



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:08 PM UTC

PDB ID : 6PSJ / pdb_00006psj
Title : Bazedoxifene in Complex with Y537S Estrogen Receptor Alpha Ligand Binding Domain
Authors : Fanning, S.W.; Greene, G.L.
Deposited on : 2019-07-12
Resolution : 1.80 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

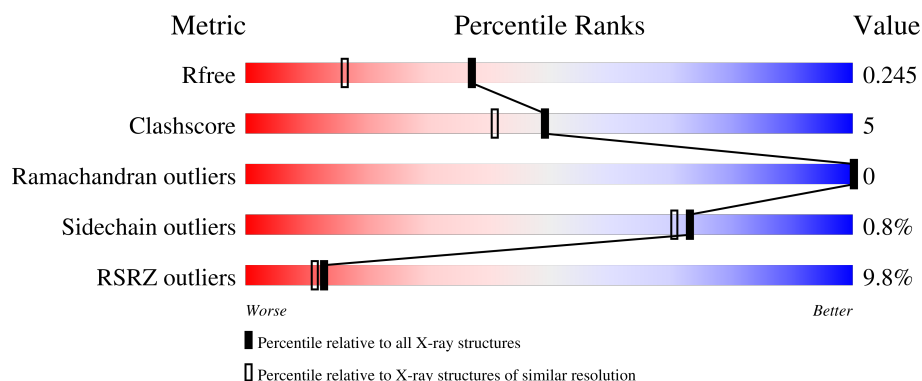
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	262	6% 66% 21% • 11%
1	B	262	10% 65% 16% • 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3966 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	8	0
			1860	1188	316	341	15			
1	B	215	Total	C	N	O	S	0	2	0
			1676	1074	288	299	15			

There are 36 discrepancies between the modelled and reference sequences:

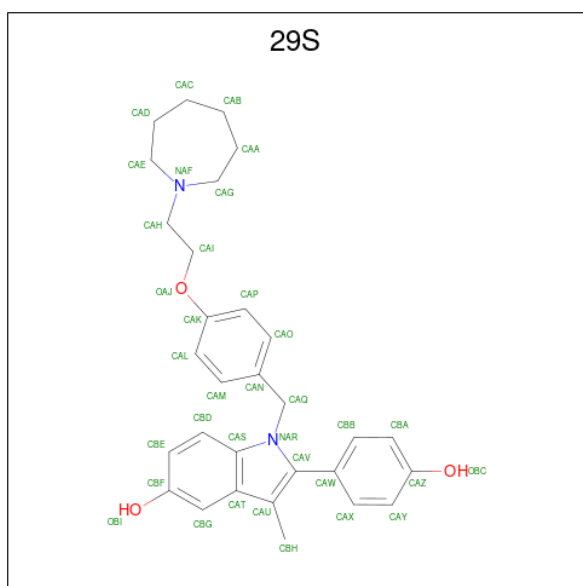
Chain	Residue	Modelled	Actual	Comment	Reference
A	293	HIS	-	expression tag	UNP P03372
A	294	HIS	-	expression tag	UNP P03372
A	295	HIS	-	expression tag	UNP P03372
A	296	HIS	-	expression tag	UNP P03372
A	297	HIS	-	expression tag	UNP P03372
A	298	HIS	-	expression tag	UNP P03372
A	299	GLU	-	expression tag	UNP P03372
A	300	ASN	-	expression tag	UNP P03372
A	301	LEU	-	expression tag	UNP P03372
A	302	TYR	-	expression tag	UNP P03372
A	303	PHE	-	expression tag	UNP P03372
A	304	GLN	-	expression tag	UNP P03372
A	305	SER	-	expression tag	UNP P03372
A	306	MET	-	expression tag	UNP P03372
A	381	SER	CYS	engineered mutation	UNP P03372
A	417	SER	CYS	engineered mutation	UNP P03372
A	530	SER	CYS	engineered mutation	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	293	HIS	-	expression tag	UNP P03372
B	294	HIS	-	expression tag	UNP P03372
B	295	HIS	-	expression tag	UNP P03372
B	296	HIS	-	expression tag	UNP P03372
B	297	HIS	-	expression tag	UNP P03372
B	298	HIS	-	expression tag	UNP P03372
B	299	GLU	-	expression tag	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
B	300	ASN	-	expression tag	UNP P03372
B	301	LEU	-	expression tag	UNP P03372
B	302	TYR	-	expression tag	UNP P03372
B	303	PHE	-	expression tag	UNP P03372
B	304	GLN	-	expression tag	UNP P03372
B	305	SER	-	expression tag	UNP P03372
B	306	MET	-	expression tag	UNP P03372
B	381	SER	CYS	engineered mutation	UNP P03372
B	417	SER	CYS	engineered mutation	UNP P03372
B	530	SER	CYS	engineered mutation	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is Bazedoxifene (CCD ID: 29S) (formula: $C_{30}H_{34}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	30	2	3		
2	B	1	Total	C	N	O	0	0
			35	30	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	188	Total	O	0	0
			188	188		
3	B	172	Total	O	0	0
			172	172		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.19Å 56.49Å 87.63Å 90.00° 104.32° 90.00°	Depositor
Resolution (Å)	29.14 – 1.80 29.14 – 1.80	Depositor EDS
% Data completeness (in resolution range)	82.1 (29.14-1.80) 82.1 (29.14-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.185 , 0.215 0.207 , 0.245	Depositor DCC
R_{free} test set	1849 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: 29S

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	1.92	35/1893 (1.8%)	0.97	0/2557
1	B	1.86	33/1705 (1.9%)	0.99	0/2306
All	All	1.89	68/3598 (1.9%)	0.98	0/4863

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	ALA	CA-CB	-8.14	1.41	1.54
1	B	405	ALA	CA-CB	-8.06	1.43	1.53
1	B	514	ILE	C-O	-7.08	1.15	1.24
1	A	378	LEU	C-O	-7.03	1.16	1.24
1	A	453	LEU	C-O	-6.94	1.16	1.24
1	A	361	ALA	CA-CB	-6.68	1.43	1.53
1	B	505	ALA	C-O	-6.63	1.16	1.24
1	A	475	ILE	C-O	-6.57	1.16	1.24
1	B	507	LEU	C-O	-6.30	1.16	1.24
1	B	517	MET	C-O	-6.29	1.16	1.24
1	A	375	GLN	C-O	-6.27	1.16	1.24
1	B	518	SER	C-O	-6.07	1.17	1.24
1	A	512	SER	C-O	-6.04	1.17	1.24
1	A	384	LEU	C-O	-6.03	1.17	1.24
1	A	426	ASP	C-O	-5.97	1.17	1.24
1	B	513	HIS	C-O	-5.95	1.17	1.24
1	A	517	MET	C-O	-5.84	1.17	1.24
1	A	328	TYR	C-O	-5.82	1.16	1.23
1	B	349	LEU	C-O	-5.80	1.17	1.24
1	B	491	ALA	CA-CB	-5.79	1.44	1.53
1	A	386	ILE	C-O	-5.76	1.17	1.24
1	B	429	LEU	C-O	-5.75	1.17	1.24
1	A	457	GLY	C-O	-5.73	1.18	1.24
1	A	344	GLY	C-O	-5.71	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	ALA	CA-CB	-5.70	1.44	1.53
1	A	349	LEU	C-O	-5.67	1.17	1.24
1	A	502	GLN	C-O	-5.59	1.17	1.24
1	B	508	LEU	C-O	-5.57	1.17	1.24
1	B	392	VAL	C-O	-5.53	1.17	1.24
1	B	380	GLU	C-O	-5.52	1.17	1.24
1	A	508	LEU	C-O	-5.50	1.17	1.24
1	A	428	LEU	C-O	-5.48	1.17	1.24
1	B	486	LEU	C-O	-5.45	1.17	1.24
1	A	377	HIS	C-O	-5.45	1.17	1.24
1	A	352	ARG	C-O	-5.43	1.17	1.24
1	B	504	LEU	C-O	-5.42	1.17	1.24
1	B	515	ARG	C-O	-5.42	1.17	1.24
1	B	451	ILE	C-O	-5.35	1.18	1.24
1	A	418	VAL	CA-CB	-5.35	1.47	1.54
1	B	320	LEU	C-O	-5.31	1.18	1.24
1	B	383	TRP	C-O	-5.31	1.18	1.24
1	B	512	SER	C-O	-5.31	1.18	1.24
1	B	316	VAL	C-O	-5.28	1.18	1.24
1	B	524	HIS	C-O	-5.26	1.18	1.24
1	A	486	LEU	C-O	-5.25	1.18	1.24
1	A	469	LEU	C-O	-5.25	1.18	1.24
1	B	378	LEU	C-O	-5.25	1.18	1.24
1	A	321	ASP	C-O	-5.22	1.17	1.24
1	A	425	PHE	C-O	-5.20	1.18	1.24
1	A	405	ALA	C-O	-5.20	1.18	1.24
1	B	519	ASN	C-O	-5.19	1.18	1.24
1	B	447	CYS	C-O	-5.19	1.18	1.24
1	B	315	MET	C-O	-5.18	1.18	1.24
1	A	396	MET	SD-CE	-5.18	1.66	1.79
1	A	427	MET	C-O	-5.18	1.18	1.24
1	A	451	ILE	C-O	-5.16	1.18	1.24
1	B	354	LEU	C-O	-5.15	1.18	1.24
1	B	427	MET	C-O	-5.15	1.18	1.24
1	A	480	ASP	C-O	-5.14	1.18	1.24
1	A	376	VAL	C-O	-5.14	1.18	1.24
1	B	506	GLN	C-O	-5.12	1.18	1.24
1	B	360	TRP	C-O	-5.11	1.18	1.24
1	A	474	HIS	C-O	-5.08	1.18	1.24
1	B	357	MET	C-O	-5.07	1.18	1.24
1	B	348	ASN	C-O	-5.05	1.18	1.24
1	B	389	ILE	C-O	-5.04	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	HIS	C-O	-5.03	1.18	1.24
1	A	388	MET	C-O	-5.01	1.18	1.24

There are no bond angle outliers.

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	1860	0	1887	28	0
1	B	1676	0	1701	11	0
2	A	35	0	34	5	0
2	B	35	0	34	3	0
3	A	188	0	0	2	0
3	B	172	0	0	1	0
All	All	3966	0	3656	39	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 5.

All (39) 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:A:524:HIS:NE2	1:A:528:MET:CE	2.39	0.86
1:A:524:HIS:CE1	1:A:528:MET:HE1	2.11	0.86
1:A:524:HIS:CD2	1:A:528:MET:HE2	2.12	0.84
1:A:524:HIS:NE2	1:A:528:MET:HE1	1.98	0.78
1:A:524:HIS:CE1	1:A:528:MET:CE	2.67	0.78
1:B:351:ASP:OD1	2:B:601:29S:H11	1.91	0.70
1:A:524:HIS:NE2	1:A:528:MET:HE2	2.05	0.69
1:A:351:ASP:OD1	2:A:601:29S:H11	1.97	0.63
1:A:412:ARG:HG2	1:A:412:ARG:HH21	1.69	0.58
1:A:412:ARG:HH21	1:A:412:ARG:CG	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.89	0.54
1:B:472:LYS:N	3:B:707:HOH:O	2.40	0.54
1:A:524:HIS:CD2	1:A:528:MET:CE	2.84	0.53
1:B:346:LEU:HB3	2:B:601:29S:H23	1.91	0.53
1:A:526:TYR:O	1:A:529:LYS:HG2	2.08	0.53
1:B:456:SER:HA	1:B:515:ARG:NH2	2.26	0.51
1:A:346:LEU:HB3	2:A:601:29S:H23	1.94	0.50
1:A:390:GLY:O	1:A:394:ARG:HG3	2.13	0.49
1:A:524:HIS:ND1	2:A:601:29S:OBC	2.20	0.48
1:A:496:THR:OG1	1:A:499:GLN:HG3	2.14	0.47
1:A:353:GLU:OE1	2:A:601:29S:OBI	2.29	0.47
1:A:547:HIS:CE1	1:A:549:LEU:HB2	2.51	0.46
1:B:414:GLN:O	1:B:417:SER:OG	2.28	0.46
3:A:841:HOH:O	1:B:498:GLN:HG3	2.16	0.46
1:A:412:ARG:CG	1:A:412:ARG:NH2	2.73	0.45
1:B:342:MET:HE1	1:B:414:GLN:O	2.17	0.45
1:A:355:VAL:HG22	1:A:543:MET:HE2	1.99	0.44
1:B:376:VAL:HG21	1:B:541:LEU:HG	2.00	0.44
1:A:416:LYS:HG2	1:A:422:VAL:HG11	1.98	0.44
1:A:343:MET:SD	1:A:421:MET:HE1	2.58	0.44
1:A:427:MET:HB3	1:A:517:MET:SD	2.58	0.43
1:B:315:MET:SD	1:B:365:PRO:HG2	2.58	0.43
1:A:396:MET:SD	1:A:435:PHE:HB3	2.59	0.43
1:A:416:LYS:CG	1:A:422:VAL:HG11	2.49	0.42
1:B:354:LEU:HD22	2:B:601:29S:H7	2.01	0.42
1:A:529:LYS:HG3	3:A:844:HOH:O	2.19	0.41
1:A:351:ASP:OD1	2:A:601:29S:CAG	2.64	0.41
1:B:437:MET:HE2	1:B:437:MET:HB2	1.82	0.40
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.94	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	233/262 (89%)	232 (100%)	1 (0%)	0	100	100
1	B	209/262 (80%)	207 (99%)	2 (1%)	0	100	100
All	All	442/524 (84%)	439 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	209/237 (88%)	206 (99%)	3 (1%)	59	52
1	B	184/237 (78%)	184 (100%)	0	100	100
All	All	393/474 (83%)	390 (99%)	3 (1%)	73	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	SER
1	A	412	ARG
1	A	528	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	ASN
1	A	476	HIS
1	A	516	HIS
1	A	519	ASN
1	B	476	HIS
1	B	488	HIS
1	B	519	ASN

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 ⓘ

2 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	29S	A	601	-	39,39,39	2.50	11 (28%)	52,54,54	1.56	9 (17%)
2	29S	B	601	-	39,39,39	2.57	13 (33%)	52,54,54	1.54	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	29S	A	601	-	-	3/14/23/23	0/5/5/5
2	29S	B	601	-	-	2/14/23/23	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	29S	CAH-NAF	-9.47	1.25	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	29S	CAH-NAF	-8.02	1.29	1.47
2	A	601	29S	CAV-NAR	-6.66	1.29	1.39
2	B	601	29S	CAG-NAF	-5.68	1.30	1.46
2	B	601	29S	CAE-NAF	-5.62	1.31	1.46
2	A	601	29S	CAG-NAF	-4.96	1.32	1.46
2	B	601	29S	CAV-NAR	-4.70	1.32	1.39
2	A	601	29S	CAE-NAF	-4.33	1.34	1.46
2	A	601	29S	CAQ-CAN	4.30	1.59	1.51
2	B	601	29S	CAQ-CAN	3.84	1.58	1.51
2	B	601	29S	CAS-NAR	-3.52	1.33	1.39
2	A	601	29S	CAV-CAU	3.21	1.39	1.37
2	B	601	29S	CBD-CAS	2.90	1.44	1.39
2	A	601	29S	CAX-CAW	-2.80	1.35	1.39
2	B	601	29S	CAQ-NAR	-2.56	1.42	1.46
2	A	601	29S	CAT-CAS	-2.41	1.37	1.41
2	B	601	29S	CAW-CAV	2.36	1.51	1.48
2	A	601	29S	CAQ-NAR	-2.27	1.43	1.46
2	A	601	29S	CAS-NAR	-2.25	1.35	1.39
2	B	601	29S	CAT-CAS	-2.23	1.38	1.41
2	B	601	29S	OAJ-CAK	2.23	1.42	1.37
2	A	601	29S	OAJ-CAI	-2.11	1.36	1.43
2	B	601	29S	CAX-CAW	-2.07	1.36	1.39
2	B	601	29S	CAM-CAL	2.05	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	29S	CAS-CAT-CAU	-4.48	103.42	107.87
2	B	601	29S	CBD-CAS-CAT	-4.15	117.32	121.95
2	A	601	29S	CBB-CAW-CAV	4.11	126.78	120.56
2	B	601	29S	CAT-CAU-CAV	-4.02	105.15	107.08
2	B	601	29S	CAD-CAE-NAF	-3.76	108.24	115.35
2	A	601	29S	CAM-CAL-CAK	3.11	123.28	119.73
2	A	601	29S	CAX-CAW-CAV	-3.09	115.89	120.56
2	A	601	29S	CBD-CAS-CAT	-3.05	118.54	121.95
2	A	601	29S	CAI-CAH-NAF	3.00	121.83	113.36
2	A	601	29S	CAN-CAQ-NAR	-2.90	108.75	113.46
2	B	601	29S	CAQ-CAN-CAM	2.84	125.98	120.75
2	B	601	29S	CAW-CAV-CAU	-2.79	124.66	128.68
2	B	601	29S	CAG-NAF-CAE	-2.37	106.86	113.22
2	B	601	29S	CAW-CAV-NAR	2.34	125.25	121.44
2	A	601	29S	CAP-CAO-CAN	2.27	123.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	29S	CAO-CAP-CAK	2.21	122.26	119.73
2	B	601	29S	CAQ-CAN-CAO	-2.16	116.77	120.75
2	B	601	29S	CAA-CAG-NAF	2.12	119.36	115.35
2	B	601	29S	CAS-CAT-CAU	-2.06	105.83	107.87
2	A	601	29S	CAQ-CAN-CAO	2.03	124.49	120.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

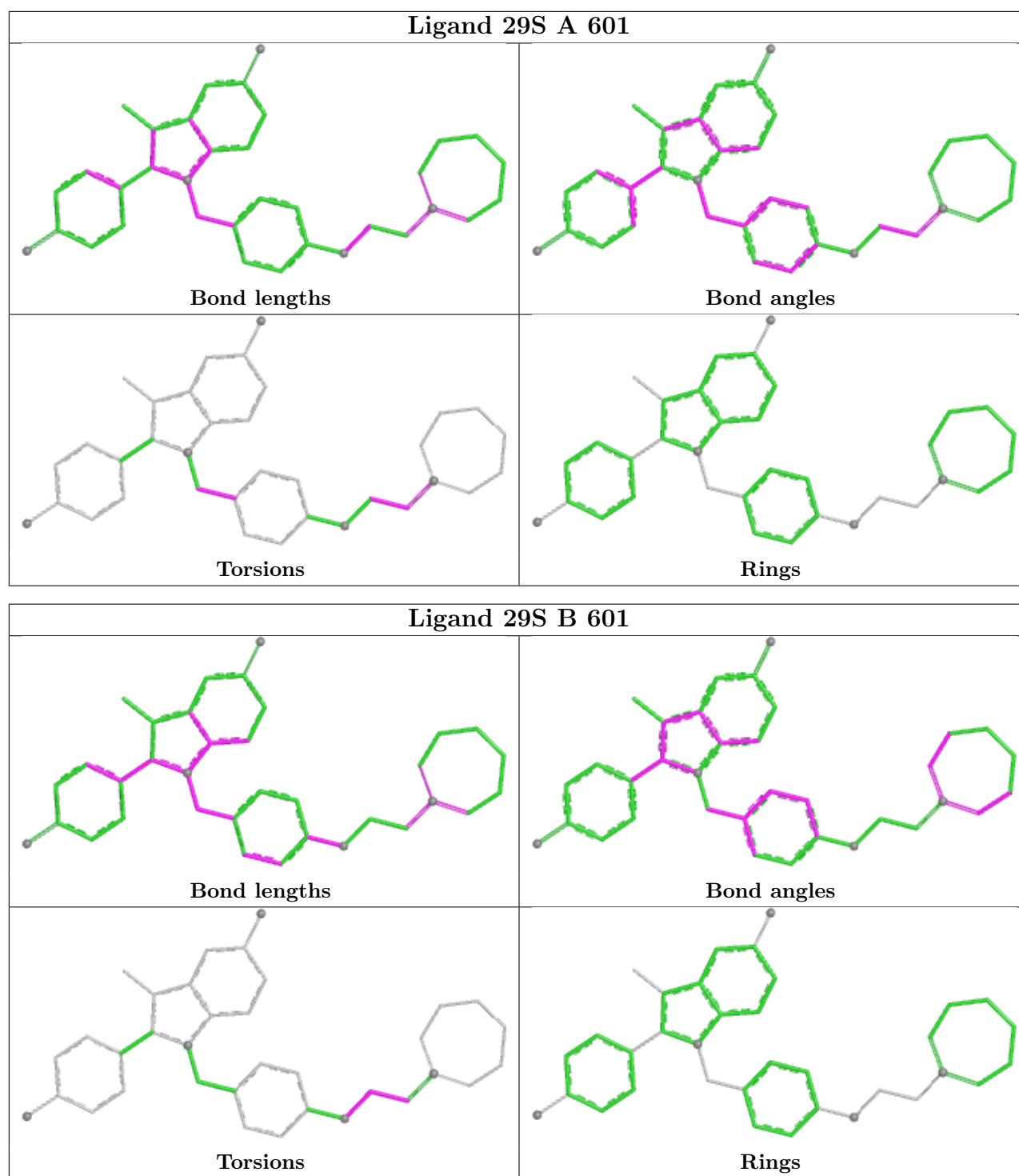
Mol	Chain	Res	Type	Atoms
2	A	601	29S	CAI-CAH-NAF-CAG
2	B	601	29S	CAH-CAI-OAJ-CAK
2	B	601	29S	NAF-CAH-CAI-OAJ
2	A	601	29S	NAF-CAH-CAI-OAJ
2	A	601	29S	CAM-CAN-CAQ-NAR

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	29S	5	0
2	B	601	29S	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	232/262 (88%)	0.26	17 (7%) 21 19	6, 23, 52, 91	8 (3%)
1	B	215/262 (82%)	0.73	27 (12%) 8 6	10, 27, 50, 81	2 (0%)
All	All	447/524 (85%)	0.49	44 (9%) 13 11	6, 25, 51, 91	10 (2%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	VAL	5.3
1	B	457	GLY	4.6
1	B	530	SER	4.6
1	B	527	SER	4.5
1	B	307	ALA	4.5
1	B	425	PHE	4.1
1	B	533	VAL	4.0
1	B	526	TYR	3.7
1	B	459	TYR	3.6
1	B	534	VAL	3.6
1	B	437	MET	3.5
1	A	538	ASP	3.5
1	A	546	ALA	3.3
1	A	462	LEU	3.3
1	B	544	LEU	3.0
1	B	476	HIS	2.9
1	A	541	LEU	2.8
1	B	456	SER	2.8
1	B	532	ASN	2.8
1	B	542	GLU	2.6
1	A	464	SER	2.6
1	B	308	LEU	2.6
1	B	473	ASP	2.6
1	A	533	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	534	VAL	2.5
1	A	529	LYS	2.5
1	B	520	LYS	2.5
1	B	432	SER	2.4
1	B	475	ILE	2.4
1	A	548	ARG	2.4
1	B	525	LEU	2.3
1	A	307	ALA	2.3
1	A	497	LEU	2.3
1	A	535	PRO	2.3
1	B	545	ASP	2.3
1	B	421	MET	2.3
1	A	341	SER	2.2
1	A	493	ALA	2.2
1	B	481	LYS	2.2
1	A	527	SER	2.1
1	B	477	ARG	2.1
1	A	528	MET	2.0
1	A	549	LEU	2.0
1	B	531	LYS	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](#)

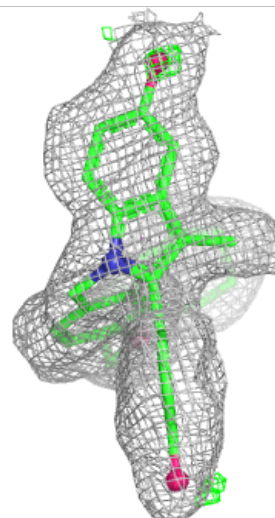
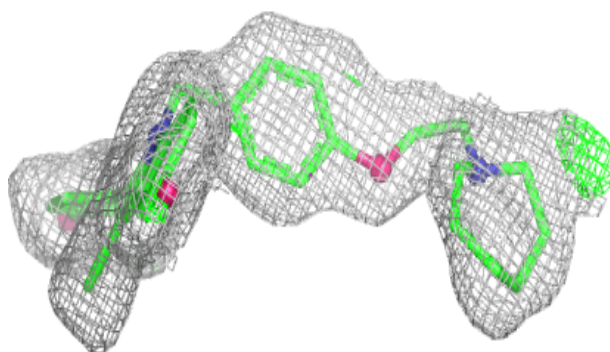
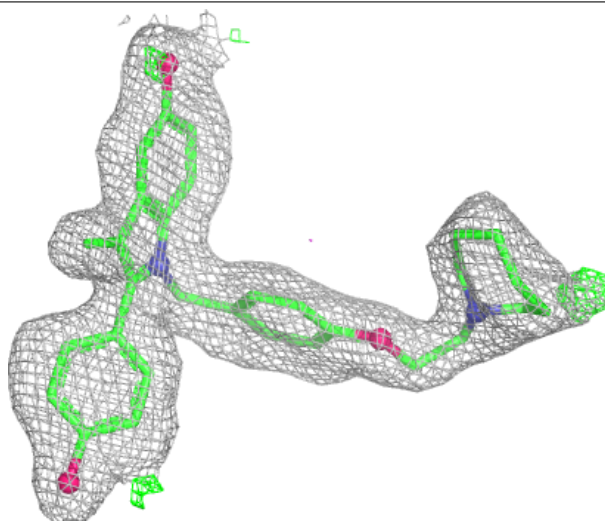
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	29S	B	601	35/35	0.92	0.09	14,23,38,39	0
2	29S	A	601	35/35	0.94	0.09	12,17,42,44	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.

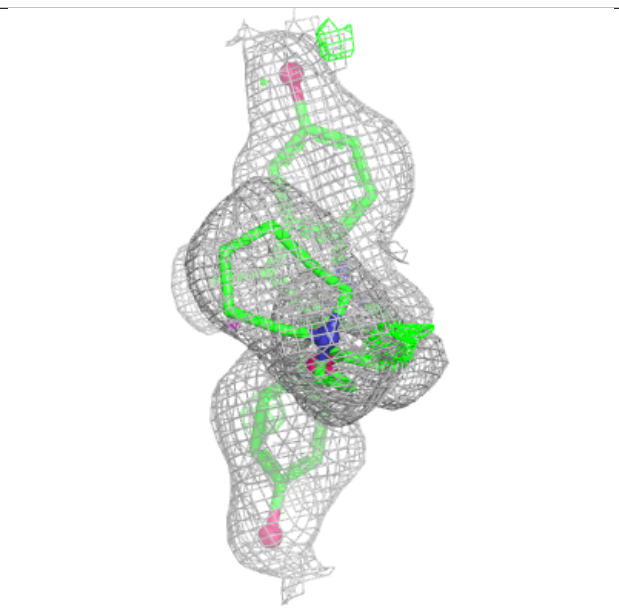
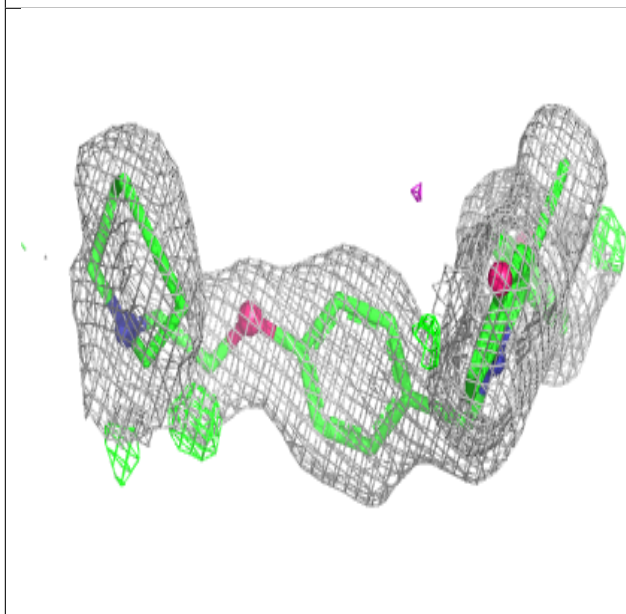
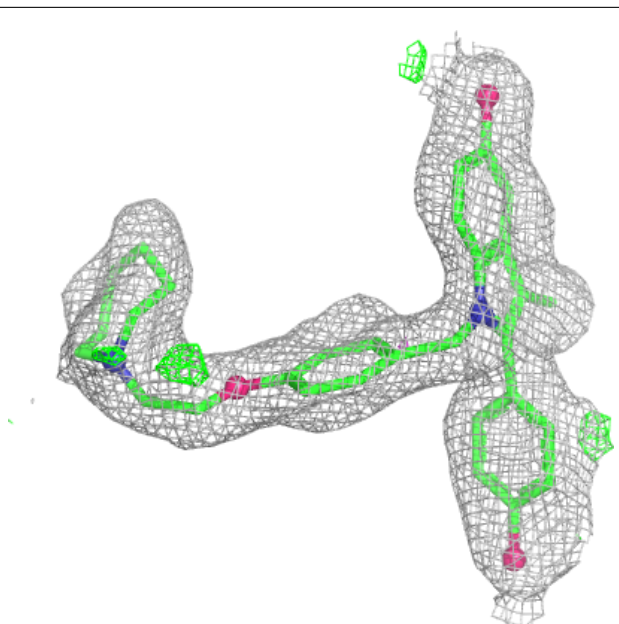
Electron density around 29S B 601:

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



Electron density around 29S A 601:

$2mF_o-DF_c$ (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.