



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:28 pm BST

PDB ID : 4KOO
Title : Crystal Structure of WHY1 from Arabidopsis thaliana
Authors : Cappadocia, L.; Parent, J.S.; Brisson, N.; Sygusch, J.
Deposited on : 2013-05-12
Resolution : 1.88 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 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 : 2.11
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) : 2.11

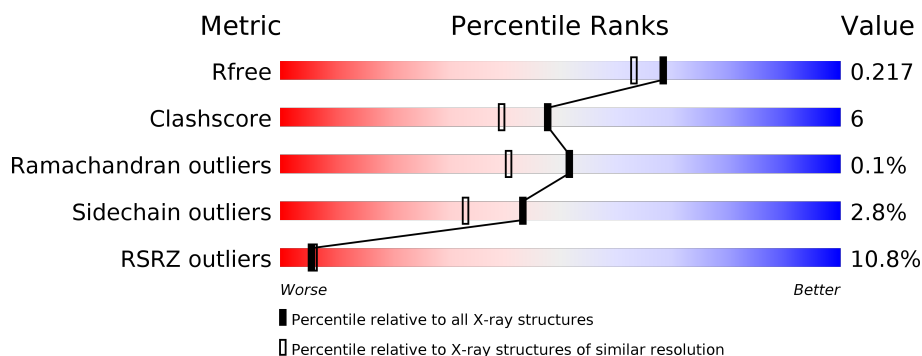
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 on 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	180	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	180	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>10%</div> </div> </div>
1	C	180	<div> <div>14%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
1	D	180	<div> <div>14%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11538 atoms, of which 5430 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 WHY1, chloroplastic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	176	Total	C	H	N	O	S	0	2	0
			2794	917	1392	240	244	1			
1	B	162	Total	C	H	N	O	S	0	0	0
			2547	836	1272	211	227	1			
1	C	165	Total	C	H	N	O	S	0	1	0
			2606	853	1306	215	231	1			
1	D	175	Total	C	H	N	O	S	0	2	0
			2777	911	1385	237	243	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	MET	-	EXPRESSION TAG	UNP Q9M9S3
A	242	ALA	-	EXPRESSION TAG	UNP Q9M9S3
A	243	ALA	-	EXPRESSION TAG	UNP Q9M9S3
A	244	ALA	-	EXPRESSION TAG	UNP Q9M9S3
A	245	LEU	-	EXPRESSION TAG	UNP Q9M9S3
A	246	GLU	-	EXPRESSION TAG	UNP Q9M9S3
A	247	HIS	-	EXPRESSION TAG	UNP Q9M9S3
A	248	HIS	-	EXPRESSION TAG	UNP Q9M9S3
A	249	HIS	-	EXPRESSION TAG	UNP Q9M9S3
A	250	HIS	-	EXPRESSION TAG	UNP Q9M9S3
A	251	HIS	-	EXPRESSION TAG	UNP Q9M9S3
A	252	HIS	-	EXPRESSION TAG	UNP Q9M9S3
B	73	MET	-	EXPRESSION TAG	UNP Q9M9S3
B	242	ALA	-	EXPRESSION TAG	UNP Q9M9S3
B	243	ALA	-	EXPRESSION TAG	UNP Q9M9S3
B	244	ALA	-	EXPRESSION TAG	UNP Q9M9S3
B	245	LEU	-	EXPRESSION TAG	UNP Q9M9S3
B	246	GLU	-	EXPRESSION TAG	UNP Q9M9S3
B	247	HIS	-	EXPRESSION TAG	UNP Q9M9S3
B	248	HIS	-	EXPRESSION TAG	UNP Q9M9S3
B	249	HIS	-	EXPRESSION TAG	UNP Q9M9S3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	250	HIS	-	EXPRESSION TAG	UNP Q9M9S3
B	251	HIS	-	EXPRESSION TAG	UNP Q9M9S3
B	252	HIS	-	EXPRESSION TAG	UNP Q9M9S3
C	73	MET	-	EXPRESSION TAG	UNP Q9M9S3
C	242	ALA	-	EXPRESSION TAG	UNP Q9M9S3
C	243	ALA	-	EXPRESSION TAG	UNP Q9M9S3
C	244	ALA	-	EXPRESSION TAG	UNP Q9M9S3
C	245	LEU	-	EXPRESSION TAG	UNP Q9M9S3
C	246	GLU	-	EXPRESSION TAG	UNP Q9M9S3
C	247	HIS	-	EXPRESSION TAG	UNP Q9M9S3
C	248	HIS	-	EXPRESSION TAG	UNP Q9M9S3
C	249	HIS	-	EXPRESSION TAG	UNP Q9M9S3
C	250	HIS	-	EXPRESSION TAG	UNP Q9M9S3
C	251	HIS	-	EXPRESSION TAG	UNP Q9M9S3
C	252	HIS	-	EXPRESSION TAG	UNP Q9M9S3
D	73	MET	-	EXPRESSION TAG	UNP Q9M9S3
D	242	ALA	-	EXPRESSION TAG	UNP Q9M9S3
D	243	ALA	-	EXPRESSION TAG	UNP Q9M9S3
D	244	ALA	-	EXPRESSION TAG	UNP Q9M9S3
D	245	LEU	-	EXPRESSION TAG	UNP Q9M9S3
D	246	GLU	-	EXPRESSION TAG	UNP Q9M9S3
D	247	HIS	-	EXPRESSION TAG	UNP Q9M9S3
D	248	HIS	-	EXPRESSION TAG	UNP Q9M9S3
D	249	HIS	-	EXPRESSION TAG	UNP Q9M9S3
D	250	HIS	-	EXPRESSION TAG	UNP Q9M9S3
D	251	HIS	-	EXPRESSION TAG	UNP Q9M9S3
D	252	HIS	-	EXPRESSION TAG	UNP Q9M9S3

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
2	A	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
2	B	1	Total 25	C 6	H 13	N 1	O 4	S 1	0	0
2	C	1	Total 24	C 6	H 12	N 1	O 4	S 1	0	0
2	D	1	Total 24	C 6	H 12	N 1	O 4	S 1	0	0
2	D	1	Total 24	C 6	H 12	N 1	O 4	S 1	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		

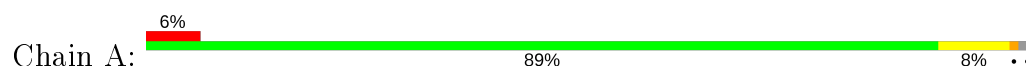
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		
5	B	176	Total	O	0	0
			176	176		
5	C	143	Total	O	0	0
			143	143		
5	D	139	Total	O	0	0
			139	139		

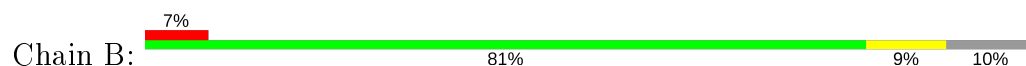
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

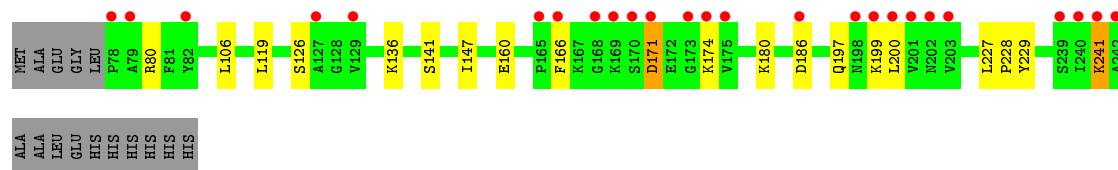
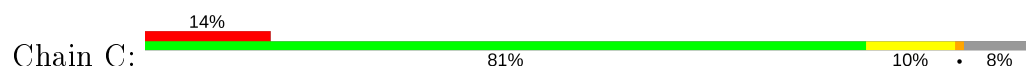
- Molecule 1: Single-stranded DNA-binding protein WHY1, chloroplastic



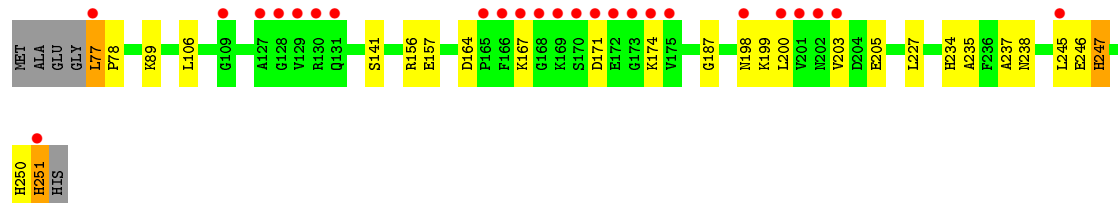
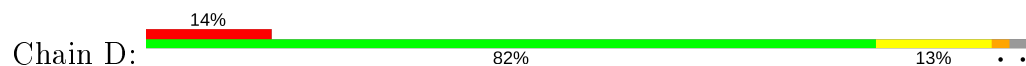
- Molecule 1: Single-stranded DNA-binding protein WHY1, chloroplastic



- Molecule 1: Single-stranded DNA-binding protein WHY1, chloroplastic



- Molecule 1: Single-stranded DNA-binding protein WHY1, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.59Å 180.69Å 116.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.28 – 1.88 48.46 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.28-1.88) 98.0 (48.46-1.88)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.176 , 0.215 0.178 , 0.217	Depositor DCC
R_{free} test set	2000 reflections (2.87%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11538	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2419e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NI, PO4, MES

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	0.60	0/1452	0.69	1/1968 (0.1%)
1	B	0.62	0/1312	0.69	0/1777
1	C	0.54	0/1340	0.62	0/1814
1	D	0.53	0/1441	0.63	0/1953
All	All	0.57	0/5545	0.66	1/7512 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH2	5.30	122.95	120.30

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	1402	1392	1391	11	0
1	B	1275	1272	1271	10	0
1	C	1300	1306	1305	18	0
1	D	1392	1385	1384	27	0
2	A	24	26	26	3	0
2	B	12	13	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	12	12	1	0
2	D	24	24	24	2	0
3	A	1	0	0	0	0
4	B	5	0	0	0	0
5	A	203	0	0	4	0
5	B	176	0	0	3	0
5	C	143	0	0	5	0
5	D	139	0	0	2	0
All	All	6108	5430	5426	66	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 6.

All (66) 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:D:238:ASN:ND2	5:D:500:HOH:O	2.20	0.74
1:C:136:LYS:NZ	5:C:498:HOH:O	2.24	0.70
1:C:171:ASP:OD1	1:C:171:ASP:N	2.25	0.69
1:C:200:LEU:O	5:C:523:HOH:O	2.10	0.69
1:D:174:LYS:HD3	1:D:200:LEU:HD21	1.74	0.69
1:A:80:ARG:NH2	1:B:108:SER:O	2.29	0.65
1:B:236:PHE:O	5:B:574:HOH:O	2.13	0.65
1:A:248:HIS:N	5:A:489:HOH:O	2.29	0.65
1:B:238:ASN:O	1:B:239:SER:CB	2.46	0.62
1:A:141[B]:SER:OG	2:A:302:MES:H71	2.00	0.61
1:D:174:LYS:HD3	1:D:200:LEU:HD11	1.82	0.61
1:C:141[A]:SER:OG	2:C:301:MES:H51	2.01	0.61
1:D:251:HIS:O	5:D:526:HOH:O	2.17	0.57
1:A:234[B]:HIS:CG	1:A:235:ALA:N	2.74	0.55
1:B:164:ASP:HB3	1:B:167:LYS:HG2	1.88	0.54
1:D:234[B]:HIS:CG	1:D:235:ALA:N	2.76	0.54
1:D:174:LYS:CD	1:D:200:LEU:HD21	2.39	0.53
1:C:227:LEU:HB3	1:C:228:PRO:HD3	1.91	0.52
1:C:166:PHE:CB	1:C:171:ASP:HB2	2.40	0.52
1:D:164:ASP:HB3	1:D:167:LYS:HG2	1.91	0.52
1:B:238:ASN:O	1:B:239:SER:HB2	2.10	0.51
1:D:77:LEU:N	1:D:78:PRO:CD	2.74	0.51
1:A:248:HIS:CA	5:A:489:HOH:O	2.58	0.51
1:C:160:GLU:CG	1:C:180:LYS:HG2	2.40	0.51
1:C:197:GLN:NE2	5:C:455:HOH:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141[B]:SER:OG	2:D:302:MES:H72	2.11	0.49
1:D:174:LYS:HD3	1:D:200:LEU:CD2	2.41	0.49
1:C:160:GLU:HG3	1:C:180:LYS:HG2	1.95	0.48
1:C:174:LYS:HA	1:C:199:LYS:HE2	1.94	0.48
1:C:229:TYR:CD1	1:D:237:ALA:HB1	2.50	0.47
1:D:198:ASN:HB3	1:D:203:VAL:HG12	1.97	0.47
1:A:79:ALA:HA	5:B:492:HOH:O	2.15	0.47
1:D:250:HIS:O	1:D:251:HIS:CB	2.63	0.47
1:D:77:LEU:HD12	1:D:78:PRO:HD3	1.95	0.47
1:B:156:ARG:NH2	1:D:157:GLU:OE2	2.46	0.47
1:D:250:HIS:O	1:D:251:HIS:HB2	2.16	0.46
1:D:203:VAL:HG22	1:D:205:GLU:HG2	1.96	0.46
2:A:302:MES:C6	5:A:432:HOH:O	2.63	0.46
1:B:122:GLN:HG2	1:B:139:VAL:HG12	1.97	0.46
1:B:227:LEU:HB3	1:B:228:PRO:HD3	1.98	0.46
1:A:203:VAL:HG13	1:A:205:GLU:HG2	1.97	0.45
1:A:227:LEU:HB3	1:A:228:PRO:HD3	1.97	0.45
1:D:174:LYS:HD3	1:D:200:LEU:CD1	2.47	0.45
1:D:174:LYS:CD	1:D:200:LEU:HD11	2.46	0.45
1:D:171:ASP:HA	1:D:174:LYS:HD2	1.98	0.45
1:D:246:GLU:C	1:D:247:HIS:ND1	2.69	0.45
1:D:174:LYS:CG	1:D:200:LEU:HD21	2.46	0.44
1:C:119:LEU:HG	1:C:147:ILE:HD11	1.99	0.44
2:D:302:MES:H52	2:D:302:MES:H81	1.78	0.44
1:A:129:VAL:O	1:A:129:VAL:HG13	2.18	0.43
1:B:205:GLU:HG2	5:B:424:HOH:O	2.18	0.43
1:C:174:LYS:HD3	1:C:200:LEU:CD2	2.49	0.43
1:C:241:LYS:N	1:C:241:LYS:CD	2.82	0.43
1:A:245:LEU:HD12	1:A:245:LEU:HA	1.82	0.43
2:A:302:MES:H62	5:A:432:HOH:O	2.18	0.42
1:C:171:ASP:HA	5:C:490:HOH:O	2.20	0.42
1:D:156:ARG:NH2	1:D:187:GLY:O	2.48	0.42
1:D:174:LYS:HB3	1:D:200:LEU:HG	2.02	0.42
1:B:141:SER:O	1:B:163:HIS:HE1	2.03	0.41
1:C:241:LYS:N	1:C:241:LYS:HD2	2.35	0.41
1:A:160:GLU:OE2	1:A:180:LYS:HE2	2.21	0.41
1:C:166:PHE:HB3	1:C:171:ASP:HB2	2.03	0.41
1:D:174:LYS:HB3	1:D:200:LEU:HD21	2.02	0.41
1:D:199:LYS:O	1:D:200:LEU:HD23	2.20	0.41
1:D:89:LYS:HA	1:D:89:LYS:HD3	1.90	0.40
1:C:171:ASP:HB3	5:C:469:HOH:O	2.21	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	176/180 (98%)	169 (96%)	7 (4%)	0	100	100
1	B	160/180 (89%)	157 (98%)	3 (2%)	0	100	100
1	C	164/180 (91%)	159 (97%)	4 (2%)	1 (1%)	25	14
1	D	175/180 (97%)	169 (97%)	6 (3%)	0	100	100
All	All	675/720 (94%)	654 (97%)	20 (3%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	186	ASP

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	150/150 (100%)	147 (98%)	3 (2%)	55	47
1	B	137/150 (91%)	135 (98%)	2 (2%)	65	59
1	C	140/150 (93%)	135 (96%)	5 (4%)	35	23
1	D	149/150 (99%)	143 (96%)	6 (4%)	31	19
All	All	576/600 (96%)	560 (97%)	16 (3%)	43	33

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	245	LEU
1	A	252	HIS
1	B	80	ARG
1	B	97	ASP
1	C	80	ARG
1	C	106	LEU
1	C	126	SER
1	C	171	ASP
1	C	241	LYS
1	D	77	LEU
1	D	106	LEU
1	D	227	LEU
1	D	245	LEU
1	D	247	HIS
1	D	251	HIS

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	MES	D	301	-	12,12,12	2.38	1 (8%)	14,16,16	2.36	6 (42%)
2	MES	B	301	-	12,12,12	2.32	1 (8%)	14,16,16	2.31	6 (42%)
2	MES	A	302	-	12,12,12	1.96	1 (8%)	14,16,16	1.75	2 (14%)
4	PO4	B	302	-	4,4,4	1.27	1 (25%)	6,6,6	0.61	0
2	MES	C	301	-	12,12,12	2.30	1 (8%)	14,16,16	2.81	5 (35%)
2	MES	A	301	-	12,12,12	2.29	1 (8%)	14,16,16	1.80	4 (28%)
2	MES	D	302	-	12,12,12	2.12	1 (8%)	14,16,16	2.61	5 (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	MES	D	301	-	-	4/6/14/14	0/1/1/1
2	MES	B	301	-	-	5/6/14/14	0/1/1/1
2	MES	A	302	-	-	2/6/14/14	0/1/1/1
2	MES	C	301	-	-	2/6/14/14	0/1/1/1
2	MES	A	301	-	-	0/6/14/14	0/1/1/1
2	MES	D	302	-	-	1/6/14/14	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	MES	C8-S	-7.96	1.66	1.77
2	C	301	MES	C8-S	-7.75	1.66	1.77
2	A	301	MES	C8-S	-7.62	1.66	1.77
2	B	301	MES	C8-S	-7.60	1.66	1.77
2	D	302	MES	C8-S	-7.12	1.67	1.77
2	A	302	MES	C8-S	-6.49	1.68	1.77
4	B	302	PO4	P-O4	-2.47	1.47	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	MES	O1S-S-C8	8.08	116.64	106.92
2	D	302	MES	O1S-S-C8	5.81	113.91	106.92
2	D	302	MES	C5-N4-C3	5.57	121.38	108.83
2	D	301	MES	C5-N4-C3	5.31	120.79	108.83
2	A	302	MES	O3S-S-C8	5.06	113.96	105.77
2	D	302	MES	C7-N4-C5	4.05	121.58	111.23
2	B	301	MES	C6-C5-N4	-3.99	104.05	110.10
2	A	301	MES	O2S-S-C8	3.88	111.58	106.92
2	D	301	MES	O1S-S-C8	3.79	111.48	106.92
2	D	301	MES	C7-N4-C5	3.64	120.55	111.23
2	B	301	MES	C6-O1-C2	3.53	121.69	109.89
2	B	301	MES	O3S-S-C8	3.48	111.40	105.77
2	C	301	MES	C5-N4-C3	3.42	116.54	108.83
2	A	301	MES	C6-C5-N4	-3.07	105.44	110.10
2	C	301	MES	C7-N4-C3	2.87	118.57	111.23
2	B	301	MES	O2S-S-C8	2.72	110.20	106.92
2	B	301	MES	O1-C2-C3	2.71	117.75	111.80
2	C	301	MES	O3S-S-C8	2.54	109.87	105.77
2	A	301	MES	C5-N4-C3	2.51	114.49	108.83
2	C	301	MES	C7-N4-C5	2.29	117.09	111.23
2	D	302	MES	O2S-S-O1S	-2.28	106.05	113.95
2	D	302	MES	C7-N4-C3	2.19	116.83	111.23
2	D	301	MES	C6-C5-N4	-2.18	106.80	110.10
2	D	301	MES	C7-N4-C3	2.16	116.76	111.23
2	A	301	MES	O1S-S-C8	2.16	109.52	106.92
2	D	301	MES	O3S-S-C8	2.15	109.24	105.77
2	B	301	MES	C5-N4-C3	2.13	113.63	108.83
2	A	302	MES	C5-N4-C3	2.01	113.36	108.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	MES	C8-C7-N4-C5
2	B	301	MES	C8-C7-N4-C3
2	B	301	MES	C7-C8-S-O1S
2	C	301	MES	N4-C7-C8-S
2	D	302	MES	C8-C7-N4-C5
2	B	301	MES	C7-C8-S-O3S
2	A	302	MES	C8-C7-N4-C5
2	D	301	MES	C7-C8-S-O3S
2	D	301	MES	C7-C8-S-O1S
2	D	301	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
2	B	301	MES	C7-C8-S-O2S
2	B	301	MES	C8-C7-N4-C5
2	A	302	MES	C8-C7-N4-C3
2	C	301	MES	C8-C7-N4-C5

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	MES	3	0
2	C	301	MES	1	0
2	D	302	MES	2	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	176/180 (97%)	0.37	11 (6%) 20 21	11, 22, 64, 103	0
1	B	162/180 (90%)	0.41	12 (7%) 14 15	12, 22, 61, 82	0
1	C	165/180 (91%)	0.60	25 (15%) 2 2	16, 27, 72, 89	0
1	D	175/180 (97%)	0.72	25 (14%) 2 2	16, 29, 85, 103	0
All	All	678/720 (94%)	0.53	73 (10%) 5 6	11, 25, 74, 103	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	168	GLY	9.1
1	A	252	HIS	8.9
1	D	166	PHE	7.8
1	D	171	ASP	6.6
1	D	203	VAL	6.5
1	D	201	VAL	6.5
1	D	129	VAL	6.0
1	C	170	SER	5.8
1	A	129	VAL	5.5
1	C	168	GLY	5.5
1	D	77	LEU	5.5
1	A	77	LEU	5.4
1	C	166	PHE	5.4
1	D	169	LYS	5.2
1	D	200	LEU	5.2
1	C	203	VAL	5.1
1	B	168	GLY	5.0
1	C	171	ASP	4.9
1	B	237	ALA	4.7
1	C	174	LYS	4.4
1	A	107	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	170	SER	4.3
1	C	242	ALA	4.3
1	C	200	LEU	4.2
1	D	198	ASN	4.2
1	D	202	ASN	4.0
1	A	128	GLY	3.9
1	C	127	ALA	3.9
1	A	251	HIS	3.8
1	C	240	ILE	3.8
1	C	199	LYS	3.8
1	A	106	LEU	3.7
1	C	239	SER	3.6
1	C	78	PRO	3.6
1	D	127	ALA	3.5
1	B	200	LEU	3.4
1	A	130	ARG	3.4
1	D	130	ARG	3.4
1	D	165	PRO	3.4
1	C	165	PRO	3.3
1	C	175	VAL	3.2
1	D	174	LYS	3.1
1	C	79	ALA	3.1
1	B	170	SER	3.0
1	C	169	LYS	3.0
1	D	167	LYS	3.0
1	B	78	PRO	2.9
1	C	129	VAL	2.9
1	C	173	GLY	2.8
1	D	175	VAL	2.8
1	C	202	ASN	2.7
1	D	131	GLN	2.7
1	D	109	GLY	2.6
1	D	251	HIS	2.6
1	B	174	LYS	2.5
1	D	128	GLY	2.5
1	A	111	PHE	2.5
1	C	241	LYS	2.5
1	D	173	GLY	2.4
1	D	172	GLU	2.4
1	B	129	VAL	2.3
1	D	245	LEU	2.3
1	B	239	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	201	VAL	2.3
1	B	169	LYS	2.3
1	B	166	PHE	2.2
1	C	186	ASP	2.2
1	A	247	HIS	2.2
1	C	198	ASN	2.1
1	C	82	TYR	2.1
1	A	131	GLN	2.1
1	B	236	PHE	2.1
1	B	171	ASP	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	MES	B	301	12/12	0.92	0.14	40,51,61,68	0
2	MES	D	301	12/12	0.94	0.14	48,58,66,67	0
2	MES	C	301	12/12	0.94	0.22	30,55,69,78	0
2	MES	A	301	12/12	0.94	0.14	40,50,60,60	0
2	MES	D	302	12/12	0.94	0.29	36,72,90,97	0
2	MES	A	302	12/12	0.95	0.26	20,46,72,86	0
4	PO4	B	302	5/5	0.97	0.10	24,29,37,48	0
3	NI	A	303	1/1	0.98	0.07	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.