Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 01:05 AM EDT

PDB ID	:	3ET2
Title	:	Structure of PPARdelta with 3-[5-Methoxy-1-(4-methoxy-benzenesulfonyl)-1 H-indol-3-yl]-propionic acid
Authors	:	Zhang, K.Y.J.; Wang, W.
Deposited on	:	2008-10-06
Resolution	:	2.24 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 (i) 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 (i)) were used in the production of this report:

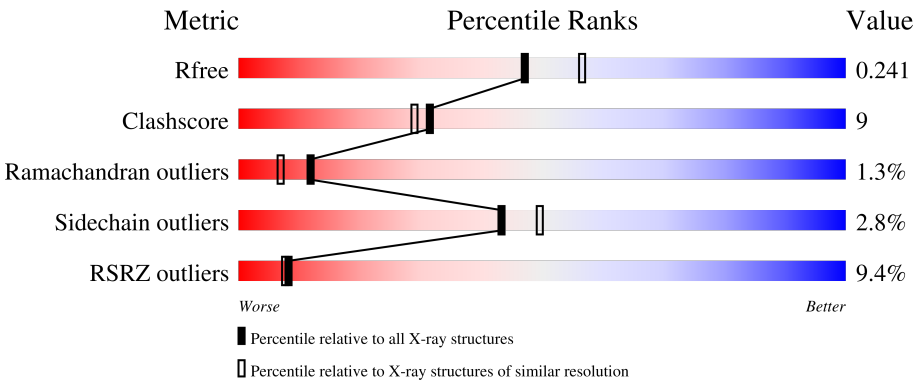
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 <=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	287	6% 70% 22% • 7%
1	B	287	12% 77% 14% •• 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4728 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.

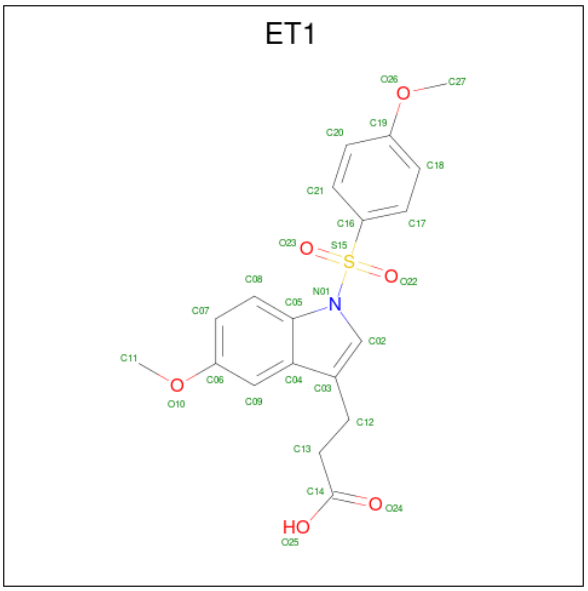
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2136	1383	360	383	10	0	0	0
1	B	267	2151	1393	362	386	10	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

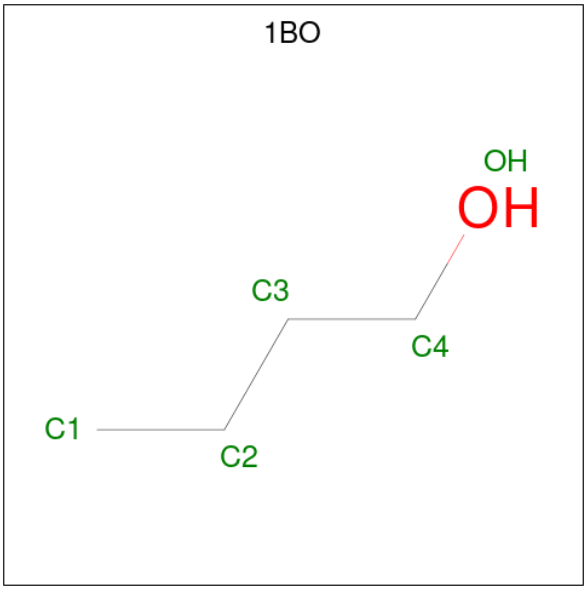
Chain	Residue	Modelled	Actual	Comment	Reference
A	155	MET	-	expression tag	UNP Q03181
A	156	LYS	-	expression tag	UNP Q03181
A	157	LYS	-	expression tag	UNP Q03181
A	158	GLY	-	expression tag	UNP Q03181
A	159	HIS	-	expression tag	UNP Q03181
A	160	HIS	-	expression tag	UNP Q03181
A	161	HIS	-	expression tag	UNP Q03181
A	162	HIS	-	expression tag	UNP Q03181
A	163	HIS	-	expression tag	UNP Q03181
A	164	HIS	-	expression tag	UNP Q03181
B	155	MET	-	expression tag	UNP Q03181
B	156	LYS	-	expression tag	UNP Q03181
B	157	LYS	-	expression tag	UNP Q03181
B	158	GLY	-	expression tag	UNP Q03181
B	159	HIS	-	expression tag	UNP Q03181
B	160	HIS	-	expression tag	UNP Q03181
B	161	HIS	-	expression tag	UNP Q03181
B	162	HIS	-	expression tag	UNP Q03181
B	163	HIS	-	expression tag	UNP Q03181
B	164	HIS	-	expression tag	UNP Q03181

- Molecule 2 is 3-{5-methoxy-1-[(4-methoxyphenyl)sulfonyl]-1H-indol-3-yl}propanoic acid (three-letter code: ET1) (formula: $C_{19}H_{19}NO_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	27	19	1	6	1	0	0
			Total	C	N	O	S		
2	B	1	27	19	1	6	1	0	0

- Molecule 3 is 1-BUTANOL (three-letter code: 1BO) (formula: $C_4H_{10}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	5	4	1	0	0
			Total	C	O		
3	A	1	5	4	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	5	4	1	0	0

- Molecule 4 is water.

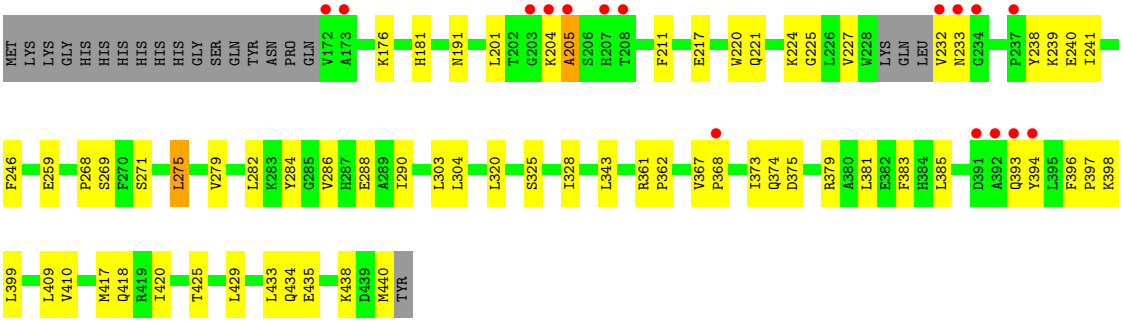
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	203	203	203	0	0
			Total	O		
4	B	169	169	169	0	0

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.

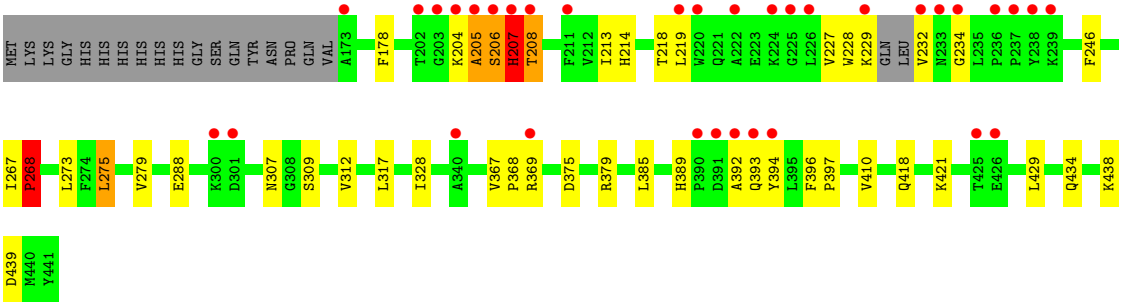
• Molecule 1: Peroxisome proliferator-activated receptor delta

Chain A:



• Molecule 1: Peroxisome proliferator-activated receptor delta

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.40Å 94.35Å 97.18Å 90.00° 98.27° 90.00°	Depositor
Resolution (Å)	38.99 – 2.24 38.99 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.99-2.24) 98.7 (38.99-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.185 , 0.242 0.181 , 0.241	Depositor DCC
R_{free} test set	1689 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4728	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ET1, 1BO

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	0.46	0/2182	0.55	0/2950
1	B	0.42	0/2198	0.54	0/2969
All	All	0.44	0/4380	0.54	0/5919

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2136	0	2177	43	0
1	B	2151	0	2190	36	0
2	A	27	0	18	2	0
2	B	27	0	18	2	0
3	A	15	0	30	3	0
4	A	203	0	0	5	0
4	B	169	0	0	7	0
All	All	4728	0	4433	79	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 9.

All (79) 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:178:PHE:CE1	1:B:268:PRO:HG2	2.22	0.75
1:B:393:GLN:HA	4:B:593:HOH:O	1.87	0.73
1:B:389:HIS:HB3	1:B:392:ALA:HB3	1.69	0.72
1:B:396:PHE:HB3	1:B:397:PRO:HD3	1.73	0.71
1:A:225:GLY:HA2	4:A:642:HOH:O	1.93	0.69
1:B:204:LYS:O	4:B:601:HOH:O	2.10	0.69
1:B:207:HIS:HA	4:B:601:HOH:O	1.94	0.68
1:B:421:LYS:HE2	1:B:434:GLN:OE1	1.95	0.67
1:A:279:VAL:HG22	1:B:275:LEU:HB3	1.78	0.66
1:A:201:LEU:HD21	1:A:304:LEU:HG	1.78	0.65
1:A:181:HIS:NE2	1:A:268:PRO:HD3	2.13	0.63
1:A:232:VAL:HG12	1:A:233:ASN:H	1.66	0.60
1:A:396:PHE:HB3	1:A:397:PRO:HD3	1.83	0.60
1:A:204:LYS:O	1:A:205:ALA:CB	2.52	0.57
1:B:438:LYS:O	1:B:439:ASP:HB2	2.05	0.57
1:A:204:LYS:O	1:A:205:ALA:HB3	2.07	0.55
1:B:232:VAL:HG12	1:B:234:GLY:H	1.72	0.55
1:A:191:ASN:HB2	1:A:259:GLU:OE2	2.06	0.55
1:A:284:TYR:HB3	1:A:361:ARG:HD2	1.89	0.55
1:A:385:LEU:HD11	1:A:399:LEU:HD12	1.90	0.54
1:B:389:HIS:HB3	1:B:392:ALA:CB	2.37	0.54
2:B:2:ET1:H18	4:B:576:HOH:O	2.07	0.53
1:B:206:SER:O	1:B:207:HIS:HB2	2.10	0.52
1:A:381:LEU:O	1:A:385:LEU:HG	2.09	0.51
1:B:208:THR:HB	4:B:594:HOH:O	2.10	0.51
1:B:227:VAL:HG12	1:B:228:TRP:CE3	2.46	0.51
1:A:238:TYR:OH	1:A:241:ILE:HD13	2.11	0.51
1:B:267:ILE:O	4:B:581:HOH:O	2.20	0.50
1:A:393:GLN:O	1:A:394:TYR:HB2	2.10	0.50
1:A:417:MET:HE1	1:A:420:ILE:HD12	1.93	0.50
1:B:214:HIS:CD2	1:B:218:THR:HG21	2.47	0.50
1:B:229:LYS:HD3	1:B:232:VAL:CG2	2.42	0.50
1:B:288:GLU:HG3	1:B:410:VAL:HG21	1.93	0.50
1:B:273:LEU:HD21	1:B:369:ARG:HG2	1.93	0.50
1:A:343:LEU:HD11	1:A:399:LEU:HD21	1.95	0.49
1:A:284:TYR:CB	1:A:361:ARG:HD2	2.43	0.49
2:A:1:ET1:H08	2:A:1:ET1:H21	1.95	0.48
1:B:213:ILE:HB	1:B:312:VAL:HG22	1.95	0.48
1:B:273:LEU:CD2	1:B:369:ARG:HG2	2.43	0.48
1:A:282:LEU:HD13	3:A:3:1BO:H41	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HB2	1:A:383:PHE:HE2	1.79	0.47
1:A:269:SER:HB2	1:A:373:ILE:CD1	2.44	0.47
1:B:393:GLN:O	1:B:394:TYR:HB2	2.15	0.47
1:A:275:LEU:HB3	1:B:279:VAL:HG22	1.97	0.47
1:A:374:GLN:NE2	4:A:629:HOH:O	2.47	0.47
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.79	0.46
1:A:246:PHE:CD1	2:A:1:ET1:H09	2.51	0.46
1:A:328:ILE:HG22	4:A:496:HOH:O	2.14	0.46
1:B:421:LYS:HG3	1:B:429:LEU:HD12	1.98	0.46
1:B:246:PHE:CD1	2:B:2:ET1:H09	2.52	0.45
1:B:229:LYS:N	1:B:229:LYS:HD2	2.31	0.45
1:A:232:VAL:HG12	1:A:233:ASN:N	2.32	0.45
1:A:394:TYR:O	1:A:398:LYS:HG3	2.17	0.45
1:A:375:ASP:O	1:A:379:ARG:HG3	2.17	0.44
1:B:309:SER:HB2	4:B:591:HOH:O	2.18	0.44
1:A:220:TRP:HD1	3:A:6:1BO:H22	1.83	0.44
1:A:241:ILE:CD1	3:A:6:1BO:H13	2.47	0.44
1:A:320:LEU:O	1:A:325:SER:HB3	2.18	0.43
1:A:286:VAL:O	1:A:290:ILE:HG13	2.17	0.43
1:B:317:LEU:HD13	1:B:328:ILE:HG21	1.99	0.43
1:A:239:LYS:O	1:A:240:GLU:HB3	2.19	0.43
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.67	0.43
1:A:211:PHE:HB3	1:A:227:VAL:CG2	2.49	0.42
1:A:435:GLU:OE2	1:A:438:LYS:HE3	2.18	0.42
1:B:204:LYS:HB3	1:B:205:ALA:H	1.65	0.42
1:B:207:HIS:O	1:B:208:THR:HB	2.20	0.42
1:A:268:PRO:HD2	4:A:469:HOH:O	2.20	0.42
1:A:367:VAL:HB	1:A:368:PRO:HD3	2.02	0.42
1:B:232:VAL:HG12	1:B:234:GLY:N	2.34	0.42
1:A:394:TYR:C	1:A:397:PRO:HD2	2.40	0.42
1:A:361:ARG:HA	1:A:362:PRO:HD3	1.95	0.41
1:B:438:LYS:O	1:B:439:ASP:CB	2.67	0.41
1:B:367:VAL:HB	1:B:368:PRO:HD3	2.01	0.41
1:A:288:GLU:HG3	1:A:410:VAL:HG21	2.03	0.40
1:A:394:TYR:N	4:A:644:HOH:O	2.43	0.40
1:B:375:ASP:O	1:B:379:ARG:HG3	2.22	0.40
1:A:217:GLU:O	1:A:221:GLN:HG2	2.22	0.40
1:A:429:LEU:HD13	1:A:434:GLN:NE2	2.37	0.40
1:B:213:ILE:HG23	1:B:219:LEU:HA	2.02	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	262/287 (91%)	252 (96%)	9 (3%)	1 (0%)	34 35
1	B	263/287 (92%)	243 (92%)	14 (5%)	6 (2%)	6 2
All	All	525/574 (92%)	495 (94%)	23 (4%)	7 (1%)	12 7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	206	SER
1	B	268	PRO
1	B	307	ASN
1	A	205	ALA
1	B	207	HIS
1	B	205	ALA
1	B	208	THR

5.3.2 Protein sidechains (i)

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	234/253 (92%)	226 (97%)	8 (3%)	37 42
1	B	235/253 (93%)	230 (98%)	5 (2%)	53 60
All	All	469/506 (93%)	456 (97%)	13 (3%)	43 49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	LYS
1	A	271	SER
1	A	275	LEU
1	A	303	LEU
1	A	418	GLN
1	A	425	THR
1	A	433	LEU
1	A	440	MET
1	B	207	HIS
1	B	268	PRO
1	B	275	LEU
1	B	385	LEU
1	B	418	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	GLN
1	B	418	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	ET1	A	1	-	24,29,29	1.32	3 (12%)	30,42,42	2.25	8 (26%)
3	1BO	A	3	-	4,4,4	0.21	0	3,3,3	0.37	0
3	1BO	A	4	-	4,4,4	0.25	0	3,3,3	0.50	0
3	1BO	A	6	-	4,4,4	0.23	0	3,3,3	0.32	0
2	ET1	B	2	-	24,29,29	1.33	4 (16%)	30,42,42	2.07	6 (20%)

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	ET1	A	1	-	-	4/15/21/21	0/3/3/3
3	1BO	A	3	-	-	1/2/2/2	-
3	1BO	A	4	-	-	0/2/2/2	-
3	1BO	A	6	-	-	2/2/2/2	-
2	ET1	B	2	-	-	3/15/21/21	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ET1	C02-N01	3.36	1.45	1.38
2	B	2	ET1	C02-N01	2.97	1.44	1.38
2	B	2	ET1	C09-C06	2.39	1.41	1.37
2	A	1	ET1	C17-C16	2.30	1.42	1.38
2	B	2	ET1	C21-C16	2.30	1.42	1.38
2	A	1	ET1	C16-S15	-2.23	1.66	1.77
2	B	2	ET1	C16-S15	-2.07	1.67	1.77

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	ET1	C20-C21-C16	7.32	127.02	119.45
2	B	2	ET1	C20-C21-C16	6.22	125.89	119.45
2	A	1	ET1	C21-C16-C17	-5.40	112.90	120.44
2	B	2	ET1	C21-C16-C17	-5.36	112.96	120.44
2	B	2	ET1	C21-C16-S15	3.90	124.10	119.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	ET1	C18-C17-C16	3.48	123.05	119.45
2	A	1	ET1	C21-C16-S15	3.32	123.45	119.77
2	A	1	ET1	C17-C16-S15	2.77	122.84	119.77
2	B	2	ET1	C17-C16-S15	2.69	122.75	119.77
2	A	1	ET1	C16-S15-N01	-2.46	102.39	104.95
2	A	1	ET1	C18-C17-C16	2.26	121.79	119.45
2	A	1	ET1	C08-C05-C04	-2.16	118.01	120.94
2	B	2	ET1	O25-C14-O24	-2.03	118.25	123.30
2	A	1	ET1	O25-C14-O24	-2.01	118.28	123.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ET1	C18-C19-O26-C27
2	A	1	ET1	C20-C19-O26-C27
2	B	2	ET1	C09-C06-O10-C11
2	B	2	ET1	C07-C06-O10-C11
3	A	6	1BO	C1-C2-C3-C4
3	A	3	1BO	C2-C3-C4-OH
2	A	1	ET1	C12-C13-C14-O24
2	A	1	ET1	C12-C13-C14-O25
3	A	6	1BO	C2-C3-C4-OH
2	B	2	ET1	C21-C16-S15-N01

There are no ring outliers.

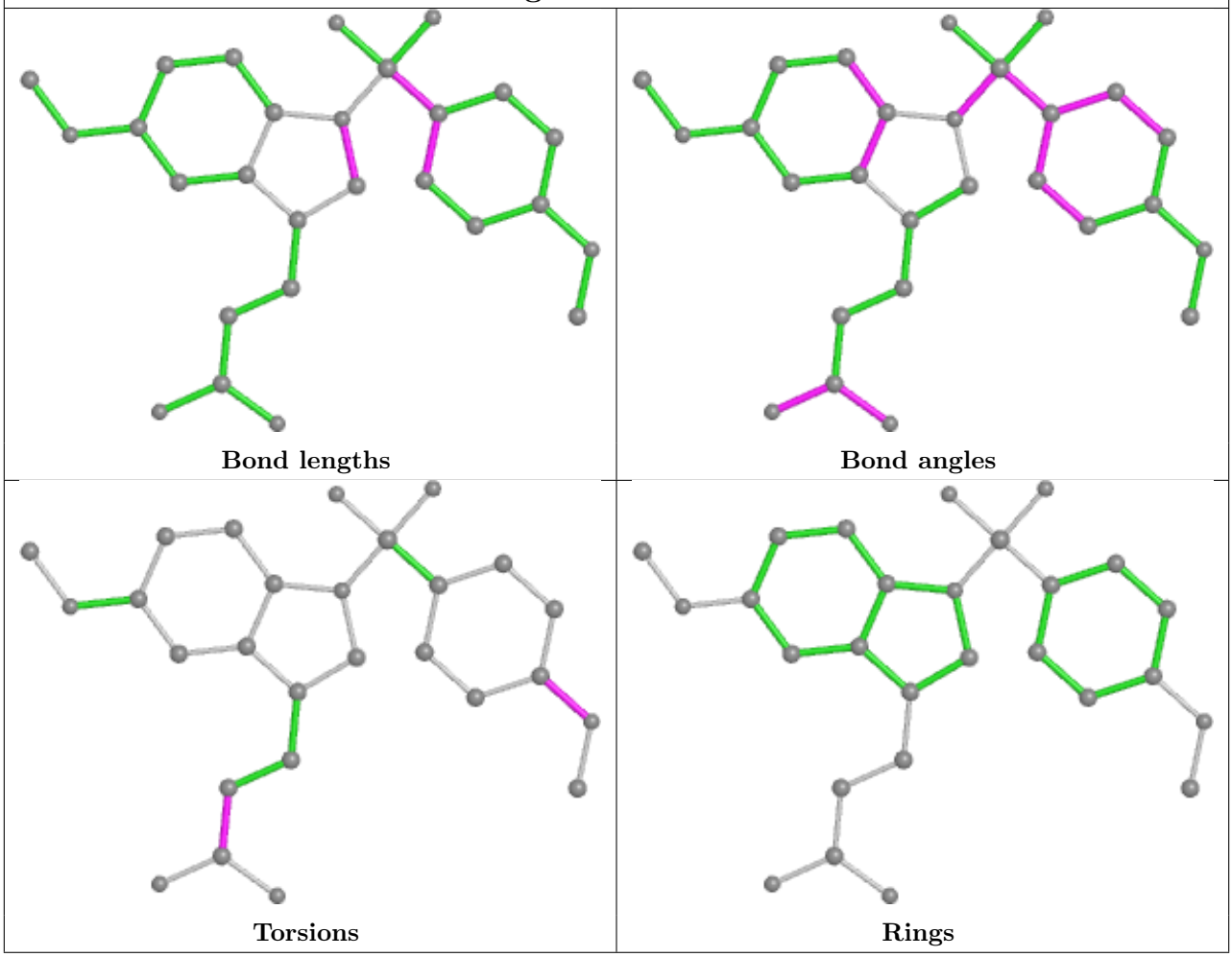
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ET1	2	0
3	A	3	1BO	1	0
3	A	6	1BO	2	0
2	B	2	ET1	2	0

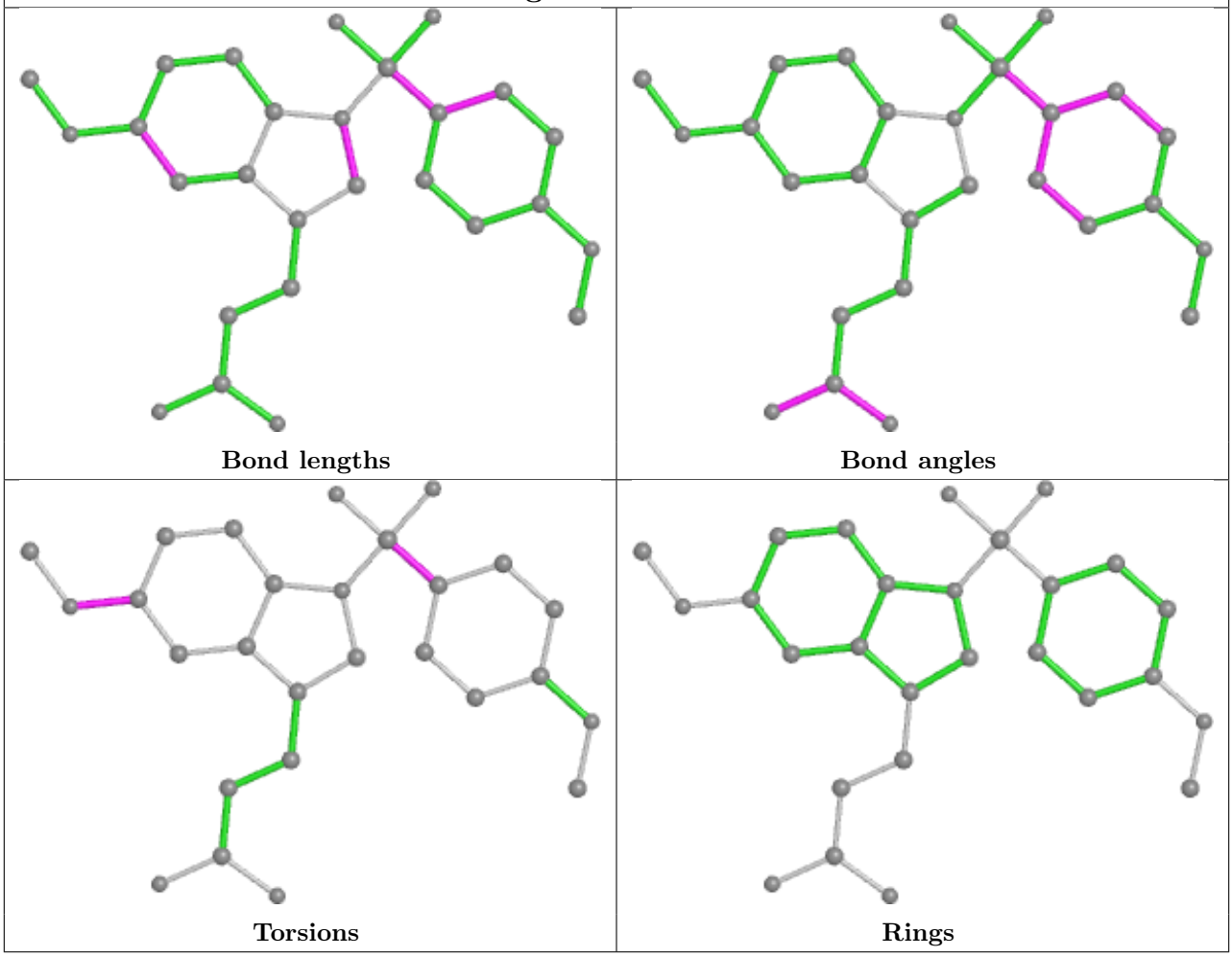
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 ET1 A 1



Ligand ET1 B 2



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	266/287 (92%)	0.31	16 (6%) 21 21	17, 35, 73, 149	0
1	B	267/287 (93%)	0.55	34 (12%) 3 2	19, 40, 86, 153	0
All	All	533/574 (92%)	0.43	50 (9%) 8 8	17, 37, 83, 153	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	ASN	12.1
1	B	226	LEU	11.6
1	A	172	VAL	8.1
1	B	234	GLY	6.5
1	B	237	PRO	6.5
1	A	205	ALA	6.1
1	B	208	THR	5.9
1	A	234	GLY	5.6
1	A	208	THR	5.5
1	A	207	HIS	5.2
1	B	229	LYS	5.2
1	A	173	ALA	4.8
1	B	211	PHE	4.7
1	B	225	GLY	4.6
1	A	204	LYS	4.6
1	B	204	LYS	4.3
1	B	238	TYR	4.2
1	B	394	TYR	3.9
1	B	205	ALA	3.7
1	A	393	GLN	3.7
1	A	394	TYR	3.6
1	A	233	ASN	3.6
1	B	425	THR	3.3
1	B	207	HIS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	300	LYS	3.2
1	B	392	ALA	3.2
1	B	220	TRP	3.1
1	B	219	LEU	3.1
1	B	391	ASP	3.0
1	A	392	ALA	2.9
1	A	203	GLY	2.9
1	A	232	VAL	2.9
1	B	222	ALA	2.8
1	B	426	GLU	2.8
1	B	203	GLY	2.7
1	B	393	GLN	2.7
1	B	206	SER	2.7
1	A	237	PRO	2.7
1	B	236	PRO	2.5
1	B	239	LYS	2.4
1	B	202	THR	2.3
1	A	368	PRO	2.3
1	A	391	ASP	2.3
1	B	173	ALA	2.2
1	B	390	PRO	2.2
1	B	369	ARG	2.1
1	B	232	VAL	2.1
1	B	224	LYS	2.1
1	B	301	ASP	2.1
1	B	340	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

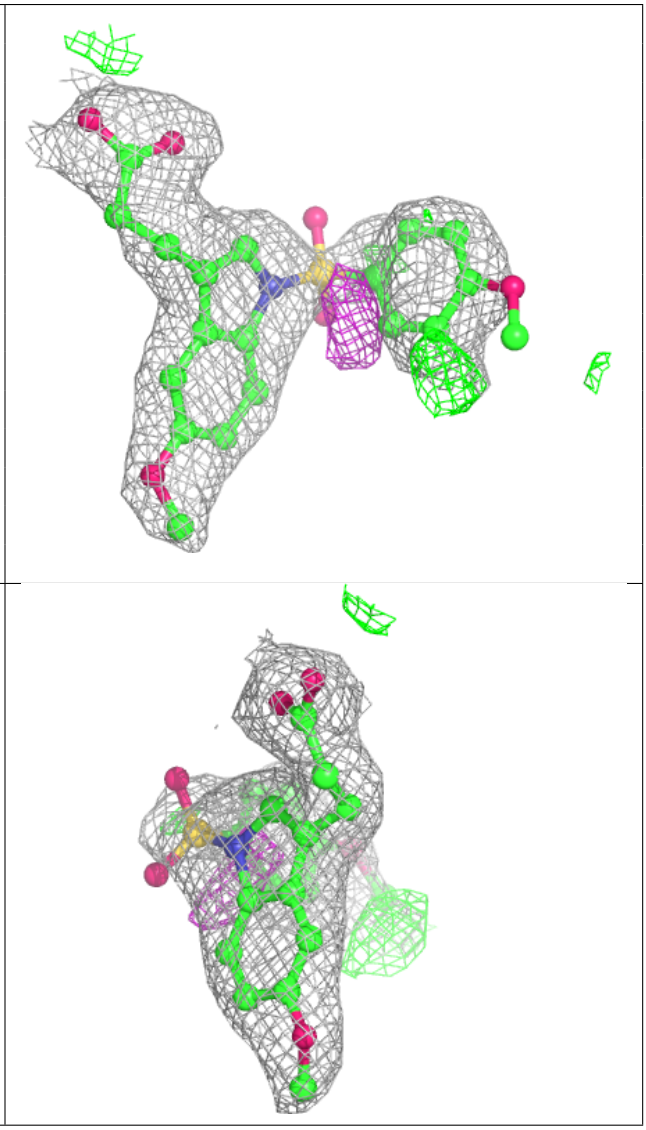
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ET1	B	2	27/27	0.90	0.20	30,54,210,211	0
3	1BO	A	3	5/5	0.92	0.22	42,47,49,59	0
2	ET1	A	1	27/27	0.93	0.18	19,34,119,130	0
3	1BO	A	6	5/5	0.93	0.17	49,49,54,55	0
3	1BO	A	4	5/5	0.97	0.13	26,26,36,48	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.

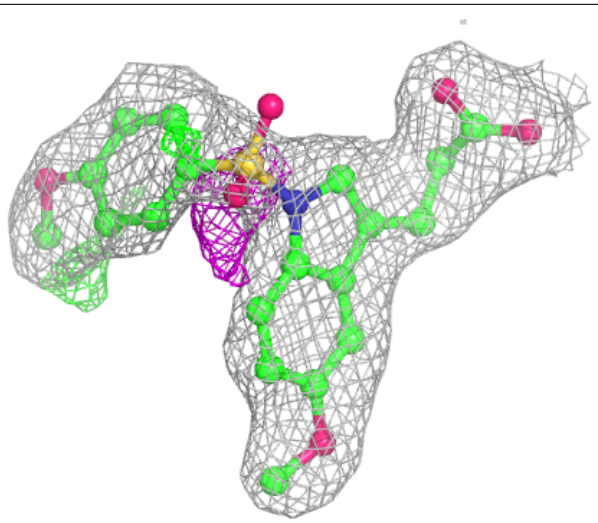
Electron density around ET1 B 2:

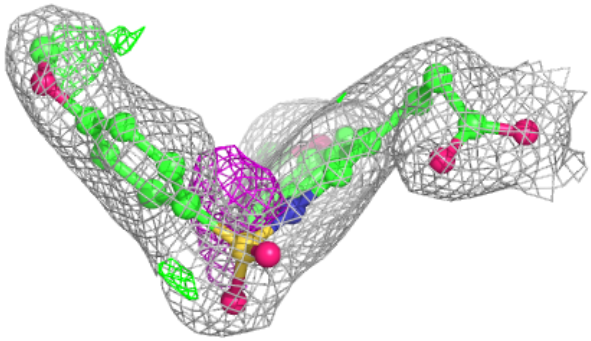
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

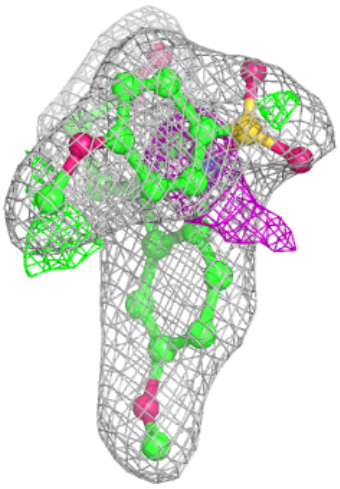


Electron density around ET1 A 1:

$2mF_o$-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.