



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 01:49 pm GMT

PDB ID : 9FIO
Title : Structure-guided discovery of selective USP7 inhibitors with in vivo activity
Authors : Baker, L.M.; Murray, J.; Hubbard, R.E.; Whitehead, N.
Deposited on : 2024-05-29
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

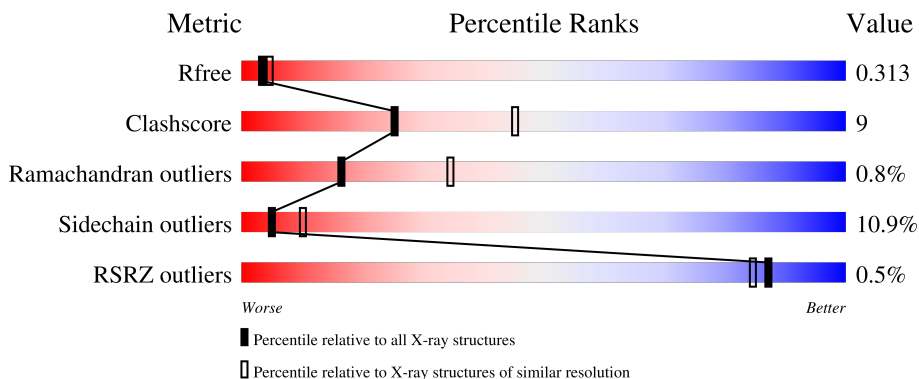
1 Overall quality at a glance

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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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	355	 % 62% 26% 5% • 6%
1	B	355	 65% 24% • • 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10862 atoms, of which 5374 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.

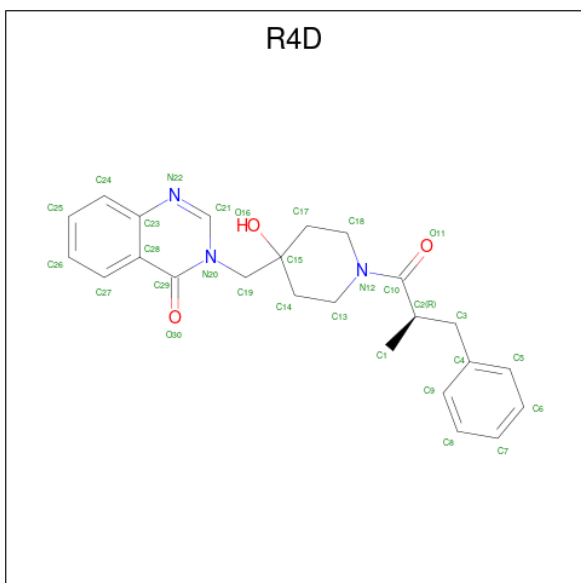
- Molecule 1 is a protein called Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	332	5353	1709	2657	457	514	16	76	0	0
1	B	332	5360	1708	2663	458	515	16	76	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	GLY	-	expression tag	UNP Q93009
A	207	SER	-	expression tag	UNP Q93009
B	206	GLY	-	expression tag	UNP Q93009
B	207	SER	-	expression tag	UNP Q93009

- Molecule 2 is 3-({4-hydroxy-1-[(2R)-2-methyl-3-phenylpropanoyl]piperidin-4-yl}methyl)quinazolin-4(3H)-one (three-letter code: R4D) (formula: C₂₄H₂₇N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	1	0
			57	24	27	3	3		
2	B	1	Total	C	H	N	O	1	0
			57	24	27	3	3		

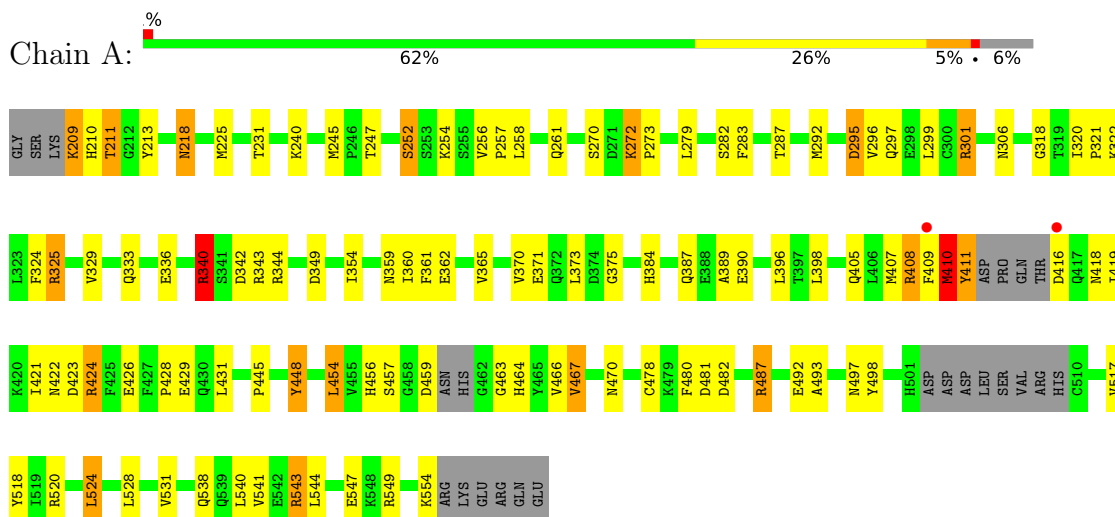
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	19	Total	O	0	0
			19	19		

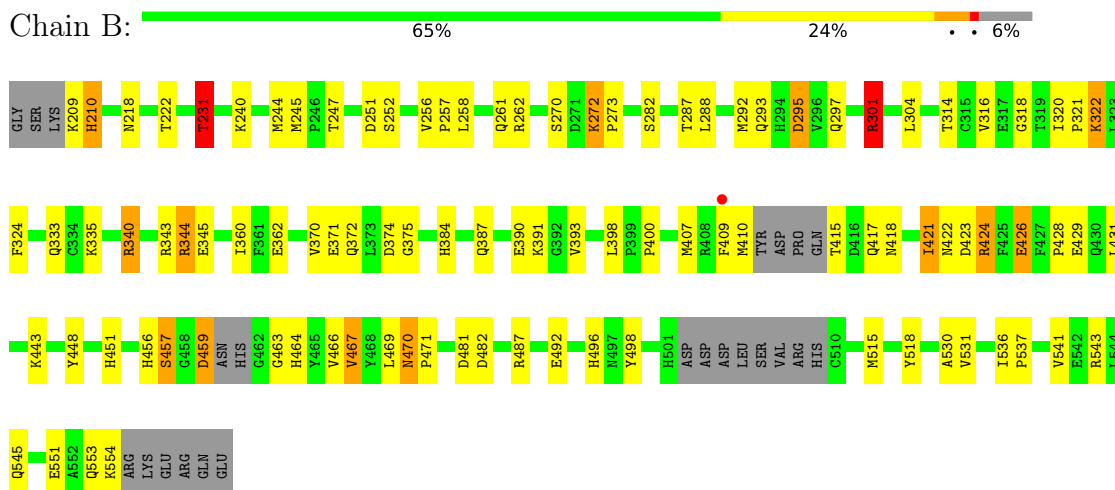
3 Residue-property plots

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: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.26Å 69.91Å 75.55Å 90.00° 132.31° 90.00°	Depositor
Resolution (Å)	29.19 – 2.60 29.19 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.19-2.60) 98.3 (29.19-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.224 , 0.321 0.224 , 0.313	Depositor DCC
R_{free} test set	1268 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.004 for h+2*k,-h-l 0.039 for -h-2*k,-k,l 0.026 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10862	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3556e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: R4D

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	0.80	3/2750 (0.1%)	1.37	27/3703 (0.7%)
1	B	0.78	4/2753 (0.1%)	1.34	22/3707 (0.6%)
All	All	0.79	7/5503 (0.1%)	1.36	49/7410 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	426	GLU	CD-OE1	6.32	1.32	1.25
1	A	492	GLU	CD-OE2	6.32	1.32	1.25
1	A	429	GLU	CD-OE2	5.84	1.32	1.25
1	B	492	GLU	CD-OE2	5.77	1.32	1.25
1	B	362	GLU	CD-OE1	5.73	1.31	1.25
1	B	429	GLU	CD-OE1	5.54	1.31	1.25
1	A	547	GLU	CD-OE1	5.02	1.31	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ARG	NE-CZ-NH1	-9.57	115.52	120.30
1	A	492	GLU	OE1-CD-OE2	8.78	133.83	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	B	515	MET	CG-SD-CE	8.38	113.61	100.20
1	A	407	MET	CG-SD-CE	8.19	113.31	100.20
1	A	487	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	231	THR	OG1-CB-CG2	-8.07	91.43	110.00
1	A	408	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	B	426	GLU	OE1-CD-OE2	7.88	132.76	123.30
1	A	292	MET	CG-SD-CE	7.55	112.28	100.20
1	B	492	GLU	OE1-CD-OE2	7.37	132.15	123.30
1	B	407	MET	CG-SD-CE	7.28	111.85	100.20
1	A	398	LEU	CB-CG-CD2	7.25	123.32	111.00
1	A	408	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	B	398	LEU	CB-CG-CD2	6.98	122.87	111.00
1	B	301	ARG	CB-CA-C	6.81	124.03	110.40
1	A	520	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	362	GLU	CG-CD-OE2	-6.56	105.17	118.30
1	A	398	LEU	CB-CG-CD1	-6.50	99.96	111.00
1	A	272	LYS	N-CA-CB	-6.46	98.98	110.60
1	A	426	GLU	OE1-CD-OE2	6.33	130.90	123.30
1	B	467	VAL	N-CA-CB	6.21	125.17	111.50
1	B	292	MET	CG-SD-CE	6.18	110.08	100.20
1	B	424	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	A	410	MET	CG-SD-CE	6.13	110.01	100.20
1	A	543	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	398	LEU	CB-CG-CD1	-6.00	100.80	111.00
1	A	492	GLU	CG-CD-OE1	-5.86	106.58	118.30
1	A	362	GLU	CG-CD-OE1	5.84	129.98	118.30
1	B	293[A]	GLN	CB-CA-C	-5.83	98.75	110.40
1	B	293[B]	GLN	CB-CA-C	-5.83	98.75	110.40
1	A	344	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	B	301	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	467	VAL	N-CA-CB	5.74	124.12	111.50
1	B	362	GLU	CG-CD-OE1	5.72	129.74	118.30
1	B	297	GLN	N-CA-CB	5.64	120.75	110.60
1	B	324	PHE	CB-CA-C	-5.63	99.14	110.40
1	A	498	TYR	N-CA-CB	-5.60	100.53	110.60
1	B	222	THR	OG1-CB-CG2	-5.51	97.33	110.00
1	A	362	GLU	CG-CD-OE2	-5.44	107.42	118.30
1	A	324	PHE	CB-CA-C	-5.40	99.60	110.40
1	A	297	GLN	N-CA-CB	5.37	120.26	110.60
1	A	549	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	301	ARG	NE-CZ-NH1	-5.33	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	TYR	CB-CA-C	5.33	121.05	110.40
1	A	301	ARG	CB-CA-C	5.30	120.99	110.40
1	A	424	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	426	GLU	CG-CD-OE2	-5.22	107.87	118.30
1	A	342	ASP	CB-CG-OD2	-5.21	113.61	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	ARG	Sidechain
1	A	340	ARG	Sidechain
1	A	424	ARG	Sidechain
1	B	262	ARG	Sidechain
1	B	424	ARG	Sidechain

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	2696	2657	2642	48	0
1	B	2697	2663	2648	54	0
2	A	30	27	0	2	0
2	B	30	27	0	3	0
3	A	16	0	0	0	0
3	B	19	0	0	2	0
All	All	5488	5374	5290	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (102) 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:340:ARG:HH11	1:B:340:ARG:HG3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:HIS:O	1:B:387:GLN:NE2	2.18	0.77
1:A:211:THR:HG22	1:A:213:TYR:H	1.49	0.76
1:B:457:SER:O	1:B:463:GLY:HA2	1.87	0.75
1:A:333:GLN:OE1	1:A:340:ARG:NH1	2.20	0.74
1:B:301:ARG:HG2	1:B:301:ARG:HH21	1.52	0.74
1:A:457:SER:O	1:A:463:GLY:HA2	1.92	0.70
1:A:384:HIS:O	1:A:387:GLN:NE2	2.23	0.70
1:A:329:VAL:CG2	1:A:396:LEU:HD21	2.22	0.69
1:A:218:ASN:C	1:A:218:ASN:ND2	2.49	0.66
1:B:252:SER:OG	1:B:543:ARG:NH2	2.29	0.66
1:A:493:ALA:O	1:A:497:ASN:ND2	2.29	0.66
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.78	0.66
1:B:231:THR:HG23	3:B:710:HOH:O	1.98	0.64
1:A:252:SER:OG	1:A:543:ARG:NH2	2.27	0.63
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.80	0.63
1:A:218:ASN:C	1:A:218:ASN:HD22	2.02	0.63
1:A:540:LEU:CD2	1:A:544:LEU:HD12	2.32	0.60
1:A:240:LYS:HD2	1:A:531:VAL:HG22	1.84	0.60
1:A:464:HIS:NE2	1:A:481:ASP:OD1	2.37	0.58
1:B:360:ILE:HG21	1:B:431:LEU:HD11	1.86	0.58
1:B:301:ARG:HG2	1:B:301:ARG:NH2	2.19	0.57
1:B:456:HIS:CD2	1:B:457:SER:N	2.73	0.57
1:B:314:THR:HG22	1:B:316:VAL:H	1.70	0.56
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.86	0.56
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.85	0.56
1:A:456:HIS:CE1	1:A:457:SER:O	2.60	0.54
1:B:218:ASN:OD1	1:B:218:ASN:C	2.46	0.54
1:B:240:LYS:HD2	1:B:531:VAL:HG22	1.92	0.52
1:B:295:ASP:CB	2:B:601:R4D:O16	2.58	0.52
1:A:272:LYS:O	1:A:273:PRO:C	2.46	0.51
1:A:295:ASP:HB3	2:A:601:R4D:O16	2.10	0.51
1:A:538:GLN:O	1:A:541:VAL:HG22	2.10	0.51
1:B:333:GLN:OE1	1:B:340:ARG:HG3	2.11	0.51
1:A:295:ASP:CB	2:A:601:R4D:O16	2.59	0.50
1:B:370:VAL:CG1	1:B:390:GLU:HB2	2.42	0.50
1:B:371:GLU:O	1:B:390:GLU:HA	2.12	0.50
1:B:451:HIS:HA	1:B:470:ASN:HD21	1.76	0.49
1:A:349:ASP:HB2	1:A:405:GLN:HE22	1.76	0.49
1:A:360:ILE:HG21	1:A:431:LEU:HD11	1.93	0.49
1:A:538:GLN:HA	1:A:541:VAL:HG22	1.94	0.49
1:B:272:LYS:O	1:B:273:PRO:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HD2	1:A:209:LYS:N	2.27	0.49
1:B:537:PRO:O	1:B:541:VAL:HG23	2.12	0.49
1:B:456:HIS:CG	1:B:457:SER:N	2.81	0.49
1:B:301:ARG:NE	1:B:301:ARG:HA	2.28	0.48
1:B:258:LEU:HA	1:B:261:GLN:OE1	2.13	0.48
1:B:318:GLY:C	1:B:321:PRO:HD2	2.33	0.48
1:B:320:ILE:N	1:B:321:PRO:CD	2.76	0.48
1:A:524:LEU:HD22	1:A:528:LEU:HD12	1.95	0.47
1:A:320:ILE:N	1:A:321:PRO:CD	2.76	0.47
1:B:464:HIS:NE2	1:B:481:ASP:OD1	2.45	0.47
1:A:258:LEU:HA	1:A:261:GLN:OE1	2.15	0.47
1:A:454:LEU:N	1:A:454:LEU:HD23	2.30	0.47
1:B:256:VAL:HA	1:B:282:SER:OG	2.14	0.47
1:B:287:THR:O	1:B:288:LEU:C	2.49	0.47
1:B:421:ILE:HG22	1:B:422:ASN:N	2.29	0.46
1:B:464:HIS:HE2	1:B:481:ASP:CG	2.19	0.46
1:A:318:GLY:C	1:A:321:PRO:HD2	2.36	0.46
1:B:333:GLN:OE1	1:B:340:ARG:NH1	2.47	0.46
1:B:295:ASP:HB3	2:B:601:R4D:O16	2.16	0.46
1:B:256:VAL:HB	1:B:257:PRO:HD3	1.97	0.46
1:A:359:ASN:ND2	1:A:361:PHE:HB3	2.31	0.45
1:B:301:ARG:NH2	1:B:301:ARG:CG	2.78	0.45
1:A:540:LEU:HD22	1:A:544:LEU:HD12	1.99	0.45
1:B:335:LYS:CE	1:B:372:GLN:HE22	2.30	0.45
1:B:344:ARG:HG2	1:B:345:GLU:N	2.32	0.44
1:B:536:ILE:HG22	1:B:541:VAL:HG22	2.00	0.44
1:B:295:ASP:HB2	2:B:601:R4D:O16	2.17	0.44
1:A:245:MET:O	1:A:247:THR:N	2.51	0.44
1:B:340:ARG:HH11	1:B:340:ARG:CG	2.25	0.44
1:B:421:ILE:HD12	1:B:421:ILE:N	2.32	0.44
1:A:478:CYS:HB2	1:A:480:PHE:HE1	1.81	0.44
1:B:335:LYS:HE2	1:B:372:GLN:HE22	1.82	0.44
1:B:426:GLU:HG2	1:B:498:TYR:CD2	2.53	0.44
1:A:411:TYR:HA	1:A:418:ASN:HA	2.00	0.43
1:A:373:LEU:HD12	1:A:389:ALA:HB3	1.99	0.43
1:A:408:ARG:NH1	1:A:423:ASP:O	2.48	0.43
1:B:240:LYS:NZ	1:B:530:ALA:O	2.51	0.43
1:B:322:LYS:HE3	3:B:713:HOH:O	2.18	0.43
1:B:210:HIS:CD2	1:B:210:HIS:H	2.35	0.43
1:A:456:HIS:CG	1:A:457:SER:N	2.87	0.42
1:B:469:LEU:C	1:B:471:PRO:HD3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:O	1:A:390:GLU:HA	2.18	0.42
1:B:466:VAL:HG12	1:B:467:VAL:N	2.35	0.41
1:A:225:MET:HG3	1:A:299:LEU:HD21	2.00	0.41
1:A:231:THR:HG21	1:A:517:VAL:HG21	2.02	0.41
1:A:466:VAL:HG12	1:A:467:VAL:N	2.34	0.41
1:A:279:LEU:HG	1:A:283:PHE:HE1	1.85	0.41
1:A:421:ILE:HG22	1:A:422:ASN:N	2.34	0.41
1:B:459:ASP:N	1:B:459:ASP:OD1	2.53	0.41
1:A:329:VAL:HG21	1:A:396:LEU:HD21	2.01	0.41
1:A:410:MET:HG3	1:A:421:ILE:HD11	2.03	0.41
1:B:245:MET:O	1:B:247:THR:N	2.53	0.41
1:A:256:VAL:HA	1:A:282:SER:OG	2.21	0.41
1:B:335:LYS:CE	1:B:372:GLN:NE2	2.84	0.41
1:B:451:HIS:HA	1:B:470:ASN:ND2	2.35	0.41
1:A:256:VAL:HB	1:A:257:PRO:HD3	2.02	0.40
1:A:209:LYS:N	1:A:209:LYS:CD	2.85	0.40
1:A:454:LEU:HD22	1:A:467:VAL:CG2	2.52	0.40
1:B:301:ARG:HH11	1:B:304:LEU:HB2	1.86	0.40
1:B:421:ILE:HG22	1:B:423:ASP:H	1.86	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	324/355 (91%)	298 (92%)	23 (7%)	3 (1%)	14	31
1	B	325/355 (92%)	301 (93%)	22 (7%)	2 (1%)	22	43
All	All	649/710 (91%)	599 (92%)	45 (7%)	5 (1%)	16	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	GLY
1	B	375	GLY
1	A	482	ASP
1	B	482	ASP
1	A	336	GLU

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	299/321 (93%)	267 (89%)	32 (11%)	5	11
1	B	300/321 (94%)	267 (89%)	33 (11%)	5	10
All	All	599/642 (93%)	534 (89%)	65 (11%)	5	10

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	LYS
1	A	210	HIS
1	A	211	THR
1	A	218	ASN
1	A	252	SER
1	A	254	LYS
1	A	270	SER
1	A	287	THR
1	A	295	ASP
1	A	296	VAL
1	A	301	ARG
1	A	306	ASN
1	A	322	LYS
1	A	325	ARG
1	A	340	ARG
1	A	343	ARG
1	A	354	ILE
1	A	365	VAL
1	A	370	VAL

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Mol	Chain	Res	Type
1	A	409	PHE
1	A	410	MET
1	A	411	TYR
1	A	416	ASP
1	A	419	ILE
1	A	428	PRO
1	A	445	PRO
1	A	454	LEU
1	A	459	ASP
1	A	470	ASN
1	A	487	ARG
1	A	524	LEU
1	A	554	LYS
1	B	209	LYS
1	B	210	HIS
1	B	231	THR
1	B	244	MET
1	B	251	ASP
1	B	270	SER
1	B	272	LYS
1	B	295	ASP
1	B	301	ARG
1	B	322	LYS
1	B	340	ARG
1	B	343	ARG
1	B	374	ASP
1	B	391	LYS
1	B	393	VAL
1	B	400	PRO
1	B	409	PHE
1	B	410	MET
1	B	415	THR
1	B	417	GLN
1	B	418	ASN
1	B	421	ILE
1	B	428	PRO
1	B	443	LYS
1	B	457	SER
1	B	459	ASP
1	B	470	ASN
1	B	487	ARG
1	B	496	HIS

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Mol	Chain	Res	Type
1	B	545	GLN
1	B	551	GLU
1	B	553	GLN
1	B	554	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	A	359	ASN
1	A	403	HIS
1	A	405	GLN
1	A	456	HIS
1	A	529	GLN
1	B	210	HIS
1	B	268	GLN
1	B	309	ASN
1	B	372	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	R4D	B	601	-	33,33,33	0.77	0	40,47,47	1.28	5 (12%)
2	R4D	A	601	-	33,33,33	0.67	0	40,47,47	1.39	3 (7%)

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	R4D	B	601	-	-	6/17/29/29	0/4/4/4
2	R4D	A	601	-	-	5/17/29/29	0/4/4/4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	R4D	C1-C2-C3	4.26	117.70	111.98
2	A	601	R4D	C28-C29-N20	3.72	115.97	113.80
2	B	601	R4D	C28-C29-N20	3.69	115.95	113.80
2	A	601	R4D	C1-C2-C10	-3.26	103.25	109.00
2	B	601	R4D	O16-C15-C14	-2.79	101.53	108.19
2	B	601	R4D	C1-C2-C3	2.55	115.41	111.98
2	B	601	R4D	C13-N12-C18	2.38	117.21	112.62
2	B	601	R4D	O16-C15-C17	2.27	113.60	108.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	R4D	C2-C10-N12-C18
2	A	601	R4D	O11-C10-N12-C18
2	B	601	R4D	C1-C2-C3-C4
2	B	601	R4D	C2-C10-N12-C18
2	B	601	R4D	O11-C10-N12-C18
2	A	601	R4D	O11-C10-N12-C13
2	B	601	R4D	O11-C10-N12-C13

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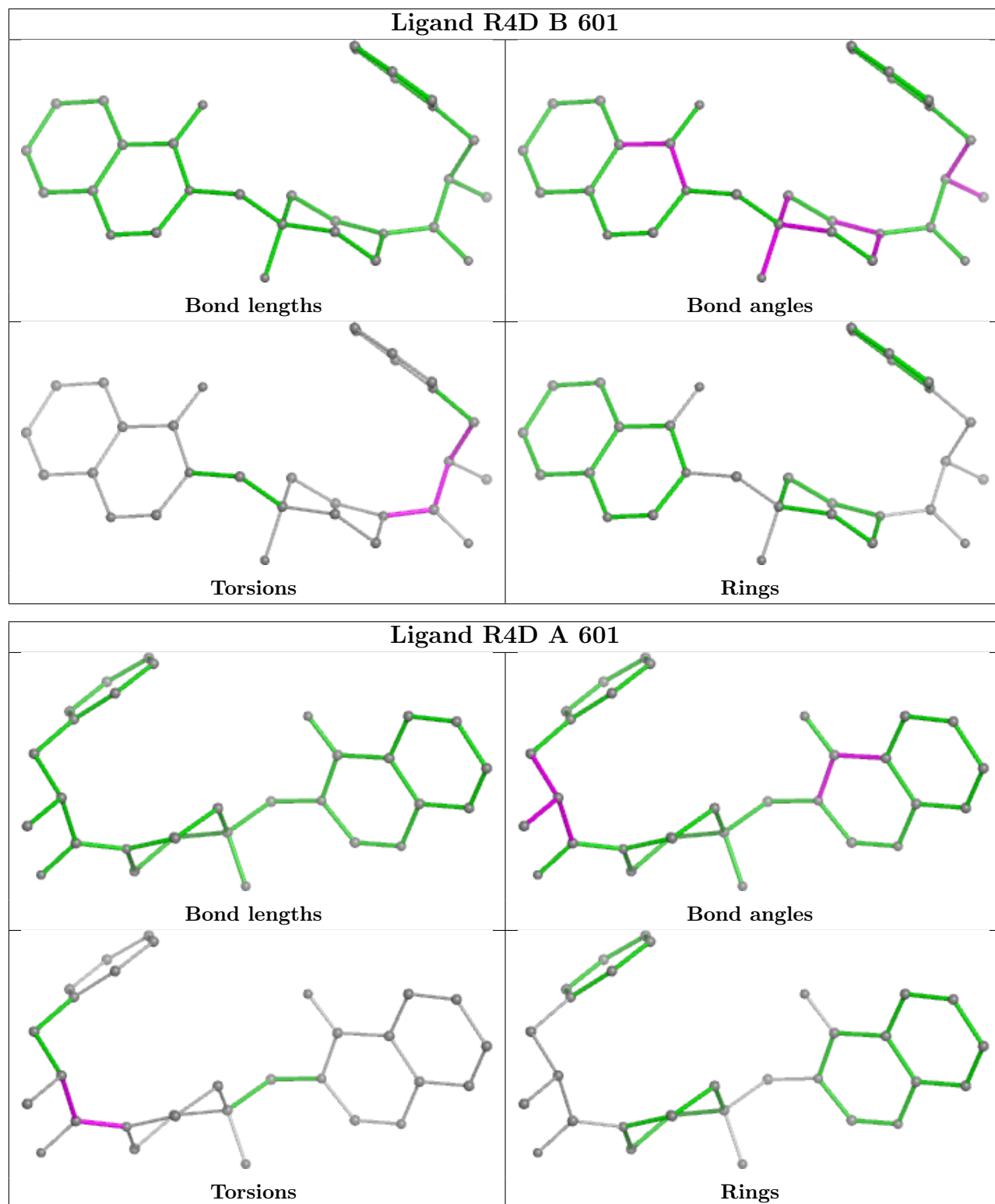
Mol	Chain	Res	Type	Atoms
2	A	601	R4D	C2-C10-N12-C13
2	B	601	R4D	C2-C10-N12-C13
2	A	601	R4D	N12-C10-C2-C3
2	B	601	R4D	N12-C10-C2-C3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	R4D	3	0
2	A	601	R4D	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 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	332/355 (93%)	-0.97	2 (0%) 85 83	49, 85, 136, 184	0
1	B	332/355 (93%)	-1.01	1 (0%) 90 88	49, 84, 135, 182	1 (0%)
All	All	664/710 (93%)	-0.99	3 (0%) 87 84	49, 85, 136, 184	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	PHE	2.8
1	A	409	PHE	2.2
1	A	416	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

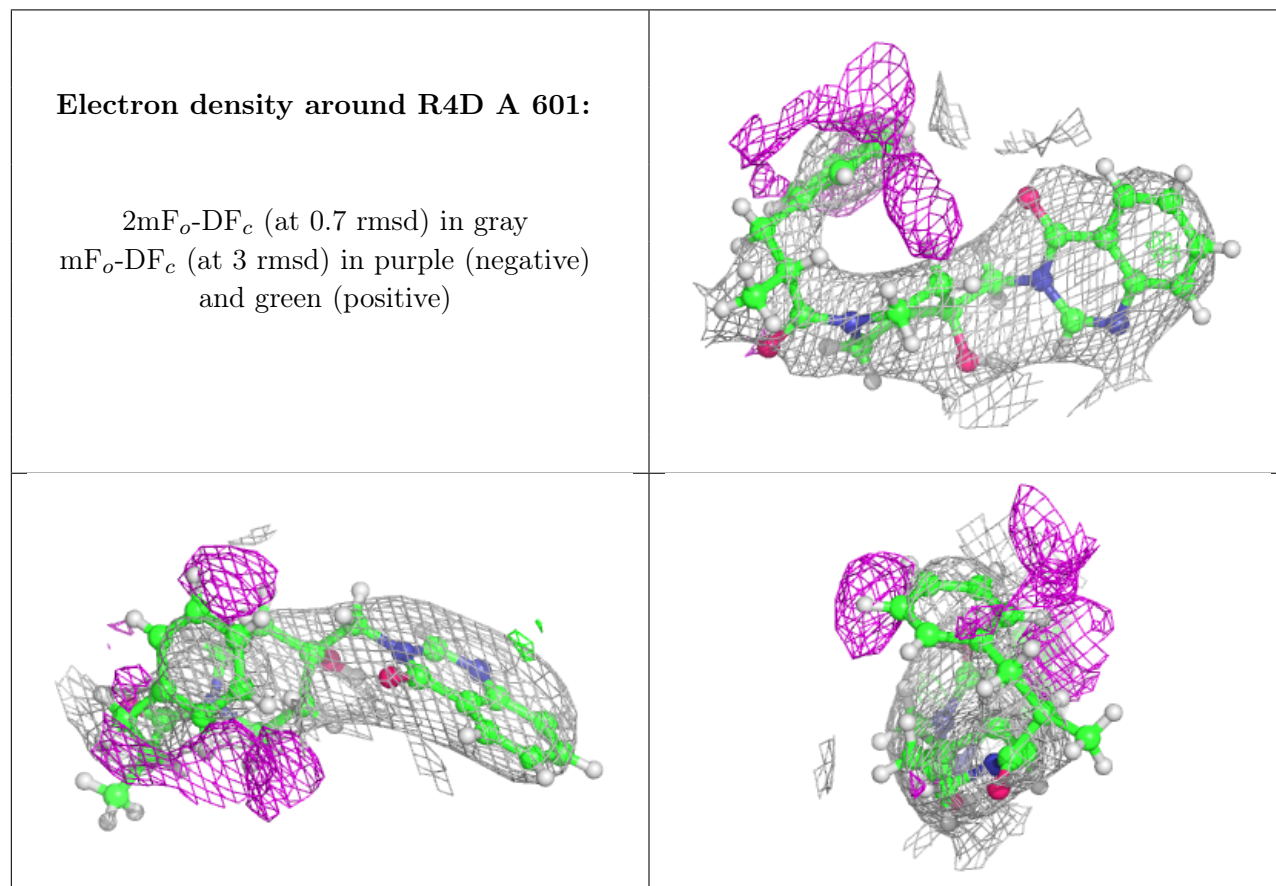
There are no monosaccharides in this entry.

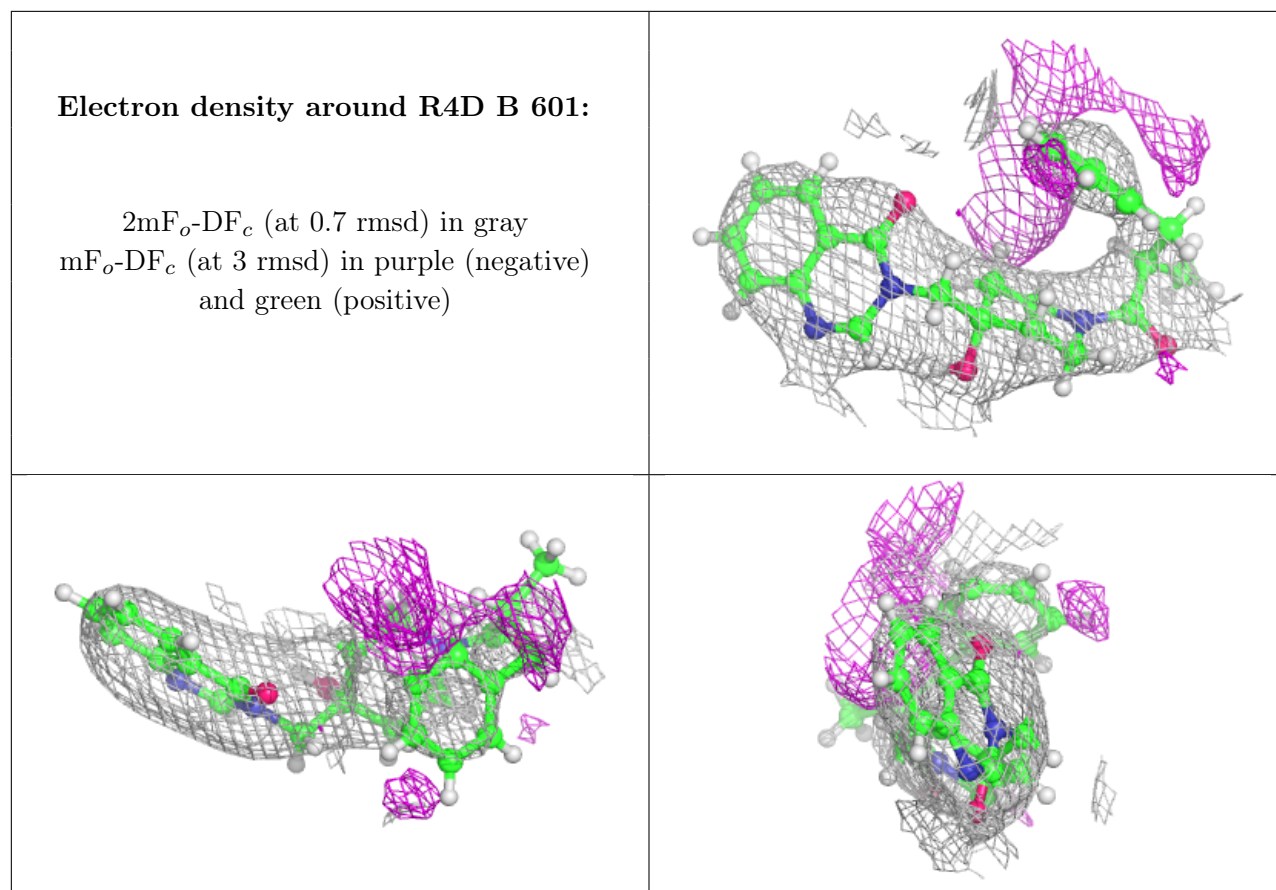
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	R4D	A	601	30/30	0.91	0.12	76,95,129,136	1
2	R4D	B	601	30/30	0.92	0.10	76,94,118,123	1

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.





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.