



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:53 PM UTC

PDB ID : 8DDV / pdb_00008ddv
EMDB ID : EMD-27343
Title : Cryo-EM structure of TRPM3 ion channel in the presence of PIP2, state4
Authors : Zhao, C.; MacKinnon, R.
Deposited on : 2022-06-19
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

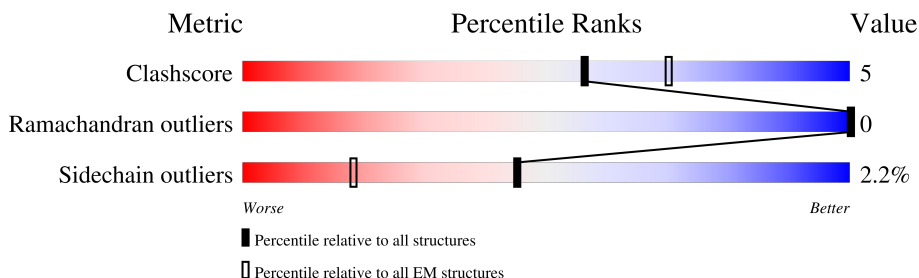
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1370	61% 9% . 29%
1	B	1370	62% 9% 29%
1	C	1370	62% 8% 29%
1	D	1370	62% 8% 29%
2	E	17	94% 6%
2	F	17	100%
2	G	17	94% 6%
2	H	17	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32230 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

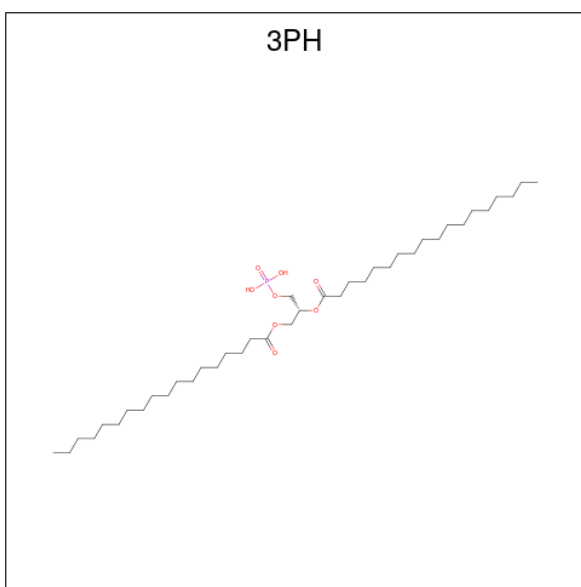
- Molecule 1 is a protein called Transient receptor potential cation channel, subfamily M, member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	B	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	C	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		
1	D	968	Total	C	N	O	S	2	0
			7841	5083	1327	1373	58		

- Molecule 2 is a protein called Unidentified segment at the N-terminus of TRPM3.

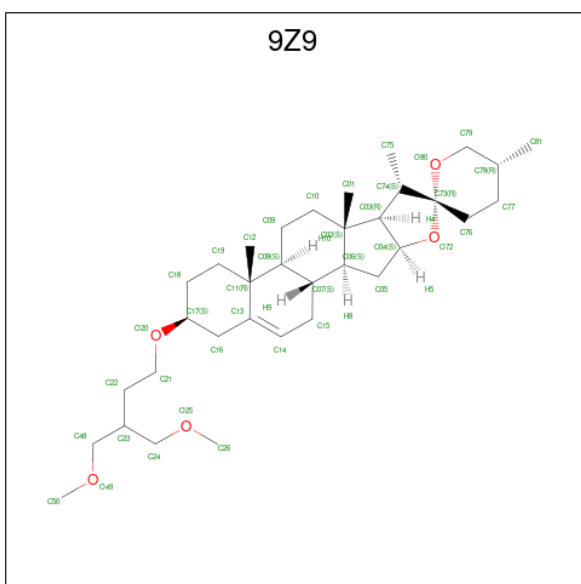
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	17	Total	C	N	O	0	0
			85	51	17	17		
2	F	17	Total	C	N	O	0	0
			85	51	17	17		
2	G	17	Total	C	N	O	0	0
			85	51	17	17		
2	H	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 3 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



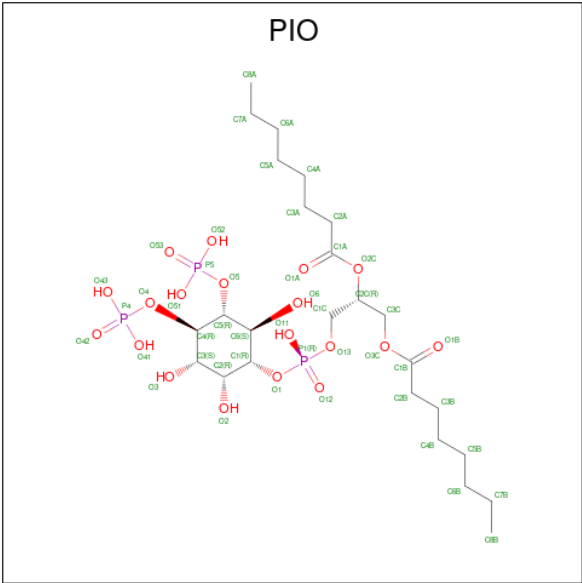
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			45	36	8	1	
3	B	1	Total	C	O	P	0
			45	36	8	1	
3	C	1	Total	C	O	P	0
			45	36	8	1	
3	D	1	Total	C	O	P	0
			45	36	8	1	

- Molecule 4 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (CCD ID: 9Z9) (formula: C₃₄H₅₆O₅).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			39	34	5	
4	A	1	Total	C	O	0
			39	34	5	
4	C	1	Total	C	O	0
			39	34	5	
4	C	1	Total	C	O	0
			39	34	5	

- Molecule 5 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			47	25	19	3	
5	B	1	Total	C	O	P	0
			47	25	19	3	
5	C	1	Total	C	O	P	0
			47	25	19	3	
5	D	1	Total	C	O	P	0
			47	25	19	3	

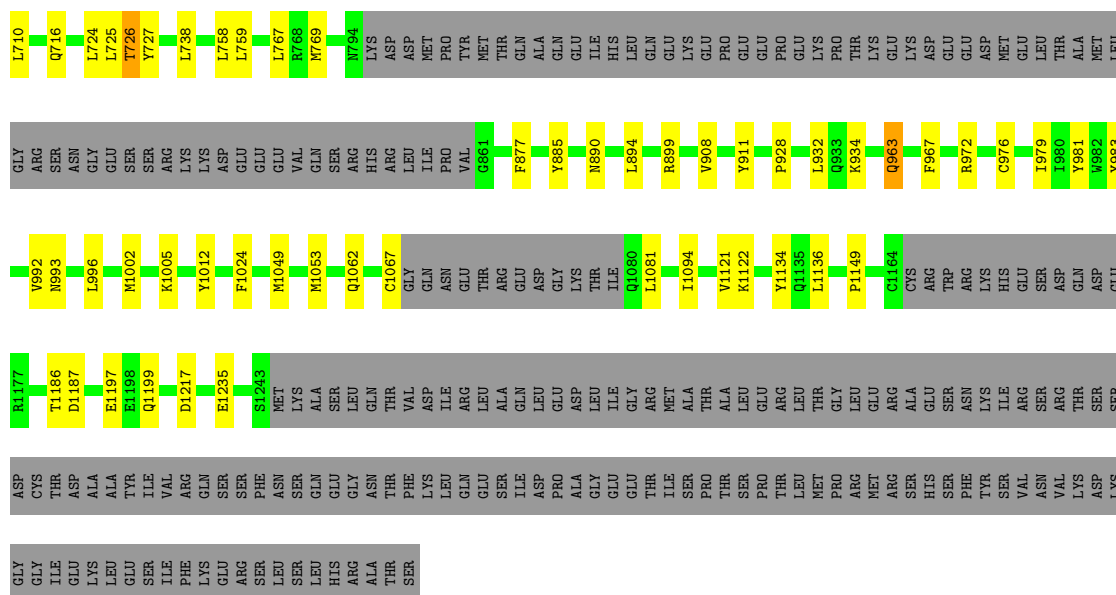
- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Na	0
			1	1	

Continued on next page...

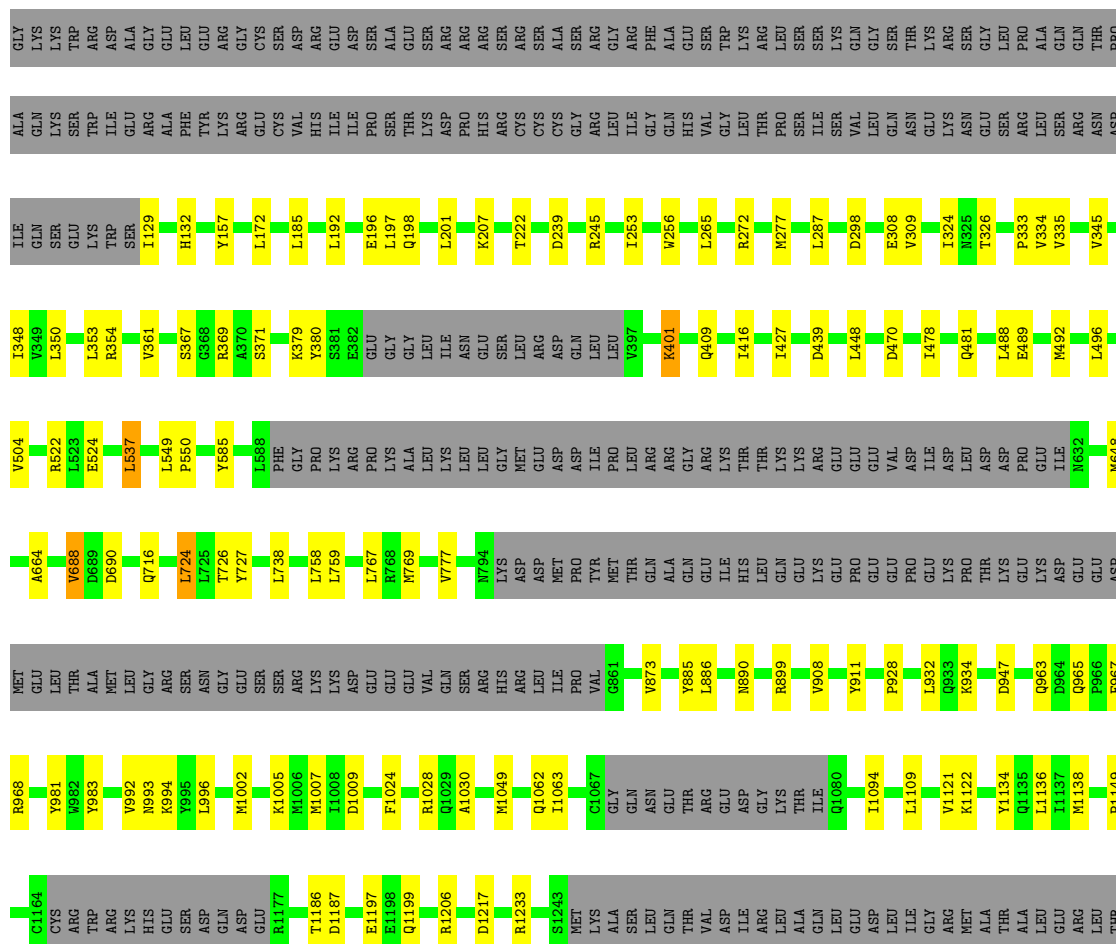
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
6	C	1	1	1	0



- Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

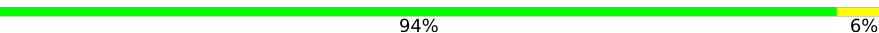
Chain D: 62% 8% 29%

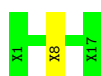


GLY LEU ARG MET ARG SER HIS SER PHE TYR SER VAL ASN ARG SER ARG THR SER SER ASP CYS THR ASP ALA ALA TYR ILE VAL ARG GLN SER PHE SER ASN SER GLN GLY ARG ALA ASN THR PHE LYS LEU GLN SER ILE ASP PRO GLY GLU THR ILE PRO SER PRO THR LEU MET

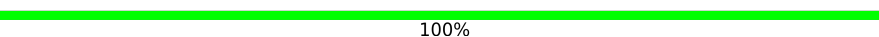
PRO ARG MET ARG SER HIS SER PHE TYR SER VAL ASN ARG SER ASP LYS GLY ILE GLU LYS LEU GLU SER ILE PHE LYS GLU SER ARG SER LEU SER LEU HIS ARG ALA THR SER

- Molecule 2: Unidentified segment at the N-terminus of TRPM3

Chain E:  94% 6%

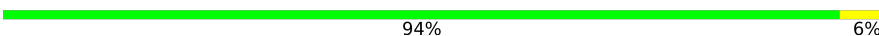
 X1 X8 X17

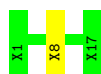
- Molecule 2: Unidentified segment at the N-terminus of TRPM3

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Unidentified segment at the N-terminus of TRPM3

Chain G:  94% 6%

 X1 X8 X17

- Molecule 2: Unidentified segment at the N-terminus of TRPM3

Chain H:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	62588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PH, 9Z9, NA, PIO

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	0.12	0/8023	0.27	0/10848
1	B	0.12	0/8023	0.28	0/10848
1	C	0.13	0/8023	0.28	0/10848
1	D	0.12	0/8023	0.28	0/10848
All	All	0.12	0/32092	0.28	0/43392

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 [i](#)

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	7841	0	7955	73	0
1	B	7841	0	7955	70	0
1	C	7841	0	7955	61	0
1	D	7841	0	7955	64	0
2	E	85	0	25	1	0
2	F	85	0	24	0	0
2	G	85	0	24	1	0
2	H	85	0	24	0	0
3	A	45	0	66	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	45	0	66	0	0
3	C	45	0	66	1	0
3	D	45	0	66	0	0
4	A	78	0	0	29	0
4	C	78	0	0	29	0
5	A	47	0	44	1	0
5	B	47	0	44	2	0
5	C	47	0	44	1	0
5	D	47	0	44	1	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
All	All	32230	0	32357	319	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 5.

All (319) 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)
4:C:1403:9Z9:C73	4:C:1403:9Z9:C74	1.81	1.58
4:A:1404:9Z9:C73	4:A:1404:9Z9:C74	1.81	1.57
4:A:1402:9Z9:C73	4:A:1402:9Z9:C74	1.80	1.56
4:C:1401:9Z9:C06	4:C:1401:9Z9:C07	1.84	1.56
4:C:1401:9Z9:C73	4:C:1401:9Z9:C74	1.81	1.55
4:A:1404:9Z9:C06	4:A:1404:9Z9:C07	1.84	1.52
4:C:1403:9Z9:C06	4:C:1403:9Z9:C07	1.84	1.51
4:A:1402:9Z9:C06	4:A:1402:9Z9:C07	1.84	1.50
4:A:1402:9Z9:C74	4:A:1402:9Z9:C75	1.90	1.49
4:A:1404:9Z9:C74	4:A:1404:9Z9:C75	1.90	1.49
4:C:1403:9Z9:C74	4:C:1403:9Z9:C75	1.90	1.47
4:C:1401:9Z9:C74	4:C:1401:9Z9:C75	1.90	1.47
4:C:1401:9Z9:C75	4:C:1401:9Z9:C03	2.31	1.08
4:A:1404:9Z9:C75	4:A:1404:9Z9:C03	2.31	1.08
4:C:1403:9Z9:C75	4:C:1403:9Z9:C03	2.32	1.08
4:A:1402:9Z9:C75	4:A:1402:9Z9:C03	2.33	1.07
4:C:1401:9Z9:C06	4:C:1401:9Z9:C02	1.78	1.01
4:A:1402:9Z9:C06	4:A:1402:9Z9:C02	1.78	1.00
4:A:1404:9Z9:C06	4:A:1404:9Z9:C02	1.78	0.96
4:A:1402:9Z9:C74	4:A:1402:9Z9:O80	2.14	0.95
4:A:1404:9Z9:C74	4:A:1404:9Z9:O80	2.15	0.94
4:C:1401:9Z9:C74	4:C:1401:9Z9:O80	2.15	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1403:9Z9:C74	4:C:1403:9Z9:O80	2.15	0.94
4:C:1403:9Z9:C06	4:C:1403:9Z9:C02	1.78	0.91
4:A:1402:9Z9:C07	4:A:1402:9Z9:C05	2.51	0.84
4:C:1403:9Z9:C07	4:C:1403:9Z9:C05	2.51	0.84
4:A:1404:9Z9:C06	4:A:1404:9Z9:C15	2.60	0.79
1:B:528:ASN:HD21	1:B:555:ILE:H	1.30	0.79
4:C:1403:9Z9:C06	4:C:1403:9Z9:C15	2.60	0.79
4:A:1402:9Z9:C06	4:A:1402:9Z9:C15	2.61	0.78
4:C:1401:9Z9:C06	4:C:1401:9Z9:C15	2.60	0.77
1:C:528:ASN:HD21	1:C:555:ILE:H	1.30	0.76
4:C:1401:9Z9:C07	4:C:1401:9Z9:C05	2.52	0.75
1:A:270:VAL:HG13	1:A:272:ARG:HH12	1.51	0.75
4:A:1404:9Z9:C07	4:A:1404:9Z9:C05	2.52	0.75
4:A:1402:9Z9:C06	4:A:1402:9Z9:C10	2.65	0.74
4:C:1401:9Z9:C06	4:C:1401:9Z9:C10	2.66	0.73
4:C:1403:9Z9:C06	4:C:1403:9Z9:C10	2.66	0.72
4:A:1404:9Z9:C06	4:A:1404:9Z9:C10	2.66	0.72
4:A:1404:9Z9:C75	4:A:1404:9Z9:O80	2.38	0.71
4:C:1403:9Z9:C75	4:C:1403:9Z9:O80	2.39	0.71
4:C:1401:9Z9:C75	4:C:1401:9Z9:O80	2.38	0.70
1:C:340:GLU:HB2	1:C:367:SER:HB3	1.73	0.70
4:C:1401:9Z9:C06	4:C:1401:9Z9:C08	2.69	0.69
4:A:1402:9Z9:C75	4:A:1402:9Z9:O80	2.41	0.69
4:A:1404:9Z9:C06	4:A:1404:9Z9:C08	2.69	0.69
4:A:1402:9Z9:C06	4:A:1402:9Z9:C08	2.69	0.69
1:B:270:VAL:H	1:B:272:ARG:HH21	1.40	0.67
4:C:1403:9Z9:C06	4:C:1403:9Z9:C08	2.69	0.67
1:C:205:PHE:HA	1:C:440:ILE:HD12	1.77	0.67
1:A:333:PRO:HB2	1:A:448:LEU:HD22	1.77	0.66
1:C:981:TYR:HB2	3:C:1402:3PH:H3C2	1.77	0.66
4:C:1401:9Z9:C06	4:C:1401:9Z9:C01	2.73	0.65
4:A:1402:9Z9:C06	4:A:1402:9Z9:C01	2.73	0.64
4:A:1404:9Z9:C06	4:A:1404:9Z9:C01	2.74	0.62
1:C:333:PRO:HB2	1:C:448:LEU:HD22	1.81	0.62
1:A:270:VAL:O	1:A:272:ARG:NH1	2.33	0.62
4:C:1403:9Z9:C06	4:C:1403:9Z9:C01	2.73	0.62
1:D:489:GLU:OE2	1:D:522:ARG:NH1	2.33	0.62
1:B:333:PRO:HB2	1:B:448:LEU:HD22	1.82	0.61
1:A:489:GLU:OE2	1:A:522:ARG:NH1	2.34	0.61
1:D:767:LEU:HD22	1:D:769:MET:HE2	1.83	0.60
1:A:767:LEU:HD22	1:A:769:MET:HE2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LEU:HD22	1:B:416:ILE:HG13	1.85	0.59
1:A:478:ILE:HG22	1:A:481:GLN:HE21	1.68	0.59
1:B:1002:MET:HE2	1:B:1122:LYS:HA	1.85	0.58
1:B:478:ILE:HG22	1:B:481:GLN:HE21	1.68	0.58
1:C:245:ARG:HD3	1:D:1206:ARG:HE	1.68	0.58
1:B:205:PHE:HA	1:B:440:ILE:HD12	1.85	0.58
1:C:341:GLY:HA3	1:C:345:VAL:HG21	1.86	0.58
1:D:478:ILE:HG22	1:D:481:GLN:HE21	1.68	0.58
1:C:767:LEU:HD22	1:C:769:MET:HE2	1.86	0.57
1:B:200:LYS:HB3	1:B:432:MET:HE1	1.85	0.57
1:C:992:VAL:HG23	1:C:1136:LEU:HD21	1.86	0.57
1:D:994:LYS:NZ	5:D:1402:PIO:O53	2.38	0.57
1:B:994:LYS:NZ	5:B:1402:PIO:O53	2.38	0.57
1:B:198:GLN:NE2	1:B:366:GLY:O	2.38	0.56
1:D:963:GLN:HG2	1:D:967:PHE:HD2	1.70	0.56
1:A:1206:ARG:HE	1:D:245:ARG:HD3	1.71	0.56
1:C:256:TRP:HB3	1:C:298:ASP:HB3	1.88	0.56
1:C:478:ILE:HG22	1:C:481:GLN:HE21	1.68	0.56
1:D:1002:MET:HE2	1:D:1122:LYS:HA	1.87	0.56
1:B:157:TYR:OH	1:B:265:LEU:O	2.23	0.56
1:D:947:ASP:OD1	1:D:981:TYR:OH	2.24	0.56
1:A:577:THR:O	1:A:582:ARG:NH1	2.39	0.56
1:D:890:ASN:ND2	1:D:983:TYR:OH	2.37	0.55
1:C:1002:MET:HE2	1:C:1122:LYS:HA	1.86	0.55
1:C:200:LYS:HB3	1:C:432:MET:HE1	1.89	0.55
1:B:963:GLN:HG2	1:B:967:PHE:HD2	1.70	0.55
1:B:890:ASN:ND2	1:B:983:TYR:OH	2.38	0.55
1:B:340:GLU:HB2	1:B:369:ARG:HB3	1.90	0.54
1:B:256:TRP:HB3	1:B:298:ASP:HB3	1.90	0.54
1:D:333:PRO:HB2	1:D:448:LEU:HD22	1.88	0.54
1:B:1067:CYS:HA	1:B:1081:LEU:HD11	1.88	0.54
1:A:245:ARG:HG2	1:B:1206:ARG:HD2	1.89	0.54
1:A:256:TRP:HB3	1:A:298:ASP:HB3	1.90	0.54
1:D:256:TRP:HB3	1:D:298:ASP:HB3	1.90	0.54
1:D:885:TYR:HE1	1:D:908:VAL:HG13	1.73	0.54
1:B:930:LYS:HG3	1:B:932:LEU:H	1.72	0.53
1:C:928:PRO:HD2	1:C:934:LYS:HG2	1.90	0.53
1:D:350:LEU:HD22	1:D:416:ILE:HG23	1.89	0.53
1:B:353:LEU:HD23	1:B:423:LYS:HB3	1.91	0.53
1:D:367:SER:OG	1:D:371:SER:OG	2.25	0.53
1:A:946:THR:HG21	3:A:1401:3PH:H331	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:MET:SD	1:C:281:MET:N	2.81	0.53
1:B:885:TYR:HE1	1:B:908:VAL:HG13	1.73	0.53
1:B:947:ASP:OD1	1:B:981:TYR:OH	2.25	0.53
1:C:885:TYR:HE1	1:C:908:VAL:HG13	1.73	0.53
1:D:992:VAL:HG23	1:D:1136:LEU:HD21	1.91	0.53
1:B:992:VAL:HG23	1:B:1136:LEU:HD21	1.91	0.53
1:A:1005:LYS:HD2	1:A:1121:VAL:HG13	1.91	0.53
1:B:965:GLN:OE1	1:B:968:ARG:NH2	2.42	0.53
1:D:965:GLN:OE1	1:D:968:ARG:NH2	2.42	0.53
1:A:1007:MET:HE1	3:A:1401:3PH:H262	1.91	0.52
1:A:992:VAL:HG23	1:A:1136:LEU:HD21	1.92	0.52
1:B:419:GLU:HG3	1:B:422:LYS:HE2	1.92	0.52
1:C:338:ILE:HB	1:C:363:VAL:HG12	1.91	0.52
1:C:993:ASN:HB3	1:C:996:LEU:HB2	1.90	0.52
1:A:885:TYR:HE1	1:A:908:VAL:HG13	1.73	0.52
1:A:759:LEU:HD21	1:A:1134:TYR:HD1	1.74	0.51
1:A:208:GLY:HA3	1:A:440:ILE:HB	1.91	0.51
1:D:759:LEU:HD21	1:D:1134:TYR:HD1	1.75	0.51
1:A:688:VAL:HG23	1:A:690:ASP:H	1.76	0.51
1:A:726:THR:HG23	1:A:758:LEU:HD21	1.93	0.51
1:B:899:ARG:NH1	1:B:963:GLN:O	2.43	0.51
1:D:726:THR:HG23	1:D:758:LEU:HD21	1.93	0.51
1:B:270:VAL:O	1:B:272:ARG:NE	2.43	0.51
1:B:549:LEU:HD12	1:B:550:PRO:HD2	1.93	0.51
1:C:129:ILE:HD12	1:C:132:HIS:HB2	1.93	0.51
1:C:726:THR:HG23	1:C:758:LEU:HD21	1.92	0.51
1:B:759:LEU:HD21	1:B:1134:TYR:HD1	1.74	0.50
1:A:963:GLN:HG2	1:A:967:PHE:HD2	1.76	0.50
1:B:345:VAL:HA	1:B:348:ILE:HG12	1.92	0.50
1:C:1002:MET:HG2	1:C:1121:VAL:HG12	1.93	0.50
1:C:963:GLN:HG2	1:C:967:PHE:HD2	1.75	0.50
1:B:1002:MET:HG2	1:B:1121:VAL:HG12	1.93	0.50
1:D:401:LYS:HE3	1:D:409:GLN:HG3	1.93	0.50
1:B:993:ASN:HB3	1:B:996:LEU:HB2	1.93	0.50
1:D:1028:ARG:HD2	1:D:1063:ILE:HG13	1.93	0.50
1:A:353:LEU:HD23	1:A:423:LYS:HB3	1.93	0.50
1:A:972:ARG:NH1	1:D:1030:ALA:O	2.44	0.50
1:C:239:ASP:O	1:C:243:LYS:NZ	2.44	0.50
1:D:185:LEU:HB3	1:D:334:VAL:HG12	1.93	0.50
1:D:928:PRO:HD2	1:D:934:LYS:HG2	1.94	0.50
1:B:1030:ALA:O	1:C:972:ARG:NH1	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:716:GLN:NE2	1:D:1199:GLN:OE1	2.44	0.49
1:A:129:ILE:HD12	1:A:132:HIS:HB2	1.94	0.49
1:A:344:ASN:OD1	1:A:347:SER:OG	2.28	0.49
1:A:353:LEU:HD21	1:A:427:ILE:HD11	1.93	0.49
1:D:1002:MET:HG2	1:D:1121:VAL:HG12	1.95	0.49
1:B:726:THR:HG23	1:B:758:LEU:HD21	1.93	0.49
1:C:335:VAL:HB	1:C:448:LEU:HD21	1.94	0.49
1:D:549:LEU:HD12	1:D:550:PRO:HD2	1.95	0.49
1:A:981:TYR:HB2	3:A:1401:3PH:H3C1	1.94	0.49
1:A:993:ASN:HB3	1:A:996:LEU:HB2	1.93	0.49
1:D:899:ARG:NH1	1:D:963:GLN:O	2.45	0.49
4:A:1402:9Z9:C06	4:A:1402:9Z9:C09	2.91	0.49
1:A:1002:MET:HG2	1:A:1121:VAL:HG12	1.95	0.49
1:D:129:ILE:HD12	1:D:132:HIS:HB2	1.95	0.48
1:B:335:VAL:HB	1:B:448:LEU:HD21	1.95	0.48
1:B:338:ILE:HB	1:B:363:VAL:HG12	1.95	0.48
4:C:1401:9Z9:C06	4:C:1401:9Z9:C09	2.91	0.48
4:C:1403:9Z9:C06	4:C:1403:9Z9:C09	2.91	0.48
1:D:335:VAL:HB	1:D:448:LEU:HD21	1.95	0.48
4:A:1404:9Z9:C06	4:A:1404:9Z9:C09	2.91	0.48
1:A:928:PRO:HD2	1:A:934:LYS:HG2	1.94	0.48
4:A:1402:9Z9:C07	4:A:1402:9Z9:C02	2.91	0.48
1:A:407:ARG:HB2	1:A:411:GLN:HB3	1.96	0.48
1:B:129:ILE:HD12	1:B:132:HIS:HB2	1.95	0.48
1:D:724:LEU:HD23	1:D:727:TYR:HE1	1.80	0.47
1:C:194:ASN:OD1	1:C:194:ASN:N	2.46	0.47
1:C:759:LEU:HD21	1:C:1134:TYR:HD1	1.79	0.47
1:C:1049:MET:HG3	1:C:1062:GLN:HE22	1.79	0.47
1:D:379:LYS:HD2	1:D:380:TYR:HB2	1.96	0.47
4:A:1404:9Z9:C07	4:A:1404:9Z9:C02	2.92	0.47
1:C:716:GLN:NE2	1:C:1199:GLN:OE1	2.44	0.47
1:A:369:ARG:HH11	1:A:405:TYR:HE1	1.62	0.47
1:C:1005:LYS:HD2	1:C:1121:VAL:HG13	1.95	0.47
1:A:890:ASN:ND2	1:A:983:TYR:OH	2.46	0.47
1:B:1005:LYS:HD2	1:B:1121:VAL:HG13	1.96	0.47
1:C:976:CYS:O	1:C:979:ILE:HG22	2.14	0.47
1:B:259:VAL:HG23	1:B:262:GLN:HG2	1.96	0.47
1:B:281:MET:SD	1:B:281:MET:N	2.84	0.47
1:A:976:CYS:O	1:A:979:ILE:HG22	2.14	0.47
1:C:313:ARG:NH2	1:C:355:ASP:OD2	2.48	0.47
1:D:993:ASN:HB3	1:D:996:LEU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:GLU:OE2	1:B:522:ARG:NE	2.37	0.46
1:C:664:ALA:N	1:C:1197:GLU:OE2	2.48	0.46
4:C:1403:9Z9:C07	4:C:1403:9Z9:C02	2.91	0.46
1:A:194:ASN:OD1	1:A:194:ASN:N	2.48	0.46
1:C:492:MET:HE1	1:C:504:VAL:HA	1.96	0.46
1:D:688:VAL:HG22	1:D:690:ASP:H	1.79	0.46
1:A:344:ASN:O	1:A:347:SER:OG	2.33	0.46
1:A:899:ARG:NH1	1:A:963:GLN:O	2.49	0.46
1:A:649:LYS:NZ	1:A:694:GLU:OE1	2.48	0.46
1:C:890:ASN:ND2	1:C:983:TYR:OH	2.46	0.46
1:D:345:VAL:HA	1:D:348:ILE:HG12	1.98	0.46
1:B:664:ALA:N	1:B:1197:GLU:OE2	2.49	0.46
1:B:649:LYS:NZ	1:B:694:GLU:OE1	2.49	0.46
1:B:190:GLY:HA3	1:B:229:VAL:HG11	1.99	0.45
1:B:928:PRO:HD2	1:B:934:LYS:HG2	1.98	0.45
4:C:1401:9Z9:C07	4:C:1401:9Z9:C02	2.92	0.45
1:C:369:ARG:HD3	1:C:369:ARG:HA	1.82	0.45
1:C:159:ARG:NH2	1:C:298:ASP:OD2	2.49	0.45
1:C:899:ARG:NH1	1:C:963:GLN:O	2.49	0.45
1:D:664:ALA:N	1:D:1197:GLU:OE2	2.49	0.45
1:A:1007:MET:HE1	3:A:1401:3PH:H281	1.98	0.45
1:A:346:ILE:HD11	1:A:370:ALA:HB1	1.99	0.45
1:B:353:LEU:HD21	1:B:427:ILE:HD11	1.99	0.45
1:A:431:ARG:HB2	1:A:434:SER:HB2	1.97	0.45
1:D:369:ARG:HD3	1:D:369:ARG:HA	1.82	0.45
1:A:205:PHE:HA	1:A:440:ILE:HG13	1.99	0.45
1:A:265:LEU:HA	1:A:272:ARG:HD3	1.99	0.45
1:C:356:THR:HB	1:C:357:PRO:HD3	1.99	0.45
1:D:157:TYR:OH	1:D:265:LEU:O	2.31	0.45
1:A:245:ARG:HH11	1:B:1206:ARG:HH11	1.65	0.44
1:A:345:VAL:HA	1:A:348:ILE:HG12	1.99	0.44
1:B:356:THR:HB	1:B:357:PRO:HD3	1.99	0.44
1:D:537:LEU:HD12	1:D:648:MET:HG2	1.99	0.44
1:C:253:ILE:HG22	1:C:308:GLU:HB2	2.00	0.44
1:D:265:LEU:HA	1:D:272:ARG:HD3	1.98	0.44
1:A:1186:THR:OG1	1:A:1187:ASP:N	2.50	0.44
1:D:207:LYS:HZ1	1:D:239:ASP:HB3	1.83	0.44
1:B:724:LEU:HD12	1:B:727:TYR:HE1	1.82	0.43
5:B:1402:PIO:H3A	5:B:1402:PIO:H3CA	2.00	0.43
1:C:508:ILE:HD11	1:C:514:MET:HE2	2.00	0.43
1:B:369:ARG:HD3	1:B:369:ARG:HA	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ALA:N	1:A:1197:GLU:OE2	2.48	0.43
5:A:1403:PIO:H8BB	5:A:1403:PIO:H5B	1.78	0.43
4:A:1402:9Z9:C05	4:A:1402:9Z9:C01	2.86	0.43
5:C:1404:PIO:H8BB	5:C:1404:PIO:H5BA	1.78	0.43
1:D:1024:PHE:HD1	1:D:1094:ILE:HG22	1.83	0.43
1:B:1041:LYS:HE3	1:B:1041:LYS:HB3	1.89	0.43
1:A:350:LEU:HD22	1:A:416:ILE:HG23	2.01	0.43
1:C:576:TYR:OH	1:C:640:GLU:HG3	2.19	0.43
1:D:963:GLN:HB3	1:D:967:PHE:HB2	2.01	0.43
1:B:421:MET:O	1:B:424:LYS:HB2	2.19	0.43
1:D:777:VAL:HG13	1:D:873:VAL:HG22	2.01	0.43
1:C:688:VAL:HG22	1:C:690:ASP:H	1.84	0.43
1:C:724:LEU:HD12	1:C:727:TYR:HE1	1.83	0.43
1:D:524:GLU:OE1	1:D:585:TYR:OH	2.30	0.43
1:A:136:SER:O	2:E:8:UNK:N	2.51	0.42
1:A:724:LEU:HD12	1:A:727:TYR:HE1	1.84	0.42
1:D:1186:THR:OG1	1:D:1187:ASP:N	2.51	0.42
1:A:133:THR:HG21	1:A:300:GLY:HA3	2.01	0.42
1:C:1186:THR:OG1	1:C:1187:ASP:N	2.51	0.42
1:A:175:LYS:O	1:A:178:GLN:NE2	2.53	0.42
1:B:1186:THR:OG1	1:B:1187:ASP:N	2.51	0.42
1:C:1067:CYS:HA	1:C:1081:LEU:HD11	2.01	0.42
4:C:1401:9Z9:C05	4:C:1401:9Z9:C01	2.86	0.42
1:D:324:ILE:HG23	1:D:326:THR:H	1.83	0.42
1:D:439:ASP:OD1	1:D:439:ASP:N	2.46	0.42
1:A:259:VAL:HG12	1:A:287:LEU:HD13	2.01	0.42
1:A:1049:MET:HE3	1:A:1062:GLN:HE22	1.84	0.42
1:A:1231:SER:HB2	1:B:1230:MET:HE2	2.02	0.42
1:A:324:ILE:O	1:A:327:ARG:NH1	2.52	0.42
1:A:738:LEU:HD23	1:A:738:LEU:HA	1.92	0.42
1:C:345:VAL:HA	1:C:348:ILE:HG12	2.00	0.42
1:B:194:ASN:OD1	1:B:194:ASN:N	2.51	0.42
1:B:963:GLN:HB3	1:B:967:PHE:HB2	2.01	0.42
1:D:492:MET:HE1	1:D:504:VAL:HA	2.01	0.42
1:A:356:THR:HB	1:A:357:PRO:HD3	2.02	0.42
1:C:324:ILE:HG23	1:C:326:THR:H	1.84	0.42
1:C:911:TYR:CE1	1:C:1149:PRO:HD3	2.55	0.42
1:A:278:SER:HB2	1:A:286:VAL:HB	2.01	0.42
1:B:710:LEU:HD13	1:B:725:LEU:HD21	2.02	0.42
1:C:738:LEU:HD23	1:C:738:LEU:HA	1.92	0.42
1:D:1049:MET:HE3	1:D:1062:GLN:HE22	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:HB3	1:B:367:SER:HB3	2.01	0.41
1:C:470:ASP:OD1	1:C:470:ASP:N	2.52	0.41
1:D:886:LEU:HD23	1:D:886:LEU:HA	1.92	0.41
1:D:1007:MET:HE2	1:D:1007:MET:HB3	2.00	0.41
1:A:1006:MET:HG3	1:D:1109:LEU:HD13	2.02	0.41
1:B:1024:PHE:HD1	1:B:1094:ILE:HG22	1.85	0.41
1:C:1053:MET:HE2	1:C:1053:MET:HB3	1.87	0.41
1:D:353:LEU:HD21	1:D:427:ILE:HD11	2.02	0.41
1:D:911:TYR:CE1	1:D:1149:PRO:HD3	2.55	0.41
1:A:1067:CYS:HA	1:A:1081:LEU:HD11	2.03	0.41
1:B:342:GLY:HA2	1:B:405:TYR:OH	2.21	0.41
1:C:1187:ASP:N	1:C:1187:ASP:OD1	2.54	0.41
1:A:549:LEU:HD12	1:A:550:PRO:HD2	2.02	0.41
1:A:865:TYR:O	1:A:869:ASN:ND2	2.53	0.41
1:C:136:SER:O	2:G:8:UNK:N	2.54	0.41
1:B:1046:ILE:HD11	1:C:894:LEU:HD11	2.03	0.41
1:D:253:ILE:HG22	1:D:308:GLU:HB2	2.03	0.41
1:B:777:VAL:HG13	1:B:873:VAL:HG22	2.02	0.41
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.93	0.41
1:B:1187:ASP:N	1:B:1187:ASP:OD1	2.53	0.41
1:C:336:ALA:HB3	1:C:361:VAL:HG12	2.03	0.41
1:A:470:ASP:OD1	1:A:470:ASP:N	2.53	0.41
1:A:1024:PHE:HD1	1:A:1094:ILE:HG22	1.84	0.41
1:B:253:ILE:HG22	1:B:308:GLU:HB2	2.02	0.41
1:B:478:ILE:HD12	1:B:478:ILE:HA	1.99	0.41
1:C:1235:GLU:OE2	1:D:1233:ARG:NE	2.54	0.41
1:D:470:ASP:N	1:D:470:ASP:OD1	2.53	0.41
1:A:640:GLU:N	1:A:640:GLU:OE1	2.54	0.41
1:A:911:TYR:CE1	1:A:1149:PRO:HD3	2.55	0.41
1:B:565:GLU:OE2	1:B:577:THR:OG1	2.29	0.41
1:B:911:TYR:CE1	1:B:1149:PRO:HD3	2.56	0.41
1:C:641:LEU:HD23	1:C:641:LEU:HA	1.94	0.41
1:C:1024:PHE:HD1	1:C:1094:ILE:HG22	1.86	0.41
1:D:738:LEU:HD23	1:D:738:LEU:HA	1.92	0.41
1:D:1005:LYS:HD2	1:D:1121:VAL:HG13	2.02	0.41
1:B:419:GLU:O	1:B:422:LYS:HG2	2.22	0.40
1:B:1002:MET:O	1:B:1006:MET:HG2	2.21	0.40
1:B:1028:ARG:HD2	1:B:1063:ILE:HG13	2.02	0.40
1:C:350:LEU:HD21	1:C:354:ARG:NH2	2.36	0.40
1:D:197:LEU:HD22	1:D:201:LEU:HD23	2.03	0.40
1:A:267:GLY:HA3	1:A:272: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:A:1028:ARG:HD2	1:A:1063:ILE:HG13	2.01	0.40
1:D:488:LEU:HD23	1:D:488:LEU:HA	1.94	0.40
1:A:324:ILE:HG23	1:A:326:THR:H	1.85	0.40
1:A:710:LEU:HD13	1:A:725:LEU:HD21	2.03	0.40
1:D:287:LEU:HD12	1:D:287:LEU:HA	1.96	0.40
1:D:350:LEU:HD21	1:D:354:ARG:NH2	2.35	0.40
1:A:207:LYS:HD3	1:A:207:LYS:HA	1.84	0.40
1:A:1041:LYS:HE3	1:A:1041:LYS:HB3	1.88	0.40
1:B:1063:ILE:HD13	1:B:1095:MET:SD	2.62	0.40
1:C:710:LEU:HD13	1:C:725:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	956/1370 (70%)	920 (96%)	36 (4%)	0	100	100
1	B	956/1370 (70%)	926 (97%)	30 (3%)	0	100	100
1	C	956/1370 (70%)	921 (96%)	35 (4%)	0	100	100
1	D	956/1370 (70%)	919 (96%)	37 (4%)	0	100	100
All	All	3824/5480 (70%)	3686 (96%)	138 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	859/1218 (70%)	836 (97%)	23 (3%)	39	68
1	B	859/1218 (70%)	840 (98%)	19 (2%)	45	71
1	C	859/1218 (70%)	843 (98%)	16 (2%)	50	73
1	D	859/1218 (70%)	842 (98%)	17 (2%)	48	72
All	All	3436/4872 (70%)	3361 (98%)	75 (2%)	45	71

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	198	GLN
1	A	222	THR
1	A	240	HIS
1	A	260	GLU
1	A	270	VAL
1	A	309	VAL
1	A	326	THR
1	A	335	VAL
1	A	353	LEU
1	A	361	VAL
1	A	397	VAL
1	A	421	MET
1	A	496	LEU
1	A	567	LEU
1	A	577	THR
1	A	726	THR
1	A	963	GLN
1	A	1012	TYR
1	A	1013	PHE
1	A	1014	VAL
1	A	1150	LEU
1	A	1217	ASP
1	B	188	VAL
1	B	194	ASN
1	B	198	GLN
1	B	222	THR
1	B	270	VAL
1	B	271	VAL
1	B	309	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	326	THR
1	B	361	VAL
1	B	380	TYR
1	B	442	LEU
1	B	496	LEU
1	B	567	LEU
1	B	726	THR
1	B	932	LEU
1	B	1012	TYR
1	B	1014	VAL
1	B	1187	ASP
1	B	1217	ASP
1	C	194	ASN
1	C	239	ASP
1	C	271	VAL
1	C	309	VAL
1	C	339	VAL
1	C	397	VAL
1	C	442	LEU
1	C	479	TYR
1	C	496	LEU
1	C	567	LEU
1	C	726	THR
1	C	877	PHE
1	C	932	LEU
1	C	963	GLN
1	C	1012	TYR
1	C	1217	ASP
1	D	172	LEU
1	D	192	LEU
1	D	196	GLU
1	D	198	GLN
1	D	222	THR
1	D	277	MET
1	D	309	VAL
1	D	361	VAL
1	D	401	LYS
1	D	496	LEU
1	D	537	LEU
1	D	688	VAL
1	D	724	LEU
1	D	932	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1009	ASP
1	D	1138	MET
1	D	1217	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	261	ASN
1	A	279	ASN
1	A	293	HIS
1	A	314	GLN
1	A	481	GLN
1	A	940	GLN
1	A	978	ASN
1	A	1062	GLN
1	A	1115	ASN
1	A	1116	ASN
1	A	1213	ASN
1	A	1229	ASN
1	A	1238	ASN
1	B	293	HIS
1	B	437	HIS
1	B	481	GLN
1	B	528	ASN
1	B	633	HIS
1	B	940	GLN
1	B	978	ASN
1	B	1115	ASN
1	B	1116	ASN
1	B	1213	ASN
1	B	1242	HIS
1	C	261	ASN
1	C	262	GLN
1	C	275	GLN
1	C	288	ASN
1	C	314	GLN
1	C	344	ASN
1	C	411	GLN
1	C	437	HIS
1	C	481	GLN
1	C	528	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	633	HIS
1	C	1115	ASN
1	C	1116	ASN
1	C	1141	HIS
1	C	1213	ASN
1	C	1238	ASN
1	D	153	ASN
1	D	232	HIS
1	D	261	ASN
1	D	293	HIS
1	D	314	GLN
1	D	437	HIS
1	D	481	GLN
1	D	731	ASN
1	D	890	ASN
1	D	978	ASN
1	D	1062	GLN
1	D	1115	ASN
1	D	1116	ASN
1	D	1155	HIS
1	D	1213	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PIO	B	1402	-	47,47,47	1.21	6 (12%)	62,65,65	0.99	2 (3%)
5	PIO	D	1402	-	47,47,47	1.22	6 (12%)	62,65,65	1.12	4 (6%)
3	3PH	D	1401	-	44,44,47	1.17	3 (6%)	47,49,52	1.16	2 (4%)
5	PIO	A	1403	-	47,47,47	1.20	6 (12%)	62,65,65	1.03	2 (3%)
5	PIO	C	1404	-	47,47,47	1.20	6 (12%)	62,65,65	1.00	2 (3%)
3	3PH	B	1401	-	44,44,47	1.16	3 (6%)	47,49,52	1.16	2 (4%)
4	9Z9	C	1403	-	44,44,44	9.36	23 (52%)	64,68,68	4.90	24 (37%)
3	3PH	C	1402	-	44,44,47	1.16	3 (6%)	47,49,52	1.17	2 (4%)
4	9Z9	A	1402	-	44,44,44	9.36	22 (50%)	64,68,68	4.93	24 (37%)
3	3PH	A	1401	-	44,44,47	1.17	3 (6%)	47,49,52	1.16	2 (4%)
4	9Z9	C	1401	-	44,44,44	9.36	22 (50%)	64,68,68	4.91	25 (39%)
4	9Z9	A	1404	-	44,44,44	9.36	23 (52%)	64,68,68	4.91	25 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PIO	B	1402	-	-	20/44/68/68	0/1/1/1
5	PIO	D	1402	-	-	21/44/68/68	0/1/1/1
3	3PH	D	1401	-	-	25/46/46/49	-
5	PIO	A	1403	-	-	18/44/68/68	0/1/1/1
5	PIO	C	1404	-	-	16/44/68/68	0/1/1/1
3	3PH	B	1401	-	-	25/46/46/49	-
4	9Z9	C	1403	-	-	2/12/100/100	0/6/6/6
3	3PH	C	1402	-	-	26/46/46/49	-
4	9Z9	A	1402	-	-	2/12/100/100	0/6/6/6
3	3PH	A	1401	-	-	24/46/46/49	-
4	9Z9	C	1401	-	-	2/12/100/100	0/6/6/6
4	9Z9	A	1404	-	-	2/12/100/100	0/6/6/6

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1401	9Z9	C02-C03	-29.60	1.01	1.56
4	A	1404	9Z9	C02-C03	-29.59	1.01	1.56
4	C	1403	9Z9	C02-C03	-29.58	1.01	1.56
4	A	1402	9Z9	C02-C03	-29.56	1.01	1.56
4	C	1401	9Z9	C03-C74	-24.99	0.83	1.54
4	A	1404	9Z9	C03-C74	-24.98	0.83	1.54
4	C	1403	9Z9	C03-C74	-24.94	0.83	1.54
4	A	1402	9Z9	C03-C74	-24.87	0.84	1.54
4	A	1402	9Z9	C05-C06	-23.14	1.04	1.54
4	C	1403	9Z9	C05-C06	-23.09	1.04	1.54
4	C	1401	9Z9	C05-C06	-23.08	1.04	1.54
4	A	1404	9Z9	C05-C06	-23.06	1.04	1.54
4	A	1402	9Z9	O72-C73	-18.58	1.03	1.42
4	C	1403	9Z9	O72-C73	-18.55	1.03	1.42
4	C	1401	9Z9	O72-C73	-18.53	1.03	1.42
4	A	1404	9Z9	O72-C73	-18.47	1.03	1.42
4	A	1402	9Z9	C75-C74	17.82	1.90	1.53
4	C	1401	9Z9	C75-C74	17.75	1.90	1.53
4	C	1403	9Z9	C75-C74	17.73	1.90	1.53
4	A	1404	9Z9	C75-C74	17.71	1.90	1.53
4	C	1401	9Z9	C07-C06	16.40	1.84	1.53
4	A	1402	9Z9	C07-C06	16.39	1.84	1.53
4	A	1404	9Z9	C07-C06	16.37	1.84	1.53
4	C	1403	9Z9	C07-C06	16.36	1.84	1.53
4	A	1404	9Z9	C73-C74	14.27	1.81	1.53
4	C	1401	9Z9	C73-C74	14.23	1.81	1.53
4	C	1403	9Z9	C73-C74	14.22	1.81	1.53
4	A	1402	9Z9	C73-C74	14.11	1.80	1.53
4	A	1402	9Z9	C02-C06	12.92	1.78	1.55
4	A	1404	9Z9	C02-C06	12.91	1.78	1.55
4	C	1403	9Z9	C02-C06	12.91	1.78	1.55
4	C	1401	9Z9	C02-C06	12.87	1.78	1.55
4	C	1403	9Z9	C10-C09	-12.18	1.29	1.53
4	A	1402	9Z9	C10-C09	-12.17	1.29	1.53
4	C	1401	9Z9	C10-C09	-12.14	1.29	1.53
4	A	1404	9Z9	C10-C09	-12.12	1.29	1.53
4	A	1404	9Z9	C15-C07	-10.00	1.37	1.53
4	C	1401	9Z9	C15-C07	-9.97	1.37	1.53
4	A	1402	9Z9	C15-C07	-9.96	1.37	1.53
4	C	1403	9Z9	C15-C07	-9.92	1.37	1.53
4	A	1404	9Z9	C10-C02	9.38	1.70	1.54
4	A	1402	9Z9	C10-C02	9.36	1.70	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1403	9Z9	C10-C02	9.36	1.70	1.54
4	C	1401	9Z9	C10-C02	9.36	1.70	1.54
4	A	1404	9Z9	C03-C04	-5.92	1.43	1.54
4	C	1401	9Z9	C03-C04	-5.91	1.43	1.54
4	C	1403	9Z9	C03-C04	-5.84	1.43	1.54
4	A	1402	9Z9	C03-C04	-5.82	1.43	1.54
4	A	1402	9Z9	C14-C13	5.73	1.44	1.33
4	C	1403	9Z9	C14-C13	5.71	1.44	1.33
4	C	1401	9Z9	C14-C13	5.68	1.44	1.33
4	A	1404	9Z9	C14-C13	5.66	1.44	1.33
4	A	1404	9Z9	C09-C08	-4.78	1.45	1.53
4	C	1403	9Z9	C09-C08	-4.77	1.45	1.53
4	C	1401	9Z9	C09-C08	-4.76	1.45	1.53
4	A	1402	9Z9	C09-C08	-4.73	1.46	1.53
4	A	1404	9Z9	C15-C14	4.14	1.58	1.50
4	C	1401	9Z9	C15-C14	4.14	1.58	1.50
4	C	1403	9Z9	C15-C14	4.13	1.58	1.50
4	A	1402	9Z9	C15-C14	4.13	1.58	1.50
4	A	1404	9Z9	C19-C18	3.77	1.60	1.53
4	C	1401	9Z9	C19-C18	3.77	1.60	1.53
4	C	1403	9Z9	C19-C18	3.76	1.60	1.53
4	A	1402	9Z9	C19-C18	3.75	1.60	1.53
5	B	1402	PIO	P4-O4	3.62	1.65	1.59
5	D	1402	PIO	P4-O4	3.57	1.65	1.59
5	D	1402	PIO	P5-O5	3.39	1.65	1.59
5	C	1404	PIO	P5-O5	3.30	1.65	1.59
5	A	1403	PIO	P5-O5	3.28	1.65	1.59
5	A	1403	PIO	P4-O4	3.27	1.65	1.59
5	C	1404	PIO	P4-O4	3.27	1.65	1.59
5	B	1402	PIO	P5-O5	3.26	1.65	1.59
4	C	1401	9Z9	C11-C08	3.24	1.61	1.56
4	A	1404	9Z9	C11-C08	3.23	1.61	1.56
4	C	1403	9Z9	C11-C08	3.21	1.61	1.56
4	A	1402	9Z9	C11-C08	3.19	1.61	1.56
4	A	1402	9Z9	C01-C02	3.17	1.59	1.54
4	C	1403	9Z9	C01-C02	3.13	1.59	1.54
4	C	1401	9Z9	C01-C02	3.09	1.59	1.54
4	A	1404	9Z9	C01-C02	3.04	1.59	1.54
3	A	1401	3PH	O31-C31	2.97	1.42	1.33
3	D	1401	3PH	O31-C31	2.92	1.41	1.33
3	C	1402	3PH	O31-C31	2.92	1.41	1.33
3	A	1401	3PH	O21-C21	2.92	1.42	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1401	3PH	O31-C31	2.91	1.41	1.33
3	D	1401	3PH	O21-C21	2.88	1.42	1.34
3	C	1402	3PH	O21-C21	2.87	1.42	1.34
4	A	1402	9Z9	C19-C11	-2.86	1.49	1.54
4	C	1403	9Z9	C19-C11	-2.85	1.49	1.54
4	C	1401	9Z9	C19-C11	-2.83	1.49	1.54
3	B	1401	3PH	O21-C21	2.83	1.42	1.34
4	C	1401	9Z9	C07-C08	-2.80	1.48	1.53
4	A	1404	9Z9	C19-C11	-2.79	1.49	1.54
4	A	1402	9Z9	C07-C08	-2.79	1.48	1.53
4	A	1402	9Z9	C18-C17	2.77	1.58	1.51
4	A	1404	9Z9	C07-C08	-2.77	1.48	1.53
4	C	1403	9Z9	C07-C08	-2.76	1.48	1.53
4	C	1403	9Z9	C18-C17	2.76	1.58	1.51
4	C	1401	9Z9	C18-C17	2.75	1.58	1.51
4	A	1404	9Z9	C18-C17	2.74	1.58	1.51
4	A	1402	9Z9	C76-C73	2.66	1.55	1.51
4	A	1404	9Z9	C76-C73	2.66	1.55	1.51
3	C	1402	3PH	O21-C2	-2.64	1.40	1.46
4	C	1403	9Z9	C76-C73	2.63	1.55	1.51
3	D	1401	3PH	O21-C2	-2.62	1.40	1.46
4	C	1401	9Z9	C76-C73	2.60	1.55	1.51
3	B	1401	3PH	O21-C2	-2.59	1.40	1.46
3	A	1401	3PH	O21-C2	-2.54	1.40	1.46
5	D	1402	PIO	O3C-C1B	2.46	1.40	1.33
5	C	1404	PIO	O3C-C1B	2.43	1.40	1.33
5	A	1403	PIO	O3C-C1B	2.42	1.40	1.33
5	A	1403	PIO	O2C-C1A	2.40	1.41	1.34
5	D	1402	PIO	O2C-C1A	2.38	1.41	1.34
5	B	1402	PIO	O3C-C1B	2.38	1.40	1.33
5	C	1404	PIO	O2C-C1A	2.38	1.41	1.34
5	B	1402	PIO	O2C-C1A	2.34	1.40	1.34
5	D	1402	PIO	O2C-C2C	-2.29	1.41	1.46
5	B	1402	PIO	O2C-C2C	-2.29	1.41	1.46
5	C	1404	PIO	O2C-C2C	-2.27	1.41	1.46
5	A	1403	PIO	O2C-C2C	-2.25	1.41	1.46
5	B	1402	PIO	O3C-C3C	-2.21	1.40	1.45
5	A	1403	PIO	O3C-C3C	-2.19	1.40	1.45
5	C	1404	PIO	O3C-C3C	-2.16	1.40	1.45
5	D	1402	PIO	O3C-C3C	-2.12	1.40	1.45
4	A	1404	9Z9	C05-C04	2.01	1.57	1.52
4	C	1403	9Z9	C05-C04	2.00	1.57	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1402	9Z9	C76-C73-C74	27.33	165.16	115.66
4	C	1401	9Z9	C76-C73-C74	27.21	164.94	115.66
4	C	1403	9Z9	C76-C73-C74	27.20	164.93	115.66
4	A	1404	9Z9	C76-C73-C74	27.18	164.89	115.66
4	A	1402	9Z9	O72-C73-C76	-18.55	70.87	108.54
4	A	1404	9Z9	O72-C73-C76	-18.54	70.89	108.54
4	C	1401	9Z9	O72-C73-C76	-18.53	70.91	108.54
4	C	1403	9Z9	O72-C73-C76	-18.40	71.17	108.54
4	A	1404	9Z9	O80-C73-O72	11.53	137.31	109.88
4	C	1401	9Z9	O80-C73-O72	11.52	137.28	109.88
4	C	1403	9Z9	O80-C73-O72	11.39	136.97	109.88
4	A	1402	9Z9	O80-C73-O72	11.34	136.87	109.88
4	A	1402	9Z9	O80-C73-C74	-8.35	82.37	107.26
4	C	1403	9Z9	O80-C73-C74	-8.23	82.74	107.26
4	C	1401	9Z9	O80-C73-C74	-8.22	82.77	107.26
4	A	1404	9Z9	O80-C73-C74	-8.20	82.81	107.26
4	A	1402	9Z9	C10-C02-C06	-5.51	99.00	107.25
4	A	1402	9Z9	C02-C06-C07	-5.46	106.67	114.41
4	C	1403	9Z9	C02-C06-C07	-5.18	107.06	114.41
4	C	1403	9Z9	C10-C02-C06	-5.08	99.64	107.25
4	C	1401	9Z9	C02-C06-C07	-5.05	107.25	114.41
4	A	1404	9Z9	C02-C06-C07	-5.03	107.27	114.41
4	A	1404	9Z9	C10-C02-C06	-4.98	99.79	107.25
4	C	1401	9Z9	C10-C02-C06	-4.97	99.81	107.25
4	A	1404	9Z9	C06-C05-C04	-4.50	94.56	102.40
4	C	1401	9Z9	C06-C05-C04	-4.49	94.58	102.40
4	C	1403	9Z9	C06-C05-C04	-4.43	94.69	102.40
4	A	1402	9Z9	C06-C05-C04	-4.39	94.75	102.40
5	A	1403	PIO	O2C-C1A-C2A	4.24	120.65	111.48
4	A	1402	9Z9	C07-C15-C14	-4.23	106.91	112.76
4	C	1401	9Z9	C07-C15-C14	-4.17	106.99	112.76
4	A	1402	9Z9	C09-C08-C11	-4.14	107.98	113.08
4	A	1404	9Z9	C07-C15-C14	-4.13	107.04	112.76
4	C	1403	9Z9	C07-C15-C14	-4.13	107.05	112.76
3	B	1401	3PH	O21-C21-C22	4.01	120.15	111.48
4	A	1404	9Z9	C09-C10-C02	-4.01	105.98	112.74
3	C	1402	3PH	O21-C21-C22	4.00	120.14	111.48
3	D	1401	3PH	O21-C21-C22	4.00	120.12	111.48
4	C	1401	9Z9	C09-C10-C02	-3.99	106.00	112.74
4	C	1403	9Z9	C09-C10-C02	-3.97	106.03	112.74
5	C	1404	PIO	O2C-C1A-C2A	3.94	120.01	111.48
4	C	1403	9Z9	C09-C08-C11	-3.91	108.26	113.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1402	9Z9	C09-C10-C02	-3.90	106.16	112.74
3	A	1401	3PH	O21-C21-C22	3.89	119.89	111.48
5	B	1402	PIO	O2C-C1A-C2A	3.75	119.59	111.48
4	C	1401	9Z9	C09-C08-C11	-3.73	108.48	113.08
4	A	1404	9Z9	C09-C08-C11	-3.72	108.50	113.08
4	A	1402	9Z9	C73-C74-C03	3.69	108.81	103.37
5	D	1402	PIO	O2C-C1A-C2A	3.68	119.44	111.48
4	C	1403	9Z9	C73-C74-C03	3.64	108.74	103.37
4	C	1401	9Z9	C73-C74-C03	3.62	108.70	103.37
4	A	1404	9Z9	C73-C74-C03	3.60	108.66	103.37
4	A	1404	9Z9	C01-C02-C03	3.45	119.08	111.58
4	C	1401	9Z9	C01-C02-C03	3.41	119.00	111.58
4	C	1403	9Z9	C01-C02-C03	3.39	118.96	111.58
4	A	1402	9Z9	C01-C02-C03	3.35	118.88	111.58
4	C	1403	9Z9	O80-C79-C78	-3.32	107.91	112.17
4	A	1402	9Z9	O80-C79-C78	-3.20	108.07	112.17
4	C	1401	9Z9	O80-C79-C78	-3.15	108.13	112.17
4	A	1404	9Z9	O80-C79-C78	-3.09	108.21	112.17
4	A	1404	9Z9	C74-C03-C04	3.04	109.17	104.27
4	C	1401	9Z9	C74-C03-C04	3.00	109.11	104.27
4	A	1404	9Z9	C15-C14-C13	-2.97	120.00	125.02
4	C	1401	9Z9	C15-C14-C13	-2.96	120.02	125.02
4	A	1402	9Z9	C15-C14-C13	-2.92	120.09	125.02
4	C	1403	9Z9	C15-C14-C13	-2.90	120.12	125.02
4	C	1403	9Z9	C74-C03-C04	2.87	108.89	104.27
5	D	1402	PIO	C6-C1-C2	2.87	114.84	110.86
5	D	1402	PIO	C5-C6-C1	2.85	114.89	109.11
5	D	1402	PIO	O3C-C1B-C2B	2.84	120.49	111.83
5	B	1402	PIO	O3C-C1B-C2B	2.81	120.41	111.83
3	A	1401	3PH	O31-C31-C32	2.75	120.21	111.83
4	C	1401	9Z9	C16-C13-C11	2.74	119.94	116.42
4	C	1403	9Z9	C16-C13-C11	2.73	119.92	116.42
4	A	1402	9Z9	C74-C03-C04	2.71	108.64	104.27
3	B	1401	3PH	O31-C31-C32	2.71	120.09	111.83
4	A	1404	9Z9	C16-C13-C11	2.71	119.89	116.42
5	A	1403	PIO	O3C-C1B-C2B	2.69	120.05	111.83
3	C	1402	3PH	O31-C31-C32	2.69	120.03	111.83
5	C	1404	PIO	O3C-C1B-C2B	2.68	120.02	111.83
4	A	1404	9Z9	C75-C74-C03	-2.68	109.14	114.50
4	C	1401	9Z9	C75-C74-C03	-2.68	109.14	114.50
3	D	1401	3PH	O31-C31-C32	2.67	119.97	111.83
4	A	1402	9Z9	O72-C73-C74	-2.64	101.05	104.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1402	9Z9	C16-C13-C11	2.60	119.75	116.42
4	C	1401	9Z9	C15-C07-C06	-2.55	107.32	110.93
4	A	1404	9Z9	C15-C07-C06	-2.53	107.35	110.93
4	A	1402	9Z9	O72-C04-C03	2.53	108.55	105.12
4	A	1402	9Z9	C73-O72-C04	-2.50	101.23	108.14
4	C	1403	9Z9	O72-C04-C03	2.45	108.44	105.12
4	C	1403	9Z9	C15-C07-C06	-2.44	107.47	110.93
4	A	1404	9Z9	O72-C04-C03	2.42	108.41	105.12
4	C	1401	9Z9	O72-C04-C03	2.42	108.41	105.12
4	C	1403	9Z9	O72-C73-C74	-2.41	101.35	104.56
4	C	1403	9Z9	C73-O72-C04	-2.40	101.51	108.14
4	C	1401	9Z9	C10-C02-C03	2.37	118.74	115.36
4	A	1404	9Z9	C10-C02-C03	2.34	118.69	115.36
4	A	1402	9Z9	C10-C09-C08	2.31	117.07	113.14
4	C	1403	9Z9	C10-C02-C03	2.29	118.63	115.36
4	C	1403	9Z9	C75-C74-C03	-2.28	109.94	114.50
4	A	1404	9Z9	C73-O72-C04	-2.27	101.87	108.14
4	C	1401	9Z9	C73-O72-C04	-2.26	101.91	108.14
4	A	1404	9Z9	O72-C73-C74	-2.23	101.59	104.56
4	C	1401	9Z9	O72-C73-C74	-2.22	101.61	104.56
4	A	1404	9Z9	C02-C03-C04	2.21	106.58	104.20
4	A	1402	9Z9	C15-C07-C06	-2.19	107.83	110.93
4	C	1403	9Z9	C10-C09-C08	2.19	116.86	113.14
4	A	1402	9Z9	C01-C02-C06	-2.19	107.71	111.68
4	C	1401	9Z9	C02-C03-C04	2.18	106.55	104.20
4	A	1404	9Z9	C79-O80-C73	2.18	117.44	113.69
4	C	1401	9Z9	C10-C09-C08	2.16	116.81	113.14
4	C	1401	9Z9	C79-O80-C73	2.16	117.42	113.69
4	A	1404	9Z9	C10-C09-C08	2.14	116.78	113.14
4	A	1402	9Z9	C10-C02-C03	2.14	118.41	115.36
4	C	1403	9Z9	C79-O80-C73	2.11	117.33	113.69
4	A	1402	9Z9	C79-O80-C73	2.08	117.28	113.69

There are no chirality outliers.

All (183) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	3PH	C22-C21-O21-C2
3	B	1401	3PH	C1-O11-P-O13
3	B	1401	3PH	C1-O11-P-O14
3	B	1401	3PH	C1-O11-P-O12
3	B	1401	3PH	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1402	3PH	C1-O11-P-O13
3	C	1402	3PH	C1-O11-P-O14
3	C	1402	3PH	C1-O11-P-O12
3	C	1402	3PH	C22-C21-O21-C2
3	D	1401	3PH	C1-O11-P-O13
3	D	1401	3PH	C1-O11-P-O14
3	D	1401	3PH	C1-O11-P-O12
3	D	1401	3PH	C22-C21-O21-C2
5	A	1403	PIO	C1-O1-P1-O12
5	A	1403	PIO	C1-O1-P1-O13
5	A	1403	PIO	C1C-O13-P1-O1
5	A	1403	PIO	C1C-O13-P1-O11
5	A	1403	PIO	C1C-O13-P1-O12
5	A	1403	PIO	C2C-C1C-O13-P1
5	A	1403	PIO	C2A-C1A-O2C-C2C
5	B	1402	PIO	C1C-O13-P1-O1
5	B	1402	PIO	C1C-O13-P1-O11
5	B	1402	PIO	C3-C4-O4-P4
5	C	1404	PIO	C1C-O13-P1-O1
5	C	1404	PIO	C1C-O13-P1-O11
5	C	1404	PIO	O1A-C1A-O2C-C2C
5	C	1404	PIO	C2A-C1A-O2C-C2C
5	C	1404	PIO	O13-C1C-C2C-O2C
5	D	1402	PIO	C3-C4-O4-P4
3	A	1401	3PH	O22-C21-O21-C2
3	B	1401	3PH	O22-C21-O21-C2
3	C	1402	3PH	O22-C21-O21-C2
3	D	1401	3PH	O22-C21-O21-C2
5	A	1403	PIO	O1A-C1A-O2C-C2C
5	B	1402	PIO	O1A-C1A-O2C-C2C
5	B	1402	PIO	C2A-C1A-O2C-C2C
3	A	1401	3PH	C32-C31-O31-C3
5	D	1402	PIO	C2B-C1B-O3C-C3C
3	A	1401	3PH	O32-C31-O31-C3
5	D	1402	PIO	O1B-C1B-O3C-C3C
3	A	1401	3PH	C21-C22-C23-C24
5	D	1402	PIO	C2A-C1A-O2C-C2C
5	B	1402	PIO	C2B-C1B-O3C-C3C
5	D	1402	PIO	O1A-C1A-O2C-C2C
3	B	1401	3PH	C31-C32-C33-C34
5	B	1402	PIO	C2C-C1C-O13-P1
3	D	1401	3PH	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1402	PIO	O1B-C1B-O3C-C3C
3	C	1402	3PH	C32-C31-O31-C3
3	C	1402	3PH	C31-C32-C33-C34
3	A	1401	3PH	C25-C26-C27-C28
3	A	1401	3PH	C3E-C3F-C3G-C3H
3	D	1401	3PH	C31-C32-C33-C34
3	A	1401	3PH	C27-C28-C29-C2A
3	B	1401	3PH	C32-C31-O31-C3
3	D	1401	3PH	C21-C22-C23-C24
3	B	1401	3PH	C21-C22-C23-C24
3	C	1402	3PH	C21-C22-C23-C24
3	C	1402	3PH	O32-C31-O31-C3
3	D	1401	3PH	O32-C31-O31-C3
3	A	1401	3PH	C26-C27-C28-C29
3	A	1401	3PH	C33-C34-C35-C36
3	B	1401	3PH	C32-C33-C34-C35
3	C	1402	3PH	C32-C33-C34-C35
3	D	1401	3PH	C32-C33-C34-C35
3	C	1402	3PH	C39-C3A-C3B-C3C
3	A	1401	3PH	C35-C36-C37-C38
3	C	1402	3PH	C26-C27-C28-C29
3	C	1402	3PH	C38-C39-C3A-C3B
3	D	1401	3PH	C24-C25-C26-C27
3	D	1401	3PH	C26-C27-C28-C29
3	B	1401	3PH	C26-C27-C28-C29
3	A	1401	3PH	C32-C33-C34-C35
3	B	1401	3PH	C24-C25-C26-C27
3	C	1402	3PH	C24-C25-C26-C27
3	B	1401	3PH	C38-C39-C3A-C3B
3	D	1401	3PH	C38-C39-C3A-C3B
3	A	1401	3PH	C23-C24-C25-C26
3	B	1401	3PH	O32-C31-O31-C3
3	A	1401	3PH	C31-C32-C33-C34
5	A	1403	PIO	C1B-C2B-C3B-C4B
5	B	1402	PIO	C1A-C2A-C3A-C4A
5	D	1402	PIO	C2A-C3A-C4A-C5A
5	A	1403	PIO	C2A-C3A-C4A-C5A
3	C	1402	3PH	C2A-C2B-C2C-C2D
3	D	1401	3PH	C23-C24-C25-C26
3	B	1401	3PH	C2A-C2B-C2C-C2D
3	A	1401	3PH	O11-C1-C2-C3
5	D	1402	PIO	O13-C1C-C2C-C3C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1401	3PH	C2A-C2B-C2C-C2D
3	B	1401	3PH	C23-C24-C25-C26
3	C	1402	3PH	C23-C24-C25-C26
3	B	1401	3PH	C1-C2-C3-O31
3	D	1401	3PH	C3A-C3B-C3C-C3D
5	C	1404	PIO	C4B-C5B-C6B-C7B
3	B	1401	3PH	C3A-C3B-C3C-C3D
5	A	1403	PIO	C1C-C2C-O2C-C1A
5	B	1402	PIO	C3C-C2C-O2C-C1A
5	C	1404	PIO	C3C-C2C-O2C-C1A
3	B	1401	3PH	C35-C36-C37-C38
3	D	1401	3PH	C35-C36-C37-C38
5	D	1402	PIO	O2C-C2C-C3C-O3C
4	A	1402	9Z9	C23-C24-O25-C26
4	A	1404	9Z9	C23-C24-O25-C26
4	C	1401	9Z9	C23-C24-O25-C26
4	C	1403	9Z9	C23-C24-O25-C26
3	C	1402	3PH	C35-C36-C37-C38
3	C	1402	3PH	C3A-C3B-C3C-C3D
3	A	1401	3PH	C24-C25-C26-C27
5	D	1402	PIO	C4A-C5A-C6A-C7A
3	D	1401	3PH	C3C-C3D-C3E-C3F
3	B	1401	3PH	C3C-C3D-C3E-C3F
3	A	1401	3PH	C1-C2-C3-O31
3	C	1402	3PH	C1-C2-C3-O31
3	D	1401	3PH	C1-C2-C3-O31
5	D	1402	PIO	C1C-C2C-C3C-O3C
3	D	1401	3PH	C39-C3A-C3B-C3C
3	C	1402	3PH	C3C-C3D-C3E-C3F
5	C	1404	PIO	C2C-C1C-O13-P1
3	B	1401	3PH	C39-C3A-C3B-C3C
3	B	1401	3PH	O21-C2-C3-O31
3	C	1402	3PH	O21-C2-C3-O31
3	D	1401	3PH	O21-C2-C3-O31
5	C	1404	PIO	C5A-C6A-C7A-C8A
5	A	1403	PIO	O13-C1C-C2C-C3C
5	C	1404	PIO	O13-C1C-C2C-C3C
5	C	1404	PIO	C4A-C5A-C6A-C7A
5	D	1402	PIO	C1C-C2C-O2C-C1A
3	A	1401	3PH	O11-C1-C2-O21
3	A	1401	3PH	C37-C38-C39-C3A
5	C	1404	PIO	C1C-C2C-C3C-O3C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1403	PIO	C3B-C4B-C5B-C6B
3	A	1401	3PH	O21-C2-C3-O31
5	B	1402	PIO	O2C-C2C-C3C-O3C
4	A	1402	9Z9	C23-C48-O49-C50
4	A	1404	9Z9	C23-C48-O49-C50
4	C	1401	9Z9	C23-C48-O49-C50
4	C	1403	9Z9	C23-C48-O49-C50
5	B	1402	PIO	C1B-C2B-C3B-C4B
3	C	1402	3PH	C27-C28-C29-C2A
5	A	1403	PIO	C3A-C4A-C5A-C6A
3	B	1401	3PH	C28-C29-C2A-C2B
3	B	1401	3PH	C27-C28-C29-C2A
3	C	1402	3PH	C28-C29-C2A-C2B
3	D	1401	3PH	C28-C29-C2A-C2B
3	D	1401	3PH	C27-C28-C29-C2A
3	A	1401	3PH	C36-C37-C38-C39
5	B	1402	PIO	O13-C1C-C2C-O2C
5	D	1402	PIO	O13-C1C-C2C-O2C
3	B	1401	3PH	C33-C34-C35-C36
3	D	1401	3PH	C33-C34-C35-C36
5	C	1404	PIO	O2C-C2C-C3C-O3C
5	B	1402	PIO	C1C-C2C-C3C-O3C
5	D	1402	PIO	C1C-O13-P1-O11
5	D	1402	PIO	C2C-C1C-O13-P1
5	D	1402	PIO	C5B-C6B-C7B-C8B
5	C	1404	PIO	C1B-C2B-C3B-C4B
5	C	1404	PIO	O2C-C1A-C2A-C3A
3	C	1402	3PH	C33-C34-C35-C36
3	B	1401	3PH	C3E-C3F-C3G-C3H
5	D	1402	PIO	C4-O4-P4-O41
3	D	1401	3PH	C3E-C3F-C3G-C3H
3	A	1401	3PH	C3A-C3B-C3C-C3D
5	D	1402	PIO	C5A-C6A-C7A-C8A
5	B	1402	PIO	C4-O4-P4-O42
5	D	1402	PIO	C4-O4-P4-O42
5	A	1403	PIO	O13-C1C-C2C-O2C
5	B	1402	PIO	O13-C1C-C2C-C3C
5	D	1402	PIO	C1A-C2A-C3A-C4A
5	A	1403	PIO	C1-O1-P1-O11
5	B	1402	PIO	C1-O1-P1-O11
5	C	1404	PIO	C1-O1-P1-O12
5	A	1403	PIO	O3C-C1B-C2B-C3B

Continued on next page...

Continued from previous page...

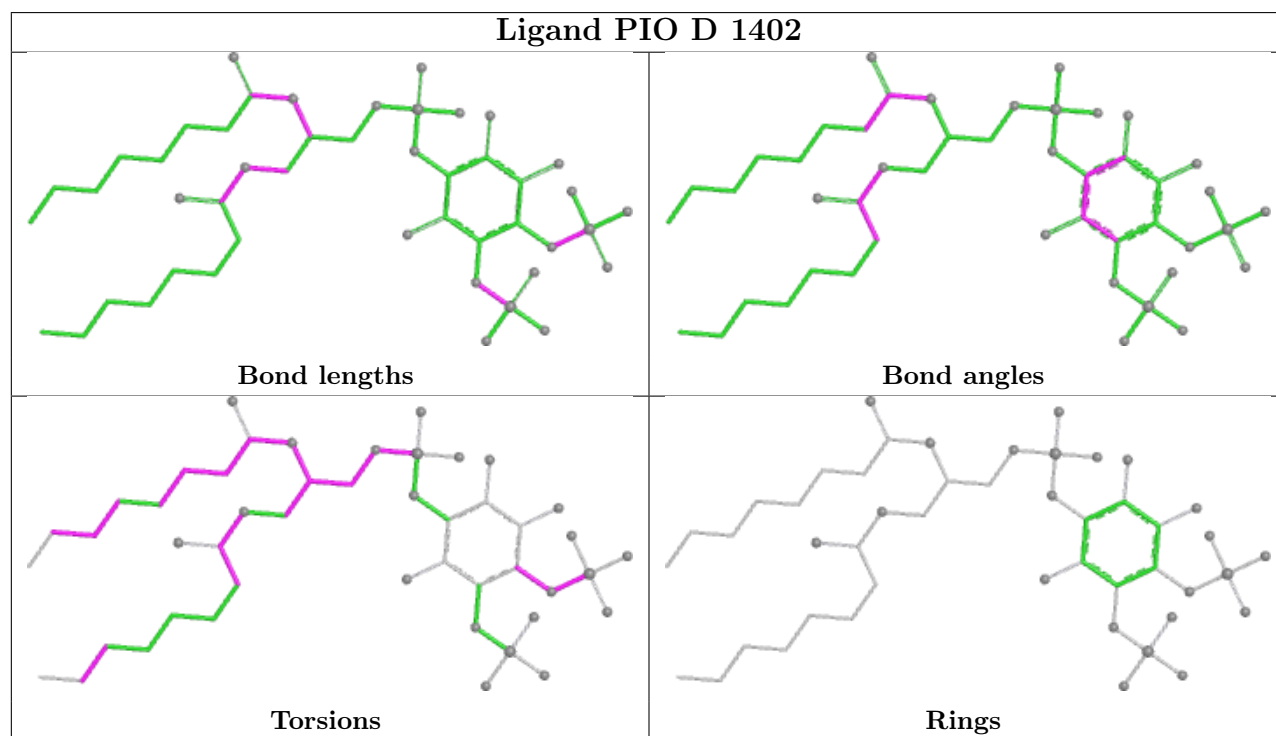
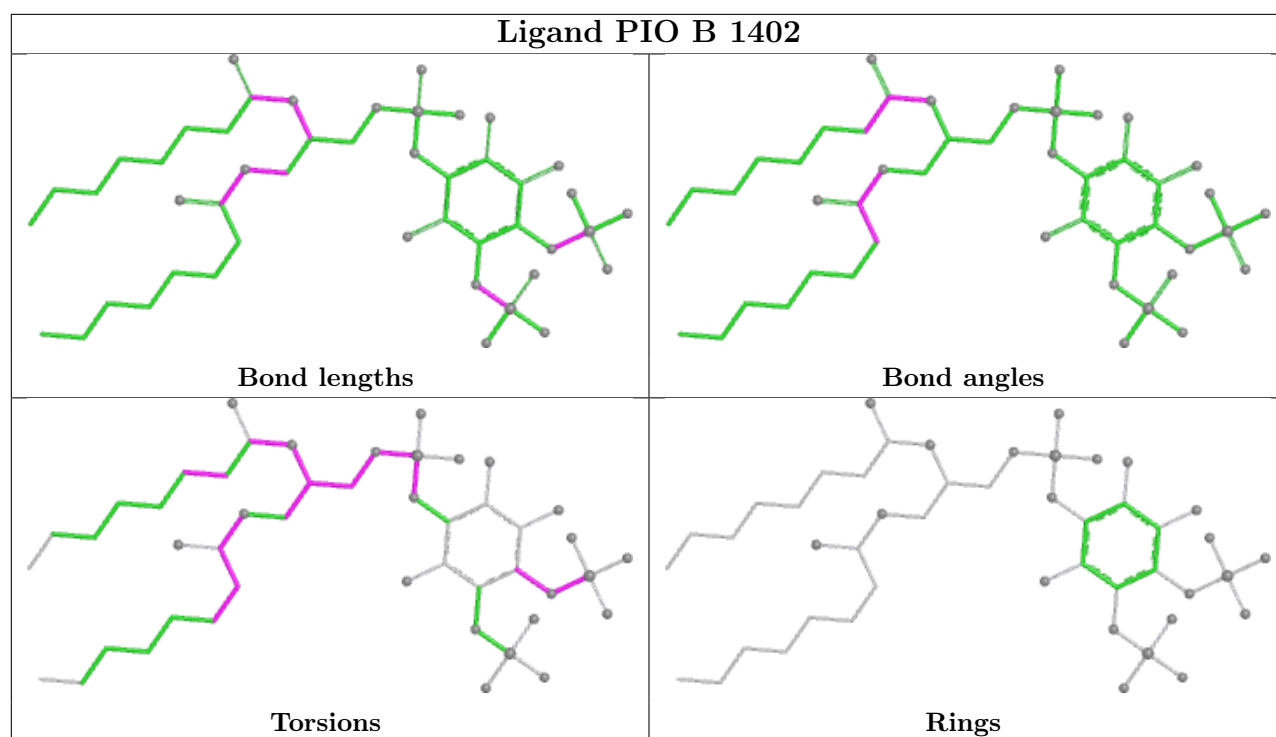
Mol	Chain	Res	Type	Atoms
5	B	1402	PIO	O3C-C1B-C2B-C3B
5	B	1402	PIO	C4-O4-P4-O43
3	A	1401	3PH	C39-C3A-C3B-C3C
3	C	1402	3PH	C3F-C3G-C3H-C3I
5	D	1402	PIO	O3C-C1B-C2B-C3B
3	C	1402	3PH	C37-C38-C39-C3A
5	A	1403	PIO	O1B-C1B-C2B-C3B
5	B	1402	PIO	O1B-C1B-C2B-C3B
3	A	1401	3PH	C2B-C2C-C2D-C2E
5	D	1402	PIO	O2C-C1A-C2A-C3A

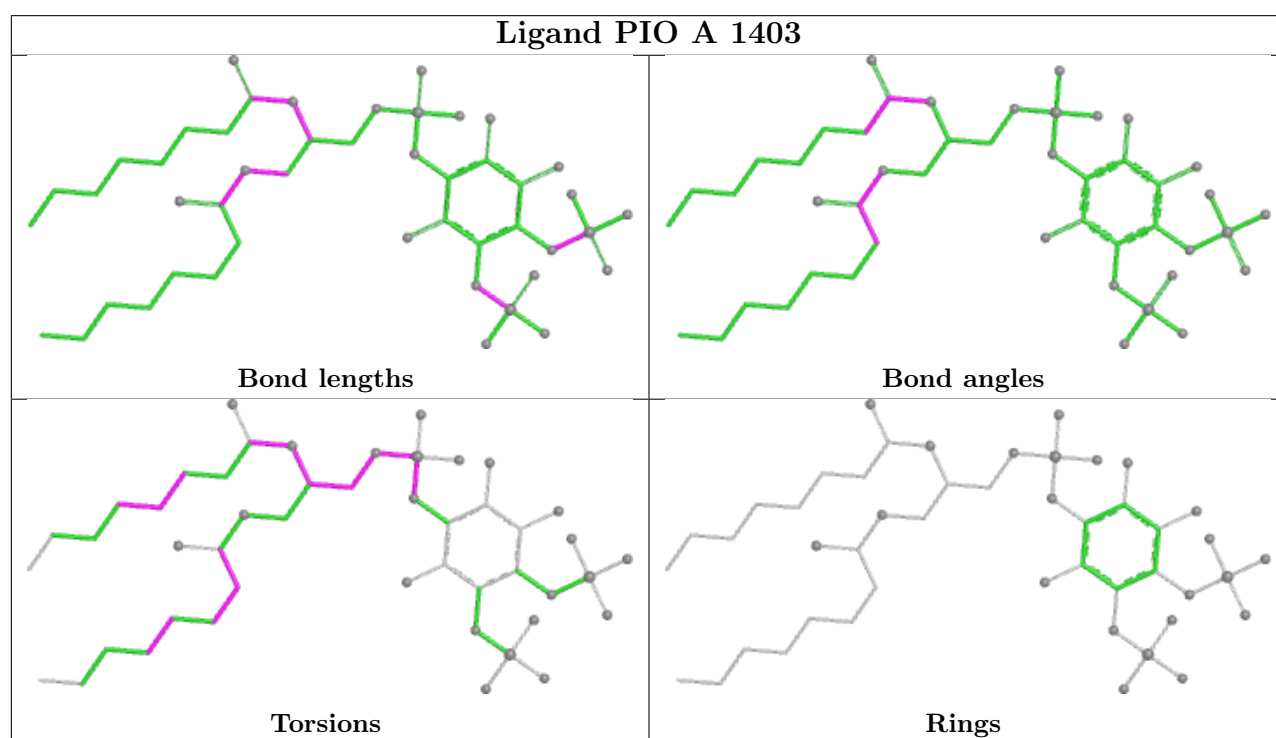
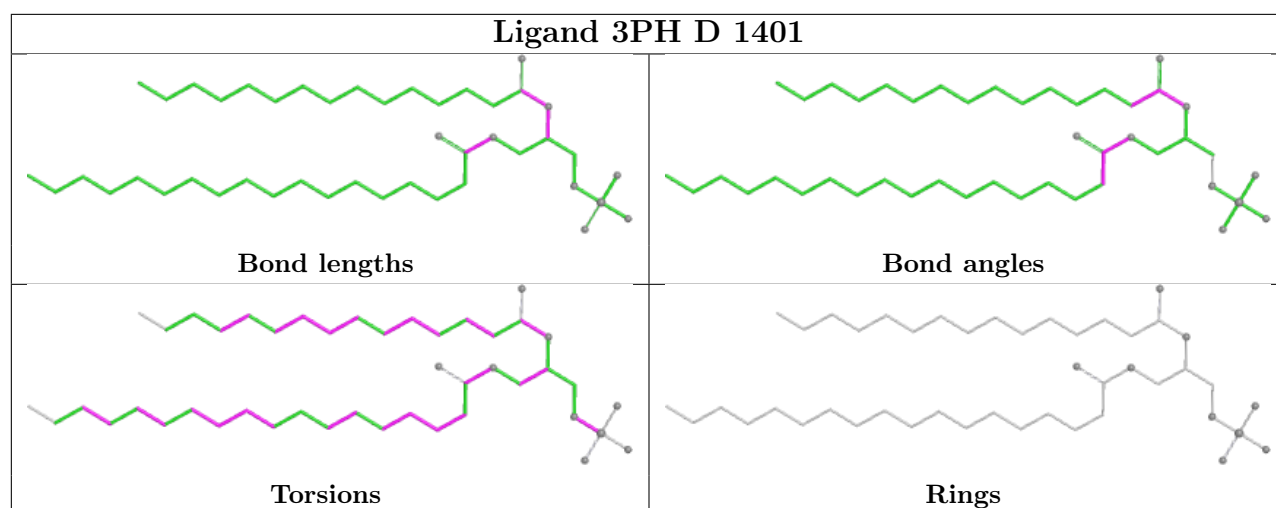
There are no ring outliers.

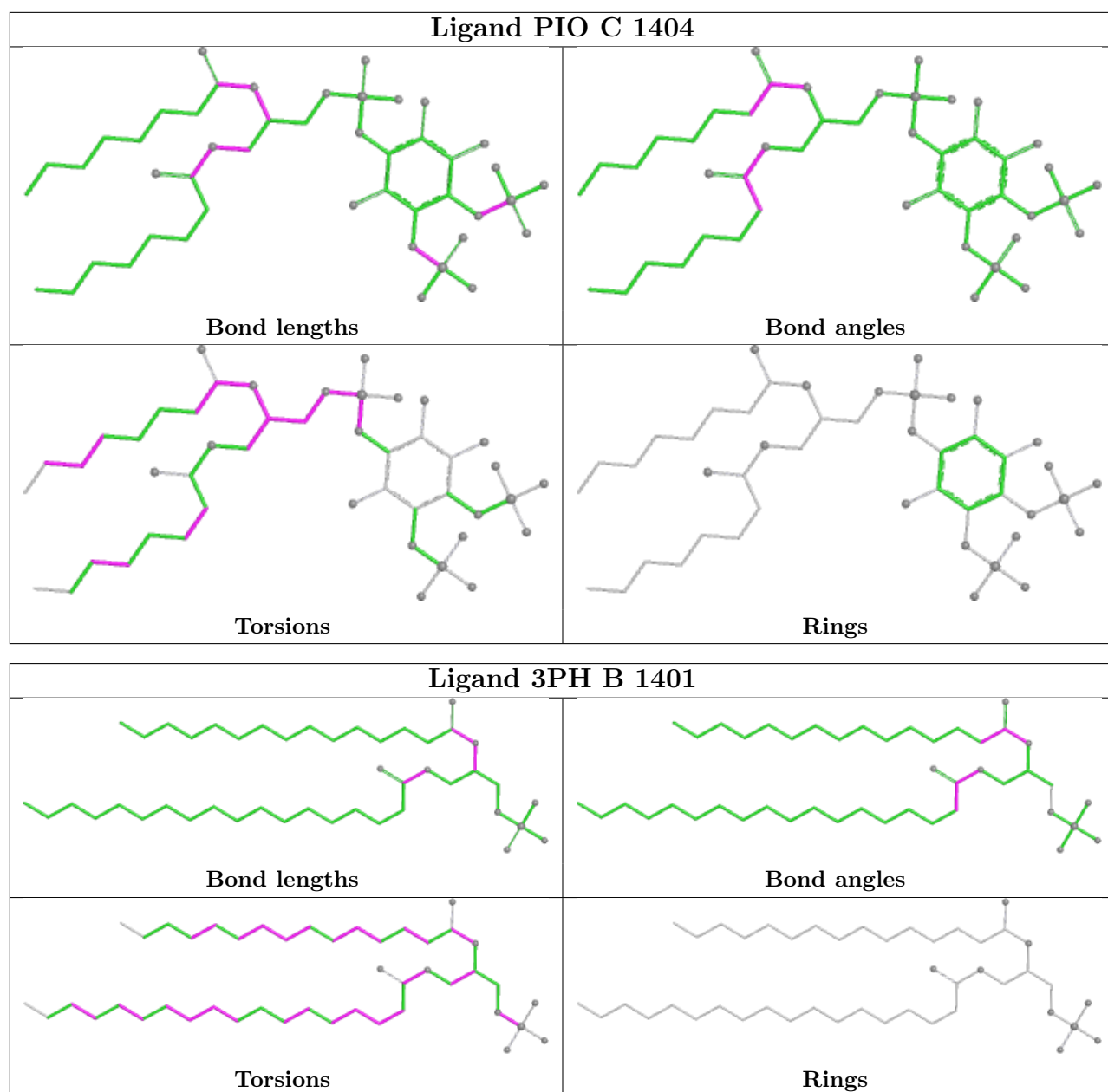
10 monomers are involved in 68 short contacts:

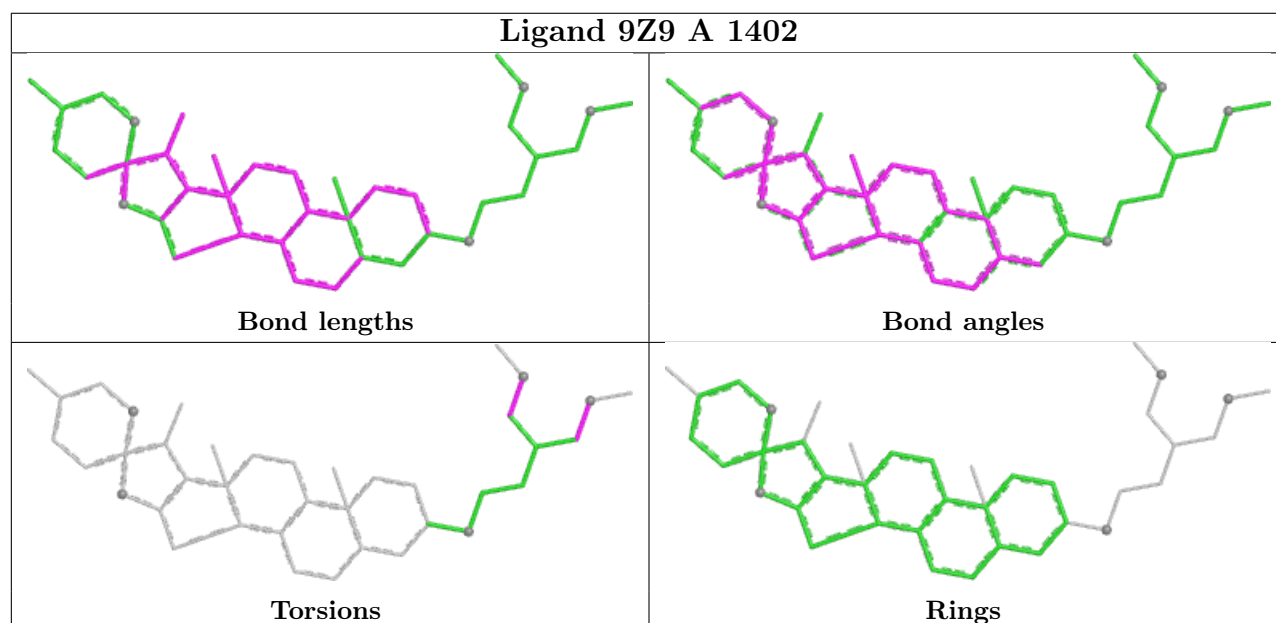
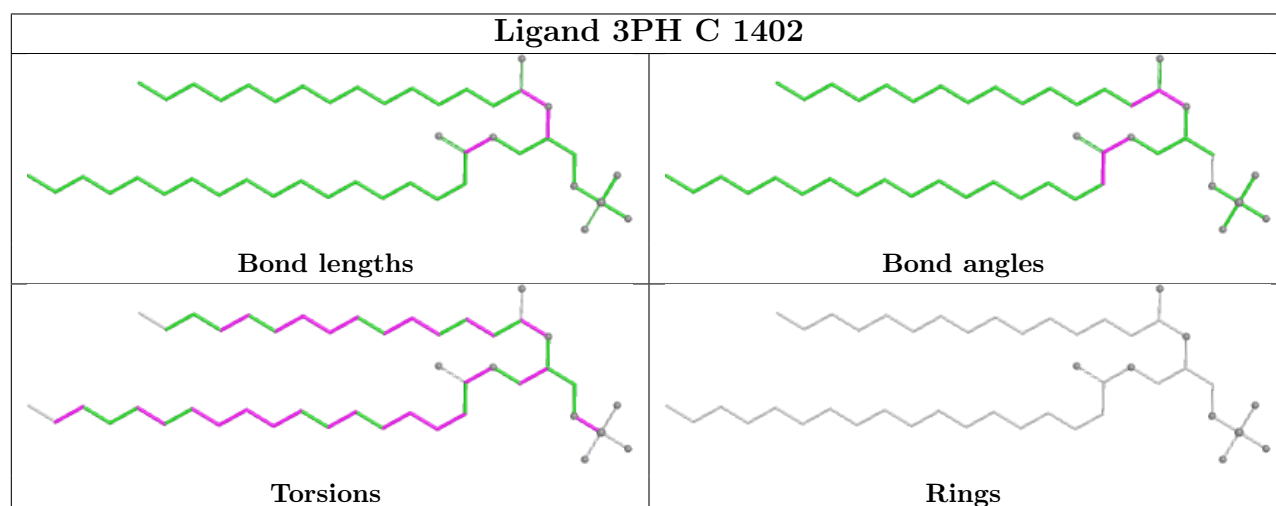
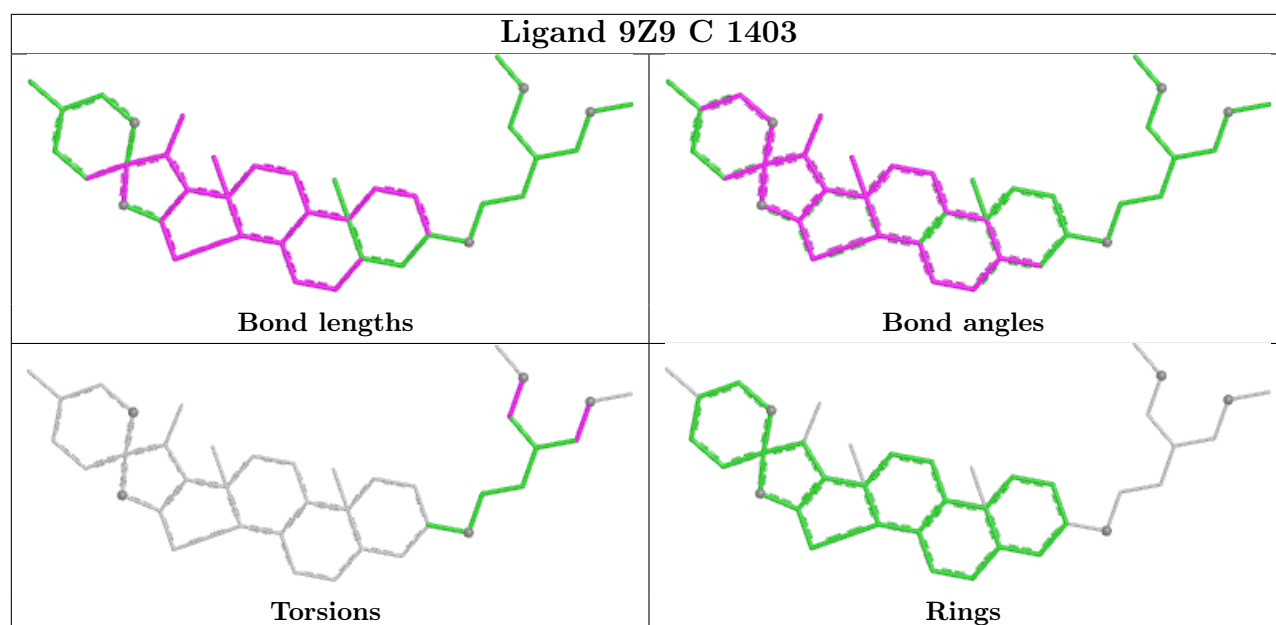
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1402	PIO	2	0
5	D	1402	PIO	1	0
5	A	1403	PIO	1	0
5	C	1404	PIO	1	0
4	C	1403	9Z9	14	0
3	C	1402	3PH	1	0
4	A	1402	9Z9	15	0
3	A	1401	3PH	4	0
4	C	1401	9Z9	15	0
4	A	1404	9Z9	14	0

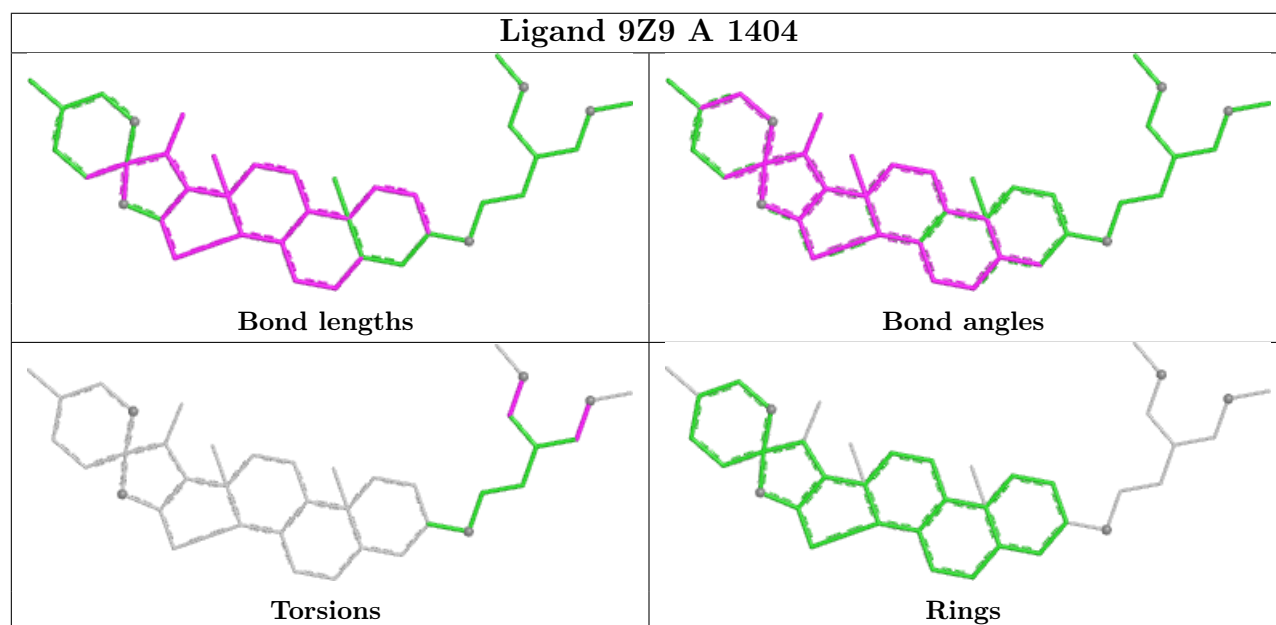
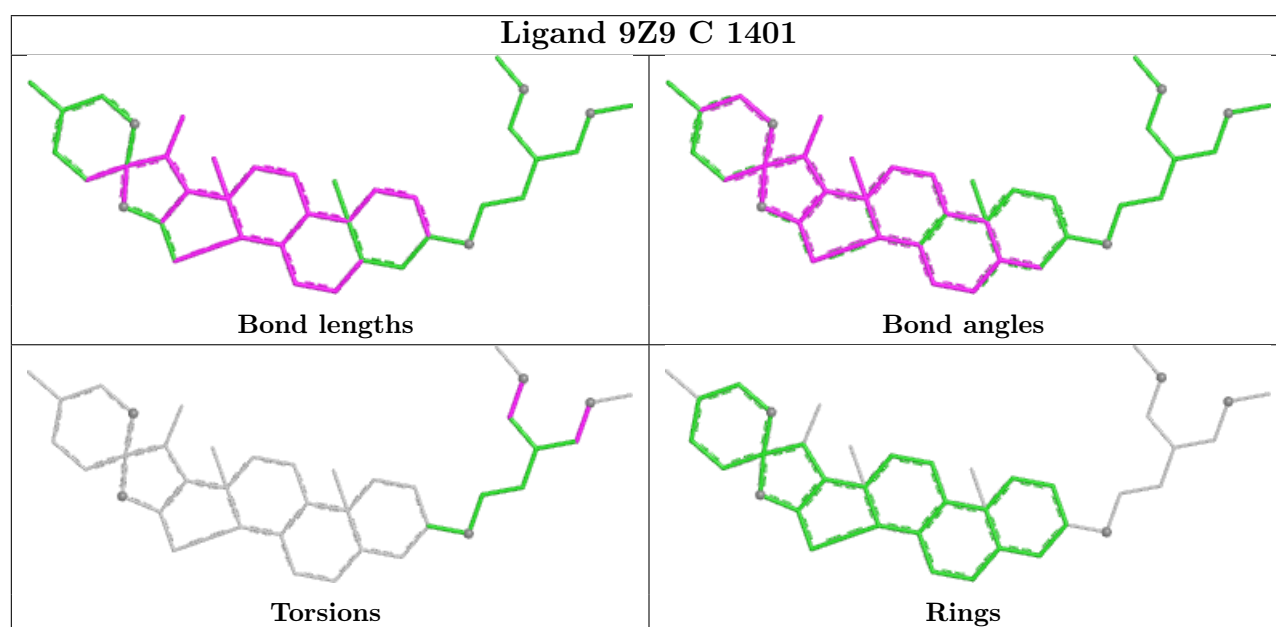
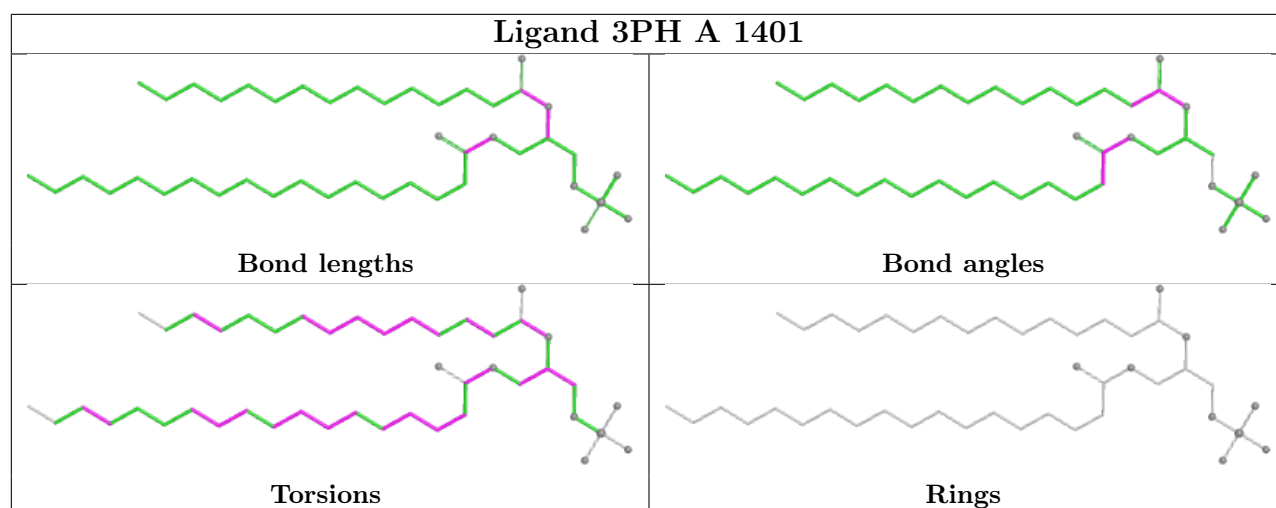
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











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 Map visualisation

This section contains visualisations of the EMDB entry EMD-27343. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.