



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:56 PM UTC

PDB ID : 2YF0 / pdb_00002yf0
Title : Human Myotubularin related protein 6 (MTMR6)
Authors : Moche, M.; Tresaugues, L.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Kouznetsova, E.; Nyman, T.; Persson, C.; Schuler, H.; Schutz, P.; Siponen, M.I.; Thorsell, A.G.; VanDenBerg, S.; Wahlberg, E.; Weigelt, J.; Welin, M.; Nordlund, P.
Deposited on : 2011-03-31
Resolution : 2.65 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)

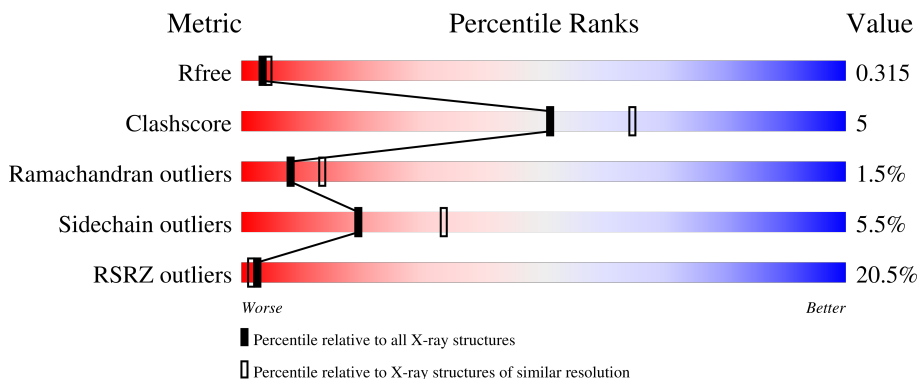
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	512	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3920 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.

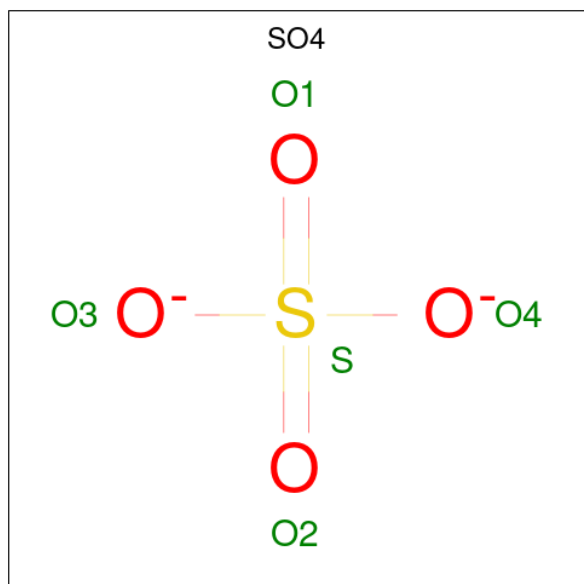
- Molecule 1 is a protein called MYOTUBULARIN-RELATED PROTEIN 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3913	2503	675	713	22	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	HIS	-	expression tag	UNP Q9Y217
A	509	HIS	-	expression tag	UNP Q9Y217
A	510	HIS	-	expression tag	UNP Q9Y217
A	511	HIS	-	expression tag	UNP Q9Y217
A	512	HIS	-	expression tag	UNP Q9Y217
A	319	VAL	ILE	cloning artifact	UNP Q9Y217

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

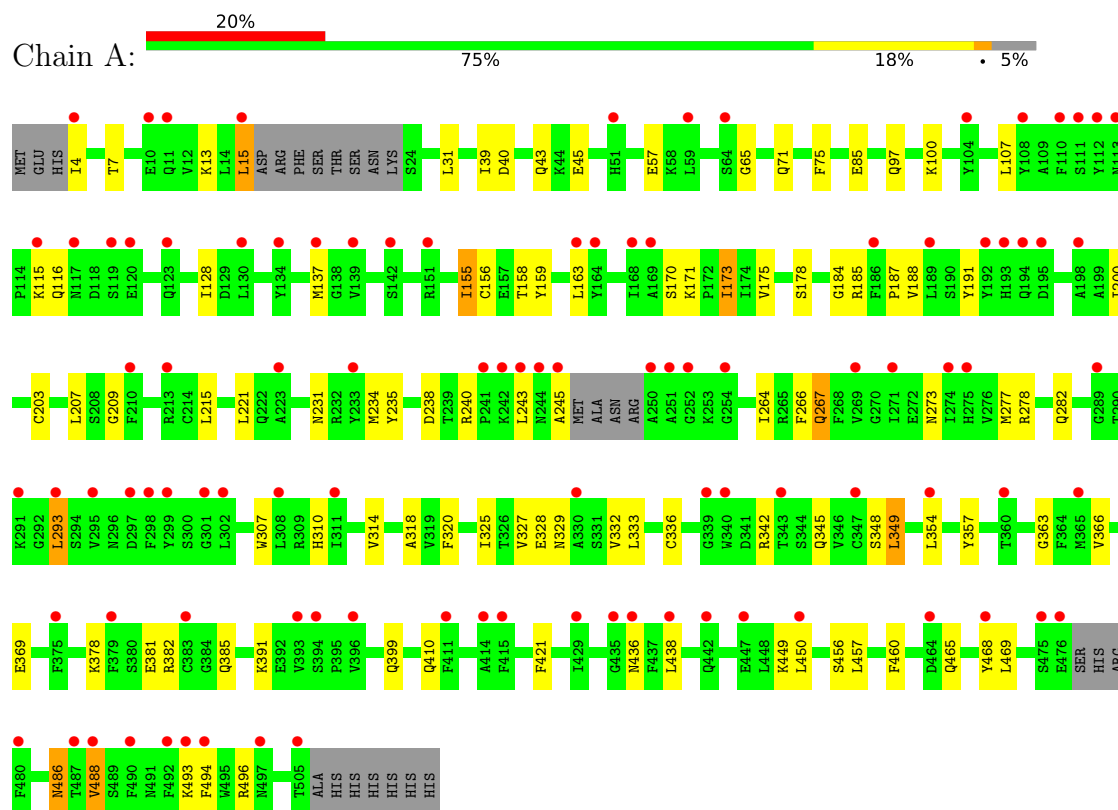
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		

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: MYOTUBULARIN-RELATED PROTEIN 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.73Å 85.73Å 448.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.77 – 2.65 29.77 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.77-2.65) 99.3 (29.77-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.64Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.258 , 0.288 0.282 , 0.315	Depositor DCC
R_{free} test set	1503 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.7	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	0.92	EDS
Total number of atoms	3920	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.83	0/4011	1.33	21/5433 (0.4%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	LYS	CA-C-N	6.36	133.70	121.54
1	A	493	LYS	C-N-CA	6.36	133.70	121.54
1	A	465	GLN	CA-C-N	5.90	128.51	120.54
1	A	465	GLN	C-N-CA	5.90	128.51	120.54
1	A	107	LEU	CA-C-N	5.73	128.28	120.54
1	A	107	LEU	C-N-CA	5.73	128.28	120.54
1	A	85	GLU	CA-C-N	5.55	128.03	120.54
1	A	85	GLU	C-N-CA	5.55	128.03	120.54
1	A	345	GLN	CA-C-N	5.26	127.14	120.72
1	A	345	GLN	C-N-CA	5.26	127.14	120.72
1	A	348	SER	CA-C-N	5.21	127.27	120.28
1	A	348	SER	C-N-CA	5.21	127.27	120.28
1	A	449	LYS	CA-C-N	5.18	127.22	120.28
1	A	449	LYS	C-N-CA	5.18	127.22	120.28
1	A	65	GLY	N-CA-C	5.16	117.56	111.63
1	A	238	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	273	ASN	CA-C-N	5.08	128.95	120.62
1	A	273	ASN	C-N-CA	5.08	128.95	120.62
1	A	200	ILE	N-CA-CB	5.05	117.82	111.46
1	A	40	ASP	CA-C-N	5.01	127.70	120.38
1	A	40	ASP	C-N-CA	5.01	127.70	120.38

There are no chirality outliers.

There are no planarity outliers.

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	3913	0	3756	40	0
2	A	5	0	0	0	0
3	A	2	0	0	0	0
All	All	3920	0	3756	40	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 (40) 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:436:ASN:HD21	1:A:456:SER:HA	1.54	0.72
1:A:277:MET:SD	1:A:310:HIS:HD2	2.19	0.65
1:A:438:LEU:HB2	1:A:450:LEU:HD21	1.79	0.65
1:A:310:HIS:O	1:A:314:VAL:HG23	2.02	0.59
1:A:13:LYS:HE3	1:A:15:LEU:HB3	1.85	0.58
1:A:156:CYS:HB3	1:A:159:TYR:HB2	1.85	0.58
1:A:245:ALA:HB2	1:A:342:ARG:HH12	1.70	0.56
1:A:277:MET:SD	1:A:310:HIS:CD2	2.99	0.56
1:A:234:MET:HE2	1:A:333:LEU:HB2	1.88	0.55
1:A:421:PHE:HB2	1:A:468:TYR:HB3	1.89	0.55
1:A:410:GLN:HE22	1:A:486:ASN:HD22	1.55	0.54
1:A:163:LEU:HD22	1:A:188:VAL:HG21	1.90	0.53
1:A:128:ILE:HG23	1:A:366:VAL:HG12	1.89	0.53
1:A:235:TYR:HB2	1:A:332:VAL:HG22	1.91	0.52
1:A:378:LYS:HD3	1:A:382:ARG:HH21	1.74	0.51
1:A:240:ARG:HH12	1:A:266:PHE:HB3	1.77	0.50
1:A:39:ILE:HG12	1:A:45:GLU:HG2	1.93	0.50
1:A:170:SER:H	1:A:173:ILE:HD13	1.77	0.49
1:A:436:ASN:ND2	1:A:457:LEU:H	2.09	0.49
1:A:155:ILE:HD11	1:A:175:VAL:HG12	1.95	0.48
1:A:187:PRO:HA	1:A:203:CYS:HB3	1.96	0.48
1:A:318:ALA:HB2	1:A:349:LEU:HB3	1.94	0.48
1:A:307:TRP:CH2	1:A:399:GLN:HG3	2.50	0.47
1:A:278:ARG:O	1:A:282:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HG21	1:A:354:LEU:HD22	1.99	0.45
1:A:231:ASN:HB2	1:A:329:ASN:O	2.16	0.44
1:A:234:MET:HB3	1:A:264:ILE:HD13	1.98	0.44
1:A:457:LEU:O	1:A:460:PHE:HB3	2.17	0.44
1:A:178:SER:O	1:A:184:GLY:HA2	2.18	0.43
1:A:4:ILE:HG23	1:A:31:LEU:HB3	2.01	0.43
1:A:496:ARG:H	1:A:496:ARG:HG2	1.53	0.42
1:A:158:THR:O	1:A:185:ARG:NH1	2.53	0.42
1:A:378:LYS:O	1:A:382:ARG:HG2	2.18	0.42
1:A:267:GLN:HG3	1:A:320:PHE:CE2	2.55	0.42
1:A:293:LEU:H	1:A:293:LEU:HG	1.77	0.41
1:A:378:LYS:HB3	1:A:381:GLU:HB2	2.02	0.41
1:A:278:ARG:NH2	1:A:391:LYS:O	2.53	0.41
1:A:191:TYR:CE2	1:A:354:LEU:HD11	2.56	0.41
1:A:357:TYR:O	1:A:363:GLY:HA3	2.21	0.41
1:A:97:GLN:HA	1:A:100:LYS:HE2	2.02	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	481/512 (94%)	433 (90%)	40 (8%)	8 (2%)	7 12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	494	PHE
1	A	209	GLY
1	A	336[A]	CYS
1	A	336[B]	CYS

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	327	VAL
1	A	488	VAL

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	420/464 (90%)	397 (94%)	23 (6%)	19	33

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	15	LEU
1	A	57	GLU
1	A	71	GLN
1	A	75	PHE
1	A	115	LYS
1	A	116	GLN
1	A	137	MET
1	A	155	ILE
1	A	171	LYS
1	A	173	ILE
1	A	207	LEU
1	A	215	LEU
1	A	221	LEU
1	A	267	GLN
1	A	293	LEU
1	A	328	GLU
1	A	349	LEU
1	A	369	GLU
1	A	385	GLN
1	A	469	LEU
1	A	486	ASN
1	A	488	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	52	HIS
1	A	71	GLN
1	A	93	ASN
1	A	244	ASN
1	A	310	HIS
1	A	335	HIS
1	A	345	GLN
1	A	426	HIS
1	A	428	HIS
1	A	436	ASN
1	A	486	ASN
1	A	491	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](#)

1 ligand is 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	SO4	A	1506	-	4,4,4	0.36	0	6,6,6	0.59	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	487/512 (95%)	1.30	100 (20%) 2 1	35, 105, 145, 171	2 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	490	PHE	6.3
1	A	245	ALA	5.4
1	A	111	SER	5.1
1	A	293	LEU	4.7
1	A	480	PHE	4.2
1	A	11	GLN	4.0
1	A	492	PHE	3.8
1	A	476	GLU	3.8
1	A	250	ALA	3.7
1	A	291	LYS	3.6
1	A	505	THR	3.6
1	A	115	LYS	3.4
1	A	243	LEU	3.4
1	A	134	TYR	3.3
1	A	192	TYR	3.3
1	A	435	GLY	3.3
1	A	168	ILE	3.2
1	A	198	ALA	3.2
1	A	113	ASN	3.2
1	A	339	GLY	3.2
1	A	210	PHE	3.2
1	A	375	PHE	3.1
1	A	104	TYR	3.1
1	A	242	LYS	3.1
1	A	164	TYR	3.1
1	A	411	PHE	3.0
1	A	394	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	4	ILE	2.9
1	A	112	TYR	2.9
1	A	299	TYR	2.9
1	A	119	SER	2.8
1	A	223	ALA	2.8
1	A	233	TYR	2.8
1	A	271	ILE	2.8
1	A	189	LEU	2.8
1	A	123	GLN	2.7
1	A	354	LEU	2.7
1	A	120	GLU	2.7
1	A	383[A]	CYS	2.7
1	A	311	ILE	2.7
1	A	110	PHE	2.7
1	A	343	THR	2.7
1	A	396	VAL	2.7
1	A	497	ASN	2.6
1	A	254	GLY	2.6
1	A	494	PHE	2.6
1	A	10	GLU	2.6
1	A	298	PHE	2.6
1	A	59	LEU	2.5
1	A	117	ASN	2.5
1	A	360	THR	2.5
1	A	302	LEU	2.5
1	A	251	ALA	2.5
1	A	415	PHE	2.5
1	A	15	LEU	2.5
1	A	213	ARG	2.5
1	A	475	SER	2.5
1	A	275	HIS	2.4
1	A	493	LYS	2.4
1	A	468	TYR	2.4
1	A	308	LEU	2.4
1	A	436	ASN	2.3
1	A	195	ASP	2.3
1	A	252	GLY	2.3
1	A	442	GLN	2.3
1	A	193	HIS	2.3
1	A	301	GLY	2.3
1	A	347	CYS	2.3
1	A	163	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	289	GLY	2.3
1	A	130	LEU	2.3
1	A	488	VAL	2.3
1	A	330	ALA	2.2
1	A	295	VAL	2.2
1	A	137	MET	2.2
1	A	241	PRO	2.2
1	A	194	GLN	2.2
1	A	64	SER	2.2
1	A	142	SER	2.2
1	A	450	LEU	2.2
1	A	365	MET	2.2
1	A	186	PHE	2.2
1	A	379	PHE	2.2
1	A	464	ASP	2.2
1	A	429	ILE	2.2
1	A	414	ALA	2.1
1	A	340	TRP	2.1
1	A	108	TYR	2.1
1	A	51	HIS	2.1
1	A	139	VAL	2.1
1	A	151	ARG	2.1
1	A	438	LEU	2.1
1	A	269	VAL	2.1
1	A	274	ILE	2.1
1	A	393	VAL	2.1
1	A	297	ASP	2.1
1	A	169	ALA	2.0
1	A	487	THR	2.0
1	A	447	GLU	2.0
1	A	244	ASN	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 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	SO4	A	1506	5/5	0.86	0.17	63,64,69,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.