



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5GNH / pdb_00005gnh
Title : Myotubularin-related protein 2
Authors : Lee, B.I.; Bong, S.M.
Deposited on : 2016-07-21
Resolution : 2.60 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

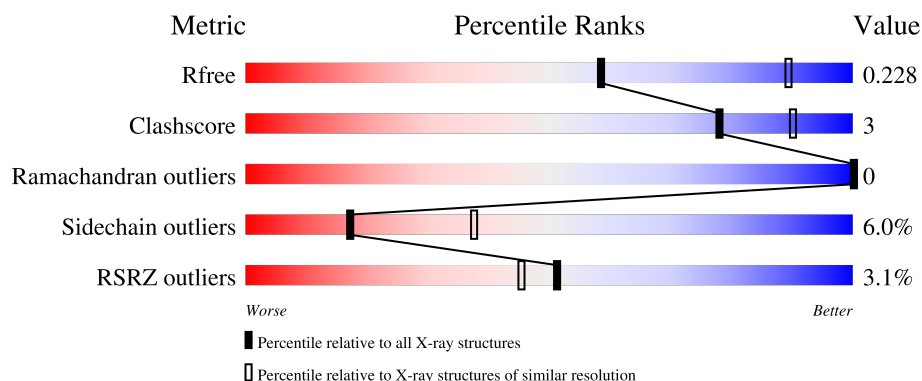
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	571	3% 78% 10% 11%
1	B	571	2% 79% 9% 11%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8330 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.

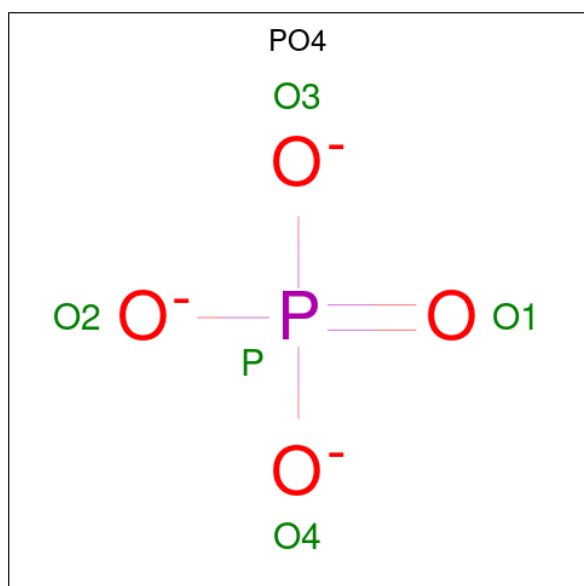
- Molecule 1 is a protein called Myotubularin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			4144	2655	719	753	17			
1	B	506	Total	C	N	O	S	0	0	0
			4139	2652	719	751	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	SER	CYS	engineered mutation	UNP Q13614
B	417	SER	CYS	engineered mutation	UNP Q13614

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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

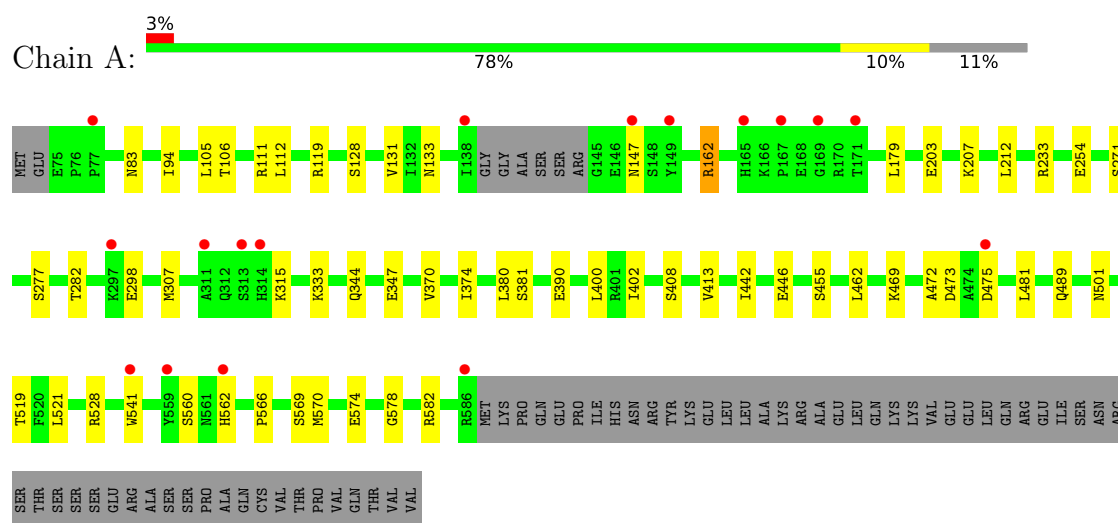
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	18	Total	O	0	0
			18	18		

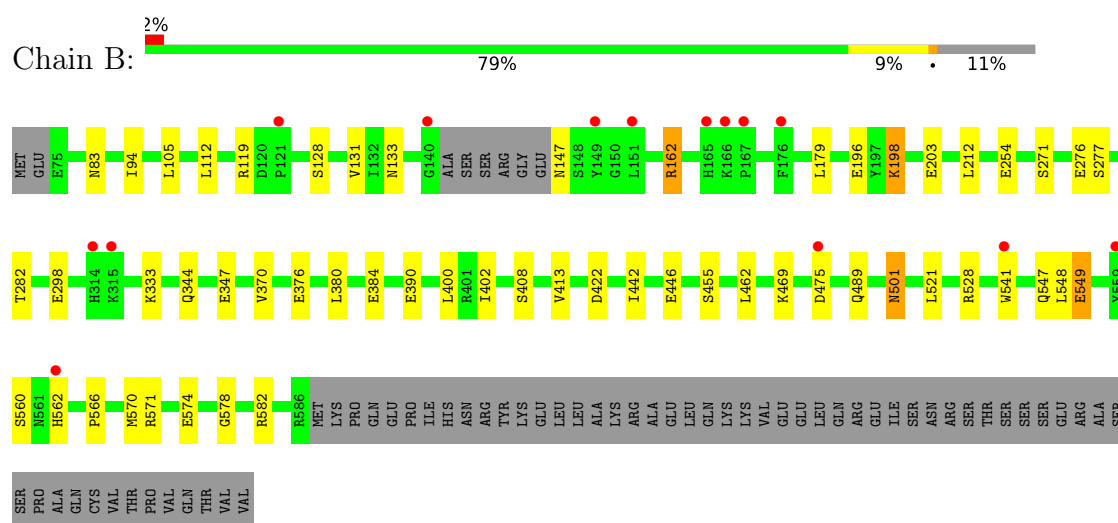
3 Residue-property plots [i](#)

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: Myotubularin-related protein 2



• Molecule 1: Myotubularin-related protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.34Å 82.82Å 99.97Å 90.00° 117.59° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.60) 95.0 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.203 , 0.258 (Not available) , 0.228	Depositor DCC
R_{free} test set	1721 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8330	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 12.16% 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: PO4

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	0.79	0/4254	0.95	1/5767 (0.0%)
1	B	0.77	0/4249	0.94	4/5760 (0.1%)
All	All	0.78	0/8503	0.95	5/11527 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	549	GLU	N-CA-C	7.15	121.45	112.87
1	B	276	GLU	N-CA-C	5.63	117.41	111.28
1	B	548	LEU	N-CA-C	5.42	116.87	111.07
1	A	111	ARG	N-CA-C	5.11	116.75	109.14
1	B	376	GLU	N-CA-C	5.10	116.84	111.28

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	4144	0	4072	29	0
1	B	4139	0	4069	20	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	0	0	0
3	B	18	0	0	0	3
All	All	8330	0	8141	46	3

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 3.

All (46) 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:446:GLU:CD	1:A:541:TRP:HD1	1.83	0.86
1:A:446:GLU:OE2	1:A:541:TRP:HD1	1.60	0.85
1:A:446:GLU:CG	1:A:541:TRP:CD1	2.69	0.75
1:A:446:GLU:CD	1:A:541:TRP:CD1	2.65	0.74
1:A:446:GLU:HB3	1:A:541:TRP:CD1	2.26	0.71
1:A:519:THR:HG21	1:A:541:TRP:CZ3	2.34	0.63
1:A:105:LEU:HD11	1:A:112:LEU:HD11	1.83	0.60
1:B:105:LEU:HD11	1:B:112:LEU:HD11	1.83	0.59
1:A:446:GLU:CB	1:A:541:TRP:CD1	2.86	0.58
1:B:442:ILE:O	1:B:446:GLU:HG3	2.04	0.58
1:A:380:LEU:HD22	1:B:380:LEU:HD22	1.85	0.58
1:A:446:GLU:OE2	1:A:541:TRP:CD1	2.51	0.57
1:A:442:ILE:O	1:A:446:GLU:HG3	2.05	0.56
1:A:519:THR:HG21	1:A:541:TRP:HZ3	1.71	0.55
1:A:402:ILE:HG23	1:A:413:VAL:HG21	1.90	0.54
1:B:402:ILE:HG23	1:B:413:VAL:HG21	1.90	0.53
1:B:196:GLU:O	1:B:198:LYS:HD2	2.10	0.52
1:A:446:GLU:HG2	1:A:541:TRP:CD1	2.44	0.51
1:A:578:GLY:O	1:A:582:ARG:HB3	2.11	0.51
1:A:112:LEU:HD13	1:A:179:LEU:HD21	1.94	0.50
1:B:578:GLY:O	1:B:582:ARG:HB3	2.11	0.50
1:B:112:LEU:HD13	1:B:179:LEU:HD21	1.93	0.50
1:A:446:GLU:HG2	1:A:541:TRP:NE1	2.28	0.49
1:A:94:ILE:HD11	1:A:147:ASN:HB3	1.96	0.48
1:A:400:LEU:HD11	1:A:566:PRO:O	2.13	0.48
1:B:94:ILE:HD11	1:B:147:ASN:HB3	1.96	0.48
1:B:400:LEU:HD11	1:B:566:PRO:O	2.15	0.47
1:A:307:MET:HE3	1:A:315:LYS:N	2.32	0.46
1:A:521:LEU:O	1:A:528:ARG:NH1	2.49	0.45
1:B:462:LEU:HD11	1:B:475:ASP:CB	2.46	0.45
1:B:462:LEU:HD11	1:B:475:ASP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:GLN:HE22	1:B:574:GLU:H	1.65	0.44
1:B:94:ILE:HD12	1:B:162:ARG:HD2	2.00	0.44
1:B:521:LEU:O	1:B:528:ARG:NH1	2.48	0.44
1:A:489:GLN:HE22	1:A:574:GLU:H	1.66	0.43
1:A:94:ILE:HD12	1:A:162:ARG:HD2	2.00	0.43
1:A:128:SER:O	1:A:131:VAL:HG22	2.18	0.43
1:A:381:SER:OG	1:B:384:GLU:OE2	2.36	0.42
1:A:519:THR:HG21	1:A:541:TRP:CE3	2.54	0.42
1:A:374:ILE:HD13	1:B:571:ARG:HD3	2.00	0.42
1:B:128:SER:O	1:B:131:VAL:HG22	2.20	0.42
1:A:462:LEU:HD11	1:A:475:ASP:CB	2.50	0.42
1:B:501:ASN:C	1:B:501:ASN:HD22	2.28	0.41
1:B:422:ASP:HB2	2:B:701:PO4:O3	2.20	0.41
1:A:472:ALA:O	1:A:473:ASP:C	2.64	0.41
1:B:446:GLU:HB3	1:B:541:TRP:CD2	2.57	0.40

All (3) 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)
3:B:807:HOH:O	3:B:810:HOH:O[4_453]	1.91	0.29
3:B:818:HOH:O	3:B:818:HOH:O[2_553]	2.04	0.16
3:B:802:HOH:O	3:B:805:HOH:O[4_453]	2.19	0.01

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	502/571 (88%)	470 (94%)	32 (6%)	0	100	100
1	B	502/571 (88%)	468 (93%)	34 (7%)	0	100	100
All	All	1004/1142 (88%)	938 (93%)	66 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	452/510 (89%)	424 (94%)	28 (6%)	16	36
1	B	451/510 (88%)	425 (94%)	26 (6%)	18	39
All	All	903/1020 (88%)	849 (94%)	54 (6%)	17	37

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	106	THR
1	A	119	ARG
1	A	133	ASN
1	A	162	ARG
1	A	203	GLU
1	A	207	LYS
1	A	212	LEU
1	A	233	ARG
1	A	254	GLU
1	A	271	SER
1	A	277	SER
1	A	282	THR
1	A	298	GLU
1	A	333	LYS
1	A	344	GLN
1	A	347	GLU
1	A	370	VAL
1	A	390	GLU
1	A	408	SER
1	A	455	SER
1	A	469	LYS
1	A	481	LEU
1	A	501	ASN
1	A	560	SER

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Mol	Chain	Res	Type
1	A	562	HIS
1	A	569	SER
1	A	570	MET
1	B	83	ASN
1	B	119	ARG
1	B	133	ASN
1	B	162	ARG
1	B	198	LYS
1	B	203	GLU
1	B	212	LEU
1	B	254	GLU
1	B	271	SER
1	B	277	SER
1	B	282	THR
1	B	298	GLU
1	B	333	LYS
1	B	344	GLN
1	B	347	GLU
1	B	370	VAL
1	B	390	GLU
1	B	408	SER
1	B	455	SER
1	B	469	LYS
1	B	501	ASN
1	B	547	GLN
1	B	549	GLU
1	B	560	SER
1	B	562	HIS
1	B	570	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	218	GLN
1	A	274	HIS
1	A	326	ASN
1	A	354	HIS
1	A	416	HIS
1	A	426	GLN
1	A	470	ASN
1	A	482	GLN

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Mol	Chain	Res	Type
1	A	489	GLN
1	A	501	ASN
1	A	526	GLN
1	A	532	ASN
1	A	545	ASN
1	B	147	ASN
1	B	218	GLN
1	B	344	GLN
1	B	416	HIS
1	B	489	GLN
1	B	501	ASN
1	B	532	ASN
1	B	545	ASN

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	$\# Z > 2$
2	PO4	B	701	-	4,4,4	1.02	0	6,6,6	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	701	-	4,4,4	1.20	0	6,6,6	0.90	0
2	PO4	B	702	-	4,4,4	0.88	0	6,6,6	1.22	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	PO4	O4-P-O3	-2.01	101.65	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	PO4	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	506/571 (88%)	0.05	17 (3%)	48 42	23, 49, 96, 162	0
1	B	506/571 (88%)	0.06	14 (2%)	55 49	24, 48, 103, 158	0
All	All	1012/1142 (88%)	0.06	31 (3%)	51 45	23, 48, 102, 162	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	562	HIS	4.1
1	A	169	GLY	3.8
1	A	167	PRO	3.6
1	A	165	HIS	3.5
1	A	559	TYR	3.2
1	B	140	GLY	3.1
1	A	475	ASP	2.9
1	B	165	HIS	2.8
1	B	559	TYR	2.7
1	B	167	PRO	2.6
1	A	149	TYR	2.5
1	B	475	ASP	2.5
1	A	314	HIS	2.5
1	A	77	PRO	2.5
1	B	176	PHE	2.5
1	B	314	HIS	2.4
1	A	311	ALA	2.4
1	A	297	LYS	2.3
1	A	313	SER	2.3
1	B	541	TRP	2.2
1	A	147	ASN	2.2
1	B	151	LEU	2.2
1	B	315	LYS	2.2
1	A	541	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	166	LYS	2.1
1	A	171	THR	2.1
1	B	562	HIS	2.1
1	A	138	ILE	2.1
1	B	121	PRO	2.1
1	A	586	ARG	2.0
1	B	149	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	B	702	5/5	0.95	0.09	51,59,60,61	0
2	PO4	A	701	5/5	0.98	0.04	29,30,31,32	0
2	PO4	B	701	5/5	0.99	0.04	35,37,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.