



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:52 AM UTC

PDB ID : 4KOP / pdb_00004kop
Title : Crystal Structure of WHY2 from Arabidopsis thaliana
Authors : Cappadocia, L.; Parent, J.S.; Brisson, N.; Sygusch, J.
Deposited on : 2013-05-12
Resolution : 1.75 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
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

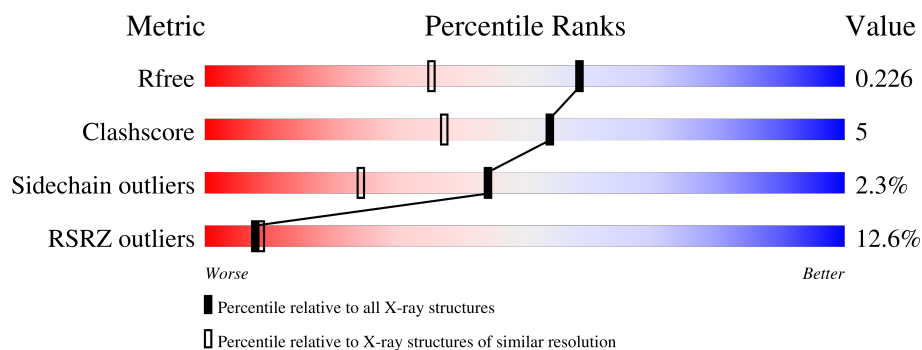
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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)
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	177	8% 79% 8% 13%
1	B	177	10% 75% 10% 15%
1	C	177	16% 77% 9% 14%
1	D	177	8% 69% 12% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10049 atoms, of which 4742 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 Single-stranded DNA-binding protein WHY2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	154	Total	C	H	N	O	S	0	0	0
			2432	785	1217	204	220	6			
1	B	151	Total	C	H	N	O	S	0	0	0
			2380	768	1192	199	215	6			
1	C	152	Total	C	H	N	O	S	0	0	0
			2387	770	1195	200	216	6			
1	D	145	Total	C	H	N	O	S	0	0	0
			2276	739	1138	186	207	6			

There are 36 discrepancies between the modelled and reference sequences:

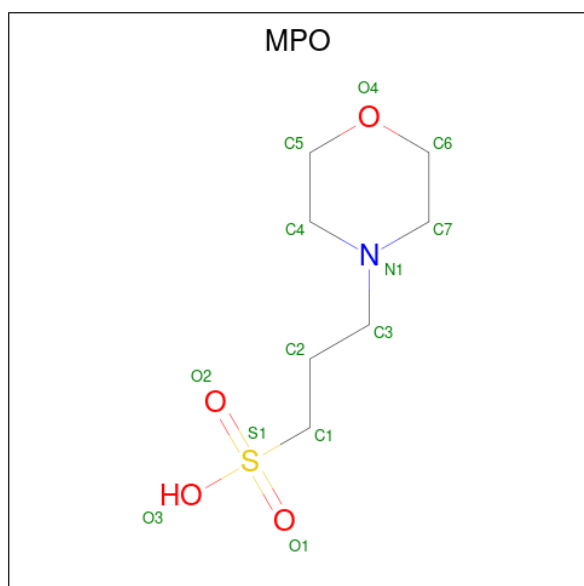
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	expression tag	UNP Q8VYF7
A	213	LEU	-	expression tag	UNP Q8VYF7
A	214	GLU	-	expression tag	UNP Q8VYF7
A	215	HIS	-	expression tag	UNP Q8VYF7
A	216	HIS	-	expression tag	UNP Q8VYF7
A	217	HIS	-	expression tag	UNP Q8VYF7
A	218	HIS	-	expression tag	UNP Q8VYF7
A	219	HIS	-	expression tag	UNP Q8VYF7
A	220	HIS	-	expression tag	UNP Q8VYF7
B	44	MET	-	expression tag	UNP Q8VYF7
B	213	LEU	-	expression tag	UNP Q8VYF7
B	214	GLU	-	expression tag	UNP Q8VYF7
B	215	HIS	-	expression tag	UNP Q8VYF7
B	216	HIS	-	expression tag	UNP Q8VYF7
B	217	HIS	-	expression tag	UNP Q8VYF7
B	218	HIS	-	expression tag	UNP Q8VYF7
B	219	HIS	-	expression tag	UNP Q8VYF7
B	220	HIS	-	expression tag	UNP Q8VYF7
C	44	MET	-	expression tag	UNP Q8VYF7
C	213	LEU	-	expression tag	UNP Q8VYF7
C	214	GLU	-	expression tag	UNP Q8VYF7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	215	HIS	-	expression tag	UNP Q8VYF7
C	216	HIS	-	expression tag	UNP Q8VYF7
C	217	HIS	-	expression tag	UNP Q8VYF7
C	218	HIS	-	expression tag	UNP Q8VYF7
C	219	HIS	-	expression tag	UNP Q8VYF7
C	220	HIS	-	expression tag	UNP Q8VYF7
D	44	MET	-	expression tag	UNP Q8VYF7
D	213	LEU	-	expression tag	UNP Q8VYF7
D	214	GLU	-	expression tag	UNP Q8VYF7
D	215	HIS	-	expression tag	UNP Q8VYF7
D	216	HIS	-	expression tag	UNP Q8VYF7
D	217	HIS	-	expression tag	UNP Q8VYF7
D	218	HIS	-	expression tag	UNP Q8VYF7
D	219	HIS	-	expression tag	UNP Q8VYF7
D	220	HIS	-	expression tag	UNP Q8VYF7

- Molecule 2 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

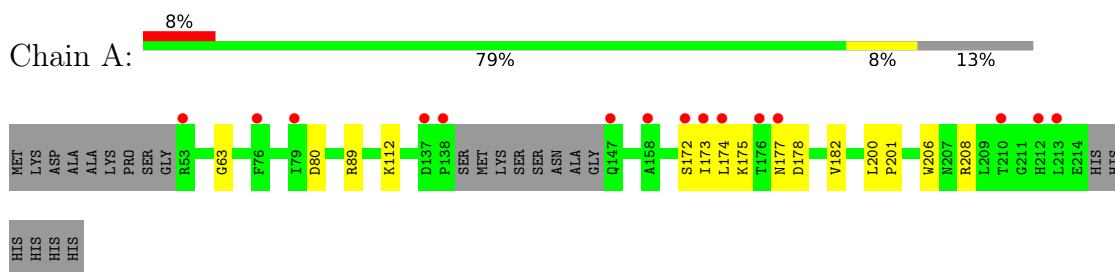
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	124	Total	O	0	0
			124	124		
3	C	97	Total	O	0	0
			97	97		
3	D	122	Total	O	0	0
			122	122		

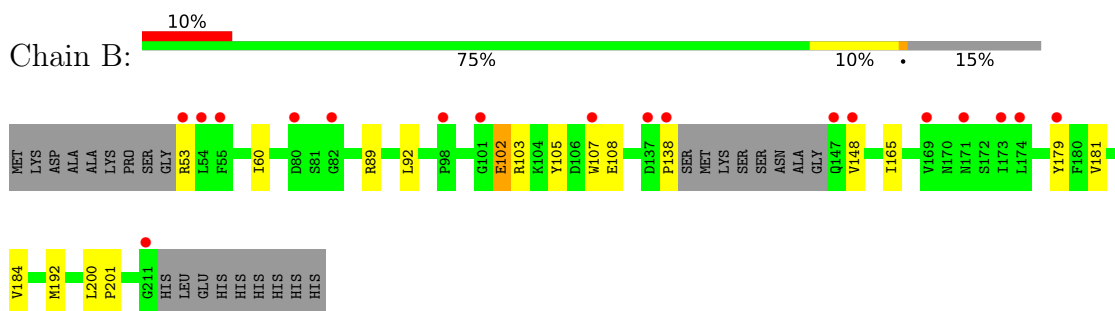
3 Residue-property plots [i](#)

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.

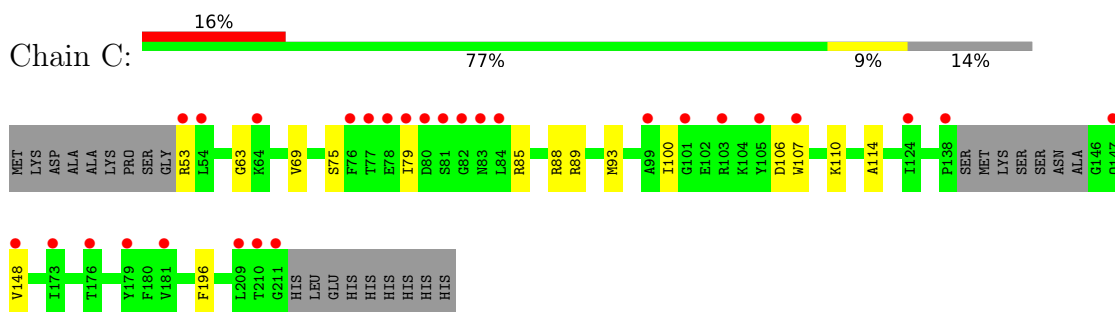
- Molecule 1: Single-stranded DNA-binding protein WHY2, mitochondrial



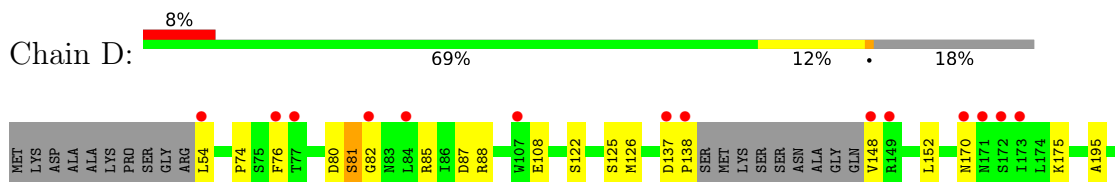
- Molecule 1: Single-stranded DNA-binding protein WHY2, mitochondrial



- Molecule 1: Single-stranded DNA-binding protein WHY2, mitochondrial



- Molecule 1: Single-stranded DNA-binding protein WHY2, mitochondrial



L200
P201
N207
ARG
LEU
THR
GLY
HIS
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.47Å 72.66Å 136.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.19 – 1.75 39.19 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.19-1.75) 94.8 (39.19-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.184 , 0.220 (Not available) , 0.226	Depositor DCC
R_{free} test set	2000 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.7	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	0.96	EDS
Total number of atoms	10049	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 3.95% 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: MPO

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	0.76	1/1246 (0.1%)	0.82	1/1679 (0.1%)
1	B	0.70	0/1218	0.78	0/1641
1	C	0.65	0/1222	0.81	1/1646 (0.1%)
1	D	0.73	0/1168	0.84	1/1575 (0.1%)
All	All	0.71	1/4854 (0.0%)	0.81	3/6541 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	VAL	CA-CB	5.76	1.58	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	SER	N-CA-C	6.60	123.54	113.51
1	C	63	GLY	N-CA-C	6.25	120.77	112.77
1	A	63	GLY	N-CA-C	5.14	118.90	112.73

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	1215	1217	1216	9	0
1	B	1188	1192	1192	15	0
1	C	1192	1195	1195	8	0
1	D	1138	1138	1137	15	0
2	A	13	0	14	0	0
2	B	26	0	28	0	0
2	C	13	0	14	1	0
2	D	26	0	28	0	0
3	A	153	0	0	3	0
3	B	124	0	0	2	0
3	C	97	0	0	1	0
3	D	122	0	0	2	0
All	All	5307	4742	4824	47	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 5.

All (47) 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:89:ARG:N	1:A:89:ARG:HD2	2.03	0.72
1:D:137:ASP:HB2	1:D:138:PRO:HA	1.75	0.69
1:B:105:TYR:O	1:B:107:TRP:CE3	2.52	0.63
1:D:125:SER:OG	3:D:462:HOH:O	2.16	0.61
1:D:81:SER:N	1:D:82:GLY:HA2	2.18	0.59
1:B:179:TYR:CE2	1:B:181:VAL:CG2	2.86	0.59
1:A:178:ASP:OD1	3:A:525:HOH:O	2.17	0.58
1:D:76:PHE:CD2	1:D:85:ARG:CZ	2.87	0.57
1:D:76:PHE:CD2	1:D:85:ARG:NH2	2.72	0.57
1:C:79:ILE:CD1	1:C:85:ARG:NH1	2.68	0.56
1:D:76:PHE:CE2	1:D:87:ASP:OD2	2.59	0.56
1:D:200:LEU:HB3	1:D:201:PRO:HD3	1.86	0.56
1:B:102:GLU:CG	1:B:103:ARG:H	2.18	0.55
1:D:170:ASN:HB2	3:D:515:HOH:O	2.06	0.54
1:A:112:LYS:NZ	3:A:471:HOH:O	2.41	0.53
1:B:92:LEU:C	1:B:92:LEU:HD13	2.34	0.53
1:A:174:LEU:O	1:A:175:LYS:CG	2.57	0.52
1:B:60:ILE:HD11	1:B:192:MET:HE3	1.91	0.52
1:B:165:ILE:HD12	1:B:184:VAL:HG21	1.93	0.50
1:B:179:TYR:CE2	1:B:181:VAL:HG23	2.46	0.50
1:B:138:PRO:HD2	1:B:148:VAL:O	2.12	0.49
1:D:74:PRO:HA	1:D:88:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:MET:HE1	1:C:114:ALA:HB2	1.95	0.47
3:B:475:HOH:O	1:D:207:ASN:HB2	2.15	0.47
1:B:60:ILE:CD1	1:B:192:MET:CE	2.92	0.47
1:B:60:ILE:CD1	1:B:192:MET:HE3	2.46	0.46
1:C:100:ILE:CG2	1:C:106:ASP:HB2	2.46	0.46
1:B:200:LEU:HB3	1:B:201:PRO:HD3	1.97	0.46
1:D:76:PHE:HE2	1:D:87:ASP:OD2	1.99	0.45
2:C:301:MPO:H21	2:C:301:MPO:H41	1.63	0.45
1:B:108:GLU:HG3	1:B:108:GLU:O	2.17	0.45
1:C:89:ARG:NH1	3:C:436:HOH:O	2.47	0.44
1:A:174:LEU:O	1:A:175:LYS:HG2	2.18	0.44
1:A:206:TRP:CZ3	1:D:195:ALA:HB1	2.52	0.43
1:B:102:GLU:CG	1:B:103:ARG:N	2.80	0.43
1:D:122:SER:O	1:D:126:MET:HG3	2.19	0.43
1:A:177:ASN:ND2	3:A:493:HOH:O	2.52	0.42
1:B:89:ARG:HG2	3:B:479:HOH:O	2.19	0.42
1:C:107:TRP:HB2	1:C:110:LYS:HE3	2.02	0.42
1:B:60:ILE:HD12	1:B:192:MET:CE	2.48	0.42
1:D:80:ASP:O	1:D:81:SER:HB2	2.19	0.42
1:C:79:ILE:HD13	1:C:85:ARG:NH1	2.34	0.42
1:A:173:ILE:HG22	1:A:174:LEU:N	2.34	0.42
1:A:200:LEU:HB3	1:A:201:PRO:HD3	2.01	0.42
1:C:69:VAL:HG21	1:C:196:PHE:CZ	2.55	0.41
1:C:75:SER:OG	1:C:88:ARG:CG	2.68	0.41
1:D:80:ASP:C	1:D:82:GLY:HA2	2.46	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	134/152 (88%)	131 (98%)	3 (2%)	45	26
1	B	131/152 (86%)	129 (98%)	2 (2%)	57	41
1	C	131/152 (86%)	129 (98%)	2 (2%)	57	41
1	D	126/152 (83%)	121 (96%)	5 (4%)	28	9
All	All	522/608 (86%)	510 (98%)	12 (2%)	44	24

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASP
1	A	172	SER
1	A	208	ARG
1	B	53	ARG
1	B	102	GLU
1	C	53	ARG
1	C	148	VAL
1	D	54	LEU
1	D	108	GLU
1	D	148	VAL
1	D	152	LEU
1	D	175	LYS

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

Mol	Chain	Res	Type
1	D	83	ASN
1	D	111	GLN
1	D	170	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	MPO	B	301	-	13,13,13	1.41	3 (23%)	17,17,17	1.98	6 (35%)
2	MPO	A	301	-	13,13,13	1.47	2 (15%)	17,17,17	1.46	1 (5%)
2	MPO	D	302	-	13,13,13	1.42	2 (15%)	17,17,17	1.88	6 (35%)
2	MPO	D	301	-	13,13,13	1.15	1 (7%)	17,17,17	2.32	6 (35%)
2	MPO	B	302	-	13,13,13	1.15	2 (15%)	17,17,17	2.20	8 (47%)
2	MPO	C	301	-	13,13,13	1.20	2 (15%)	17,17,17	1.84	6 (35%)

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	MPO	B	301	-	-	4/7/15/15	0/1/1/1
2	MPO	A	301	-	-	3/7/15/15	0/1/1/1
2	MPO	D	302	-	-	5/7/15/15	0/1/1/1
2	MPO	D	301	-	-	5/7/15/15	0/1/1/1
2	MPO	B	302	-	-	1/7/15/15	0/1/1/1
2	MPO	C	301	-	-	6/7/15/15	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	MPO	C1-S1	-3.32	1.72	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302	MPO	C1-S1	-3.11	1.73	1.77
2	B	301	MPO	C1-S1	-3.03	1.73	1.77
2	D	302	MPO	C4-N1	-2.72	1.39	1.46
2	A	301	MPO	C4-N1	-2.65	1.39	1.46
2	B	301	MPO	C4-N1	-2.58	1.39	1.46
2	B	302	MPO	C1-S1	-2.52	1.74	1.77
2	C	301	MPO	C4-N1	-2.45	1.40	1.46
2	D	301	MPO	C4-N1	-2.29	1.40	1.46
2	B	302	MPO	C4-N1	-2.14	1.41	1.46
2	B	301	MPO	C7-N1	-2.08	1.41	1.46
2	C	301	MPO	C1-S1	-2.02	1.74	1.77

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	MPO	C2-C1-S1	4.19	119.67	113.25
2	D	301	MPO	O1-S1-C1	3.78	112.44	106.73
2	C	301	MPO	O2-S1-O1	-3.70	101.78	113.82
2	D	301	MPO	C6-C7-N1	3.66	115.69	110.12
2	A	301	MPO	O2-S1-O1	-3.61	102.07	113.82
2	D	302	MPO	O2-S1-O1	-3.61	102.09	113.82
2	B	301	MPO	O2-S1-O1	-3.56	102.23	113.82
2	B	302	MPO	O3-S1-C1	3.52	112.89	106.00
2	B	302	MPO	O2-S1-C1	3.50	112.02	106.73
2	D	302	MPO	O1-S1-C1	3.47	111.97	106.73
2	B	301	MPO	O1-S1-C1	3.46	111.96	106.73
2	B	301	MPO	C3-N1-C7	3.46	120.46	111.24
2	C	301	MPO	C3-N1-C7	3.39	120.28	111.24
2	D	301	MPO	O2-S1-O1	-3.33	103.00	113.82
2	B	302	MPO	O1-S1-C1	3.08	111.38	106.73
2	B	302	MPO	O2-S1-O1	-3.06	103.88	113.82
2	B	302	MPO	C2-C1-S1	3.00	117.84	113.25
2	D	301	MPO	C5-C4-N1	2.97	114.64	110.12
2	D	302	MPO	C3-N1-C7	2.94	119.08	111.24
2	D	301	MPO	C2-C3-N1	2.93	122.18	113.93
2	B	301	MPO	C7-N1-C4	2.87	115.02	108.84
2	B	302	MPO	C3-N1-C7	2.73	118.52	111.24
2	D	302	MPO	O2-S1-C1	2.72	110.83	106.73
2	D	302	MPO	C3-N1-C4	2.65	118.30	111.24
2	B	301	MPO	C3-N1-C4	2.61	118.18	111.24
2	B	302	MPO	C3-N1-C4	2.49	117.88	111.24
2	B	301	MPO	O2-S1-C1	2.32	110.23	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	MPO	C2-C3-N1	2.32	120.45	113.93
2	C	301	MPO	C5-C4-N1	2.21	113.48	110.12
2	C	301	MPO	C2-C1-S1	2.20	116.62	113.25
2	C	301	MPO	O3-S1-C1	2.15	110.20	106.00
2	D	302	MPO	O3-S1-C1	2.04	109.99	106.00
2	C	301	MPO	O2-S1-C1	2.04	109.81	106.73

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	MPO	C1-C2-C3-N1
2	C	301	MPO	C2-C1-S1-O2
2	C	301	MPO	C1-C2-C3-N1
2	C	301	MPO	C2-C3-N1-C4
2	B	301	MPO	C2-C3-N1-C7
2	C	301	MPO	C2-C1-S1-O3
2	D	301	MPO	C2-C1-S1-O3
2	A	301	MPO	C2-C3-N1-C4
2	B	301	MPO	C2-C3-N1-C4
2	D	302	MPO	C2-C1-S1-O3
2	A	301	MPO	C2-C3-N1-C7
2	D	302	MPO	C2-C3-N1-C7
2	B	302	MPO	C2-C3-N1-C4
2	D	302	MPO	C2-C3-N1-C4
2	A	301	MPO	S1-C1-C2-C3
2	C	301	MPO	C2-C1-S1-O1
2	D	301	MPO	C2-C1-S1-O1
2	D	301	MPO	C2-C1-S1-O2
2	D	301	MPO	S1-C1-C2-C3
2	D	301	MPO	C1-C2-C3-N1
2	D	302	MPO	C2-C1-S1-O2
2	C	301	MPO	C2-C3-N1-C7
2	D	302	MPO	C1-C2-C3-N1
2	B	301	MPO	S1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	MPO	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	154/177 (87%)	0.44	15 (9%) 13 15	20, 30, 69, 107	0
1	B	151/177 (85%)	0.67	18 (11%) 9 10	20, 36, 84, 114	0
1	C	152/177 (85%)	0.81	28 (18%) 3 3	24, 36, 90, 145	0
1	D	145/177 (81%)	0.47	15 (10%) 12 13	22, 33, 65, 82	0
All	All	602/708 (85%)	0.60	76 (12%) 8 9	20, 34, 80, 145	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	PRO	6.0
1	A	173	ILE	4.9
1	C	107	TRP	4.9
1	C	79	ILE	4.6
1	B	173	ILE	4.4
1	A	210	THR	4.3
1	D	170	ASN	4.3
1	B	55	PHE	4.2
1	C	148	VAL	4.2
1	C	82	GLY	4.2
1	C	211	GLY	4.0
1	A	137	ASP	4.0
1	C	77	THR	4.0
1	B	54	LEU	3.9
1	D	138	PRO	3.7
1	C	76	PHE	3.6
1	B	171	ASN	3.6
1	B	107	TRP	3.6
1	D	54	LEU	3.6
1	C	210	THR	3.5
1	A	213	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	138	PRO	3.4
1	A	138	PRO	3.4
1	A	212	HIS	3.3
1	C	173	ILE	3.2
1	C	105	TYR	3.2
1	A	174	LEU	3.2
1	C	78	GLU	3.2
1	C	81	SER	3.2
1	B	174	LEU	3.1
1	B	148	VAL	3.1
1	D	173	ILE	3.0
1	A	172	SER	3.0
1	B	80	ASP	2.9
1	C	64	LYS	2.9
1	D	76	PHE	2.9
1	C	124	ILE	2.8
1	D	149	ARG	2.7
1	D	84	LEU	2.7
1	B	82	GLY	2.6
1	A	53	ARG	2.6
1	B	101	GLY	2.6
1	B	53	ARG	2.6
1	B	179	TYR	2.5
1	A	147	GLN	2.5
1	D	82	GLY	2.5
1	C	54	LEU	2.5
1	B	98	PRO	2.5
1	B	169	VAL	2.4
1	D	172	SER	2.4
1	C	80	ASP	2.4
1	D	107	TRP	2.4
1	C	103	ARG	2.4
1	C	83	ASN	2.3
1	D	207	ASN	2.3
1	A	76	PHE	2.3
1	A	158	ALA	2.2
1	C	101	GLY	2.2
1	C	53	ARG	2.2
1	C	176	THR	2.2
1	A	177	ASN	2.2
1	C	209	LEU	2.2
1	C	147	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	176	THR	2.2
1	C	181	VAL	2.2
1	B	147	GLN	2.2
1	C	84	LEU	2.2
1	D	148	VAL	2.1
1	C	99	ALA	2.1
1	B	211	GLY	2.1
1	C	179	TYR	2.1
1	A	79	ILE	2.1
1	D	171	ASN	2.1
1	D	137	ASP	2.1
1	D	77	THR	2.0
1	B	137	ASP	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
2	MPO	B	301	13/13	0.72	0.21	41,46,67,85	13
2	MPO	C	301	13/13	0.72	0.27	50,53,69,70	13
2	MPO	D	301	13/13	0.85	0.25	31,78,102,102	13
2	MPO	B	302	13/13	0.89	0.21	34,63,92,94	13
2	MPO	A	301	13/13	0.93	0.23	24,48,85,90	13
2	MPO	D	302	13/13	0.94	0.11	35,39,51,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.