



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:33 AM UTC

PDB ID : 8HF8 / pdb_00008hf8
Title : Human PPAR delta ligand binding domain in complex with a synthetic agonist V1
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Deposited on : 2022-11-09
Resolution : 2.11 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

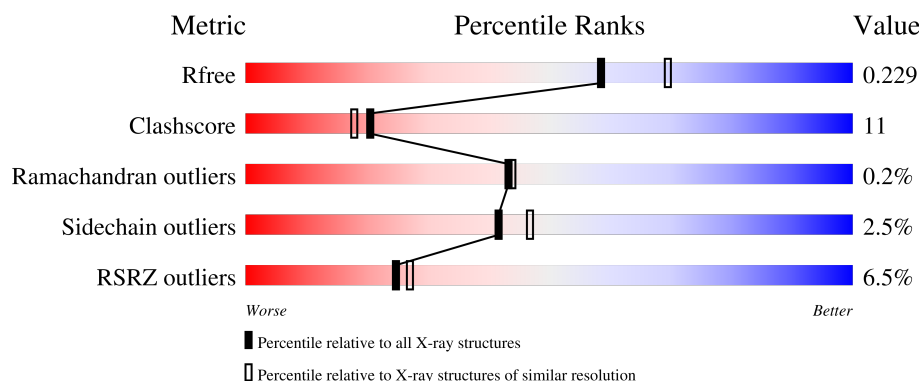
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	282	5% 78% 14% • 7%
1	B	282	7% 70% 21% •• 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4553 atoms, of which 56 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	262	Total	C	N	O	S	0	0	0
			2089	1354	350	376	9			
1	B	259	Total	C	N	O	S	0	0	0
			2062	1336	346	371	9			

There are 26 discrepancies between the modelled and reference sequences:

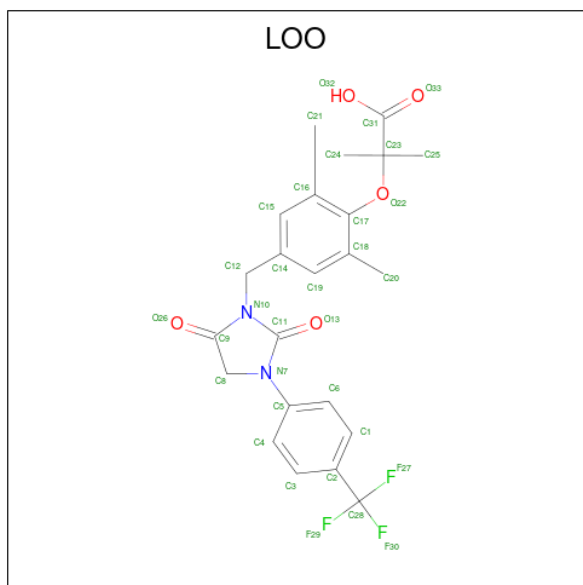
Chain	Residue	Modelled	Actual	Comment	Reference
A	196	MET	-	initiating methionine	UNP Q03181
A	197	HIS	-	expression tag	UNP Q03181
A	198	HIS	-	expression tag	UNP Q03181
A	199	HIS	-	expression tag	UNP Q03181
A	200	HIS	-	expression tag	UNP Q03181
A	201	HIS	-	expression tag	UNP Q03181
A	202	HIS	-	expression tag	UNP Q03181
A	203	LEU	-	expression tag	UNP Q03181
A	204	VAL	-	expression tag	UNP Q03181
A	205	PRO	-	expression tag	UNP Q03181
A	206	ARG	-	expression tag	UNP Q03181
A	207	GLY	-	expression tag	UNP Q03181
A	208	SER	-	expression tag	UNP Q03181
B	196	MET	-	initiating methionine	UNP Q03181
B	197	HIS	-	expression tag	UNP Q03181
B	198	HIS	-	expression tag	UNP Q03181
B	199	HIS	-	expression tag	UNP Q03181
B	200	HIS	-	expression tag	UNP Q03181
B	201	HIS	-	expression tag	UNP Q03181
B	202	HIS	-	expression tag	UNP Q03181
B	203	LEU	-	expression tag	UNP Q03181
B	204	VAL	-	expression tag	UNP Q03181
B	205	PRO	-	expression tag	UNP Q03181
B	206	ARG	-	expression tag	UNP Q03181
B	207	GLY	-	expression tag	UNP Q03181

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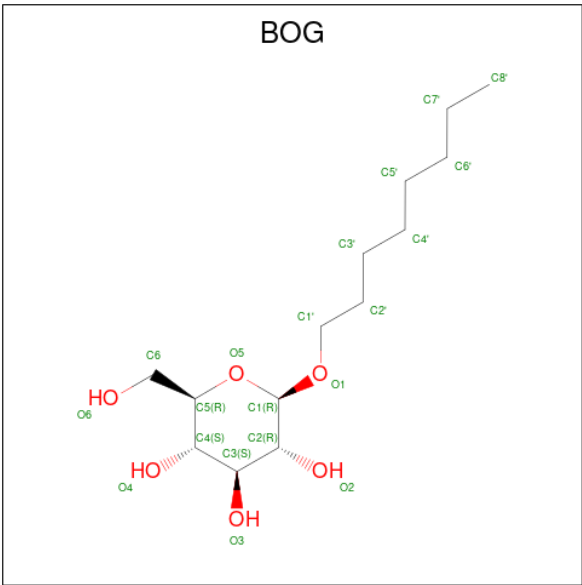
Chain	Residue	Modelled	Actual	Comment	Reference
B	208	SER	-	expression tag	UNP Q03181

- Molecule 2 is 2-[4-[[2,5-bis(oxidanylidene)-3-[4-(trifluoromethyl)phenyl]imidazolidin-1-yl]methyl]-2,6-dimethyl-phenoxy]-2-methyl-propanoic acid (CCD ID: LOO) (formula: $C_{23}H_{23}F_3N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			33	23	3	2	5		
2	B	1	Total	C	F	N	O	0	0
			33	23	3	2	5		

- Molecule 3 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			48	14	28	6		
3	B	1	Total	C	H	O	0	0
			48	14	28	6		

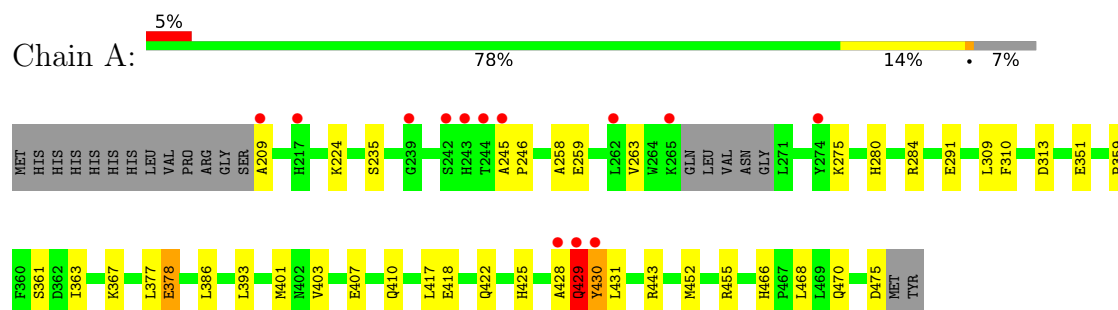
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		
4	B	91	Total	O	0	0
			91	91		

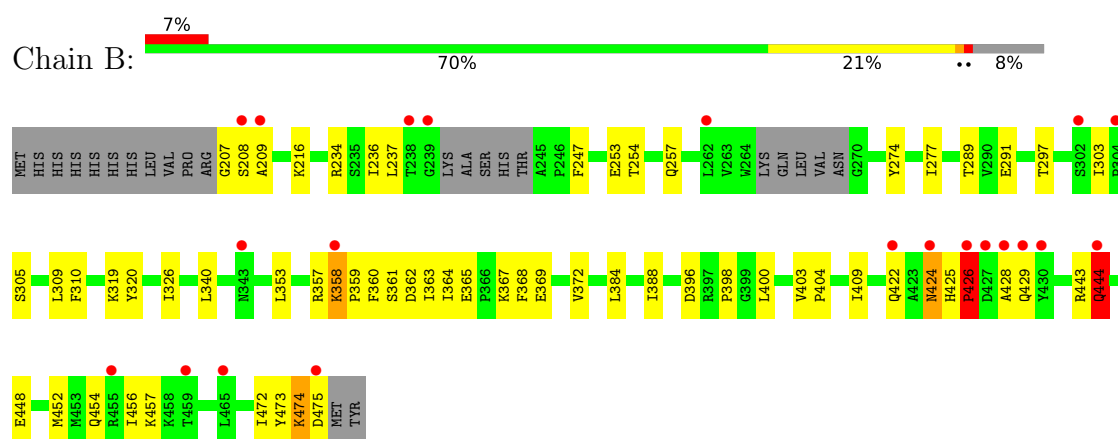
3 Residue-property plots

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	39.80Å 92.97Å 96.72Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	32.26 – 2.11 32.26 – 2.11	Depositor EDS
% Data completeness (in resolution range)	94.2 (32.26-2.11) 94.2 (32.26-2.11)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.230 0.199 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4553	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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: LOO, BOG

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	0.87	2/2134 (0.1%)	0.73	3/2889 (0.1%)
1	B	0.56	0/2106	0.95	8/2849 (0.3%)
All	All	0.73	2/4240 (0.0%)	0.85	11/5738 (0.2%)

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	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	TYR	C-N	-29.40	0.95	1.33
1	A	429	GLN	C-N	-12.05	1.16	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	PRO	CB-CA-C	14.96	136.25	111.56
1	B	474	LYS	CB-CA-C	-12.81	91.91	109.71
1	B	443	ARG	CA-C-N	-9.96	103.53	122.06
1	B	443	ARG	C-N-CA	-9.96	103.53	122.06
1	B	444	GLN	CB-CG-CD	-9.92	95.74	112.60
1	B	357	ARG	CA-C-N	-9.46	103.68	122.40
1	B	357	ARG	C-N-CA	-9.46	103.68	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	LYS	CA-CB-CG	-7.59	98.93	114.10
1	A	378	GLU	N-CA-CB	-6.87	102.03	112.47
1	A	430	TYR	O-C-N	-6.64	111.94	121.91
1	A	378	GLU	CG-CD-OE2	-5.10	106.67	118.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	429	GLN	Mainchain
1	B	358	LYS	Peptide

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	2089	0	2100	40	0
1	B	2062	0	2071	56	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0
3	A	20	28	28	5	0
3	B	20	28	28	2	0
4	A	149	0	0	14	1
4	B	91	0	0	5	0
All	All	4497	56	4227	95	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (95) 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:474:LYS:HE3	1:B:475:ASP:OD1	1.16	1.33
1:B:474:LYS:CE	1:B:475:ASP:OD1	2.12	0.96
1:A:209:ALA:O	4:A:601:HOH:O	1.82	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LYS:HE3	1:B:475:ASP:CG	1.89	0.96
1:A:418:GLU:OE2	4:A:602:HOH:O	1.91	0.88
1:B:400:LEU:O	4:B:601:HOH:O	1.92	0.87
1:B:425:HIS:HB2	1:B:428:ALA:HB2	1.55	0.86
1:A:224:LYS:NZ	4:A:603:HOH:O	2.09	0.86
1:B:474:LYS:HG2	1:B:475:ASP:N	1.87	0.85
1:B:360:PHE:O	1:B:363:ILE:HG22	1.79	0.83
1:B:358:LYS:HD2	1:B:362:ASP:OD1	1.79	0.82
1:A:209:ALA:C	4:A:601:HOH:O	2.22	0.80
1:A:209:ALA:HB1	4:A:601:HOH:O	1.84	0.77
1:A:430:TYR:HE1	4:A:696:HOH:O	1.67	0.76
1:A:430:TYR:CE1	4:A:696:HOH:O	2.39	0.75
1:B:358:LYS:HD3	1:B:361:SER:OG	1.86	0.74
1:B:363:ILE:HG23	1:B:364:ILE:HG13	1.72	0.71
1:A:367:LYS:N	1:A:367:LYS:HD2	2.03	0.71
1:B:303:ILE:O	4:B:602:HOH:O	2.09	0.69
1:A:351:GLU:HB2	4:A:614:HOH:O	1.91	0.69
1:B:474:LYS:CE	1:B:475:ASP:CG	2.64	0.69
1:A:393:LEU:O	1:A:410:GLN:HB2	1.94	0.66
1:B:457:LYS:HD2	1:B:457:LYS:O	1.95	0.66
1:B:425:HIS:O	1:B:426:PRO:C	2.37	0.65
1:B:208:SER:O	4:B:604:HOH:O	2.13	0.65
1:B:363:ILE:HD12	1:B:452:MET:HE3	1.77	0.65
1:A:377:LEU:O	1:A:378:GLU:HB2	1.97	0.63
1:B:358:LYS:HB3	1:B:361:SER:H	1.61	0.63
1:A:403:VAL:O	1:A:407:GLU:HG3	2.00	0.62
1:B:253:GLU:O	1:B:257:GLN:HG3	2.00	0.62
1:A:284:ARG:HD3	4:A:684:HOH:O	1.99	0.61
1:B:444:GLN:O	1:B:448:GLU:HG3	2.01	0.60
1:A:245:ALA:HB1	1:A:246:PRO:HD2	1.84	0.59
3:A:502:BOG:H7'2	1:B:319:LYS:HB2	1.84	0.58
1:B:353:LEU:O	1:B:361:SER:HB3	2.03	0.58
1:B:234:ARG:NH1	4:B:605:HOH:O	2.32	0.57
1:B:289:THR:HG23	1:B:326:ILE:HD13	1.86	0.57
1:A:468:LEU:HD11	3:B:502:BOG:H6'1	1.86	0.56
1:A:310:PHE:HD1	3:A:502:BOG:H1'1	1.69	0.56
1:A:475:ASP:HB2	4:A:610:HOH:O	2.05	0.55
1:A:429:GLN:O	1:A:430:TYR:HB2	2.08	0.54
1:B:274:TYR:OH	1:B:277:ILE:HD12	2.08	0.54
1:B:291:GLU:HA	1:B:291:GLU:OE1	2.08	0.54
1:B:319:LYS:HD3	1:B:320:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:LYS:HA	1:B:360:PHE:H	1.73	0.52
1:A:367:LYS:HD2	1:A:367:LYS:H	1.71	0.52
1:A:430:TYR:O	1:A:431:LEU:C	2.50	0.52
1:B:368:PHE:O	1:B:372:VAL:HG22	2.09	0.51
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.46	0.51
1:A:309:LEU:O	3:A:502:BOG:H4	2.12	0.50
1:A:455:ARG:NH2	4:A:604:HOH:O	2.12	0.50
1:B:208:SER:O	1:B:209:ALA:HB3	2.10	0.50
1:B:444:GLN:NE2	1:B:448:GLU:HG2	2.26	0.50
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.94	0.49
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.77	0.49
1:B:358:LYS:HB3	1:B:361:SER:OG	2.12	0.49
1:B:474:LYS:HD3	1:B:475:ASP:OD2	2.12	0.49
1:B:365:GLU:O	1:B:369:GLU:HG3	2.13	0.49
1:B:454:GLN:O	1:B:457:LYS:HB3	2.12	0.49
1:B:424:ASN:HB3	1:B:425:HIS:CD2	2.48	0.48
1:A:209:ALA:CB	4:A:601:HOH:O	2.54	0.48
1:B:424:ASN:HB3	1:B:425:HIS:HD2	1.79	0.48
1:B:237:LEU:CD1	1:B:340:LEU:HD11	2.44	0.47
1:B:473:TYR:O	1:B:474:LYS:C	2.55	0.47
1:A:468:LEU:HD22	1:B:310:PHE:CE1	2.50	0.47
1:B:247:PHE:C	1:B:247:PHE:CD1	2.92	0.47
1:B:309:LEU:O	3:B:502:BOG:H4	2.16	0.46
1:B:367:LYS:HD2	1:B:367:LYS:N	2.29	0.46
1:B:403:VAL:HB	1:B:404:PRO:HD3	1.96	0.46
1:A:466:HIS:O	1:A:470:GLN:HG3	2.15	0.46
1:A:418:GLU:O	1:A:422:GLN:HG3	2.16	0.46
1:B:457:LYS:HD2	1:B:457:LYS:C	2.39	0.45
1:A:258:ALA:HB1	1:A:263:VAL:HB	1.97	0.45
1:A:359:PRO:HB2	4:A:673:HOH:O	2.16	0.45
1:A:313:ASP:OD1	1:A:401:MET:HB2	2.17	0.45
1:B:247:PHE:HE1	1:B:254:THR:HB	1.81	0.44
1:B:384:LEU:O	1:B:388:ILE:HG12	2.17	0.44
1:B:474:LYS:HG2	1:B:475:ASP:CG	2.44	0.43
3:A:502:BOG:H7'1	1:B:472:ILE:HG12	1.99	0.43
1:B:305:SER:HB3	1:B:409:ILE:HD11	2.00	0.43
3:A:502:BOG:H2'1	1:B:297:THR:OG1	2.19	0.43
1:A:363:ILE:HA	1:A:452:MET:CE	2.48	0.42
1:A:363:ILE:HD12	1:A:452:MET:HB2	2.01	0.42
1:A:425:HIS:O	1:A:428:ALA:HB2	2.19	0.42
1:B:207:GLY:N	4:B:614:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LYS:CD	1:B:475:ASP:CG	2.92	0.42
1:B:216:LYS:HD2	1:B:216:LYS:C	2.45	0.42
1:A:224:LYS:O	1:A:224:LYS:HG3	2.19	0.41
1:A:363:ILE:HA	1:A:452:MET:HE1	2.03	0.41
1:A:291:GLU:OE1	1:A:291:GLU:HA	2.20	0.41
1:A:359:PRO:HB2	4:A:641:HOH:O	2.21	0.41
1:A:363:ILE:HG13	1:A:452:MET:HE3	2.02	0.40
1:B:237:LEU:HD11	1:B:340:LEU:HG	2.03	0.40
1:B:359:PRO:HA	1:B:362:ASP:OD2	2.22	0.40
1:A:259:GLU:OE2	1:A:280:HIS:NE2	2.42	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:694:HOH:O	4:A:739:HOH:O[1_655]	1.83	0.37

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	258/282 (92%)	249 (96%)	9 (4%)	0	100	100
1	B	253/282 (90%)	244 (96%)	8 (3%)	1 (0%)	30	28
All	All	511/564 (91%)	493 (96%)	17 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	426	PRO

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	224/249 (90%)	220 (98%)	4 (2%)	51	59
1	B	221/249 (89%)	214 (97%)	7 (3%)	34	37
All	All	445/498 (89%)	434 (98%)	11 (2%)	42	47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	SER
1	A	275	LYS
1	A	361	SER
1	A	429	GLN
1	B	236	ILE
1	B	396	ASP
1	B	422	GLN
1	B	424	ASN
1	B	429	GLN
1	B	444	GLN
1	B	456	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	410	GLN
1	B	422	GLN
1	B	429	GLN
1	B	451	GLN

5.3.3 RNA ⓘ

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](#)

4 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$
3	BOG	A	502	-	20,20,20	1.26	1 (5%)	25,25,25	1.52	7 (28%)
2	LOO	B	501	-	35,35,35	5.00	20 (57%)	49,54,54	1.78	9 (18%)
2	LOO	A	501	-	35,35,35	4.92	20 (57%)	49,54,54	1.98	16 (32%)
3	BOG	B	502	-	20,20,20	1.24	2 (10%)	25,25,25	1.12	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BOG	A	502	-	-	7/11/31/31	0/1/1/1
2	LOO	B	501	-	-	3/25/41/41	0/3/3/3
2	LOO	A	501	-	-	6/25/41/41	0/3/3/3
3	BOG	B	502	-	-	4/11/31/31	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	LOO	C19-C18	9.70	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LOO	C19-C18	9.41	1.52	1.39
2	A	501	LOO	C15-C16	9.30	1.52	1.39
2	B	501	LOO	C15-C16	9.20	1.52	1.39
2	A	501	LOO	C19-C14	8.51	1.53	1.39
2	B	501	LOO	C4-C3	8.32	1.52	1.38
2	B	501	LOO	C6-C1	8.20	1.52	1.38
2	B	501	LOO	C19-C14	7.85	1.52	1.39
2	B	501	LOO	C3-C2	7.84	1.52	1.39
2	A	501	LOO	C6-C1	7.75	1.51	1.38
2	B	501	LOO	C1-C2	7.75	1.52	1.39
2	B	501	LOO	C15-C14	7.67	1.52	1.39
2	B	501	LOO	C17-C16	7.42	1.53	1.40
2	A	501	LOO	C11-N7	7.41	1.47	1.38
2	A	501	LOO	C17-C18	7.37	1.53	1.40
2	A	501	LOO	C3-C2	7.36	1.51	1.39
2	B	501	LOO	C17-C18	7.32	1.52	1.40
2	A	501	LOO	C4-C3	7.31	1.50	1.38
2	A	501	LOO	C1-C2	7.31	1.51	1.39
2	A	501	LOO	C17-C16	7.30	1.52	1.40
2	B	501	LOO	C11-N7	7.24	1.46	1.38
2	B	501	LOO	C6-C5	7.00	1.52	1.39
2	B	501	LOO	C4-C5	6.85	1.52	1.39
2	A	501	LOO	C4-C5	6.80	1.52	1.39
2	A	501	LOO	C6-C5	6.71	1.52	1.39
2	A	501	LOO	C15-C14	6.48	1.50	1.39
2	A	501	LOO	C9-N10	3.97	1.44	1.38
2	A	501	LOO	C8-N7	-3.94	1.42	1.46
3	B	502	BOG	O5-C1	3.79	1.51	1.41
3	A	502	BOG	O5-C1	3.53	1.50	1.41
2	B	501	LOO	C11-N10	3.34	1.46	1.39
2	A	501	LOO	O22-C23	-3.32	1.40	1.45
2	B	501	LOO	C9-N10	3.30	1.43	1.38
2	B	501	LOO	O22-C23	-2.78	1.40	1.45
2	B	501	LOO	C8-N7	-2.58	1.44	1.46
2	A	501	LOO	O26-C9	-2.54	1.17	1.23
2	A	501	LOO	O22-C17	2.41	1.42	1.38
2	B	501	LOO	O13-C11	-2.36	1.18	1.22
2	A	501	LOO	C11-N10	2.30	1.44	1.39
2	B	501	LOO	O26-C9	-2.24	1.18	1.23
2	A	501	LOO	C12-N10	-2.15	1.43	1.47
2	B	501	LOO	C12-N10	-2.08	1.43	1.47
3	B	502	BOG	O3-C3	2.06	1.48	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	LOO	C9-N10-C11	-5.14	108.51	111.83
2	A	501	LOO	C14-C12-N10	-5.05	104.63	113.09
2	A	501	LOO	C9-N10-C11	-4.65	108.83	111.83
2	B	501	LOO	C8-N7-C5	4.58	124.93	121.21
2	B	501	LOO	C14-C12-N10	-4.56	105.46	113.09
2	B	501	LOO	C9-C8-N7	4.37	107.19	102.36
2	A	501	LOO	C12-N10-C9	4.26	128.45	123.23
2	A	501	LOO	F29-C28-C2	-3.83	104.70	112.90
3	A	502	BOG	O5-C5-C4	3.44	115.89	109.70
2	A	501	LOO	C3-C2-C1	3.09	122.64	118.03
3	A	502	BOG	C1'-O1-C1	3.01	118.83	113.68
2	A	501	LOO	F30-C28-F27	2.90	116.23	105.77
2	A	501	LOO	O13-C11-N7	2.83	129.76	126.91
2	A	501	LOO	C6-C5-C4	2.81	124.54	119.18
2	A	501	LOO	C8-N7-C5	2.79	123.48	121.21
2	A	501	LOO	C3-C4-C5	-2.70	116.88	120.30
2	B	501	LOO	C12-N10-C9	2.70	126.53	123.23
2	A	501	LOO	C9-C8-N7	2.68	105.33	102.36
2	A	501	LOO	O26-C9-N10	2.58	126.71	123.94
2	A	501	LOO	C4-C5-N7	-2.52	116.56	120.18
2	A	501	LOO	C15-C16-C17	2.45	121.49	117.94
2	A	501	LOO	C1-C6-C5	-2.43	117.23	120.30
3	B	502	BOG	C1-O5-C5	2.41	118.44	113.72
2	A	501	LOO	C16-C15-C14	-2.36	119.56	122.22
3	A	502	BOG	C3-C4-C5	-2.31	106.04	110.23
3	A	502	BOG	O4-C4-C3	-2.22	105.13	110.38
3	A	502	BOG	C4-C3-C2	2.21	114.71	110.83
2	B	501	LOO	C18-C19-C14	-2.18	119.76	122.22
2	B	501	LOO	O26-C9-N10	2.12	126.21	123.94
2	B	501	LOO	C3-C2-C1	2.07	121.12	118.03
2	B	501	LOO	F27-C28-C2	-2.04	108.53	112.90
3	A	502	BOG	C1-C2-C3	2.03	114.28	110.01
3	A	502	BOG	C1-O5-C5	2.00	117.63	113.72

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LOO	O22-C23-C31-O33
3	A	502	BOG	O5-C5-C6-O6
3	A	502	BOG	O1-C1'-C2'-C3'

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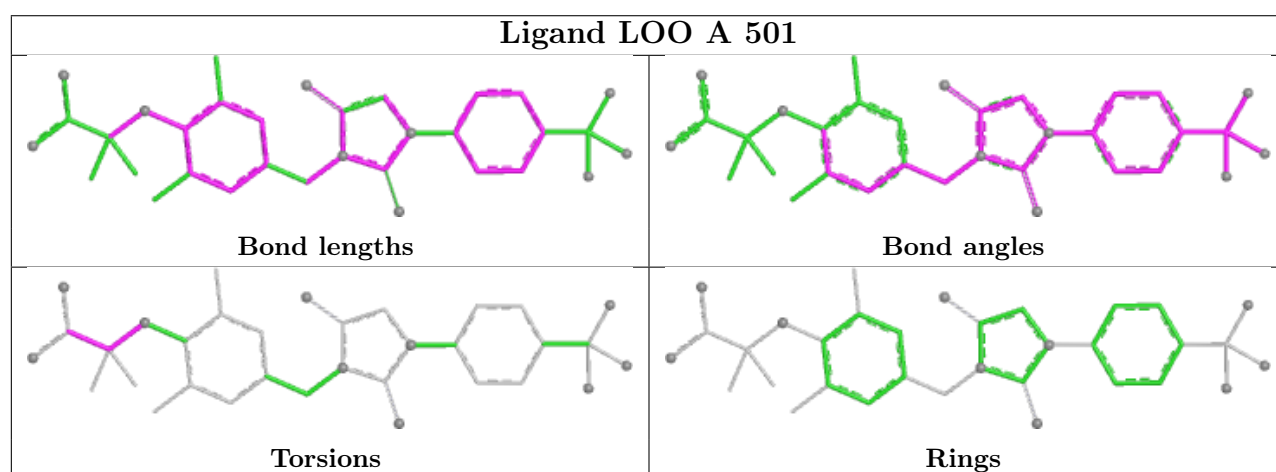
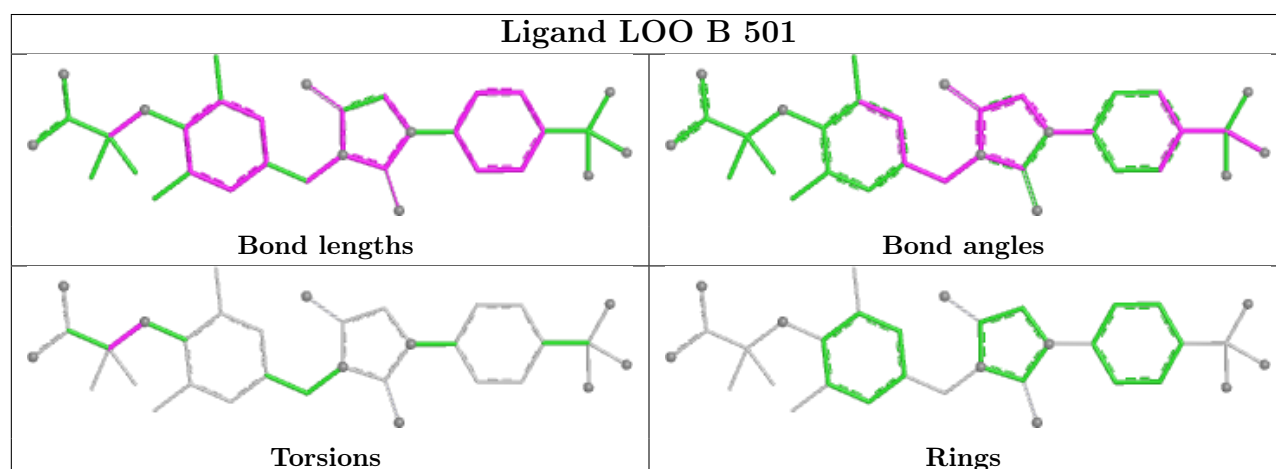
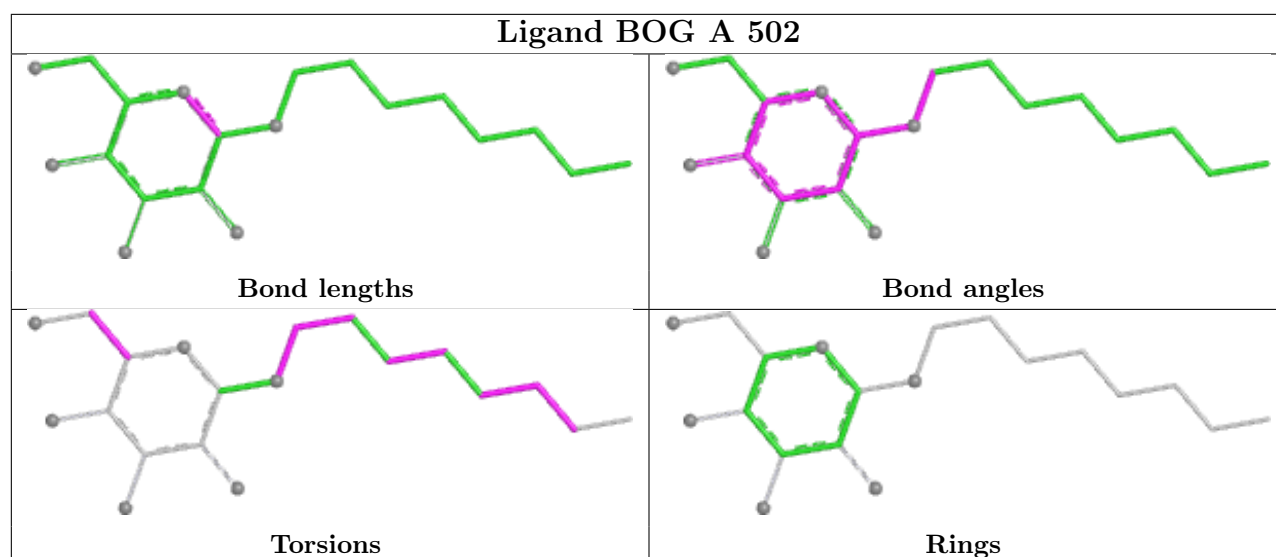
Mol	Chain	Res	Type	Atoms
3	A	502	BOG	C4-C5-C6-O6
3	B	502	BOG	O1-C1'-C2'-C3'
3	B	502	BOG	C2'-C3'-C4'-C5'
3	B	502	BOG	C3'-C4'-C5'-C6'
2	A	501	LOO	C24-C23-O22-C17
2	A	501	LOO	C25-C23-O22-C17
2	B	501	LOO	C24-C23-O22-C17
2	B	501	LOO	C25-C23-O22-C17
3	A	502	BOG	C2'-C1'-O1-C1
3	A	502	BOG	C4'-C5'-C6'-C7'
2	A	501	LOO	C31-C23-O22-C17
2	B	501	LOO	C31-C23-O22-C17
3	A	502	BOG	C2'-C3'-C4'-C5'
3	B	502	BOG	C4-C5-C6-O6
2	A	501	LOO	C25-C23-C31-O32
3	A	502	BOG	C5'-C6'-C7'-C8'
2	A	501	LOO	O22-C23-C31-O32

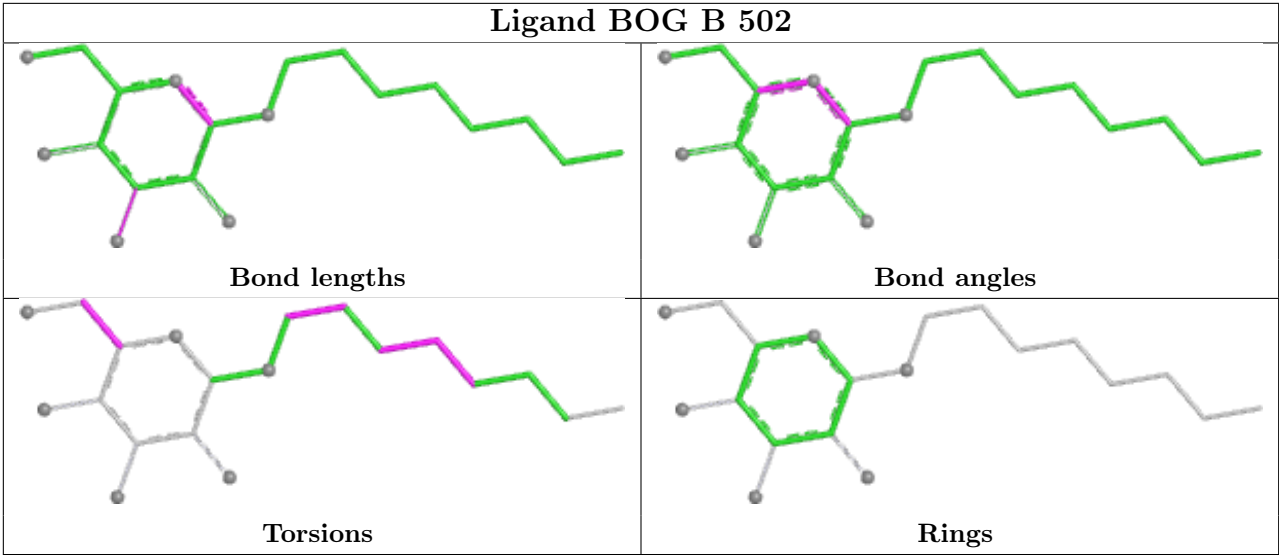
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	BOG	5	0
3	B	502	BOG	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	429:GLN	C	430:TYR	N	1.16
1	A	430:TYR	C	431:LEU	N	0.95

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	262/282 (92%)	0.30	13 (4%) 34 37	24, 40, 72, 103	0
1	B	259/282 (91%)	0.51	21 (8%) 18 19	28, 46, 73, 92	0
All	All	521/564 (92%)	0.41	34 (6%) 25 27	24, 42, 73, 103	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ALA	8.5
1	B	430	TYR	6.8
1	A	430	TYR	6.6
1	A	429	GLN	6.0
1	A	244	THR	5.8
1	B	429	GLN	5.8
1	A	274	TYR	5.1
1	A	428	ALA	4.6
1	B	426	PRO	4.4
1	A	239	GLY	4.4
1	A	209	ALA	3.8
1	B	427	ASP	3.6
1	B	208	SER	3.2
1	B	209	ALA	3.2
1	B	239	GLY	3.0
1	A	242	SER	3.0
1	B	444	GLN	3.0
1	B	455	ARG	3.0
1	B	424	ASN	3.0
1	B	304	PRO	2.9
1	B	262	LEU	2.7
1	B	302	SER	2.6
1	B	343	ASN	2.5
1	A	243	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	265	LYS	2.5
1	B	238	THR	2.5
1	B	465	LEU	2.5
1	A	217	HIS	2.4
1	A	262	LEU	2.4
1	B	422	GLN	2.4
1	B	358	LYS	2.3
1	A	245	ALA	2.3
1	B	475	ASP	2.1
1	B	459	THR	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](#)

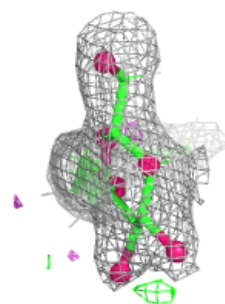
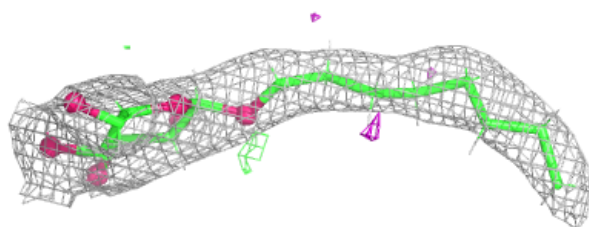
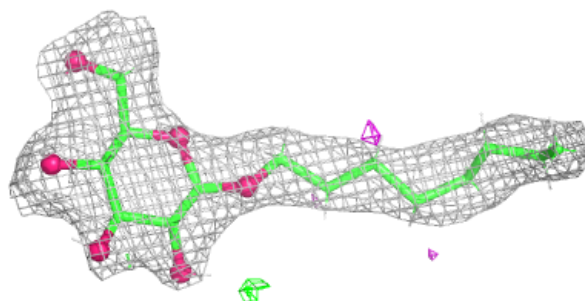
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BOG	A	502	20/20	0.89	0.10	41,56,71,88	0
2	LOO	B	501	33/33	0.91	0.11	31,41,52,63	0
3	BOG	B	502	20/20	0.91	0.10	40,56,69,70	0
2	LOO	A	501	33/33	0.95	0.07	26,32,40,43	0

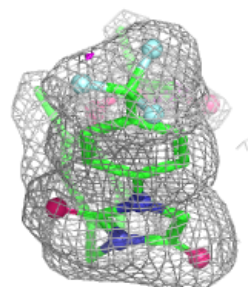
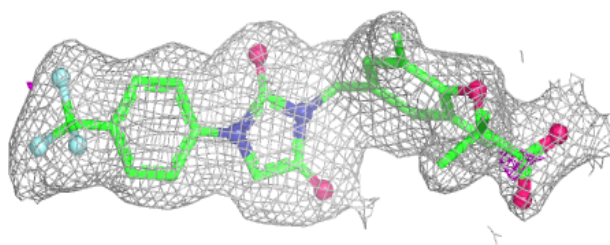
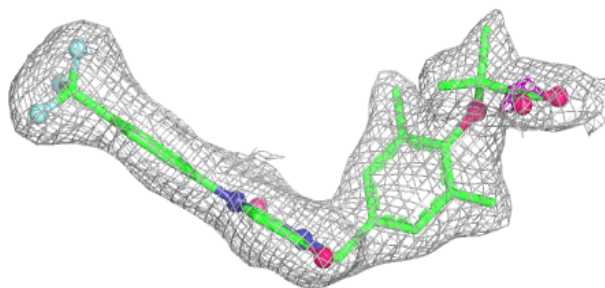
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 502:

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

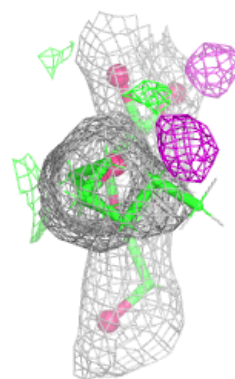
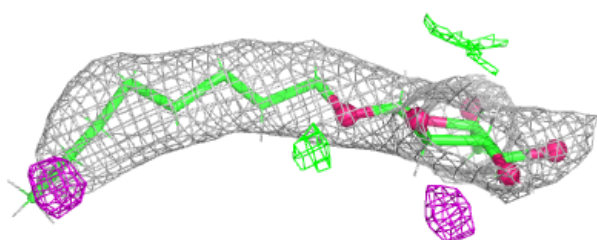
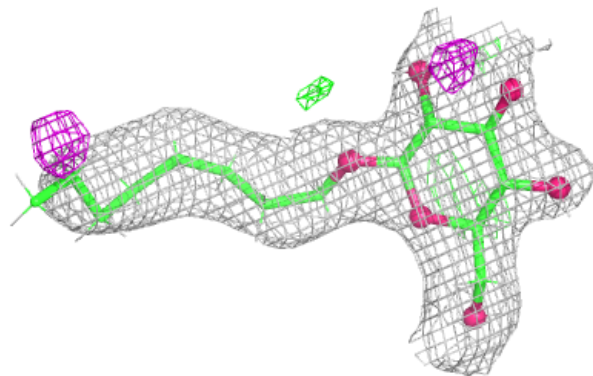
**Electron density around LOO B 501:**

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

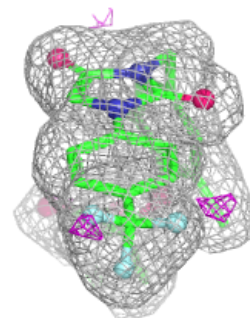
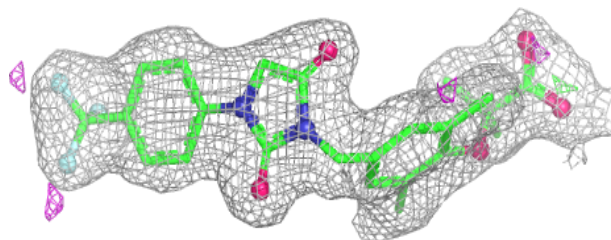
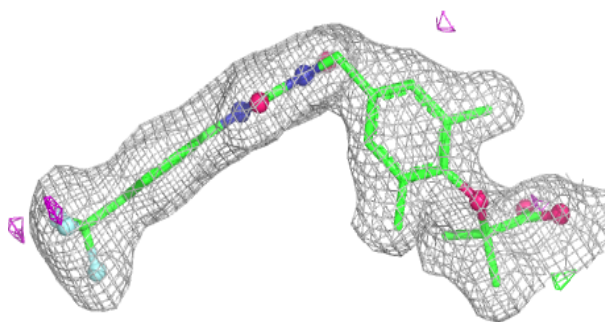


Electron density around BOG B 502:

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

**Electron density around LOO 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 [i](#)

There are no such residues in this entry.