



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 02:07 PM EDT

PDB ID : 1ERR  
Title : HUMAN ESTROGEN RECEPTOR LIGAND-BINDING DOMAIN IN COMPLEX WITH RALOXIFENE  
Authors : Brzozowski, A.M.; Pike, A.C.W.  
Deposited on : 1997-09-08  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

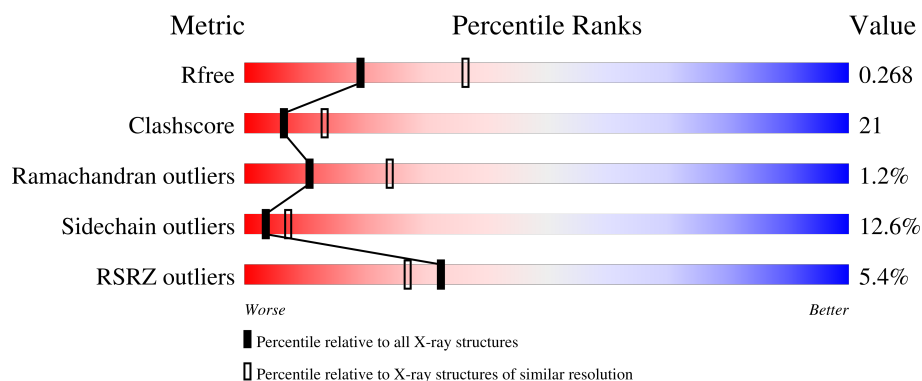
# 1 Overall quality at a glance

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  $\geq 3$ , 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	253	<div> <div>4%</div> <div>46%34%9%11%</div> </div>
1	B	253	<div> <div>5%</div> <div>48%32%7%12%</div> </div>

## 2 Entry composition [i](#)

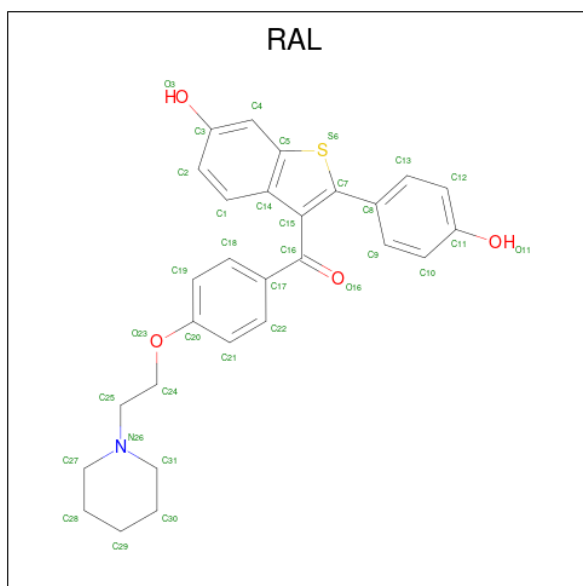
There are 3 unique types of molecules in this entry. The entry contains 3733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	225	Total	C	N	O	S	0	5	0
			1790	1146	308	317	19			
1	B	223	Total	C	N	O	S	0	5	0
			1775	1139	304	314	18			

- Molecule 2 is RALOXIFENE (three-letter code: RAL) (formula:  $C_{28}H_{27}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	28	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			34	28	1	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	49	Total	O	0	0
			49	49		



- Molecule 1: ESTROGEN RECEPTOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.53Å 53.68Å 102.71Å 90.00° 116.79° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 25.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (25.00-2.60) 97.1 (25.00-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.219 , 0.299 0.196 , 0.268	Depositor DCC
$R_{free}$ test set	1565 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CCS, RAL

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	0.78	0/1825	1.49	18/2469 (0.7%)
1	B	0.76	0/1800	1.53	22/2432 (0.9%)
All	All	0.77	0/3625	1.51	40/4901 (0.8%)

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	B	363	ARG	NE-CZ-NH1	10.83	125.71	120.30
1	B	503	ARG	NE-CZ-NH1	-9.97	115.31	120.30
1	A	515	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	B	436	ARG	CD-NE-CZ	9.11	136.36	123.60
1	A	421	MET	CA-CB-CG	8.43	127.62	113.30
1	A	394	ARG	CD-NE-CZ	-8.20	112.11	123.60
1	B	432	SER	N-CA-CB	7.41	121.61	110.50
1	B	394	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	B	359	ASN	OD1-CG-ND2	6.56	136.99	121.90
1	A	432	SER	N-CA-CB	6.53	120.29	110.50
1	B	313	ASP	CB-CG-OD2	-6.48	112.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	B	434	ARG	CD-NE-CZ	6.24	132.34	123.60
1	B	359	ASN	CA-CB-CG	-6.18	99.81	113.40
1	B	385	GLU	OE1-CD-OE2	-6.06	116.03	123.30
1	B	313	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	446	VAL	CA-CB-CG1	6.00	119.91	110.90
1	B	363	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	394	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	B	321	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	A	437	MET	CA-CB-CG	5.62	122.86	113.30
1	B	511	LEU	CA-C-N	5.61	129.54	117.20
1	A	446	VAL	N-CA-CB	-5.60	99.18	111.50
1	B	412	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	374	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	523	GLU	CA-CB-CG	5.57	125.65	113.40
1	A	352	ARG	NH1-CZ-NH2	5.56	125.51	119.40
1	A	431	THR	O-C-N	-5.34	114.16	122.70
1	B	446	VAL	N-CA-CB	-5.32	99.81	111.50
1	B	363	ARG	CD-NE-CZ	5.25	130.96	123.60
1	A	389	ILE	CA-C-N	5.23	126.66	116.20
1	A	502	GLN	O-C-N	5.23	131.07	122.70
1	B	480	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	421	MET	N-CA-CB	5.21	119.98	110.60
1	B	446	VAL	CB-CA-C	5.19	121.27	111.40
1	A	501[A]	HIS	CA-CB-CG	5.17	122.38	113.60
1	A	501[B]	HIS	CA-CB-CG	5.17	122.38	113.60
1	A	405	ALA	N-CA-CB	5.13	117.28	110.10
1	A	480	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	473[B]	ASP	Mainchain
1	B	457[B]	GLY	Mainchain
1	B	501[B]	HIS	Mainchain

## 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	1790	0	1784	90	0
1	B	1775	0	1770	70	0
2	A	34	0	27	1	0
2	B	34	0	27	1	0
3	A	51	0	0	1	0
3	B	49	0	0	0	0
All	All	3733	0	3608	155	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 21.

All (155) 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:455[A]:ASN:O	1:B:458:VAL:HG12	1.70	0.92
1:A:401:LYS:HB3	1:A:409:LEU:HD21	1.55	0.86
1:A:373[A]:HIS:CD2	1:A:377[A]:HIS:HE1	1.97	0.82
1:A:424:ILE:HA	1:A:427:MET:HE3	1.61	0.82
1:A:373[A]:HIS:CD2	1:A:377[A]:HIS:CE1	2.71	0.79
1:B:343:MET:HG3	1:B:528:MET:HE1	1.64	0.78
1:B:310:LEU:O	1:B:481:LYS:HE2	1.84	0.77
1:A:315:MET:HE3	1:A:365:PRO:HG2	1.67	0.76
1:A:315:MET:CE	1:A:365:PRO:HG2	2.17	0.74
1:B:368:VAL:HA	1:B:375:GLN:NE2	2.01	0.74
1:B:319:LEU:HB3	1:B:446:VAL:HG13	1.68	0.73
1:B:347:THR:HG23	2:B:600:RAL:H242	1.71	0.72
1:A:539:LEU:HD22	1:A:543:MET:CE	2.18	0.72
1:B:401:LYS:HB3	1:B:409:LEU:HD22	1.71	0.71
1:A:335:ARG:HG3	1:A:336:PRO:HA	1.74	0.69
1:A:358:ILE:HD13	1:A:543:MET:HB3	1.74	0.69
1:B:398:HIS:CD2	1:B:409:LEU:HD11	2.29	0.68
1:A:421:MET:HB3	1:A:524:HIS:CE1	2.29	0.67
1:A:311:THR:HG23	1:A:314:GLN:OE1	1.96	0.65
1:A:319:LEU:HB3	1:A:446:VAL:HG13	1.79	0.65
1:B:382:ALA:HB2	1:B:456[B]:SER:HB3	1.78	0.65
1:A:421:MET:HB3	1:A:524:HIS:HE1	1.62	0.65
1:A:424:ILE:HA	1:A:427:MET:CE	2.28	0.64
1:A:498:GLN:HA	1:A:501[A]:HIS:CE1	2.33	0.63
1:A:312:ALA:O	1:A:316:VAL:HG23	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LEU:HD22	1:A:543:MET:HE2	1.81	0.63
1:A:498:GLN:O	1:A:502:GLN:HG3	2.00	0.62
1:B:370:LEU:HD11	1:B:475:ILE:HD11	1.81	0.62
1:A:539:LEU:HD22	1:A:543:MET:HE1	1.81	0.62
1:B:341:SER:OG	1:B:342:MET:N	2.32	0.61
1:A:392:VAL:O	1:A:432:SER:HB3	2.01	0.61
1:A:401:LYS:HB3	1:A:409:LEU:CD2	2.30	0.61
1:A:497:LEU:HD13	1:B:497:LEU:HD21	1.82	0.61
1:B:398:HIS:HD2	1:B:409:LEU:HD11	1.65	0.60
1:A:347:THR:HG23	2:A:600:RAL:H241	1.84	0.60
1:B:498:GLN:O	1:B:502:GLN:HG3	2.01	0.60
1:A:496:THR:OG1	1:A:499:GLN:HG3	2.02	0.59
1:B:536:LEU:HD12	1:B:539:LEU:HB3	1.85	0.59
1:A:381[B]:CCS:OZ2	1:A:381[B]:CCS:HB2	2.01	0.59
1:A:409:LEU:C	1:A:409:LEU:HD23	2.23	0.59
1:B:315:MET:HE2	1:B:319:LEU:HD11	1.86	0.58
1:B:368:VAL:HA	1:B:375:GLN:HE22	1.67	0.58
1:A:436:ARG:O	1:A:437:MET:C	2.42	0.58
1:A:418:VAL:HB	1:A:421:MET:HG2	1.84	0.58
1:A:362:LYS:HD2	1:A:547:HIS:ND1	2.19	0.58
1:B:539:LEU:O	1:B:543:MET:HG3	2.03	0.57
1:B:372:LEU:O	1:B:376:VAL:HG23	2.05	0.57
1:A:335:ARG:HD3	1:A:337:PHE:CZ	2.40	0.57
1:A:509:LEU:HD22	1:B:455[A]:ASN:ND2	2.19	0.57
1:B:424:ILE:HA	1:B:427:MET:CE	2.34	0.57
1:A:392:VAL:HG11	1:A:431:THR:HG22	1.88	0.56
1:B:434:ARG:O	1:B:438:MET:HG3	2.05	0.56
1:B:421:MET:O	1:B:425:PHE:HB2	2.06	0.56
1:A:389:ILE:HG13	1:A:514:ILE:HD13	1.89	0.55
1:A:339:GLU:HG3	1:A:418:VAL:HA	1.89	0.54
1:A:372:LEU:HD21	1:A:541:LEU:CD1	2.38	0.53
1:B:362:LYS:HG3	1:B:547:HIS:CE1	2.43	0.53
1:A:342:MET:CE	1:A:418:VAL:HG23	2.39	0.53
1:A:376:VAL:HG22	1:A:544:LEU:HD12	1.91	0.53
1:A:333:PRO:HG3	1:A:345:LEU:HD21	1.89	0.53
1:B:312:ALA:O	1:B:315:MET:HB3	2.09	0.53
1:A:329:SER:O	1:A:330:GLU:C	2.47	0.53
1:A:516:HIS:CE1	1:B:519:ASN:HD21	2.27	0.53
1:B:424:ILE:HA	1:B:427:MET:HE3	1.90	0.53
1:A:405:ALA:HB1	1:A:406:PRO:CD	2.38	0.52
1:B:473:ASP:O	1:B:477:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373[A]:HIS:NE2	1:A:377[A]:HIS:CE1	2.78	0.52
1:A:405:ALA:HB1	1:A:406:PRO:HD2	1.92	0.51
1:A:502:GLN:O	1:A:506:GLN:HG3	2.11	0.51
1:A:372:LEU:HD21	1:A:541:LEU:HD11	1.93	0.51
1:A:360:TRP:O	1:A:361:ALA:C	2.48	0.51
1:B:528:MET:O	1:B:529:LYS:CB	2.57	0.51
1:A:509:LEU:HD22	1:B:455[A]:ASN:HD22	1.75	0.51
1:B:376:VAL:HG22	1:B:544:LEU:HD12	1.92	0.51
1:A:478:VAL:O	1:A:482:ILE:HG13	2.10	0.51
1:B:323:GLU:HA	1:B:323:GLU:OE1	2.11	0.50
1:A:389:ILE:HG13	1:A:514:ILE:CD1	2.41	0.50
1:B:315:MET:HE1	1:B:365:PRO:HG2	1.94	0.50
1:A:392:VAL:HG13	1:A:432:SER:CA	2.42	0.50
1:A:401:LYS:CB	1:A:409:LEU:HD21	2.34	0.50
1:B:315:MET:CE	1:B:365:PRO:HG2	2.42	0.49
1:A:415:GLY:O	1:A:421:MET:HG3	2.13	0.49
1:A:394:ARG:HG3	1:A:403:LEU:HD23	1.95	0.49
1:B:402:LEU:HD12	1:B:425:PHE:CZ	2.48	0.49
1:B:539:LEU:HD11	1:B:543:MET:HE2	1.95	0.48
1:A:319:LEU:HB3	1:A:446:VAL:CG1	2.42	0.48
1:B:398:HIS:N	1:B:399:PRO:CD	2.76	0.48
1:A:317:SER:O	1:A:318:ALA:C	2.49	0.48
1:B:435:PHE:CE1	1:B:510:ILE:HG21	2.48	0.48
1:A:396:MET:HA	1:A:432:SER:HB2	1.96	0.48
1:A:342:MET:HE1	1:A:418:VAL:HG23	1.95	0.47
1:B:358:ILE:O	1:B:361:ALA:HB3	2.14	0.47
1:B:445:PHE:CZ	1:B:449:LYS:HE2	2.49	0.47
1:B:311:THR:OG1	1:B:314:GLN:HG3	2.14	0.47
1:A:442:GLY:O	1:A:445:PHE:HB3	2.15	0.47
1:B:359:ASN:HD22	1:B:363:ARG:HH21	1.63	0.47
1:A:335:ARG:HA	1:A:336:PRO:C	2.35	0.47
1:B:478:VAL:O	1:B:482:ILE:HG13	2.15	0.47
1:A:315:MET:HE1	1:A:365:PRO:HG2	1.92	0.46
1:B:395:SER:O	1:B:396:MET:C	2.53	0.46
1:B:403:LEU:HD11	1:B:406:PRO:HA	1.98	0.46
1:A:402:LEU:HD12	1:A:425:PHE:CZ	2.51	0.46
1:A:419:GLU:O	1:A:524:HIS:NE2	2.49	0.46
1:B:522:MET:O	1:B:526[A]:TYR:HD2	1.99	0.46
1:A:363:ARG:O	1:A:365:PRO:HD3	2.16	0.45
1:A:365:PRO:O	1:A:478:VAL:HG11	2.16	0.45
1:B:315:MET:HG2	1:B:485:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ALA:O	1:A:315:MET:HB3	2.16	0.45
1:A:520:LYS:HA	1:A:520:LYS:HD2	1.67	0.45
1:B:405:ALA:HB1	1:B:406:PRO:HD2	1.98	0.44
1:B:394:ARG:HG3	1:B:403:LEU:HD23	1.99	0.44
1:A:392:VAL:HG13	1:A:432:SER:N	2.33	0.44
1:A:546:ALA:O	1:A:547:HIS:C	2.54	0.44
1:A:447:CYS:CB	1:A:486:LEU:HD13	2.48	0.44
1:B:434:ARG:HD2	1:B:437:MET:HE2	1.99	0.43
1:A:440:LEU:HD11	1:A:444:GLU:HB2	2.00	0.43
1:A:372:LEU:O	1:A:375:GLN:HB2	2.17	0.43
1:A:320:LEU:HD11	1:A:443:GLU:HG3	2.01	0.43
1:B:359:ASN:ND2	1:B:363:ARG:HH21	2.16	0.43
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.82	0.43
1:B:424:ILE:HA	1:B:427:MET:HE2	2.00	0.43
1:A:368:VAL:HA	1:A:375:GLN:NE2	2.34	0.43
1:B:367:PHE:O	1:B:375:GLN:NE2	2.49	0.43
1:A:330:GLU:OE1	1:A:345:LEU:HD23	2.18	0.43
1:A:496:THR:HG23	1:A:499:GLN:OE1	2.19	0.43
1:B:319:LEU:HD23	1:B:319:LEU:HA	1.82	0.42
1:A:343:MET:CE	1:A:528:MET:HE1	2.50	0.42
1:A:373[A]:HIS:HD2	1:A:377[A]:HIS:HE1	1.61	0.42
1:B:323:GLU:OE1	1:B:449:LYS:NZ	2.37	0.42
1:A:392:VAL:HG13	1:A:432:SER:HA	2.01	0.42
1:A:435:PHE:HE1	1:A:510:ILE:HG21	1.85	0.42
1:A:440:LEU:HD12	1:A:444:GLU:OE1	2.19	0.42
1:B:343:MET:CG	1:B:528:MET:HE1	2.43	0.42
1:B:362:LYS:HG3	1:B:547:HIS:ND1	2.35	0.42
1:B:363:ARG:O	1:B:365:PRO:HD3	2.20	0.42
1:B:405:ALA:HB1	1:B:406:PRO:CD	2.49	0.42
1:A:319:LEU:CB	1:A:446:VAL:CG1	2.97	0.42
1:A:330:GLU:HG3	3:A:33:HOH:O	2.19	0.42
1:B:392:VAL:HG13	1:B:432:SER:HA	2.02	0.42
1:B:411:ASP:O	1:B:412:ARG:C	2.56	0.42
1:A:379:LEU:O	1:A:380:GLU:C	2.54	0.41
1:A:434:ARG:O	1:A:438:MET:HG3	2.20	0.41
1:A:497:LEU:HD13	1:B:497:LEU:CD2	2.49	0.41
1:B:353:GLU:O	1:B:354:LEU:C	2.55	0.41
1:A:539:LEU:CD2	1:A:543:MET:HE2	2.49	0.41
1:A:421:MET:O	1:A:425:PHE:HB2	2.20	0.41
1:A:491:ALA:O	1:A:492:LYS:C	2.58	0.41
1:A:423:GLU:H	1:A:423:GLU:HG2	1.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:VAL:O	1:A:365:PRO:C	2.59	0.41
1:B:388:MET:O	1:B:389:ILE:C	2.59	0.41
1:B:381:CCS:HB2	1:B:456[B]:SER:HB2	2.04	0.40
1:B:434:ARG:HD2	1:B:434:ARG:HA	1.91	0.40
1:B:509:LEU:HD23	1:B:509:LEU:HA	1.84	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	222/253 (88%)	212 (96%)	7 (3%)	3 (1%)	9	19
1	B	219/253 (87%)	208 (95%)	8 (4%)	3 (1%)	9	19
All	All	441/506 (87%)	420 (95%)	15 (3%)	6 (1%)	11	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	PRO
1	B	528	MET
1	A	419	GLU
1	B	456[A]	SER
1	B	456[B]	SER
1	A	332	ASP

### 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	193/227 (85%)	173 (90%)	20 (10%)	5	11
1	B	188/227 (83%)	160 (85%)	28 (15%)	2	4
All	All	381/454 (84%)	333 (87%)	48 (13%)	3	7

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	SER
1	A	321	ASP
1	A	334	THR
1	A	335	ARG
1	A	341	SER
1	A	365	PRO
1	A	373[A]	HIS
1	A	373[B]	HIS
1	A	412	ARG
1	A	422	VAL
1	A	424	ILE
1	A	434	ARG
1	A	486	LEU
1	A	495	LEU
1	A	512	SER
1	A	518	SER
1	A	520	LYS
1	A	525	LEU
1	A	539	LEU
1	A	541	LEU
1	B	306	LEU
1	B	309	SER
1	B	321	ASP
1	B	331	TYR
1	B	359	ASN
1	B	360	TRP
1	B	368	VAL
1	B	370	LEU
1	B	389	ILE
1	B	394	ARG
1	B	396	MET
1	B	409	LEU
1	B	412	ARG

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Mol	Chain	Res	Type
1	B	432	SER
1	B	446	VAL
1	B	447	CYS
1	B	473	ASP
1	B	475	ILE
1	B	481	LYS
1	B	486	LEU
1	B	497	LEU
1	B	512	SER
1	B	515	ARG
1	B	523	GLU
1	B	525	LEU
1	B	538	ASP
1	B	541	LEU
1	B	543	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	B	398	HIS
1	B	502	GLN
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 ⓘ

3 non-standard protein/DNA/RNA residues 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
1	CCS	A	381[B]	-	8,9,10	1.71	2 (25%)	7,10,12	2.19	2 (28%)
1	CCS	A	381[A]	-	8,9,10	1.71	2 (25%)	7,10,12	3.00	3 (42%)
1	CCS	B	381	1	8,9,10	1.69	3 (37%)	7,10,12	2.08	2 (28%)

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
1	CCS	A	381[B]	-	-	3/6/8/10	-
1	CCS	A	381[A]	-	-	2/6/8/10	-
1	CCS	B	381	1	-	4/6/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	CCS	OZ1-CE	3.35	1.33	1.22
1	A	381[B]	CCS	OZ2-CE	-3.27	1.20	1.30
1	A	381[A]	CCS	OZ1-CE	3.21	1.32	1.22
1	A	381[B]	CCS	OZ1-CE	2.84	1.31	1.22
1	A	381[A]	CCS	OZ2-CE	-2.83	1.21	1.30
1	B	381	CCS	OZ2-CE	-2.36	1.23	1.30
1	B	381	CCS	CD-SG	-2.18	1.76	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381[A]	CCS	OZ1-CE-CD	-6.26	105.92	122.85
1	A	381[B]	CCS	OZ1-CE-CD	-4.37	111.03	122.85
1	B	381	CCS	OZ1-CE-CD	-4.24	111.38	122.85
1	A	381[A]	CCS	OZ2-CE-OZ1	3.24	131.67	123.33
1	A	381[B]	CCS	OZ2-CE-CD	3.10	123.45	113.38
1	A	381[A]	CCS	OZ2-CE-CD	2.77	122.37	113.38
1	B	381	CCS	OZ2-CE-CD	2.20	120.51	113.38

There are no chirality outliers.

All (9) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
1	A	381[B]	CCS	CE-CD-SG-CB
1	B	381	CCS	N-CA-CB-SG
1	B	381	CCS	C-CA-CB-SG
1	B	381	CCS	CA-CB-SG-CD
1	B	381	CCS	CE-CD-SG-CB
1	A	381[A]	CCS	SG-CD-CE-OZ1
1	A	381[A]	CCS	SG-CD-CE-OZ2
1	A	381[B]	CCS	SG-CD-CE-OZ1
1	A	381[B]	CCS	SG-CD-CE-OZ2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	381[B]	CCS	1	0
1	B	381	CCS	1	0

## 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	RAL	B	600	-	32,38,38	1.65	4 (12%)	40,53,53	2.01	13 (32%)
2	RAL	A	600	-	32,38,38	2.21	3 (9%)	40,53,53	1.88	9 (22%)

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	RAL	B	600	-	-	4/11/26/26	0/5/5/5
2	RAL	A	600	-	-	2/11/26/26	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	RAL	C5-S6	-10.81	1.65	1.74
2	B	600	RAL	C5-S6	-6.24	1.69	1.74
2	A	600	RAL	C1-C14	-3.73	1.34	1.42
2	B	600	RAL	C1-C14	-3.01	1.36	1.42
2	B	600	RAL	C13-C8	-2.69	1.36	1.42
2	A	600	RAL	C13-C8	-2.19	1.37	1.42
2	B	600	RAL	C17-C16	-2.17	1.45	1.49

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	RAL	C1-C14-C15	-6.32	128.25	135.95
2	A	600	RAL	C1-C14-C15	-5.73	128.97	135.95
2	A	600	RAL	C24-C25-N26	5.57	129.11	113.36
2	B	600	RAL	C31-N26-C27	4.33	118.18	108.84
2	B	600	RAL	C28-C27-N26	3.21	116.29	111.30
2	B	600	RAL	C29-C30-C31	-3.20	105.26	111.19
2	B	600	RAL	C4-C5-S6	3.01	131.13	125.10
2	B	600	RAL	C22-C17-C18	2.96	122.33	118.57
2	A	600	RAL	C25-N26-C31	2.84	118.81	111.24
2	B	600	RAL	O16-C16-C17	-2.77	115.72	120.15
2	B	600	RAL	C18-C17-C16	-2.71	114.59	120.55
2	B	600	RAL	C18-C19-C20	-2.69	116.66	119.73
2	B	600	RAL	C21-C22-C17	-2.53	118.10	120.80
2	A	600	RAL	C30-C29-C28	-2.46	103.89	111.19
2	A	600	RAL	C29-C28-C27	-2.41	106.74	111.19
2	B	600	RAL	O23-C24-C25	-2.34	101.89	107.79
2	A	600	RAL	C29-C30-C31	-2.30	106.93	111.19
2	B	600	RAL	C15-C16-C17	2.29	122.85	119.24
2	A	600	RAL	C15-C16-C17	2.25	122.79	119.24
2	A	600	RAL	C1-C2-C3	2.21	122.47	120.08
2	A	600	RAL	C4-C5-S6	2.20	129.50	125.10
2	B	600	RAL	C21-C20-C19	2.01	123.09	120.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

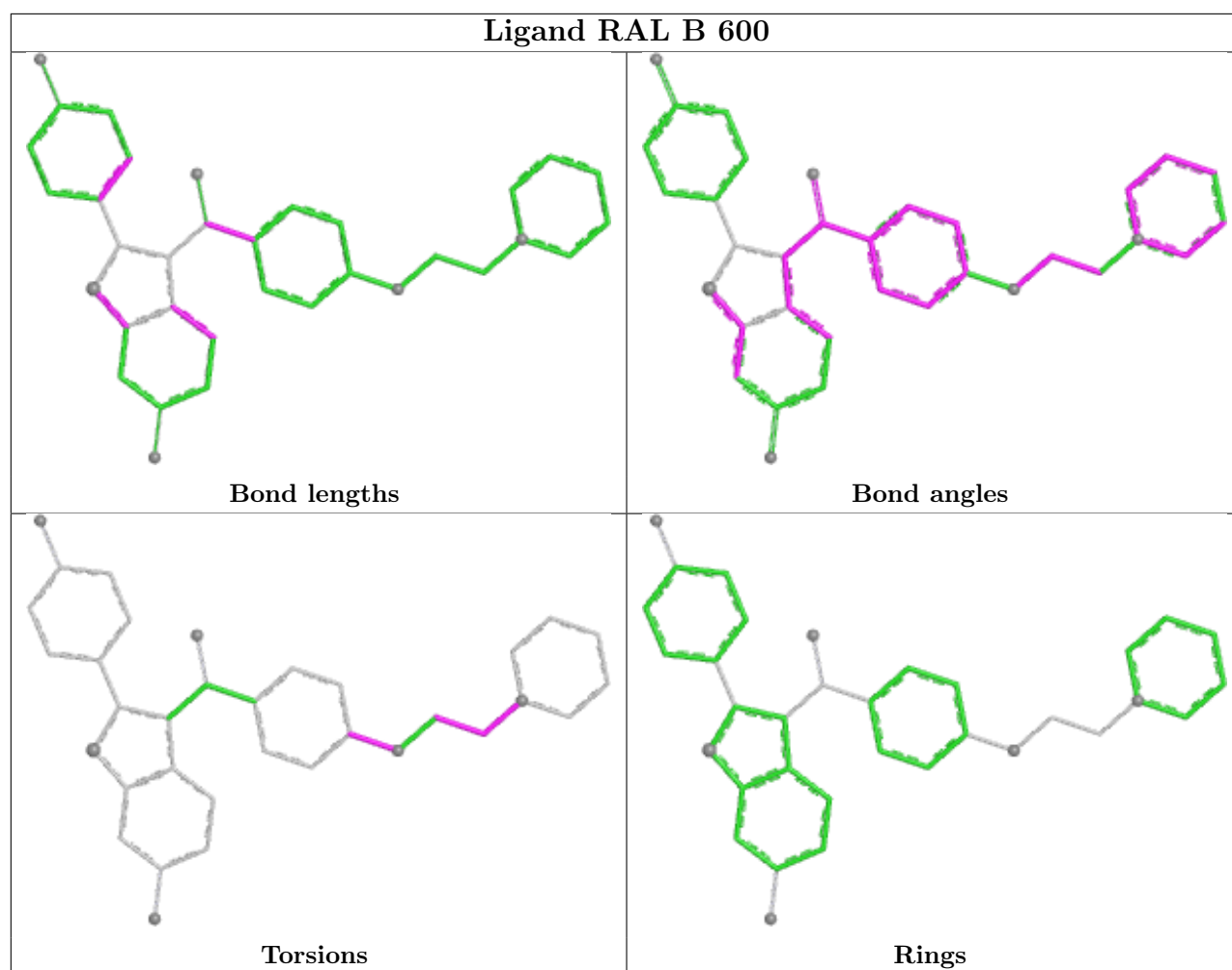
Mol	Chain	Res	Type	Atoms
2	B	600	RAL	C21-C20-O23-C24
2	B	600	RAL	C19-C20-O23-C24
2	B	600	RAL	C24-C25-N26-C31
2	A	600	RAL	C24-C25-N26-C31
2	B	600	RAL	O23-C24-C25-N26
2	A	600	RAL	O23-C24-C25-N26

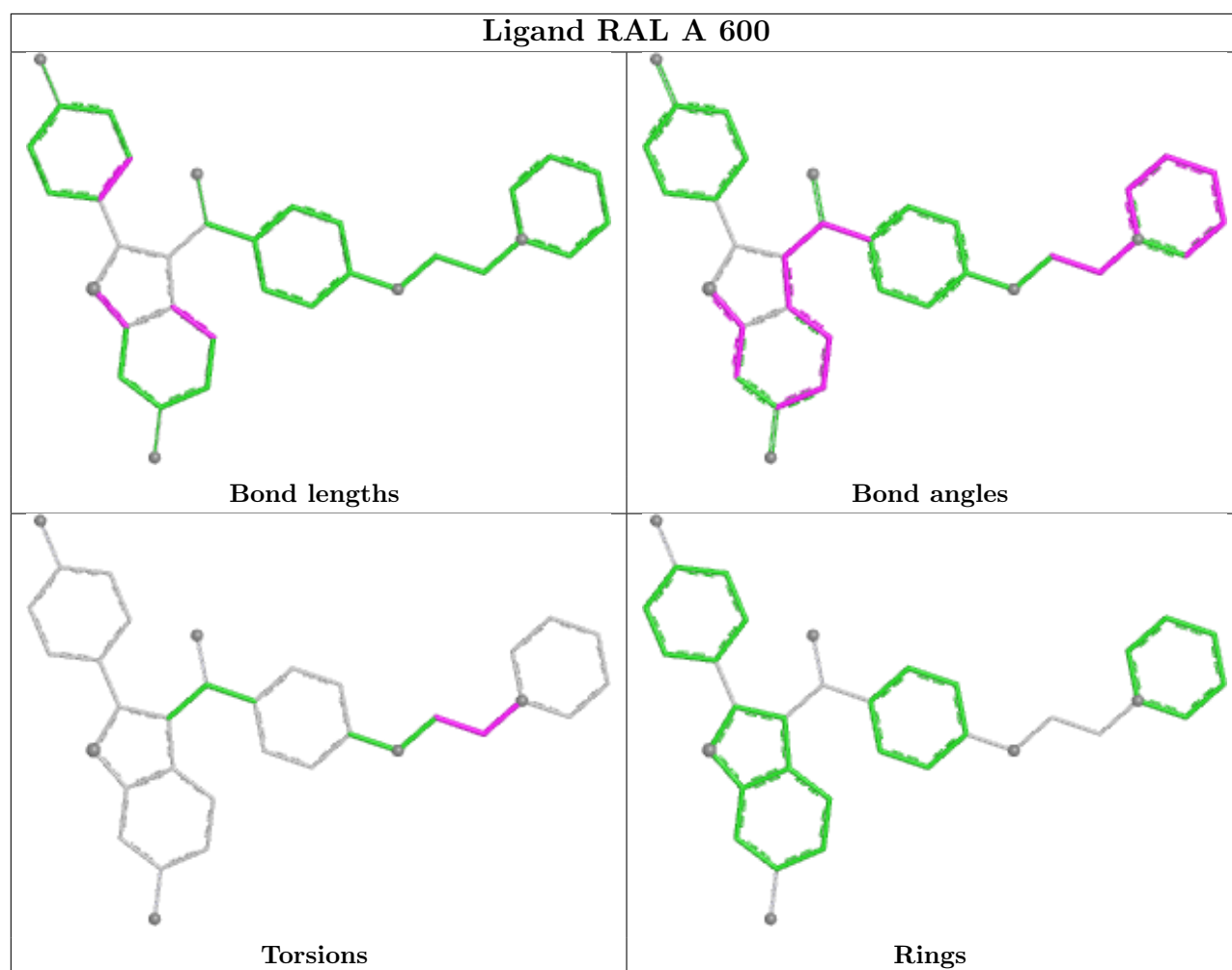
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	RAL	1	0
2	A	600	RAL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	224/253 (88%)	-0.04	11 (4%) 36 30	27, 48, 101, 130	4 (1%)
1	B	222/253 (87%)	-0.02	13 (5%) 29 24	22, 46, 102, 139	5 (2%)
All	All	446/506 (88%)	-0.03	24 (5%) 32 27	22, 47, 101, 139	9 (2%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456[A]	SER	4.6
1	A	337	PHE	4.5
1	B	546	ALA	4.5
1	B	551	ALA	4.1
1	B	458	VAL	3.9
1	A	334	THR	3.7
1	A	336	PRO	3.7
1	A	331	TYR	3.6
1	A	373[A]	HIS	3.6
1	A	459	TYR	3.3
1	A	332	ASP	3.1
1	B	526[A]	TYR	2.9
1	A	333	PRO	2.9
1	B	331	TYR	2.7
1	B	547	HIS	2.6
1	A	335	ARG	2.6
1	B	548	ARG	2.5
1	B	340	ALA	2.3
1	B	459	TYR	2.3
1	B	550	HIS	2.2
1	B	471	GLU	2.2
1	A	535	PRO	2.1
1	A	413	ASN	2.1
1	B	306	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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
1	CCS	B	381	10/11	0.86	0.14	37,52,71,73	0
1	CCS	A	381[B]	10/11	0.87	0.13	37,51,59,65	5
1	CCS	A	381[A]	10/11	0.87	0.13	37,51,61,62	5

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

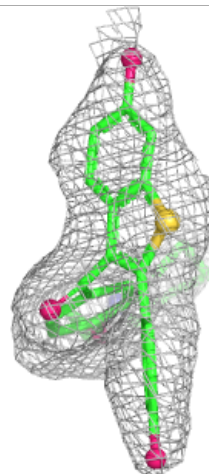
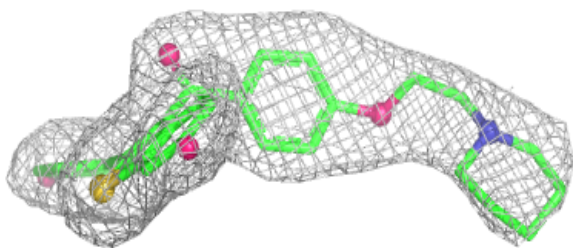
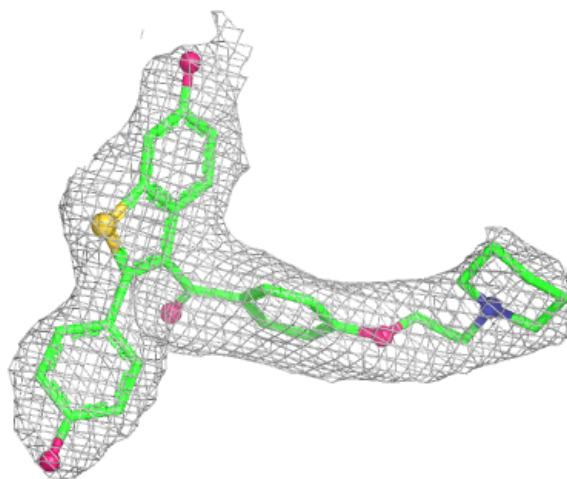
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	RAL	B	600	34/34	0.93	0.09	34,40,45,50	0
2	RAL	A	600	34/34	0.96	0.07	30,36,50,50	0

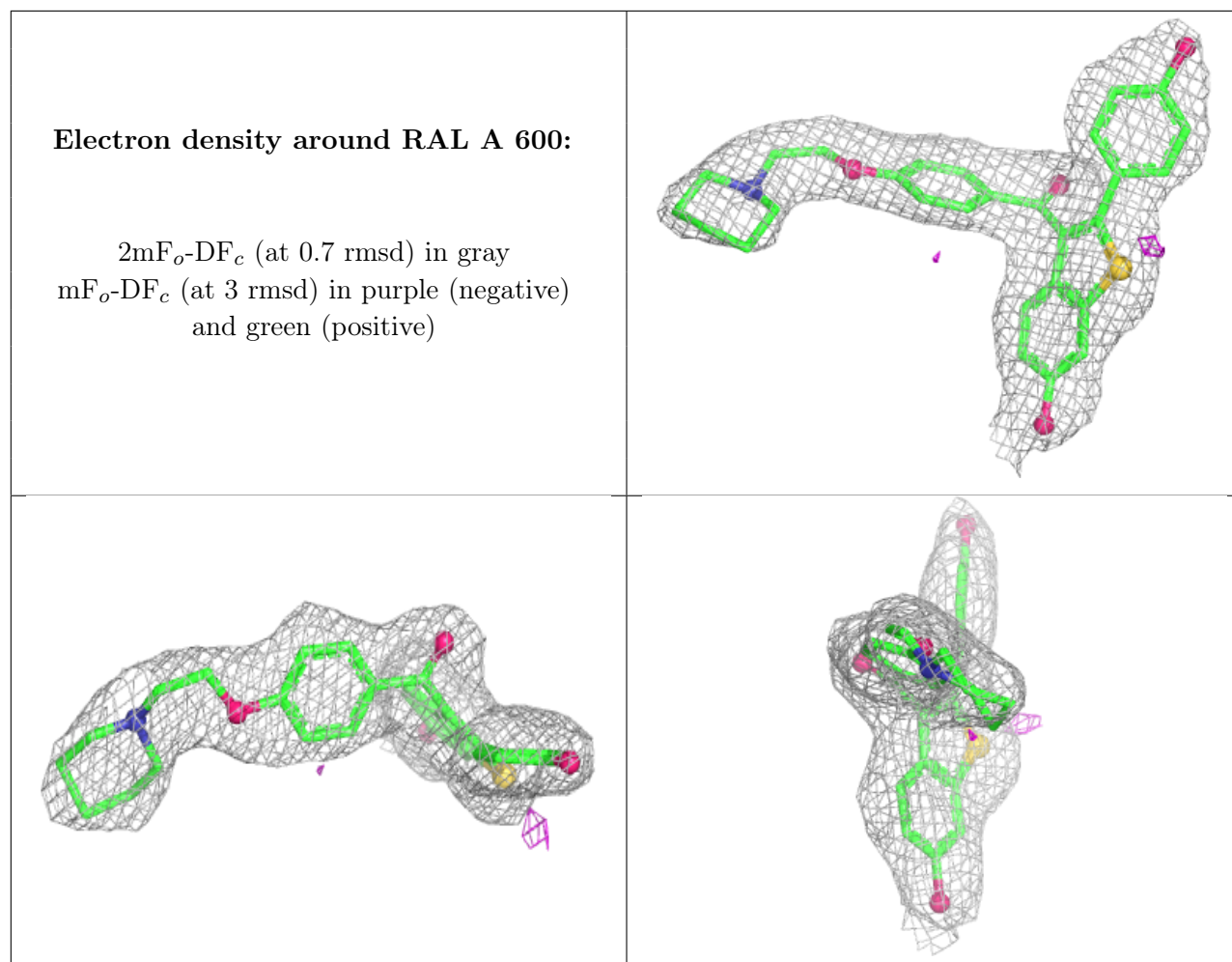
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around RAL B 600:**

$2mF_o-DF_c$  (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.