



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2020 – 06:37 am BST

PDB ID : 5UHI
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 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

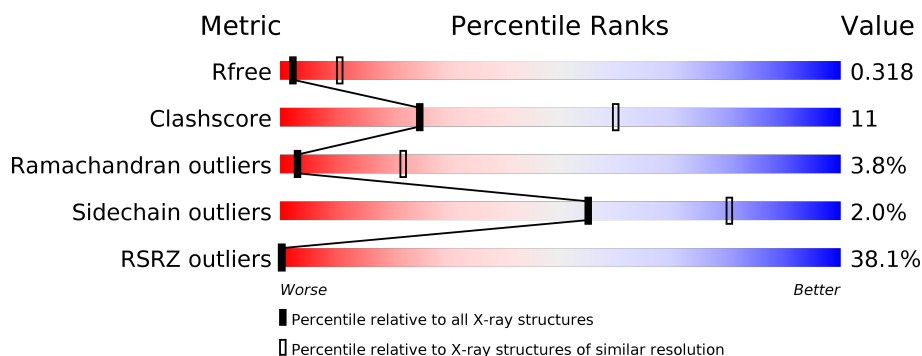
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 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	258	
1	B	258	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	8A4	A	601	-	-	-	X
2	8A4	B	601	-	-	-	X

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:

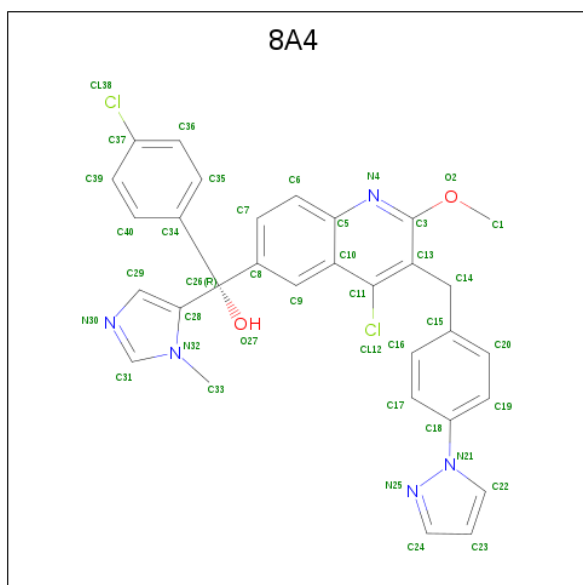
Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	expression tag	UNP P51449
A	251	HIS	-	expression tag	UNP P51449
A	252	HIS	-	expression tag	UNP P51449
A	253	HIS	-	expression tag	UNP P51449
A	254	HIS	-	expression tag	UNP P51449
A	255	HIS	-	expression tag	UNP P51449
A	256	HIS	-	expression tag	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 (three-letter code: 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		

- Molecule 1: Nuclear receptor ROR-gamma



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 48.06 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.86-3.20) 82.6 (48.06-3.20)	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 0.257 , 0.318	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)	0.28 , 104.9	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	0.26	0/1851	0.58	3/2488 (0.1%)
1	B	0.25	0/1847	0.47	1/2483 (0.0%)
All	All	0.25	0/3698	0.53	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($^{\circ}$)	Ideal($^{\circ}$)
1	A	466	LEU	CA-CB-CG	7.63	132.85	115.30
1	A	483	LEU	CA-CB-CG	6.43	130.10	115.30
1	A	296	ARG	C-N-CA	6.24	137.31	121.70
1	B	483	LEU	CA-CB-CG	5.01	126.83	115.30

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	46	0
1	B	1812	0	1807	34	0
2	A	40	0	0	0	0
2	B	40	0	0	0	0
All	All	3708	0	3618	79	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 (79) 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:296:ARG:NH2	1:B:293:LEU:O	2.37	0.57
1:A:454:LEU:HD11	1:A:460:GLN:HA	1.90	0.54
1:A:288:ARG:HH12	1:A:291:ASP:CG	2.10	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:A:348:ASP:O	1:A:352:LEU:HD23	2.09	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ALA:HB1	1:A:377:PHE:HB3	1.93	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: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: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:366:CYS:SG	1:A:367:ARG:N	2.87	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:B:267:LEU:HD23	1:B:267:LEU:H	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:297:SER:C	1:B:299:ILE:HD12	2.35	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:295:GLN:C	1:B:297:SER:H	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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	18
1	B	221/258 (86%)	199 (90%)	15 (7%)	7 (3%)	4	26
All	All	442/516 (86%)	394 (89%)	31 (7%)	17 (4%)	3	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	ARG
1	A	289	LEU
1	A	467	PRO

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Mol	Chain	Res	Type
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%)	195 (99%)	2 (1%)	76	90
1	B	196/229 (86%)	190 (97%)	6 (3%)	40	72
All	All	393/458 (86%)	385 (98%)	8 (2%)	55	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	ARG
1	A	481	GLU
1	B	298	ASN
1	B	338	LEU
1	B	437	ARG
1	B	444	TYR
1	B	466	LEU
1	B	482	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

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

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 ⓘ

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	B	601	-	40,45,45	1.46	7 (17%)	57,66,66	2.20	3 (5%)
2	8A4	A	601	-	40,45,45	1.47	7 (17%)	57,66,66	2.21	3 (5%)

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	B	601	-	-	8/22/28/28	0/6/6/6
2	8A4	A	601	-	-	5/22/28/28	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	8A4	C26-C34	-3.28	1.48	1.53
2	B	601	8A4	C26-C34	-3.11	1.49	1.53
2	B	601	8A4	C11-C10	-3.11	1.37	1.42
2	A	601	8A4	C26-C8	-3.08	1.49	1.53
2	B	601	8A4	C26-C8	-3.08	1.49	1.53
2	A	601	8A4	C11-C10	-3.06	1.37	1.42
2	B	601	8A4	C10-C5	-2.77	1.37	1.42
2	A	601	8A4	C10-C5	-2.71	1.38	1.42
2	B	601	8A4	C5-N4	-2.33	1.33	1.37
2	A	601	8A4	C6-C5	-2.31	1.37	1.41
2	A	601	8A4	C5-N4	-2.25	1.33	1.37
2	B	601	8A4	C6-C5	-2.23	1.38	1.41
2	B	601	8A4	C9-C10	-2.13	1.37	1.42
2	A	601	8A4	C9-C10	-2.13	1.37	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	8A4	C1-O2-C3	-14.81	102.54	117.21
2	A	601	8A4	C1-O2-C3	-14.73	102.62	117.21
2	A	601	8A4	C11-C10-C5	3.41	118.44	116.41
2	B	601	8A4	C11-C10-C5	3.39	118.42	116.41
2	A	601	8A4	C22-N21-N25	2.85	113.86	111.94
2	B	601	8A4	O2-C3-N4	-2.02	117.37	120.11

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	8A4	C13-C3-O2-C1
2	A	601	8A4	C17-C18-N21-N25
2	A	601	8A4	N4-C3-O2-C1
2	B	601	8A4	N4-C3-O2-C1
2	A	601	8A4	C13-C3-O2-C1
2	A	601	8A4	C3-C13-C14-C15
2	B	601	8A4	C17-C18-N21-N25

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Mol	Chain	Res	Type	Atoms
2	B	601	8A4	C19-C18-N21-N25
2	A	601	8A4	C19-C18-N21-N25
2	B	601	8A4	C3-C13-C14-C15
2	B	601	8A4	C17-C18-N21-C22
2	B	601	8A4	C19-C18-N21-C22
2	B	601	8A4	C13-C14-C15-C20

There are no ring outliers.

No monomer is involved in short contacts.

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%)	1.87	87 (39%) 0 0	98, 157, 232, 307	0
1	B	223/258 (86%)	1.86	83 (37%) 0 0	109, 163, 242, 291	0
All	All	446/516 (86%)	1.86	170 (38%) 0 0	98, 160, 237, 307	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	CYS	7.9
1	B	278	CYS	6.2
1	A	468	PRO	6.1
1	B	339	SER	5.9
1	B	474	SER	5.7
1	A	380	GLY	5.4
1	B	265	ALA	5.3
1	B	413	SER	5.2
1	A	473	ARG	5.2
1	A	339	SER	4.9
1	B	266	SER	4.9
1	B	463	LEU	4.8
1	A	472	LEU	4.7
1	B	298	ASN	4.6
1	B	291	ASP	4.6
1	B	475	LEU	4.6
1	B	462	ILE	4.5
1	A	469	LYS	4.4
1	B	469	LYS	4.3
1	B	461	SER	4.3
1	B	412	PHE	4.3
1	A	461	SER	4.3
1	B	452	HIS	4.3
1	A	463	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	476	CYS	4.2
1	B	372	ASP	4.1
1	B	477	SER	4.1
1	A	467	PRO	4.1
1	A	308	TYR	4.0
1	A	457	THR	3.9
1	A	297	SER	3.9
1	B	290	GLU	3.8
1	B	284	THR	3.8
1	A	462	ILE	3.8
1	A	394	SER	3.7
1	A	408	SER	3.7
1	A	268	THR	3.7
1	A	422	ALA	3.6
1	B	283	GLU	3.6
1	A	421	THR	3.6
1	B	482	ARG	3.6
1	A	445	ASN	3.6
1	A	280	SER	3.5
1	B	468	PRO	3.5
1	B	280	SER	3.5
1	B	282	ARG	3.5
1	A	289	LEU	3.5
1	A	290	GLU	3.5
1	B	464	ALA	3.5
1	A	295	GLN	3.5
1	A	366	CYS	3.5
1	B	297	SER	3.4
1	B	425	LEU	3.4
1	A	356	GLY	3.3
1	A	393	CYS	3.3
1	B	467	PRO	3.3
1	B	448	LEU	3.3
1	A	420	TYR	3.3
1	B	465	LYS	3.3
1	A	475	LEU	3.3
1	B	366	CYS	3.3
1	A	278	CYS	3.2
1	A	373	ASN	3.2
1	A	442	LEU	3.2
1	B	337	ARG	3.2
1	B	334	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	298	ASN	3.1
1	A	340	GLY	3.1
1	A	288	ARG	3.1
1	B	479	HIS	3.1
1	A	460	GLN	3.0
1	A	267	LEU	3.0
1	A	418	ALA	3.0
1	A	424	VAL	3.0
1	B	274	VAL	3.0
1	B	277	VAL	3.0
1	B	330	TYR	3.0
1	A	368	ALA	3.0
1	A	464	ALA	2.9
1	A	272	HIS	2.9
1	B	447	GLU	2.9
1	A	409	ALA	2.9
1	B	338	LEU	2.9
1	B	437	ARG	2.9
1	A	470	GLY	2.9
1	B	268	THR	2.9
1	B	445	ASN	2.9
1	B	329	GLN	2.9
1	B	294	ARG	2.9
1	B	380	GLY	2.9
1	A	471	LYS	2.8
1	A	406	SER	2.8
1	A	474	SER	2.8
1	A	343	GLU	2.8
1	B	460	GLN	2.8
1	B	453	HIS	2.8
1	A	405	HIS	2.7
1	A	411	HIS	2.7
1	B	466	LEU	2.7
1	B	293	LEU	2.7
1	A	271	GLU	2.7
1	A	466	LEU	2.7
1	A	302	ARG	2.6
1	A	455	CYS	2.6
1	B	289	LEU	2.6
1	A	458	HIS	2.6
1	A	447	GLU	2.6
1	B	478	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	292	LEU	2.6
1	A	388	PHE	2.6
1	B	444	TYR	2.6
1	A	419	LEU	2.6
1	A	359	GLU	2.5
1	A	446	LEU	2.5
1	A	459	ARG	2.5
1	A	448	LEU	2.5
1	B	424	VAL	2.5
1	B	410	LEU	2.5
1	B	423	LEU	2.5
1	A	428	ALA	2.5
1	A	443	GLN	2.5
1	B	472	LEU	2.5
1	A	300	PHE	2.4
1	A	423	LEU	2.4
1	B	343	GLU	2.4
1	B	459	ARG	2.4
1	A	287	LEU	2.4
1	A	377	PHE	2.4
1	A	482	ARG	2.4
1	A	372	ASP	2.4
1	A	450	PHE	2.4
1	B	449	ALA	2.3
1	B	438	LYS	2.3
1	A	341	PHE	2.3
1	B	409	ALA	2.3
1	A	342	MET	2.3
1	B	301	SER	2.3
1	A	487	GLN	2.3
1	B	299	ILE	2.2
1	B	487	GLN	2.2
1	A	478	GLN	2.2
1	A	452	HIS	2.2
1	B	458	HIS	2.2
1	B	370	ASN	2.2
1	B	471	LYS	2.2
1	B	333	GLU	2.2
1	B	367	ARG	2.2
1	B	451	HIS	2.2
1	B	371	ALA	2.2
1	A	426	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	421	THR	2.2
1	B	470	GLY	2.2
1	B	267	LEU	2.2
1	B	387	LEU	2.1
1	B	302	ARG	2.1
1	A	334	PHE	2.1
1	B	405	HIS	2.1
1	B	352	LEU	2.1
1	A	391	LEU	2.1
1	A	444	TYR	2.1
1	A	402	ASP	2.1
1	A	453	HIS	2.1
1	A	379	GLU	2.1
1	B	279	LYS	2.0
1	A	265	ALA	2.0
1	B	484	GLN	2.0
1	B	308	TYR	2.0
1	A	338	LEU	2.0
1	A	436	LYS	2.0
1	A	279	LYS	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](#)

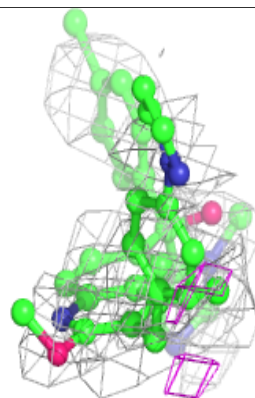
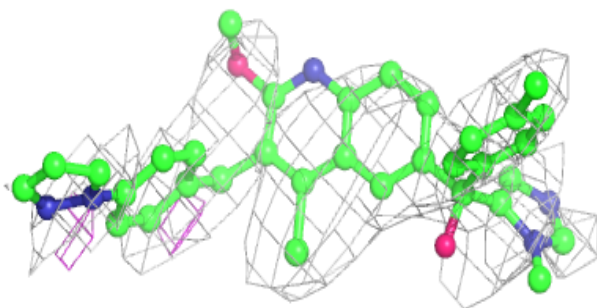
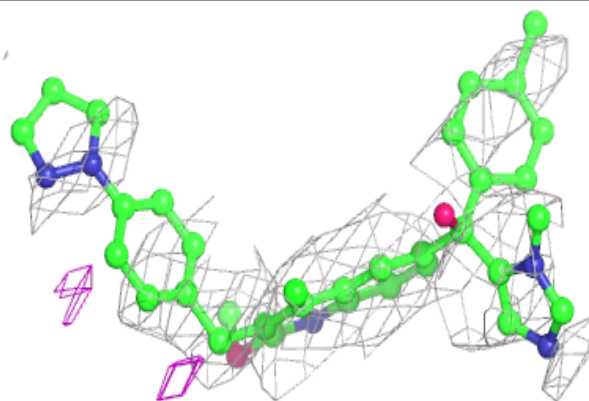
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	8A4	B	601	40/40	0.67	0.51	104,131,160,168	0
2	8A4	A	601	40/40	0.74	0.49	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.

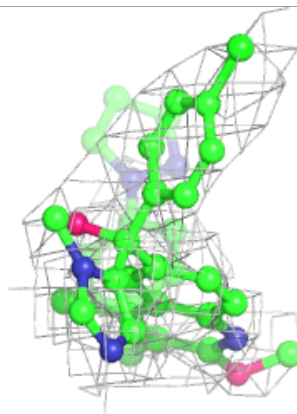
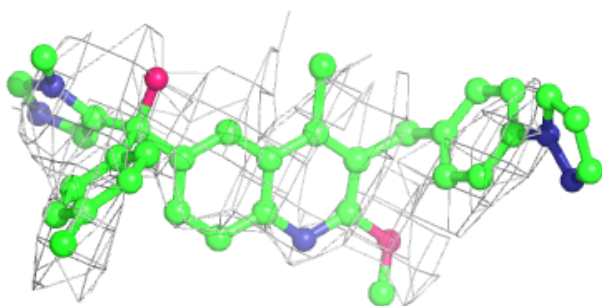
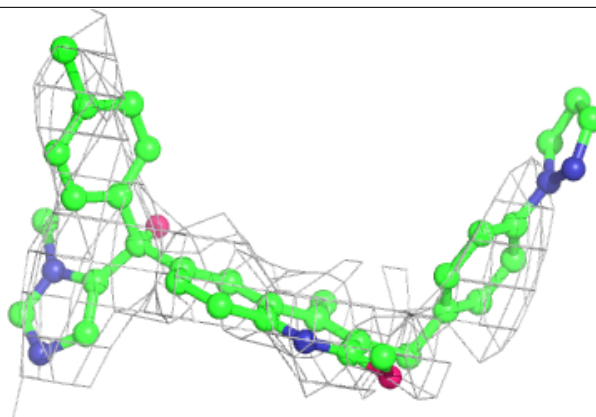
Electron density around 8A4 B 601:

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 [i](#)

There are no such residues in this entry.