Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 11:22 PM JST

PDB ID	:	7Y8F
Title	:	Estrogen Receptor Alpha Ligand Binding Domain Y537S Mutant in Complex with an Inhibitor 30o and GRIP Peptide
Authors	:	Min, J.; Hu, H.B.; Yang, Y.; Dong, C.E.; Zhou, H.B.; Chen, C.-C.; Guo, R.-T.
Deposited on	:	2022-06-23
Resolution	:	2.22 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:

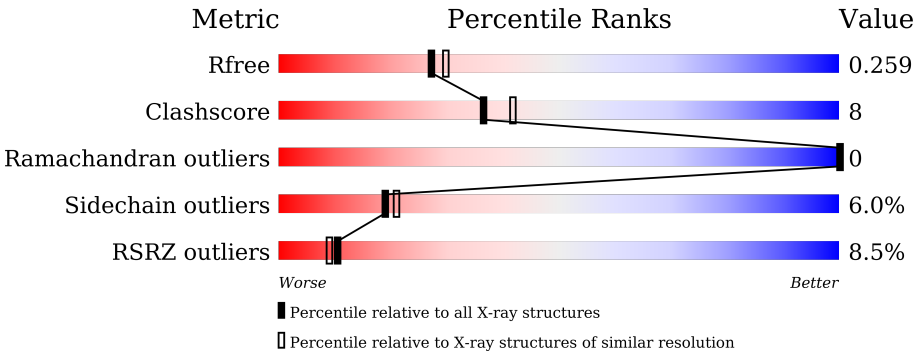
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 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	260	6%, 75%, 15%, 9%
1	B	260	7%, 66%, 17%, 15%
2	C	8	88%, 12%
2	D	8	88%, 62%, 38%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3977 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	236	Total	C	N	O	S	0	2	0
			1878	1200	326	333	19			
1	B	220	Total	C	N	O	S	0	0	0
			1751	1124	300	311	16			

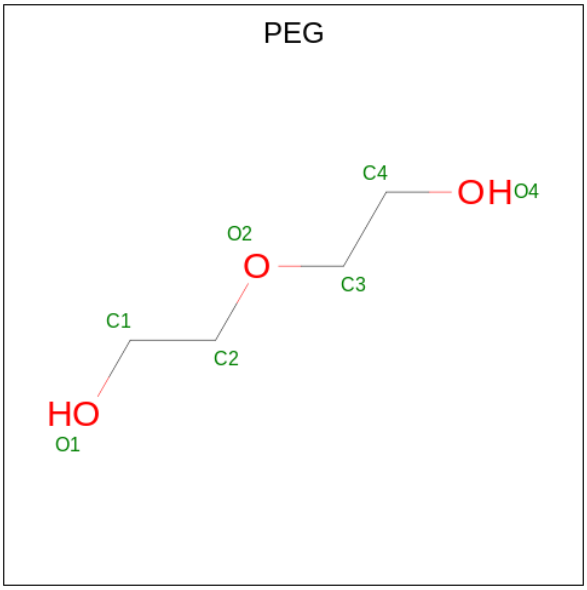
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	ALA	-	linker	UNP P03372
A	296	GLY	-	linker	UNP P03372
A	297	ALA	-	linker	UNP P03372
A	298	GLY	-	linker	UNP P03372
A	299	ALA	-	linker	UNP P03372
A	300	GLY	-	linker	UNP P03372
A	301	ALA	-	linker	UNP P03372
A	302	GLY	-	linker	UNP P03372
A	303	ALA	-	linker	UNP P03372
A	304	GLY	-	linker	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	295	ALA	-	linker	UNP P03372
B	296	GLY	-	linker	UNP P03372
B	297	ALA	-	linker	UNP P03372
B	298	GLY	-	linker	UNP P03372
B	299	ALA	-	linker	UNP P03372
B	300	GLY	-	linker	UNP P03372
B	301	ALA	-	linker	UNP P03372
B	302	GLY	-	linker	UNP P03372
B	303	ALA	-	linker	UNP P03372
B	304	GLY	-	linker	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called Grip peptide.

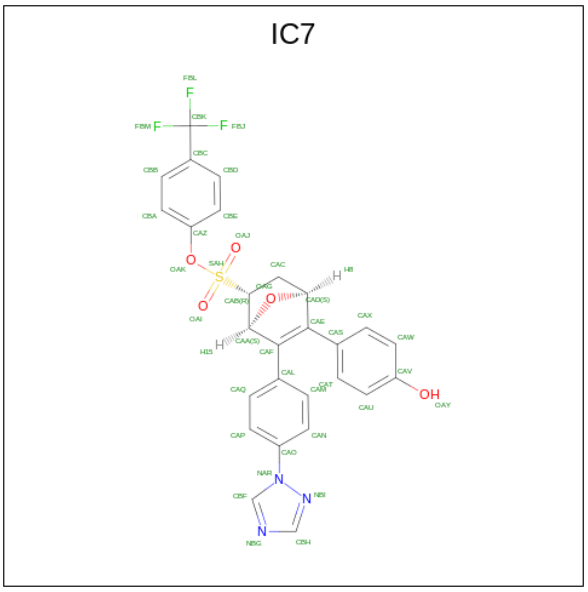
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	8	Total C N O 67 44 14 9	0	0	0
2	D	8	Total C N O 64 41 14 9	0	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



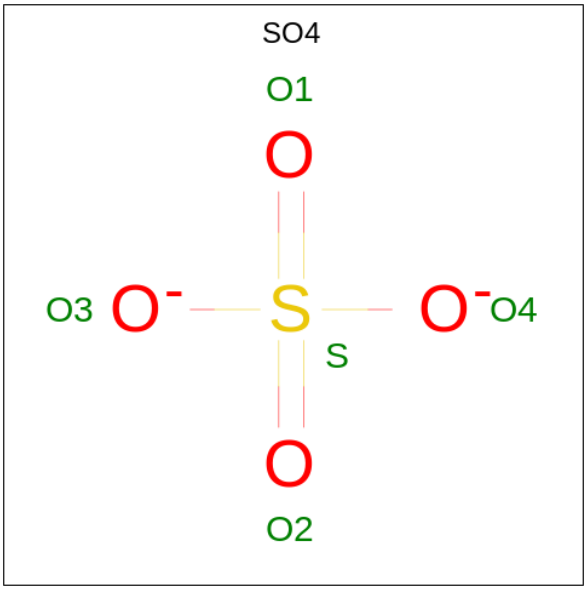
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0

- Molecule 4 is [4-(trifluoromethyl)phenyl] (1 {S},2 {R},4 {S})-5-(4-hydroxyphenyl)-6-[4-(1,2,4-triazol-1-yl)phenyl]-7-oxabicyclo[2.2.1]heptane-2-sulfonate (three-letter code: IC7) (formula: $C_{27}H_{20}F_3N_3O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	S	0	0
			39	27	3	3	5	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	O	S		0	0
			5	4	1			

- Molecule 6 is water.

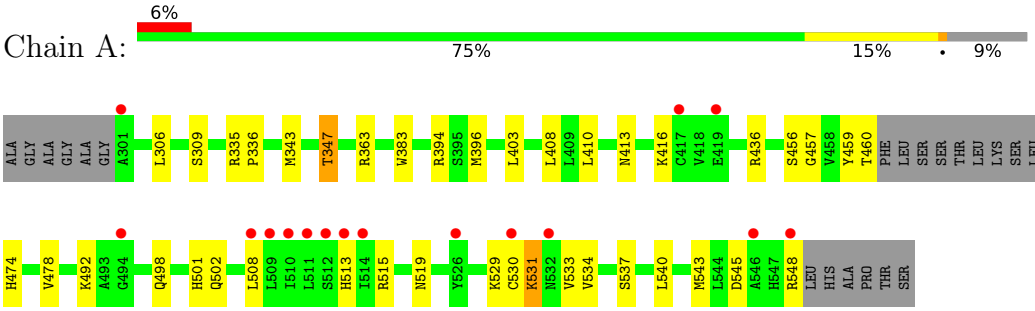
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	82	Total O 82 82	0	0
6	C	6	Total O 6 6	0	0
6	B	78	Total O 78 78	0	0

3 Residue-property plots

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.

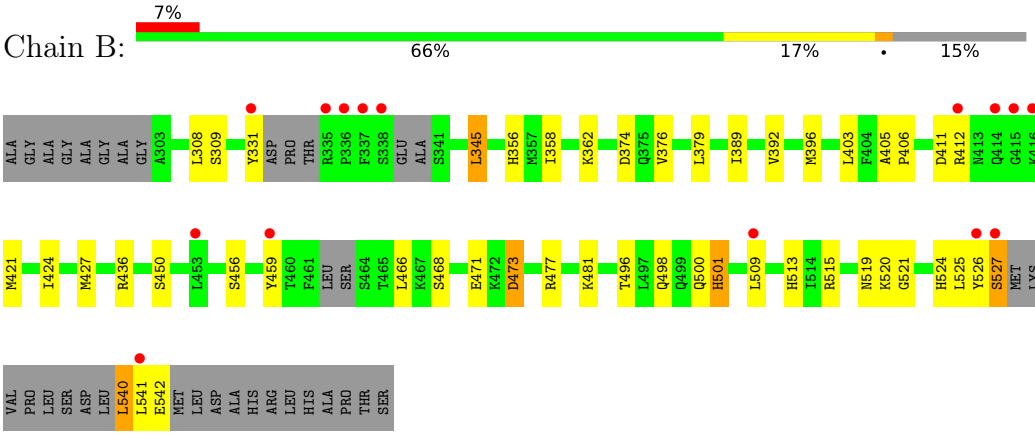
• Molecule 1: Estrogen receptor

Chain A:



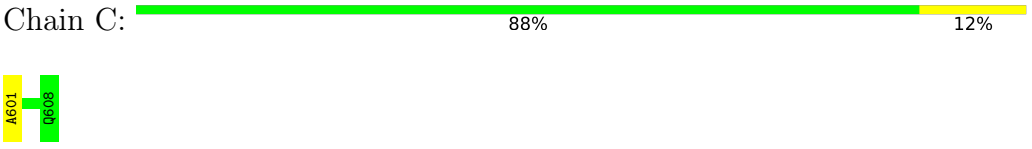
• Molecule 1: Estrogen receptor

Chain B:



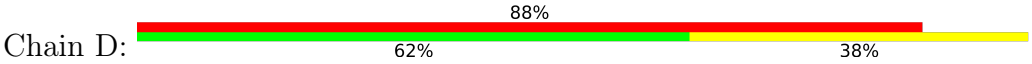
• Molecule 2: Grip peptide

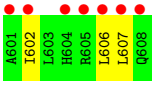
Chain C:



• Molecule 2: Grip peptide

Chain D:




A601
I602
L603
H604
R605
L606
L607
Q608

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	52.74Å 101.58Å 195.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.22 – 2.22 35.20 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.22-2.22) 99.8 (35.20-2.22)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.188 , 0.251 0.196 , 0.259	Depositor DCC
R_{free} test set	1322 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.9	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	3977	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IC7, PEG, 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	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.76	0/1920	0.87	0/2595
1	B	0.76	0/1779	0.86	0/2395
2	C	0.68	0/67	0.97	0/89
2	D	0.79	0/64	0.77	0/85
All	All	0.76	0/3830	0.86	0/5164

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

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	1878	0	1924	25	0
1	B	1751	0	1798	43	0
2	C	67	0	76	1	0
2	D	64	0	67	8	0
3	A	7	0	10	0	0
4	B	39	0	0	2	0
5	B	5	0	0	0	0
6	A	82	0	0	2	0
6	B	78	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	6	0	0	1	0
All	All	3977	0	3875	61	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 8.

All (61) 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:519:ASN:HD22	1:B:519:ASN:HD22	0.98	0.90
1:B:331:TYR:CD2	1:B:345:LEU:HD23	2.09	0.87
1:A:519:ASN:ND2	1:B:519:ASN:HD22	1.80	0.78
1:A:519:ASN:HD22	1:B:519:ASN:ND2	1.79	0.77
1:B:331:TYR:CG	1:B:345:LEU:HD23	2.20	0.75
1:B:308:LEU:O	1:B:481:LYS:HE3	1.95	0.67
1:B:331:TYR:CB	1:B:345:LEU:CD2	2.75	0.64
2:C:601:ALA:HB1	6:C:704:HOH:O	1.98	0.63
1:B:496:THR:O	1:B:500:GLN:HG3	1.98	0.63
1:B:540:LEU:HD21	4:B:601:IC7:CBH	2.30	0.61
1:B:456:SER:HA	1:B:515:ARG:NH2	2.16	0.60
1:B:331:TYR:CD2	1:B:345:LEU:CD2	2.84	0.60
1:A:396:MET:O	1:A:436:ARG:HD3	2.03	0.58
1:A:531:LYS:HB3	1:A:533:VAL:HG23	1.85	0.57
1:A:459:TYR:CD2	1:B:513:HIS:CD2	2.92	0.57
1:B:540:LEU:HD13	1:B:541:LEU:N	2.19	0.56
1:A:457:GLY:HA2	1:A:460:THR:HB	1.87	0.56
1:B:389:ILE:HA	1:B:392:VAL:HG22	1.92	0.52
1:B:521:GLY:O	1:B:525:LEU:HB2	2.10	0.51
1:A:474:HIS:O	1:A:478:VAL:HG23	2.11	0.50
1:B:374:ASP:OD2	1:B:471:GLU:OE1	2.30	0.50
1:B:424:ILE:HA	1:B:427:MET:HE3	1.94	0.50
1:B:403:LEU:HD12	1:B:405:ALA:O	2.12	0.49
1:A:383:TRP:NE1	1:A:543:MET:HB3	2.28	0.48
1:A:456:SER:HA	1:A:515:ARG:NH2	2.29	0.48
1:A:529:LYS:NZ	6:A:701:HOH:O	2.25	0.48
1:B:331:TYR:HB3	1:B:345:LEU:CD2	2.43	0.48
1:B:331:TYR:CG	1:B:345:LEU:CD2	2.92	0.47
1:B:358:ILE:HD13	2:D:606:LEU:CB	2.44	0.47
1:B:358:ILE:HD13	2:D:606:LEU:HB3	1.95	0.47
1:B:362:LYS:HE3	2:D:607:LEU:HD23	1.97	0.46
1:B:421:MET:HG2	4:B:601:IC7:CBE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:HB3	1:A:403:LEU:HD23	1.98	0.46
1:A:513[B]:HIS:CD2	1:B:459:TYR:CD2	3.03	0.46
1:B:376:VAL:HG22	2:D:607:LEU:HD12	1.98	0.46
1:B:527:SER:C	6:B:751:HOH:O	2.55	0.45
1:A:459:TYR:HD2	1:B:513:HIS:CD2	2.34	0.45
1:B:403:LEU:HD11	1:B:406:PRO:HA	1.99	0.45
1:A:459:TYR:CE2	1:B:513:HIS:CD2	3.04	0.45
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.52	0.45
2:D:602:ILE:O	2:D:606:LEU:HD23	2.16	0.44
1:A:537:SER:OG	1:A:540:LEU:HB2	2.17	0.43
1:B:331:TYR:HB2	1:B:345:LEU:HD22	2.00	0.43
1:A:498:GLN:O	1:A:502:GLN:HG3	2.19	0.43
1:A:413:ASN:OD1	1:A:416:LYS:NZ	2.52	0.42
1:B:356:HIS:HD2	6:B:701:HOH:O	2.03	0.42
1:B:358:ILE:HG21	2:D:606:LEU:HB3	2.01	0.42
1:B:379:LEU:HD12	2:D:607:LEU:HD11	2.02	0.42
1:B:540:LEU:O	1:B:541:LEU:HB2	2.20	0.42
1:A:363:ARG:NH1	6:A:706:HOH:O	2.50	0.41
1:A:335:ARG:HA	1:A:336:PRO:HA	1.90	0.41
1:B:308:LEU:O	1:B:481:LYS:CE	2.67	0.41
1:B:396:MET:HE2	1:B:436:ARG:HA	2.02	0.41
1:A:408:LEU:CD1	1:A:410:LEU:HD21	2.50	0.41
1:B:542:GLU:OE1	2:D:602:ILE:CB	2.69	0.41
1:A:408:LEU:HD12	1:A:410:LEU:HD21	2.02	0.41
1:A:513[B]:HIS:CD2	1:B:459:TYR:HD2	2.39	0.41
1:A:343:MET:O	1:A:347:THR:HB	2.21	0.40
1:A:508:LEU:HD22	1:B:509:LEU:HD21	2.02	0.40
1:B:473:ASP:OD2	1:B:477:ARG:NH2	2.54	0.40
1:B:331:TYR:CB	1:B:345:LEU:HD22	2.50	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	234/260 (90%)	229 (98%)	5 (2%)	0	100	100
1	B	208/260 (80%)	201 (97%)	7 (3%)	0	100	100
2	C	6/8 (75%)	6 (100%)	0	0	100	100
2	D	6/8 (75%)	6 (100%)	0	0	100	100
All	All	454/536 (85%)	442 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	210/225 (93%)	199 (95%)	11 (5%)	23	27
1	B	196/225 (87%)	181 (92%)	15 (8%)	13	12
2	C	7/7 (100%)	7 (100%)	0	100	100
2	D	6/7 (86%)	6 (100%)	0	100	100
All	All	419/464 (90%)	393 (94%)	26 (6%)	19	19

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	309	SER
1	A	347	THR
1	A	492	LYS
1	A	501[A]	HIS
1	A	501[B]	HIS
1	A	530	CYS
1	A	531	LYS
1	A	534	VAL
1	A	545	ASP
1	A	548	ARG
1	B	309	SER
1	B	345	LEU

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Mol	Chain	Res	Type
1	B	411	ASP
1	B	412	ARG
1	B	418	VAL
1	B	450	SER
1	B	466	LEU
1	B	468	SER
1	B	473	ASP
1	B	501	HIS
1	B	520	LYS
1	B	524	HIS
1	B	526	TYR
1	B	527	SER
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	398	HIS
1	B	513	HIS
1	B	519	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEG	A	601	-	6,6,6	0.27	0	5,5,5	0.13	0
4	IC7	B	601	-	40,44,44	3.66	13 (32%)	55,67,67	4.45	18 (32%)
5	SO4	B	602	-	4,4,4	0.39	0	6,6,6	0.20	0

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
3	PEG	A	601	-	-	0/4/4/4	-
4	IC7	B	601	-	-	5/27/53/53	0/7/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	IC7	CAA-CAF	-11.29	1.38	1.50
4	B	601	IC7	OAI-SAH	8.27	1.56	1.43
4	B	601	IC7	CAL-CAF	-8.01	1.33	1.48
4	B	601	IC7	CAS-CAE	-7.20	1.34	1.48
4	B	601	IC7	CAB-SAH	7.10	1.94	1.79
4	B	601	IC7	OAJ-SAH	6.30	1.53	1.43
4	B	601	IC7	FBM-CBK	-5.55	1.12	1.32
4	B	601	IC7	CAD-CAE	-5.15	1.44	1.51
4	B	601	IC7	CBK-CBC	-4.15	1.41	1.49
4	B	601	IC7	OAK-SAH	-3.80	1.54	1.60
4	B	601	IC7	CAO-NAR	-3.61	1.33	1.44
4	B	601	IC7	FBJ-CBK	-3.44	1.20	1.32
4	B	601	IC7	NBI-NAR	-2.11	1.33	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	IC7	OAJ-SAH-CAB	-22.57	79.97	109.33
4	B	601	IC7	OAI-SAH-CAB	-17.72	86.28	109.33
4	B	601	IC7	CAO-NAR-NBI	6.07	124.19	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	IC7	CBH-NBI-NAR	6.00	107.60	102.85
4	B	601	IC7	FBL-CBK-CBC	-5.33	101.21	112.93
4	B	601	IC7	CAD-CAC-CAB	-5.06	96.15	100.61
4	B	601	IC7	OAK-SAH-OAJ	3.92	118.91	106.82
4	B	601	IC7	CAZ-OAK-SAH	-3.30	111.80	119.85
4	B	601	IC7	CAP-CAO-NAR	3.27	122.02	119.15
4	B	601	IC7	OAG-CAD-CAC	-2.96	98.82	104.64
4	B	601	IC7	CBF-NBG-CBH	2.89	105.60	102.34
4	B	601	IC7	FBJ-CBK-CBC	2.84	119.17	112.93
4	B	601	IC7	OAK-SAH-OAI	2.80	115.46	106.82
4	B	601	IC7	FBJ-CBK-FBM	2.60	115.27	105.72
4	B	601	IC7	OAJ-SAH-OAI	2.53	124.84	118.01
4	B	601	IC7	NBG-CBF-NAR	-2.35	110.24	113.30
4	B	601	IC7	CBD-CBE-CAZ	2.04	122.23	119.73
4	B	601	IC7	CAT-CAS-CAE	-2.02	118.30	120.91

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	IC7	CAP-CAO-NAR-NBI
4	B	601	IC7	CAN-CAO-NAR-NBI
4	B	601	IC7	CAZ-OAK-SAH-OAJ
4	B	601	IC7	CAP-CAO-NAR-CBF
4	B	601	IC7	CAN-CAO-NAR-CBF

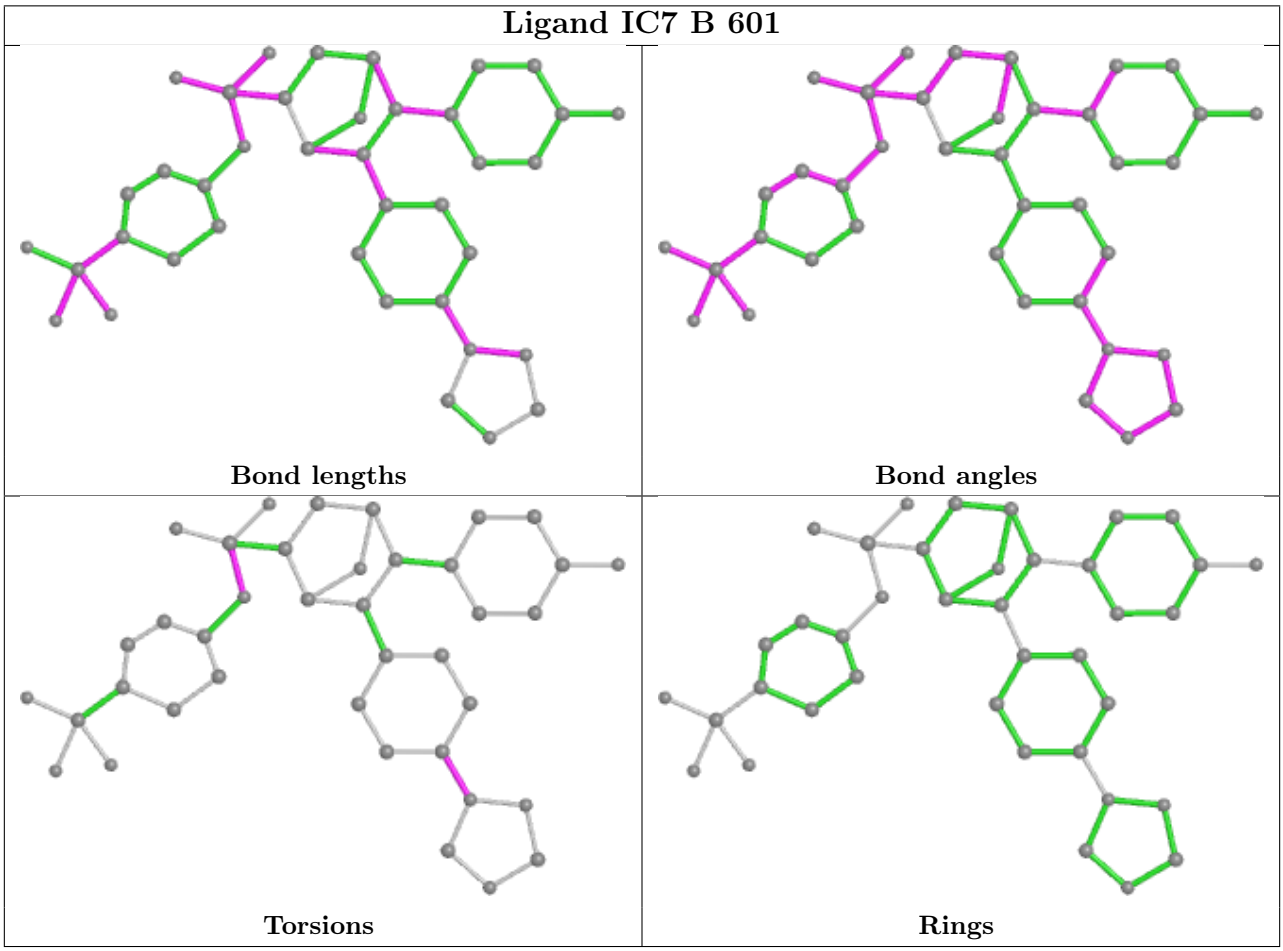
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	IC7	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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	236/260 (90%)	0.10	16 (6%) 17 16	23, 41, 82, 101	0
1	B	220/260 (84%)	0.24	17 (7%) 13 12	27, 43, 99, 125	0
2	C	8/8 (100%)	-0.53	0 100 100	36, 41, 47, 54	0
2	D	8/8 (100%)	3.81	7 (87%) 0 0	83, 97, 101, 110	0
All	All	472/536 (88%)	0.22	40 (8%) 10 9	23, 43, 93, 125	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	CYS	8.1
1	B	337	PHE	7.0
1	B	526	TYR	6.8
2	D	604	HIS	6.6
2	D	605	ARG	5.4
2	D	601	ALA	5.2
1	B	541	LEU	4.9
1	A	513[A]	HIS	4.6
1	B	418	VAL	4.3
1	B	336	PRO	4.2
2	D	608	GLN	4.2
1	B	415	GLY	4.0
1	A	548	ARG	3.8
1	A	510	ILE	3.5
1	B	338	SER	3.5
1	A	546	ALA	3.4
1	A	511	LEU	3.3
1	B	459	TYR	3.3
2	D	602	ILE	3.3
1	A	526	TYR	3.2
1	B	331	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	527	SER	2.7
1	A	532	ASN	2.7
1	B	412	ARG	2.7
1	A	530	CYS	2.6
1	A	509	LEU	2.4
1	A	301	ALA	2.4
1	A	494	GLY	2.3
1	B	335	ARG	2.3
1	A	514	ILE	2.3
1	A	512	SER	2.3
2	D	606	LEU	2.2
1	A	417	CYS	2.2
1	B	509	LEU	2.2
1	B	416	LYS	2.1
1	A	508	LEU	2.1
1	A	419	GLU	2.1
1	B	453	LEU	2.1
2	D	607	LEU	2.0
1	B	414	GLN	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)

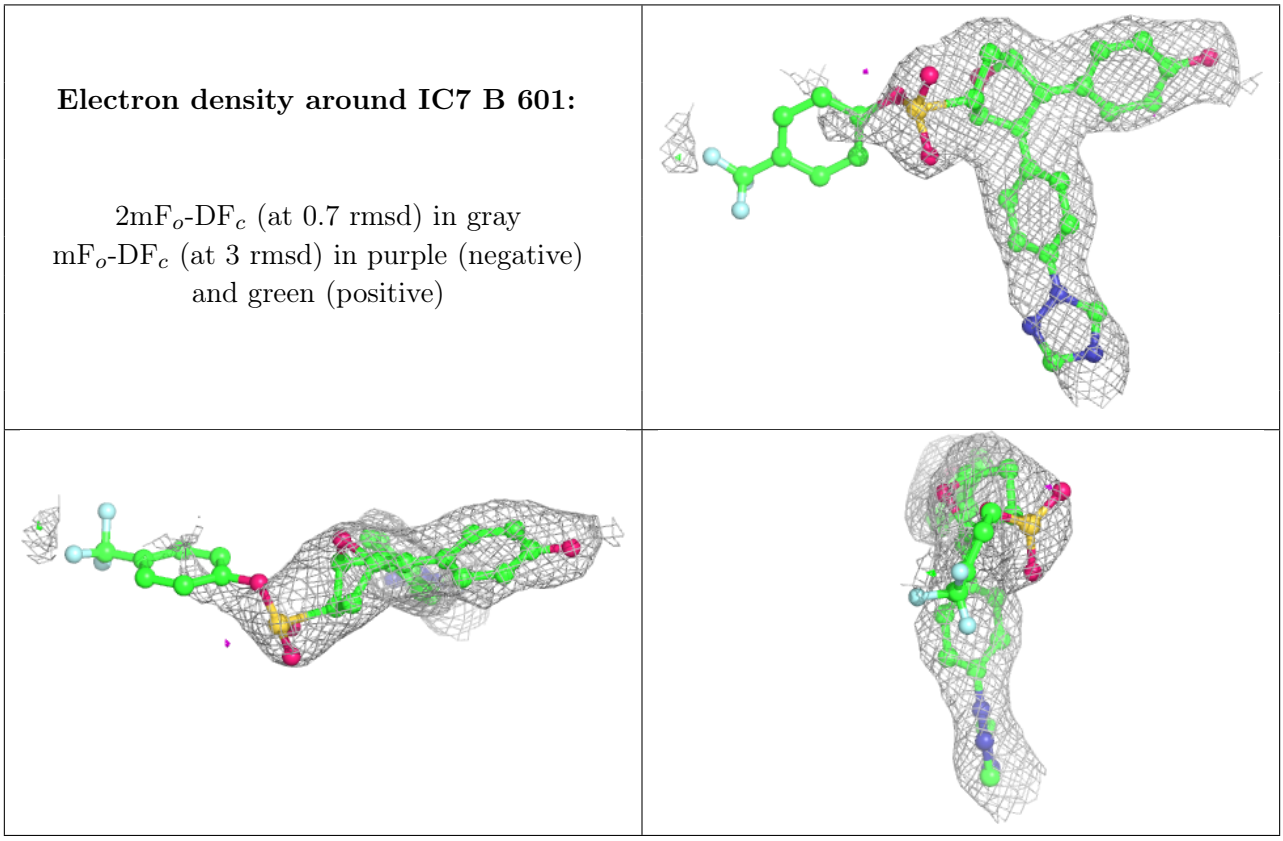
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	A	601	7/7	0.80	0.40	56,67,73,73	0
4	IC7	B	601	39/39	0.87	0.25	43,81,225,237	0
5	SO4	B	602	5/5	0.92	0.36	84,85,93,114	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 IC7 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)



6.5 Other polymers

There are no such residues in this entry.