



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 02:24 am BST

PDB ID : 1WM0
Title : PPARgamma in complex with a 2-BABA compound
Authors : Ostberg, T.; Svensson, S.; Selen, G.; Uppenberg, J.; Thor, M.; Sundbom, M.;
Sydow-Backman, M.; Gustavsson, A.L.; Jendeberg, L.
Deposited on : 2004-07-01
Resolution : 2.90 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 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)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

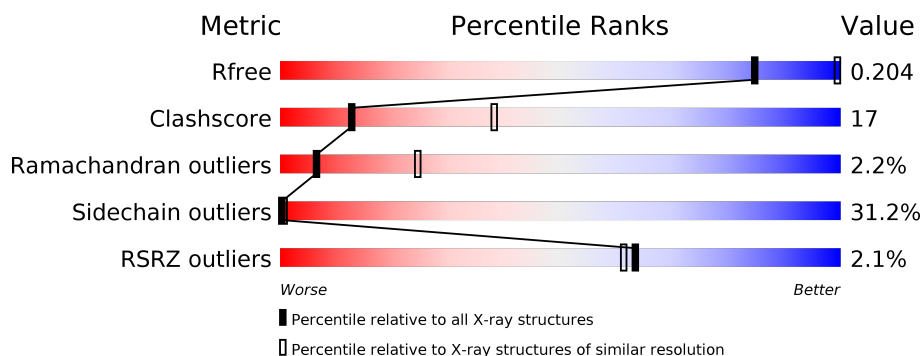
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	X	292	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>33%</div> <div>12%</div> <div>• 7%</div> </div> </div>
2	Y	14	<div> <div>43%</div> <div>21%</div> <div>7%</div> <div>29%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2297 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	X	272	Total	C	N	O	S	0	0	0
			2184	1410	358	406	10			

There are 18 discrepancies between the modelled and reference sequences:

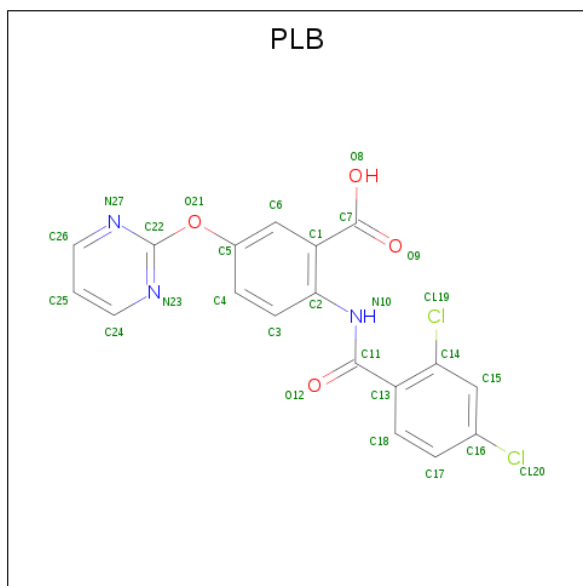
Chain	Residue	Modelled	Actual	Comment	Reference
X	186	GLY	-	EXPRESSION TAG	UNP Q96J12
X	187	SER	-	EXPRESSION TAG	UNP Q96J12
X	188	SER	-	EXPRESSION TAG	UNP Q96J12
X	189	HIS	-	EXPRESSION TAG	UNP Q96J12
X	190	HIS	-	EXPRESSION TAG	UNP Q96J12
X	191	HIS	-	EXPRESSION TAG	UNP Q96J12
X	192	HIS	-	EXPRESSION TAG	UNP Q96J12
X	193	HIS	-	EXPRESSION TAG	UNP Q96J12
X	194	HIS	-	EXPRESSION TAG	UNP Q96J12
X	195	SER	-	EXPRESSION TAG	UNP Q96J12
X	196	GLY	-	EXPRESSION TAG	UNP Q96J12
X	197	SER	-	EXPRESSION TAG	UNP Q96J12
X	198	GLY	-	EXPRESSION TAG	UNP Q96J12
X	199	THR	-	EXPRESSION TAG	UNP Q96J12
X	200	ILE	-	EXPRESSION TAG	UNP Q96J12
X	201	GLU	-	EXPRESSION TAG	UNP Q96J12
X	202	GLY	-	EXPRESSION TAG	UNP Q96J12
X	203	ARG	-	EXPRESSION TAG	UNP Q96J12

- Molecule 2 is a protein called 14-mer from Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Y	10	Total	C	N	O	0	0	0
			86	56	19	11			

- Molecule 3 is 2-[(2,4-DICHLOROBENZOYL)AMINO]-5-(PYRIMIDIN-2-YLOXY)BENZOI

C ACID (three-letter code: PLB) (formula: $C_{18}H_{11}Cl_2N_3O_4$).

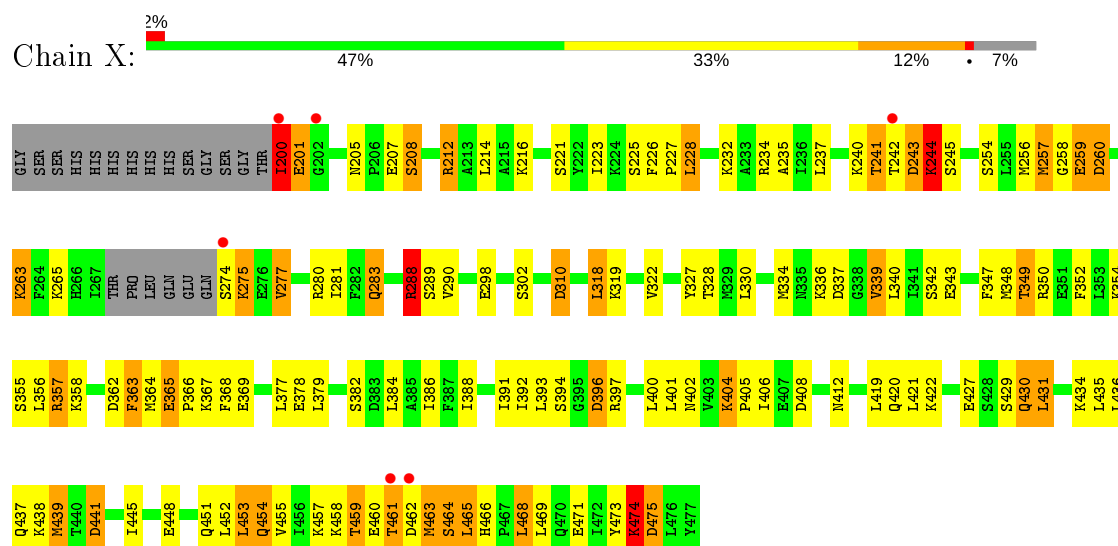


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	X	1	27	18	2	3	4	0	0

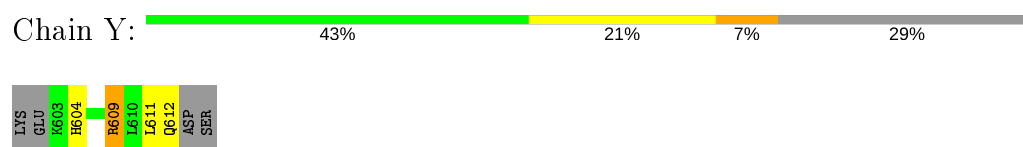
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 2: 14-mer from Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.17Å 66.32Å 122.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.70 – 2.90 14.83 – 2.81	Depositor EDS
% Data completeness (in resolution range)	87.7 (14.70-2.90) 87.7 (14.83-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.191 , 0.295 0.190 , 0.204	Depositor DCC
R_{free} test set	449 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2297	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: 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	X	1.13	2/2221 (0.1%)	1.18	12/2989 (0.4%)
2	Y	1.29	0/87	1.04	0/115
All	All	1.13	2/2308 (0.1%)	1.18	12/3104 (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	X	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	347	PHE	CE1-CZ	6.27	1.49	1.37
1	X	327	TYR	CE1-CZ	5.16	1.45	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	310	ASP	CB-CG-OD2	8.00	125.50	118.30
1	X	339	VAL	CB-CA-C	-6.61	98.84	111.40
1	X	396	ASP	CB-CA-C	-6.54	97.32	110.40
1	X	362	ASP	CB-CG-OD2	6.48	124.13	118.30
1	X	212	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	X	212	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	X	475	ASP	CB-CG-OD2	5.89	123.60	118.30
1	X	228	LEU	CB-CG-CD2	5.77	120.80	111.00
1	X	337	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	408	ASP	CB-CG-OD2	5.28	123.05	118.30
1	X	441	ASP	CB-CG-OD2	5.05	122.85	118.30
1	X	288	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	200	ILE	Peptide
1	X	244	LYS	Peptide
1	X	265	LYS	Peptide

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	X	2184	0	2250	76	1
2	Y	86	0	93	7	1
3	X	27	0	10	2	0
All	All	2297	0	2353	77	1

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 (77) 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:X:256:MET:CE	1:X:256:MET:SD	2.04	1.45
1:X:275:LYS:N	1:X:275:LYS:HD3	1.65	1.11
1:X:275:LYS:H	1:X:275:LYS:CD	1.64	1.10
1:X:430:GLN:NE2	1:X:430:GLN:HA	1.71	1.06
1:X:349:THR:HG22	1:X:352:PHE:H	1.15	1.05
1:X:275:LYS:H	1:X:275:LYS:HD3	0.81	0.95
1:X:319:LYS:HE2	2:Y:604:HIS:CE1	2.02	0.94
1:X:430:GLN:HE21	1:X:430:GLN:HA	1.24	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:330:LEU:HD22	1:X:334:MET:HE3	1.50	0.92
1:X:319:LYS:NZ	1:X:319:LYS:HB2	1.85	0.91
1:X:259:GLU:OE1	1:X:280:ARG:NH1	2.05	0.90
1:X:319:LYS:HZ2	1:X:319:LYS:HB2	1.42	0.82
1:X:212:ARG:NH2	1:X:420:GLN:OE1	2.17	0.77
1:X:319:LYS:CE	2:Y:604:HIS:CE1	2.69	0.76
1:X:330:LEU:HD22	1:X:334:MET:CE	2.16	0.74
1:X:350:ARG:HD2	1:X:365:GLU:OE1	1.90	0.72
1:X:451:GLN:O	1:X:454:GLN:HB2	1.90	0.72
1:X:319:LYS:CB	1:X:319:LYS:NZ	2.52	0.71
1:X:200:ILE:HD12	1:X:201:GLU:HG2	1.72	0.71
1:X:319:LYS:CE	2:Y:604:HIS:NE2	2.55	0.69
1:X:441:ASP:O	1:X:445:ILE:HG12	1.94	0.66
1:X:259:GLU:CD	1:X:280:ARG:HH11	1.99	0.65
1:X:283:GLN:OE1	1:X:283:GLN:HA	1.97	0.65
1:X:349:THR:CG2	1:X:352:PHE:H	2.02	0.65
1:X:275:LYS:N	1:X:275:LYS:CD	2.40	0.63
1:X:349:THR:HG22	1:X:352:PHE:N	2.00	0.62
1:X:277:VAL:O	1:X:281:ILE:HG13	2.01	0.60
1:X:421:LEU:HD11	1:X:435:LEU:HD12	1.82	0.60
1:X:319:LYS:HE2	2:Y:604:HIS:NE2	2.17	0.59
1:X:363:PHE:CE1	1:X:364:MET:HG2	2.37	0.58
1:X:318:LEU:HD21	2:Y:611:LEU:HD21	1.85	0.58
1:X:461:THR:O	1:X:462:ASP:HB2	2.04	0.57
1:X:382:SER:HB3	1:X:420:GLN:NE2	2.22	0.55
1:X:319:LYS:HZ3	1:X:319:LYS:CB	2.18	0.54
1:X:438:LYS:HE3	1:X:441:ASP:OD1	2.08	0.54
1:X:288:ARG:HG3	3:X:1:PLB:O9	2.07	0.54
1:X:244:LYS:HB3	1:X:244:LYS:NZ	2.23	0.54
1:X:319:LYS:HE3	2:Y:604:HIS:NE2	2.22	0.53
1:X:318:LEU:CD2	2:Y:611:LEU:HD21	2.37	0.53
1:X:319:LYS:HZ3	1:X:319:LYS:HB2	1.67	0.53
1:X:386:ILE:HD12	1:X:420:GLN:HG2	1.90	0.53
1:X:473:TYR:O	1:X:474:LYS:O	2.27	0.53
1:X:465:LEU:HD21	1:X:469:LEU:HB3	1.91	0.51
1:X:379:LEU:HD11	1:X:435:LEU:HD21	1.92	0.51
1:X:471:GLU:O	1:X:474:LYS:HB2	2.11	0.51
1:X:258:GLY:C	1:X:260:ASP:H	2.13	0.51
1:X:404:LYS:N	1:X:405:PRO:HD2	2.27	0.49
1:X:365:GLU:N	1:X:366:PRO:CD	2.75	0.49
3:X:1:PLB:O12	3:X:1:PLB:H3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:464:SER:OG	1:X:464:SER:O	2.30	0.49
1:X:235:ALA:HB1	1:X:241:THR:HG22	1.94	0.49
1:X:205:ASN:CB	1:X:208:SER:HB3	2.43	0.48
1:X:459:THR:HG22	1:X:460:GLU:OE2	2.13	0.48
1:X:263:LYS:H	1:X:263:LYS:HG2	1.46	0.48
1:X:474:LYS:HA	1:X:474:LYS:HD2	1.39	0.47
1:X:466:HIS:CE1	1:X:468:LEU:HB2	2.50	0.47
1:X:391:ILE:HG22	1:X:392:ILE:N	2.29	0.46
1:X:384:LEU:O	1:X:388:ILE:HD12	2.16	0.46
1:X:382:SER:HB3	1:X:420:GLN:HE22	1.81	0.45
1:X:226:PHE:HA	1:X:227:PRO:HD2	1.84	0.45
1:X:350:ARG:HD3	1:X:368:PHE:CG	2.51	0.45
1:X:377:LEU:HB3	1:X:431:LEU:HD21	1.99	0.45
1:X:205:ASN:HB3	1:X:208:SER:HB3	1.98	0.44
1:X:237:LEU:HD21	1:X:340:LEU:HG	1.99	0.44
1:X:257:MET:HB3	1:X:257:MET:HE2	1.91	0.43
1:X:436:LEU:CD2	1:X:439:MET:HE1	2.48	0.43
1:X:254:SER:HA	1:X:257:MET:HG3	2.00	0.43
1:X:404:LYS:N	1:X:405:PRO:CD	2.81	0.43
1:X:350:ARG:NH1	1:X:365:GLU:OE2	2.52	0.42
1:X:400:LEU:HD13	1:X:406:ILE:HD13	2.01	0.42
1:X:256:MET:CE	1:X:256:MET:CG	2.94	0.42
1:X:234:ARG:HD3	1:X:234:ARG:HA	1.73	0.42
1:X:436:LEU:HA	1:X:439:MET:CE	2.49	0.41
1:X:474:LYS:HB3	1:X:475:ASP:H	1.69	0.41
1:X:357:ARG:HE	1:X:357:ARG:HB2	1.79	0.40
1:X:460:GLU:O	1:X:463:MET:HB2	2.21	0.40
1:X:365:GLU:O	1:X:369:GLU:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:400:LEU:O	2:Y:609:ARG:NH1[4_455]	2.12	0.08

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	X	268/292 (92%)	239 (89%)	23 (9%)	6 (2%)	6	24
2	Y	8/14 (57%)	7 (88%)	1 (12%)	0	100	100
All	All	276/306 (90%)	246 (89%)	24 (9%)	6 (2%)	6	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	243	ASP
1	X	455	VAL
1	X	474	LYS
1	X	259	GLU
1	X	453	LEU
1	X	464	SER

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	X	244/261 (94%)	167 (68%)	77 (32%)	0	0
2	Y	9/14 (64%)	7 (78%)	2 (22%)	1	3
All	All	253/275 (92%)	174 (69%)	79 (31%)	0	1

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	200	ILE
1	X	201	GLU
1	X	207	GLU
1	X	208	SER
1	X	214	LEU
1	X	216	LYS
1	X	221	SER
1	X	223	ILE
1	X	225	SER
1	X	228	LEU
1	X	232	LYS
1	X	240	LYS
1	X	241	THR
1	X	242	THR
1	X	243	ASP
1	X	244	LYS
1	X	245	SER
1	X	257	MET
1	X	260	ASP
1	X	263	LYS
1	X	274	SER
1	X	275	LYS
1	X	277	VAL
1	X	283	GLN
1	X	288	ARG
1	X	289	SER
1	X	290	VAL
1	X	298	GLU
1	X	302	SER
1	X	310	ASP
1	X	318	LEU
1	X	322	VAL
1	X	328	THR
1	X	336	LYS
1	X	339	VAL
1	X	342	SER
1	X	343	GLU
1	X	348	MET
1	X	349	THR
1	X	354	LYS
1	X	355	SER
1	X	356	LEU
1	X	357	ARG

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Mol	Chain	Res	Type
1	X	358	LYS
1	X	363	PHE
1	X	365	GLU
1	X	367	LYS
1	X	378	GLU
1	X	393	LEU
1	X	394	SER
1	X	396	ASP
1	X	397	ARG
1	X	401	LEU
1	X	402	ASN
1	X	404	LYS
1	X	412	ASN
1	X	419	LEU
1	X	422	LYS
1	X	427	GLU
1	X	429	SER
1	X	430	GLN
1	X	431	LEU
1	X	434	LYS
1	X	437	GLN
1	X	439	MET
1	X	448	GLU
1	X	452	LEU
1	X	453	LEU
1	X	454	GLN
1	X	457	LYS
1	X	458	LYS
1	X	459	THR
1	X	461	THR
1	X	463	MET
1	X	465	LEU
1	X	468	LEU
1	X	474	LYS
2	Y	609	ARG
2	Y	612	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	444	GLN
1	X	470	GLN

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Mol	Chain	Res	Type
2	Y	612	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	X	1	-	27,29,29	3.61	5 (18%)	35,40,40	4.16	15 (42%)

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	X	1	-	-	2/12/16/16	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	1	PLB	C22-N27	12.48	1.48	1.32
3	X	1	PLB	C22-N23	12.20	1.47	1.32
3	X	1	PLB	C1-C7	4.65	1.51	1.47
3	X	1	PLB	C14-CL19	2.41	1.79	1.73
3	X	1	PLB	C2-N10	-2.23	1.37	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	1	PLB	C26-N27-C22	13.63	121.19	114.41
3	X	1	PLB	C24-N23-C22	13.37	121.06	114.41
3	X	1	PLB	N23-C22-N27	-9.23	115.48	127.99
3	X	1	PLB	C15-C16-CL20	-5.88	111.80	119.15
3	X	1	PLB	C24-C25-C26	4.67	123.37	116.67
3	X	1	PLB	C17-C16-CL20	4.24	125.98	119.35
3	X	1	PLB	O12-C11-C13	-3.52	114.58	121.01
3	X	1	PLB	C14-C13-C11	-2.85	118.04	122.58
3	X	1	PLB	C18-C13-C14	2.82	121.08	117.78
3	X	1	PLB	C17-C18-C13	-2.69	116.57	120.94
3	X	1	PLB	C25-C24-N23	-2.55	119.26	123.43
3	X	1	PLB	C25-C26-N27	-2.48	119.38	123.43
3	X	1	PLB	O12-C11-N10	2.40	129.18	123.71
3	X	1	PLB	C15-C14-CL19	-2.10	115.11	118.49
3	X	1	PLB	C18-C17-C16	2.03	121.38	119.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	1	PLB	N27-C22-O21-C5
3	X	1	PLB	C13-C11-N10-C2

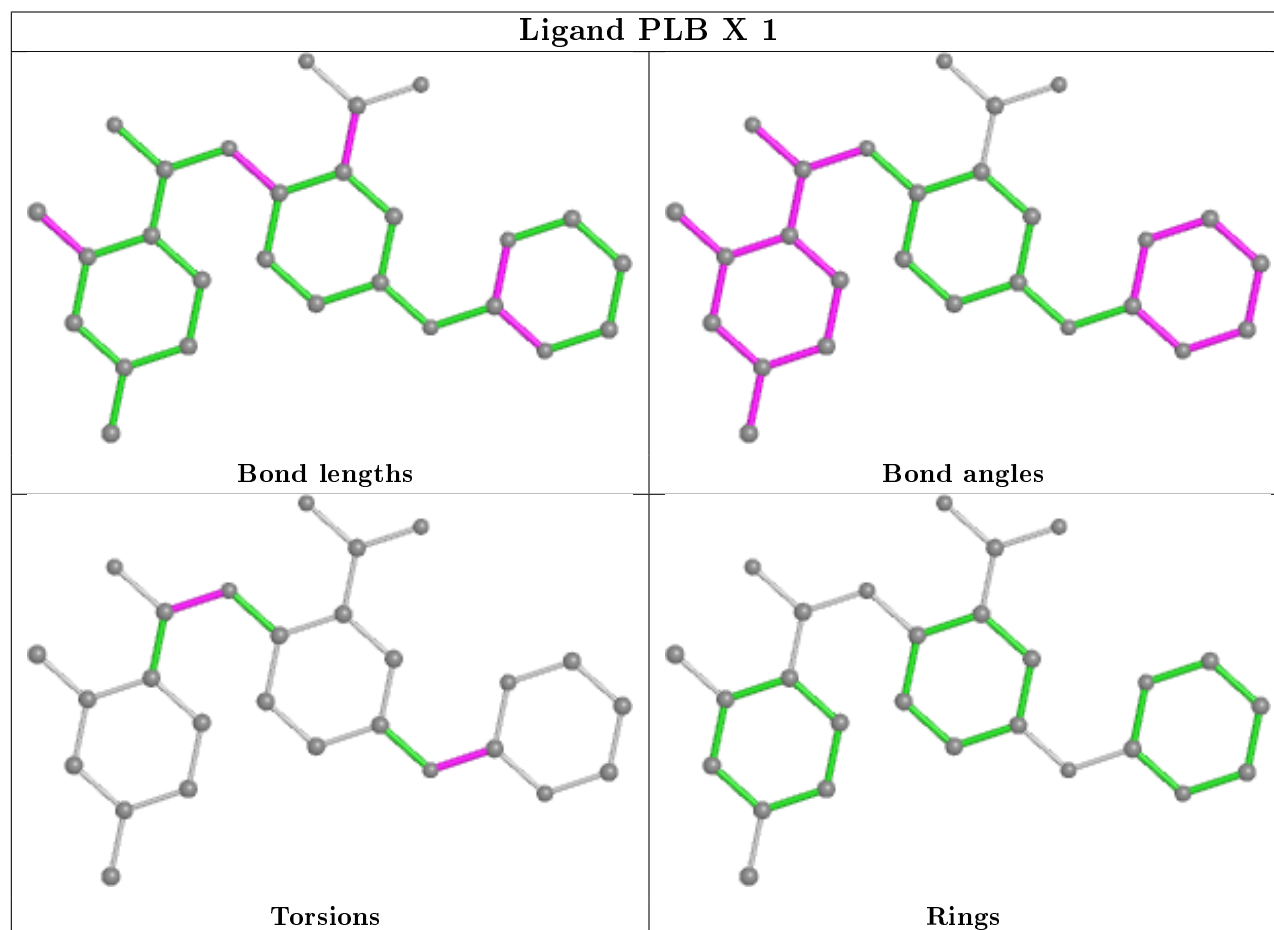
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	1	PLB	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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	272/292 (93%)	-0.64	6 (2%) 62 59	27, 46, 86, 104	0
2	Y	10/14 (71%)	-0.48	0 100 100	40, 52, 57, 62	0
All	All	282/306 (92%)	-0.64	6 (2%) 63 61	27, 46, 85, 104	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	274	SER	3.7
1	X	242	THR	3.1
1	X	200	ILE	3.0
1	X	461	THR	2.6
1	X	462	ASP	2.4
1	X	202	GLY	2.4

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](#)

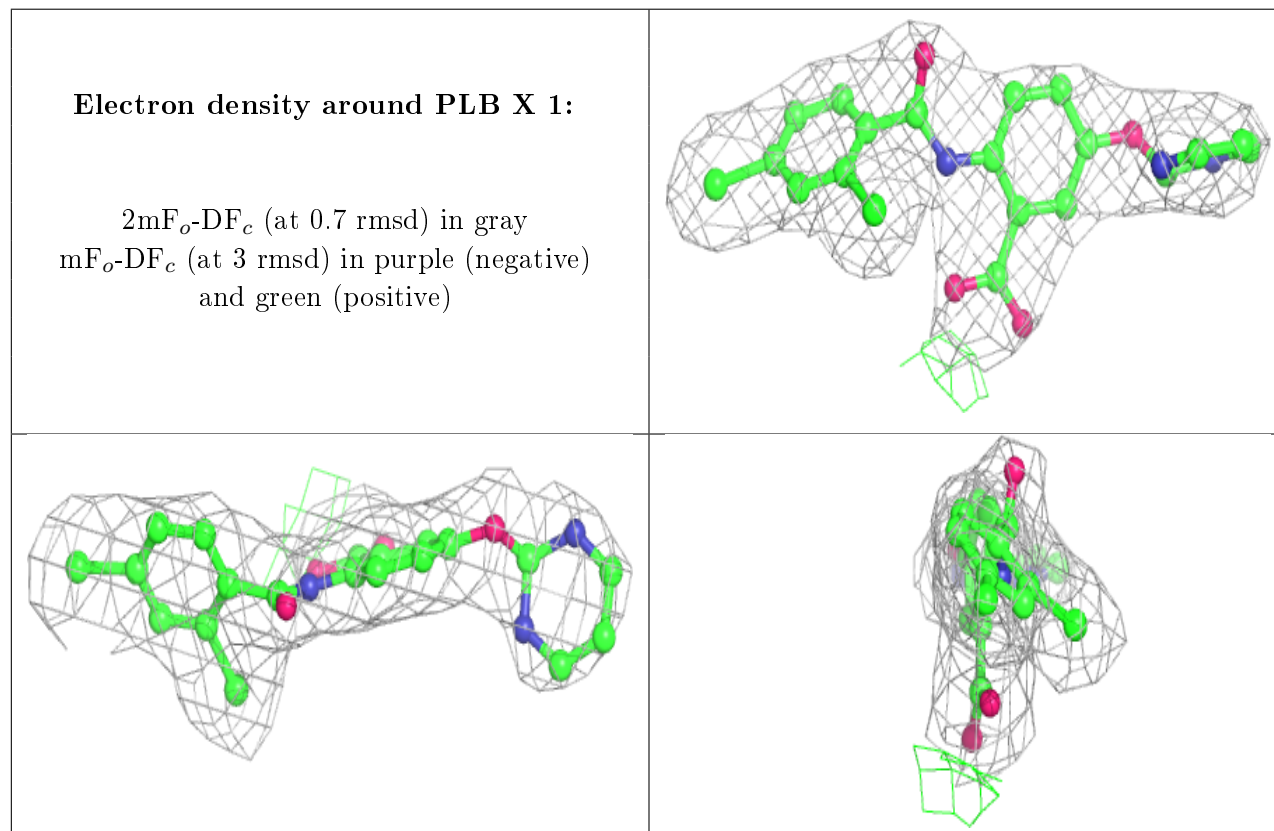
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
3	PLB	X	1	27/27	0.97	0.11	46,52,64,66	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.