



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:41 AM UTC

PDB ID : 8DUS / pdb_00008dus
Title : Estrogen Receptor Alpha Ligand Binding Domain in Complex with (1'-(4-(2-(ethylamino)ethoxy)phenyl)-6'-hydroxy-1',4'-dihydro-2'-H</i>-spiro[cyclopropane-1,3'-isoquinolin]-2'-yl)(phenyl)methanone
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Deposited on : 2022-07-27
Resolution : 1.90 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](#) ①) 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

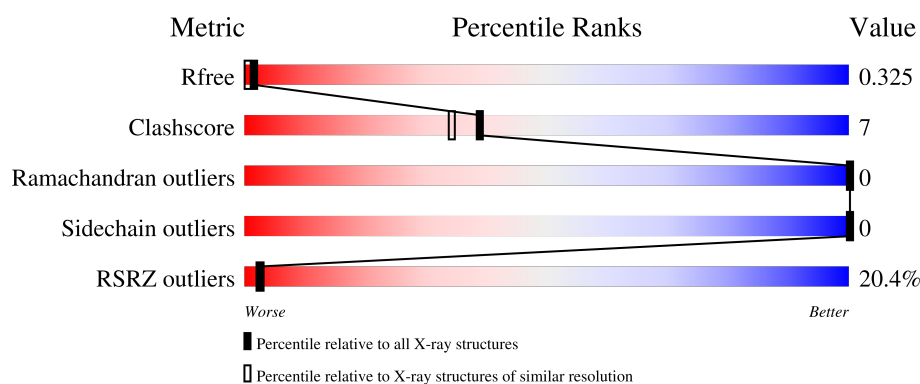
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	255	26% 79% 13% 8%
1	B	255	18% 74% 13% 13%
1	E	255	24% 75% 16% 9%
1	F	255	23% 74% 12% 14%
1	G	255	9% 79% 13% 8%

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Mol	Chain	Length	Quality of chain
1	H	255	10% 77% 11% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11334 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	235	Total	C	N	O	S	3	2	0
			1821	1159	311	336	15			
1	B	221	Total	C	N	O	S	0	0	0
			1721	1108	294	305	14			
1	E	232	Total	C	N	O	S	1	4	0
			1808	1155	310	329	14			
1	F	220	Total	C	N	O	S	0	0	0
			1732	1115	295	307	15			
1	G	234	Total	C	N	O	S	0	2	0
			1817	1161	309	332	15			
1	H	224	Total	C	N	O	S	1	1	0
			1748	1120	300	313	15			

There are 30 discrepancies between the modelled and reference sequences:

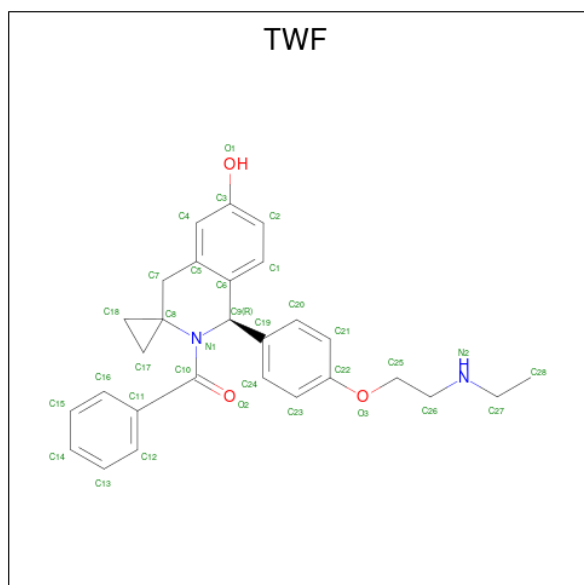
Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	-	initiating methionine	UNP P03372
A	381	SER	CYS	engineered mutation	UNP P03372
A	417	SER	CYS	engineered mutation	UNP P03372
A	530	SER	CYS	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	300	MET	-	initiating methionine	UNP P03372
B	381	SER	CYS	engineered mutation	UNP P03372
B	417	SER	CYS	engineered mutation	UNP P03372
B	530	SER	CYS	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
E	300	MET	-	initiating methionine	UNP P03372
E	381	SER	CYS	engineered mutation	UNP P03372
E	417	SER	CYS	engineered mutation	UNP P03372
E	530	SER	CYS	engineered mutation	UNP P03372
E	536	SER	LEU	engineered mutation	UNP P03372
F	300	MET	-	initiating methionine	UNP P03372
F	381	SER	CYS	engineered mutation	UNP P03372

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Chain	Residue	Modelled	Actual	Comment	Reference
F	417	SER	CYS	engineered mutation	UNP P03372
F	530	SER	CYS	engineered mutation	UNP P03372
F	536	SER	LEU	engineered mutation	UNP P03372
G	300	MET	-	initiating methionine	UNP P03372
G	381	SER	CYS	engineered mutation	UNP P03372
G	417	SER	CYS	engineered mutation	UNP P03372
G	530	SER	CYS	engineered mutation	UNP P03372
G	536	SER	LEU	engineered mutation	UNP P03372
H	300	MET	-	initiating methionine	UNP P03372
H	381	SER	CYS	engineered mutation	UNP P03372
H	417	SER	CYS	engineered mutation	UNP P03372
H	530	SER	CYS	engineered mutation	UNP P03372
H	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is [(1'R)-1'-{4-[2-(ethylamino)ethoxy]phenyl}-6'-hydroxy-1',4'-dihydro-2'H-spiro[cyclopropane-1,3'-isoquinolin]-2'-yl](phenyl)methanone (CCD ID: TWF) (formula: C₂₈H₃₀N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	28	2	3		
2	B	1	Total	C	N	O	0	0
			33	28	2	3		
2	E	1	Total	C	N	O	0	0
			33	28	2	3		
2	F	1	Total	C	N	O	0	0
			33	28	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			33	28	2	3		
2	H	1	Total	C	N	O	0	0
			33	28	2	3		

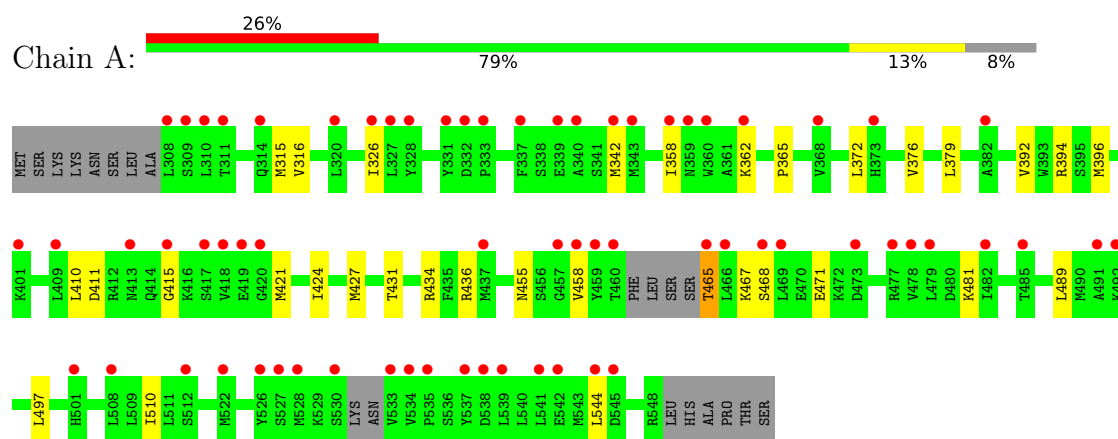
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	80	Total	O	0	0
			80	80		
3	E	79	Total	O	0	0
			79	79		
3	F	88	Total	O	0	0
			88	88		
3	G	78	Total	O	0	0
			78	78		
3	H	83	Total	O	0	0
			83	83		

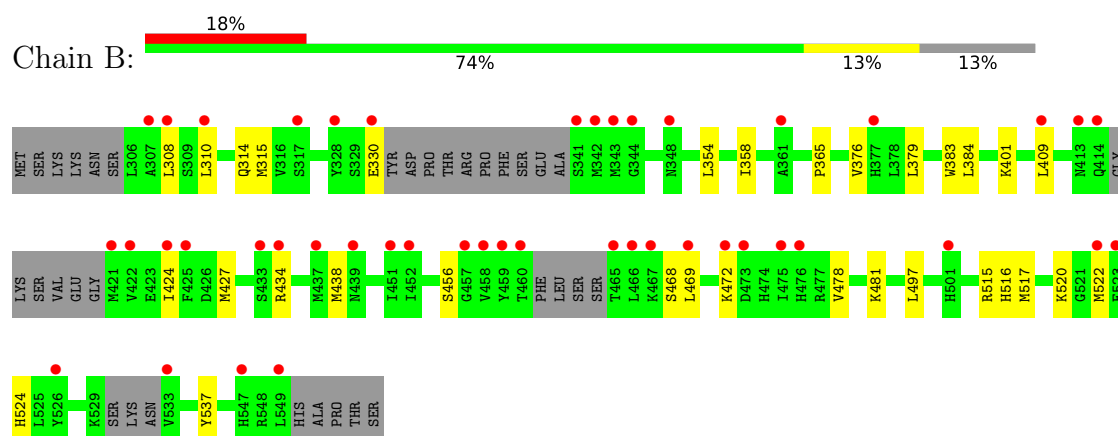
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

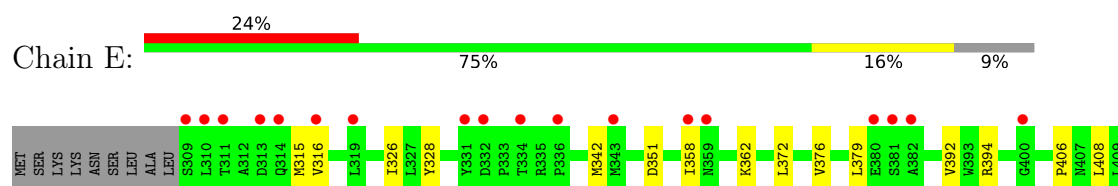
• Molecule 1: Estrogen receptor

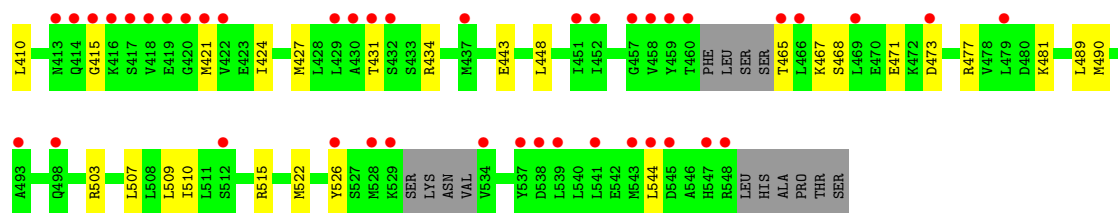


• Molecule 1: Estrogen receptor

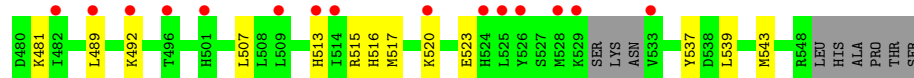
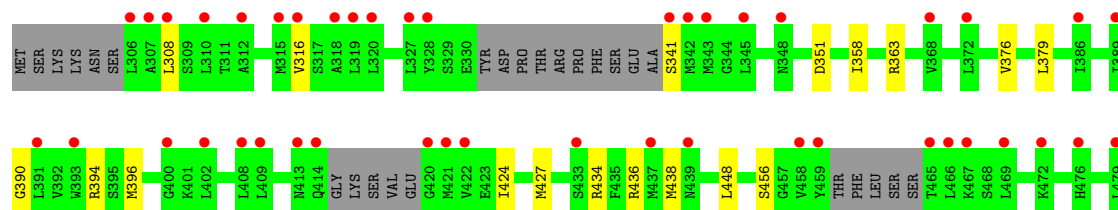
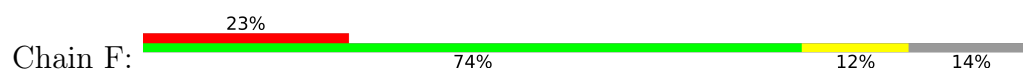


• Molecule 1: Estrogen receptor

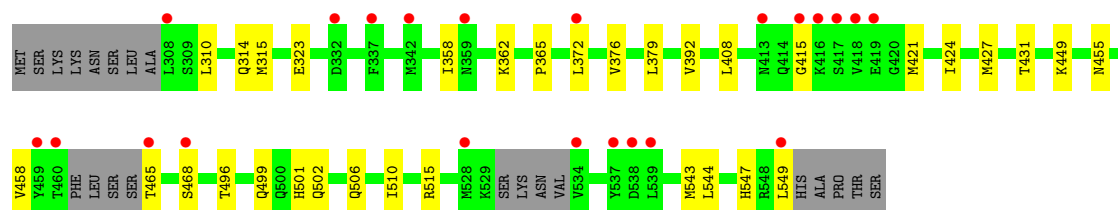
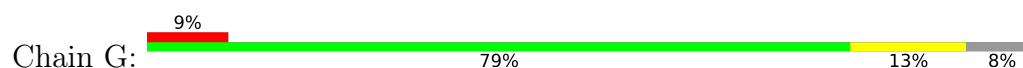




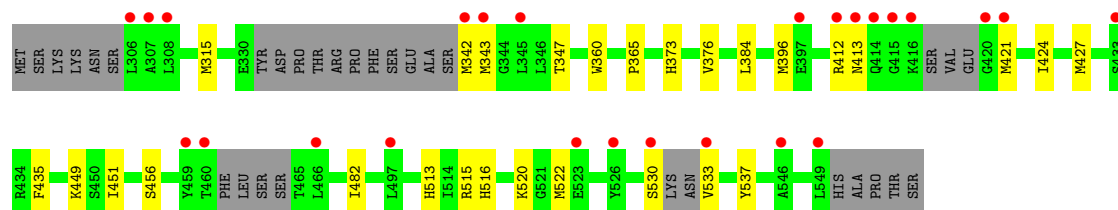
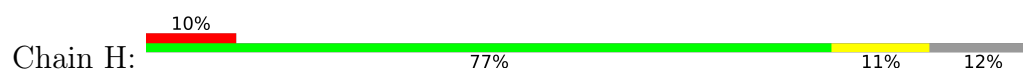
● Molecule 1: Estrogen receptor



● Molecule 1: Estrogen receptor



● Molecule 1: Estrogen receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.04Å 57.67Å 259.87Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	49.91 – 1.90 49.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.5 (49.91-1.90) 85.0 (49.91-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.285 , 0.327 0.285 , 0.325	Depositor DCC
R_{free} test set	5082 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11334	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 85.01 % 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 1.4204e-07. 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

5.1 Standard geometry

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

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	0.49	0/1853	0.73	1/2511 (0.0%)
1	B	0.44	0/1747	0.68	0/2361
1	E	0.43	0/1843	0.63	0/2498
1	F	0.41	0/1759	0.62	0/2374
1	G	0.52	0/1852	0.74	0/2510
1	H	0.51	0/1774	0.74	0/2396
All	All	0.47	0/10828	0.69	1/14650 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	465	THR	OG1-CB-CG2	5.88	121.07	109.30

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	1821	0	1795	26	0
1	B	1721	0	1744	25	0
1	E	1808	0	1791	30	0
1	F	1732	0	1764	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1817	0	1806	26	0
1	H	1748	0	1764	24	0
2	A	33	0	0	1	0
2	B	33	0	0	0	0
2	E	33	0	0	2	0
2	F	33	0	0	1	0
2	G	33	0	0	1	0
2	H	33	0	0	0	0
3	A	81	0	0	0	0
3	B	80	0	0	3	0
3	E	79	0	0	0	0
3	F	88	0	0	3	0
3	G	78	0	0	0	0
3	H	83	0	0	4	0
All	All	11334	0	10664	146	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 7.

All (146) 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:384:LEU:HD22	1:B:522:MET:HE3	1.48	0.92
1:G:415:GLY:HA2	1:G:421:MET:HE2	1.50	0.91
1:A:415:GLY:HA2	1:A:421:MET:HE2	1.55	0.87
1:E:372:LEU:HD23	1:G:372:LEU:HD23	1.58	0.84
1:G:358:ILE:HG13	1:G:543:MET:HE2	1.63	0.81
1:E:342:MET:HE3	1:E:410:LEU:HD13	1.64	0.79
1:G:424:ILE:HA	1:G:427:MET:HE3	1.70	0.74
1:E:415:GLY:HA2	1:E:421:MET:HE2	1.71	0.72
1:A:465:THR:HG23	1:A:468:SER:HB2	1.71	0.72
1:E:515:ARG:HH22	1:F:513:HIS:CE1	2.07	0.71
1:F:489:LEU:HD23	1:F:492:LYS:HE2	1.77	0.67
1:B:383:TRP:CZ2	1:B:522:MET:HE1	2.30	0.66
1:B:310:LEU:HD22	1:B:314:GLN:HB3	1.77	0.65
1:E:351:ASP:OD1	2:E:601:TWF:N2	2.30	0.64
1:H:384:LEU:HD23	1:H:522:MET:HG2	1.80	0.63
1:E:415:GLY:HA2	1:E:421:MET:CE	2.28	0.62
1:B:434:ARG:NH2	3:B:702:HOH:O	2.32	0.62
1:B:524:HIS:HB2	3:B:729:HOH:O	2.00	0.62
1:F:424:ILE:HD11	1:F:520:LYS:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:ILE:HD12	1:F:379:LEU:HD13	1.83	0.60
1:H:396:MET:HE3	1:H:435:PHE:C	2.26	0.60
1:A:342:MET:HE3	1:A:410:LEU:HD13	1.83	0.60
1:F:516:HIS:CE1	1:F:520:LYS:HE2	2.35	0.60
1:A:342:MET:HE3	1:A:410:LEU:CD1	2.32	0.60
1:G:310:LEU:HD22	1:G:314:GLN:HB3	1.84	0.59
1:H:516:HIS:CE1	1:H:520:LYS:HE2	2.37	0.59
1:E:424:ILE:HA	1:E:427:MET:HE3	1.83	0.59
1:B:456:SER:HA	1:B:515:ARG:NH2	2.18	0.58
1:E:392:VAL:HG11	1:E:431:THR:HG22	1.85	0.58
1:G:455:ASN:O	1:G:458:VAL:HG12	2.04	0.58
1:H:360:TRP:CH2	1:H:449:LYS:HG2	2.39	0.58
1:G:465:THR:HG23	1:G:468:SER:OG	2.05	0.57
1:F:456:SER:HA	1:F:515:ARG:NH2	2.19	0.57
1:G:515:ARG:HH12	1:H:513:HIS:CD2	2.22	0.57
1:F:520:LYS:O	1:F:523:GLU:HG2	2.04	0.57
1:F:341:SER:N	3:F:704:HOH:O	2.38	0.56
1:A:342:MET:CE	1:A:421:MET:HE1	2.36	0.56
1:H:373:HIS:NE2	3:H:702:HOH:O	2.33	0.56
1:A:342:MET:HE2	1:A:421:MET:HE1	1.88	0.56
1:B:434:ARG:NH1	1:B:438:MET:SD	2.79	0.56
1:G:379:LEU:HD12	1:G:544:LEU:HD11	1.87	0.56
1:A:465:THR:HG23	1:A:468:SER:CB	2.35	0.55
1:A:392:VAL:HG11	1:A:431:THR:HG22	1.87	0.55
1:E:473:ASP:OD1	1:E:477[B]:ARG:NE	2.41	0.54
1:B:516:HIS:CE1	1:B:520:LYS:HE2	2.43	0.54
1:A:455:ASN:O	1:A:458:VAL:HG12	2.09	0.53
1:G:392:VAL:HG11	1:G:431:THR:HG22	1.91	0.53
1:B:308:LEU:HD21	1:B:478:VAL:HG22	1.89	0.53
1:H:424:ILE:HD11	1:H:520:LYS:HD2	1.91	0.52
1:B:354:LEU:O	1:B:358:ILE:HG12	2.09	0.52
1:E:326:ILE:HD12	1:E:394:ARG:HD3	1.92	0.52
1:B:358:ILE:HD12	1:B:379:LEU:HD13	1.90	0.52
1:E:465:THR:HA	1:E:468:SER:OG	2.09	0.52
1:G:496:THR:OG1	1:G:499:GLN:HG3	2.10	0.52
1:B:376:VAL:HG11	1:B:537:TYR:CD2	2.44	0.51
1:B:384:LEU:CD2	1:B:522:MET:HE3	2.32	0.51
1:F:316:VAL:HG21	1:F:489:LEU:HD21	1.94	0.50
1:G:372:LEU:O	1:G:376:VAL:HG23	2.12	0.50
1:B:468:SER:O	1:B:472:LYS:HG3	2.11	0.50
1:A:434:ARG:HG2	1:A:510:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:MET:HE3	1:E:410:LEU:CD1	2.38	0.50
1:G:323:GLU:OE1	1:G:449:LYS:NZ	2.41	0.50
1:A:421:MET:HG3	2:A:601:TWF:C15	2.42	0.50
1:E:490:MET:HE2	1:E:503:ARG:HG2	1.94	0.50
1:A:315:MET:HE3	1:A:481:LYS:HG2	1.93	0.49
1:A:326:ILE:HD12	1:A:394:ARG:HD3	1.94	0.49
1:A:415:GLY:CA	1:A:421:MET:HE2	2.34	0.49
1:B:384:LEU:HD22	1:B:522:MET:CE	2.31	0.49
1:H:315:MET:HE1	1:H:365:PRO:HB2	1.93	0.49
1:F:363:ARG:NH2	3:F:701:HOH:O	2.32	0.49
1:G:358:ILE:HG13	1:G:543:MET:CE	2.38	0.49
1:G:421:MET:HG3	2:G:601:TWF:C15	2.43	0.49
1:E:379:LEU:HD12	1:E:544:LEU:HD11	1.93	0.49
1:E:434:ARG:HG2	1:E:510:ILE:HD11	1.95	0.49
1:B:522:MET:HA	1:B:522:MET:HE2	1.96	0.48
1:E:467:LYS:O	1:E:471:GLU:HG2	2.14	0.48
1:H:396:MET:HE3	1:H:435:PHE:HB3	1.94	0.48
1:H:376:VAL:HG11	1:H:537:TYR:CD2	2.48	0.48
1:A:372:LEU:O	1:A:376:VAL:HG23	2.13	0.47
1:H:451:ILE:HG13	1:H:482:ILE:HG21	1.96	0.47
1:B:330:GLU:HG3	3:B:774:HOH:O	2.13	0.47
1:F:539:LEU:HG	1:F:543:MET:HE3	1.95	0.47
1:F:427:MET:HB3	1:F:517:MET:SD	2.55	0.47
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.96	0.47
1:B:469:LEU:HD23	1:B:472:LYS:HE2	1.97	0.46
1:E:421:MET:HG3	2:E:601:TWF:C15	2.45	0.46
1:B:401:LYS:HB3	1:B:409:LEU:HD22	1.96	0.46
1:G:501:HIS:HD2	3:H:777:HOH:O	1.98	0.46
1:H:456:SER:HA	1:H:515:ARG:NH2	2.29	0.46
1:A:358:ILE:O	1:A:362:LYS:HG3	2.15	0.46
1:B:424:ILE:HD11	1:B:520:LYS:HB2	1.98	0.46
1:G:315:MET:SD	1:G:365:PRO:HG2	2.56	0.46
1:G:515:ARG:HH12	1:H:513:HIS:HD2	1.61	0.46
1:A:424:ILE:HA	1:A:427:MET:HE3	1.98	0.46
1:F:434:ARG:NH2	3:F:709:HOH:O	2.49	0.46
1:H:343:MET:HE3	1:H:347:THR:OG1	2.16	0.45
1:E:328:TYR:CE2	1:E:406:PRO:HB2	2.51	0.45
1:H:342:MET:HE2	1:H:421:MET:HE1	1.98	0.45
1:A:379:LEU:HD12	1:A:544:LEU:HD11	1.98	0.45
1:H:516:HIS:NE2	1:H:520:LYS:HE2	2.30	0.45
1:E:507:LEU:HD23	1:E:507:LEU:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LYS:O	1:A:471:GLU:HG2	2.17	0.44
1:E:372:LEU:O	1:E:376:VAL:HG23	2.17	0.44
1:E:448:LEU:HD21	1:E:507:LEU:HB3	2.00	0.44
1:A:497:LEU:HD11	1:B:497:LEU:HD11	2.00	0.44
1:E:316:VAL:HG21	1:E:489:LEU:HD21	1.99	0.44
1:G:465:THR:HG23	1:G:468:SER:CB	2.48	0.44
1:E:315:MET:HE3	1:E:481:LYS:HG2	2.01	0.43
1:H:412:ARG:HG2	1:H:412:ARG:HH11	1.84	0.43
1:F:390:GLY:O	1:F:394:ARG:HG3	2.19	0.43
1:H:522:MET:HE3	1:H:522:MET:HB3	1.86	0.43
1:H:373:HIS:CE1	3:H:702:HOH:O	2.68	0.43
1:F:351:ASP:OD1	2:F:601:TWF:N2	2.51	0.43
1:G:358:ILE:O	1:G:362:LYS:HG3	2.19	0.43
1:G:502:GLN:O	1:G:506:GLN:HG3	2.18	0.43
1:G:310:LEU:HA	1:G:314:GLN:OE1	2.18	0.42
1:G:506:GLN:O	1:G:510:ILE:HG12	2.18	0.42
1:F:434:ARG:NH1	1:F:438:MET:SD	2.91	0.42
1:H:315:MET:SD	1:H:365:PRO:HG2	2.59	0.42
1:H:530:SER:HB3	1:H:533:VAL:HG21	2.01	0.42
1:B:424:ILE:HD13	1:B:427:MET:HE3	2.00	0.42
1:E:515:ARG:HH12	1:F:513:HIS:HD1	1.68	0.42
1:H:413:ASN:ND2	3:H:701:HOH:O	2.24	0.42
1:H:427:MET:HE1	1:H:520:LYS:HE3	2.02	0.42
1:E:358:ILE:O	1:E:362:LYS:HG3	2.20	0.42
1:G:408:LEU:HA	1:G:408:LEU:HD12	1.76	0.42
1:B:308:LEU:HA	1:B:481:LYS:HE3	2.02	0.41
1:F:396:MET:HE3	1:F:436:ARG:HA	2.02	0.41
1:A:376:VAL:HG22	1:A:544:LEU:HD12	2.01	0.41
1:A:510:ILE:HD13	1:A:510:ILE:HA	1.83	0.41
1:B:315:MET:SD	1:B:365:PRO:HG2	2.61	0.41
1:B:427:MET:HB3	1:B:517:MET:SD	2.60	0.41
1:E:434:ARG:HG2	1:E:510:ILE:CD1	2.51	0.41
1:E:509:LEU:HD23	1:E:509:LEU:HA	1.87	0.41
1:E:522:MET:HE3	1:E:526:TYR:CE2	2.56	0.41
1:F:448:LEU:HD11	1:F:507:LEU:HD22	2.02	0.41
1:G:547:HIS:CE1	1:G:549:LEU:HB2	2.56	0.41
1:A:315:MET:SD	1:A:365:PRO:HG2	2.60	0.41
1:A:411:ASP:OD1	1:A:411:ASP:C	2.63	0.41
1:E:408:LEU:HD12	1:E:408:LEU:HA	1.86	0.41
1:F:308:LEU:O	1:F:481:LYS:HE2	2.20	0.41
1:H:360:TRP:CZ2	1:H:449:LYS:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:GLU:H	1:E:443:GLU:CD	2.28	0.41
1:F:376:VAL:HG11	1:F:537:TYR:CD2	2.56	0.40
1:G:515:ARG:HE	1:G:515:ARG:HB2	1.76	0.40
1:A:396:MET:O	1:A:436:ARG:HD3	2.22	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	231/255 (91%)	227 (98%)	4 (2%)	0	100	100
1	B	211/255 (83%)	207 (98%)	4 (2%)	0	100	100
1	E	230/255 (90%)	227 (99%)	3 (1%)	0	100	100
1	F	210/255 (82%)	206 (98%)	4 (2%)	0	100	100
1	G	230/255 (90%)	227 (99%)	3 (1%)	0	100	100
1	H	215/255 (84%)	211 (98%)	4 (2%)	0	100	100
All	All	1327/1530 (87%)	1305 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/230 (86%)	197 (100%)	0	100	100
1	B	185/230 (80%)	185 (100%)	0	100	100
1	E	194/230 (84%)	194 (100%)	0	100	100
1	F	188/230 (82%)	188 (100%)	0	100	100
1	G	197/230 (86%)	197 (100%)	0	100	100
1	H	188/230 (82%)	188 (100%)	0	100	100
All	All	1149/1380 (83%)	1149 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	A	498	GLN
1	A	501	HIS
1	B	476	HIS
1	F	375	GLN
1	F	455	ASN
1	G	356	HIS
1	G	455	ASN
1	G	501	HIS
1	H	375	GLN
1	H	455	ASN
1	H	513	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

6 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	TWF	E	601	-	36,37,37	5.34	24 (66%)	42,53,53	2.08	18 (42%)
2	TWF	H	601	-	36,37,37	5.51	26 (72%)	42,53,53	2.14	18 (42%)
2	TWF	B	601	-	36,37,37	5.49	23 (63%)	42,53,53	1.88	13 (30%)
2	TWF	G	601	-	36,37,37	5.36	27 (75%)	42,53,53	2.13	18 (42%)
2	TWF	A	601	-	36,37,37	5.40	28 (77%)	42,53,53	1.81	11 (26%)
2	TWF	F	601	-	36,37,37	5.60	26 (72%)	42,53,53	1.80	12 (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
2	TWF	E	601	-	-	6/18/41/41	0/5/5/5
2	TWF	H	601	-	-	5/18/41/41	0/5/5/5
2	TWF	B	601	-	-	6/18/41/41	0/5/5/5
2	TWF	G	601	-	-	5/18/41/41	0/5/5/5
2	TWF	A	601	-	-	7/18/41/41	0/5/5/5
2	TWF	F	601	-	-	6/18/41/41	0/5/5/5

All (154) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	TWF	C21-C20	11.67	1.57	1.38
2	F	601	TWF	C1-C6	11.13	1.53	1.39
2	G	601	TWF	C1-C6	10.95	1.53	1.39
2	H	601	TWF	C24-C19	10.85	1.56	1.39
2	G	601	TWF	C24-C19	10.83	1.56	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TWF	C1-C6	10.81	1.52	1.39
2	H	601	TWF	C1-C6	10.72	1.52	1.39
2	F	601	TWF	C24-C19	10.64	1.55	1.39
2	B	601	TWF	C16-C11	10.59	1.55	1.39
2	F	601	TWF	C16-C11	10.50	1.55	1.39
2	H	601	TWF	C16-C11	10.40	1.55	1.39
2	F	601	TWF	C21-C20	10.38	1.55	1.38
2	B	601	TWF	C24-C19	10.32	1.55	1.39
2	E	601	TWF	C1-C6	10.12	1.52	1.39
2	A	601	TWF	C24-C19	10.09	1.55	1.39
2	B	601	TWF	C13-C12	10.01	1.56	1.38
2	A	601	TWF	C21-C20	9.96	1.54	1.38
2	A	601	TWF	C16-C11	9.91	1.54	1.39
2	E	601	TWF	C16-C11	9.80	1.54	1.39
2	H	601	TWF	C13-C12	9.59	1.55	1.38
2	F	601	TWF	C10-N1	9.57	1.57	1.36
2	F	601	TWF	C13-C12	9.55	1.55	1.38
2	B	601	TWF	C21-C20	9.46	1.54	1.38
2	B	601	TWF	C10-N1	9.46	1.57	1.36
2	G	601	TWF	C16-C11	9.45	1.53	1.39
2	B	601	TWF	C4-C5	9.41	1.54	1.39
2	H	601	TWF	C10-N1	9.40	1.57	1.36
2	H	601	TWF	C21-C20	9.38	1.54	1.38
2	E	601	TWF	C24-C19	9.27	1.53	1.39
2	F	601	TWF	C4-C5	9.18	1.53	1.39
2	H	601	TWF	C4-C5	9.17	1.53	1.39
2	G	601	TWF	C13-C12	9.02	1.54	1.38
2	G	601	TWF	C10-N1	8.99	1.56	1.36
2	E	601	TWF	C13-C12	8.97	1.54	1.38
2	A	601	TWF	C1-C6	8.91	1.50	1.39
2	G	601	TWF	C21-C20	8.83	1.53	1.38
2	E	601	TWF	C10-N1	8.44	1.54	1.36
2	G	601	TWF	C23-C22	8.29	1.54	1.38
2	A	601	TWF	C12-C11	-8.21	1.27	1.39
2	A	601	TWF	C23-C22	8.12	1.53	1.38
2	H	601	TWF	C23-C22	8.09	1.53	1.38
2	B	601	TWF	C23-C22	8.05	1.53	1.38
2	F	601	TWF	C2-C3	7.99	1.54	1.39
2	E	601	TWF	C4-C5	7.97	1.52	1.39
2	F	601	TWF	C23-C22	7.96	1.53	1.38
2	H	601	TWF	C2-C3	7.85	1.53	1.39
2	B	601	TWF	C2-C3	7.80	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TWF	C10-N1	7.78	1.53	1.36
2	A	601	TWF	C4-C5	7.75	1.51	1.39
2	G	601	TWF	C2-C3	7.74	1.53	1.39
2	G	601	TWF	C4-C5	7.69	1.51	1.39
2	A	601	TWF	C13-C12	7.66	1.52	1.38
2	E	601	TWF	C2-C3	7.65	1.53	1.39
2	E	601	TWF	C23-C22	7.12	1.52	1.38
2	F	601	TWF	C12-C11	-7.00	1.28	1.39
2	G	601	TWF	C12-C11	-6.92	1.28	1.39
2	H	601	TWF	C12-C11	-6.82	1.29	1.39
2	A	601	TWF	C2-C3	6.76	1.51	1.39
2	B	601	TWF	C14-C15	6.68	1.52	1.38
2	E	601	TWF	C12-C11	-6.52	1.29	1.39
2	B	601	TWF	C12-C11	-6.33	1.29	1.39
2	E	601	TWF	C14-C15	6.31	1.52	1.38
2	H	601	TWF	C14-C15	6.15	1.51	1.38
2	G	601	TWF	C14-C15	6.15	1.51	1.38
2	F	601	TWF	C14-C15	6.02	1.51	1.38
2	A	601	TWF	C4-C3	-5.60	1.30	1.39
2	A	601	TWF	C15-C16	-5.28	1.29	1.38
2	A	601	TWF	C8-N1	-5.27	1.43	1.51
2	A	601	TWF	C5-C6	-5.12	1.31	1.40
2	A	601	TWF	C2-C1	-4.91	1.30	1.38
2	A	601	TWF	C11-C10	4.74	1.58	1.50
2	F	601	TWF	C7-C5	4.73	1.59	1.50
2	F	601	TWF	C11-C10	4.68	1.57	1.50
2	E	601	TWF	C8-N1	-4.61	1.44	1.51
2	B	601	TWF	C11-C10	4.59	1.57	1.50
2	A	601	TWF	C20-C19	-4.47	1.32	1.39
2	E	601	TWF	C7-C5	4.46	1.59	1.50
2	G	601	TWF	C4-C3	-4.44	1.32	1.39
2	H	601	TWF	C5-C6	-4.43	1.32	1.40
2	B	601	TWF	C18-C8	4.43	1.57	1.50
2	F	601	TWF	C18-C8	4.41	1.57	1.50
2	H	601	TWF	C11-C10	4.38	1.57	1.50
2	A	601	TWF	C14-C15	4.37	1.47	1.38
2	H	601	TWF	C18-C8	4.35	1.57	1.50
2	F	601	TWF	C5-C6	-4.32	1.32	1.40
2	A	601	TWF	O2-C10	-4.30	1.13	1.22
2	B	601	TWF	C5-C6	-4.25	1.33	1.40
2	E	601	TWF	C23-C24	-4.25	1.31	1.38
2	A	601	TWF	C14-C13	-4.25	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	TWF	C7-C5	4.22	1.58	1.50
2	E	601	TWF	C4-C3	-4.21	1.32	1.39
2	E	601	TWF	C5-C6	-4.20	1.33	1.40
2	H	601	TWF	C7-C5	4.19	1.58	1.50
2	E	601	TWF	C11-C10	4.18	1.57	1.50
2	F	601	TWF	C2-C1	-4.17	1.32	1.38
2	G	601	TWF	C15-C16	-4.09	1.31	1.38
2	B	601	TWF	C7-C5	4.08	1.58	1.50
2	G	601	TWF	C11-C10	4.05	1.56	1.50
2	F	601	TWF	C15-C16	-3.92	1.32	1.38
2	E	601	TWF	C17-C8	3.91	1.56	1.50
2	E	601	TWF	C15-C16	-3.83	1.32	1.38
2	H	601	TWF	C15-C16	-3.81	1.32	1.38
2	H	601	TWF	C2-C1	-3.80	1.32	1.38
2	H	601	TWF	C17-C8	3.79	1.56	1.50
2	G	601	TWF	C17-C8	3.75	1.56	1.50
2	A	601	TWF	C23-C24	-3.69	1.32	1.38
2	G	601	TWF	C5-C6	-3.69	1.33	1.40
2	B	601	TWF	C4-C3	-3.68	1.33	1.39
2	E	601	TWF	C18-C8	3.67	1.56	1.50
2	B	601	TWF	C15-C16	-3.62	1.32	1.38
2	F	601	TWF	C17-C8	3.62	1.55	1.50
2	G	601	TWF	C8-N1	-3.58	1.45	1.51
2	B	601	TWF	C2-C1	-3.54	1.33	1.38
2	A	601	TWF	C21-C22	-3.53	1.32	1.38
2	A	601	TWF	C18-C8	3.52	1.55	1.50
2	B	601	TWF	C17-C8	3.48	1.55	1.50
2	B	601	TWF	C8-N1	-3.42	1.46	1.51
2	H	601	TWF	C8-N1	-3.39	1.46	1.51
2	E	601	TWF	C2-C1	-3.33	1.33	1.38
2	H	601	TWF	C20-C19	-3.27	1.34	1.39
2	G	601	TWF	C20-C19	-3.24	1.34	1.39
2	H	601	TWF	C4-C3	-3.23	1.34	1.39
2	F	601	TWF	C4-C3	-3.22	1.34	1.39
2	F	601	TWF	C8-N1	-3.15	1.46	1.51
2	G	601	TWF	C18-C8	3.10	1.55	1.50
2	G	601	TWF	O3-C22	3.05	1.44	1.37
2	G	601	TWF	C2-C1	-3.03	1.33	1.38
2	F	601	TWF	C23-C24	-3.01	1.33	1.38
2	G	601	TWF	C19-C9	-2.98	1.48	1.52
2	G	601	TWF	C14-C13	-2.97	1.31	1.38
2	A	601	TWF	C7-C5	2.94	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	TWF	C14-C13	-2.89	1.31	1.38
2	B	601	TWF	C20-C19	-2.80	1.34	1.39
2	H	601	TWF	C23-C24	-2.80	1.34	1.38
2	F	601	TWF	C20-C19	-2.72	1.34	1.39
2	B	601	TWF	C14-C13	-2.66	1.32	1.38
2	H	601	TWF	C14-C13	-2.66	1.32	1.38
2	A	601	TWF	C19-C9	-2.62	1.48	1.52
2	A	601	TWF	C6-C9	-2.52	1.49	1.51
2	G	601	TWF	C23-C24	-2.49	1.34	1.38
2	F	601	TWF	C14-C13	-2.46	1.32	1.38
2	G	601	TWF	C21-C22	-2.44	1.34	1.38
2	B	601	TWF	C23-C24	-2.40	1.34	1.38
2	E	601	TWF	O3-C22	2.39	1.43	1.37
2	G	601	TWF	C6-C9	-2.39	1.49	1.51
2	H	601	TWF	O1-C3	2.34	1.42	1.37
2	H	601	TWF	C6-C9	-2.31	1.49	1.51
2	F	601	TWF	C21-C22	-2.26	1.34	1.38
2	F	601	TWF	C6-C9	-2.24	1.49	1.51
2	A	601	TWF	C17-C8	2.18	1.53	1.50
2	A	601	TWF	O3-C22	2.17	1.42	1.37
2	H	601	TWF	C21-C22	-2.13	1.34	1.38
2	E	601	TWF	O2-C10	-2.08	1.18	1.22
2	F	601	TWF	O1-C3	2.05	1.41	1.37

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	TWF	C7-C5-C4	-5.37	109.79	121.18
2	B	601	TWF	C7-C5-C4	-4.82	110.96	121.18
2	H	601	TWF	C7-C5-C4	-4.60	111.42	121.18
2	A	601	TWF	C7-C5-C4	-4.55	111.54	121.18
2	F	601	TWF	C7-C5-C4	-4.33	112.01	121.18
2	G	601	TWF	C7-C5-C6	4.29	127.08	120.67
2	E	601	TWF	C7-C5-C4	-4.12	112.44	121.18
2	A	601	TWF	C18-C17-C8	4.10	62.48	59.67
2	H	601	TWF	C21-C20-C19	-3.92	117.27	121.18
2	E	601	TWF	C24-C19-C9	-3.88	112.58	120.67
2	H	601	TWF	C3-C4-C5	-3.87	116.42	120.77
2	E	601	TWF	C15-C16-C11	-3.83	116.60	120.36
2	G	601	TWF	C24-C19-C20	3.69	122.88	118.30
2	E	601	TWF	C21-C20-C19	-3.67	117.52	121.18
2	A	601	TWF	O2-C10-N1	-3.50	116.82	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	TWF	C21-C20-C19	-3.43	117.76	121.18
2	H	601	TWF	C25-O3-C22	-3.40	109.09	117.93
2	H	601	TWF	C26-N2-C27	-3.40	106.19	113.43
2	F	601	TWF	C3-C4-C5	-3.39	116.97	120.77
2	B	601	TWF	C18-C17-C8	3.36	61.97	59.67
2	B	601	TWF	C25-O3-C22	-3.35	109.23	117.93
2	F	601	TWF	C7-C5-C6	3.32	125.64	120.67
2	B	601	TWF	C4-C5-C6	3.32	123.67	119.49
2	H	601	TWF	C24-C19-C20	3.28	122.38	118.30
2	E	601	TWF	C3-C4-C5	-3.25	117.12	120.77
2	F	601	TWF	C18-C17-C8	3.18	61.85	59.67
2	F	601	TWF	C25-O3-C22	-3.17	109.69	117.93
2	B	601	TWF	C7-C5-C6	3.14	125.37	120.67
2	G	601	TWF	C15-C16-C11	-3.13	117.28	120.36
2	H	601	TWF	C7-C5-C6	3.11	125.32	120.67
2	E	601	TWF	C12-C11-C10	-3.02	112.53	120.28
2	A	601	TWF	C7-C5-C6	3.01	125.18	120.67
2	A	601	TWF	C4-C5-C6	3.00	123.27	119.49
2	B	601	TWF	O2-C10-N1	-2.99	117.55	121.84
2	H	601	TWF	C4-C5-C6	2.99	123.25	119.49
2	E	601	TWF	O2-C10-N1	-2.97	117.59	121.84
2	G	601	TWF	C25-O3-C22	-2.92	110.34	117.93
2	H	601	TWF	C18-C17-C8	2.91	61.66	59.67
2	G	601	TWF	C4-C5-C6	2.89	123.13	119.49
2	B	601	TWF	C3-C4-C5	-2.87	117.54	120.77
2	H	601	TWF	C16-C11-C10	-2.86	112.94	120.28
2	H	601	TWF	C16-C11-C12	2.86	122.20	118.57
2	B	601	TWF	C15-C16-C11	-2.85	117.56	120.36
2	G	601	TWF	C23-C24-C19	-2.82	118.37	121.18
2	G	601	TWF	C12-C11-C10	-2.74	113.26	120.28
2	B	601	TWF	C19-C9-N1	2.73	115.82	112.60
2	E	601	TWF	C7-C5-C6	2.72	124.74	120.67
2	G	601	TWF	C11-C10-N1	2.68	122.76	117.83
2	G	601	TWF	C20-C19-C9	-2.66	115.12	120.67
2	G	601	TWF	O2-C10-N1	-2.64	118.05	121.84
2	E	601	TWF	C4-C5-C6	2.64	122.82	119.49
2	H	601	TWF	C24-C23-C22	-2.64	116.72	119.73
2	E	601	TWF	C20-C19-C9	2.63	126.16	120.67
2	F	601	TWF	C21-C20-C19	-2.59	118.59	121.18
2	A	601	TWF	C12-C11-C10	-2.59	113.64	120.28
2	E	601	TWF	C16-C11-C12	2.56	121.83	118.57
2	E	601	TWF	C17-C18-C8	2.56	61.43	59.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	TWF	C16-C11-C12	2.54	121.79	118.57
2	H	601	TWF	C1-C2-C3	2.53	122.56	119.88
2	E	601	TWF	C14-C13-C12	-2.50	117.15	120.24
2	F	601	TWF	C26-N2-C27	-2.49	108.14	113.43
2	E	601	TWF	C25-C26-N2	-2.46	105.45	111.43
2	G	601	TWF	C17-C18-C8	2.46	61.36	59.67
2	B	601	TWF	C1-C2-C3	2.40	122.42	119.88
2	A	601	TWF	C16-C11-C10	2.38	126.38	120.28
2	G	601	TWF	C3-C4-C5	-2.37	118.10	120.77
2	F	601	TWF	O2-C10-N1	-2.35	118.46	121.84
2	H	601	TWF	C13-C12-C11	-2.35	118.05	120.36
2	E	601	TWF	C11-C10-N1	2.33	122.12	117.83
2	F	601	TWF	C16-C11-C12	2.31	121.51	118.57
2	E	601	TWF	C24-C19-C20	2.30	121.16	118.30
2	A	601	TWF	C11-C10-N1	2.30	122.06	117.83
2	F	601	TWF	C4-C5-C6	2.25	122.32	119.49
2	F	601	TWF	C11-C10-N1	2.23	121.94	117.83
2	B	601	TWF	C14-C13-C12	-2.22	117.49	120.24
2	H	601	TWF	O2-C10-N1	-2.20	118.68	121.84
2	A	601	TWF	C15-C16-C11	-2.19	118.21	120.36
2	G	601	TWF	C14-C13-C12	-2.19	117.54	120.24
2	E	601	TWF	C18-C17-C8	2.16	61.16	59.67
2	H	601	TWF	C1-C6-C9	-2.16	115.94	121.22
2	A	601	TWF	C1-C2-C3	2.12	122.12	119.88
2	H	601	TWF	C23-C22-C21	2.09	123.21	120.16
2	G	601	TWF	C19-C9-N1	-2.08	110.15	112.60
2	F	601	TWF	C1-C6-C9	-2.05	116.19	121.22
2	E	601	TWF	C16-C11-C10	2.05	125.54	120.28
2	B	601	TWF	C26-N2-C27	-2.05	109.07	113.43
2	G	601	TWF	C26-N2-C27	-2.04	109.09	113.43
2	A	601	TWF	C23-C24-C19	-2.04	119.15	121.18
2	H	601	TWF	C2-C1-C6	-2.02	117.77	121.12
2	B	601	TWF	C11-C10-N1	2.02	121.55	117.83

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TWF	C11-C10-N1-C8
2	A	601	TWF	O2-C10-N1-C8
2	B	601	TWF	C11-C10-N1-C8
2	B	601	TWF	O2-C10-N1-C8

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Mol	Chain	Res	Type	Atoms
2	E	601	TWF	C11-C10-N1-C8
2	E	601	TWF	O2-C10-N1-C8
2	E	601	TWF	C25-C26-N2-C27
2	F	601	TWF	C11-C10-N1-C8
2	F	601	TWF	O2-C10-N1-C8
2	G	601	TWF	C11-C10-N1-C8
2	G	601	TWF	O2-C10-N1-C8
2	H	601	TWF	C11-C10-N1-C8
2	H	601	TWF	O2-C10-N1-C8
2	A	601	TWF	O3-C25-C26-N2
2	E	601	TWF	O3-C25-C26-N2
2	G	601	TWF	C25-C26-N2-C27
2	H	601	TWF	O3-C25-C26-N2
2	H	601	TWF	C21-C22-O3-C25
2	F	601	TWF	C21-C22-O3-C25
2	B	601	TWF	C23-C22-O3-C25
2	A	601	TWF	C23-C22-O3-C25
2	A	601	TWF	C21-C22-O3-C25
2	F	601	TWF	C23-C22-O3-C25
2	H	601	TWF	C23-C22-O3-C25
2	B	601	TWF	C21-C22-O3-C25
2	E	601	TWF	C28-C27-N2-C26
2	E	601	TWF	C26-C25-O3-C22
2	A	601	TWF	C25-C26-N2-C27
2	G	601	TWF	C21-C22-O3-C25
2	F	601	TWF	O3-C25-C26-N2
2	G	601	TWF	C23-C22-O3-C25
2	A	601	TWF	C26-C25-O3-C22
2	B	601	TWF	O3-C25-C26-N2
2	B	601	TWF	C25-C26-N2-C27
2	F	601	TWF	C25-C26-N2-C27

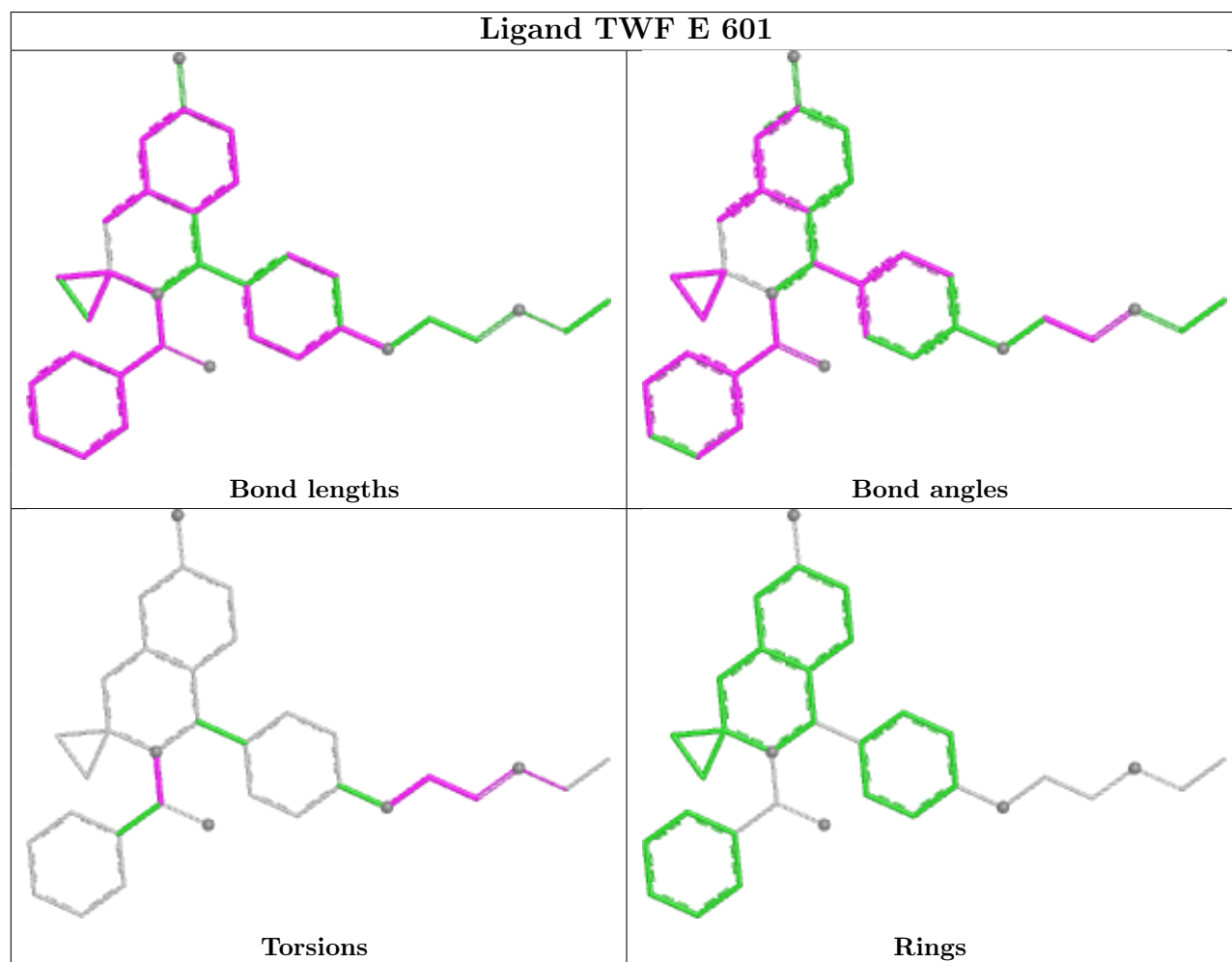
There are no ring outliers.

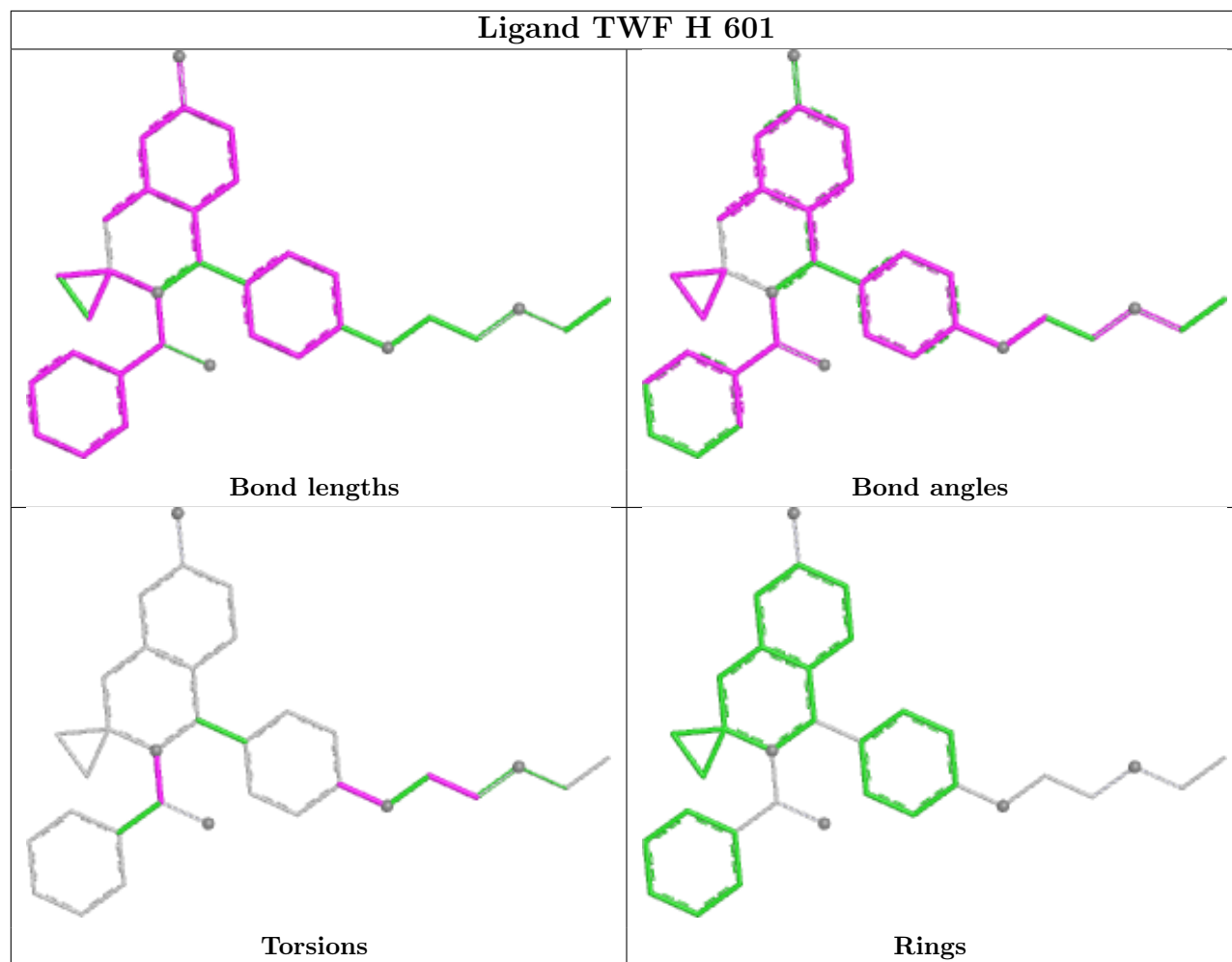
4 monomers are involved in 5 short contacts:

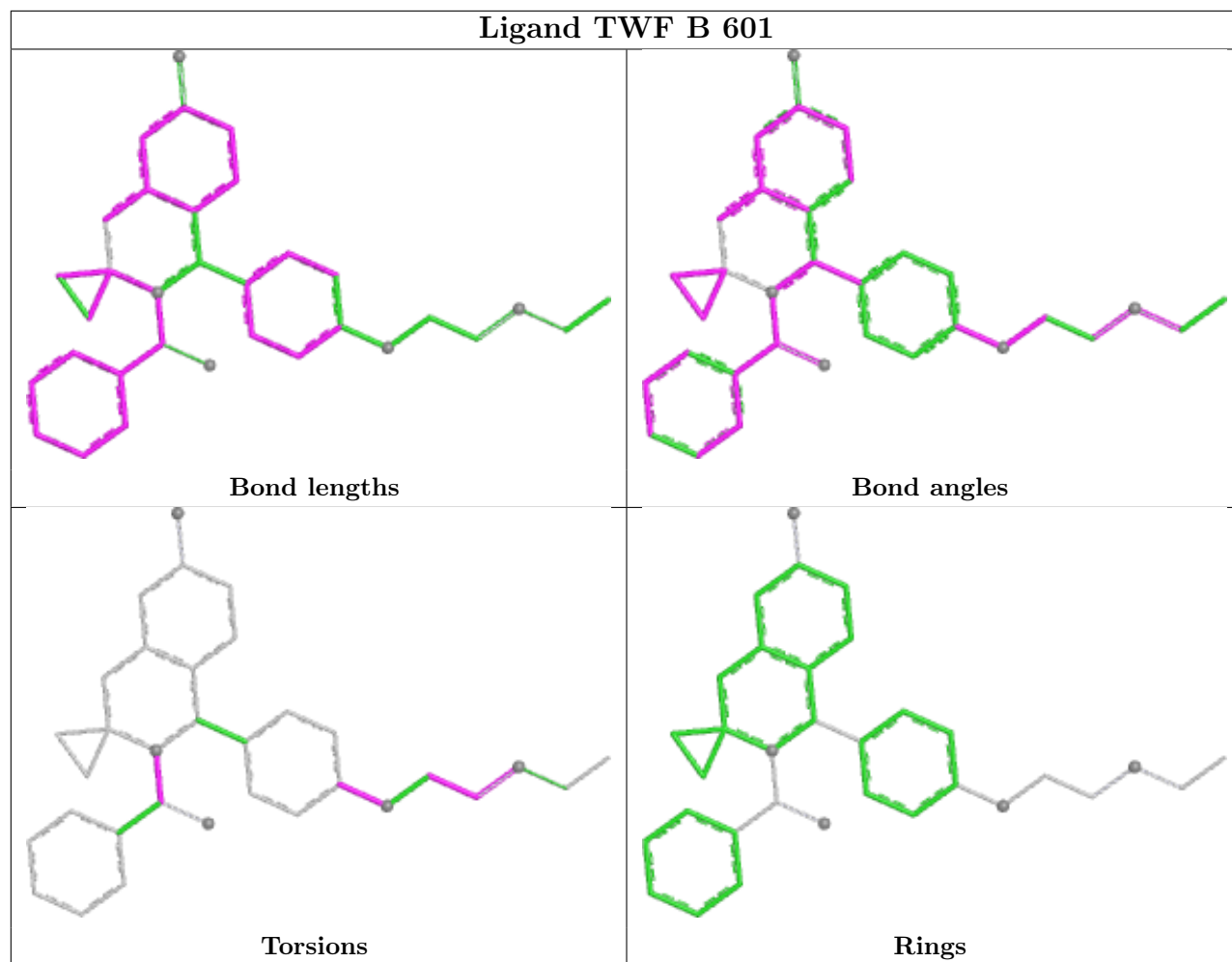
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	TWF	2	0
2	G	601	TWF	1	0
2	A	601	TWF	1	0
2	F	601	TWF	1	0

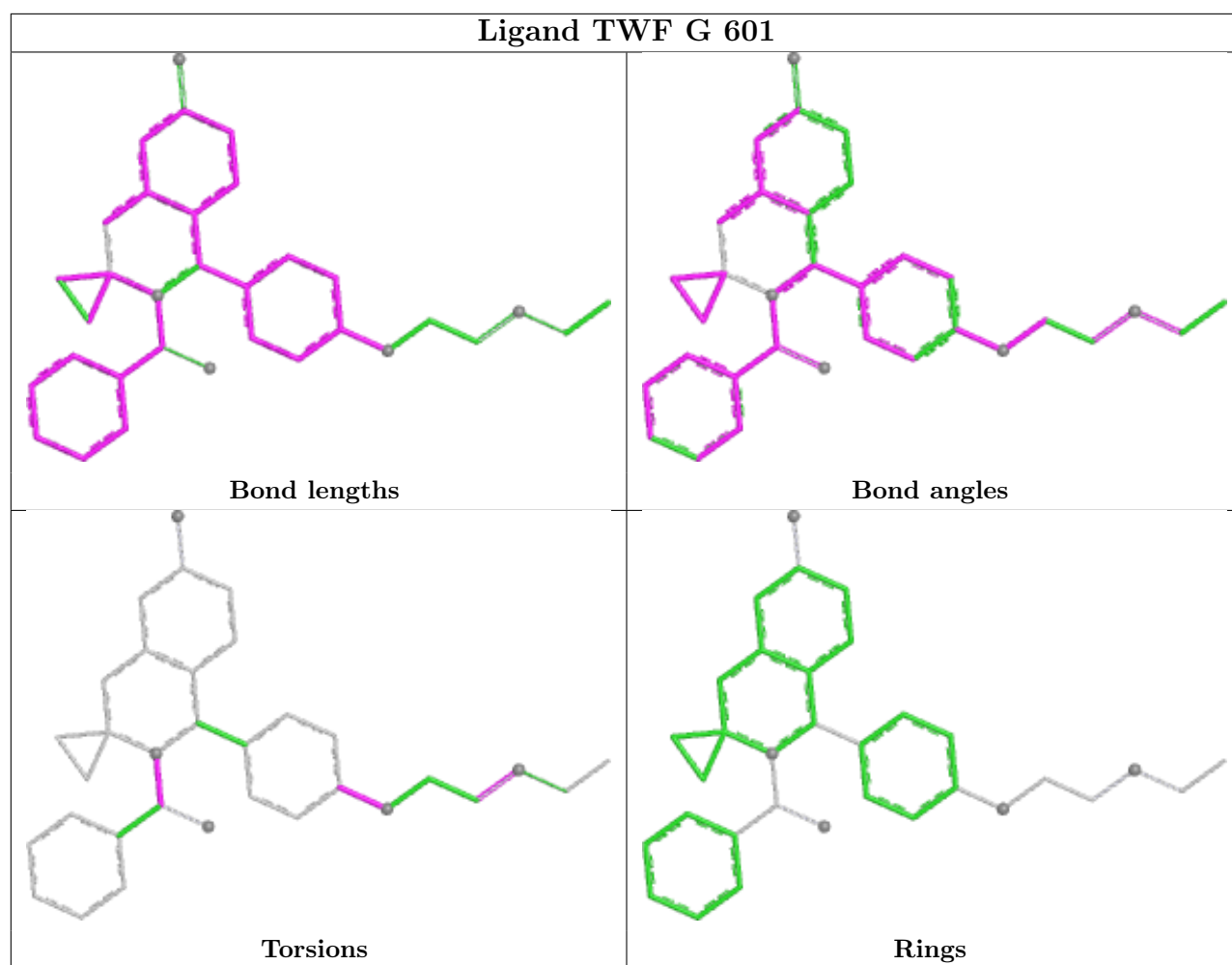
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

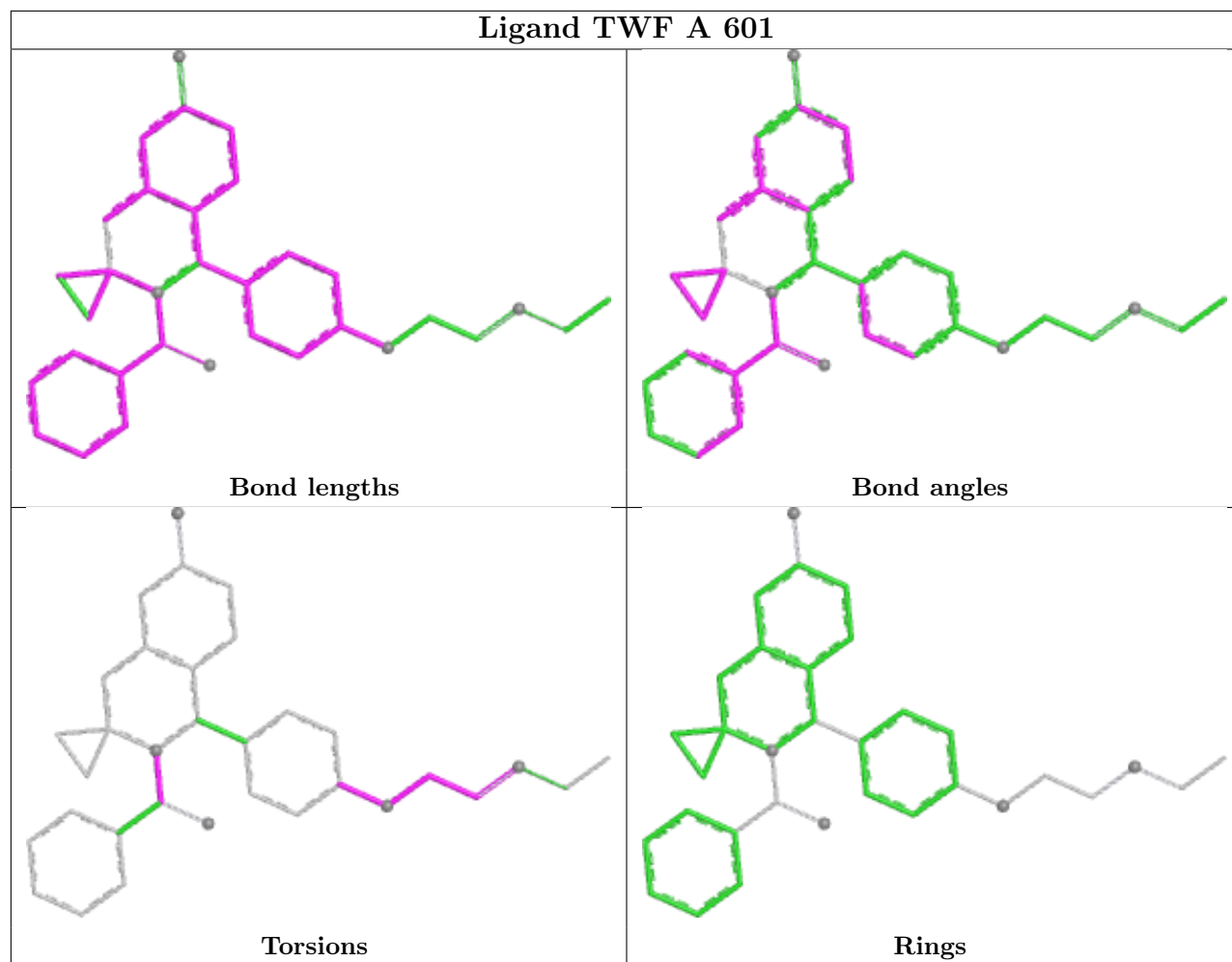
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

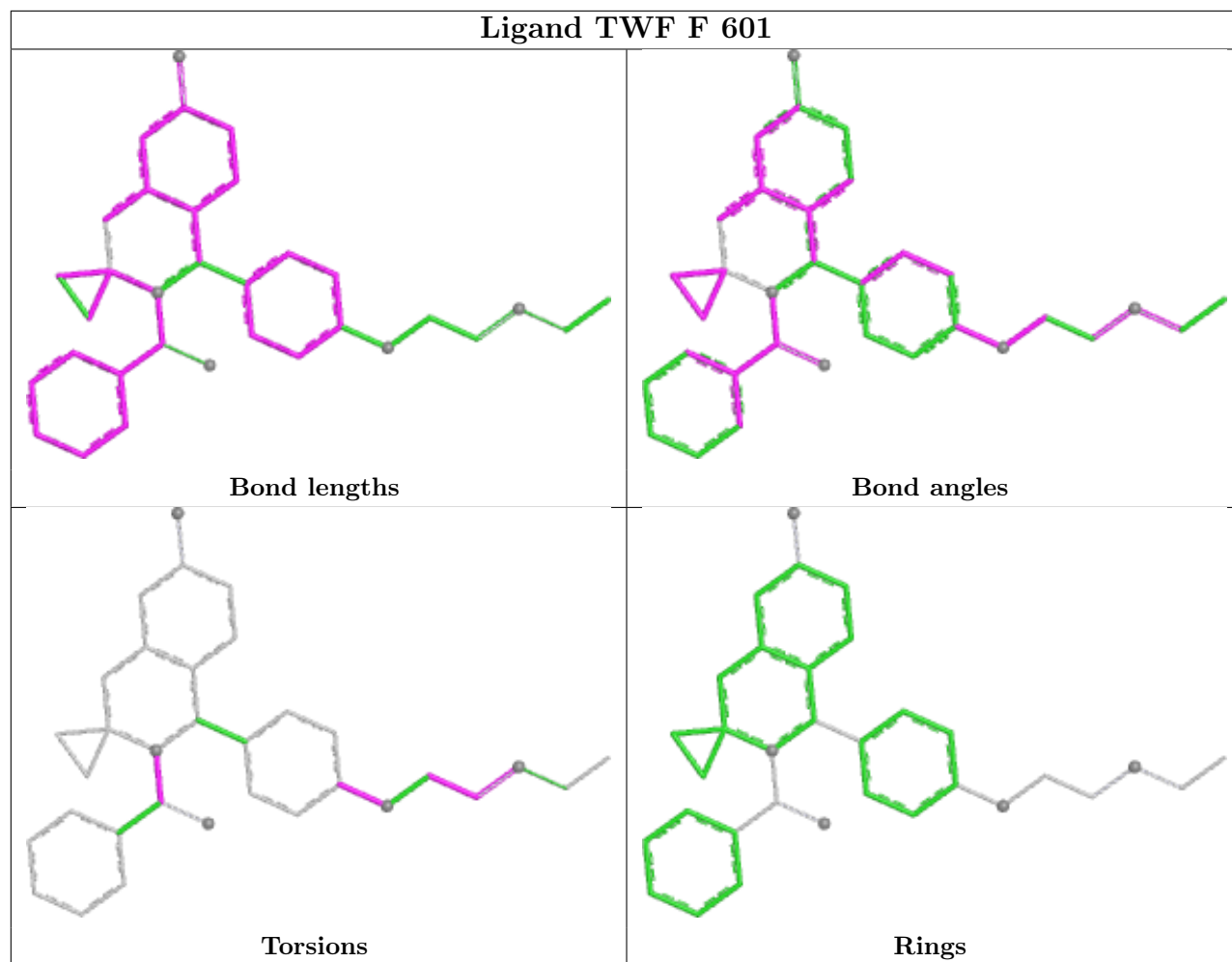












5.7 Other polymers [i](#)

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	235/255 (92%)	1.65	67 (28%) 1 1	11, 28, 47, 61	3 (1%)
1	B	221/255 (86%)	1.30	45 (20%) 3 2	20, 25, 39, 51	0
1	E	232/255 (90%)	1.55	60 (25%) 1 1	10, 25, 45, 56	5 (2%)
1	F	220/255 (86%)	1.54	59 (26%) 1 1	19, 27, 42, 52	1 (0%)
1	G	234/255 (91%)	0.67	22 (9%) 14 14	7, 17, 42, 52	2 (0%)
1	H	224/255 (87%)	0.79	25 (11%) 10 10	9, 19, 43, 61	2 (0%)
All	All	1366/1530 (89%)	1.25	278 (20%) 3 2	7, 25, 43, 61	13 (0%)

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	THR	6.6
1	F	341	SER	6.5
1	E	418	VAL	6.5
1	A	537	TYR	6.2
1	A	533	VAL	5.8
1	B	523	GLU	5.8
1	B	459	TYR	5.3
1	A	310	LEU	5.2
1	F	414	GLN	5.2
1	A	331	TYR	5.2
1	F	459	TYR	5.2
1	E	310	LEU	5.1
1	H	308	LEU	5.0
1	E	465	THR	5.0
1	H	460	THR	5.0
1	H	415	GLY	4.9
1	B	342	MET	4.7
1	E	544	LEU	4.5
1	A	465	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	530	SER	4.5
1	F	312	ALA	4.5
1	H	342	MET	4.3
1	B	414	GLN	4.2
1	E	331	TYR	4.2
1	B	344	GLY	4.2
1	A	460	THR	4.2
1	G	465	THR	4.2
1	E	309	SER	4.2
1	A	359	ASN	4.1
1	F	437	MET	4.1
1	G	418	VAL	4.1
1	F	526	TYR	4.1
1	B	547	HIS	4.0
1	H	416	LYS	4.0
1	E	534	VAL	4.0
1	A	526	TYR	4.0
1	H	459	TYR	3.9
1	E	460	THR	3.9
1	E	419	GLU	3.9
1	F	529	LYS	3.9
1	E	548	ARG	3.8
1	B	330	GLU	3.8
1	A	479	LEU	3.8
1	G	549	LEU	3.8
1	G	534	VAL	3.8
1	A	512	SER	3.8
1	A	437	MET	3.8
1	A	528	MET	3.7
1	A	326	ILE	3.7
1	G	308	LEU	3.7
1	F	525	LEU	3.6
1	E	537	TYR	3.6
1	A	309	SER	3.6
1	B	421	MET	3.6
1	A	308	LEU	3.6
1	F	320	LEU	3.6
1	A	340	ALA	3.6
1	A	541	LEU	3.6
1	H	307	ALA	3.5
1	F	342	MET	3.5
1	G	528	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	439	ASN	3.5
1	H	497	LEU	3.5
1	F	413	ASN	3.4
1	E	528	MET	3.4
1	A	419	GLU	3.3
1	A	418	VAL	3.3
1	E	319	LEU	3.3
1	F	343	MET	3.3
1	E	313	ASP	3.3
1	G	417	SER	3.3
1	B	307	ALA	3.3
1	G	416	LYS	3.3
1	B	413	ASN	3.3
1	G	359	ASN	3.3
1	A	542	GLU	3.2
1	E	459	TYR	3.2
1	H	420	GLY	3.2
1	B	522	MET	3.2
1	A	534	VAL	3.2
1	A	527	SER	3.2
1	H	414	GLN	3.2
1	B	466	LEU	3.1
1	G	415	GLY	3.1
1	E	538	ASP	3.1
1	F	420	GLY	3.1
1	G	459	TYR	3.1
1	G	537	TYR	3.1
1	F	319	LEU	3.1
1	F	472	LYS	3.1
1	E	417	SER	3.1
1	F	306	LEU	3.1
1	A	413	ASN	3.1
1	A	333	PRO	3.1
1	B	424	ILE	3.0
1	H	421	MET	3.0
1	E	547	HIS	3.0
1	A	477	ARG	3.0
1	E	343	MET	3.0
1	F	458	VAL	3.0
1	B	473	ASP	3.0
1	E	430	ALA	3.0
1	F	391	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	458	VAL	3.0
1	F	465	THR	3.0
1	E	457	GLY	3.0
1	A	466	LEU	2.9
1	H	306	LEU	2.9
1	F	310	LEU	2.9
1	H	345	LEU	2.9
1	B	341	SER	2.9
1	B	476	HIS	2.9
1	A	314	GLN	2.9
1	B	475	ILE	2.9
1	B	469	LEU	2.9
1	B	465	THR	2.9
1	E	451	ILE	2.9
1	E	452	ILE	2.9
1	F	422	VAL	2.8
1	A	459	TYR	2.8
1	A	535	PRO	2.8
1	E	545	ASP	2.8
1	A	468	SER	2.8
1	B	343	MET	2.8
1	B	501	HIS	2.8
1	A	339	GLU	2.8
1	A	417	SER	2.8
1	E	432	SER	2.8
1	E	400	GLY	2.8
1	A	311	THR	2.8
1	B	533	VAL	2.8
1	G	419	GLU	2.7
1	E	334	THR	2.7
1	F	469	LEU	2.7
1	G	539	LEU	2.7
1	E	332	ASP	2.7
1	E	336	PRO	2.7
1	H	533	VAL	2.7
1	A	337	PHE	2.7
1	F	528	MET	2.7
1	A	409	LEU	2.7
1	F	433	SER	2.7
1	E	458	VAL	2.7
1	B	377	HIS	2.7
1	E	382	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	420	GLY	2.7
1	B	437	MET	2.7
1	A	485	THR	2.7
1	G	460	THR	2.7
1	A	539	LEU	2.7
1	F	409	LEU	2.7
1	F	476	HIS	2.7
1	H	343	MET	2.6
1	E	526	TYR	2.6
1	H	412	ARG	2.6
1	B	425	PHE	2.6
1	F	492	LYS	2.6
1	A	508	LEU	2.6
1	F	509	LEU	2.6
1	A	358	ILE	2.6
1	A	373	HIS	2.6
1	A	544	LEU	2.6
1	B	452	ILE	2.6
1	G	332	ASP	2.6
1	B	361	ALA	2.6
1	E	311	THR	2.6
1	A	457	GLY	2.6
1	F	533	VAL	2.6
1	E	359	ASN	2.6
1	B	328	TYR	2.5
1	E	479	LEU	2.5
1	A	492	LYS	2.5
1	F	520	LYS	2.5
1	B	526	TYR	2.5
1	E	429	LEU	2.5
1	G	468	SER	2.5
1	A	343	MET	2.5
1	A	368	VAL	2.5
1	G	538	ASP	2.5
1	E	420	GLY	2.5
1	E	466	LEU	2.5
1	H	466	LEU	2.5
1	F	421	MET	2.5
1	A	415	GLY	2.4
1	F	489	LEU	2.4
1	F	501	HIS	2.4
1	E	380	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	342	MET	2.4
1	F	467	LYS	2.4
1	E	473	ASP	2.4
1	F	400	GLY	2.4
1	H	413	ASN	2.4
1	A	501	HIS	2.4
1	H	526	TYR	2.4
1	B	434	ARG	2.4
1	A	482	ILE	2.4
1	F	514	ILE	2.4
1	H	397	GLU	2.4
1	F	513	HIS	2.4
1	A	360	TRP	2.4
1	F	372	LEU	2.3
1	H	523	GLU	2.3
1	E	414	GLN	2.3
1	E	381[A]	SER	2.3
1	H	530	SER	2.3
1	A	538	ASP	2.3
1	A	327	LEU	2.3
1	E	539	LEU	2.3
1	F	308	LEU	2.3
1	F	466	LEU	2.3
1	E	358	ILE	2.3
1	E	543	MET	2.3
1	A	362	LYS	2.3
1	B	457	GLY	2.3
1	E	512	SER	2.3
1	A	545	ASP	2.3
1	B	422	VAL	2.3
1	E	541	LEU	2.3
1	F	393	TRP	2.3
1	E	529	LYS	2.3
1	G	337	PHE	2.3
1	A	491	ALA	2.3
1	E	422	VAL	2.3
1	B	549	LEU	2.3
1	F	315	MET	2.3
1	F	327	LEU	2.3
1	F	408	LEU	2.3
1	H	546	ALA	2.2
1	B	458	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	469	LEU	2.2
1	B	310	LEU	2.2
1	F	345	LEU	2.2
1	F	479	LEU	2.2
1	A	332	ASP	2.2
1	F	386	ILE	2.2
1	F	439	ASN	2.2
1	G	413	ASN	2.2
1	E	316	VAL	2.2
1	E	314	GLN	2.2
1	E	498	GLN	2.2
1	A	473	ASP	2.2
1	A	382	ALA	2.2
1	E	493	ALA	2.2
1	B	348	ASN	2.2
1	E	416	LYS	2.2
1	G	342	MET	2.2
1	F	316	VAL	2.2
1	F	368	VAL	2.2
1	B	451	ILE	2.1
1	E	469	LEU	2.1
1	B	472	LYS	2.1
1	E	437	MET	2.1
1	F	482	ILE	2.1
1	B	433	SER	2.1
1	E	421	MET	2.1
1	F	524	HIS	2.1
1	F	402	LEU	2.1
1	F	318	ALA	2.1
1	A	328	TYR	2.1
1	F	328	TYR	2.1
1	F	496	THR	2.1
1	E	415	GLY	2.1
1	F	348	ASN	2.1
1	A	320	LEU	2.1
1	B	409	LEU	2.1
1	G	372	LEU	2.1
1	H	549	LEU	2.1
1	F	307	ALA	2.1
1	F	389	ILE	2.0
1	H	433	SER	2.0
1	A	522	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	478	VAL	2.0
1	B	308	LEU	2.0
1	A	401	LYS	2.0
1	B	467	LYS	2.0
1	B	317	SER	2.0
1	E	431	THR	2.0
1	E	413	ASN	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](#)

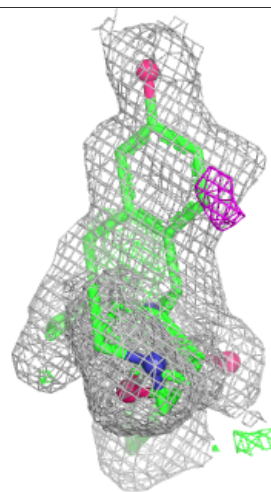
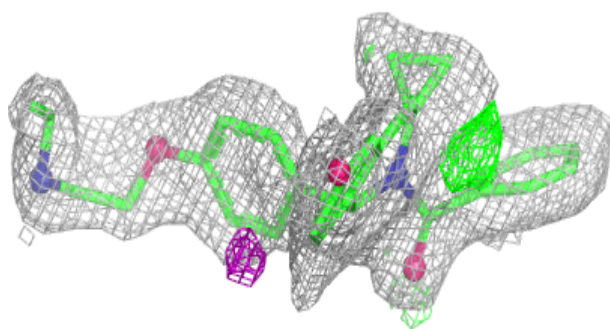
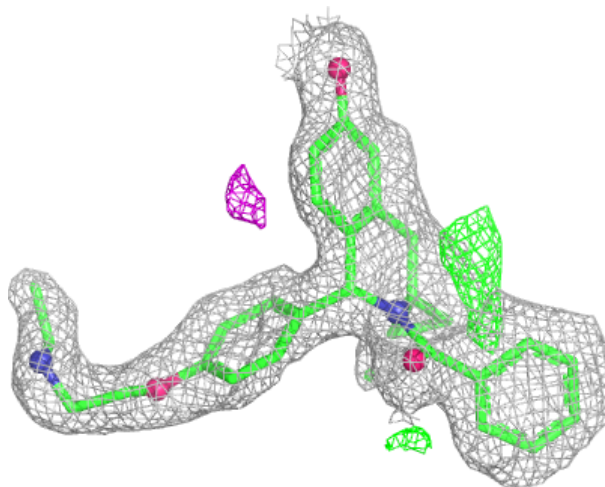
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	TWF	F	601	33/33	0.88	0.11	12,21,31,33	0
2	TWF	H	601	33/33	0.88	0.13	10,17,33,39	0
2	TWF	A	601	33/33	0.89	0.11	11,17,27,30	0
2	TWF	E	601	33/33	0.89	0.12	11,17,26,29	0
2	TWF	B	601	33/33	0.90	0.12	11,19,32,37	0
2	TWF	G	601	33/33	0.93	0.09	8,16,25,34	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.

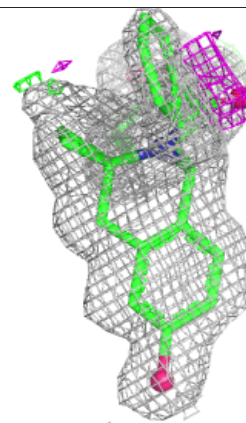
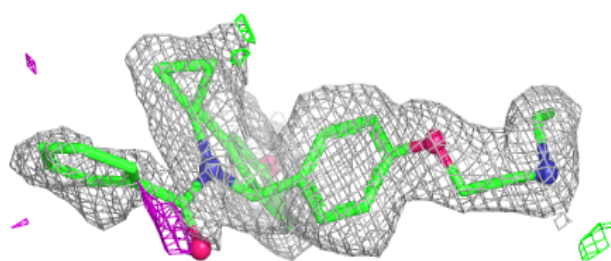
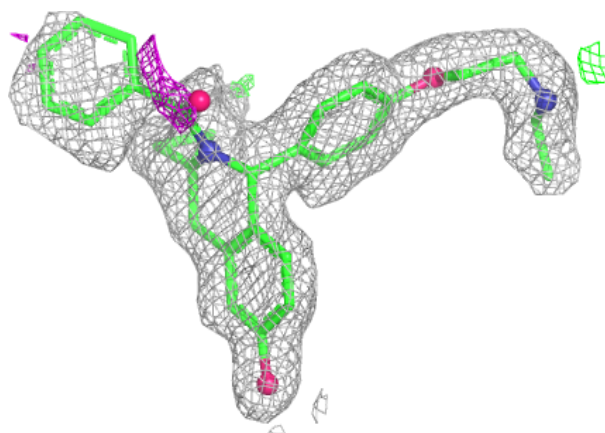
Electron density around TWF F 601:

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

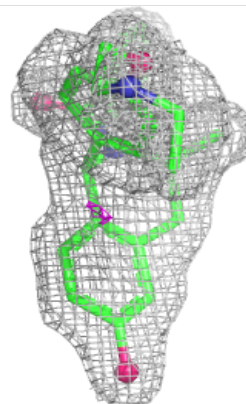
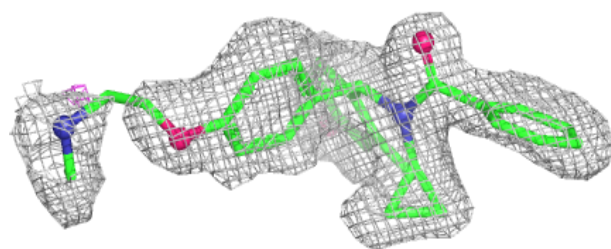
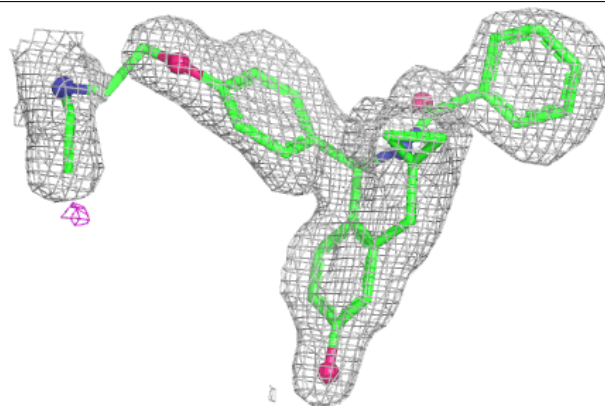


Electron density around TWF H 601:

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

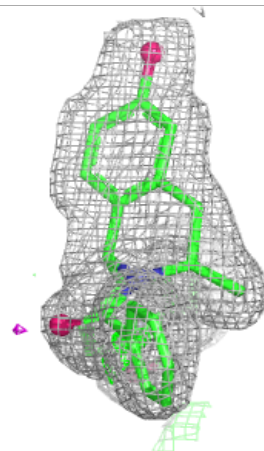
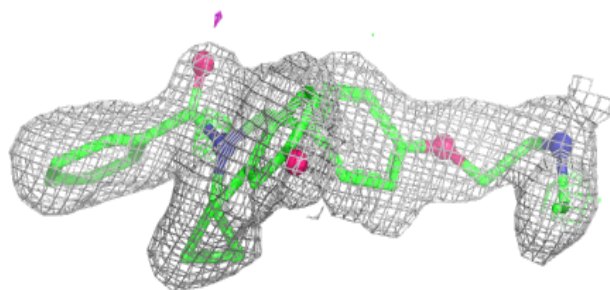
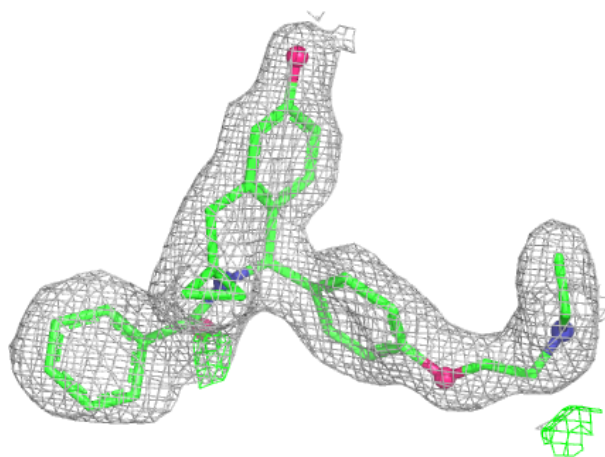
**Electron density around TWF A 601:**

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



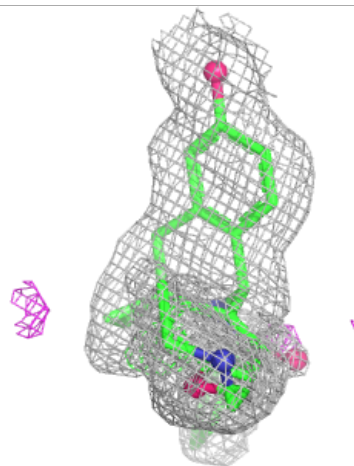
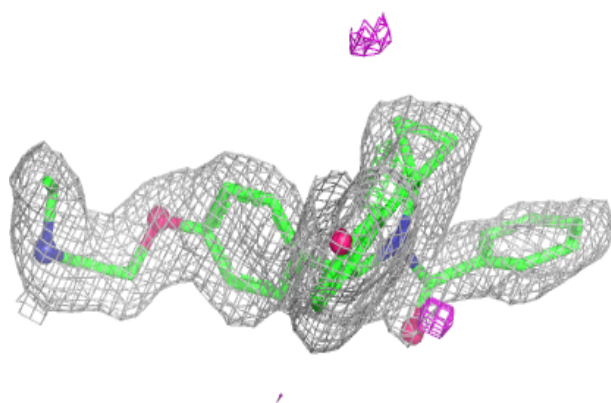
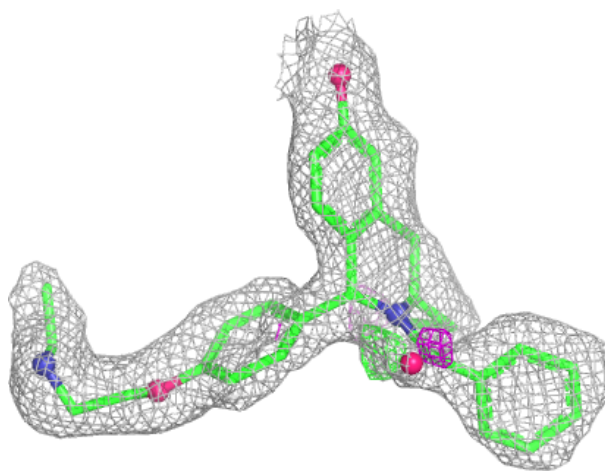
Electron density around TWF E 601:

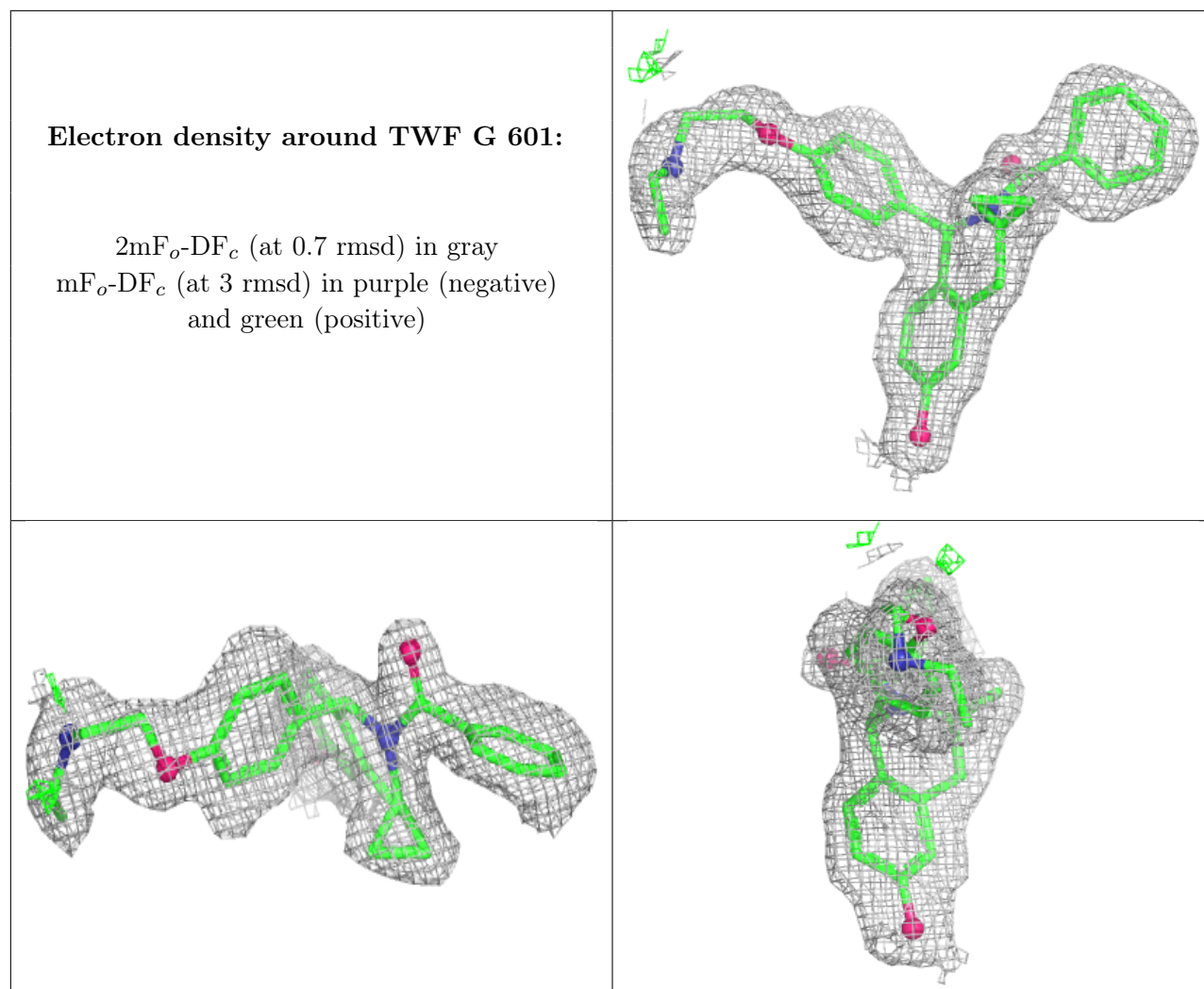
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TWF 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.