



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 AM UTC

PDB ID : 6NX1 / pdb_00006nx1
Title : STRUCTURE OF HUMAN PREGNANE X RECEPTOR LIGAND BINDING DOMAIN BOUND TETHERED WITH SRC CO-ACTIVATOR PEPTIDE AND COMPOUND-3 AKA 1,1,1,3,3,3-HEXAFLUORO-2-{4-[1-(4-LUOROBENZENESULFONYL)CYCLOPENTYL]PHENYL}PROPAN-2-OL
Authors : Khan, J.A.
Deposited on : 2019-02-07
Resolution : 2.27 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](#) ①) 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

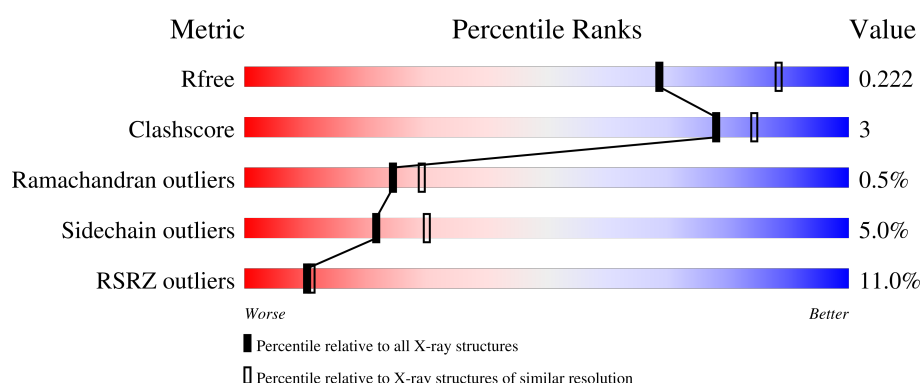
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	351	9% 72% 10% 18%
1	B	351	9% 77% 7% 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4686 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 Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1 fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	2	0
			2263	1464	380	399	20			
1	B	294	Total	C	N	O	S	0	1	0
			2275	1463	386	408	18			

There are 26 discrepancies between the modelled and reference sequences:

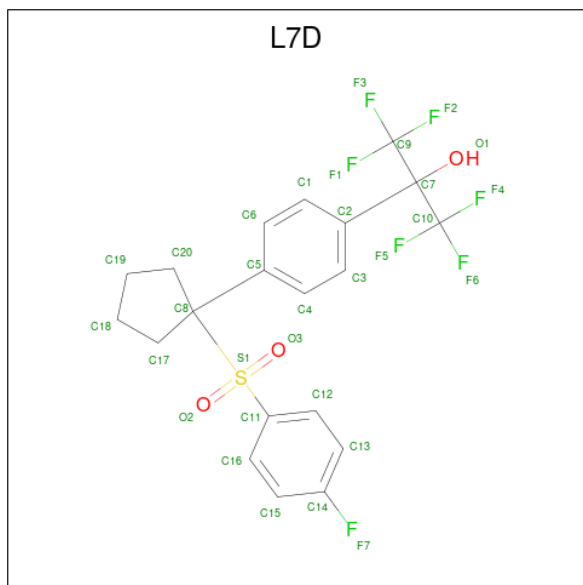
Chain	Residue	Modelled	Actual	Comment	Reference
A	123	HIS	-	expression tag	UNP O75469
A	124	HIS	-	expression tag	UNP O75469
A	125	HIS	-	expression tag	UNP O75469
A	126	HIS	-	expression tag	UNP O75469
A	127	HIS	-	expression tag	UNP O75469
A	128	HIS	-	expression tag	UNP O75469
A	129	GLY	-	expression tag	UNP O75469
A	432C	SER	-	linker	UNP O75469
A	432D	GLY	-	linker	UNP O75469
A	432E	GLY	-	linker	UNP O75469
A	432F	SER	-	linker	UNP O75469
A	432G	GLY	-	linker	UNP O75469
A	432H	GLY	-	linker	UNP O75469
B	123	HIS	-	expression tag	UNP O75469
B	124	HIS	-	expression tag	UNP O75469
B	125	HIS	-	expression tag	UNP O75469
B	126	HIS	-	expression tag	UNP O75469
B	127	HIS	-	expression tag	UNP O75469
B	128	HIS	-	expression tag	UNP O75469
B	129	GLY	-	expression tag	UNP O75469
B	432C	SER	-	linker	UNP O75469
B	432D	GLY	-	linker	UNP O75469
B	432E	GLY	-	linker	UNP O75469
B	432F	SER	-	linker	UNP O75469

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Chain	Residue	Modelled	Actual	Comment	Reference
B	432G	GLY	-	linker	UNP O75469
B	432H	GLY	-	linker	UNP O75469

- Molecule 2 is 1,1,1,3,3,3-hexafluoro-2-(4-{1-[(4-fluorophenyl)sulfonyl]cyclopentyl}phenyl)propan-2-ol (CCD ID: L7D) (formula: C₂₀H₁₇F₇O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	O	S	0	1
			62	40	14	6	2		
2	B	1	Total	C	F	O	S	0	0
			25	15	6	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	29	Total	O	0	0
			29	29		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.19Å 89.61Å 106.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.10 – 2.27 42.10 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.10-2.27) 99.8 (42.10-2.27)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.02	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.211 , 0.240 0.218 , 0.222	Depositor DCC
R_{free} test set	1842 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4686	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: L7D

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	0.84	0/2315	1.29	4/3130 (0.1%)
1	B	0.85	0/2328	1.31	2/3151 (0.1%)
All	All	0.84	0/4643	1.30	6/6281 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	GLY	CA-C-N	5.91	132.33	121.70
1	B	314	GLY	C-N-CA	5.91	132.33	121.70
1	A	155	MET	CA-C-N	5.46	127.54	120.44
1	A	155	MET	C-N-CA	5.46	127.54	120.44
1	A	450	LYS	N-CA-C	5.20	116.94	111.28
1	A	162	PHE	CA-CB-CG	5.19	118.99	113.80

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	2263	0	2204	15	0
1	B	2275	0	2176	10	0
2	A	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	0	0	0
3	A	32	0	0	0	0
3	B	29	0	0	0	0
All	All	4686	0	4380	25	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 3.

All (25) 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:289:ASN:HD22	1:B:327:HIS:HD1	1.41	0.68
1:B:214:GLN:HE21	1:B:216:ARG:HH11	1.41	0.66
1:B:155:MET:HA	1:B:155:MET:CE	2.28	0.64
1:B:254:ILE:HD12	1:B:283:LEU:HB3	1.80	0.63
1:A:202:VAL:HG11	1:A:417:ILE:HD11	1.82	0.61
1:B:445:LEU:O	1:B:449:HIS:HD2	1.88	0.56
1:A:445:LEU:O	1:A:449:HIS:CD2	2.59	0.56
1:A:213:LEU:HD21	1:A:304:LEU:HD23	1.89	0.55
1:A:445:LEU:O	1:A:449:HIS:HD2	1.90	0.55
1:B:254:ILE:HD11	1:B:287:ARG:HD2	1.89	0.54
1:A:214:GLN:HE21	1:A:216:ARG:HH11	1.57	0.53
1:A:289:ASN:HD22	1:A:327:HIS:HD1	1.56	0.53
1:B:202:VAL:HG11	1:B:417:ILE:HD11	1.90	0.53
1:B:155:MET:HA	1:B:155:MET:HE3	1.90	0.53
1:A:254:ILE:HD11	1:A:287:ARG:HD2	1.91	0.52
1:A:150:MET:HE1	1:A:368:GLN:HB3	1.92	0.51
1:A:254:ILE:HD12	1:A:283:LEU:HB3	1.95	0.48
1:A:159:MET:HE3	1:A:160:LYS:HG3	1.96	0.47
1:A:279:ALA:HB1	1:A:283:LEU:HD13	1.98	0.45
1:A:163:ASP:OD2	1:A:249:TYR:OH	2.31	0.45
1:A:277:LYS:HD2	1:A:449:HIS:CE1	2.51	0.45
1:A:285:GLN:NE2	1:A:327:HIS:NE2	2.68	0.42
1:B:254:ILE:CD1	1:B:287:ARG:HD2	2.50	0.42
1:B:445:LEU:O	1:B:449:HIS:CD2	2.70	0.41
1:A:202:VAL:HG21	1:A:417:ILE:HG12	2.03	0.41

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	282/351 (80%)	271 (96%)	10 (4%)	1 (0%)	30	36
1	B	289/351 (82%)	277 (96%)	10 (4%)	2 (1%)	18	21
All	All	571/702 (81%)	548 (96%)	20 (4%)	3 (0%)	24	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	LYS
1	A	230	ASP
1	B	315	PHE

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	235/310 (76%)	223 (95%)	12 (5%)	21	29
1	B	231/310 (74%)	220 (95%)	11 (5%)	23	32
All	All	466/620 (75%)	443 (95%)	23 (5%)	22	31

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LEU
1	A	207	CYS
1	A	213	LEU

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Mol	Chain	Res	Type
1	A	243	MET
1	A	260	VAL
1	A	308	LEU
1	A	317	GLN
1	A	358	GLN
1	A	402	SER
1	A	406	GLN
1	A	444	SER
1	A	457	GLN
1	B	155	MET
1	B	167	SER
1	B	213	LEU
1	B	224	ASN
1	B	243	MET
1	B	265	ARG
1	B	269	ILE
1	B	308	LEU
1	B	341	VAL
1	B	381	ARG
1	B	460	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	272	GLN
1	A	285	GLN
1	A	289	ASN
1	A	449	HIS
1	A	457	GLN
1	B	214	GLN
1	B	224	ASN
1	B	272	GLN
1	B	289	ASN
1	B	383	GLN
1	B	404	ASN
1	B	449	HIS

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](#)

3 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	L7D	A	501[B]	-	32,33,33	0.64	1 (3%)	48,54,54	0.74	2 (4%)
2	L7D	B	501	-	24,26,33	0.56	0	35,44,54	1.02	3 (8%)
2	L7D	A	501[A]	-	32,33,33	1.04	2 (6%)	48,54,54	0.94	2 (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
2	L7D	A	501[B]	-	-	9/45/54/54	0/3/3/3
2	L7D	B	501	-	-	4/36/48/54	0/2/2/3
2	L7D	A	501[A]	-	-	4/45/54/54	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	L7D	C17-C8	5.08	1.59	1.55
2	A	501[B]	L7D	C17-C8	2.64	1.57	1.55
2	A	501[A]	L7D	C7-C2	2.47	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	L7D	C6-C5-C8	4.14	123.17	120.61
2	A	501[B]	L7D	C9-C7-C2	3.23	115.89	110.42
2	A	501[A]	L7D	C9-C7-C2	3.07	115.61	110.42
2	A	501[A]	L7D	C4-C5-C8	2.96	122.44	120.61
2	B	501	L7D	C4-C5-C8	-2.29	119.19	120.61
2	B	501	L7D	C9-C7-C2	2.28	114.28	110.42
2	A	501[B]	L7D	C6-C5-C8	2.14	121.93	120.61

There are no chirality outliers.

All (17) torsion outliers are listed below:

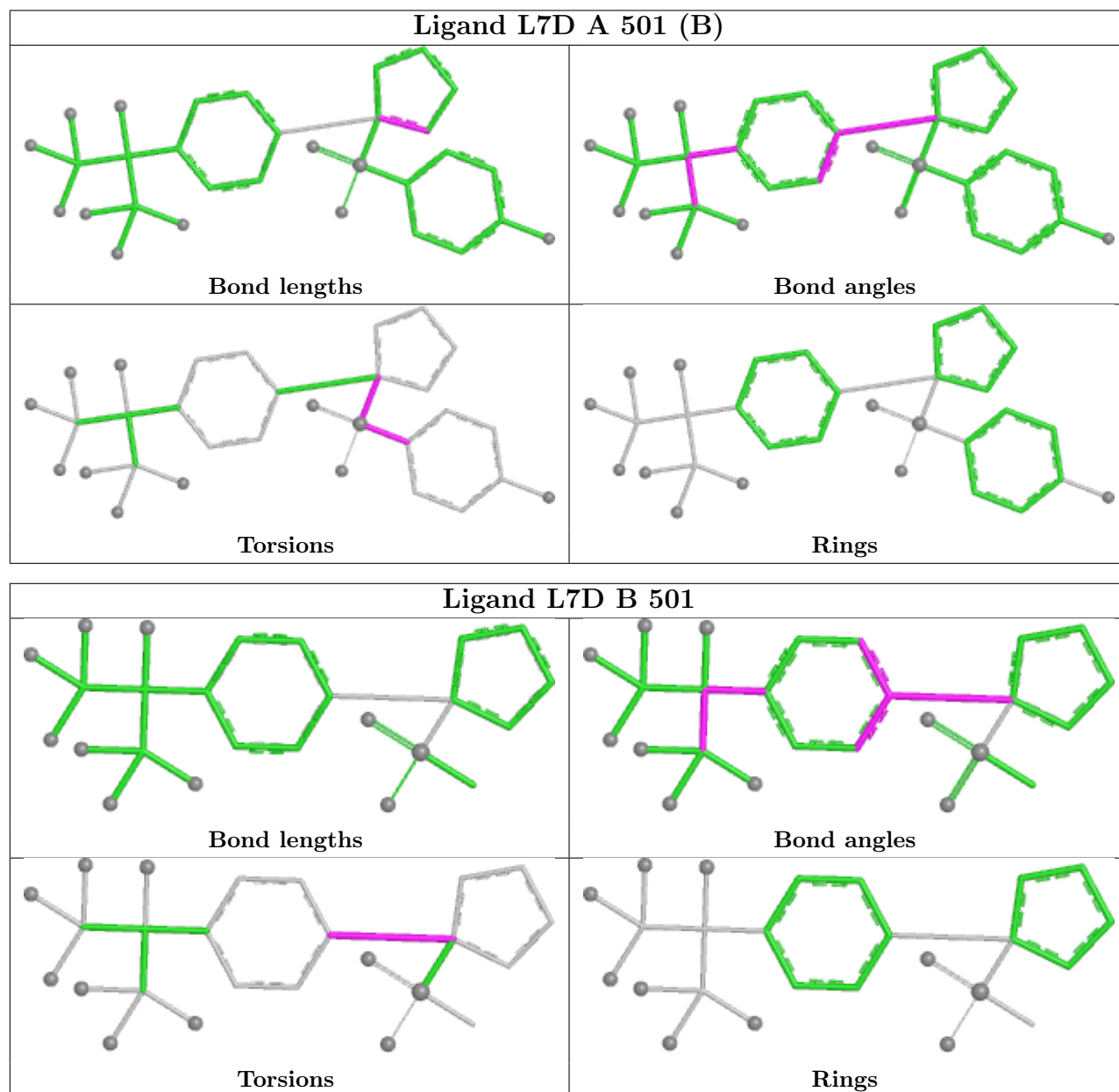
Mol	Chain	Res	Type	Atoms
2	A	501[B]	L7D	C17-C8-S1-O2
2	A	501[B]	L7D	C20-C8-S1-O2
2	A	501[B]	L7D	C20-C8-S1-O3
2	A	501[B]	L7D	C5-C8-S1-O2
2	B	501	L7D	C6-C5-C8-C20
2	A	501[B]	L7D	C20-C8-S1-C11
2	A	501[A]	L7D	C4-C5-C8-C20
2	A	501[A]	L7D	C4-C5-C8-C17
2	A	501[A]	L7D	C6-C5-C8-C17
2	B	501	L7D	C4-C5-C8-C17
2	B	501	L7D	C4-C5-C8-C20
2	B	501	L7D	C6-C5-C8-C17
2	A	501[A]	L7D	C6-C5-C8-S1
2	A	501[B]	L7D	C17-C8-S1-C11
2	A	501[B]	L7D	C5-C8-S1-C11
2	A	501[B]	L7D	C12-C11-S1-O2
2	A	501[B]	L7D	C16-C11-S1-O2

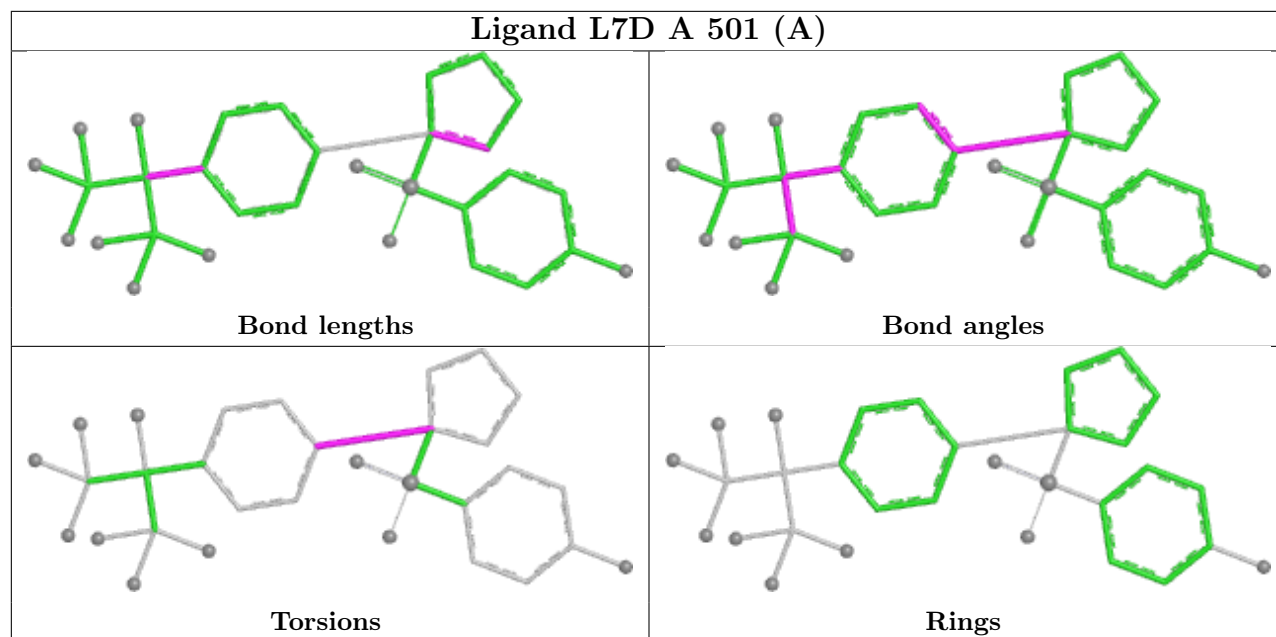
There are no ring outliers.

No monomer is involved in short contacts.

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	288/351 (82%)	0.71	32 (11%)	10 11	22, 60, 95, 136	2 (0%)
1	B	294/351 (83%)	0.68	32 (10%)	10 11	28, 61, 97, 119	1 (0%)
All	All	582/702 (82%)	0.69	64 (10%)	10 11	22, 60, 96, 136	3 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	8.1
1	B	178	LEU	5.7
1	A	310	ASP	5.5
1	B	460	SER	5.3
1	B	445	LEU	5.3
1	A	318	LEU	5.2
1	A	432	THR	5.0
1	A	311	THR	4.9
1	B	357	LEU	4.3
1	A	199	TRP	4.2
1	B	385	ALA	4.1
1	A	357	LEU	4.0
1	B	432	THR	4.0
1	B	234	LYS	3.9
1	A	458	GLU	3.8
1	A	177	VAL	3.7
1	A	312	ALA	3.5
1	B	315	PHE	3.5
1	A	195	GLU	3.5
1	B	143	LEU	3.1
1	A	320	LEU	2.9
1	A	144	THR	2.9
1	B	195	GLU	2.9
1	B	384	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	149	MET	2.8
1	A	229	ALA	2.6
1	A	444	SER	2.6
1	A	143	LEU	2.6
1	A	141	GLN	2.6
1	B	215	LEU	2.6
1	A	309	GLU	2.6
1	B	199	TRP	2.6
1	B	229	ALA	2.6
1	A	361	VAL	2.6
1	B	150	MET	2.6
1	A	316	GLN	2.5
1	A	359	HIS	2.5
1	B	192	SER	2.5
1	A	384	PRO	2.5
1	B	231	SER	2.5
1	B	266	ASP	2.5
1	B	177	VAL	2.4
1	B	417	ILE	2.4
1	A	148	ARG	2.4
1	B	263	TYR	2.3
1	B	270	GLU	2.3
1	B	194	GLU	2.3
1	B	316	GLN	2.3
1	B	379	CYS	2.2
1	B	151	ILE	2.2
1	B	232	GLY	2.2
1	A	308	LEU	2.1
1	B	317	GLN	2.1
1	A	323	MET	2.1
1	A	445	LEU	2.1
1	B	455	LEU	2.1
1	A	263	TYR	2.1
1	B	237	PHE	2.1
1	B	142	GLY	2.1
1	B	448	ARG	2.1
1	A	385	ALA	2.1
1	A	362	VAL	2.1
1	A	201	GLN	2.0
1	A	203	ARG	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](#)

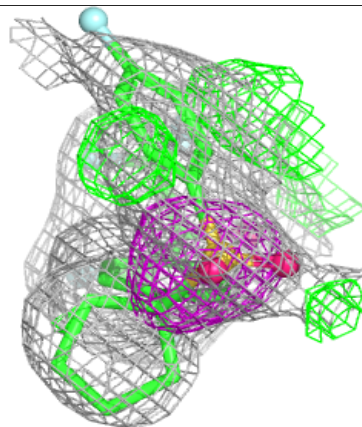
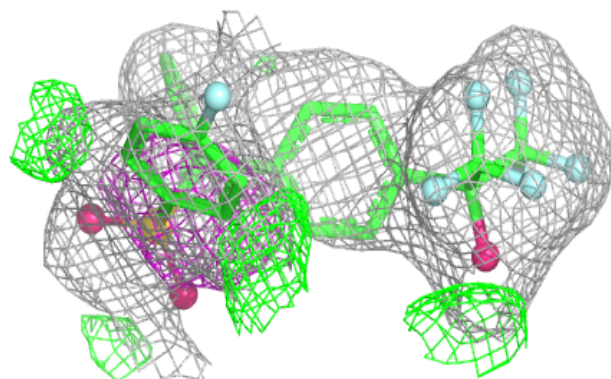
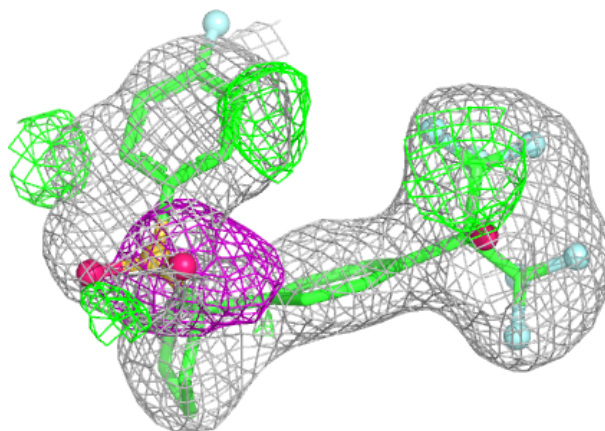
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	L7D	A	501[A]	31/31	0.86	0.18	51,62,84,87	31
2	L7D	A	501[B]	31/31	0.86	0.18	91,95,96,96	31
2	L7D	B	501	25/31	0.89	0.14	60,67,94,96	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.

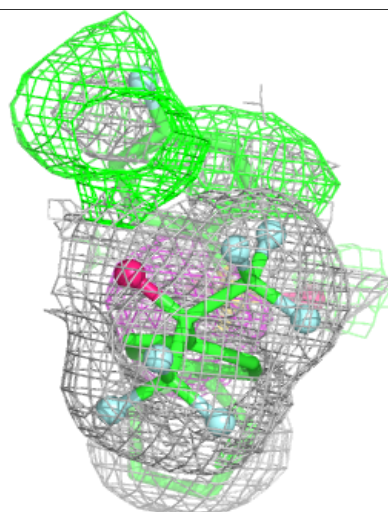
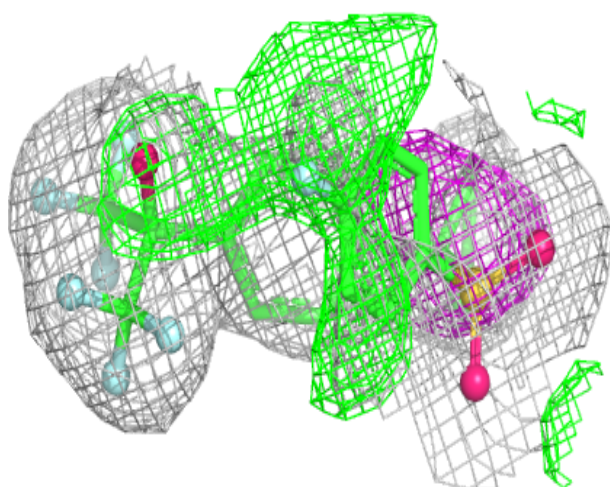
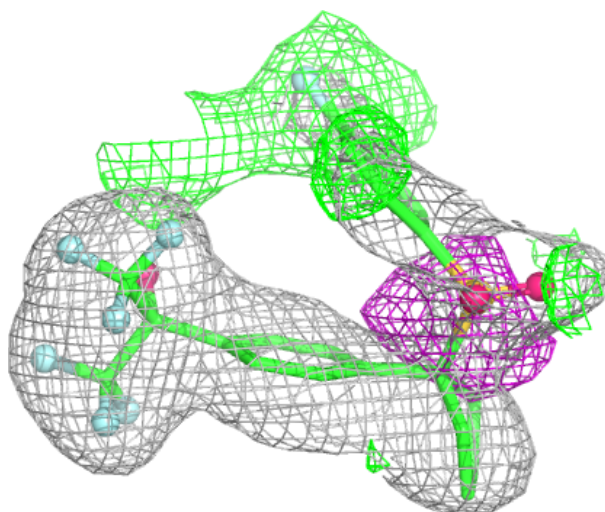
Electron density around L7D A 501 (A):

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



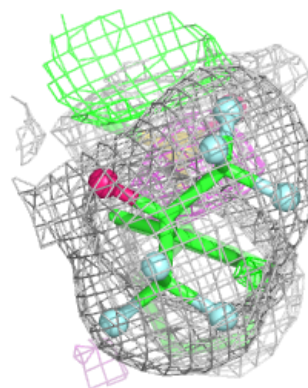
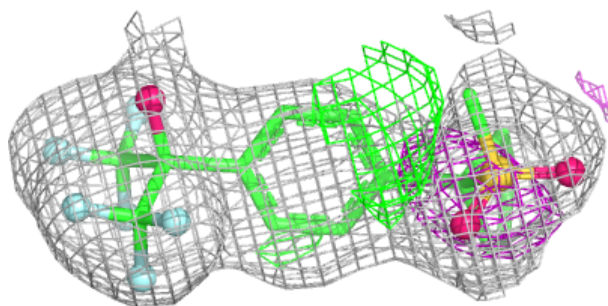
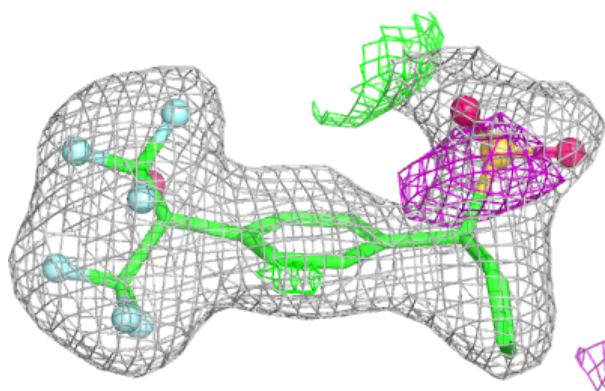
Electron density around L7D A 501 (B):

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



Electron density around L7D 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.