



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:45 PM UTC

PDB ID : 4WZ8 / pdb_00004wz8
Title : Crystal structure of human-yeast chimera acetyl coA carboxylase CT domain bound to Compound 6
Authors : Vajdos, F.F.
Deposited on : 2014-11-18
Resolution : 2.23 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

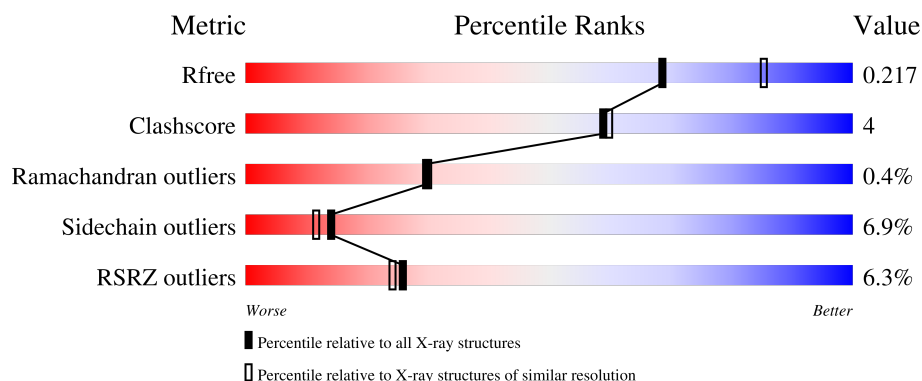
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

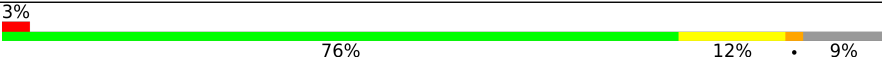
The reported resolution of this entry is 2.23 Å.

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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	B	769	
1	C	769	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12728 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 Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	698	Total	C	N	O	S	0	0	0
			5579	3548	964	1050	17			
1	C	698	Total	C	N	O	S	0	0	0
			5570	3536	965	1052	17			

There are 40 discrepancies between the modelled and reference sequences:

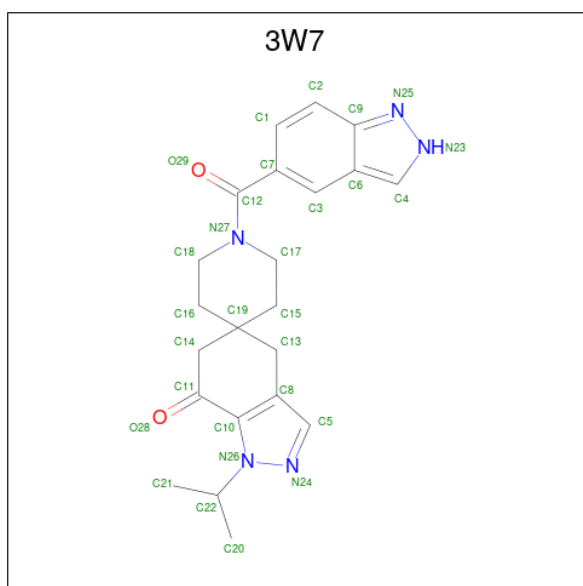
Chain	Residue	Modelled	Actual	Comment	Reference
B	1473	MET	-	initiating methionine	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
B	1919	GLN	GLU	engineered mutation	UNP Q00955
B	1920	ALA	PRO	engineered mutation	UNP Q00955
B	1925	PHE	HIS	engineered mutation	UNP Q00955
B	2028	GLU	GLN	engineered mutation	UNP Q00955
B	2030	THR	MET	engineered mutation	UNP Q00955
B	2032	GLU	GLY	engineered mutation	UNP Q00955
B	2234	LEU	-	expression tag	UNP Q00955
B	2235	GLU	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955
B	2240	HIS	-	expression tag	UNP Q00955
B	2241	HIS	-	expression tag	UNP Q00955
C	1473	MET	-	initiating methionine	UNP Q00955
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	1760	SER	PRO	engineered mutation	UNP Q00955
C	1762	LEU	ILE	engineered mutation	UNP Q00955

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1765	VAL	MET	engineered mutation	UNP Q00955
C	1919	GLN	GLU	engineered mutation	UNP Q00955
C	1920	ALA	PRO	engineered mutation	UNP Q00955
C	1925	PHE	HIS	engineered mutation	UNP Q00955
C	2028	GLU	GLN	engineered mutation	UNP Q00955
C	2030	THR	MET	engineered mutation	UNP Q00955
C	2032	GLU	GLY	engineered mutation	UNP Q00955
C	2234	LEU	-	expression tag	UNP Q00955
C	2235	GLU	-	expression tag	UNP Q00955
C	2236	HIS	-	expression tag	UNP Q00955
C	2237	HIS	-	expression tag	UNP Q00955
C	2238	HIS	-	expression tag	UNP Q00955
C	2239	HIS	-	expression tag	UNP Q00955
C	2240	HIS	-	expression tag	UNP Q00955
C	2241	HIS	-	expression tag	UNP Q00955

- Molecule 2 is 1'-(2H-indazol-5-ylcarbonyl)-1-(propan-2-yl)-1,4-dihydrospiro[indazole-5,4'-pi peridin]-7(6H)-one (CCD ID: 3W7) (formula: C₂₂H₂₅N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			29	22	5	2		
2	C	1	Total	C	N	O	0	0
			29	22	5	2		

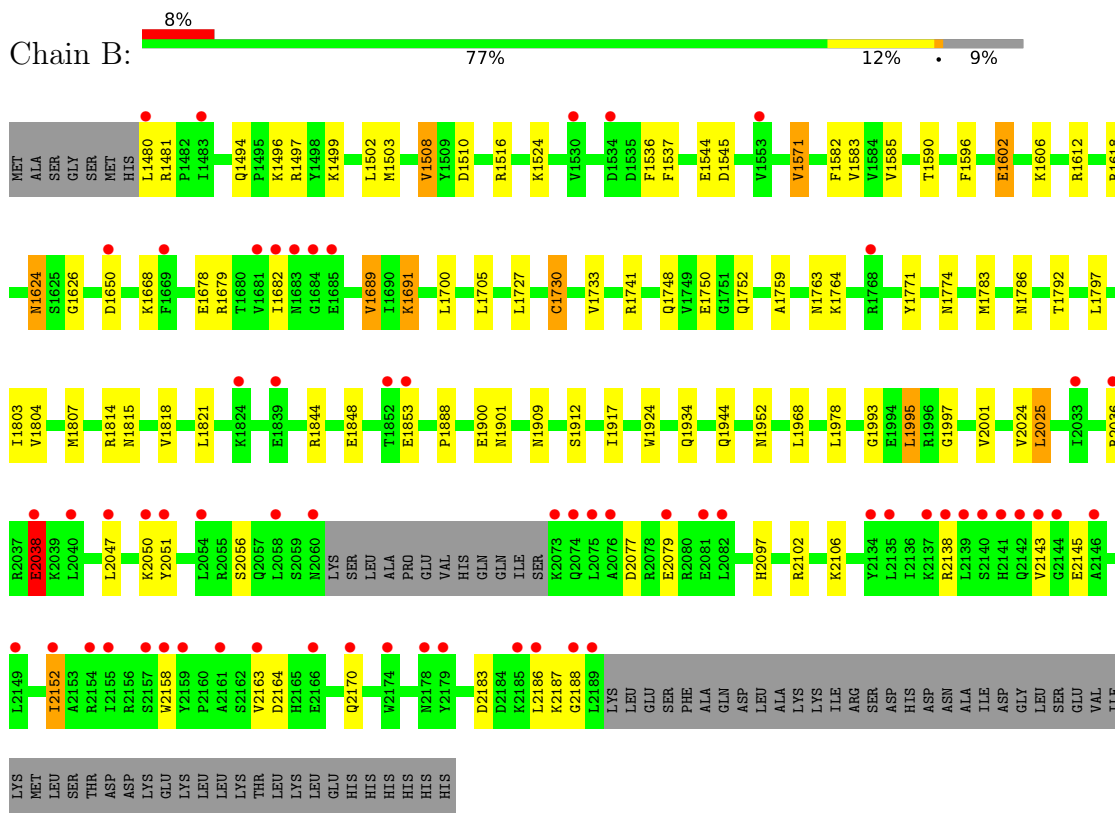
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	743	Total 743	O 743	0	0
3	C	778	Total 778	O 778	0	0

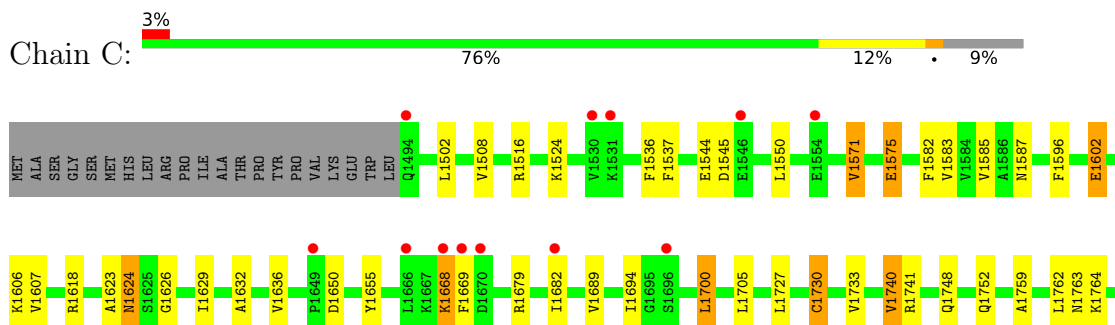
3 Residue-property plots

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: Acetyl-CoA carboxylase



• Molecule 1: Acetyl-CoA carboxylase



GLU	T1992	Y1771
SER	G1993	
PHE	E1994	N1774
ALA	L1995	
GLN	R1996	M1783
ASP	G1997	V1788
LEU		
ALA	V2001	
LYS		L1797
LYS	V2018	
ILE		I1803
ARG	L2025	V1804
SER		
ASP	L2040	M1807
HIS		
ASP	M2044	N1815
ASN		
ALA	L2047	V1818
ILE		
ASP	Y2051	V1843
GLY		R1844
LEU	L2054	
SER	R2055	E1848
GLU		
VAL	M2060	T1852
ILE	K2061	E1853
LYS	S2062	
MET		V1879
LEU	E2066	
SER	V2067	P1888
THR	H2068	
ASP	H2069	E1900
ASP	Q2070	N1901
LYS	I2071	
LYS	S2072	A1908
LEU		N1909
LEU	E2079	PH910
LYS		N1911
LYS		S1912
THR	L2083	
LEU		I1917
LYS		
LEU	Q2142	Q1922
GLU	V2143	V1923
HIS	G2144	W1924
HIS	E2145	
HIS	L2149	K1931
HIS		
HIS	L2152	Q1934
	D2164	Q1944
	Q2170	N1952
	K2185	L1968
	L2189	L1978
	K2190	
	L2191	P1990
		P1991

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.52Å 138.03Å 184.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.59 – 2.23 110.59 – 2.23	Depositor EDS
% Data completeness (in resolution range)	97.8 (110.59-2.23) 97.8 (110.59-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.22Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5	Depositor
R, R_{free}	0.177 , 0.209 0.182 , 0.217	Depositor DCC
R_{free} test set	5766 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12728	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: 3W7

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	B	0.84	0/5699	1.24	10/7718 (0.1%)
1	C	0.84	1/5687 (0.0%)	1.22	13/7698 (0.2%)
All	All	0.84	1/11386 (0.0%)	1.23	23/15416 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1636	VAL	CA-C	5.66	1.59	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1740	VAL	N-CA-CB	6.39	120.16	110.58
1	B	1508	VAL	N-CA-CB	6.24	117.43	110.51
1	B	1596	PHE	CA-CB-CG	6.04	119.84	113.80
1	C	1596	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	1730	CYS	N-CA-C	-5.88	100.63	108.74
1	B	2152	ILE	N-CA-CB	5.85	119.35	110.58
1	C	2142	GLN	CA-C-N	5.81	132.43	121.97
1	C	2142	GLN	C-N-CA	5.81	132.43	121.97
1	B	1786	ASN	CA-CB-CG	5.72	118.33	112.60
1	C	1843	VAL	CB-CA-C	-5.68	103.75	112.05
1	C	2189	LEU	CA-C-N	5.67	132.36	121.54
1	C	2189	LEU	C-N-CA	5.67	132.36	121.54
1	C	1545	ASP	CA-C-N	5.65	127.85	120.28
1	C	1545	ASP	C-N-CA	5.65	127.85	120.28
1	C	2152	ILE	N-CA-CB	5.64	119.04	110.58
1	C	1788	VAL	N-CA-C	-5.63	105.03	110.72
1	C	1730	CYS	N-CA-C	-5.41	101.27	108.74
1	B	2056	SER	CA-C-N	5.25	127.27	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2056	SER	C-N-CA	5.25	127.27	120.44
1	B	1545	ASP	CA-C-N	5.17	127.21	120.28
1	B	1545	ASP	C-N-CA	5.17	127.21	120.28
1	B	1624	ASN	N-CA-C	5.17	115.87	108.74
1	C	1624	ASN	N-CA-C	5.00	115.65	108.74

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	B	5579	0	5519	52	0
1	C	5570	0	5513	54	0
2	B	29	0	25	2	0
2	C	29	0	25	3	0
3	B	743	0	0	3	0
3	C	778	0	0	3	0
All	All	12728	0	11082	98	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 4.

All (98) 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:1763:ASN:HD21	1:B:1771:TYR:H	1.19	0.89
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.20	0.87
1:B:1764:LYS:HE3	2:C:2301:3W7:H25	1.40	0.84
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.28	0.80
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.35	0.74
1:B:1821:LEU:HD22	3:B:2782:HOH:O	1.87	0.74
1:C:1730:CYS:HA	1:C:1752:GLN:HE21	1.56	0.70
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.08	0.69
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1497:ARG:HD3	1:B:1510:ASP:OD2	1.97	0.65
1:C:1550:LEU:HD21	1:C:1607:VAL:HG22	1.80	0.63
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.63	0.63
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.97	0.63
1:C:1537:PHE:HD2	1:C:1571:VAL:HG13	1.65	0.61
1:B:1759:ALA:H	1:B:1774:ASN:ND2	1.98	0.61
1:C:2051:TYR:HE2	1:C:2079:GLU:HG3	1.66	0.61
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.67	0.60
1:B:2138:ARG:HH12	1:B:2183:ASP:HA	1.66	0.59
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.38	0.58
1:C:1537:PHE:CD2	1:C:1571:VAL:HG13	2.39	0.58
1:C:2185:LYS:HG3	1:C:2189:LEU:HD13	1.87	0.57
1:B:2102:ARG:HH21	1:C:1700:LEU:HB2	1.71	0.56
1:B:2102:ARG:NH1	1:B:2106:LYS:HD3	2.21	0.56
1:C:1668:LYS:HG3	1:C:1669:PHE:HD1	1.69	0.56
1:B:2102:ARG:NH2	1:C:1700:LEU:HB2	2.21	0.55
1:B:2102:ARG:HH12	1:B:2106:LYS:HD3	1.71	0.55
1:B:1678:GLU:HB3	1:B:1689:VAL:HG13	1.89	0.55
1:B:2051:TYR:HE1	1:B:2079:GLU:HG3	1.72	0.53
1:C:2051:TYR:HE2	1:C:2079:GLU:CG	2.21	0.53
1:C:1922:GLN:NE2	3:C:2708:HOH:O	2.40	0.53
1:B:1612:ARG:O	1:B:1814:ARG:NH2	2.43	0.52
1:C:1748:GLN:HE22	1:C:1783:MET:HB2	1.73	0.52
1:C:2060:ASN:HD22	1:C:2062:SER:H	1.58	0.51
2:B:2301:3W7:H25	1:C:1764:LYS:HZ2	1.57	0.51
1:C:2060:ASN:ND2	1:C:2062:SER:H	2.10	0.50
1:C:1624:ASN:HD21	1:C:1733:VAL:H	1.60	0.49
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.10	0.49
1:C:2044:MET:HE1	1:C:2083:LEU:HD13	1.93	0.49
1:B:1815:ASN:ND2	1:B:1944:GLN:HE22	2.10	0.49
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.59	0.49
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.10	0.48
1:C:2025:LEU:HD22	2:C:2301:3W7:H1	1.95	0.48
1:C:2142:GLN:HB3	1:C:2190:LYS:HG3	1.95	0.48
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	2.11	0.48
1:B:2050:LYS:HB3	3:B:3109:HOH:O	2.14	0.48
1:B:1750:GLU:HG3	1:B:1792:THR:CG2	2.44	0.48
1:B:2158:TRP:CH2	1:B:2186:LEU:HD21	2.49	0.48
1:C:1741:ARG:HH22	1:C:1934:GLN:NE2	2.11	0.48
2:C:2301:3W7:H16	2:C:2301:3W7:C3	2.42	0.48
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1689:VAL:HG22	1:B:1691:LYS:HE3	1.97	0.47
1:C:1575:GLU:HG2	3:C:2551:HOH:O	2.14	0.47
1:C:2068:HIS:HE1	3:C:2403:HOH:O	1.98	0.47
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	1.95	0.47
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.15	0.46
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.15	0.46
1:C:1624:ASN:ND2	1:C:1733:VAL:H	2.14	0.46
1:B:1759:ALA:H	1:B:1774:ASN:HD21	1.62	0.46
1:B:1741:ARG:HH22	1:B:1934:GLN:HE22	1.64	0.46
1:B:2024:VAL:HG12	1:B:2025:LEU:HD13	1.98	0.45
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.99	0.45
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.14	0.44
1:B:1544:GLU:OE1	1:B:1602:GLU:OE2	2.35	0.44
1:B:1909:ASN:HB3	1:B:1912:SER:HB2	2.00	0.44
1:C:1990:PRO:HB2	1:C:1991:PRO:HD2	1.99	0.44
1:C:1741:ARG:HH22	1:C:1934:GLN:HE22	1.64	0.44
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.65	0.44
1:C:1909:ASN:HB3	1:C:1912:SER:HB2	1.99	0.44
1:C:1544:GLU:OE1	1:C:1602:GLU:OE2	2.35	0.43
1:B:2164:ASP:H	1:B:2170:GLN:NE2	2.16	0.43
1:B:2102:ARG:HD2	1:C:1694:ILE:HA	2.00	0.43
1:C:1582:PHE:CD1	1:C:1807:MET:HE1	2.54	0.43
1:B:1582:PHE:CD1	1:B:1807:MET:HE1	2.54	0.43
1:C:1624:ASN:HD22	1:C:1626:GLY:H	1.67	0.43
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.66	0.43
1:C:1655:TYR:CE1	1:C:1689:VAL:HG22	2.54	0.43
1:C:1952:ASN:OD1	1:C:1993:GLY:HA2	2.20	0.42
1:B:1705:LEU:HD22	1:C:1997:GLY:HA2	2.02	0.42
1:B:1995:LEU:HD12	1:B:1995:LEU:HA	1.98	0.42
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.68	0.42
1:B:2038:GLU:HG3	3:B:2520:HOH:O	2.19	0.42
1:B:2158:TRP:HH2	1:B:2186:LEU:HD21	1.85	0.42
1:C:1727:LEU:HB2	1:C:1803:ILE:HD11	2.02	0.42
1:C:1900:GLU:HA	1:C:1917:ILE:O	2.20	0.42
1:B:1900:GLU:HA	1:B:1917:ILE:O	2.20	0.41
1:C:2152:ILE:H	1:C:2152:ILE:HG13	1.71	0.41
1:B:2187:LYS:HA	1:B:2188:GLY:HA2	1.82	0.41
1:B:1499:LYS:HD3	1:B:1590:THR:HB	2.01	0.41
1:B:1997:GLY:HA2	1:C:1705:LEU:CD2	2.50	0.41
1:B:2025:LEU:HD21	1:C:1629:ILE:HD13	2.03	0.41
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1879:VAL:HG13	1:C:1931:LYS:HE2	2.02	0.41
1:C:2136:ILE:HD11	1:C:2152:ILE:HG23	2.03	0.41
1:C:1730:CYS:HA	1:C:1752:GLN:NE2	2.31	0.40
1:B:1997:GLY:HA2	1:C:1705:LEU:HD22	2.02	0.40
2:B:2301:3W7:H25	1:C:1764:LYS:NZ	2.20	0.40
1:B:1952:ASN:OD1	1:B:1993:GLY:HA2	2.22	0.40
1:B:2163:VAL:HG13	1:B:2170:GLN:HG2	2.04	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	B	694/769 (90%)	672 (97%)	19 (3%)	3 (0%)	30	30
1	C	696/769 (90%)	679 (98%)	15 (2%)	2 (0%)	36	38
All	All	1390/1538 (90%)	1351 (97%)	34 (2%)	5 (0%)	30	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2143	VAL
1	C	2190	LYS
1	C	2143	VAL
1	B	1481	ARG
1	B	2038	GLU

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	B	594/658 (90%)	558 (94%)	36 (6%)	17	15
1	C	594/658 (90%)	548 (92%)	46 (8%)	12	9
All	All	1188/1316 (90%)	1106 (93%)	82 (7%)	14	11

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1480	LEU
1	B	1502	LEU
1	B	1503	MET
1	B	1508	VAL
1	B	1516	ARG
1	B	1524	LYS
1	B	1536	PHE
1	B	1571	VAL
1	B	1583	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1606	LYS
1	B	1618	ARG
1	B	1650	ASP
1	B	1668	LYS
1	B	1679	ARG
1	B	1682	ILE
1	B	1689	VAL
1	B	1691	LYS
1	B	1700	LEU
1	B	1797	LEU
1	B	1804	VAL
1	B	1853	GLU
1	B	1901	ASN
1	B	1924	TRP
1	B	1968	LEU
1	B	1978	LEU
1	B	1995	LEU
1	B	2001	VAL
1	B	2025	LEU
1	B	2036	ARG
1	B	2038	GLU
1	B	2047	LEU

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Mol	Chain	Res	Type
1	B	2077	ASP
1	B	2145	GLU
1	B	2152	ILE
1	C	1502	LEU
1	C	1508	VAL
1	C	1516	ARG
1	C	1524	LYS
1	C	1536	PHE
1	C	1571	VAL
1	C	1575	GLU
1	C	1583	VAL
1	C	1585	VAL
1	C	1602	GLU
1	C	1606	LYS
1	C	1618	ARG
1	C	1650	ASP
1	C	1668	LYS
1	C	1679	ARG
1	C	1682	ILE
1	C	1700	LEU
1	C	1740	VAL
1	C	1762	LEU
1	C	1797	LEU
1	C	1804	VAL
1	C	1843	VAL
1	C	1853	GLU
1	C	1879	VAL
1	C	1901	ASN
1	C	1924	TRP
1	C	1968	LEU
1	C	1978	LEU
1	C	1994	GLU
1	C	1995	LEU
1	C	2001	VAL
1	C	2018	VAL
1	C	2040	LEU
1	C	2047	LEU
1	C	2054	LEU
1	C	2055	ARG
1	C	2060	ASN
1	C	2061	LYS
1	C	2066	GLU

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Mol	Chain	Res	Type
1	C	2070	GLN
1	C	2071	ILE
1	C	2072	SER
1	C	2083	LEU
1	C	2145	GLU
1	C	2152	ILE
1	C	2191	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1540	ASN
1	B	1587	ASN
1	B	1624	ASN
1	B	1640	GLN
1	B	1648	ASN
1	B	1673	ASN
1	B	1683	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1774	ASN
1	B	1815	ASN
1	B	1837	ASN
1	B	1909	ASN
1	B	1919	GLN
1	B	1934	GLN
1	B	1937	ASN
1	B	1960	GLN
1	B	2019	ASN
1	B	2045	ASN
1	B	2092	GLN
1	B	2097	HIS
1	B	2170	GLN
1	C	1517	GLN
1	C	1522	GLN
1	C	1525	ASN
1	C	1587	ASN
1	C	1605	ASN

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Mol	Chain	Res	Type
1	C	1624	ASN
1	C	1673	ASN
1	C	1683	ASN
1	C	1748	GLN
1	C	1752	GLN
1	C	1763	ASN
1	C	1774	ASN
1	C	1815	ASN
1	C	1909	ASN
1	C	1922	GLN
1	C	1934	GLN
1	C	1937	ASN
1	C	1941	ASN
1	C	2060	ASN
1	C	2068	HIS
1	C	2074	GLN
1	C	2142	GLN
1	C	2165	HIS
1	C	2170	GLN
1	C	2178	ASN

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	3W7	B	2301	-	31,33,33	1.25	5 (16%)	36,50,50	2.66	14 (38%)
2	3W7	C	2301	-	31,33,33	1.25	4 (12%)	36,50,50	2.77	11 (30%)

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	3W7	B	2301	-	-	0/12/38/38	0/5/5/5
2	3W7	C	2301	-	-	0/12/38/38	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2301	3W7	C13-C8	-3.35	1.46	1.50
2	B	2301	3W7	C9-N25	3.19	1.37	1.33
2	C	2301	3W7	C9-N25	2.96	1.37	1.33
2	B	2301	3W7	C9-C6	-2.44	1.38	1.43
2	B	2301	3W7	C12-N27	2.42	1.39	1.34
2	B	2301	3W7	C13-C8	-2.40	1.47	1.50
2	B	2301	3W7	C2-C9	-2.09	1.38	1.40
2	C	2301	3W7	C2-C9	-2.07	1.38	1.40
2	C	2301	3W7	C9-C6	-2.06	1.39	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2301	3W7	C7-C3-C6	-9.52	114.21	121.92
2	B	2301	3W7	C7-C3-C6	-8.25	115.23	121.92
2	C	2301	3W7	C1-C2-C9	-6.64	112.86	120.80
2	B	2301	3W7	C4-N23-N25	-5.81	103.70	112.59
2	B	2301	3W7	C1-C2-C9	-5.23	114.54	120.80
2	C	2301	3W7	C4-N23-N25	-4.87	105.13	112.59
2	B	2301	3W7	C13-C8-C10	4.50	123.97	120.36
2	C	2301	3W7	C13-C8-C10	4.32	123.82	120.36
2	B	2301	3W7	C9-N25-N23	4.12	114.01	105.24
2	C	2301	3W7	C1-C7-C3	4.05	123.93	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2301	3W7	C9-N25-N23	3.80	113.34	105.24
2	B	2301	3W7	C1-C7-C3	3.71	123.54	119.25
2	B	2301	3W7	C6-C4-N23	3.67	112.28	108.93
2	C	2301	3W7	C15-C19-C14	-2.95	106.77	110.32
2	C	2301	3W7	C18-N27-C17	2.88	118.57	112.68
2	C	2301	3W7	C13-C8-C5	-2.85	130.16	133.84
2	B	2301	3W7	C19-C13-C8	-2.83	109.89	113.11
2	B	2301	3W7	C15-C19-C14	-2.53	107.28	110.32
2	C	2301	3W7	C19-C13-C8	-2.47	110.30	113.11
2	B	2301	3W7	C16-C19-C13	2.46	113.28	110.32
2	B	2301	3W7	C13-C8-C5	-2.41	130.72	133.84
2	B	2301	3W7	C18-N27-C17	2.40	117.57	112.68
2	C	2301	3W7	C6-C4-N23	2.17	110.91	108.93
2	B	2301	3W7	O29-C12-N27	2.07	125.61	122.35
2	B	2301	3W7	O29-C12-C7	-2.01	116.30	120.29

There are no chirality outliers.

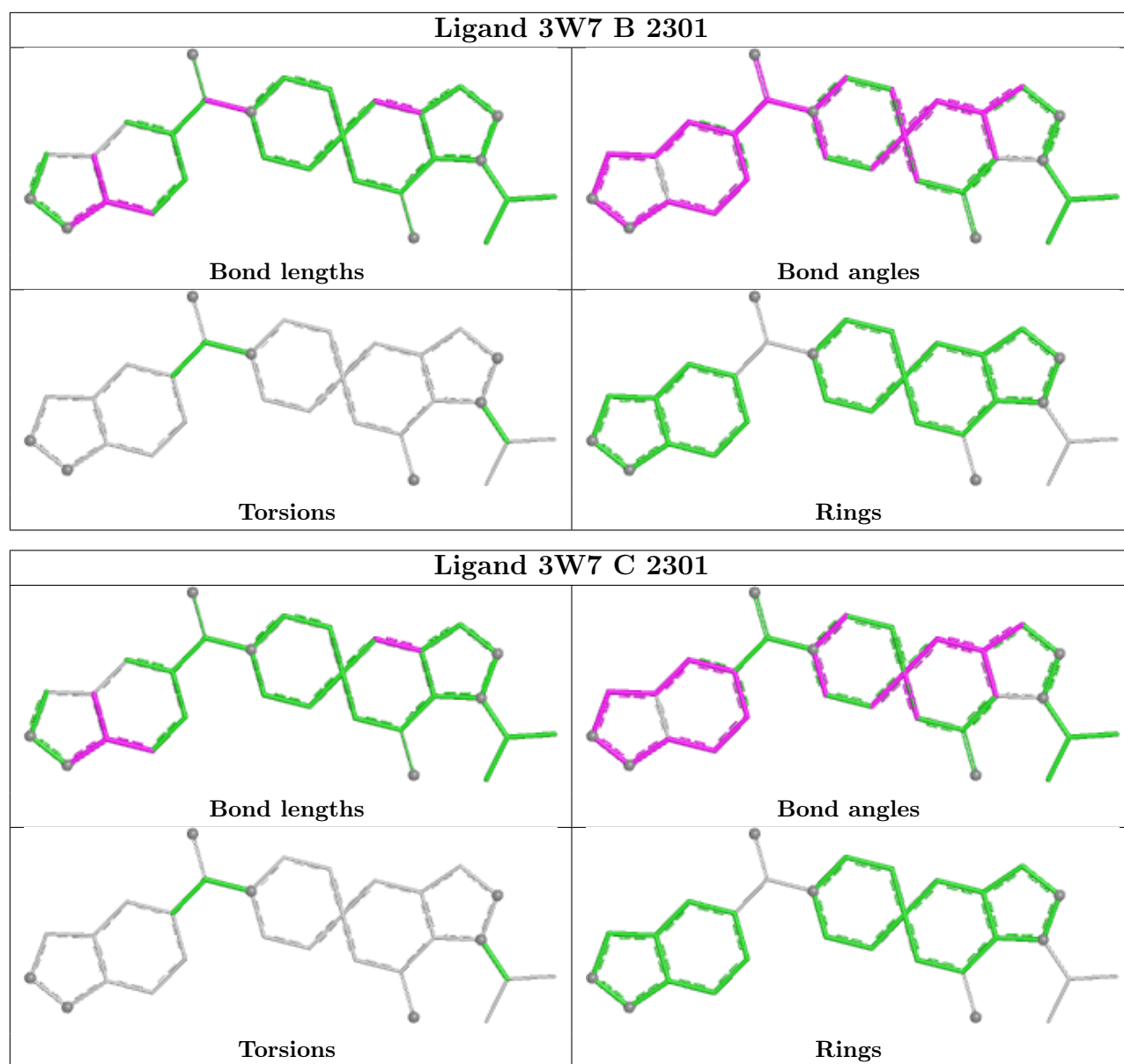
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2301	3W7	2	0
2	C	2301	3W7	3	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	B	698/769 (90%)	0.15	63 (9%) 15 14	19, 35, 80, 118	0
1	C	698/769 (90%)	0.02	25 (3%) 46 46	19, 35, 68, 126	0
All	All	1396/1538 (90%)	0.08	88 (6%) 26 24	19, 35, 74, 126	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2191	LEU	8.1
1	C	2189	LEU	7.2
1	B	2189	LEU	6.8
1	B	2143	VAL	6.2
1	B	2139	LEU	4.8
1	C	2144	GLY	4.7
1	B	2073	LYS	4.6
1	C	2143	VAL	4.4
1	B	2075	LEU	4.3
1	B	2179	TYR	4.3
1	B	2186	LEU	4.2
1	B	2185	LYS	4.1
1	B	2144	GLY	3.9
1	B	1553	VAL	3.9
1	B	2079	GLU	3.8
1	B	2054	LEU	3.8
1	B	1683	ASN	3.7
1	B	2074	GLN	3.7
1	B	2163	VAL	3.5
1	B	2058	LEU	3.5
1	C	1669	PHE	3.5
1	C	2190	LYS	3.4
1	B	2076	ALA	3.4
1	B	2154	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1682	ILE	3.2
1	B	2033	ILE	3.1
1	B	2138	ARG	3.1
1	B	1480	LEU	3.0
1	B	2060	ASN	3.0
1	B	1669	PHE	3.0
1	B	2134	TYR	3.0
1	B	2038	GLU	2.9
1	B	1650	ASP	2.8
1	B	2051	TYR	2.8
1	B	1685	GLU	2.8
1	B	2157	SER	2.7
1	B	2146	ALA	2.7
1	B	2158	TRP	2.7
1	B	2161	ALA	2.7
1	B	2142	GLN	2.6
1	B	2140	SER	2.6
1	B	1534	ASP	2.6
1	B	1483	ILE	2.6
1	C	1670	ASP	2.5
1	B	1684	GLY	2.5
1	C	1530	VAL	2.5
1	B	2166	GLU	2.5
1	C	1546	GLU	2.5
1	B	2159	TYR	2.5
1	C	2149	LEU	2.5
1	B	1852	THR	2.4
1	B	1681	VAL	2.4
1	B	1530	VAL	2.4
1	B	2174	TRP	2.4
1	B	2141	HIS	2.4
1	B	2082	LEU	2.3
1	C	1910	PRO	2.3
1	B	1853	GLU	2.3
1	C	2145	GLU	2.3
1	C	1852	THR	2.3
1	B	2050	LYS	2.3
1	B	1768	ARG	2.2
1	B	2152	ILE	2.2
1	B	2040	LEU	2.2
1	B	2178	ASN	2.2
1	B	2170	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	1668	LYS	2.2
1	C	1649	PRO	2.2
1	B	1839	GLU	2.2
1	B	2188	GLY	2.2
1	C	1554	GLU	2.1
1	B	2135	LEU	2.1
1	C	2152	ILE	2.1
1	C	2070	GLN	2.1
1	C	1696	SER	2.1
1	C	1494	GLN	2.1
1	C	1682	ILE	2.1
1	B	2036	ARG	2.0
1	B	1824	LYS	2.0
1	B	2137	LYS	2.0
1	C	1531	LYS	2.0
1	B	2081	GLU	2.0
1	C	1912	SER	2.0
1	C	1908	ALA	2.0
1	B	2047	LEU	2.0
1	B	2149	LEU	2.0
1	C	1666	LEU	2.0
1	B	2155	ILE	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.

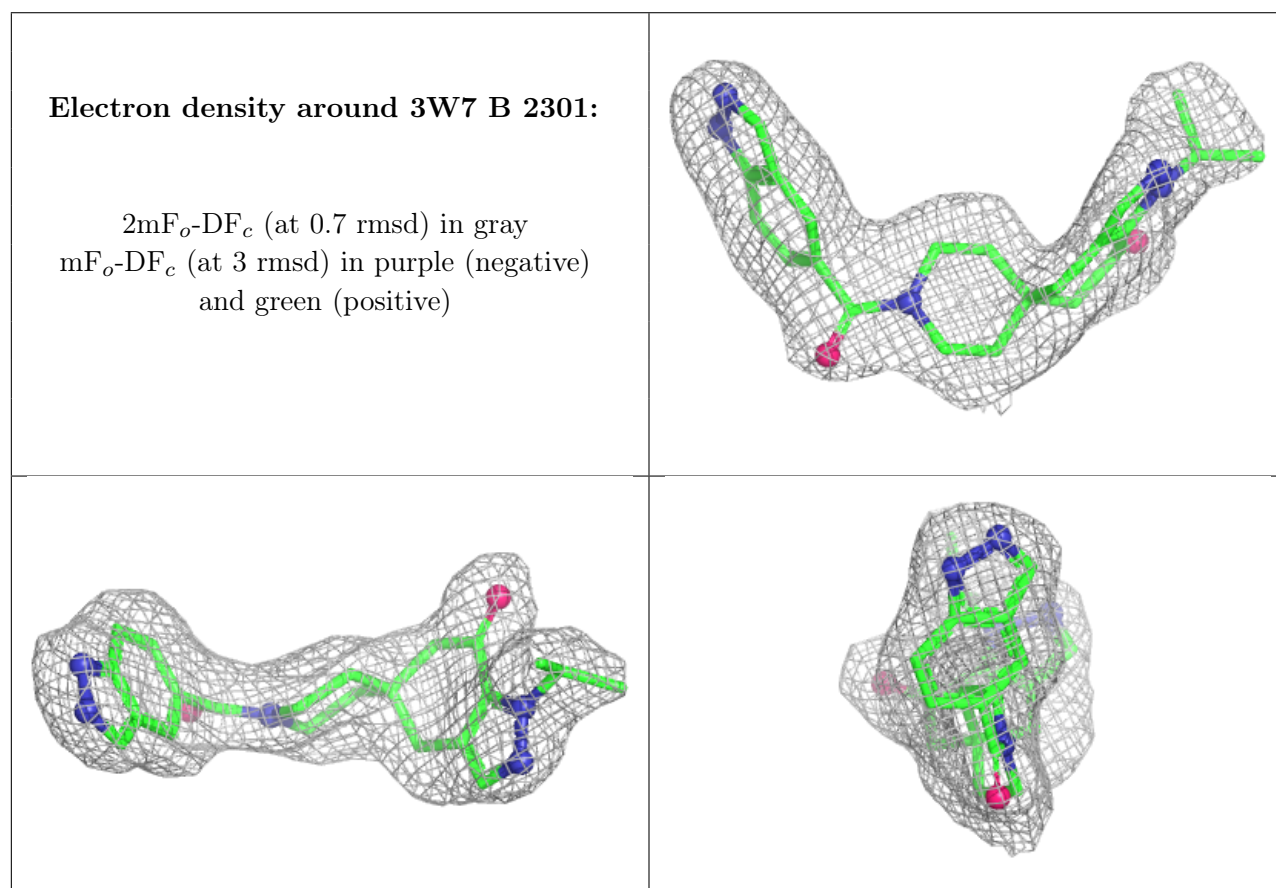
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3W7	B	2301	29/29	0.96	0.08	27,34,45,46	0

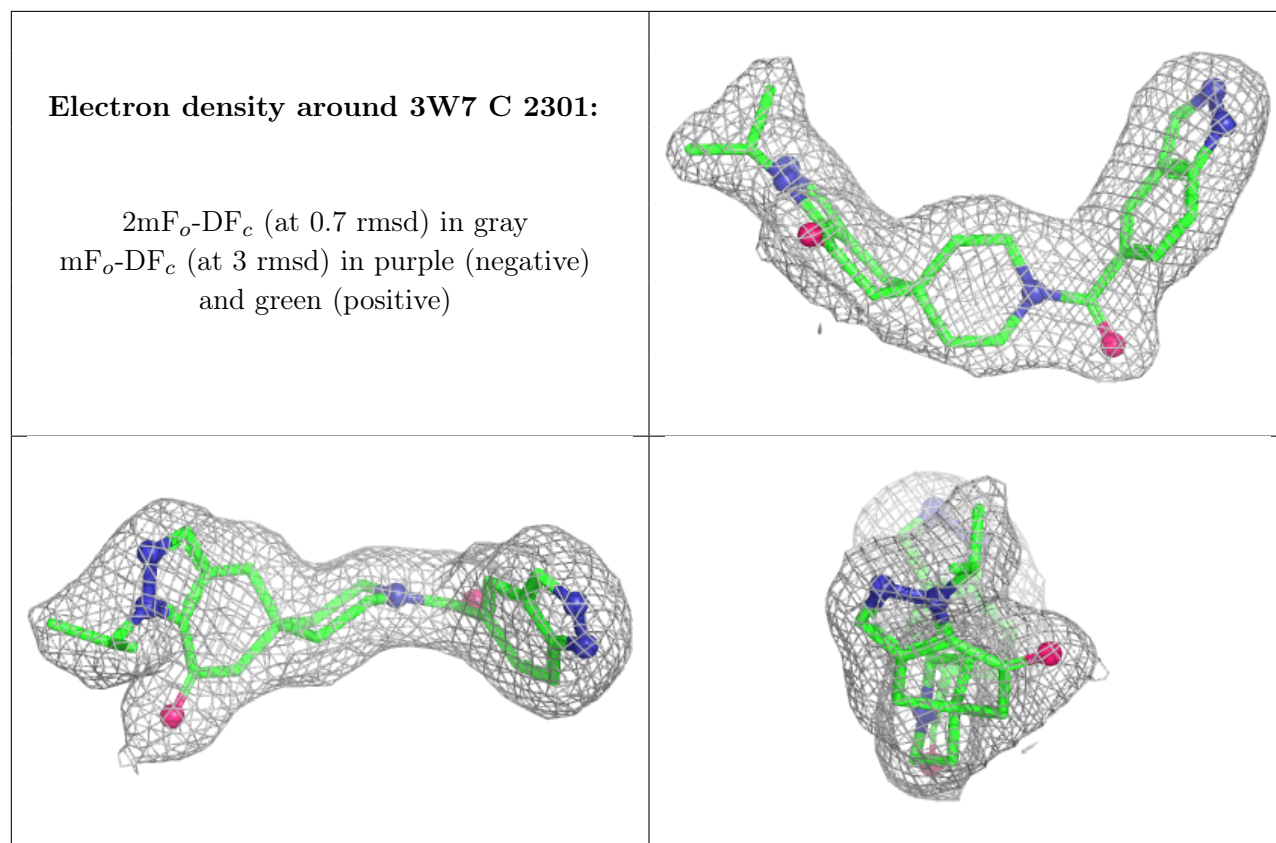
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3W7	C	2301	29/29	0.97	0.06	24,29,34,36	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.