



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:53 PM UTC

PDB ID : 3FP3 / pdb_00003fp3
Title : Crystal structure of Tom71
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Deposited on : 2009-01-03
Resolution : 1.98 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

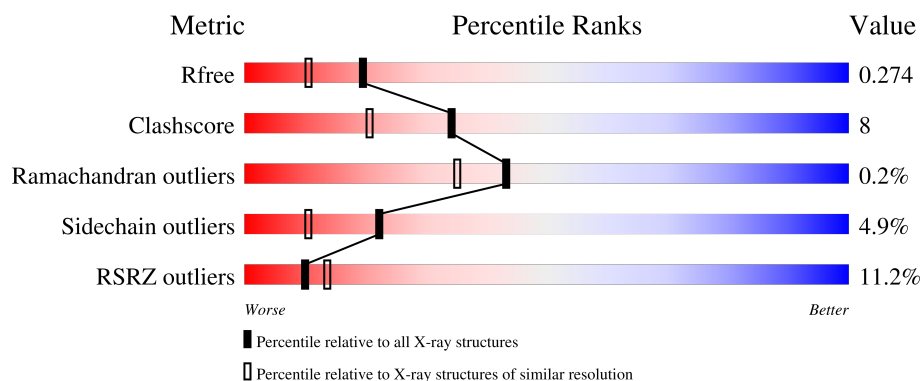
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	537	10% 80% 10% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	4	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	641	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4669 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.

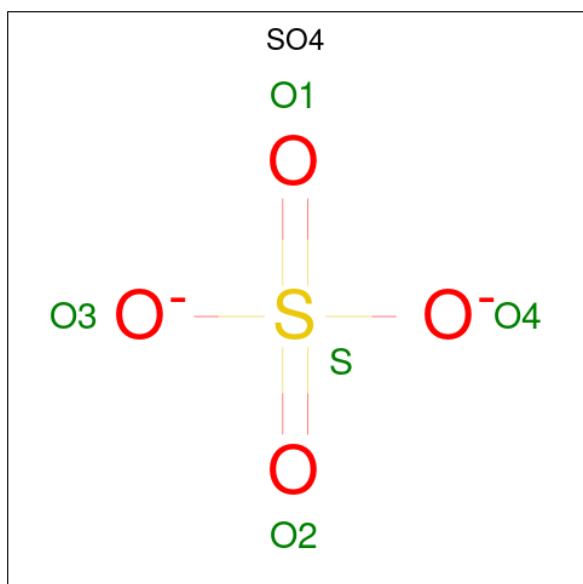
- Molecule 1 is a protein called TPR repeat-containing protein YHR117W.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	498	4108	2615	671	808	14	0	19	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	expression tag	UNP P38825
A	104	SER	-	expression tag	UNP P38825
A	105	HIS	-	expression tag	UNP P38825
A	106	MET	-	expression tag	UNP P38825

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



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

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		

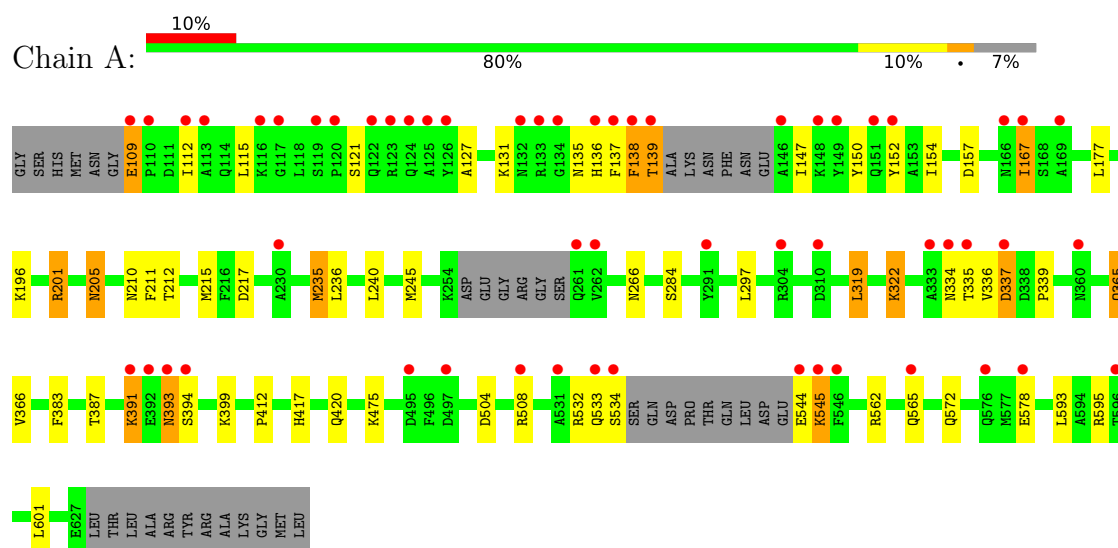
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	542	Total	O	0	0
			542	542		

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: TPR repeat-containing protein YHR117W



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.90Å 83.42Å 109.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.63 – 1.98 19.63 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.63-1.98) 99.8 (19.63-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.79 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.227 (Not available) , 0.274	Depositor DCC
R_{free} test set	2508 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4669	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: SO4, CL

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	0.98	2/4184 (0.0%)	0.96	4/5656 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ALA	C-O	5.89	1.31	1.24
1	A	412	PRO	CA-C	5.27	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	MET	CG-SD-CE	-7.29	84.86	100.90
1	A	109	GLU	CA-C-N	-6.26	113.33	119.78
1	A	109	GLU	C-N-CA	-6.26	113.33	119.78
1	A	593	LEU	N-CA-C	5.09	116.91	111.36

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	4108	0	4043	61	0
2	A	15	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	5	0
4	A	542	0	0	14	0
All	All	4669	0	4043	62	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 8.

All (62) 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:578:GLU:O	1:A:578:GLU:HG3	1.68	0.94
1:A:245[B]:MET:HG3	3:A:641:CL:CL	2.16	0.81
1:A:135:ASN:O	1:A:138:PHE:HB2	1.82	0.80
1:A:215[A]:MET:HE3	1:A:236:LEU:O	1.82	0.78
1:A:201:ARG:HD2	1:A:217:ASP:OD2	1.85	0.77
1:A:365:GLN:HG3	1:A:366:VAL:N	2.00	0.75
1:A:201:ARG:CD	1:A:217:ASP:OD2	2.37	0.72
1:A:322:LYS:NZ	4:A:1072:HOH:O	2.26	0.67
1:A:533:GLN:O	1:A:534:SER:HB2	1.93	0.67
1:A:391:LYS:HE2	1:A:391:LYS:H	1.60	0.65
1:A:138:PHE:O	1:A:139:THR:C	2.39	0.65
1:A:112:ILE:HG13	1:A:152:TYR:CD1	2.32	0.64
1:A:383:PHE:O	1:A:387[B]:THR:HG23	1.97	0.64
1:A:420:GLN:HG2	4:A:910:HOH:O	2.00	0.62
1:A:139:THR:HA	4:A:834:HOH:O	1.99	0.61
1:A:109:GLU:N	4:A:825:HOH:O	2.34	0.61
1:A:147:ILE:HG23	1:A:167[B]:ILE:HD11	1.85	0.58
1:A:136:HIS:C	1:A:138:PHE:H	2.13	0.57
1:A:399:LYS:HE3	4:A:899:HOH:O	2.05	0.56
1:A:391:LYS:HE2	1:A:391:LYS:N	2.21	0.55
1:A:115:LEU:HD11	3:A:1:CL:CL	2.44	0.54
1:A:150:TYR:CB	1:A:167[A]:ILE:HG13	2.39	0.53
1:A:284:SER:HB3	4:A:872:HOH:O	2.07	0.53
1:A:177:LEU:HD23	4:A:842:HOH:O	2.07	0.53
1:A:201:ARG:HD3	1:A:217:ASP:OD2	2.07	0.52
1:A:205:ASN:HD22	1:A:210:ASN:HD22	1.56	0.52
1:A:365:GLN:HB3	4:A:883:HOH:O	2.09	0.52
1:A:136:HIS:C	1:A:138:PHE:N	2.68	0.51
1:A:215[A]:MET:CE	1:A:240:LEU:HB2	2.41	0.51
1:A:565[B]:GLN:HE21	1:A:565[B]:GLN:H	1.59	0.51
1:A:215[A]:MET:HE1	1:A:240:LEU:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLN:CB	4:A:883:HOH:O	2.59	0.50
1:A:475:LYS:HE2	4:A:746:HOH:O	2.11	0.50
1:A:365:GLN:HG3	1:A:366:VAL:H	1.75	0.50
1:A:266:ASN:ND2	1:A:562:ARG:HH22	2.11	0.49
1:A:157:ASP:O	3:A:640:CL:CL	2.68	0.49
1:A:335:THR:HG22	4:A:763:HOH:O	2.11	0.49
1:A:365:GLN:C	1:A:365:GLN:HE21	2.21	0.48
1:A:508:ARG:N	1:A:508:ARG:HD2	2.29	0.47
1:A:297:LEU:HD11	1:A:319:LEU:HG	1.95	0.47
1:A:578:GLU:HB2	4:A:1073:HOH:O	2.14	0.47
1:A:150:TYR:HB2	1:A:167[A]:ILE:HG13	1.98	0.45
1:A:136:HIS:O	1:A:138:PHE:N	2.50	0.45
1:A:545:LYS:HB3	1:A:545:LYS:HE3	1.69	0.44
3:A:642:CL:CL	4:A:784:HOH:O	2.59	0.44
1:A:154:ILE:HD12	1:A:167[A]:ILE:HD12	2.00	0.43
1:A:211:PHE:O	1:A:215[B]:MET:HG3	2.19	0.43
1:A:212:THR:HA	1:A:215[B]:MET:HE3	2.00	0.43
1:A:196:LYS:HB2	1:A:196:LYS:HE2	1.76	0.43
1:A:391:LYS:H	1:A:391:LYS:CE	2.29	0.43
1:A:504:ASP:O	1:A:508:ARG:CD	2.66	0.43
1:A:565[B]:GLN:H	1:A:565[B]:GLN:NE2	2.16	0.43
1:A:417:HIS:CE1	4:A:667:HOH:O	2.71	0.43
1:A:215[A]:MET:CE	2:A:4:SO4:O1	2.67	0.43
1:A:393:ASN:C	1:A:393:ASN:HD22	2.27	0.43
1:A:578:GLU:O	1:A:578:GLU:CG	2.50	0.42
1:A:601:LEU:HD11	3:A:641:CL:CL	2.57	0.42
1:A:215[A]:MET:HE1	2:A:4:SO4:O1	2.19	0.41
1:A:337:ASP:HB3	1:A:339:PRO:HD2	2.02	0.41
1:A:572[A]:GLN:OE1	1:A:572[A]:GLN:HA	2.21	0.41
1:A:504:ASP:O	1:A:508:ARG:HD2	2.21	0.41
1:A:205:ASN:ND2	1:A:210:ASN:HD22	2.18	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	510/537 (95%)	504 (99%)	5 (1%)	1 (0%)	43	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PHE

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	452/463 (98%)	430 (95%)	22 (5%)	22	10

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	131	LYS
1	A	138	PHE
1	A	139	THR
1	A	167[A]	ILE
1	A	167[B]	ILE
1	A	201	ARG
1	A	205	ASN
1	A	235	MET
1	A	319	LEU
1	A	322	LYS
1	A	334	ASN
1	A	336	VAL
1	A	337	ASP
1	A	365	GLN
1	A	391	LYS
1	A	393	ASN
1	A	394	SER

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Mol	Chain	Res	Type
1	A	532	ARG
1	A	544	GLU
1	A	545	LYS
1	A	595	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	239	ASN
1	A	249	ASN
1	A	266	ASN
1	A	303	GLN
1	A	365	GLN
1	A	369	GLN
1	A	393	ASN
1	A	417	HIS
1	A	420	GLN
1	A	430	ASN
1	A	451	GLN
1	A	459	GLN
1	A	547	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](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	SO4	A	4	-	4,4,4	0.30	0	6,6,6	0.47	0
2	SO4	A	3	-	4,4,4	0.26	0	6,6,6	0.11	0
2	SO4	A	2	-	4,4,4	0.27	0	6,6,6	0.11	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4	SO4	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	498/537 (92%)	0.97	56 (11%)	10 14	10, 33, 49, 64	19 (3%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	PHE	9.9
1	A	139	THR	6.8
1	A	136	HIS	4.8
1	A	334	ASN	4.5
1	A	149	TYR	4.5
1	A	392	GLU	4.1
1	A	393	ASN	3.5
1	A	578	GLU	3.4
1	A	146	ALA	3.4
1	A	262	VAL	3.3
1	A	531	ALA	3.3
1	A	137	PHE	3.3
1	A	508	ARG	3.2
1	A	120	PRO	3.2
1	A	230	ALA	3.0
1	A	123	ARG	3.0
1	A	337	ASP	3.0
1	A	304	ARG	3.0
1	A	534	SER	2.9
1	A	291	TYR	2.9
1	A	576	GLN	2.8
1	A	544	GLU	2.8
1	A	360	ASN	2.7
1	A	119	SER	2.7
1	A	113	ALA	2.6
1	A	333	ALA	2.6
1	A	110	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	112	ILE	2.6
1	A	116	LYS	2.6
1	A	126	TYR	2.6
1	A	565[A]	GLN	2.6
1	A	133	ARG	2.5
1	A	391	LYS	2.5
1	A	310	ASP	2.5
1	A	497	ASP	2.4
1	A	124	GLN	2.4
1	A	169	ALA	2.4
1	A	261	GLN	2.3
1	A	495	ASP	2.3
1	A	148	LYS	2.3
1	A	151	GLN	2.2
1	A	394	SER	2.2
1	A	132	ASN	2.2
1	A	125	ALA	2.2
1	A	167[A]	ILE	2.2
1	A	166	ASN	2.2
1	A	335	THR	2.1
1	A	545	LYS	2.1
1	A	122	GLN	2.1
1	A	117	GLY	2.1
1	A	134	GLY	2.1
1	A	109	GLU	2.1
1	A	533	GLN	2.1
1	A	152	TYR	2.1
1	A	596	THR	2.0
1	A	546	PHE	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(Å ²)	Q<0.9
2	SO4	A	3	5/5	0.65	0.23	161,161,161,161	0
2	SO4	A	4	5/5	0.68	0.17	62,65,66,66	0
2	SO4	A	2	5/5	0.73	0.22	59,60,61,61	0
3	CL	A	1	1/1	0.89	0.46	58,58,58,58	0
3	CL	A	642	1/1	0.89	0.28	51,51,51,51	0
3	CL	A	641	1/1	0.92	0.33	44,44,44,44	0
3	CL	A	640	1/1	0.94	0.39	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.