



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:28 pm BST

PDB ID : 1R5K
Title : Human Estrogen Receptor alpha Ligand-Binding Domain In Complex With GW5638
Authors : Wu, Y.-L.; Yang, X.; Ren, Z.; McDonnell, D.P.; Norris, J.D.; Willson, T.M.; Greene, G.L.
Deposited on : 2003-10-10
Resolution : 2.70 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 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 : 2.11
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) : 2.11

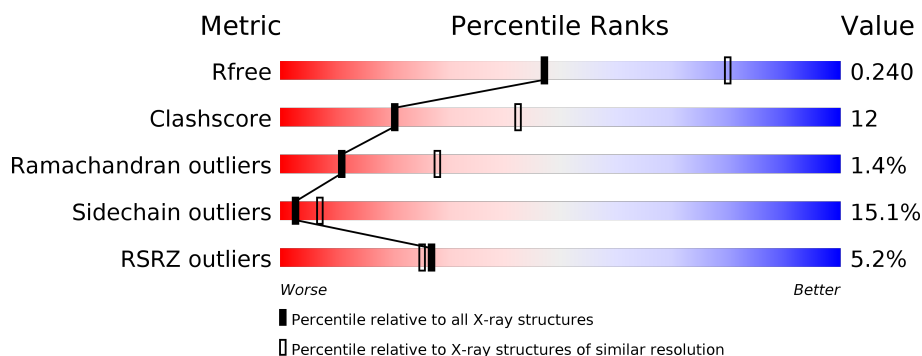
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	261	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	261	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>• •</div> <div>10%</div> </div> </div>
1	C	261	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>22%</div> <div>6%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5756 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.

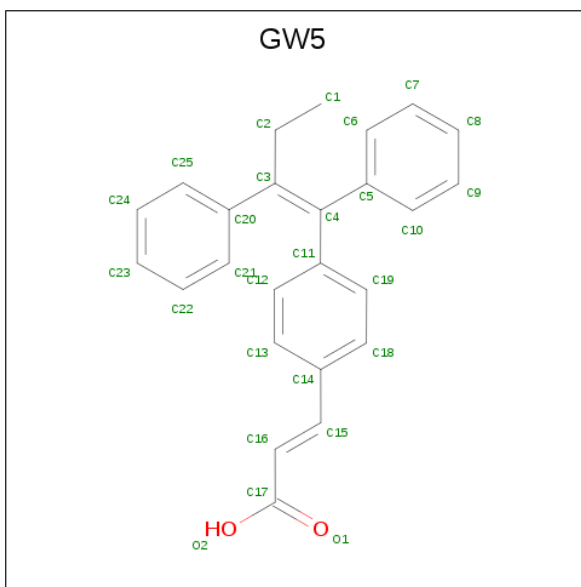
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1884	1210	316	339	19			
1	B	235	Total	C	N	O	S	0	0	0
			1876	1206	315	336	19			
1	C	235	Total	C	N	O	S	0	0	0
			1876	1206	315	336	19			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	MET	-	CLONING ARTIFACT	UNP P03372
A	295	ASP	-	CLONING ARTIFACT	UNP P03372
A	296	PRO	-	CLONING ARTIFACT	UNP P03372
B	294	MET	-	CLONING ARTIFACT	UNP P03372
B	295	ASP	-	CLONING ARTIFACT	UNP P03372
B	296	PRO	-	CLONING ARTIFACT	UNP P03372
C	294	MET	-	CLONING ARTIFACT	UNP P03372
C	295	ASP	-	CLONING ARTIFACT	UNP P03372
C	296	PRO	-	CLONING ARTIFACT	UNP P03372

- Molecule 2 is (2E)-3-{4-[(1E)-1,2-DIPHENYLBUT-1-ENYL]PHENYL}ACRYLIC ACID (three-letter code: GW5) (formula: C₂₅H₂₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			27	25	2		
2	B	1	Total	C	O	0	0
			27	25	2		
2	C	1	Total	C	O	0	0
			27	25	2		

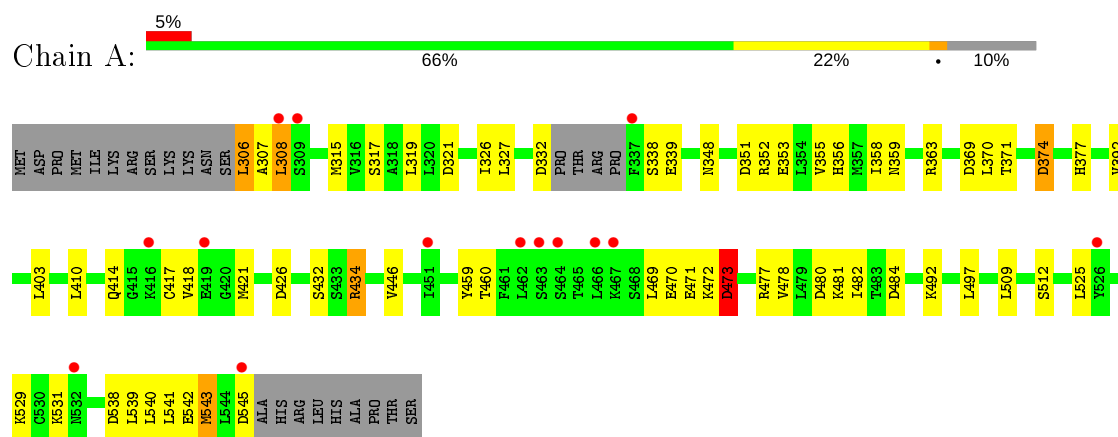
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	12	Total	O	0	0
			12	12		
3	C	12	Total	O	0	0
			12	12		

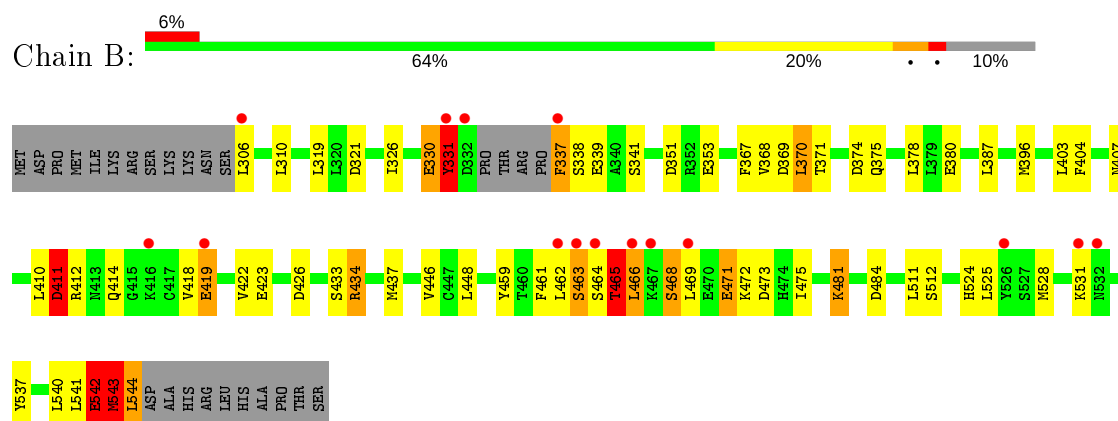
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

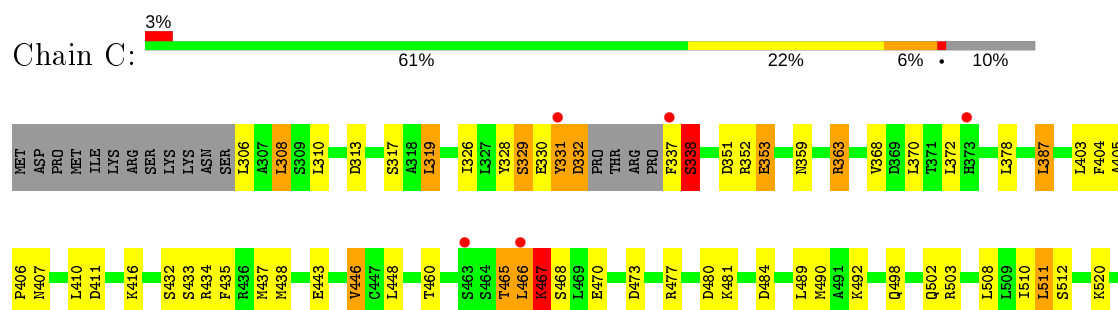
• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor



• Molecule 1: Estrogen receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	136.03Å 136.03Å 357.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.95 – 2.70 27.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.8 (27.95-2.70) 92.6 (27.93-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.236 0.208 , 0.240	Depositor DCC
R_{free} test set	5160 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5756	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GW5

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	0.61	0/1917	0.78	8/2588 (0.3%)
1	B	0.60	0/1909	0.77	6/2577 (0.2%)
1	C	0.64	0/1909	0.82	7/2577 (0.3%)
All	All	0.62	0/5735	0.79	21/7742 (0.3%)

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ASP	CB-CG-OD2	8.03	125.52	118.30
1	B	411	ASP	CB-CG-OD2	6.85	124.47	118.30
1	B	351	ASP	CB-CG-OD2	6.82	124.43	118.30
1	C	351	ASP	CB-CG-OD2	6.62	124.25	118.30
1	A	369	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	321	ASP	CB-CG-OD2	6.47	124.13	118.30
1	B	484	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	484	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	369	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	332	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	484	ASP	CB-CG-OD2	5.68	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	545	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	374	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	480	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	473	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	473	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	411	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	313	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	480	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	426	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	473	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	330	GLU	Peptide
1	C	467	LYS	Peptide

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	1884	0	1936	31	0
1	B	1876	0	1932	50	0
1	C	1876	0	1932	58	0
2	A	27	0	21	5	0
2	B	27	0	21	1	0
2	C	27	0	21	3	0
3	A	15	0	0	0	0
3	B	12	0	0	0	0
3	C	12	0	0	5	0
All	All	5756	0	5863	144	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 12.

All (144) 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:543:MET:O	1:B:543:MET:HG3	1.44	1.10
1:B:463:SER:HB3	1:B:472:LYS:NZ	1.67	1.09
1:B:465:THR:HG23	1:B:468:SER:HB2	1.46	0.98
1:B:524:HIS:CD2	1:B:528:MET:HE2	2.01	0.95
1:C:468:SER:HA	3:C:732:HOH:O	1.67	0.94
1:B:463:SER:HB3	1:B:472:LYS:HZ1	1.23	0.94
1:A:319:LEU:HB3	1:A:446:VAL:HG13	1.49	0.94
1:B:319:LEU:HB3	1:B:446:VAL:HG13	1.50	0.94
1:C:467:LYS:HG3	1:C:470:GLU:HG3	1.49	0.93
1:B:462:LEU:O	1:B:464:SER:N	2.04	0.90
1:B:463:SER:CB	1:B:472:LYS:HZ1	1.86	0.88
1:B:463:SER:CB	1:B:472:LYS:NZ	2.36	0.88
2:A:600:GW5:H22A	2:A:600:GW5:C10	2.02	0.87
1:C:467:LYS:C	3:C:732:HOH:O	2.15	0.85
1:C:466:LEU:O	3:C:733:HOH:O	1.96	0.84
1:A:319:LEU:HB3	1:A:446:VAL:CG1	2.07	0.84
1:B:319:LEU:HB3	1:B:446:VAL:CG1	2.08	0.83
1:B:465:THR:CG2	1:B:468:SER:HB2	2.08	0.83
1:C:468:SER:CA	3:C:732:HOH:O	2.21	0.83
1:A:374:ASP:OD1	1:A:471:GLU:HG2	1.81	0.80
1:C:438:MET:O	1:C:503:ARG:NH2	2.15	0.80
1:B:374:ASP:OD1	1:B:471:GLU:HG2	1.83	0.79
1:C:331:TYR:HE1	1:C:407:ASN:HD22	1.31	0.79
1:C:540:LEU:O	1:C:543:MET:HB2	1.83	0.78
1:C:329:SER:OG	1:C:330:GLU:N	2.15	0.78
1:B:463:SER:HB3	1:B:472:LYS:HZ3	1.50	0.77
1:C:466:LEU:CD1	1:C:466:LEU:H	2.00	0.74
1:C:319:LEU:HB3	1:C:446:VAL:CG1	2.19	0.73
1:A:473:ASP:OD1	1:A:477:ARG:NH2	2.22	0.73
1:B:330:GLU:O	1:B:331:TYR:HB2	1.89	0.71
1:C:467:LYS:HG3	1:C:470:GLU:CG	2.20	0.70
1:B:524:HIS:CD2	1:B:528:MET:CE	2.75	0.69
1:B:542:GLU:O	1:B:544:LEU:N	2.25	0.68
1:C:542:GLU:O	1:C:543:MET:CG	2.42	0.68
1:B:543:MET:CG	1:B:543:MET:O	2.27	0.66
2:C:602:GW5:H22A	2:C:602:GW5:C10	2.25	0.66
1:C:310:LEU:O	1:C:481:LYS:HE3	1.96	0.65
1:C:541:LEU:O	1:C:543:MET:N	2.29	0.65
1:C:319:LEU:HB3	1:C:446:VAL:HG13	1.79	0.65
1:B:310:LEU:O	1:B:481:LYS:HE3	1.97	0.64
1:C:538:ASP:O	1:C:542:GLU:HG3	1.98	0.64
1:C:465:THR:HG22	1:C:468:SER:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ARG:HD3	1:B:426:ASP:OD2	1.99	0.63
1:C:328:TYR:O	1:C:352:ARG:NH1	2.29	0.60
1:C:498:GLN:O	1:C:502:GLN:HG3	2.00	0.60
1:C:331:TYR:HE1	1:C:407:ASN:ND2	1.98	0.59
1:C:466:LEU:HD12	1:C:466:LEU:H	1.66	0.59
1:A:319:LEU:CB	1:A:446:VAL:CG1	2.80	0.57
2:B:601:GW5:H22A	2:B:601:GW5:C10	2.35	0.57
1:C:466:LEU:HD12	1:C:466:LEU:N	2.20	0.57
1:B:380:GLU:HG3	1:B:541:LEU:HD13	1.87	0.56
1:C:319:LEU:HB3	1:C:446:VAL:HG11	1.88	0.55
1:C:465:THR:O	1:C:467:LYS:N	2.40	0.55
1:C:532:ASN:H	1:C:532:ASN:ND2	2.05	0.55
1:C:404:PHE:CE2	1:C:410:LEU:HD12	2.43	0.54
1:C:331:TYR:CE1	1:C:407:ASN:ND2	2.64	0.53
1:B:411:ASP:HB2	1:B:414:GLN:HG3	1.89	0.53
1:B:339:GLU:HG2	1:B:418:VAL:HA	1.89	0.53
1:C:465:THR:HG22	1:C:468:SER:OG	2.08	0.53
2:C:602:GW5:C12	2:C:602:GW5:C20	2.86	0.52
1:A:538:ASP:O	1:A:542:GLU:HG3	2.10	0.52
2:A:600:GW5:H10	2:A:600:GW5:H22A	1.90	0.52
1:C:353:GLU:HB3	1:C:387:LEU:HD11	1.92	0.52
1:C:337:PHE:O	1:C:338:SER:HB3	2.10	0.51
2:C:602:GW5:H12	2:C:602:GW5:C20	2.39	0.51
1:B:464:SER:O	1:B:465:THR:CB	2.58	0.51
1:C:466:LEU:O	1:C:467:LYS:CG	2.58	0.51
1:C:542:GLU:O	1:C:543:MET:HG2	2.10	0.51
1:C:466:LEU:O	1:C:467:LYS:HG2	2.11	0.51
1:B:331:TYR:HE1	1:B:407:ASN:HD22	1.59	0.50
1:C:337:PHE:O	1:C:338:SER:CB	2.59	0.50
1:B:337:PHE:HE2	1:B:414:GLN:NE2	2.09	0.50
1:A:371:THR:HG23	1:A:471:GLU:OE2	2.11	0.49
1:B:464:SER:O	1:B:465:THR:HB	2.12	0.49
1:B:370:LEU:HD21	1:B:475:ILE:HD11	1.94	0.49
1:C:537:TYR:O	1:C:541:LEU:HD22	2.11	0.49
1:C:508:LEU:O	1:C:511:LEU:HB2	2.12	0.49
1:B:463:SER:CB	1:B:472:LYS:HZ3	2.17	0.49
1:A:414:GLN:O	1:A:417:CYS:HB2	2.12	0.49
1:C:465:THR:HG22	1:C:468:SER:H	1.76	0.49
1:A:327:LEU:HD21	1:A:356:HIS:CD2	2.48	0.49
1:B:371:THR:HG23	1:B:471:GLU:OE2	2.13	0.49
1:A:377:HIS:HE1	1:A:460:THR:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HD12	1:A:353:GLU:HG3	1.94	0.48
1:C:435:PHE:CE2	1:C:510:ILE:HD13	2.49	0.48
1:C:467:LYS:HB3	1:C:470:GLU:HB2	1.95	0.48
1:A:434:ARG:HD3	1:B:459:TYR:HE1	1.79	0.48
1:B:537:TYR:O	1:B:541:LEU:HG	2.14	0.47
1:B:418:VAL:O	1:B:419:GLU:C	2.53	0.47
1:A:377:HIS:CE1	1:A:460:THR:O	2.68	0.47
1:B:367:PHE:CE2	1:B:375:GLN:HG2	2.49	0.47
1:C:337:PHE:HB3	1:C:338:SER:H	1.62	0.46
1:A:348:ASN:ND2	1:A:352:ARG:HE	2.12	0.46
1:A:355:VAL:HA	1:A:358:ILE:HD12	1.98	0.46
1:B:404:PHE:CE2	1:B:410:LEU:HD12	2.51	0.46
1:C:465:THR:C	1:C:467:LYS:N	2.67	0.46
1:B:331:TYR:HD1	1:B:331:TYR:HA	1.53	0.46
2:A:600:GW5:C2	2:A:600:GW5:C10	2.76	0.45
1:A:359:ASN:O	1:A:363:ARG:HG3	2.16	0.45
1:B:422:VAL:HG13	1:B:423:GLU:N	2.31	0.45
1:C:477:ARG:HG2	1:C:477:ARG:HH11	1.82	0.45
1:C:405:ALA:HB1	1:C:406:PRO:HD2	1.98	0.45
1:A:308:LEU:HA	1:A:308:LEU:HD12	1.70	0.45
1:A:327:LEU:HD12	1:A:353:GLU:CG	2.46	0.45
1:A:509:LEU:HD23	1:A:509:LEU:HA	1.86	0.45
1:B:466:LEU:HD23	1:B:466:LEU:O	2.18	0.44
1:A:315:MET:HE2	1:A:319:LEU:HD11	1.99	0.44
1:B:319:LEU:CB	1:B:446:VAL:CG1	2.88	0.44
1:B:524:HIS:CE1	1:B:528:MET:HE1	2.51	0.44
1:C:540:LEU:HD23	1:C:543:MET:CE	2.48	0.44
1:A:459:TYR:HE1	1:B:434:ARG:HD3	1.83	0.43
1:C:541:LEU:HD12	1:C:541:LEU:HA	1.91	0.43
2:A:600:GW5:H10	2:A:600:GW5:C2	2.48	0.43
1:C:308:LEU:HA	1:C:308:LEU:HD13	1.81	0.43
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.80	0.42
2:A:600:GW5:C20	2:A:600:GW5:C12	2.95	0.42
1:B:464:SER:C	1:B:465:THR:HG22	2.39	0.42
1:A:492:LYS:HD3	1:A:492:LYS:HA	1.89	0.42
1:C:468:SER:N	3:C:732:HOH:O	2.33	0.42
1:C:466:LEU:HD13	1:C:466:LEU:H	1.80	0.42
1:A:470:GLU:HA	1:A:473:ASP:HB2	2.00	0.42
1:B:524:HIS:NE2	1:B:528:MET:CE	2.83	0.42
1:B:524:HIS:CG	1:B:528:MET:HE2	2.51	0.42
1:B:380:GLU:HG3	1:B:541:LEU:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HB3	1:A:446:VAL:HG11	1.98	0.41
1:B:544:LEU:HD23	1:B:544:LEU:HA	1.84	0.41
1:B:411:ASP:O	1:B:412:ARG:C	2.58	0.41
1:B:310:LEU:O	1:B:481:LYS:CE	2.64	0.41
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.82	0.41
1:B:422:VAL:CG1	1:B:423:GLU:N	2.84	0.41
1:B:337:PHE:HD1	1:B:337:PHE:HA	1.74	0.41
1:A:539:LEU:HD12	1:C:352:ARG:HG2	2.03	0.41
1:C:443:GLU:HB3	1:C:489:LEU:CD1	2.50	0.41
1:A:478:VAL:O	1:A:482:ILE:HG13	2.20	0.41
1:C:359:ASN:O	1:C:363:ARG:HG3	2.20	0.41
1:C:490:MET:CE	1:C:503:ARG:HG2	2.51	0.41
1:C:465:THR:HG23	1:C:467:LYS:H	1.87	0.40
1:C:540:LEU:HD23	1:C:543:MET:HE2	2.02	0.40
1:B:463:SER:HB2	1:B:472:LYS:NZ	2.29	0.40
1:A:355:VAL:HG11	1:C:539:LEU:HB3	2.04	0.40
1:C:319:LEU:HA	1:C:319:LEU:HD12	1.87	0.40
1:A:306:LEU:HD12	1:A:307:ALA:H	1.86	0.40
1:A:543:MET:HB3	1:A:543:MET:HE3	1.78	0.40
1:C:529:LYS:HG3	1:C:530:CYS:O	2.22	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	232/261 (89%)	223 (96%)	9 (4%)	0	100	100
1	B	231/261 (88%)	216 (94%)	9 (4%)	6 (3%)	5	13
1	C	231/261 (88%)	218 (94%)	9 (4%)	4 (2%)	9	23
All	All	694/783 (89%)	657 (95%)	27 (4%)	10 (1%)	11	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	TYR
1	B	463	SER
1	B	543	MET
1	C	338	SER
1	C	542	GLU
1	B	465	THR
1	B	542	GLU
1	C	331	TYR
1	B	461	PHE
1	C	467	LYS

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	213/236 (90%)	187 (88%)	26 (12%)	5	11
1	B	212/236 (90%)	179 (84%)	33 (16%)	2	7
1	C	212/236 (90%)	175 (82%)	37 (18%)	2	4
All	All	637/708 (90%)	541 (85%)	96 (15%)	3	7

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	308	LEU
1	A	317	SER
1	A	321	ASP
1	A	326	ILE
1	A	332	ASP
1	A	338	SER
1	A	339	GLU
1	A	370	LEU
1	A	392	VAL
1	A	403	LEU

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Mol	Chain	Res	Type
1	A	418	VAL
1	A	421	MET
1	A	432	SER
1	A	434	ARG
1	A	469	LEU
1	A	472	LYS
1	A	473	ASP
1	A	481	LYS
1	A	512	SER
1	A	525	LEU
1	A	529	LYS
1	A	531	LYS
1	A	540	LEU
1	A	541	LEU
1	A	543	MET
1	B	306	LEU
1	B	326	ILE
1	B	331	TYR
1	B	337	PHE
1	B	338	SER
1	B	341	SER
1	B	353	GLU
1	B	368	VAL
1	B	370	LEU
1	B	378	LEU
1	B	387	LEU
1	B	396	MET
1	B	403	LEU
1	B	411	ASP
1	B	419	GLU
1	B	433	SER
1	B	434	ARG
1	B	437	MET
1	B	448	LEU
1	B	465	THR
1	B	466	LEU
1	B	468	SER
1	B	469	LEU
1	B	471	GLU
1	B	481	LYS
1	B	511	LEU
1	B	512	SER

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Mol	Chain	Res	Type
1	B	525	LEU
1	B	531	LYS
1	B	540	LEU
1	B	542	GLU
1	B	543	MET
1	B	544	LEU
1	C	306	LEU
1	C	308	LEU
1	C	317	SER
1	C	319	LEU
1	C	326	ILE
1	C	329	SER
1	C	332	ASP
1	C	338	SER
1	C	353	GLU
1	C	363	ARG
1	C	368	VAL
1	C	370	LEU
1	C	372	LEU
1	C	378	LEU
1	C	387	LEU
1	C	403	LEU
1	C	416	LYS
1	C	432	SER
1	C	433	SER
1	C	434	ARG
1	C	437	MET
1	C	446	VAL
1	C	448	LEU
1	C	460	THR
1	C	465	THR
1	C	466	LEU
1	C	467	LYS
1	C	492	LYS
1	C	511	LEU
1	C	512	SER
1	C	520	LYS
1	C	525	LEU
1	C	527	SER
1	C	532	ASN
1	C	536	LEU
1	C	541	LEU

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Mol	Chain	Res	Type
1	C	543	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	ASN
1	A	356	HIS
1	A	359	ASN
1	A	502	GLN
1	A	519	ASN
1	B	377	HIS
1	B	474	HIS
1	B	488	HIS
1	B	498	GLN
1	B	519	ASN
1	B	524	HIS
1	C	348	ASN
1	C	356	HIS
1	C	359	ASN
1	C	502	GLN
1	C	524	HIS
1	C	532	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
2	GW5	C	602	-	26,29,29	1.90	4 (15%)	35,38,38	1.39	4 (11%)
2	GW5	A	600	-	26,29,29	2.05	5 (19%)	35,38,38	1.73	5 (14%)
2	GW5	B	601	-	26,29,29	1.98	5 (19%)	35,38,38	1.71	6 (17%)

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	GW5	C	602	-	-	3/21/23/23	0/3/3/3
2	GW5	A	600	-	-	4/21/23/23	0/3/3/3
2	GW5	B	601	-	-	4/21/23/23	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GW5	C20-C3	-5.89	1.38	1.49
2	A	600	GW5	C5-C4	-5.58	1.39	1.49
2	A	600	GW5	C11-C4	-5.55	1.39	1.49
2	B	601	GW5	C5-C4	-5.43	1.40	1.49
2	C	602	GW5	C5-C4	-5.17	1.40	1.49
2	C	602	GW5	C20-C3	-5.14	1.40	1.49
2	A	600	GW5	C20-C3	-4.84	1.40	1.49
2	C	602	GW5	C11-C4	-4.49	1.41	1.49
2	B	601	GW5	C11-C4	-4.42	1.41	1.49
2	A	600	GW5	C14-C15	-2.83	1.39	1.47
2	C	602	GW5	C14-C15	-2.72	1.39	1.47
2	B	601	GW5	C14-C15	-2.57	1.40	1.47
2	A	600	GW5	C4-C3	2.51	1.39	1.35
2	B	601	GW5	C4-C3	2.36	1.39	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	GW5	C5-C4-C3	-5.76	116.43	122.86
2	B	601	GW5	C5-C4-C3	-5.66	116.54	122.86
2	B	601	GW5	C2-C3-C20	4.18	120.44	114.45
2	A	600	GW5	C2-C3-C20	4.10	120.34	114.45
2	C	602	GW5	C2-C3-C4	-4.09	119.20	123.47
2	B	601	GW5	C2-C3-C4	-3.87	119.44	123.47
2	A	600	GW5	C1-C2-C3	-3.69	107.47	112.88
2	C	602	GW5	C5-C4-C3	-3.47	118.98	122.86
2	C	602	GW5	C2-C3-C20	3.44	119.38	114.45
2	A	600	GW5	C2-C3-C4	-3.19	120.14	123.47
2	A	600	GW5	C20-C3-C4	-2.77	119.48	122.33
2	B	601	GW5	C17-C16-C15	-2.51	118.33	123.69
2	C	602	GW5	C7-C6-C5	2.19	122.93	120.34
2	B	601	GW5	C20-C3-C4	-2.15	120.12	122.33
2	B	601	GW5	C21-C20-C3	-2.05	118.39	121.01

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	GW5	C20-C3-C4-C11
2	A	600	GW5	C2-C3-C4-C11
2	B	601	GW5	C20-C3-C4-C11
2	B	601	GW5	C2-C3-C4-C11
2	C	602	GW5	C1-C2-C3-C20
2	C	602	GW5	C1-C2-C3-C4
2	A	600	GW5	C11-C4-C5-C10
2	C	602	GW5	C12-C11-C4-C3
2	B	601	GW5	C12-C11-C4-C3
2	A	600	GW5	C11-C4-C5-C6
2	B	601	GW5	C19-C11-C4-C3

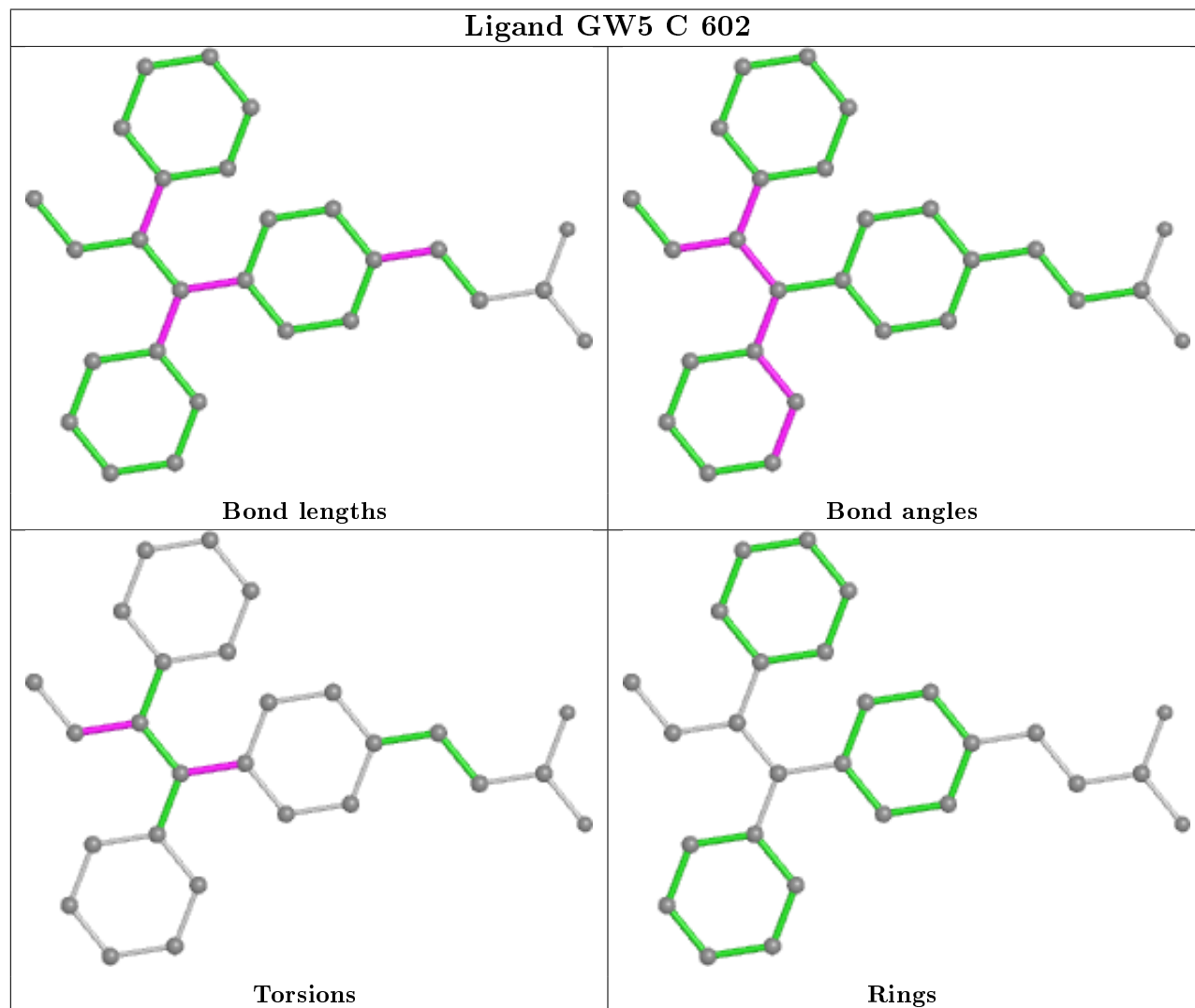
There are no ring outliers.

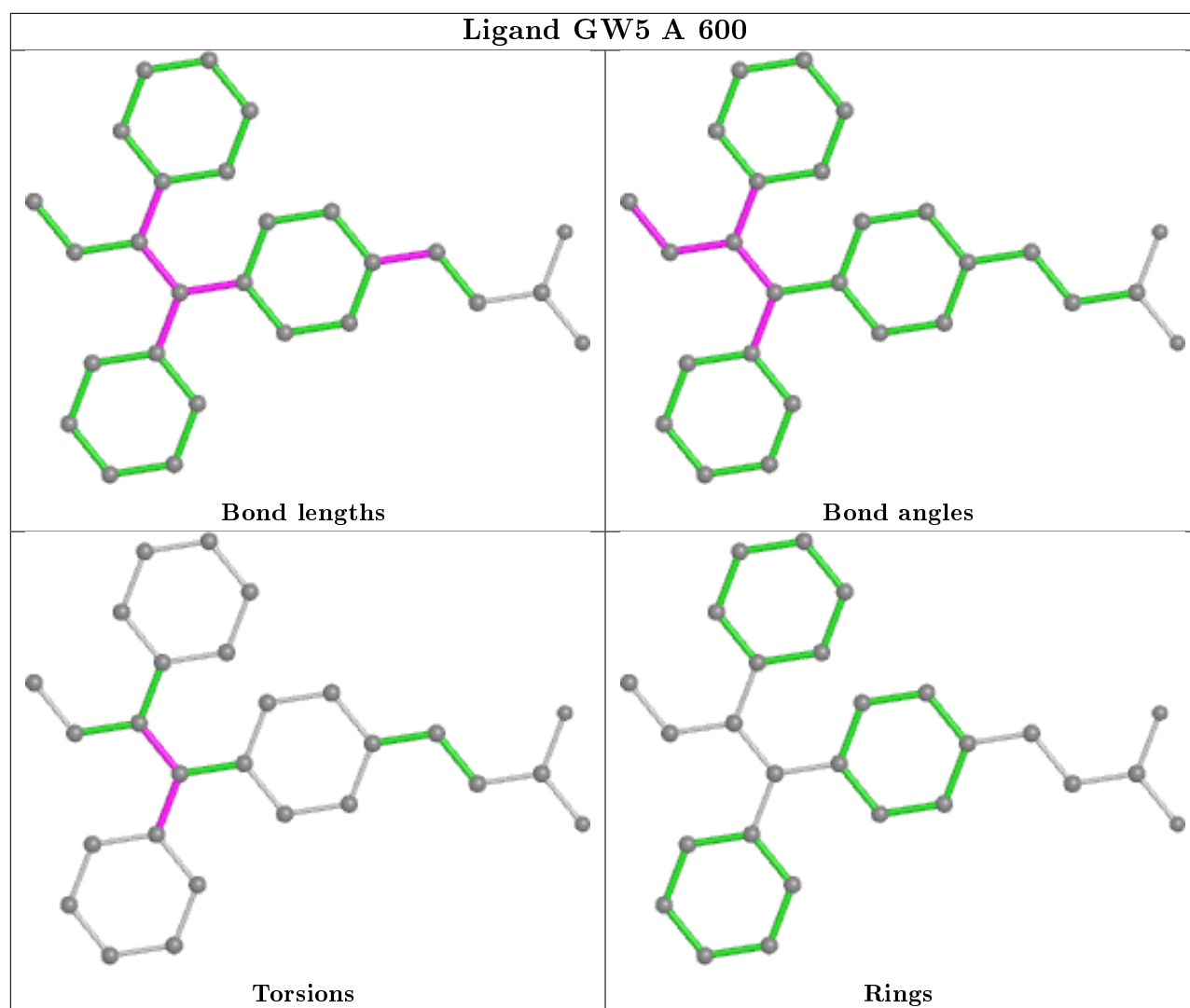
3 monomers are involved in 9 short contacts:

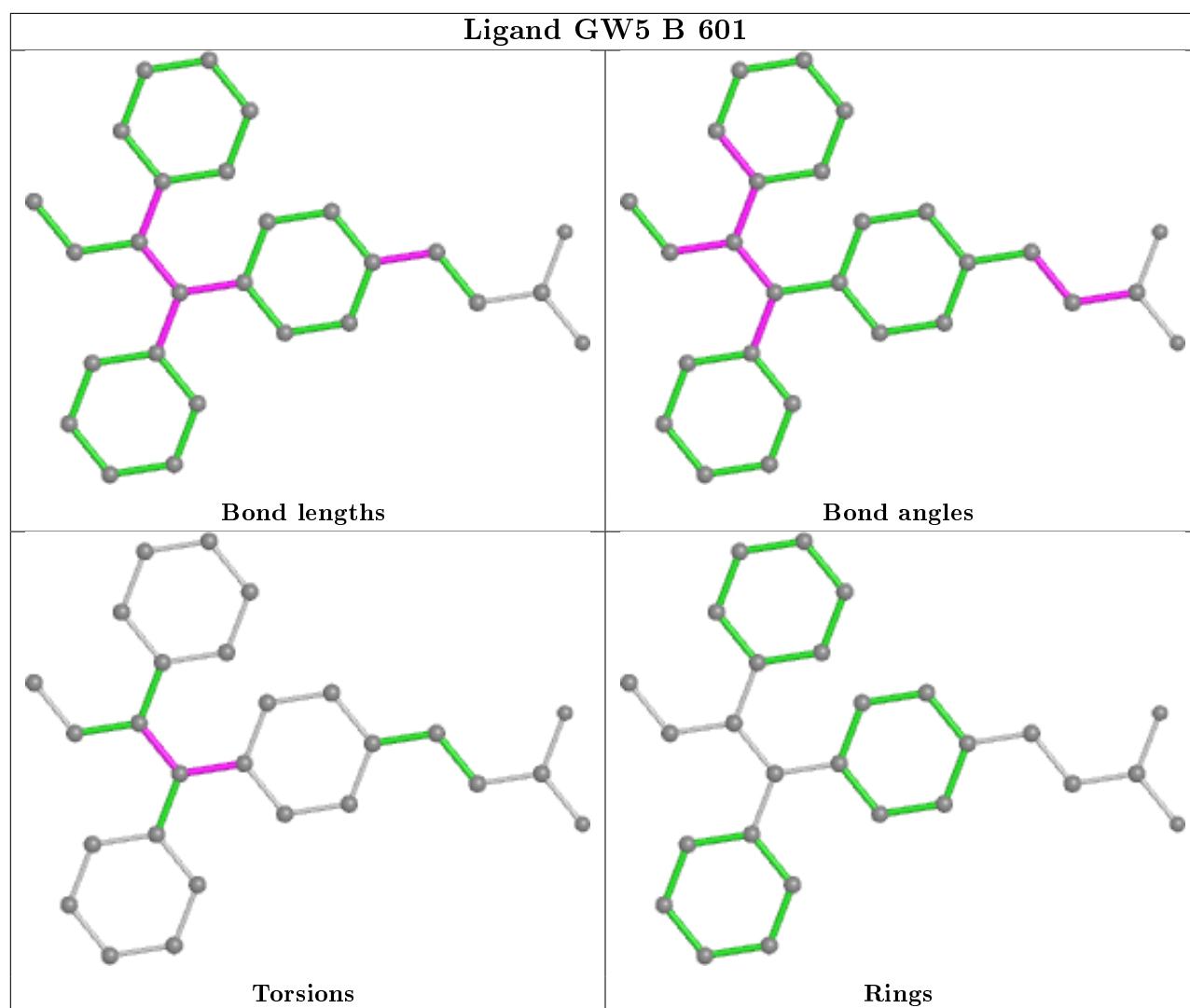
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GW5	3	0
2	A	600	GW5	5	0
2	B	601	GW5	1	0

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	236/261 (90%)	0.17	14 (5%)	22 21	33, 45, 63, 74	0
1	B	235/261 (90%)	0.24	15 (6%)	19 18	33, 46, 64, 77	0
1	C	235/261 (90%)	0.05	8 (3%)	45 45	34, 45, 60, 82	0
All	All	706/783 (90%)	0.15	37 (5%)	27 25	33, 45, 63, 82	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	LEU	6.6
1	C	544	LEU	5.4
1	B	337	PHE	5.4
1	B	462	LEU	5.3
1	B	332	ASP	5.0
1	C	331	TYR	4.3
1	C	466	LEU	3.8
1	A	545	ASP	3.7
1	B	466	LEU	3.6
1	A	466	LEU	3.5
1	B	532	ASN	3.5
1	A	526	TYR	3.4
1	C	337	PHE	3.3
1	B	331	TYR	3.1
1	B	463	SER	3.1
1	A	337	PHE	3.0
1	A	467	LYS	2.9
1	C	531	LYS	2.9
1	A	532	ASN	2.7
1	A	463	SER	2.7
1	B	419	GLU	2.6
1	A	309	SER	2.6
1	C	532	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	416	LYS	2.6
1	A	419	GLU	2.5
1	B	469	LEU	2.5
1	B	464	SER	2.4
1	C	463	SER	2.3
1	B	467	LYS	2.3
1	C	373	HIS	2.3
1	B	526	TYR	2.3
1	B	416	LYS	2.3
1	B	531	LYS	2.3
1	B	306	LEU	2.2
1	A	464	SER	2.1
1	A	451	ILE	2.0
1	A	308	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

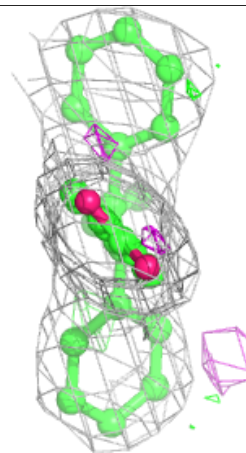
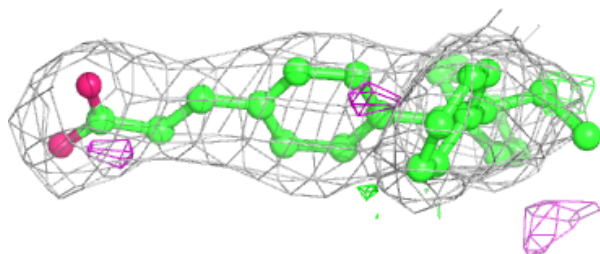
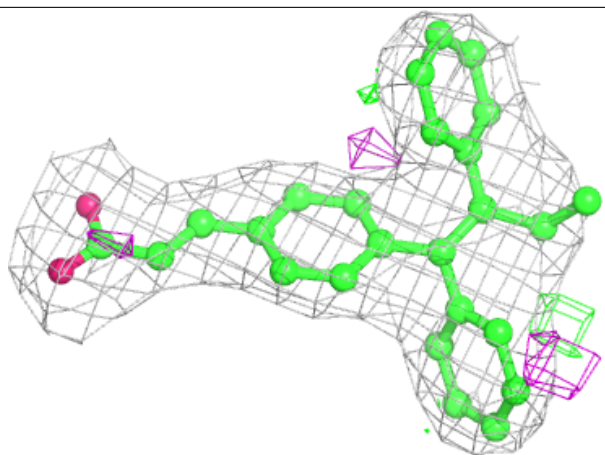
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GW5	B	601	27/27	0.94	0.23	67,70,76,77	0
2	GW5	A	600	27/27	0.95	0.27	69,71,75,77	0
2	GW5	C	602	27/27	0.97	0.21	58,61,70,72	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.

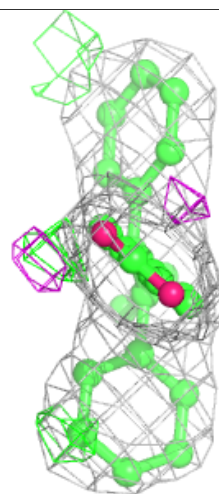
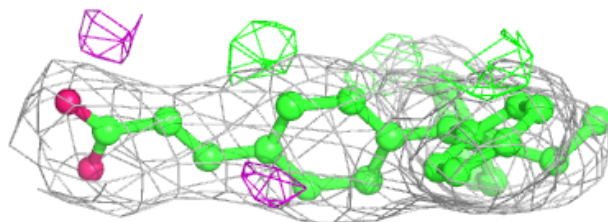
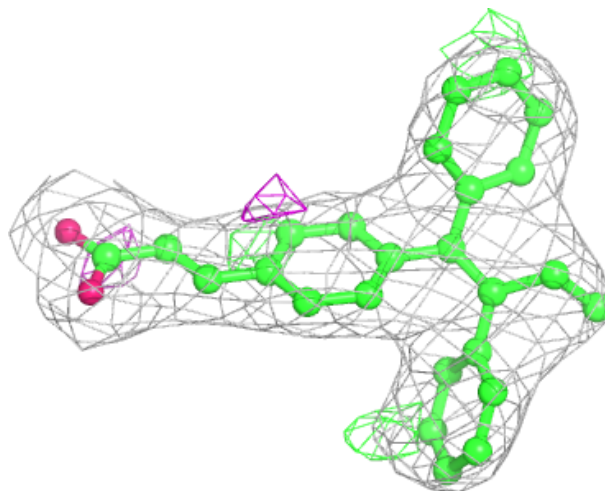
Electron density around GW5 B 601:

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



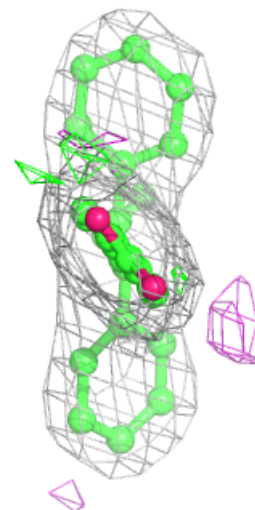
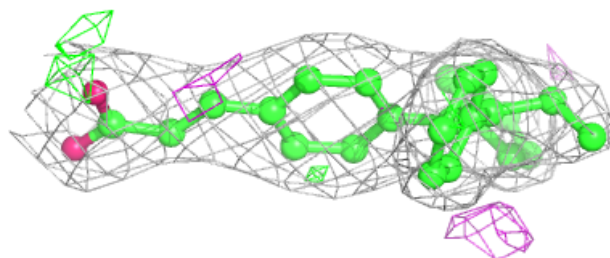
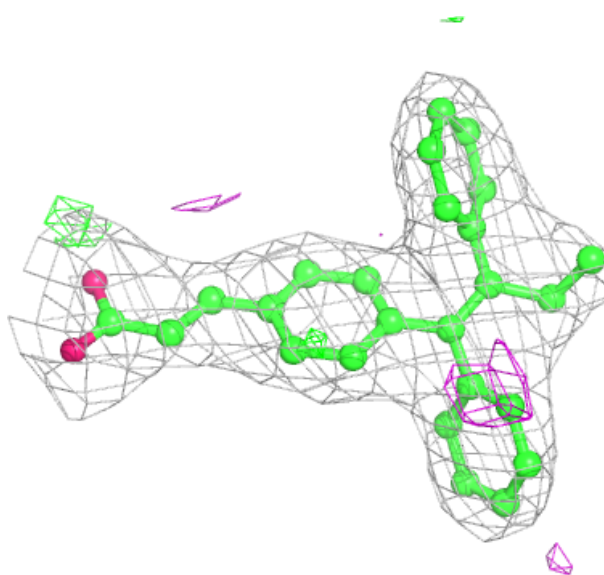
Electron density around GW5 A 600:

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



Electron density around GW5 C 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.