



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:53 PM UTC

PDB ID : 4I9N / pdb_00004i9n
Title : Crystal structure of rabbit LDHA in complex with AP28161 and AP28122
Authors : Zhou, T.; Kohlmann, A.; Stephan, Z.G.; Li, F.; Commodore, L.; Greenfield, M.T.; Shakespeare, W.C.; Zhu, X.; Dalgarno, D.C.
Deposited on : 2012-12-05
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

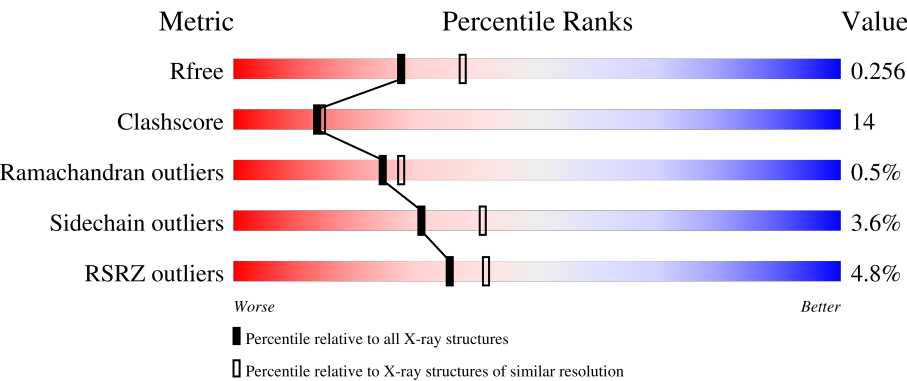
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	331	3% 73% 23% ..
1	B	331	4% 67% 29% ..
1	C	331	5% 74% 23% ..
1	D	331	3% 68% 31% .
1	E	331	8% 68% 30% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	331	5% 73% 24% ..
1	G	331	6% 68% 30% ..
1	H	331	4% 69% 26% ..

2 Entry composition

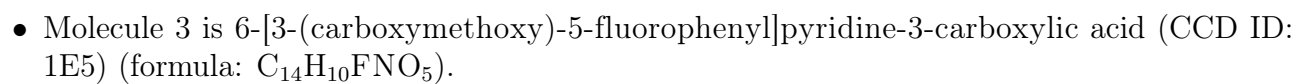
There are 4 unique types of molecules in this entry. The entry contains 20952 atoms, of which 0 are hydrogens and 0 are deuteriums.

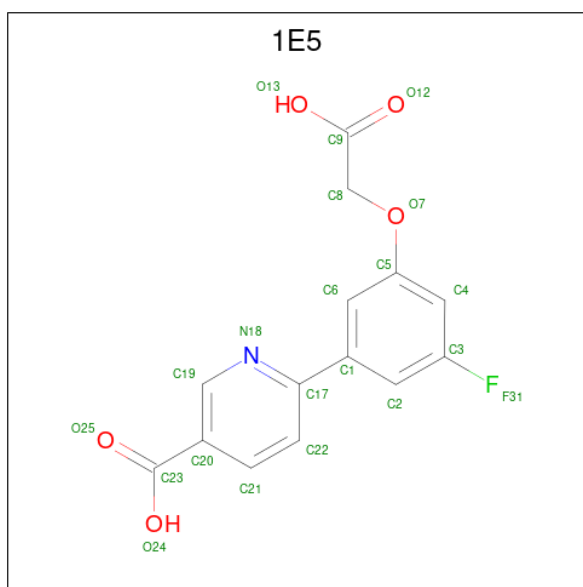
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2502	1602	429	457	14			
1	B	324	Total	C	N	O	S	0	0	0
			2502	1602	429	457	14			
1	C	328	Total	C	N	O	S	0	0	0
			2532	1618	436	464	14			
1	D	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	E	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	F	329	Total	C	N	O	S	0	0	0
			2540	1622	437	467	14			
1	G	328	Total	C	N	O	S	0	0	0
			2537	1621	437	465	14			
1	H	325	Total	C	N	O	S	0	0	0
			2508	1605	430	459	14			

- Molecule 2 is 6-({2-[(5-chloro-4-{[(2S)-2,3-dihydroxypropyl]oxy})-2-methoxyphenyl]amino}-2-oxoethyl)sulfanyl)pyridine-3-carboxylic acid (CCD ID: 1E6) (formula: C₁₈H₁₉ClN₂O₇S).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			21	14	1	1	5		
3	B	1	Total	C	F	N	O	0	0
			21	14	1	1	5		
3	C	1	Total	C	F	N	O	0	0
			21	14	1	1	5		
3	D	1	Total	C	F	N	O	0	0
			21	14	1	1	5		
3	E	1	Total	C	F	N	O	0	0
			21	14	1	1	5		
3	F	1	Total	C	F	N	O	0	0
			21	14	1	1	5		
3	G	1	Total	C	F	N	O	0	0
			21	14	1	1	5		
3	H	1	Total	C	F	N	O	0	0
			21	14	1	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	41	Total	O	0	0
			41	41		
4	C	36	Total	O	0	0
			36	36		
4	D	43	Total	O	0	0
			43	43		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	26	Total 26	O 26	0	0
4	F	32	Total 32	O 32	0	0
4	G	42	Total 42	O 42	0	0
4	H	39	Total 39	O 39	0	0

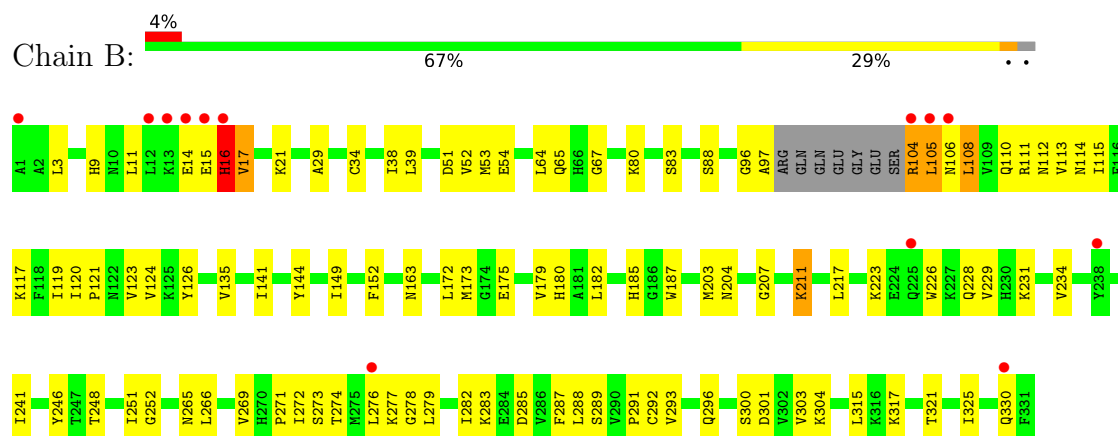
3 Residue-property plots

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

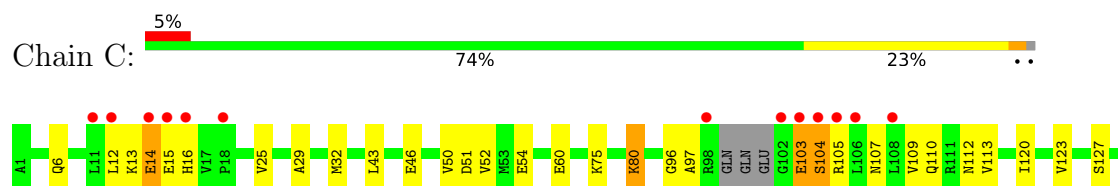
- Molecule 1: L-lactate dehydrogenase A chain

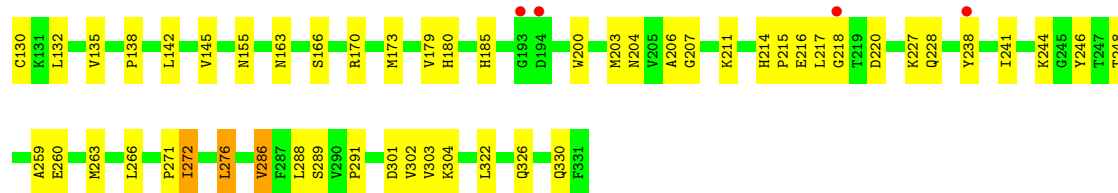


- Molecule 1: L-lactate dehydrogenase A chain

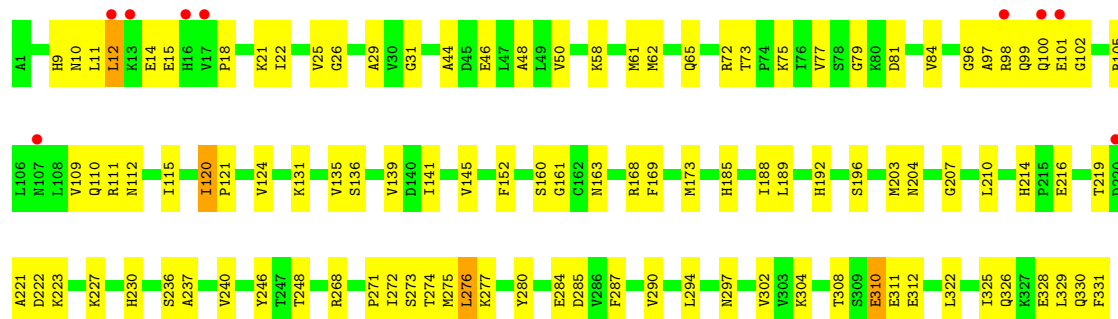


- Molecule 1: L-lactate dehydrogenase A chain

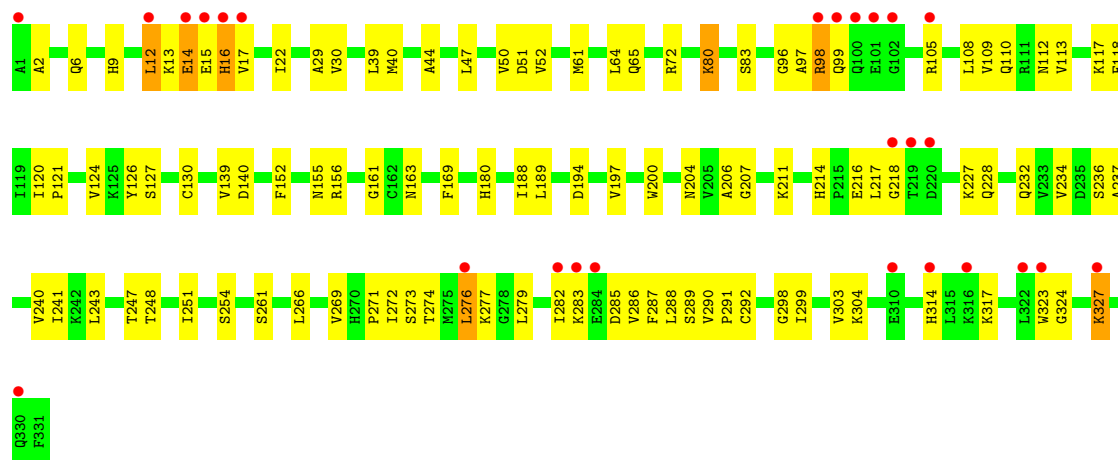




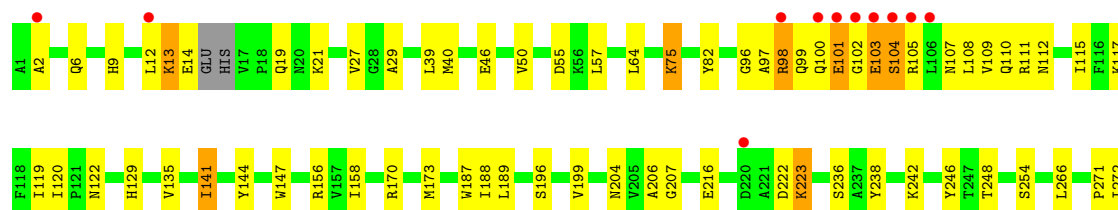
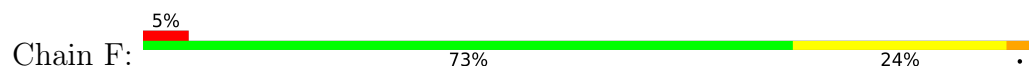
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain

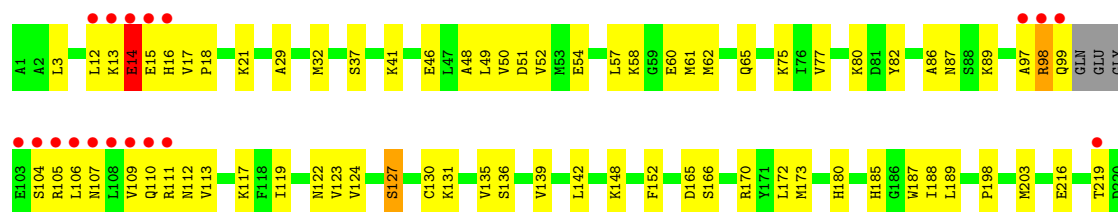


• Molecule 1: L-lactate dehydrogenase A chain

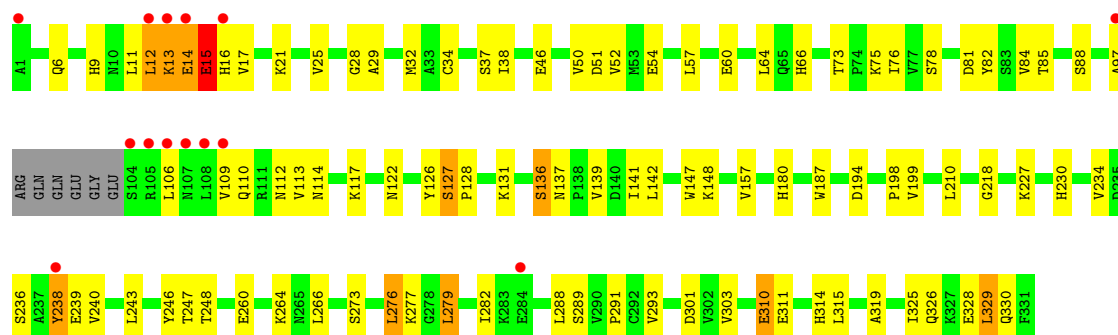




- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.04Å 139.81Å 138.93Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 50.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-2.35) 94.7 (50.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.264 0.213 , 0.256	Depositor DCC
R_{free} test set	7246 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20952	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1E5, 1E6

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	0.44	0/2547	0.80	4/3445 (0.1%)
1	B	0.45	0/2547	0.82	4/3445 (0.1%)
1	C	0.42	0/2577	0.77	0/3484
1	D	0.42	0/2605	0.77	3/3523 (0.1%)
1	E	0.39	0/2605	0.75	2/3523 (0.1%)
1	F	0.41	0/2584	0.78	1/3493 (0.0%)
1	G	0.41	0/2582	0.79	2/3491 (0.1%)
1	H	0.44	0/2553	0.80	6/3453 (0.2%)
All	All	0.42	0/20600	0.78	22/27857 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	H	0	1
All	All	0	3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ASN	N-CA-C	-8.28	102.49	112.59
1	G	127	SER	CA-C-N	7.65	127.36	119.56
1	G	127	SER	C-N-CA	7.65	127.36	119.56
1	A	197	VAL	N-CA-C	6.42	114.47	107.60
1	E	127	SER	CA-C-N	5.94	125.81	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	127	SER	C-N-CA	5.94	125.81	119.28
1	D	120	ILE	CB-CA-C	-5.82	108.18	114.35
1	H	199	VAL	N-CA-C	5.82	112.44	106.21
1	H	54	GLU	N-CA-C	5.75	117.54	111.28
1	A	135	VAL	N-CA-C	-5.68	107.73	113.47
1	B	108	LEU	N-CA-C	-5.64	105.90	112.89
1	F	120	ILE	CB-CA-C	-5.60	108.42	114.35
1	H	127	SER	CA-C-N	5.50	125.33	119.28
1	H	127	SER	C-N-CA	5.50	125.33	119.28
1	H	73	THR	CA-C-N	5.46	125.55	119.87
1	H	73	THR	C-N-CA	5.46	125.55	119.87
1	D	73	THR	CA-C-N	5.31	124.92	119.56
1	D	73	THR	C-N-CA	5.31	124.92	119.56
1	B	17	VAL	CA-C-N	5.29	125.05	119.76
1	B	17	VAL	C-N-CA	5.29	125.05	119.76
1	A	127	SER	CA-C-N	5.16	125.45	119.47
1	A	127	SER	C-N-CA	5.16	125.45	119.47

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ASN	Peptide
1	B	16	HIS	Peptide
1	H	15	GLU	Peptide

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	2502	0	2589	63	0
1	B	2502	0	2589	78	0
1	C	2532	0	2616	66	0
1	D	2559	0	2639	93	0
1	E	2559	0	2639	91	0
1	F	2540	0	2625	87	0
1	G	2537	0	2621	85	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2508	0	2594	95	0
2	A	29	0	18	0	0
2	B	29	0	18	0	0
2	C	29	0	18	0	0
2	D	29	0	18	0	0
2	E	29	0	18	1	0
2	F	29	0	18	0	0
2	G	29	0	18	0	0
2	H	29	0	18	0	0
3	A	21	0	8	1	0
3	B	21	0	9	1	0
3	C	21	0	8	1	0
3	D	21	0	8	1	0
3	E	21	0	8	1	0
3	F	21	0	8	1	0
3	G	21	0	9	1	0
3	H	21	0	9	1	0
4	A	54	0	0	1	0
4	B	41	0	0	0	0
4	C	36	0	0	0	0
4	D	43	0	0	2	0
4	E	26	0	0	0	0
4	F	32	0	0	0	0
4	G	42	0	0	0	0
4	H	39	0	0	3	0
All	All	20952	0	21123	604	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 14.

All (604) 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:304:LYS:HD2	1:D:9:HIS:HB2	1.45	0.95
1:D:97:ALA:H	1:D:112:ASN:HD21	1.11	0.94
1:F:276:LEU:HD21	1:F:288:LEU:HD12	1.48	0.94
1:H:110:GLN:HE22	1:H:330:GLN:H	1.10	0.93
1:E:98:ARG:H	1:E:98:ARG:HE	0.94	0.91
1:A:97:ALA:H	1:A:112:ASN:HD21	1.18	0.91
1:D:110:GLN:HE22	1:D:330:GLN:H	1.18	0.90
1:E:29:ALA:HB1	1:E:248:THR:HG21	1.54	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:LEU:HD21	1:E:288:LEU:HD12	1.55	0.88
1:G:29:ALA:HB1	1:G:248:THR:CG2	2.04	0.87
1:D:97:ALA:H	1:D:112:ASN:ND2	1.72	0.87
1:C:104:SER:HB3	1:C:107:ASN:HD22	1.39	0.86
1:F:104:SER:HA	1:F:107:ASN:HB2	1.57	0.86
1:H:97:ALA:H	1:H:112:ASN:HD21	1.24	0.85
1:E:29:ALA:HB1	1:E:248:THR:CG2	2.08	0.83
1:E:98:ARG:HE	1:E:98:ARG:N	1.74	0.82
1:B:29:ALA:HB1	1:B:248:THR:CG2	2.10	0.81
1:D:29:ALA:HB1	1:D:248:THR:CG2	2.11	0.80
1:A:109:VAL:O	1:A:113:VAL:HG23	1.81	0.80
1:E:163:ASN:HA	1:E:271:PRO:HG2	1.64	0.79
1:G:14:GLU:O	1:G:15:GLU:HG3	1.84	0.78
1:A:29:ALA:HB1	1:A:248:THR:CG2	2.14	0.78
1:G:219:THR:HG23	1:G:221:ALA:H	1.47	0.78
1:C:103:GLU:O	1:C:104:SER:HB3	1.82	0.77
1:B:97:ALA:H	1:B:112:ASN:HD21	1.30	0.77
1:G:219:THR:HG23	1:G:221:ALA:N	1.98	0.77
1:C:29:ALA:HB1	1:C:248:THR:CG2	2.14	0.77
1:E:13:LYS:O	1:E:14:GLU:HB2	1.83	0.77
1:D:97:ALA:N	1:D:112:ASN:HD21	1.83	0.77
1:B:97:ALA:H	1:B:112:ASN:ND2	1.84	0.76
1:D:101:GLU:H	1:D:102:GLY:HA3	1.50	0.76
1:H:85:THR:HG22	4:H:501:HOH:O	1.86	0.75
1:H:29:ALA:HB1	1:H:248:THR:CG2	2.17	0.75
1:F:29:ALA:HB1	1:F:248:THR:CG2	2.16	0.75
1:H:291:PRO:HB2	1:H:303:VAL:HB	1.70	0.74
1:F:277:LYS:HD3	1:F:285:ASP:OD2	1.87	0.74
1:H:29:ALA:HB1	1:H:248:THR:HG21	1.67	0.73
1:E:98:ARG:H	1:E:98:ARG:NE	1.79	0.73
1:D:330:GLN:HG2	1:F:99:GLN:NE2	2.04	0.72
1:C:110:GLN:HE22	1:C:330:GLN:H	1.37	0.72
1:H:110:GLN:NE2	1:H:330:GLN:H	1.85	0.72
1:H:282:ILE:HD13	1:H:319:ALA:HB2	1.71	0.72
1:A:297:ASN:OD1	1:B:14:GLU:HG2	1.90	0.71
1:D:100:GLN:HB3	1:D:101:GLU:CD	2.16	0.71
1:F:96:GLY:HA2	1:F:112:ASN:ND2	2.06	0.71
1:F:189:LEU:HD22	1:F:290:VAL:HA	1.72	0.70
1:B:228:GLN:HE22	1:B:231:LYS:HD3	1.56	0.70
1:D:101:GLU:OE1	1:D:102:GLY:HA3	1.91	0.70
1:G:61:MET:O	1:G:65:GLN:HG3	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:ASN:HD22	1:F:207:GLY:H	1.39	0.69
1:D:98:ARG:HE	1:D:99:GLN:H	1.40	0.69
1:E:97:ALA:H	1:E:112:ASN:HD21	1.40	0.68
1:F:291:PRO:HB2	1:F:303:VAL:HB	1.76	0.68
1:C:97:ALA:H	1:C:112:ASN:ND2	1.92	0.68
1:D:135:VAL:HG12	3:D:402:1E5:H1	1.75	0.68
1:G:98:ARG:HD3	1:G:98:ARG:H	1.59	0.68
1:G:300:SER:HA	1:H:12:LEU:HB2	1.76	0.68
1:G:29:ALA:HB1	1:G:248:THR:HG21	1.73	0.68
1:E:236:SER:O	1:E:240:VAL:HG23	1.94	0.67
1:C:97:ALA:H	1:C:112:ASN:HD21	1.43	0.67
1:G:13:LYS:HE2	1:G:14:GLU:OE1	1.93	0.67
1:B:14:GLU:HG3	1:B:15:GLU:H	1.58	0.67
1:D:277:LYS:HB2	1:D:284:GLU:O	1.95	0.67
1:A:97:ALA:H	1:A:112:ASN:ND2	1.91	0.67
1:A:3:LEU:HD13	1:C:214:HIS:HB2	1.77	0.66
1:F:96:GLY:HA2	1:F:112:ASN:HD21	1.60	0.66
1:D:204:ASN:HA	1:D:210:LEU:HD13	1.77	0.66
1:E:15:GLU:O	1:E:16:HIS:HB2	1.96	0.66
1:F:13:LYS:HE2	1:F:14:GLU:HG3	1.77	0.66
1:E:277:LYS:HD3	1:E:285:ASP:OD2	1.96	0.65
1:A:187:TRP:CZ3	1:A:271:PRO:HD3	2.32	0.65
1:C:276:LEU:HD21	1:C:288:LEU:HB2	1.77	0.65
1:G:302:VAL:HG13	1:H:11:LEU:HD11	1.77	0.65
1:A:204:ASN:HA	1:A:210:LEU:HD13	1.77	0.65
1:E:228:GLN:O	1:E:232:GLN:HG3	1.97	0.65
1:A:283:LYS:H	1:A:316:LYS:HZ1	1.44	0.65
1:H:276:LEU:CD1	1:H:282:ILE:HD12	2.27	0.65
1:E:206:ALA:HA	1:H:187:TRP:CZ2	2.32	0.65
1:G:304:LYS:HD2	1:H:9:HIS:HB2	1.79	0.65
1:H:198:PRO:HG3	1:H:230:HIS:CG	2.33	0.64
1:H:236:SER:O	1:H:240:VAL:HG23	1.97	0.64
1:E:22:ILE:O	1:E:47:LEU:HD12	1.97	0.64
1:B:317:LYS:O	1:B:321:THR:HG23	1.96	0.64
1:B:29:ALA:HB1	1:B:248:THR:HG21	1.80	0.64
1:A:117:LYS:HE2	1:A:149:ILE:HD13	1.80	0.64
1:F:238:TYR:CZ	1:F:242:LYS:HD2	2.33	0.64
1:E:324:GLY:HA2	1:E:327:LYS:HE3	1.78	0.63
1:F:277:LYS:HB2	1:F:284:GLU:O	1.99	0.63
1:E:97:ALA:H	1:E:112:ASN:ND2	1.97	0.62
1:D:81:ASP:O	1:D:84:VAL:HG22	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:GLU:O	1:D:219:THR:HG22	1.98	0.62
1:H:82:TYR:O	1:H:85:THR:HB	1.99	0.62
1:A:304:LYS:HD2	1:B:9:HIS:HB2	1.81	0.62
1:F:55:ASP:O	1:H:243:LEU:HB3	2.00	0.62
1:A:204:ASN:HA	1:A:210:LEU:CD1	2.31	0.61
1:H:198:PRO:HD3	1:H:230:HIS:CE1	2.35	0.61
1:F:82:TYR:OH	1:F:119:ILE:HG23	2.00	0.61
1:F:141:ILE:CD1	1:F:322:LEU:HD22	2.30	0.61
1:F:103:GLU:O	1:F:104:SER:CB	2.49	0.61
1:B:265:ASN:OD1	1:B:296:GLN:HG2	2.01	0.61
1:D:29:ALA:HB1	1:D:248:THR:HG21	1.83	0.60
1:G:29:ALA:HB1	1:G:248:THR:HG22	1.82	0.60
1:B:97:ALA:N	1:B:112:ASN:HD21	2.00	0.60
1:D:236:SER:O	1:D:240:VAL:HG23	2.02	0.60
1:E:261:SER:HA	1:E:266:LEU:HD12	1.83	0.59
1:D:25:VAL:HG22	1:D:50:VAL:CG2	2.32	0.59
1:A:246:TYR:CD2	1:A:248:THR:HG23	2.37	0.59
1:B:14:GLU:HG3	1:B:15:GLU:N	2.17	0.59
1:G:109:VAL:O	1:G:113:VAL:HG23	2.02	0.59
1:B:119:ILE:O	1:B:123:VAL:HG23	2.02	0.59
1:F:98:ARG:HH11	1:F:111:ARG:HH21	1.51	0.58
1:A:50:VAL:HG11	1:A:82:TYR:CZ	2.37	0.58
1:G:302:VAL:HG13	1:H:11:LEU:CD1	2.33	0.58
1:H:25:VAL:HG22	1:H:50:VAL:CG2	2.33	0.58
1:E:292:CYS:HB3	1:E:299:ILE:HG23	1.84	0.58
1:H:81:ASP:O	1:H:84:VAL:HG22	2.03	0.58
1:C:204:ASN:HD22	1:C:207:GLY:H	1.51	0.58
1:G:246:TYR:CD2	1:G:248:THR:HG23	2.38	0.58
1:G:98:ARG:HD3	1:G:98:ARG:N	2.17	0.58
1:B:277:LYS:HD2	1:B:285:ASP:OD2	2.03	0.58
1:E:9:HIS:HB2	1:F:304:LYS:HD3	1.85	0.58
1:E:204:ASN:HD22	1:E:207:GLY:H	1.51	0.58
1:G:50:VAL:HG11	1:G:82:TYR:CZ	2.39	0.58
1:C:43:LEU:HD21	1:C:260:GLU:HG3	1.86	0.58
1:H:97:ALA:H	1:H:112:ASN:ND2	1.98	0.58
1:D:101:GLU:N	1:D:102:GLY:HA3	2.12	0.57
1:E:40:MET:HE1	1:G:37:SER:HA	1.86	0.57
1:E:61:MET:O	1:E:65:GLN:HG3	2.04	0.57
1:B:248:THR:O	1:B:251:ILE:HG22	2.04	0.57
1:F:2:ALA:O	1:F:6:GLN:HG3	2.04	0.57
1:F:325:ILE:O	1:F:329:LEU:HD13	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:VAL:HG12	3:B:402:1E5:H1	1.87	0.57
1:C:103:GLU:O	1:C:104:SER:CB	2.52	0.57
1:F:135:VAL:HG12	3:F:402:1E5:H1	1.85	0.57
1:A:259:ALA:O	1:A:263:MET:HG2	2.04	0.57
1:B:223:LYS:CD	1:B:223:LYS:H	2.17	0.57
1:C:110:GLN:NE2	1:C:330:GLN:H	2.01	0.57
1:D:275:MET:HE1	1:D:277:LYS:HB3	1.85	0.57
1:H:246:TYR:CD2	1:H:248:THR:HG23	2.39	0.57
1:B:111:ARG:O	1:B:115:ILE:HG13	2.05	0.57
1:F:223:LYS:HD3	1:F:223:LYS:H	1.68	0.56
1:H:276:LEU:HD21	1:H:288:LEU:HD12	1.86	0.56
1:E:17:VAL:HG23	1:E:17:VAL:O	2.06	0.56
1:F:223:LYS:HD3	1:F:223:LYS:N	2.19	0.56
1:B:104:ARG:C	1:B:105:LEU:HD23	2.30	0.56
1:D:196:SER:OG	1:D:230:HIS:HE1	1.87	0.56
1:G:17:VAL:O	1:G:17:VAL:HG23	2.06	0.56
1:H:218:GLY:O	1:H:227:LYS:HD2	2.05	0.56
1:G:82:TYR:CG	1:G:122:ASN:HB3	2.40	0.56
1:G:104:SER:OG	1:G:106:LEU:HB3	2.05	0.56
1:C:204:ASN:ND2	1:C:207:GLY:H	2.03	0.56
1:E:269:VAL:HA	1:E:292:CYS:O	2.05	0.56
1:E:13:LYS:O	1:E:14:GLU:CB	2.52	0.56
1:H:97:ALA:N	1:H:112:ASN:HD21	2.00	0.56
1:H:106:LEU:HD11	1:H:328:GLU:HB2	1.87	0.56
1:B:15:GLU:HB3	1:B:16:HIS:HD2	1.71	0.56
1:E:276:LEU:H	1:E:276:LEU:HD12	1.71	0.56
1:F:236:SER:HB3	1:H:66:HIS:HE1	1.71	0.56
1:G:104:SER:C	1:G:106:LEU:H	2.14	0.56
1:F:170:ARG:HA	1:F:173:MET:HE3	1.86	0.56
1:E:323:TRP:O	1:E:327:LYS:HG3	2.04	0.55
1:F:104:SER:O	1:F:105:ARG:HB3	2.07	0.55
1:F:316:LYS:HE2	1:F:316:LYS:HA	1.87	0.55
1:D:219:THR:HG23	1:D:222:ASP:H	1.72	0.55
1:E:276:LEU:HD22	1:E:282:ILE:HG13	1.87	0.55
1:F:158:ILE:HD12	1:F:158:ILE:N	2.21	0.55
1:H:276:LEU:HD21	1:H:288:LEU:HB2	1.89	0.55
1:H:310:GLU:O	1:H:314:HIS:HB2	2.06	0.55
1:G:32:MET:HE2	1:G:60:GLU:HB3	1.89	0.55
1:G:97:ALA:H	1:G:112:ASN:ND2	2.05	0.55
1:H:260:GLU:HG3	1:H:264:LYS:HD2	1.88	0.55
1:H:14:GLU:C	1:H:15:GLU:HG2	2.31	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:VAL:HG23	1:H:17:VAL:O	2.07	0.55
1:E:237:ALA:O	1:E:241:ILE:HG13	2.07	0.55
1:A:120:ILE:HB	1:A:121:PRO:HD3	1.89	0.54
1:H:141:ILE:HD13	1:H:325:ILE:HG21	1.88	0.54
1:G:166:SER:O	1:G:170:ARG:HG3	2.08	0.54
1:F:105:ARG:O	1:F:109:VAL:HG23	2.07	0.54
1:H:246:TYR:HD2	1:H:248:THR:HG23	1.73	0.54
1:E:105:ARG:O	1:E:109:VAL:HG23	2.08	0.54
1:E:155:ASN:ND2	1:F:12:LEU:HD11	2.23	0.54
1:F:236:SER:HB3	1:H:66:HIS:CE1	2.43	0.54
1:H:131:LYS:HD3	1:H:131:LYS:N	2.22	0.54
1:H:51:ASP:OD1	1:H:52:VAL:N	2.41	0.54
1:D:101:GLU:HB2	1:D:102:GLY:CA	2.37	0.54
1:D:310:GLU:HG3	1:D:311:GLU:N	2.18	0.53
1:H:326:GLN:HA	1:H:329:LEU:HD22	1.89	0.53
1:E:276:LEU:HD11	1:E:286:VAL:HG23	1.90	0.53
1:A:117:LYS:HE2	1:A:117:LYS:HA	1.91	0.53
1:F:29:ALA:HB1	1:F:248:THR:HG21	1.89	0.53
1:F:96:GLY:CA	1:F:112:ASN:HD21	2.21	0.53
1:G:127:SER:HB3	1:G:130:CYS:HB3	1.91	0.53
1:D:15:GLU:HG3	1:D:15:GLU:O	2.08	0.53
1:B:223:LYS:H	1:B:223:LYS:HD2	1.73	0.53
1:G:98:ARG:NH2	1:G:98:ARG:HB2	2.23	0.53
1:E:39:LEU:HD11	1:E:64:LEU:HD13	1.91	0.53
1:E:80:LYS:NZ	1:E:80:LYS:HB3	2.24	0.53
1:F:46:GLU:OE1	1:F:75:LYS:HG2	2.08	0.53
1:F:50:VAL:HG11	1:F:82:TYR:CZ	2.44	0.53
1:G:272:ILE:O	1:G:289:SER:HA	2.09	0.53
1:C:272:ILE:O	1:C:289:SER:HA	2.08	0.53
1:G:279:LEU:HD11	1:H:11:LEU:HD21	1.91	0.53
1:F:189:LEU:HD12	1:F:199:VAL:HG21	1.91	0.53
1:F:204:ASN:ND2	1:F:207:GLY:H	2.07	0.53
1:H:114:ASN:HA	1:H:117:LYS:HD3	1.90	0.53
1:A:288:LEU:HD13	1:A:315:LEU:CD1	2.39	0.52
1:A:218:GLY:O	1:A:227:LYS:HE3	2.09	0.52
1:B:272:ILE:O	1:B:289:SER:HA	2.09	0.52
1:E:130:CYS:O	1:E:156:ARG:HD2	2.09	0.52
1:F:223:LYS:H	1:F:223:LYS:CD	2.22	0.52
1:B:29:ALA:C	1:B:248:THR:HG22	2.33	0.52
1:F:100:GLN:O	1:F:101:GLU:O	2.28	0.52
1:F:108:LEU:HD13	1:F:108:LEU:C	2.34	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:GLY:O	1:E:227:LYS:HD2	2.09	0.52
1:H:276:LEU:CD2	1:H:288:LEU:HB2	2.40	0.52
1:E:214:HIS:HB2	1:G:3:LEU:HD13	1.91	0.52
1:G:216:GLU:O	1:G:219:THR:HG22	2.09	0.52
1:B:83:SER:HA	1:B:126:TYR:CD2	2.45	0.52
1:D:61:MET:O	1:D:65:GLN:HG3	2.09	0.52
1:E:274:THR:O	1:E:287:PHE:HA	2.10	0.52
1:G:246:TYR:HD2	1:G:248:THR:HG23	1.74	0.52
1:A:297:ASN:CG	1:B:14:GLU:HG2	2.35	0.52
1:G:41:LYS:HD3	1:G:256:ALA:HB1	1.91	0.52
1:G:124:VAL:HG22	1:G:152:PHE:CZ	2.45	0.52
1:G:110:GLN:OE1	1:G:329:LEU:HA	2.10	0.52
1:F:97:ALA:H	1:F:112:ASN:ND2	2.09	0.51
1:D:46:GLU:OE1	1:D:75:LYS:HD3	2.11	0.51
1:F:97:ALA:H	1:F:112:ASN:HD21	1.57	0.51
1:F:187:TRP:CZ3	1:F:271:PRO:HD3	2.45	0.51
1:C:14:GLU:HB2	1:C:16:HIS:ND1	2.25	0.51
1:D:246:TYR:CD2	1:D:248:THR:HG23	2.46	0.51
1:G:32:MET:HE2	1:G:60:GLU:OE1	2.10	0.51
1:F:103:GLU:O	1:F:104:SER:HB2	2.10	0.51
1:B:39:LEU:HD11	1:B:64:LEU:HD13	1.92	0.51
1:F:273:SER:OG	1:F:287:PHE:HB3	2.11	0.51
1:H:276:LEU:HD11	1:H:282:ILE:HD12	1.92	0.51
1:C:97:ALA:N	1:C:112:ASN:HD21	2.07	0.51
1:E:211:LYS:HD2	1:E:217:LEU:HB3	1.92	0.51
1:A:110:GLN:OE1	1:A:329:LEU:HA	2.11	0.51
1:A:225:GLN:HB3	1:A:228:GLN:HG2	1.93	0.51
1:B:21:LYS:HB3	1:B:88:SER:HA	1.92	0.51
1:C:51:ASP:OD1	1:C:52:VAL:N	2.42	0.51
1:F:104:SER:CA	1:F:107:ASN:HB2	2.36	0.51
1:D:219:THR:HG22	1:D:222:ASP:HB2	1.92	0.50
1:E:51:ASP:OD1	1:E:52:VAL:N	2.37	0.50
1:A:277:LYS:HD3	1:A:285:ASP:OD2	2.12	0.50
1:G:321:THR:O	1:G:325:ILE:HD12	2.11	0.50
1:D:216:GLU:O	1:D:222:ASP:HB2	2.11	0.50
1:D:246:TYR:CE2	1:D:248:THR:HG23	2.46	0.50
1:H:32:MET:HE2	1:H:60:GLU:HB3	1.91	0.50
1:A:28:GLY:HA3	3:A:402:1E5:O12	2.10	0.50
1:D:98:ARG:NE	1:D:99:GLN:H	2.08	0.50
1:F:39:LEU:CD1	1:F:64:LEU:HD22	2.42	0.50
1:D:169:PHE:O	1:D:173:MET:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:LEU:HD13	1:F:108:LEU:O	2.11	0.50
1:G:16:HIS:NE2	1:G:75:LYS:HD2	2.26	0.50
1:E:243:LEU:HD13	1:G:58:LYS:HG2	1.93	0.50
1:C:123:VAL:HG11	1:C:132:LEU:HD21	1.94	0.50
1:D:100:GLN:HB3	1:D:101:GLU:OE2	2.12	0.50
1:A:58:LYS:O	1:A:62:MET:HG3	2.12	0.50
1:E:109:VAL:O	1:E:113:VAL:HG23	2.12	0.49
1:F:141:ILE:HD11	1:F:322:LEU:HD22	1.93	0.49
1:H:110:GLN:HE22	1:H:330:GLN:N	1.93	0.49
1:H:46:GLU:OE1	1:H:75:LYS:HD3	2.12	0.49
1:D:96:GLY:HA2	1:D:112:ASN:ND2	2.28	0.49
1:F:115:ILE:O	1:F:119:ILE:HG13	2.13	0.49
1:B:51:ASP:OD1	1:B:52:VAL:N	2.45	0.49
1:B:204:ASN:ND2	1:B:207:GLY:H	2.10	0.49
1:C:29:ALA:HB1	1:C:248:THR:HG21	1.93	0.49
1:H:194:ASP:HA	1:H:234:VAL:HG11	1.94	0.49
1:E:98:ARG:O	1:E:98:ARG:HG2	2.13	0.49
1:D:219:THR:HG23	1:D:222:ASP:N	2.28	0.49
1:C:276:LEU:CD2	1:C:288:LEU:HB2	2.42	0.49
1:G:189:LEU:HD22	1:G:290:VAL:HA	1.93	0.49
1:E:272:ILE:O	1:E:289:SER:HA	2.13	0.49
1:G:32:MET:CE	1:G:60:GLU:HB3	2.43	0.49
1:G:54:GLU:CD	1:G:80:LYS:HD3	2.37	0.49
1:A:282:ILE:HD13	1:A:319:ALA:HB2	1.94	0.48
1:B:266:LEU:O	1:C:180:HIS:HB2	2.12	0.48
1:B:278:GLY:C	1:B:279:LEU:HD22	2.38	0.48
1:D:120:ILE:HB	1:D:121:PRO:HD3	1.95	0.48
1:E:22:ILE:HD12	1:E:44:ALA:HB2	1.94	0.48
1:F:40:MET:HE1	1:H:37:SER:HA	1.95	0.48
1:G:18:PRO:HB2	1:G:21:LYS:HB2	1.95	0.48
1:G:97:ALA:H	1:G:112:ASN:HD21	1.60	0.48
1:H:34:CYS:O	1:H:38:ILE:HG13	2.12	0.48
1:B:17:VAL:O	1:B:17:VAL:HG13	2.12	0.48
1:B:187:TRP:CZ2	1:C:206:ALA:HA	2.48	0.48
1:E:96:GLY:HA2	1:E:112:ASN:HD21	1.79	0.48
1:F:98:ARG:NH1	1:F:111:ARG:HH21	2.11	0.48
1:F:276:LEU:CD2	1:F:288:LEU:HB2	2.43	0.48
1:G:302:VAL:CG1	1:H:11:LEU:HD11	2.42	0.48
1:A:17:VAL:HG13	1:A:17:VAL:O	2.13	0.48
1:E:96:GLY:HA2	1:E:112:ASN:ND2	2.28	0.48
1:G:98:ARG:HB2	1:G:98:ARG:CZ	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:LEU:HB3	1:H:76:ILE:HD13	1.95	0.48
1:A:6:GLN:O	1:B:304:LYS:HE3	2.13	0.48
1:B:117:LYS:HA	1:B:149:ILE:HD13	1.94	0.48
1:C:200:TRP:CH2	1:C:227:LYS:HA	2.48	0.48
1:A:328:GLU:O	1:A:329:LEU:O	2.30	0.48
1:E:12:LEU:HD22	1:E:13:LYS:O	2.14	0.48
1:E:15:GLU:O	1:E:16:HIS:CB	2.61	0.48
1:G:104:SER:C	1:G:106:LEU:N	2.72	0.48
1:B:97:ALA:HB1	1:B:111:ARG:NH1	2.28	0.48
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.95	0.48
1:F:223:LYS:N	1:F:223:LYS:CD	2.77	0.48
1:D:141:ILE:HG13	1:D:322:LEU:HD22	1.96	0.48
1:F:100:GLN:O	1:F:101:GLU:C	2.56	0.48
1:F:102:GLY:HA2	1:F:103:GLU:O	2.12	0.48
1:F:216:GLU:O	1:F:222:ASP:HB2	2.14	0.48
1:B:114:ASN:HA	1:B:117:LYS:HD3	1.94	0.48
1:C:185:HIS:O	1:C:203:MET:HA	2.14	0.48
1:E:189:LEU:HD22	1:E:290:VAL:HA	1.95	0.48
1:H:109:VAL:O	1:H:113:VAL:HG23	2.13	0.48
1:B:211:LYS:O	1:B:211:LYS:HG3	2.14	0.48
1:A:110:GLN:O	1:A:113:VAL:HB	2.14	0.47
4:A:521:HOH:O	1:B:11:LEU:HD13	2.14	0.47
1:C:291:PRO:HB2	1:C:303:VAL:HB	1.96	0.47
1:C:163:ASN:HA	1:C:271:PRO:HG2	1.96	0.47
1:D:26:GLY:O	1:D:31:GLY:HA3	2.14	0.47
1:A:127:SER:HB3	1:A:130:CYS:HB3	1.97	0.47
1:E:194:ASP:HA	1:E:234:VAL:HG11	1.96	0.47
1:D:163:ASN:HA	1:D:271:PRO:HG2	1.96	0.47
1:H:194:ASP:HA	1:H:234:VAL:CG1	2.44	0.47
1:C:25:VAL:HG22	1:C:50:VAL:CG2	2.45	0.47
1:C:322:LEU:O	1:C:326:GLN:HG3	2.14	0.47
1:F:276:LEU:CD1	1:F:276:LEU:C	2.88	0.47
1:E:273:SER:OG	1:E:287:PHE:HB3	2.14	0.47
1:G:185:HIS:O	1:G:203:MET:HA	2.14	0.47
1:A:117:LYS:HE2	1:A:149:ILE:CD1	2.45	0.47
1:C:216:GLU:OE2	1:C:216:GLU:HA	2.15	0.47
1:D:22:ILE:HD12	1:D:44:ALA:HB2	1.95	0.47
1:D:131:LYS:HE2	1:D:131:LYS:HB2	1.77	0.47
1:D:189:LEU:HD22	1:D:290:VAL:HA	1.95	0.47
1:D:192:HIS:HE1	4:D:519:HOH:O	1.98	0.47
1:E:200:TRP:CH2	1:E:227:LYS:HA	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:SER:HB2	1:H:142:LEU:CD1	2.44	0.47
1:H:137:ASN:HA	1:H:139:VAL:N	2.29	0.47
1:B:228:GLN:NE2	1:B:231:LYS:HD3	2.28	0.47
1:G:106:LEU:CD1	1:G:328:GLU:HB3	2.45	0.47
1:E:169:PHE:HB2	1:E:188:ILE:HD11	1.97	0.46
1:F:238:TYR:CE2	1:F:242:LYS:HD2	2.51	0.46
1:B:120:ILE:HB	1:B:121:PRO:HD3	1.97	0.46
1:C:155:ASN:ND2	1:D:12:LEU:HD11	2.29	0.46
1:H:238:TYR:CE2	1:H:239:GLU:OE2	2.69	0.46
1:C:96:GLY:HA2	1:C:112:ASN:ND2	2.29	0.46
1:C:173:MET:HE3	1:C:173:MET:HB2	1.68	0.46
1:E:155:ASN:HD22	1:F:12:LEU:HD11	1.78	0.46
1:H:136:SER:HB2	1:H:142:LEU:HD12	1.98	0.46
1:B:34:CYS:O	1:B:38:ILE:HG13	2.14	0.46
1:G:280:TYR:O	1:G:282:ILE:HD12	2.15	0.46
1:G:304:LYS:HE2	1:H:6:GLN:O	2.15	0.46
1:A:276:LEU:HD12	1:A:276:LEU:H	1.80	0.46
1:G:51:ASP:OD1	1:G:52:VAL:N	2.45	0.46
1:A:117:LYS:HA	1:A:117:LYS:CE	2.45	0.46
1:B:96:GLY:HA2	1:B:112:ASN:ND2	2.31	0.46
1:B:241:ILE:HG12	1:B:246:TYR:HA	1.97	0.46
1:E:304:LYS:HE3	1:F:6:GLN:O	2.15	0.46
1:F:276:LEU:HD21	1:F:288:LEU:CD1	2.32	0.46
1:A:29:ALA:HB1	1:A:248:THR:HG22	1.93	0.46
1:E:206:ALA:HA	1:H:187:TRP:CE2	2.50	0.46
1:D:22:ILE:CD1	1:D:44:ALA:HB2	2.46	0.46
1:D:48:ALA:HA	1:D:77:VAL:O	2.16	0.46
1:C:244:LYS:HG3	1:C:246:TYR:O	2.16	0.46
1:D:145:VAL:HG22	1:D:331:PHE:CZ	2.51	0.46
1:E:97:ALA:N	1:E:112:ASN:HD21	2.12	0.46
1:F:21:LYS:HD2	1:F:46:GLU:OE2	2.16	0.46
1:D:112:ASN:HD22	1:D:115:ILE:HD12	1.81	0.46
1:G:98:ARG:NH2	1:G:98:ARG:C	2.74	0.46
1:G:142:LEU:HA	1:G:142:LEU:HD23	1.69	0.46
1:A:282:ILE:CD1	1:A:288:LEU:HD12	2.45	0.45
1:D:185:HIS:O	1:D:203:MET:HA	2.16	0.45
1:F:117:LYS:HB3	1:F:117:LYS:HE2	1.83	0.45
1:D:58:LYS:O	1:D:62:MET:HG3	2.16	0.45
1:E:16:HIS:HD2	1:F:296:GLN:NE2	2.15	0.45
1:B:144:TYR:HA	1:B:287:PHE:CE2	2.52	0.45
1:E:6:GLN:O	1:F:304:LYS:HE2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LYS:HD3	1:C:217:LEU:HB3	1.96	0.45
1:D:275:MET:HG2	1:D:287:PHE:CE2	2.51	0.45
1:E:180:HIS:HB2	1:H:266:LEU:O	2.17	0.45
1:A:155:ASN:O	1:A:298:GLY:HA3	2.16	0.45
1:C:241:ILE:HG12	1:C:246:TYR:HA	1.97	0.45
1:D:275:MET:SD	1:D:277:LYS:HB3	2.56	0.45
1:H:12:LEU:HD22	1:H:13:LYS:N	2.32	0.45
1:H:293:VAL:HB	1:H:301:ASP:HB2	1.97	0.45
1:C:246:TYR:CD2	1:C:248:THR:HG23	2.52	0.45
1:C:260:GLU:OE2	1:D:72:ARG:NH1	2.49	0.45
1:G:98:ARG:C	1:G:98:ARG:HH21	2.24	0.45
1:G:251:ILE:O	1:G:255:VAL:HG23	2.17	0.45
1:B:265:ASN:CG	1:B:296:GLN:HG2	2.42	0.45
1:D:168:ARG:HD3	1:D:236:SER:OG	2.17	0.45
1:F:129:HIS:HA	1:F:156:ARG:NH1	2.32	0.45
1:G:18:PRO:HB3	1:G:46:GLU:OE1	2.17	0.45
1:H:310:GLU:HG3	1:H:311:GLU:N	2.32	0.45
1:A:292:CYS:HB3	1:A:299:ILE:HG23	1.98	0.45
1:E:279:LEU:HD21	1:F:9:HIS:ND1	2.32	0.45
1:G:98:ARG:NH1	1:G:99:GLN:NE2	2.65	0.45
1:G:216:GLU:OE1	1:G:216:GLU:HA	2.17	0.45
1:A:279:LEU:CD1	1:A:302:VAL:HG21	2.47	0.45
1:E:266:LEU:O	1:H:180:HIS:HB2	2.17	0.45
1:B:185:HIS:O	1:B:203:MET:HA	2.16	0.44
1:B:187:TRP:CE2	1:C:206:ALA:HA	2.52	0.44
1:E:117:LYS:O	1:E:121:PRO:HG2	2.17	0.44
1:E:276:LEU:HD12	1:E:276:LEU:N	2.31	0.44
1:D:97:ALA:HB1	1:D:111:ARG:CZ	2.48	0.44
1:H:276:LEU:O	1:H:277:LYS:C	2.59	0.44
1:A:173:MET:HE2	1:A:203:MET:HE3	1.98	0.44
1:B:173:MET:HE2	1:B:203:MET:HE3	2.00	0.44
1:B:223:LYS:HD2	1:B:223:LYS:N	2.33	0.44
1:B:246:TYR:CD2	1:B:248:THR:HG23	2.52	0.44
1:C:259:ALA:O	1:C:263:MET:HG2	2.18	0.44
1:G:117:LYS:HE2	1:G:117:LYS:HB3	1.88	0.44
1:G:259:ALA:O	1:G:263:MET:HG2	2.17	0.44
1:H:240:VAL:HB	1:H:247:THR:HG22	1.99	0.44
1:A:130:CYS:O	1:A:156:ARG:NH1	2.51	0.44
1:D:105:ARG:O	1:D:109:VAL:HG23	2.18	0.44
1:D:237:ALA:HB3	4:D:525:HOH:O	2.17	0.44
1:H:136:SER:O	1:H:139:VAL:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:GLU:CG	1:H:264:LYS:HD2	2.48	0.44
1:A:291:PRO:HB2	1:A:303:VAL:HB	2.00	0.44
1:C:113:VAL:HG22	1:C:145:VAL:HG21	1.99	0.44
1:D:50:VAL:HG12	1:D:79:GLY:O	2.16	0.44
1:E:30:VAL:HG21	3:E:402:1E5:C1	2.47	0.44
1:F:98:ARG:HG2	1:F:98:ARG:O	2.16	0.44
1:G:135:VAL:HG12	3:G:402:1E5:H1	2.00	0.44
1:G:172:LEU:HD23	1:G:172:LEU:HA	1.76	0.44
1:H:325:ILE:O	1:H:329:LEU:HD13	2.18	0.44
1:C:246:TYR:CE2	1:C:248:THR:HG23	2.53	0.44
1:G:49:LEU:O	1:G:57:LEU:HD11	2.17	0.44
1:H:282:ILE:CD1	1:H:288:LEU:HD12	2.48	0.44
1:C:14:GLU:HG3	1:C:14:GLU:O	2.18	0.44
1:D:328:GLU:OE1	1:D:328:GLU:HA	2.18	0.44
1:E:248:THR:O	1:E:251:ILE:HG22	2.18	0.44
1:G:82:TYR:OH	1:G:119:ILE:HG23	2.17	0.44
1:H:28:GLY:HA3	3:H:402:1E5:O12	2.18	0.44
1:B:187:TRP:CZ3	1:B:271:PRO:HD3	2.53	0.44
1:B:211:LYS:HE3	1:B:217:LEU:HB3	2.00	0.44
1:C:46:GLU:OE1	1:C:75:LYS:HD3	2.17	0.44
1:D:276:LEU:CD1	1:D:276:LEU:C	2.91	0.44
1:G:105:ARG:HG2	1:G:105:ARG:O	2.16	0.44
1:G:165:ASP:O	1:G:188:ILE:HD12	2.18	0.44
1:G:241:ILE:HG12	1:G:246:TYR:HA	1.99	0.44
1:D:173:MET:HE2	1:D:203:MET:HE3	1.99	0.44
1:D:274:THR:O	1:D:287:PHE:HA	2.18	0.44
1:G:86:ALA:O	1:G:87:ASN:HB2	2.18	0.44
1:C:301:ASP:OD2	1:D:10:ASN:HA	2.17	0.43
1:H:273:SER:HA	1:H:289:SER:HA	1.99	0.43
1:D:330:GLN:HG2	1:F:99:GLN:HE22	1.79	0.43
1:E:276:LEU:CD1	1:E:276:LEU:C	2.92	0.43
1:H:82:TYR:CG	1:H:122:ASN:HB3	2.53	0.43
1:A:108:LEU:O	1:A:111:ARG:N	2.49	0.43
1:B:124:VAL:HG12	1:B:152:PHE:CZ	2.53	0.43
1:A:83:SER:HA	1:A:126:TYR:CD2	2.53	0.43
1:A:288:LEU:HD13	1:A:315:LEU:HD13	2.00	0.43
1:B:163:ASN:HA	1:B:271:PRO:HG2	2.00	0.43
1:H:9:HIS:HD2	1:H:11:LEU:HD23	1.84	0.43
1:B:141:ILE:HD13	1:B:325:ILE:HG21	2.00	0.43
1:B:293:VAL:HB	1:B:301:ASP:HB2	1.99	0.43
1:E:155:ASN:O	1:E:298:GLY:HA3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD22	1:A:290:VAL:HA	1.99	0.43
1:E:291:PRO:HB2	1:E:303:VAL:HB	2.00	0.43
1:H:12:LEU:O	1:H:13:LYS:HB3	2.18	0.43
1:A:246:TYR:HD2	1:A:248:THR:HG23	1.79	0.43
1:B:29:ALA:O	1:B:248:THR:HG22	2.19	0.43
1:C:286:VAL:HG13	1:C:322:LEU:HD23	2.01	0.43
1:D:325:ILE:O	1:D:329:LEU:HG	2.19	0.43
1:A:274:THR:HB	1:A:299:ILE:HD13	2.01	0.43
1:B:3:LEU:HD13	1:D:214:HIS:HB2	2.00	0.43
1:G:110:GLN:NE2	1:G:330:GLN:O	2.49	0.43
1:H:25:VAL:HG22	1:H:50:VAL:HG21	2.00	0.43
1:H:32:MET:CE	1:H:60:GLU:HB3	2.49	0.43
1:H:148:LYS:HD2	1:H:148:LYS:HA	1.86	0.43
1:H:276:LEU:CD1	1:H:282:ILE:HG21	2.49	0.43
1:B:282:ILE:CD1	1:B:288:LEU:HD12	2.49	0.43
1:D:219:THR:HG23	1:D:221:ALA:N	2.34	0.43
1:A:97:ALA:N	1:A:112:ASN:ND2	2.64	0.42
1:C:13:LYS:HD3	1:C:14:GLU:N	2.33	0.42
1:C:54:GLU:CG	1:C:80:LYS:HD3	2.49	0.42
1:D:188:ILE:HG22	1:D:196:SER:HB2	2.00	0.42
1:D:204:ASN:HD22	1:D:207:GLY:H	1.64	0.42
1:H:276:LEU:CD2	1:H:282:ILE:HD12	2.49	0.42
1:A:14:GLU:OE1	1:B:300:SER:HB3	2.20	0.42
1:C:135:VAL:HG12	3:C:402:1E5:H1	2.01	0.42
1:E:139:VAL:HG21	1:E:161:GLY:H	1.83	0.42
1:E:276:LEU:CD2	1:E:288:LEU:HB2	2.49	0.42
1:G:107:ASN:O	1:G:111:ARG:HG3	2.18	0.42
1:A:282:ILE:HA	1:A:316:LYS:NZ	2.34	0.42
1:B:274:THR:O	1:B:287:PHE:HA	2.19	0.42
1:C:13:LYS:HD3	1:C:14:GLU:O	2.19	0.42
1:H:13:LYS:N	4:H:503:HOH:O	2.52	0.42
1:B:223:LYS:CD	1:B:223:LYS:N	2.83	0.42
1:C:12:LEU:HD21	1:D:297:ASN:HB3	2.01	0.42
1:D:18:PRO:HB2	1:D:21:LYS:HB2	2.01	0.42
1:F:276:LEU:C	1:F:276:LEU:HD12	2.44	0.42
1:C:96:GLY:HA2	1:C:112:ASN:HD22	1.85	0.42
1:D:276:LEU:HD12	1:D:276:LEU:H	1.84	0.42
1:E:99:GLN:HA	1:E:108:LEU:HD13	2.02	0.42
1:F:144:TYR:O	1:F:147:TRP:HB3	2.19	0.42
1:H:276:LEU:HD13	1:H:282:ILE:HD12	2.00	0.42
1:B:269:VAL:HA	1:B:292:CYS:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:SER:O	1:D:161:GLY:C	2.63	0.42
1:E:9:HIS:CD2	1:F:279:LEU:HD11	2.55	0.42
1:F:13:LYS:O	1:F:14:GLU:HB2	2.18	0.42
1:B:172:LEU:O	1:B:175:GLU:HB2	2.20	0.42
1:A:302:VAL:HG13	1:B:11:LEU:HD12	2.02	0.42
1:C:218:GLY:O	1:C:227:LYS:HD2	2.20	0.42
1:D:280:TYR:CE1	1:D:290:VAL:HG11	2.54	0.42
1:G:62:MET:HE2	1:G:62:MET:HB3	1.90	0.42
1:H:57:LEU:HG	1:H:78:SER:HB2	2.02	0.42
1:H:106:LEU:HD11	1:H:328:GLU:CB	2.50	0.42
1:A:273:SER:OG	1:A:287:PHE:HB3	2.20	0.42
1:D:112:ASN:HA	1:D:115:ILE:HD12	2.02	0.42
1:G:13:LYS:HD3	1:G:14:GLU:O	2.20	0.42
1:G:89:LYS:O	1:G:131:LYS:HE2	2.19	0.42
1:G:136:SER:O	1:G:139:VAL:HA	2.20	0.42
1:H:46:GLU:OE1	1:H:75:LYS:CD	2.67	0.42
1:A:86:ALA:O	1:A:87:ASN:HB2	2.20	0.41
1:B:65:GLN:C	1:B:67:GLY:N	2.77	0.41
1:D:276:LEU:C	1:D:276:LEU:HD13	2.45	0.41
1:A:68:SER:O	1:A:69:LEU:C	2.63	0.41
1:C:43:LEU:HD22	1:C:260:GLU:HA	2.00	0.41
1:F:266:LEU:O	1:G:180:HIS:HB2	2.20	0.41
1:C:166:SER:O	1:C:170:ARG:HG3	2.20	0.41
1:D:46:GLU:CD	1:D:75:LYS:HD3	2.44	0.41
1:E:276:LEU:CD2	1:E:288:LEU:HD12	2.38	0.41
1:H:85:THR:O	1:H:85:THR:CG2	2.67	0.41
1:H:147:TRP:HB2	1:H:157:VAL:HG11	2.01	0.41
1:H:279:LEU:HD13	1:H:279:LEU:HA	1.73	0.41
1:A:54:GLU:CD	1:A:80:LYS:HD3	2.45	0.41
1:C:138:PRO:O	1:C:142:LEU:HG	2.19	0.41
1:E:117:LYS:HB3	1:E:117:LYS:HE3	1.88	0.41
1:F:13:LYS:O	1:F:13:LYS:HG3	2.16	0.41
1:A:182:LEU:HD13	1:D:268:ARG:HD3	2.02	0.41
1:B:204:ASN:HD22	1:B:207:GLY:H	1.69	0.41
1:D:216:GLU:HB3	1:D:222:ASP:HA	2.02	0.41
1:E:9:HIS:HB2	1:F:304:LYS:CD	2.48	0.41
1:F:246:TYR:CD2	1:F:248:THR:HG23	2.55	0.41
1:B:180:HIS:HB2	1:C:266:LEU:O	2.20	0.41
1:C:32:MET:HE2	1:C:60:GLU:OE1	2.21	0.41
1:C:127:SER:HB3	1:C:130:CYS:HB3	2.01	0.41
1:C:211:LYS:O	1:C:215:PRO:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:VAL:HG13	1:C:322:LEU:CD2	2.50	0.41
1:F:272:ILE:O	1:F:289:SER:HA	2.20	0.41
1:F:304:LYS:HE2	1:F:304:LYS:HB2	1.84	0.41
1:G:119:ILE:O	1:G:123:VAL:HG23	2.21	0.41
1:G:198:PRO:HD3	1:G:230:HIS:CE1	2.55	0.41
1:H:12:LEU:C	1:H:13:LYS:HG2	2.46	0.41
1:A:136:SER:O	1:A:139:VAL:HA	2.21	0.41
1:D:219:THR:HG23	1:D:221:ALA:H	1.86	0.41
1:D:272:ILE:HD13	1:D:294:LEU:HD22	2.03	0.41
1:E:9:HIS:CG	1:F:279:LEU:HD11	2.55	0.41
1:E:232:GLN:O	1:E:236:SER:HB3	2.20	0.41
1:F:27:VAL:HG11	1:F:57:LEU:HD12	2.03	0.41
1:G:48:ALA:HA	1:G:77:VAL:O	2.21	0.41
1:G:173:MET:HE3	1:G:173:MET:HB2	1.78	0.41
1:H:210:LEU:N	1:H:210:LEU:HD23	2.36	0.41
1:A:82:TYR:CG	1:A:122:ASN:HB3	2.56	0.41
1:D:308:THR:O	1:D:312:GLU:HG3	2.20	0.41
1:E:139:VAL:HG13	1:E:140:ASP:N	2.35	0.41
1:E:279:LEU:HD21	1:F:9:HIS:CG	2.56	0.41
1:H:85:THR:CG2	4:H:501:HOH:O	2.57	0.41
1:A:248:THR:O	1:A:251:ILE:HG22	2.21	0.41
1:A:279:LEU:HD13	1:A:302:VAL:HG21	2.02	0.41
1:B:110:GLN:O	1:B:113:VAL:HB	2.21	0.41
1:B:226:TRP:O	1:B:229:VAL:HB	2.21	0.41
1:C:6:GLN:O	1:D:304:LYS:HE3	2.21	0.41
1:D:124:VAL:HG22	1:D:152:PHE:CZ	2.55	0.41
1:D:273:SER:OG	1:D:287:PHE:HB3	2.21	0.41
1:E:120:ILE:HB	1:E:121:PRO:HD3	2.02	0.41
1:E:188:ILE:HA	1:E:197:VAL:O	2.21	0.41
1:F:82:TYR:CG	1:F:122:ASN:HB3	2.56	0.41
1:F:206:ALA:HA	1:G:187:TRP:CZ2	2.56	0.41
1:G:110:GLN:HE22	1:G:330:GLN:H	1.68	0.41
1:H:9:HIS:CD2	1:H:11:LEU:HD23	2.56	0.41
1:H:21:LYS:HB3	1:H:88:SER:HA	2.03	0.41
1:H:126:TYR:C	1:H:128:PRO:HD3	2.45	0.41
1:A:279:LEU:HD21	1:B:9:HIS:ND1	2.36	0.41
1:B:54:GLU:OE2	1:B:80:LYS:HE2	2.20	0.41
1:C:120:ILE:HD13	1:C:120:ILE:HA	1.91	0.41
1:C:105:ARG:O	1:C:109:VAL:HG23	2.20	0.40
1:C:228:GLN:NE2	1:C:228:GLN:HA	2.35	0.40
1:D:97:ALA:HB1	1:D:111:ARG:NH2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:SER:O	1:D:139:VAL:HA	2.20	0.40
1:D:227:LYS:HE2	1:D:227:LYS:HB3	1.88	0.40
1:E:2:ALA:O	1:E:6:GLN:HG3	2.21	0.40
1:E:124:VAL:HG22	1:E:152:PHE:CZ	2.57	0.40
1:E:204:ASN:ND2	1:E:207:GLY:H	2.17	0.40
1:D:29:ALA:HB1	1:D:248:THR:HG22	1.97	0.40
1:E:194:ASP:HA	1:E:234:VAL:CG1	2.52	0.40
1:C:302:VAL:HG23	1:D:11:LEU:HD11	2.04	0.40
1:E:29:ALA:C	1:E:248:THR:HG22	2.47	0.40
1:G:105:ARG:HD3	1:G:325:ILE:HG12	2.03	0.40
1:B:251:ILE:HG23	1:B:252:GLY:N	2.36	0.40
1:D:25:VAL:HG22	1:D:50:VAL:HG21	2.04	0.40
1:F:188:ILE:HG22	1:F:196:SER:HB2	2.03	0.40
1:G:148:LYS:HD2	1:G:148:LYS:HA	1.77	0.40
1:H:127:SER:N	1:H:128:PRO:HD3	2.36	0.40
1:A:302:VAL:O	1:A:302:VAL:HG23	2.21	0.40
1:B:53:MET:HE2	1:B:53:MET:HB3	1.94	0.40
1:B:65:GLN:C	1:B:67:GLY:H	2.28	0.40
1:B:180:HIS:CE1	1:B:182:LEU:HG	2.57	0.40
1:E:83:SER:HA	1:E:126:TYR:CD2	2.56	0.40
1:E:118:PHE:CD2	2:E:401:1E6:H6	2.56	0.40
1:G:274:THR:HB	1:G:299:ILE:HD13	2.03	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	320/331 (97%)	305 (95%)	12 (4%)	3 (1%)	14	14
1	B	320/331 (97%)	307 (96%)	12 (4%)	1 (0%)	36	43
1	C	324/331 (98%)	310 (96%)	13 (4%)	1 (0%)	36	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	329/331 (99%)	314 (95%)	15 (5%)	0	100	100
1	E	329/331 (99%)	317 (96%)	10 (3%)	2 (1%)	21	24
1	F	325/331 (98%)	311 (96%)	11 (3%)	3 (1%)	14	14
1	G	324/331 (98%)	312 (96%)	11 (3%)	1 (0%)	36	43
1	H	321/331 (97%)	309 (96%)	10 (3%)	2 (1%)	21	24
All	All	2592/2648 (98%)	2485 (96%)	94 (4%)	13 (0%)	24	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	329	LEU
1	E	14	GLU
1	E	16	HIS
1	F	101	GLU
1	F	104	SER
1	H	13	LYS
1	C	104	SER
1	A	108	LEU
1	B	16	HIS
1	F	103	GLU
1	G	14	GLU
1	H	16	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/284 (98%)	269 (97%)	9 (3%)	34	46
1	B	278/284 (98%)	267 (96%)	11 (4%)	28	37
1	C	281/284 (99%)	271 (96%)	10 (4%)	31	41
1	D	284/284 (100%)	276 (97%)	8 (3%)	38	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	284/284 (100%)	270 (95%)	14 (5%)	22	28
1	F	282/284 (99%)	271 (96%)	11 (4%)	28	39
1	G	282/284 (99%)	274 (97%)	8 (3%)	38	51
1	H	279/284 (98%)	269 (96%)	10 (4%)	31	41
All	All	2248/2272 (99%)	2167 (96%)	81 (4%)	31	41

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

Mol	Chain	Res	Type
1	A	107	ASN
1	A	117	LYS
1	A	133	LEU
1	A	211	LYS
1	A	276	LEU
1	A	282	ILE
1	A	310	GLU
1	A	316	LYS
1	A	331	PHE
1	B	104	ARG
1	B	105	LEU
1	B	108	LEU
1	B	179	VAL
1	B	211	LYS
1	B	234	VAL
1	B	273	SER
1	B	276	LEU
1	B	283	LYS
1	B	315	LEU
1	B	330	GLN
1	C	14	GLU
1	C	15	GLU
1	C	80	LYS
1	C	103	GLU
1	C	179	VAL
1	C	220	ASP
1	C	238	TYR
1	C	272	ILE
1	C	276	LEU
1	C	286	VAL
1	D	12	LEU
1	D	14	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	223	LYS
1	D	276	LEU
1	D	285	ASP
1	D	302	VAL
1	D	310	GLU
1	D	326	GLN
1	E	12	LEU
1	E	50	VAL
1	E	72	ARG
1	E	80	LYS
1	E	98	ARG
1	E	110	GLN
1	E	216	GLU
1	E	247	THR
1	E	254	SER
1	E	276	LEU
1	E	283	LYS
1	E	314	HIS
1	E	317	LYS
1	E	327	LYS
1	F	13	LYS
1	F	19	GLN
1	F	75	LYS
1	F	98	ARG
1	F	110	GLN
1	F	141	ILE
1	F	223	LYS
1	F	254	SER
1	F	276	LEU
1	F	283	LYS
1	F	316	LYS
1	G	12	LEU
1	G	14	GLU
1	G	98	ARG
1	G	236	SER
1	G	276	LEU
1	G	314	HIS
1	G	322	LEU
1	G	330	GLN
1	H	12	LEU
1	H	14	GLU
1	H	15	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	136	SER
1	H	238	TYR
1	H	276	LEU
1	H	279	LEU
1	H	310	GLU
1	H	315	LEU
1	H	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	107	ASN
1	A	112	ASN
1	A	122	ASN
1	A	192	HIS
1	A	204	ASN
1	A	228	GLN
1	A	230	HIS
1	A	330	GLN
1	B	10	ASN
1	B	16	HIS
1	B	106	ASN
1	B	112	ASN
1	B	185	HIS
1	B	204	ASN
1	B	228	GLN
1	B	230	HIS
1	B	296	GLN
1	B	297	ASN
1	B	314	HIS
1	C	6	GLN
1	C	20	ASN
1	C	87	ASN
1	C	107	ASN
1	C	110	GLN
1	C	112	ASN
1	C	204	ASN
1	C	230	HIS
1	C	297	ASN
1	C	326	GLN
1	D	20	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	100	GLN
1	D	107	ASN
1	D	110	GLN
1	D	112	ASN
1	D	137	ASN
1	D	192	HIS
1	D	204	ASN
1	D	230	HIS
1	D	297	ASN
1	D	330	GLN
1	E	16	HIS
1	E	20	ASN
1	E	100	GLN
1	E	107	ASN
1	E	112	ASN
1	E	137	ASN
1	E	185	HIS
1	E	204	ASN
1	E	230	HIS
1	E	297	ASN
1	F	6	GLN
1	F	20	ASN
1	F	87	ASN
1	F	99	GLN
1	F	112	ASN
1	F	192	HIS
1	F	204	ASN
1	F	228	GLN
1	F	230	HIS
1	F	232	GLN
1	F	297	ASN
1	F	326	GLN
1	G	6	GLN
1	G	20	ASN
1	G	112	ASN
1	G	129	HIS
1	G	163	ASN
1	G	185	HIS
1	G	192	HIS
1	G	204	ASN
1	G	228	GLN
1	G	297	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	9	HIS
1	H	10	ASN
1	H	20	ASN
1	H	110	GLN
1	H	112	ASN
1	H	114	ASN
1	H	297	ASN
1	H	314	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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	1E5	C	402	-	22,22,22	3.11	12 (54%)	30,30,30	1.46	5 (16%)
3	1E5	E	402	-	22,22,22	3.14	13 (59%)	30,30,30	1.44	6 (20%)
3	1E5	G	402	-	22,22,22	2.75	9 (40%)	30,30,30	1.33	3 (10%)
3	1E5	H	402	-	22,22,22	2.73	10 (45%)	30,30,30	1.39	4 (13%)
2	1E6	H	401	-	30,30,30	3.91	12 (40%)	39,40,40	2.46	8 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1E6	E	401	-	30,30,30	4.13	14 (46%)	39,40,40	2.55	8 (20%)
2	1E6	C	401	-	30,30,30	4.01	11 (36%)	39,40,40	2.42	7 (17%)
2	1E6	D	401	-	30,30,30	4.11	14 (46%)	39,40,40	2.47	9 (23%)
2	1E6	F	401	-	30,30,30	3.97	11 (36%)	39,40,40	2.45	7 (17%)
3	1E5	A	402	-	22,22,22	2.84	9 (40%)	30,30,30	1.33	4 (13%)
3	1E5	B	402	-	22,22,22	2.73	11 (50%)	30,30,30	1.38	4 (13%)
2	1E6	A	401	-	30,30,30	3.89	13 (43%)	39,40,40	2.50	7 (17%)
2	1E6	B	401	-	30,30,30	3.90	11 (36%)	39,40,40	2.51	8 (20%)
3	1E5	F	402	-	22,22,22	3.04	10 (45%)	30,30,30	1.46	7 (23%)
3	1E5	D	402	-	22,22,22	2.96	8 (36%)	30,30,30	1.50	6 (20%)
2	1E6	G	401	-	30,30,30	3.91	13 (43%)	39,40,40	2.40	7 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1E5	C	402	-	-	2/13/13/13	0/2/2/2
3	1E5	E	402	-	-	3/13/13/13	0/2/2/2
3	1E5	G	402	-	-	2/13/13/13	0/2/2/2
3	1E5	H	402	-	-	4/13/13/13	0/2/2/2
2	1E6	H	401	-	-	5/22/22/22	0/2/2/2
2	1E6	E	401	-	-	6/22/22/22	0/2/2/2
2	1E6	C	401	-	-	5/22/22/22	0/2/2/2
2	1E6	D	401	-	-	4/22/22/22	0/2/2/2
2	1E6	F	401	-	-	5/22/22/22	0/2/2/2
3	1E5	A	402	-	-	2/13/13/13	0/2/2/2
3	1E5	B	402	-	-	2/13/13/13	0/2/2/2
2	1E6	A	401	-	-	4/22/22/22	0/2/2/2
2	1E6	B	401	-	-	2/22/22/22	0/2/2/2
3	1E5	F	402	-	-	2/13/13/13	0/2/2/2
3	1E5	D	402	-	-	2/13/13/13	0/2/2/2
2	1E6	G	401	-	-	1/22/22/22	0/2/2/2

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	1E6	C11-C12	15.56	1.69	1.51
2	C	401	1E6	C11-C12	15.27	1.68	1.51
2	D	401	1E6	C11-C12	14.80	1.68	1.51
2	G	401	1E6	C11-C12	14.73	1.68	1.51
2	F	401	1E6	C11-C12	14.66	1.68	1.51
2	A	401	1E6	C11-C12	14.31	1.67	1.51
2	B	401	1E6	C11-C12	14.16	1.67	1.51
2	H	401	1E6	C11-C12	14.13	1.67	1.51
2	H	401	1E6	C11-S10	-11.12	1.55	1.80
2	B	401	1E6	C11-S10	-10.98	1.55	1.80
2	A	401	1E6	C11-S10	-10.92	1.55	1.80
2	C	401	1E6	C11-S10	-10.88	1.55	1.80
2	D	401	1E6	C11-S10	-10.83	1.55	1.80
2	F	401	1E6	C11-S10	-10.82	1.55	1.80
2	G	401	1E6	C11-S10	-10.78	1.55	1.80
2	E	401	1E6	C11-S10	-10.49	1.56	1.80
3	C	402	1E5	O25-C23	7.14	1.43	1.22
3	E	402	1E5	O25-C23	7.03	1.42	1.22
3	A	402	1E5	O25-C23	6.76	1.42	1.22
3	F	402	1E5	O25-C23	6.60	1.41	1.22
2	B	401	1E6	C17-C16	6.52	1.49	1.39
2	A	401	1E6	C17-C16	6.46	1.49	1.39
3	F	402	1E5	C2-C1	6.37	1.50	1.39
3	D	402	1E5	O25-C23	6.34	1.40	1.22
2	D	401	1E6	C17-C16	6.28	1.49	1.39
3	D	402	1E5	C8-C9	6.24	1.69	1.50
3	H	402	1E5	C2-C1	6.21	1.50	1.39
2	F	401	1E6	C17-C16	6.18	1.49	1.39
2	G	401	1E6	C17-C16	6.10	1.49	1.39
3	E	402	1E5	C2-C1	6.09	1.50	1.39
3	G	402	1E5	C2-C1	6.08	1.50	1.39
2	C	401	1E6	C17-C16	6.03	1.49	1.39
3	D	402	1E5	C2-C1	5.97	1.50	1.39
3	E	402	1E5	C8-C9	5.96	1.68	1.50
3	B	402	1E5	C8-C9	5.94	1.68	1.50
3	A	402	1E5	C8-C9	5.93	1.68	1.50
2	E	401	1E6	C17-C16	5.88	1.48	1.39
3	C	402	1E5	C2-C1	5.77	1.49	1.39
2	H	401	1E6	C17-C16	5.77	1.48	1.39
3	C	402	1E5	C8-C9	5.65	1.67	1.50
3	F	402	1E5	C8-C9	5.64	1.67	1.50
3	H	402	1E5	C8-C9	5.57	1.67	1.50
3	A	402	1E5	C2-C1	5.52	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	402	1E5	C8-C9	5.49	1.67	1.50
3	B	402	1E5	C2-C1	5.38	1.49	1.39
3	H	402	1E5	O25-C23	4.57	1.35	1.22
3	G	402	1E5	O25-C23	4.54	1.35	1.22
2	D	401	1E6	O4-C1	4.32	1.35	1.22
2	F	401	1E6	O37-C21	4.26	1.44	1.37
2	H	401	1E6	O37-C21	4.17	1.43	1.37
3	C	402	1E5	O12-C9	4.06	1.35	1.22
3	B	402	1E5	O25-C23	4.01	1.34	1.22
2	E	401	1E6	O4-C1	3.98	1.34	1.22
3	E	402	1E5	O12-C9	3.97	1.35	1.22
2	F	401	1E6	C19-C18	3.97	1.46	1.39
2	B	401	1E6	C17-C18	3.96	1.45	1.38
2	D	401	1E6	O37-C21	3.95	1.43	1.37
2	D	401	1E6	C17-C18	3.87	1.44	1.38
3	F	402	1E5	O12-C9	3.86	1.34	1.22
2	E	401	1E6	C17-C18	3.85	1.44	1.38
3	E	402	1E5	C21-C20	3.85	1.45	1.39
2	B	401	1E6	O37-C21	3.84	1.43	1.37
3	D	402	1E5	O12-C9	3.82	1.34	1.22
2	F	401	1E6	C17-C18	3.80	1.44	1.38
3	B	402	1E5	C21-C20	3.79	1.45	1.39
3	B	402	1E5	O24-C23	3.79	1.41	1.30
3	A	402	1E5	C21-C20	3.78	1.45	1.39
3	H	402	1E5	O24-C23	3.73	1.41	1.30
2	D	401	1E6	C20-C21	3.72	1.45	1.38
3	C	402	1E5	O13-C9	-3.67	1.18	1.30
2	C	401	1E6	O37-C21	3.62	1.43	1.37
3	G	402	1E5	O24-C23	3.62	1.41	1.30
2	H	401	1E6	C9-C2	3.56	1.44	1.39
2	A	401	1E6	C17-C18	3.56	1.44	1.38
2	E	401	1E6	O37-C21	3.54	1.42	1.37
3	D	402	1E5	O13-C9	-3.51	1.19	1.30
2	G	401	1E6	O37-C21	3.51	1.42	1.37
3	F	402	1E5	O13-C9	-3.50	1.19	1.30
2	F	401	1E6	C20-C21	3.49	1.44	1.38
3	C	402	1E5	C21-C20	3.49	1.44	1.39
2	E	401	1E6	C19-C18	3.45	1.45	1.39
2	G	401	1E6	C19-C18	3.45	1.45	1.39
2	C	401	1E6	C17-C18	3.45	1.44	1.38
2	A	401	1E6	O37-C21	3.44	1.42	1.37
3	E	402	1E5	O13-C9	-3.44	1.19	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	1E6	C20-C21	3.41	1.44	1.38
2	A	401	1E6	C19-C18	3.40	1.45	1.39
2	B	401	1E6	C9-C2	3.38	1.44	1.39
2	E	401	1E6	O3-C1	-3.37	1.20	1.30
2	C	401	1E6	C19-C18	3.36	1.45	1.39
3	G	402	1E5	C21-C20	3.35	1.44	1.39
3	H	402	1E5	C21-C20	3.35	1.44	1.39
2	H	401	1E6	C19-C18	3.34	1.45	1.39
3	C	402	1E5	C4-C5	3.34	1.44	1.39
2	G	401	1E6	C9-C2	3.34	1.44	1.39
2	C	401	1E6	C9-C2	3.33	1.44	1.39
3	A	402	1E5	C4-C5	3.32	1.44	1.39
2	A	401	1E6	C9-C2	3.31	1.44	1.39
2	C	401	1E6	C20-C21	3.31	1.44	1.38
2	H	401	1E6	C20-C21	3.30	1.44	1.38
2	D	401	1E6	C9-C2	3.28	1.44	1.39
2	E	401	1E6	C9-C2	3.27	1.44	1.39
3	G	402	1E5	C4-C5	3.25	1.44	1.39
3	F	402	1E5	C21-C20	3.24	1.44	1.39
3	D	402	1E5	C21-C20	3.20	1.44	1.39
2	D	401	1E6	O3-C1	-3.19	1.21	1.30
3	D	402	1E5	C4-C5	3.19	1.44	1.39
2	D	401	1E6	C19-C18	3.17	1.45	1.39
3	H	402	1E5	C4-C5	3.14	1.44	1.39
2	G	401	1E6	C17-C18	3.14	1.43	1.38
2	H	401	1E6	C17-C18	3.10	1.43	1.38
3	E	402	1E5	C4-C5	3.09	1.44	1.39
3	F	402	1E5	C4-C5	3.09	1.44	1.39
3	B	402	1E5	C4-C5	3.04	1.44	1.39
2	F	401	1E6	C9-C2	3.00	1.44	1.39
3	G	402	1E5	C6-C5	2.98	1.43	1.39
2	B	401	1E6	C20-C21	2.92	1.43	1.38
3	G	402	1E5	C19-C20	2.81	1.43	1.39
3	C	402	1E5	C6-C5	2.81	1.43	1.39
3	B	402	1E5	C6-C5	2.78	1.43	1.39
3	H	402	1E5	C6-C5	2.71	1.43	1.39
2	B	401	1E6	C19-C18	2.71	1.44	1.39
2	C	401	1E6	C9-C8	2.60	1.43	1.38
2	G	401	1E6	C20-C21	2.58	1.43	1.38
3	E	402	1E5	C6-C5	2.56	1.43	1.39
2	E	401	1E6	C5-N6	2.53	1.39	1.34
3	G	402	1E5	C17-N18	2.52	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	1E5	C6-C5	2.51	1.43	1.39
2	B	401	1E6	C9-C8	2.48	1.42	1.38
2	G	401	1E6	C5-C2	2.46	1.43	1.39
2	A	401	1E6	C5-N6	2.45	1.39	1.34
2	D	401	1E6	C20-C19	2.42	1.43	1.38
3	B	402	1E5	C17-N18	2.41	1.40	1.35
3	A	402	1E5	C19-C20	2.36	1.42	1.39
3	B	402	1E5	C19-C20	2.36	1.42	1.39
2	C	401	1E6	C5-N6	2.36	1.39	1.34
2	A	401	1E6	C16-C21	2.35	1.45	1.40
2	C	401	1E6	C20-C19	2.33	1.42	1.38
2	E	401	1E6	C16-C21	2.32	1.45	1.40
2	B	401	1E6	C5-N6	2.31	1.39	1.34
2	H	401	1E6	C9-C8	2.31	1.42	1.38
2	A	401	1E6	C20-C21	2.30	1.42	1.38
2	A	401	1E6	C5-C2	2.30	1.42	1.39
3	C	402	1E5	C17-N18	2.29	1.39	1.35
3	E	402	1E5	C17-N18	2.29	1.39	1.35
2	G	401	1E6	C9-C8	2.27	1.42	1.38
2	G	401	1E6	C5-N6	2.27	1.39	1.34
2	D	401	1E6	C5-C2	2.26	1.42	1.39
3	A	402	1E5	C6-C5	2.26	1.42	1.39
2	H	401	1E6	C5-C2	2.26	1.42	1.39
2	E	401	1E6	C5-C2	2.25	1.42	1.39
2	F	401	1E6	C20-C19	2.25	1.42	1.38
2	H	401	1E6	C5-N6	2.24	1.39	1.34
3	E	402	1E5	C19-C20	2.24	1.42	1.39
2	G	401	1E6	C7-N6	2.23	1.38	1.34
3	E	402	1E5	C22-C21	2.22	1.42	1.38
3	B	402	1E5	C22-C21	2.19	1.42	1.38
3	F	402	1E5	C2-C3	2.18	1.41	1.37
2	A	401	1E6	C7-N6	2.17	1.38	1.34
3	C	402	1E5	C19-C20	2.17	1.42	1.39
2	F	401	1E6	C16-C21	2.16	1.44	1.40
2	H	401	1E6	C20-C19	2.14	1.42	1.38
3	C	402	1E5	C22-C21	2.14	1.42	1.38
3	B	402	1E5	O7-C5	2.14	1.42	1.37
3	H	402	1E5	C4-C3	2.13	1.41	1.37
2	B	401	1E6	C5-C2	2.11	1.42	1.39
2	D	401	1E6	C16-C21	2.11	1.44	1.40
2	E	401	1E6	C20-C19	2.11	1.42	1.38
3	E	402	1E5	C2-C3	2.10	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	402	1E5	C17-N18	2.10	1.39	1.35
3	H	402	1E5	C19-C20	2.10	1.42	1.39
2	A	401	1E6	C9-C8	2.09	1.42	1.38
3	F	402	1E5	C19-C20	2.08	1.42	1.39
3	A	402	1E5	C17-N18	2.07	1.39	1.35
2	D	401	1E6	C5-N6	2.07	1.38	1.34
3	D	402	1E5	C6-C5	2.06	1.42	1.39
3	E	402	1E5	C4-C3	2.04	1.41	1.37
3	A	402	1E5	C22-C21	2.04	1.42	1.38
2	F	401	1E6	C5-N6	2.03	1.38	1.34
3	C	402	1E5	C2-C3	2.02	1.41	1.37
2	G	401	1E6	C20-C19	2.01	1.42	1.38

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	1E6	O43-C12-C11	-10.98	102.82	121.44
2	H	401	1E6	O43-C12-C11	-10.95	102.88	121.44
2	B	401	1E6	O43-C12-C11	-10.91	102.95	121.44
2	F	401	1E6	O43-C12-C11	-10.75	103.21	121.44
2	D	401	1E6	O43-C12-C11	-10.75	103.22	121.44
2	A	401	1E6	O43-C12-C11	-10.75	103.22	121.44
2	C	401	1E6	O43-C12-C11	-10.54	103.56	121.44
2	G	401	1E6	O43-C12-C11	-10.38	103.84	121.44
2	D	401	1E6	O43-C12-N15	7.25	136.65	123.64
2	F	401	1E6	O43-C12-N15	7.21	136.57	123.64
2	C	401	1E6	O43-C12-N15	7.11	136.38	123.64
2	A	401	1E6	O43-C12-N15	7.05	136.28	123.64
2	H	401	1E6	O43-C12-N15	7.02	136.23	123.64
2	E	401	1E6	O43-C12-N15	6.94	136.09	123.64
2	B	401	1E6	O43-C12-N15	6.93	136.07	123.64
2	G	401	1E6	O43-C12-N15	6.69	135.63	123.64
2	E	401	1E6	C11-C12-N15	4.45	121.08	114.55
2	B	401	1E6	C11-C12-N15	4.38	120.97	114.55
2	H	401	1E6	C11-C12-N15	4.32	120.88	114.55
2	A	401	1E6	O22-C19-C18	4.14	121.32	116.39
2	G	401	1E6	O22-C19-C18	4.11	121.29	116.39
2	G	401	1E6	C11-C12-N15	4.08	120.53	114.55
2	A	401	1E6	C11-C12-N15	4.06	120.50	114.55
2	B	401	1E6	O22-C19-C18	4.02	121.18	116.39
2	E	401	1E6	O22-C19-C18	3.95	121.09	116.39
2	F	401	1E6	O22-C19-C18	3.90	121.04	116.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	1E6	C11-C12-N15	3.86	120.21	114.55
2	D	401	1E6	C11-C12-N15	3.81	120.13	114.55
2	C	401	1E6	C11-C12-N15	3.75	120.05	114.55
2	C	401	1E6	O22-C19-C18	3.70	120.79	116.39
3	E	402	1E5	C19-N18-C17	3.55	122.55	117.93
3	C	402	1E5	C19-N18-C17	3.51	122.50	117.93
3	H	402	1E5	C19-N18-C17	3.49	122.47	117.93
3	A	402	1E5	C19-N18-C17	3.47	122.44	117.93
3	D	402	1E5	C19-N18-C17	3.45	122.41	117.93
3	F	402	1E5	C19-N18-C17	3.38	122.33	117.93
2	A	401	1E6	O37-C21-C16	3.31	118.93	114.81
2	H	401	1E6	O22-C19-C18	3.30	120.32	116.39
2	D	401	1E6	O22-C19-C18	3.24	120.25	116.39
3	B	402	1E5	C19-N18-C17	3.21	122.11	117.93
3	G	402	1E5	C19-N18-C17	3.17	122.05	117.93
2	D	401	1E6	O37-C21-C16	2.90	118.43	114.81
2	E	401	1E6	O37-C21-C16	2.80	118.30	114.81
2	B	401	1E6	C21-C20-C19	2.78	124.35	118.98
2	B	401	1E6	O37-C21-C16	2.72	118.20	114.81
2	G	401	1E6	O37-C21-C16	2.69	118.17	114.81
2	C	401	1E6	C5-N6-C7	2.69	120.03	117.08
2	B	401	1E6	C5-N6-C7	2.60	119.93	117.08
2	D	401	1E6	O3-C1-C2	2.60	121.51	114.84
2	A	401	1E6	C21-C20-C19	2.59	123.98	118.98
2	H	401	1E6	O37-C21-C16	2.54	117.97	114.81
2	F	401	1E6	O37-C21-C16	2.53	117.96	114.81
3	D	402	1E5	C22-C21-C20	-2.52	118.11	120.80
2	H	401	1E6	C5-N6-C7	2.51	119.84	117.08
2	E	401	1E6	O3-C1-C2	2.50	121.26	114.84
2	E	401	1E6	C5-N6-C7	2.50	119.83	117.08
2	E	401	1E6	C21-C20-C19	2.49	123.79	118.98
2	G	401	1E6	C21-C20-C19	2.45	123.72	118.98
2	C	401	1E6	C21-C20-C19	2.45	123.72	118.98
3	F	402	1E5	O12-C9-C8	-2.43	111.88	121.99
2	D	401	1E6	C5-N6-C7	2.42	119.73	117.08
2	A	401	1E6	C5-N6-C7	2.39	119.70	117.08
2	H	401	1E6	C21-C20-C19	2.38	123.59	118.98
3	F	402	1E5	C22-C21-C20	-2.38	118.26	120.80
2	D	401	1E6	C21-C20-C19	2.38	123.57	118.98
3	E	402	1E5	O12-C9-C8	-2.38	112.10	121.99
2	F	401	1E6	C5-N6-C7	2.35	119.66	117.08
3	H	402	1E5	C1-C6-C5	2.34	122.67	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	1E5	C22-C21-C20	-2.33	118.31	120.80
3	G	402	1E5	C6-C1-C17	2.31	123.83	120.59
2	F	401	1E6	C21-C20-C19	2.30	123.43	118.98
2	G	401	1E6	C5-N6-C7	2.30	119.61	117.08
3	D	402	1E5	O12-C9-C8	-2.28	112.48	121.99
2	C	401	1E6	O37-C21-C16	2.25	117.61	114.81
3	C	402	1E5	C6-C1-C17	2.24	123.73	120.59
3	G	402	1E5	C22-C17-N18	-2.23	118.93	122.24
3	A	402	1E5	C22-C21-C20	-2.22	118.43	120.80
3	H	402	1E5	C22-C17-N18	-2.22	118.94	122.24
3	C	402	1E5	O12-C9-C8	-2.21	112.80	121.99
3	A	402	1E5	C1-C6-C5	2.20	122.49	119.85
3	E	402	1E5	C22-C21-C20	-2.17	118.48	120.80
3	C	402	1E5	C22-C17-N18	-2.16	119.03	122.24
3	B	402	1E5	C1-C6-C5	2.15	122.43	119.85
3	F	402	1E5	C22-C17-N18	-2.10	119.12	122.24
3	B	402	1E5	C6-C1-C17	2.10	123.53	120.59
3	F	402	1E5	C6-C1-C17	2.10	123.52	120.59
3	F	402	1E5	O13-C9-C8	2.07	123.45	113.66
3	D	402	1E5	O13-C9-C8	2.07	123.44	113.66
3	H	402	1E5	C20-C19-N18	-2.07	120.55	123.59
3	E	402	1E5	C22-C17-N18	-2.06	119.17	122.24
3	A	402	1E5	C22-C17-N18	-2.04	119.20	122.24
3	E	402	1E5	C20-C19-N18	-2.04	120.59	123.59
3	E	402	1E5	C1-C6-C5	2.03	122.30	119.85
3	C	402	1E5	C1-C6-C5	2.02	122.28	119.85
3	F	402	1E5	C5-C4-C3	2.01	120.07	117.55
2	B	401	1E6	O22-C23-C24	2.01	111.27	107.64
3	D	402	1E5	C1-C6-C5	2.01	122.27	119.85
2	D	401	1E6	O4-C1-C2	-2.01	116.19	121.46
3	D	402	1E5	C5-C4-C3	2.00	120.05	117.55
2	H	401	1E6	O22-C23-C24	2.00	111.25	107.64

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	401	1E6	C23-C24-C27-O28
2	H	401	1E6	O44-C24-C27-O28
3	H	402	1E5	C19-C20-C23-O24
3	H	402	1E5	C21-C20-C23-O24
2	A	401	1E6	C18-C19-O22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	401	1E6	C18-C19-O22-C23
3	G	402	1E5	C21-C20-C23-O24
2	D	401	1E6	C16-C21-O37-C38
2	C	401	1E6	O4-C1-C2-C9
2	C	401	1E6	O3-C1-C2-C9
2	E	401	1E6	C18-C19-O22-C23
3	F	402	1E5	C21-C20-C23-O25
2	C	401	1E6	O3-C1-C2-C5
2	C	401	1E6	O4-C1-C2-C5
3	G	402	1E5	C19-C20-C23-O24
3	B	402	1E5	C21-C20-C23-O24
2	B	401	1E6	C23-C24-C27-O28
2	D	401	1E6	C20-C21-O37-C38
3	B	402	1E5	C19-C20-C23-O24
2	D	401	1E6	C18-C19-O22-C23
2	E	401	1E6	O3-C1-C2-C9
2	E	401	1E6	O4-C1-C2-C9
3	F	402	1E5	C19-C20-C23-O25
3	D	402	1E5	C21-C20-C23-O25
3	A	402	1E5	C21-C20-C23-O25
3	C	402	1E5	C21-C20-C23-O25
2	E	401	1E6	O3-C1-C2-C5
2	F	401	1E6	C16-C21-O37-C38
2	E	401	1E6	O4-C1-C2-C5
3	A	402	1E5	C19-C20-C23-O25
3	D	402	1E5	C19-C20-C23-O25
3	H	402	1E5	C21-C20-C23-O25
2	A	401	1E6	C16-C21-O37-C38
3	C	402	1E5	C19-C20-C23-O25
2	F	401	1E6	C20-C21-O37-C38
2	A	401	1E6	C20-C19-O22-C23
2	H	401	1E6	C24-C23-O22-C19
2	F	401	1E6	C20-C19-O22-C23
3	E	402	1E5	C21-C20-C23-O25
2	B	401	1E6	O44-C24-C27-O28
2	H	401	1E6	O22-C23-C24-O44
2	A	401	1E6	C20-C21-O37-C38
2	F	401	1E6	O22-C23-C24-O44
2	H	401	1E6	O22-C23-C24-C27
3	H	402	1E5	C19-C20-C23-O25
3	E	402	1E5	C19-C20-C23-O25
2	C	401	1E6	C18-C19-O22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	401	1E6	C20-C19-O22-C23
3	E	402	1E5	O7-C8-C9-O13
2	G	401	1E6	C16-C21-O37-C38
2	D	401	1E6	C20-C19-O22-C23

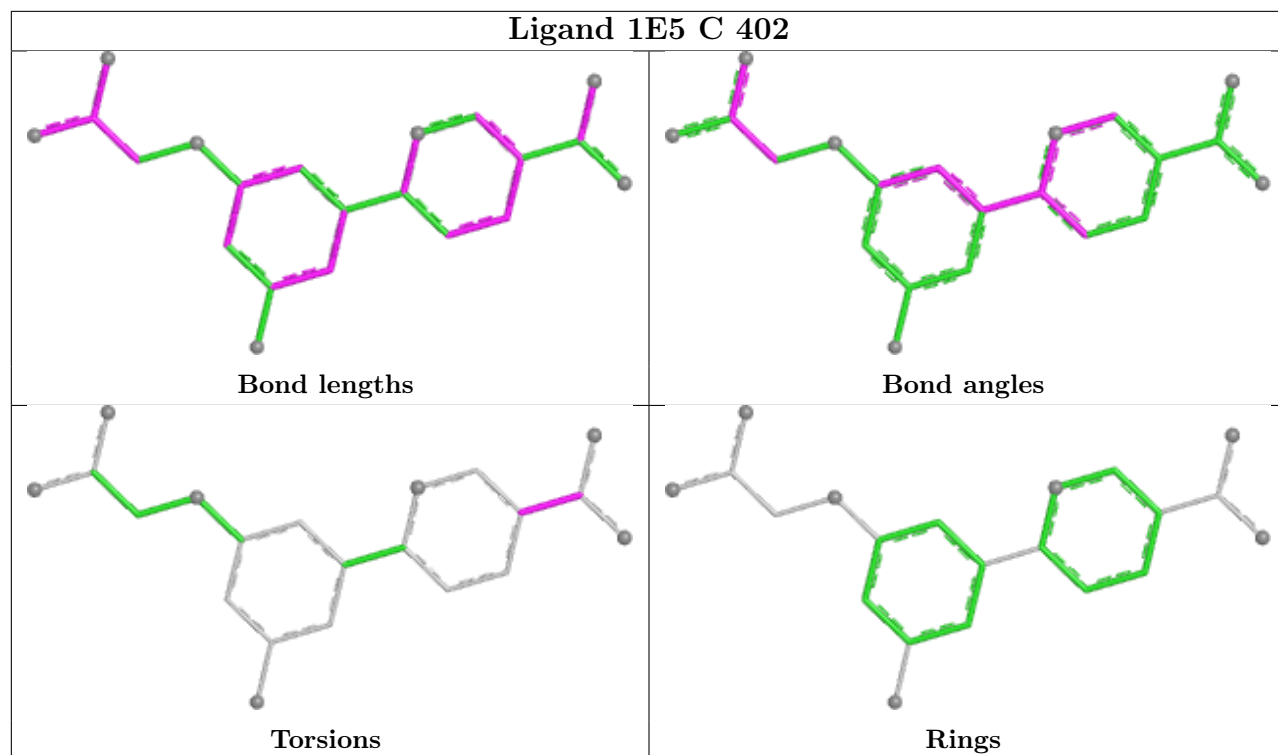
There are no ring outliers.

9 monomers are involved in 9 short contacts:

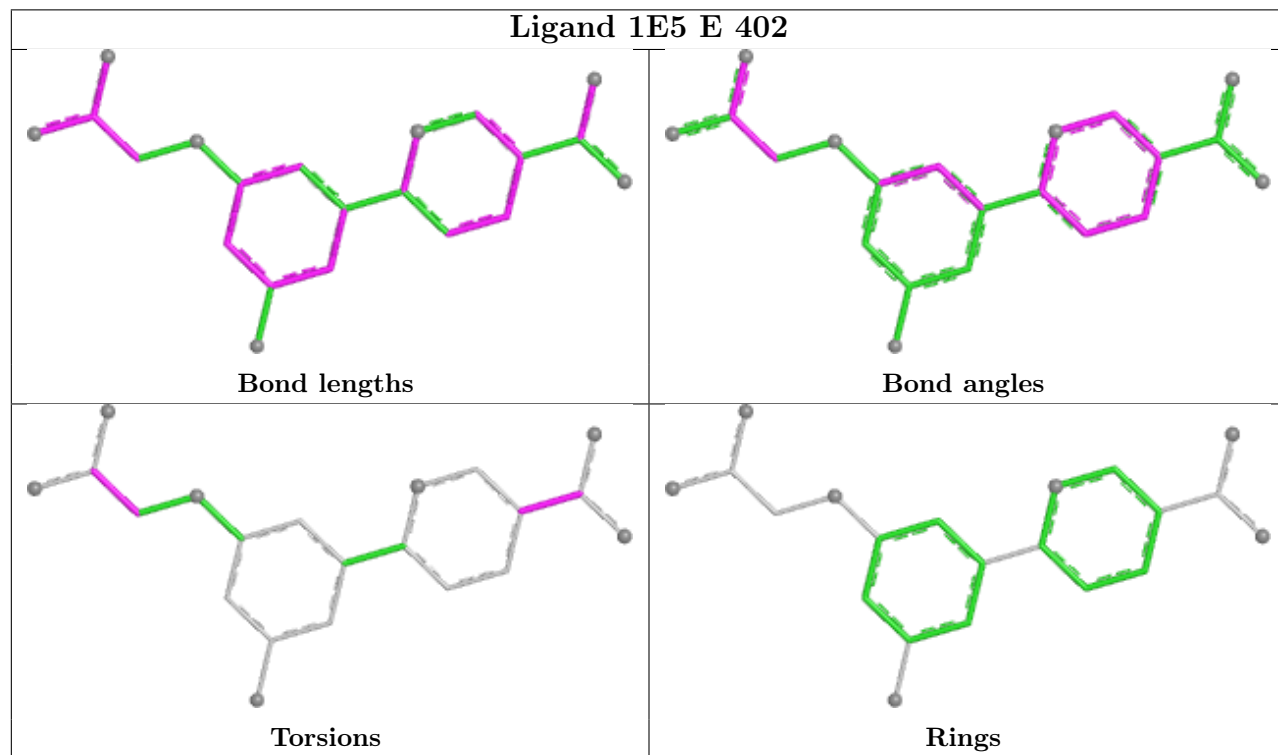
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	1E5	1	0
3	E	402	1E5	1	0
3	G	402	1E5	1	0
3	H	402	1E5	1	0
2	E	401	1E6	1	0
3	A	402	1E5	1	0
3	B	402	1E5	1	0
3	F	402	1E5	1	0
3	D	402	1E5	1	0

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.

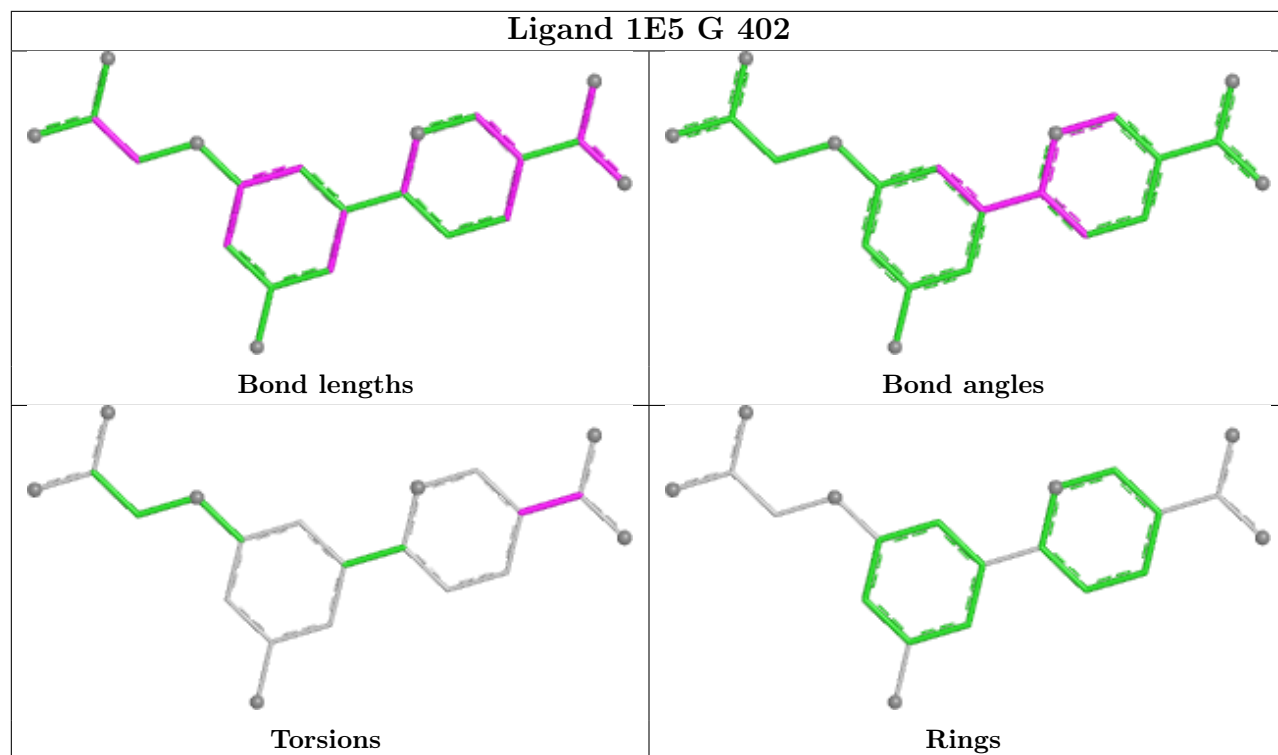
Ligand 1E5 C 402



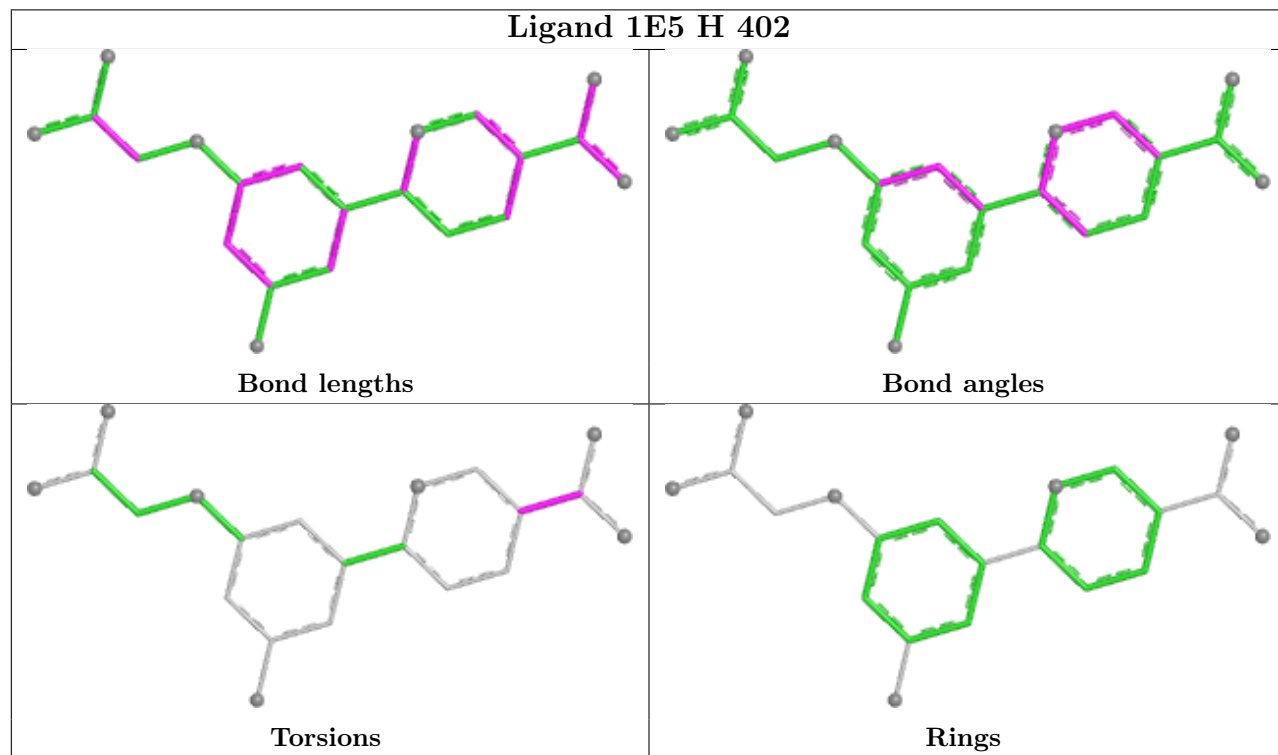
Ligand 1E5 E 402



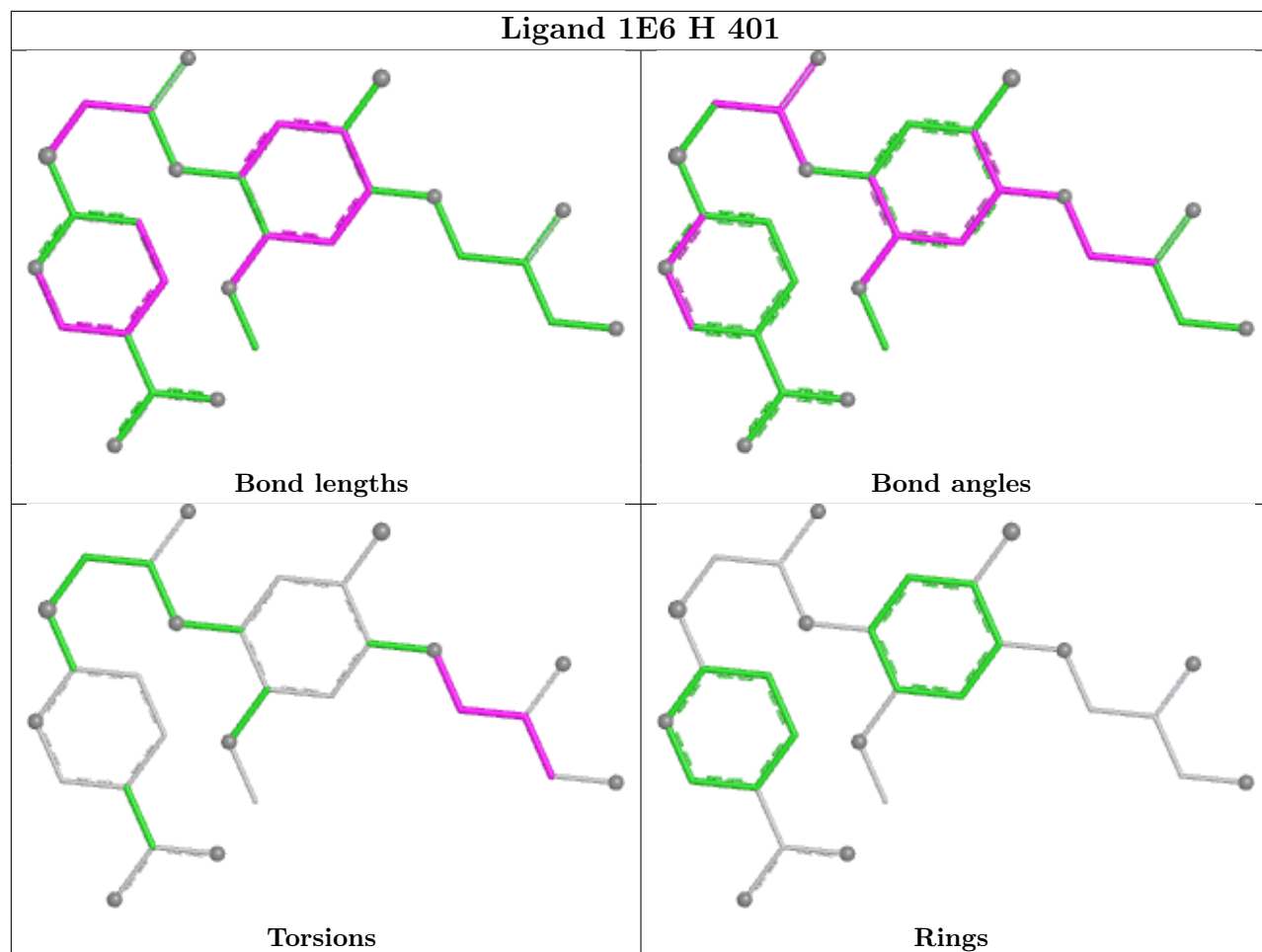
Ligand 1E5 G 402



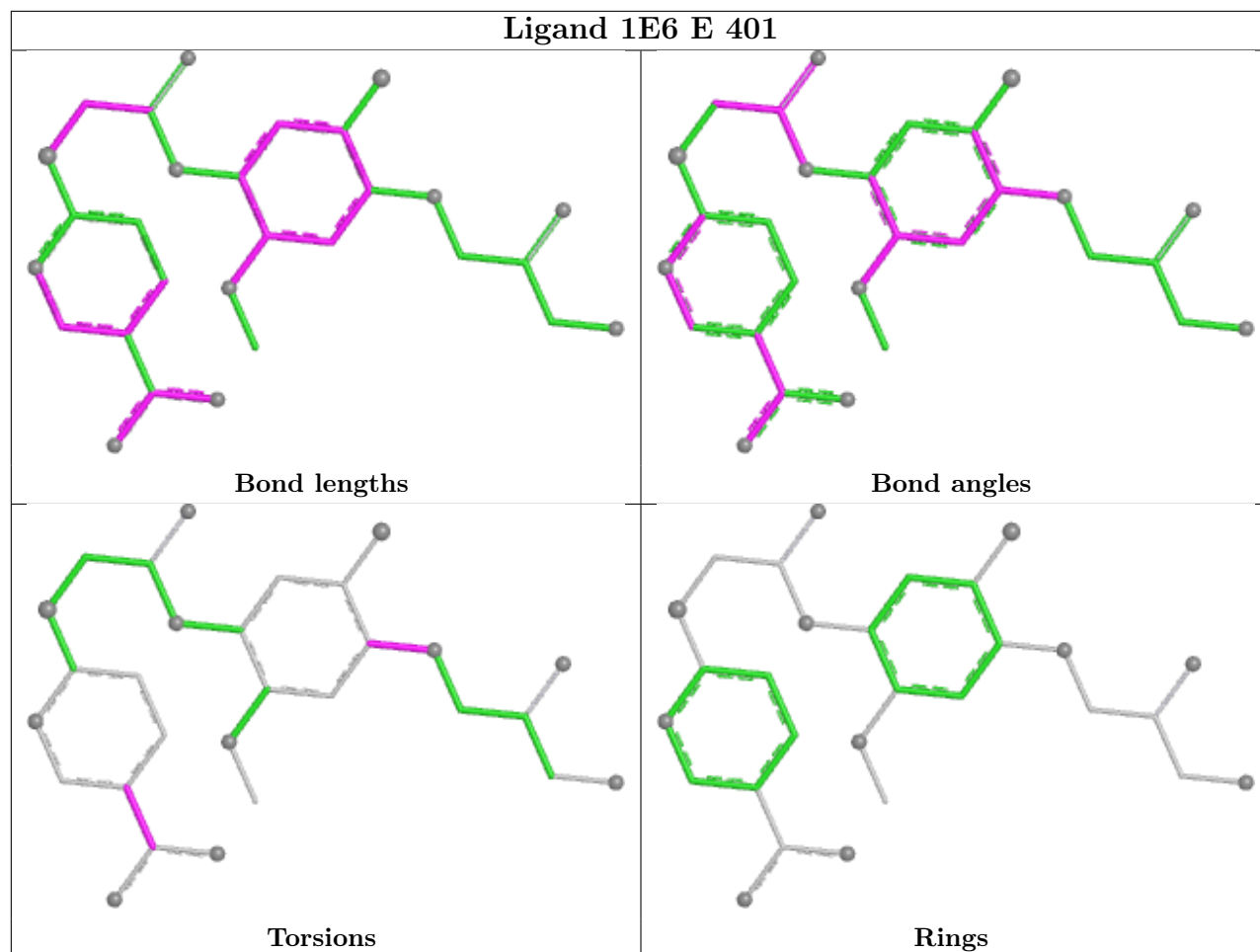
Ligand 1E5 H 402



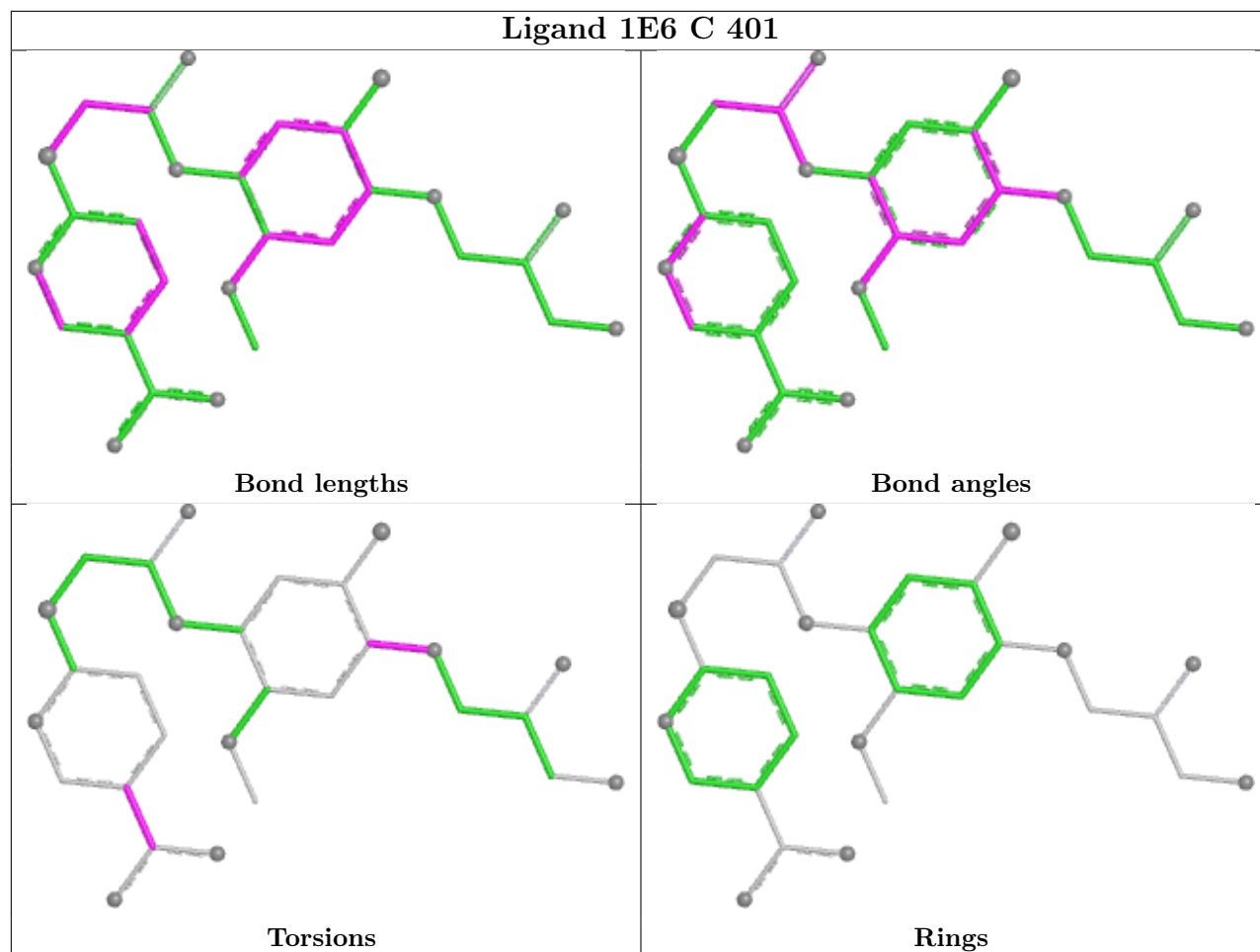
Ligand 1E6 H 401



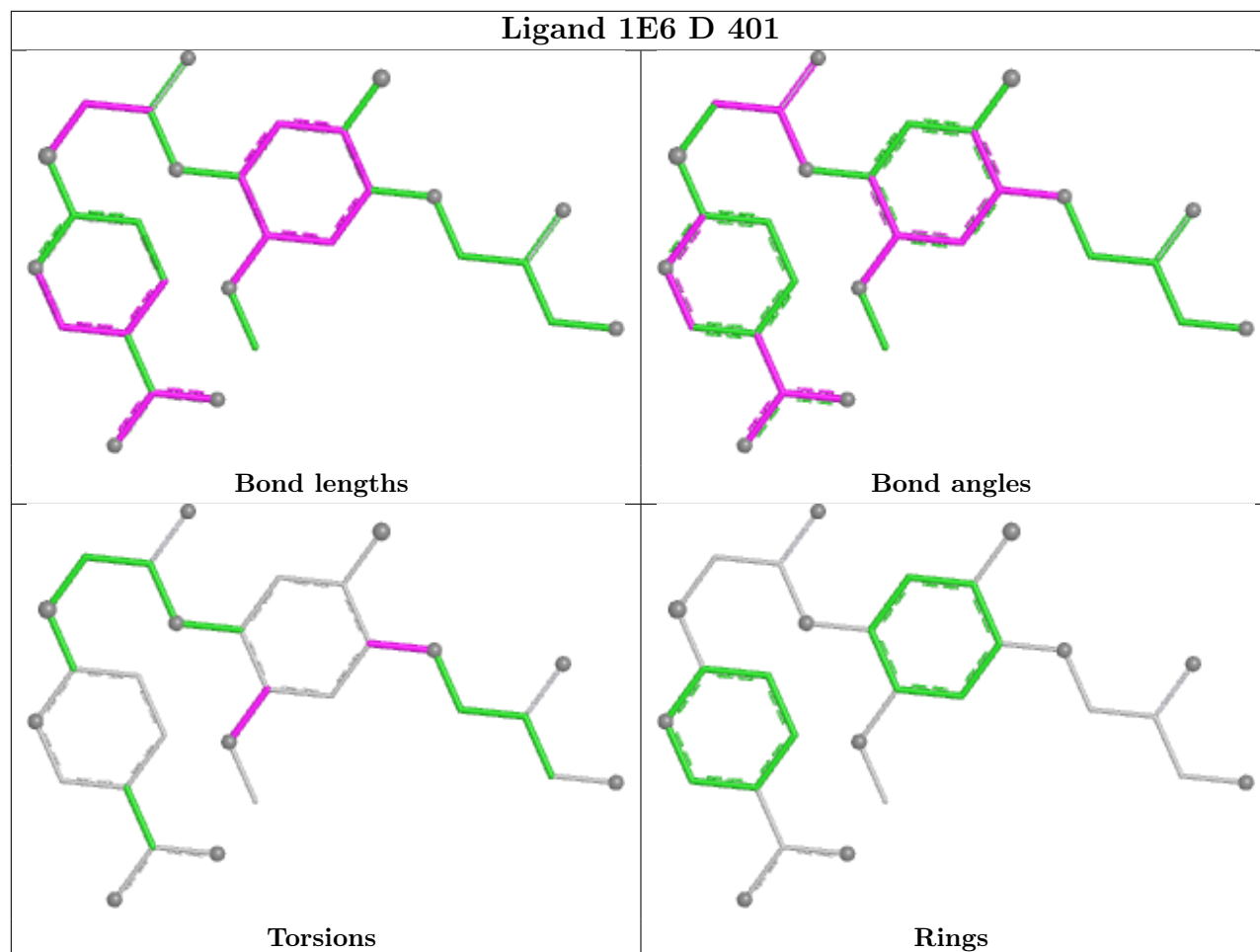
Ligand 1E6 E 401



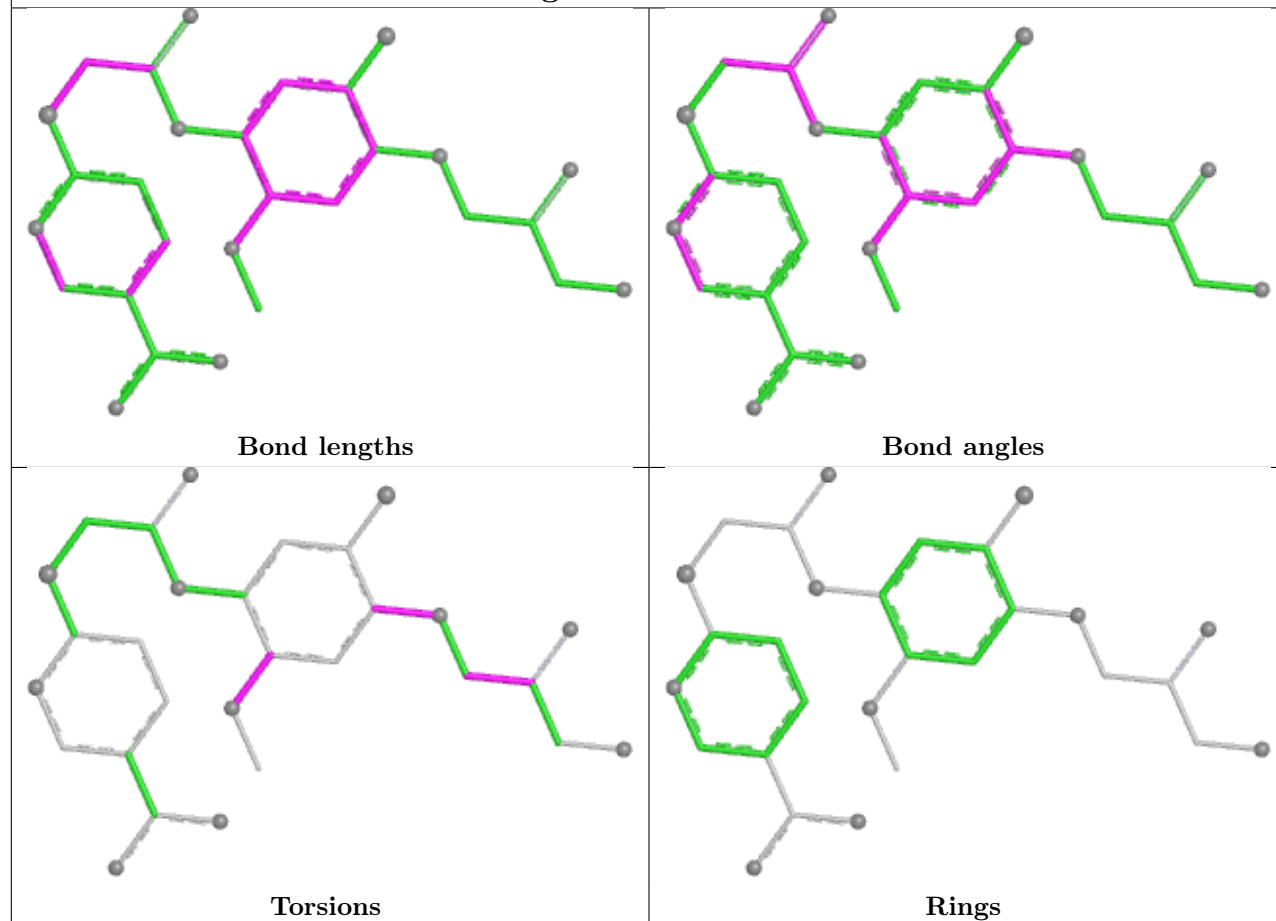
Ligand 1E6 C 401



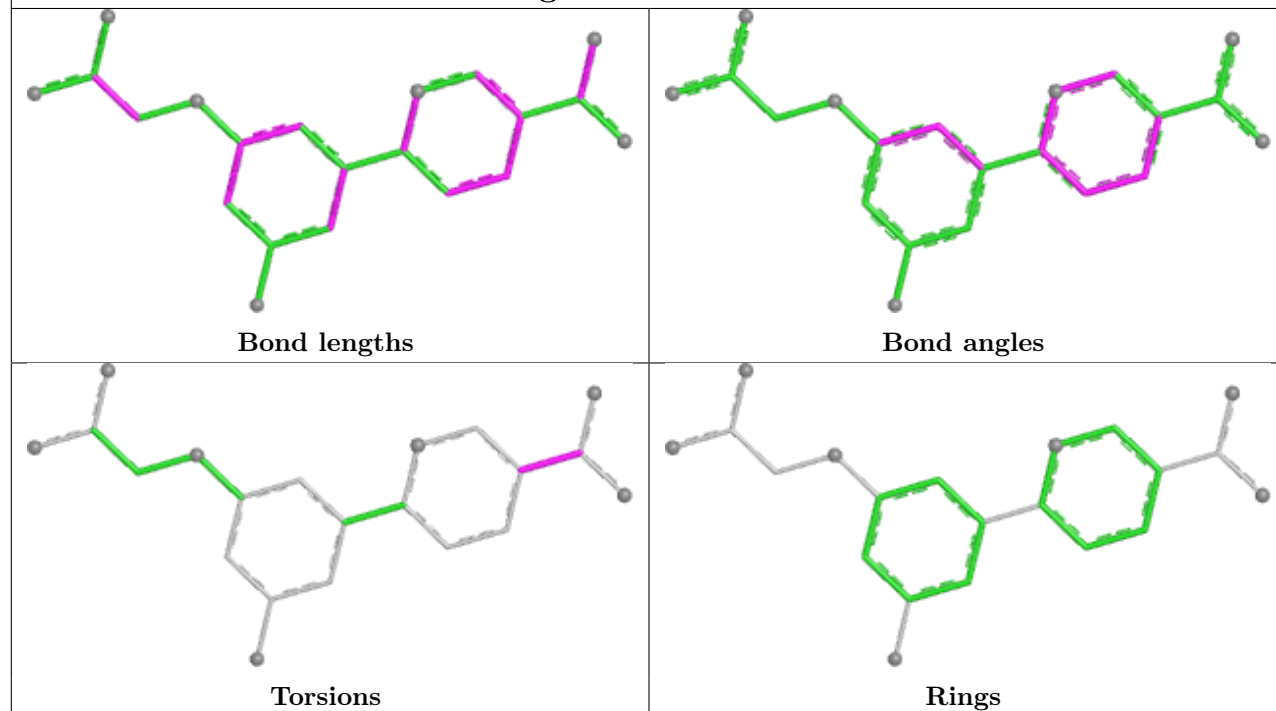
Ligand 1E6 D 401



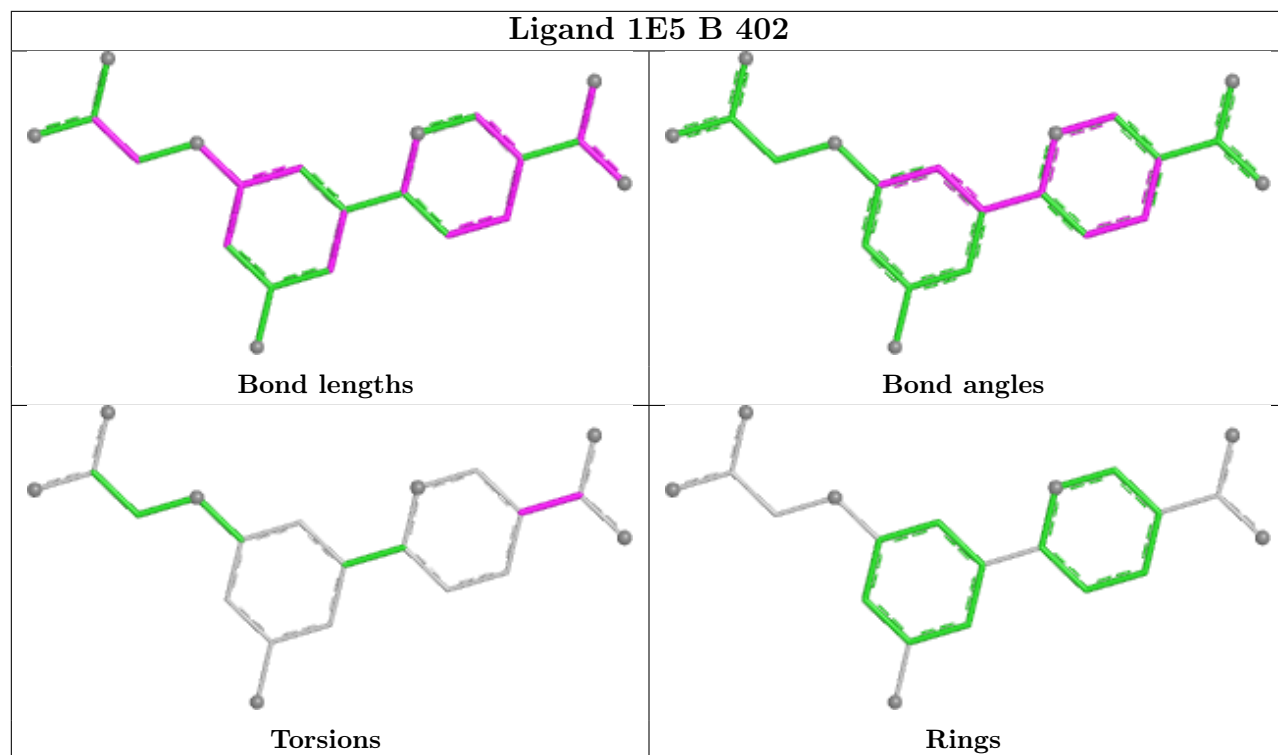
Ligand 1E6 F 401



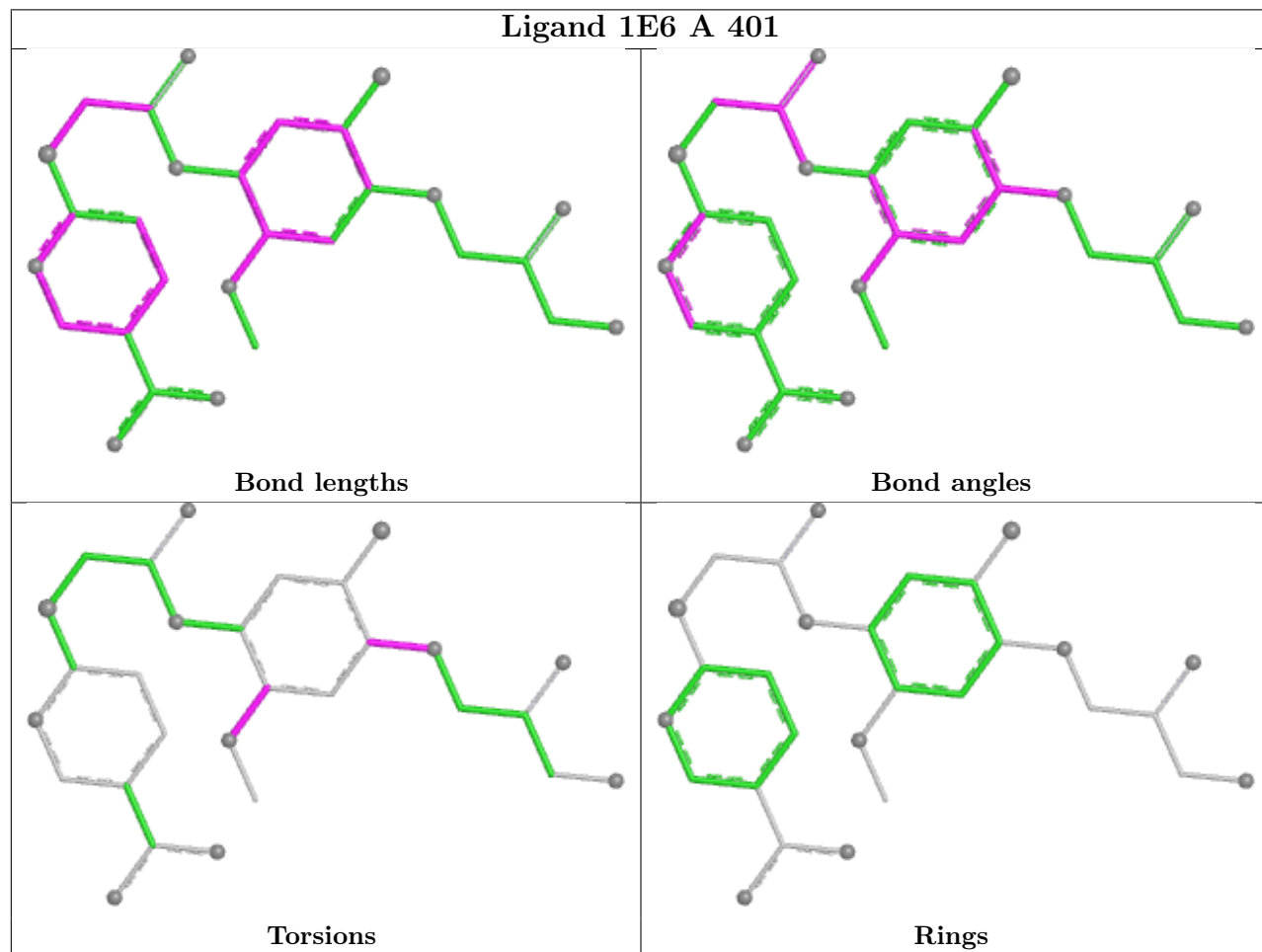
Ligand 1E5 A 402



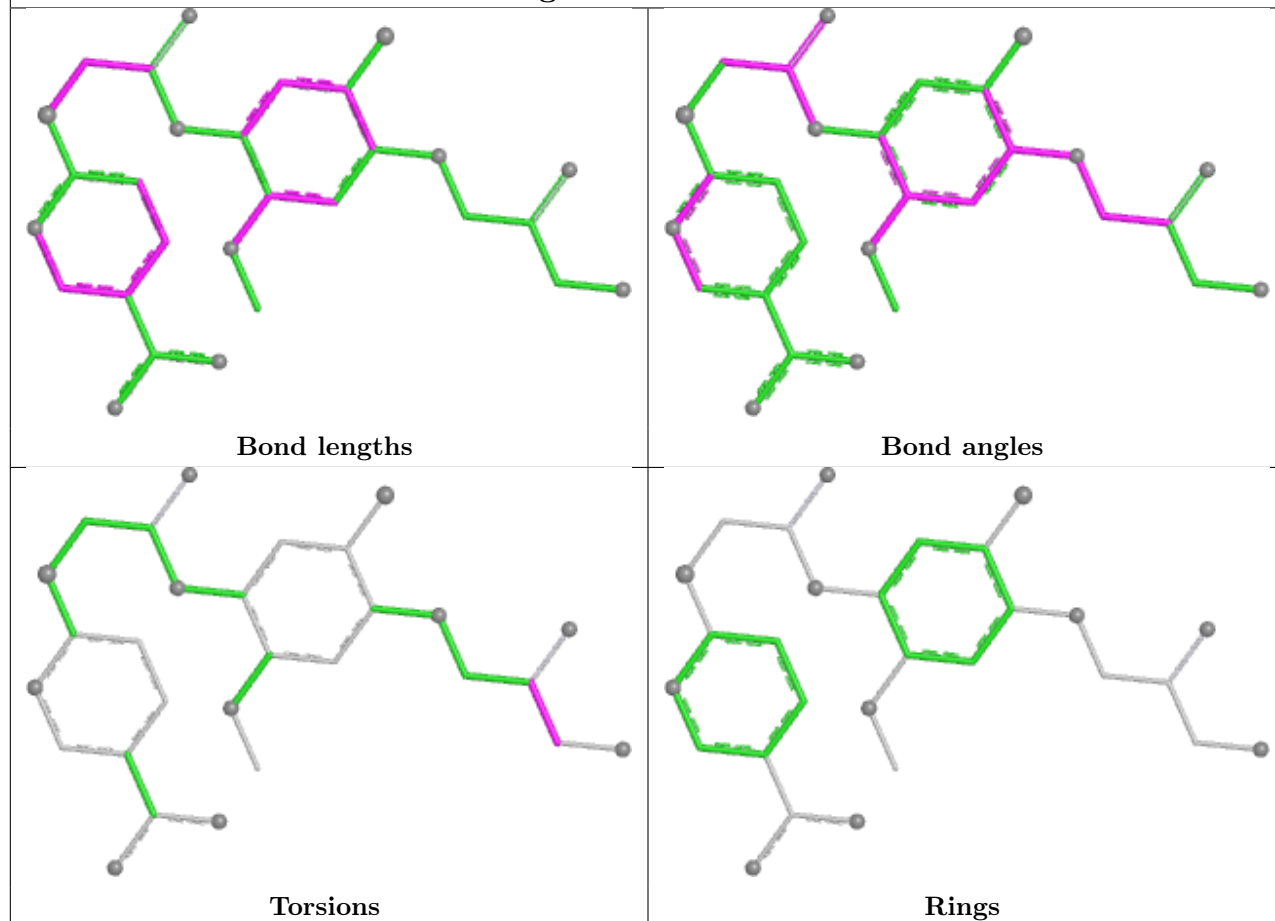
Ligand 1E5 B 402



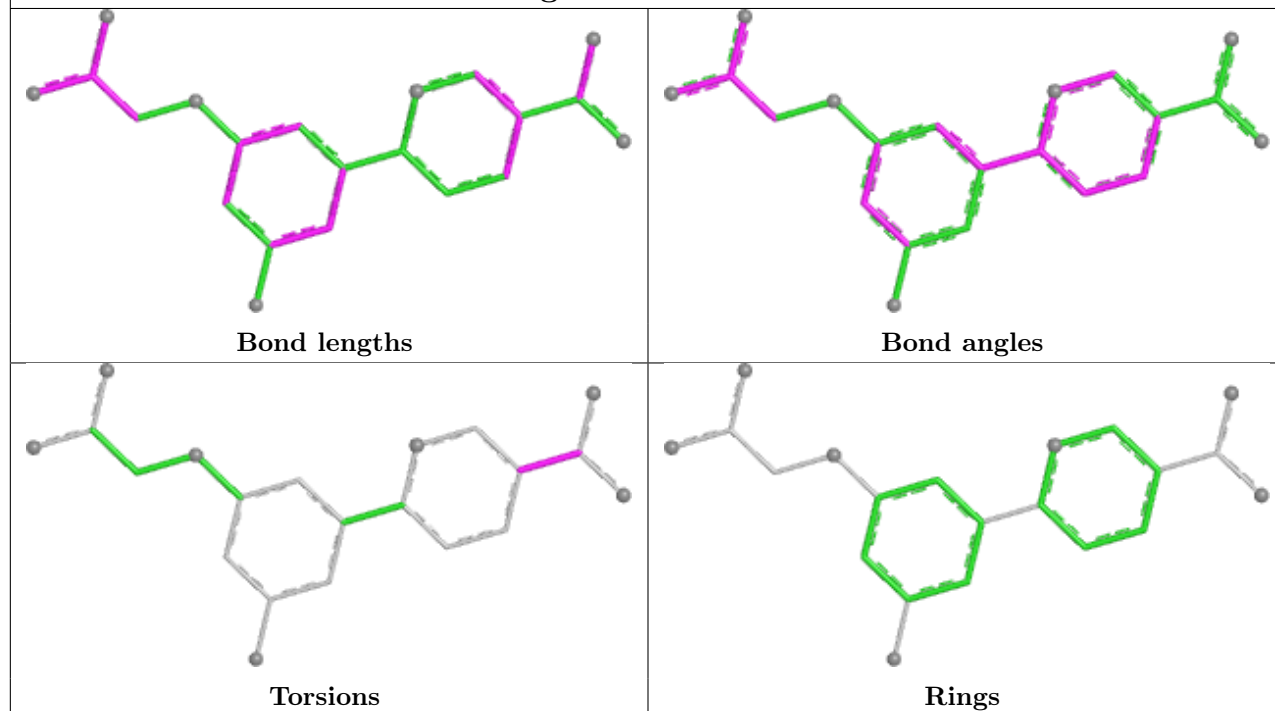
Ligand 1E6 A 401



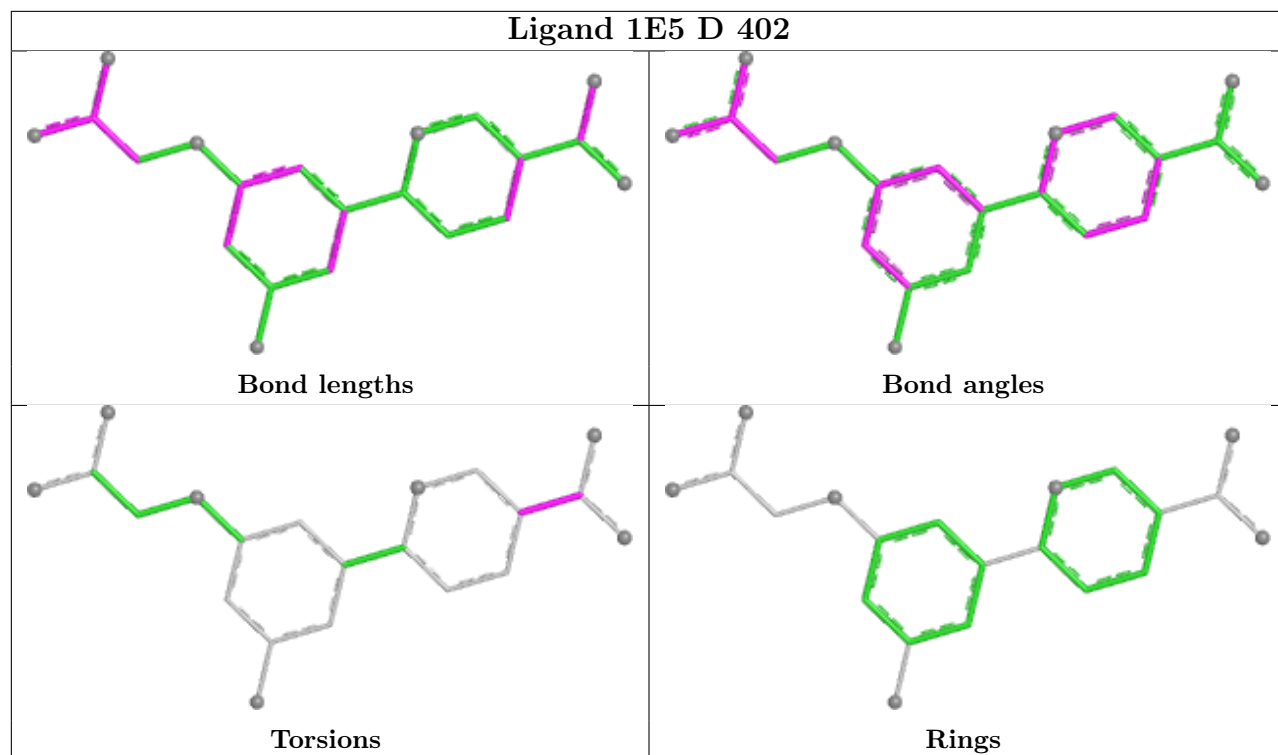
Ligand 1E6 B 401



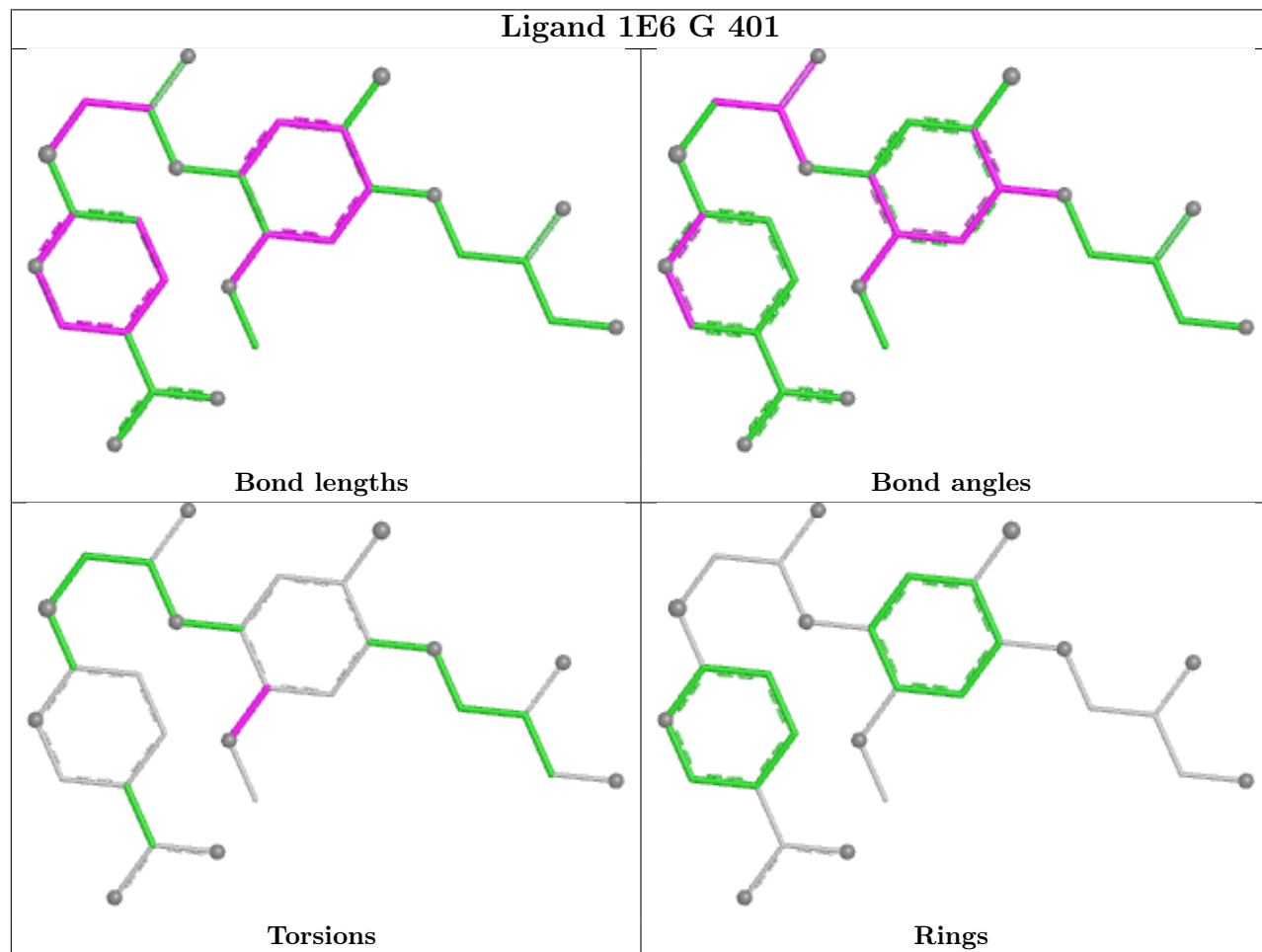
Ligand 1E5 F 402



Ligand 1E5 D 402



Ligand 1E6 G 401



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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	324/331 (97%)	0.05	9 (2%)	55	61	9, 25, 44, 65	1 (0%)
1	B	324/331 (97%)	0.02	13 (4%)	42	48	14, 24, 45, 63	1 (0%)
1	C	328/331 (99%)	0.31	17 (5%)	33	38	17, 30, 50, 85	1 (0%)
1	D	331/331 (100%)	0.07	9 (2%)	56	63	15, 26, 48, 72	1 (0%)
1	E	331/331 (100%)	0.55	26 (7%)	18	21	19, 33, 61, 77	1 (0%)
1	F	329/331 (99%)	0.36	18 (5%)	30	36	13, 30, 59, 79	1 (0%)
1	G	328/331 (99%)	0.23	21 (6%)	25	28	15, 27, 55, 86	1 (0%)
1	H	325/331 (98%)	0.13	14 (4%)	40	45	13, 26, 47, 94	1 (0%)
All	All	2620/2648 (98%)	0.21	127 (4%)	35	41	9, 27, 53, 94	8 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	12	LEU	9.5
1	B	12	LEU	9.2
1	C	12	LEU	8.8
1	D	12	LEU	8.5
1	H	12	LEU	8.4
1	F	12	LEU	8.4
1	G	12	LEU	8.0
1	G	106	LEU	7.2
1	C	102	GLY	7.0
1	A	12	LEU	6.7
1	H	106	LEU	5.6
1	H	104	SER	5.6
1	G	104	SER	5.4
1	B	14	GLU	5.0
1	G	98	ARG	5.0
1	H	105	ARG	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	108	LEU	4.7
1	D	101	GLU	4.5
1	C	105	ARG	4.5
1	F	102	GLY	4.4
1	C	16	HIS	4.3
1	G	105	ARG	4.2
1	G	107	ASN	4.2
1	G	97	ALA	4.2
1	B	105	LEU	4.2
1	A	16	HIS	4.1
1	B	13	LYS	4.1
1	C	238	TYR	4.0
1	F	104	SER	4.0
1	A	106	LEU	4.0
1	C	103	GLU	4.0
1	H	16	HIS	3.9
1	E	99	GLN	3.9
1	F	103	GLU	3.8
1	H	238	TYR	3.7
1	H	108	LEU	3.7
1	E	323	TRP	3.6
1	F	98	ARG	3.5
1	G	109	VAL	3.4
1	A	108	LEU	3.4
1	C	218	GLY	3.4
1	G	99	GLN	3.3
1	C	104	SER	3.3
1	E	102	GLY	3.3
1	F	330	GLN	3.3
1	E	330	GLN	3.1
1	E	14	GLU	3.1
1	G	103	GLU	3.1
1	E	314	HIS	3.1
1	H	97	ALA	3.1
1	E	100	GLN	3.0
1	F	323	TRP	3.0
1	E	15	GLU	3.0
1	E	282	ILE	2.9
1	A	107	ASN	2.9
1	D	100	GLN	2.8
1	E	322	LEU	2.8
1	E	219	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	98	ARG	2.7
1	E	284	GLU	2.7
1	C	193	GLY	2.7
1	H	13	LYS	2.7
1	C	108	LEU	2.7
1	A	238	TYR	2.7
1	B	238	TYR	2.7
1	E	316	LYS	2.7
1	E	218	GLY	2.7
1	E	101	GLU	2.6
1	H	14	GLU	2.6
1	H	284	GLU	2.6
1	H	109	VAL	2.6
1	F	105	ARG	2.6
1	G	111	ARG	2.6
1	A	329	LEU	2.6
1	B	1	ALA	2.6
1	G	16	HIS	2.6
1	B	225	GLN	2.5
1	B	104	ARG	2.5
1	E	17	VAL	2.5
1	E	276	LEU	2.5
1	F	314	HIS	2.5
1	D	98	ARG	2.5
1	F	2	ALA	2.5
1	B	15	GLU	2.5
1	C	14	GLU	2.5
1	G	238	TYR	2.5
1	F	101	GLU	2.4
1	C	106	LEU	2.4
1	B	330	GLN	2.4
1	E	283	LYS	2.4
1	B	106	ASN	2.4
1	D	107	ASN	2.4
1	G	110	GLN	2.4
1	C	11	LEU	2.4
1	E	105	ARG	2.3
1	F	106	LEU	2.3
1	F	284	GLU	2.3
1	G	14	GLU	2.3
1	G	15	GLU	2.3
1	A	109	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	16	HIS	2.3
1	E	327	LYS	2.3
1	F	220	ASP	2.3
1	C	15	GLU	2.3
1	F	100	GLN	2.3
1	D	17	VAL	2.3
1	C	18	PRO	2.2
1	E	16	HIS	2.2
1	F	279	LEU	2.2
1	E	220	ASP	2.2
1	H	107	ASN	2.2
1	E	98	ARG	2.2
1	H	1	ALA	2.2
1	F	331	PHE	2.2
1	C	194	ASP	2.1
1	D	220	ASP	2.1
1	A	331	PHE	2.1
1	G	219	THR	2.1
1	E	310	GLU	2.1
1	B	16	HIS	2.1
1	D	13	LYS	2.1
1	E	1	ALA	2.1
1	F	283	LYS	2.1
1	G	284	GLU	2.1
1	G	314	HIS	2.0
1	B	276	LEU	2.0
1	G	13	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

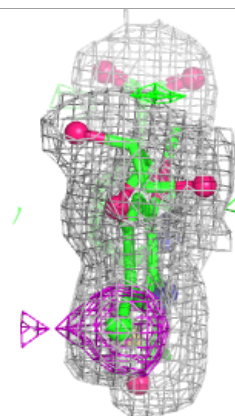
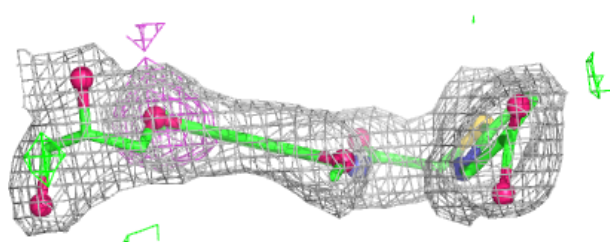
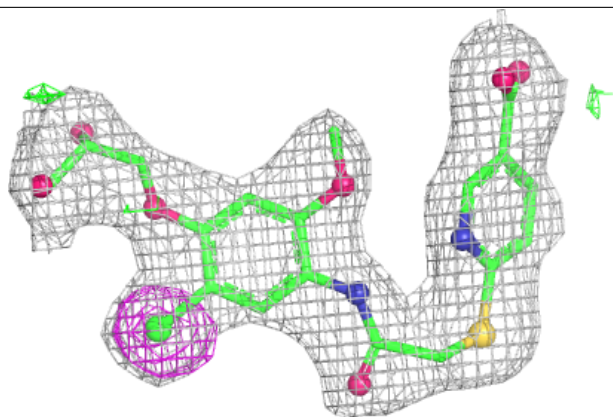
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	1E6	E	401	29/29	0.90	0.11	22,37,40,44	0
3	1E5	F	402	21/21	0.91	0.10	23,27,29,31	0
2	1E6	B	401	29/29	0.92	0.10	3,28,33,34	0
3	1E5	E	402	21/21	0.92	0.10	29,32,35,36	0
2	1E6	C	401	29/29	0.92	0.11	18,36,40,41	0
3	1E5	G	402	21/21	0.92	0.10	24,27,28,30	0
3	1E5	H	402	21/21	0.92	0.10	22,25,27,28	0
3	1E5	B	402	21/21	0.93	0.08	19,22,24,26	0
3	1E5	C	402	21/21	0.93	0.08	22,23,28,31	0
2	1E6	D	401	29/29	0.93	0.10	17,34,35,37	0
2	1E6	F	401	29/29	0.93	0.10	14,33,40,43	0
2	1E6	G	401	29/29	0.93	0.10	13,28,35,39	0
2	1E6	H	401	29/29	0.93	0.09	11,31,39,42	0
3	1E5	A	402	21/21	0.94	0.09	22,25,31,33	0
3	1E5	D	402	21/21	0.94	0.08	18,23,24,28	0
2	1E6	A	401	29/29	0.94	0.09	17,31,35,36	0

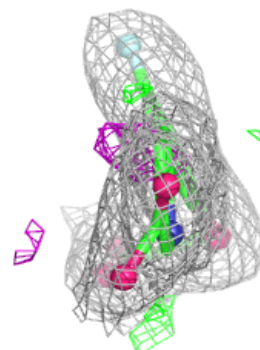
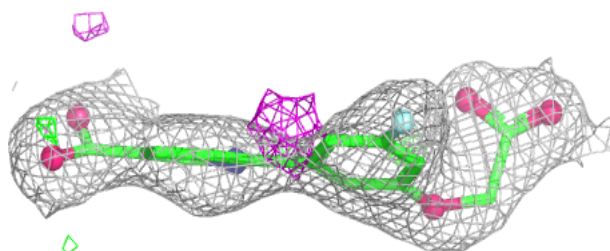
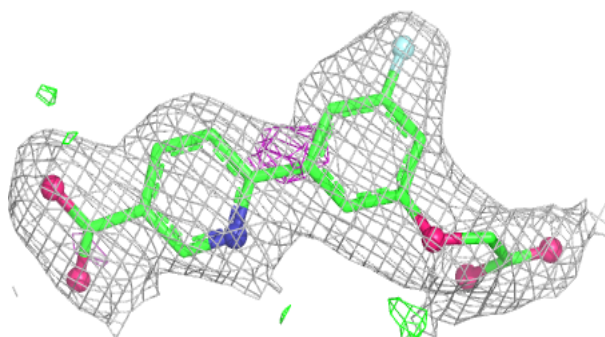
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1E6 E 401:

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

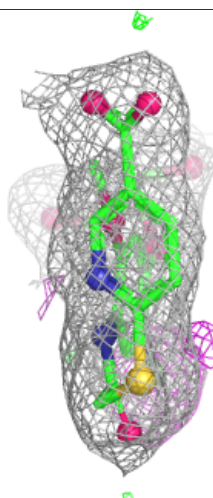
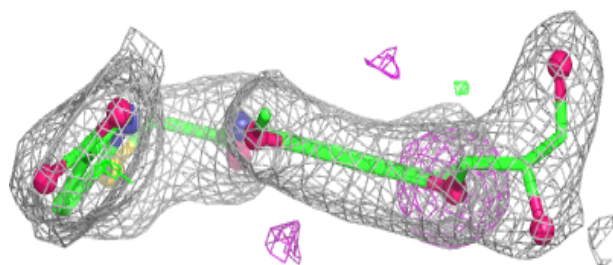
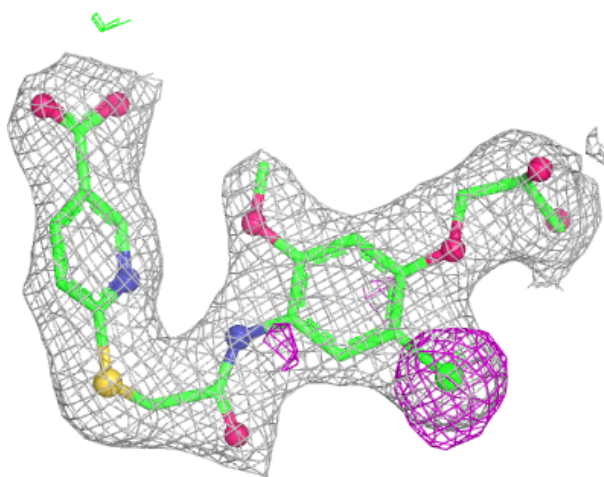
**Electron density around 1E5 F 402:**

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



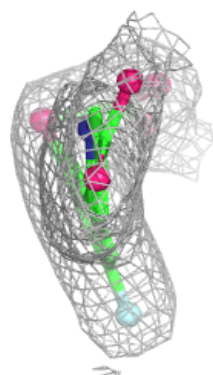
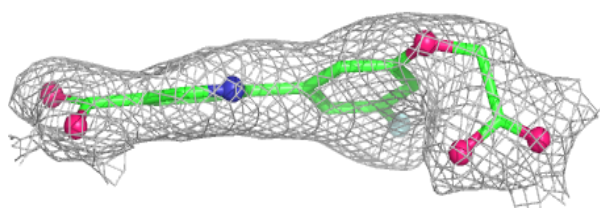
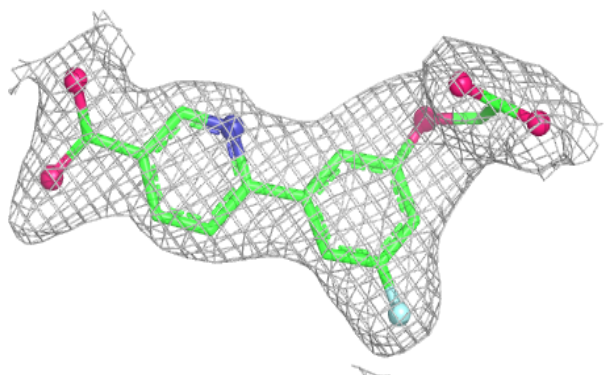
Electron density around 1E6 B 401:

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

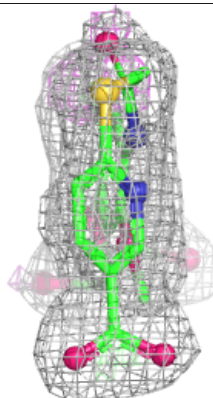
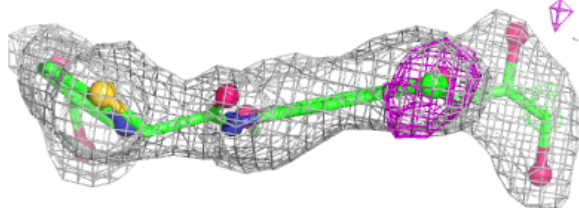
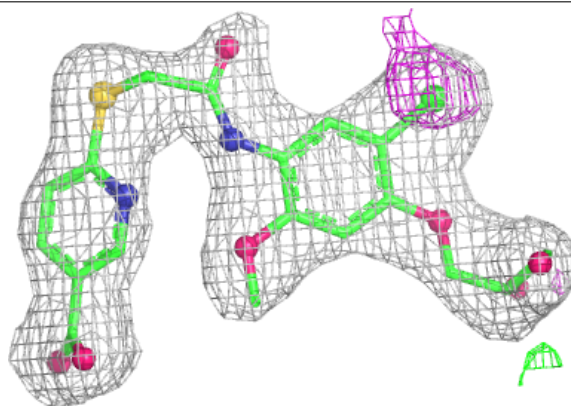


Electron density around 1E5 E 402:

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

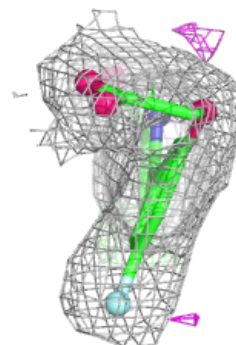
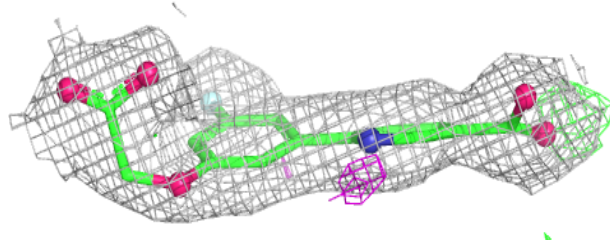
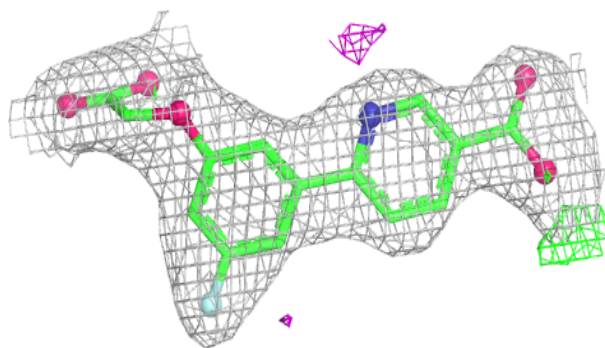
**Electron density around 1E6 C 401:**

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

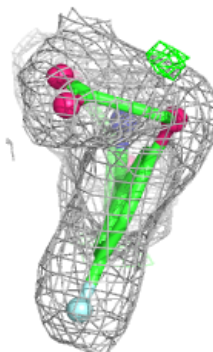
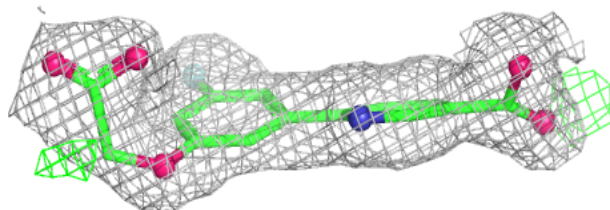
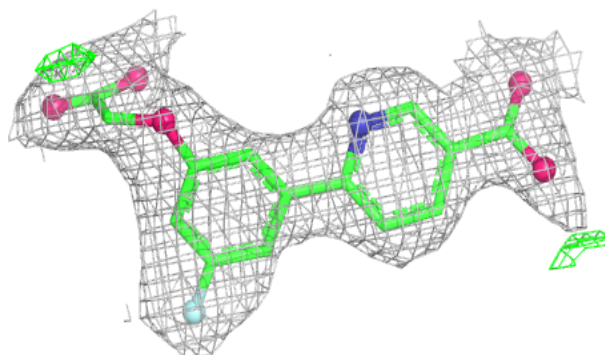


Electron density around 1E5 G 402:

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

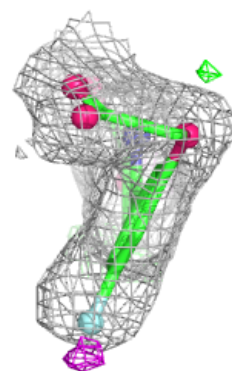
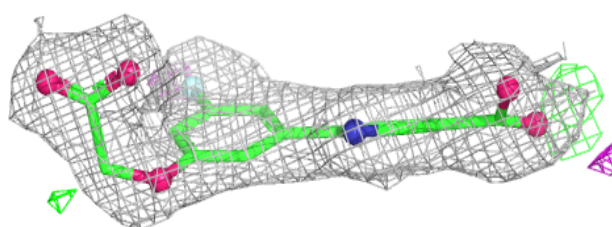
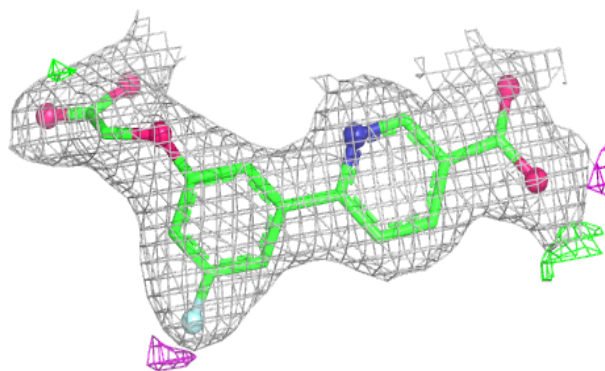
**Electron density around 1E5 H 402:**

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

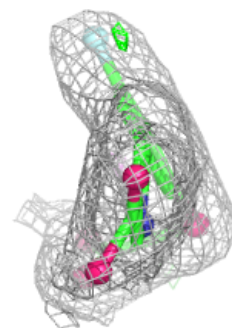
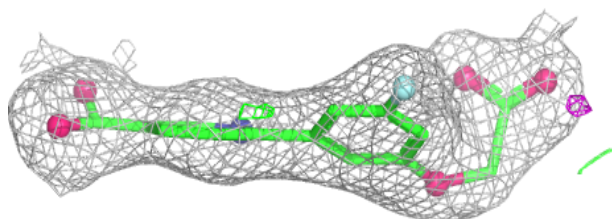


Electron density around 1E5 B 402:

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

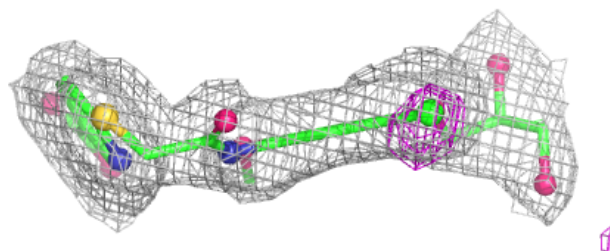
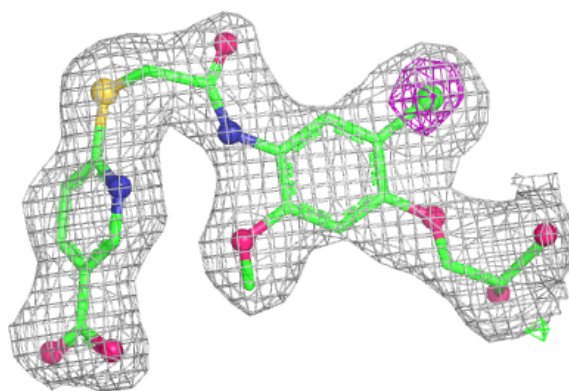
**Electron density around 1E5 C 402:**

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

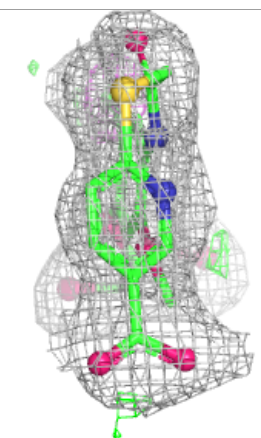
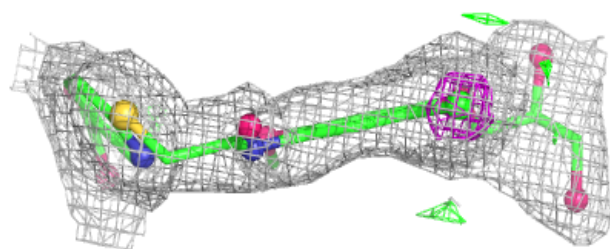
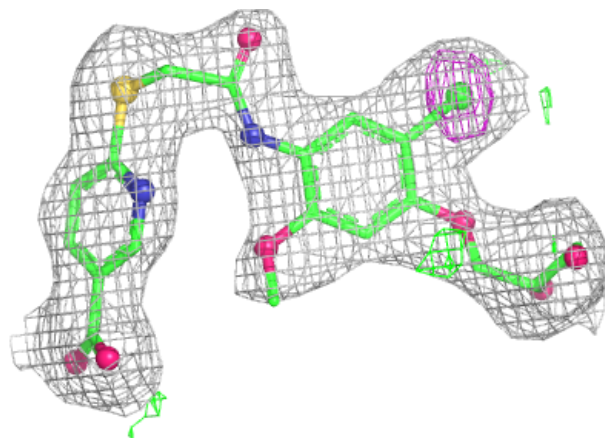


Electron density around 1E6 D 401:

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

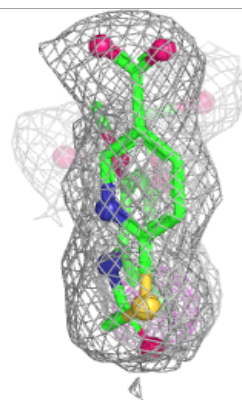
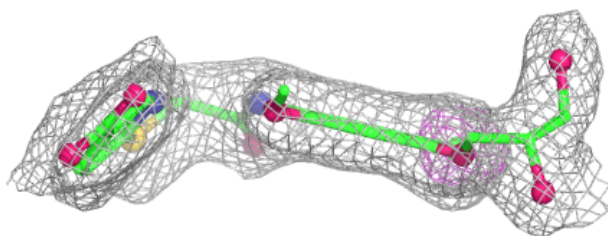
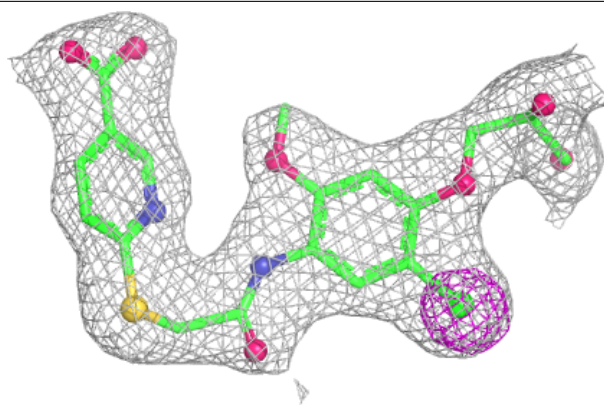
**Electron density around 1E6 F 401:**

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

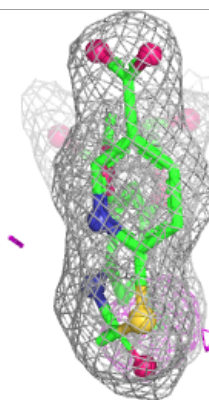
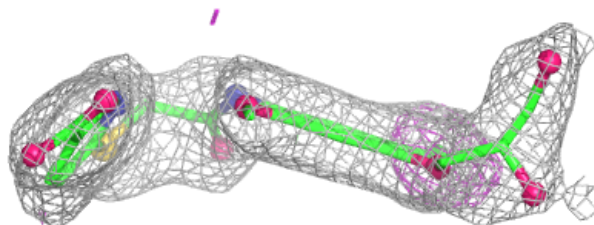
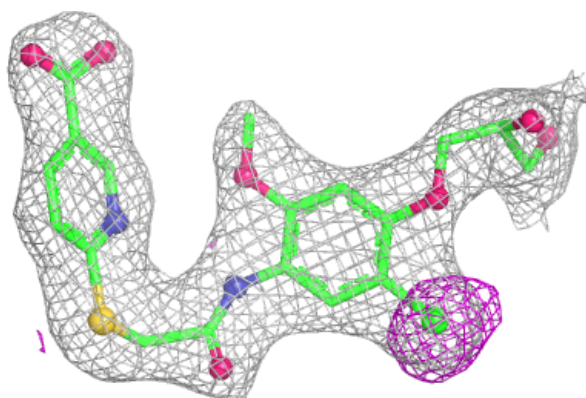


Electron density around 1E6 G 401:

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

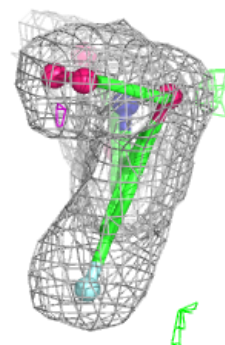
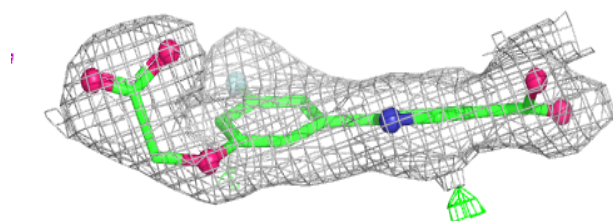
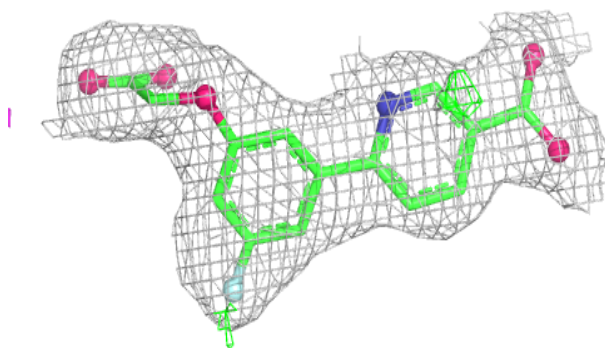
**Electron density around 1E6 H 401:**

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

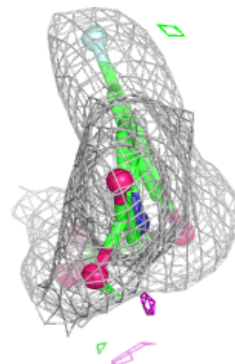
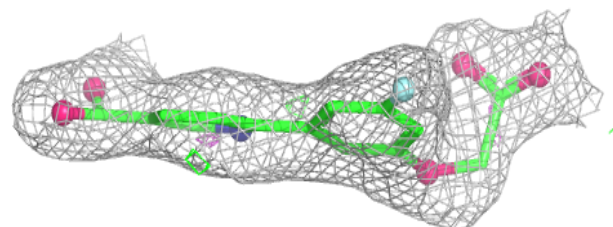
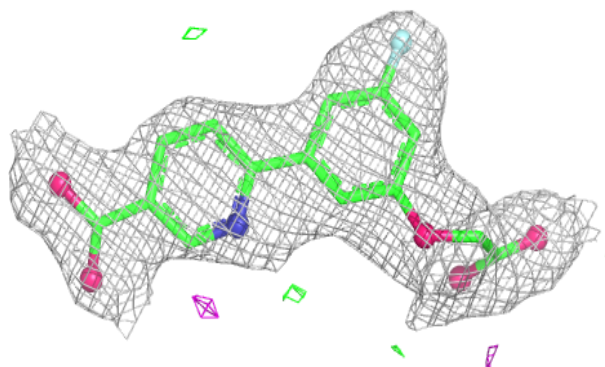


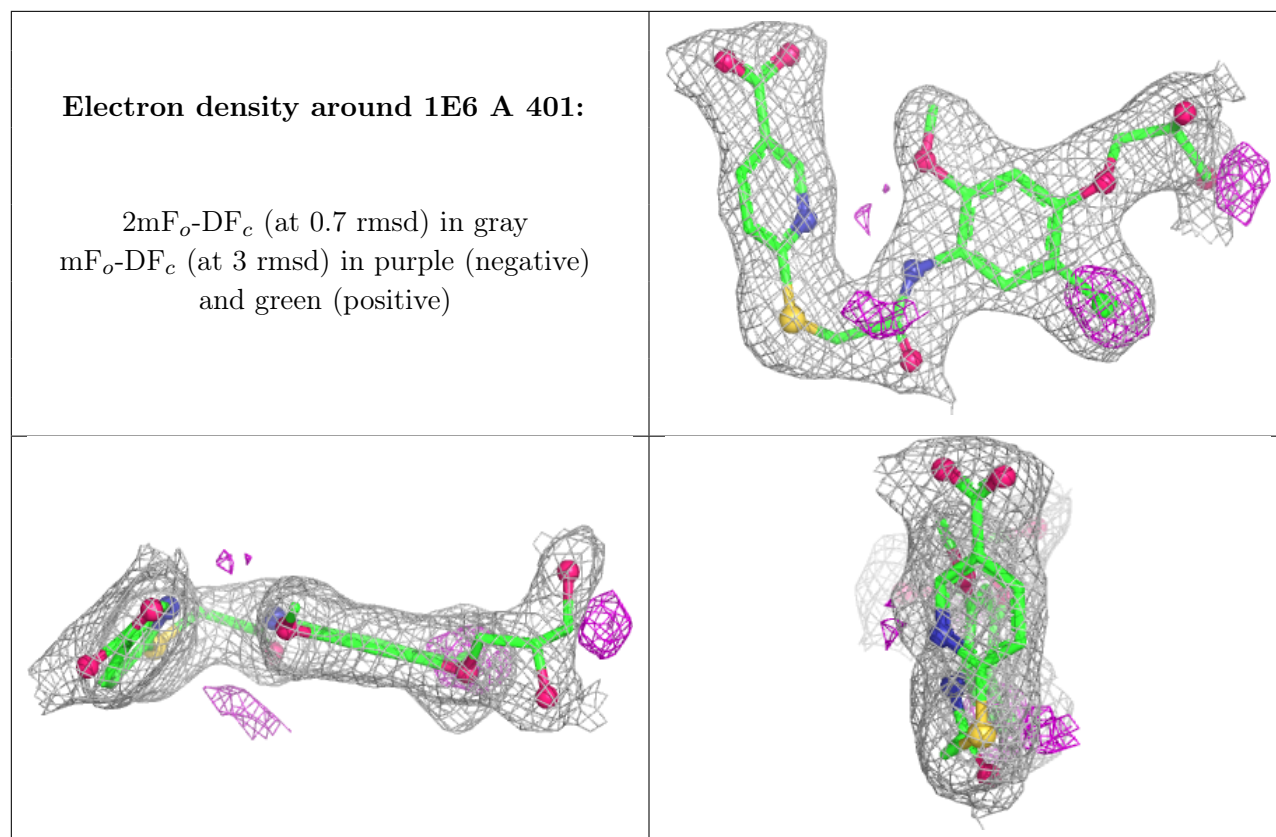
Electron density around 1E5 A 402:

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

**Electron density around 1E5 D 402:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.