



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:29 PM EDT

PDB ID : 7FOR / pdb_00007for
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P08C12 from the F2X-Universal Library
Authors : Barthel, T.; Wollenhaupt, J.; Lima, G.M.A.; Wahl, M.C.; Weiss, M.S.
Deposited on : 2022-08-26
Resolution : 2.03 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

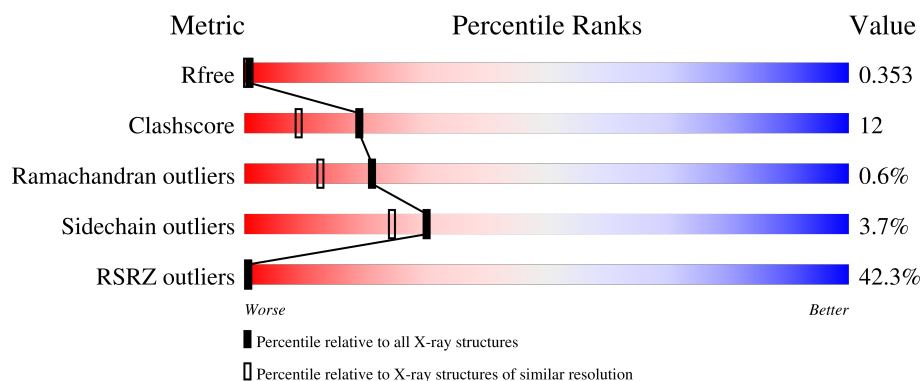
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	
2	B	308	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4642 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	2008	1287	336	373	12	8	12	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	GLY	-	expression tag	UNP P33334
A	1834	ALA	-	expression tag	UNP P33334
A	1835	MET	-	expression tag	UNP P33334

- Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	300	2580	1654	421	485	20	0	9	0

There are 20 discrepancies between the modelled and reference sequences:

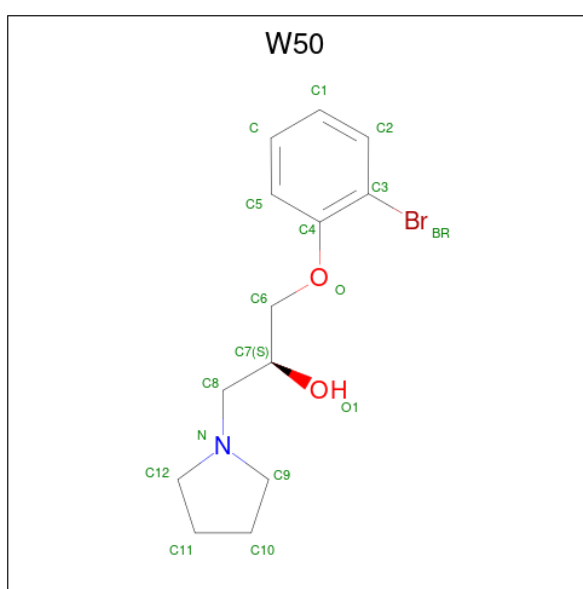
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	GLY	deletion	UNP P32357
B	?	-	SER	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ASN	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	170	SER	ASP	conflict	UNP P32357

- Molecule 3 is (2S)-1-(2-bromophenoxy)-3-(pyrrolidin-1-yl)propan-2-ol (CCD ID: W50) (formula: C₁₃H₁₈BrNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			17	1	13	1	2		

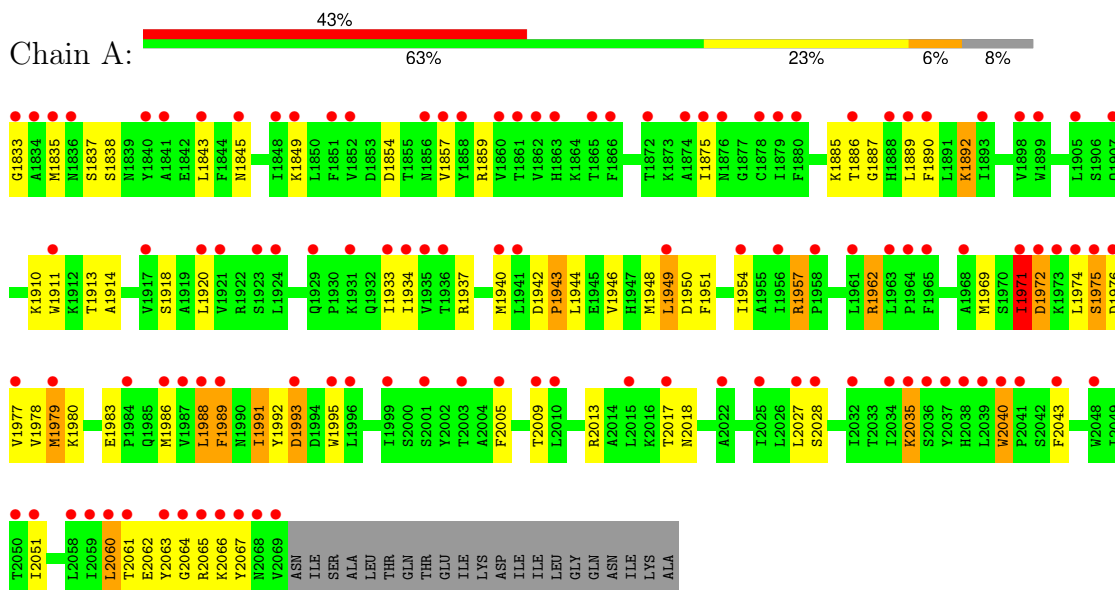
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	21	Total	O	0	0
			21	21		

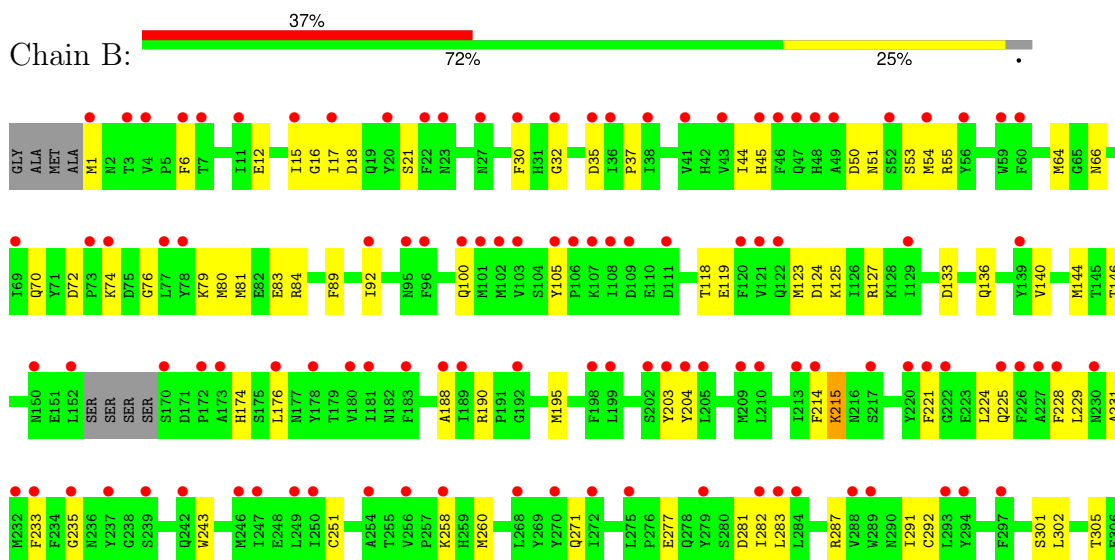
3 Residue-property plots

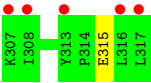
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pre-mRNA-splicing factor 8



• Molecule 2: A1 cistron-splicing factor AAR2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.23Å 82.31Å 92.22Å 90.00° 107.62° 90.00°	Depositor
Resolution (Å)	44.89 – 2.03 44.89 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.89-2.03) 99.1 (44.89-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.334 , 0.378 0.312 , 0.353	Depositor DCC
R_{free} test set	2039 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4642	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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: W50

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	0.87	3/2055 (0.1%)	1.13	10/2784 (0.4%)
2	B	0.73	0/2651	0.92	4/3581 (0.1%)
All	All	0.79	3/4706 (0.1%)	1.01	14/6365 (0.2%)

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	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2040	TRP	C-N	8.15	1.52	1.33
1	A	1887	GLY	C-O	-6.40	1.15	1.24
1	A	1957	ARG	C-N	5.35	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1992	TYR	CA-C-O	-8.86	109.49	119.95
1	A	2040	TRP	CA-C-N	7.85	129.66	119.84
1	A	2040	TRP	C-N-CA	7.85	129.66	119.84
1	A	1993	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	1972	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	1989	PHE	CA-C-O	-5.98	114.76	120.56
1	A	1971	ILE	CA-C-N	5.72	132.46	121.54
1	A	1971	ILE	C-N-CA	5.72	132.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1992	TYR	CA-CB-CG	5.46	123.74	113.90
1	A	1886	THR	CA-CB-OG1	-5.46	101.41	109.60
2	B	76	GLY	CA-C-N	-5.44	112.34	121.75
2	B	76	GLY	C-N-CA	-5.44	112.34	121.75
2	B	30	PHE	CA-C-N	-5.34	112.79	122.50
2	B	30	PHE	C-N-CA	-5.34	112.79	122.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1885	LYS	Mainchain
1	A	1971	ILE	Mainchain
1	A	1978	VAL	Mainchain
1	A	1979[B]	MET	Mainchain
1	A	1993	ASP	Mainchain

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	2008	0	2041	55	0
2	B	2580	0	2450	54	0
3	A	17	0	0	1	0
4	A	16	0	0	0	0
4	B	21	0	0	3	0
All	All	4642	0	4491	107	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 12.

All (107) 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:1890:PHE:HD2	1:A:1988:LEU:HD13	1.18	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1890:PHE:CD2	1:A:1988:LEU:HD13	1.97	0.99
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.52	0.88
2:B:50:ASP:OD1	2:B:51:ASN:N	2.07	0.87
1:A:1911:TRP:CD2	2:B:195:MET:HB2	2.15	0.82
1:A:1890:PHE:HD2	1:A:1988:LEU:CD1	1.95	0.80
1:A:1889:LEU:HD23	1:A:1989:PHE:CZ	2.18	0.79
1:A:1995:TRP:CZ2	1:A:2040:TRP:CD1	2.72	0.76
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.20	0.74
1:A:1890:PHE:CD2	1:A:1988:LEU:CD1	2.69	0.73
2:B:74:LYS:NZ	4:B:401:HOH:O	2.09	0.72
1:A:1845:ASN:OD1	1:A:1849:LYS:NZ	2.30	0.65
1:A:1911:TRP:CG	2:B:195:MET:HB2	2.31	0.64
2:B:1:MET:N	4:B:402:HOH:O	2.30	0.64
1:A:1991:ILE:O	1:A:1991:ILE:HD13	2.00	0.62
1:A:1910:LYS:HG2	1:A:1940:MET:SD	2.40	0.61
2:B:221:PHE:O	2:B:225:GLN:HG3	2.00	0.61
1:A:1934:ILE:HA	1:A:1957:ARG:O	2.01	0.61
1:A:1962:ARG:H	1:A:1962:ARG:CD	2.13	0.60
1:A:2018:ASN:HB2	1:A:2062:GLU:HG3	1.83	0.60
1:A:1920:LEU:HD13	1:A:1986:MET:HE1	1.85	0.57
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.40	0.57
1:A:1946:VAL:O	1:A:1949:LEU:HG	2.06	0.56
2:B:258:LYS:HD2	2:B:258:LYS:H	1.70	0.56
1:A:1911:TRP:CE3	2:B:195:MET:HB2	2.39	0.56
1:A:2063:TYR:C	1:A:2063:TYR:CD1	2.84	0.56
2:B:64[B]:MET:HE3	2:B:136:GLN:OE1	2.07	0.55
2:B:83:GLU:OE2	2:B:84:ARG:N	2.40	0.54
3:A:2101:W50:C12	3:A:2101:W50:C6	2.85	0.54
1:A:1889:LEU:HD23	1:A:1989:PHE:HZ	1.70	0.54
2:B:224:LEU:HD23	2:B:224:LEU:O	2.08	0.54
2:B:282:ILE:HG13	2:B:283:LEU:HG	1.89	0.54
2:B:6:PHE:CD1	2:B:32:GLY:HA2	2.43	0.53
2:B:228:PHE:CD2	2:B:271:GLN:HG2	2.45	0.52
1:A:1974:LEU:HA	1:A:1977:VAL:HG12	1.92	0.52
2:B:225:GLN:O	2:B:229:LEU:HG	2.10	0.52
1:A:2061:THR:O	1:A:2064:GLY:N	2.44	0.51
1:A:1889:LEU:HD23	1:A:1989:PHE:CE1	2.47	0.50
2:B:251:CYS:HG	2:B:292:CYS:HG	1.57	0.50
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.12	0.50
2:B:277:GLU:CD	2:B:277:GLU:H	2.20	0.49
2:B:301:SER:O	2:B:302:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1857:VAL:HG21	1:A:1913:THR:OG1	2.13	0.49
2:B:302:LEU:HB3	2:B:305:THR:HB	1.94	0.49
1:A:1975:SER:O	1:A:1979[A]:MET:HE2	2.12	0.48
2:B:1:MET:HB3	2:B:35:ASP:HA	1.95	0.48
2:B:251:CYS:HG	2:B:292:CYS:HB3	1.77	0.48
1:A:2060:LEU:HG	1:A:2061:THR:N	2.28	0.48
1:A:1859:ARG:NH1	1:A:1979[A]:MET:HE1	2.28	0.48
2:B:17:ILE:O	2:B:18:ASP:C	2.55	0.48
2:B:188:ALA:HA	2:B:204:TYR:CD1	2.47	0.48
2:B:251:CYS:SG	2:B:292:CYS:SG	3.09	0.48
2:B:72:ASP:OD2	2:B:79:LYS:NZ	2.32	0.48
2:B:146:THR:HG22	2:B:176:LEU:HB2	1.96	0.48
2:B:16:GLY:HA3	2:B:45:HIS:NE2	2.28	0.47
2:B:287:ARG:O	2:B:291:ILE:HD13	2.14	0.47
1:A:1854:ASP:CG	1:A:1937:ARG:HH21	2.19	0.47
2:B:80:MET:O	2:B:81:MET:HG2	2.15	0.47
1:A:2005:PHE:O	1:A:2009:THR:HG23	2.14	0.47
1:A:2035:LYS:HD3	1:A:2035:LYS:HA	1.68	0.46
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.50	0.46
2:B:224:LEU:HD23	2:B:224:LEU:C	2.41	0.46
2:B:55:ARG:HD2	2:B:233:PHE:O	2.15	0.46
1:A:1892:LYS:HD2	1:A:1892:LYS:HA	1.73	0.45
1:A:1948:MET:O	1:A:1949:LEU:C	2.59	0.45
2:B:51:ASN:ND2	2:B:53:SER:O	2.49	0.45
2:B:251:CYS:HG	2:B:292:CYS:CB	2.29	0.45
2:B:72:ASP:OD1	2:B:72:ASP:C	2.58	0.45
1:A:2066:LYS:HD2	1:A:2067:TYR:CE1	2.52	0.44
2:B:214:PHE:O	2:B:215:LYS:HB2	2.17	0.44
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	1.99	0.44
2:B:124:ASP:OD2	2:B:125:LYS:HD3	2.18	0.44
1:A:1940:MET:HB3	1:A:1940:MET:HE3	1.55	0.44
1:A:1914:ALA:HB1	1:A:1944:LEU:HA	2.00	0.43
1:A:2013:ARG:O	1:A:2017[A]:THR:HG23	2.18	0.43
1:A:2017[B]:THR:HG22	1:A:2062:GLU:HB3	2.00	0.43
1:A:1933:ILE:HD12	1:A:1948:MET:HE2	1.99	0.43
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.48	0.43
1:A:1875:ILE:HB	1:A:1979[C]:MET:HE1	1.99	0.43
2:B:260:MET:HE2	2:B:260:MET:HB3	1.81	0.43
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	2.00	0.43
1:A:1995:TRP:CH2	1:A:2040:TRP:CD1	3.06	0.43
2:B:127:ARG:NH1	2:B:133:ASP:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1951:PHE:HB3	1:A:1954:ILE:HD12	2.00	0.43
2:B:140:VAL:HA	2:B:144:MET:SD	2.59	0.43
1:A:1971:ILE:HB	1:A:1974:LEU:HD12	2.00	0.43
2:B:17:ILE:O	2:B:17:ILE:HG23	2.19	0.42
1:A:1918[A]:SER:HB3	1:A:1948:MET:SD	2.59	0.42
2:B:100:GLN:HA	4:B:411:HOH:O	2.18	0.42
1:A:1890:PHE:CD1	1:A:1890:PHE:N	2.88	0.42
1:A:1969:MET:HA	1:A:1969:MET:HE2	2.02	0.42
1:A:2027:LEU:O	1:A:2028:SER:C	2.62	0.42
1:A:2043:PHE:CZ	1:A:2051:ILE:HG13	2.55	0.42
2:B:66:ASN:HB3	2:B:89:PHE:CE1	2.55	0.42
1:A:1890:PHE:CE2	1:A:1988:LEU:CD1	3.03	0.41
1:A:1833:GLY:O	1:A:1957:ARG:NE	2.44	0.41
1:A:1948:MET:O	1:A:1950:ASP:N	2.53	0.41
1:A:2062:GLU:OE1	1:A:2065:ARG:NH1	2.53	0.41
2:B:15:ILE:O	2:B:21:SER:HA	2.21	0.41
2:B:16:GLY:HA3	2:B:45:HIS:CD2	2.56	0.41
2:B:231:ALA:O	2:B:235:GLY:HA2	2.21	0.41
2:B:118:THR:O	2:B:119:GLU:C	2.63	0.41
2:B:228:PHE:HB2	2:B:243:TRP:CD1	2.56	0.40
1:A:1976:ASP:HB3	1:A:1980:LYS:NZ	2.36	0.40
2:B:17:ILE:HD13	2:B:44[B]:ILE:HG13	2.03	0.40
1:A:2061:THR:O	1:A:2063:TYR:N	2.54	0.40
2:B:70:GLN:HB3	2:B:81:MET:CE	2.37	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	248/258 (96%)	230 (93%)	16 (6%)	2 (1%)	16 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	306/308 (99%)	292 (95%)	13 (4%)	1 (0%)	36	31
All	All	554/566 (98%)	522 (94%)	29 (5%)	3 (0%)	21	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1972	ASP
2	B	215	LYS
1	A	1949	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	228/233 (98%)	216 (95%)	12 (5%)	20	13
2	B	287/284 (101%)	281 (98%)	6 (2%)	47	47
All	All	515/517 (100%)	497 (96%)	18 (4%)	30	27

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1837	SER
1	A	1838	SER
1	A	1892	LYS
1	A	1943	PRO
1	A	1962	ARG
1	A	1975	SER
1	A	1983	GLU
1	A	1988	LEU
1	A	1991	ILE
1	A	2035	LYS
1	A	2060	LEU
2	B	12	GLU

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Mol	Chain	Res	Type
2	B	92	ILE
2	B	123	MET
2	B	174	HIS
2	B	281	ASP
2	B	315	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1876	ASN
1	A	1947	HIS
1	A	2054	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](#)

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	$\# Z > 2$
3	W50	A	2101	-	18,18,18	2.69	8 (44%)	23,23,23	1.95	7 (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
3	W50	A	2101	-	-	3/9/16/16	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2101	W50	BR-C3	-5.32	1.78	1.89
3	A	2101	W50	C5-C4	-4.84	1.29	1.39
3	A	2101	W50	C2-C3	-4.09	1.31	1.38
3	A	2101	W50	C-C1	-3.60	1.30	1.38
3	A	2101	W50	C1-C2	-3.54	1.32	1.38
3	A	2101	W50	C4-C3	-2.91	1.33	1.39
3	A	2101	W50	C12-N	2.89	1.53	1.47
3	A	2101	W50	O1-C7	-2.21	1.36	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2101	W50	O-C4-C3	4.23	122.04	116.89
3	A	2101	W50	C12-N-C8	4.21	118.85	113.07
3	A	2101	W50	C12-N-C9	3.63	108.33	104.04
3	A	2101	W50	O1-C7-C8	-3.20	100.69	109.91
3	A	2101	W50	C8-C7-C6	-2.45	106.12	111.59
3	A	2101	W50	O-C4-C5	-2.42	118.67	123.95
3	A	2101	W50	O1-C7-C6	2.11	116.98	109.70

There are no chirality outliers.

All (3) torsion outliers are listed below:

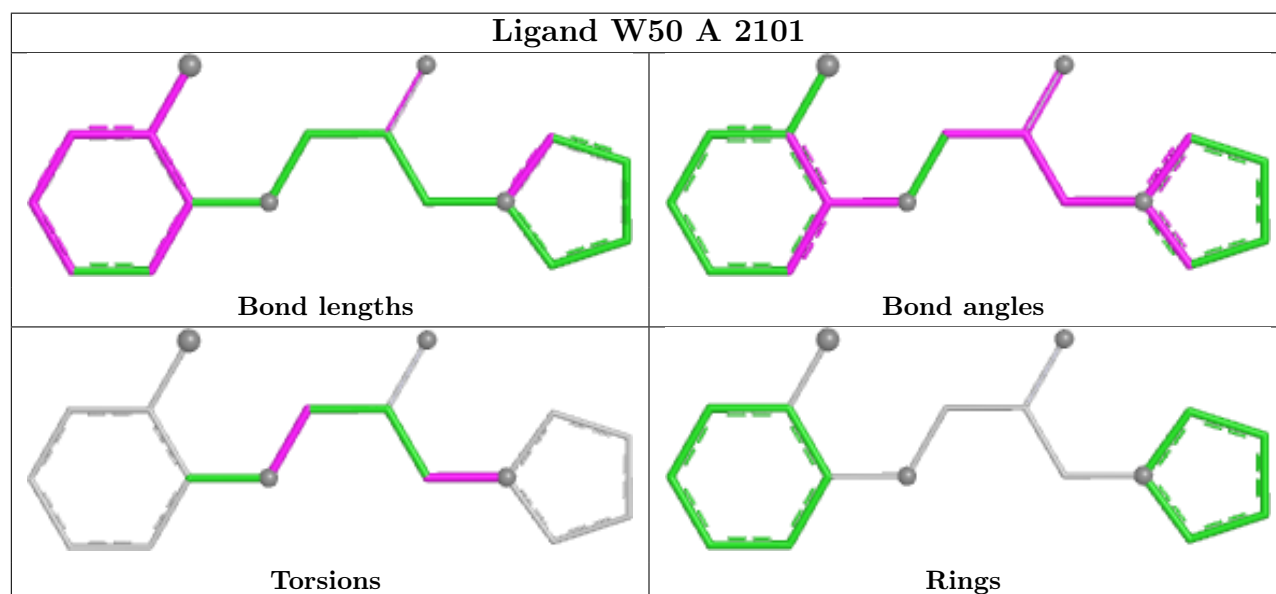
Mol	Chain	Res	Type	Atoms
3	A	2101	W50	C7-C8-N-C9
3	A	2101	W50	C7-C8-N-C12
3	A	2101	W50	C7-C6-O-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2101	W50	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/258 (91%)	2.10	112 (47%) 0 0	28, 93, 144, 278	12 (5%)
2	B	300/308 (97%)	1.88	115 (38%) 1 1	30, 92, 147, 241	9 (3%)
All	All	537/566 (94%)	1.98	227 (42%) 0 0	28, 92, 145, 278	21 (3%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1989	PHE	8.9
1	A	1940	MET	6.3
1	A	2040	TRP	6.2
1	A	2037	TYR	6.0
1	A	1988	LEU	5.6
2	B	54[A]	MET	5.6
1	A	2039	LEU	5.5
1	A	1878	CYS	5.4
2	B	246	MET	5.4
2	B	17	ILE	5.3
2	B	77	LEU	5.3
1	A	1889	LEU	5.2
1	A	2060	LEU	5.0
1	A	1890	PHE	5.0
1	A	1987	VAL	4.9
2	B	313	TYR	4.5
2	B	316	LEU	4.5
1	A	1857	VAL	4.3
1	A	1840	TYR	4.2
2	B	69	ILE	4.1
2	B	220	TYR	4.1
2	B	1	MET	4.1
1	A	1931[A]	LYS	4.0
2	B	4	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1979[A]	MET	4.0
2	B	226	PHE	3.9
1	A	1949	LEU	3.9
2	B	256	VAL	3.8
1	A	1834	ALA	3.8
2	B	106	PRO	3.7
1	A	2069	VAL	3.7
2	B	203[A]	TYR	3.7
2	B	15	ILE	3.7
2	B	46	PHE	3.7
2	B	282	ILE	3.6
2	B	92	ILE	3.6
2	B	294	TYR	3.6
1	A	2064	GLY	3.5
2	B	272	ILE	3.5
1	A	2063	TYR	3.5
2	B	139	TYR	3.5
2	B	199	LEU	3.5
2	B	237	TYR	3.5
1	A	1860	VAL	3.5
2	B	3	THR	3.5
2	B	178	TYR	3.4
2	B	181	ILE	3.4
1	A	1866	PHE	3.4
2	B	233	PHE	3.4
1	A	1852	VAL	3.4
2	B	108	ILE	3.4
1	A	1973	LYS	3.3
1	A	2051	ILE	3.3
1	A	1995	TRP	3.3
1	A	1977	VAL	3.3
2	B	22	PHE	3.3
2	B	101	MET	3.3
2	B	45	HIS	3.2
2	B	214	PHE	3.2
1	A	1954	ILE	3.2
1	A	1974	LEU	3.2
2	B	38	ILE	3.2
2	B	247	ILE	3.2
1	A	2043	PHE	3.2
2	B	249	LEU	3.2
2	B	183	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	2001[A]	SER	3.2
1	A	2068	ASN	3.2
1	A	1879	ILE	3.1
1	A	2025	ILE	3.1
2	B	210	LEU	3.1
1	A	2005	PHE	3.1
1	A	2034	ILE	3.1
1	A	1874	ALA	3.1
2	B	41[A]	VAL	3.1
1	A	1888	HIS	3.1
2	B	20	TYR	3.1
2	B	105	TYR	3.1
2	B	120	PHE	3.1
2	B	172	PRO	3.1
2	B	121	VAL	3.1
2	B	307	LYS	3.1
1	A	2058	LEU	3.0
1	A	1961	LEU	3.0
1	A	1872	THR	3.0
1	A	1845	ASN	3.0
1	A	1843	LEU	2.9
2	B	288	VAL	2.9
2	B	250	ILE	2.9
2	B	204	TYR	2.9
2	B	230[A]	ASN	2.9
1	A	1935	VAL	2.9
1	A	1976	ASP	2.9
2	B	308	ILE	2.9
2	B	7	THR	2.9
2	B	73	PRO	2.9
2	B	279	TYR	2.9
1	A	1968	ALA	2.9
2	B	293	LEU	2.8
1	A	2017[A]	THR	2.8
1	A	2050	THR	2.8
2	B	198	PHE	2.8
2	B	270	TYR	2.8
1	A	1941	LEU	2.8
2	B	268	LEU	2.8
1	A	2066	LYS	2.8
1	A	2022	ALA	2.8
2	B	56	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	283	LEU	2.8
2	B	180	VAL	2.8
1	A	1880	PHE	2.7
2	B	221	PHE	2.7
1	A	1865	THR	2.7
1	A	1851	PHE	2.7
1	A	1920	LEU	2.7
1	A	1996	LEU	2.7
2	B	152	LEU	2.7
2	B	176	LEU	2.7
2	B	59	TRP	2.7
2	B	205	LEU	2.6
2	B	297	PHE	2.6
2	B	170	SER	2.6
1	A	2038	HIS	2.6
1	A	1893	ILE	2.6
1	A	1933	ILE	2.6
1	A	1934	ILE	2.6
1	A	2059	ILE	2.6
2	B	74	LYS	2.6
1	A	2065	ARG	2.6
2	B	49	ALA	2.6
2	B	35	ASP	2.6
1	A	1924	LEU	2.6
2	B	284	LEU	2.6
1	A	2032	ILE	2.5
2	B	232	MET	2.5
2	B	32	GLY	2.5
1	A	2009	THR	2.5
1	A	1958	PRO	2.5
1	A	2015	LEU	2.5
2	B	317	LEU	2.5
1	A	1898[A]	VAL	2.5
2	B	150	ASN	2.5
1	A	2041	PRO	2.5
2	B	188	ALA	2.5
1	A	2027	LEU	2.5
2	B	30	PHE	2.5
2	B	129	ILE	2.5
1	A	1986	MET	2.4
2	B	102	MET	2.4
1	A	1905	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2010	LEU	2.4
2	B	48	HIS	2.4
2	B	47	GLN	2.4
2	B	100	GLN	2.4
1	A	1972	ASP	2.4
2	B	189	ILE	2.4
1	A	1886	THR	2.4
1	A	1964	PRO	2.4
2	B	225	GLN	2.4
1	A	1921	VAL	2.4
2	B	217	SER	2.4
2	B	258	LYS	2.4
1	A	1841	ALA	2.4
2	B	60	PHE	2.4
2	B	96	PHE	2.4
1	A	1956	ILE	2.4
2	B	103	VAL	2.4
2	B	213	ILE	2.4
1	A	2067	TYR	2.3
1	A	2035	LYS	2.3
1	A	2036	SER	2.3
1	A	1936	THR	2.3
1	A	2061	THR	2.3
2	B	289	TRP	2.3
2	B	254	ALA	2.3
1	A	1963	LEU	2.3
1	A	1975	SER	2.3
1	A	1971	ILE	2.3
2	B	11	ILE	2.3
1	A	2003	THR	2.3
1	A	1899	TRP	2.3
1	A	1911	TRP	2.3
1	A	1862	VAL	2.3
1	A	1984	PRO	2.3
2	B	192	GLY	2.3
1	A	1999	ILE	2.2
2	B	36	ILE	2.2
1	A	1849	LYS	2.2
2	B	222	GLY	2.2
1	A	1907	GLN	2.2
2	B	228	PHE	2.2
1	A	1836	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	107	LYS	2.2
1	A	1923	SER	2.2
2	B	202	SER	2.2
1	A	1856	ASN	2.2
2	B	6	PHE	2.2
1	A	1917	VAL	2.2
2	B	122[A]	GLN	2.2
2	B	52	SER	2.2
1	A	1858	TYR	2.2
2	B	27	ASN	2.2
1	A	1929	GLN	2.1
2	B	173	ALA	2.1
2	B	275	LEU	2.1
2	B	242	GLN	2.1
1	A	1965	PHE	2.1
2	B	109	ASP	2.1
2	B	111	ASP	2.1
2	B	78	TYR	2.1
1	A	1833	GLY	2.1
1	A	2028	SER	2.1
1	A	1861	THR	2.1
1	A	1848	ILE	2.1
1	A	1875	ILE	2.1
2	B	43	VAL	2.1
1	A	2048	TRP	2.1
2	B	239	SER	2.1
2	B	209	MET	2.0
2	B	23	ASN	2.0
2	B	95	ASN	2.0
1	A	1993	ASP	2.0
1	A	1863	HIS	2.0
1	A	1835	MET	2.0
2	B	227	ALA	2.0
1	A	1876	ASN	2.0
2	B	235	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

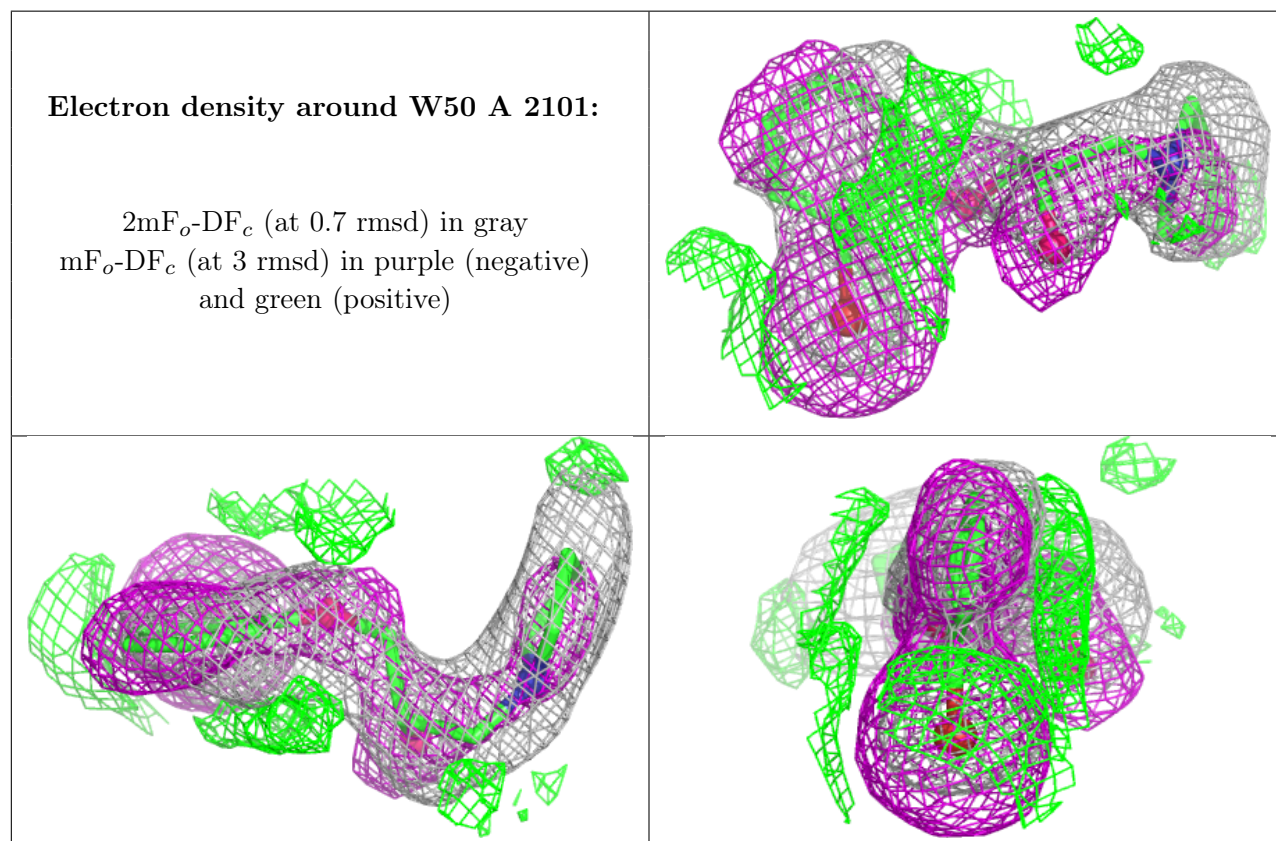
There are no oligosaccharides in this entry.

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
3	W50	A	2101	17/17	0.78	0.22	20,20,20,20	17

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.