



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:15 PM EDT

PDB ID : 3D5F / pdb_00003d5f
Title : Crystal Structure of PPAR-delta complex
Authors : Amano, Y.
Deposited on : 2008-05-16
Resolution : 2.20 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

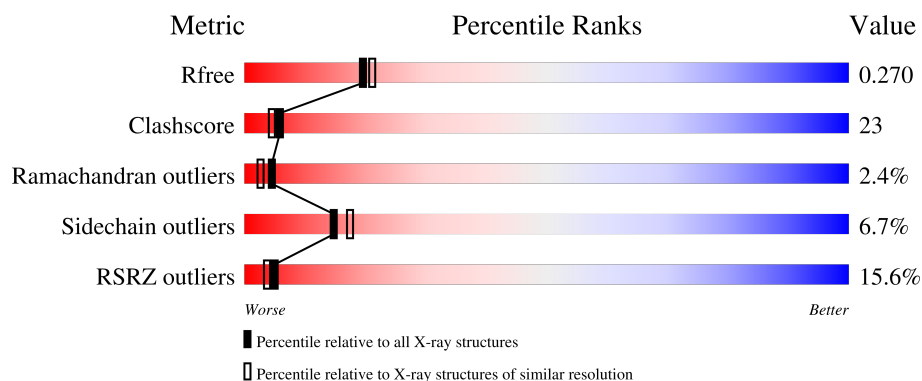
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	267	
1	B	267	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4245 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.

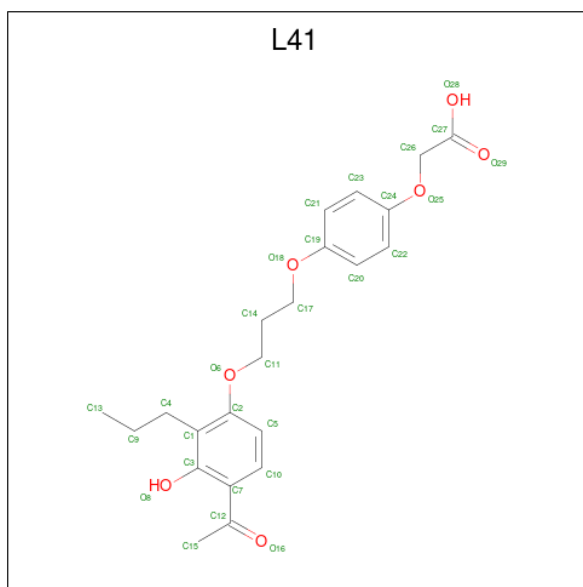
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2048	1329	345	364	10			
1	B	254	Total	C	N	O	S	0	0	0
			2052	1332	343	367	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	430	GLN	TYR	engineered mutation	UNP Q03181
B	430	GLN	TYR	engineered mutation	UNP Q03181

- Molecule 2 is {4-[3-(4-acetyl-3-hydroxy-2-propylphenoxy)propoxy]phenoxy}acetic acid (CCD ID: L41) (formula: C₂₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			29	22	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			29	22	7		

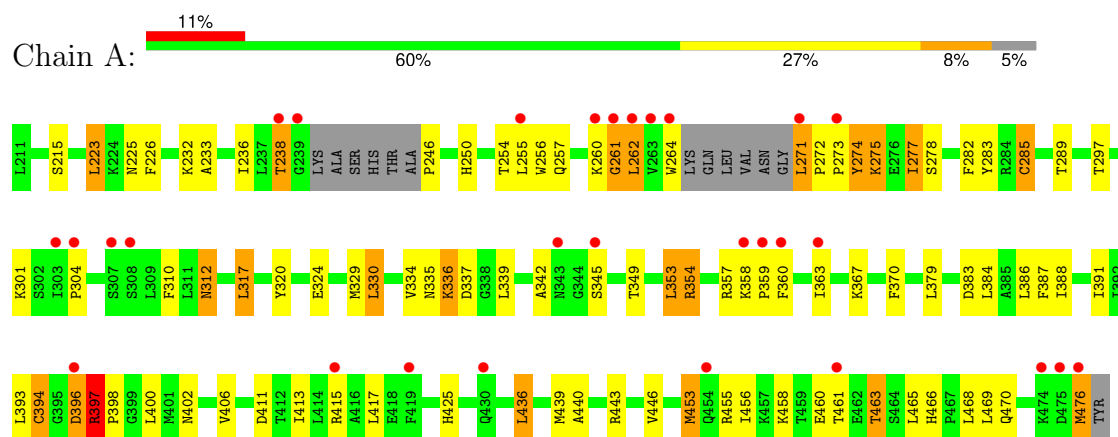
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	37	Total	O	0	0
			37	37		

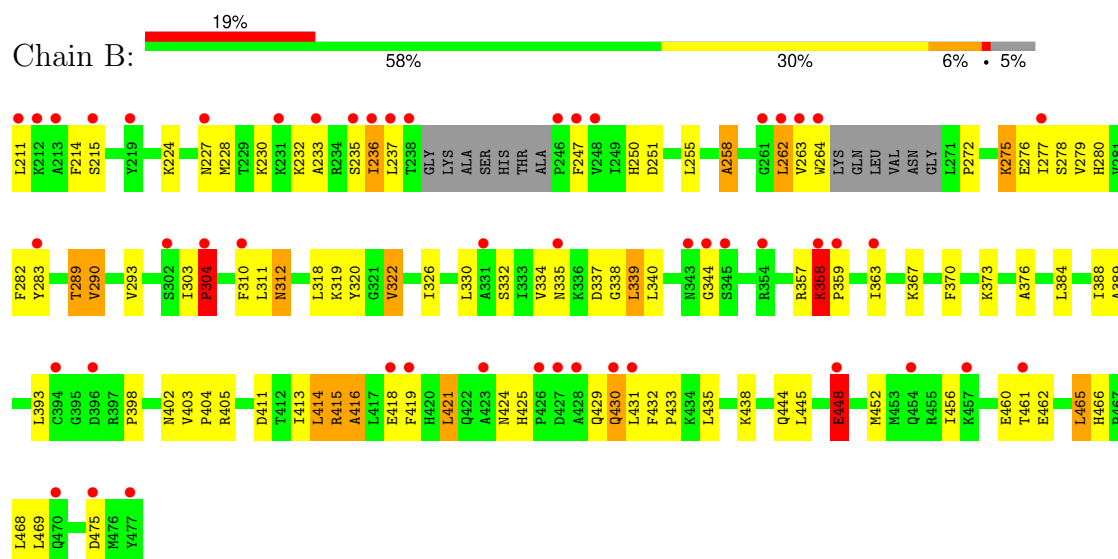
3 Residue-property plots [i](#)

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 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	39.46Å 92.83Å 96.45Å 90.00° 98.02° 90.00°	Depositor
Resolution (Å)	42.47 – 2.20 42.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (42.47-2.20) 97.0 (42.47-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.281 0.270 , 0.270	Depositor DCC
R_{free} test set	1698 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4245	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.64% 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: L41

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	0.50	1/2091 (0.0%)	1.04	12/2823 (0.4%)
1	B	0.48	0/2096	1.01	7/2832 (0.2%)
All	All	0.49	1/4187 (0.0%)	1.02	19/5655 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	453	MET	SD-CE	-5.36	1.66	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	ARG	N-CA-C	8.11	119.54	109.57
1	B	233	ALA	N-CA-C	-7.82	103.19	112.89
1	B	215	SER	CA-C-O	6.57	127.71	120.82
1	A	285	CYS	N-CA-C	-6.49	104.12	111.07
1	B	416	ALA	N-CA-C	-6.26	104.38	111.07
1	A	396	ASP	N-CA-C	6.02	118.80	111.82
1	B	322	VAL	N-CA-C	5.80	116.45	110.36
1	B	258	ALA	N-CA-C	-5.73	104.65	111.69
1	B	358	LYS	N-CA-C	5.71	122.42	109.81
1	A	436	LEU	N-CA-C	-5.70	105.15	111.36
1	A	337	ASP	N-CA-C	5.68	120.27	113.23
1	A	277	ILE	N-CA-C	5.66	116.31	110.36
1	A	225	ASN	N-CA-C	5.57	120.23	113.38
1	A	440	ALA	N-CA-C	-5.48	105.38	111.36
1	A	397	ARG	CA-C-N	5.39	126.58	119.84
1	A	397	ARG	C-N-CA	5.39	126.58	119.84
1	B	448	GLU	N-CA-C	-5.21	105.68	111.36
1	A	425	HIS	CA-C-N	5.14	125.18	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	425	HIS	C-N-CA	5.14	125.18	119.32

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	2048	0	2094	89	0
1	B	2052	0	2079	104	0
2	A	29	0	24	2	0
2	B	29	0	24	2	0
3	A	50	0	0	3	0
3	B	37	0	0	1	0
All	All	4245	0	4221	193	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 23.

All (193) 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:293:VAL:HG22	1:B:322:VAL:HG11	1.23	1.13
1:B:247:PHE:HB3	1:B:262:LEU:HD11	1.48	0.95
1:B:275:LYS:HD3	1:B:275:LYS:H	1.32	0.93
1:B:275:LYS:HD3	1:B:275:LYS:N	1.84	0.92
1:A:465:LEU:HD23	1:A:470:GLN:HG2	1.53	0.90
1:A:312:ASN:HD22	1:A:312:ASN:H	1.18	0.90
1:B:275:LYS:H	1:B:275:LYS:CD	1.83	0.90
1:B:363:ILE:HG22	1:B:452:MET:SD	2.14	0.88
1:B:358:LYS:HE2	1:B:358:LYS:H	1.39	0.84
1:B:411:ASP:O	1:B:415:ARG:HG2	1.76	0.84
1:B:358:LYS:HE2	1:B:358:LYS:N	1.96	0.81
1:A:436:LEU:HA	1:A:439:MET:HE3	1.64	0.80
1:B:237:LEU:HD21	1:B:335:ASN:HD21	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:HD12	1:B:344:GLY:HA3	1.66	0.77
1:B:358:LYS:H	1:B:358:LYS:CE	1.98	0.76
1:A:312:ASN:HD22	1:A:312:ASN:N	1.85	0.75
1:A:285:CYS:O	1:A:289:THR:HG23	1.88	0.74
1:B:255:LEU:HD13	1:B:277:ILE:HD11	1.69	0.74
1:B:264:TRP:H	1:B:264:TRP:CD1	2.05	0.73
1:B:293:VAL:HG22	1:B:322:VAL:CG1	2.14	0.73
1:A:257:GLN:HG3	1:A:262:LEU:HD11	1.70	0.73
1:B:289:THR:HG21	2:B:501:L41:O28	1.88	0.72
1:B:456:ILE:O	1:B:460:GLU:HB2	1.90	0.71
1:B:335:ASN:HB3	1:B:337:ASP:H	1.55	0.71
1:A:460:GLU:HB3	1:A:463:THR:HG23	1.72	0.70
1:A:411:ASP:OD2	1:A:415:ARG:HD2	1.90	0.70
1:A:363:ILE:CD1	1:A:453:MET:HE3	2.22	0.70
1:B:415:ARG:O	1:B:418:GLU:HB3	1.92	0.70
1:A:282:PHE:HE1	1:A:453:MET:HE1	1.57	0.69
1:B:237:LEU:O	1:B:237:LEU:HD23	1.93	0.69
1:A:466:HIS:CD2	1:A:468:LEU:H	2.11	0.69
1:B:461:THR:O	1:B:462:GLU:HB2	1.92	0.68
1:B:310:PHE:HB3	1:B:312:ASN:ND2	2.09	0.67
1:B:312:ASN:HD22	1:B:312:ASN:N	1.92	0.67
1:B:275:LYS:HG3	1:B:279:VAL:CG1	2.24	0.67
1:A:466:HIS:HD2	1:A:468:LEU:H	1.42	0.66
1:A:310:PHE:HB3	1:A:312:ASN:ND2	2.11	0.66
1:B:255:LEU:HD13	1:B:277:ILE:CD1	2.25	0.66
1:A:274:TYR:O	1:A:275:LYS:HG3	1.97	0.65
1:A:246:PRO:HA	1:A:345:SER:O	1.96	0.65
1:A:367:LYS:N	1:A:367:LYS:HD2	2.11	0.65
1:B:312:ASN:HD22	1:B:312:ASN:H	1.42	0.65
1:A:363:ILE:HD13	1:A:453:MET:HE3	1.79	0.64
1:B:424:ASN:HD22	1:B:425:HIS:CE1	2.15	0.64
1:A:310:PHE:CB	1:A:312:ASN:HD21	2.11	0.64
1:A:236:ILE:C	1:A:238:THR:H	2.05	0.64
1:A:256:TRP:CZ2	1:A:260:LYS:HD2	2.33	0.63
1:A:272:PRO:HG2	1:A:283:TYR:CE2	2.34	0.62
1:A:310:PHE:HB3	1:A:312:ASN:HD21	1.65	0.61
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.82	0.61
1:B:373:LYS:HB2	3:B:66:HOH:O	2.00	0.61
1:B:310:PHE:HB3	1:B:312:ASN:HD21	1.65	0.60
1:A:470:GLN:HG3	3:A:42:HOH:O	2.02	0.60
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:HG2	1:B:276:GLU:H	1.67	0.60
1:A:402:ASN:O	1:A:406:VAL:HG23	2.02	0.59
1:B:264:TRP:H	1:B:264:TRP:HD1	1.49	0.59
1:B:255:LEU:C	1:B:255:LEU:HD23	2.28	0.59
1:A:282:PHE:CE1	1:A:453:MET:HE1	2.36	0.58
1:B:432:PHE:HB3	1:B:433:PRO:HD3	1.85	0.58
1:A:363:ILE:HD13	1:A:453:MET:CE	2.34	0.58
1:B:214:PHE:CE2	1:B:304:PRO:HG2	2.39	0.57
1:A:215:SER:OG	1:A:386:LEU:HD11	2.04	0.56
1:A:363:ILE:CD1	1:A:453:MET:CE	2.84	0.55
1:A:336:LYS:HE3	3:A:29:HOH:O	2.06	0.55
1:B:275:LYS:HD2	1:B:283:TYR:HE2	1.70	0.55
1:B:430:GLN:O	1:B:433:PRO:HD2	2.08	0.54
1:A:255:LEU:C	1:A:255:LEU:HD23	2.33	0.53
1:A:320:TYR:HD1	1:A:476:MET:HE3	1.74	0.53
1:A:393:LEU:HD13	1:A:413:ILE:HD11	1.90	0.53
1:B:465:LEU:CD1	1:B:469:LEU:HB2	2.39	0.53
1:B:236:ILE:CD1	1:B:344:GLY:HA3	2.37	0.53
1:A:317:LEU:HD13	1:A:400:LEU:HD21	1.91	0.53
1:B:275:LYS:HE3	1:B:280:HIS:HA	1.90	0.53
1:B:389:ALA:O	1:B:393:LEU:HD23	2.09	0.52
1:A:250:HIS:CD2	1:A:254:THR:HG21	2.44	0.52
1:A:357:ARG:HB3	1:A:359:PRO:HD2	1.91	0.52
1:A:310:PHE:CB	1:A:312:ASN:ND2	2.72	0.52
1:B:358:LYS:HB2	1:B:359:PRO:CD	2.40	0.52
1:B:340:LEU:HB3	1:B:344:GLY:HA2	1.91	0.52
1:A:465:LEU:HD23	1:A:470:GLN:HE21	1.75	0.52
1:A:312:ASN:N	1:A:312:ASN:ND2	2.56	0.52
1:B:237:LEU:HD21	1:B:335:ASN:ND2	2.18	0.52
1:A:324:GLU:HG3	1:A:446:VAL:HG21	1.92	0.51
1:A:411:ASP:O	1:A:415:ARG:HG3	2.10	0.51
1:B:319:LYS:HZ3	1:B:475:ASP:HB2	1.75	0.51
1:B:235:SER:C	1:B:237:LEU:H	2.18	0.51
1:A:226:PHE:CE1	1:A:329:MET:HE1	2.46	0.51
1:A:277:ILE:HG23	1:A:278:SER:N	2.25	0.51
1:B:318:LEU:O	1:B:322:VAL:HG23	2.11	0.50
1:B:258:ALA:HB1	1:B:262:LEU:HD12	1.93	0.50
1:B:384:LEU:O	1:B:388:ILE:HG12	2.12	0.50
1:A:289:THR:HG22	2:A:501:L41:H13	1.93	0.50
1:B:340:LEU:HD22	1:B:344:GLY:HA2	1.94	0.50
1:B:319:LYS:NZ	1:B:475:ASP:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:GLN:C	1:B:433:PRO:HD2	2.38	0.49
1:A:394:CYS:SG	1:A:396:ASP:HB2	2.52	0.49
1:B:211:LEU:HD23	1:B:419:PHE:CD2	2.48	0.49
1:B:262:LEU:O	1:B:264:TRP:N	2.46	0.49
1:B:393:LEU:HD22	1:B:393:LEU:N	2.27	0.49
1:B:444:GLN:NE2	1:B:448:GLU:OE2	2.45	0.49
1:A:363:ILE:HD11	1:A:453:MET:HE3	1.94	0.49
1:A:379:LEU:HB3	1:A:383:ASP:HB2	1.95	0.49
1:B:465:LEU:HD12	1:B:469:LEU:HB2	1.94	0.49
1:B:403:VAL:HB	1:B:404:PRO:HD3	1.95	0.48
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.48	0.48
1:B:264:TRP:CD1	1:B:264:TRP:N	2.78	0.48
1:B:275:LYS:HE3	1:B:283:TYR:HD2	1.79	0.48
1:A:236:ILE:C	1:A:238:THR:N	2.71	0.48
1:A:310:PHE:HB2	1:A:312:ASN:HD21	1.79	0.48
1:B:461:THR:O	1:B:462:GLU:CB	2.60	0.48
1:A:312:ASN:H	1:A:312:ASN:ND2	1.97	0.47
1:B:339:LEU:HD12	1:B:340:LEU:O	2.13	0.47
1:B:444:GLN:HE21	1:B:448:GLU:CD	2.22	0.47
1:A:255:LEU:HD13	1:A:277:ILE:HD11	1.96	0.47
1:A:465:LEU:HD23	1:A:470:GLN:CG	2.36	0.47
1:B:230:LYS:HA	1:B:332:SER:HB3	1.97	0.47
1:A:334:VAL:CG1	1:A:335:ASN:N	2.77	0.47
1:A:367:LYS:HG2	2:A:501:L41:H17	1.96	0.47
1:B:312:ASN:ND2	1:B:312:ASN:N	2.62	0.47
1:A:357:ARG:C	1:A:359:PRO:HD2	2.40	0.47
1:A:396:ASP:CG	1:A:443:ARG:HH12	2.23	0.47
1:A:384:LEU:O	1:A:388:ILE:HG12	2.15	0.46
1:B:335:ASN:HB2	1:B:338:GLY:O	2.15	0.46
1:A:317:LEU:HD12	1:A:397:ARG:HG3	1.98	0.46
1:A:360:PHE:O	1:A:363:ILE:HG22	2.15	0.46
1:A:466:HIS:CD2	1:A:468:LEU:HB3	2.51	0.46
1:B:367:LYS:HD2	1:B:367:LYS:N	2.29	0.46
1:A:264:TRP:CE2	1:A:342:ALA:HB2	2.50	0.46
1:A:396:ASP:CB	1:A:443:ARG:HH22	2.28	0.46
1:A:466:HIS:HD2	1:A:468:LEU:N	2.10	0.46
1:B:272:PRO:O	1:B:275:LYS:NZ	2.49	0.46
1:B:330:LEU:HD21	2:B:501:L41:H14A	1.97	0.46
1:A:297:THR:HG22	1:A:301:LYS:HD3	1.98	0.46
1:B:279:VAL:HG12	1:B:283:TYR:CE2	2.50	0.46
1:A:330:LEU:HD21	1:A:339:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LYS:HE2	1:B:358:LYS:CA	2.46	0.46
1:A:354:ARG:HD2	3:A:59:HOH:O	2.17	0.45
1:A:397:ARG:H	1:A:397:ARG:HG2	1.38	0.45
1:B:414:LEU:O	1:B:418:GLU:N	2.41	0.45
1:B:303:ILE:HG23	1:B:304:PRO:HD2	1.99	0.45
1:A:317:LEU:CD1	1:A:400:LEU:HD21	2.46	0.44
1:A:320:TYR:CD1	1:A:476:MET:HE3	2.52	0.44
1:A:393:LEU:CD1	1:A:413:ILE:HD11	2.47	0.44
1:A:274:TYR:CG	1:A:275:LYS:N	2.84	0.44
1:B:322:VAL:HG12	1:B:326:ILE:CD1	2.48	0.44
1:A:367:LYS:N	1:A:367:LYS:CD	2.80	0.44
1:B:320:TYR:CE2	1:B:398:PRO:HG2	2.52	0.44
1:B:310:PHE:CB	1:B:312:ASN:HD21	2.30	0.44
1:A:272:PRO:O	1:A:273:PRO:C	2.60	0.44
1:A:261:GLY:O	1:A:262:LEU:C	2.60	0.44
1:B:224:LYS:HE2	1:B:224:LYS:HB3	1.83	0.43
1:B:415:ARG:HG2	1:B:415:ARG:H	1.62	0.43
1:A:272:PRO:HG2	1:A:283:TYR:CD2	2.54	0.43
1:B:373:LYS:O	1:B:376:ALA:HB3	2.18	0.43
1:B:275:LYS:HG3	1:B:279:VAL:HG12	1.98	0.43
1:B:393:LEU:N	1:B:393:LEU:CD2	2.81	0.43
1:A:387:PHE:CE2	1:A:391:ILE:HD11	2.52	0.43
1:B:465:LEU:O	1:B:466:HIS:C	2.61	0.43
1:B:430:GLN:HE21	1:B:430:GLN:HB3	1.63	0.43
1:B:277:ILE:HG23	1:B:278:SER:N	2.34	0.43
1:B:466:HIS:HB3	1:B:469:LEU:HG	2.01	0.43
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.81	0.42
1:B:421:LEU:HD21	1:B:435:LEU:HD12	2.01	0.42
1:B:272:PRO:HG2	1:B:283:TYR:CE2	2.53	0.42
1:A:226:PHE:CD1	1:A:329:MET:HE1	2.55	0.42
1:A:273:PRO:O	1:A:274:TYR:O	2.38	0.42
1:B:438:LYS:HD3	1:B:438:LYS:HA	1.84	0.42
1:A:349:THR:O	1:A:353:LEU:HD22	2.20	0.42
1:B:290:VAL:HG21	1:B:466:HIS:CD2	2.55	0.42
1:B:322:VAL:HG12	1:B:326:ILE:HD12	2.00	0.42
1:A:232:LYS:O	1:A:233:ALA:C	2.63	0.41
1:B:413:ILE:O	1:B:416:ALA:HB3	2.20	0.41
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.87	0.41
1:B:275:LYS:HG3	1:B:279:VAL:HG11	1.99	0.41
1:B:227:ASN:CG	1:B:228:MET:N	2.77	0.41
1:B:370:PHE:CD1	1:B:370:PHE:C	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLU:HB3	1:A:463:THR:CG2	2.47	0.41
1:B:402:ASN:CG	1:B:405:ARG:HB2	2.46	0.41
1:B:250:HIS:CE1	1:B:251:ASP:OD2	2.74	0.41
1:A:257:GLN:CG	1:A:262:LEU:HD11	2.46	0.41
1:A:271:LEU:N	1:A:272:PRO:HD2	2.36	0.41
1:A:455:ARG:NH1	1:A:458:LYS:HG2	2.36	0.41
1:B:429:GLN:O	1:B:430:GLN:HB2	2.21	0.41
1:B:311:LEU:HA	1:B:311:LEU:HD12	1.84	0.41
1:B:357:ARG:HG2	1:B:359:PRO:HD2	2.03	0.40
1:B:334:VAL:CG1	1:B:335:ASN:N	2.82	0.40
1:B:402:ASN:C	1:B:402:ASN:HD22	2.30	0.40
1:A:367:LYS:HD2	1:A:367:LYS:H	1.85	0.40
1:A:370:PHE:CD1	1:A:370:PHE:C	2.99	0.40
1:A:456:ILE:O	1:A:460:GLU:HB2	2.22	0.40
1:B:275:LYS:HE3	1:B:283:TYR:CD2	2.56	0.40
1:B:279:VAL:O	1:B:282:PHE:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	248/267 (93%)	228 (92%)	14 (6%)	6 (2%)	4	3
1	B	248/267 (93%)	226 (91%)	16 (6%)	6 (2%)	4	3
All	All	496/534 (93%)	454 (92%)	30 (6%)	12 (2%)	4	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	TYR
1	B	263	VAL

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Mol	Chain	Res	Type
1	B	304	PRO
1	B	358	LYS
1	A	275	LYS
1	B	232	LYS
1	A	238	THR
1	A	261	GLY
1	B	236	ILE
1	B	262	LEU
1	A	262	LEU
1	A	358	LYS

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	225/236 (95%)	210 (93%)	15 (7%)	15	17
1	B	224/236 (95%)	209 (93%)	15 (7%)	15	17
All	All	449/472 (95%)	419 (93%)	30 (7%)	15	17

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	LEU
1	A	271	LEU
1	A	304	PRO
1	A	312	ASN
1	A	317	LEU
1	A	330	LEU
1	A	336	LYS
1	A	353	LEU
1	A	354	ARG
1	A	394	CYS
1	A	397	ARG
1	A	461	THR
1	A	463	THR

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Mol	Chain	Res	Type
1	A	469	LEU
1	A	476	MET
1	B	275	LYS
1	B	289	THR
1	B	290	VAL
1	B	304	PRO
1	B	312	ASN
1	B	339	LEU
1	B	414	LEU
1	B	415	ARG
1	B	421	LEU
1	B	430	GLN
1	B	431	LEU
1	B	445	LEU
1	B	448	GLU
1	B	465	LEU
1	B	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	250	HIS
1	A	257	GLN
1	A	312	ASN
1	A	314	GLN
1	A	343	ASN
1	A	402	ASN
1	A	420	HIS
1	A	424	ASN
1	A	437	GLN
1	A	466	HIS
1	A	470	GLN
1	B	220	ASN
1	B	225	ASN
1	B	250	HIS
1	B	257	GLN
1	B	312	ASN
1	B	335	ASN
1	B	375	ASN
1	B	402	ASN
1	B	422	GLN

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Mol	Chain	Res	Type
1	B	424	ASN
1	B	425	HIS
1	B	430	GLN
1	B	444	GLN
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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	L41	B	501	-	30,30,30	2.34	12 (40%)	39,39,39	1.36	7 (17%)
2	L41	A	501	-	30,30,30	2.40	10 (33%)	39,39,39	1.63	9 (23%)

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	L41	B	501	-	-	0/20/20/20	0/2/2/2
2	L41	A	501	-	-	0/20/20/20	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	L41	O8-C3	-5.92	1.23	1.36
2	B	501	L41	O8-C3	-5.26	1.24	1.36
2	A	501	L41	C20-C19	4.78	1.47	1.38
2	B	501	L41	C20-C19	4.68	1.47	1.38
2	B	501	L41	C22-C20	4.39	1.45	1.38
2	B	501	L41	C21-C19	4.29	1.46	1.38
2	A	501	L41	C22-C20	3.99	1.45	1.38
2	B	501	L41	C23-C24	3.68	1.45	1.38
2	A	501	L41	O18-C19	3.66	1.46	1.37
2	A	501	L41	C3-C1	3.65	1.45	1.40
2	A	501	L41	C22-C24	3.56	1.45	1.38
2	A	501	L41	C10-C7	3.52	1.45	1.39
2	A	501	L41	C21-C19	3.31	1.44	1.38
2	B	501	L41	C23-C21	3.18	1.43	1.38
2	B	501	L41	C22-C24	3.05	1.44	1.38
2	A	501	L41	C23-C24	2.81	1.44	1.38
2	B	501	L41	O18-C19	2.59	1.43	1.37
2	B	501	L41	O25-C26	2.41	1.48	1.42
2	B	501	L41	C15-C12	2.38	1.56	1.49
2	B	501	L41	C3-C1	2.32	1.43	1.40
2	B	501	L41	O28-C27	-2.22	1.23	1.30
2	A	501	L41	C2-C1	2.10	1.43	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	L41	C26-O25-C24	4.34	125.41	117.63
2	B	501	L41	C7-C3-C1	-3.54	118.18	121.35
2	A	501	L41	O16-C12-C7	3.44	125.34	120.56
2	B	501	L41	C2-C1-C3	2.91	120.58	117.49
2	A	501	L41	C7-C3-C1	-2.72	118.91	121.35
2	A	501	L41	C23-C24-C22	2.72	124.12	120.16
2	A	501	L41	C21-C19-C20	2.56	123.89	120.16
2	B	501	L41	C23-C24-C22	2.45	123.73	120.16
2	B	501	L41	C4-C1-C2	-2.36	118.11	121.44
2	B	501	L41	C11-O6-C2	2.35	123.36	117.69
2	A	501	L41	C22-C20-C19	-2.27	117.14	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	L41	C20-C22-C24	-2.24	117.17	119.73
2	A	501	L41	C10-C7-C3	2.23	120.92	118.76
2	B	501	L41	O16-C12-C7	2.20	123.62	120.56
2	B	501	L41	O16-C12-C15	-2.09	115.74	120.19
2	A	501	L41	C17-C14-C11	-2.05	107.04	113.67

There are no chirality outliers.

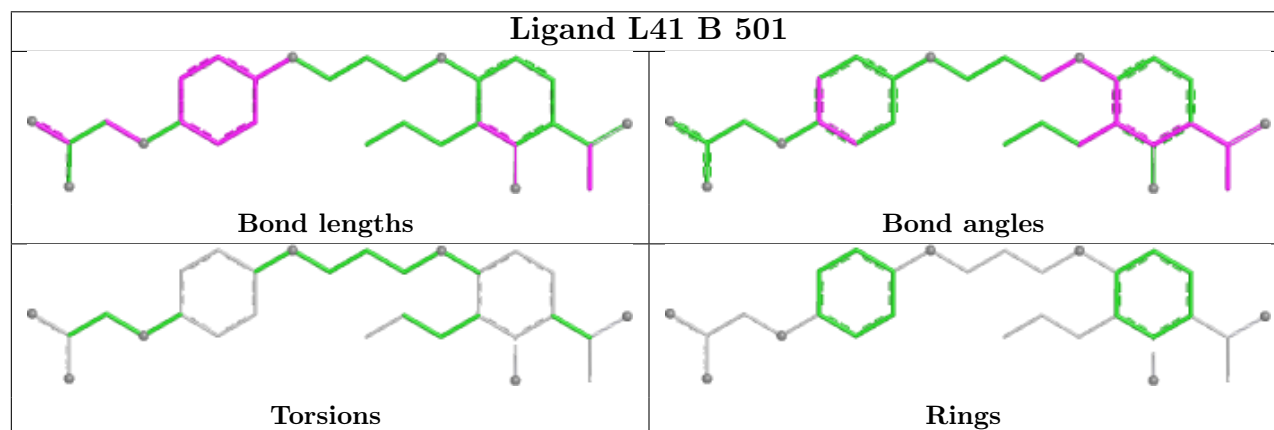
There are no torsion outliers.

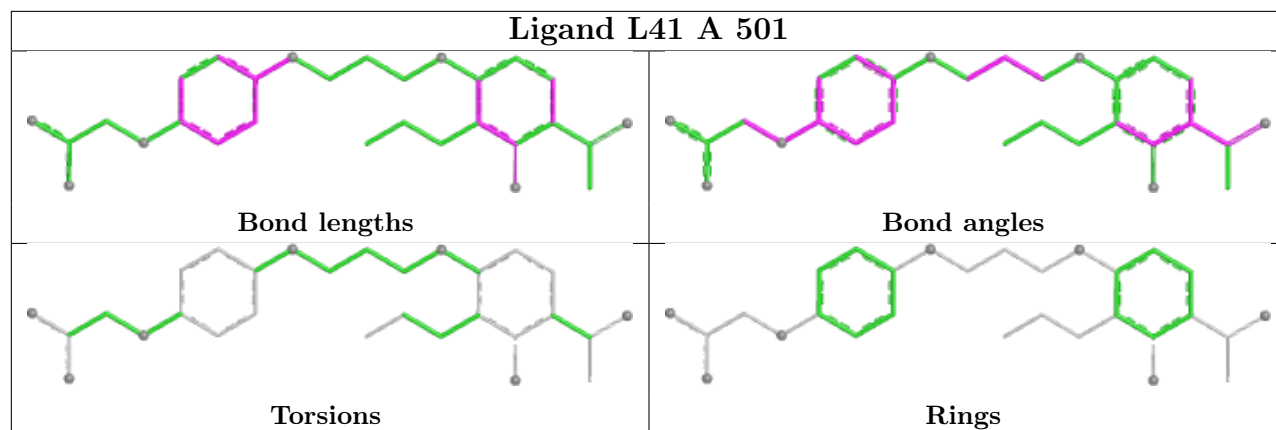
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	L41	2	0
2	A	501	L41	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

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	254/267 (95%)	0.92	29 (11%) 10 7	20, 34, 54, 72	0
1	B	254/267 (95%)	1.25	50 (19%) 3 2	23, 38, 64, 78	0
All	All	508/534 (95%)	1.09	79 (15%) 5 4	20, 36, 62, 78	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	LEU	6.8
1	B	263	VAL	6.8
1	B	212	LYS	5.4
1	A	239	GLY	5.2
1	B	236	ILE	5.1
1	A	271	LEU	4.9
1	B	264	TRP	4.7
1	B	358	LYS	4.3
1	A	262	LEU	4.3
1	B	418	GLU	4.3
1	B	213	ALA	4.0
1	B	428	ALA	3.9
1	B	227	ASN	3.9
1	B	345	SER	3.9
1	B	233	ALA	3.7
1	A	263	VAL	3.7
1	B	277	ILE	3.7
1	A	475	ASP	3.7
1	B	477	TYR	3.7
1	B	475	ASP	3.6
1	B	211	LEU	3.6
1	B	261	GLY	3.5
1	A	461	THR	3.4
1	A	261	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	474	LYS	3.3
1	B	461	THR	3.3
1	B	215	SER	3.2
1	A	264	TRP	3.2
1	B	247	PHE	3.1
1	B	231	LYS	3.1
1	A	260	LYS	3.0
1	B	304	PRO	3.0
1	B	359	PRO	3.0
1	A	476	MET	2.9
1	B	419	PHE	2.9
1	B	238	THR	2.9
1	B	219	TYR	2.9
1	B	344	GLY	2.9
1	A	307	SER	2.7
1	B	302	SER	2.7
1	B	283	TYR	2.7
1	B	454	GLN	2.7
1	B	246	PRO	2.7
1	B	354	ARG	2.7
1	B	237	LEU	2.7
1	B	426	PRO	2.6
1	A	273	PRO	2.6
1	A	238	THR	2.6
1	A	308	SER	2.6
1	B	396	ASP	2.6
1	A	419	PHE	2.5
1	B	235	SER	2.5
1	B	448	GLU	2.5
1	A	430	GLN	2.5
1	B	430	GLN	2.4
1	B	335	ASN	2.4
1	B	248	VAL	2.4
1	A	396	ASP	2.3
1	B	331	ALA	2.3
1	A	359	PRO	2.3
1	B	363	ILE	2.3
1	A	454	GLN	2.3
1	B	394	CYS	2.3
1	B	423	ALA	2.3
1	B	470	GLN	2.3
1	A	415	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	304	PRO	2.2
1	A	255	LEU	2.1
1	B	457	LYS	2.1
1	A	358	LYS	2.1
1	A	343	ASN	2.1
1	B	427	ASP	2.1
1	A	303	ILE	2.1
1	B	310	PHE	2.1
1	A	345	SER	2.0
1	B	343	ASN	2.0
1	A	360	PHE	2.0
1	B	431	LEU	2.0
1	A	363	ILE	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](#)

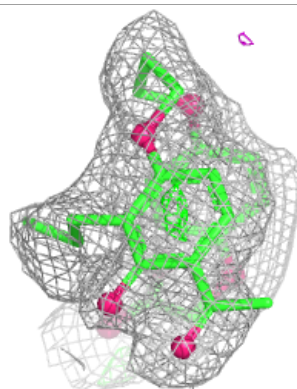
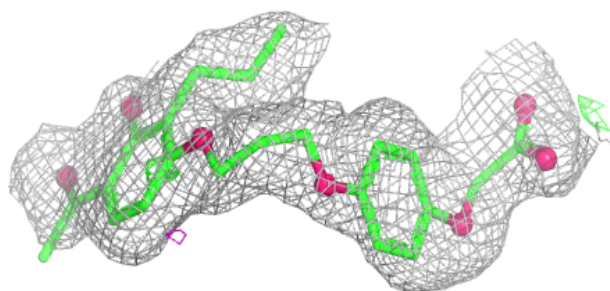
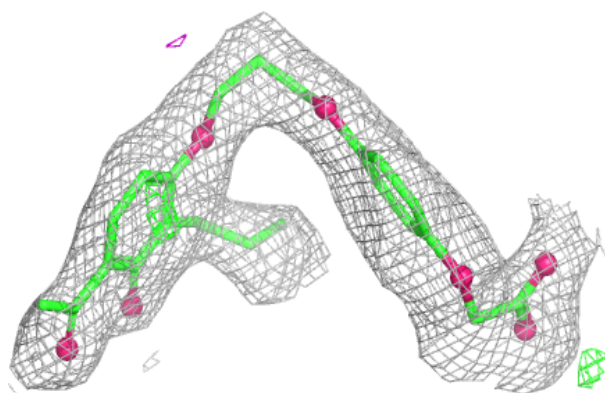
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	L41	B	501	29/29	0.91	0.11	23,29,34,40	0
2	L41	A	501	29/29	0.94	0.08	16,25,31,32	0

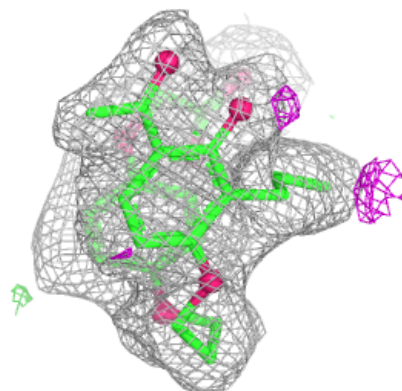
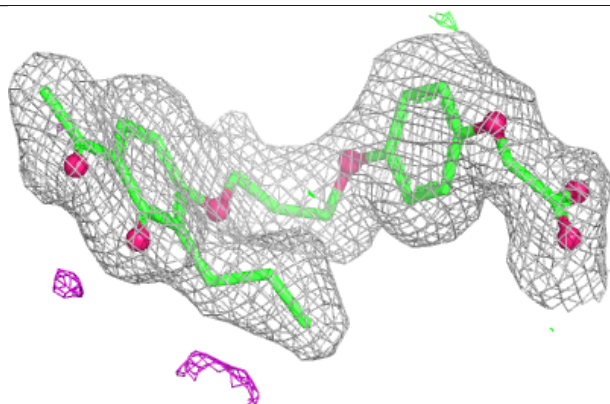
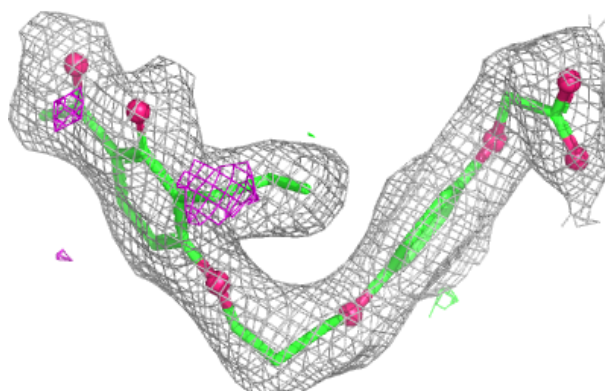
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L41 B 501:

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

**Electron density around L41 A 501:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.