



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID : 2F4B / pdb_00002f4b
Title : Crystal structure of the ligand binding domain of human PPAR-gamma in complex with an agonist
Authors : Lu, I.L.; Peng, Y.H.; Mahindroo, N.; Hsieh, H.P.; Wu, S.Y.
Deposited on : 2005-11-23
Resolution : 2.07 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

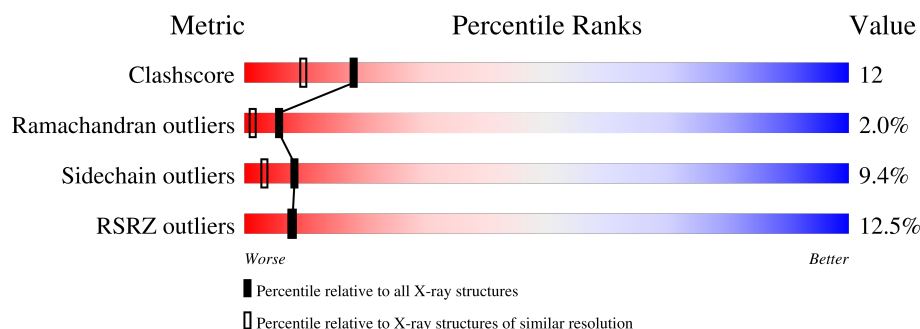
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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.



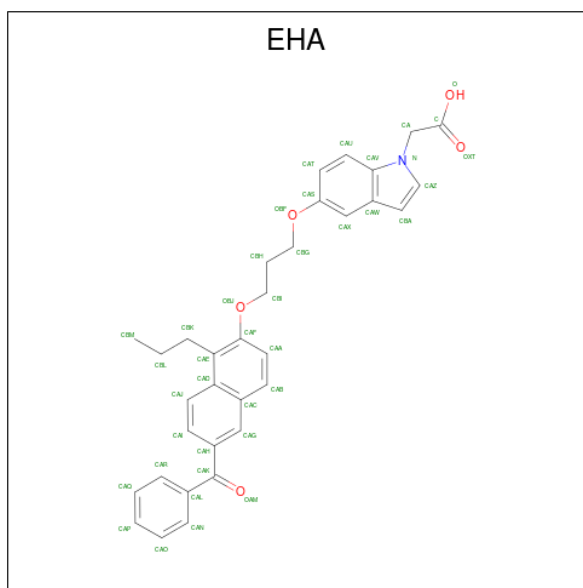
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	271	9% 70% 24% 5%
1	B	271	16% 71% 23% 6%

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 2 is (5-{3-[(6-BENZOYL-1-PROPYL-2-NAPHTHYL)OXY]PROPOXY}-1H-INDOL-1-YL)ACETIC ACID (CCD ID: EHA) (formula: $C_{33}H_{31}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	33	1	5		

- | | | | | | |
|---|---|----|-------|----|---|
| 3 | A | 59 | Total | 0 | 0 |
| | | | 50 | 50 | |

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	59	Total O 59 59	0	0

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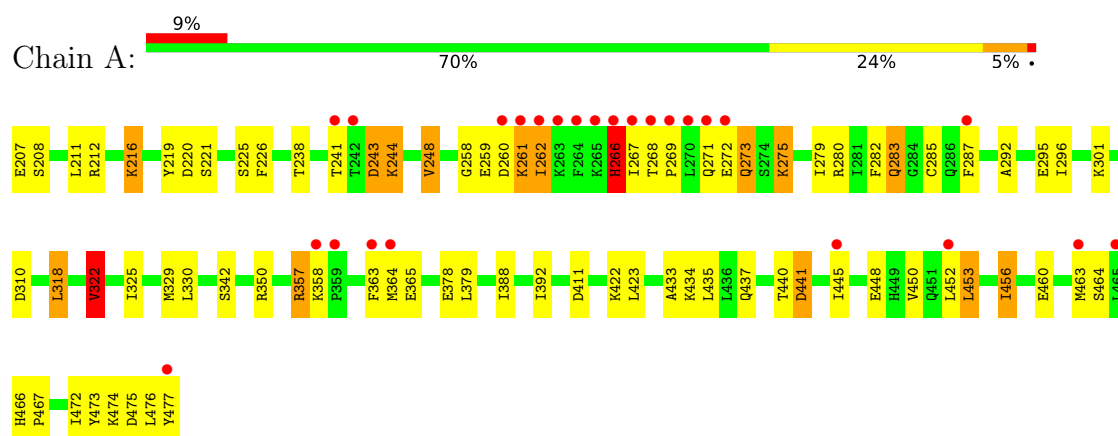
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	81	Total	O	0	0
			81	81		

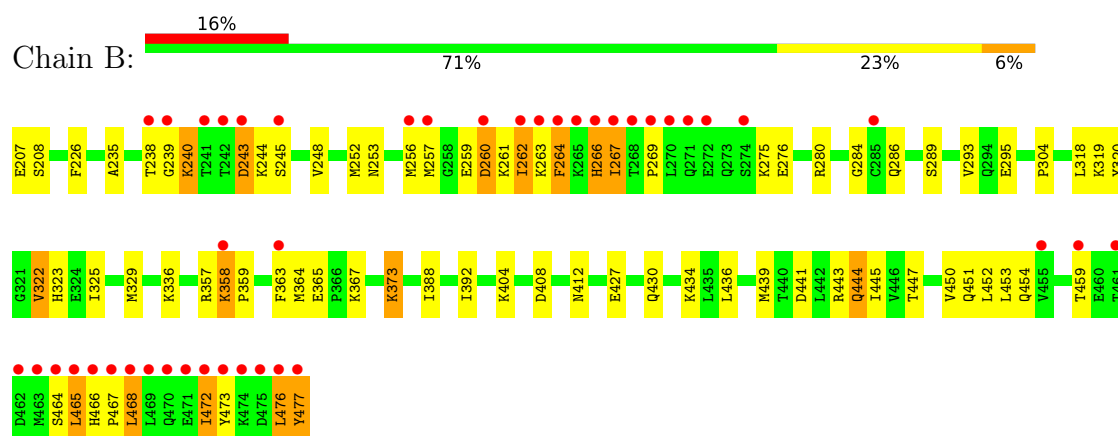
3 Residue-property plots [i](#)

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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.97Å 88.64Å 57.88Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	30.00 – 2.07 30.00 – 2.07	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-2.07) 93.2 (30.00-2.07)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.219 , 0.288 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.034 for h,-k,-l 0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4535	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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: EHA

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	1.21	3/2216 (0.1%)	1.25	9/2985 (0.3%)
1	B	1.23	2/2216 (0.1%)	1.23	12/2985 (0.4%)
All	All	1.22	5/4432 (0.1%)	1.24	21/5970 (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	A	0	2
1	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	THR	C-O	8.68	1.34	1.24
1	A	266	HIS	CE1-NE2	7.59	1.40	1.32
1	A	267	ILE	CA-CB	5.57	1.61	1.54
1	A	266	HIS	CG-CD2	5.29	1.41	1.35
1	B	295	GLU	C-O	-5.13	1.18	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	HIS	CA-C-O	-13.57	106.89	119.91
1	A	266	HIS	O-C-N	-11.57	110.75	123.13
1	A	267	ILE	N-CA-C	7.74	120.64	108.87
1	B	358	LYS	CA-C-N	-7.49	110.74	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	LYS	C-N-CA	-7.49	110.74	119.05
1	A	266	HIS	N-CA-C	6.84	118.94	109.29
1	B	262	ILE	N-CA-C	-6.67	106.29	112.43
1	A	248	VAL	N-CA-C	6.64	118.15	108.58
1	B	365	GLU	CA-C-N	-6.51	112.98	119.56
1	B	365	GLU	C-N-CA	-6.51	112.98	119.56
1	B	459	THR	N-CA-C	6.26	120.93	113.16
1	A	295	GLU	N-CA-C	-5.87	104.80	111.14
1	A	266	HIS	CB-CA-C	-5.86	107.08	114.40
1	B	261	LYS	N-CA-C	-5.81	104.70	113.89
1	A	208	SER	N-CA-C	5.79	118.08	111.02
1	B	445	ILE	CB-CA-C	-5.49	104.86	112.04
1	A	322	VAL	N-CA-CB	-5.45	103.12	110.54
1	B	264	PHE	N-CA-C	-5.39	105.92	112.88
1	B	322	VAL	N-CA-CB	-5.35	103.26	110.54
1	B	358	LYS	N-CA-C	5.21	120.65	113.77
1	B	284	GLY	N-CA-C	-5.09	106.55	113.37

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	HIS	Mainchain
1	A	357	ARG	Peptide
1	B	245	SER	Mainchain

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	2178	0	2241	60	0
1	B	2178	0	2241	50	0
2	A	39	0	30	5	0
3	A	59	0	0	3	0
3	B	81	0	0	11	0
All	All	4535	0	4512	109	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 12.

All (109) 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:444:GLN:HB3	3:B:98:HOH:O	1.47	1.11
1:B:412:ASN:HB3	3:B:3:HOH:O	1.60	1.01
1:A:216:LYS:HZ1	1:A:219:TYR:HD2	0.98	0.95
1:A:275:LYS:HD3	1:A:279:ILE:HG21	1.52	0.90
1:A:243:ASP:HB2	1:A:244:LYS:HG2	1.58	0.84
1:A:216:LYS:NZ	1:A:219:TYR:CD2	2.44	0.83
1:B:243:ASP:CG	1:B:244:LYS:N	2.37	0.83
1:B:256:MET:HG2	3:B:129:HOH:O	1.79	0.81
1:A:216:LYS:NZ	1:A:219:TYR:HD2	1.76	0.81
1:A:330:LEU:HD21	2:A:201:EHA:HBG1	1.63	0.78
1:A:273:GLN:HB3	1:A:280:ARG:CD	2.13	0.77
1:B:243:ASP:OD1	1:B:244:LYS:N	2.19	0.74
1:A:273:GLN:CB	1:A:280:ARG:HD3	2.18	0.73
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.72	0.69
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.73	0.69
1:A:279:ILE:O	1:A:283:GLN:HG3	1.93	0.69
1:A:448:GLU:O	1:A:452:LEU:HD13	1.92	0.68
1:B:259:GLU:OE1	1:B:280:ARG:NH2	2.26	0.68
1:A:422:LYS:HG3	3:A:95:HOH:O	1.93	0.68
1:A:301:LYS:HD2	1:B:468:LEU:HD13	1.76	0.67
1:A:411:ASP:HB2	3:A:77:HOH:O	1.97	0.65
1:B:319:LYS:NZ	1:B:472:ILE:O	2.30	0.64
1:A:325:ILE:HG12	1:A:388:ILE:HG23	1.79	0.64
1:B:235:ALA:HA	1:B:240:LYS:HE3	1.82	0.62
1:A:279:ILE:O	1:A:283:GLN:CG	2.48	0.62
1:B:439:MET:O	1:B:443:ARG:HG3	1.99	0.62
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.31	0.60
1:A:272:GLU:O	1:A:280:ARG:HD2	2.02	0.59
1:A:441:ASP:O	1:A:445:ILE:HG12	2.02	0.59
1:B:364:MET:O	1:B:367:LYS:HB2	2.02	0.59
1:B:319:LYS:HE3	1:B:320:TYR:CZ	2.38	0.58
1:A:273:GLN:HB3	1:A:280:ARG:HD2	1.83	0.58
1:A:330:LEU:CD2	2:A:201:EHA:HBG1	2.31	0.58
1:A:262:ILE:HG23	1:A:266:HIS:HA	1.86	0.58
1:B:286:GLN:HE22	1:B:465:LEU:HB3	1.67	0.58
1:A:287:PHE:CD2	1:A:287:PHE:C	2.82	0.57
1:A:463:MET:HG3	1:A:464:SER:H	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.86	0.56
1:B:260:ASP:O	1:B:264:PHE:HB2	2.06	0.55
1:A:216:LYS:HE3	1:A:216:LYS:O	2.06	0.55
1:B:263:LYS:O	1:B:263:LYS:HD3	2.07	0.54
1:A:273:GLN:CB	1:A:280:ARG:CD	2.79	0.54
1:A:241:THR:OG1	1:A:243:ASP:OD1	2.25	0.54
1:B:430:GLN:O	1:B:434:LYS:HG3	2.08	0.54
1:A:280:ARG:HA	1:A:283:GLN:HG3	1.89	0.54
1:A:261:LYS:O	1:A:262:ILE:C	2.51	0.53
1:A:357:ARG:NH2	1:A:460:GLU:OE1	2.41	0.53
1:B:357:ARG:HG3	1:B:359:PRO:HD2	1.91	0.53
1:A:357:ARG:HH22	1:A:460:GLU:CD	2.16	0.53
1:B:262:ILE:HB	3:B:85:HOH:O	2.08	0.53
1:B:275:LYS:HG3	1:B:276:GLU:H	1.74	0.52
1:B:253:ASN:HA	1:B:256:MET:HE2	1.93	0.51
1:B:427:GLU:HG2	3:B:38:HOH:O	2.09	0.51
1:B:363:PHE:CE2	1:B:364:MET:HG2	2.47	0.50
1:B:404:LYS:HE2	1:B:408:ASP:OD1	2.12	0.50
1:B:450:VAL:HG21	1:B:476:LEU:HD22	1.94	0.50
1:B:263:LYS:HA	1:B:266:HIS:O	2.12	0.50
1:A:259:GLU:C	1:A:261:LYS:H	2.20	0.49
1:B:243:ASP:OD1	1:B:244:LYS:HG2	2.13	0.49
1:A:434:LYS:HA	1:A:437:GLN:HE21	1.78	0.49
1:B:275:LYS:HG3	1:B:276:GLU:N	2.28	0.48
1:A:318:LEU:O	1:A:322:VAL:HB	2.14	0.48
1:A:330:LEU:HD21	2:A:201:EHA:CBG	2.39	0.48
1:B:451:GLN:HG3	1:B:477:TYR:OXT	2.13	0.47
1:B:363:PHE:CE2	1:B:364:MET:HE3	2.50	0.47
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.79	0.47
1:B:451:GLN:O	1:B:454:GLN:HB2	2.14	0.47
1:A:474:LYS:O	1:A:475:ASP:C	2.58	0.46
1:B:434:LYS:HE3	3:B:140:HOH:O	2.16	0.45
1:B:275:LYS:NZ	3:B:88:HOH:O	2.50	0.45
1:A:466:HIS:CG	1:A:467:PRO:HD2	2.52	0.44
1:A:272:GLU:O	1:A:273:GLN:HB3	2.17	0.44
1:B:289:SER:O	1:B:293:VAL:HG23	2.17	0.44
1:B:226:PHE:CG	1:B:329:MET:HE1	2.52	0.44
1:B:466:HIS:HA	1:B:467:PRO:HD3	1.89	0.44
1:A:258:GLY:O	1:A:261:LYS:HB2	2.18	0.44
1:B:467:PRO:HD3	3:B:127:HOH:O	2.16	0.44
1:A:364:MET:SD	2:A:201:EHA:HBH1	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LYS:O	1:B:359:PRO:C	2.59	0.43
1:A:433:ALA:O	1:A:437:GLN:HG3	2.19	0.43
1:A:243:ASP:C	1:A:244:LYS:HG2	2.43	0.43
1:B:235:ALA:HB3	3:B:125:HOH:O	2.18	0.43
3:A:50:HOH:O	1:B:466:HIS:CE1	2.71	0.43
1:A:216:LYS:O	1:A:216:LYS:CE	2.67	0.43
1:A:279:ILE:O	1:A:283:GLN:HG2	2.19	0.43
1:A:350:ARG:NH2	1:A:365:GLU:OE2	2.41	0.43
1:A:259:GLU:C	1:A:261:LYS:N	2.77	0.43
1:A:325:ILE:HG12	1:A:388:ILE:HD12	2.01	0.42
1:A:310:ASP:OD2	1:B:269:PRO:HD2	2.20	0.42
2:A:201:EHA:HAA	2:A:201:EHA:HBI1	1.76	0.42
1:B:373:LYS:HB2	3:B:68:HOH:O	2.19	0.42
1:B:262:ILE:HD12	3:B:72:HOH:O	2.19	0.42
1:A:473:TYR:O	1:A:474:LYS:C	2.63	0.42
1:B:476:LEU:HD23	1:B:477:TYR:H	1.84	0.42
1:A:266:HIS:CD2	1:A:266:HIS:N	2.87	0.42
1:B:266:HIS:HB3	1:B:267:ILE:H	1.59	0.42
1:A:207:GLU:O	1:A:211:LEU:HG	2.20	0.42
1:B:436:LEU:O	1:B:439:MET:HB2	2.20	0.41
1:A:273:GLN:HB2	1:A:280:ARG:HD3	1.99	0.41
1:A:450:VAL:O	1:A:453:LEU:HB2	2.20	0.41
1:B:267:ILE:C	1:B:269:PRO:HD3	2.46	0.41
1:A:212:ARG:HD3	1:A:423:LEU:HD11	2.03	0.41
1:A:226:PHE:CG	1:A:329:MET:HE1	2.55	0.41
1:A:472:ILE:O	1:A:476:LEU:HD13	2.20	0.41
1:B:319:LYS:HG3	1:B:472:ILE:HG23	2.02	0.41
1:A:282:PHE:O	1:A:285:CYS:HB2	2.21	0.41
1:A:325:ILE:HG23	1:A:388:ILE:HD12	2.03	0.40
1:A:292:ALA:O	1:A:296:ILE:HG13	2.22	0.40
1:B:444:GLN:HA	1:B:447:THR:OG1	2.22	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	269/271 (99%)	249 (93%)	13 (5%)	7 (3%)	4	0
1	B	269/271 (99%)	254 (94%)	11 (4%)	4 (2%)	8	2
All	All	538/542 (99%)	503 (94%)	24 (4%)	11 (2%)	6	1

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ILE
1	B	266	HIS
1	A	260	ASP
1	B	473	TYR
1	A	271	GLN
1	B	239	GLY
1	A	358	LYS
1	B	243	ASP
1	A	244	LYS
1	A	269	PRO
1	A	273	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/244 (100%)	223 (91%)	21 (9%)	10	4
1	B	244/244 (100%)	219 (90%)	25 (10%)	7	2
All	All	488/488 (100%)	442 (91%)	46 (9%)	8	3

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	220	ASP

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Mol	Chain	Res	Type
1	A	221	SER
1	A	225	SER
1	A	238	THR
1	A	243	ASP
1	A	248	VAL
1	A	261	LYS
1	A	266	HIS
1	A	268	THR
1	A	275	LYS
1	A	283	GLN
1	A	318	LEU
1	A	322	VAL
1	A	342	SER
1	A	378	GLU
1	A	440	THR
1	A	441	ASP
1	A	453	LEU
1	A	456	ILE
1	A	477	TYR
1	B	207	GLU
1	B	208	SER
1	B	240	LYS
1	B	248	VAL
1	B	252	MET
1	B	257	MET
1	B	260	ASP
1	B	267	ILE
1	B	304	PRO
1	B	318	LEU
1	B	322	VAL
1	B	323	HIS
1	B	336	LYS
1	B	373	LYS
1	B	388	ILE
1	B	441	ASP
1	B	444	GLN
1	B	452	LEU
1	B	453	LEU
1	B	464	SER
1	B	465	LEU
1	B	468	LEU
1	B	472	ILE

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Mol	Chain	Res	Type
1	B	476	LEU
1	B	477	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	271	GLN
1	A	294	GLN
1	A	437	GLN
1	A	451	GLN
1	B	273	GLN
1	B	283	GLN
1	B	286	GLN
1	B	323	HIS
1	B	466	HIS
1	B	470	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](#)

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	$\# Z > 2$
2	EHA	A	201	-	43,43,43	1.47	6 (13%)	59,59,59	0.97	3 (5%)

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	EHA	A	201	-	-	13/23/23/23	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	EHA	CAL-CAK	4.39	1.56	1.49
2	A	201	EHA	CAW-CBA	-3.55	1.33	1.43
2	A	201	EHA	CAH-CAK	3.53	1.55	1.49
2	A	201	EHA	CAV-N	-2.76	1.34	1.39
2	A	201	EHA	CAF-CAE	2.23	1.41	1.38
2	A	201	EHA	CBK-CAE	2.19	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	EHA	CAU-CAV-N	2.39	134.85	131.50
2	A	201	EHA	OBF-CBG-CBH	2.37	117.04	108.30
2	A	201	EHA	CAW-CAV-N	-2.14	105.50	107.62

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	EHA	OXT-C-CA-N
2	A	201	EHA	O-C-CA-N
2	A	201	EHA	OAM-CAK-CAL-CAN
2	A	201	EHA	OAM-CAK-CAL-CAR
2	A	201	EHA	CAH-CAK-CAL-CAN
2	A	201	EHA	CAH-CAK-CAL-CAR
2	A	201	EHA	CAX-CAS-OBF-CBG

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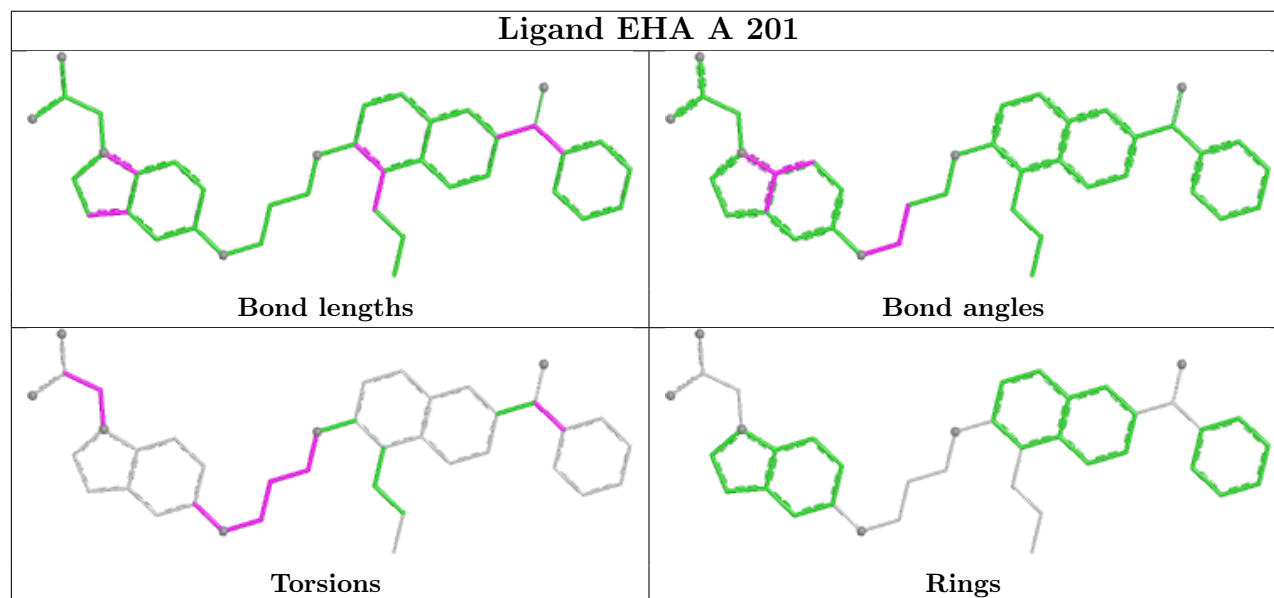
Mol	Chain	Res	Type	Atoms
2	A	201	EHA	CAT-CAS-OBF-CBG
2	A	201	EHA	CBG-CBH-CBI-OBJ
2	A	201	EHA	CBH-CBG-OBF-CAS
2	A	201	EHA	CBH-CBI-OBJ-CAF
2	A	201	EHA	C-CA-N-CAZ
2	A	201	EHA	OBF-CBG-CBH-CBI

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	EHA	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.



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

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	271/271 (100%)	0.53	25 (9%)	14 15	17, 33, 69, 99	0
1	B	271/271 (100%)	0.83	43 (15%)	5 5	15, 31, 99, 130	0
All	All	542/542 (100%)	0.68	68 (12%)	8 8	15, 32, 94, 130	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	LEU	9.1
1	B	262	ILE	8.6
1	B	477	TYR	8.1
1	B	476	LEU	7.0
1	B	467	PRO	6.6
1	A	262	ILE	6.6
1	B	472	ILE	6.5
1	B	270	LEU	6.4
1	A	359	PRO	6.4
1	A	270	LEU	6.3
1	B	473	TYR	6.1
1	B	468	LEU	5.6
1	A	267	ILE	5.6
1	B	469	LEU	5.4
1	A	264	PHE	5.4
1	B	269	PRO	5.3
1	B	264	PHE	5.1
1	B	241	THR	5.0
1	B	274	SER	4.4
1	B	463	MET	4.0
1	B	466	HIS	3.9
1	B	266	HIS	3.8
1	B	243	ASP	3.8
1	B	265	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	470	GLN	3.8
1	A	268	THR	3.7
1	A	269	PRO	3.7
1	B	268	THR	3.7
1	A	263	LYS	3.6
1	A	477	TYR	3.3
1	B	260	ASP	3.3
1	B	257	MET	3.2
1	B	267	ILE	3.2
1	A	242	THR	3.0
1	B	263	LYS	3.0
1	B	455	VAL	2.9
1	B	271	GLN	2.9
1	A	272	GLU	2.8
1	B	471	GLU	2.8
1	B	363	PHE	2.7
1	B	285	CYS	2.7
1	B	239	GLY	2.7
1	A	465	LEU	2.6
1	B	272	GLU	2.6
1	A	364	MET	2.6
1	B	242	THR	2.6
1	A	452	LEU	2.6
1	A	271	GLN	2.5
1	B	256	MET	2.5
1	B	475	ASP	2.5
1	A	363	PHE	2.5
1	B	245	SER	2.4
1	B	459	THR	2.4
1	A	261	LYS	2.3
1	B	474	LYS	2.3
1	A	287	PHE	2.3
1	A	241	THR	2.3
1	A	265	LYS	2.3
1	B	461	THR	2.2
1	B	238	THR	2.2
1	B	358	LYS	2.1
1	A	260	ASP	2.1
1	B	462	ASP	2.1
1	A	445	ILE	2.1
1	A	266	HIS	2.1
1	B	464	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	463	MET	2.0
1	A	358	LYS	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](#)

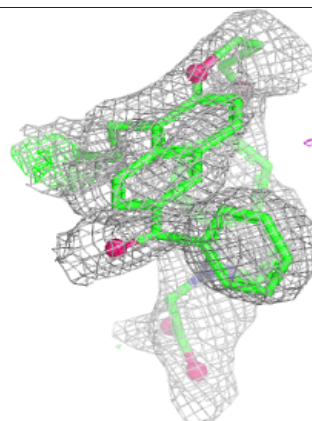
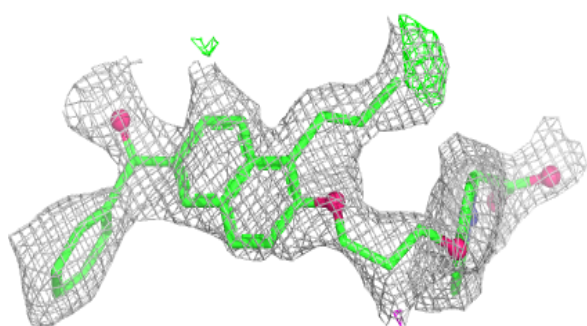
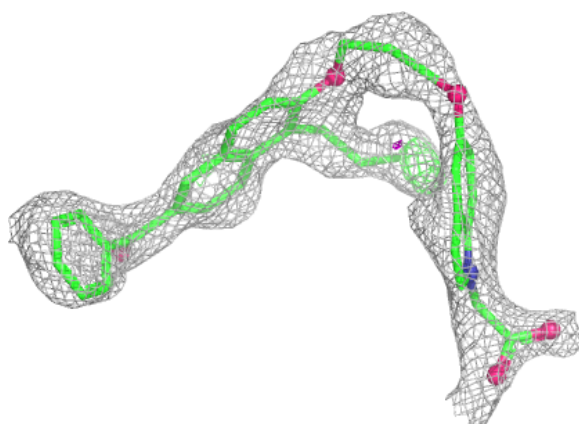
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	EHA	A	201	39/39	0.71	0.17	58,62,64,64	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 EHA A 201:

$2mF_o-DF_c$ (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.