



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6IAR / pdb_00006iar
Title : Tricyclic indazoles a novel class of selective estrogen receptor degrader antagonists
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Deposited on : 2018-11-27
Resolution : 1.84 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	: 1.8.4, CSD as541be (2020)
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	: 9.0.015 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)

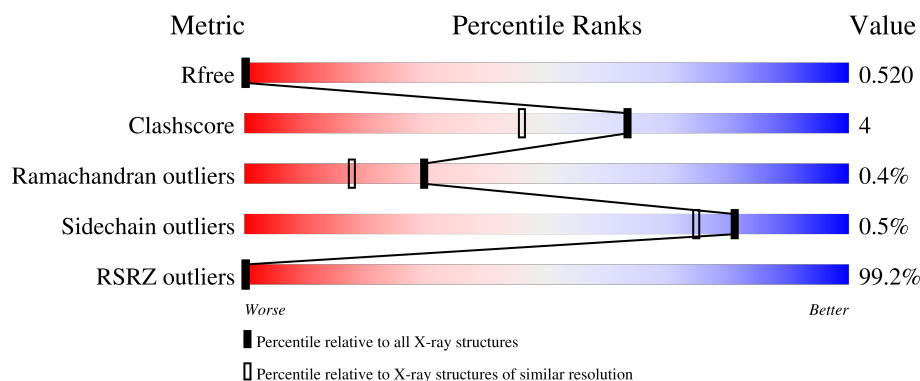
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	237	99% 93%7%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1992 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.

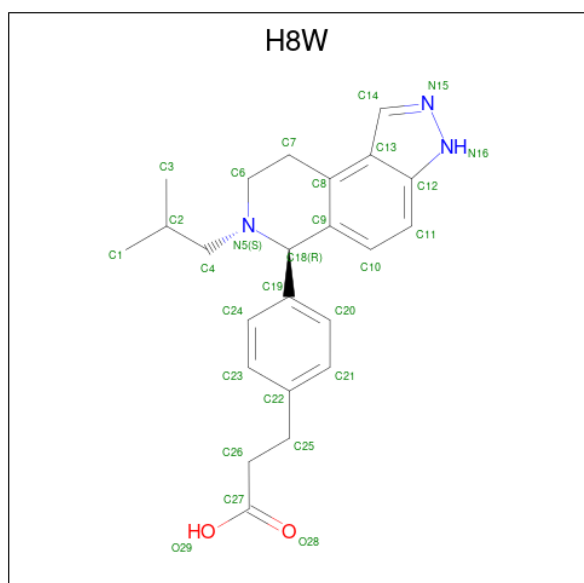
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	1865	1195	314	339	17	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P03372
A	?	-	GLU	deletion	UNP P03372
A	?	-	ALA	deletion	UNP P03372
A	381	SER	CYS	conflict	UNP P03372
A	417	SER	CYS	conflict	UNP P03372
A	?	-	LEU	deletion	UNP P03372
A	536	SER	LEU	conflict	UNP P03372

- Molecule 2 is 3-[4-[(6 {R})-7-(2-methylpropyl)-3,6,8,9-tetrahydropyrazolo[4,3-f]isoquinolin-6-yl]phenyl]propanoic acid (CCD ID: H8W) (formula: C₂₃H₂₇N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	23	3	2		

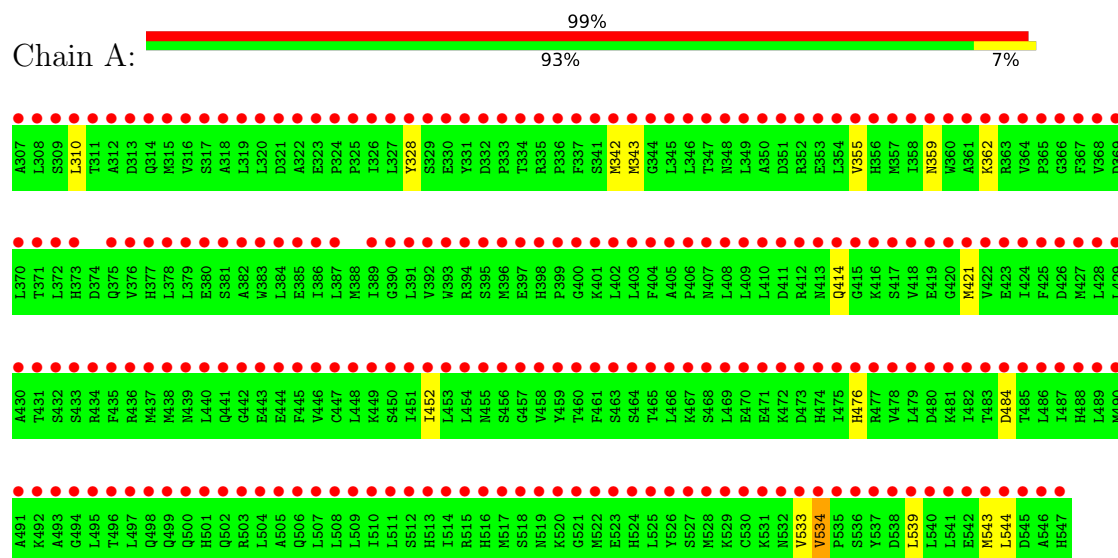
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	58.35Å 58.35Å 275.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.53 – 1.84 50.53 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.53-1.84) 99.9 (50.53-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.190 , 0.239 0.548 , 0.520	Depositor DCC
R_{free} test set	1293 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.49	EDS
Total number of atoms	1992	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H8W

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	1.22	2/1900 (0.1%)	1.08	0/2573

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	452	ILE	N-CA	5.97	1.53	1.46
1	A	484	ASP	N-CA	5.37	1.52	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1865	0	1871	15	1
2	A	28	0	0	5	0
3	A	99	0	0	1	0
All	All	1992	0	1871	15	1

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 4.

All (15) 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:343:MET:HE1	1:A:421:MET:CE	2.04	0.87
1:A:533:VAL:HG13	2:A:601:H8W:O28	1.84	0.78
1:A:533:VAL:HA	2:A:601:H8W:O28	1.85	0.76
1:A:343:MET:HE1	1:A:421:MET:HE1	1.76	0.65
1:A:355:VAL:HG22	1:A:543:MET:HE1	1.77	0.64
1:A:476:HIS:HE1	3:A:787:HOH:O	1.86	0.58
1:A:362:LYS:HE2	1:A:544:LEU:HD23	1.88	0.56
1:A:534:VAL:H	2:A:601:H8W:C27	2.23	0.52
1:A:533:VAL:CG1	2:A:601:H8W:O28	2.60	0.47
1:A:533:VAL:CA	2:A:601:H8W:O28	2.59	0.45
1:A:539:LEU:O	1:A:543:MET:HG3	2.16	0.45
1:A:342:MET:HE1	1:A:414:GLN:O	2.17	0.44
1:A:343:MET:CE	1:A:421:MET:CE	2.89	0.43
1:A:343:MET:HE1	1:A:421:MET:HE3	1.92	0.42
1:A:362:LYS:HE2	1:A:544:LEU:CD2	2.50	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TYR:OH	1:A:359:ASN:ND2[11_655]	2.14	0.06

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	231/237 (98%)	227 (98%)	3 (1%)	1 (0%)	30 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	534	VAL

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	207/214 (97%)	206 (100%)	1 (0%)	81	75

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU

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

Mol	Chain	Res	Type
1	A	398	HIS
1	A	476	HIS
1	A	488	HIS
1	A	513	HIS

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

1 ligand is 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	H8W	A	601	-	31,31,31	2.08	7 (22%)	36,44,44	3.83	7 (19%)

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	H8W	A	601	-	-	2/13/26/26	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	H8W	C14-N15	6.40	1.36	1.32
2	A	601	H8W	C19-C18	-4.13	1.47	1.52
2	A	601	H8W	C18-N5	3.80	1.53	1.47
2	A	601	H8W	C25-C26	-3.63	1.34	1.52
2	A	601	H8W	N16-N15	-3.37	1.34	1.36
2	A	601	H8W	C13-C14	-3.16	1.38	1.42
2	A	601	H8W	C11-C12	-2.77	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	H8W	C13-C14-N15	18.55	117.29	111.41
2	A	601	H8W	C14-N15-N16	-10.60	100.40	106.02
2	A	601	H8W	C19-C18-C9	-2.98	107.65	112.78
2	A	601	H8W	O28-C27-C26	-2.64	114.59	123.08
2	A	601	H8W	C10-C11-C12	-2.39	115.03	119.64
2	A	601	H8W	C26-C25-C22	2.16	120.58	112.70
2	A	601	H8W	C2-C4-N5	-2.02	110.53	115.91

There are no chirality outliers.

All (2) torsion outliers are listed below:

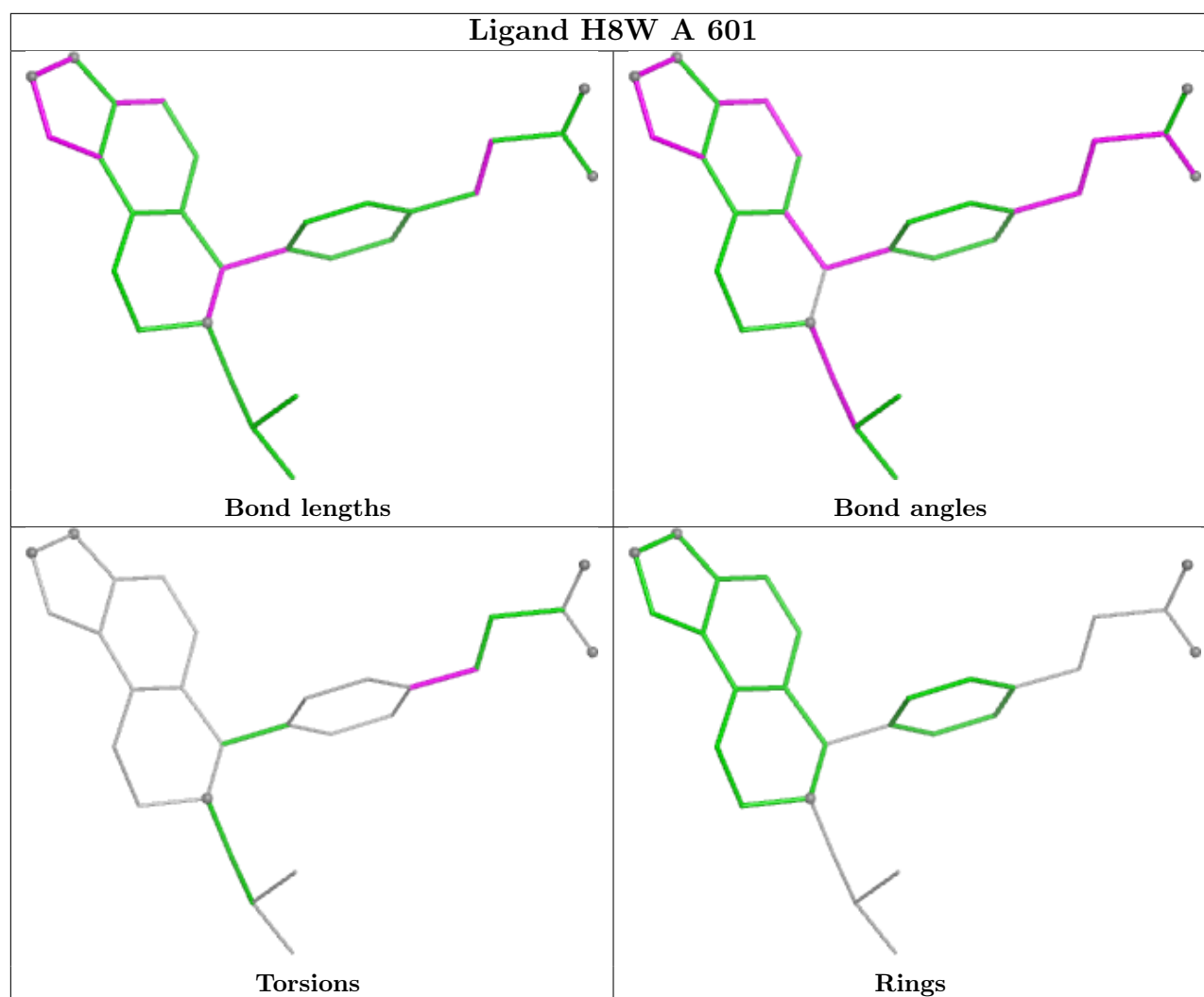
Mol	Chain	Res	Type	Atoms
2	A	601	H8W	C21-C22-C25-C26
2	A	601	H8W	C23-C22-C25-C26

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	H8W	5	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	337:PHE	C	341:SER	N	6.90
1	A	461:PHE	C	463:SER	N	3.20

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	237/237 (100%)	6.57	235 (99%) 0 0	15, 28, 50, 96	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	422	VAL	15.2
1	A	540	LEU	13.6
1	A	438	MET	13.0
1	A	537	TYR	12.6
1	A	326	ILE	12.5
1	A	335	ARG	12.1
1	A	348	ASN	11.9
1	A	341	SER	11.6
1	A	514	ILE	11.6
1	A	428	LEU	11.4
1	A	517	MET	11.4
1	A	521	GLY	11.2
1	A	418	VAL	11.0
1	A	482	ILE	11.0
1	A	541	LEU	11.0
1	A	526	TYR	10.7
1	A	485	THR	10.7
1	A	531	LYS	10.6
1	A	416	LYS	10.3
1	A	477	ARG	10.3
1	A	525	LEU	10.3
1	A	367	PHE	10.2
1	A	500	GLN	10.2
1	A	355	VAL	10.1
1	A	435	PHE	10.0
1	A	368	VAL	10.0
1	A	498	GLN	9.9

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Mol	Chain	Res	Type	RSRZ
1	A	410	LEU	9.9
1	A	320	LEU	9.8
1	A	459	TYR	9.8
1	A	501	HIS	9.7
1	A	522	MET	9.6
1	A	460	THR	9.5
1	A	533	VAL	9.4
1	A	405	ALA	9.3
1	A	475	ILE	9.3
1	A	386	ILE	9.2
1	A	544	LEU	9.2
1	A	532	ASN	9.1
1	A	539	LEU	9.1
1	A	495	LEU	9.1
1	A	461	PHE	9.1
1	A	490	MET	9.0
1	A	379	LEU	8.8
1	A	309	SER	8.8
1	A	354	LEU	8.8
1	A	380	GLU	8.7
1	A	349	LEU	8.6
1	A	392	VAL	8.6
1	A	481	LYS	8.6
1	A	487	ILE	8.6
1	A	351	ASP	8.6
1	A	372	LEU	8.6
1	A	440	LEU	8.5
1	A	316	VAL	8.5
1	A	318	ALA	8.5
1	A	382	ALA	8.4
1	A	397	GLU	8.3
1	A	409	LEU	8.3
1	A	464	SER	8.2
1	A	423	GLU	8.2
1	A	478	VAL	8.1
1	A	486	LEU	8.1
1	A	518	SER	8.1
1	A	535	PRO	8.1
1	A	408	LEU	8.0
1	A	387	LEU	7.9
1	A	337	PHE	7.9
1	A	534	VAL	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	321	ASP	7.8
1	A	331	TYR	7.8
1	A	458	VAL	7.7
1	A	404	PHE	7.7
1	A	370	LEU	7.4
1	A	512	SER	7.4
1	A	439	ASN	7.4
1	A	463	SER	7.4
1	A	317	SER	7.3
1	A	431	THR	7.3
1	A	342	MET	7.3
1	A	333	PRO	7.2
1	A	417	SER	7.2
1	A	543	MET	7.2
1	A	429	LEU	7.1
1	A	436	ARG	7.1
1	A	383	TRP	7.0
1	A	508	LEU	7.0
1	A	528	MET	7.0
1	A	313	ASP	7.0
1	A	538	ASP	7.0
1	A	491	ALA	6.9
1	A	365	PRO	6.9
1	A	310	LEU	6.9
1	A	530	CYS	6.9
1	A	507	LEU	6.8
1	A	414	GLN	6.8
1	A	510	ILE	6.8
1	A	542	GLU	6.8
1	A	473	ASP	6.6
1	A	504	LEU	6.6
1	A	346	LEU	6.6
1	A	415	GLY	6.5
1	A	373	HIS	6.5
1	A	446	VAL	6.5
1	A	381	SER	6.4
1	A	356	HIS	6.4
1	A	412	ARG	6.4
1	A	449	LYS	6.4
1	A	369	ASP	6.4
1	A	546	ALA	6.4
1	A	420	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	536	SER	6.4
1	A	403	LEU	6.4
1	A	419	GLU	6.4
1	A	492	LYS	6.4
1	A	442	GLY	6.3
1	A	319	LEU	6.3
1	A	520	LYS	6.3
1	A	332	ASP	6.3
1	A	413	ASN	6.3
1	A	497	LEU	6.3
1	A	437	MET	6.2
1	A	494	GLY	6.2
1	A	366	GLY	6.2
1	A	424	ILE	6.2
1	A	393	TRP	6.2
1	A	345	LEU	6.1
1	A	448	LEU	6.1
1	A	358	ILE	6.1
1	A	480	ASP	6.1
1	A	307	ALA	6.1
1	A	519	ASN	6.1
1	A	376	VAL	6.1
1	A	524	HIS	6.0
1	A	328	TYR	6.0
1	A	308	LEU	6.0
1	A	425	PHE	6.0
1	A	324	PRO	6.0
1	A	336	PRO	6.0
1	A	445	PHE	5.9
1	A	493	ALA	5.9
1	A	364	VAL	5.9
1	A	529	LYS	5.8
1	A	406	PRO	5.7
1	A	399	PRO	5.6
1	A	427	MET	5.6
1	A	433	SER	5.5
1	A	468	SER	5.5
1	A	456	SER	5.5
1	A	489	LEU	5.4
1	A	311	THR	5.4
1	A	402	LEU	5.3
1	A	359	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	479	LEU	5.2
1	A	396	MET	5.1
1	A	394	ARG	5.1
1	A	447	CYS	5.1
1	A	389	ILE	5.1
1	A	443	GLU	5.1
1	A	401	LYS	5.0
1	A	343	MET	5.0
1	A	362	LYS	5.0
1	A	474	HIS	4.9
1	A	323	GLU	4.9
1	A	506	GLN	4.8
1	A	421	MET	4.8
1	A	360	TRP	4.8
1	A	450	SER	4.8
1	A	411	ASP	4.8
1	A	314	GLN	4.7
1	A	471	GLU	4.7
1	A	391	LEU	4.7
1	A	378	LEU	4.7
1	A	469	LEU	4.7
1	A	353	GLU	4.6
1	A	476	HIS	4.6
1	A	545	ASP	4.6
1	A	527	SER	4.6
1	A	453	LEU	4.6
1	A	398	HIS	4.6
1	A	347	THR	4.6
1	A	466	LEU	4.6
1	A	509	LEU	4.5
1	A	426	ASP	4.5
1	A	472	LYS	4.4
1	A	363	ARG	4.4
1	A	434	ARG	4.4
1	A	407	ASN	4.4
1	A	344	GLY	4.4
1	A	451	ILE	4.4
1	A	330	GLU	4.4
1	A	484	ASP	4.4
1	A	377	HIS	4.4
1	A	513	HIS	4.4
1	A	325	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	432	SER	4.3
1	A	322	ALA	4.3
1	A	505	ALA	4.3
1	A	467	LYS	4.3
1	A	454	LEU	4.3
1	A	523	GLU	4.3
1	A	327	LEU	4.2
1	A	452	ILE	4.2
1	A	352	ARG	4.2
1	A	496	THR	4.1
1	A	334	THR	4.0
1	A	488	HIS	3.9
1	A	350	ALA	3.9
1	A	444	GLU	3.9
1	A	511	LEU	3.8
1	A	483	THR	3.8
1	A	357	MET	3.8
1	A	499	GLN	3.7
1	A	547	HIS	3.7
1	A	465	THR	3.7
1	A	395	SER	3.6
1	A	312	ALA	3.5
1	A	400	GLY	3.5
1	A	384	LEU	3.5
1	A	455	ASN	3.4
1	A	315	MET	3.4
1	A	375	GLN	3.3
1	A	515	ARG	3.2
1	A	441	GLN	3.1
1	A	329	SER	3.1
1	A	385	GLU	3.1
1	A	361	ALA	3.1
1	A	502	GLN	2.8
1	A	516	HIS	2.8
1	A	390	GLY	2.7
1	A	503	ARG	2.6
1	A	457	GLY	2.5
1	A	430	ALA	2.4
1	A	470	GLU	2.2
1	A	371	THR	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](#)

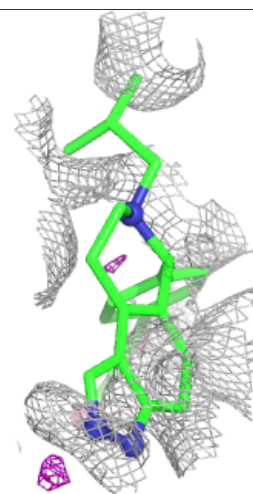
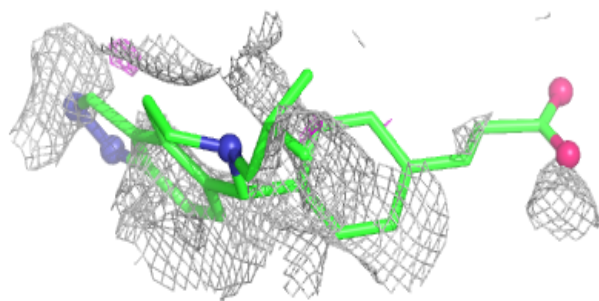
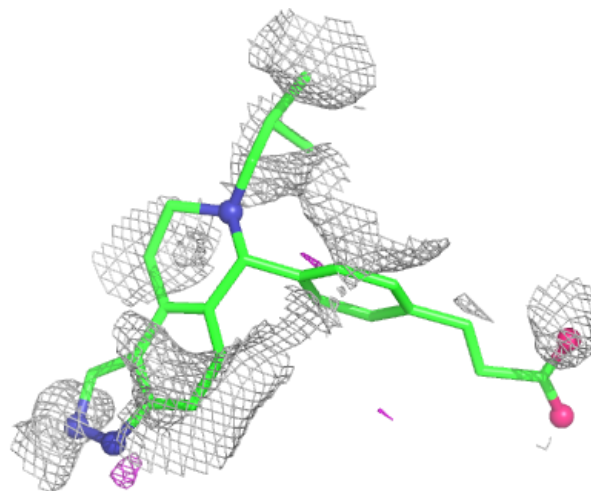
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	H8W	A	601	28/28	0.39	0.26	18,24,45,57	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 H8W 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.