



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:07 PM UTC

PDB ID : 1Y0S / pdb_00001y0s
Title : Crystal structure of PPAR delta complexed with GW2331
Authors : Takada, I.; Yu, R.T.; Xu, H.E.; Xu, R.X.; Lambert, M.H.; Montana, V.G.;
Kliwer, S.A.; Evans, R.M.; Umesono, K.
Deposited on : 2004-11-16
Resolution : 2.65 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

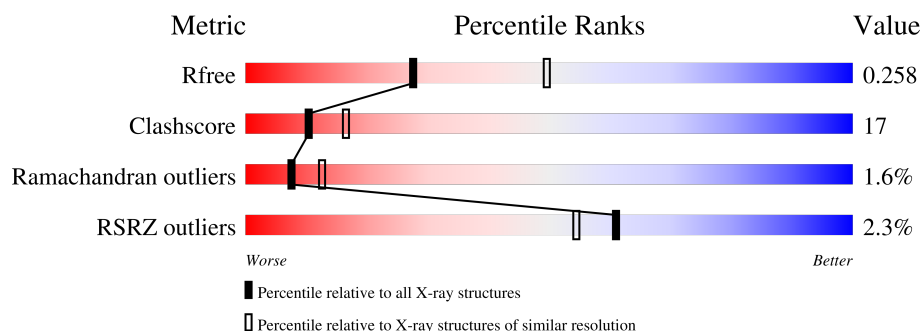
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	272	2% 59% 33% • •
1	B	272	3% 59% 32% • 5%

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
4	B7G	A	483	X	-	-	-
4	B7G	B	480	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4452 atoms, of which 70 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.

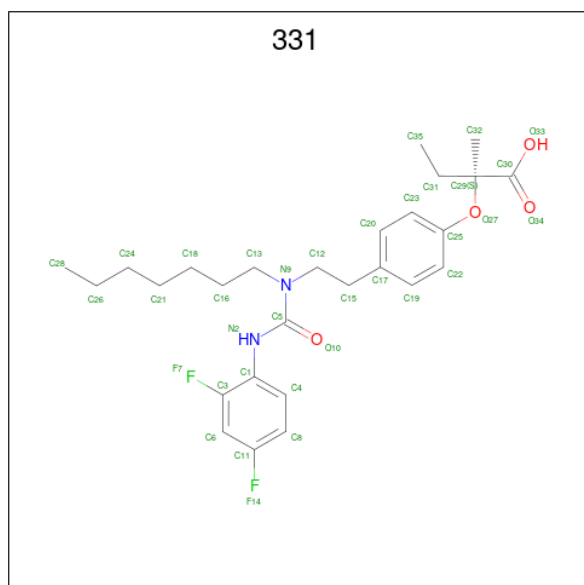
- Molecule 1 is a protein called Peroxisome proliferator activated receptor delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2069	1341	347	372	9			
1	B	258	Total	C	N	O	S	0	0	0
			2032	1316	340	366	10			

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

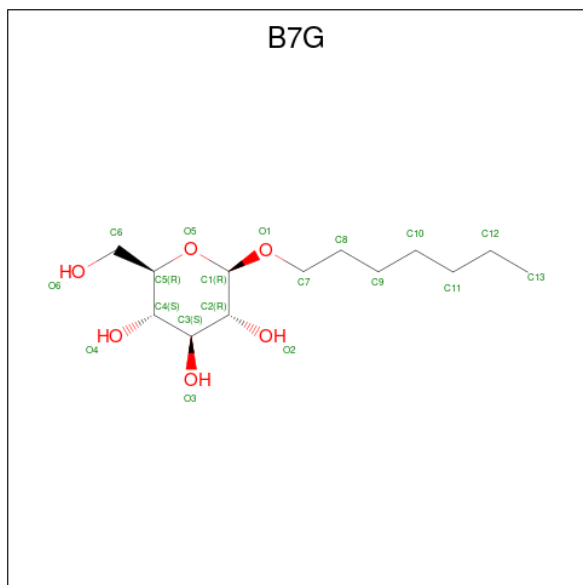
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	I	0	0
			7	7		
2	B	4	Total	I	0	0
			4	4		

- Molecule 3 is (2S)-2-(4-[2-(3-[2,4-DIFLUOROPHENYL]-1-HEPTYLUREIDO)ETHYL]PHENOXY)-2-METHYLBUTYRIC ACID (CCD ID: 331) (formula: C₂₇H₃₆F₂N₂O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	0	0
			70	27	2	35	2	4		
3	B	1	Total	C	F	H	N	O	0	0
			70	27	2	35	2	4		

- Molecule 4 is heptyl beta-D-glucopyranoside (CCD ID: B7G) (formula: C₁₃H₂₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	13	6		
4	B	1	Total	C	O	0	0
			19	13	6		

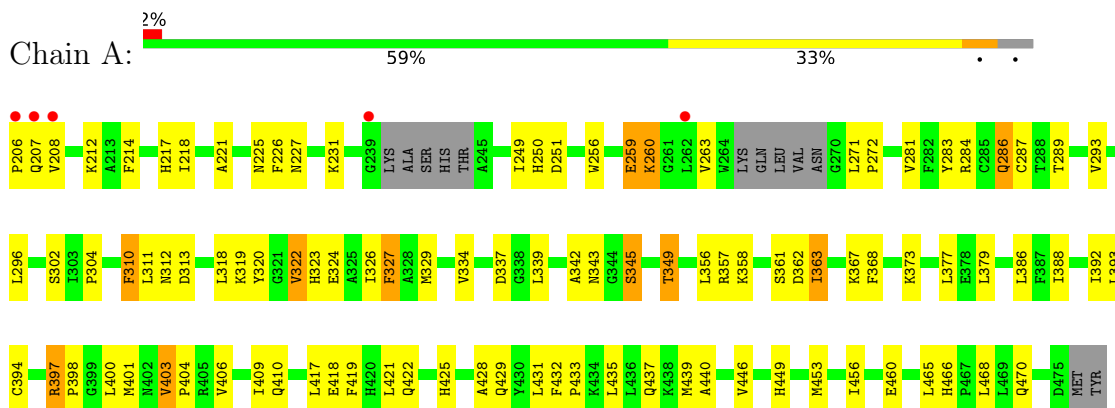
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	78	Total	O	0	0
			78	78		

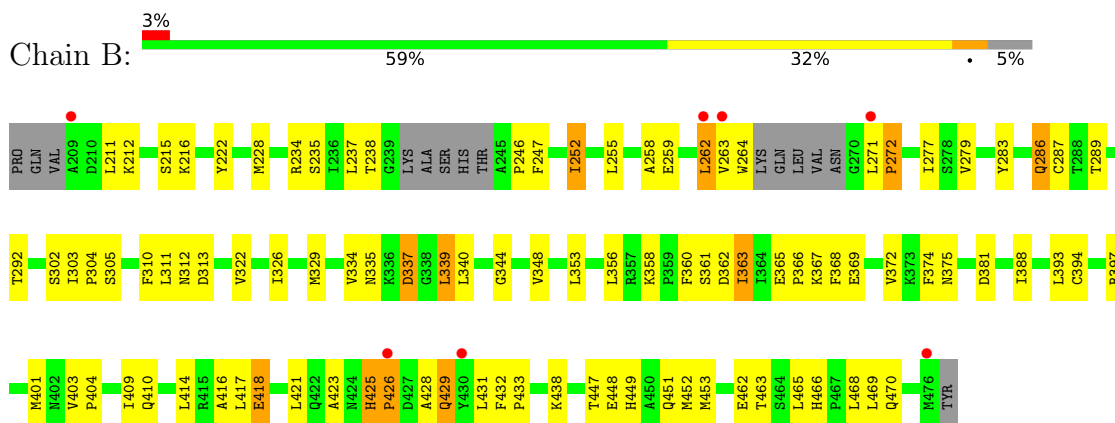
3 Residue-property plots

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 delta



- Molecule 1: Peroxisome proliferator activated receptor delta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.36Å 94.52Å 96.49Å 90.00° 97.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 50.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-2.65) 94.7 (50.00-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.261 0.203 , 0.258	Depositor DCC
R_{free} test set	1198 reflections (5.85%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.0	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	0.94	EDS
Total number of atoms	4452	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.10% 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: IOD, 331, B7G

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	0.93	14/2114 (0.7%)	0.96	9/2862 (0.3%)
1	B	0.92	7/2075 (0.3%)	0.95	6/2811 (0.2%)
All	All	0.93	21/4189 (0.5%)	0.96	15/5673 (0.3%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	PHE	CA-C	-9.02	1.40	1.52
1	A	226	PHE	CA-C	-7.27	1.43	1.52
1	B	339	LEU	CA-C	-7.17	1.43	1.52
1	B	425	HIS	CA-C	-6.82	1.46	1.52
1	A	349	THR	CA-C	-6.45	1.44	1.52
1	A	343	ASN	CA-C	6.42	1.61	1.53
1	A	310	PHE	CA-C	-6.34	1.44	1.52
1	A	362	ASP	CA-C	-6.33	1.44	1.52
1	B	365	GLU	CA-C	6.17	1.60	1.52
1	A	439	MET	CA-C	-5.84	1.45	1.52
1	B	286	GLN	CA-C	-5.83	1.45	1.52
1	A	296	LEU	CA-C	-5.69	1.45	1.52
1	A	345	SER	CA-C	5.66	1.60	1.52
1	A	342	ALA	CA-C	-5.64	1.46	1.53
1	A	323	HIS	CA-C	-5.51	1.45	1.52
1	A	286	GLN	CA-C	-5.50	1.45	1.52
1	B	303	ILE	CA-C	5.47	1.57	1.53
1	A	373	LYS	CA-C	-5.35	1.46	1.52
1	A	227	ASN	CA-C	-5.21	1.46	1.52
1	B	252	ILE	CA-C	-5.06	1.46	1.52
1	B	418	GLU	CA-C	-5.01	1.46	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	HIS	CA-C-N	7.34	129.02	119.84
1	B	425	HIS	C-N-CA	7.34	129.02	119.84
1	A	322	VAL	N-CA-C	7.07	117.83	110.62
1	A	225	ASN	N-CA-C	6.75	122.18	113.88
1	B	363	ILE	N-CA-C	6.31	117.87	111.00
1	B	337	ASP	N-CA-C	6.28	121.02	113.23
1	B	322	VAL	N-CA-C	6.11	116.85	110.62
1	A	397	ARG	CA-C-N	5.91	126.21	119.83
1	A	397	ARG	C-N-CA	5.91	126.21	119.83
1	A	363	ILE	N-CA-C	5.73	115.86	110.30
1	A	231	LYS	N-CA-C	-5.62	104.84	110.97
1	A	337	ASP	N-CA-C	5.45	120.20	113.50
1	B	431	LEU	N-CA-C	5.36	117.12	111.28
1	A	212	LYS	N-CA-C	-5.23	105.48	111.07
1	A	403	VAL	CB-CA-C	-5.09	108.86	113.70

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	2069	0	2079	66	0
1	B	2032	0	2024	77	0
2	A	7	0	0	0	0
2	B	4	0	0	1	0
3	A	35	35	35	6	0
3	B	35	35	35	6	0
4	A	19	0	19	0	0
4	B	19	0	19	0	0
5	A	84	0	0	2	0
5	B	78	0	0	5	0
All	All	4382	70	4211	143	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 (143) 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:286:GLN:HA	3:B:479:331:H69	1.50	0.91
1:A:286:GLN:HA	3:A:482:331:H69	1.53	0.88
1:B:432:PHE:HB3	1:B:433:PRO:HD3	1.64	0.79
1:B:258:ALA:HB1	1:B:263:VAL:HG22	1.68	0.75
1:A:356:LEU:O	1:A:361:SER:HB3	1.86	0.75
1:A:334:VAL:HG22	1:A:339:LEU:HB3	1.74	0.70
1:A:256:TRP:CZ2	1:A:260:LYS:HD2	2.27	0.69
1:A:363:ILE:HD12	1:A:453:MET:HE1	1.72	0.69
1:A:421:LEU:HD11	1:A:435:LEU:HD12	1.74	0.69
1:B:334:VAL:HG22	1:B:339:LEU:HB3	1.75	0.68
1:B:448:GLU:HA	1:B:451:GLN:HG3	1.75	0.67
1:A:319:LYS:HE3	1:A:320:TYR:CZ	2.31	0.66
1:B:463:THR:HG23	5:B:57:HOH:O	1.96	0.64
1:B:234:ARG:O	1:B:238:THR:HG23	1.97	0.64
1:B:363:ILE:HD12	1:B:453:MET:HE1	1.79	0.64
1:B:289:THR:OG1	3:B:479:331:H70	1.98	0.63
1:B:258:ALA:HA	1:B:262:LEU:CB	2.28	0.63
1:B:292:THR:HG21	1:B:326:ILE:HG12	1.82	0.61
1:A:466:HIS:HD2	1:A:468:LEU:H	1.48	0.61
1:B:277:ILE:HD12	5:B:162:HOH:O	1.98	0.61
1:A:357:ARG:HD2	1:A:358:LYS:O	2.00	0.61
1:B:466:HIS:CD2	1:B:468:LEU:H	2.19	0.61
1:B:366:PRO:HA	1:B:369:GLU:OE1	2.00	0.60
1:A:421:LEU:HD22	1:A:431:LEU:HD23	1.83	0.60
1:A:363:ILE:HD11	3:A:482:331:H54	1.84	0.60
1:B:356:LEU:O	1:B:361:SER:HB3	2.02	0.60
1:B:305:SER:HB2	1:B:409:ILE:HD13	1.84	0.59
1:B:449:HIS:O	1:B:453:MET:HG2	2.02	0.58
1:A:388:ILE:O	1:A:392:ILE:HD12	2.03	0.58
1:A:322:VAL:O	1:A:326:ILE:HG13	2.03	0.58
1:B:211:LEU:HD22	1:B:416:ALA:HB2	1.86	0.57
1:B:211:LEU:HD13	1:B:416:ALA:HA	1.85	0.57
1:B:258:ALA:HB1	1:B:263:VAL:CG2	2.34	0.57
1:A:456:ILE:O	1:A:460:GLU:HB2	2.05	0.57
1:B:447:THR:O	1:B:451:GLN:HG2	2.04	0.57
1:A:289:THR:O	1:A:293:VAL:HG23	2.05	0.57
1:A:324:GLU:HG3	1:A:446:VAL:HG21	1.86	0.57
1:B:329:MET:HG2	1:B:388:ILE:HD11	1.87	0.57
1:B:228:MET:HE3	1:B:340:LEU:HD13	1.87	0.56
1:B:466:HIS:HD2	1:B:468:LEU:H	1.51	0.56
1:B:462:GLU:HB3	5:B:57:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:O	1:B:410:GLN:HB2	2.07	0.55
1:A:313:ASP:OD2	1:A:401:MET:HB3	2.07	0.55
1:A:271:LEU:HD12	1:A:283:TYR:HB3	1.89	0.55
1:B:363:ILE:HD12	1:B:453:MET:CE	2.36	0.55
1:A:363:ILE:HD11	3:A:482:331:C22	2.37	0.55
1:A:310:PHE:HB3	1:A:312:ASN:OD1	2.06	0.55
1:B:286:GLN:CA	3:B:479:331:H69	2.30	0.55
1:B:305:SER:HB2	1:B:409:ILE:CD1	2.38	0.54
1:B:465:LEU:HD23	1:B:470:GLN:HG2	1.89	0.54
1:A:363:ILE:HD12	1:A:453:MET:CE	2.37	0.54
1:A:432:PHE:HB3	1:A:433:PRO:CD	2.38	0.54
1:B:358:LYS:HE2	1:B:362:ASP:OD2	2.08	0.54
1:A:449:HIS:O	1:A:453:MET:HG2	2.09	0.53
1:B:262:LEU:CB	5:B:13:HOH:O	2.56	0.53
1:A:281:VAL:HG13	3:A:482:331:H57	1.91	0.53
1:A:339:LEU:HD23	1:A:368:PHE:CZ	2.44	0.53
1:A:393:LEU:O	1:A:410:GLN:HB2	2.09	0.52
1:B:263:VAL:HG23	1:B:264:TRP:CD2	2.45	0.51
1:B:310:PHE:HB3	1:B:312:ASN:OD1	2.10	0.51
1:B:237:LEU:HD21	1:B:340:LEU:HG	1.91	0.51
1:A:466:HIS:CD2	1:A:468:LEU:H	2.28	0.50
1:B:428:ALA:O	1:B:429:GLN:O	2.29	0.50
1:A:400:LEU:HD21	1:A:406:VAL:HG21	1.94	0.49
1:B:418:GLU:HB2	1:B:432:PHE:CE1	2.46	0.49
1:B:348:VAL:HG21	3:B:479:331:H61	1.93	0.49
1:A:394:CYS:HB2	5:A:63:HOH:O	2.13	0.49
1:A:289:THR:HA	5:A:155:HOH:O	2.12	0.49
1:B:252:ILE:HD11	1:B:277:ILE:HD13	1.93	0.49
1:A:466:HIS:HD2	1:A:468:LEU:N	2.11	0.48
1:B:292:THR:CG2	1:B:326:ILE:HG12	2.41	0.48
1:B:360:PHE:O	1:B:363:ILE:HG22	2.14	0.48
1:B:368:PHE:O	1:B:372:VAL:HG23	2.13	0.48
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.95	0.48
1:A:418:GLU:HB2	1:A:432:PHE:CE1	2.49	0.47
1:B:466:HIS:HD2	1:B:468:LEU:N	2.12	0.47
1:B:452:MET:HB2	1:B:453:MET:HE2	1.97	0.47
1:B:363:ILE:HD11	3:B:479:331:H54	1.96	0.47
1:A:403:VAL:HB	1:A:404:PRO:HD3	1.97	0.47
1:A:327:PHE:CZ	1:A:367:LYS:HE2	2.51	0.46
1:B:271:LEU:HD22	1:B:287:CYS:SG	2.56	0.46
1:A:263:VAL:HG13	1:A:345:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:VAL:HB	1:B:404:PRO:HD3	1.98	0.46
1:B:246:PRO:HB3	1:B:344:GLY:O	2.16	0.46
1:B:263:VAL:HG23	1:B:264:TRP:N	2.31	0.46
1:A:214:PHE:CE1	1:A:218:ILE:HD11	2.51	0.46
1:A:250:HIS:CE1	1:A:251:ASP:OD2	2.69	0.45
1:A:259:GLU:CD	1:A:284:ARG:HH11	2.24	0.45
1:B:367:LYS:HD2	1:B:367:LYS:N	2.31	0.45
1:A:465:LEU:HD23	1:A:470:GLN:HG2	1.99	0.45
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.50	0.45
1:A:393:LEU:HD22	1:A:409:ILE:HG21	1.98	0.45
1:A:256:TRP:CE2	1:A:260:LYS:HD2	2.51	0.45
1:B:313:ASP:OD2	1:B:401:MET:HB3	2.17	0.45
1:B:425:HIS:HA	1:B:426:PRO:HD2	1.57	0.45
1:A:272:PRO:HB2	1:A:283:TYR:CE2	2.51	0.44
1:B:255:LEU:O	1:B:259:GLU:HB2	2.17	0.44
1:A:249:ILE:O	1:A:349:THR:HG23	2.17	0.44
1:A:320:TYR:HB3	1:A:397:ARG:HD2	1.99	0.44
1:A:425:HIS:HB3	1:A:428:ALA:HB2	2.00	0.44
1:B:375:ASN:HA	5:B:75:HOH:O	2.17	0.44
1:A:206:PRO:HB2	1:A:207:GLN:H	1.61	0.44
1:A:271:LEU:HD13	1:A:287:CYS:SG	2.58	0.43
1:A:394:CYS:O	1:A:397:ARG:HG2	2.18	0.43
1:B:235:SER:O	1:B:238:THR:OG1	2.36	0.43
1:B:247:PHE:CE2	1:B:258:ALA:HB2	2.53	0.43
1:B:353:LEU:O	1:B:356:LEU:HG	2.18	0.43
1:B:335:ASN:HA	2:B:201:IOD:I	2.88	0.43
1:B:469:LEU:HD13	3:B:479:331:H64	1.99	0.43
1:A:377:LEU:HB2	1:A:379:LEU:HD13	2.01	0.43
1:B:448:GLU:HA	1:B:451:GLN:CG	2.44	0.43
1:A:318:LEU:O	1:A:322:VAL:HG22	2.18	0.43
1:A:329:MET:HG2	1:A:388:ILE:HD11	2.01	0.42
1:A:329:MET:HE3	1:A:388:ILE:CD1	2.49	0.42
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.69	0.42
1:B:279:VAL:HG12	1:B:283:TYR:CE2	2.54	0.42
1:A:320:TYR:CB	1:A:397:ARG:HD2	2.48	0.42
1:B:263:VAL:CG2	1:B:264:TRP:CE3	3.03	0.42
1:B:271:LEU:O	1:B:272:PRO:C	2.61	0.42
1:A:208:VAL:O	1:A:208:VAL:HG12	2.20	0.42
1:A:286:GLN:HG2	3:A:482:331:H64	2.01	0.42
1:B:417:LEU:O	1:B:421:LEU:HG	2.19	0.42
1:A:388:ILE:O	1:A:392:ILE:CD1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:OD1	1:B:337:ASP:N	2.51	0.42
1:A:419:PHE:HD2	1:A:422:GLN:OE1	2.02	0.42
1:A:289:THR:OG1	3:A:482:331:H71	2.20	0.42
1:B:360:PHE:HZ	1:B:463:THR:HG21	1.85	0.42
1:B:452:MET:CB	1:B:453:MET:HE2	2.49	0.42
1:A:217:HIS:CE1	1:A:304:PRO:HD3	2.55	0.42
1:B:311:LEU:HD12	1:B:311:LEU:HA	1.83	0.41
1:A:425:HIS:HB3	1:A:428:ALA:CB	2.50	0.41
1:B:394:CYS:O	1:B:397:ARG:HG2	2.20	0.41
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.85	0.41
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.80	0.41
1:B:234:ARG:HD3	1:B:234:ARG:HA	1.59	0.41
1:A:221:ALA:HB1	1:A:302:SER:HB2	2.03	0.41
1:A:437:GLN:O	1:A:440:ALA:HB3	2.20	0.41
1:B:302:SER:O	1:B:304:PRO:HD3	2.21	0.40
1:B:363:ILE:HD11	1:B:449:HIS:HE1	1.86	0.40
1:B:414:LEU:HA	1:B:414:LEU:HD23	1.84	0.40
1:B:211:LEU:O	1:B:212:LYS:C	2.64	0.40
1:B:215:SER:O	1:B:216:LYS:C	2.64	0.40
1:B:374:PHE:HD1	1:B:438:LYS:HD2	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	254/272 (93%)	237 (93%)	14 (6%)	3 (1%)	10	17
1	B	252/272 (93%)	229 (91%)	18 (7%)	5 (2%)	6	10
All	All	506/544 (93%)	466 (92%)	32 (6%)	8 (2%)	7	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	LYS
1	A	429	GLN
1	B	426	PRO
1	B	429	GLN
1	A	259	GLU
1	B	423	ALA
1	B	262	LEU
1	B	272	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
4	B7G	A	483	-	19,19,19	3.26	4 (21%)	24,24,24	2.82	9 (37%)
3	331	A	482	-	35,36,36	1.20	3 (8%)	44,48,48	1.58	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	331	B	479	-	35,36,36	1.11	2 (5%)	44,48,48	1.36	7 (15%)
4	B7G	B	480	-	19,19,19	3.24	5 (26%)	24,24,24	2.97	11 (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
4	B7G	A	483	-	3/3/5/5	0/10/30/30	0/1/1/1
3	331	A	482	-	-	8/34/34/34	0/2/2/2
3	331	B	479	-	-	7/34/34/34	0/2/2/2
4	B7G	B	480	-	3/3/5/5	1/10/30/30	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	483	B7G	O2-C2	-7.97	1.23	1.43
4	B	480	B7G	O2-C2	-7.92	1.23	1.43
4	A	483	B7G	O4-C4	-7.85	1.23	1.43
4	B	480	B7G	O4-C4	-7.75	1.23	1.43
4	B	480	B7G	O3-C3	-7.63	1.24	1.43
4	A	483	B7G	O3-C3	-7.56	1.24	1.43
3	B	479	331	C6-C3	3.32	1.43	1.37
3	A	482	331	C1-N2	-3.25	1.35	1.41
3	A	482	331	C1-C3	2.73	1.42	1.39
4	B	480	B7G	O6-C6	-2.72	1.31	1.42
4	A	483	B7G	O6-C6	-2.70	1.31	1.42
4	B	480	B7G	O1-C1	2.52	1.44	1.40
3	A	482	331	C8-C11	2.15	1.41	1.37
3	B	479	331	C1-C3	2.13	1.41	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	483	B7G	O3-C3-C2	5.94	124.38	110.38
4	B	480	B7G	O3-C3-C4	5.63	123.64	110.38
4	A	483	B7G	O4-C4-C3	5.45	123.21	110.38
4	B	480	B7G	O3-C3-C2	5.04	122.27	110.38
4	A	483	B7G	O4-C4-C5	4.96	121.55	109.32
4	A	483	B7G	O2-C2-C3	4.85	121.82	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	480	B7G	O4-C4-C3	4.73	121.52	110.38
4	B	480	B7G	O4-C4-C5	4.63	120.73	109.32
4	B	480	B7G	C1-C2-C3	4.46	119.39	110.01
4	B	480	B7G	O2-C2-C1	4.33	120.38	110.08
4	A	483	B7G	O2-C2-C1	4.26	120.23	110.08
4	A	483	B7G	O3-C3-C4	4.26	120.42	110.38
4	B	480	B7G	O2-C2-C3	4.18	120.22	110.38
4	B	480	B7G	C3-C4-C5	4.14	117.74	110.23
4	A	483	B7G	C1-C2-C3	3.77	117.95	110.01
3	A	482	331	O33-C30-C29	3.68	124.10	114.26
3	B	479	331	O33-C30-C29	3.64	123.98	114.26
3	A	482	331	C31-C29-C30	3.59	118.49	109.41
4	B	480	B7G	O1-C1-C2	-3.46	103.02	108.27
3	A	482	331	C32-C29-C30	-2.96	99.29	110.02
3	A	482	331	C12-C15-C17	-2.83	104.17	112.15
4	B	480	B7G	C7-O1-C1	2.78	118.43	113.68
4	A	483	B7G	C3-C4-C5	2.76	115.23	110.23
3	A	482	331	C3-C1-N2	-2.58	113.72	118.51
3	B	479	331	C1-N2-C5	2.54	132.15	125.66
3	A	482	331	C19-C22-C25	2.52	122.61	119.73
3	B	479	331	O27-C29-C30	2.49	113.23	109.97
4	A	483	B7G	C4-C3-C2	2.49	115.20	110.83
3	B	479	331	C12-C15-C17	-2.49	105.13	112.15
3	B	479	331	F14-C11-C6	2.36	121.63	118.28
3	A	482	331	C4-C1-N2	2.30	127.15	121.82
3	A	482	331	O34-C30-C29	-2.28	115.05	121.63
3	A	482	331	C18-C16-C13	-2.17	103.32	113.17
4	B	480	B7G	O5-C1-O1	2.11	115.02	110.04
3	A	482	331	F14-C11-C6	-2.09	115.31	118.28
3	A	482	331	F14-C11-C8	2.08	121.87	118.55
3	B	479	331	C19-C22-C25	2.02	122.04	119.73
3	B	479	331	C31-C29-C30	-2.00	104.35	109.41

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	483	B7G	C2
4	A	483	B7G	C3
4	A	483	B7G	C4
4	B	480	B7G	C2
4	B	480	B7G	C3
4	B	480	B7G	C4

All (16) torsion outliers are listed below:

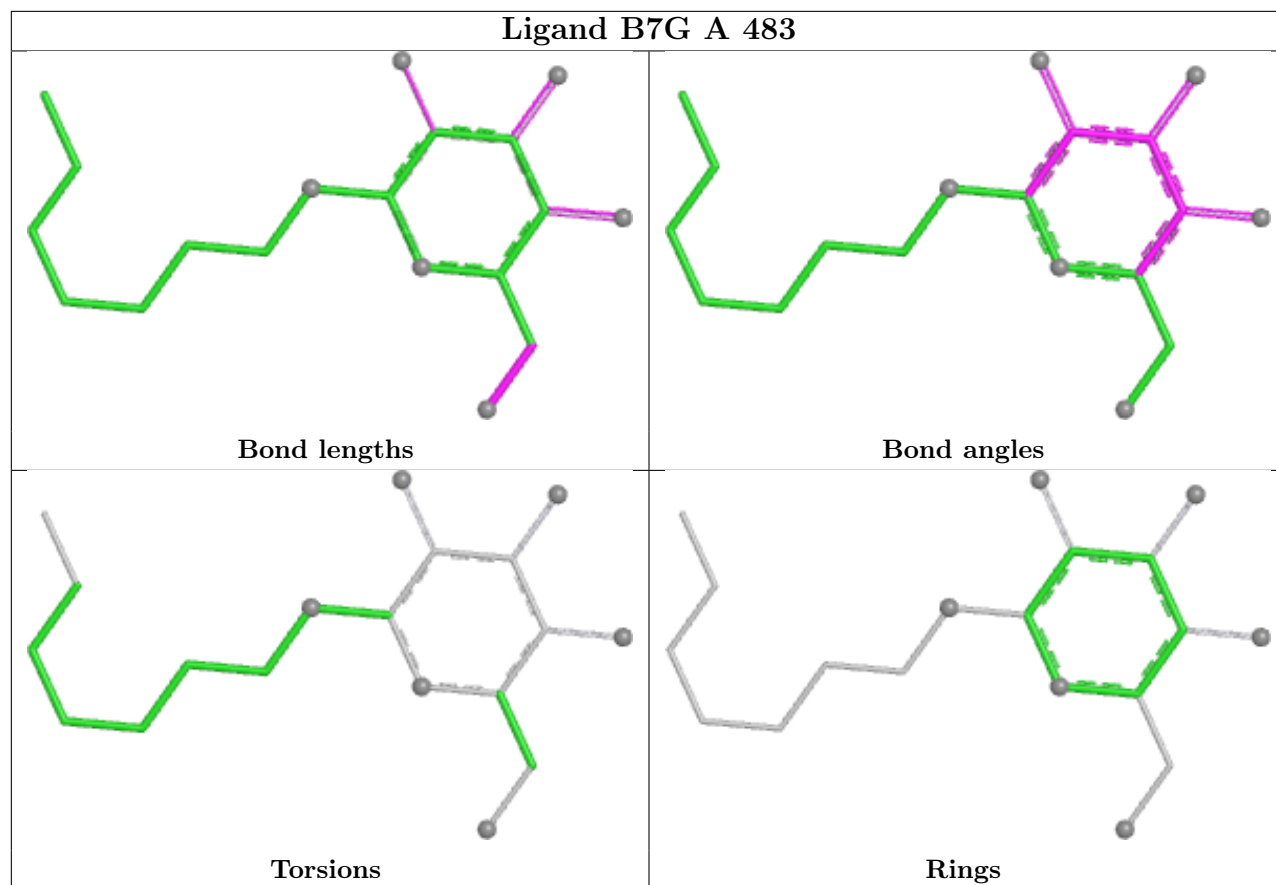
Mol	Chain	Res	Type	Atoms
3	A	482	331	C31-C29-C30-O33
3	A	482	331	C31-C29-C30-O34
3	A	482	331	O27-C29-C31-C35
3	A	482	331	C30-C29-C31-C35
3	A	482	331	C32-C29-C31-C35
3	B	479	331	C31-C29-C30-O33
3	B	479	331	C31-C29-C30-O34
3	A	482	331	C23-C25-O27-C29
3	B	479	331	C22-C25-O27-C29
3	B	479	331	C23-C25-O27-C29
3	A	482	331	C22-C25-O27-C29
4	B	480	B7G	C8-C7-O1-C1
3	B	479	331	C32-C29-C31-C35
3	B	479	331	C30-C29-C31-C35
3	B	479	331	O27-C29-C30-O34
3	A	482	331	C21-C24-C26-C28

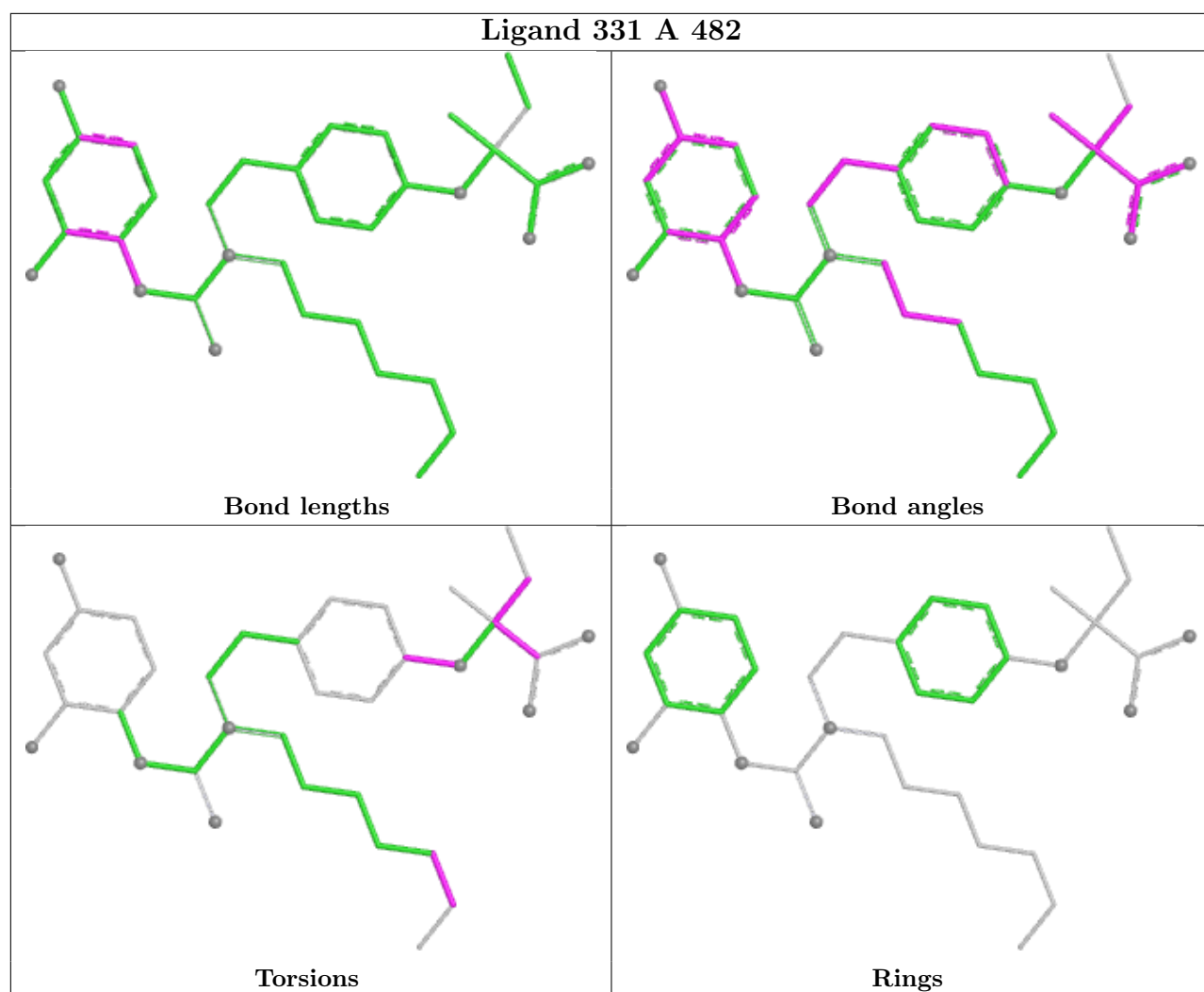
There are no ring outliers.

2 monomers are involved in 12 short contacts:

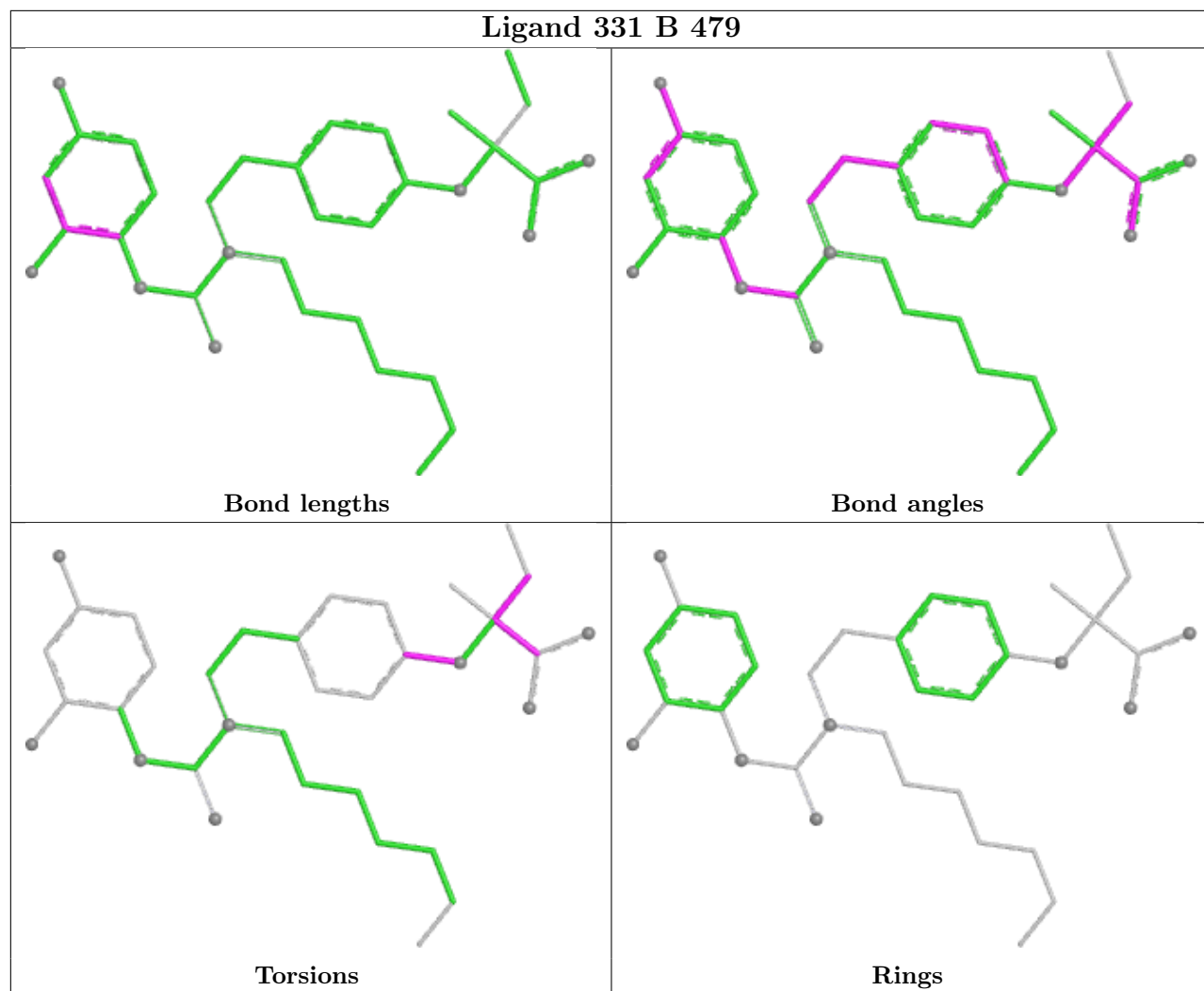
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	482	331	6	0
3	B	479	331	6	0

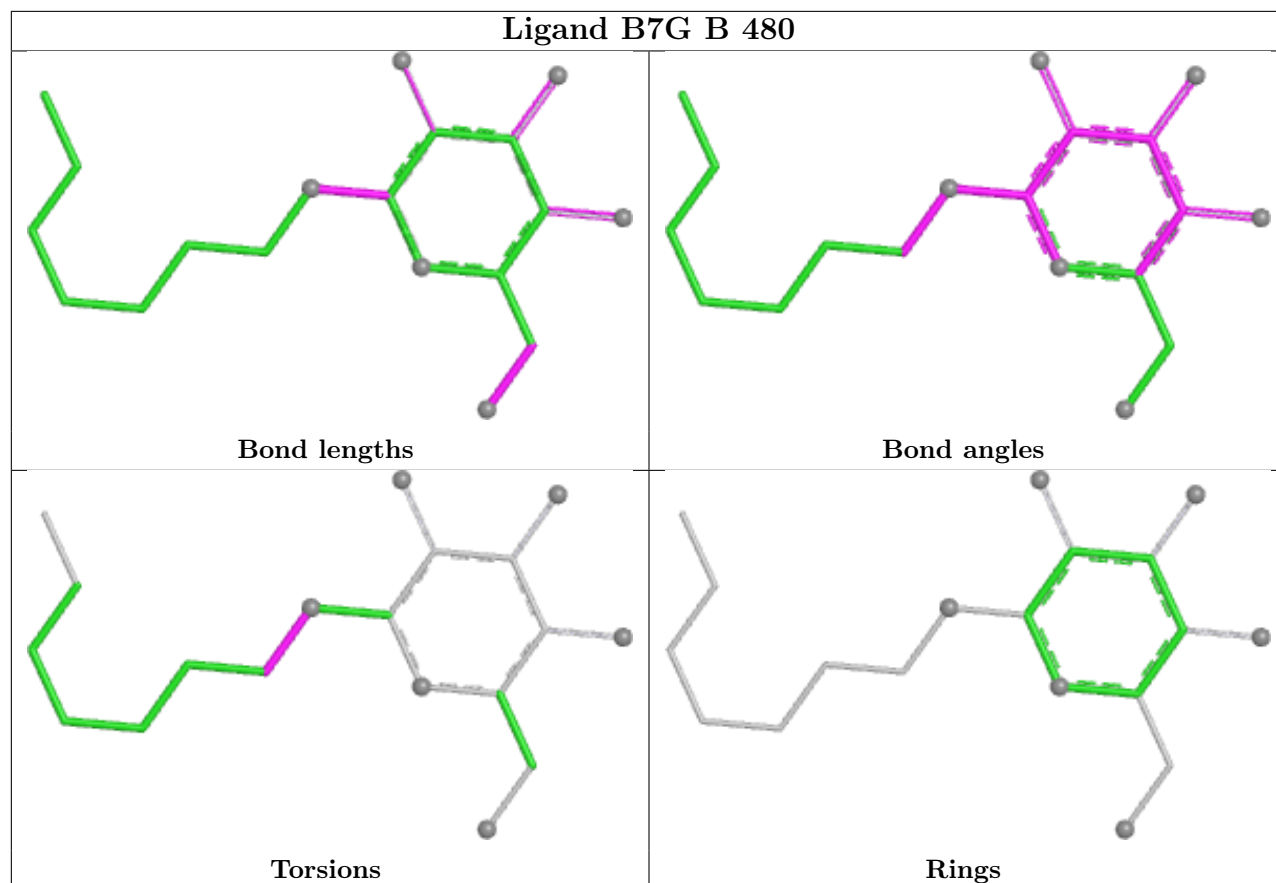
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 331 B 479





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	A	260/272 (95%)	-0.22	5 (1%) 66 61	27, 43, 69, 90	0
1	B	258/272 (94%)	-0.01	7 (2%) 56 49	28, 49, 77, 92	0
All	All	518/544 (95%)	-0.12	12 (2%) 61 54	27, 46, 73, 92	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	PRO	3.6
1	B	426	PRO	3.0
1	A	208	VAL	3.0
1	B	262	LEU	2.9
1	A	207	GLN	2.7
1	B	209	ALA	2.5
1	B	263	VAL	2.5
1	B	430	TYR	2.3
1	A	262	LEU	2.3
1	B	271	LEU	2.3
1	B	476	MET	2.2
1	A	239	GLY	2.1

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

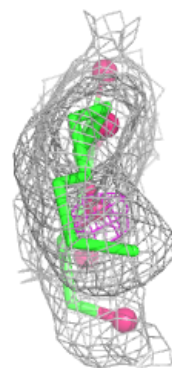
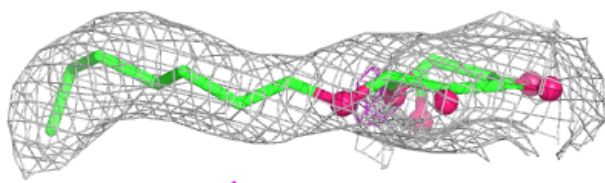
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IOD	A	479	1/1	0.81	0.19	200,200,200,200	0
2	IOD	B	478	1/1	0.84	0.18	200,200,200,200	0
4	B7G	A	483	19/19	0.85	0.12	43,58,62,63	0
2	IOD	A	478	1/1	0.86	0.14	158,158,158,158	0
4	B7G	B	480	19/19	0.88	0.11	35,60,62,63	0
2	IOD	A	203	1/1	0.90	0.18	167,167,167,167	0
3	331	B	479	35/35	0.92	0.07	39,46,55,56	0
3	331	A	482	35/35	0.94	0.07	29,36,43,48	0
2	IOD	B	204	1/1	0.94	0.08	158,158,158,158	0
2	IOD	B	205	1/1	0.95	0.09	106,106,106,106	0
2	IOD	A	481	1/1	0.97	0.06	96,96,96,96	0
2	IOD	B	201	1/1	0.97	0.06	80,80,80,80	0
2	IOD	A	202	1/1	0.97	0.09	85,85,85,85	0
2	IOD	A	480	1/1	0.99	0.04	91,91,91,91	0
2	IOD	A	200	1/1	0.99	0.03	64,64,64,64	0

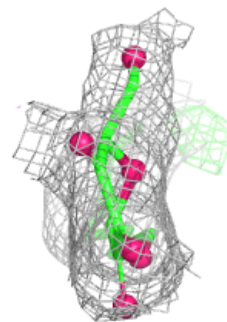
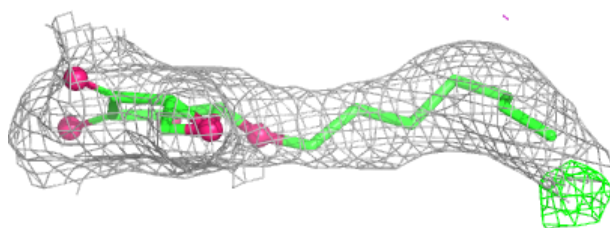
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B7G A 483:

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

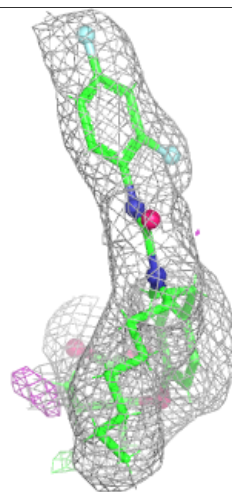
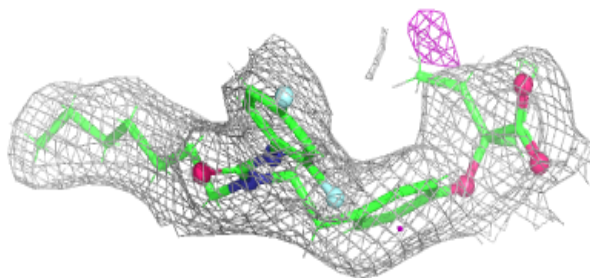
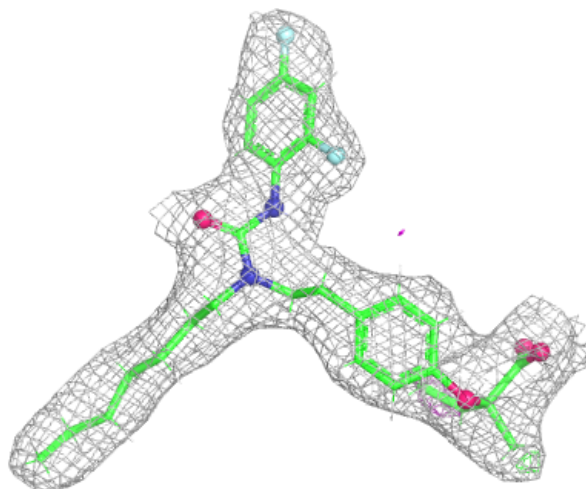
**Electron density around B7G B 480:**

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



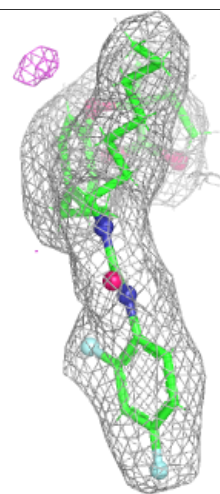
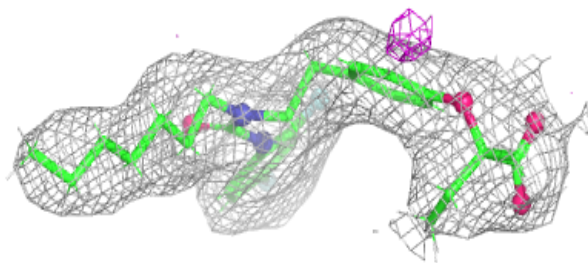
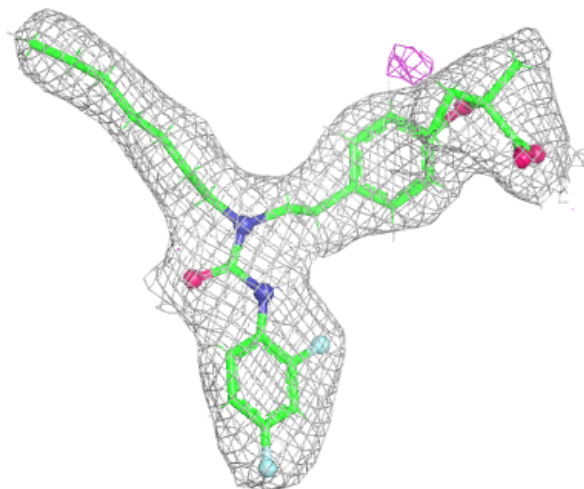
Electron density around 331 B 479:

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



Electron density around 331 A 482:

$2mF_o-DF_c$ (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.