



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:40 PM UTC

PDB ID : 2ATH / pdb_00002ath
Title : Crystal structure of the ligand binding domain of human PPAR-gamma im
complex with an agonist
Authors : Mahindroo, N.; Huang, C.-F.; Wu, S.-Y.; Hsieh, H.-P.
Deposited on : 2005-08-25
Resolution : 2.28 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

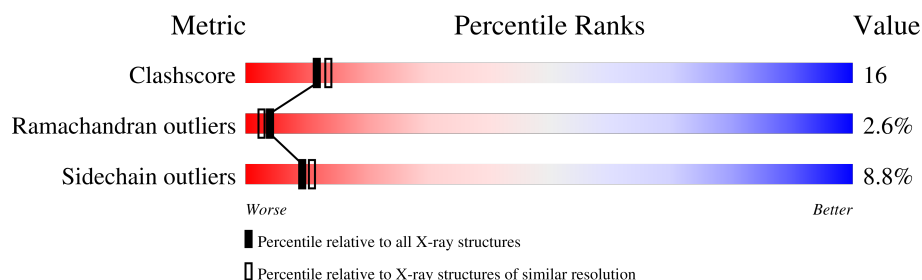
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)

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	271	 64% 30% 6% •
1	B	271	 60% 31% 7% •

2 Entry composition [i](#)

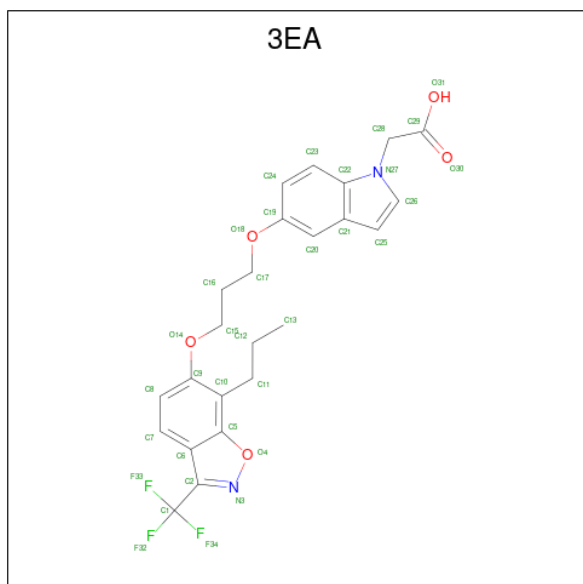
There are 3 unique types of molecules in this entry. The entry contains 4547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2178	1406	355	407	10			
1	B	271	Total	C	N	O	S	0	0	0
			2178	1406	355	407	10			

- Molecule 2 is 2-{5-[3-(7-PROPYL-3-TRIFLUOROMETHYLBENZO[D]ISOXAZOL-6-YLOXY)PROPOXY]INDOL-1-YL}ETHANOIC ACID (CCD ID: 3EA) (formula: C₂₄H₂₃F₃N₂O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			34	24	3	2	5		
2	B	1	Total	C	F	N	O	0	0
			34	24	3	2	5		

- Molecule 3 is water.

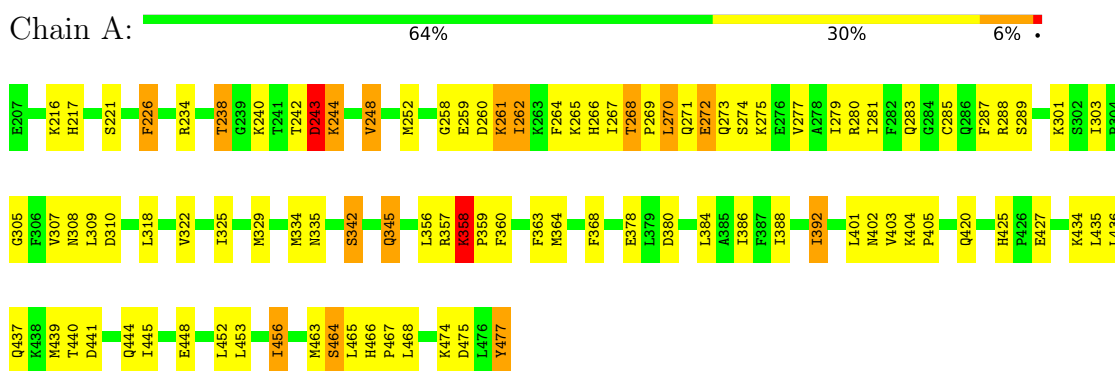
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total 58	O 58	0	0
3	B	65	Total 65	O 65	0	0

3 Residue-property plots

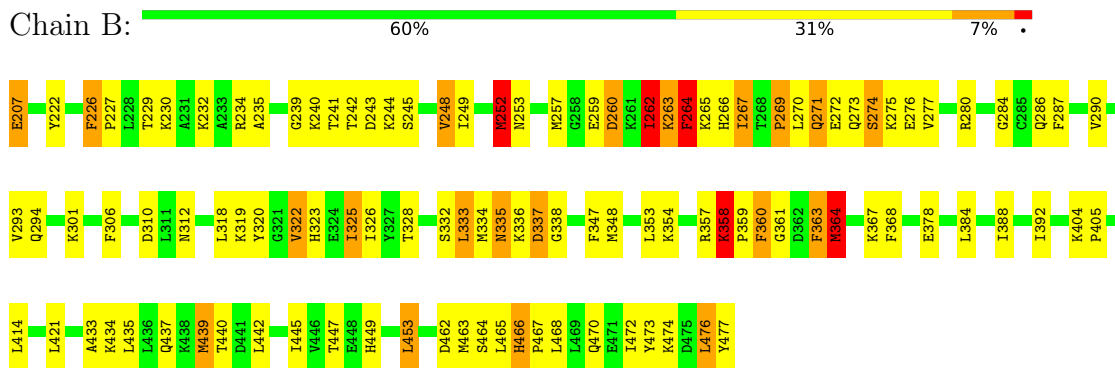
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: Peroxisome proliferator activated receptor gamma



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.78Å 88.52Å 57.56Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	20.00 – 2.28	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.28)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4547	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: 3EA

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	1.06	2/2216 (0.1%)	1.13	12/2985 (0.4%)
1	B	1.07	4/2216 (0.2%)	1.12	14/2985 (0.5%)
All	All	1.06	6/4432 (0.1%)	1.12	26/5970 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	MET	SD-CE	-7.62	1.60	1.79
1	B	439	MET	SD-CE	6.98	1.97	1.79
1	A	364	MET	SD-CE	5.38	1.93	1.79
1	B	325	ILE	CA-CB	5.05	1.60	1.54
1	B	252	MET	SD-CE	5.03	1.92	1.79
1	A	303	ILE	CA-CB	5.02	1.60	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ASN	N-CA-C	-10.09	94.81	108.74
1	A	403	VAL	N-CA-C	8.60	118.62	110.53
1	B	262	ILE	N-CA-C	-7.10	105.59	111.91
1	A	226	PHE	CA-C-N	6.68	126.18	119.24
1	A	226	PHE	C-N-CA	6.68	126.18	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ASP	N-CA-C	6.46	121.95	113.30
1	B	335	ASN	N-CA-C	-6.38	100.12	109.18
1	B	306	PHE	N-CA-C	6.29	117.80	111.07
1	B	360	PHE	N-CA-C	6.07	117.97	111.36
1	B	322	VAL	N-CA-C	5.69	116.42	110.62
1	A	425	HIS	CA-C-N	5.56	125.23	119.56
1	A	425	HIS	C-N-CA	5.56	125.23	119.56
1	A	264	PHE	N-CA-C	-5.50	106.73	113.50
1	B	363	PHE	N-CA-C	-5.50	106.74	113.50
1	A	364	MET	N-CA-C	5.48	119.68	111.96
1	B	263	LYS	N-CA-C	-5.45	107.88	114.75
1	B	264	PHE	N-CA-C	-5.43	105.47	111.71
1	A	392	ILE	N-CA-C	5.39	116.12	110.62
1	A	363	PHE	N-CA-C	-5.30	106.32	112.89
1	B	440	THR	N-CA-C	-5.24	105.57	111.28
1	B	226	PHE	CA-C-N	5.18	124.63	119.24
1	B	226	PHE	C-N-CA	5.18	124.63	119.24
1	B	414	LEU	N-CA-C	-5.16	105.73	111.36
1	A	248	VAL	N-CA-C	5.12	115.68	108.36
1	B	284	GLY	N-CA-C	-5.06	106.59	113.37
1	A	358	LYS	N-CA-C	5.04	120.96	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	222	TYR	Sidechain

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	2178	0	2241	66	0
1	B	2178	0	2241	85	0
2	A	34	0	22	0	0
2	B	34	0	22	1	0
3	A	58	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	65	0	0	4	0
All	All	4547	0	4526	142	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 16.

All (142) 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:293:VAL:HG22	1:B:322:VAL:HG11	1.49	0.95
1:B:286:GLN:HE22	1:B:465:LEU:HD23	1.35	0.91
1:A:268:THR:HG22	1:A:269:PRO:HD2	1.59	0.85
1:A:301:LYS:HE2	1:B:468:LEU:HB2	1.61	0.81
1:B:433:ALA:O	1:B:437:GLN:HG3	1.81	0.81
1:B:473:TYR:HD1	1:B:476:LEU:HD13	1.47	0.79
1:A:463:MET:HG3	1:A:464:SER:H	1.49	0.78
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.65	0.77
1:B:290:VAL:HG22	1:B:468:LEU:HD23	1.67	0.76
1:A:448:GLU:O	1:A:452:LEU:HD13	1.85	0.76
1:B:363:PHE:HZ	1:B:453:LEU:HD13	1.52	0.75
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.70	0.74
1:A:345:GLN:HE21	1:A:345:GLN:HA	1.53	0.73
1:A:358:LYS:HB3	1:A:359:PRO:HD3	1.69	0.73
1:A:358:LYS:HB3	1:A:359:PRO:CD	2.18	0.72
1:A:217:HIS:ND1	1:B:301:LYS:HE2	2.05	0.72
1:A:238:THR:CG2	1:A:240:LYS:HG3	2.19	0.72
1:A:252:MET:SD	1:A:277:VAL:HG21	2.30	0.71
1:B:325:ILE:HD11	1:B:392:ILE:HG12	1.75	0.68
1:A:444:GLN:HG2	3:A:115:HOH:O	1.94	0.67
1:B:322:VAL:O	1:B:326:ILE:HG13	1.93	0.67
1:B:293:VAL:HG22	1:B:322:VAL:CG1	2.24	0.67
1:B:363:PHE:HE1	1:B:449:HIS:CE1	2.14	0.66
1:B:275:LYS:HE3	1:B:462:ASP:HB2	1.78	0.65
1:A:401:LEU:HB3	1:B:267:ILE:HD13	1.78	0.65
1:B:319:LYS:HG3	1:B:472:ILE:HG23	1.76	0.65
1:A:262:ILE:HD13	1:A:267:ILE:HG12	1.78	0.64
1:A:238:THR:HG22	1:A:240:LYS:HG3	1.79	0.64
1:B:473:TYR:CD1	1:B:476:LEU:HD13	2.31	0.64
1:A:342:SER:O	1:A:345:GLN:HG2	1.98	0.63
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.29	0.63
1:A:345:GLN:HA	1:A:345:GLN:NE2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PRO:C	1:B:270:LEU:HD12	2.26	0.60
1:B:229:THR:OG1	1:B:232:LYS:HG3	2.01	0.60
1:A:384:LEU:O	1:A:388:ILE:HG12	2.01	0.60
1:B:353:LEU:HD22	1:B:364:MET:HG2	1.83	0.60
1:B:336:LYS:HE2	3:B:110:HOH:O	2.00	0.60
1:A:273:GLN:HB3	1:A:280:ARG:HD2	1.83	0.59
1:B:235:ALA:HA	1:B:240:LYS:HE3	1.83	0.59
1:A:358:LYS:CB	1:A:359:PRO:CD	2.81	0.59
1:A:477:TYR:O	1:A:477:TYR:HD1	1.87	0.57
1:B:269:PRO:O	1:B:270:LEU:HD12	2.04	0.57
1:A:238:THR:HG21	1:A:240:LYS:HG3	1.85	0.57
1:B:263:LYS:HA	1:B:266:HIS:O	2.04	0.57
1:B:270:LEU:O	1:B:271:GLN:HB2	2.05	0.56
1:B:230:LYS:O	1:B:234:ARG:HG2	2.05	0.56
1:A:301:LYS:NZ	1:B:467:PRO:HD2	2.21	0.56
1:A:279:ILE:O	1:A:283:GLN:HG3	2.06	0.56
1:B:325:ILE:HG23	1:B:388:ILE:HD12	1.88	0.55
1:A:345:GLN:HE21	1:A:345:GLN:CA	2.20	0.55
1:A:342:SER:HB2	1:A:345:GLN:HB2	1.89	0.55
1:A:301:LYS:HZ1	1:B:467:PRO:HD2	1.72	0.54
1:A:268:THR:HB	1:A:270:LEU:HG	1.88	0.54
1:B:253:ASN:O	1:B:257:MET:HB2	2.08	0.54
1:B:328:THR:OG1	1:B:442:LEU:HD11	2.07	0.54
1:A:301:LYS:HZ1	1:B:467:PRO:CD	2.20	0.53
1:A:360:PHE:CE1	1:A:456:ILE:HD11	2.43	0.53
1:A:307:VAL:HG22	3:A:72:HOH:O	2.07	0.53
1:B:259:GLU:O	1:B:262:ILE:HG13	2.08	0.53
1:B:333:LEU:HD23	1:B:333:LEU:N	2.24	0.53
1:A:262:ILE:HG23	1:A:265:LYS:O	2.10	0.52
1:A:273:GLN:CB	1:A:280:ARG:HD2	2.40	0.52
1:B:465:LEU:HD22	1:B:470:GLN:OE1	2.10	0.52
1:A:466:HIS:CG	1:A:467:PRO:HD2	2.44	0.52
1:B:275:LYS:HG3	1:B:276:GLU:H	1.74	0.51
1:A:288:ARG:NE	3:A:107:HOH:O	2.40	0.51
1:B:334:MET:HE2	1:B:368:PHE:CE1	2.46	0.51
1:A:301:LYS:CE	1:B:468:LEU:HB2	2.37	0.51
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.41	0.51
1:B:354:LYS:HE2	3:B:123:HOH:O	2.11	0.51
1:B:361:GLY:C	1:B:363:PHE:H	2.19	0.51
1:B:260:ASP:O	1:B:264:PHE:HB2	2.11	0.50
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLY:O	1:A:261:LYS:HB2	2.12	0.49
1:A:280:ARG:HH11	1:A:280:ARG:HB2	1.76	0.49
1:A:436:LEU:O	1:A:439:MET:HB2	2.12	0.49
1:B:270:LEU:HD23	1:B:287:PHE:HB3	1.94	0.49
1:B:242:THR:O	1:B:242:THR:HG23	2.12	0.49
1:A:309:LEU:O	1:A:310:ASP:C	2.56	0.48
1:B:252:MET:SD	1:B:277:VAL:HG11	2.53	0.48
1:A:386:ILE:HD12	1:A:420:GLN:HG2	1.96	0.48
1:B:447:THR:HG22	1:B:477:TYR:OXT	2.13	0.48
1:B:367:LYS:HD2	1:B:367:LYS:N	2.29	0.48
1:A:259:GLU:O	1:A:262:ILE:HG13	2.14	0.48
1:B:421:LEU:HD11	1:B:435:LEU:HD23	1.96	0.47
1:A:301:LYS:HE2	1:B:468:LEU:CB	2.39	0.47
1:B:275:LYS:CE	1:B:462:ASP:HB2	2.44	0.47
1:B:290:VAL:HG22	1:B:468:LEU:HB3	1.96	0.47
1:A:301:LYS:HZ1	1:B:467:PRO:N	2.14	0.46
1:A:404:LYS:N	1:A:405:PRO:HD2	2.30	0.46
1:A:427:GLU:HB2	3:A:52:HOH:O	2.16	0.46
1:B:364:MET:HG3	2:B:1002:3EA:H161	1.98	0.46
1:A:441:ASP:O	1:A:445:ILE:HG12	2.15	0.46
1:A:226:PHE:CG	1:A:329:MET:HE1	2.51	0.46
1:B:274:SER:O	1:B:275:LYS:HB2	2.15	0.45
1:B:241:THR:O	1:B:242:THR:C	2.58	0.45
1:B:248:VAL:HG13	3:B:116:HOH:O	2.15	0.45
1:B:273:GLN:O	1:B:274:SER:HB2	2.15	0.45
1:A:242:THR:HG23	1:A:242:THR:O	2.17	0.45
1:A:243:ASP:O	1:A:244:LYS:HB3	2.17	0.45
1:A:270:LEU:HB3	1:A:287:PHE:CG	2.52	0.45
1:B:357:ARG:C	1:B:359:PRO:HD2	2.41	0.45
1:A:260:ASP:C	1:A:262:ILE:N	2.74	0.45
1:B:359:PRO:HG2	1:B:360:PHE:H	1.82	0.45
1:A:463:MET:HG3	1:A:464:SER:N	2.26	0.45
1:A:474:LYS:HE2	1:A:475:ASP:OD2	2.16	0.45
1:B:244:LYS:O	1:B:245:SER:C	2.60	0.45
1:B:474:LYS:C	1:B:476:LEU:H	2.24	0.45
1:B:319:LYS:NZ	1:B:320:TYR:CZ	2.85	0.44
1:A:380:ASP:C	1:A:380:ASP:OD1	2.60	0.44
1:B:434:LYS:HA	1:B:437:GLN:HE21	1.83	0.44
1:A:466:HIS:CE1	1:A:468:LEU:H	2.35	0.44
1:B:226:PHE:HA	1:B:227:PRO:HD2	1.84	0.44
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:HIS:HA	1:B:467:PRO:HD3	1.86	0.43
1:B:265:LYS:O	1:B:266:HIS:CG	2.72	0.43
1:A:466:HIS:CE1	1:A:467:PRO:HG2	2.53	0.43
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.99	0.43
1:B:404:LYS:HB3	1:B:405:PRO:CD	2.48	0.43
1:B:267:ILE:H	1:B:267:ILE:HG13	1.61	0.42
1:B:272:GLU:HA	1:B:280:ARG:NH2	2.33	0.42
1:B:335:ASN:OD1	1:B:337:ASP:N	2.46	0.42
1:B:249:ILE:HG21	1:B:348:MET:HE2	2.01	0.42
1:A:272:GLU:HB2	1:A:273:GLN:H	1.51	0.42
1:B:272:GLU:HA	1:B:280:ARG:HH21	1.84	0.42
1:B:263:LYS:HD3	1:B:263:LYS:C	2.44	0.42
1:B:310:ASP:OD1	1:B:312:ASN:HB2	2.19	0.42
1:A:356:LEU:O	1:A:357:ARG:C	2.59	0.42
1:B:269:PRO:HG3	1:B:272:GLU:OE2	2.20	0.42
1:B:332:SER:C	1:B:333:LEU:HD23	2.45	0.42
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.83	0.42
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.85	0.41
1:B:207:GLU:HG3	3:B:4:HOH:O	2.20	0.41
1:B:474:LYS:C	1:B:476:LEU:N	2.77	0.41
1:A:435:LEU:O	1:A:435:LEU:HD12	2.21	0.41
1:B:384:LEU:O	1:B:388:ILE:HG12	2.20	0.41
1:B:445:ILE:HD13	1:B:445:ILE:HA	1.90	0.41
1:A:434:LYS:HA	1:A:437:GLN:HE21	1.85	0.41
1:A:285:CYS:O	1:A:289:SER:HB3	2.21	0.41
1:A:334:MET:HE2	1:A:368:PHE:CZ	2.56	0.41
1:B:465:LEU:HD12	1:B:465:LEU:N	2.36	0.40
1:B:334:MET:HE2	1:B:368:PHE:CZ	2.56	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	269/271 (99%)	252 (94%)	9 (3%)	8 (3%)	3	2
1	B	269/271 (99%)	244 (91%)	19 (7%)	6 (2%)	5	3
All	All	538/542 (99%)	496 (92%)	28 (5%)	14 (3%)	4	2

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	SER
1	A	358	LYS
1	B	269	PRO
1	B	274	SER
1	B	358	LYS
1	A	243	ASP
1	A	244	LYS
1	A	262	ILE
1	A	266	HIS
1	A	464	SER
1	B	271	GLN
1	A	272	GLU
1	B	243	ASP
1	B	239	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 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	244/244 (100%)	221 (91%)	23 (9%)	8	9
1	B	244/244 (100%)	224 (92%)	20 (8%)	10	12
All	All	488/488 (100%)	445 (91%)	43 (9%)	9	11

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	221	SER

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Mol	Chain	Res	Type
1	A	234	ARG
1	A	238	THR
1	A	243	ASP
1	A	248	VAL
1	A	261	LYS
1	A	268	THR
1	A	270	LEU
1	A	271	GLN
1	A	275	LYS
1	A	281	ILE
1	A	318	LEU
1	A	322	VAL
1	A	342	SER
1	A	345	GLN
1	A	378	GLU
1	A	402	ASN
1	A	440	THR
1	A	453	LEU
1	A	456	ILE
1	A	465	LEU
1	A	477	TYR
1	B	207	GLU
1	B	248	VAL
1	B	252	MET
1	B	260	ASP
1	B	262	ILE
1	B	264	PHE
1	B	267	ILE
1	B	294	GLN
1	B	318	LEU
1	B	323	HIS
1	B	333	LEU
1	B	358	LYS
1	B	364	MET
1	B	378	GLU
1	B	439	MET
1	B	453	LEU
1	B	463	MET
1	B	464	SER
1	B	466	HIS
1	B	476	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	294	GLN
1	A	308	ASN
1	A	345	GLN
1	A	402	ASN
1	A	415	GLN
1	A	437	GLN
1	B	273	GLN
1	B	283	GLN
1	B	286	GLN
1	B	402	ASN
1	B	437	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	3EA	B	1002	-	36,37,37	1.28	4 (11%)	47,53,53	1.29	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3EA	A	1001	-	36,37,37	1.33	5 (13%)	47,53,53	1.17	5 (10%)

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
2	3EA	B	1002	-	-	5/21/21/21	0/4/4/4
2	3EA	A	1001	-	-	4/21/21/21	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	3EA	C21-C25	-3.50	1.33	1.43
2	B	1002	3EA	C21-C25	-3.49	1.33	1.43
2	A	1001	3EA	C6-C2	-3.48	1.39	1.46
2	A	1001	3EA	C22-N27	-3.44	1.33	1.39
2	B	1002	3EA	C6-C2	-3.27	1.39	1.46
2	B	1002	3EA	C22-N27	-3.04	1.33	1.39
2	A	1001	3EA	C2-N3	2.86	1.33	1.28
2	B	1002	3EA	C2-N3	2.81	1.33	1.28
2	A	1001	3EA	O4-N3	-2.04	1.41	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	3EA	C17-O18-C19	-3.55	108.69	117.93
2	A	1001	3EA	C17-O18-C19	-2.77	110.73	117.93
2	B	1002	3EA	C29-C28-N27	-2.63	107.91	112.24
2	A	1001	3EA	C17-C16-C15	-2.55	105.44	113.67
2	A	1001	3EA	O4-N3-C2	-2.48	107.58	108.74
2	A	1001	3EA	C25-C26-N27	-2.48	107.71	110.54
2	B	1002	3EA	C17-C16-C15	-2.48	105.67	113.67
2	B	1002	3EA	O4-N3-C2	-2.41	107.62	108.74
2	B	1002	3EA	C21-C22-N27	-2.28	105.37	107.62
2	A	1001	3EA	F32-C1-C2	-2.26	108.14	112.42
2	B	1002	3EA	C25-C26-N27	-2.23	108.00	110.54
2	B	1002	3EA	F34-C1-C2	-2.03	108.57	112.42
2	B	1002	3EA	C6-C2-N3	-2.00	109.69	111.36

There are no chirality outliers.

All (9) torsion outliers are listed below:

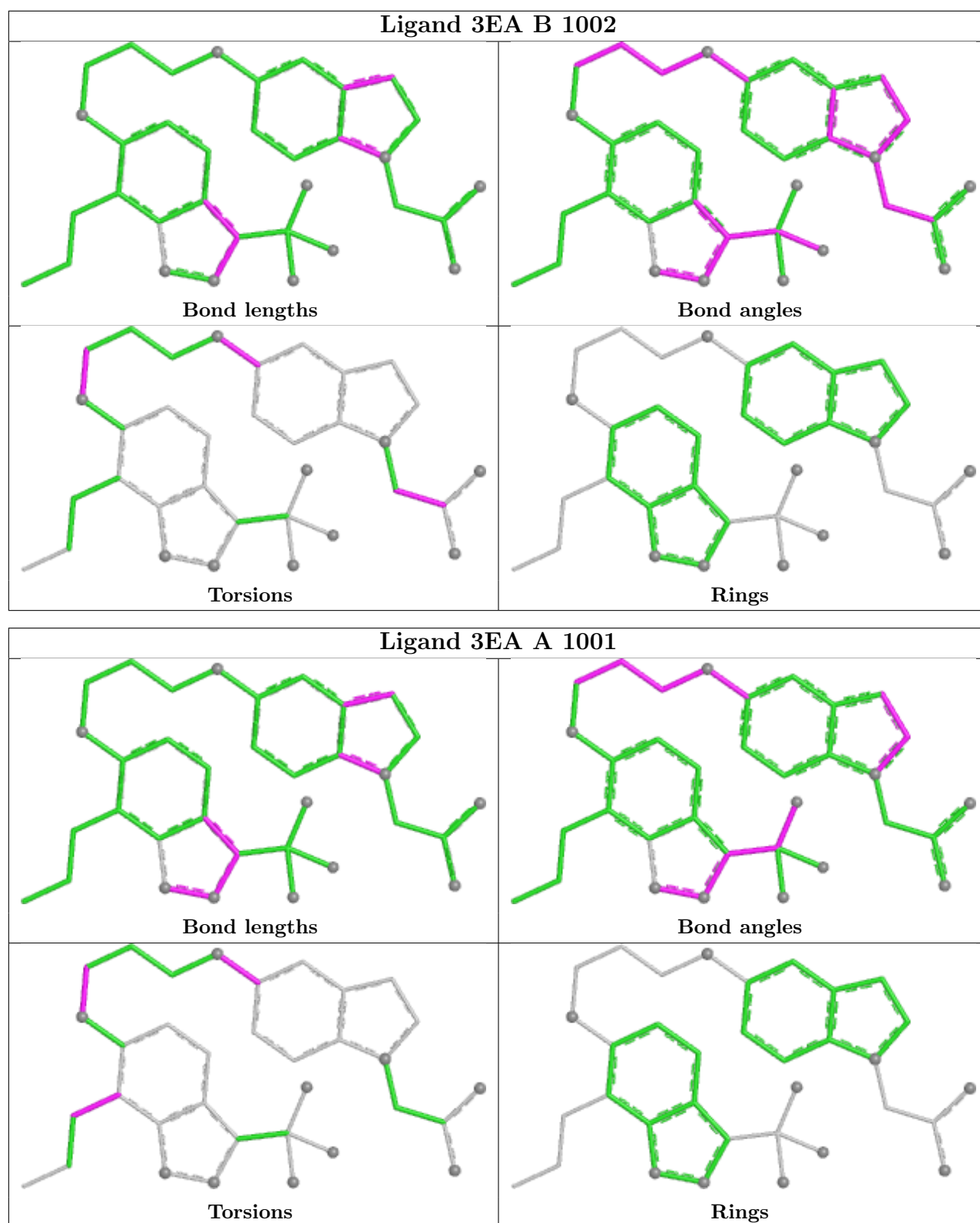
Mol	Chain	Res	Type	Atoms
2	B	1002	3EA	N27-C28-C29-O31
2	B	1002	3EA	N27-C28-C29-O30
2	A	1001	3EA	C24-C19-O18-C17
2	A	1001	3EA	C20-C19-O18-C17
2	B	1002	3EA	C20-C19-O18-C17
2	B	1002	3EA	C24-C19-O18-C17
2	A	1001	3EA	C16-C15-O14-C9
2	B	1002	3EA	C16-C15-O14-C9
2	A	1001	3EA	C9-C10-C11-C12

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	3EA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.