



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:30 AM UTC

PDB ID : 5UHI / pdb_00005uhi
Title : Structure of RORgt bound to
Authors : Spurlino, J.; Abad, M.
Deposited on : 2017-01-11
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

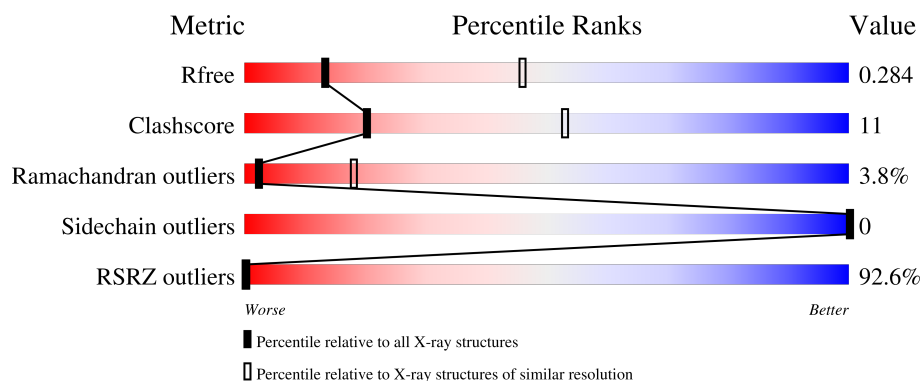
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	258	81% 62% 21% • 14%
1	B	258	79% 64% 19% • 14%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3708 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 Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1816	1149	328	325	14			
1	B	223	Total	C	N	O	S	0	0	0
			1812	1147	328	323	14			

There are 30 discrepancies between the modelled and reference sequences:

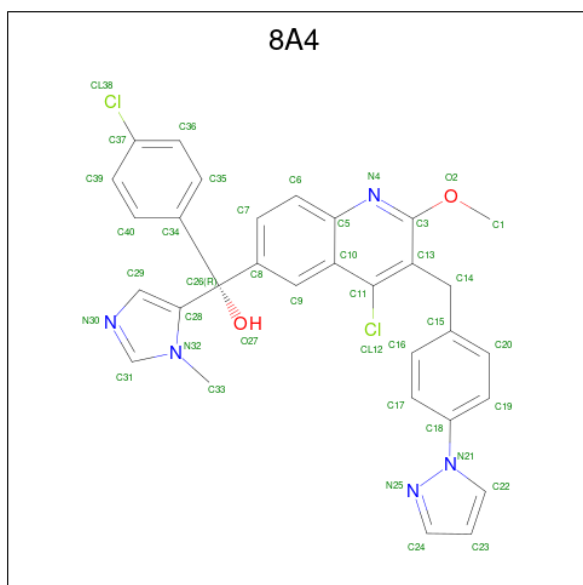
Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	expression tag	UNP P51449
A	251	HIS	-	expression tag	UNP P51449
A	252	HIS	-	expression tag	UNP P51449
A	253	HIS	-	expression tag	UNP P51449
A	254	HIS	-	expression tag	UNP P51449
A	255	HIS	-	expression tag	UNP P51449
A	256	HIS	-	expression tag	UNP P51449
A	257	GLY	-	expression tag	UNP P51449
A	258	GLU	-	expression tag	UNP P51449
A	259	ASN	-	expression tag	UNP P51449
A	260	LEU	-	expression tag	UNP P51449
A	261	TYR	-	expression tag	UNP P51449
A	262	PHE	-	expression tag	UNP P51449
A	263	GLN	-	expression tag	UNP P51449
A	264	GLY	-	expression tag	UNP P51449
B	250	GLY	-	expression tag	UNP P51449
B	251	HIS	-	expression tag	UNP P51449
B	252	HIS	-	expression tag	UNP P51449
B	253	HIS	-	expression tag	UNP P51449
B	254	HIS	-	expression tag	UNP P51449
B	255	HIS	-	expression tag	UNP P51449
B	256	HIS	-	expression tag	UNP P51449
B	257	GLY	-	expression tag	UNP P51449
B	258	GLU	-	expression tag	UNP P51449
B	259	ASN	-	expression tag	UNP P51449

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Chain	Residue	Modelled	Actual	Comment	Reference
B	260	LEU	-	expression tag	UNP P51449
B	261	TYR	-	expression tag	UNP P51449
B	262	PHE	-	expression tag	UNP P51449
B	263	GLN	-	expression tag	UNP P51449
B	264	GLY	-	expression tag	UNP P51449

- Molecule 2 is (R)-(4-chloro-2-methoxy-3-{{4-(1H-pyrazol-1-yl)phenyl}methyl}quinolin-6-yl)(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl)methanol (CCD ID: 8A4) (formula: $C_{31}H_{25}Cl_2N_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			40	31	2	5	2		
2	B	1	Total	C	Cl	N	O	0	0
			40	31	2	5	2		

VAL
VAL
GLN
ALA
ALA
PHE
PRO
PRO
LEU
TYR
LYS
GLU
LEU
PHE
SER

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.35Å 104.32Å 123.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.86 – 3.20 39.86 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.86-3.20) 82.6 (39.86-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.257 , 0.318 (Not available) , 0.284	Depositor DCC
R_{free} test set	1102 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 116.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3708	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8A4

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	0.18	0/1851	0.58	3/2488 (0.1%)
1	B	0.14	0/1847	0.44	1/2483 (0.0%)
All	All	0.16	0/3698	0.52	4/4971 (0.1%)

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	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	CA-C-N	8.67	137.31	121.70
1	A	296	ARG	C-N-CA	8.67	137.31	121.70
1	A	296	ARG	N-CA-C	6.90	119.39	111.11
1	B	413	SER	CB-CA-C	-5.68	110.05	116.63

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	467	PRO	Peptide
1	B	338	LEU	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	1816	0	1811	47	0
1	B	1812	0	1807	37	0
2	A	40	0	0	0	0
2	B	40	0	0	0	0
All	All	3708	0	3618	83	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 11.

All (83) 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:A:430:ARG:HB2	1:A:433:LEU:HD21	1.70	0.73
1:B:297:SER:O	1:B:298:ASN:ND2	2.24	0.70
1:B:318:GLU:HG2	1:B:486:PHE:HB3	1.72	0.70
1:A:456:LYS:HD2	1:A:457:THR:HG23	1.74	0.69
1:A:468:PRO:HD2	1:A:471:LYS:NZ	2.08	0.68
1:A:284:THR:O	1:A:364:ARG:NH2	2.28	0.65
1:A:287:LEU:HB3	1:A:292:LEU:HD11	1.79	0.65
1:B:455:CYS:HA	1:B:460:GLN:NE2	2.14	0.62
1:B:447:GLU:O	1:B:451:HIS:ND1	2.33	0.61
1:A:463:LEU:HA	1:A:466:LEU:HD23	1.82	0.60
1:A:288:ARG:HH12	1:A:291:ASP:CG	2.10	0.59
1:A:296:ARG:NH2	1:B:293:LEU:O	2.37	0.57
1:A:385:MET:HE1	1:A:398:SER:HB3	1.88	0.55
1:A:454:LEU:HD11	1:A:460:GLN:HA	1.90	0.54
1:A:456:LYS:O	1:A:457:THR:OG1	2.24	0.54
1:B:284:THR:O	1:B:364:ARG:NH2	2.41	0.54
1:B:388:PHE:HB3	1:B:391:LEU:HD23	1.90	0.54
1:A:289:LEU:HD13	1:A:293:LEU:HD23	1.89	0.54
1:A:296:ARG:N	1:A:297:SER:HB3	2.23	0.53
1:A:281:TYR:OH	1:A:417:ILE:HD11	2.09	0.52
1:B:269:GLU:HA	1:B:272:HIS:HB2	1.91	0.52
1:B:297:SER:C	1:B:299:ILE:HD12	2.35	0.51
1:A:348:ASP:O	1:A:352:LEU:HD23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LYS:O	1:B:457:THR:HG22	2.11	0.51
1:A:293:LEU:HD12	1:A:296:ARG:HE	1.76	0.50
1:A:368:ALA:HB1	1:A:377:PHE:HB3	1.93	0.50
1:B:324:LEU:HD22	1:B:358:MET:HE1	1.92	0.50
1:A:466:LEU:HD12	1:A:466:LEU:O	2.11	0.50
1:A:468:PRO:HD2	1:A:471:LYS:HZ1	1.76	0.50
1:B:385:MET:HE1	1:B:398:SER:HB3	1.94	0.50
1:A:425:LEU:O	1:A:427:ASN:N	2.45	0.50
1:B:266:SER:O	1:B:270:ILE:HG12	2.12	0.49
1:B:295:GLN:C	1:B:297:SER:H	2.20	0.49
1:B:297:SER:O	1:B:299:ILE:N	2.45	0.49
1:A:293:LEU:HD12	1:A:296:ARG:NE	2.27	0.49
1:B:481:GLU:O	1:B:483:LEU:N	2.46	0.48
1:A:334:PHE:O	1:A:338:LEU:HD12	2.13	0.48
1:A:288:ARG:NH1	1:A:291:ASP:OD2	2.45	0.48
1:A:471:LYS:HB3	1:A:471:LYS:HE3	1.69	0.48
1:A:388:PHE:HB3	1:A:391:LEU:HD23	1.95	0.47
1:A:346:GLN:O	1:A:350:ILE:HG12	2.14	0.47
1:A:305:VAL:O	1:A:309:GLN:HG3	2.14	0.47
1:B:284:THR:HG21	1:B:334:PHE:HB2	1.94	0.47
1:A:366:CYS:SG	1:A:367:ARG:N	2.87	0.47
1:B:267:LEU:H	1:B:267:LEU:HD23	1.79	0.47
1:A:447:GLU:O	1:A:451:HIS:ND1	2.48	0.47
1:B:430:ARG:HB2	1:B:433:LEU:HD11	1.96	0.47
1:B:482:ARG:O	1:B:484:GLN:HG3	2.15	0.47
1:B:317:TRP:CE2	1:B:391:LEU:HD12	2.51	0.46
1:A:309:GLN:HB3	1:A:389:ARG:HD3	1.97	0.46
1:B:368:ALA:HB1	1:B:377:PHE:HB3	1.96	0.46
1:B:413:SER:OG	1:B:414:GLU:N	2.47	0.46
1:A:266:SER:O	1:A:270:ILE:HG12	2.16	0.46
1:B:425:LEU:O	1:B:427:ASN:N	2.49	0.45
1:A:481:GLU:O	1:A:483:LEU:N	2.51	0.44
1:A:468:PRO:HD2	1:A:471:LYS:CE	2.47	0.44
1:B:329:GLN:HA	1:B:332:VAL:HG22	1.99	0.44
1:A:420:TYR:O	1:A:424:VAL:HG23	2.17	0.43
1:B:348:ASP:O	1:B:352:LEU:HD23	2.17	0.43
1:A:403:PHE:CE2	1:A:407:LEU:HD11	2.53	0.43
1:B:419:LEU:HD13	1:B:450:PHE:HA	2.01	0.43
1:A:292:LEU:HD23	1:A:368:ALA:HB2	2.00	0.43
1:B:450:PHE:O	1:B:454:LEU:HB2	2.18	0.43
1:A:296:ARG:HB2	1:A:297:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TRP:CE2	1:A:391:LEU:HD12	2.53	0.43
1:A:375:THR:HG23	1:A:382:TYR:CD1	2.54	0.43
1:A:482:ARG:O	1:A:483:LEU:HD23	2.19	0.42
1:A:301:SER:OG	1:A:302:ARG:N	2.53	0.42
1:A:286:GLN:HB2	1:A:330:TYR:CD2	2.55	0.42
1:A:368:ALA:HB1	1:A:377:PHE:CB	2.50	0.42
1:B:420:TYR:O	1:B:424:VAL:HG23	2.19	0.42
1:A:403:PHE:O	1:A:407:LEU:HG	2.20	0.42
1:B:317:TRP:CD2	1:B:391:LEU:HD12	2.55	0.41
1:B:295:GLN:OE1	1:B:298:ASN:ND2	2.54	0.41
1:A:373:ASN:OD1	1:A:375:THR:HG22	2.20	0.41
1:B:281:TYR:HA	1:B:284:THR:HG22	2.01	0.41
1:B:298:ASN:CG	1:B:299:ILE:N	2.79	0.41
1:A:286:GLN:O	1:A:287:LEU:HD23	2.20	0.41
1:B:273:LEU:O	1:B:277:VAL:HG23	2.21	0.41
1:A:465:LYS:HE3	1:A:465:LYS:HB3	1.82	0.40
1:B:482:ARG:O	1:B:484:GLN:N	2.54	0.40
1:B:287:LEU:HB3	1:B:292:LEU:HD21	2.04	0.40
1:B:267:LEU:HG	1:B:268:THR:HG23	2.02	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	221/258 (86%)	195 (88%)	16 (7%)	10 (4%)	2	15
1	B	221/258 (86%)	199 (90%)	15 (7%)	7 (3%)	3	21
All	All	442/516 (86%)	394 (89%)	31 (7%)	17 (4%)	2	18

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ARG
1	A	289	LEU
1	A	467	PRO
1	A	468	PRO
1	B	483	LEU
1	A	297	SER
1	A	426	ILE
1	A	482	ARG
1	B	299	ILE
1	B	338	LEU
1	B	426	ILE
1	B	482	ARG
1	A	430	ARG
1	A	431	PRO
1	B	266	SER
1	B	298	ASN
1	A	466	LEU

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	197/229 (86%)	197 (100%)	0	100	100
1	B	196/229 (86%)	196 (100%)	0	100	100
All	All	393/458 (86%)	393 (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 (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
1	A	295	GLN
1	A	309	GLN
1	A	322	HIS
1	A	323	HIS

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Mol	Chain	Res	Type
1	A	460	GLN
1	B	323	HIS
1	B	460	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	8A4	A	601	-	42,45,45	1.40	9 (21%)	55,66,66	2.39	5 (9%)
2	8A4	B	601	-	42,45,45	1.38	9 (21%)	55,66,66	2.39	4 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8A4	A	601	-	-	5/28/28/28	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8A4	B	601	-	-	3/28/28/28	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	8A4	C11-C10	-3.17	1.37	1.42
2	A	601	8A4	C11-C10	-3.13	1.37	1.42
2	B	601	8A4	C10-C5	-2.90	1.37	1.42
2	A	601	8A4	C26-C34	-2.87	1.48	1.53
2	A	601	8A4	C10-C5	-2.84	1.38	1.42
2	B	601	8A4	C26-C34	-2.71	1.49	1.53
2	A	601	8A4	C26-C8	-2.68	1.49	1.53
2	B	601	8A4	C26-C8	-2.68	1.49	1.53
2	B	601	8A4	C5-N4	-2.43	1.33	1.37
2	A	601	8A4	C6-C5	-2.41	1.37	1.41
2	A	601	8A4	C5-N4	-2.34	1.33	1.37
2	B	601	8A4	C6-C5	-2.33	1.38	1.41
2	A	601	8A4	C18-N21	-2.23	1.39	1.43
2	A	601	8A4	C13-C3	-2.14	1.37	1.39
2	B	601	8A4	C9-C10	-2.11	1.37	1.42
2	A	601	8A4	C9-C10	-2.11	1.37	1.42
2	B	601	8A4	C18-N21	-2.10	1.39	1.43
2	B	601	8A4	C13-C3	-2.00	1.37	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	8A4	C1-O2-C3	-15.68	102.54	117.20
2	A	601	8A4	C1-O2-C3	-15.59	102.62	117.20
2	A	601	8A4	C11-C10-C5	3.73	118.44	116.35
2	B	601	8A4	C11-C10-C5	3.70	118.42	116.35
2	A	601	8A4	N32-C31-N30	-2.92	111.20	112.94
2	B	601	8A4	N32-C31-N30	-2.85	111.25	112.94
2	A	601	8A4	C22-N21-N25	2.44	113.86	111.83
2	B	601	8A4	C18-N21-C22	-2.09	123.83	128.39
2	A	601	8A4	C14-C13-C11	2.05	121.91	118.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

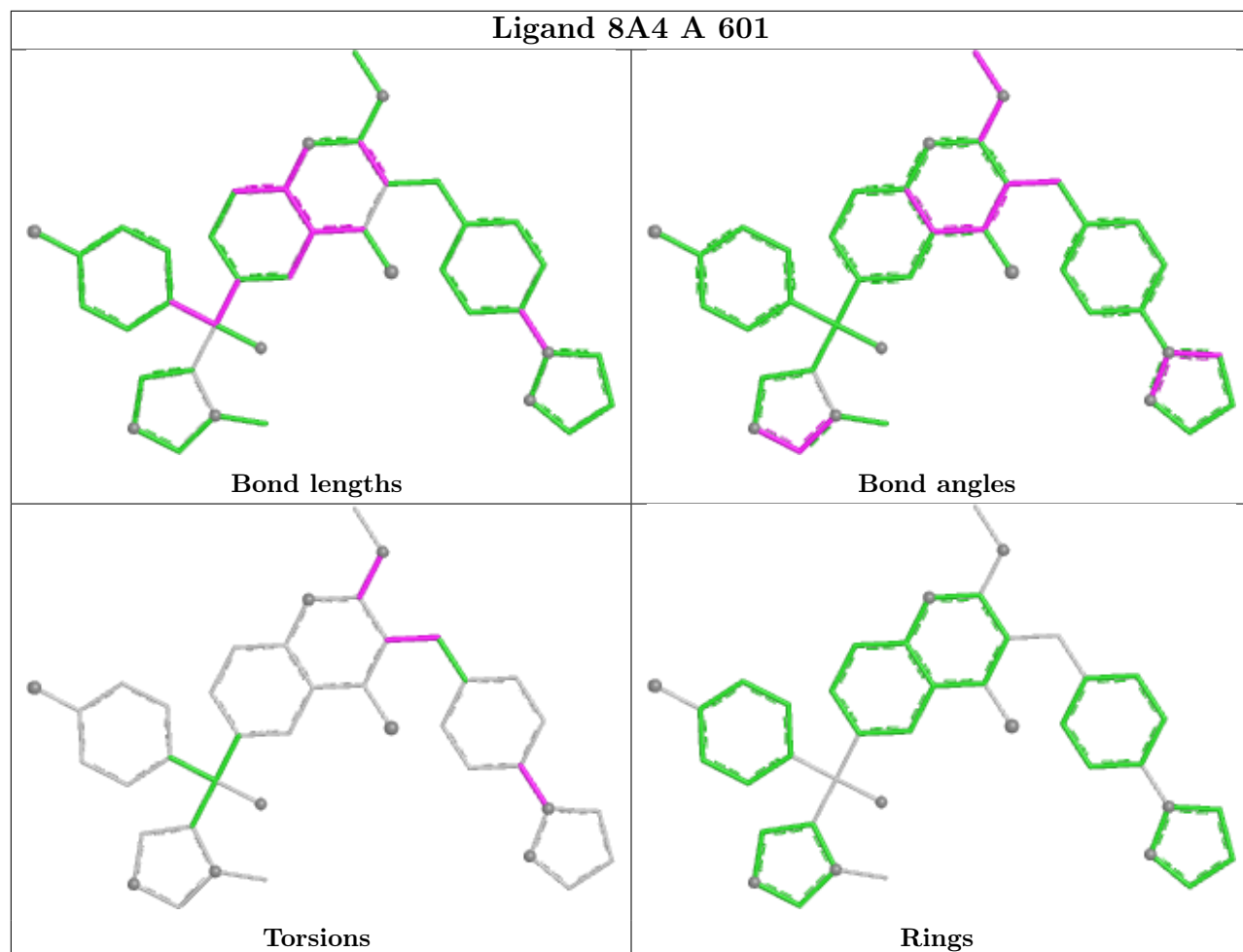
Mol	Chain	Res	Type	Atoms
2	A	601	8A4	N4-C3-O2-C1
2	B	601	8A4	C13-C3-O2-C1
2	B	601	8A4	N4-C3-O2-C1
2	A	601	8A4	C13-C3-O2-C1
2	A	601	8A4	C19-C18-N21-C22
2	A	601	8A4	C17-C18-N21-C22
2	A	601	8A4	C3-C13-C14-C15
2	B	601	8A4	C3-C13-C14-C15

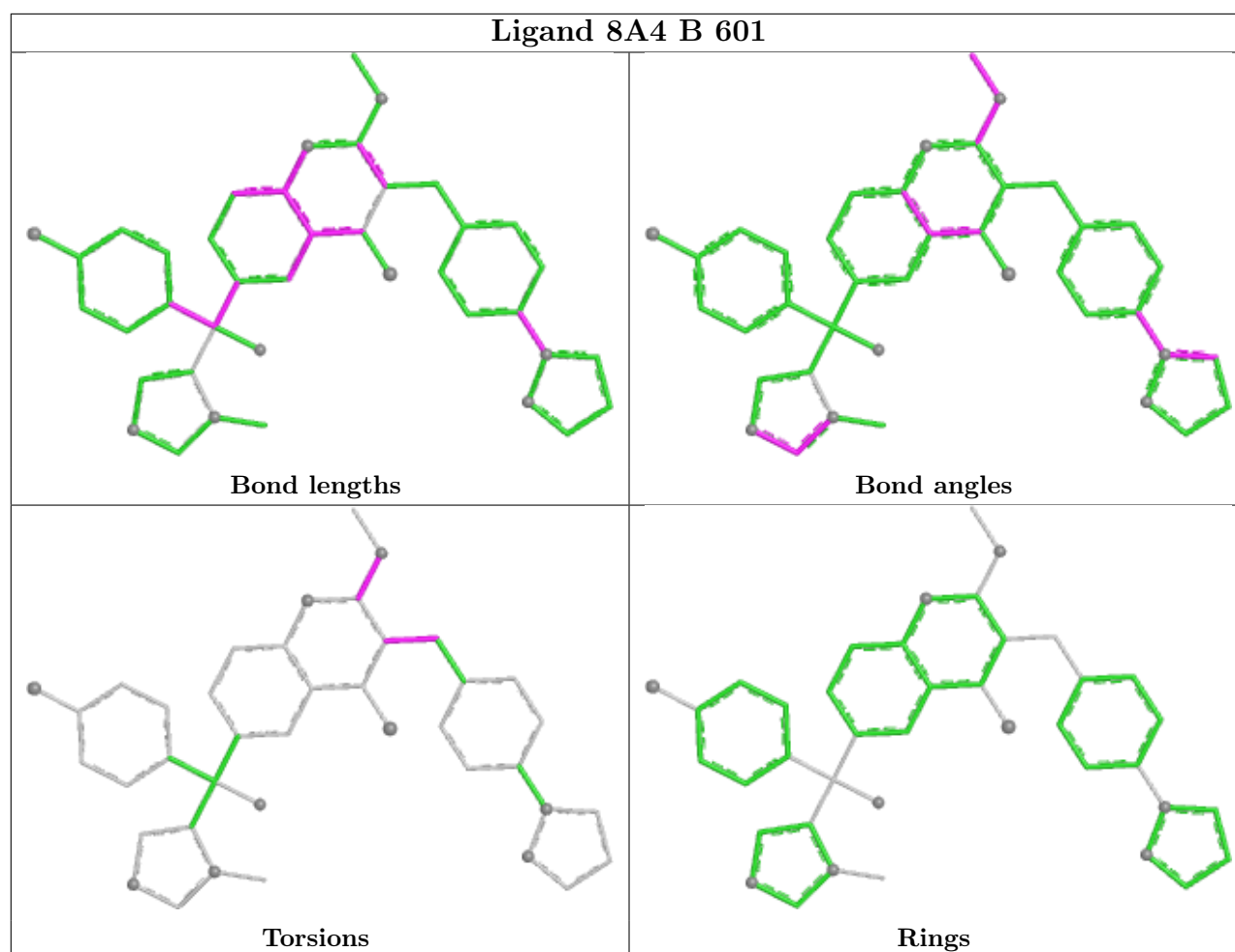
There are no ring outliers.

No monomer is involved in short contacts.

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.

Ligand 8A4 A 601





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	223/258 (86%)	5.00	209 (93%) 0 0	98, 157, 232, 307	0
1	B	223/258 (86%)	4.97	204 (91%) 0 0	109, 163, 242, 291	0
All	All	446/516 (86%)	4.98	413 (92%) 0 0	98, 160, 237, 307	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	ASP	12.5
1	A	408	SER	12.2
1	A	339	SER	12.2
1	B	413	SER	11.8
1	B	476	CYS	11.7
1	A	297	SER	11.4
1	B	462	ILE	11.3
1	A	290	GLU	11.2
1	B	372	ASP	11.1
1	B	412	PHE	10.8
1	B	339	SER	10.8
1	B	463	LEU	10.4
1	A	472	LEU	10.1
1	B	425	LEU	10.0
1	A	420	TYR	10.0
1	A	411	HIS	9.8
1	B	294	ARG	9.7
1	A	468	PRO	9.6
1	B	278	CYS	9.5
1	B	290	GLU	9.5
1	A	289	LEU	9.5
1	B	343	GLU	9.3
1	B	298	ASN	9.2
1	B	461	SER	9.2

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Mol	Chain	Res	Type	RSRZ
1	B	474	SER	9.2
1	B	452	HIS	9.2
1	A	409	ALA	9.2
1	A	280	SER	9.0
1	B	446	LEU	9.0
1	A	393	CYS	9.0
1	A	457	THR	9.0
1	A	424	VAL	8.8
1	A	373	ASN	8.8
1	A	394	SER	8.8
1	B	283	GLU	8.7
1	A	439	VAL	8.7
1	A	288	ARG	8.7
1	B	297	SER	8.7
1	B	475	LEU	8.6
1	A	442	LEU	8.6
1	A	421	THR	8.5
1	A	458	HIS	8.4
1	B	459	ARG	8.4
1	B	277	VAL	8.3
1	B	426	ILE	8.3
1	B	293	LEU	8.3
1	B	334	PHE	8.2
1	A	446	LEU	8.2
1	A	428	ALA	8.2
1	B	477	SER	8.1
1	A	419	LEU	8.1
1	B	289	LEU	8.1
1	B	464	ALA	8.1
1	A	466	LEU	8.0
1	A	464	ALA	8.0
1	B	441	GLN	8.0
1	A	272	HIS	8.0
1	A	340	GLY	7.9
1	B	299	ILE	7.8
1	B	447	GLU	7.8
1	A	470	GLY	7.8
1	A	334	PHE	7.7
1	A	461	SER	7.7
1	A	343	GLU	7.7
1	B	448	LEU	7.7
1	B	466	LEU	7.7

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Mol	Chain	Res	Type	RSRZ
1	A	456	LYS	7.6
1	B	338	LEU	7.5
1	B	423	LEU	7.5
1	B	330	TYR	7.5
1	B	292	LEU	7.4
1	A	366	CYS	7.4
1	A	295	GLN	7.4
1	A	316	MET	7.4
1	A	302	ARG	7.3
1	B	371	ALA	7.3
1	B	280	SER	7.3
1	A	443	GLN	7.2
1	A	388	PHE	7.2
1	B	282	ARG	7.2
1	B	373	ASN	7.1
1	B	460	GLN	7.1
1	B	467	PRO	7.1
1	A	273	LEU	7.1
1	B	268	THR	7.1
1	A	331	VAL	7.1
1	B	265	ALA	7.0
1	A	447	GLU	7.0
1	B	422	ALA	7.0
1	A	469	LYS	6.9
1	B	472	LEU	6.9
1	B	333	GLU	6.9
1	B	411	HIS	6.9
1	B	267	LEU	6.8
1	A	303	GLU	6.8
1	A	406	SER	6.8
1	B	284	THR	6.8
1	A	418	ALA	6.7
1	A	460	GLN	6.7
1	B	366	CYS	6.7
1	A	476	CYS	6.7
1	B	410	LEU	6.7
1	B	302	ARG	6.7
1	A	333	GLU	6.6
1	B	316	MET	6.6
1	B	453	HIS	6.6
1	B	443	GLN	6.6
1	A	359	GLU	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	445	ASN	6.5
1	B	428	ALA	6.5
1	A	287	LEU	6.5
1	A	467	PRO	6.4
1	B	367	ARG	6.4
1	A	379	GLU	6.4
1	A	426	ILE	6.4
1	A	429	HIS	6.4
1	B	352	LEU	6.4
1	A	267	LEU	6.4
1	A	422	ALA	6.3
1	A	445	ASN	6.3
1	A	391	LEU	6.3
1	A	368	ALA	6.3
1	A	278	CYS	6.2
1	B	266	SER	6.2
1	A	279	LYS	6.2
1	A	423	LEU	6.2
1	B	396	LEU	6.2
1	A	405	HIS	6.1
1	B	269	GLU	6.1
1	A	360	VAL	6.1
1	B	274	VAL	6.1
1	A	395	GLU	6.1
1	B	308	TYR	6.1
1	A	453	HIS	6.1
1	B	407	LEU	6.1
1	A	277	VAL	6.0
1	B	437	ARG	6.0
1	B	363	VAL	6.0
1	A	298	ASN	6.0
1	B	370	ASN	6.0
1	B	420	TYR	6.0
1	A	337	ARG	6.0
1	A	283	GLU	5.9
1	A	268	THR	5.9
1	B	465	LYS	5.9
1	B	340	GLY	5.9
1	B	320	CYS	5.9
1	A	478	GLN	5.9
1	A	320	CYS	5.8
1	B	405	HIS	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	448	LEU	5.8
1	B	444	TYR	5.8
1	B	419	LEU	5.8
1	A	397	ILE	5.8
1	A	374	ARG	5.7
1	A	271	GLU	5.7
1	B	456	LYS	5.7
1	A	392	GLY	5.7
1	A	407	LEU	5.7
1	A	454	LEU	5.7
1	B	479	HIS	5.6
1	A	473	ARG	5.6
1	A	416	GLU	5.6
1	B	451	HIS	5.6
1	A	276	SER	5.6
1	A	425	LEU	5.6
1	B	332	VAL	5.5
1	A	293	LEU	5.5
1	A	452	HIS	5.5
1	A	292	LEU	5.5
1	B	286	GLN	5.5
1	B	272	HIS	5.5
1	A	367	ARG	5.5
1	B	276	SER	5.5
1	B	317	TRP	5.4
1	B	480	VAL	5.4
1	B	424	VAL	5.4
1	A	450	PHE	5.4
1	A	463	LEU	5.4
1	B	337	ARG	5.4
1	A	404	SER	5.4
1	A	342	MET	5.4
1	A	363	VAL	5.3
1	A	357	ALA	5.3
1	A	438	LYS	5.3
1	B	438	LYS	5.3
1	A	344	LEU	5.3
1	B	331	VAL	5.3
1	A	296	ARG	5.3
1	A	378	PHE	5.2
1	A	358	MET	5.2
1	A	308	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	388	PHE	5.2
1	B	427	ASN	5.2
1	A	402	ASP	5.2
1	B	329	GLN	5.2
1	A	299	ILE	5.1
1	B	353	LEU	5.1
1	B	287	LEU	5.1
1	B	319	ARG	5.1
1	B	397	ILE	5.1
1	A	372	ASP	5.1
1	A	444	TYR	5.1
1	A	440	GLU	5.0
1	B	375	THR	5.0
1	B	378	PHE	5.0
1	A	284	THR	5.0
1	B	279	LYS	5.0
1	A	412	PHE	5.0
1	A	270	ILE	4.9
1	A	338	LEU	4.9
1	B	483	LEU	4.9
1	A	415	ASP	4.9
1	A	332	VAL	4.9
1	A	319	ARG	4.9
1	B	273	LEU	4.9
1	A	455	CYS	4.9
1	B	429	HIS	4.9
1	B	342	MET	4.8
1	A	317	TRP	4.8
1	A	484	GLN	4.8
1	A	282	ARG	4.8
1	B	485	ILE	4.8
1	A	433	LEU	4.7
1	A	281	TYR	4.7
1	B	384	GLY	4.7
1	A	390	ALA	4.7
1	B	335	ALA	4.7
1	B	458	HIS	4.7
1	A	471	LYS	4.7
1	B	470	GLY	4.7
1	B	271	GLU	4.7
1	A	329	GLN	4.6
1	B	311	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	482	ARG	4.6
1	A	474	SER	4.6
1	B	394	SER	4.6
1	A	400	ILE	4.6
1	A	356	GLY	4.6
1	A	301	SER	4.6
1	A	364	ARG	4.6
1	A	348	ASP	4.5
1	A	403	PHE	4.5
1	A	462	ILE	4.5
1	A	436	LYS	4.5
1	A	369	TYR	4.5
1	B	281	TYR	4.5
1	B	368	ALA	4.5
1	A	485	ILE	4.4
1	B	357	ALA	4.4
1	B	484	GLN	4.4
1	B	409	ALA	4.4
1	A	323	HIS	4.3
1	A	341	PHE	4.3
1	A	387	LEU	4.3
1	B	400	ILE	4.3
1	B	487	GLN	4.3
1	A	396	LEU	4.3
1	A	417	ILE	4.3
1	B	374	ARG	4.3
1	B	421	THR	4.2
1	B	364	ARG	4.2
1	A	294	ARG	4.2
1	B	387	LEU	4.2
1	B	442	LEU	4.2
1	A	475	LEU	4.1
1	B	327	ALA	4.1
1	A	477	SER	4.1
1	B	270	ILE	4.1
1	B	391	LEU	4.1
1	B	450	PHE	4.1
1	B	415	ASP	4.0
1	B	325	THR	4.0
1	B	275	GLN	4.0
1	B	383	GLY	4.0
1	B	385	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	449	ALA	4.0
1	B	418	ALA	4.0
1	B	362	LEU	3.9
1	B	365	MET	3.9
1	B	328	ILE	3.8
1	A	434	GLN	3.8
1	A	326	GLU	3.8
1	B	414	GLU	3.8
1	B	440	GLU	3.8
1	B	377	PHE	3.8
1	A	383	GLY	3.7
1	A	269	GLU	3.7
1	A	481	GLU	3.7
1	B	416	GLU	3.7
1	B	324	LEU	3.7
1	A	483	LEU	3.7
1	B	341	PHE	3.7
1	A	330	TYR	3.7
1	B	288	ARG	3.6
1	B	417	ILE	3.6
1	A	310	ARG	3.6
1	A	382	TYR	3.6
1	B	408	SER	3.6
1	B	393	CYS	3.6
1	A	414	GLU	3.6
1	A	479	HIS	3.6
1	A	482	ARG	3.6
1	A	427	ASN	3.6
1	B	454	LEU	3.6
1	B	356	GLY	3.5
1	A	385	MET	3.5
1	B	457	THR	3.5
1	B	471	LYS	3.5
1	A	441	GLN	3.4
1	B	369	TYR	3.4
1	A	370	ASN	3.4
1	A	459	ARG	3.4
1	B	304	GLU	3.4
1	B	380	GLY	3.4
1	B	401	PHE	3.3
1	B	379	GLU	3.3
1	A	451	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	322	HIS	3.3
1	B	295	GLN	3.3
1	A	321	ALA	3.3
1	A	345	CYS	3.2
1	B	285	CYS	3.2
1	B	296	ARG	3.2
1	A	432	GLY	3.2
1	A	480	VAL	3.2
1	B	399	SER	3.2
1	B	402	ASP	3.2
1	A	449	ALA	3.2
1	B	468	PRO	3.2
1	B	314	TRP	3.1
1	A	291	ASP	3.1
1	B	354	LYS	3.1
1	A	300	PHE	3.1
1	A	324	LEU	3.1
1	B	395	GLU	3.1
1	A	285	CYS	3.1
1	A	398	SER	3.0
1	A	365	MET	3.0
1	B	455	CYS	3.0
1	A	309	GLN	3.0
1	B	431	PRO	3.0
1	B	473	ARG	3.0
1	B	355	ALA	3.0
1	A	305	VAL	3.0
1	A	362	LEU	3.0
1	B	303	GLU	2.9
1	B	323	HIS	2.9
1	B	392	GLY	2.9
1	B	406	SER	2.9
1	B	478	GLN	2.9
1	B	430	ARG	2.9
1	B	390	ALA	2.9
1	A	327	ALA	2.9
1	A	389	ARG	2.9
1	A	353	LEU	2.9
1	A	354	LYS	2.9
1	B	336	LYS	2.8
1	B	358	MET	2.8
1	B	439	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	328	ILE	2.8
1	A	275	GLN	2.8
1	B	403	PHE	2.7
1	A	306	THR	2.7
1	B	398	SER	2.7
1	A	349	GLN	2.7
1	B	469	LYS	2.7
1	A	380	GLY	2.7
1	A	286	GLN	2.6
1	A	431	PRO	2.6
1	A	266	SER	2.6
1	B	326	GLU	2.6
1	A	325	THR	2.6
1	B	310	ARG	2.6
1	A	313	MET	2.6
1	B	350	ILE	2.5
1	B	300	PHE	2.5
1	B	321	ALA	2.5
1	A	401	PHE	2.5
1	A	399	SER	2.5
1	B	435	GLU	2.5
1	A	361	VAL	2.5
1	A	371	ALA	2.4
1	A	410	LEU	2.4
1	B	382	TYR	2.4
1	A	352	LEU	2.4
1	B	306	THR	2.4
1	B	322	HIS	2.4
1	A	465	LYS	2.4
1	A	375	THR	2.3
1	B	389	ARG	2.3
1	B	481	GLU	2.3
1	B	376	VAL	2.3
1	B	344	LEU	2.3
1	A	435	GLU	2.3
1	A	355	ALA	2.3
1	A	376	VAL	2.3
1	B	351	VAL	2.2
1	A	381	LYS	2.2
1	B	312	SER	2.2
1	A	318	GLU	2.2
1	A	386	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	ARG	2.1
1	B	361	VAL	2.1
1	B	301	SER	2.1
1	A	314	TRP	2.1
1	A	311	LYS	2.1
1	A	265	ALA	2.1
1	A	335	ALA	2.0
1	A	304	GLU	2.0
1	A	347	ASN	2.0
1	B	436	LYS	2.0
1	B	318	GLU	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](#)

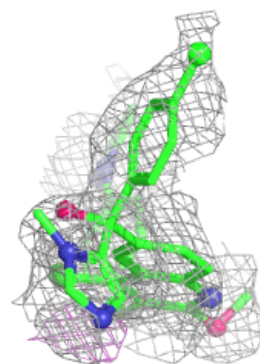
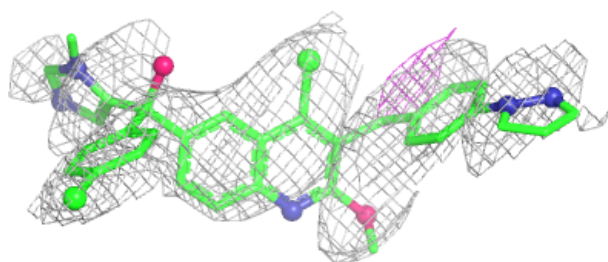
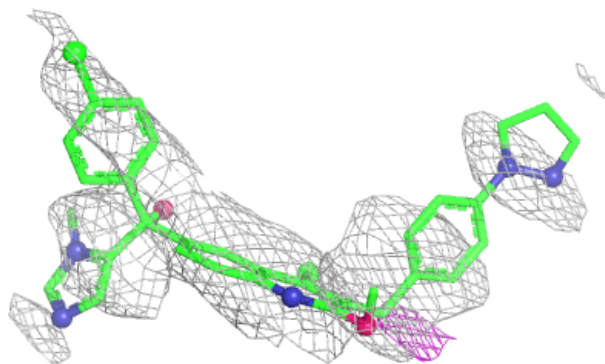
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	8A4	B	601	40/40	0.64	0.38	104,131,160,168	0
2	8A4	A	601	40/40	0.67	0.29	107,134,187,191	0

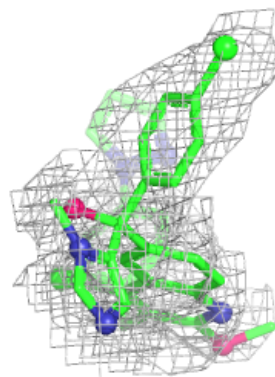
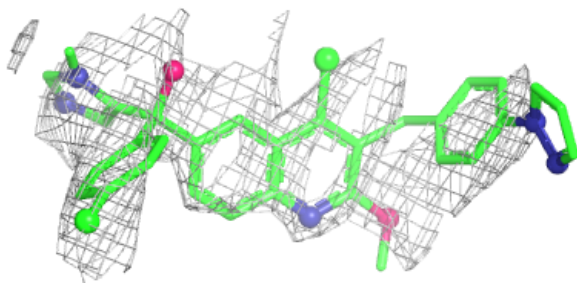
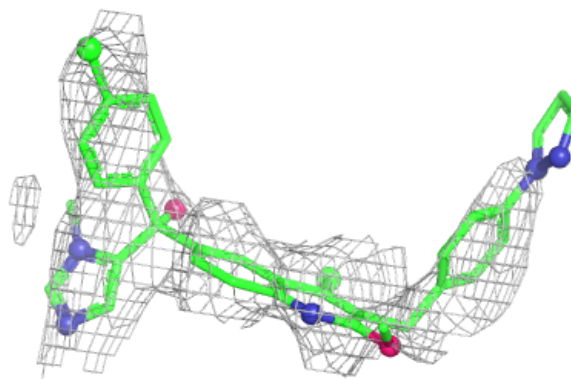
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8A4 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 8A4 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.