



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 PM UTC

PDB ID : 7FK1 / pdb_00007fk1
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P04A06 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 : 1.76 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

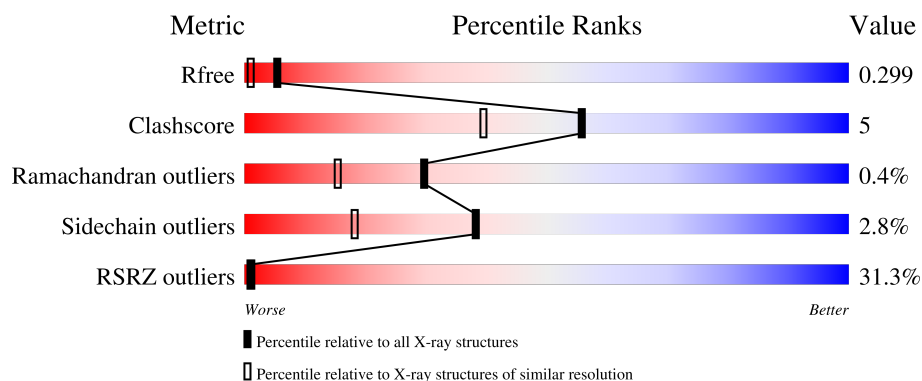
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 4694 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	1997	1281	332	372	12	0	11	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:

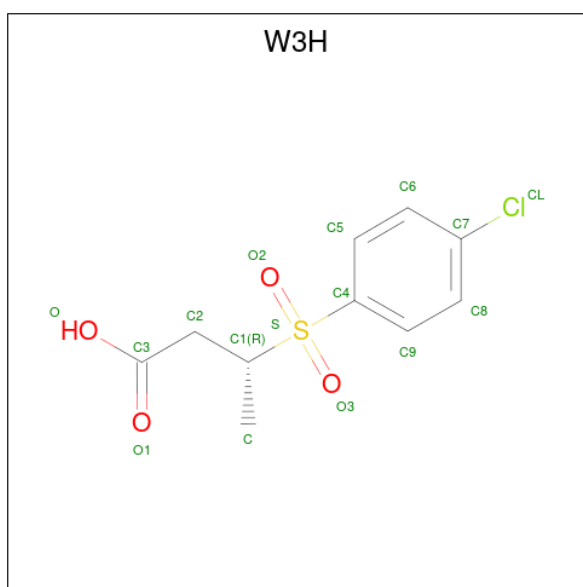
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 (3R)-3-(4-chlorobenzene-1-sulfonyl)butanoic acid (CCD ID: W3H) (formula: $C_{10}H_{11}ClO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	S	0	1
			32	20	2	8	2		
3	B	1	Total	C	Cl	O	S	0	0
			16	10	1	4	1		

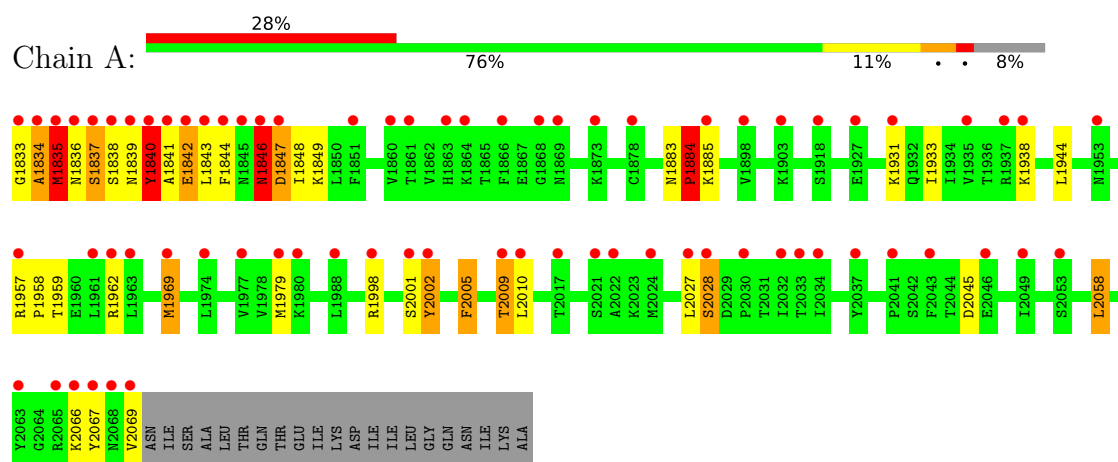
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	29	Total	O	0	0
			29	29		

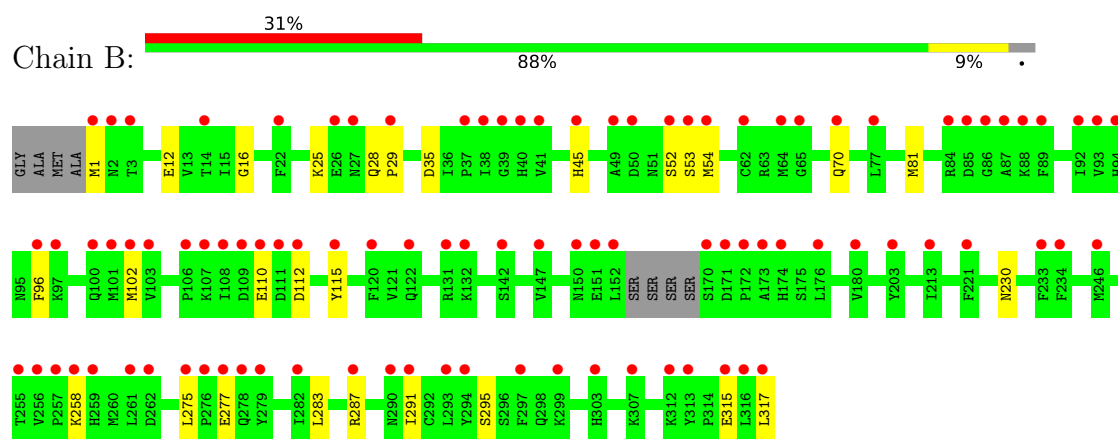
3 Residue-property plots

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	89.61Å 82.69Å 94.59Å 90.00° 108.02° 90.00°	Depositor
Resolution (Å)	45.26 – 1.76 45.26 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.26-1.76) 98.9 (45.26-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.280 , 0.315 0.265 , 0.299	Depositor DCC
R_{free} test set	2101 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4694	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: W3H

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	0.93	9/2044 (0.4%)	1.20	30/2770 (1.1%)
2	B	0.63	2/2651 (0.1%)	0.79	4/3581 (0.1%)
All	All	0.77	11/4695 (0.2%)	0.99	34/6351 (0.5%)

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	2
2	B	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1884	PRO	N-CA	15.16	1.67	1.47
1	A	2002	TYR	N-CA	7.91	1.56	1.46
1	A	1884	PRO	C-O	-7.80	1.14	1.24
1	A	2001[A]	SER	C-N	6.93	1.43	1.33
1	A	2001[B]	SER	C-N	6.93	1.43	1.33
1	A	1883	ASN	C-N	6.71	1.43	1.34
2	B	230[A]	ASN	C-O	6.39	1.31	1.24
2	B	230[B]	ASN	C-O	6.39	1.31	1.24
1	A	1843	LEU	C-O	-5.67	1.17	1.24
1	A	2005	PHE	C-O	-5.57	1.17	1.24
1	A	1836	ASN	N-CA	5.18	1.52	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1883	ASN	CA-C-N	13.03	133.51	119.05
1	A	1883	ASN	C-N-CA	13.03	133.51	119.05
1	A	1884	PRO	CB-CA-C	12.54	133.31	112.62
2	B	230[A]	ASN	CA-C-O	10.80	132.00	120.55
2	B	230[B]	ASN	CA-C-O	10.80	132.00	120.55
1	A	1884	PRO	N-CA-CB	-8.77	93.69	103.33
1	A	1836	ASN	CA-C-N	8.13	134.30	120.72
1	A	1836	ASN	C-N-CA	8.13	134.30	120.72
1	A	1883	ASN	O-C-N	-7.83	114.89	121.23
1	A	1884	PRO	N-CA-C	-7.57	103.01	113.53
1	A	1842	GLU	CB-CA-C	-6.78	98.31	110.23
1	A	1837	SER	CA-C-N	6.38	133.81	121.18
1	A	1837	SER	C-N-CA	6.38	133.81	121.18
1	A	1835	MET	CA-C-O	-6.36	114.17	121.68
2	B	230[A]	ASN	O-C-N	-6.27	115.47	122.12
2	B	230[B]	ASN	O-C-N	-6.27	115.47	122.12
1	A	1846	ASN	CB-CA-C	-6.03	98.42	110.42
1	A	1844	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	1836	ASN	CA-CB-CG	5.89	118.49	112.60
1	A	1840	TYR	CA-C-N	5.77	132.21	123.04
1	A	1840	TYR	C-N-CA	5.77	132.21	123.04
1	A	2001[A]	SER	CA-C-N	-5.75	112.50	120.38
1	A	2001[A]	SER	C-N-CA	-5.75	112.50	120.38
1	A	2001[B]	SER	CA-C-N	-5.75	112.50	120.38
1	A	2001[B]	SER	C-N-CA	-5.75	112.50	120.38
1	A	1843	LEU	N-CA-C	-5.51	105.37	111.71
1	A	1847	ASP	CA-C-O	-5.51	114.77	121.05
1	A	1838	SER	CA-C-N	5.47	134.89	122.20
1	A	1838	SER	C-N-CA	5.47	134.89	122.20
1	A	1835	MET	CA-C-N	5.43	131.12	122.10
1	A	1835	MET	C-N-CA	5.43	131.12	122.10
1	A	1846	ASN	N-CA-CB	5.39	119.59	110.49
1	A	1834	ALA	CA-C-O	-5.29	115.38	121.47
1	A	2010	LEU	N-CA-C	-5.21	105.28	111.69

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1959	THR	Mainchain
2	B	54[A]	MET	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	1997	0	2028	27	4
2	B	2580	0	2450	15	4
3	A	32	0	0	1	0
3	B	16	0	0	1	0
4	A	40	0	0	2	0
4	B	29	0	0	2	0
All	All	4694	0	4478	43	4

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 5.

All (43) 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:1884:PRO:N	1:A:1884:PRO:CA	1.67	1.36
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.20	0.89
1:A:1846:ASN:ND2	1:A:1846:ASN:O	2.06	0.89
2:B:70:GLN:HB3	2:B:81:MET:HE1	1.67	0.77
1:A:1834:ALA:HB2	1:A:1958:PRO:HG2	1.76	0.68
2:B:53:SER:O	4:B:501:HOH:O	2.13	0.67
1:A:1833:GLY:O	1:A:1957:ARG:HB3	1.95	0.66
1:A:1884:PRO:N	1:A:1884:PRO:C	2.53	0.64
1:A:1835:MET:HA	1:A:1835:MET:HE3	1.80	0.63
1:A:1840:TYR:CE2	3:A:2101[A]:W3H:CL	2.92	0.60
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.29	0.58
1:A:2069:VAL:C	4:A:2224:HOH:O	2.48	0.56
1:A:1842:GLU:O	1:A:1842:GLU:HG3	2.05	0.56
2:B:12:GLU:HG3	2:B:25:LYS:HA	1.86	0.55
1:A:2027:LEU:O	1:A:2028:SER:C	2.49	0.55
2:B:277:GLU:CD	2:B:277:GLU:H	2.14	0.55
1:A:1938:LYS:NZ	4:A:2201:HOH:O	2.34	0.54
3:B:401:W3H:C	3:B:401:W3H:C5	2.85	0.54
2:B:275:LEU:CD2	2:B:283:LEU:HD13	2.40	0.52
1:A:1847:ASP:HB3	1:A:1931[A]:LYS:HB2	1.90	0.52
2:B:16:GLY:HA3	2:B:45:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:O	2:B:291:ILE:HD13	2.09	0.52
1:A:1834:ALA:CB	1:A:1958:PRO:HG2	2.39	0.51
1:A:1848:ILE:N	1:A:1931[A]:LYS:HZ2	1.99	0.50
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.92	0.50
1:A:1835:MET:SD	1:A:1957:ARG:NH2	2.84	0.50
1:A:1847:ASP:HB3	1:A:1931[B]:LYS:HG3	1.94	0.48
2:B:275:LEU:HD22	2:B:283:LEU:HD13	1.95	0.48
1:A:1998:ARG:NH1	1:A:2045:ASP:OD2	2.41	0.47
2:B:110:GLU:HG2	2:B:110:GLU:O	2.15	0.47
1:A:1969:MET:HA	1:A:1969:MET:HE2	1.98	0.46
2:B:258:LYS:HD2	2:B:258:LYS:H	1.82	0.45
1:A:1835:MET:SD	1:A:1842:GLU:HG2	2.57	0.45
1:A:1979[B]:MET:HA	1:A:1979[B]:MET:HE2	1.98	0.44
1:A:1933:ILE:HG21	1:A:1944:LEU:HD21	2.00	0.44
2:B:28:GLN:CG	2:B:29:PRO:HD2	2.49	0.43
1:A:2002:TYR:C	1:A:2002:TYR:CD1	2.96	0.43
2:B:1:MET:N	4:B:504:HOH:O	2.52	0.42
2:B:96:PHE:CB	2:B:102:MET:HE3	2.50	0.42
2:B:1:MET:HB3	2:B:35:ASP:HA	2.02	0.42
1:A:2066:LYS:HD3	1:A:2067:TYR:CZ	2.55	0.42
1:A:2005:PHE:O	1:A:2009:THR:HG23	2.21	0.41
1:A:2066:LYS:HD3	1:A:2067:TYR:CE1	2.56	0.40

All (4) 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:1841:ALA:O	2:B:115:TYR:CE1[4_555]	1.53	0.67
1:A:1846:ASN:CB	2:B:112:ASP:OD2[4_555]	1.75	0.45
1:A:2069:VAL:O	2:B:52:SER:OG[2_655]	1.98	0.22
1:A:1846:ASN:CG	2:B:112:ASP:OD2[4_555]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	247/258 (96%)	236 (96%)	9 (4%)	2 (1%)	16	5
2	B	306/308 (99%)	293 (96%)	13 (4%)	0	100	100
All	All	553/566 (98%)	529 (96%)	22 (4%)	2 (0%)	30	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1846	ASN
1	A	2028	SER

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	227/233 (97%)	216 (95%)	11 (5%)	23	6
2	B	287/284 (101%)	284 (99%)	3 (1%)	68	56
All	All	514/517 (99%)	500 (97%)	14 (3%)	38	19

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1837	SER
1	A	1839	ASN
1	A	1840	TYR
1	A	1849	LYS
1	A	1884	PRO
1	A	1885	LYS
1	A	1962	ARG
1	A	1969	MET
1	A	2009	THR
1	A	2058	LEU

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Mol	Chain	Res	Type
2	B	295	SER
2	B	315	GLU
2	B	317	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	2054	GLN
2	B	23	ASN
2	B	47	GLN
2	B	94	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 [i](#)

3 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	$\# Z > 2$
3	W3H	A	2101[A]	-	14,16,16	0.71	0	21,23,23	1.93	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	W3H	A	2101[B]	-	14,16,16	0.53	0	21,23,23	0.63	0
3	W3H	B	401	-	14,16,16	7.22	4 (28%)	21,23,23	2.73	11 (52%)

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	W3H	A	2101[A]	-	-	4/16/16/16	0/1/1/1
3	W3H	A	2101[B]	-	-	1/16/16/16	0/1/1/1
3	W3H	B	401	-	-	0/16/16/16	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	W3H	O2-S	-20.85	1.25	1.44
3	B	401	W3H	O3-S	-12.39	1.33	1.44
3	B	401	W3H	C1-S	-11.00	1.58	1.79
3	B	401	W3H	O-C3	-3.13	1.20	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2101[A]	W3H	C-C1-S	-6.30	91.97	109.66
3	B	401	W3H	O2-S-O3	-6.09	113.22	118.72
3	B	401	W3H	C5-C4-S	5.56	124.14	119.43
3	A	2101[A]	W3H	C4-S-C1	4.28	113.19	105.15
3	B	401	W3H	C5-C4-C9	-3.89	115.39	120.47
3	B	401	W3H	C4-S-C1	-3.72	98.15	105.15
3	B	401	W3H	O3-S-C1	3.42	113.13	108.14
3	B	401	W3H	C6-C5-C4	3.40	122.75	119.44
3	B	401	W3H	C8-C9-C4	2.92	122.28	119.44
3	B	401	W3H	O2-S-C1	2.64	111.99	108.14
3	B	401	W3H	O2-S-C4	2.46	110.57	108.19
3	B	401	W3H	O1-C3-C2	-2.30	115.79	122.84
3	A	2101[A]	W3H	O2-S-C1	-2.19	104.94	108.14
3	A	2101[A]	W3H	C1-C2-C3	-2.17	108.03	113.14
3	B	401	W3H	O-C3-O1	2.04	128.58	123.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2101[A]	W3H	C5-C4-S-O3
3	A	2101[A]	W3H	C5-C4-S-C1
3	A	2101[A]	W3H	C9-C4-S-O3
3	A	2101[A]	W3H	C9-C4-S-C1
3	A	2101[B]	W3H	C-C1-C2-C3

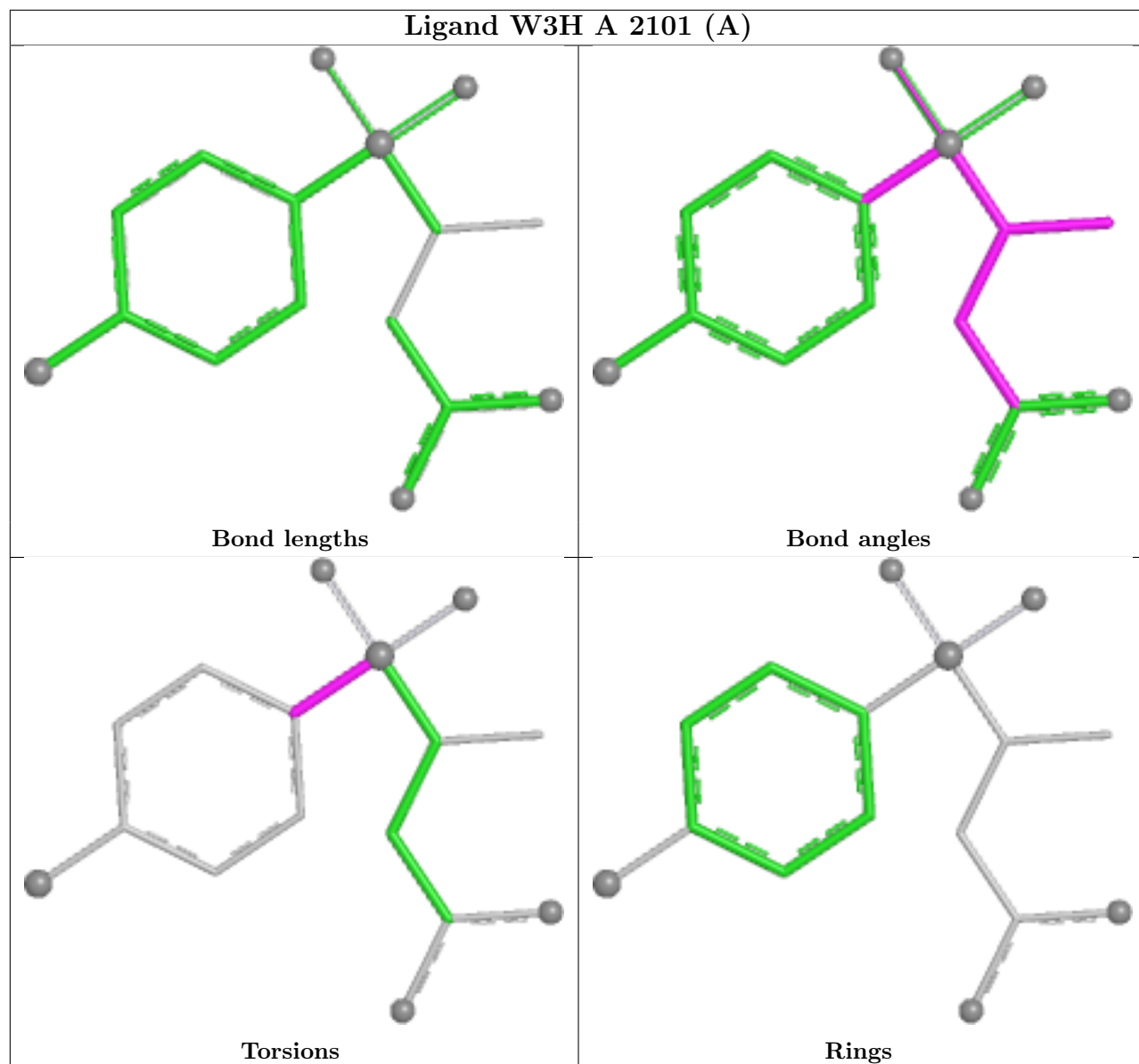
There are no ring outliers.

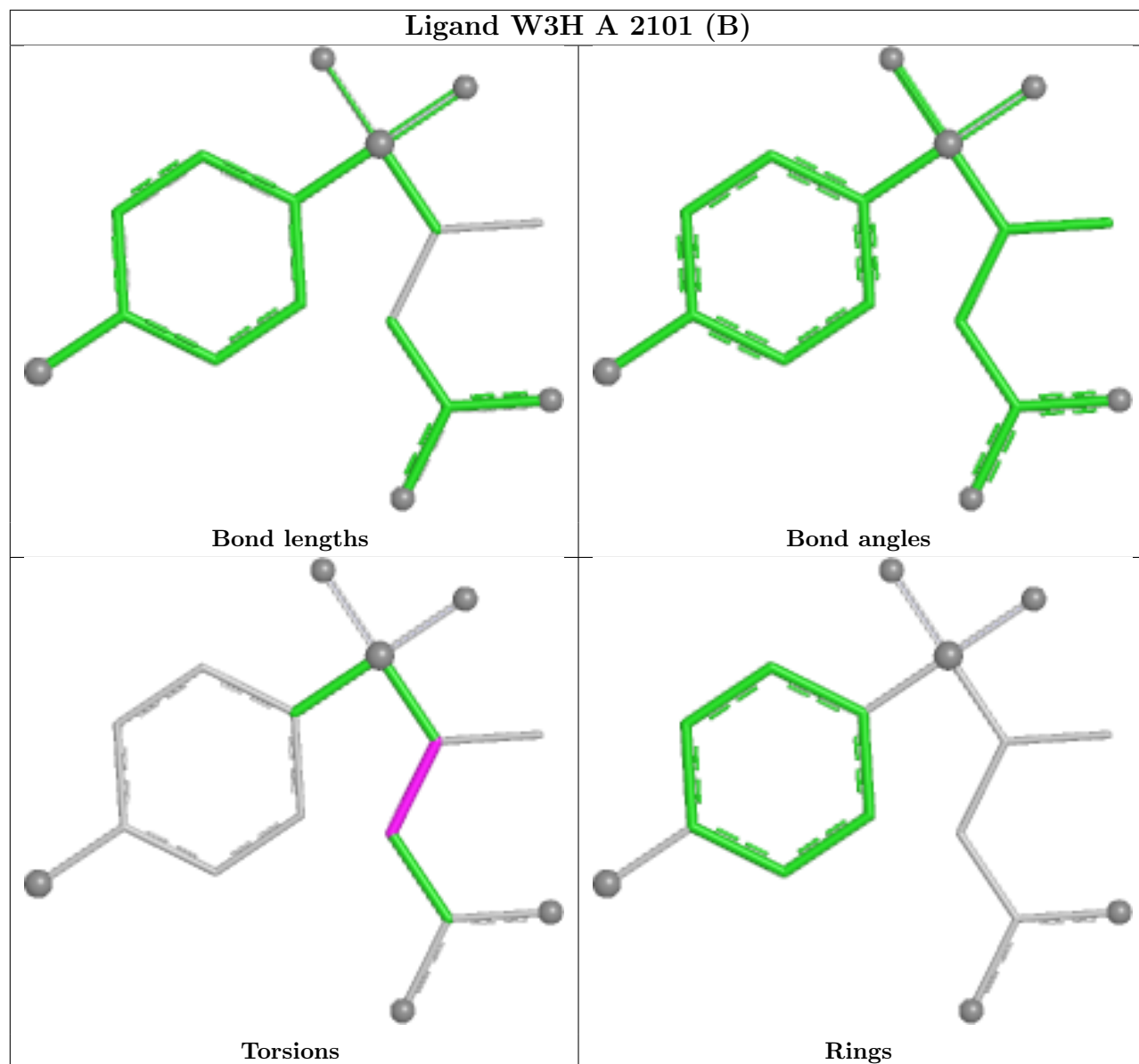
2 monomers are involved in 2 short contacts:

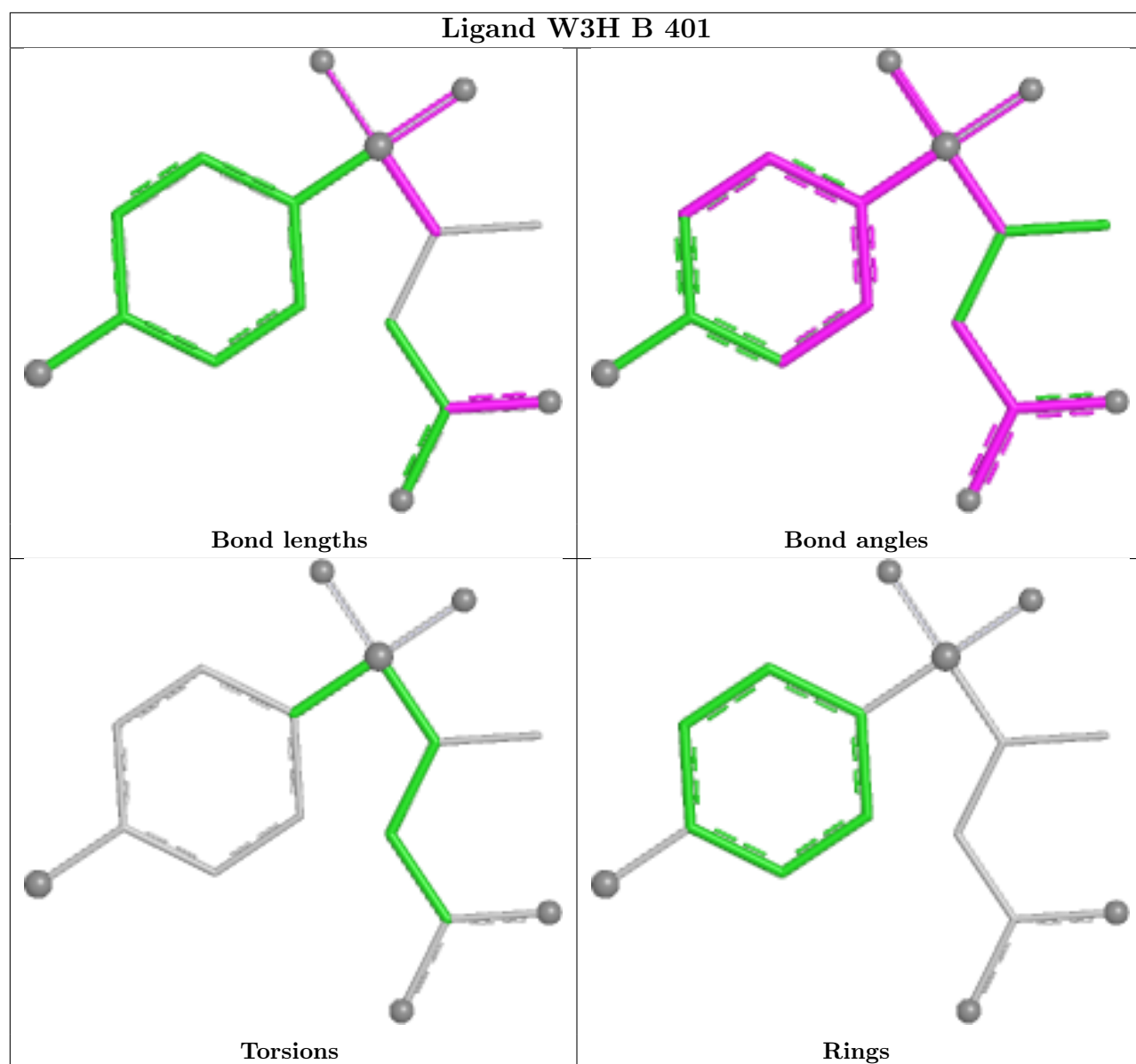
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2101[A]	W3H	1	0
3	B	401	W3H	1	0

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.

Ligand W3H A 2101 (A)







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%)	1.88	72 (30%) 1 1	17, 47, 89, 193	11 (4%)
2	B	300/308 (97%)	1.66	96 (32%) 1 1	16, 50, 97, 136	9 (3%)
All	All	537/566 (94%)	1.76	168 (31%) 1 1	16, 49, 96, 193	20 (3%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1841	ALA	15.7
1	A	1844	PHE	11.4
1	A	1843	LEU	10.4
1	A	1979[A]	MET	7.6
1	A	1840	TYR	7.4
1	A	1846	ASN	7.3
1	A	1839	ASN	7.0
1	A	1845	ASN	7.0
1	A	1835	MET	6.5
1	A	2017[A]	THR	6.4
2	B	316	LEU	6.0
1	A	1898[A]	VAL	5.8
2	B	275	LEU	5.8
2	B	54[A]	MET	5.5
1	A	1863	HIS	5.4
2	B	203[A]	TYR	5.3
2	B	172	PRO	5.1
2	B	115	TYR	5.1
2	B	108	ILE	5.0
2	B	152	LEU	4.9
1	A	1842	GLU	4.7
1	A	1834	ALA	4.6
2	B	170	SER	4.4
1	A	1833	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	38	ILE	4.4
2	B	1	MET	4.4
1	A	2069	VAL	4.4
2	B	317	LEU	4.3
2	B	174	HIS	4.2
2	B	50	ASP	4.2
1	A	2001[A]	SER	4.2
2	B	176	LEU	4.2
1	A	2027	LEU	4.1
1	A	2030	PRO	3.9
2	B	92	ILE	3.8
2	B	93	VAL	3.8
1	A	1838	SER	3.7
2	B	259	HIS	3.6
1	A	1836	ASN	3.6
1	A	1962	ARG	3.6
2	B	173	ALA	3.5
1	A	2022	ALA	3.5
2	B	39	GLY	3.5
2	B	111	ASP	3.4
1	A	1837	SER	3.4
2	B	293	LEU	3.4
1	A	2063	TYR	3.4
2	B	291	ILE	3.3
2	B	106	PRO	3.3
1	A	1957	ARG	3.3
1	A	2049	ILE	3.3
2	B	147	VAL	3.3
1	A	1866	PHE	3.2
2	B	258	LYS	3.2
1	A	1969	MET	3.2
2	B	77	LEU	3.2
2	B	131	ARG	3.2
2	B	279	TYR	3.1
2	B	313	TYR	3.1
1	A	1961	LEU	3.1
2	B	213	ILE	3.1
1	A	1878	CYS	3.1
1	A	1847	ASP	3.1
1	A	2037	TYR	3.1
1	A	2032	ILE	3.1
2	B	294	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	171	ASP	3.0
2	B	299	LYS	3.0
1	A	1860	VAL	3.0
2	B	85	ASP	3.0
1	A	2033	THR	3.0
2	B	142	SER	3.0
2	B	107	LYS	3.0
2	B	278	GLN	2.9
1	A	1927	GLU	2.9
2	B	234	PHE	2.9
1	A	1963	LEU	2.9
2	B	88	LYS	2.9
2	B	221	PHE	2.8
2	B	41[A]	VAL	2.8
2	B	2	ASN	2.8
1	A	1873	LYS	2.8
2	B	65	GLY	2.8
2	B	86	GLY	2.8
1	A	1977	VAL	2.8
2	B	103	VAL	2.8
2	B	276	PRO	2.8
2	B	64[A]	MET	2.8
2	B	27	ASN	2.7
2	B	89	PHE	2.7
1	A	1864	LYS	2.7
2	B	282	ILE	2.7
1	A	2065	ARG	2.7
1	A	2067	TYR	2.7
1	A	1937	ARG	2.7
2	B	120	PHE	2.7
2	B	94	HIS	2.7
1	A	2009	THR	2.7
2	B	3	THR	2.7
1	A	1868	GLY	2.7
2	B	246	MET	2.7
2	B	312	LYS	2.7
1	A	2010	LEU	2.6
2	B	53	SER	2.6
1	A	1974	LEU	2.6
1	A	1998	ARG	2.6
1	A	2046	GLU	2.6
1	A	1885	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1861	THR	2.6
2	B	151	GLU	2.6
2	B	22	PHE	2.6
1	A	1918[A]	SER	2.6
1	A	2028	SER	2.6
2	B	45	HIS	2.5
2	B	52	SER	2.5
2	B	101	MET	2.5
1	A	1851	PHE	2.5
1	A	1869	ASN	2.5
1	A	2002	TYR	2.5
1	A	2034	ILE	2.5
2	B	307	LYS	2.5
1	A	2068	ASN	2.5
2	B	87	ALA	2.5
1	A	1988	LEU	2.4
2	B	29	PRO	2.4
2	B	150	ASN	2.4
2	B	180	VAL	2.4
1	A	1953	ASN	2.3
2	B	84	ARG	2.3
2	B	261	LEU	2.3
1	A	1903	LYS	2.3
1	A	1931[A]	LYS	2.3
1	A	1980	LYS	2.3
2	B	40	HIS	2.3
1	A	2021	SER	2.3
2	B	109	ASP	2.3
2	B	262	ASP	2.3
1	A	2024[A]	MET	2.3
2	B	303	HIS	2.3
2	B	290	ASN	2.3
2	B	112	ASP	2.2
2	B	26	GLU	2.2
2	B	110	GLU	2.2
2	B	255	THR	2.2
2	B	62	CYS	2.2
2	B	14	THR	2.2
2	B	100	GLN	2.1
2	B	277	GLU	2.1
2	B	49	ALA	2.1
1	A	1938	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	97	LYS	2.1
1	A	2043	PHE	2.1
2	B	256	VAL	2.1
1	A	2066	LYS	2.1
2	B	70	GLN	2.1
2	B	37	PRO	2.1
2	B	257	PRO	2.1
2	B	287	ARG	2.1
2	B	96	PHE	2.1
2	B	315	GLU	2.1
2	B	297	PHE	2.1
2	B	102	MET	2.0
1	A	2053[A]	SER	2.0
1	A	2041	PRO	2.0
2	B	132	LYS	2.0
2	B	122[A]	GLN	2.0
2	B	233	PHE	2.0
1	A	1935	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

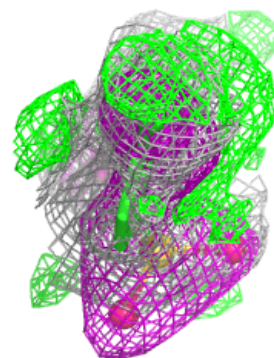
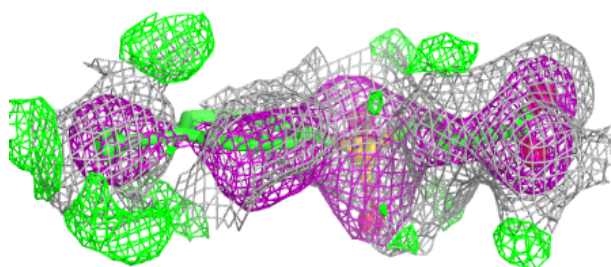
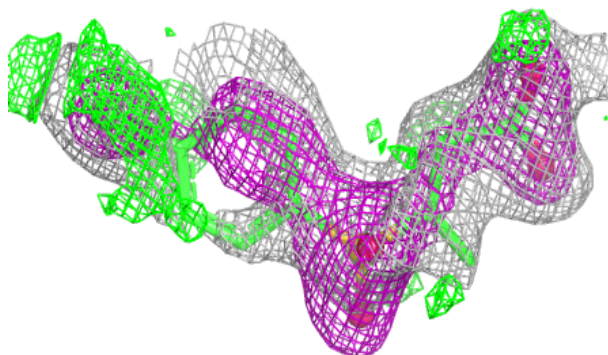
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	W3H	A	2101[A]	16/16	0.70	0.22	20,20,20,20	16
3	W3H	A	2101[B]	16/16	0.70	0.22	30,30,30,30	16
3	W3H	B	401	16/16	0.72	0.20	20,20,20,20	0

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.

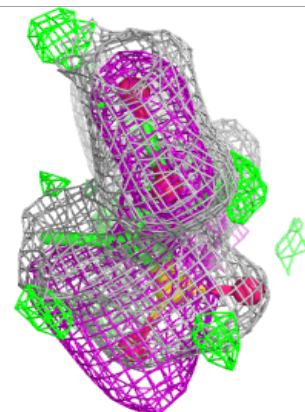
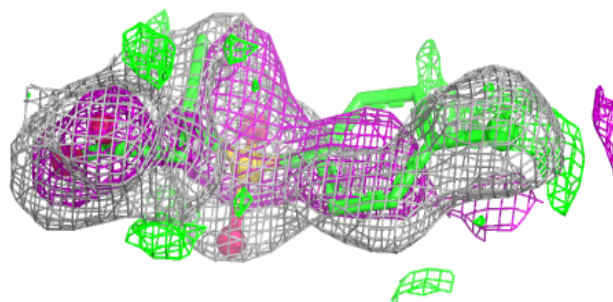
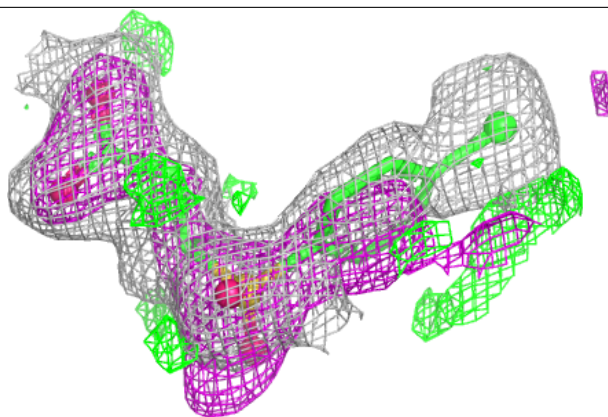
Electron density around W3H A 2101 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

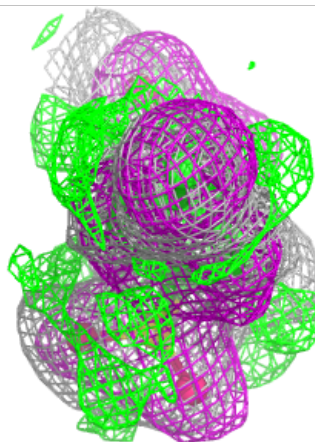
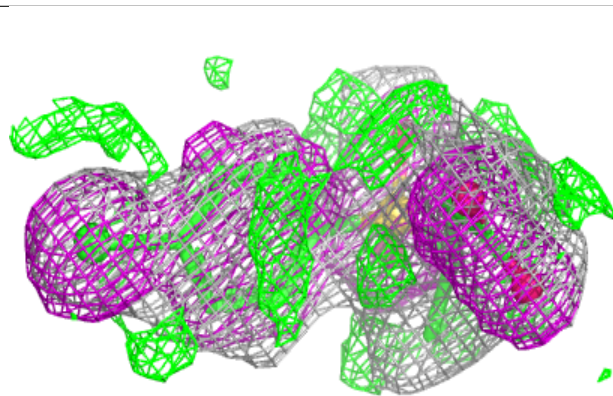
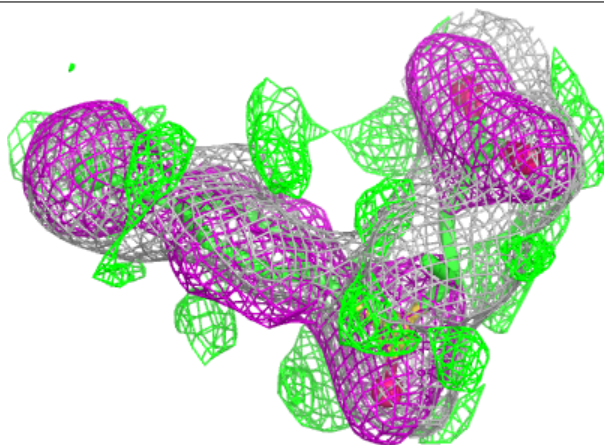


Electron density around W3H A 2101 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around W3H B 401:**

$2mF_o-DF_c$ (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.