



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:39 AM UTC

PDB ID : 1PQC / pdb_00001pqc
Title : HUMAN LXR BETA HORMONE RECEPTOR COMPLEXED WITH
T0901317
Authors : Farnegardh, M.; Bonn, T.; Sun, S.; Ljunggren, J.; Ahola, H.; Wilhelmsson, A.;
Gustafsson, J.-A.; Carlquist, M.
Deposited on : 2003-06-18
Resolution : 2.80 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

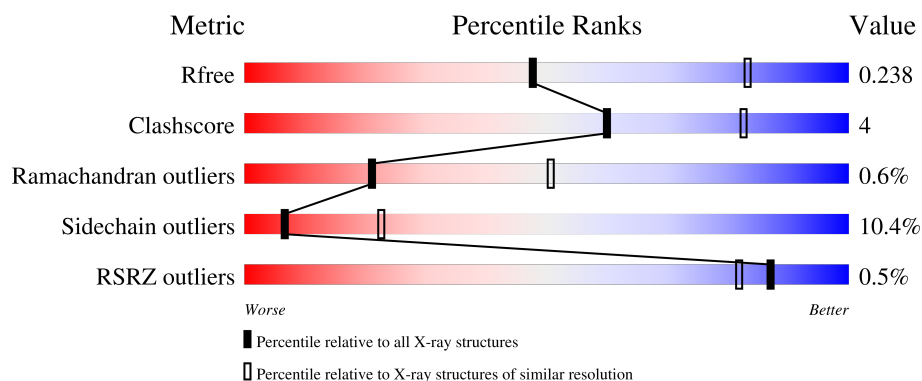
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	253	% 76% 14% • 8%
1	B	253	78% 15% 6%
1	C	253	70% 19% • 9%
1	D	253	% 69% 16% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7782 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.

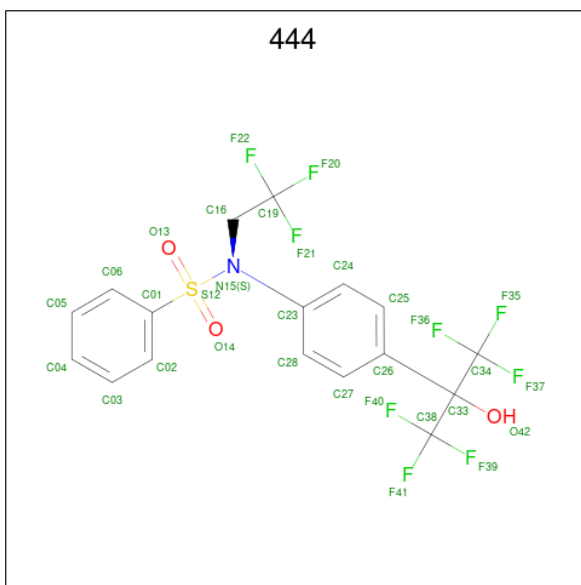
- Molecule 1 is a protein called Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1891	1210	331	343	7			
1	B	238	Total	C	N	O	S	0	0	0
			1925	1230	337	351	7			
1	C	231	Total	C	N	O	S	0	0	0
			1887	1207	333	340	7			
1	D	219	Total	C	N	O	S	0	0	0
			1774	1133	313	321	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	insertion	UNP P55055
A	210	SER	-	insertion	UNP P55055
A	211	HIS	-	insertion	UNP P55055
A	212	MET	-	insertion	UNP P55055
B	209	GLY	-	insertion	UNP P55055
B	210	SER	-	insertion	UNP P55055
B	211	HIS	-	insertion	UNP P55055
B	212	MET	-	insertion	UNP P55055
C	209	GLY	-	insertion	UNP P55055
C	210	SER	-	insertion	UNP P55055
C	211	HIS	-	insertion	UNP P55055
C	212	MET	-	insertion	UNP P55055
D	209	GLY	-	insertion	UNP P55055
D	210	SER	-	insertion	UNP P55055
D	211	HIS	-	insertion	UNP P55055
D	212	MET	-	insertion	UNP P55055

- Molecule 2 is N-(2,2,2-TRIFLUOROETHYL)-N-{4-[2,2,2-TRIFLUORO-1-HYDROXY-1-(TRIFLUOROMETHYL)ETHYL]PHENYL}BENZENESULFONAMIDE (CCD ID: 444) (formula: C₁₇H₁₂F₉NO₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 31	C 17	F 9	N 1	O 3	S 1	0	0
2	B	1	Total 31	C 17	F 9	N 1	O 3	S 1	0	0
2	C	1	Total 31	C 17	F 9	N 1	O 3	S 1	0	0
2	D	1	Total 31	C 17	F 9	N 1	O 3	S 1	0	0

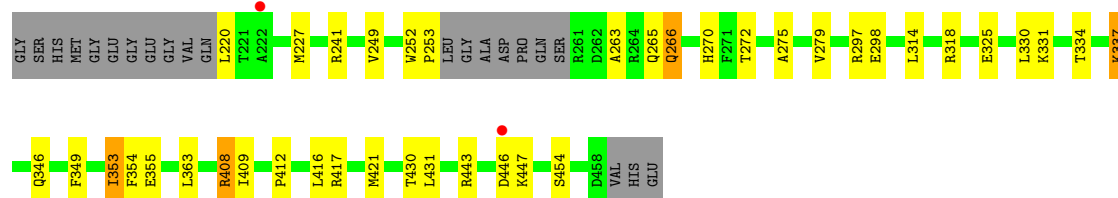
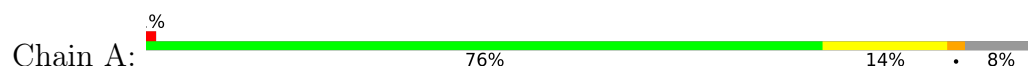
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	72	Total	O	0	0
			72	72		
3	C	52	Total	O	0	0
			52	52		
3	D	21	Total	O	0	0
			21	21		

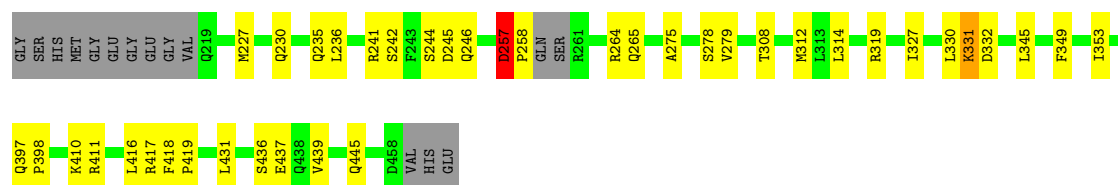
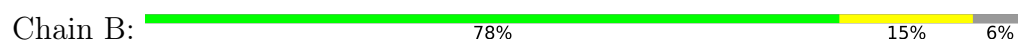
3 Residue-property plots [i](#)

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.

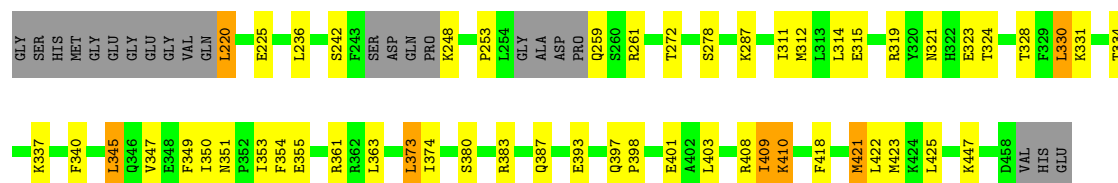
- Molecule 1: Oxysterols receptor LXR-beta



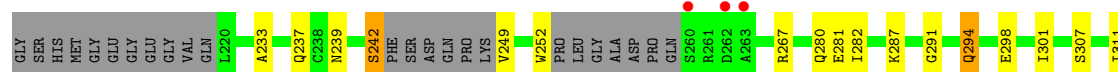
- Molecule 1: Oxysterols receptor LXR-beta



- Molecule 1: Oxysterols receptor LXR-beta



- Molecule 1: Oxysterols receptor LXR-beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.72Å 103.26Å 176.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.80) 99.9 (40.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.195 , 0.262 0.242 , 0.238	Depositor DCC
R_{free} test set	1353 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 20.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7782	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
444

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	0.90	1/1928 (0.1%)	1.05	2/2607 (0.1%)
1	B	0.94	1/1963 (0.1%)	1.01	0/2656
1	C	0.94	1/1922 (0.1%)	1.05	2/2595 (0.1%)
1	D	0.91	0/1804	1.04	1/2436 (0.0%)
All	All	0.92	3/7617 (0.0%)	1.04	5/10294 (0.0%)

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	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	312	MET	SD-CE	-7.24	1.61	1.79
1	A	421	MET	SD-CE	-6.88	1.62	1.79
1	C	421	MET	SD-CE	-6.17	1.64	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	361	ARG	CA-C-N	5.34	127.70	120.38
1	C	361	ARG	C-N-CA	5.34	127.70	120.38
1	A	346	GLN	N-CA-C	5.24	117.06	110.24
1	D	387	GLN	N-CA-C	5.05	116.87	111.36
1	A	297	ARG	N-CA-C	5.00	117.38	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	248	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	1891	0	1913	11	0
1	B	1925	0	1936	18	0
1	C	1887	0	1914	26	0
1	D	1774	0	1788	16	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
3	A	36	0	0	0	0
3	B	72	0	0	1	0
3	C	52	0	0	0	0
3	D	21	0	0	0	0
All	All	7782	0	7599	66	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 4.

All (66) 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:257:ASP:HB3	1:B:258:PRO:HD2	1.67	0.77
1:B:257:ASP:CB	1:B:258:PRO:HD2	2.18	0.73
1:C:409:ILE:O	1:C:410:LYS:C	2.35	0.68
1:C:351:ASN:O	1:C:355:GLU:HG3	1.98	0.64
1:C:403:LEU:HD11	1:C:421:MET:HE1	1.81	0.62
1:B:257:ASP:HB3	1:B:258:PRO:CD	2.30	0.61
1:B:257:ASP:CB	1:B:258:PRO:CD	2.78	0.60
1:D:233:ALA:O	1:D:237:GLN:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:MET:HE2	1:C:423:MET:HA	1.83	0.60
1:B:437:GLU:OE2	3:B:50:HOH:O	2.16	0.59
1:C:423:MET:HE1	1:D:425:LEU:HD12	1.85	0.58
1:A:349:PHE:CE1	1:A:353:ILE:HD11	2.38	0.58
1:D:252:TRP:CZ2	1:D:267:ARG:HD3	2.41	0.55
1:B:418:PHE:HB3	1:B:419:PRO:HD3	1.89	0.55
1:C:373:LEU:HD22	1:C:425:LEU:HD21	1.90	0.53
1:B:241:ARG:NH1	1:B:245:ASP:OD2	2.41	0.53
1:C:321:ASN:HD22	1:C:324:THR:H	1.56	0.53
1:D:242:SER:OG	1:D:281:GLU:OE2	2.19	0.53
1:C:418:PHE:CZ	1:C:422:LEU:HD11	2.44	0.52
1:B:246:GLN:HE22	1:B:332:ASP:HB2	1.75	0.52
1:C:315:GLU:OE1	1:C:319:ARG:NH1	2.42	0.52
1:A:253:PRO:HG2	1:A:263:ALA:HB1	1.91	0.52
1:C:330:LEU:O	1:C:331:LYS:C	2.50	0.51
1:C:349:PHE:CZ	1:C:353:ILE:HD11	2.46	0.51
1:D:291:GLY:O	1:D:294:GLN:HG2	2.11	0.51
1:C:311:ILE:HG12	1:C:374:ILE:HG23	1.92	0.51
1:D:252:TRP:CE2	1:D:267:ARG:HD3	2.46	0.50
1:A:416:LEU:CD1	1:B:397:GLN:HE21	2.25	0.50
1:C:401:GLU:HG2	1:D:416:LEU:HD21	1.93	0.49
1:C:397:GLN:HB3	1:C:398:PRO:HD3	1.93	0.49
1:B:397:GLN:HB3	1:B:398:PRO:HD3	1.94	0.49
1:A:263:ALA:HA	1:A:266:GLN:HB2	1.95	0.48
1:D:311:ILE:HG12	1:D:374:ILE:HG23	1.96	0.48
1:A:416:LEU:HD13	1:B:397:GLN:HE21	1.79	0.48
1:D:360:MET:HE1	1:D:424:LYS:HD2	1.93	0.48
1:B:410:LYS:HG2	1:B:411:ARG:HG2	1.96	0.48
1:C:345:LEU:N	1:C:345:LEU:HD23	2.29	0.48
1:C:409:ILE:HG22	1:C:410:LYS:N	2.30	0.47
1:C:220:LEU:HD13	1:C:225:GLU:CG	2.43	0.47
1:C:328:THR:HG23	1:C:334:THR:HG22	1.96	0.47
1:B:246:GLN:NE2	1:B:330:LEU:O	2.49	0.45
1:C:220:LEU:HD13	1:C:225:GLU:HG3	1.98	0.45
1:B:416:LEU:C	1:B:419:PRO:HD2	2.41	0.45
1:C:337:LYS:HG2	1:C:354:PHE:CD1	2.52	0.45
1:A:252:TRP:HE3	1:A:270:HIS:CD2	2.35	0.45
1:D:388:GLU:CD	1:D:391:ARG:HD3	2.42	0.44
1:C:321:ASN:HD21	1:C:323:GLU:HB3	1.83	0.44
1:C:401:GLU:CG	1:D:416:LEU:HD21	2.48	0.44
1:D:417:ARG:O	1:D:421:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LYS:HG3	1:A:354:PHE:CD1	2.53	0.43
1:B:257:ASP:O	1:B:258:PRO:C	2.62	0.43
1:D:349:PHE:CE1	1:D:353:ILE:HD11	2.53	0.43
1:C:380:SER:O	1:C:383:ARG:HG2	2.19	0.43
1:D:314:LEU:HD13	1:D:428:LEU:HD11	2.01	0.42
1:C:340:PHE:HB3	1:C:350:ILE:HG12	2.01	0.42
1:C:278:SER:HB2	1:C:312:MET:HE2	2.01	0.42
1:D:351:ASN:HB2	1:D:352:PRO:HD3	2.01	0.42
1:C:363:LEU:HD23	1:C:363:LEU:HA	1.93	0.41
1:D:282:ILE:HG12	1:D:311:ILE:HG21	2.01	0.41
1:A:252:TRP:CE3	1:A:270:HIS:CD2	3.09	0.41
1:A:275:ALA:O	1:A:279:VAL:HG23	2.20	0.41
1:B:275:ALA:O	1:B:279:VAL:HG23	2.20	0.41
1:A:408:ARG:O	1:A:412:PRO:HA	2.21	0.41
1:B:349:PHE:CZ	1:B:353:ILE:HD11	2.55	0.41
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.96	0.40
1:B:436:SER:HA	1:B:439:VAL:HG22	2.02	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	228/253 (90%)	221 (97%)	6 (3%)	1 (0%)	30	60
1	B	234/253 (92%)	227 (97%)	5 (2%)	2 (1%)	14	41
1	C	225/253 (89%)	216 (96%)	7 (3%)	2 (1%)	14	41
1	D	209/253 (83%)	202 (97%)	7 (3%)	0	100	100
All	All	896/1012 (88%)	866 (97%)	25 (3%)	5 (1%)	21	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	ASP
1	C	410	LYS
1	B	331	LYS
1	B	257	ASP
1	C	253	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	206/222 (93%)	181 (88%)	25 (12%)	5	16
1	B	208/222 (94%)	189 (91%)	19 (9%)	9	28
1	C	205/222 (92%)	188 (92%)	17 (8%)	10	32
1	D	191/222 (86%)	168 (88%)	23 (12%)	5	17
All	All	810/888 (91%)	726 (90%)	84 (10%)	7	22

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	LEU
1	A	227	MET
1	A	241	ARG
1	A	249	VAL
1	A	265	GLN
1	A	266	GLN
1	A	272	THR
1	A	298	GLU
1	A	314	LEU
1	A	318	ARG
1	A	325	GLU
1	A	330	LEU
1	A	331	LYS
1	A	334	THR
1	A	337	LYS
1	A	353	ILE
1	A	355	GLU

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Mol	Chain	Res	Type
1	A	408	ARG
1	A	409	ILE
1	A	417	ARG
1	A	430	THR
1	A	431	LEU
1	A	443	ARG
1	A	447	LYS
1	A	454	SER
1	B	227	MET
1	B	230	GLN
1	B	235	GLN
1	B	236	LEU
1	B	242	SER
1	B	244	SER
1	B	257	ASP
1	B	264	ARG
1	B	265	GLN
1	B	278	SER
1	B	308	THR
1	B	314	LEU
1	B	319	ARG
1	B	327	ILE
1	B	331	LYS
1	B	345	LEU
1	B	417	ARG
1	B	431	LEU
1	B	445	GLN
1	C	220	LEU
1	C	236	LEU
1	C	242	SER
1	C	259	GLN
1	C	261	ARG
1	C	272	THR
1	C	287	LYS
1	C	314	LEU
1	C	330	LEU
1	C	345	LEU
1	C	347	VAL
1	C	373	LEU
1	C	387	GLN
1	C	393	GLU
1	C	408	ARG

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Mol	Chain	Res	Type
1	C	409	ILE
1	C	447	LYS
1	D	239	ASN
1	D	242	SER
1	D	249	VAL
1	D	280	GLN
1	D	287	LYS
1	D	294	GLN
1	D	298	GLU
1	D	301	ILE
1	D	307	SER
1	D	314	LEU
1	D	321	ASN
1	D	342	ARG
1	D	348	GLU
1	D	353	ILE
1	D	408	ARG
1	D	411	ARG
1	D	413	GLN
1	D	423	MET
1	D	439	VAL
1	D	442	LEU
1	D	443	ARG
1	D	448	LYS
1	D	455	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	237	GLN
1	A	266	GLN
1	A	300	GLN
1	A	377	ASN
1	B	239	ASN
1	B	246	GLN
1	B	280	GLN
1	B	341	HIS
1	B	397	GLN
1	C	259	GLN
1	C	280	GLN
1	C	321	ASN

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Mol	Chain	Res	Type
1	C	397	GLN
1	D	235	GLN
1	D	265	GLN
1	D	294	GLN
1	D	387	GLN
1	D	396	GLN
1	D	415	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	444	C	3500	-	31,32,32	2.34	8 (25%)	52,52,52	1.97	11 (21%)
2	444	A	1500	-	31,32,32	2.61	10 (32%)	52,52,52	2.49	12 (23%)
2	444	B	2500	-	31,32,32	2.48	9 (29%)	52,52,52	2.30	10 (19%)
2	444	D	4500	-	31,32,32	2.04	8 (25%)	52,52,52	1.92	11 (21%)

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	444	C	3500	-	-	0/45/45/45	0/2/2/2
2	444	A	1500	-	-	1/45/45/45	0/2/2/2
2	444	B	2500	-	-	2/45/45/45	0/2/2/2
2	444	D	4500	-	-	4/45/45/45	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	444	S12-N15	11.01	1.80	1.65
2	B	2500	444	S12-N15	10.50	1.80	1.65
2	C	3500	444	S12-N15	9.04	1.77	1.65
2	D	4500	444	S12-N15	7.01	1.75	1.65
2	A	1500	444	C23-N15	4.18	1.50	1.44
2	B	2500	444	C23-N15	3.81	1.50	1.44
2	C	3500	444	C02-C01	3.62	1.44	1.38
2	A	1500	444	C02-C01	3.50	1.44	1.38
2	D	4500	444	C02-C01	3.48	1.44	1.38
2	C	3500	444	C25-C26	3.33	1.44	1.39
2	D	4500	444	C25-C26	3.26	1.44	1.39
2	C	3500	444	C23-N15	3.08	1.49	1.44
2	B	2500	444	C27-C26	2.96	1.44	1.39
2	B	2500	444	C02-C01	2.83	1.43	1.38
2	C	3500	444	C28-C23	2.79	1.44	1.39
2	D	4500	444	O42-C33	2.65	1.47	1.41
2	D	4500	444	C27-C26	2.61	1.43	1.39
2	B	2500	444	C33-C26	2.61	1.57	1.53
2	C	3500	444	C27-C26	2.56	1.43	1.39
2	A	1500	444	C28-C23	2.52	1.44	1.39
2	C	3500	444	C05-C04	2.49	1.43	1.38
2	D	4500	444	C28-C23	2.46	1.43	1.39
2	B	2500	444	C28-C23	2.42	1.43	1.39
2	A	1500	444	C05-C04	2.40	1.43	1.38
2	A	1500	444	C25-C26	2.40	1.43	1.39
2	A	1500	444	C27-C26	2.32	1.43	1.39
2	B	2500	444	O14-S12	2.26	1.45	1.43
2	D	4500	444	C05-C04	2.19	1.43	1.38
2	B	2500	444	C25-C26	2.16	1.42	1.39
2	A	1500	444	C33-C26	2.11	1.56	1.53
2	A	1500	444	C05-C06	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3500	444	O14-S12	2.09	1.45	1.43
2	B	2500	444	C05-C04	2.09	1.42	1.38
2	D	4500	444	C33-C26	2.05	1.56	1.53
2	A	1500	444	O42-C33	2.01	1.46	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	444	O13-S12-N15	9.26	117.47	106.69
2	B	2500	444	O14-S12-N15	8.61	116.72	106.69
2	A	1500	444	O14-S12-O13	-6.82	108.94	119.59
2	D	4500	444	C19-C16-N15	-6.61	105.72	112.14
2	C	3500	444	O14-S12-N15	6.55	114.31	106.69
2	A	1500	444	O14-S12-N15	6.11	113.80	106.69
2	B	2500	444	C16-N15-C23	-5.84	109.96	117.63
2	B	2500	444	O13-S12-N15	5.69	113.32	106.69
2	D	4500	444	O13-S12-N15	5.28	112.84	106.69
2	C	3500	444	C16-N15-C23	-5.24	110.76	117.63
2	D	4500	444	O13-S12-C01	-5.10	101.76	108.10
2	A	1500	444	C16-N15-C23	-5.05	110.99	117.63
2	A	1500	444	O13-S12-C01	-4.80	102.14	108.10
2	C	3500	444	O13-S12-N15	4.77	112.24	106.69
2	B	2500	444	O13-S12-C01	-4.55	102.44	108.10
2	C	3500	444	O14-S12-O13	-4.36	112.79	119.59
2	B	2500	444	O14-S12-O13	-4.25	112.96	119.59
2	B	2500	444	C38-C33-C34	-4.17	105.20	110.23
2	D	4500	444	C38-C33-C34	-4.02	105.38	110.23
2	C	3500	444	C01-S12-N15	-3.77	102.04	106.97
2	B	2500	444	C28-C23-N15	3.59	125.38	120.15
2	A	1500	444	F41-C38-C33	3.18	117.82	111.84
2	A	1500	444	C28-C23-N15	3.16	124.76	120.15
2	B	2500	444	C01-S12-N15	-3.10	102.91	106.97
2	C	3500	444	C38-C33-C34	-3.10	106.49	110.23
2	A	1500	444	C38-C33-C34	-3.08	106.51	110.23
2	C	3500	444	C28-C23-N15	3.06	124.61	120.15
2	D	4500	444	C16-N15-C23	-2.96	113.74	117.63
2	C	3500	444	F41-C38-C33	2.93	117.34	111.84
2	D	4500	444	C23-N15-S12	-2.83	112.03	117.72
2	A	1500	444	C27-C26-C33	2.77	126.53	120.35
2	A	1500	444	F22-C19-C16	-2.69	106.97	112.04
2	B	2500	444	C27-C26-C33	2.66	126.27	120.35
2	C	3500	444	C27-C26-C33	2.65	126.25	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	444	C16-N15-S12	-2.63	113.48	116.97
2	A	1500	444	C38-C33-C26	-2.47	106.25	110.42
2	D	4500	444	C24-C23-N15	-2.36	116.72	120.15
2	C	3500	444	C24-C23-N15	-2.29	116.81	120.15
2	B	2500	444	C24-C23-N15	-2.25	116.87	120.15
2	D	4500	444	F39-C38-C33	2.21	116.00	111.84
2	D	4500	444	F22-C19-C16	-2.13	108.02	112.04
2	D	4500	444	C34-C33-C26	2.09	113.96	110.42
2	C	3500	444	C34-C33-C26	2.01	113.81	110.42
2	D	4500	444	F40-C38-C33	-2.00	108.07	111.84

There are no chirality outliers.

All (7) torsion outliers are listed below:

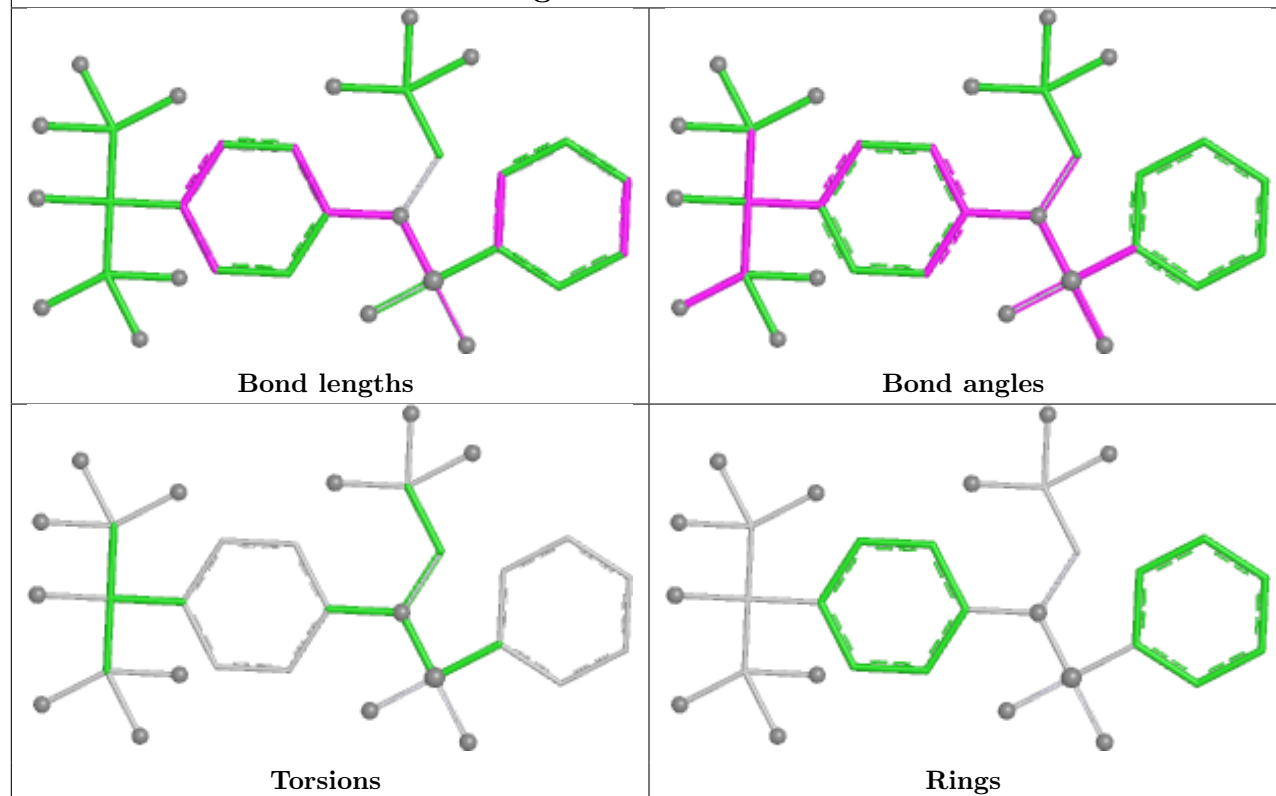
Mol	Chain	Res	Type	Atoms
2	D	4500	444	C16-N15-S12-O14
2	D	4500	444	C16-N15-S12-C01
2	D	4500	444	N15-C16-C19-F20
2	A	1500	444	C19-C16-N15-S12
2	B	2500	444	C25-C26-C33-C34
2	B	2500	444	C27-C26-C33-C34
2	D	4500	444	C19-C16-N15-S12

There are no ring outliers.

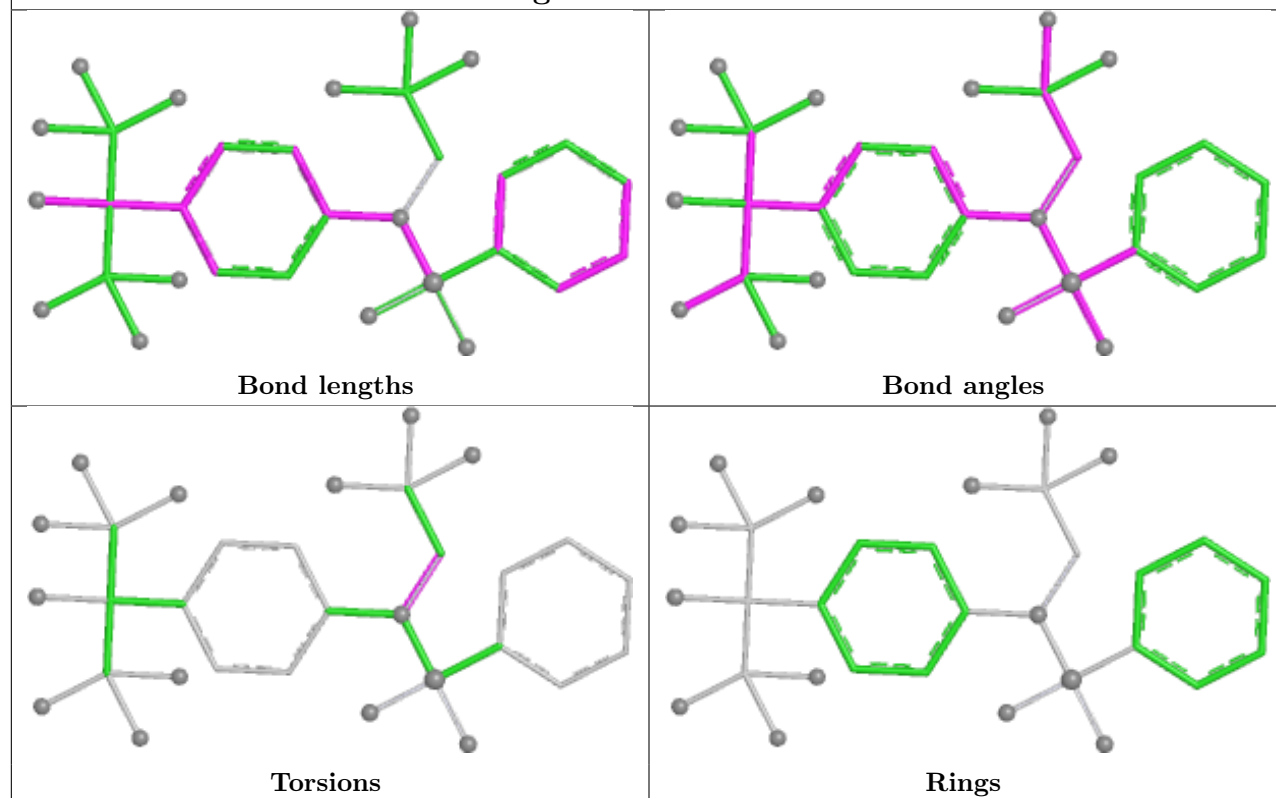
No monomer is involved in short contacts.

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.

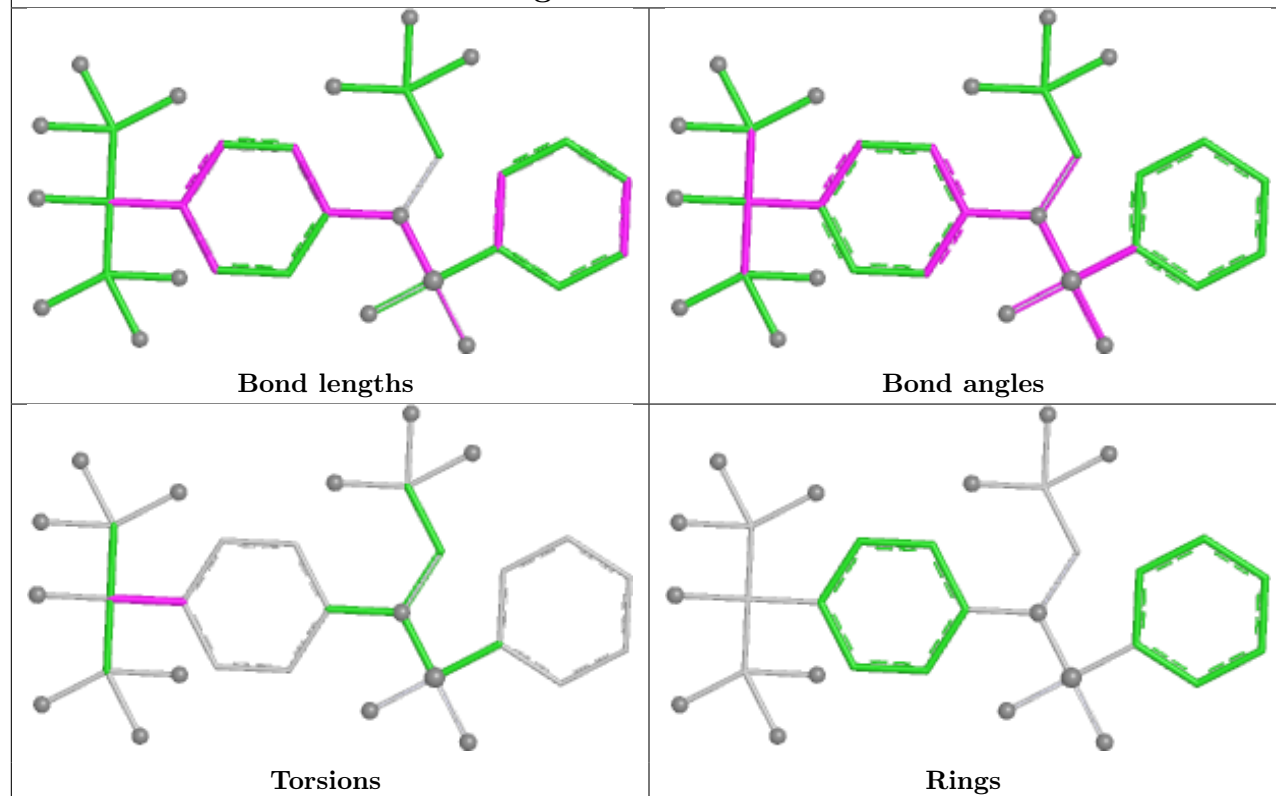
Ligand 444 C 3500



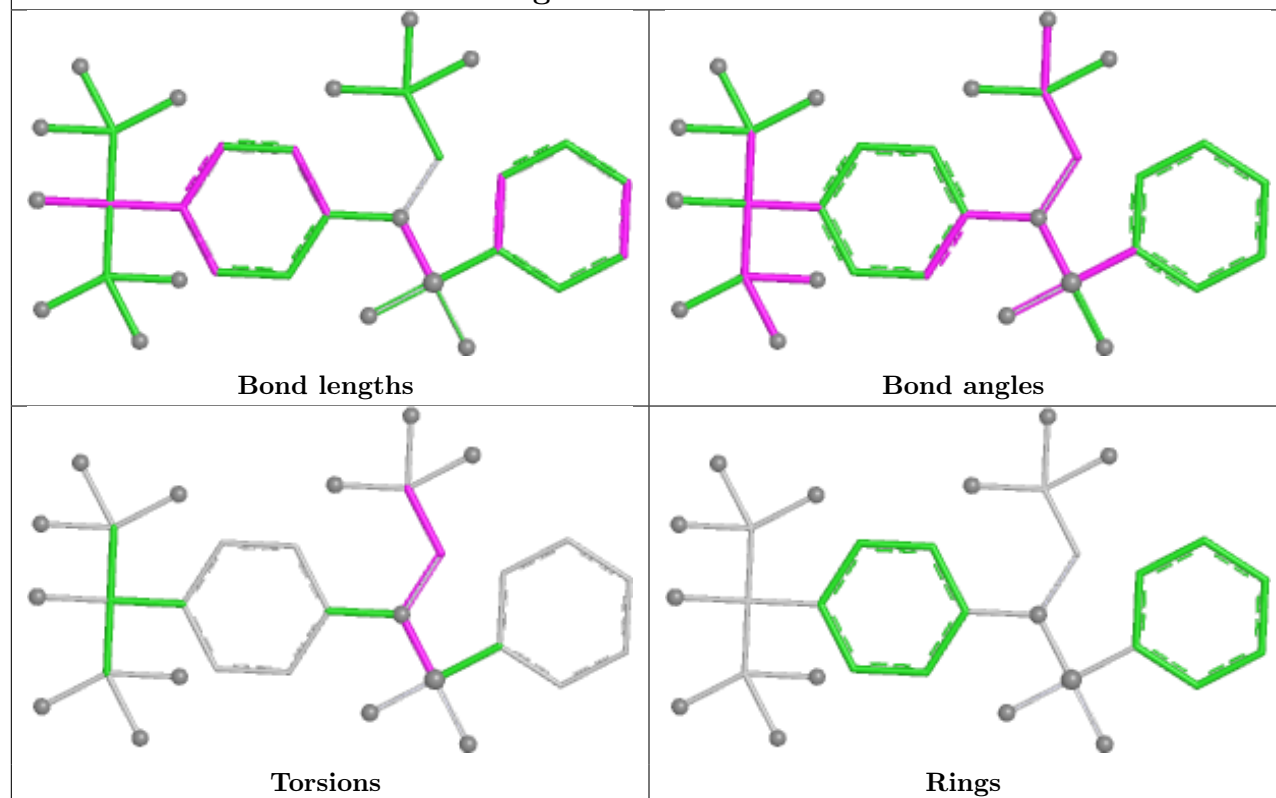
Ligand 444 A 1500



Ligand 444 B 2500



Ligand 444 D 4500



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	232/253 (91%)	-0.06	2 (0%) 81 74	13, 25, 36, 42	0
1	B	238/253 (94%)	-0.15	0 100 100	12, 23, 44, 57	0
1	C	231/253 (91%)	-0.12	0 100 100	13, 24, 39, 62	0
1	D	219/253 (86%)	0.05	3 (1%) 73 64	16, 23, 34, 48	0
All	All	920/1012 (90%)	-0.08	5 (0%) 87 82	12, 23, 39, 62	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	262	ASP	3.0
1	A	222	ALA	2.9
1	A	446	ASP	2.6
1	D	260	SER	2.4
1	D	263	ALA	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 [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,

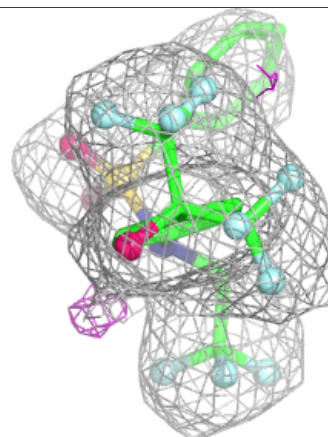
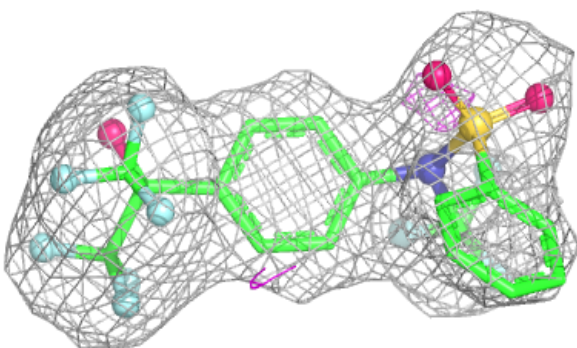
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	444	B	2500	31/31	0.94	0.09	18,27,51,52	0
2	444	D	4500	31/31	0.94	0.07	15,27,47,47	0
2	444	C	3500	31/31	0.95	0.09	19,27,51,51	0
2	444	A	1500	31/31	0.95	0.07	14,22,36,38	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.

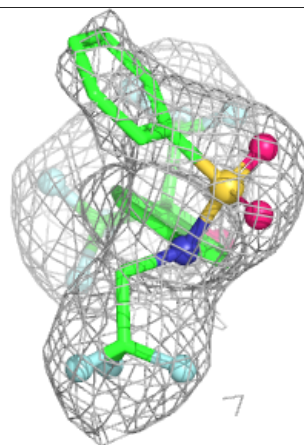
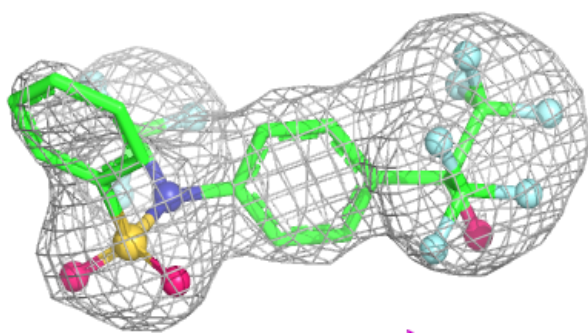
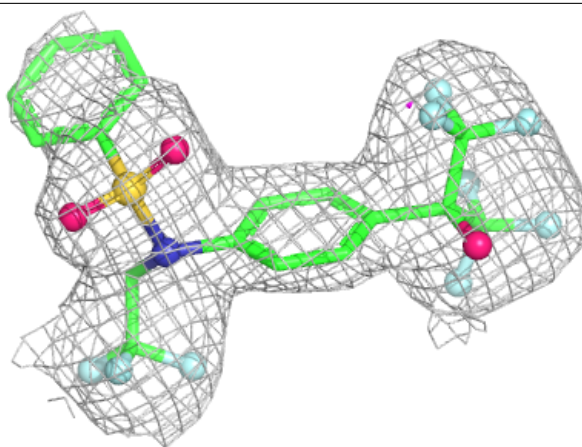
Electron density around 444 B 2500:

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



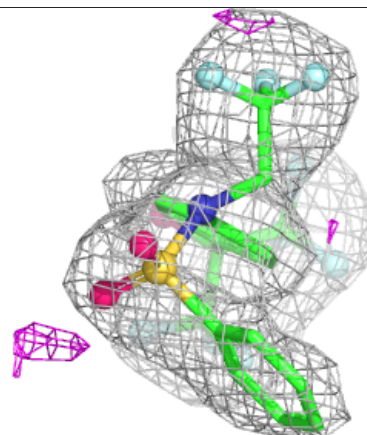
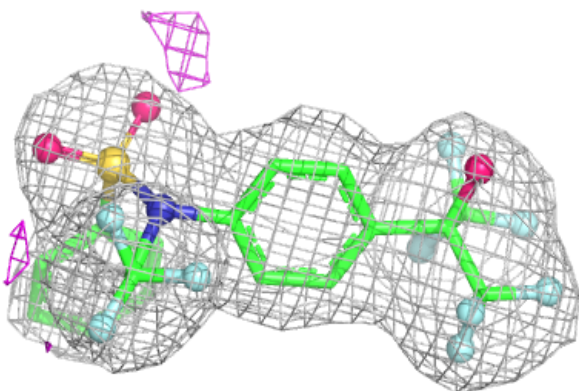
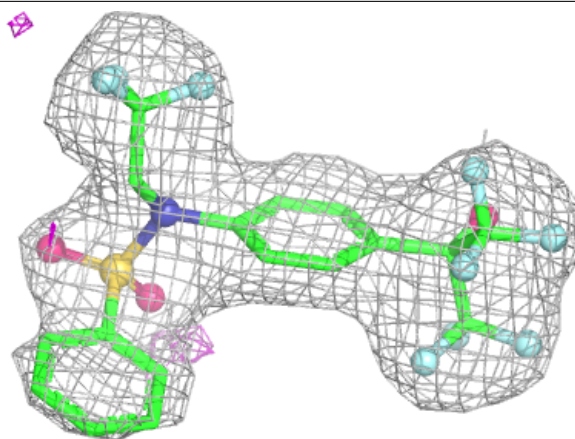
Electron density around 444 D 4500:

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



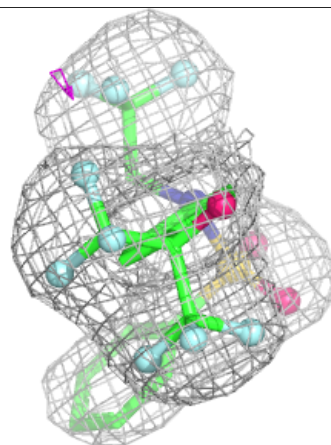
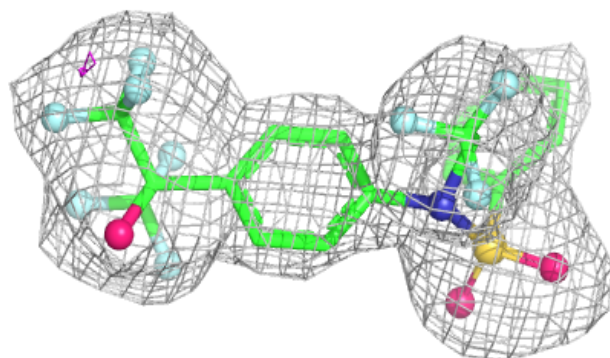
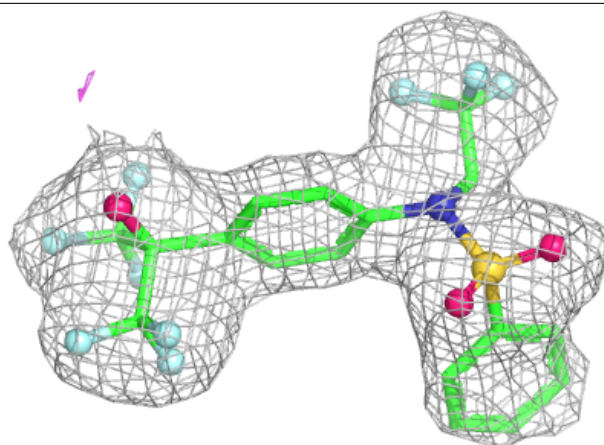
Electron density around 444 C 3500:

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



Electron density around 444 A 1500:

$2mF_o - DF_c$ (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.