



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 05:32 PM EST

PDB ID : 4KOP
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

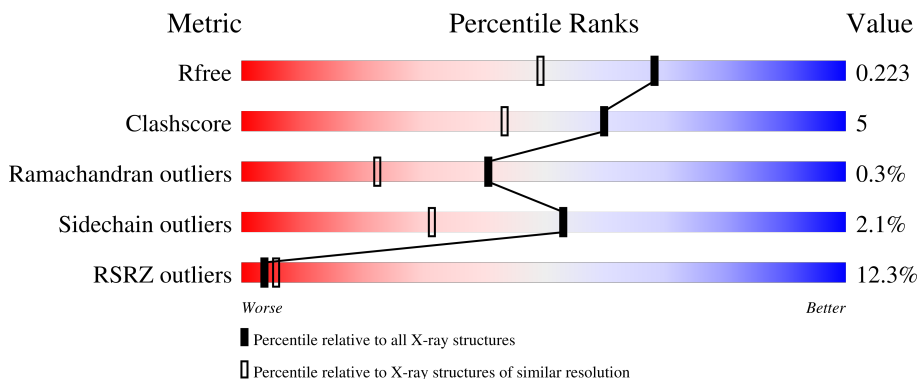
1 Overall quality at a glance

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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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	 10% 80% 7% • 13%
1	B	177	 7% 75% 11% 15%
1	C	177	 16% 79% 7% • 14%
1	D	177	 9% 69% 12% 18%

2 Entry composition [i](#)

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

There are 36 discrepancies between the modelled and reference sequences:

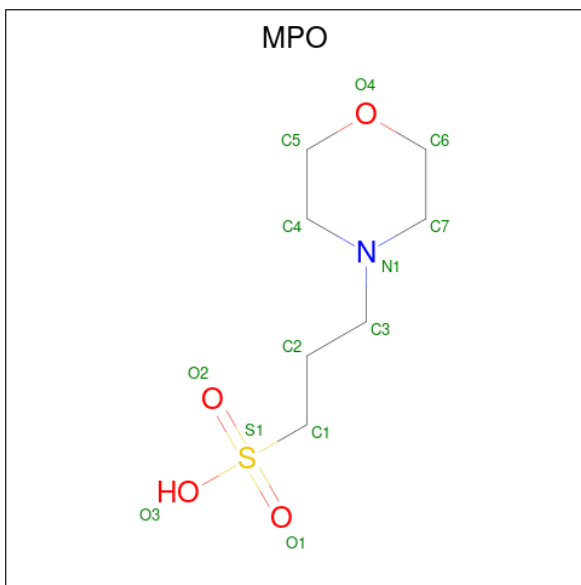
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	expression tag	UNP Q8VYF7
A	213	LEU	-	expression tag	UNP Q8VYF7
A	214	GLU	-	expression tag	UNP Q8VYF7
A	215	HIS	-	expression tag	UNP Q8VYF7
A	216	HIS	-	expression tag	UNP Q8VYF7
A	217	HIS	-	expression tag	UNP Q8VYF7
A	218	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

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 (three-letter code: MPO) (formula: C₇H₁₅NO₄S).



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

Continued on next page...

Continued from previous page...

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.

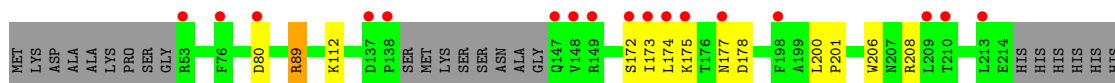
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	124	Total	O	0	0
			124	124		
3	C	97	Total	O	0	0
			97	97		
3	D	122	Total	O	0	0
			122	122		

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

Chain A: 




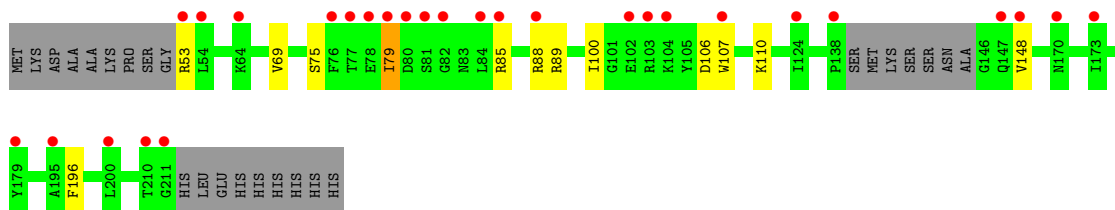
- Molecule 1: Single-stranded DNA-binding protein WHY2, mitochondrial

Chain B: 



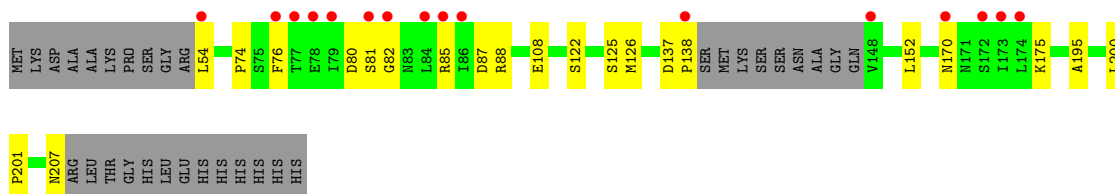
- Molecule 1: Single-stranded DNA-binding protein WHY2, mitochondrial

Chain C: 



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

Chain D: 



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 39.18 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.19-1.75) 94.3 (39.18-1.74)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.74Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.184 , 0.220 0.185 , 0.223	Depositor DCC
R_{free} test set	2000 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtrriage
Anisotropy	0.262	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.65	0/1246	0.66	0/1679
1	B	0.56	0/1218	0.61	0/1641
1	C	0.51	0/1222	0.62	0/1646
1	D	0.59	0/1168	0.67	0/1575
All	All	0.58	0/4854	0.64	0/6541

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1215	1217	1216	9	0
1	B	1188	1192	1192	14	0
1	C	1192	1195	1195	7	0
1	D	1138	1138	1137	14	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	44	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 (44) 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:A:174:LEU:O	1:A:175:LYS:CG	2.57	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
1:B:92:LEU:C	1:B:92:LEU:HD13	2.34	0.48
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: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:B:102:GLU:CG	1:B:103:ARG:N	2.80	0.44
1:C:89:ARG:NH1	3:C:436:HOH:O	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:60:ILE:CD1	1:B:192:MET:HE3	2.51	0.41

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	150/177 (85%)	148 (99%)	2 (1%)	0	100	100
1	B	147/177 (83%)	144 (98%)	2 (1%)	1 (1%)	22	8
1	C	148/177 (84%)	143 (97%)	4 (3%)	1 (1%)	22	8
1	D	141/177 (80%)	137 (97%)	4 (3%)	0	100	100
All	All	586/708 (83%)	572 (98%)	12 (2%)	2 (0%)	41	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	79	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	79	ILE

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%)	130 (97%)	4 (3%)	41	18
1	B	131/152 (86%)	130 (99%)	1 (1%)	81	72
1	C	131/152 (86%)	129 (98%)	2 (2%)	65	49
1	D	126/152 (83%)	122 (97%)	4 (3%)	39	16
All	All	522/608 (86%)	511 (98%)	11 (2%)	53	31

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASP
1	A	89	ARG
1	A	172	SER
1	A	208	ARG
1	B	53	ARG
1	C	53	ARG
1	C	148	VAL
1	D	54	LEU
1	D	108	GLU
1	D	152	LEU
1	D	175	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	302	-	13,13,13	1.14	2 (15%)	17,17,17	2.43	8 (47%)
2	MPO	C	301	-	13,13,13	1.19	1 (7%)	17,17,17	1.93	7 (41%)
2	MPO	A	301	-	13,13,13	1.46	2 (15%)	17,17,17	1.52	4 (23%)
2	MPO	D	302	-	13,13,13	1.40	2 (15%)	17,17,17	2.05	6 (35%)
2	MPO	D	301	-	13,13,13	1.14	1 (7%)	17,17,17	2.46	8 (47%)
2	MPO	B	301	-	13,13,13	1.38	3 (23%)	17,17,17	2.11	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	302	-	-	1/7/15/15	0/1/1/1
2	MPO	C	301	-	-	6/7/15/15	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	301	-	-	4/7/15/15	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	MPO	C1-S1	-3.22	1.72	1.77
2	D	302	MPO	C1-S1	-3.01	1.73	1.77
2	B	301	MPO	C1-S1	-2.94	1.73	1.77
2	D	302	MPO	C4-N1	-2.67	1.39	1.46
2	A	301	MPO	C4-N1	-2.60	1.39	1.46
2	B	301	MPO	C4-N1	-2.53	1.39	1.46
2	B	302	MPO	C1-S1	-2.43	1.74	1.77
2	C	301	MPO	C4-N1	-2.40	1.40	1.46
2	D	301	MPO	C4-N1	-2.25	1.40	1.46
2	B	302	MPO	C4-N1	-2.10	1.41	1.46
2	B	301	MPO	C7-N1	-2.04	1.41	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	MPO	O1-S1-C1	4.58	112.44	106.92
2	B	302	MPO	O3-S1-C1	4.41	112.89	105.77
2	B	302	MPO	O2-S1-C1	4.24	112.02	106.92
2	D	302	MPO	O1-S1-C1	4.19	111.97	106.92
2	D	301	MPO	C2-C1-S1	4.19	119.67	113.25
2	B	301	MPO	O1-S1-C1	4.19	111.96	106.92
2	B	302	MPO	O1-S1-C1	3.71	111.38	106.92
2	D	301	MPO	C6-C7-N1	3.68	115.69	110.10
2	B	301	MPO	C3-N1-C7	3.61	120.46	111.23
2	C	301	MPO	C3-N1-C7	3.54	120.28	111.23
2	C	301	MPO	O2-S1-O1	-3.52	101.78	113.95
2	A	301	MPO	O2-S1-O1	-3.43	102.07	113.95
2	D	302	MPO	O2-S1-O1	-3.43	102.09	113.95
2	B	301	MPO	O2-S1-O1	-3.38	102.23	113.95
2	D	301	MPO	C2-C3-N1	3.30	122.18	113.84
2	D	302	MPO	O2-S1-C1	3.25	110.83	106.92
2	D	301	MPO	O2-S1-O1	-3.16	103.00	113.95
2	D	302	MPO	C3-N1-C7	3.07	119.08	111.23
2	B	302	MPO	C2-C1-S1	3.00	117.84	113.25
2	D	301	MPO	C5-C4-N1	2.99	114.64	110.10
2	B	302	MPO	O2-S1-O1	-2.91	103.88	113.95
2	B	302	MPO	C3-N1-C7	2.85	118.52	111.23
2	D	302	MPO	C3-N1-C4	2.76	118.30	111.23
2	B	301	MPO	O2-S1-C1	2.75	110.23	106.92
2	B	301	MPO	C7-N1-C4	2.75	115.02	108.83
2	C	301	MPO	O3-S1-C1	2.74	110.20	105.77
2	B	301	MPO	C3-N1-C4	2.72	118.18	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	MPO	C2-C3-N1	2.62	120.45	113.84
2	D	302	MPO	O3-S1-C1	2.61	109.99	105.77
2	B	302	MPO	C3-N1-C4	2.60	117.88	111.23
2	D	301	MPO	O3-S1-C1	2.51	109.83	105.77
2	A	301	MPO	O3-S1-C1	2.51	109.83	105.77
2	C	301	MPO	O2-S1-C1	2.40	109.81	106.92
2	C	301	MPO	O1-S1-C1	2.26	109.64	106.92
2	C	301	MPO	C5-C4-N1	2.23	113.48	110.10
2	C	301	MPO	C2-C1-S1	2.20	116.62	113.25
2	D	301	MPO	O2-S1-C1	2.09	109.43	106.92
2	A	301	MPO	O2-S1-C1	2.04	109.37	106.92
2	A	301	MPO	C3-N1-C7	2.02	116.40	111.23

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-C3-N1-C7
2	A	301	MPO	C2-C3-N1-C7
2	B	302	MPO	C2-C3-N1-C4
2	D	302	MPO	C2-C1-S1-O3
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	302	MPO	C2-C1-S1-O2
2	D	301	MPO	S1-C1-C2-C3
2	D	301	MPO	C1-C2-C3-N1
2	C	301	MPO	C2-C3-N1-C7
2	B	301	MPO	S1-C1-C2-C3
2	D	302	MPO	C1-C2-C3-N1

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

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	154/177 (87%)	0.57	17 (11%) 5 7	18, 27, 64, 93	0
1	B	151/177 (85%)	0.62	13 (8%) 10 13	19, 33, 79, 107	0
1	C	152/177 (85%)	0.77	28 (18%) 1 1	22, 33, 85, 137	0
1	D	145/177 (81%)	0.46	16 (11%) 5 7	19, 29, 59, 74	0
All	All	602/708 (85%)	0.61	74 (12%) 4 6	18, 31, 72, 137	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	82	GLY	8.7
1	A	173	ILE	7.8
1	C	79	ILE	7.3
1	D	173	ILE	7.1
1	B	53	ARG	7.0
1	C	107	TRP	6.6
1	B	173	ILE	6.4
1	D	138	PRO	5.8
1	C	148	VAL	5.7
1	C	78	GLU	5.6
1	B	54	LEU	5.4
1	D	76	PHE	5.4
1	A	172	SER	5.2
1	C	77	THR	5.0
1	B	55	PHE	5.0
1	B	175	LYS	4.8
1	A	174	LEU	4.8
1	D	148	VAL	4.5
1	D	77	THR	4.2
1	D	174	LEU	4.2
1	C	102	GLU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	103	ARG	4.1
1	A	137	ASP	3.8
1	A	147	GLN	3.6
1	A	213	LEU	3.6
1	D	84	LEU	3.6
1	A	138	PRO	3.5
1	D	54	LEU	3.5
1	A	148	VAL	3.4
1	B	107	TRP	3.4
1	A	53	ARG	3.4
1	B	171	ASN	3.3
1	C	81	SER	3.3
1	B	172	SER	3.3
1	D	79	ILE	3.2
1	C	53	ARG	3.1
1	B	147	GLN	3.1
1	B	100	ILE	3.1
1	C	210	THR	3.1
1	C	80	ASP	2.9
1	C	211	GLY	2.8
1	C	170	ASN	2.8
1	A	175	LYS	2.7
1	B	102	GLU	2.7
1	C	138	PRO	2.7
1	C	76	PHE	2.6
1	C	173	ILE	2.6
1	D	81	SER	2.6
1	D	170	ASN	2.5
1	B	108	GLU	2.5
1	D	172	SER	2.5
1	A	210	THR	2.4
1	C	147	GLN	2.4
1	D	82	GLY	2.4
1	C	64	LYS	2.4
1	A	209	LEU	2.3
1	D	78	GLU	2.3
1	C	124	ILE	2.3
1	A	76	PHE	2.3
1	A	149	ARG	2.3
1	A	80	ASP	2.3
1	A	198	PHE	2.3
1	C	84	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	200	LEU	2.2
1	B	124	ILE	2.2
1	D	86	ILE	2.2
1	D	85	ARG	2.2
1	A	177	ASN	2.1
1	C	54	LEU	2.1
1	C	195	ALA	2.0
1	C	104	LYS	2.0
1	C	85	ARG	2.0
1	C	88	ARG	2.0
1	C	179	TYR	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 monosaccharides 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	C	301	13/13	0.74	0.22	50,53,69,70	13
2	MPO	B	301	13/13	0.78	0.18	41,46,67,85	13
2	MPO	D	301	13/13	0.94	0.19	31,78,102,102	13
2	MPO	B	302	13/13	0.95	0.24	34,63,92,94	13
2	MPO	A	301	13/13	0.97	0.23	24,48,85,90	13
2	MPO	D	302	13/13	0.97	0.10	35,39,51,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.