



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:23 AM UTC

PDB ID : 1ECG / pdb_00001ecg
Title : DON INACTIVATED ESCHERICHIA COLI GLUTAMINE PHOSPHORIBOSYL PYROPHOSPHATE (PRPP) AMIDOTRANSFERASE
Authors : Krahn, J.M.
Deposited on : 1996-04-23
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

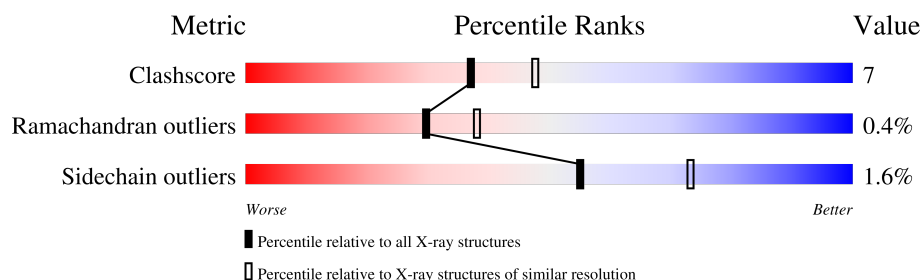
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	504	 79% 18% ..
1	B	504	 79% 18% ..

2 Entry composition [i](#)

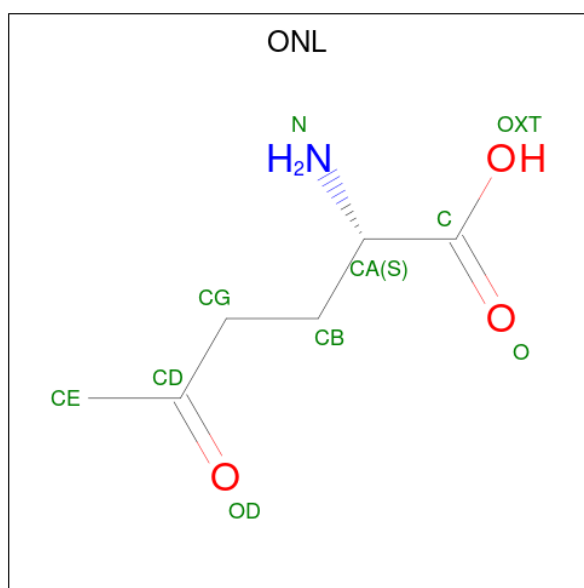
There are 4 unique types of molecules in this entry. The entry contains 9126 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE.

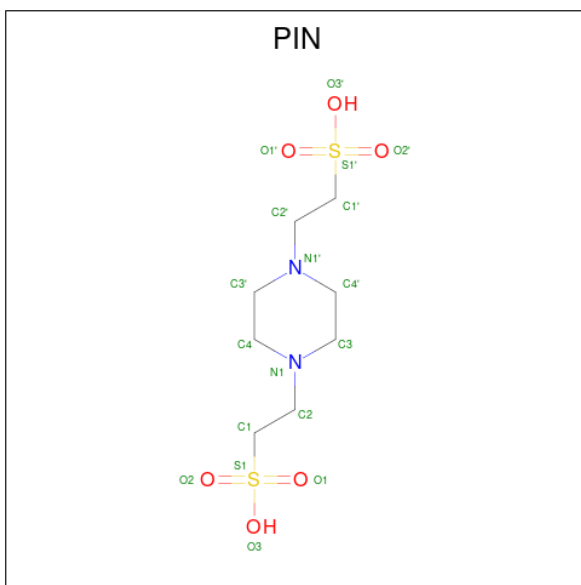
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	17	0
			3997	2513	708	759	17			
1	B	500	Total	C	N	O	S	0	13	0
			4042	2537	723	764	18			

- Molecule 2 is 5-OXO-L-NORLEUCINE (CCD ID: ONL) (formula: $C_6H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	B	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is PIPERAZINE-N,N'-BIS(2-ETHANESULFONIC ACID) (CCD ID: PIN) (formula: $C_8H_{18}N_2O_6S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			18	8	2	6	2		
3	A	1	Total	C	N	O	S	0	0
			18	8	2	6	2		
3	A	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			18	8	2	6	2		
3	B	1	Total	C	N	O	S	0	0
			18	8	2	6	2		
3	B	1	Total	C	N	O	S	0	0
			9	4	1	3	1		

- Molecule 4 is water.

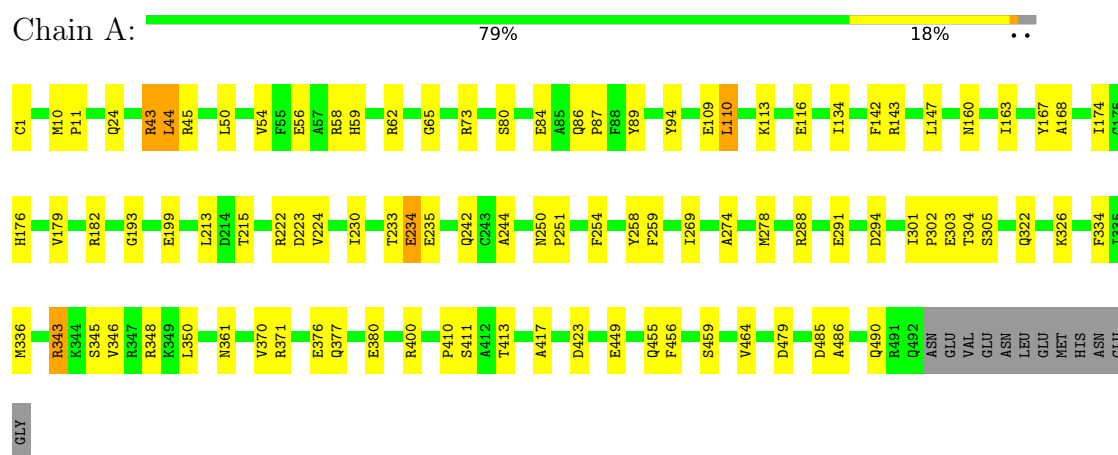
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	501	Total	O	0	0
			501	501		
4	B	478	Total	O	0	0
			478	478		

3 Residue-property plots

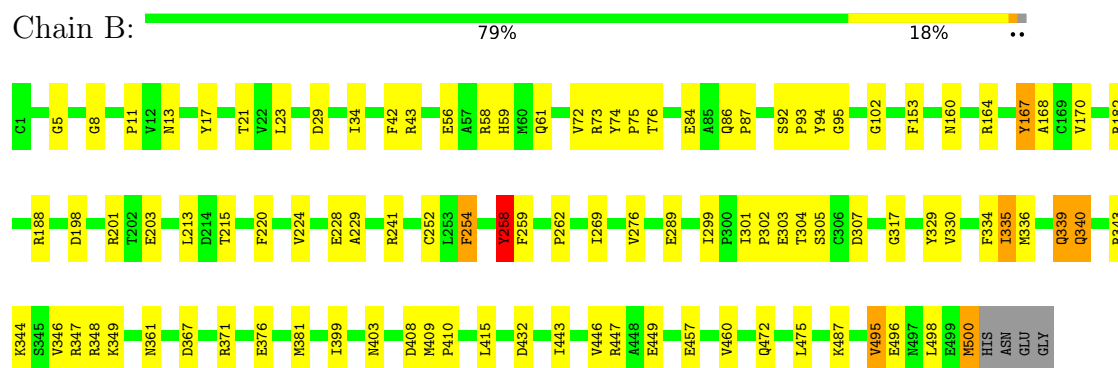
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

- Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE



- Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	116.90Å 157.50Å 106.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30	Depositor
% Data completeness (in resolution range)	91.8 (30.00-2.30)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.147 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9126	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PIN, ONL

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	0.94	5/4068 (0.1%)	1.40	23/5509 (0.4%)
1	B	0.77	2/4112 (0.0%)	1.05	20/5565 (0.4%)
All	All	0.86	7/8180 (0.1%)	1.24	43/11074 (0.4%)

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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GLU	C-N	26.46	1.73	1.33
1	A	234	GLU	CA-C	-21.05	1.24	1.52
1	B	500	MET	C-O	-16.53	0.90	1.23
1	A	233	THR	C-N	-12.81	1.17	1.33
1	B	299	ILE	CA-CB	5.86	1.59	1.54
1	A	234	GLU	C-O	-5.78	1.17	1.24
1	A	464	VAL	CA-CB	5.44	1.60	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GLU	CA-C-O	52.65	177.49	120.63
1	A	234	GLU	O-C-N	-40.41	79.29	122.12
1	A	234	GLU	N-CA-C	15.18	129.69	111.33
1	B	301	ILE	N-CA-C	-11.38	96.28	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	THR	O-C-N	9.31	134.01	122.65
1	B	496	GLU	N-CA-C	-8.61	101.83	111.82
1	A	301	ILE	N-CA-C	-8.32	99.31	107.55
1	A	459	SER	N-CA-C	8.20	121.25	111.33
1	B	289	GLU	N-CA-C	7.68	121.91	112.23
1	B	224	VAL	N-CA-C	-7.54	98.94	108.89
1	B	74	TYR	N-CA-C	-7.14	97.22	109.15
1	A	345	SER	N-CA-C	6.97	120.94	110.14
1	A	305	SER	N-CA-C	6.87	121.25	113.01
1	A	343	ARG	N-CA-C	6.79	125.27	110.80
1	A	168	ALA	N-CA-C	-6.70	97.48	108.41
1	B	168	ALA	N-CA-C	-6.62	97.48	108.34
1	A	234	GLU	CA-C-N	6.54	134.22	122.38
1	A	234	GLU	C-N-CA	6.54	134.22	122.38
1	A	116	GLU	N-CA-C	6.41	118.35	111.36
1	A	361	ASN	N-CA-C	-6.24	97.54	108.20
1	B	361	ASN	N-CA-C	-6.19	98.44	108.41
1	B	73	ARG	N-CA-C	6.13	119.46	109.59
1	A	346	VAL	N-CA-C	-6.09	104.09	113.16
1	A	73	ARG	N-CA-C	5.96	119.53	109.76
1	B	167	TYR	N-CA-C	5.62	116.95	108.46
1	B	500	MET	CA-C-O	5.59	130.30	120.80
1	A	134	ILE	N-CA-C	-5.53	105.33	110.53
1	A	223	ASP	N-CA-C	-5.53	102.29	110.48
1	A	259	PHE	N-CA-C	5.46	117.03	111.14
1	B	259	PHE	N-CA-C	5.39	117.23	111.36
1	B	304	THR	N-CA-C	5.38	117.14	111.28
1	B	305	SER	N-CA-C	5.32	119.64	113.20
1	B	43	ARG	N-CA-C	-5.26	99.86	108.76
1	A	224	VAL	N-CA-C	-5.18	100.88	108.54
1	A	43	ARG	N-CA-C	-5.16	100.49	108.90
1	B	276	VAL	N-CA-C	-5.13	105.53	110.72
1	A	44	LEU	N-CA-C	5.11	117.58	109.50
1	B	13	ASN	N-CA-C	5.11	116.54	111.07
1	B	72	VAL	N-CA-C	-5.11	101.12	108.48
1	B	94	TYR	N-CA-C	5.10	121.67	110.80
1	B	95	GLY	N-CA-C	-5.07	101.16	113.18
1	B	432	ASP	N-CA-C	-5.06	106.62	112.89
1	A	142	PHE	N-CA-C	5.01	117.14	109.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	258	TYR	Sidechain

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	3997	0	3937	64	0
1	B	4042	0	4002	58	0
2	A	10	0	9	2	0
2	B	10	0	8	0	0
3	A	43	0	36	4	0
3	B	45	0	36	3	0
4	A	501	0	0	9	0
4	B	478	0	0	9	0
All	All	9126	0	8028	115	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 7.

All (115) 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:A:234:GLU:C	1:A:235[A]:GLU:N	1.73	1.44
1:A:234:GLU:C	1:A:235[B]:GLU:N	1.74	1.42
1:A:234:GLU:O	1:A:235[B]:GLU:N	1.89	1.04
1:A:234:GLU:O	1:A:235[A]:GLU:N	1.90	1.02
1:A:56:GLU:H	1:A:59:HIS:HD2	1.13	0.93
1:A:234:GLU:CA	1:A:235[A]:GLU:N	2.31	0.93
1:A:234:GLU:CA	1:A:235[B]:GLU:N	2.34	0.90
1:A:10:MET:SD	1:B:340:GLN:HB3	2.20	0.82
1:A:58:ARG:HA	1:B:500:MET:HE1	1.64	0.80
1:B:254:PHE:CE2	1:B:258:TYR:HE1	1.99	0.80
1:A:291[B]:GLU:HB2	4:A:966:HOH:O	1.87	0.75
1:B:76:THR:HG22	1:B:408:ASP:HB2	1.69	0.74
1:B:86:GLN:HB3	1:B:87:PRO:HA	1.72	0.71
1:A:89[A]:TYR:O	3:A:508:PIN:H21	1.91	0.71
1:A:10:MET:HB2	1:B:340:GLN:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLU:H	1:B:59:HIS:HD2	1.39	0.70
1:A:242:GLN:HE21	1:A:244:ALA:H	1.40	0.68
1:A:348:ARG:NE	1:A:348:ARG:HA	2.08	0.68
1:A:109:GLU:HG3	1:A:113[A]:LYS:HE2	1.76	0.68
1:A:486:ALA:O	1:A:490:GLN:HG2	1.97	0.65
1:A:10:MET:SD	1:B:340:GLN:CB	2.84	0.64
1:A:1:CYS:N	2:A:505:ONL:HE1	2.12	0.64
1:B:334:PHE:HB3	1:B:336:MET:HE3	1.80	0.63
1:A:89[B]:TYR:OH	4:A:904:HOH:O	2.16	0.60
1:B:346:VAL:HG13	1:B:381:MET:HE3	1.82	0.60
1:A:1:CYS:H1	2:A:505:ONL:HE1	1.68	0.58
1:B:8:GLY:HA2	1:B:203:GLU:HG2	1.85	0.57
1:A:234:GLU:O	1:A:235[B]:GLU:CA	2.51	0.57
1:B:410:PRO:HG2	1:B:415:LEU:HD21	1.87	0.57
1:B:269:ILE:HD13	1:B:446:VAL:HG12	1.87	0.56
1:A:94:TYR:OH	1:A:147:LEU:HD21	2.06	0.56
1:B:58:ARG:HA	1:B:61:GLN:HE21	1.70	0.56
1:B:371:ARG:HH11	1:B:371:ARG:HG2	1.71	0.55
1:A:176:HIS:O	1:A:234:GLU:HG3	2.05	0.55
1:B:153:PHE:HB3	1:B:241[A]:ARG:HD3	1.89	0.55
1:A:89[B]:TYR:O	3:A:508:PIN:H21	2.06	0.55
1:A:288:ARG:O	1:A:291[B]:GLU:HG3	2.07	0.54
1:A:411:SER:HB3	1:A:479:ASP:OD1	2.07	0.54
1:B:410:PRO:HG2	1:B:415:LEU:CD2	2.38	0.53
1:B:330[B]:VAL:HG22	4:B:834:HOH:O	2.09	0.53
1:B:254:PHE:CE2	1:B:258:TYR:CE1	2.90	0.52
1:A:250:ASN:HA	1:A:455:GLN:O	2.09	0.52
1:A:348:ARG:NH2	1:B:215:THR:OG1	2.42	0.52
1:B:317:GLY:HA2	4:B:552:HOH:O	2.09	0.52
1:A:251:PRO:HG2	1:A:456:PHE:CD2	2.44	0.51
1:A:56:GLU:H	1:A:59:HIS:CD2	2.06	0.51
1:A:380:GLU:HG3	4:A:849:HOH:O	2.11	0.51
1:A:302:PRO:HB2	1:A:326:LYS:HB2	1.93	0.51
1:B:344:LYS:HE3	1:B:347:ARG:CZ	2.41	0.51
1:B:182:ARG:NH2	4:B:869:HOH:O	2.42	0.50
1:B:367:ASP:OD2	3:B:506:PIN:H1'2	2.12	0.50
1:B:84:GLU:HG3	3:B:507:PIN:H4'2	1.93	0.50
1:B:269:ILE:HG23	1:B:449:GLU:HB2	1.93	0.50
1:A:322:GLN:HE22	1:B:262:PRO:HB2	1.77	0.50
1:B:198:ASP:OD1	1:B:201:ARG:HB2	2.12	0.49
1:B:495:VAL:HA	1:B:498:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASP:HB3	4:A:601:HOH:O	2.13	0.49
1:B:17:TYR:O	1:B:21:THR:HG23	2.12	0.49
1:A:44:LEU:HD23	4:A:829:HOH:O	2.14	0.48
1:A:50:LEU:O	1:A:54:VAL:HG23	2.14	0.48
1:A:199:GLU:H	1:A:199:GLU:CD	2.22	0.47
1:A:86:GLN:HB3	1:A:87:PRO:HA	1.96	0.47
1:A:423:ASP:HB3	4:A:604:HOH:O	2.13	0.47
1:A:44:LEU:HG	1:A:45:ARG:N	2.30	0.46
1:A:400:ARG:NH1	1:A:417:ALA:O	2.48	0.46
1:A:371:ARG:NH2	1:A:410:PRO:HB3	2.31	0.46
1:B:343:ARG:NH1	1:B:348[A]:ARG:HG3	2.29	0.46
1:B:307:ASP:HB2	4:B:719:HOH:O	2.16	0.46
1:A:84:GLU:HG3	3:A:507:PIN:H4'2	1.98	0.46
1:B:34:ILE:HD11	1:B:42:PHE:HB3	1.98	0.46
1:B:241[A]:ARG:NH1	4:B:940:HOH:O	2.48	0.46
1:B:153:PHE:CB	1:B:241[A]:ARG:HD3	2.46	0.46
1:A:179:VAL:HA	1:A:230:ILE:O	2.16	0.45
1:A:193:GLY:HA3	1:A:213:LEU:HD13	1.99	0.45
1:B:56:GLU:H	1:B:59:HIS:CD2	2.26	0.45
1:B:160:ASN:ND2	1:B:167:TYR:OH	2.50	0.45
1:B:5:GLY:HA3	1:B:170:VAL:HG21	1.99	0.45
1:A:24:GLN:HB3	1:B:329:TYR:CD2	2.52	0.45
1:A:182:ARG:NH2	4:A:781:HOH:O	2.49	0.45
1:B:399:ILE:HG21	1:B:409:MET:CE	2.47	0.44
1:A:269:ILE:HG12	1:A:449:GLU:HB2	1.98	0.44
1:B:84:GLU:HG3	3:B:507:PIN:C4'	2.48	0.44
1:B:443:ILE:O	1:B:447:ARG:HB2	2.18	0.44
1:B:376:GLU:HG2	4:B:893:HOH:O	2.17	0.44
1:B:252:CYS:HA	1:B:457:GLU:HB3	1.99	0.43
1:B:336:MET:O	1:B:339:GLN:HG3	2.18	0.43
1:B:102:GLY:HA2	1:B:188:ARG:HD2	2.00	0.43
1:B:29:ASP:CG	1:B:75:PRO:HG3	2.43	0.43
1:B:241[A]:ARG:HB2	4:B:982:HOH:O	2.18	0.43
1:A:222:ARG:HG3	1:A:222:ARG:HH11	1.83	0.43
1:A:110:LEU:HD21	1:A:163:ILE:HG22	2.00	0.42
1:B:335:ILE:HA	1:B:339:GLN:OE1	2.19	0.42
1:A:254:PHE:CZ	1:A:258:TYR:CE2	3.07	0.42
1:A:291[A]:GLU:HB3	4:A:966:HOH:O	2.18	0.42
1:A:302:PRO:HD2	1:A:350:LEU:HD11	2.02	0.42
1:A:370:VAL:HB	3:A:506:PIN:O2	2.18	0.42
1:A:377:GLN:O	1:A:380:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:PHE:HB3	1:A:336:MET:HE3	2.01	0.42
1:A:58:ARG:O	1:A:62:ARG:HG3	2.20	0.42
1:A:80:SER:HB3	1:A:485:ASP:HB3	2.01	0.42
1:B:228:GLU:HG2	1:B:229:ALA:N	2.35	0.42
1:B:213:LEU:HD23	1:B:220:PHE:HA	2.02	0.42
1:B:403:ASN:HB2	1:B:460:VAL:CG1	2.50	0.41
1:B:487:LYS:HE2	1:B:487:LYS:HB3	1.92	0.41
1:A:160:ASN:ND2	1:A:167:TYR:OH	2.53	0.41
1:A:348:ARG:NH1	4:A:602:HOH:O	2.54	0.41
1:B:92[B]:SER:HA	1:B:93:PRO:C	2.45	0.41
1:A:274:ALA:O	1:A:278:MET:HG3	2.20	0.41
1:B:164:ARG:HD3	4:B:816:HOH:O	2.20	0.41
1:A:302:PRO:HA	1:A:303:GLU:HA	1.61	0.41
1:B:349:LYS:HG3	4:B:976:HOH:O	2.21	0.40
1:A:11:PRO:HA	1:A:65:GLY:O	2.22	0.40
1:A:94:TYR:O	1:A:174[B]:ILE:HB	2.21	0.40
1:B:302:PRO:HA	1:B:303:GLU:HA	1.78	0.40
1:B:475:LEU:HD23	1:B:475:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/504 (101%)	489 (96%)	17 (3%)	1 (0%)	43	55
1	B	511/504 (101%)	490 (96%)	18 (4%)	3 (1%)	21	27
All	All	1018/1008 (101%)	979 (96%)	35 (3%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	ARG
1	B	340	GLN
1	B	258	TYR
1	B	339	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/422 (101%)	418 (98%)	8 (2%)	50	69
1	B	432/422 (102%)	426 (99%)	6 (1%)	59	76
All	All	858/844 (102%)	844 (98%)	14 (2%)	55	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	110	LEU
1	A	143	ARG
1	A	215	THR
1	A	304[A]	THR
1	A	304[B]	THR
1	A	376	GLU
1	A	413	THR
1	B	11	PRO
1	B	23	LEU
1	B	254	PHE
1	B	335	ILE
1	B	472	GLN
1	B	495	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS

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Mol	Chain	Res	Type
1	A	61	GLN
1	A	103	ASN
1	A	160	ASN
1	A	185	ASN
1	A	242	GLN
1	A	322	GLN
1	A	427	GLN
1	A	437	GLN
1	B	59	HIS
1	B	61	GLN
1	B	160	ASN
1	B	492	GLN
1	B	493	ASN
1	B	497	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PIN	B	508	-	8,8,18	1.14	1 (12%)	10,11,26	0.43	0
3	PIN	A	507	-	18,18,18	1.83	4 (22%)	24,26,26	0.44	0
3	PIN	A	506	-	18,18,18	0.97	1 (5%)	24,26,26	0.46	0
2	ONL	B	505	1	8,9,9	0.72	0	8,11,11	0.89	1 (12%)
3	PIN	B	506	-	18,18,18	0.56	0	24,26,26	0.52	0
2	ONL	A	505	1	8,9,9	0.74	0	8,11,11	1.00	1 (12%)
3	PIN	B	507	-	18,18,18	1.15	3 (16%)	24,26,26	0.42	0
3	PIN	A	508	-	6,6,18	1.77	1 (16%)	7,8,26	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PIN	B	508	-	-	3/6/6/22	-
3	PIN	A	507	-	-	1/12/22/22	0/1/1/1
3	PIN	A	506	-	-	4/12/22/22	0/1/1/1
2	ONL	B	505	1	-	3/9/9/9	-
3	PIN	B	506	-	-	1/12/22/22	0/1/1/1
2	ONL	A	505	1	-	0/9/9/9	-
3	PIN	B	507	-	-	2/12/22/22	0/1/1/1
3	PIN	A	508	-	-	3/4/4/22	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	PIN	C1'-S1'	5.34	1.85	1.77
3	A	508	PIN	C1-S1	4.06	1.83	1.77
3	A	507	PIN	C1-S1	3.91	1.83	1.77
3	B	507	PIN	C1'-S1'	3.04	1.81	1.77
3	A	507	PIN	C2-N1	2.80	1.53	1.47
3	A	506	PIN	C1-S1	2.43	1.81	1.77
3	A	507	PIN	C2'-N1'	2.42	1.52	1.47
3	B	508	PIN	C1-S1	2.34	1.80	1.77
3	B	507	PIN	C1-S1	2.17	1.80	1.77
3	B	507	PIN	C2'-N1'	2.17	1.52	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	ONL	CB-CG-CD	-2.71	110.55	114.77
2	B	505	ONL	CB-CG-CD	-2.07	111.53	114.77

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	PIN	C2-C1-S1-O1
3	A	508	PIN	C2-C1-S1-O2
3	A	508	PIN	C2-C1-S1-O3
3	B	508	PIN	C2-C1-S1-O1
3	B	508	PIN	C2-C1-S1-O2
3	B	508	PIN	C2-C1-S1-O3
3	A	506	PIN	C2-C1-S1-O3
3	A	506	PIN	S1'-C1'-C2'-N1'
3	A	507	PIN	S1'-C1'-C2'-N1'
3	B	506	PIN	S1-C1-C2-N1
3	B	507	PIN	S1'-C1'-C2'-N1'
3	A	506	PIN	C2-C1-S1-O2
3	A	508	PIN	C2-C1-S1-O1
2	B	505	ONL	CE-CD-CG-CB
3	B	507	PIN	C2-C1-S1-O3
2	B	505	ONL	OD-CD-CG-CB
2	B	505	ONL	CA-CB-CG-CD

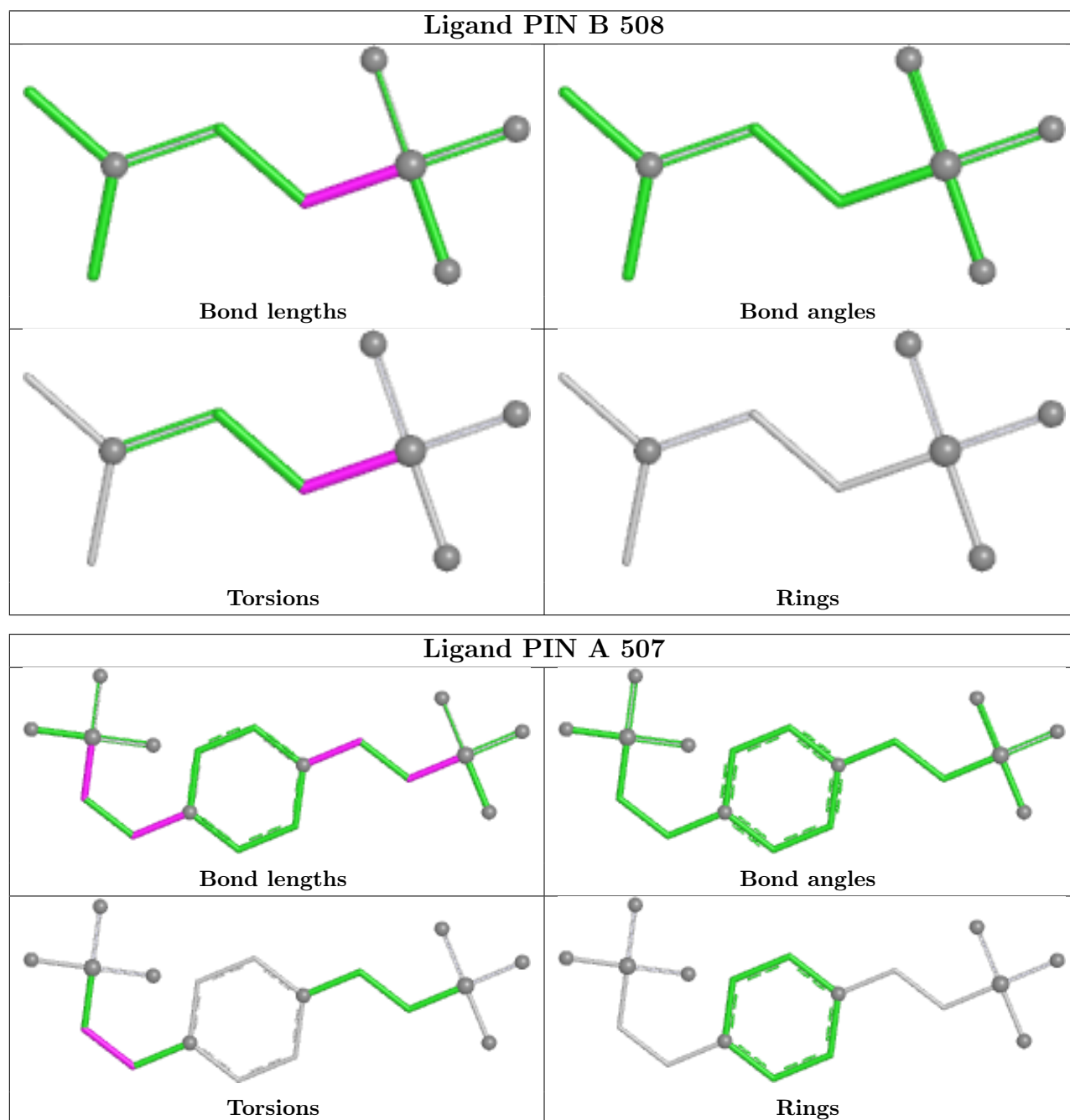
There are no ring outliers.

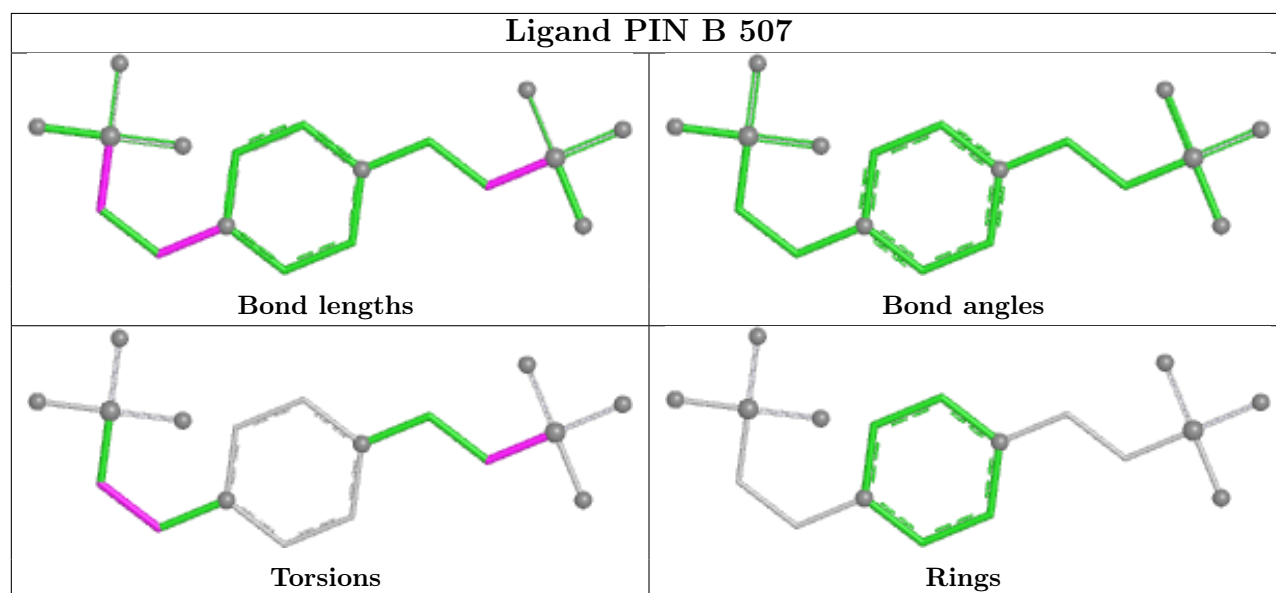
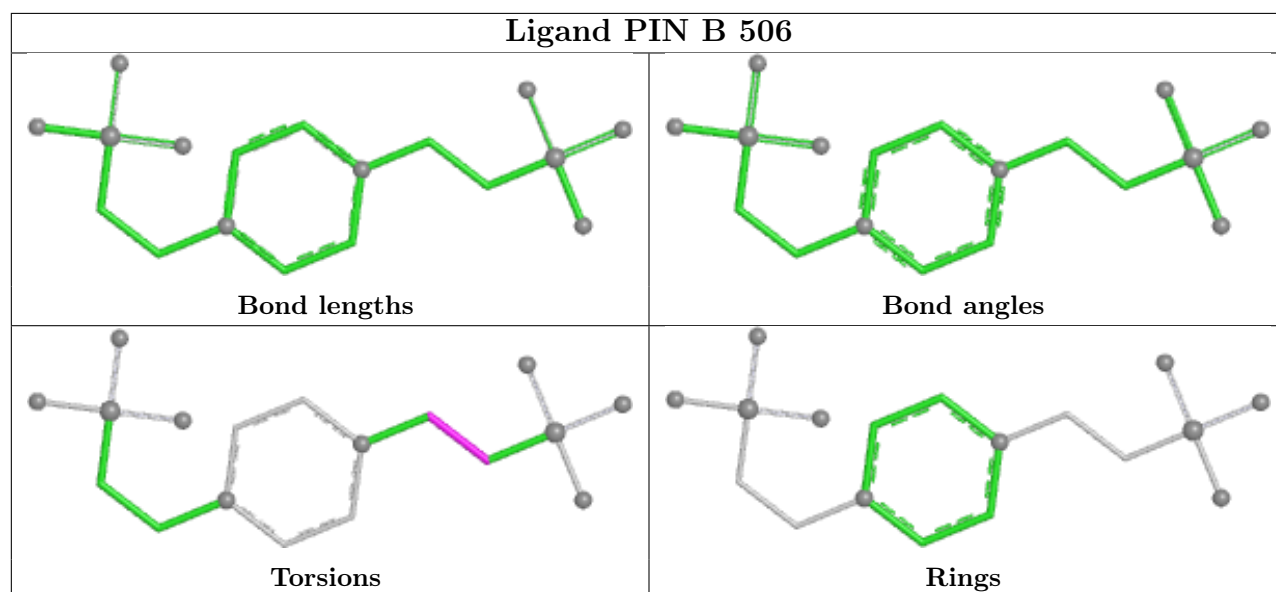
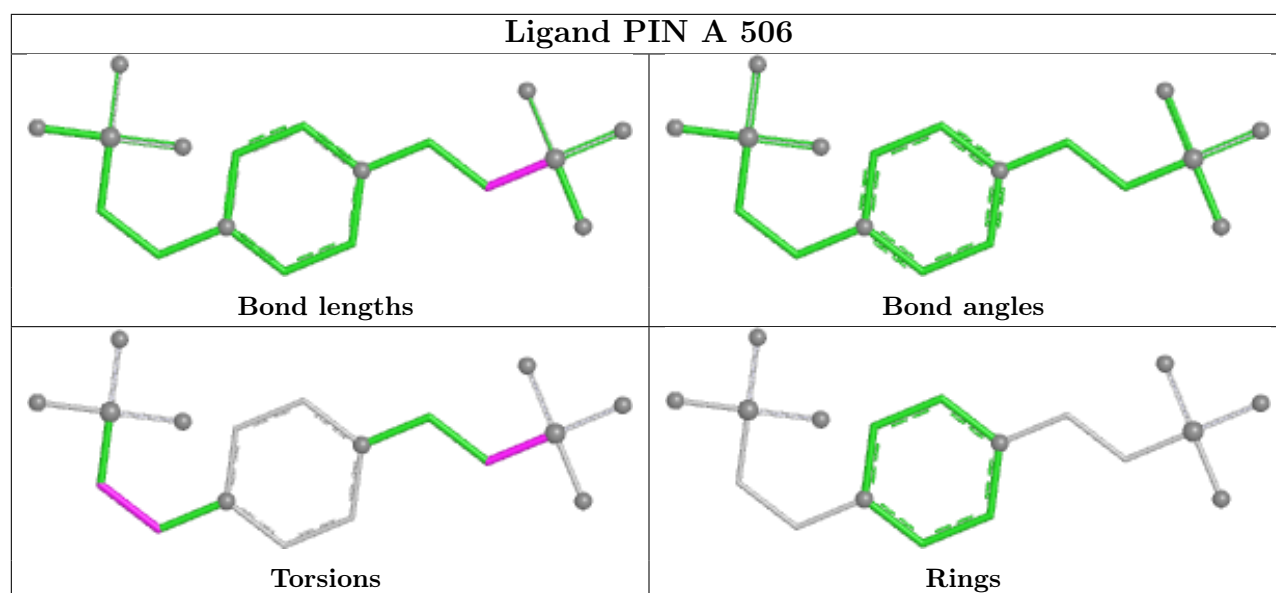
6 monomers are involved in 9 short contacts:

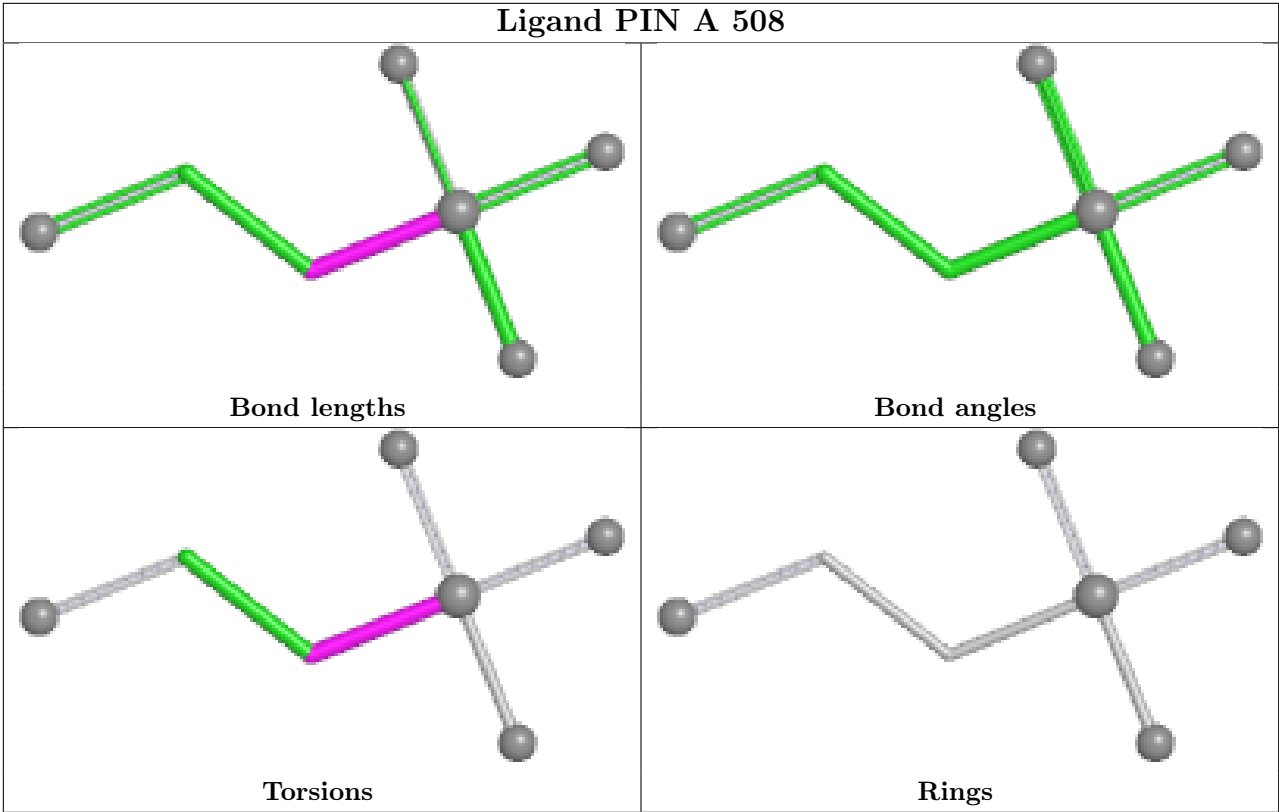
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	PIN	1	0
3	A	506	PIN	1	0
3	B	506	PIN	1	0
2	A	505	ONL	2	0
3	B	507	PIN	2	0
3	A	508	PIN	2	0

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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	234:GLU	C	235[B]:GLU	N	1.74
1	A	234:GLU	C	235[A]:GLU	N	1.73
1	A	233:THR	C	234:GLU	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.