



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:15 PM UTC

PDB ID : 3GBK / pdb_00003gbk
Title : Crystal Structure of Human PPAR-gamma Ligand Binding Domain Complexed with a Potent and Selective Agonist
Authors : Peng, Y.-H.; Lin, C.-H.; Hsieh, H.-P.; Wu, S.-Y.
Deposited on : 2009-02-19
Resolution : 2.30 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

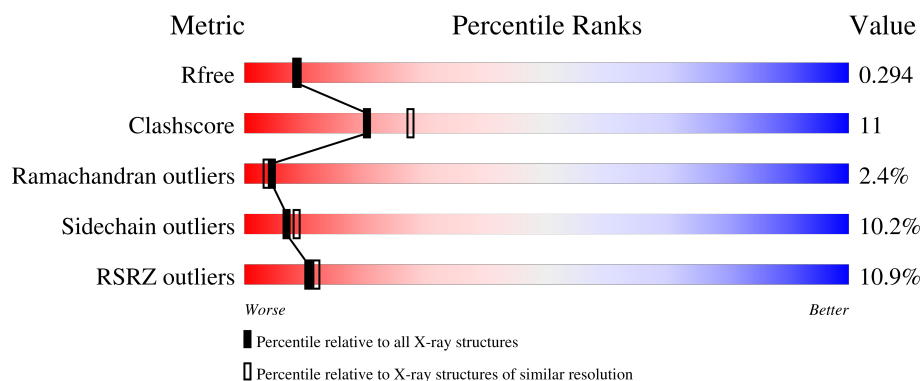
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



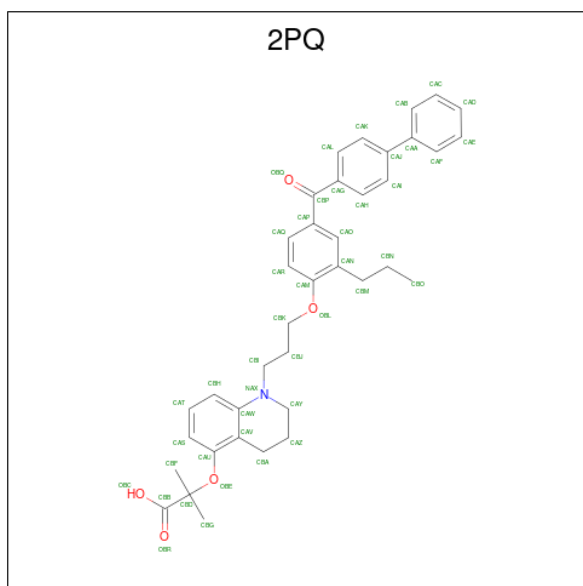
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	7% 75% 18% 7%
1	B	271	14% 69% 24% 5%

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 2-[(1-{3-[4-(biphenyl-4-ylcarbonyl)-2-propylphenoxy]propyl}-1,2,3,4-tetrahydroquinolin-5-yl)oxy]-2-methylpropanoic acid (CCD ID: 2PQ) (formula: $C_{38}H_{41}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	38	1	5		

- | | | |
|---|---|----|
| 3 | A | 34 |
|---|---|----|

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0

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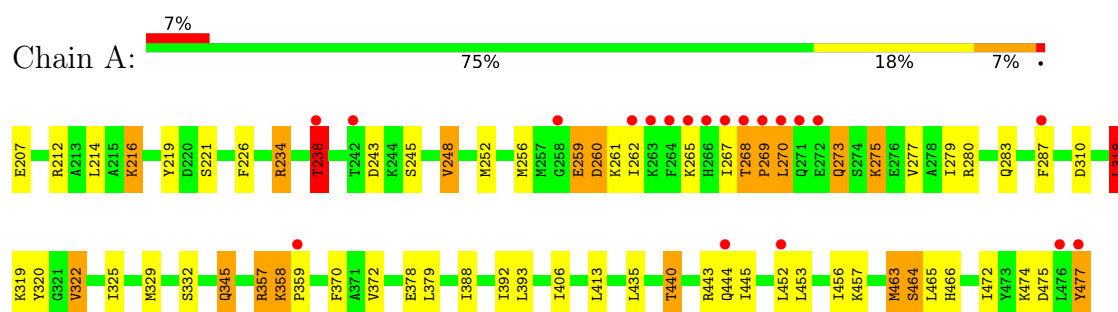
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	39	Total	O	0	0
			39	39		

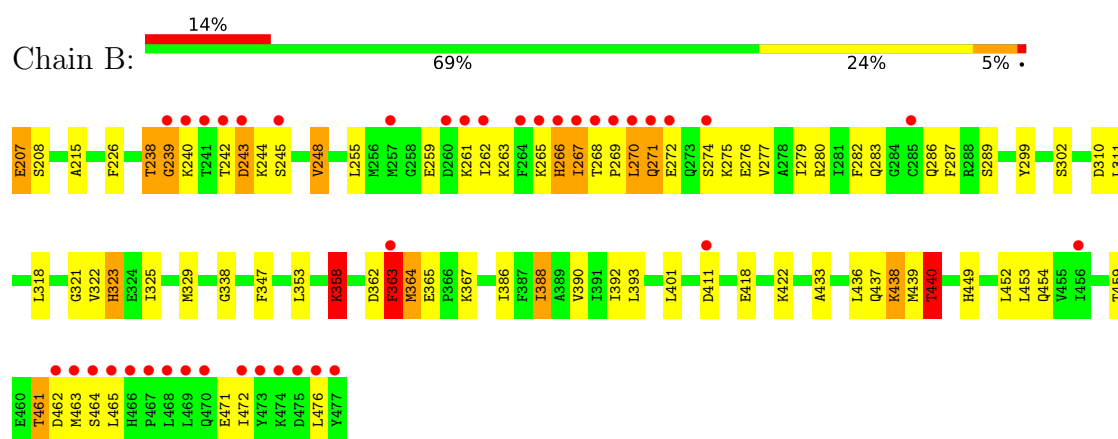
3 Residue-property plots [i](#)

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	56.50Å 88.89Å 58.37Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	26.12 – 2.30 26.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (26.12-2.30) 98.1 (26.12-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.32 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.298 0.229 , 0.294	Depositor DCC
R_{free} test set	1279 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for l,k,-h 0.034 for h,-k,-l 0.026 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4473	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: 2PQ

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	1.17	3/2216 (0.1%)	1.23	12/2985 (0.4%)
1	B	1.20	1/2216 (0.0%)	1.29	13/2985 (0.4%)
All	All	1.19	4/4432 (0.1%)	1.26	25/5970 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	VAL	CA-CB	6.51	1.61	1.54
1	A	318	LEU	CB-CG	-6.10	1.41	1.53
1	B	440	THR	CA-CB	5.47	1.62	1.53
1	A	318	LEU	CA-CB	-5.03	1.45	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	SER	N-CA-C	7.26	118.50	109.57
1	A	318	LEU	CD1-CG-CD2	7.24	126.73	110.80
1	B	268	THR	CA-C-N	-6.81	113.49	120.85
1	B	268	THR	C-N-CA	-6.81	113.49	120.85
1	A	268	THR	CA-C-N	6.20	127.59	119.84
1	A	268	THR	C-N-CA	6.20	127.59	119.84
1	A	466	HIS	CA-C-N	6.10	127.46	119.84
1	A	466	HIS	C-N-CA	6.10	127.46	119.84
1	A	245	SER	N-CA-C	6.07	118.43	109.50
1	B	248	VAL	CB-CA-C	6.06	118.43	110.91
1	A	275	LYS	N-CA-C	5.93	115.84	108.19
1	B	459	THR	N-CA-C	5.84	120.56	113.38
1	B	363	PHE	N-CA-C	5.66	117.25	111.14
1	A	248	VAL	N-CA-C	5.62	116.67	108.58
1	A	273	GLN	N-CA-C	5.44	117.26	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	LYS	CA-C-N	-5.29	113.22	119.84
1	B	358	LYS	C-N-CA	-5.29	113.22	119.84
1	B	261	LYS	N-CA-C	-5.27	106.91	113.55
1	A	277	VAL	N-CA-C	5.24	115.86	110.36
1	B	248	VAL	N-CA-C	5.23	116.11	108.58
1	A	406	ILE	N-CA-C	5.21	115.42	110.42
1	B	243	ASP	N-CA-C	5.15	120.03	113.18
1	B	323	HIS	CA-C-N	5.11	127.13	120.28
1	B	323	HIS	C-N-CA	5.11	127.13	120.28
1	A	238	THR	CB-CA-C	5.04	117.54	109.07

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	2178	0	2241	48	0
1	B	2178	0	2241	54	0
2	A	44	0	40	5	0
3	A	34	0	0	7	0
3	B	39	0	0	6	0
All	All	4473	0	4522	101	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 11.

All (101) 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:207:GLU:HG3	3:B:38:HOH:O	1.50	1.09
1:B:270:LEU:HB2	3:B:56:HOH:O	1.55	1.05
1:A:345:GLN:HG3	3:A:22:HOH:O	1.62	1.00
1:A:440:THR:O	1:A:444:GLN:HG3	1.75	0.87
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLN:HB3	3:A:51:HOH:O	1.81	0.80
1:A:269:PRO:HB2	1:A:287:PHE:CZ	2.20	0.77
1:A:444:GLN:CB	3:A:51:HOH:O	2.34	0.76
1:A:477:TYR:O	1:A:477:TYR:CD1	2.38	0.76
1:A:259:GLU:OE2	1:A:280:ARG:NH2	2.20	0.74
1:B:461:THR:HA	3:B:58:HOH:O	1.88	0.73
1:A:463:MET:HG3	1:A:464:SER:H	1.55	0.72
1:A:279:ILE:O	1:A:283:GLN:HG3	1.91	0.70
1:B:275:LYS:HG3	1:B:276:GLU:H	1.57	0.69
1:A:234:ARG:O	1:A:238:THR:HB	1.94	0.68
1:B:270:LEU:HD23	1:B:287:PHE:CD2	2.31	0.65
1:A:256:MET:O	1:A:260:ASP:HB2	1.96	0.64
1:A:268:THR:O	1:A:270:LEU:N	2.31	0.63
1:A:269:PRO:HB2	1:A:287:PHE:HZ	1.64	0.61
1:A:259:GLU:CD	2:A:1385:2PQ:HAD	2.27	0.59
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.36	0.59
1:A:310:ASP:OD2	1:B:269:PRO:HD2	2.03	0.59
1:B:321:GLY:O	1:B:325:ILE:HD12	2.02	0.58
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.86	0.58
1:B:259:GLU:HG3	1:B:280:ARG:HH22	1.68	0.58
1:B:353:LEU:HD22	1:B:364:MET:HG2	1.86	0.57
1:B:363:PHE:CE1	1:B:449:HIS:CE1	2.91	0.57
1:B:270:LEU:O	1:B:271:GLN:HB2	2.03	0.57
1:B:363:PHE:CZ	1:B:452:LEU:HB3	2.38	0.57
1:B:358:LYS:O	1:B:362:ASP:OD2	2.23	0.57
1:B:438:LYS:HE3	3:B:65:HOH:O	2.04	0.57
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.87	0.56
1:B:226:PHE:CG	1:B:329:MET:HE1	2.39	0.56
1:B:270:LEU:CB	3:B:56:HOH:O	2.29	0.56
1:A:474:LYS:HE2	1:A:475:ASP:OD2	2.05	0.55
1:A:477:TYR:O	1:A:477:TYR:HD1	1.86	0.55
1:B:275:LYS:HE3	1:B:462:ASP:HB2	1.87	0.55
1:B:437:GLN:O	1:B:440:THR:HG23	2.07	0.54
1:B:226:PHE:CD1	1:B:329:MET:HE1	2.43	0.54
1:B:279:ILE:O	1:B:283:GLN:HG3	2.07	0.54
1:A:216:LYS:CE	3:A:61:HOH:O	2.56	0.53
1:A:259:GLU:C	1:A:261:LYS:H	2.17	0.53
1:A:322:VAL:HG11	1:A:472:ILE:HD13	1.90	0.53
1:B:263:LYS:O	1:B:263:LYS:HD3	2.09	0.52
1:B:364:MET:O	1:B:367:LYS:HB2	2.10	0.51
1:A:392:ILE:HG22	1:A:393:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:HG2	2:A:1385:2PQ:HAD	1.91	0.50
1:A:357:ARG:HH11	1:A:357:ARG:HB2	1.75	0.50
1:A:275:LYS:HG2	1:A:279:ILE:HG21	1.94	0.50
1:A:318:LEU:O	1:A:322:VAL:HB	2.11	0.50
1:A:216:LYS:HE3	3:A:61:HOH:O	2.12	0.50
1:B:242:THR:O	1:B:242:THR:HG23	2.12	0.50
1:B:310:ASP:OD2	1:B:401:LEU:HD12	2.12	0.50
1:B:271:GLN:HG2	1:B:272:GLU:H	1.77	0.49
1:A:259:GLU:O	1:A:261:LYS:N	2.46	0.48
1:A:319:LYS:NZ	1:A:474:LYS:O	2.34	0.48
1:A:457:LYS:HG2	1:A:463:MET:SD	2.53	0.48
1:B:275:LYS:HG3	1:B:276:GLU:N	2.25	0.47
1:B:238:THR:HB	1:B:239:GLY:H	1.25	0.47
1:A:329:MET:O	1:A:332:SER:HB2	2.14	0.46
1:B:392:ILE:HG22	1:B:393:LEU:HD22	1.97	0.46
1:A:259:GLU:C	1:A:261:LYS:N	2.73	0.46
1:A:259:GLU:CG	2:A:1385:2PQ:HAD	2.46	0.46
2:A:1385:2PQ:HBJ	2:A:1385:2PQ:HAY	1.71	0.45
1:B:259:GLU:CG	1:B:280:ARG:HH22	2.29	0.45
1:B:436:LEU:O	1:B:439:MET:HB2	2.16	0.45
1:B:390:VAL:HG12	1:B:439:MET:HE1	1.97	0.45
1:B:364:MET:HE2	1:B:365:GLU:H	1.82	0.45
1:B:418:GLU:HG2	1:B:422:LYS:HE2	1.99	0.45
1:B:255:LEU:CD2	1:B:277:VAL:CG1	2.95	0.44
1:A:310:ASP:OD2	1:B:269:PRO:CD	2.64	0.44
2:A:1385:2PQ:HBM	2:A:1385:2PQ:HBI	1.98	0.44
1:B:433:ALA:O	1:B:437:GLN:HG3	2.18	0.44
1:B:438:LYS:HA	1:B:438:LYS:HD2	1.71	0.44
1:B:325:ILE:HD11	1:B:392:ILE:HG13	2.00	0.44
1:B:463:MET:SD	1:B:465:LEU:HD13	2.57	0.44
1:B:255:LEU:CD2	1:B:277:VAL:HG13	2.48	0.44
1:A:310:ASP:CG	1:B:269:PRO:HD2	2.44	0.43
1:A:219:TYR:CD2	3:A:61:HOH:O	2.57	0.43
1:B:276:GLU:O	1:B:280:ARG:HG3	2.19	0.43
1:B:363:PHE:HE1	1:B:449:HIS:CE1	2.36	0.43
1:A:275:LYS:HB2	3:A:45:HOH:O	2.18	0.42
1:B:270:LEU:HD12	3:B:17:HOH:O	2.18	0.42
1:B:259:GLU:CD	1:B:280:ARG:HH22	2.27	0.42
1:A:320:TYR:HE2	1:A:477:TYR:H	1.68	0.42
1:A:214:LEU:HD21	1:A:413:LEU:HD23	2.01	0.42
1:A:226:PHE:CG	1:A:329:MET:HE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASP:CG	1:B:244:LYS:HG2	2.45	0.42
1:B:255:LEU:HD21	1:B:277:VAL:HG13	2.02	0.42
1:A:358:LYS:HB3	1:A:359:PRO:HD3	2.03	0.41
1:B:282:PHE:O	1:B:286:GLN:HG3	2.21	0.41
1:B:299:TYR:O	1:B:302:SER:OG	2.35	0.41
1:B:388:ILE:HD13	1:B:388:ILE:HA	1.84	0.41
1:A:379:LEU:HD11	1:A:435:LEU:HD13	2.03	0.41
1:B:215:ALA:CB	1:B:386:ILE:HD11	2.51	0.41
1:A:212:ARG:HD2	1:A:212:ARG:HA	1.83	0.41
1:A:463:MET:HG3	1:A:464:SER:N	2.29	0.41
1:A:477:TYR:CD1	1:A:477:TYR:C	2.97	0.40
1:B:265:LYS:HG3	1:B:266:HIS:H	1.86	0.40
1:B:362:ASP:OD1	1:B:452:LEU:HD21	2.22	0.40
1:A:345:GLN:HE21	1:A:345:GLN:HA	1.86	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%)	248 (92%)	14 (5%)	7 (3%)	4	3
1	B	269/271 (99%)	243 (90%)	20 (7%)	6 (2%)	5	4
All	All	538/542 (99%)	491 (91%)	34 (6%)	13 (2%)	4	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	ASP
1	A	269	PRO
1	A	464	SER
1	B	464	SER

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Mol	Chain	Res	Type
1	A	358	LYS
1	B	267	ILE
1	B	271	GLN
1	A	243	ASP
1	B	274	SER
1	B	266	HIS
1	A	262	ILE
1	B	239	GLY
1	A	267	ILE

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%)	220 (90%)	24 (10%)	7	10
1	B	244/244 (100%)	218 (89%)	26 (11%)	6	8
All	All	488/488 (100%)	438 (90%)	50 (10%)	7	8

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	216	LYS
1	A	221	SER
1	A	234	ARG
1	A	238	THR
1	A	248	VAL
1	A	252	MET
1	A	259	GLU
1	A	265	LYS
1	A	270	LEU
1	A	273	GLN
1	A	318	LEU
1	A	322	VAL
1	A	345	GLN

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Mol	Chain	Res	Type
1	A	357	ARG
1	A	378	GLU
1	A	440	THR
1	A	443	ARG
1	A	452	LEU
1	A	453	LEU
1	A	456	ILE
1	A	463	MET
1	A	465	LEU
1	A	477	TYR
1	B	207	GLU
1	B	208	SER
1	B	238	THR
1	B	240	LYS
1	B	248	VAL
1	B	262	ILE
1	B	267	ILE
1	B	270	LEU
1	B	289	SER
1	B	311	LEU
1	B	318	LEU
1	B	322	VAL
1	B	323	HIS
1	B	358	LYS
1	B	363	PHE
1	B	364	MET
1	B	388	ILE
1	B	411	ASP
1	B	438	LYS
1	B	440	THR
1	B	453	LEU
1	B	454	GLN
1	B	461	THR
1	B	471	GLU
1	B	472	ILE
1	B	476	LEU

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	294	GLN
1	A	345	GLN

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Mol	Chain	Res	Type
1	A	412	ASN
1	A	451	GLN
1	B	253	ASN
1	B	271	GLN
1	B	273	GLN
1	B	412	ASN
1	B	454	GLN
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	2PQ	A	1385	-	48,48,48	1.19	3 (6%)	65,67,67	1.23	9 (13%)

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	2PQ	A	1385	-	-	15/33/43/43	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1385	2PQ	CAJ-CAA	-4.19	1.39	1.49
2	A	1385	2PQ	CBA-CAV	2.22	1.55	1.51
2	A	1385	2PQ	CAP-CBP	2.19	1.53	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1385	2PQ	CBK-OBL-CAM	3.42	125.94	117.69
2	A	1385	2PQ	CBD-OBE-CAU	3.32	128.89	121.65
2	A	1385	2PQ	CAK-CAL-CAG	-2.64	117.98	120.80
2	A	1385	2PQ	CAH-CAI-CAJ	-2.45	117.98	121.12
2	A	1385	2PQ	CAH-CAG-CAL	2.42	121.64	118.57
2	A	1385	2PQ	CAI-CAJ-CAK	2.41	122.00	117.68
2	A	1385	2PQ	CAF-CAA-CAB	2.21	121.63	117.68
2	A	1385	2PQ	CAV-CAW-NAX	-2.20	119.91	122.07
2	A	1385	2PQ	CAE-CAF-CAA	-2.03	118.23	120.54

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1385	2PQ	NAX-CBI-CBJ-CBK
2	A	1385	2PQ	CBJ-CBI-NAX-CAY
2	A	1385	2PQ	CBI-CBJ-CBK-OBL
2	A	1385	2PQ	OBR-CBB-CBD-CBF
2	A	1385	2PQ	CBJ-CBI-NAX-CAW
2	A	1385	2PQ	CAO-CAN-CBM-CBN
2	A	1385	2PQ	OBC-CBB-CBD-CBF
2	A	1385	2PQ	CAM-CAN-CBM-CBN
2	A	1385	2PQ	CAF-CAA-CAJ-CAK
2	A	1385	2PQ	CBJ-CBK-OBL-CAM
2	A	1385	2PQ	OBR-CBB-CBD-OBE
2	A	1385	2PQ	OBC-CBB-CBD-OBE
2	A	1385	2PQ	CAB-CAA-CAJ-CAI

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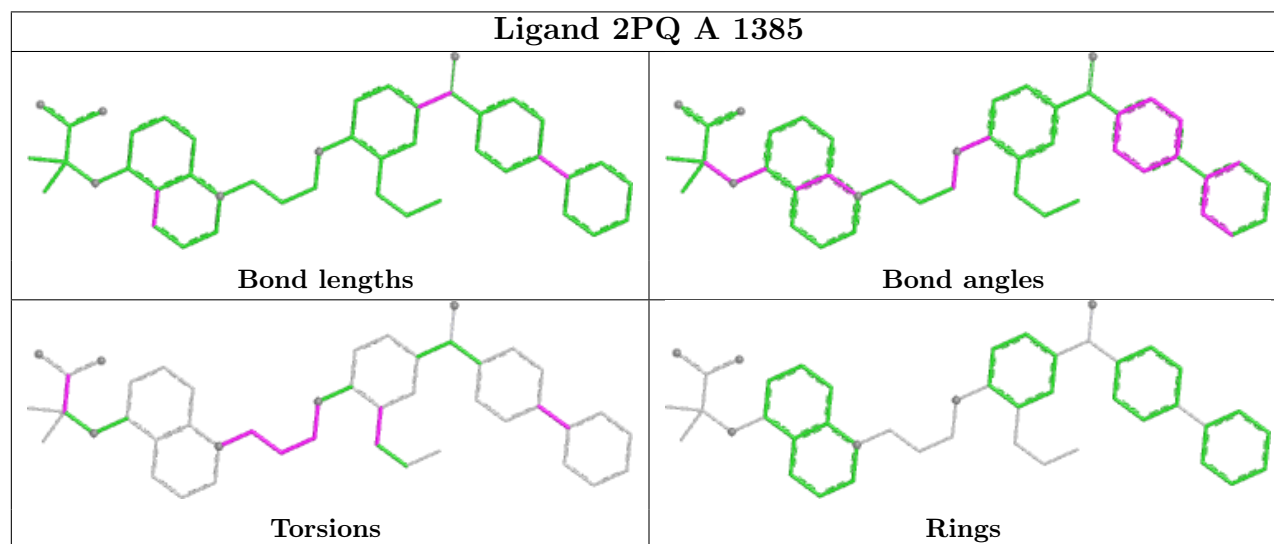
Mol	Chain	Res	Type	Atoms
2	A	1385	2PQ	CAB-CAA-CAJ-CAK
2	A	1385	2PQ	CAF-CAA-CAJ-CAI

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1385	2PQ	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 ⓘ

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	271/271 (100%)	0.37	20 (7%) 20 22	22, 36, 77, 101	0
1	B	271/271 (100%)	0.77	39 (14%) 6 7	20, 36, 97, 121	0
All	All	542/542 (100%)	0.57	59 (10%) 10 12	20, 36, 92, 121	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	ILE	8.8
1	B	477	TYR	7.9
1	B	476	LEU	7.6
1	B	475	ASP	6.5
1	B	467	PRO	6.4
1	A	270	LEU	6.0
1	B	465	LEU	5.8
1	B	472	ILE	5.6
1	B	468	LEU	5.2
1	B	363	PHE	5.2
1	B	469	LEU	5.0
1	B	270	LEU	4.9
1	B	269	PRO	4.8
1	A	268	THR	4.5
1	A	477	TYR	4.3
1	A	262	ILE	4.0
1	A	267	ILE	3.9
1	B	240	LYS	3.8
1	B	241	THR	3.7
1	B	267	ILE	3.6
1	B	268	THR	3.6
1	B	473	TYR	3.6
1	A	265	LYS	3.6
1	B	274	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	272	GLU	3.4
1	B	264	PHE	3.4
1	B	466	HIS	3.3
1	B	260	ASP	3.3
1	A	238	THR	3.3
1	A	287	PHE	3.3
1	B	242	THR	3.3
1	A	271	GLN	3.3
1	B	272	GLU	3.2
1	A	264	PHE	3.2
1	B	411	ASP	3.1
1	B	271	GLN	3.1
1	B	265	LYS	3.0
1	B	239	GLY	3.0
1	B	243	ASP	3.0
1	A	452	LEU	2.9
1	B	462	ASP	2.9
1	B	463	MET	2.8
1	A	476	LEU	2.7
1	B	266	HIS	2.7
1	B	245	SER	2.7
1	A	269	PRO	2.7
1	A	359	PRO	2.7
1	A	263	LYS	2.6
1	B	470	GLN	2.5
1	B	261	LYS	2.4
1	B	474	LYS	2.4
1	B	257	MET	2.4
1	B	464	SER	2.4
1	B	456	ILE	2.3
1	A	266	HIS	2.3
1	A	242	THR	2.1
1	B	285	CYS	2.1
1	A	444	GLN	2.0
1	A	258	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

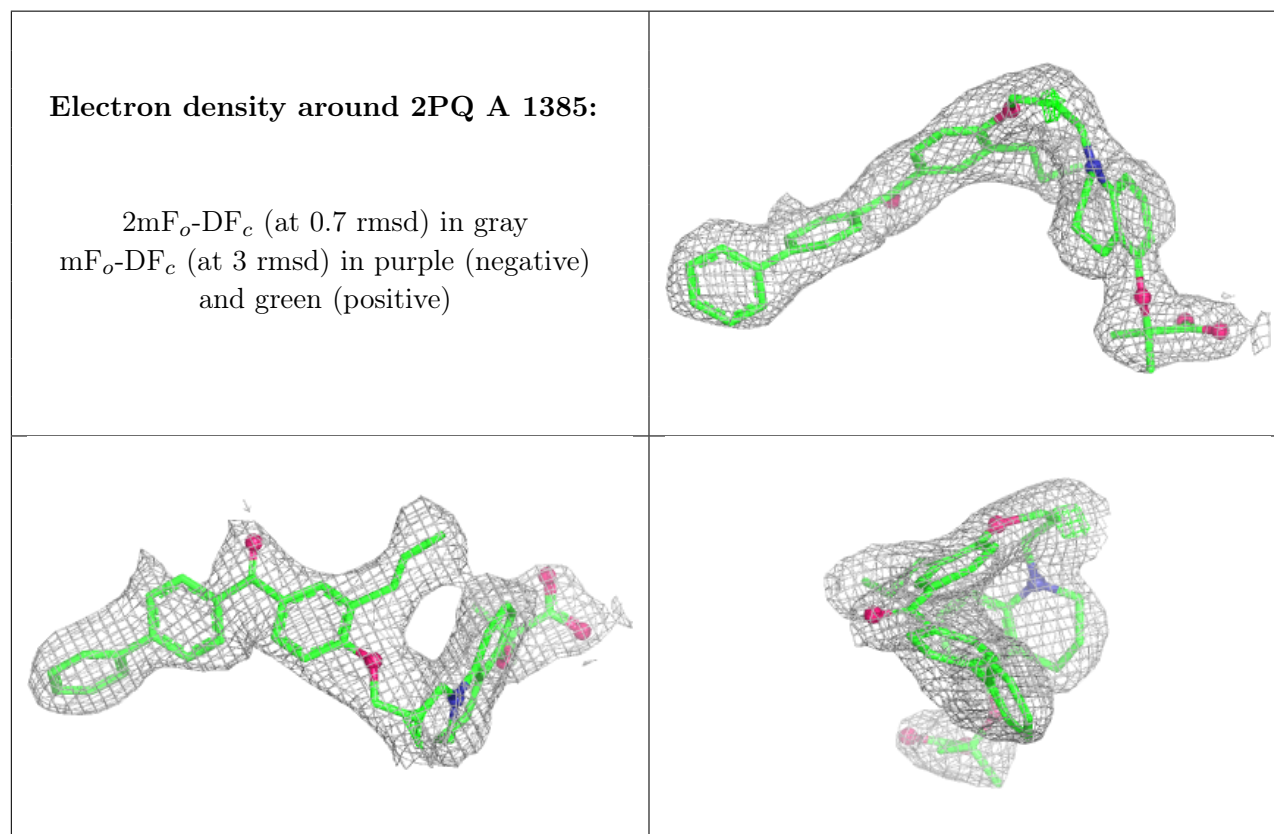
There are no oligosaccharides in this entry.

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	2PQ	A	1385	44/44	0.85	0.11	39,48,59,60	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 [i](#)

There are no such residues in this entry.