



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:00 AM UTC

PDB ID : 7FD4 / pdb_00007fd4
EMDB ID : EMD-31534
Title : A complete three-dimensional structure of the Lon protease translocating a protein substrate (conformation 1)
Authors : Li, S.; Hsieh, K.; Kuo, C.; Lee, S.; Pintilie, G.; Zhang, K.; Chang, C.
Deposited on : 2021-07-16
Resolution : 2.40 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

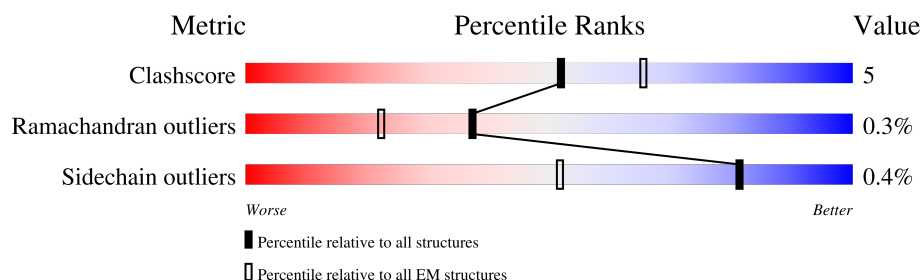
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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	793	87% 11% .
1	B	793	84% 14% .
1	C	793	87% 11% ..
1	D	793	86% 12% .
1	E	793	84% 14% ..
1	F	793	82% 16% .
2	S	22	100%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	4KZ	B	802	-	-	X	-
4	4KZ	D	802	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37182 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.

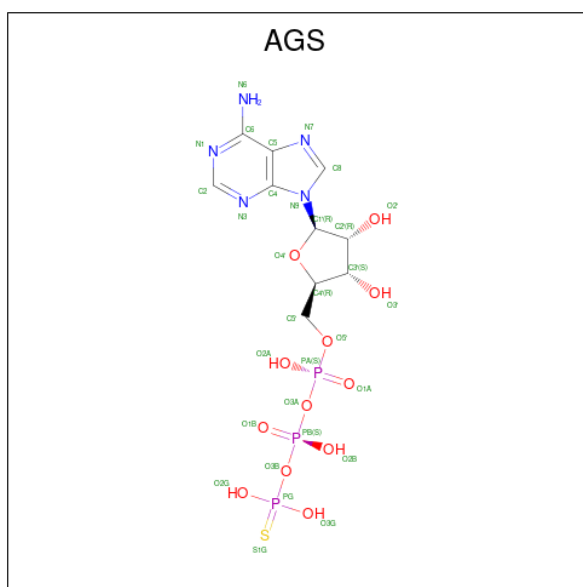
- Molecule 1 is a protein called Lon protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	C	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	D	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	E	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	F	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		
1	A	779	Total	C	N	O	S	0	0
			6118	3867	1073	1156	22		

- Molecule 2 is a protein called Alpha-S1-casein.

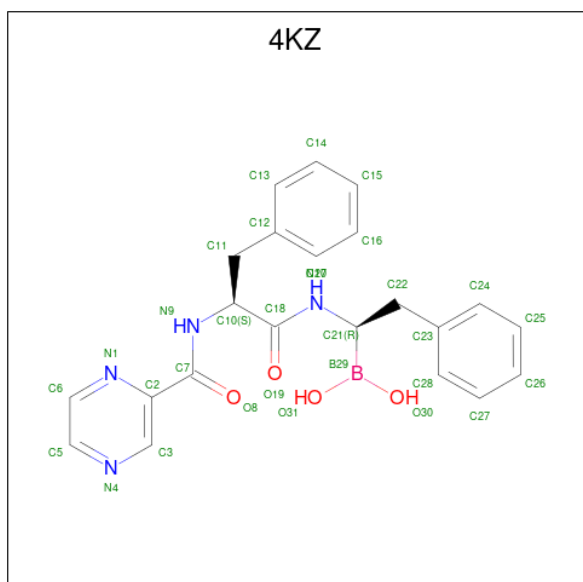
Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



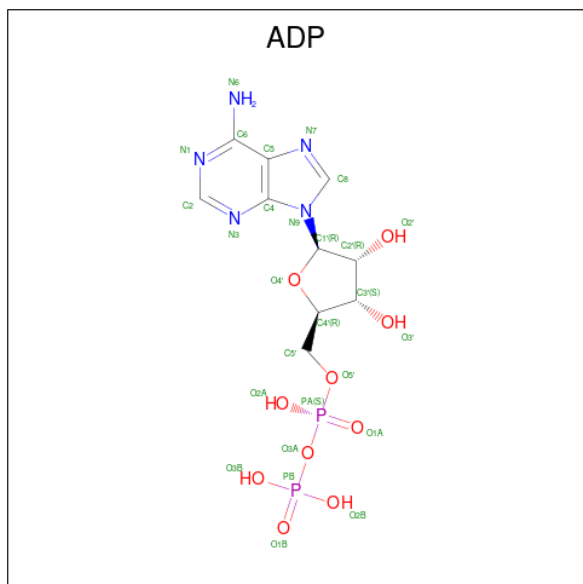
Mol	Chain	Residues	Atoms					AltConf	
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 4 is N-[(1R)-1-(dihydroxyboranyl)-2-phenylethyl]-Nalpha-(pyrazin-2-ylcarbon yl)-L-phenylalaninamide (CCD ID: 4KZ) (formula: C₂₂H₂₃BN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	C	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	D	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	E	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	F	1	Total	B	C	N	O	0
			31	1	22	4	4	
4	A	1	Total	B	C	N	O	0
			31	1	22	4	4	

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

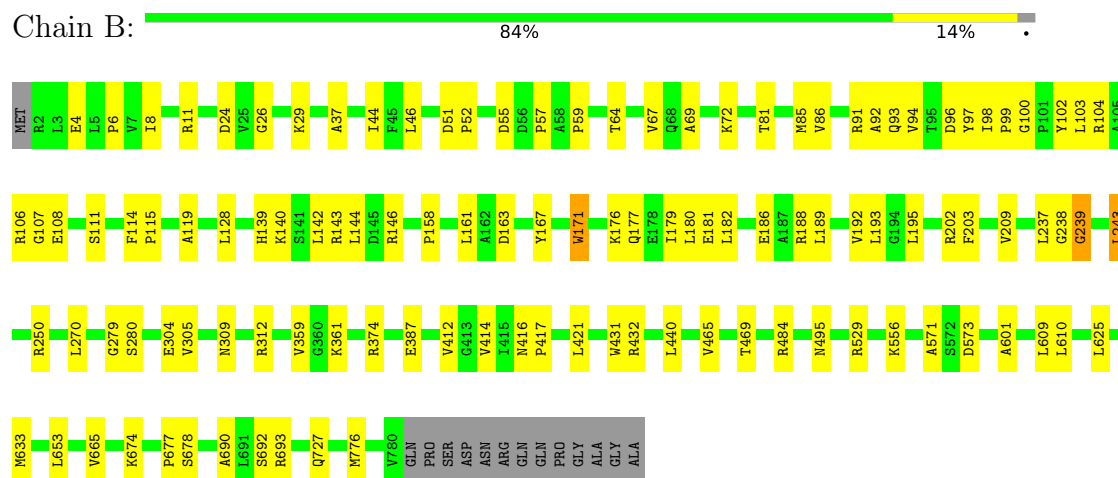


Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

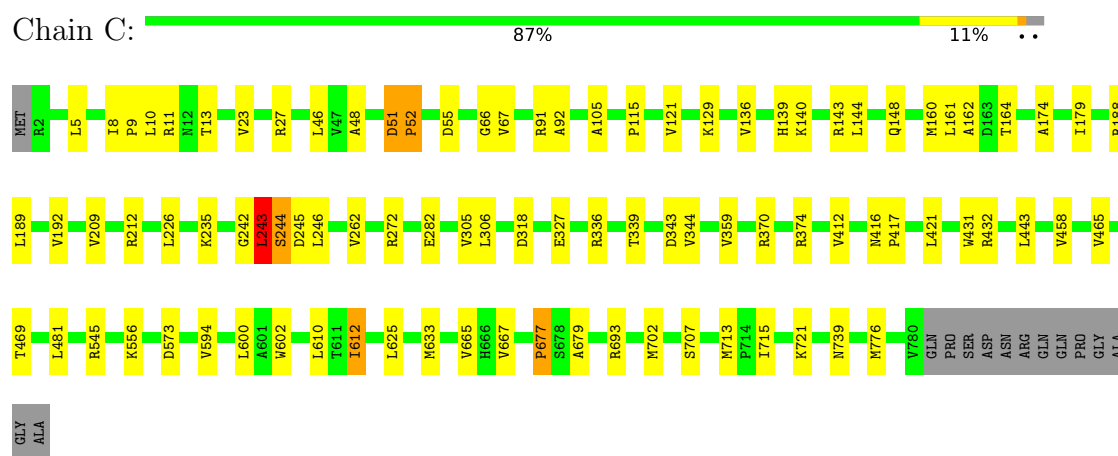
3 Residue-property plots

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

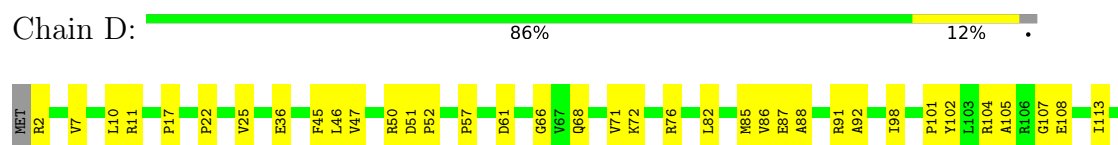
- Molecule 1: Lon protease

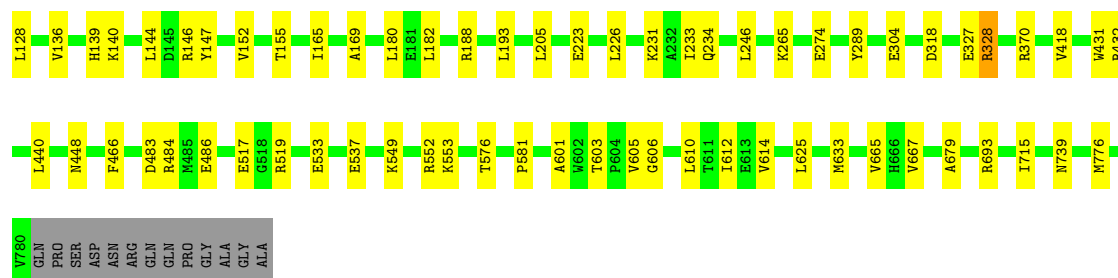


- Molecule 1: Lon protease



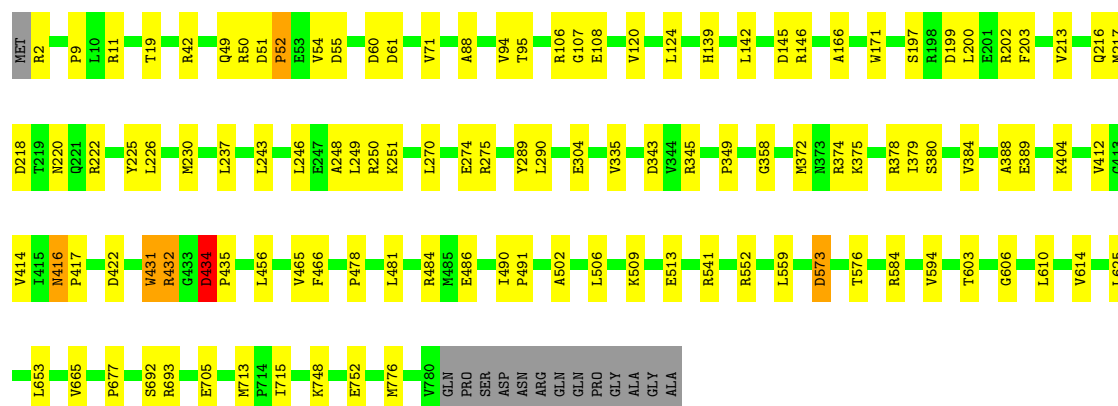
- Molecule 1: Lon protease





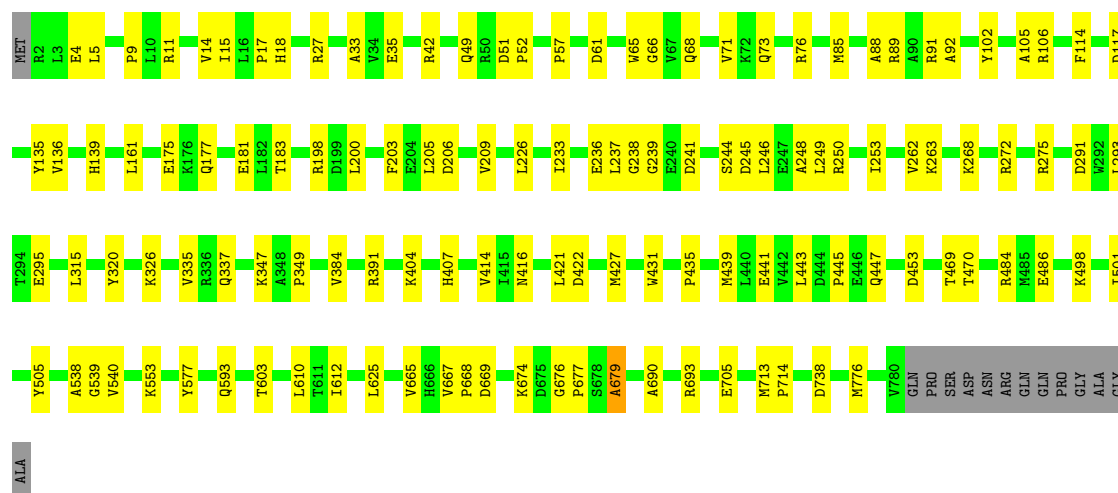
- Molecule 1: Lon protease

Chain E: 84% 14% ..



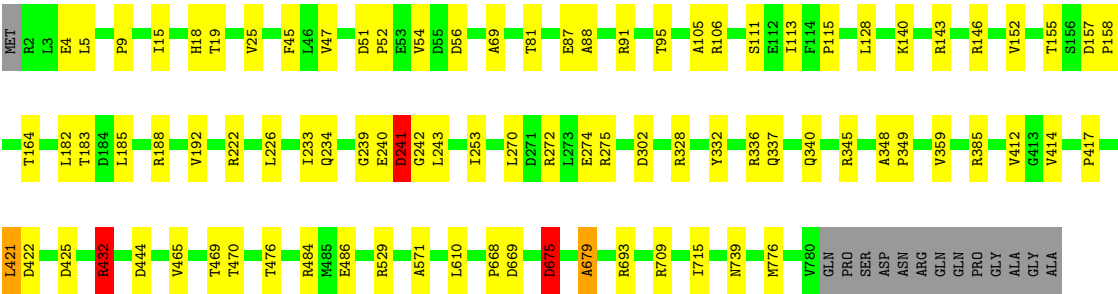
- Molecule 1: Lon protease

Chain F: 82% 16% .



- Molecule 1: Lon protease

Chain A: 87% 11% .



● Molecule 2: Alpha-S1-casein



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	158553	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, ADP, 4KZ

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	0.45	1/6229 (0.0%)	0.68	10/8444 (0.1%)
1	B	0.48	1/6229 (0.0%)	0.69	10/8444 (0.1%)
1	C	0.47	2/6229 (0.0%)	0.66	8/8444 (0.1%)
1	D	0.42	1/6229 (0.0%)	0.75	5/8444 (0.1%)
1	E	0.39	0/6229	0.66	8/8444 (0.1%)
1	F	0.40	2/6229 (0.0%)	0.69	6/8444 (0.1%)
All	All	0.44	7/37374 (0.0%)	0.69	47/50664 (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	4
1	B	0	2
1	C	0	2
1	D	0	4
1	E	0	6
1	F	0	4
All	All	0	22

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	679	ALA	C-N	8.81	1.44	1.33
1	F	679	ALA	C-N	7.39	1.44	1.33
1	C	677	PRO	N-CA	-6.62	1.43	1.47
1	A	432	ARG	C-O	-5.44	1.17	1.24
1	B	677	PRO	C-O	-5.11	1.17	1.24
1	F	676	GLY	C-O	-5.06	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	677	PRO	C-O	-5.03	1.17	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	679	ALA	O-C-N	-23.14	85.16	122.42
1	D	679	ALA	CA-C-N	21.74	143.91	120.00
1	D	679	ALA	C-N-CA	21.74	143.91	120.00
1	A	679	ALA	O-C-N	-15.02	102.98	122.20
1	C	679	ALA	O-C-N	-14.50	103.48	122.19
1	F	679	ALA	O-C-N	-11.83	107.22	122.37
1	E	434	ASP	CA-C-N	10.77	133.30	119.84
1	E	434	ASP	C-N-CA	10.77	133.30	119.84
1	F	676	GLY	CA-C-N	-9.88	107.49	119.84
1	F	676	GLY	C-N-CA	-9.88	107.49	119.84
1	A	243	LEU	N-CA-C	-9.70	103.56	114.62
1	A	241	ASP	N-CA-C	-9.12	95.45	109.95
1	A	242	GLY	N-CA-C	-8.69	103.22	115.30
1	E	432	ARG	N-CA-C	-7.99	98.11	110.17
1	F	246	LEU	N-CA-C	-7.84	101.13	111.24
1	A	240	GLU	CB-CA-C	7.82	117.58	109.83
1	B	239	GLY	N-CA-C	-7.32	103.95	112.73
1	A	240	GLU	N-CA-C	-6.92	102.99	113.51
1	F	676	GLY	O-C-N	-6.86	114.91	121.77
1	B	243	LEU	CA-C-N	-6.63	109.64	120.72
1	B	243	LEU	C-N-CA	-6.63	109.64	120.72
1	C	677	PRO	N-CA-CB	-6.59	96.29	101.83
1	A	675	ASP	CA-C-N	-6.53	111.61	121.87
1	A	675	ASP	C-N-CA	-6.53	111.61	121.87
1	A	679	ALA	CA-C-N	6.45	134.06	121.41
1	A	679	ALA	C-N-CA	6.45	134.06	121.41
1	C	573	ASP	CA-C-N	6.30	124.21	120.24
1	C	573	ASP	C-N-CA	6.30	124.21	120.24
1	D	328	ARG	CB-CG-CD	6.30	125.79	111.30
1	B	677	PRO	CB-CA-C	-6.05	103.26	109.92
1	B	677	PRO	N-CA-CB	-5.97	96.81	101.83
1	B	279	GLY	CA-C-N	5.77	132.09	121.70
1	B	279	GLY	C-N-CA	5.77	132.09	121.70
1	C	243	LEU	N-CA-C	-5.74	98.57	110.80
1	B	573	ASP	CA-C-N	5.71	123.84	120.24
1	B	573	ASP	C-N-CA	5.71	123.84	120.24
1	E	573	ASP	CA-C-N	5.49	123.69	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	573	ASP	C-N-CA	5.49	123.69	120.24
1	B	280	SER	N-CA-C	-5.44	95.76	111.00
1	F	241	ASP	N-CA-C	-5.42	105.47	112.68
1	C	679	ALA	CA-C-N	5.38	131.95	121.41
1	C	679	ALA	C-N-CA	5.38	131.95	121.41
1	E	52	PRO	CA-C-N	5.36	131.78	121.54
1	E	52	PRO	C-N-CA	5.36	131.78	121.54
1	D	328	ARG	CG-CD-NE	-5.35	100.22	112.00
1	C	306	LEU	N-CA-C	5.19	118.66	111.71
1	E	677	PRO	N-CA-CB	-5.06	96.77	101.88

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	421	LEU	Peptide
1	A	51	ASP	Peptide
1	A	52	PRO	Peptide
1	A	675	ASP	Mainchain
1	B	171	TRP	Peptide
1	B	51	ASP	Peptide
1	C	51	ASP	Peptide
1	C	52	PRO	Peptide
1	D	139	HIS	Peptide
1	D	147	TYR	Peptide
1	D	304	GLU	Peptide
1	D	51	ASP	Peptide
1	E	145	ASP	Peptide
1	E	416	ASN	Peptide
1	E	434	ASP	Peptide
1	E	484	ARG	Peptide
1	E	51	ASP	Peptide
1	E	60	ASP	Peptide
1	F	114	PHE	Peptide
1	F	15	ILE	Peptide
1	F	51	ASP	Peptide
1	F	679	ALA	Mainchain

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	6118	0	6235	63	0
1	B	6118	0	6235	81	0
1	C	6118	0	6235	62	0
1	D	6118	0	6235	67	0
1	E	6118	0	6235	81	0
1	F	6118	0	6235	79	0
2	S	110	0	28	0	0
3	A	31	0	12	1	0
3	B	31	0	12	2	0
3	C	31	0	12	3	0
3	F	31	0	12	1	0
4	A	31	0	0	4	0
4	B	31	0	0	16	0
4	C	31	0	0	4	0
4	D	31	0	0	9	0
4	E	31	0	0	3	0
4	F	31	0	0	5	0
5	D	27	0	12	0	0
5	E	27	0	12	0	0
All	All	37182	0	37510	400	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 (400) 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:B:610:LEU:HD22	4:B:802:4KZ:C25	1.41	1.48
1:B:610:LEU:CD2	4:B:802:4KZ:C25	2.32	1.06
1:B:610:LEU:HD22	4:B:802:4KZ:C26	1.85	1.06
1:D:610:LEU:HD12	4:D:802:4KZ:C26	1.99	0.91
1:F:610:LEU:HD12	4:F:802:4KZ:C26	1.99	0.91
1:B:610:LEU:CD2	4:B:802:4KZ:C26	2.49	0.90
1:D:610:LEU:CD1	4:D:802:4KZ:C26	2.57	0.83
1:A:432:ARG:HG2	1:A:432:ARG:HH21	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ARG:HG2	1:E:270:LEU:HD13	1.62	0.80
1:D:603:THR:HG22	4:D:802:4KZ:N4	1.97	0.78
1:B:163:ASP:O	1:B:167:TYR:HB2	1.84	0.77
1:A:432:ARG:HG2	1:A:432:ARG:NH2	1.98	0.77
1:E:388:ALA:HB2	1:E:432:ARG:NH2	2.01	0.74
1:F:244:SER:C	1:F:248:ALA:HB2	2.13	0.73
1:D:603:THR:HG22	4:D:802:4KZ:C3	2.20	0.72
1:A:610:LEU:HD11	4:A:802:4KZ:C26	2.21	0.71
1:C:715:ILE:H	1:C:739:ASN:HD21	1.37	0.70
1:D:610:LEU:HD12	4:D:802:4KZ:C27	2.21	0.70
1:E:380:SER:HA	1:E:422:ASP:HB3	1.74	0.69
1:C:417:PRO:HD2	1:C:465:VAL:HG12	1.72	0.69
1:A:432:ARG:HD2	1:A:432:ARG:O	1.91	0.69
1:F:35:GLU:HG2	1:F:76:ARG:HE	1.57	0.68
1:F:610:LEU:CD1	4:F:802:4KZ:C26	2.70	0.68
1:C:431:TRP:CH2	1:D:432:ARG:NH2	2.61	0.68
1:D:205:LEU:HD11	1:A:226:LEU:HD21	1.77	0.67
1:D:715:ILE:H	1:D:739:ASN:HD21	1.44	0.66
1:C:633:MET:HE3	4:C:802:4KZ:C25	2.26	0.66
1:A:715:ILE:H	1:A:739:ASN:HD21	1.44	0.66
1:C:431:TRP:HH2	1:D:432:ARG:HH21	1.43	0.66
1:B:412:VAL:HG11	1:B:417:PRO:HB3	1.78	0.66
1:C:633:MET:CE	4:C:802:4KZ:C25	2.74	0.65
1:F:4:GLU:HG2	1:F:106:ARG:HB2	1.77	0.65
1:A:140:LYS:HE2	1:A:146:ARG:HE	1.61	0.65
1:A:412:VAL:HG11	1:A:417:PRO:HB3	1.80	0.64
1:E:610:LEU:HD12	4:E:802:4KZ:C25	2.28	0.63
1:A:345:ARG:NH1	1:A:349:PRO:O	2.29	0.63
1:D:10:LEU:HD21	1:D:46:LEU:HB3	1.80	0.63
1:F:49:GLN:HB2	1:F:61:ASP:HB3	1.78	0.63
1:C:421:LEU:HB2	1:C:469:THR:HG22	1.81	0.63
1:D:603:THR:CG2	4:D:802:4KZ:N4	2.62	0.63
1:B:29:LYS:NZ	1:B:55:ASP:O	2.30	0.63
1:E:250:ARG:HG2	1:E:270:LEU:CD1	2.28	0.62
1:D:11:ARG:HH21	1:D:25:VAL:HG13	1.64	0.62
1:C:51:ASP:HB2	1:C:174:ALA:HB2	1.81	0.62
1:F:244:SER:O	1:F:248:ALA:HB2	1.99	0.62
1:A:421:LEU:HB2	1:A:469:THR:HG22	1.80	0.62
1:A:25:VAL:O	1:A:81:THR:HA	1.98	0.62
1:F:253:ILE:O	1:F:263:LYS:NZ	2.32	0.62
1:D:182:LEU:O	1:D:188:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:PRO:O	1:F:27:ARG:NH1	2.33	0.62
1:F:693:ARG:HD2	1:F:776:MET:HB2	1.81	0.62
1:D:328:ARG:NH1	1:D:486:GLU:OE1	2.33	0.61
1:E:230:MET:SD	1:E:274:GLU:OE1	2.59	0.61
1:E:250:ARG:NH2	1:E:274:GLU:OE2	2.33	0.61
1:A:158:PRO:HB2	1:A:185:LEU:HD21	1.83	0.61
1:E:552:ARG:HG2	1:F:335:VAL:HG21	1.81	0.60
1:E:412:VAL:HG22	1:E:414:VAL:H	1.66	0.60
1:A:610:LEU:HD11	4:A:802:4KZ:C25	2.32	0.60
1:D:234:GLN:OE1	1:E:274:GLU:HB3	2.02	0.60
1:C:412:VAL:HG11	1:C:417:PRO:HB3	1.84	0.60
1:B:421:LEU:HB2	1:B:469:THR:HG22	1.83	0.59
1:F:226:LEU:HD22	1:A:233:ILE:HD12	1.85	0.59
1:D:98:ILE:HB	1:D:104:ARG:HB2	1.85	0.59
1:C:115:PRO:HG2	1:C:121:VAL:HG11	1.84	0.59
1:C:179:ILE:HG23	1:C:188:ARG:HB2	1.85	0.59
1:E:216:GLN:OE1	1:E:220:ASN:ND2	2.35	0.59
1:B:601:ALA:HB2	4:B:802:4KZ:C25	2.32	0.59
1:F:439:MET:O	1:F:443:LEU:HB2	2.02	0.59
1:A:115:PRO:HG2	1:A:158:PRO:HD2	1.85	0.59
1:F:272:ARG:HD3	1:F:275:ARG:HH12	1.67	0.58
1:E:559:LEU:HD13	1:F:337:GLN:HE21	1.68	0.58
1:F:498:LYS:NZ	1:F:539:GLY:O	2.37	0.58
1:E:414:VAL:HG12	1:E:416:ASN:H	1.68	0.58
1:F:445:PRO:HD2	1:F:484:ARG:HH21	1.67	0.58
1:B:192:VAL:HA	1:B:195:LEU:HD12	1.85	0.58
1:C:143:ARG:HB3	1:F:117:ASP:HB2	1.86	0.58
1:F:91:ARG:HD3	1:F:183:THR:HG22	1.84	0.58
1:B:8:ILE:HD12	1:B:44:ILE:HG23	1.87	0.57
1:A:332:TYR:O	1:A:336:ARG:NH1	2.38	0.57
1:B:609:LEU:C	1:B:610:LEU:HD12	2.30	0.57
1:F:245:ASP:HA	1:F:248:ALA:HB3	1.87	0.56
1:B:610:LEU:HD23	4:B:802:4KZ:C26	2.35	0.56
1:E:304:GLU:OE1	1:E:374:ARG:NH2	2.39	0.56
1:E:431:TRP:CZ3	1:F:431:TRP:CE3	2.94	0.56
1:A:95:THR:HB	1:A:106:ARG:HG2	1.87	0.56
1:E:375:LYS:HD3	1:E:412:VAL:HG23	1.87	0.56
1:F:236:GLU:O	1:A:222:ARG:NH2	2.38	0.56
1:B:361:LYS:NZ	3:B:801:AGS:O2G	2.38	0.56
1:D:17:PRO:HA	1:D:88:ALA:HB3	1.86	0.56
1:B:4:GLU:HA	1:B:107:GLY:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:VAL:O	3:C:801:AGS:O2B	2.24	0.55
1:D:72:LYS:HD2	1:D:87:GLU:HB2	1.88	0.55
1:A:9:PRO:HA	1:A:47:VAL:O	2.06	0.55
1:B:171:TRP:O	1:B:176:LYS:NZ	2.39	0.55
1:E:384:VAL:HG11	1:E:389:GLU:HG3	1.87	0.55
1:F:42:ARG:HE	1:F:71:VAL:HB	1.70	0.55
1:B:237:LEU:O	1:B:239:GLY:N	2.37	0.55
1:D:68:GLN:NE2	1:D:108:GLU:O	2.39	0.55
1:F:73:GLN:HG2	1:F:85:MET:H	1.70	0.55
1:C:242:GLY:H	1:C:245:ASP:HB2	1.72	0.55
1:C:556:LYS:NZ	1:D:327:GLU:OE1	2.40	0.55
1:C:140:LYS:NZ	1:C:144:LEU:O	2.40	0.55
1:D:140:LYS:HE3	1:D:146:ARG:HE	1.71	0.55
1:D:610:LEU:HD13	4:D:802:4KZ:C26	2.35	0.55
1:B:495:ASN:OD1	1:B:727:GLN:NE2	2.40	0.55
1:C:431:TRP:CE3	1:C:432:ARG:HB2	2.42	0.54
1:A:91:ARG:HD2	1:A:183:THR:HG22	1.88	0.54
1:D:91:ARG:NE	1:D:180:LEU:O	2.39	0.54
1:D:418:VAL:HG12	1:D:466:PHE:HB3	1.90	0.54
1:A:337:GLN:O	1:A:340:GLN:NE2	2.41	0.54
3:C:801:AGS:O2G	3:C:801:AGS:O1B	2.25	0.54
1:F:603:THR:HG22	4:F:802:4KZ:C6	2.38	0.54
1:B:92:ALA:HB1	1:B:108:GLU:HB2	1.90	0.54
1:D:537:GLU:HA	1:D:605:VAL:HG22	1.89	0.54
1:A:422:ASP:O	1:A:470:THR:OG1	2.23	0.54
1:C:272:ARG:NH1	1:C:282:GLU:OE2	2.40	0.54
1:C:209:VAL:HG22	1:C:212:ARG:HH21	1.73	0.54
1:A:359:VAL:O	3:A:801:AGS:O2B	2.26	0.54
1:C:602:TRP:N	4:C:802:4KZ:O19	2.40	0.53
1:E:610:LEU:HD12	4:E:802:4KZ:C26	2.38	0.53
1:B:119:ALA:HB3	1:E:146:ARG:HG3	1.89	0.53
1:E:389:GLU:HB3	1:E:404:LYS:HE2	1.91	0.53
1:F:625:LEU:HD23	1:F:665:VAL:HB	1.91	0.53
1:B:59:PRO:HG3	1:B:99:PRO:HB3	1.91	0.53
1:B:57:PRO:HB2	1:B:103:LEU:HD13	1.91	0.52
1:B:440:LEU:O	1:B:484:ARG:NH1	2.38	0.52
1:B:678:SER:CB	4:B:802:4KZ:O31	2.56	0.52
1:A:675:ASP:O	4:A:802:4KZ:C17	2.56	0.52
1:A:679:ALA:HB2	4:A:802:4KZ:C24	2.39	0.52
1:C:545:ARG:NH2	1:D:483:ASP:O	2.38	0.52
1:B:182:LEU:O	1:B:188:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:553:LYS:NZ	1:D:576:THR:O	2.37	0.52
1:F:347:LYS:HE3	1:F:349:PRO:HG3	1.91	0.52
1:F:674:LYS:HG2	4:F:802:4KZ:C3	2.39	0.52
1:B:609:LEU:O	1:B:610:LEU:HD12	2.09	0.52
1:E:412:VAL:HG11	1:E:417:PRO:HG3	1.91	0.52
1:B:529:ARG:NH1	1:B:571:ALA:O	2.42	0.52
1:F:68:GLN:HE21	1:F:89:ARG:H	1.57	0.52
1:C:243:LEU:C	1:C:245:ASP:N	2.69	0.51
1:D:57:PRO:HD2	1:D:101:PRO:HG3	1.91	0.51
1:D:440:LEU:O	1:D:484:ARG:NH1	2.43	0.51
1:D:71:VAL:HA	1:D:86:VAL:HG12	1.91	0.51
1:B:11:ARG:NH2	1:B:24:ASP:O	2.44	0.51
1:E:748:LYS:NZ	1:E:752:GLU:OE2	2.42	0.51
1:A:54:VAL:HG12	1:A:56:ASP:H	1.76	0.51
1:B:693:ARG:HD2	1:B:776:MET:HB2	1.92	0.51
1:D:318:ASP:OD2	1:D:370:ARG:NH2	2.44	0.51
1:F:593:GLN:OE1	1:A:709:ARG:NH2	2.43	0.51
1:A:328:ARG:NH1	1:A:486:GLU:OE2	2.44	0.51
1:B:431:TRP:CZ3	1:B:432:ARG:HB2	2.45	0.51
1:E:552:ARG:HH12	1:F:486:GLU:HG3	1.76	0.51
1:A:91:ARG:HH12	1:A:113:ILE:HG22	1.76	0.51
1:A:182:LEU:O	1:A:188:ARG:NH1	2.44	0.51
1:E:19:THR:H	1:E:88:ALA:HB3	1.74	0.51
1:B:186:GLU:HG3	1:B:189:LEU:HD12	1.93	0.50
1:E:417:PRO:HD2	1:E:465:VAL:HG12	1.93	0.50
1:E:603:THR:OG1	1:E:606:GLY:O	2.26	0.50
1:B:140:LYS:HB3	1:B:143:ARG:HH11	1.75	0.50
1:E:166:ALA:O	1:E:171:TRP:NE1	2.45	0.50
1:A:693:ARG:HD2	1:A:776:MET:HB2	1.93	0.50
1:B:431:TRP:CE3	1:B:432:ARG:HB2	2.46	0.50
1:F:505:TYR:CD2	3:F:801:AGS:H2	2.46	0.50
1:A:529:ARG:NH1	1:A:571:ALA:O	2.44	0.50
1:C:129:LYS:HZ1	1:C:161:LEU:HD21	1.77	0.50
1:B:91:ARG:HG3	1:B:111:SER:HB2	1.93	0.50
1:B:158:PRO:HA	1:B:161:LEU:HB2	1.93	0.50
1:B:633:MET:HE3	4:B:802:4KZ:C28	2.42	0.50
1:F:553:LYS:NZ	1:F:577:TYR:O	2.45	0.50
1:B:64:THR:O	1:B:93:GLN:NE2	2.45	0.49
1:E:197:SER:HA	1:E:200:LEU:HD12	1.94	0.49
1:E:431:TRP:CZ3	1:F:431:TRP:CD2	3.00	0.49
1:B:601:ALA:HB2	4:B:802:4KZ:C24	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLU:O	1:B:104:ARG:NH1	2.45	0.49
1:B:556:LYS:NZ	1:C:327:GLU:OE2	2.34	0.49
1:C:336:ARG:HH21	1:C:339:THR:HG21	1.77	0.49
1:A:69:ALA:HA	1:A:87:GLU:O	2.11	0.49
1:B:633:MET:HE1	4:B:802:4KZ:C27	2.42	0.49
1:C:633:MET:HE1	4:C:802:4KZ:C25	2.43	0.49
1:D:102:TYR:OH	1:D:104:ARG:NH1	2.46	0.49
1:D:231:LYS:NZ	1:E:275:ARG:HA	2.28	0.49
1:F:291:ASP:O	1:F:295:GLU:HB2	2.13	0.49
1:F:705:GLU:HB3	1:F:713:MET:HB2	1.95	0.49
1:B:374:ARG:HH12	1:B:416:ASN:HB2	1.78	0.48
1:B:128:LEU:HB2	1:B:193:LEU:HD21	1.96	0.48
1:C:431:TRP:NE1	1:D:431:TRP:HE3	2.11	0.48
1:F:391:ARG:HE	1:F:453:ASP:HA	1.78	0.48
1:B:359:VAL:O	3:B:801:AGS:O2B	2.31	0.48
1:D:66:GLY:O	1:D:92:ALA:N	2.45	0.48
1:F:315:LEU:HB3	1:F:326:LYS:HZ2	1.78	0.48
1:F:439:MET:O	1:F:443:LEU:CB	2.61	0.48
1:C:67:VAL:HA	1:C:91:ARG:HA	1.94	0.48
1:D:633:MET:HE1	4:D:802:4KZ:C25	2.42	0.48
1:E:199:ASP:OD1	1:E:202:ARG:NH1	2.46	0.48
1:F:233:ILE:HG23	1:A:226:LEU:HD22	1.95	0.48
1:B:72:LYS:HB2	1:B:85:MET:HB3	1.96	0.48
1:B:144:LEU:O	1:B:146:ARG:NH2	2.46	0.48
1:F:65:TRP:HB2	1:F:181:GLU:HG2	1.96	0.48
1:D:36:GLU:OE1	1:D:102:TYR:OH	2.25	0.48
1:D:223:GLU:HG3	1:E:237:LEU:HD22	1.95	0.48
1:D:614:VAL:HG22	1:D:665:VAL:HG22	1.96	0.48
1:F:237:LEU:C	1:F:239:GLY:H	2.21	0.48
1:D:136:VAL:HG23	1:D:144:LEU:HD23	1.96	0.47
1:F:66:GLY:N	1:F:92:ALA:O	2.45	0.47
1:A:234:GLN:CG	1:A:274:GLU:OE1	2.62	0.47
1:A:234:GLN:HG3	1:A:274:GLU:OE1	2.14	0.47
1:B:8:ILE:HD11	1:B:37:ALA:HB2	1.95	0.47
1:D:246:LEU:HD13	1:D:274:GLU:HG2	1.96	0.47
1:E:246:LEU:O	1:E:250:ARG:HG3	2.14	0.47
1:E:120:VAL:O	1:E:124:LEU:CB	2.62	0.47
1:E:374:ARG:NH1	1:E:416:ASN:O	2.47	0.47
1:E:95:THR:OG1	1:E:108:GLU:OE2	2.28	0.47
1:E:50:ARG:HD3	1:E:61:ASP:HA	1.97	0.47
1:A:185:LEU:HA	1:A:188:ARG:HE	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:705:GLU:HB2	1:E:713:MET:HB2	1.97	0.47
1:F:501:ILE:HD11	1:F:540:VAL:HG11	1.96	0.47
1:B:179:ILE:O	1:B:188:ARG:NH1	2.48	0.46
1:D:57:PRO:HB2	1:D:101:PRO:HB3	1.96	0.46
1:D:533:GLU:HG3	1:D:581:PRO:HB3	1.97	0.46
1:B:653:LEU:HD23	1:B:692:SER:HB3	1.98	0.46
1:B:432:ARG:HH12	1:A:385:ARG:HD3	1.80	0.46
1:E:509:LYS:O	1:E:513:GLU:HB2	2.15	0.46
1:A:425:ASP:HB2	1:A:476:THR:HG23	1.96	0.46
1:E:478:PRO:HD2	1:E:481:LEU:HD12	1.96	0.46
1:C:9:PRO:HA	1:C:48:ALA:HA	1.97	0.46
1:E:289:TYR:HE1	1:E:456:LEU:HA	1.80	0.46
1:E:349:PRO:HG2	1:E:486:GLU:HB2	1.98	0.46
1:F:5:LEU:O	1:F:105:ALA:N	2.43	0.46
1:B:209:VAL:HG11	1:D:233:ILE:HD13	1.98	0.46
1:B:625:LEU:HD23	1:B:665:VAL:HB	1.96	0.46
1:E:243:LEU:HD21	1:F:268:LYS:HE2	1.98	0.46
1:A:4:GLU:HG2	1:A:106:ARG:HB3	1.98	0.46
1:A:15:ILE:HG23	1:A:19:THR:HB	1.97	0.46
1:B:678:SER:HB3	4:B:802:4KZ:O31	2.16	0.46
1:E:614:VAL:HG22	1:E:665:VAL:HG22	1.97	0.46
1:F:17:PRO:HA	1:F:88:ALA:HB3	1.98	0.46
1:F:427:MET:HE3	1:F:435:PRO:HG2	1.96	0.46
1:D:76:ARG:HD3	1:D:82:LEU:HD22	1.98	0.46
1:F:414:VAL:HG12	1:F:416:ASN:H	1.81	0.46
1:F:498:LYS:NZ	1:F:538:ALA:O	2.45	0.46
1:B:177:GLN:NE2	1:B:181:GLU:OE2	2.48	0.46
1:F:175:GLU:OE2	1:F:198:ARG:NH1	2.41	0.46
1:F:245:ASP:CA	1:F:248:ALA:HB3	2.45	0.45
1:B:6:PRO:HA	1:B:104:ARG:HA	1.98	0.45
1:B:690:ALA:O	1:B:693:ARG:NH1	2.49	0.45
1:C:51:ASP:OD2	1:C:174:ALA:N	2.49	0.45
1:E:584:ARG:NH1	1:F:738:ASP:O	2.47	0.45
1:E:610:LEU:CD1	4:E:802:4KZ:C25	2.94	0.45
1:F:612:ILE:HG12	1:F:667:VAL:HG22	1.98	0.45
1:F:714:PRO:HG3	1:F:738:ASP:HB2	1.99	0.45
1:A:417:PRO:HD2	1:A:465:VAL:HG22	1.98	0.45
1:B:633:MET:CE	4:B:802:4KZ:C27	2.94	0.45
1:B:674:LYS:HE2	1:B:674:LYS:HB2	1.84	0.45
1:E:246:LEU:O	1:E:250:ARG:HD2	2.17	0.45
1:F:603:THR:CG2	4:F:802:4KZ:C6	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:VAL:HG23	1:C:458:VAL:HG11	1.98	0.45
1:A:4:GLU:HA	1:A:105:ALA:O	2.17	0.45
1:B:46:LEU:N	1:B:67:VAL:O	2.48	0.45
1:C:431:TRP:HH2	1:D:432:ARG:NH2	2.07	0.45
1:C:693:ARG:HB3	1:C:776:MET:HB3	1.97	0.45
1:D:113:ILE:HD11	1:A:143:ARG:HH12	1.81	0.45
1:D:603:THR:OG1	1:D:606:GLY:O	2.28	0.45
1:F:441:GLU:HA	1:F:447:GLN:HE21	1.82	0.45
1:B:59:PRO:HB3	1:B:97:TYR:HE2	1.81	0.45
1:E:246:LEU:O	1:E:250:ARG:CD	2.65	0.45
1:E:372:MET:HG3	1:E:374:ARG:HG2	1.98	0.45
1:F:11:ARG:HA	1:F:49:GLN:HE21	1.81	0.45
1:B:309:ASN:OD1	1:B:312:ARG:NH2	2.50	0.45
1:E:248:ALA:HA	1:E:251:LYS:HE3	1.98	0.45
1:B:139:HIS:HB3	1:B:142:LEU:HD23	1.99	0.44
1:F:136:VAL:HA	1:F:139:HIS:HB3	1.99	0.44
1:F:404:LYS:HA	1:F:407:HIS:HD2	1.82	0.44
1:A:155:THR:HG22	1:A:157:ASP:H	1.81	0.44
1:B:202:ARG:HH22	1:E:226:LEU:HD23	1.83	0.44
1:C:443:LEU:HD12	1:C:481:LEU:HD11	1.99	0.44
1:E:249:LEU:HD13	1:E:290:LEU:HD11	2.00	0.44
1:F:347:LYS:HG3	1:F:349:PRO:HD3	1.99	0.44
1:A:345:ARG:HD3	1:A:348:ALA:HB3	2.00	0.44
1:E:94:VAL:HG22	1:E:107:GLY:HA2	2.00	0.44
1:E:358:GLY:HA2	1:E:541:ARG:HG3	1.99	0.44
1:B:412:VAL:HG12	1:B:414:VAL:H	1.82	0.44
1:C:5:LEU:O	1:C:105:ALA:N	2.50	0.44
1:C:612:ILE:HG13	1:C:667:VAL:HG22	2.00	0.44
1:B:202:ARG:NH2	1:E:225:TYR:HB3	2.33	0.44
1:E:9:PRO:O	1:E:11:ARG:NH1	2.51	0.44
1:A:128:LEU:HD11	1:A:192:VAL:HG12	1.99	0.44
1:A:302:ASP:OD1	1:A:302:ASP:N	2.47	0.44
1:B:26:GLY:HA2	1:B:81:THR:HA	1.99	0.44
1:C:610:LEU:HD23	1:C:610:LEU:HA	1.85	0.44
1:B:633:MET:CE	4:B:802:4KZ:C28	2.97	0.43
1:C:8:ILE:HB	1:C:46:LEU:HD23	2.01	0.43
1:C:11:ARG:HD3	1:C:27:ARG:HD2	2.01	0.43
1:C:707:SER:HB3	1:C:713:MET:HE1	1.99	0.43
1:E:2:ARG:HD3	1:E:106:ARG:HD3	2.00	0.43
1:E:139:HIS:HD2	1:E:142:LEU:HG	1.83	0.43
1:B:96:ASP:H	1:B:106:ARG:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:VAL:HG22	1:D:45:PHE:HD2	1.83	0.43
1:D:50:ARG:HG2	1:D:61:ASP:HB3	1.98	0.43
1:A:253:ILE:HD12	1:A:270:LEU:HD22	2.00	0.43
1:D:693:ARG:HD2	1:D:776:MET:HB2	2.00	0.43
1:F:200:LEU:HD23	1:F:203:PHE:HD2	1.83	0.43
1:A:444:ASP:OD1	1:A:484:ARG:NH1	2.51	0.43
1:D:165:ILE:O	1:D:169:ALA:N	2.51	0.43
1:E:653:LEU:HD23	1:E:692:SER:HB3	2.01	0.43
1:F:66:GLY:O	1:F:92:ALA:N	2.46	0.43
1:F:421:LEU:HB2	1:F:469:THR:HG22	2.01	0.43
1:A:152:VAL:HG11	1:A:164:THR:HG21	2.01	0.43
1:C:66:GLY:O	1:C:92:ALA:N	2.52	0.43
1:E:434:ASP:HA	1:E:435:PRO:HD3	1.52	0.43
1:F:250:ARG:HA	1:F:253:ILE:HG22	2.01	0.43
1:C:243:LEU:O	1:C:244:SER:C	2.62	0.43
1:E:55:ASP:OD1	1:E:55:ASP:N	2.52	0.43
1:E:374:ARG:HH12	1:E:466:PHE:HD2	1.66	0.43
1:E:502:ALA:HA	1:E:506:LEU:HB2	2.00	0.43
1:F:320:TYR:HB3	1:F:501:ILE:HG22	2.01	0.43
1:A:5:LEU:HB2	1:A:45:PHE:CD2	2.54	0.43
1:C:243:LEU:HB3	1:C:244:SER:H	1.69	0.42
1:D:549:LYS:HG2	1:D:552:ARG:HH21	1.83	0.42
1:B:250:ARG:HE	1:B:270:LEU:HD23	1.84	0.42
1:D:265:LYS:NZ	1:D:289:TYR:OH	2.51	0.42
1:A:432:ARG:HH21	1:A:432:ARG:CG	2.15	0.42
1:F:18:HIS:NE2	1:F:89:ARG:O	2.53	0.42
1:F:690:ALA:O	1:F:693:ARG:NH1	2.52	0.42
1:A:239:GLY:C	1:A:241:ASP:H	2.27	0.42
1:D:152:VAL:O	1:D:155:THR:OG1	2.32	0.42
1:B:143:ARG:HA	1:B:146:ARG:HH12	1.83	0.42
1:C:226:LEU:HD11	1:F:205:LEU:HD21	2.01	0.42
1:D:612:ILE:HG12	1:D:667:VAL:HG22	2.02	0.42
1:E:573:ASP:O	1:E:576:THR:OG1	2.30	0.42
1:E:625:LEU:HD23	1:E:665:VAL:HB	2.02	0.42
1:A:18:HIS:H	1:A:88:ALA:HB3	1.83	0.42
1:A:91:ARG:HG3	1:A:111:SER:HB3	2.01	0.42
1:C:136:VAL:HG23	1:C:144:LEU:HD23	2.01	0.42
1:C:243:LEU:O	1:C:246:LEU:N	2.53	0.42
1:C:343:ASP:OD1	1:C:343:ASP:N	2.53	0.42
1:E:49:GLN:NE2	1:E:54:VAL:O	2.46	0.42
1:E:250:ARG:NH1	1:E:270:LEU:HD13	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:802:4KZ:C22	4:B:802:4KZ:O30	2.65	0.42
1:E:218:ASP:O	1:E:222:ARG:HB2	2.20	0.42
1:C:162:ALA:HB1	1:C:189:LEU:HD21	2.00	0.42
1:C:625:LEU:HD23	1:C:665:VAL:HB	2.02	0.42
1:D:226:LEU:HB2	1:E:237:LEU:HD21	2.01	0.42
1:E:120:VAL:O	1:E:124:LEU:HB2	2.20	0.42
1:F:9:PRO:HG3	1:F:57:PRO:HB3	2.02	0.42
1:F:262:VAL:HG13	1:F:293:LEU:HD11	2.02	0.42
1:B:177:GLN:O	1:B:180:LEU:N	2.53	0.42
1:C:243:LEU:HA	1:C:243:LEU:HD23	1.84	0.42
1:C:318:ASP:OD2	1:C:370:ARG:NH2	2.42	0.42
1:E:199:ASP:O	1:E:203:PHE:HB2	2.20	0.42
1:E:412:VAL:HG21	1:E:417:PRO:HG3	2.02	0.42
1:B:69:ALA:HB1	1:B:86:VAL:HB	2.01	0.41
1:C:235:LYS:HE2	1:C:235:LYS:HB3	1.92	0.41
1:A:332:TYR:OH	1:A:486:GLU:OE1	2.31	0.41
1:C:10:LEU:HD11	1:C:23:VAL:HG13	2.02	0.41
1:C:160:MET:O	1:C:164:THR:OG1	2.29	0.41
1:B:387:GLU:H	1:A:385:ARG:NH2	2.18	0.41
1:C:600:LEU:HD13	1:C:721:LYS:HB3	2.02	0.41
1:D:47:VAL:HG22	1:D:66:GLY:HA3	2.03	0.41
1:F:14:VAL:HG21	1:F:177:GLN:HE21	1.85	0.41
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.83	0.41
1:A:668:PRO:HA	1:A:669:ASP:HA	1.81	0.41
1:C:702:MET:HE3	1:C:702:MET:HB2	1.91	0.41
3:C:801:AGS:S1G	1:D:484:ARG:NH2	2.77	0.41
1:D:517:GLU:O	1:D:519:ARG:N	2.47	0.41
1:E:213:VAL:HG12	1:E:217:MET:HE2	2.03	0.41
1:F:33:ALA:HA	1:F:102:TYR:HE1	1.86	0.41
1:A:272:ARG:O	1:A:275:ARG:NH1	2.54	0.41
1:A:412:VAL:HG12	1:A:414:VAL:H	1.86	0.41
1:B:139:HIS:CE1	1:B:203:PHE:HB2	2.56	0.41
1:C:55:ASP:OD1	1:C:55:ASP:N	2.40	0.41
1:C:374:ARG:HH21	1:C:416:ASN:HB2	1.85	0.41
1:D:7:VAL:HG21	1:D:105:ALA:HB3	2.02	0.41
1:D:601:ALA:HB2	4:D:802:4KZ:C27	2.51	0.41
1:E:490:ILE:HA	1:E:491:PRO:HD3	1.93	0.41
1:E:345:ARG:H	1:E:345:ARG:HD2	1.85	0.41
1:E:431:TRP:CH2	1:F:431:TRP:CE3	3.09	0.41
1:B:100:GLY:HA3	1:B:102:TYR:C	2.45	0.41
1:B:114:PHE:HA	1:B:115:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HD11	1:C:148:GLN:HG3	2.02	0.41
1:D:128:LEU:HA	1:D:193:LEU:HD13	2.02	0.41
1:D:552:ARG:HG2	1:E:335:VAL:HG21	2.03	0.41
1:E:42:ARG:HH21	1:E:71:VAL:HG11	1.86	0.41
1:F:206:ASP:HA	1:F:209:VAL:HG12	2.02	0.41
1:F:422:ASP:OD1	1:F:470:THR:OG1	2.33	0.41
1:E:343:ASP:O	1:E:345:ARG:NH1	2.54	0.41
1:E:693:ARG:HD2	1:E:776:MET:HB2	2.03	0.41
1:F:135:TYR:HA	1:F:200:LEU:HD21	2.03	0.41
1:C:189:LEU:HA	1:C:192:VAL:HB	2.03	0.40
1:C:10:LEU:HD13	1:C:13:THR:HB	2.03	0.40
1:C:136:VAL:HA	1:C:139:HIS:HB3	2.03	0.40
1:D:22:PRO:HB3	1:D:85:MET:HE1	2.03	0.40
1:D:625:LEU:HD23	1:D:665:VAL:HB	2.02	0.40
1:F:668:PRO:HA	1:F:669:ASP:HA	1.75	0.40
1:B:432:ARG:HH22	1:A:385:ARG:HB2	1.86	0.40
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.81	0.40
1:B:94:VAL:HG11	1:B:97:TYR:HD1	1.86	0.40
1:B:98:ILE:HA	1:B:99:PRO:HD3	1.91	0.40
1:B:678:SER:CB	4:B:802:4KZ:O30	2.66	0.40
1:B:678:SER:N	4:B:802:4KZ:O30	2.45	0.40
1:D:2:ARG:HA	1:D:107:GLY:H	1.87	0.40
1:F:384:VAL:HG12	1:F:435:PRO:HG3	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 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	777/793 (98%)	733 (94%)	44 (6%)	0	100	100
1	B	777/793 (98%)	730 (94%)	43 (6%)	4 (0%)	24	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	777/793 (98%)	725 (93%)	50 (6%)	2 (0%)	36	50
1	D	777/793 (98%)	727 (94%)	48 (6%)	2 (0%)	36	50
1	E	777/793 (98%)	715 (92%)	60 (8%)	2 (0%)	36	50
1	F	777/793 (98%)	717 (92%)	57 (7%)	3 (0%)	30	43
All	All	4662/4758 (98%)	4347 (93%)	302 (6%)	13 (0%)	37	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	244	SER
1	B	238	GLY
1	E	431	TRP
1	B	52	PRO
1	C	52	PRO
1	D	448	ASN
1	B	304	GLU
1	F	677	PRO
1	E	52	PRO
1	B	305	VAL
1	D	52	PRO
1	F	52	PRO
1	F	238	GLY

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	655/665 (98%)	653 (100%)	2 (0%)	86	93
1	B	655/665 (98%)	653 (100%)	2 (0%)	86	93
1	C	655/665 (98%)	649 (99%)	6 (1%)	70	85
1	D	655/665 (98%)	655 (100%)	0	100	100
1	E	655/665 (98%)	651 (99%)	4 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	655/665 (98%)	653 (100%)	2 (0%)	86	93
All	All	3930/3990 (98%)	3914 (100%)	16 (0%)	81	92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	243	LEU
1	B	465	VAL
1	C	243	LEU
1	C	305	VAL
1	C	344	VAL
1	C	594	VAL
1	C	612	ILE
1	C	677	PRO
1	E	378	ARG
1	E	379	ILE
1	E	594	VAL
1	E	715	ILE
1	F	161	LEU
1	F	249	LEU
1	A	241	ASP
1	A	432	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	ASN
1	B	139	HIS
1	B	220	ASN
1	B	346	ASN
1	B	598	GLN
1	B	647	HIS
1	B	666	HIS
1	C	139	HIS
1	C	310	HIS
1	C	393	HIS
1	C	598	GLN
1	C	628	GLN
1	C	638	GLN
1	C	664	HIS
1	C	726	HIS

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Mol	Chain	Res	Type
1	C	739	ASN
1	C	742	GLN
1	D	12	ASN
1	D	18	HIS
1	D	377	HIS
1	D	393	HIS
1	D	510	GLN
1	D	731	HIS
1	D	739	ASN
1	E	138	ASN
1	E	216	GLN
1	E	220	ASN
1	E	310	HIS
1	E	319	HIS
1	E	340	GLN
1	F	68	GLN
1	F	177	GLN
1	F	211	GLN
1	F	216	GLN
1	F	220	ASN
1	F	337	GLN
1	F	377	HIS
1	F	416	ASN
1	F	510	GLN
1	F	598	GLN
1	F	664	HIS
1	A	234	GLN
1	A	377	HIS
1	A	739	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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
4	4KZ	E	802	1	29,33,33	0.83	1 (3%)	38,43,43	1.63	3 (7%)
4	4KZ	A	802	1	29,33,33	0.67	0	38,43,43	1.09	3 (7%)
3	AGS	F	801	-	32,33,33	0.69	1 (3%)	45,52,52	0.68	1 (2%)
3	AGS	B	801	-	32,33,33	1.02	3 (9%)	45,52,52	0.67	1 (2%)
3	AGS	C	801	-	32,33,33	0.96	3 (9%)	45,52,52	0.85	1 (2%)
4	4KZ	D	802	1	29,33,33	0.52	0	38,43,43	1.24	5 (13%)
5	ADP	E	801	-	28,29,29	1.36	5 (17%)	43,45,45	1.84	11 (25%)
4	4KZ	C	802	1	29,33,33	0.84	1 (3%)	38,43,43	1.81	6 (15%)
3	AGS	A	801	-	32,33,33	1.13	3 (9%)	45,52,52	0.65	2 (4%)
4	4KZ	F	802	1	29,33,33	0.95	3 (10%)	38,43,43	1.73	8 (21%)
4	4KZ	B	802	1	29,33,33	0.65	0	38,43,43	1.58	4 (10%)
5	ADP	D	801	-	28,29,29	1.37	4 (14%)	43,45,45	1.79	8 (18%)

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
4	4KZ	E	802	1	-	13/23/28/28	0/3/3/3
4	4KZ	A	802	1	-	0/23/28/28	0/3/3/3
3	AGS	F	801	-	-	0/21/38/38	0/3/3/3
3	AGS	B	801	-	-	1/21/38/38	0/3/3/3
3	AGS	C	801	-	-	6/21/38/38	0/3/3/3
4	4KZ	D	802	1	-	5/23/28/28	0/3/3/3
5	ADP	E	801	-	-	0/16/32/32	0/3/3/3
4	4KZ	C	802	1	-	13/23/28/28	0/3/3/3
3	AGS	A	801	-	-	1/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4KZ	F	802	1	-	6/23/28/28	0/3/3/3
4	4KZ	B	802	1	-	9/23/28/28	0/3/3/3
5	ADP	D	801	-	-	3/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	801	ADP	C5-C4	4.18	1.46	1.39
5	D	801	ADP	C5-C4	3.94	1.46	1.39
3	A	801	AGS	PB-O3B	-3.60	1.55	1.59
3	C	801	AGS	PB-O3B	-3.32	1.55	1.59
5	D	801	ADP	C5-N7	-3.15	1.33	1.39
3	B	801	AGS	PA-O3A	-3.10	1.56	1.59
3	A	801	AGS	PB-O3A	-3.09	1.56	1.59
4	E	802	4KZ	C21-N20	-2.81	1.41	1.46
3	B	801	AGS	PB-O3B	-2.64	1.56	1.59
5	E	801	ADP	C5-N7	-2.62	1.34	1.39
3	A	801	AGS	PA-O3A	-2.56	1.56	1.59
4	F	802	4KZ	C21-N20	-2.55	1.41	1.46
5	E	801	ADP	C5-C6	2.40	1.47	1.41
4	F	802	4KZ	C10-C18	-2.39	1.46	1.52
5	D	801	ADP	C4-N9	-2.37	1.32	1.37
3	B	801	AGS	PB-O3A	-2.35	1.57	1.59
5	E	801	ADP	C4-N9	-2.27	1.33	1.37
3	C	801	AGS	PB-O3A	-2.20	1.57	1.59
3	F	801	AGS	PG-S1G	2.14	1.95	1.90
5	E	801	ADP	C8-N7	2.10	1.35	1.31
4	C	802	4KZ	C21-N20	-2.05	1.42	1.46
5	D	801	ADP	C8-N7	2.03	1.35	1.31
4	F	802	4KZ	C18-N20	-2.02	1.29	1.34
3	C	801	AGS	PA-O3A	-2.01	1.57	1.59

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	802	4KZ	C22-C21-N20	-8.30	99.66	110.39
4	F	802	4KZ	C22-C21-N20	-7.60	100.56	110.39
4	E	802	4KZ	C22-C21-N20	-6.96	101.38	110.39
4	B	802	4KZ	C22-C21-N20	-6.07	102.54	110.39
5	D	801	ADP	C5-C4-N3	-5.92	118.57	126.72
5	E	801	ADP	C5-C4-N3	-5.72	118.85	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	801	ADP	N3-C4-N9	4.78	135.31	127.17
5	E	801	ADP	N3-C4-N9	4.49	134.81	127.17
3	C	801	AGS	PB-O3B-PG	-3.73	119.51	133.17
5	E	801	ADP	C2-N3-C4	3.64	120.72	111.83
3	F	801	AGS	PB-O3B-PG	-3.58	120.06	133.17
5	D	801	ADP	C2-N3-C4	3.52	120.42	111.83
5	E	801	ADP	C4-C5-N7	-3.36	106.74	110.58
3	B	801	AGS	PB-O3B-PG	-3.28	121.18	133.17
5	E	801	ADP	N3-C2-N1	-3.03	123.99	128.58
4	B	802	4KZ	C6-N1-C2	2.96	120.74	116.93
4	D	802	4KZ	C6-N1-C2	2.95	120.73	116.93
5	D	801	ADP	N3-C2-N1	-2.83	124.30	128.58
4	C	802	4KZ	O19-C18-N20	2.81	127.99	122.96
5	D	801	ADP	O4'-C1'-N9	2.79	113.45	108.09
4	A	802	4KZ	C6-N1-C2	2.74	120.47	116.93
5	E	801	ADP	C4-N9-C8	2.72	108.59	105.74
4	F	802	4KZ	O19-C18-N20	2.70	127.79	122.96
5	D	801	ADP	C4-C5-N7	-2.68	107.51	110.58
4	F	802	4KZ	C2-C3-N4	-2.61	118.55	121.97
5	E	801	ADP	C3'-C2'-C1'	2.56	106.30	101.46
3	A	801	AGS	PB-O3B-PG	-2.53	123.90	133.17
4	D	802	4KZ	C5-N4-C3	2.52	121.26	116.85
4	B	802	4KZ	O19-C18-N20	2.51	127.46	122.96
4	C	802	4KZ	C6-N1-C2	2.49	120.14	116.93
5	E	801	ADP	C5-N7-C8	2.45	107.30	103.45
5	E	801	ADP	C2'-C1'-N9	-2.41	107.31	113.30
4	F	802	4KZ	C6-N1-C2	2.37	119.99	116.93
4	A	802	4KZ	C7-C2-N1	2.37	120.19	117.42
5	D	801	ADP	C4-N9-C8	2.35	108.20	105.74
4	E	802	4KZ	C10-C18-N20	-2.32	111.67	116.63
4	D	802	4KZ	C22-C21-N20	-2.30	107.41	110.39
4	A	802	4KZ	C5-N4-C3	2.28	120.84	116.85
4	F	802	4KZ	C5-N4-C3	2.27	120.83	116.85
4	E	802	4KZ	C6-N1-C2	2.24	119.82	116.93
4	D	802	4KZ	C6-C5-N4	-2.20	119.22	121.96
3	A	801	AGS	O2G-PG-O3B	2.19	111.96	104.64
4	B	802	4KZ	C5-N4-C3	2.17	120.65	116.85
4	D	802	4KZ	C3-C2-N1	-2.16	119.06	121.60
4	F	802	4KZ	C21-N20-C18	-2.15	117.57	122.99
5	E	801	ADP	C6-C5-N7	2.13	136.20	132.09
4	F	802	4KZ	C5-C6-N1	-2.07	119.27	122.19
4	C	802	4KZ	C18-C10-N9	-2.06	105.54	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	801	ADP	N9-C8-N7	-2.06	111.02	113.94
4	F	802	4KZ	C10-C18-N20	-2.05	112.26	116.63
4	C	802	4KZ	C5-C6-N1	-2.05	119.31	122.19
5	D	801	ADP	C5-N7-C8	2.04	106.66	103.45
4	C	802	4KZ	C10-C18-N20	-2.01	112.33	116.63

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	802	4KZ	C3-C2-C7-N9
4	B	802	4KZ	C3-C2-C7-O8
4	B	802	4KZ	O19-C18-N20-C21
4	B	802	4KZ	N20-C21-C22-C23
4	B	802	4KZ	B29-C21-C22-C23
4	C	802	4KZ	C3-C2-C7-N9
4	C	802	4KZ	C3-C2-C7-O8
4	C	802	4KZ	O19-C18-N20-C21
4	C	802	4KZ	N20-C21-C22-C23
4	C	802	4KZ	B29-C21-C22-C23
4	C	802	4KZ	C21-C22-C23-C24
4	C	802	4KZ	C21-C22-C23-C28
4	E	802	4KZ	O19-C18-N20-C21
4	E	802	4KZ	N20-C21-C22-C23
4	E	802	4KZ	B29-C21-C22-C23
4	F	802	4KZ	O19-C18-N20-C21
4	F	802	4KZ	N20-C21-C22-C23
4	F	802	4KZ	B29-C21-C22-C23
5	D	801	ADP	O4'-C1'-N9-C8
5	D	801	ADP	O4'-C1'-N9-C4
4	B	802	4KZ	C10-C18-N20-C21
4	F	802	4KZ	C10-C18-N20-C21
4	C	802	4KZ	N1-C2-C7-N9
4	C	802	4KZ	N1-C2-C7-O8
4	E	802	4KZ	N1-C2-C7-N9
4	B	802	4KZ	N1-C2-C7-O8
4	D	802	4KZ	N1-C2-C7-O8
4	E	802	4KZ	C10-C18-N20-C21
4	E	802	4KZ	N1-C2-C7-O8
4	B	802	4KZ	N1-C2-C7-N9
4	D	802	4KZ	N1-C2-C7-N9
3	C	801	AGS	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
4	D	802	4KZ	C3-C2-C7-O8
4	C	802	4KZ	C10-C18-N20-C21
3	C	801	AGS	O4'-C1'-N9-C4
4	D	802	4KZ	C3-C2-C7-N9
4	E	802	4KZ	C3-C2-C7-O8
4	E	802	4KZ	C3-C2-C7-N9
4	E	802	4KZ	N9-C10-C18-O19
4	E	802	4KZ	C11-C10-C18-O19
4	F	802	4KZ	C21-C22-C23-C24
4	F	802	4KZ	C21-C22-C23-C28
4	C	802	4KZ	C10-C11-C12-C17
3	C	801	AGS	PB-O3B-PG-O2G
4	E	802	4KZ	N9-C10-C18-N20
3	C	801	AGS	O4'-C4'-C5'-O5'
4	C	802	4KZ	C10-C11-C12-C13
3	B	801	AGS	PA-O3A-PB-O2B
3	C	801	AGS	PA-O3A-PB-O1B
3	A	801	AGS	PA-O3A-PB-O2B
4	E	802	4KZ	C22-C21-N20-C18
4	E	802	4KZ	N9-C10-C11-C12
4	B	802	4KZ	C21-C22-C23-C28
4	D	802	4KZ	C21-C22-C23-C24
5	D	801	ADP	O4'-C4'-C5'-O5'
4	C	802	4KZ	C18-C10-N9-C7
3	C	801	AGS	PA-O3A-PB-O2B

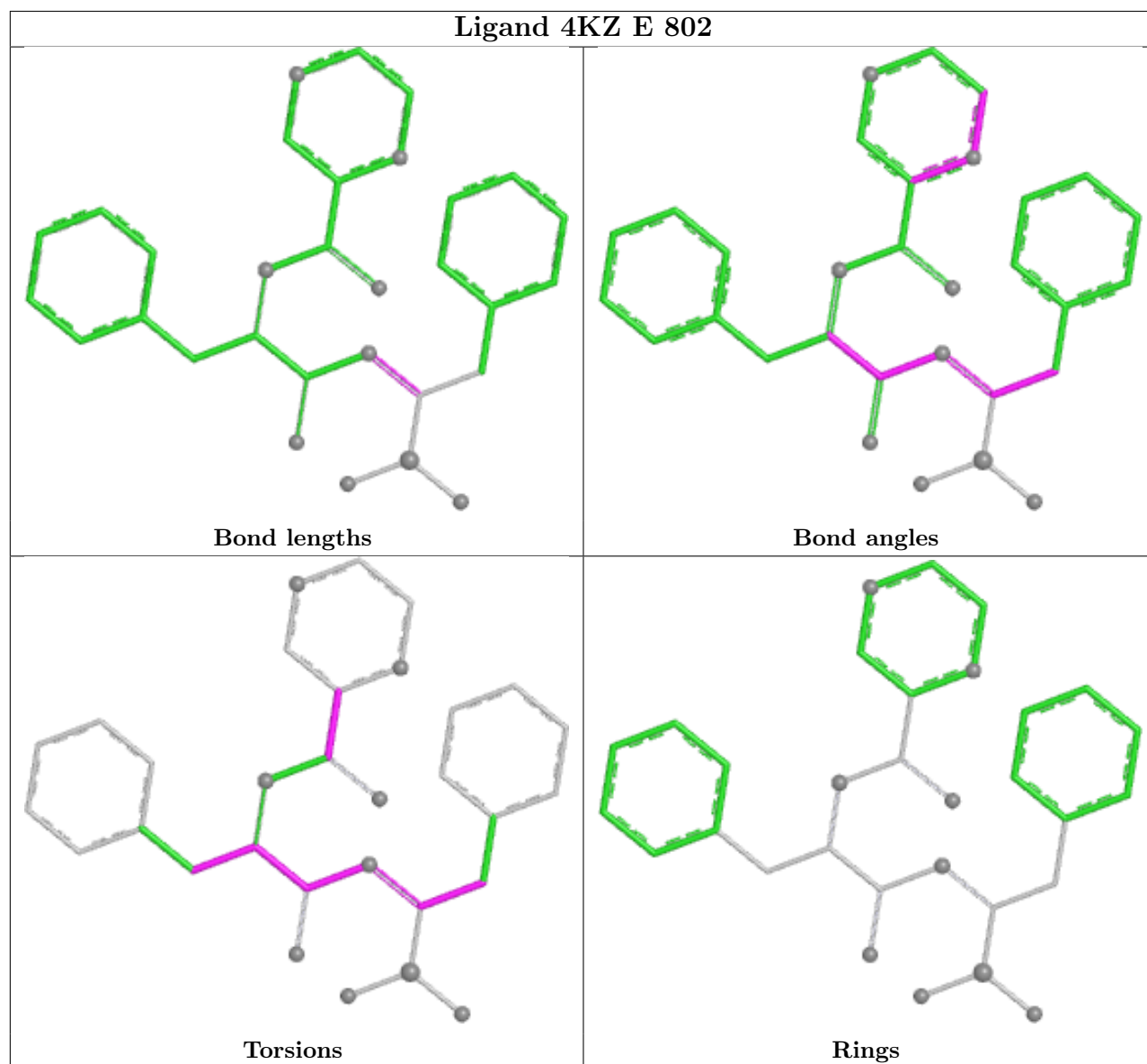
There are no ring outliers.

10 monomers are involved in 48 short contacts:

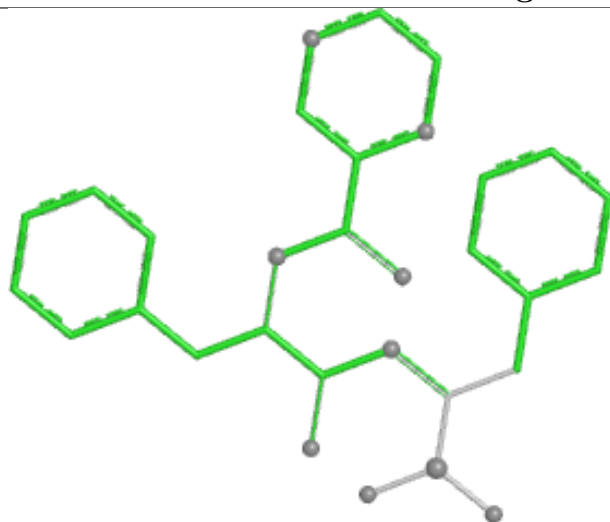
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	802	4KZ	3	0
4	A	802	4KZ	4	0
3	F	801	AGS	1	0
3	B	801	AGS	2	0
3	C	801	AGS	3	0
4	D	802	4KZ	9	0
4	C	802	4KZ	4	0
3	A	801	AGS	1	0
4	F	802	4KZ	5	0
4	B	802	4KZ	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

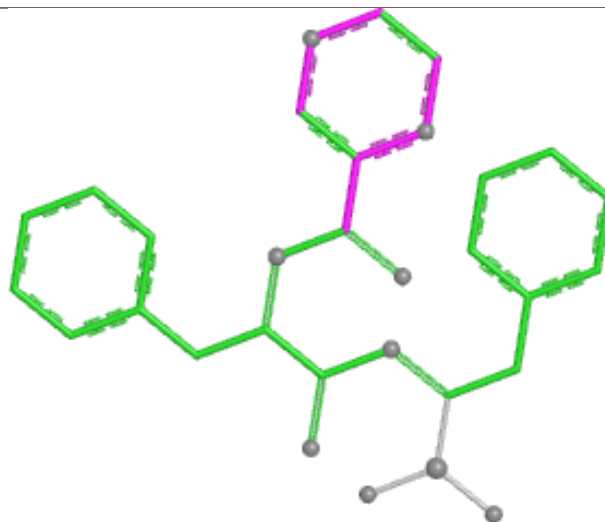
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



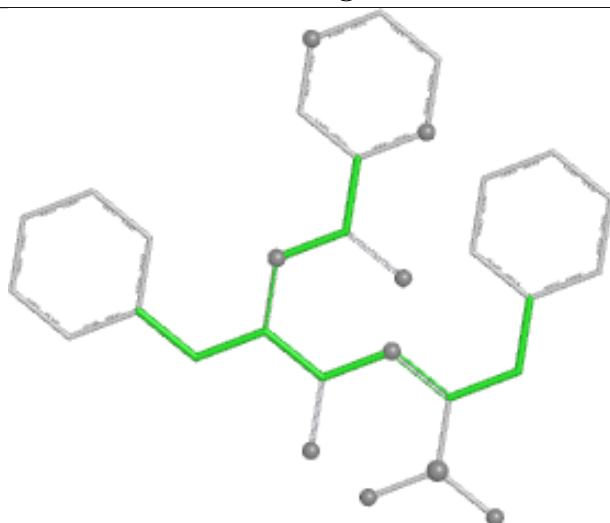
Ligand 4KZ A 802



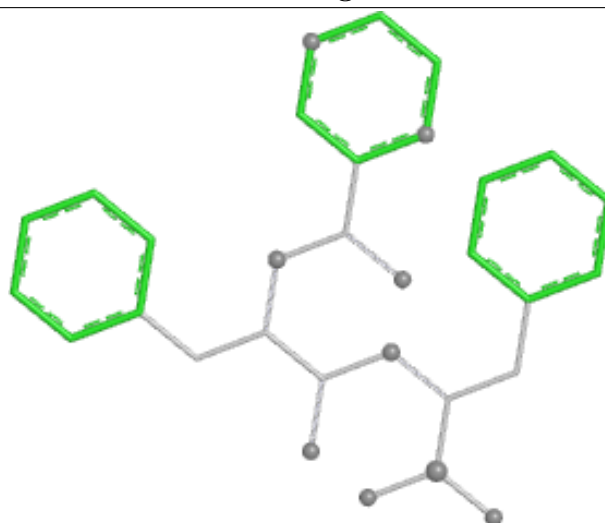
Bond lengths



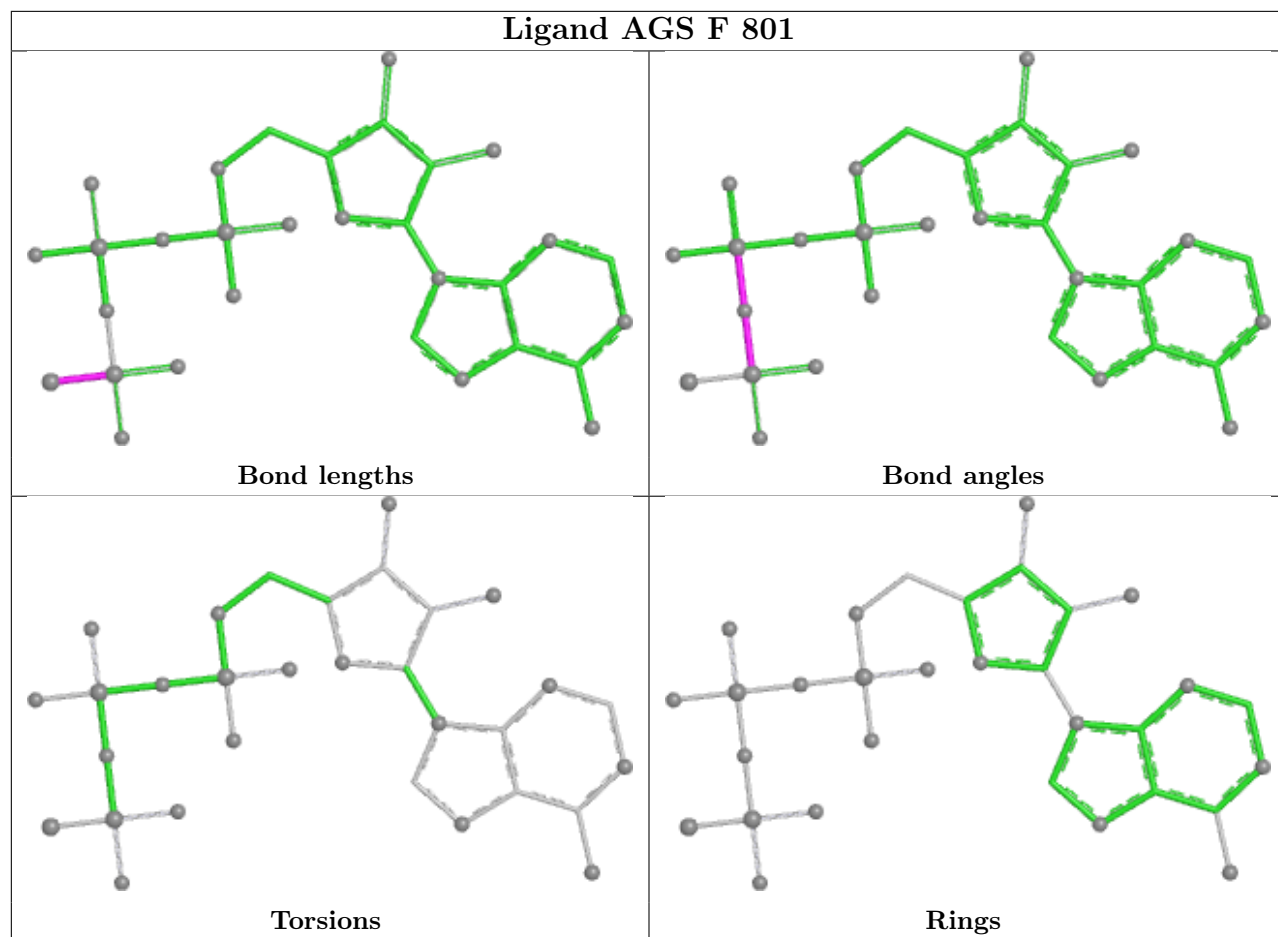
Bond angles



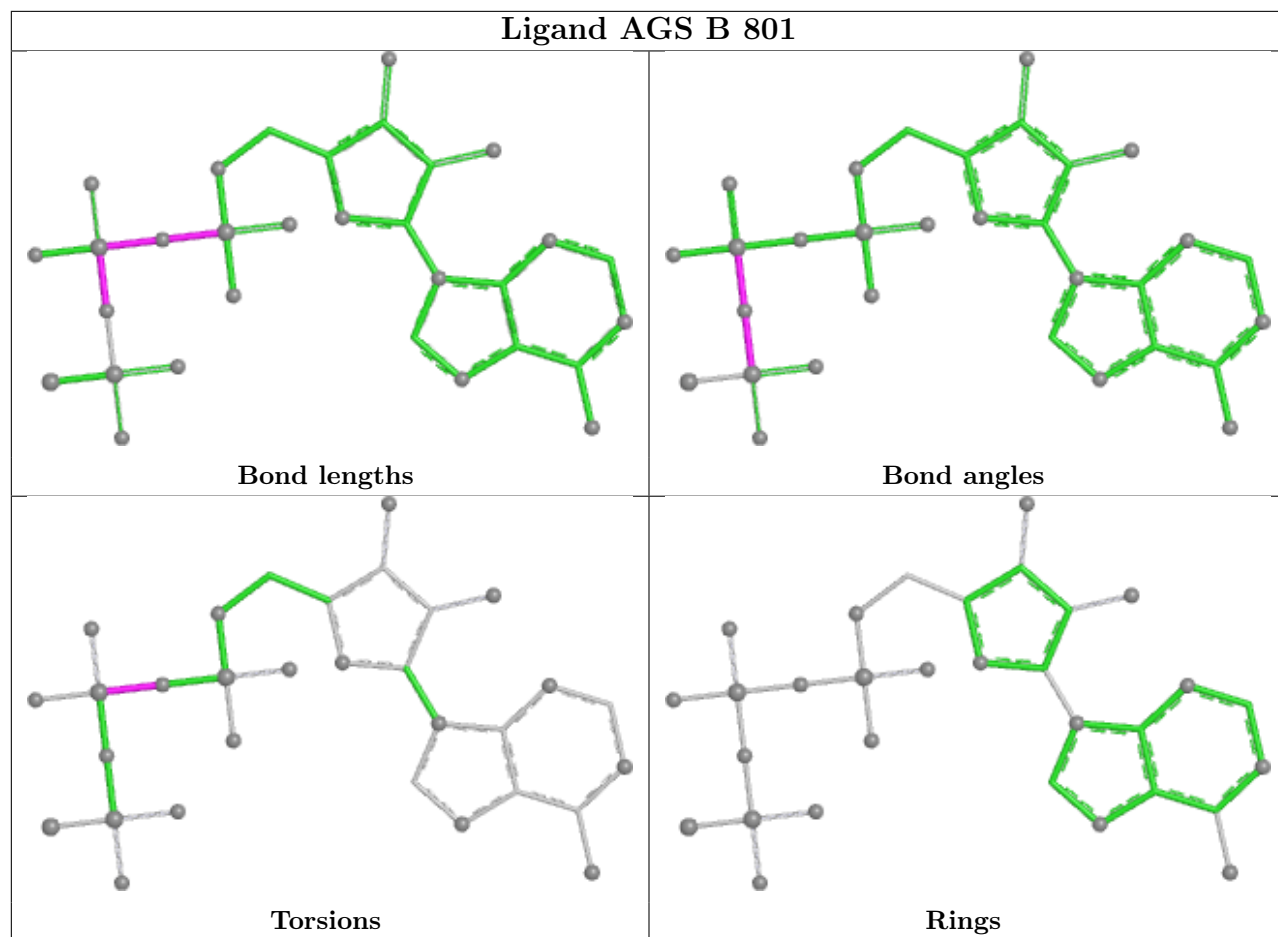
Torsions

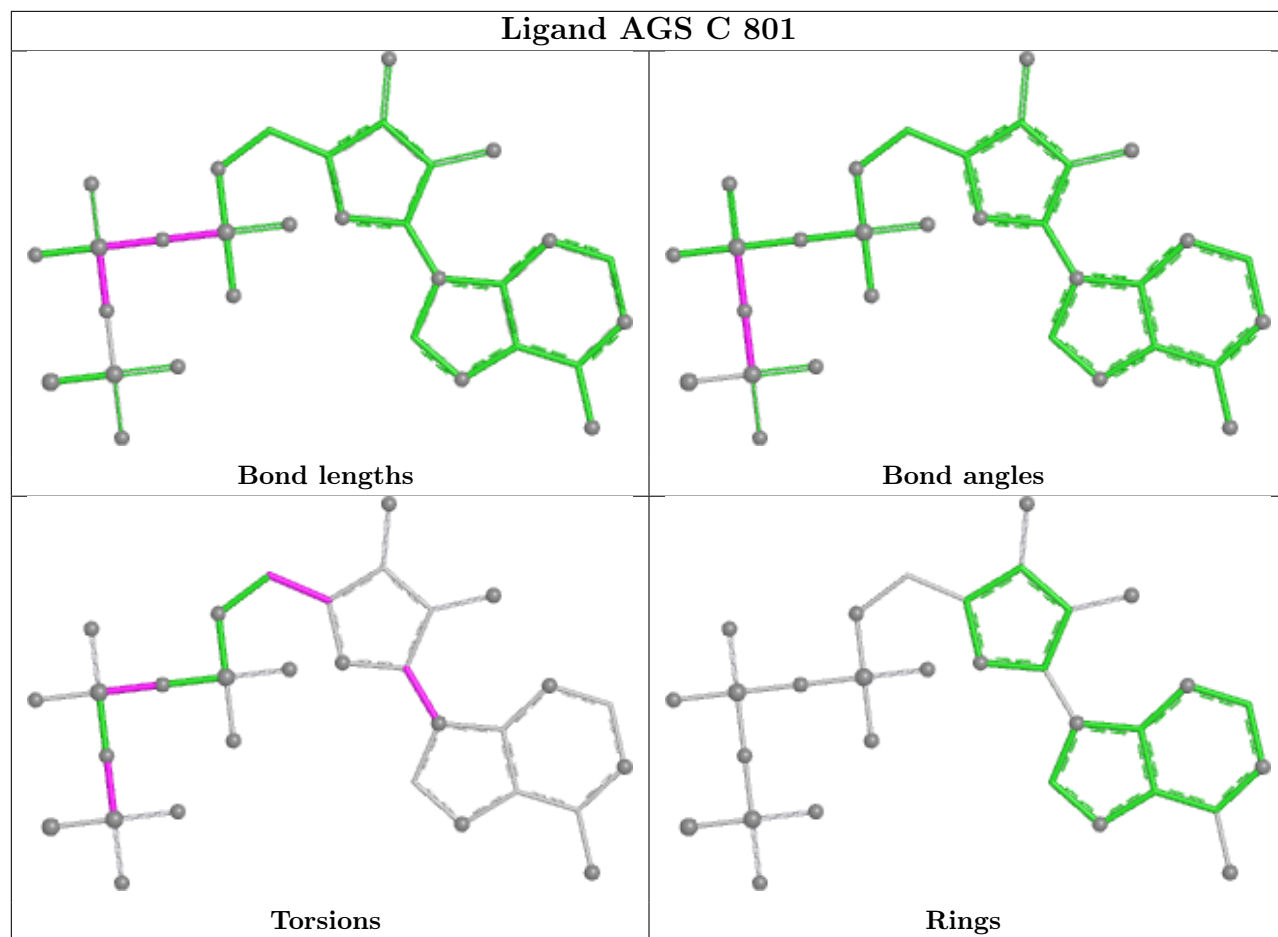


Rings

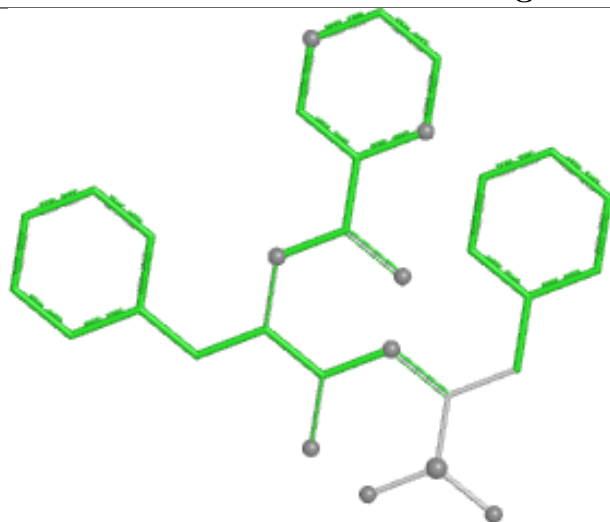


Ligand AGS B 801

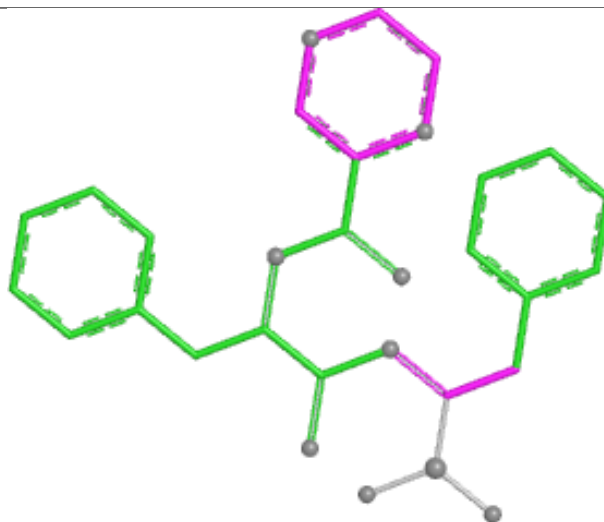




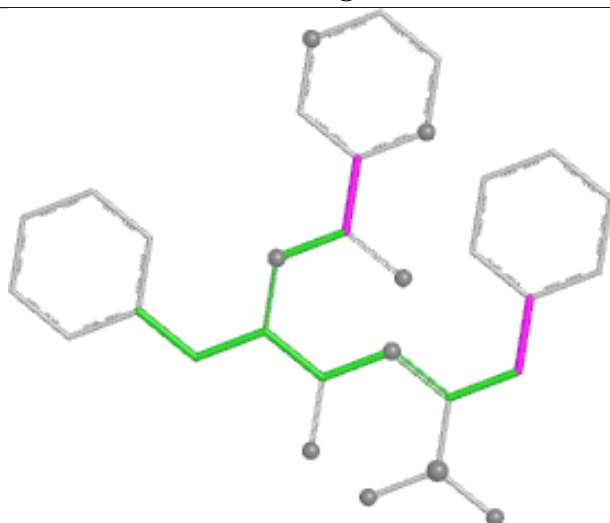
Ligand 4KZ D 802



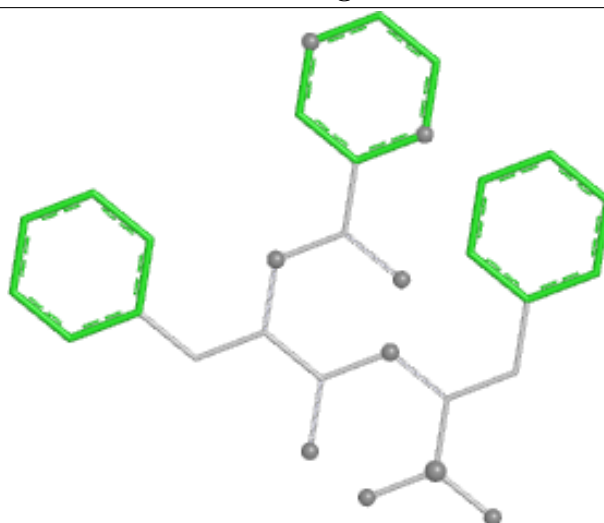
Bond lengths



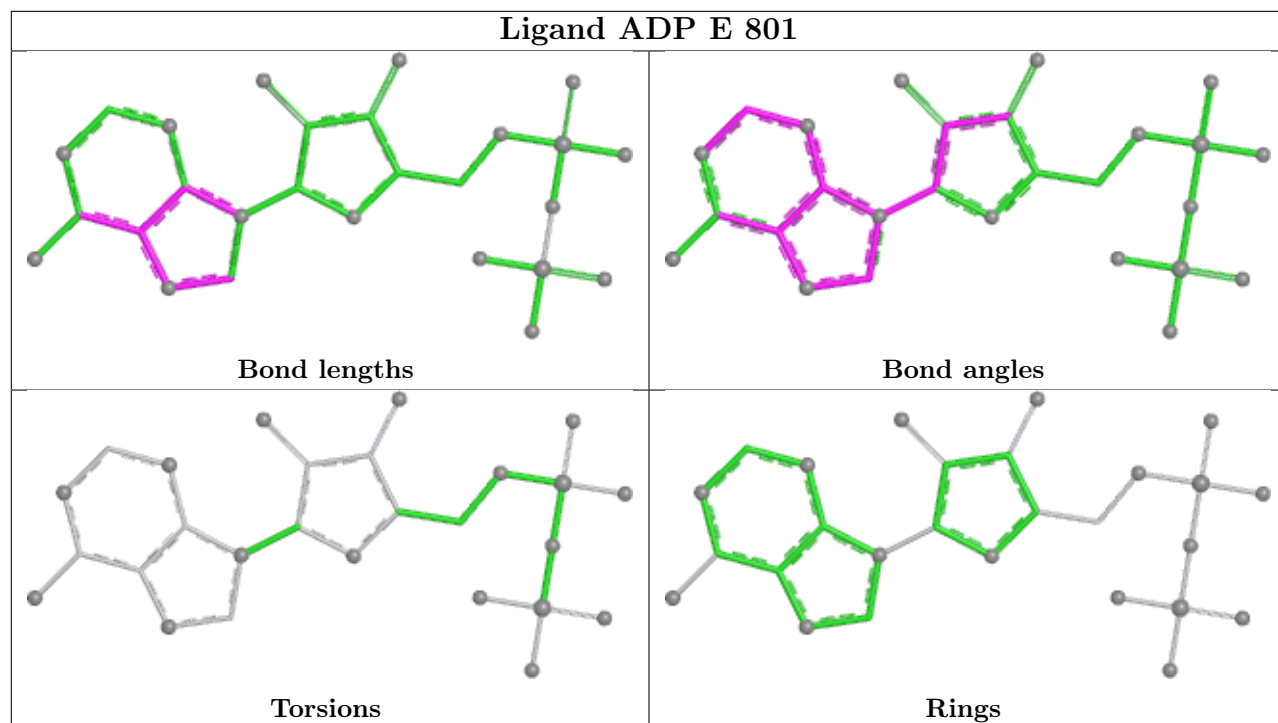
Bond angles



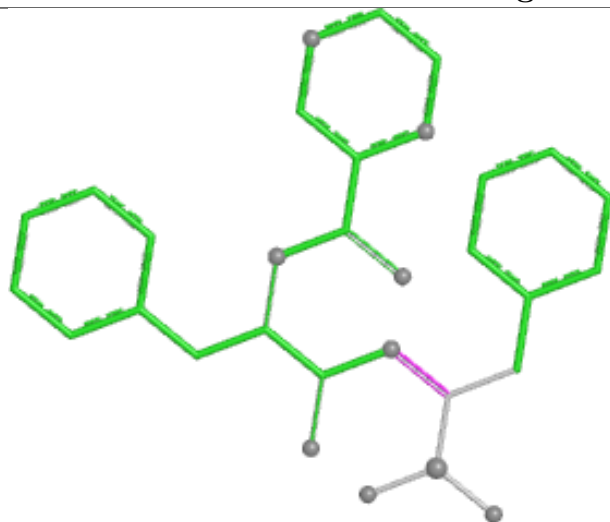
Torsions



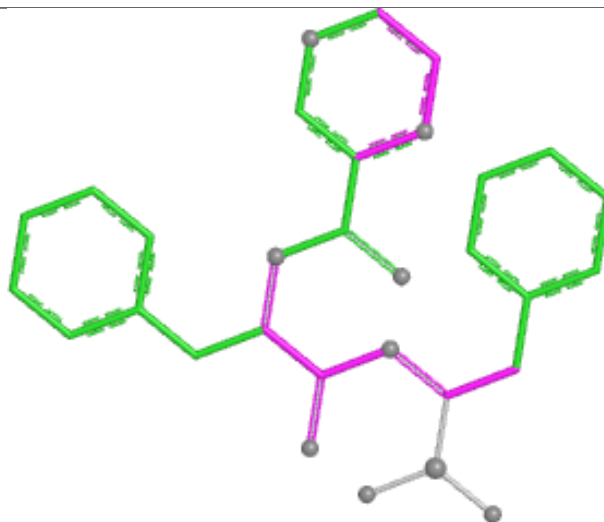
Rings



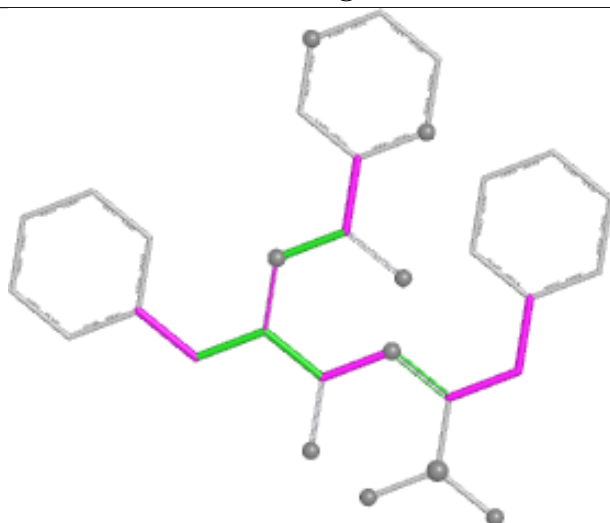
Ligand 4KZ C 802



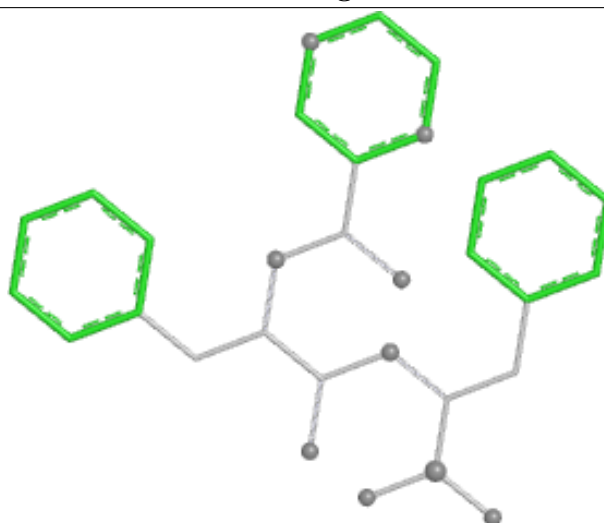
Bond lengths



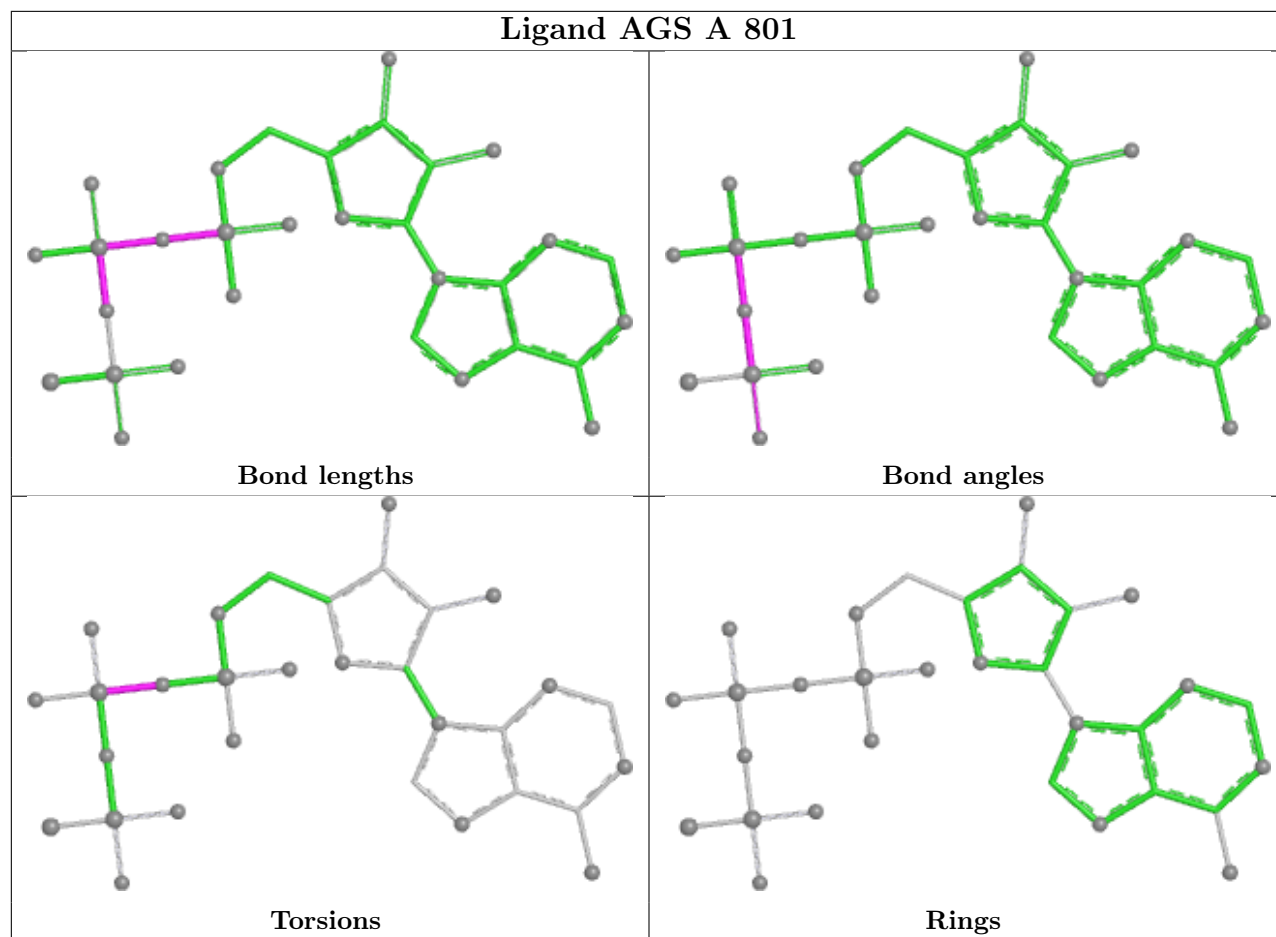
Bond angles



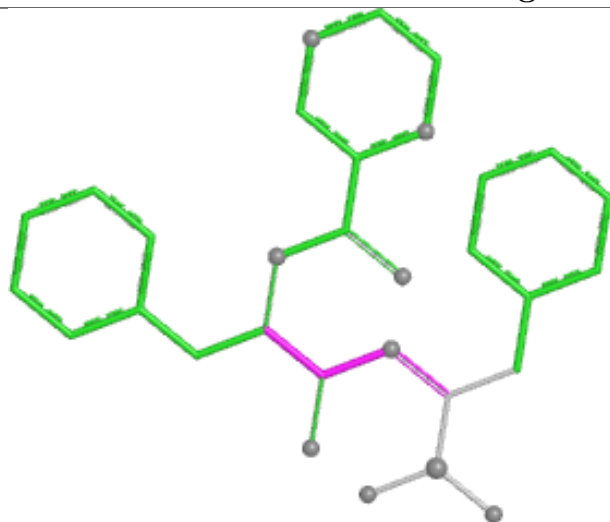
Torsions



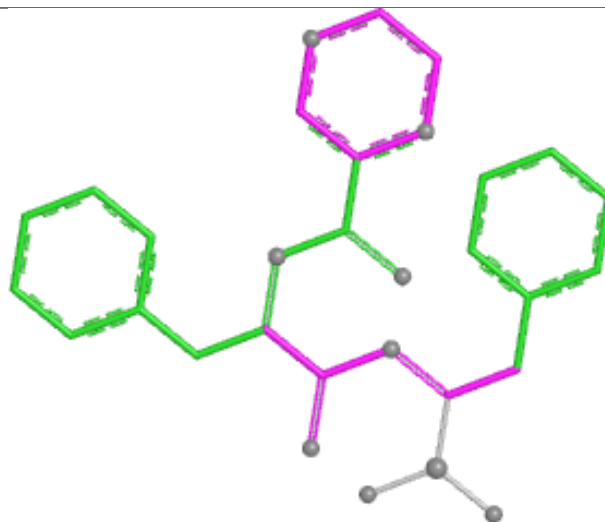
Rings



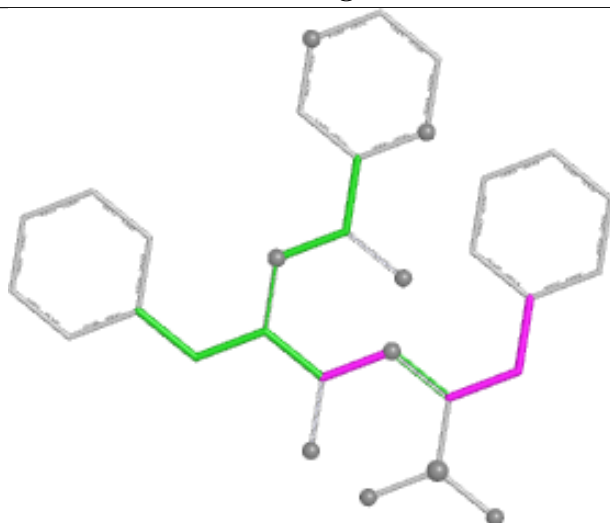
Ligand 4KZ F 802



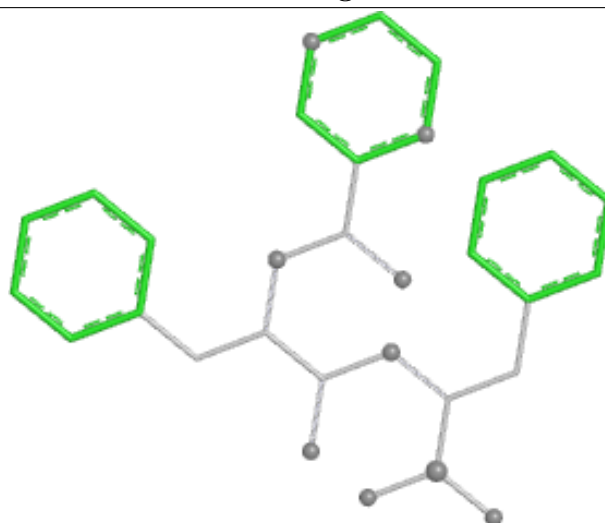
Bond lengths



Bond angles

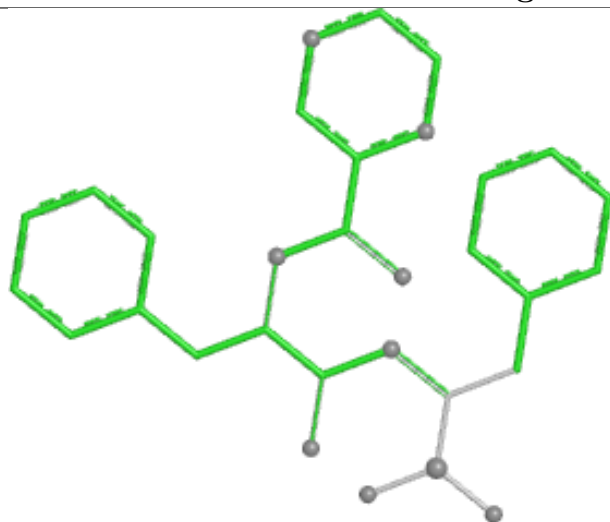


Torsions

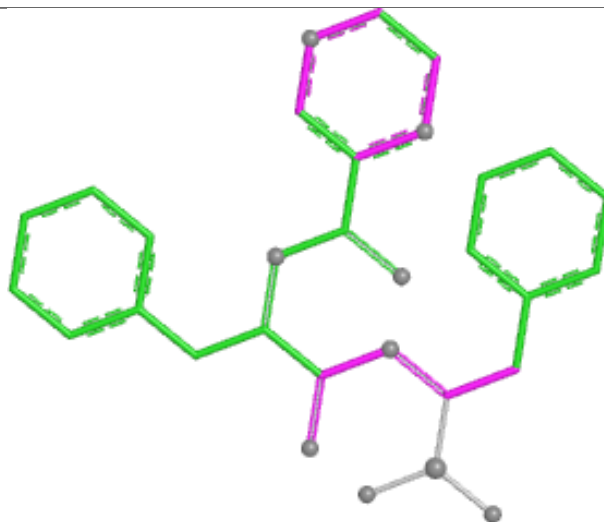


Rings

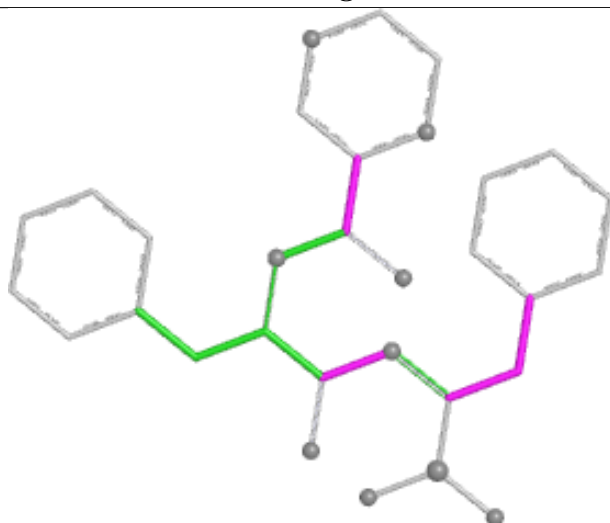
Ligand 4KZ B 802



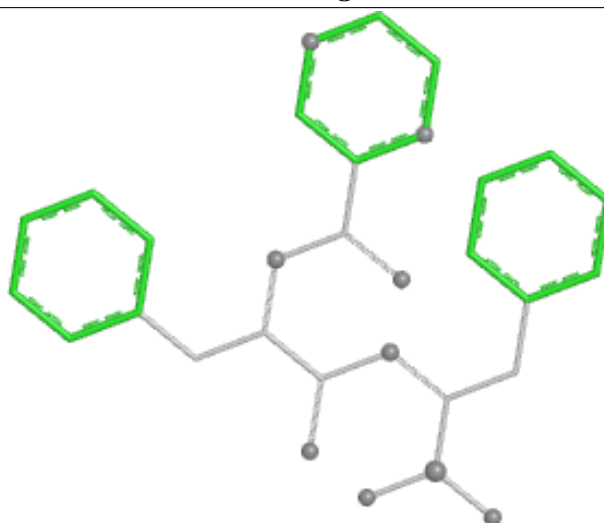
Bond lengths



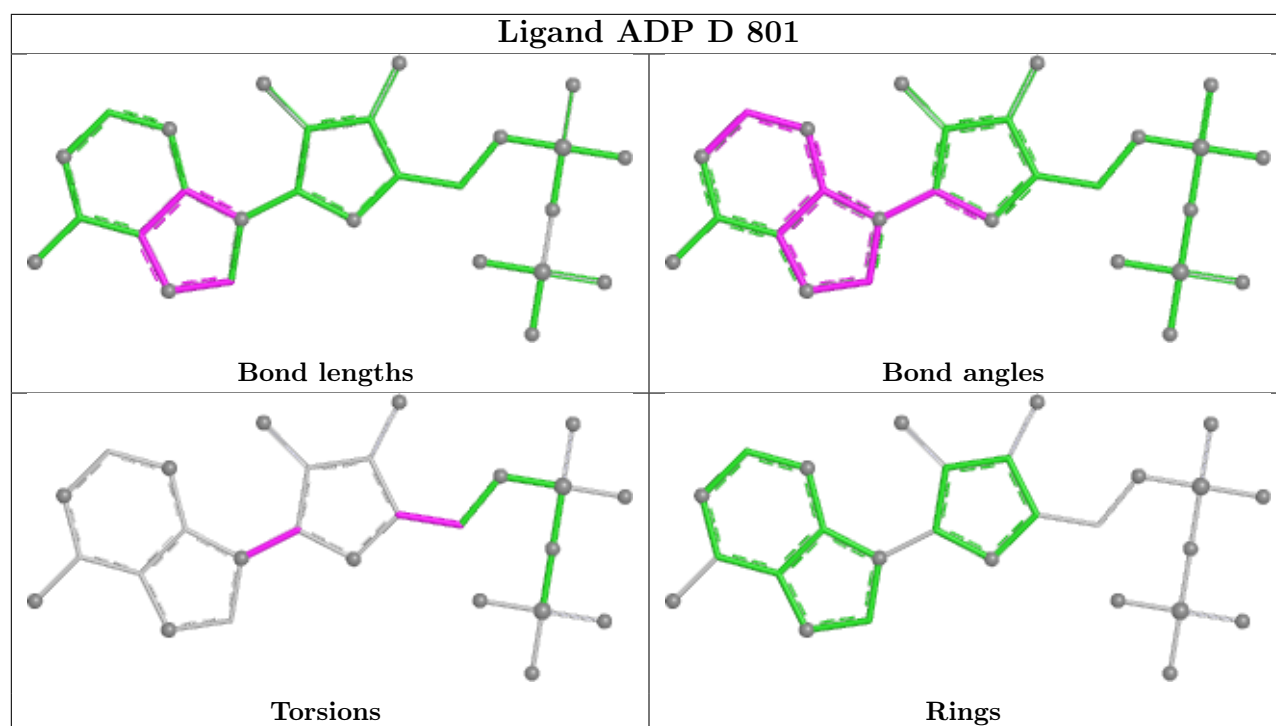
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-31534. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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.