:LYS:HB2	2.52	0.45
1:C:3122:TYR:HB2	1:C:3165:VAL:HB	1.98	0.45
1:C:3190:GLY:O	1:C:3194:GLN:HG3	2.17	0.45
1:C:3029:VAL:HG23	1:C:3204:ASN:OD1	2.16	0.45
1:C:3452:ARG:HG2	1:C:3452:ARG:HH11	1.82	0.45
1:C:3474:SER:HB3	1:C:3496:VAL:HG21	1.98	0.45
1:A:1098:SER:O	1:A:1102:THR:HB	2.17	0.45
1:B:2407:THR:HB	9:B:7200:HOH:O	2.17	0.44
1:A:1136:MET:HB3	1:A:1218:PHE:CE1	2.52	0.44
1:A:1375:GLN:OE1	1:A:1400:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3464:VAL:HG12	1:C:3467:ASP:HB2	1.99	0.44
1:A:1143:GLY:O	1:A:1144:LEU:HB2	2.18	0.44
1:A:1447:TYR:C	1:A:1447:TYR:CD2	2.90	0.44
1:B:2202:GLN:HB3	9:B:7007:HOH:O	2.16	0.44
1:A:1284:HIS:O	1:A:1288:GLN:HG2	2.18	0.44
1:B:2024:PRO:HG3	1:B:2037:PHE:CE1	2.51	0.44
1:B:2191:HIS:O	1:B:2195:VAL:HG23	2.17	0.44
1:C:3233:SER:HA	1:C:3234:PRO:HD3	1.87	0.44
1:C:3221:SER:HA	1:C:3247:SER:O	2.16	0.44
1:C:3025:VAL:CG2	1:C:3034:LEU:HD23	2.47	0.44
1:C:3343:THR:HB	1:C:3442:ALA:CB	2.44	0.44
1:A:1366:TYR:HA	1:A:1367:PRO:HD3	1.84	0.44
1:B:2379:MET:HG2	1:B:2400:THR:OG1	2.16	0.44
1:A:1052:GLY:O	3:A:182:SIA:H92	2.17	0.44
1:B:2242:ARG:CG	1:B:2242:ARG:HH11	2.31	0.44
1:B:2079:ASN:H	3:B:282:SIA:C1	2.31	0.44
1:B:2126:ASP:OD2	1:B:2129:LYS:HG2	2.18	0.44
1:B:2132:ARG:NH2	1:B:2206:ALA:HB1	2.33	0.43
1:C:3357:TRP:C	1:C:3360:PRO:HD2	2.38	0.43
1:A:1225:GLU:O	1:A:1229:VAL:HG23	2.18	0.43
1:C:3033:VAL:HG13	1:C:3080:ALA:HB2	2.00	0.43
1:B:2512:GLU:O	1:B:2512:GLU:HG3	2.18	0.43
1:C:3414:LYS:O	1:C:3418:LEU:HG	2.17	0.43
1:A:1063:LEU:HA	1:A:1063:LEU:HD23	1.89	0.43
1:A:1249:VAL:HG23	1:A:1251:LEU:H	1.83	0.43
1:A:1257:LYS:HB2	1:A:1322:VAL:HG12	2.00	0.43
1:A:1452:ARG:NE	1:A:1462:LYS:HA	2.34	0.43
1:B:2428:VAL:HG13	1:B:2544:VAL:HA	2.01	0.43
1:C:3214:SER:HA	9:C:7301:HOH:O	2.19	0.43
1:B:2452:ARG:NE	1:B:2462:LYS:HA	2.33	0.43
1:C:3199:ARG:NH1	1:C:3199:ARG:HB3	2.16	0.43
1:B:2086:MET:HE2	1:B:2110:LEU:CD1	2.44	0.43
1:B:2152:TYR:CD1	1:B:2152:TYR:N	2.86	0.43
1:A:1461:PRO:HG2	1:A:1464:VAL:HG23	2.01	0.43
1:B:2254:VAL:O	1:B:2318:LEU:HD11	2.19	0.43
1:B:2079:ASN:HB2	3:B:282:SIA:O1A	2.19	0.42
1:B:2540:LYS:HA	1:B:2543:GLU:OE2	2.18	0.42
1:B:2395:LEU:HD22	1:B:2550:LEU:CD1	2.49	0.42
1:C:3359:ILE:HB	1:C:3360:PRO:HD3	2.01	0.42
1:B:2358:LEU:HD23	1:B:2468:HIS:HB3	2.00	0.42
1:C:3078:LYS:HG3	9:C:7291:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3461:PRO:HG2	1:C:3464:VAL:CG2	2.49	0.42
1:A:1086:MET:HE2	1:A:1110:LEU:HB2	2.01	0.42
1:A:1124:PRO:HD3	1:A:1158:ALA:HB1	2.02	0.42
1:C:3339:ARG:HD2	1:C:3339:ARG:N	2.34	0.42
1:C:3097:LEU:HD11	1:C:3101:PHE:CE2	2.54	0.42
1:C:3218:PHE:HB3	1:C:3244:ILE:HB	2.02	0.42
1:C:3242:ARG:NH1	1:C:3242:ARG:CG	2.82	0.42
1:C:3375:GLN:HB3	9:C:7078:HOH:O	2.19	0.42
1:A:1292:GLU:HB2	9:A:7067:HOH:O	2.19	0.42
1:A:1103:ASN:HB3	9:A:7185:HOH:O	2.19	0.42
1:A:1131:ASN:O	1:A:1132:ARG:NH1	2.52	0.42
1:A:1187:GLY:O	1:A:1188:ASN:HB2	2.19	0.42
1:A:1138:TRP:HH2	1:A:1220:GLU:HB2	1.84	0.42
1:B:2332:PRO:O	1:B:2336:GLN:HG2	2.19	0.42
1:B:2221:SER:O	1:B:2224:GLY:N	2.52	0.42
1:A:1242:ARG:HD3	1:A:1503:PHE:O	2.20	0.42
1:B:2363:LEU:HD13	6:B:112:PLM:H72	2.02	0.42
1:B:2233:SER:HA	1:B:2234:PRO:HD3	1.90	0.42
1:C:3083:TYR:HD1	1:C:3150:SER:HG	1.67	0.42
1:C:3355:PHE:CE1	1:C:3360:PRO:HG3	2.55	0.42
1:B:2266:GLU:O	1:B:2270:ILE:HG13	2.19	0.42
1:C:3104:ARG:HD2	1:C:3108:ILE:HG12	2.02	0.42
1:C:3402:LYS:HG2	1:C:3546:PHE:CE1	2.55	0.42
1:A:1066:THR:HG22	9:A:7273:HOH:O	2.19	0.42
1:A:1080:ALA:HA	9:A:7095:HOH:O	2.19	0.42
1:A:1385:SER:O	1:A:1389:VAL:HG22	2.20	0.42
1:B:2059:PRO:HD3	1:B:2117:LEU:HD12	2.02	0.42
1:B:2364:MET:CE	1:B:2388:LEU:HD11	2.49	0.42
1:A:1034:LEU:C	1:A:1034:LEU:HD13	2.41	0.41
1:A:1355:PHE:CE2	1:A:1425:MET:HE1	2.55	0.41
1:B:2324:ASP:OD1	1:B:2326:MET:HB2	2.20	0.41
1:B:2528:GLN:O	1:B:2533:THR:HA	2.20	0.41
1:C:3149:ALA:HB1	1:C:3167:THR:HB	2.01	0.41
1:C:3290:THR:HA	4:C:185:SO4:O4	2.19	0.41
1:A:1235:LEU:HD12	1:A:1327:LEU:HD12	2.03	0.41
1:C:3064:ARG:O	1:C:3066:THR:HG23	2.20	0.41
1:C:3527:LEU:HD11	1:C:3533:THR:HG22	2.01	0.41
1:C:3268:ILE:HG12	1:C:3301:MET:CE	2.50	0.41
1:A:1229:VAL:HG13	1:A:1328:LEU:HD11	2.02	0.41
1:A:1404:LEU:HD23	1:A:1416:LEU:HB2	2.03	0.41
1:B:2330:LYS:HG3	1:B:2335:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:THR:HG23	1:A:1404:LEU:HD12	2.01	0.41
9:A:7091:HOH:O	1:B:2284:HIS:HD2	2.04	0.41
1:B:2331:THR:HB	1:B:2333:GLU:OE1	2.20	0.41
1:B:2342:HIS:HD2	9:B:7021:HOH:O	2.04	0.41
1:A:1499:PHE:CD2	1:A:1509:PRO:HB2	2.55	0.41
1:B:2278:THR:OG1	1:B:2281:VAL:HG23	2.21	0.41
1:C:3124:PRO:HD3	1:C:3158:ALA:HB1	2.02	0.41
1:A:1106:GLU:OE1	1:A:1108:ILE:HD13	2.20	0.41
1:C:3107:ASN:HA	9:C:7164:HOH:O	2.20	0.41
1:C:3348:VAL:O	1:C:3446:MET:HA	2.21	0.41
1:A:1340:ASN:O	1:A:1341:PHE:HB2	2.21	0.41
1:B:2023:PRO:HA	1:B:2024:PRO:HD3	1.85	0.41
1:B:2409:ASP:O	1:B:2413:LYS:HG3	2.20	0.41
1:B:2225:GLU:O	1:B:2229:VAL:HG23	2.21	0.41
1:C:3135:VAL:HG21	1:C:3205:ILE:HG12	2.03	0.41
1:A:1255:LEU:O	1:A:1320:GLY:HA3	2.21	0.41
1:C:3205:ILE:HD12	1:C:3205:ILE:HA	1.70	0.41
1:C:3152:TYR:CD1	1:C:3152:TYR:N	2.88	0.40
1:A:1361:MET:HA	7:A:11:HTQ:H191	2.03	0.40
1:B:2231:VAL:O	1:B:2231:VAL:HG12	2.21	0.40
1:A:1375:GLN:HG2	1:A:1413:LYS:NZ	2.36	0.40
1:A:1526:TYR:CZ	1:A:1536:ALA:HB3	2.57	0.40
1:B:2048:ALA:HB3	1:B:2123:THR:CG2	2.51	0.40
1:B:2403:TYR:CE2	1:B:2420:LEU:HA	2.57	0.40
1:C:3316:GLN:HG2	9:C:7318:HOH:O	2.21	0.40
1:A:1218:PHE:HB3	1:A:1244:ILE:HB	2.02	0.40
1:A:1398:GLU:CD	1:A:1550:LEU:HD13	2.42	0.40
1:A:1355:PHE:CD2	1:A:1425:MET:HE1	2.56	0.40
1:B:2447:TYR:C	1:B:2447:TYR:CD2	2.94	0.40
1:C:3540:LYS:O	1:C:3544:VAL:HG23	2.21	0.40
1:A:1271:THR:HG22	1:A:1297:THR:HG23	2.04	0.40
1:B:2102:THR:OG1	1:B:2104:ARG:HG2	2.22	0.40
1:C:3220:GLU:HA	1:C:3246:GLU:O	2.20	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	530/542 (98%)	485 (92%)	40 (8%)	5 (1%)	17	46
1	B	530/542 (98%)	477 (90%)	47 (9%)	6 (1%)	14	41
1	C	530/542 (98%)	490 (92%)	36 (7%)	4 (1%)	19	49
All	All	1590/1626 (98%)	1452 (91%)	123 (8%)	15 (1%)	17	46

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2105	LYS
1	A	1320	GLY
1	B	2320	GLY
1	C	3105	LYS
1	C	3406	GLY
1	A	1538	LYS
1	C	3303	PHE
1	A	1185	SER
1	A	1253	SER
1	B	2254	VAL
1	C	3185	SER
1	B	2185	SER
1	B	2515	PRO
1	B	2427	GLY
1	A	1367	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	448/457 (98%)	437 (98%)	11 (2%)	47	80
1	B	448/457 (98%)	436 (97%)	12 (3%)	44	78
1	C	448/457 (98%)	440 (98%)	8 (2%)	59	86
All	All	1344/1371 (98%)	1313 (98%)	31 (2%)	50	82

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1106	GLU
1	A	1129	LYS
1	A	1199	ARG
1	A	1218	PHE
1	A	1264	LEU
1	A	1339	ARG
1	A	1498	LYS
1	A	1499	PHE
1	A	1500	TRP
1	A	1523	LYS
1	A	1553	LYS
1	B	2132	ARG
1	B	2218	PHE
1	B	2245	SER
1	B	2264	LEU
1	B	2318	LEU
1	B	2338	GLU
1	B	2366	TYR
1	B	2372	GLN
1	B	2499	PHE
1	B	2500	TRP
1	B	2506	ASN
1	B	2551	PHE
1	C	3106	GLU
1	C	3128	THR
1	C	3132	ARG
1	C	3199	ARG
1	C	3218	PHE
1	C	3264	LEU
1	C	3339	ARG
1	C	3500	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1069	GLN
1	A	1238	ASN
1	A	1342	HIS
1	A	1450	GLN
1	B	2069	GLN
1	B	2131	ASN
1	B	2202	GLN
1	B	2372	GLN
1	B	2436	ASN
1	B	2528	GLN
1	B	2534	GLN
1	C	3537	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SIA	C	382	-	18,21,21	0.96	2 (11%)	21,31,31	1.91	4 (19%)
4	SO4	A	184	-	4,4,4	0.43	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HTQ	C	31[B]	-	22,22,22	2.66	13 (59%)	30,31,31	1.70	6 (20%)
2	NAG	A	179	1	14,14,15	0.63	0	17,19,21	0.73	0
6	PLM	B	112	-	7,10,17	0.74	0	6,10,17	0.73	0
4	SO4	A	284	-	4,4,4	0.27	0	6,6,6	0.08	0
4	SO4	B	385	-	4,4,4	0.33	0	6,6,6	0.06	0
4	SO4	C	185	-	4,4,4	0.37	0	6,6,6	0.08	0
4	SO4	B	285	-	4,4,4	0.34	0	6,6,6	0.05	0
2	NAG	B	279	1	14,14,15	0.50	0	17,19,21	0.86	1 (5%)
3	SIA	A	182	-	18,21,21	0.99	2 (11%)	21,31,31	0.81	0
3	SIA	B	282	-	18,21,21	0.74	0	21,31,31	1.24	2 (9%)
4	SO4	C	384	-	4,4,4	0.38	0	6,6,6	0.10	0
4	SO4	B	286	-	4,4,4	0.47	0	6,6,6	0.07	0
7	HTQ	B	21	-	22,22,22	2.70	13 (59%)	30,31,31	1.72	6 (20%)
7	HTQ	A	11	-	22,22,22	2.81	13 (59%)	30,31,31	1.76	6 (20%)
6	PLM	A	111	-	7,10,17	0.76	0	6,10,17	0.72	0
7	HTQ	C	31[A]	-	22,22,22	2.64	12 (54%)	30,31,31	1.84	5 (16%)
8	COA	C	1	-	5,6,50	4.32	2 (40%)	5,6,75	4.53	4 (80%)
2	NAG	C	379	1	14,14,15	0.79	0	17,19,21	0.68	0
6	PLM	C	113	-	7,10,17	0.88	0	6,10,17	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HTQ	C	31[B]	-	-	0/12/33/33	0/4/3/3
6	PLM	B	112	-	-	4/6/8/15	-
3	SIA	B	282	-	-	4/14/38/38	0/1/1/1
2	NAG	B	279	1	-	4/6/23/26	0/1/1/1
3	SIA	A	182	-	-	3/14/38/38	0/1/1/1
3	SIA	C	382	-	-	6/14/38/38	0/1/1/1
2	NAG	A	179	1	-	3/6/23/26	0/1/1/1
7	HTQ	B	21	-	-	0/12/33/33	0/4/3/3
7	HTQ	A	11	-	-	1/12/33/33	0/4/3/3
6	PLM	A	111	-	-	3/6/8/15	-
7	HTQ	C	31[A]	-	-	0/12/33/33	0/4/3/3
8	COA	C	1	-	-	2/4/4/64	-
2	NAG	C	379	1	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLM	C	113	-	-	4/6/8/15	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1	COA	O5P-C5P	8.03	1.41	1.23
7	C	31[A]	HTQ	C9-N8	5.15	1.55	1.47
7	C	31[B]	HTQ	C9-N8	5.07	1.55	1.47
7	B	21	HTQ	C9-N8	5.00	1.54	1.47
7	A	11	HTQ	C9-N8	4.94	1.54	1.47
8	C	1	COA	C5P-N4P	4.91	1.48	1.34
7	A	11	HTQ	C15-C14	4.45	1.46	1.39
7	A	11	HTQ	C16-C14	4.42	1.46	1.39
7	A	11	HTQ	C4-C3	4.34	1.63	1.52
7	B	21	HTQ	C16-C14	4.32	1.46	1.39
7	C	31[B]	HTQ	C16-C14	4.26	1.45	1.39
7	C	31[A]	HTQ	C16-C14	4.14	1.45	1.39
7	C	31[B]	HTQ	C4-C5	4.00	1.61	1.53
7	B	21	HTQ	C15-C14	3.99	1.45	1.39
7	C	31[A]	HTQ	C4-C5	3.92	1.60	1.53
7	B	21	HTQ	C4-C5	3.90	1.60	1.53
7	C	31[B]	HTQ	C2-C1	3.87	1.60	1.53
7	A	11	HTQ	C4-C5	3.81	1.60	1.53
7	C	31[A]	HTQ	C4-C3	3.79	1.61	1.52
7	B	21	HTQ	C4-C3	3.79	1.61	1.52
7	C	31[B]	HTQ	C15-C14	3.70	1.45	1.39
7	C	31[B]	HTQ	C4-C3	3.70	1.61	1.52
7	C	31[A]	HTQ	C15-C14	3.69	1.45	1.39
7	C	31[A]	HTQ	C2-C1	3.65	1.60	1.53
7	A	11	HTQ	C2-C1	3.44	1.60	1.53
7	B	21	HTQ	C2-C1	3.38	1.59	1.53
7	A	11	HTQ	C17-C15	3.06	1.45	1.38
7	A	11	HTQ	C7-C1	2.95	1.61	1.53
7	A	11	HTQ	C18-C16	2.92	1.45	1.38
7	B	21	HTQ	C17-C15	2.81	1.44	1.38
7	C	31[A]	HTQ	C17-C15	2.78	1.44	1.38
7	B	21	HTQ	C18-C16	2.77	1.44	1.38
7	C	31[B]	HTQ	C17-C15	2.74	1.44	1.38
7	C	31[A]	HTQ	O10-C11	2.72	1.40	1.34
7	B	21	HTQ	C19-C18	2.70	1.45	1.38
7	C	31[B]	HTQ	C19-C17	2.68	1.45	1.38
3	C	382	SIA	C4-C5	2.67	1.55	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	31[A]	HTQ	C18-C16	2.66	1.44	1.38
7	C	31[B]	HTQ	C18-C16	2.66	1.44	1.38
7	A	11	HTQ	C19-C18	2.65	1.45	1.38
7	A	11	HTQ	C19-C17	2.61	1.44	1.38
7	B	21	HTQ	C19-C17	2.59	1.44	1.38
7	A	11	HTQ	O10-C11	2.59	1.40	1.34
7	B	21	HTQ	C7-C1	2.59	1.60	1.53
7	C	31[B]	HTQ	O10-C11	2.57	1.40	1.34
7	C	31[A]	HTQ	C19-C17	2.56	1.44	1.38
7	C	31[B]	HTQ	C19-C18	2.52	1.44	1.38
7	C	31[A]	HTQ	C19-C18	2.50	1.44	1.38
3	A	182	SIA	O6-C2	2.44	1.45	1.43
7	C	31[B]	HTQ	C7-C1	2.43	1.59	1.53
7	A	11	HTQ	C5-N8	2.36	1.51	1.48
7	B	21	HTQ	O10-C11	2.35	1.39	1.34
7	C	31[A]	HTQ	C7-C1	2.35	1.59	1.53
7	B	21	HTQ	C5-N8	2.33	1.51	1.48
3	C	382	SIA	C6-C5	2.05	1.56	1.53
7	C	31[B]	HTQ	C5-N8	2.00	1.51	1.48
3	A	182	SIA	C3-C2	2.00	1.54	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	31[A]	HTQ	C3-O10-C11	7.07	129.29	117.69
8	C	1	COA	O5P-C5P-C6P	-6.41	110.15	122.06
7	A	11	HTQ	C3-O10-C11	6.20	127.86	117.69
8	C	1	COA	O5P-C5P-N4P	-6.11	104.53	121.74
7	B	21	HTQ	C3-O10-C11	6.04	127.59	117.69
7	C	31[B]	HTQ	C3-O10-C11	5.76	127.13	117.69
3	C	382	SIA	O6-C6-C5	4.86	114.52	109.78
3	C	382	SIA	C4-C5-C6	3.91	118.98	109.10
3	C	382	SIA	C3-C4-C5	3.61	115.53	109.98
7	C	31[B]	HTQ	C15-C14-C13	-3.57	114.63	120.53
8	C	1	COA	C3P-N4P-C5P	-3.56	117.09	122.56
7	A	11	HTQ	C15-C14-C13	-3.53	114.70	120.53
7	B	21	HTQ	C15-C14-C13	-3.46	114.82	120.53
7	C	31[A]	HTQ	C15-C14-C13	-3.40	114.92	120.53
8	C	1	COA	C6P-C5P-N4P	-3.14	110.53	116.09
7	A	11	HTQ	C16-C14-C13	3.08	125.61	120.53
7	C	31[B]	HTQ	C16-C14-C13	2.73	125.05	120.53
2	B	279	NAG	C2-N2-C7	-2.65	119.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	21	HTQ	C7-C6-C5	2.59	107.92	104.05
7	C	31[A]	HTQ	C16-C14-C13	2.57	124.78	120.53
3	B	282	SIA	O6-C6-C5	2.57	112.28	109.78
3	C	382	SIA	C9-C8-C7	-2.57	106.85	112.41
7	C	31[B]	HTQ	C7-C6-C5	2.55	107.85	104.05
7	C	31[A]	HTQ	C7-C6-C5	2.54	107.84	104.05
7	B	21	HTQ	C16-C14-C13	2.54	124.73	120.53
3	B	282	SIA	C4-C5-C6	2.49	115.40	109.10
7	B	21	HTQ	C4-C3-C2	2.40	116.68	112.07
7	C	31[A]	HTQ	C3-C2-C1	2.34	116.20	112.69
7	A	11	HTQ	C7-C6-C5	2.33	107.53	104.05
7	C	31[B]	HTQ	C3-C2-C1	2.24	116.05	112.69
7	B	21	HTQ	C3-C2-C1	2.06	115.79	112.69
7	C	31[B]	HTQ	C4-C3-C2	2.05	116.00	112.07
7	A	11	HTQ	O10-C11-O12	2.00	127.68	123.94
7	A	11	HTQ	C4-C3-C2	2.00	115.91	112.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	379	NAG	C1

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	179	NAG	C8-C7-N2-C2
2	A	179	NAG	O7-C7-N2-C2
2	B	279	NAG	C8-C7-N2-C2
2	B	279	NAG	O7-C7-N2-C2
3	C	382	SIA	C5-C6-C7-C8
3	C	382	SIA	C5-C6-C7-O7
3	C	382	SIA	O6-C6-C7-O7
3	A	182	SIA	C11-C10-N5-C5
3	A	182	SIA	O10-C10-N5-C5
8	C	1	COA	C6P-C5P-N4P-C3P
8	C	1	COA	O5P-C5P-N4P-C3P
6	C	113	PLM	C1-C2-C3-C4
2	C	379	NAG	C4-C5-C6-O6
3	C	382	SIA	C11-C10-N5-C5
2	C	379	NAG	C8-C7-N2-C2
2	C	379	NAG	O5-C5-C6-O6
2	C	379	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	C	382	SIA	O10-C10-N5-C5
3	B	282	SIA	C7-C8-C9-O9
6	C	113	PLM	C5-C6-C7-C8
6	B	112	PLM	C4-C5-C6-C7
6	A	111	PLM	C3-C4-C5-C6
6	C	113	PLM	C4-C5-C6-C7
6	A	111	PLM	C4-C5-C6-C7
6	C	113	PLM	C2-C3-C4-C5
6	A	111	PLM	C2-C3-C4-C5
3	B	282	SIA	C11-C10-N5-C5
2	B	279	NAG	C4-C5-C6-O6
6	B	112	PLM	C2-C3-C4-C5
6	B	112	PLM	C3-C4-C5-C6
6	B	112	PLM	C5-C6-C7-C8
2	B	279	NAG	O5-C5-C6-O6
3	B	282	SIA	O10-C10-N5-C5
3	B	282	SIA	O8-C8-C9-O9
2	A	179	NAG	O5-C5-C6-O6
3	C	382	SIA	C4-C5-N5-C10
3	A	182	SIA	C4-C5-N5-C10
7	A	11	HTQ	C4-C3-O10-C11

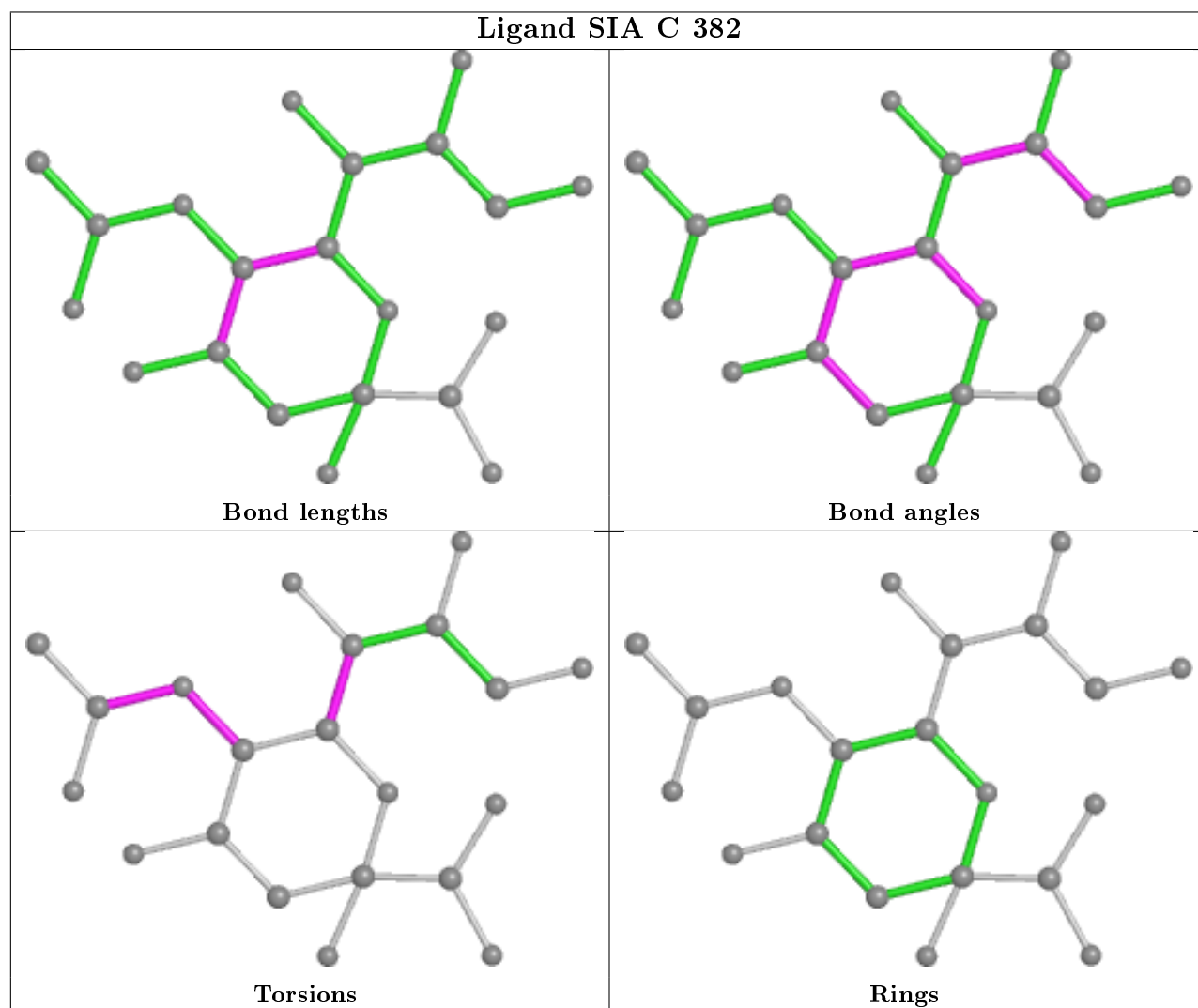
There are no ring outliers.

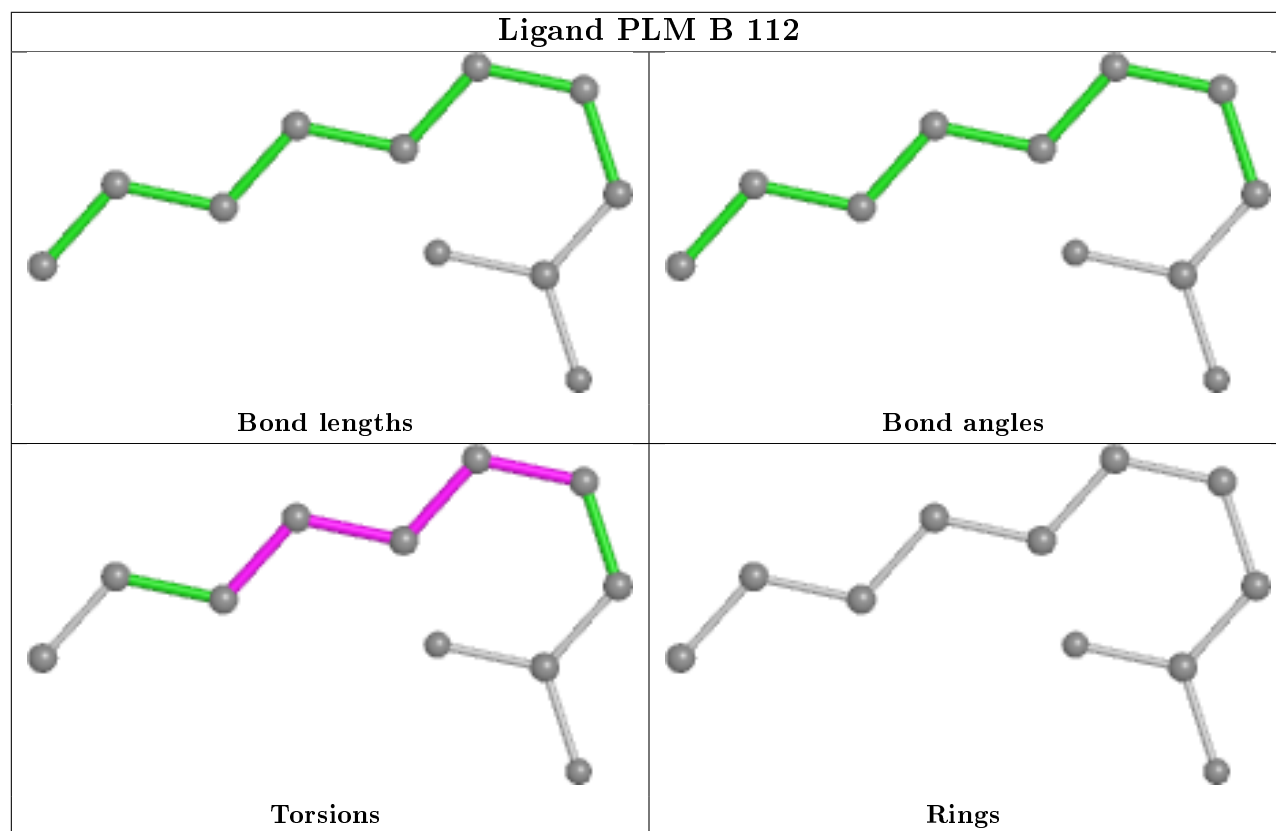
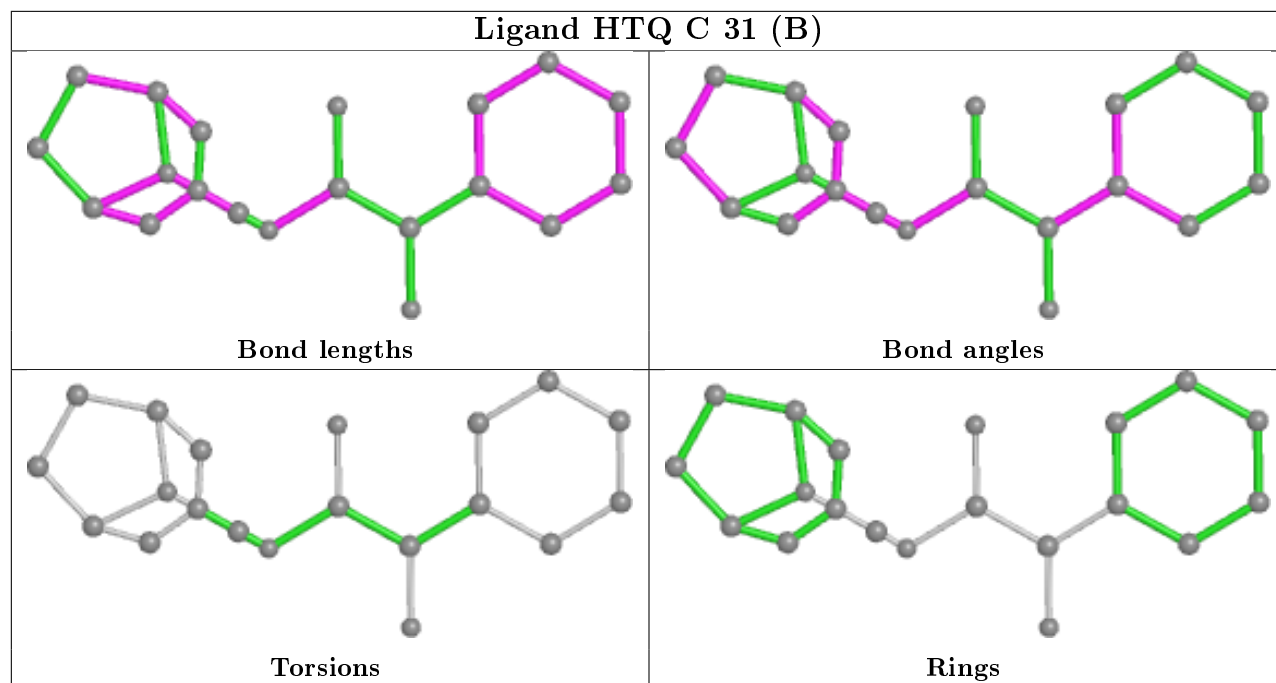
9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	382	SIA	4	0
2	A	179	NAG	1	0
6	B	112	PLM	2	0
4	C	185	SO4	1	0
2	B	279	NAG	2	0
3	A	182	SIA	5	0
3	B	282	SIA	6	0
7	A	11	HTQ	2	0
2	C	379	NAG	1	0

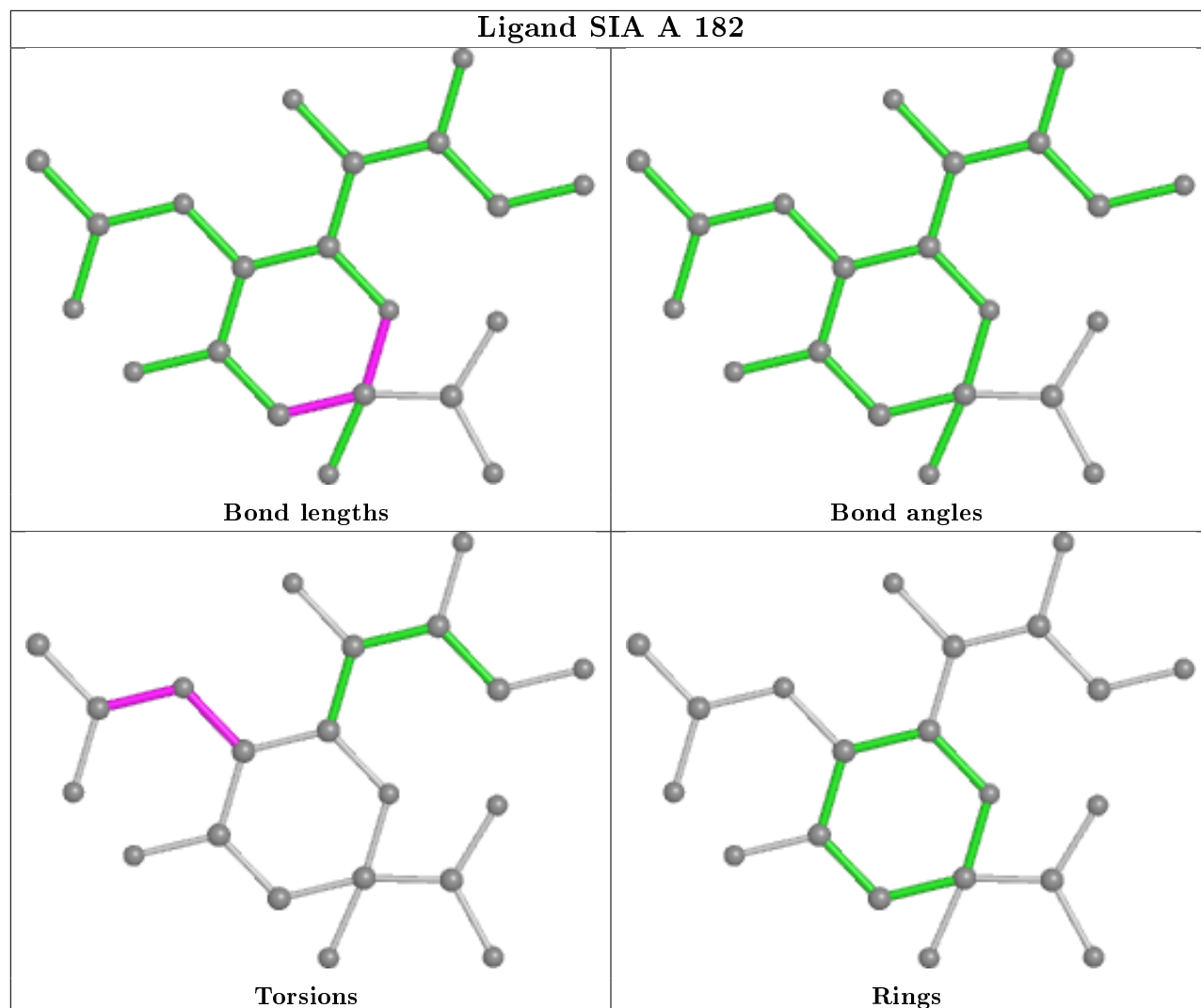
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

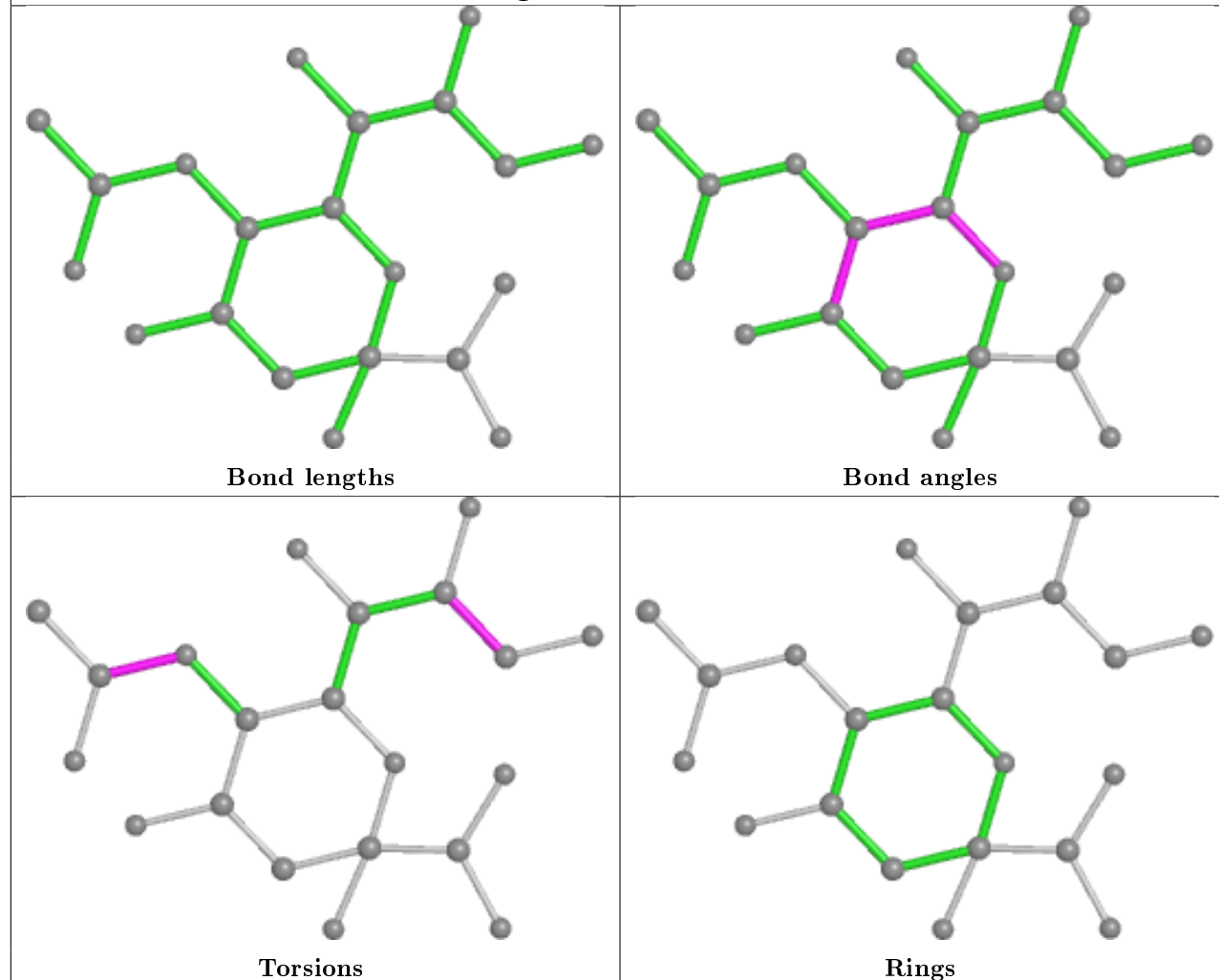




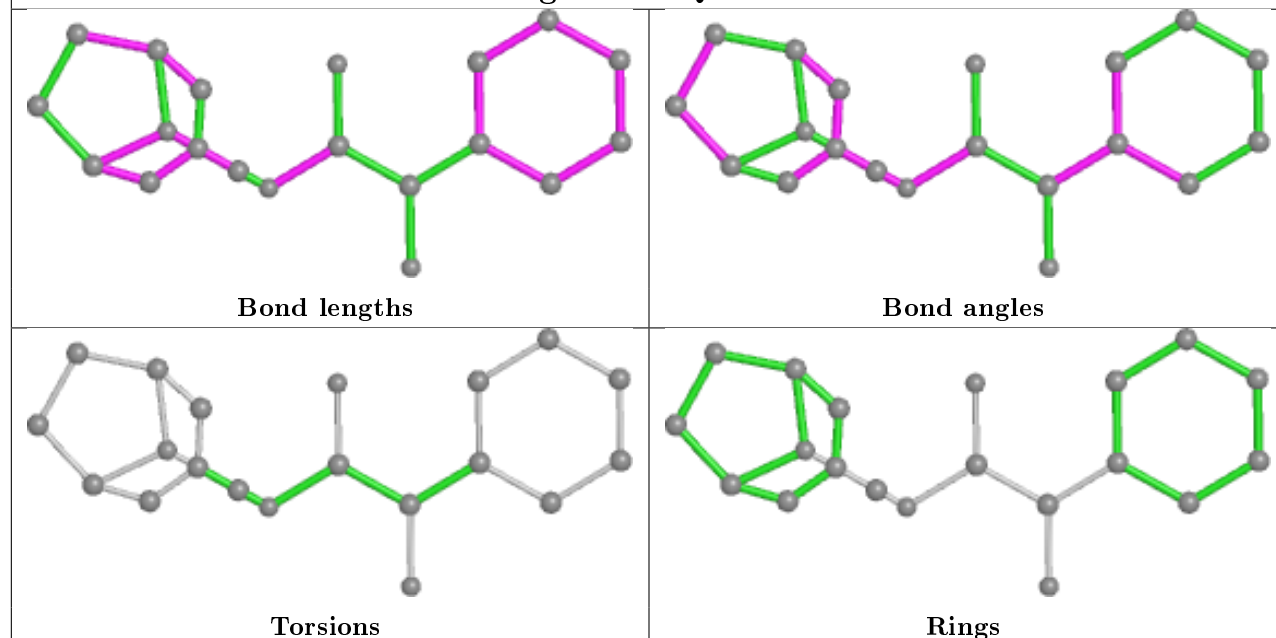
Ligand SIA A 182

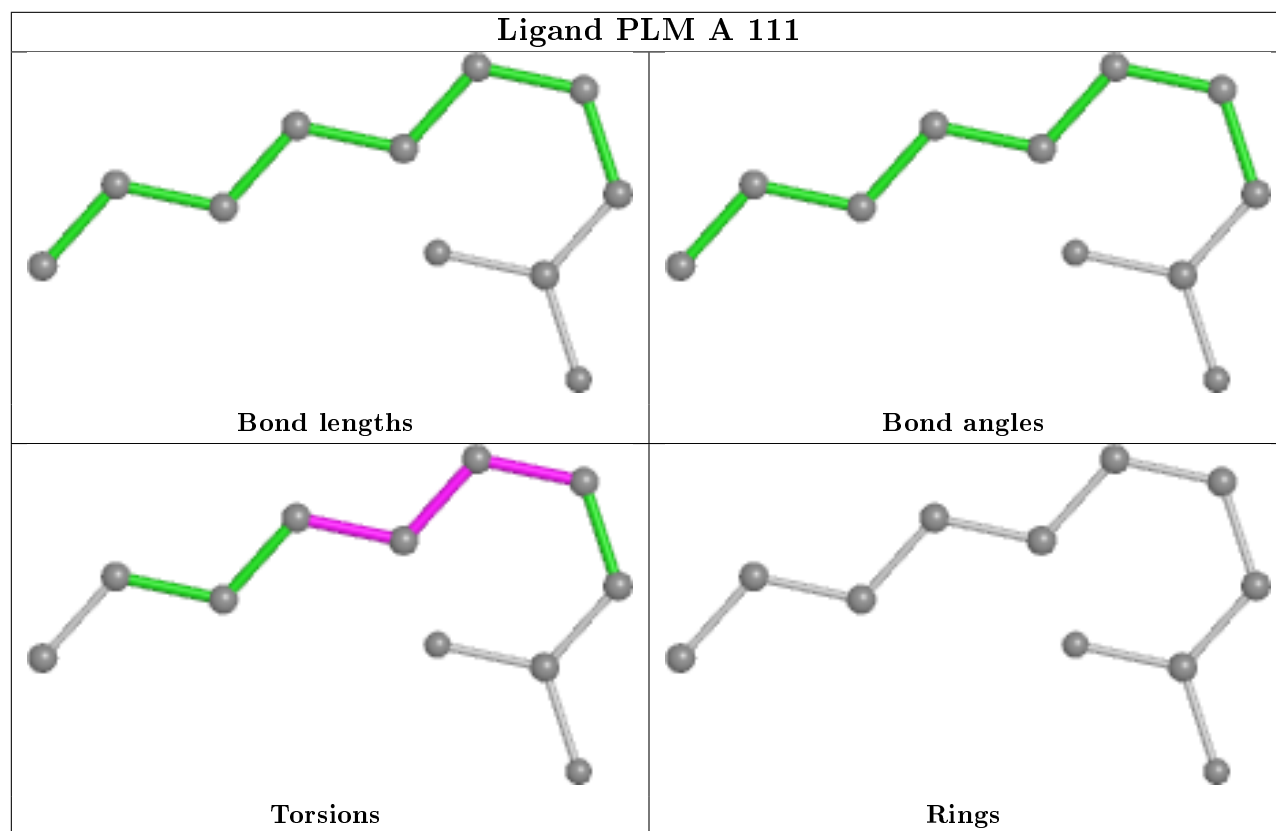
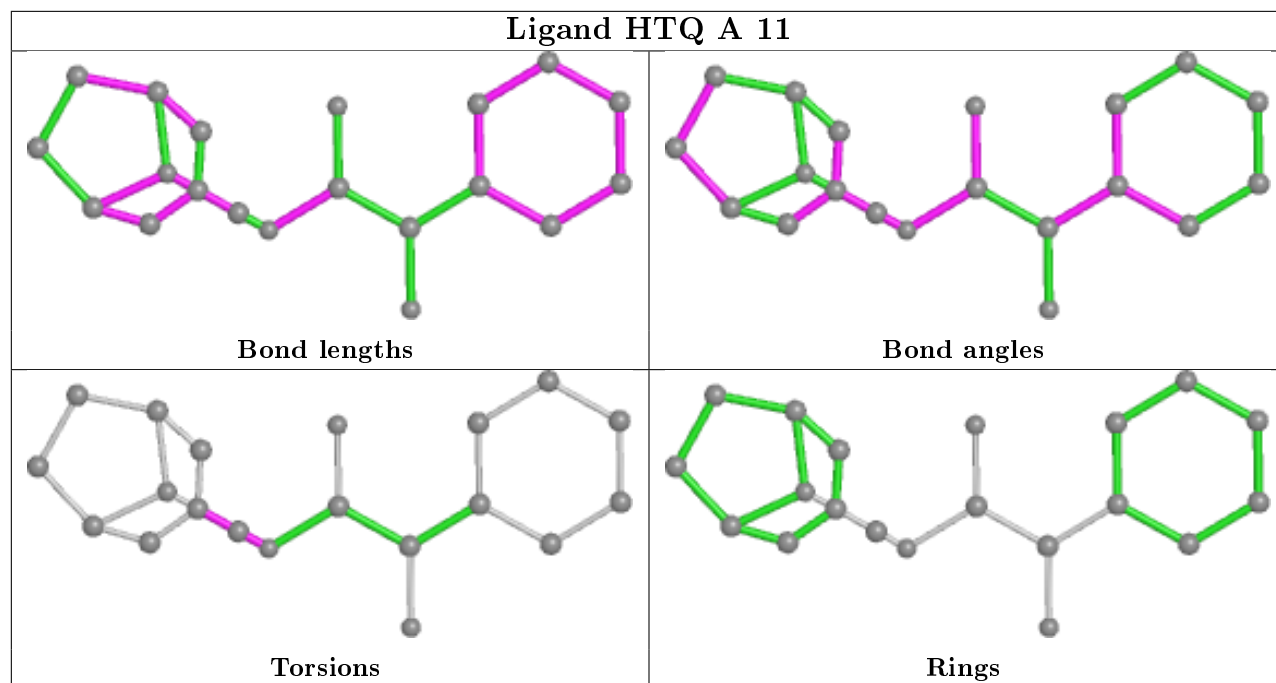


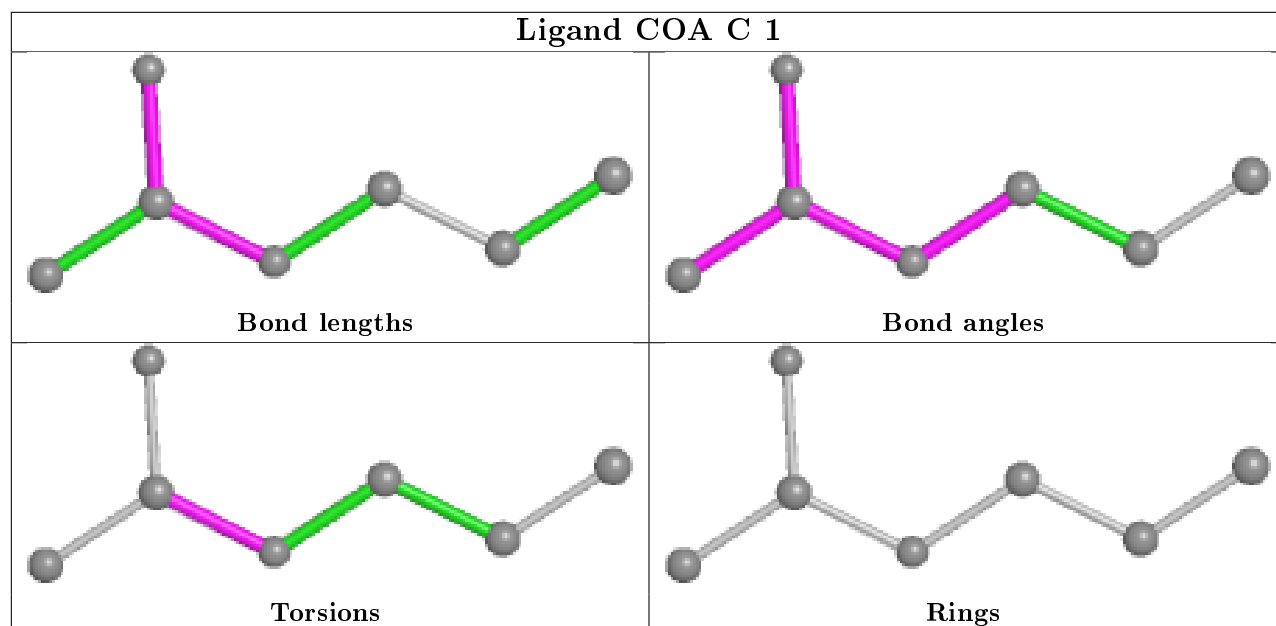
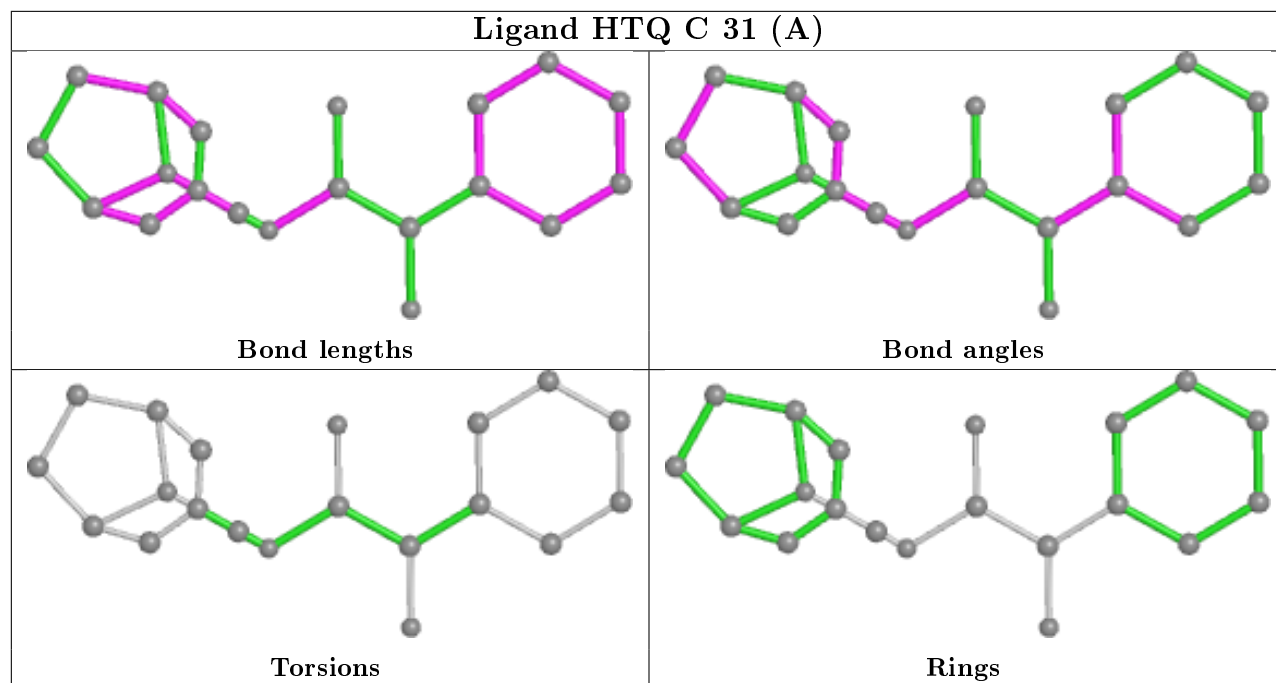
Ligand SIA B 282

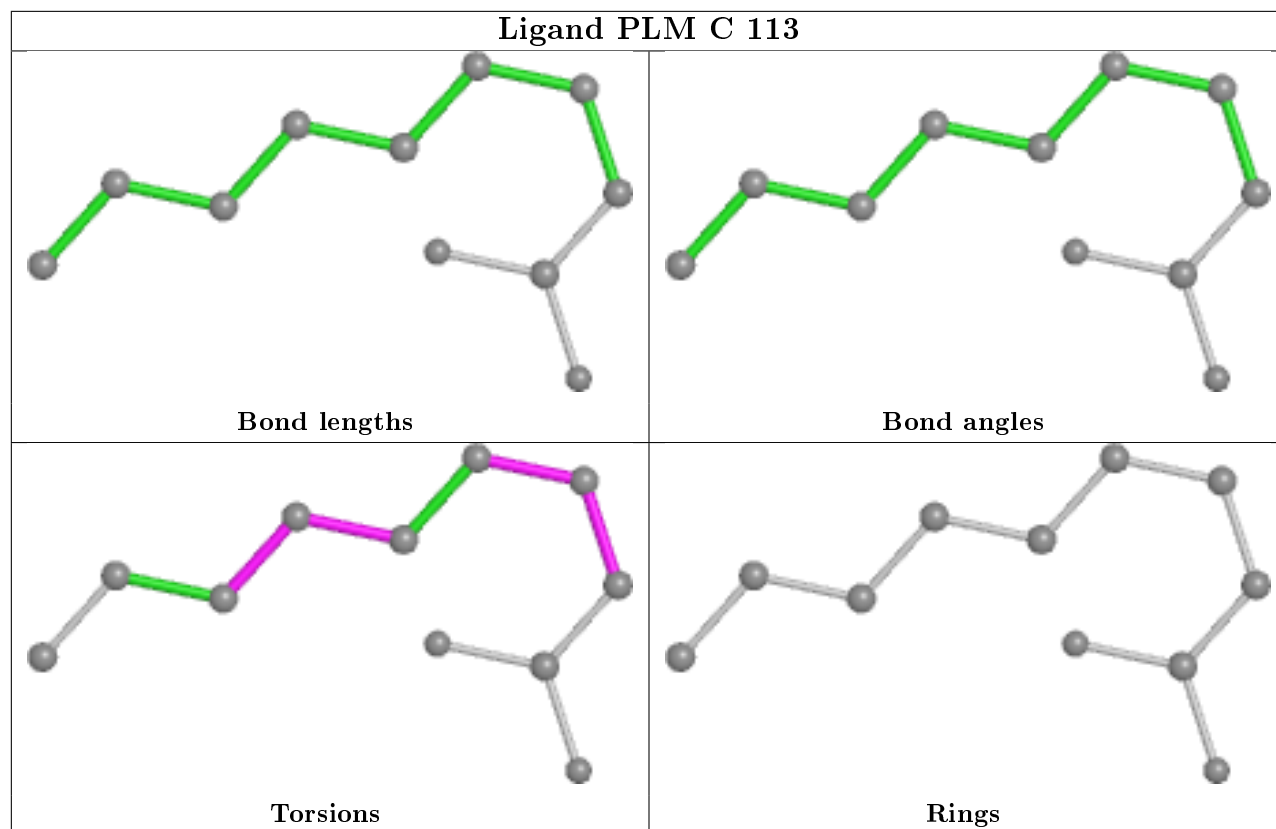


Ligand HTQ B 21









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.