



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2023 – 11:01 PM EDT

PDB ID : 1I7G
Title : CRYSTAL STRUCTURE OF THE LIGAND BINDING DOMAIN FROM HUMAN PPAR-ALPHA IN COMPLEX WITH THE AGONIST AZ 242
Authors : Petersen, J.F.W.; Cronet, P.; Folmer, R.; Blomberg, N.; Sjoblom, K.; Karlsson, U.; Lindstedt, E.-L.; Bamberg, K.
Deposited on : 2001-03-09
Resolution : 2.20 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

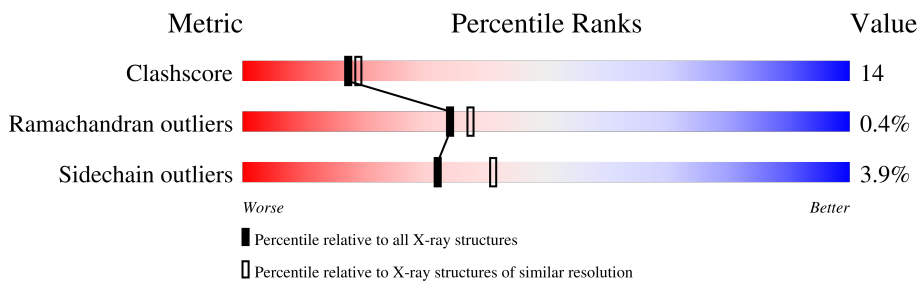
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	287	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 2188 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 PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	2064	1322	344	380	18	0	0	0

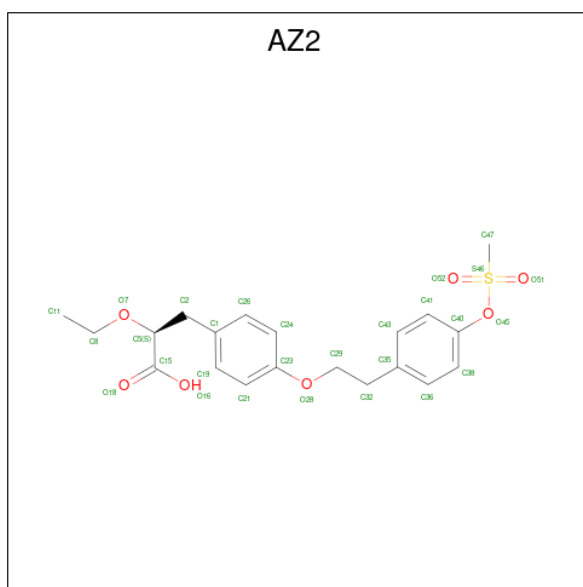
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	GLY	-	cloning artifact	UNP Q07869
A	183	SER	-	cloning artifact	UNP Q07869
A	184	HIS	-	cloning artifact	UNP Q07869
A	185	MET	-	cloning artifact	UNP Q07869
A	186	SER	-	cloning artifact	UNP Q07869
A	187	GLY	-	cloning artifact	UNP Q07869
A	188	GLU	-	cloning artifact	UNP Q07869
A	189	ASP	-	cloning artifact	UNP Q07869
A	190	SER	-	cloning artifact	UNP Q07869
A	191	GLU	-	cloning artifact	UNP Q07869
A	192	THR	-	cloning artifact	UNP Q07869
A	193	GLU	-	cloning artifact	UNP Q07869
A	194	ALA	-	cloning artifact	UNP Q07869
A	195	ASP	-	cloning artifact	UNP Q07869

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

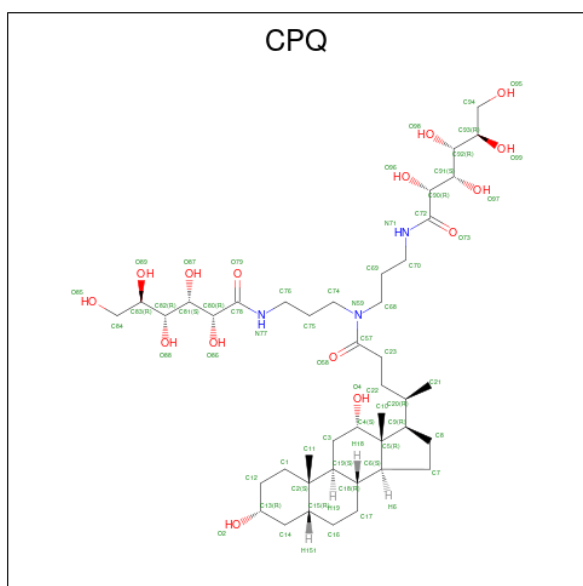
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is (2S)-2-ETHOXY-3-[4-(2-{4-[(METHYLSULFONYL)OXY]PHENYL}ETHOXY)PHENYL]PROPANOIC ACID (three-letter code: AZ2) (formula: C₂₀H₂₄O₇S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	A	1	28	20	7	1	0	0

- Molecule 4 is N,N-BIS(3-D-GLUCONAMIDOPROPYL)DEOXYCHOLAMIDE (three-letter code: CPQ) (formula: $C_{42}H_{75}N_3O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	A	1	25	23	2	0	0	

- Molecule 5 is water.

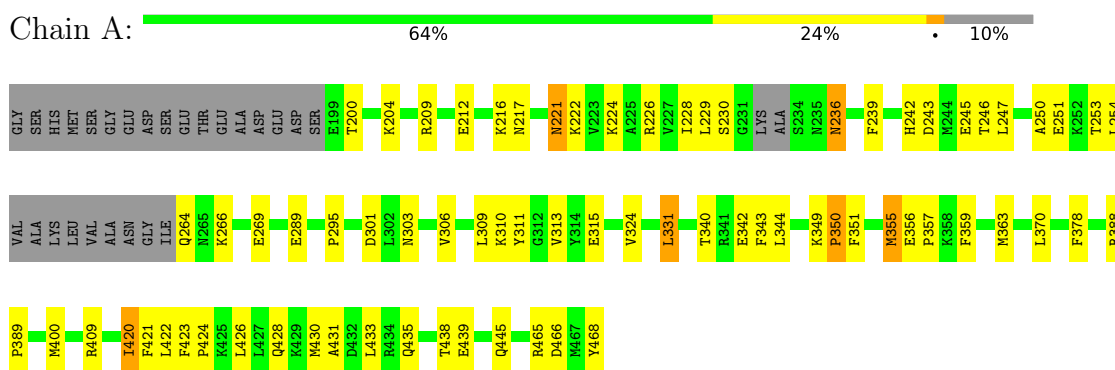
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		

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: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR ALPHA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.97Å 76.97Å 100.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.64 – 2.20	Depositor
% Data completeness (in resolution range)	99.3 (23.64-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.237 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2188	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

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: CPQ, AZ2, NA

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	0.36	0/2100	0.56	0/2828

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	2064	0	2087	59	0
2	A	1	0	0	0	0
3	A	28	0	23	0	0
4	A	25	0	34	0	0
5	A	70	0	0	7	0
All	All	2188	0	2144	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (59) 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:433:LEU:HB3	5:A:538:HOH:O	1.73	0.86
1:A:264:GLN:HE21	1:A:266:LYS:HB2	1.46	0.78
1:A:423:PHE:HB3	1:A:424:PRO:HD3	1.70	0.74
1:A:200:THR:HG22	1:A:204:LYS:NZ	2.03	0.73
1:A:309:LEU:O	1:A:313:VAL:HG13	1.92	0.70
1:A:310:LYS:HD2	1:A:466:ASP:CB	2.23	0.69
1:A:340:THR:HG22	1:A:343:PHE:H	1.59	0.68
1:A:221:ASN:ND2	1:A:224:LYS:H	1.92	0.67
1:A:253:THR:O	1:A:254:LEU:HG	1.95	0.66
1:A:229:LEU:HD21	1:A:331:LEU:HD13	1.81	0.63
1:A:221:ASN:HD22	1:A:221:ASN:C	2.02	0.62
1:A:310:LYS:HD2	1:A:466:ASP:HB2	1.83	0.61
1:A:200:THR:HG22	1:A:204:LYS:HZ1	1.68	0.59
1:A:221:ASN:HD21	1:A:224:LYS:HG3	1.70	0.57
1:A:243:ASP:OD2	1:A:245:GLU:HB2	2.05	0.56
1:A:359:PHE:O	1:A:363:MET:HG2	2.06	0.54
1:A:254:LEU:HD21	5:A:519:HOH:O	2.07	0.53
1:A:228:ILE:C	1:A:230:SER:H	2.12	0.53
1:A:264:GLN:NE2	1:A:266:LYS:HD2	2.24	0.53
1:A:435:GLN:O	1:A:439:GLU:HG3	2.10	0.52
1:A:239:PHE:CE2	1:A:250:ALA:HB2	2.45	0.52
1:A:221:ASN:HD21	1:A:224:LYS:H	1.56	0.51
1:A:315:GLU:HA	5:A:538:HOH:O	2.10	0.51
1:A:209:ARG:HH11	1:A:209:ARG:HG2	1.76	0.50
1:A:356:GLU:HB3	1:A:357:PRO:HD3	1.94	0.50
1:A:209:ARG:HE	1:A:295:PRO:HG3	1.77	0.49
1:A:315:GLU:HG2	5:A:538:HOH:O	2.12	0.49
1:A:217:ASN:ND2	1:A:289:GLU:HB3	2.28	0.49
1:A:344:LEU:HD13	1:A:355:MET:HG2	1.94	0.49
1:A:306:VAL:HG23	5:A:509:HOH:O	2.11	0.49
1:A:438:THR:HG22	1:A:468:TYR:OH	2.14	0.48
1:A:247:LEU:O	1:A:251:GLU:HG3	2.14	0.48
1:A:250:ALA:O	1:A:254:LEU:N	2.47	0.47
1:A:340:THR:HG22	1:A:342:GLU:N	2.30	0.46
1:A:212:GLU:HB3	1:A:216:LYS:NZ	2.30	0.45
1:A:428:GLN:O	1:A:431:ALA:HB3	2.15	0.45
1:A:311:TYR:CZ	1:A:389:PRO:HG2	2.51	0.45
1:A:209:ARG:NE	1:A:295:PRO:HG3	2.32	0.45
1:A:421:PHE:O	1:A:424:PRO:HD2	2.17	0.45
1:A:445:GLN:HG2	5:A:495:HOH:O	2.17	0.45
1:A:349:LYS:HG3	1:A:350:PRO:HA	1.98	0.44
1:A:295:PRO:O	1:A:400:MET:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:ND2	1:A:221:ASN:C	2.71	0.43
1:A:269:GLU:HB3	1:A:351:PHE:CG	2.53	0.43
1:A:229:LEU:HD21	1:A:331:LEU:CD1	2.48	0.43
1:A:264:GLN:HG3	1:A:266:LYS:H	1.84	0.42
1:A:242:HIS:CE1	1:A:246:THR:HG21	2.54	0.42
1:A:324:VAL:HB	1:A:331:LEU:HB2	2.00	0.42
1:A:370:LEU:HD11	1:A:426:LEU:HD13	2.01	0.42
1:A:222:LYS:O	1:A:226:ARG:HG2	2.19	0.41
1:A:239:PHE:HE2	1:A:250:ALA:HB2	1.85	0.41
1:A:420:ILE:N	1:A:420:ILE:HD13	2.35	0.41
1:A:301:ASP:OD2	1:A:303:ASN:HB2	2.21	0.41
1:A:311:TYR:HB3	1:A:388:ARG:HD2	2.03	0.41
1:A:217:ASN:ND2	1:A:289:GLU:CB	2.84	0.41
1:A:378:PHE:CE1	1:A:430:MET:HG3	2.56	0.41
1:A:378:PHE:HE1	1:A:430:MET:HG3	1.86	0.40
1:A:228:ILE:C	1:A:230:SER:N	2.73	0.40
1:A:226:ARG:NH1	5:A:520:HOH:O	2.55	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	253/287 (88%)	241 (95%)	11 (4%)	1 (0%)	34 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	229/250 (92%)	220 (96%)	9 (4%)	32 41

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	236	ASN
1	A	331	LEU
1	A	350	PRO
1	A	355	MET
1	A	409	ARG
1	A	420	ILE
1	A	422	LEU
1	A	465	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	221	ASN
1	A	236	ASN
1	A	264	GLN
1	A	305	GLN
1	A	336	ASN
1	A	396	HIS
1	A	445	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AZ2	A	469	-	29,29,29	1.50	4 (13%)	37,39,39	1.02	1 (2%)
4	CPQ	A	470	-	28,28,63	4.79	15 (53%)	45,45,92	5.01	26 (57%)

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	AZ2	A	469	-	-	1/22/22/22	0/2/2/2
4	CPQ	A	470	-	-	4/6/68/125	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	470	CPQ	O4-C4	-13.33	1.21	1.43
4	A	470	CPQ	C10-C5	12.16	1.74	1.54
4	A	470	CPQ	C18-C19	8.27	1.69	1.53
4	A	470	CPQ	C5-C9	-8.12	1.41	1.55
4	A	470	CPQ	C17-C18	6.10	1.64	1.53
4	A	470	CPQ	C3-C4	5.34	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	470	CPQ	C8-C9	4.50	1.63	1.54
4	A	470	CPQ	C14-C15	4.02	1.60	1.53
3	A	469	AZ2	O45-C40	-3.63	1.36	1.42
4	A	470	CPQ	C8-C7	3.53	1.63	1.54
4	A	470	CPQ	C5-C4	-3.17	1.49	1.54
4	A	470	CPQ	O2-C13	3.08	1.52	1.43
4	A	470	CPQ	C14-C13	2.72	1.56	1.51
4	A	470	CPQ	C11-C2	2.72	1.59	1.54
4	A	470	CPQ	C20-C9	2.66	1.59	1.54
4	A	470	CPQ	C16-C15	-2.64	1.46	1.53
3	A	469	AZ2	C24-C23	2.52	1.43	1.38
3	A	469	AZ2	C19-C1	2.33	1.43	1.38
3	A	469	AZ2	C38-C40	2.29	1.43	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	470	CPQ	C5-C6-C18	13.20	129.27	114.71
4	A	470	CPQ	C5-C9-C20	10.30	131.80	119.50
4	A	470	CPQ	C9-C5-C4	9.84	126.65	117.67
4	A	470	CPQ	C9-C5-C6	9.19	109.36	100.09
4	A	470	CPQ	C17-C18-C19	-9.07	99.25	110.49
4	A	470	CPQ	C17-C18-C6	8.55	126.69	112.08
4	A	470	CPQ	C19-C3-C4	8.41	125.41	114.30
4	A	470	CPQ	C10-C5-C6	-8.31	98.21	111.21
4	A	470	CPQ	C2-C19-C18	8.03	120.86	112.42
4	A	470	CPQ	C7-C6-C5	6.46	109.89	103.55
4	A	470	CPQ	C10-C5-C4	-5.73	103.24	109.07
4	A	470	CPQ	C10-C5-C9	-5.61	102.43	111.21
4	A	470	CPQ	C6-C5-C4	5.09	112.14	107.40
4	A	470	CPQ	O4-C4-C5	-4.98	102.61	111.03
4	A	470	CPQ	C21-C20-C9	4.74	120.18	112.92
4	A	470	CPQ	C8-C9-C5	4.58	108.05	103.55
4	A	470	CPQ	C1-C12-C13	4.25	115.93	110.47
4	A	470	CPQ	C12-C1-C2	3.86	119.40	112.78
4	A	470	CPQ	O4-C4-C3	-3.66	101.67	109.12
4	A	470	CPQ	C3-C19-C18	-3.21	105.61	110.82
3	A	469	AZ2	O45-C40-C41	3.16	124.85	118.64
4	A	470	CPQ	C19-C2-C15	-2.79	104.66	108.58
4	A	470	CPQ	C17-C16-C15	2.65	117.17	111.84
4	A	470	CPQ	C11-C2-C1	2.45	112.21	108.26
4	A	470	CPQ	C7-C6-C18	-2.22	115.42	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	470	CPQ	C14-C15-C16	-2.20	107.71	111.74
4	A	470	CPQ	C14-C15-C2	2.15	114.94	112.66

There are no chirality outliers.

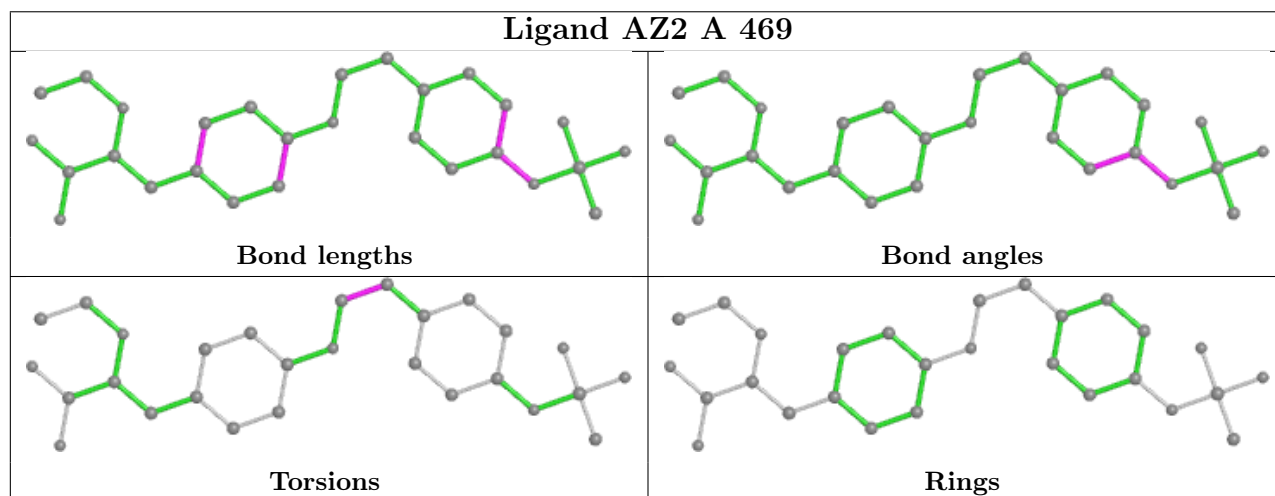
All (5) torsion outliers are listed below:

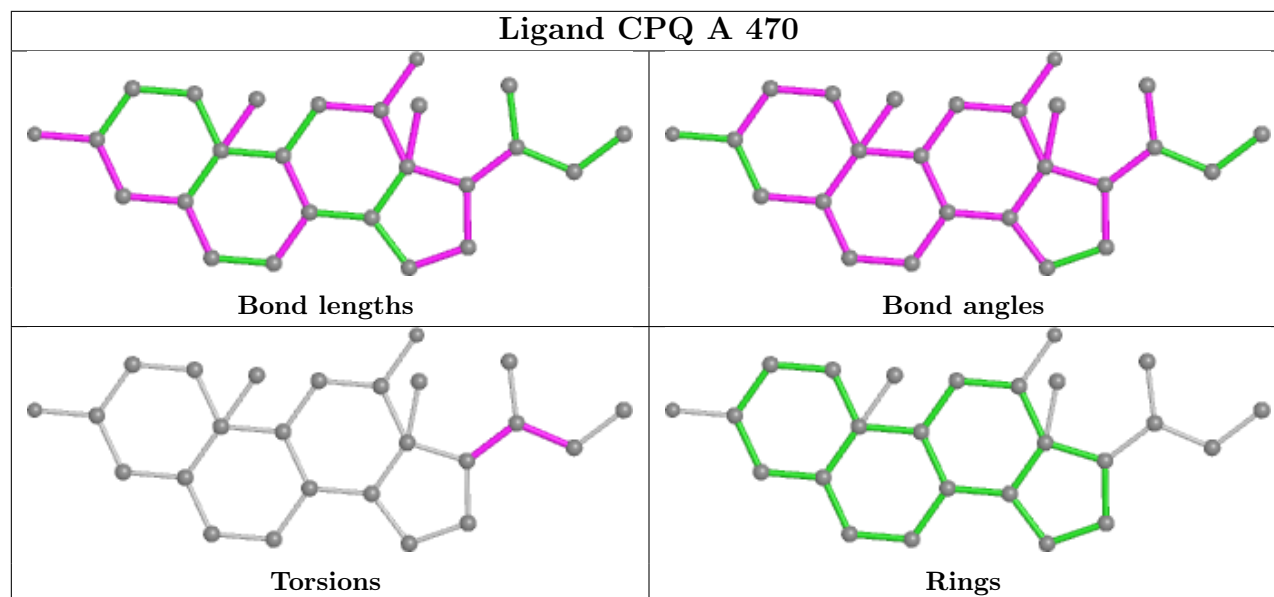
Mol	Chain	Res	Type	Atoms
4	A	470	CPQ	C21-C20-C9-C5
4	A	470	CPQ	C9-C20-C22-C23
3	A	469	AZ2	O28-C29-C32-C35
4	A	470	CPQ	C22-C20-C9-C5
4	A	470	CPQ	C21-C20-C22-C23

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.