



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 08:41 AM EDT

PDB ID : 7UJW / pdb_00007ujw
Title : Estrogen Receptor Alpha Ligand Binding Domain Y537S Mutant in Complex with a Methylated Lasofoxifene Derivative that Possesses Selective Estrogen Receptor Degradation Activities
Authors : Hosfield, D.J.; Greene, G.L.; Fanning, S.W.
Deposited on : 2022-03-31
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

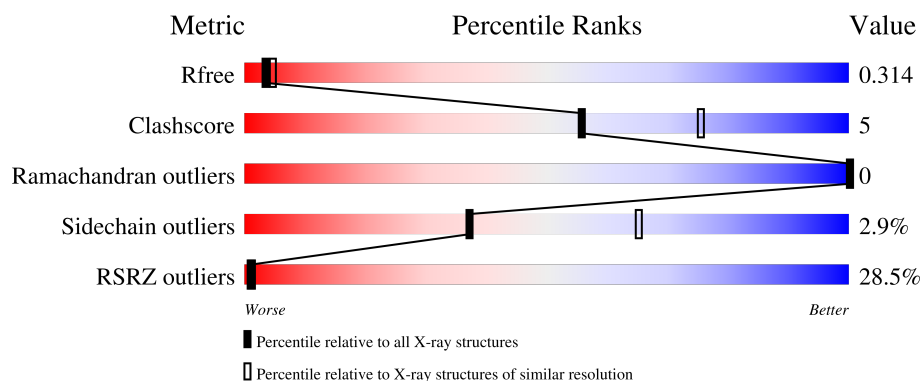
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	263	29% 68% 12% 20%
1	B	263	10% 70% 11% 19%
1	C	263	27% 68% 11% 21%
1	D	263	26% 73% 9% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6682 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	B	212	Total	C	N	O	S	0	0	0
			1621	1039	280	287	15			
1	D	218	Total	C	N	O	S	0	0	0
			1646	1052	285	294	15			
1	C	208	Total	C	N	O	S	0	0	0
			1589	1020	276	280	13			
1	A	210	Total	C	N	O	S	0	0	0
			1612	1034	278	286	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	292	HIS	-	expression tag	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	GLU	-	expression tag	UNP P03372
B	299	ASN	-	expression tag	UNP P03372
B	300	LEU	-	expression tag	UNP P03372
B	301	TYR	-	expression tag	UNP P03372
B	302	PHE	-	expression tag	UNP P03372
B	303	GLN	-	expression tag	UNP P03372
B	304	SER	-	expression tag	UNP P03372
B	305	MET	-	expression tag	UNP P03372
B	381	SER	CYS	conflict	UNP P03372
B	417	SER	CYS	conflict	UNP P03372
B	530	SER	CYS	conflict	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372
D	292	HIS	-	expression tag	UNP P03372
D	293	HIS	-	expression tag	UNP P03372
D	294	HIS	-	expression tag	UNP P03372

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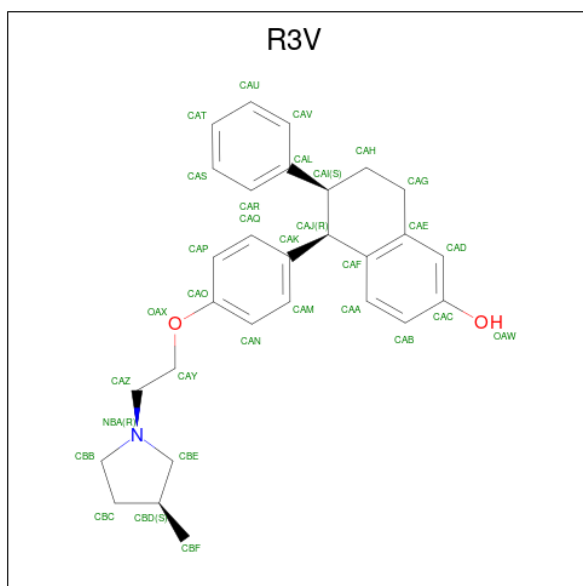
Chain	Residue	Modelled	Actual	Comment	Reference
D	295	HIS	-	expression tag	UNP P03372
D	296	HIS	-	expression tag	UNP P03372
D	297	HIS	-	expression tag	UNP P03372
D	298	GLU	-	expression tag	UNP P03372
D	299	ASN	-	expression tag	UNP P03372
D	300	LEU	-	expression tag	UNP P03372
D	301	TYR	-	expression tag	UNP P03372
D	302	PHE	-	expression tag	UNP P03372
D	303	GLN	-	expression tag	UNP P03372
D	304	SER	-	expression tag	UNP P03372
D	305	MET	-	expression tag	UNP P03372
D	381	SER	CYS	conflict	UNP P03372
D	417	SER	CYS	conflict	UNP P03372
D	530	SER	CYS	conflict	UNP P03372
D	537	SER	TYR	engineered mutation	UNP P03372
C	292	HIS	-	expression tag	UNP P03372
C	293	HIS	-	expression tag	UNP P03372
C	294	HIS	-	expression tag	UNP P03372
C	295	HIS	-	expression tag	UNP P03372
C	296	HIS	-	expression tag	UNP P03372
C	297	HIS	-	expression tag	UNP P03372
C	298	GLU	-	expression tag	UNP P03372
C	299	ASN	-	expression tag	UNP P03372
C	300	LEU	-	expression tag	UNP P03372
C	301	TYR	-	expression tag	UNP P03372
C	302	PHE	-	expression tag	UNP P03372
C	303	GLN	-	expression tag	UNP P03372
C	304	SER	-	expression tag	UNP P03372
C	305	MET	-	expression tag	UNP P03372
C	381	SER	CYS	conflict	UNP P03372
C	417	SER	CYS	conflict	UNP P03372
C	530	SER	CYS	conflict	UNP P03372
C	537	SER	TYR	engineered mutation	UNP P03372
A	292	HIS	-	expression tag	UNP P03372
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	GLU	-	expression tag	UNP P03372
A	299	ASN	-	expression tag	UNP P03372
A	300	LEU	-	expression tag	UNP P03372

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

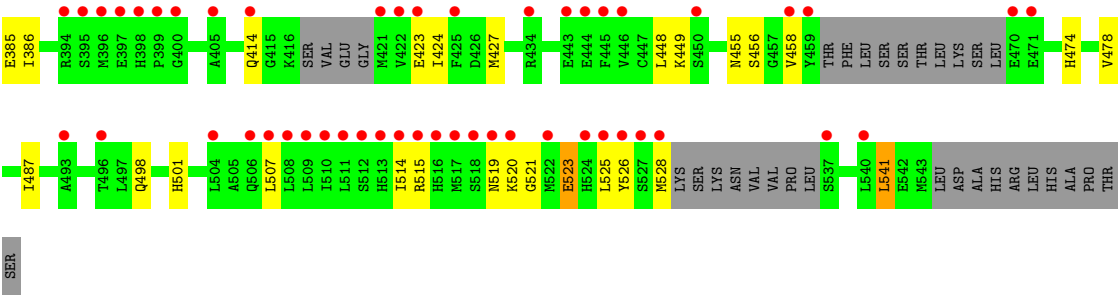
- Molecule 2 is (5R,6S)-5-(4-{2-[(3S)-3-methylpyrrolidin-1-yl]ethoxy}phenyl)-6-phenyl-5,6,7,8-tetrahydronaphthalen-2-ol (CCD ID: R3V) (formula: C₂₉H₃₃NO₂) (labeled as "Ligand of Interest" by depositor).



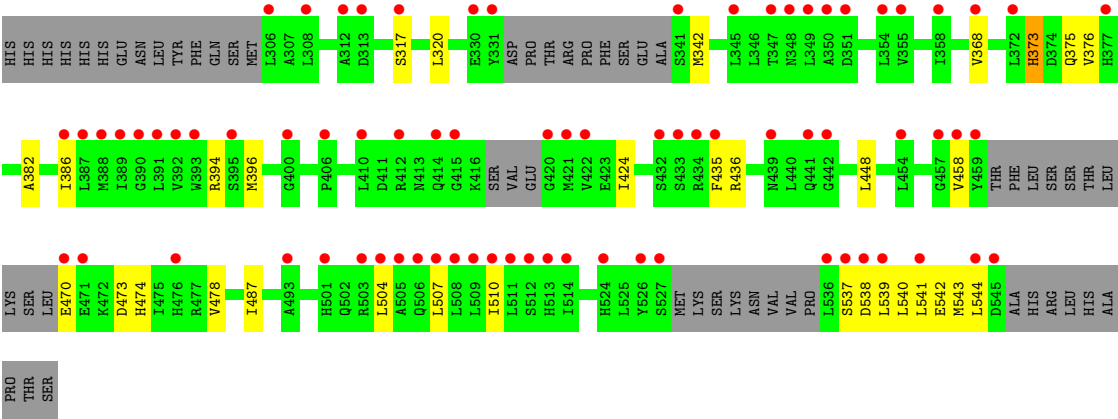
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			32	29	1	2		
2	D	1	Total	C	N	O	0	0
			32	29	1	2		
2	C	1	Total	C	N	O	0	0
			32	29	1	2		
2	A	1	Total	C	N	O	0	0
			32	29	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	24	Total 24	O 24	0	0
3	D	19	Total 19	O 19	0	0
3	C	24	Total 24	O 24	0	0
3	A	19	Total 19	O 19	0	0



• Molecule 1: Estrogen receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.95Å 58.97Å 88.99Å 91.46° 102.06° 117.23°	Depositor
Resolution (Å)	47.59 – 2.60 47.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.1 (47.59-2.60) 87.4 (47.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.82	Depositor
R, R_{free}	0.215 , 0.263 0.292 , 0.314	Depositor DCC
R_{free} test set	1251 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6682	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% 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: R3V

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	0.38	0/1637	0.81	0/2214
1	B	0.52	0/1645	0.82	1/2224 (0.0%)
1	C	0.47	0/1614	0.84	1/2184 (0.0%)
1	D	0.39	0/1671	0.81	1/2262 (0.0%)
All	All	0.44	0/6567	0.82	3/8884 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	414	GLN	N-CA-C	-8.41	103.02	113.28
1	D	341	SER	N-CA-C	-6.42	105.27	113.23
1	B	341	SER	N-CA-C	-5.15	105.75	111.36

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	1612	0	1594	18	0
1	B	1621	0	1601	16	0
1	C	1589	0	1562	16	0
1	D	1646	0	1611	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	32	0	0	1	0
2	B	32	0	0	1	0
2	C	32	0	0	1	0
2	D	32	0	0	1	0
3	A	19	0	0	0	0
3	B	24	0	0	0	0
3	C	24	0	0	1	0
3	D	19	0	0	0	0
All	All	6682	0	6368	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 5.

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:B:540:LEU:O	1:B:544:LEU:HD12	1.81	0.81
1:A:373:HIS:O	1:A:373:HIS:ND1	2.16	0.79
1:C:376:VAL:HG21	1:C:541:LEU:HG	1.70	0.74
1:B:539:LEU:O	1:B:543:MET:HB2	1.89	0.73
1:A:538:ASP:O	1:A:542:GLU:HG3	1.92	0.69
1:A:317:SER:HA	1:A:320:LEU:HB2	1.76	0.66
1:A:539:LEU:O	1:A:543:MET:HG3	2.00	0.62
1:B:343:MET:HE2	1:B:528:MET:SD	2.43	0.59
1:D:456:SER:HA	1:D:515:ARG:NH2	2.18	0.58
1:A:540:LEU:O	1:A:544:LEU:HG	2.05	0.56
1:A:368:VAL:HA	1:A:375:GLN:NE2	2.21	0.56
1:D:439:ASN:O	1:D:441:GLN:NE2	2.39	0.55
2:C:601:R3V:CAV	2:C:601:R3V:CAK	2.85	0.55
1:C:385:GLU:HG2	1:C:514:ILE:HG22	1.87	0.54
1:D:455:ASN:O	1:D:458:VAL:HG12	2.09	0.53
1:A:487:ILE:HD11	1:A:504:LEU:HD22	1.91	0.52
1:B:456:SER:HA	1:B:515:ARG:NH2	2.24	0.52
1:D:448:LEU:HD11	1:D:507:LEU:HD22	1.92	0.52
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.46	0.51
1:A:396:MET:HE3	1:A:436:ARG:HA	1.92	0.51
1:B:424:ILE:HA	1:B:427:MET:HE3	1.93	0.51
1:D:525:LEU:HD13	2:D:601:R3V:CAS	2.41	0.50
1:A:448:LEU:HD11	1:A:507:LEU:HD22	1.93	0.50
1:A:470:GLU:HA	1:A:473:ASP:HB3	1.92	0.50
1:B:541:LEU:HG	1:D:373:HIS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:SER:HA	1:C:515:ARG:NH2	2.26	0.50
1:B:342:MET:O	1:B:346:LEU:HG	2.12	0.49
1:B:382:ALA:O	1:B:386:ILE:HG12	2.13	0.47
1:A:470:GLU:O	1:A:474:HIS:N	2.28	0.47
1:C:382:ALA:O	1:C:386:ILE:HG12	2.14	0.47
1:B:509:LEU:O	1:B:512:SER:OG	2.33	0.47
1:D:454:LEU:HD22	1:D:475:ILE:HG23	1.97	0.47
1:C:455:ASN:O	1:C:458:VAL:HG12	2.15	0.47
1:A:435:PHE:CE1	1:A:510:ILE:HG21	2.50	0.47
1:C:448:LEU:HD11	1:C:507:LEU:HD22	1.97	0.46
1:C:449:LYS:NZ	3:C:702:HOH:O	2.42	0.46
1:B:392:VAL:HG11	1:B:431:THR:HG22	1.98	0.46
1:C:519:ASN:O	1:C:523:GLU:HG2	2.16	0.45
1:C:526:TYR:HA	1:C:528:MET:HG2	1.97	0.45
1:D:537:SER:HB2	1:D:538:ASP:H	1.61	0.45
1:A:394:ARG:NH2	2:A:601:R3V:OAW	2.48	0.45
1:D:396:MET:HE3	1:D:436:ARG:HA	1.98	0.45
1:A:537:SER:O	1:A:541:LEU:N	2.36	0.45
1:A:382:ALA:O	1:A:386:ILE:HG12	2.18	0.44
1:D:516:HIS:O	1:D:520:LYS:HG2	2.18	0.44
1:D:545:ASP:OD1	1:D:545:ASP:N	2.50	0.44
1:A:376:VAL:HG11	1:A:537:SER:OG	2.18	0.44
1:D:373:HIS:CD2	1:D:373:HIS:C	2.96	0.43
1:B:501:HIS:CD2	1:C:487:ILE:HG13	2.53	0.43
1:C:521:GLY:O	1:C:525:LEU:HB2	2.19	0.43
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.99	0.43
1:C:423:GLU:O	1:C:427:MET:HG3	2.19	0.43
1:C:474:HIS:O	1:C:478:VAL:HG23	2.19	0.43
1:C:498:GLN:HA	1:C:501:HIS:NE2	2.33	0.43
1:B:353:GLU:OE2	2:B:601:R3V:OAW	2.38	0.42
1:B:501:HIS:CG	1:C:487:ILE:HG13	2.56	0.41
1:A:539:LEU:O	1:A:543:MET:CG	2.69	0.41
1:C:372:LEU:O	1:C:376:VAL:HG23	2.20	0.40
1:B:524:HIS:O	1:B:524:HIS:CD2	2.74	0.40
1:A:474:HIS:O	1:A:478:VAL:HG23	2.20	0.40
1:D:328:TYR:CE2	1:D:406:PRO:HB2	2.56	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	200/263 (76%)	196 (98%)	4 (2%)	0	100	100
1	B	202/263 (77%)	201 (100%)	1 (0%)	0	100	100
1	C	198/263 (75%)	195 (98%)	3 (2%)	0	100	100
1	D	210/263 (80%)	204 (97%)	6 (3%)	0	100	100
All	All	810/1052 (77%)	796 (98%)	14 (2%)	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	168/238 (71%)	164 (98%)	4 (2%)	43	70
1	B	167/238 (70%)	163 (98%)	4 (2%)	43	70
1	C	163/238 (68%)	159 (98%)	4 (2%)	42	69
1	D	168/238 (71%)	161 (96%)	7 (4%)	26	52
All	All	666/952 (70%)	647 (97%)	19 (3%)	37	65

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	421	MET
1	B	425	PHE

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Mol	Chain	Res	Type
1	B	543	MET
1	B	545	ASP
1	D	330	GLU
1	D	362	LYS
1	D	365	PRO
1	D	368	VAL
1	D	373	HIS
1	D	525	LEU
1	D	537	SER
1	C	424	ILE
1	C	520	LYS
1	C	523	GLU
1	C	541	LEU
1	A	342	MET
1	A	373	HIS
1	A	424	ILE
1	A	458	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	474	HIS
1	B	500	GLN
1	B	501	HIS
1	B	519	ASN
1	D	359	ASN
1	D	373	HIS
1	D	474	HIS
1	D	501	HIS
1	D	513	HIS
1	C	356	HIS
1	C	414	GLN
1	C	516	HIS
1	C	519	ASN
1	A	348	ASN
1	A	359	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	R3V	C	601	-	35,36,36	0.82	2 (5%)	44,50,50	1.22	3 (6%)
2	R3V	A	601	-	35,36,36	3.59	16 (45%)	44,50,50	2.51	16 (36%)
2	R3V	B	601	-	35,36,36	0.88	1 (2%)	44,50,50	1.01	4 (9%)
2	R3V	D	601	-	35,36,36	0.83	2 (5%)	44,50,50	0.80	1 (2%)

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	R3V	C	601	-	-	2/14/36/36	0/5/5/5
2	R3V	A	601	-	-	3/14/36/36	0/5/5/5
2	R3V	B	601	-	-	3/14/36/36	0/5/5/5
2	R3V	D	601	-	-	5/14/36/36	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	R3V	CAA-CAF	9.03	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	R3V	CAM-CAN	7.75	1.51	1.38
2	A	601	R3V	CAB-CAC	7.21	1.52	1.39
2	A	601	R3V	CAQ-CAK	6.04	1.48	1.39
2	A	601	R3V	CAP-CAO	5.92	1.49	1.38
2	A	601	R3V	CAF-CAJ	-5.76	1.43	1.51
2	A	601	R3V	CAD-CAE	5.24	1.47	1.39
2	A	601	R3V	CAZ-NBA	-4.44	1.37	1.47
2	A	601	R3V	CAD-CAC	-4.23	1.32	1.39
2	A	601	R3V	CAE-CAF	-4.09	1.33	1.40
2	B	601	R3V	CAH-CAI	-3.56	1.49	1.53
2	D	601	R3V	CAH-CAI	-3.35	1.49	1.53
2	C	601	R3V	CAH-CAI	-3.30	1.49	1.53
2	A	601	R3V	CBE-NBA	-3.22	1.42	1.47
2	A	601	R3V	CAK-CAJ	-3.03	1.49	1.52
2	A	601	R3V	CAM-CAK	-2.79	1.34	1.39
2	A	601	R3V	CAN-CAO	-2.69	1.33	1.38
2	A	601	R3V	OAW-CAC	2.40	1.42	1.37
2	A	601	R3V	CAH-CAG	2.25	1.57	1.52
2	C	601	R3V	CBC-CBB	-2.14	1.48	1.52
2	D	601	R3V	CBC-CBB	-2.11	1.48	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	R3V	CAC-CAD-CAE	-8.03	111.75	120.77
2	C	601	R3V	CAK-CAJ-CAF	-6.27	103.30	112.95
2	A	601	R3V	CAD-CAE-CAF	6.26	127.38	119.49
2	A	601	R3V	CAG-CAE-CAD	-6.02	108.03	119.91
2	A	601	R3V	CAK-CAJ-CAF	-4.58	105.90	112.95
2	A	601	R3V	CAB-CAC-CAD	4.04	124.61	120.19
2	A	601	R3V	CBB-NBA-CBE	3.69	108.36	104.02
2	A	601	R3V	CAB-CAA-CAF	-3.45	115.41	121.12
2	B	601	R3V	CAH-CAI-CAL	-3.31	106.46	112.54
2	A	601	R3V	CAA-CAF-CAJ	-3.20	116.52	124.80
2	B	601	R3V	CAK-CAJ-CAF	-2.99	108.35	112.95
2	A	601	R3V	CAV-CAL-CAR	2.90	121.90	118.30
2	C	601	R3V	CAA-CAF-CAJ	-2.53	118.27	124.80
2	B	601	R3V	CAA-CAF-CAJ	-2.38	118.65	124.80
2	D	601	R3V	CAA-CAF-CAJ	-2.35	118.73	124.80
2	A	601	R3V	CAG-CAE-CAF	2.34	124.59	121.11
2	A	601	R3V	CAV-CAL-CAI	-2.28	116.71	121.08
2	A	601	R3V	CAP-CAQ-CAK	-2.24	118.95	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	R3V	CAH-CAG-CAE	-2.22	108.65	112.87
2	A	601	R3V	CAZ-NBA-CBB	-2.13	108.19	113.25
2	A	601	R3V	CAY-CAZ-NBA	-2.09	107.44	113.36
2	A	601	R3V	CAZ-NBA-CBE	-2.07	108.38	113.18
2	B	601	R3V	CBB-NBA-CBE	2.06	106.45	104.02
2	C	601	R3V	CBB-NBA-CBE	2.01	106.39	104.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	R3V	CAY-CAZ-NBA-CBE
2	D	601	R3V	CAY-CAZ-NBA-CBB
2	C	601	R3V	CAJ-CAI-CAL-CAV
2	D	601	R3V	OAX-CAY-CAZ-NBA
2	C	601	R3V	CAJ-CAI-CAL-CAR
2	B	601	R3V	OAX-CAY-CAZ-NBA
2	A	601	R3V	CAP-CAO-OAX-CAY
2	A	601	R3V	CAN-CAO-OAX-CAY
2	D	601	R3V	CAP-CAO-OAX-CAY
2	D	601	R3V	CAN-CAO-OAX-CAY
2	B	601	R3V	CAP-CAO-OAX-CAY
2	B	601	R3V	CAN-CAO-OAX-CAY
2	A	601	R3V	OAX-CAY-CAZ-NBA

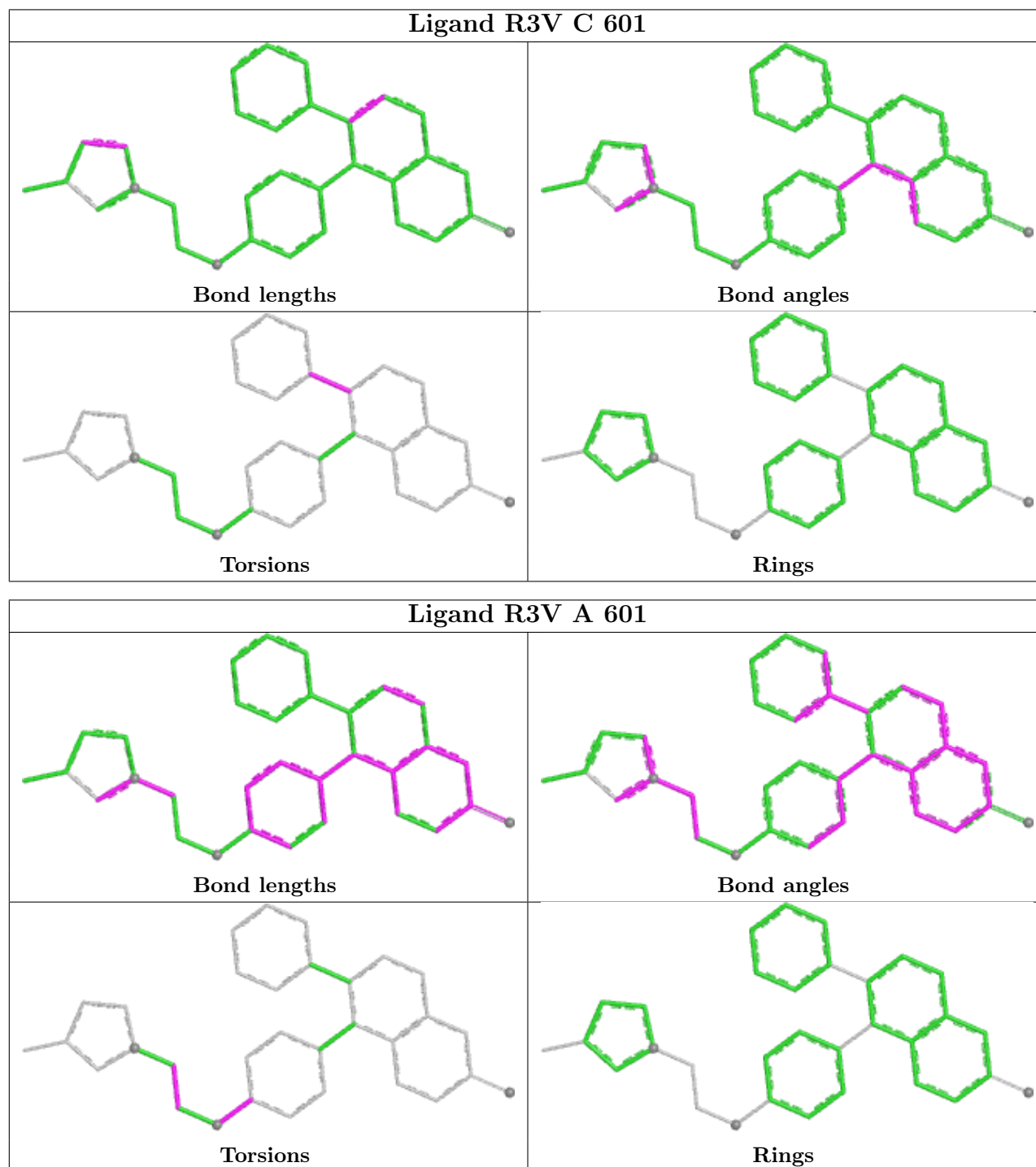
There are no ring outliers.

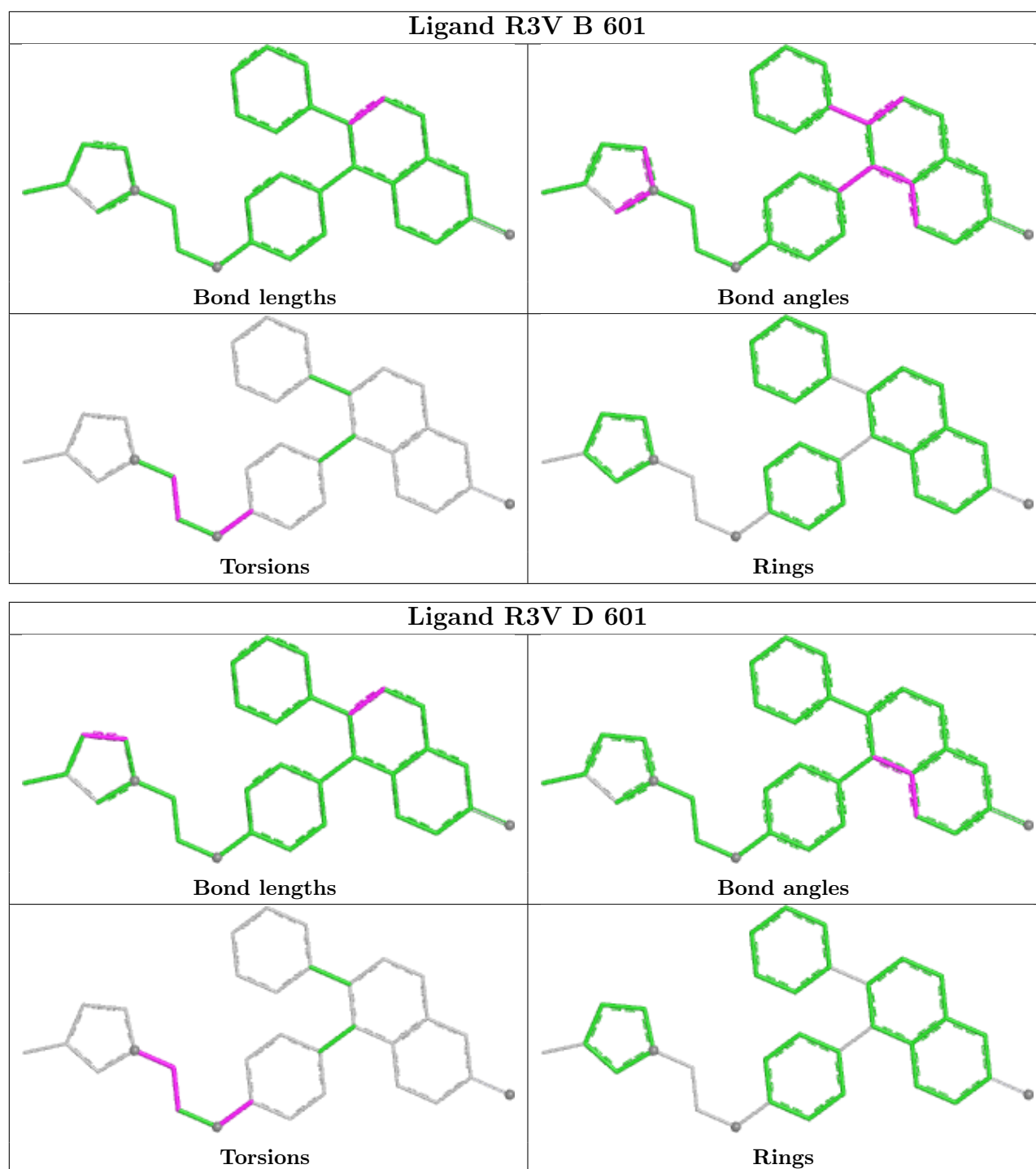
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	R3V	1	0
2	A	601	R3V	1	0
2	B	601	R3V	1	0
2	D	601	R3V	1	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 [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, 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	210/263 (79%)	1.68	76 (36%) 1 0	28, 49, 88, 115	0
1	B	212/263 (80%)	0.74	26 (12%) 8 6	25, 46, 82, 109	0
1	C	208/263 (79%)	1.76	71 (34%) 1 1	27, 49, 94, 129	0
1	D	218/263 (82%)	1.59	69 (31%) 1 1	28, 50, 90, 116	1 (0%)
All	All	848/1052 (80%)	1.44	242 (28%) 1 1	25, 49, 90, 129	1 (0%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	513	HIS	7.1
1	C	512	SER	6.7
1	D	450	SER	6.5
1	D	471	GLU	6.2
1	A	504	LEU	5.8
1	A	470	GLU	5.7
1	C	509	LEU	5.7
1	C	514	ILE	5.6
1	C	511	LEU	5.6
1	A	536	LEU	5.4
1	C	510	ILE	5.3
1	B	471	GLU	5.2
1	C	518	SER	5.0
1	D	452	ILE	4.9
1	C	421	MET	4.6
1	C	332	ASP	4.6
1	C	470	GLU	4.5
1	A	390	GLY	4.5
1	D	449	LYS	4.5
1	C	444	GLU	4.4
1	D	546	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	526	TYR	4.2
1	D	418	VAL	4.2
1	D	451	ILE	4.2
1	D	309	SER	4.2
1	C	306	LEU	4.2
1	D	528	MET	4.1
1	D	453	LEU	4.1
1	A	442	GLY	4.1
1	A	513	HIS	4.0
1	A	508	LEU	4.0
1	A	545	ASP	4.0
1	A	389	ILE	4.0
1	D	454	LEU	3.9
1	D	415	GLY	3.9
1	C	458	VAL	3.8
1	A	471	GLU	3.8
1	A	538	ASP	3.8
1	D	389	ILE	3.8
1	B	544	LEU	3.7
1	C	540	LEU	3.7
1	D	537	SER	3.7
1	A	392	VAL	3.7
1	D	470	GLU	3.7
1	A	507	LEU	3.7
1	B	536	LEU	3.6
1	D	459	TYR	3.6
1	D	543	MET	3.6
1	C	397	GLU	3.6
1	D	472	LYS	3.6
1	C	519	ASN	3.5
1	C	508	LEU	3.5
1	A	511	LEU	3.5
1	D	521	GLY	3.5
1	D	425	PHE	3.5
1	C	398	HIS	3.5
1	A	350	ALA	3.4
1	D	545	ASP	3.4
1	C	423	GLU	3.4
1	D	527	SER	3.4
1	A	391	LEU	3.3
1	C	405	ALA	3.3
1	C	516	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	505	ALA	3.3
1	C	527	SER	3.3
1	A	537	SER	3.3
1	A	512	SER	3.3
1	D	538	ASP	3.3
1	A	387	LEU	3.2
1	A	501	HIS	3.2
1	A	527	SER	3.2
1	B	419	GLU	3.2
1	A	388	MET	3.1
1	D	518	SER	3.1
1	C	395	SER	3.1
1	A	331	TYR	3.1
1	B	545	ASP	3.1
1	B	459	TYR	3.1
1	D	406	PRO	3.1
1	C	358	ILE	3.0
1	D	307	ALA	3.0
1	C	357	MET	3.0
1	C	517	MET	3.0
1	C	354	LEU	3.0
1	A	330	GLU	3.0
1	A	406	PRO	3.0
1	D	517	MET	3.0
1	A	347	THR	3.0
1	C	445	PHE	3.0
1	D	402	LEU	3.0
1	A	393	TRP	3.0
1	C	520	LYS	3.0
1	C	374	ASP	3.0
1	A	434	ARG	3.0
1	A	386	ILE	3.0
1	D	404	PHE	3.0
1	A	509	LEU	2.9
1	B	307	ALA	2.9
1	D	408	LEU	2.9
1	B	470	GLU	2.9
1	A	459	TYR	2.9
1	A	514	ILE	2.9
1	A	510	ILE	2.9
1	D	483	THR	2.9
1	A	308	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	330	GLU	2.9
1	A	544	LEU	2.9
1	C	394	ARG	2.8
1	A	503	ARG	2.8
1	D	475	ILE	2.8
1	A	354	LEU	2.8
1	D	547	HIS	2.8
1	C	368	VAL	2.8
1	A	458	VAL	2.8
1	B	309	SER	2.8
1	A	349	LEU	2.8
1	C	515	ARG	2.8
1	C	414	GLN	2.8
1	A	306	LEU	2.8
1	C	493	ALA	2.8
1	D	448	LEU	2.8
1	D	479	LEU	2.8
1	A	368	VAL	2.8
1	B	308	LEU	2.7
1	D	340	ALA	2.7
1	C	496	THR	2.7
1	B	525	LEU	2.7
1	C	373	HIS	2.7
1	A	348	ASN	2.7
1	C	425	PHE	2.7
1	D	409	LEU	2.7
1	C	400	GLY	2.7
1	D	413	ASN	2.7
1	C	459	TYR	2.6
1	D	386	ILE	2.6
1	D	478	VAL	2.6
1	A	493	ALA	2.6
1	C	396	MET	2.6
1	C	522	MET	2.6
1	B	537	SER	2.6
1	B	526	TYR	2.6
1	A	506	GLN	2.6
1	D	310	LEU	2.5
1	A	345	LEU	2.5
1	D	512	SER	2.5
1	C	537	SER	2.5
1	A	341	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	525	LEU	2.5
1	C	526	TYR	2.5
1	D	473	ASP	2.5
1	B	330	GLU	2.5
1	C	364	VAL	2.5
1	B	340	ALA	2.5
1	D	419	GLU	2.4
1	D	401	LYS	2.4
1	B	306	LEU	2.4
1	D	487	ILE	2.4
1	A	410	LEU	2.4
1	A	526	TYR	2.4
1	A	539	LEU	2.4
1	D	417	SER	2.4
1	A	420	GLY	2.4
1	A	355	VAL	2.4
1	D	403	LEU	2.4
1	C	372	LEU	2.4
1	C	507	LEU	2.4
1	C	314	GLN	2.4
1	C	446	VAL	2.4
1	C	307	ALA	2.4
1	C	525	LEU	2.3
1	D	524	HIS	2.3
1	A	377	HIS	2.3
1	A	476	HIS	2.3
1	D	519	ASN	2.3
1	B	473	ASP	2.3
1	C	506	GLN	2.3
1	A	441	GLN	2.3
1	A	372	LEU	2.3
1	A	454	LEU	2.3
1	D	490	MET	2.3
1	A	421	MET	2.3
1	B	472	LYS	2.3
1	D	308	LEU	2.3
1	B	416	LYS	2.3
1	B	359	ASN	2.3
1	A	317	SER	2.3
1	C	434	ARG	2.3
1	B	310	LEU	2.3
1	C	308	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	501	HIS	2.3
1	C	369	ASP	2.3
1	C	450	SER	2.3
1	A	312	ALA	2.2
1	D	331	TYR	2.2
1	A	412	ARG	2.2
1	A	395	SER	2.2
1	A	432	SER	2.2
1	A	400	GLY	2.2
1	A	439	ASN	2.2
1	D	324	PRO	2.2
1	A	541	LEU	2.2
1	C	316	VAL	2.2
1	D	322	ALA	2.2
1	A	457	GLY	2.2
1	A	422	VAL	2.2
1	C	524	HIS	2.2
1	B	415	GLY	2.2
1	A	415	GLY	2.2
1	A	351	ASP	2.2
1	C	422	VAL	2.2
1	D	455	ASN	2.1
1	C	504	LEU	2.1
1	A	313	ASP	2.1
1	C	382	ALA	2.1
1	D	360	TRP	2.1
1	C	383	TRP	2.1
1	C	443	GLU	2.1
1	C	471	GLU	2.1
1	D	515	ARG	2.1
1	B	485	THR	2.1
1	D	311	THR	2.1
1	C	528	MET	2.1
1	D	456	SER	2.1
1	A	433	SER	2.1
1	C	399	PRO	2.1
1	B	421	MET	2.1
1	D	421	MET	2.1
1	D	390	GLY	2.1
1	A	358	ILE	2.1
1	C	371	THR	2.1
1	A	414	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	372	LEU	2.1
1	D	429	LEU	2.1
1	C	327	LEU	2.1
1	B	413	ASN	2.1
1	D	476	HIS	2.1
1	C	318	ALA	2.0
1	D	315	MET	2.0
1	C	353	GLU	2.0
1	A	435	PHE	2.0
1	D	516	HIS	2.0
1	A	524	HIS	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](#)

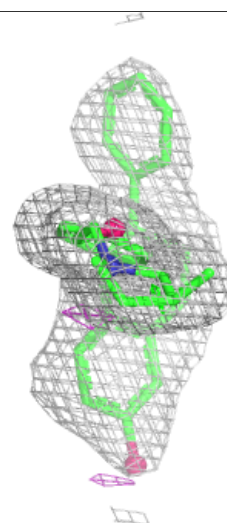
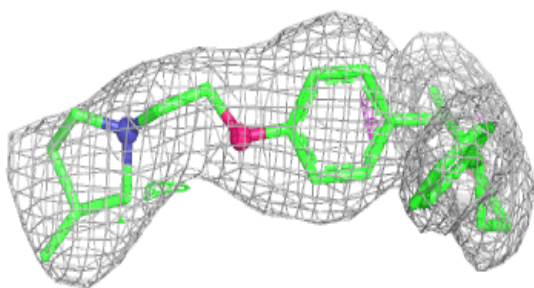
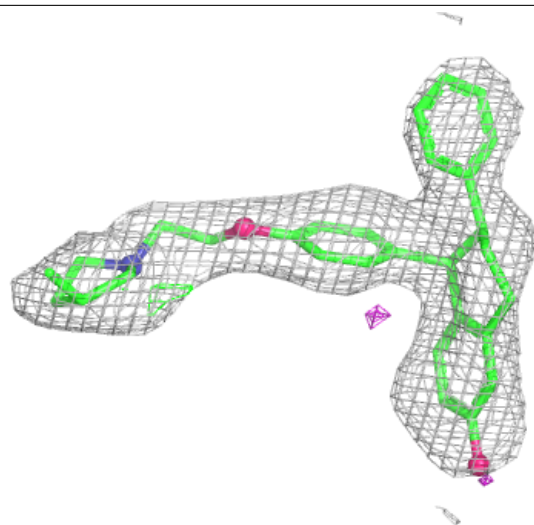
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	R3V	D	601	32/32	0.82	0.17	24,44,66,81	0
2	R3V	C	601	32/32	0.82	0.15	41,50,65,66	0
2	R3V	B	601	32/32	0.86	0.28	24,39,69,71	0
2	R3V	A	601	32/32	0.87	0.14	41,48,56,59	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.

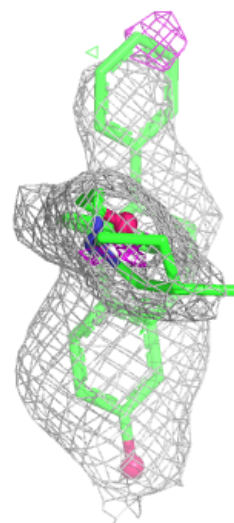
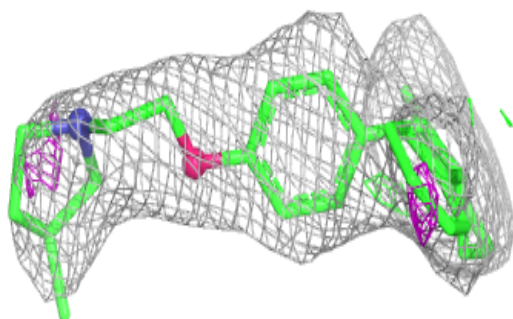
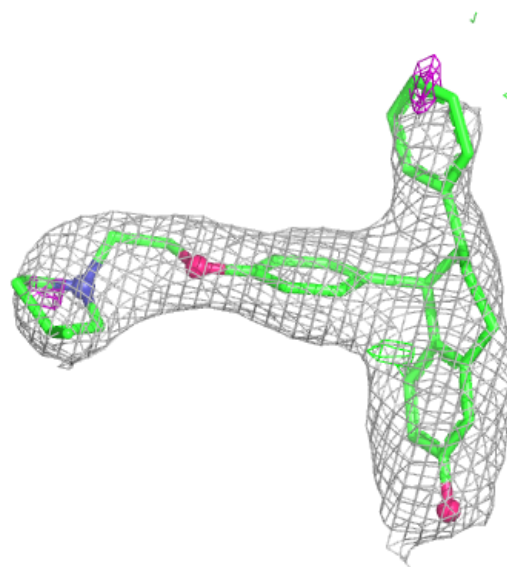
Electron density around R3V D 601:

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



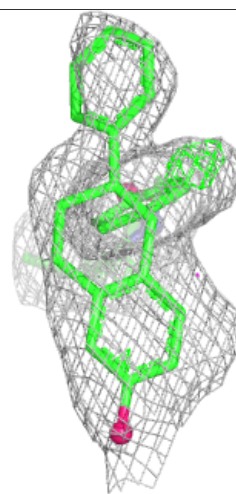
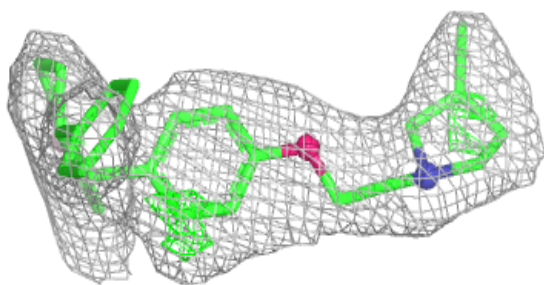
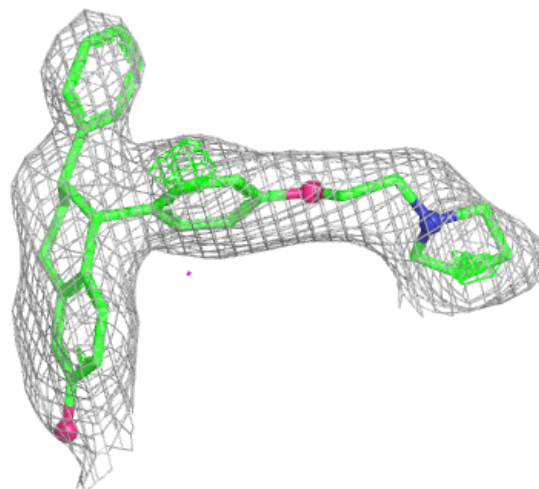
Electron density around R3V C 601:

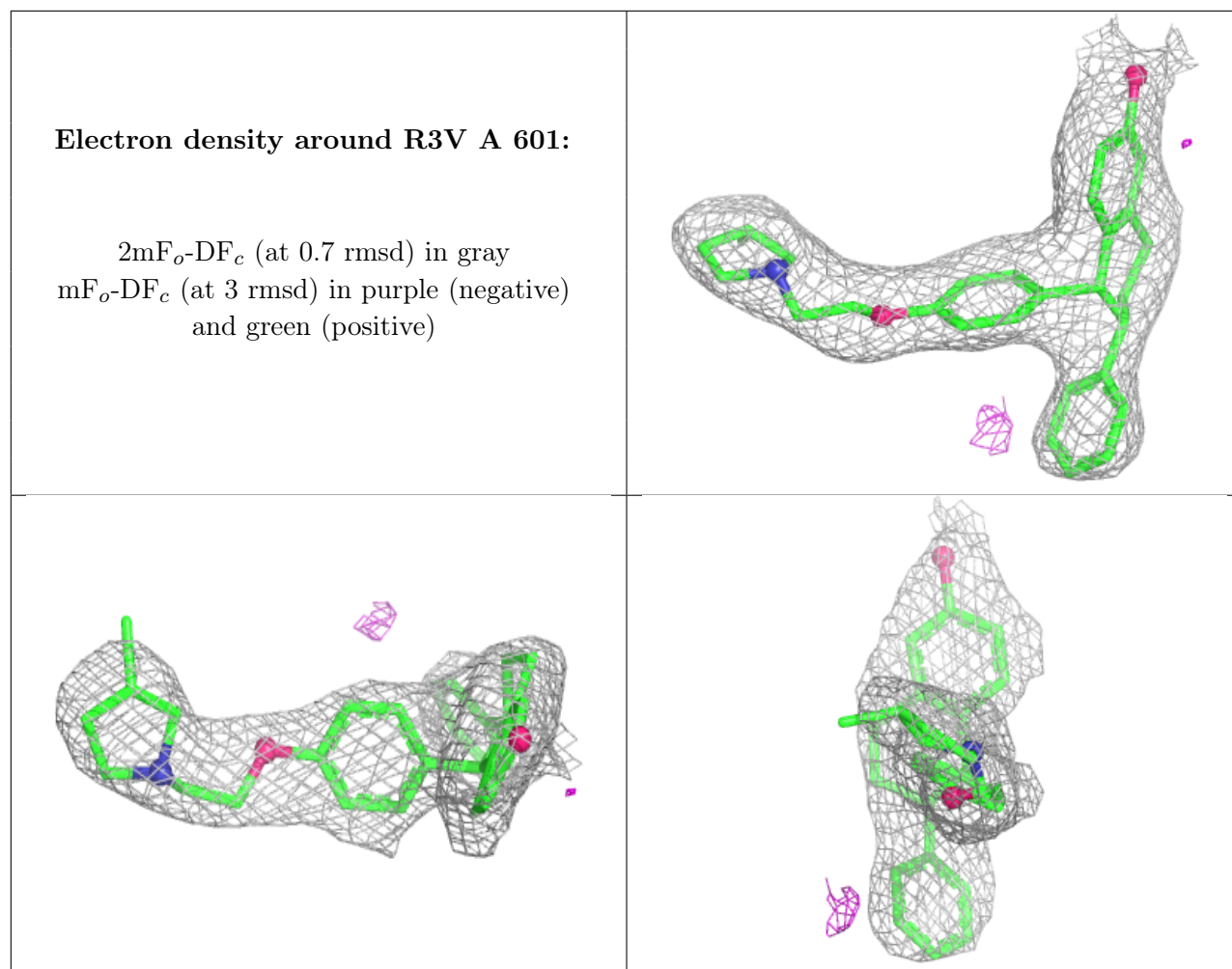
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around R3V 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.