



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:54 PM UTC

PDB ID : 8ZFQ / pdb_00008zfq
Title : Crystal Structure of Human PPARgamma Ligand Binding Domain in Complex with T0070907 and BVT.13
Authors : Shang, J.; Kojetin, D.J.
Deposited on : 2024-05-08
Resolution : 2.49 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

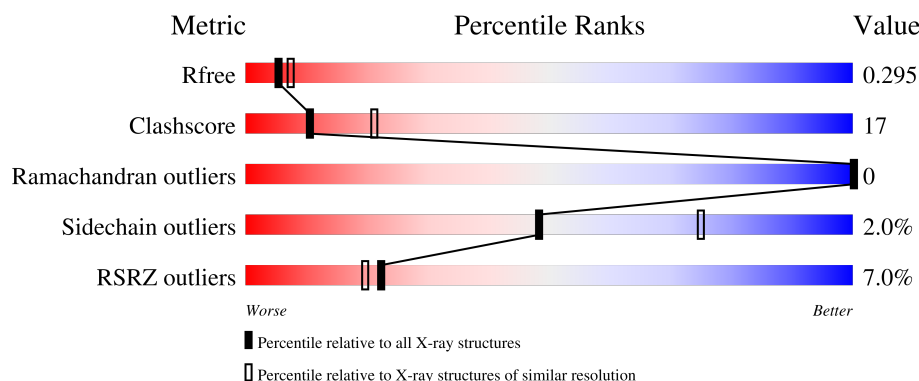
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	8% 63% 30% 6%
1	B	275	5% 67% 25% 7%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLB	A	502	-	-	X	-

2 Entry composition [i](#)

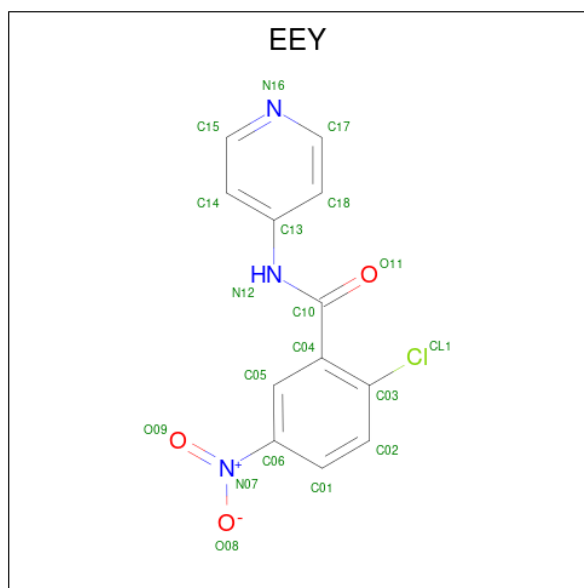
There are 4 unique types of molecules in this entry. The entry contains 4256 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

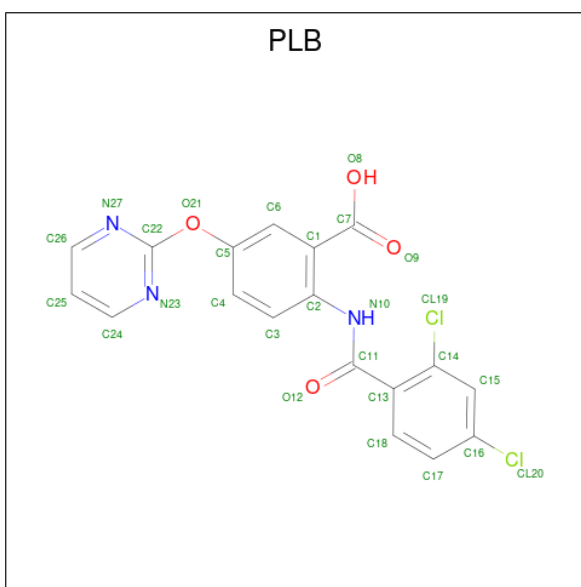
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2075	1340	338	387	10			
1	B	255	Total	C	N	O	S	0	0	0
			2048	1324	336	379	9			

- Molecule 2 is 2-chloro-5-nitro-N-(pyridin-4-yl)benzamide (CCD ID: EEY) (formula: $C_{12}H_8ClN_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	12	3	3		
2	B	1	Total	C	N	O	0	0
			18	12	3	3		

- Molecule 3 is 2-[(2,4-DICHLOROBENZOYL)AMINO]-5-(PYRIMIDIN-2-YLOXY)BENZ OIC ACID (CCD ID: PLB) (formula: $C_{18}H_{11}Cl_2N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			27	18	2	3	4	
3	B	1	Total	C	Cl	N	O	0
			27	18	2	3	4	

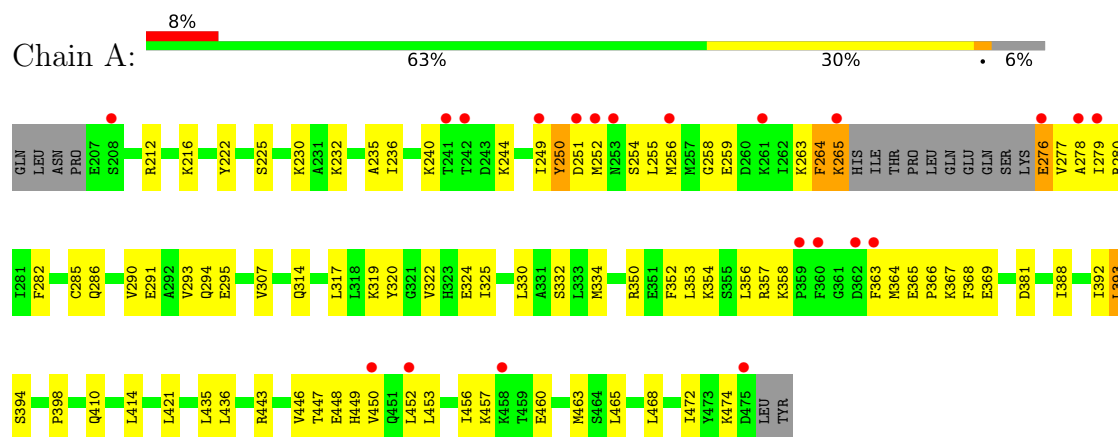
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	23	Total	O	0	0
			23	23		

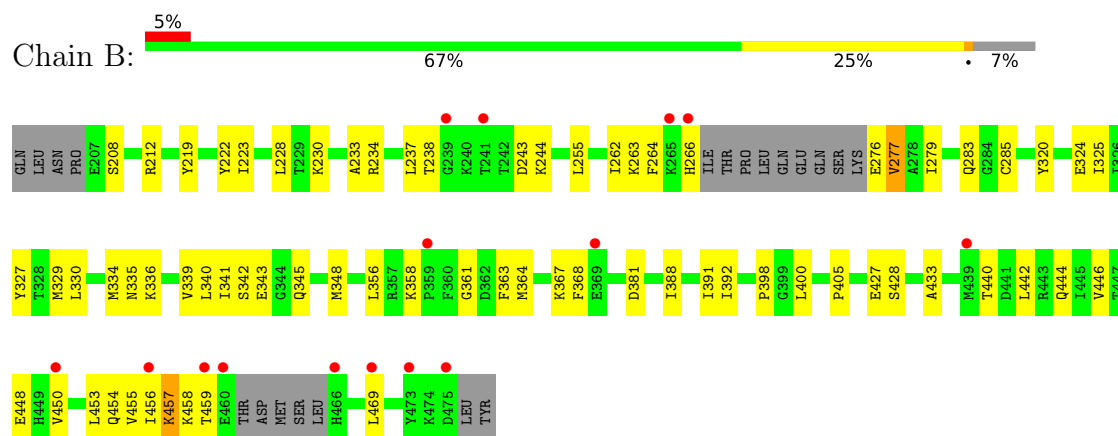
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.64Å 61.77Å 119.13Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	51.02 – 2.49 51.02 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (51.02-2.49) 99.1 (51.02-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.231 , 0.304 0.239 , 0.295	Depositor DCC
R_{free} test set	1114 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4256	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/2109	0.77	2/2839 (0.1%)
1	B	0.62	2/2082 (0.1%)	0.75	3/2801 (0.1%)
All	All	0.57	2/4191 (0.0%)	0.76	5/5640 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	PRO	C-O	-5.70	1.17	1.24
1	B	391	ILE	C-O	-5.36	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	GLU	CB-CG-CD	5.71	122.31	112.60
1	B	343	GLU	N-CA-C	-5.28	106.61	112.57
1	B	342	SER	CA-C-N	-5.12	114.94	122.83
1	B	342	SER	C-N-CA	-5.12	114.94	122.83
1	A	264	PHE	CA-CB-CG	5.02	118.82	113.80

There are no chirality outliers.

There are no planarity outliers.

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	2075	0	2137	86	0
1	B	2048	0	2106	55	0
2	A	18	0	0	3	0
2	B	18	0	0	0	0
3	A	27	0	10	11	0
3	B	27	0	10	5	0
4	A	20	0	0	2	0
4	B	23	0	0	2	0
All	All	4256	0	4263	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 17.

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:A:285:CYS:SG	2:A:501:EEY:C03	2.28	1.21
1:A:252:MET:O	1:A:256:MET:HG2	1.51	1.10
1:B:285:CYS:SG	4:B:617:HOH:O	2.31	0.87
1:A:448:GLU:O	1:A:452:LEU:HG	1.76	0.86
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.61	0.82
1:A:259:GLU:HA	1:A:264:PHE:HE1	1.44	0.81
1:A:252:MET:O	1:A:256:MET:CG	2.30	0.79
1:B:264:PHE:HB3	1:B:266:HIS:CE1	2.17	0.79
1:B:276:GLU:HB3	1:B:279:ILE:HB	1.65	0.78
1:B:262:ILE:HG21	1:B:264:PHE:CE1	2.21	0.76
1:A:319:LYS:HZ1	1:A:474:LYS:HB2	1.51	0.75
1:B:457:LYS:HA	1:B:457:LYS:HE2	1.67	0.75
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.70	0.73
1:A:319:LYS:NZ	1:A:474:LYS:HB2	2.03	0.72
1:A:244:LYS:NZ	4:A:602:HOH:O	2.25	0.69
1:A:364:MET:HG3	3:A:502:PLB:H15	1.75	0.69
1:B:444:GLN:O	1:B:448:GLU:HG2	1.93	0.68
1:B:262:ILE:CG2	1:B:264:PHE:CE1	2.76	0.68
1:A:254:SER:O	1:A:258:GLY:N	2.27	0.67
1:A:259:GLU:OE1	1:A:280:ARG:NH1	2.29	0.66
3:A:502:PLB:O12	3:A:502:PLB:H3	1.95	0.66
1:B:457:LYS:HA	1:B:457:LYS:CE	2.26	0.65
1:A:449:HIS:HA	1:A:452:LEU:HD12	1.80	0.63
1:A:235:ALA:HA	1:A:240:LYS:HG3	1.80	0.62
1:B:276:GLU:HG2	1:B:279:ILE:H	1.64	0.62
1:A:334:MET:HE1	3:A:502:PLB:CL20	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:HG23	1:A:255:LEU:N	2.16	0.61
1:A:285:CYS:SG	2:A:501:EEY:C04	2.89	0.61
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.83	0.61
1:A:250:TYR:CD2	1:A:250:TYR:N	2.69	0.60
1:B:262:ILE:HG21	1:B:264:PHE:HE1	1.67	0.60
1:B:356:LEU:HB2	1:B:361:GLY:HA2	1.83	0.59
1:A:225:SER:O	1:A:295:GLU:HG2	2.01	0.59
1:B:364:MET:CG	3:B:502:PLB:H15	2.32	0.59
1:A:364:MET:HE3	1:A:367:LYS:HG3	1.84	0.58
1:A:259:GLU:HA	1:A:264:PHE:CE1	2.33	0.58
1:A:264:PHE:CE2	3:A:502:PLB:N27	2.72	0.58
1:A:472:ILE:HG22	1:A:472:ILE:O	2.03	0.58
1:A:421:LEU:HD11	1:A:435:LEU:HD23	1.86	0.57
1:B:243:ASP:OD1	1:B:244:LYS:N	2.36	0.57
1:B:219:TYR:CZ	1:B:223:ILE:HD11	2.40	0.57
1:A:453:LEU:O	1:A:456:ILE:N	2.37	0.57
1:A:468:LEU:O	1:A:472:ILE:HG13	2.05	0.56
1:A:393:LEU:O	1:A:410:GLN:NE2	2.39	0.56
1:B:358:LYS:N	1:B:358:LYS:HD3	2.21	0.56
1:A:357:ARG:NH1	1:A:460:GLU:OE1	2.39	0.56
1:A:443:ARG:HH11	1:A:443:ARG:HG2	1.71	0.55
1:A:249:ILE:HD11	1:A:258:GLY:HA3	1.89	0.54
1:B:262:ILE:HG12	1:B:345:GLN:HG3	1.90	0.54
1:B:363:PHE:CD2	1:B:364:MET:HE2	2.43	0.54
1:A:364:MET:CG	3:A:502:PLB:H15	2.36	0.54
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.88	0.54
1:A:414:LEU:HD21	1:A:436:LEU:HD21	1.89	0.54
1:B:450:VAL:O	1:B:454:GLN:HG2	2.07	0.54
1:A:249:ILE:HG21	1:A:255:LEU:HA	1.90	0.53
1:A:350:ARG:NH2	1:A:365:GLU:OE2	2.27	0.53
1:B:325:ILE:HD13	1:B:388:ILE:HG23	1.90	0.53
1:A:364:MET:HE1	1:A:367:LYS:HE2	1.91	0.53
1:A:230:LYS:HG3	1:A:332:SER:HB3	1.92	0.52
1:A:353:LEU:HA	1:A:356:LEU:HD12	1.92	0.52
1:A:394:SER:HA	1:A:410:GLN:NE2	2.25	0.52
1:A:212:ARG:O	1:A:216:LYS:HG3	2.10	0.52
1:B:230:LYS:O	1:B:234:ARG:HG2	2.11	0.51
1:A:285:CYS:SG	2:A:501:EEY:C10	2.98	0.51
1:B:336:LYS:HG2	1:B:336:LYS:O	2.10	0.51
1:A:414:LEU:HD22	1:B:433:ALA:HB1	1.91	0.51
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:MET:HG3	3:B:502:PLB:H15	1.93	0.50
1:A:354:LYS:O	1:A:354:LYS:HD2	2.12	0.50
1:A:222:TYR:CE2	1:A:381:ASP:HB3	2.47	0.50
1:A:320:TYR:CZ	1:A:398:PRO:HG2	2.47	0.49
1:B:237:LEU:HD13	1:B:335:ASN:HD22	1.77	0.49
1:B:255:LEU:CD1	1:B:277:VAL:CG1	2.91	0.49
1:B:341:ILE:HG21	1:B:348:MET:HE3	1.95	0.48
3:A:502:PLB:O12	3:A:502:PLB:C3	2.58	0.48
1:B:255:LEU:HD12	1:B:277:VAL:CG1	2.44	0.48
1:B:324:GLU:HG3	1:B:446:VAL:HG21	1.95	0.48
1:A:330:LEU:O	1:A:334:MET:HG3	2.13	0.48
1:A:357:ARG:HG2	1:A:358:LYS:N	2.28	0.48
1:A:474:LYS:O	1:A:474:LYS:HG2	2.13	0.48
1:B:339:VAL:HG22	1:B:340:LEU:O	2.14	0.48
1:A:290:VAL:O	1:A:294:GLN:HG3	2.14	0.47
1:B:400:LEU:HA	4:B:601:HOH:O	2.13	0.47
1:A:278:ALA:HA	1:A:356:LEU:HD22	1.97	0.47
1:B:208:SER:O	1:B:212:ARG:HG2	2.15	0.47
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.45	0.47
1:B:228:LEU:CD2	1:B:233:ALA:HB2	2.45	0.47
1:A:443:ARG:O	1:A:447:THR:HG23	2.15	0.46
1:A:286:GLN:OE1	1:A:465:LEU:HA	2.15	0.46
1:B:327:TYR:CZ	1:B:367:LYS:HE3	2.50	0.46
1:B:334:MET:HE2	1:B:368:PHE:CD1	2.50	0.46
1:A:264:PHE:HE2	3:A:502:PLB:N27	2.13	0.46
1:A:250:TYR:HA	1:A:352:PHE:HB2	1.97	0.46
1:A:364:MET:HE2	3:A:502:PLB:CL20	2.53	0.46
1:B:234:ARG:O	1:B:238:THR:HG23	2.16	0.46
1:B:255:LEU:HD21	3:B:502:PLB:H25	1.96	0.46
1:A:457:LYS:O	1:A:457:LYS:HG3	2.15	0.46
1:A:277:VAL:HG12	1:A:280:ARG:NH2	2.31	0.46
1:A:388:ILE:O	1:A:392:ILE:HG13	2.16	0.46
1:B:279:ILE:O	1:B:283:GLN:HG3	2.17	0.45
1:A:443:ARG:HH11	1:A:443:ARG:CG	2.30	0.45
1:A:363:PHE:CE2	1:A:452:LEU:HB3	2.52	0.45
1:A:443:ARG:HG3	1:B:440:THR:HG23	1.97	0.45
1:A:264:PHE:HB2	1:A:265:LYS:H	1.59	0.45
1:B:222:TYR:CE2	1:B:381:ASP:HB3	2.52	0.45
1:A:250:TYR:N	1:A:250:TYR:HD2	2.14	0.45
3:B:502:PLB:N10	3:B:502:PLB:O8	2.48	0.45
1:A:286:GLN:HE21	1:A:286:GLN:HB2	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:MET:HE2	1:A:368:PHE:CE1	2.53	0.44
1:A:334:MET:CE	3:A:502:PLB:CL20	3.01	0.44
3:A:502:PLB:O12	3:A:502:PLB:CL19	2.73	0.44
1:A:251:ASP:O	1:A:255:LEU:HB2	2.18	0.44
1:A:364:MET:CE	1:A:367:LYS:HE2	2.48	0.44
1:B:329:MET:HE2	1:B:329:MET:HB3	1.92	0.43
1:B:453:LEU:HA	1:B:456:ILE:HD12	1.99	0.43
1:B:356:LEU:HB2	1:B:361:GLY:CA	2.46	0.43
1:A:307:VAL:HG22	4:A:609:HOH:O	2.18	0.43
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.45	0.43
1:B:327:TYR:CE2	1:B:367:LYS:HE3	2.53	0.43
1:B:228:LEU:HD22	1:B:233:ALA:HB2	2.01	0.43
1:B:334:MET:HG2	1:B:339:VAL:HB	2.01	0.42
1:B:276:GLU:CD	1:B:279:ILE:HD13	2.45	0.42
1:A:317:LEU:HD13	1:A:393:LEU:HD13	2.01	0.42
1:A:367:LYS:H	1:A:367:LYS:HG2	1.66	0.42
1:A:244:LYS:HD2	1:A:244:LYS:HA	1.82	0.42
1:A:291:GLU:HA	1:A:294:GLN:OE1	2.20	0.42
1:B:348:MET:HE3	1:B:348:MET:HB2	1.65	0.42
1:A:443:ARG:HG3	1:B:440:THR:CG2	2.50	0.41
1:A:232:LYS:O	1:A:236:ILE:HG13	2.19	0.41
1:A:366:PRO:HA	1:A:369:GLU:HG3	2.02	0.41
1:B:427:GLU:HG2	1:B:428:SER:N	2.36	0.41
1:A:276:GLU:O	1:A:279:ILE:HG12	2.21	0.41
1:A:307:VAL:O	1:A:314:GLN:NE2	2.53	0.41
1:B:330:LEU:HD11	3:B:502:PLB:H17	2.03	0.41
1:A:363:PHE:HD1	1:A:364:MET:SD	2.43	0.41
1:A:212:ARG:HA	1:A:212:ARG:HD2	1.77	0.41
1:A:282:PHE:CD2	1:A:463:MET:HE1	2.56	0.41
1:A:324:GLU:OE2	1:A:443:ARG:HD3	2.21	0.41
1:A:446:VAL:O	1:A:450:VAL:HG23	2.21	0.41
1:B:455:VAL:HA	1:B:458:LYS:HE2	2.02	0.40
1:B:442:LEU:O	1:B:446:VAL:HG23	2.21	0.40
1:A:364:MET:HE2	3:A:502:PLB:C15	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	255/275 (93%)	245 (96%)	10 (4%)	0	100	100
1	B	249/275 (90%)	242 (97%)	7 (3%)	0	100	100
All	All	504/550 (92%)	487 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	232/248 (94%)	228 (98%)	4 (2%)	53	78
1	B	228/248 (92%)	223 (98%)	5 (2%)	45	73
All	All	460/496 (93%)	451 (98%)	9 (2%)	48	75

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

Mol	Chain	Res	Type
1	A	250	TYR
1	A	263	LYS
1	A	265	LYS
1	A	393	LEU
1	B	263	LYS
1	B	277	VAL
1	B	457	LYS
1	B	459	THR

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Mol	Chain	Res	Type
1	B	469	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	ASN
1	A	410	GLN
1	A	449	HIS
1	B	323	HIS
1	B	437	GLN

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 ⓘ

4 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	PLB	A	502	-	29,29,29	1.72	6 (20%)	40,40,40	3.07	14 (35%)
2	EEY	A	501	-	19,19,20	3.07	4 (21%)	23,25,27	1.08	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EEY	B	501	1	19,19,20	3.22	4 (21%)	23,25,27	1.76	5 (21%)
3	PLB	B	502	-	29,29,29	1.51	6 (20%)	40,40,40	3.09	18 (45%)

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	PLB	A	502	-	-	6/16/16/16	0/3/3/3
2	EEY	A	501	-	-	6/10/12/12	0/2/2/2
2	EEY	B	501	1	-	6/10/12/12	0/2/2/2
3	PLB	B	502	-	-	3/16/16/16	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	EEY	O09-N07	11.42	1.42	1.22
2	B	501	EEY	O09-N07	11.41	1.42	1.22
2	B	501	EEY	C10-N12	4.58	1.49	1.35
2	A	501	EEY	C10-N12	4.34	1.48	1.35
2	B	501	EEY	C04-C10	4.01	1.59	1.50
2	B	501	EEY	C13-N12	3.90	1.49	1.41
3	A	502	PLB	C11-N10	3.82	1.46	1.35
3	A	502	PLB	O21-C22	3.61	1.42	1.34
2	A	501	EEY	C13-N12	3.48	1.48	1.41
3	A	502	PLB	C22-N27	3.43	1.36	1.32
3	A	502	PLB	C22-N23	3.40	1.36	1.32
3	B	502	PLB	C22-N23	3.14	1.36	1.32
3	B	502	PLB	O21-C22	3.10	1.41	1.34
3	B	502	PLB	C22-N27	3.02	1.36	1.32
3	B	502	PLB	C11-N10	2.92	1.44	1.35
2	A	501	EEY	C04-C10	2.70	1.56	1.50
3	A	502	PLB	C14-CL19	2.50	1.79	1.73
3	A	502	PLB	C2-N10	2.32	1.46	1.41
3	B	502	PLB	C14-CL19	2.13	1.78	1.73
3	B	502	PLB	C1-C7	2.11	1.54	1.49

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PLB	C24-N23-C22	9.77	120.92	114.46
3	B	502	PLB	C24-N23-C22	9.38	120.67	114.46
3	A	502	PLB	C26-N27-C22	9.34	120.64	114.46
3	A	502	PLB	N23-C22-N27	-8.19	118.33	128.12
3	B	502	PLB	C26-N27-C22	7.57	119.47	114.46
3	B	502	PLB	N23-C22-N27	-6.84	119.95	128.12
3	B	502	PLB	C2-N10-C11	-5.16	112.55	126.90
2	B	501	EEY	C05-C06-N07	4.95	123.00	118.74
3	B	502	PLB	C14-C13-C11	-4.92	114.59	122.56
3	B	502	PLB	C18-C13-C14	4.83	123.44	117.79
3	B	502	PLB	C22-O21-C5	-3.94	108.89	118.72
3	A	502	PLB	C22-O21-C5	-3.85	109.13	118.72
2	B	501	EEY	C18-C13-C14	-3.47	114.43	119.04
3	A	502	PLB	C13-C11-N10	3.38	123.04	116.03
3	B	502	PLB	C3-C2-C1	3.23	123.59	119.37
3	A	502	PLB	O12-C11-C13	-3.07	115.41	121.03
3	B	502	PLB	C24-C25-C26	3.05	120.60	116.63
3	A	502	PLB	C2-N10-C11	-2.91	118.82	126.90
3	A	502	PLB	C17-C16-CL20	2.78	123.46	119.36
3	B	502	PLB	C2-C1-C7	-2.76	118.65	121.72
3	B	502	PLB	C25-C24-N23	-2.69	119.16	123.42
2	B	501	EEY	C15-C14-C13	2.67	122.38	118.88
2	B	501	EEY	O09-N07-C06	2.65	122.47	118.82
3	A	502	PLB	C15-C14-C13	-2.61	119.45	121.59
3	B	502	PLB	C17-C18-C13	-2.61	116.56	120.86
3	A	502	PLB	C14-C15-C16	2.50	121.55	118.72
3	B	502	PLB	C3-C2-N10	-2.42	116.22	121.82
3	B	502	PLB	C15-C14-C13	-2.39	119.63	121.59
3	B	502	PLB	C15-C16-CL20	-2.30	116.28	119.17
3	A	502	PLB	C1-C2-N10	2.25	122.76	118.70
3	A	502	PLB	C24-C25-C26	2.16	119.44	116.63
3	A	502	PLB	C25-C24-N23	-2.16	120.01	123.42
2	B	501	EEY	C01-C06-N07	-2.14	117.47	119.34
3	B	502	PLB	C25-C26-N27	-2.06	120.16	123.42
2	A	501	EEY	O09-N07-C06	2.06	121.65	118.82
3	A	502	PLB	C14-C13-C11	-2.02	119.29	122.56
3	B	502	PLB	O8-C7-O9	-2.02	119.01	123.35
3	B	502	PLB	C6-C1-C7	2.00	123.51	117.89

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	EEY	C03-C04-C10-O11
2	B	501	EEY	C05-C04-C10-O11
2	B	501	EEY	C03-C04-C10-N12
2	B	501	EEY	C05-C04-C10-N12
3	A	502	PLB	N27-C22-O21-C5
3	A	502	PLB	N23-C22-O21-C5
3	B	502	PLB	N27-C22-O21-C5
3	B	502	PLB	N23-C22-O21-C5
2	A	501	EEY	C03-C04-C10-N12
2	A	501	EEY	C03-C04-C10-O11
2	B	501	EEY	C18-C13-N12-C10
2	B	501	EEY	C14-C13-N12-C10
2	A	501	EEY	C05-C04-C10-N12
2	A	501	EEY	C18-C13-N12-C10
2	A	501	EEY	C14-C13-N12-C10
2	A	501	EEY	C05-C04-C10-O11
3	A	502	PLB	C4-C5-O21-C22
3	B	502	PLB	C4-C5-O21-C22
3	A	502	PLB	N10-C11-C13-C14
3	A	502	PLB	C6-C5-O21-C22
3	A	502	PLB	O12-C11-C13-C14

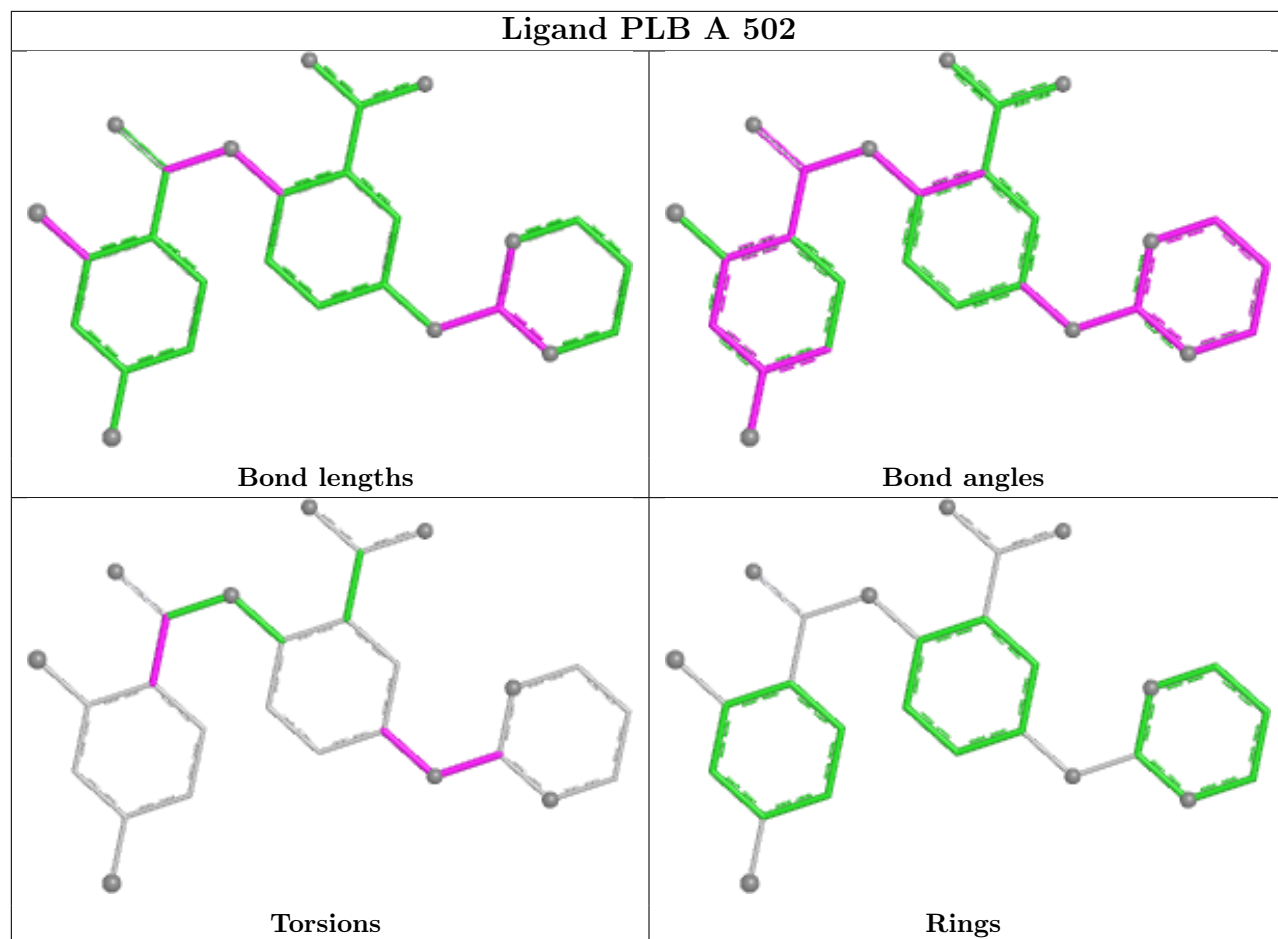
There are no ring outliers.

3 monomers are involved in 19 short contacts:

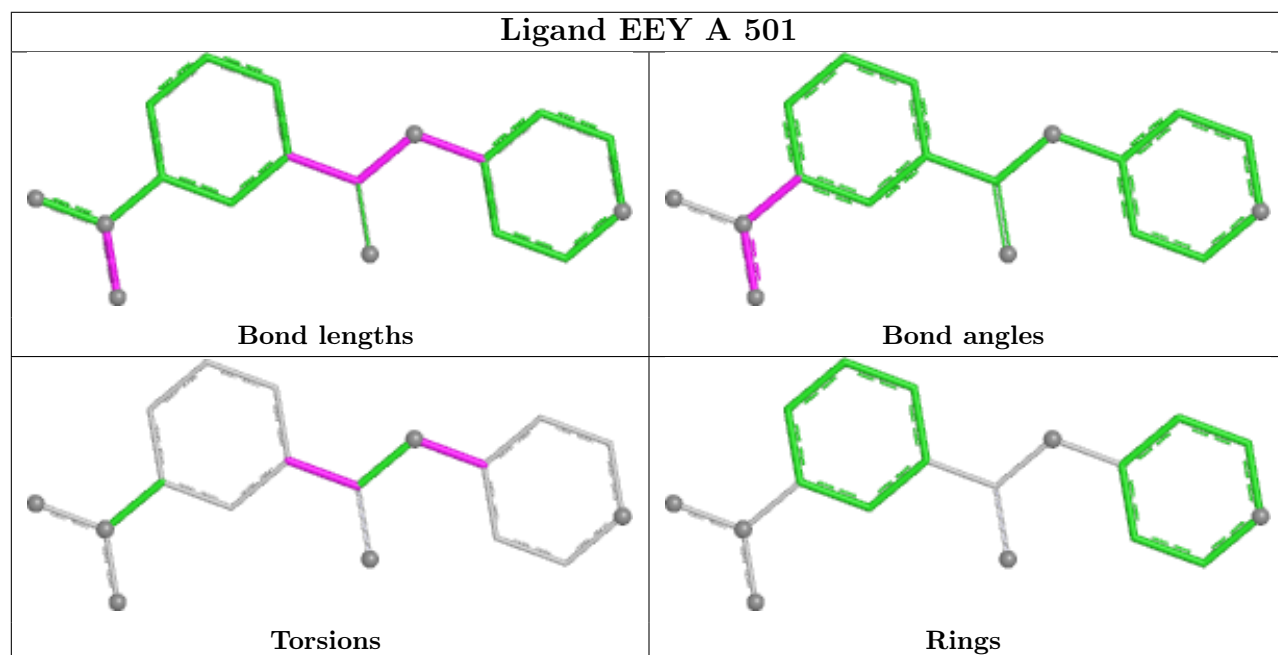
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PLB	11	0
2	A	501	EEY	3	0
3	B	502	PLB	5	0

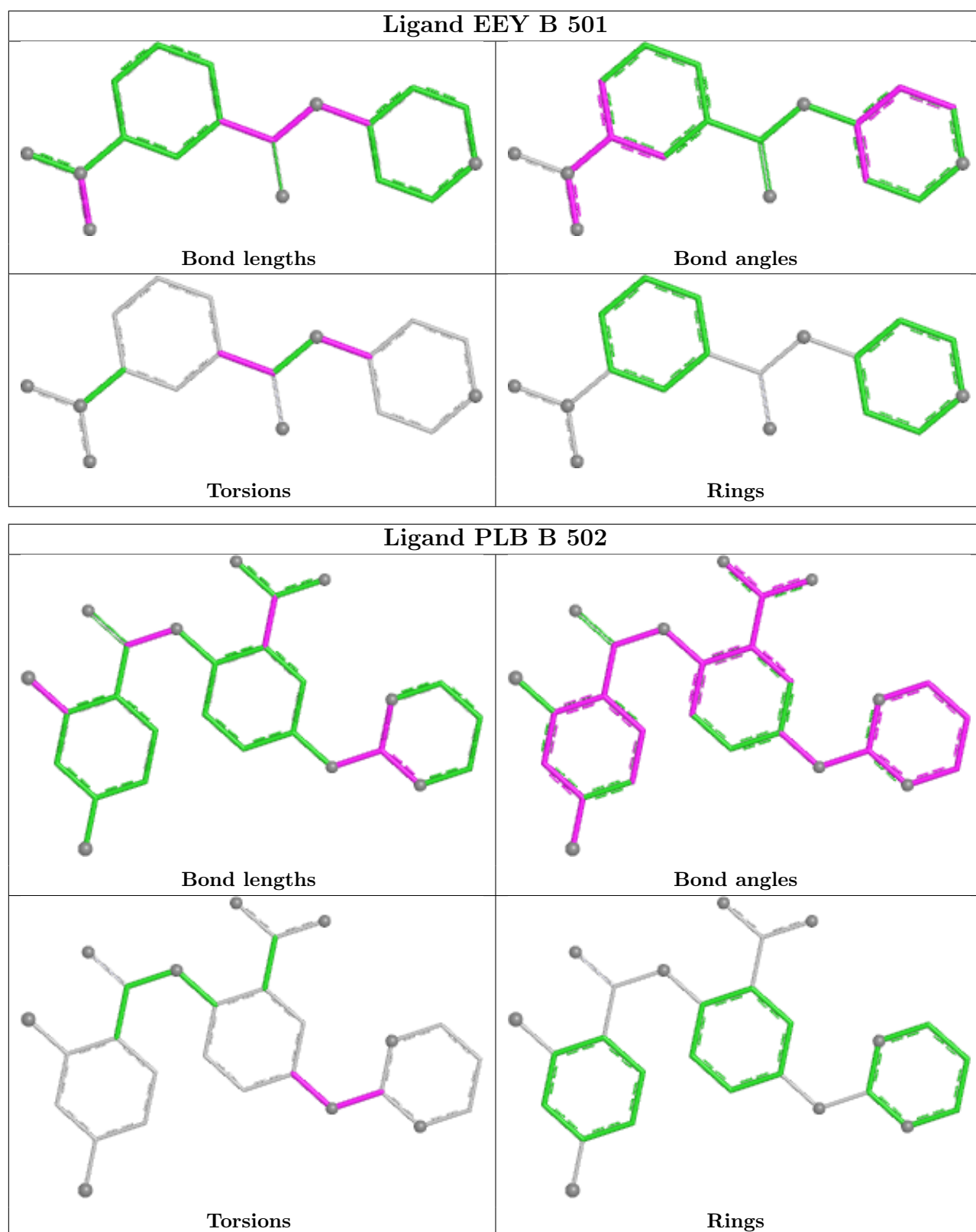
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 PLB A 502



Ligand EEY A 501





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	259/275 (94%)	0.60	21 (8%) 18 15	39, 59, 93, 111	0
1	B	255/275 (92%)	0.46	15 (5%) 28 24	39, 59, 97, 116	0
All	All	514/550 (93%)	0.53	36 (7%) 22 20	39, 59, 94, 116	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ILE	4.8
1	A	241	THR	4.6
1	B	266	HIS	3.3
1	A	253	ASN	3.2
1	B	265	LYS	3.2
1	A	265	LYS	3.2
1	A	279	ILE	2.9
1	B	241	THR	2.9
1	B	369	GLU	2.8
1	B	239	GLY	2.8
1	A	242	THR	2.7
1	A	363	PHE	2.7
1	B	460	GLU	2.6
1	B	469	LEU	2.6
1	A	458	LYS	2.6
1	A	252	MET	2.5
1	A	359	PRO	2.5
1	A	360	PHE	2.5
1	A	452	LEU	2.5
1	A	278	ALA	2.5
1	B	475	ASP	2.4
1	A	251	ASP	2.3
1	A	276	GLU	2.3
1	B	439	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	473	TYR	2.3
1	A	362	ASP	2.3
1	A	475	ASP	2.3
1	B	450	VAL	2.3
1	A	261	LYS	2.2
1	B	359	PRO	2.2
1	A	208	SER	2.2
1	B	456	ILE	2.2
1	B	459	THR	2.1
1	A	450	VAL	2.1
1	A	256	MET	2.1
1	B	466	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

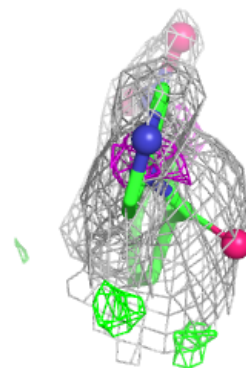
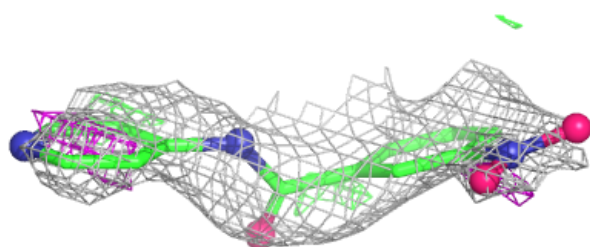
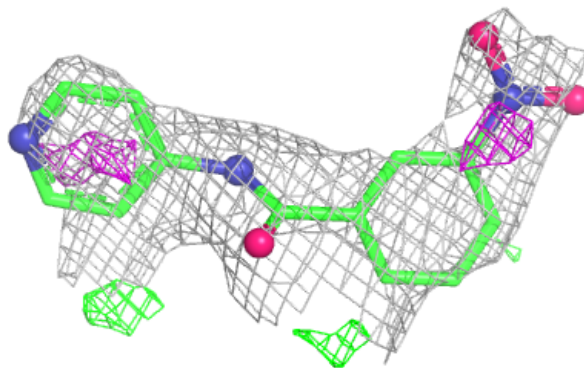
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EEY	A	501	18/19	0.67	0.19	68,87,95,97	0
2	EEY	B	501	18/19	0.80	0.13	59,75,95,97	0
3	PLB	A	502	27/27	0.81	0.15	59,70,91,94	0
3	PLB	B	502	27/27	0.88	0.11	47,65,77,87	0

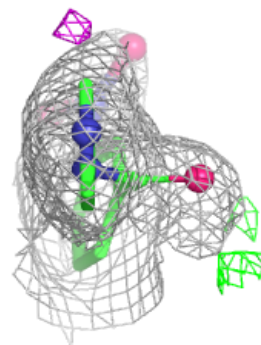
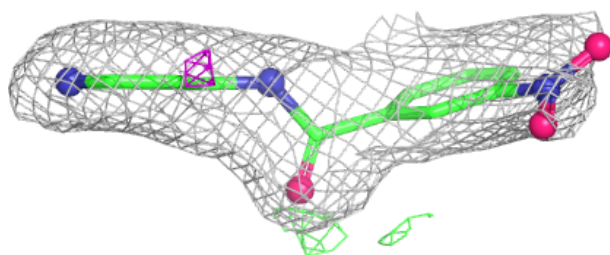
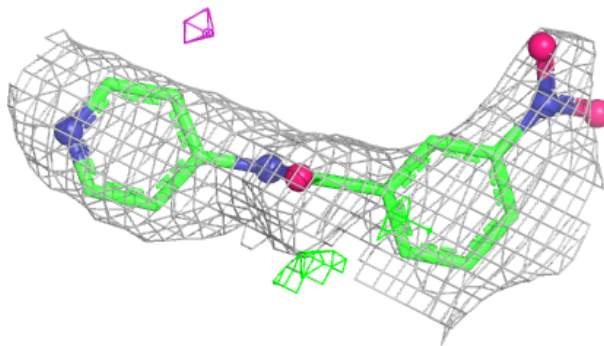
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EEY A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

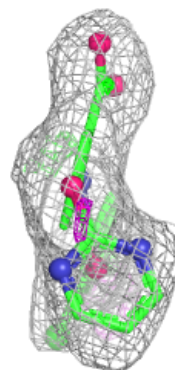
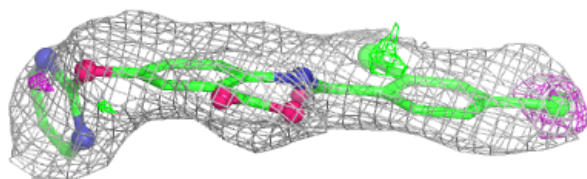
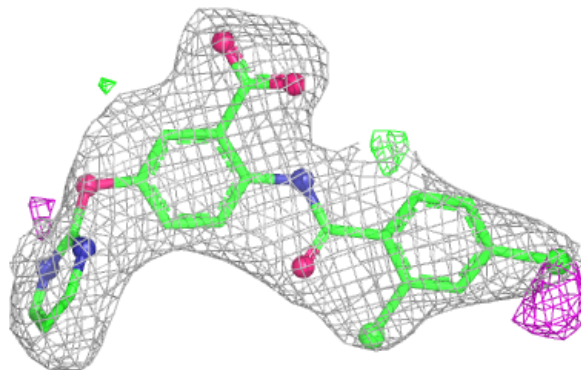
**Electron density around EEY B 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

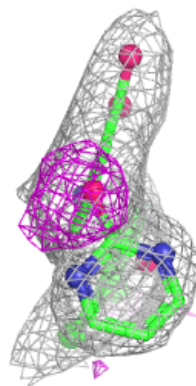
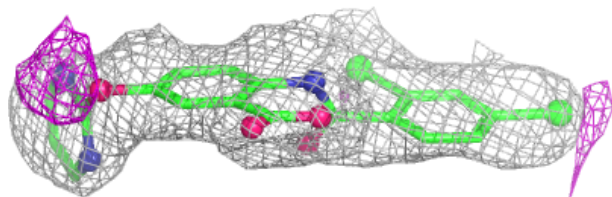
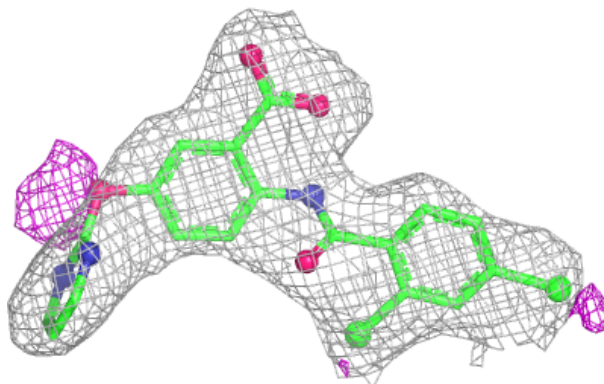


Electron density around PLB A 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PLB B 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.