

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 05:24 pm BST

PDB ID : 2YLY

Title: Sulfonamides as selective Estrogen Receptor beta Agonists.

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Deposited on : 2011-06-06

Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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 : 2.11

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)

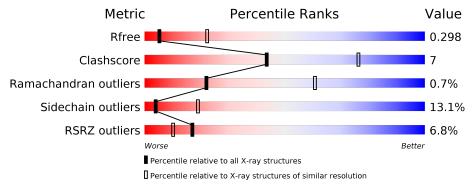
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar resolution} \\ (\#{\rm Entries, resolution range(\AA)}) \end{array}$
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	240	67%	20%	•	9%
1	В	240	68%	22%	•	8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3538 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.

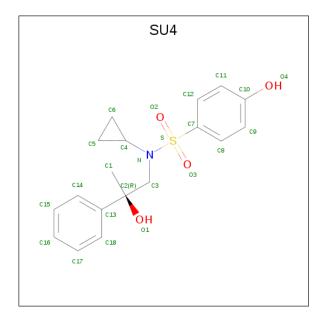
• Molecule 1 is a protein called ESTROGEN RECEPTOR BETA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	210	Total	С	N	О	S	0	0	0
1	1 A 219	219	1731	1114	290	308	19	U	0	U
1	D	221	Total	С	N	О	S	0	0	0
1	D	221	1749	1126	294	310	19	U	U	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q92731
В	?	-	ALA	deletion	UNP Q92731

• Molecule 2 is N-cyclopropyl-4-oxidanyl-N-[(2R)-2-oxidanyl-2-phenyl-propyl]benzenesulfona mide (three-letter code: SU4) (formula: C₁₈H₂₁NO₄S).



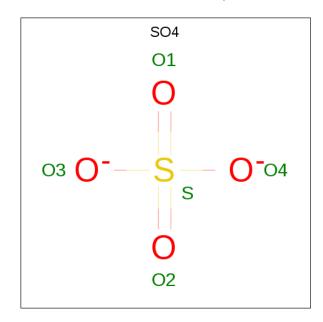
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	A	1	Total	C	N	O	S	0	0
			24	18	1	4	1		



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
9	D	1	Total	С	N	О	S	0	0
	Б	1	24	18	1	4	1	U	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



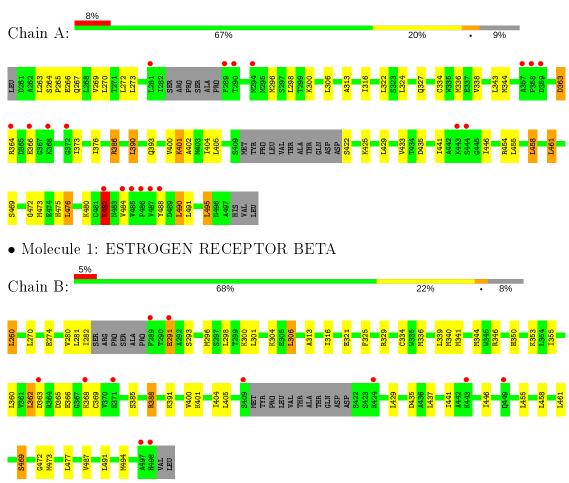
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	В	1	Total O S 5 4 1	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: ESTROGEN RECEPTOR BETA





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants	116.72Å 116.72Å 186.66Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 3.20	Depositor
Resolution (A)	29.11 - 3.20	EDS
% Data completeness	99.8 (30.00-3.20)	Depositor
(in resolution range)	99.8 (29.11-3.20)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.44 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
P. P.	0.235 , 0.275	Depositor
R, R_{free}	0.250 , 0.298	DCC
R_{free} test set	529 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	91.7	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 74.7	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3538	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: SU4, SO4

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		
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.47	0/1759	0.69	0/2371	
1	В	0.48	0/1778	0.75	0/2397	
All	All	0.47	0/3537	0.72	0/4768	

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	1731	0	1808	25	0
1	В	1749	0	1826	23	0
2	A	24	0	20	5	0
2	В	24	0	20	6	0
3	A	5	0	0	0	0
3	В	5	0	0	0	0
All	All	3538	0	3674	48	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 7.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

A	A.1 0	Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	overlap (Å)
1:B:298:LEU:HB3	2:B:1499:SU4:H52C	1.71	0.72
1:A:472:GLY:HA2	2:A:1499:SU4:H17	1.74	0.69
1:B:301:LEU:HD23	2:B:1499:SU4:H9	1.80	0.63
1:A:386:ARG:HB3	1:A:461:LEU:HD21	1.81	0.62
1:B:325:PHE:CE2	1:B:329:ARG:HD3	2.36	0.61
1:B:472:GLY:O	2:B:1499:SU4:H17	2.03	0.58
1:B:385:SER:HA	1:B:388:ARG:HD2	1.87	0.57
1:B:313:ALA:HA	1:B:316:ILE:HD12	1.91	0.53
1:A:455:LEU:HD23	1:B:455:LEU:HD23	1.90	0.53
2:B:1499:SU4:H61C	2:B:1499:SU4:C14	2.39	0.52
1:B:270:LEU:O	1:B:274:GLU:HG2	2.09	0.51
1:A:313:ALA:HA	1:A:316:ILE:HD12	1.93	0.51
1:A:401:LYS:HA	1:A:404:ILE:HD12	1.94	0.50
1:A:338:VAL:HG13	1:A:401:LYS:HD2	1.94	0.50
1:B:341:MET:HA	1:B:344:MET:HE2	1.95	0.49
1:A:472:GLY:CA	2:A:1499:SU4:H17	2.43	0.47
1:B:362:LEU:HD13	1:B:366:GLU:HG3	1.96	0.47
1:A:422:SER:HB3	1:A:425:LYS:HE2	1.95	0.47
1:A:298:LEU:HD13	2:A:1499:SU4:H12C	1.97	0.47
1:A:482:LYS:HB3	1:A:484:VAL:HG23	1.96	0.47
1:B:282:ILE:HD11	1:B:360:LEU:HD13	1.97	0.47
1:B:260:LEU:HD22	1:B:321:GLU:HG3	1.97	0.47
1:B:437:LEU:O	1:B:441:ILE:HG12	2.15	0.47
1:A:343:LEU:HB2	2:A:1499:SU4:H11	1.98	0.46
1:A:373:ILE:HD12	1:A:376:ILE:HD12	1.98	0.46
1:A:264:SER:HB3	1:A:267:GLN:HG3	1.98	0.45
1:B:291:GLU:HB2	1:B:369:CYS:HB2	1.97	0.45
1:A:376:ILE:HD11	1:A:475:HIS:CD2	2.52	0.45
1:A:363:ASP:H	1:A:366:GLU:HB2	1.82	0.44
1:B:340:MET:HE1	1:B:469:SER:N	2.33	0.44
1:B:293:SER:HA	1:B:296:MET:HB3	1.99	0.44
1:A:296:MET:O	1:A:300:LYS:HB2	2.18	0.44
1:B:346:ARG:O	1:B:355:ILE:HD13	2.18	0.44
1:B:339:LEU:O	2:B:1499:SU4:H11	2.17	0.43
1:B:401:LYS:HA	1:B:404:ILE:HD12	2.01	0.43
1:B:334:CYS:SG	1:B:405:LEU:HA	2.57	0.43
1:A:265:PRO:O	1:A:269:VAL:HG23	2.17	0.43
1:A:476:LEU:HD21	2:A:1499:SU4:H62C	2.01	0.43
1:A:322:LEU:O	1:A:327:GLN:NE2	2.51	0.43
1:B:336:MET:HE1	2:B:1499:SU4:H17	2.00	0.43
1:A:336:MET:HG2	1:A:473:MET:HG2	2.01	0.43



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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:334:CYS:SG	1:A:405:LEU:HA	2.59	0.42
1:A:390:LEU:O	1:A:454:ARG:NH1	2.50	0.42
1:B:336:MET:HG2	1:B:473:MET:HG2	2.02	0.42
1:A:402:ALA:HB3	1:A:433:VAL:HG11	2.00	0.42
1:A:458:LEU:H	1:A:458:LEU:HG	1.74	0.41
1:A:480:LYS:HD2	1:A:495:LEU:HD23	2.02	0.41
1:B:306:LEU:HD11	1:B:487:VAL:HG13	2.03	0.41

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	Perc	entiles
1	A	213/240 (89%)	200 (94%)	11 (5%)	2 (1%)	17	56
1	В	215/240 (90%)	200 (93%)	14 (6%)	1 (0%)	29	67
All	All	428/480 (89%)	400 (94%)	25 (6%)	3 (1%)	22	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	LEU
1	В	494	MET
1	A	482	LYS

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	197/216 (91%)	169 (86%)	28 (14%)	3 15
1	В	$199/216 \ (92\%)$	175 (88%)	24 (12%)	5 22
All	All	396/432 (92%)	344 (87%)	52 (13%)	4 19

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	LEU
1	A	266	GLU
1	A	270	LEU
1	A	272	LEU
1	A	273	LEU
1	A A	306	LEU
1	A A	324	LEU
1	A	344	MET
1	A	363	ASP
1	A A	364	ARG
1	A	386	ARG
1	A A A A A A	390	LEU
1	A	393	GLN
1	A	400	VAL
1	A	401	LYS
1	A	429	LEU
1	A	435	LEU ASP
1	A	441	ILE
1	A	446	ILE
1	A	458	LEU
1	A	461	LEU
1	A	469	SER
1	A	476	LEU
1	A A	482	LYS
1	A	488	TYR
1	A	490	LEU
1	A A	491	LEU
1	A	495	LEU
1	В	260	LEU
1	В	280	VAL
1	В	281	LEU
1	В	291	GLU
1	В	300	LYS
1	В	304	LYS



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Mol	Chain	Res	Type
1	В	306	LEU
1	В	350	HIS
1	В	353	LYS
1	В	362	LEU
1	В	363	ASP
1	В	365	ASP
1	В	368	LYS
1	В	388	ARG
1	В	391	LYS
1	В	400	VAL
1	В	429	LEU
1	В	435	ASP
1	В	446	ILE
1	В	458	LEU
1	В	461	LEU
1	В	469	SER
1	В	477	LEU
1	В	491	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	HIS
1	A	407	ASN
1	A	431	ASN
1	A	457	ASN
1	A	475	HIS
1	A	496	ASN
1	В	350	HIS
1	В	394	HIS
1	В	407	ASN
1	В	431	ASN
1	В	457	ASN

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 carbohydrates 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	Tuna	Chain	Pos	Ros	in Res	hain Res	Dog	Dog	Ros	Dag	ain Dag		Link Bond lengths				Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2									
3	SO4	В	1500	-	4,4,4	0.24	0	6,6,6	0.30	0									
3	SO4	A	1500	-	4,4,4	0.33	0	6,6,6	0.27	0									
2	SU4	A	1499	-	23,26,26	3.01	3 (13%)	37,39,39	1.93	8 (21%)									
2	SU4	В	1499	-	23,26,26	2.64	7 (30%)	37,39,39	2.17	10 (27%)									

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	${f Torsions}$	Rings
2	SU4	A	1499	-	-	6/25/29/29	0/3/3/3
2	SU4	В	1499	-	-	9/25/29/29	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
2	A	1499	SU4	C7-S	-12.20	1.59	1.76
2	В	1499	SU4	C7-S	-10.09	1.62	1.76
2	A	1499	SU4	S-N	-5.46	1.54	1.63
2	В	1499	SU4	S-N	-4.17	1.56	1.63



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
2	В	1499	SU4	C2-C13	-3.09	1.50	1.53
2	В	1499	SU4	C6-C4	2.65	1.54	1.48
2	A	1499	SU4	C6-C4	2.14	1.53	1.48
2	В	1499	SU4	C8-C7	2.11	1.42	1.38
2	В	1499	SU4	C12-C7	2.08	1.42	1.38
2	В	1499	SU4	O2-S	2.06	1.45	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	1499	SU4	O2-S-O3	-7.32	107.66	119.52
2	A	1499	SU4	O2-S-O3	-6.01	109.79	119.52
2	A	1499	SU4	C7-S-N	5.12	116.48	107.36
2	В	1499	SU4	C2-C3-N	4.74	119.02	112.33
2	A	1499	SU4	C2-C3-N	4.26	118.33	112.33
2	В	1499	SU4	C6-C4-N	4.10	127.72	119.32
2	В	1499	SU4	C5-C4-N	-3.53	112.08	119.32
2	В	1499	SU4	O1-C2-C1	-3.49	100.63	107.46
2	A	1499	SU4	C4-N-S	3.22	124.34	117.90
2	A	1499	SU4	O3-S-C7	-3.18	104.03	108.05
2	В	1499	SU4	O2-S-N	3.07	112.58	106.97
2	В	1499	SU4	C7-S-N	3.07	112.83	107.36
2	A	1499	SU4	O2-S-N	2.70	111.89	106.97
2	A	1499	SU4	O1-C2-C1	-2.42	102.72	107.46
2	A	1499	SU4	C5-C4-N	-2.34	114.53	119.32
2	В	1499	SU4	O2-S-C7	-2.33	105.10	108.05
2	В	1499	SU4	C1-C2-C3	2.20	115.19	109.73
2	В	1499	SU4	O1-C2-C3	2.09	113.10	108.32

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1499	SU4	C8-C7-S-N
2	В	1499	SU4	C12-C7-S-N
2	A	1499	SU4	C8-C7-S-N
2	A	1499	SU4	C12-C7-S-N
2	A	1499	SU4	C8-C7-S-O2
2	A	1499	SU4	C12-C7-S-O2
2	В	1499	SU4	C12-C7-S-O2
2	В	1499	SU4	C8-C7-S-O2
2	A	1499	SU4	C4-N-S-O3



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Mol	Chain	Res	Type	Atoms
2	В	1499	SU4	C6-C4-N-C3
2	A	1499	SU4	C4-N-S-O2
2	В	1499	SU4	C2-C3-N-S
2	В	1499	SU4	C18-C13-C2-O1
2	В	1499	SU4	C14-C13-C2-O1
2	В	1499	SU4	C4-N-S-O3

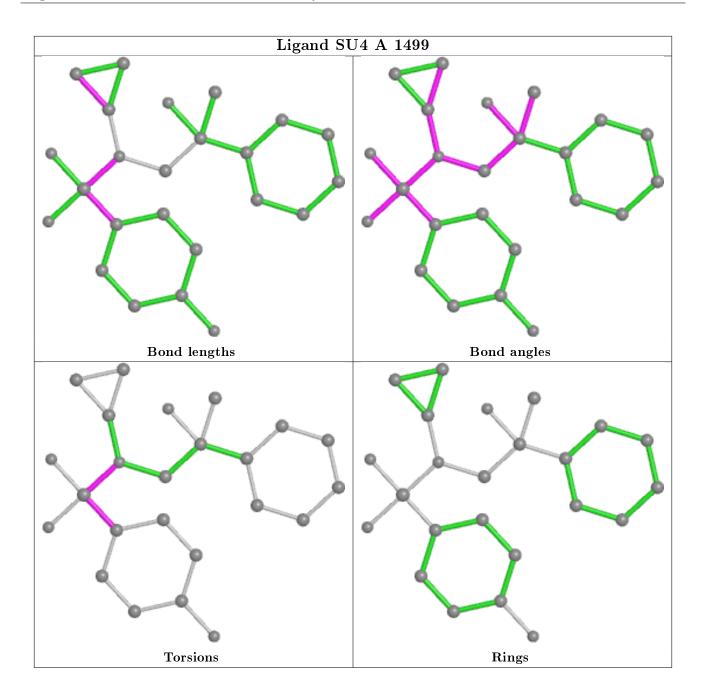
There are no ring outliers.

2 monomers are involved in 11 short contacts:

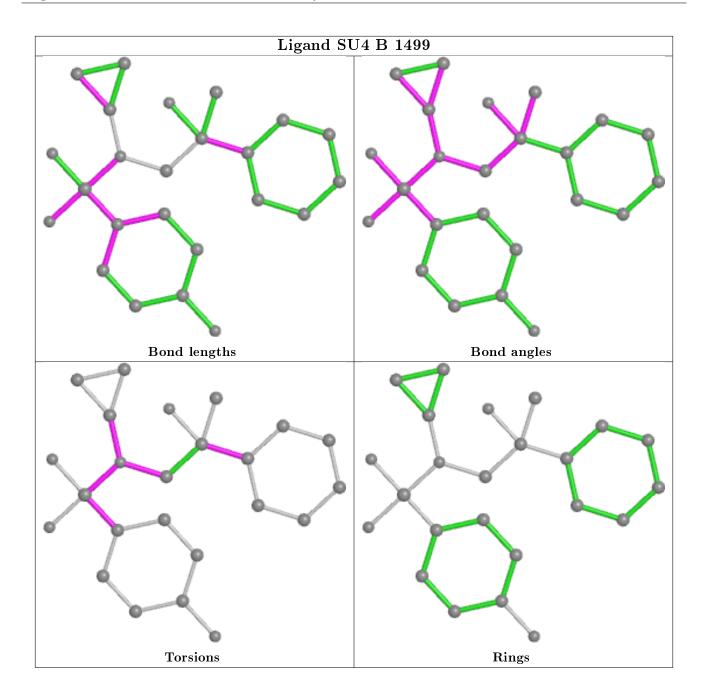
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1499	SU4	5	0
2	В	1499	SU4	6	0

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.









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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	219/240 (91%)	0.33	19 (8%) 10 5	63, 114, 166, 182	0
1	В	221/240 (92%)	-0.01	11 (4%) 28 16	44, 84, 130, 162	0
All	All	440/480 (91%)	0.16	30 (6%) 17 10	44, 99, 161, 182	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	289	PHE	5.5
1	A	484	VAL	4.3
1	A	289	PHE	4.0
1	A	366	GLU	4.0
1	A	359	ASP	3.8
1	В	363	ASP	3.6
1	В	498	HIS	3.6
1	A	486	PRO	3.3
1	A	358	PRO	3.1
1	В	291	GLU	3.0
1	В	497	ALA	3.0
1	В	368	LYS	2.9
1	A	290	THR	2.9
1	В	424	ARG	2.9
1	A	364	ARG	2.8
1	A	485	VAL	2.8
1	A	488	TYR	2.7
1	В	443	LYS	2.6
1	A	372	GLY	2.5
1	A	443	LYS	2.5
1	A	482	LYS	2.5
1	A	487	VAL	2.4
1	В	371	GLU	2.3
1	A	444	SER	2.3



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Mol	Chain	Res	Type	RSRZ
1	В	449	GLN	2.3
1	A	368	LYS	2.2
1	A	281	LEU	2.1
1	A	294	MET	2.1
1	В	409	SER	2.1
1	A	357	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 carbohydrates 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, 95^{th} 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.

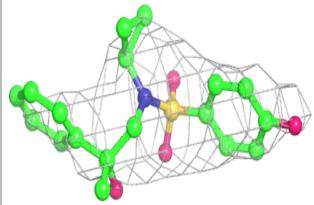
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	SO4	В	1500	5/5	0.83	0.27	138,142,143,143	0
2	SU4	A	1499	24/24	0.89	0.29	154,158,159,160	0
2	SU4	В	1499	24/24	0.92	0.29	96,103,108,108	0
3	SO4	A	1500	5/5	0.96	0.19	118,122,123,124	0

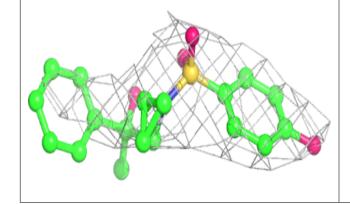
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

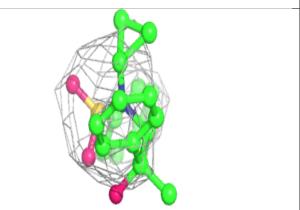


Electron density around SU4 A 1499:

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

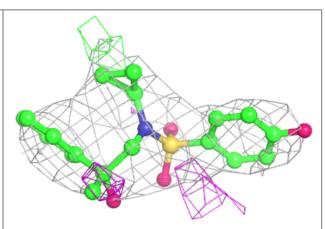


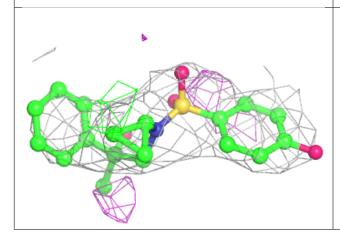


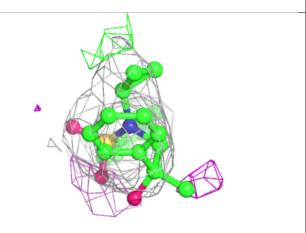


Electron density around SU4 B 1499:

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









6.5 Other polymers (i)

There are no such residues in this entry.

