



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:59 AM UTC

PDB ID : 6R65 / pdb_00006r65
Title : Crystal Structure of human TMEM16K / Anoctamin 10 (Form 2)
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Deposited on : 2019-03-26
Resolution : 3.50 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
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

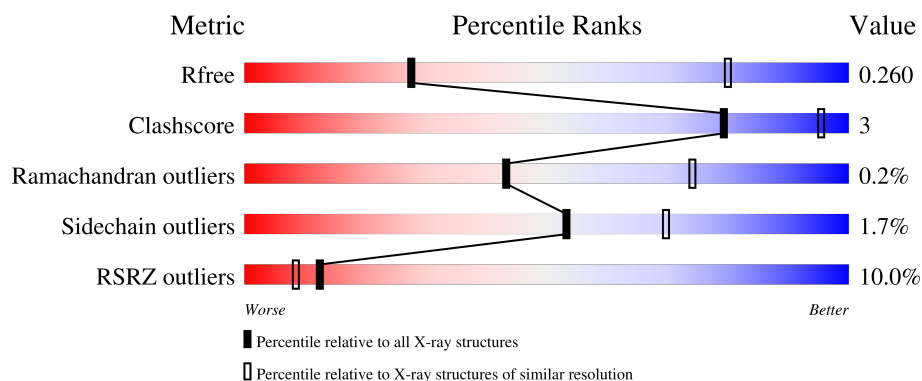
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	667	8% 83% 8% 8%
1	B	667	11% 85% 8% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9648 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 Anoctamin-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4768	3147	754	841	26			
1	B	623	Total	C	N	O	S	0	0	0
			4874	3216	773	858	27			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	661	ALA	-	expression tag	UNP Q9NW15
A	662	GLU	-	expression tag	UNP Q9NW15
A	663	ASN	-	expression tag	UNP Q9NW15
A	664	LEU	-	expression tag	UNP Q9NW15
A	665	TYR	-	expression tag	UNP Q9NW15
A	666	PHE	-	expression tag	UNP Q9NW15
A	667	GLN	-	expression tag	UNP Q9NW15
B	661	ALA	-	expression tag	UNP Q9NW15
B	662	GLU	-	expression tag	UNP Q9NW15
B	663	ASN	-	expression tag	UNP Q9NW15
B	664	LEU	-	expression tag	UNP Q9NW15
B	665	TYR	-	expression tag	UNP Q9NW15
B	666	PHE	-	expression tag	UNP Q9NW15
B	667	GLN	-	expression tag	UNP Q9NW15

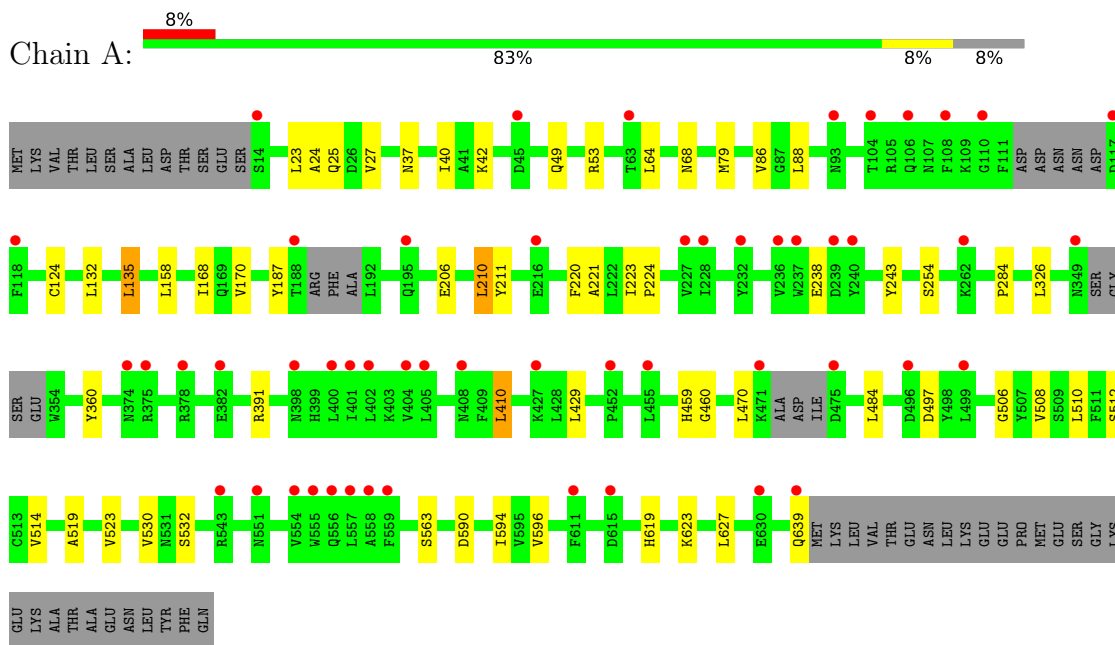
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		

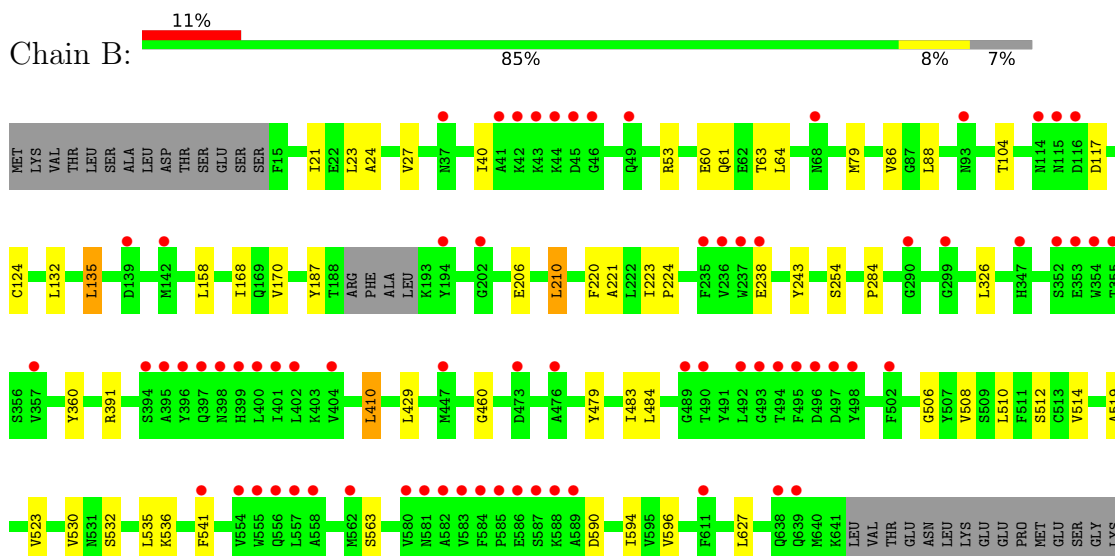
3 Residue-property plots [i](#)

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: Anoctamin-10



• Molecule 1: Anoctamin-10



GLU
LYS
ALA
THR
ALA
GLU
ASN
LEU
TYR
PHE
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.16Å 152.27Å 153.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.69 – 3.50 39.69 – 3.50	Depositor EDS
% Data completeness (in resolution range)	70.0 (39.69-3.50) 69.9 (39.69-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.49Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.237 , 0.249 0.252 , 0.260	Depositor DCC
R_{free} test set	1191 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 17.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.056 for -h,l,k	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	9648	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: CA

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	0.75	0/4882	1.36	5/6648 (0.1%)
1	B	0.75	0/4996	1.35	5/6807 (0.1%)
All	All	0.75	0/9878	1.35	10/13455 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	TYR	CA-C-N	8.32	128.41	120.43
1	B	360	TYR	C-N-CA	8.32	128.41	120.43
1	A	360	TYR	CA-C-N	8.00	128.11	120.43
1	A	360	TYR	C-N-CA	8.00	128.11	120.43
1	B	535	LEU	CA-C-N	6.06	128.31	120.44
1	B	535	LEU	C-N-CA	6.06	128.31	120.44
1	B	117	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	37	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	459	HIS	CA-C-N	5.01	125.55	119.98
1	A	459	HIS	C-N-CA	5.01	125.55	119.98

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	4768	0	4647	27	0
1	B	4874	0	4722	27	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
All	All	9648	0	9369	52	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 3.

All (52) 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:B:238:GLU:HA	1:B:243:TYR:HE1	1.61	0.63
1:B:60:GLU:H	1:B:63:THR:HB	1.65	0.61
1:A:238:GLU:HA	1:A:243:TYR:HE1	1.67	0.59
1:B:238:GLU:HA	1:B:243:TYR:CE1	2.38	0.58
1:A:429:LEU:HD23	1:A:514:VAL:HG11	1.84	0.58
1:B:429:LEU:HD23	1:B:514:VAL:HG11	1.85	0.57
1:A:506:GLY:O	1:A:510:LEU:HB2	2.09	0.53
1:A:238:GLU:HA	1:A:243:TYR:CE1	2.44	0.53
1:A:206:GLU:O	1:A:210:LEU:HB2	2.09	0.53
1:B:206:GLU:O	1:B:210:LEU:HB2	2.09	0.53
1:B:326:LEU:HG	1:B:410:LEU:HD13	1.90	0.52
1:A:596:VAL:HG21	1:B:596:VAL:HG21	1.91	0.52
1:A:326:LEU:HG	1:A:410:LEU:HD13	1.91	0.52
1:B:508:VAL:O	1:B:512:SER:HB3	2.11	0.51
1:A:460:GLY:HA2	1:A:484:LEU:HD11	1.93	0.51
1:A:79:MET:HE2	1:A:124:CYS:HA	1.93	0.50
1:A:132:LEU:HA	1:A:135:LEU:HD12	1.94	0.50
1:B:132:LEU:HA	1:B:135:LEU:HD12	1.94	0.49
1:A:508:VAL:O	1:A:512:SER:HB3	2.12	0.49
1:A:211:TYR:CZ	1:A:497:ASP:HB3	2.48	0.49
1:A:221:ALA:O	1:A:224:PRO:HD2	2.14	0.48
1:B:220:PHE:HA	1:B:223:ILE:HD12	1.96	0.48
1:B:221:ALA:O	1:B:224:PRO:HD2	2.14	0.48
1:B:519:ALA:O	1:B:523:VAL:HG23	2.14	0.48
1:A:220:PHE:HA	1:A:223:ILE:HD12	1.96	0.48
1:B:79:MET:HE2	1:B:124:CYS:HA	1.94	0.48
1:B:61:GLN:HA	1:B:64:LEU:HD12	1.95	0.47
1:B:506:GLY:O	1:B:510:LEU:HB2	2.15	0.47
1:B:590:ASP:O	1:B:594:ILE:HG12	2.14	0.47
1:A:519:ALA:O	1:A:523:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ASP:O	1:A:594:ILE:HG12	2.15	0.46
1:A:639:GLN:HG3	1:B:104:THR:HG21	1.96	0.46
1:B:460:GLY:HA2	1:B:484:LEU:HD11	1.98	0.46
1:B:21:ILE:HG12	1:B:170:VAL:HG22	1.97	0.46
1:A:254:SER:HB3	1:A:563:SER:HB2	1.98	0.45
1:B:86:VAL:HG23	1:B:88:LEU:HG	1.99	0.45
1:B:254:SER:HB3	1:B:563:SER:HB2	1.99	0.45
1:A:86:VAL:HG23	1:A:88:LEU:HG	1.99	0.45
1:A:23:LEU:HD23	1:A:27:VAL:HG11	1.99	0.44
1:A:64:LEU:HD11	1:A:470:LEU:HD13	1.99	0.44
1:A:23:LEU:HB2	1:A:68:ASN:HB3	2.01	0.43
1:A:619:HIS:HB2	1:A:623:LYS:NZ	2.34	0.43
1:B:479:TYR:O	1:B:483:ILE:HG12	2.19	0.42
1:A:24:ALA:HA	1:A:168:ILE:HD11	2.02	0.42
1:B:536:LYS:HE2	1:B:541:PHE:HE2	1.85	0.41
1:A:158:LEU:HD11	1:A:170:VAL:HG21	2.03	0.41
1:B:23:LEU:HD23	1:B:27:VAL:HG11	2.02	0.41
1:B:284:PRO:HB3	1:B:391:ARG:HG2	2.03	0.41
1:A:42:LYS:HA	1:A:49:GLN:HG3	2.03	0.40
1:A:284:PRO:HB3	1:A:391:ARG:HG2	2.03	0.40
1:B:24:ALA:HA	1:B:168:ILE:HD11	2.03	0.40
1:B:158:LEU:HD11	1:B:170:VAL:HG21	2.03	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	601/667 (90%)	581 (97%)	19 (3%)	1 (0%)	43	74
1	B	619/667 (93%)	597 (96%)	21 (3%)	1 (0%)	43	74
All	All	1220/1334 (92%)	1178 (97%)	40 (3%)	2 (0%)	43	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	TYR
1	B	187	TYR

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	485/591 (82%)	476 (98%)	9 (2%)	50	68
1	B	490/591 (83%)	482 (98%)	8 (2%)	55	70
All	All	975/1182 (82%)	958 (98%)	17 (2%)	53	70

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	40	ILE
1	A	53	ARG
1	A	135	LEU
1	A	210	LEU
1	A	410	LEU
1	A	530	VAL
1	A	532	SER
1	A	627	LEU
1	B	40	ILE
1	B	53	ARG
1	B	135	LEU
1	B	210	LEU
1	B	410	LEU
1	B	530	VAL
1	B	532	SER
1	B	627	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	441	GLN
1	A	459	HIS
1	A	504	GLN
1	A	526	ASN
1	A	638	GLN
1	A	639	GLN
1	B	49	GLN
1	B	67	GLN
1	B	456	GLN
1	B	504	GLN
1	B	526	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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	611/667 (91%)	0.56	52 (8%) 16 11	63, 91, 140, 211	0
1	B	623/667 (93%)	0.76	72 (11%) 9 6	60, 87, 118, 139	0
All	All	1234/1334 (92%)	0.66	124 (10%) 12 8	60, 89, 127, 211	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	ASP	9.4
1	B	398	ASN	9.0
1	B	585	PRO	8.4
1	B	496	ASP	7.3
1	B	581	ASN	7.1
1	B	586	GLU	6.3
1	B	582	ALA	6.3
1	B	237	TRP	6.2
1	B	588	LYS	6.2
1	A	475	ASP	6.1
1	B	587	SER	6.0
1	A	558	ALA	5.8
1	B	353	GLU	5.8
1	B	37	ASN	5.4
1	B	473	ASP	5.3
1	B	558	ALA	5.2
1	B	584	PHE	5.1
1	B	555	TRP	5.1
1	B	49	GLN	5.0
1	B	194	TYR	5.0
1	A	455	LEU	5.0
1	B	557	LEU	4.9
1	B	397	GLN	4.8
1	B	495	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	401	ILE	4.7
1	A	611	PHE	4.6
1	B	41	ALA	4.5
1	B	396	TYR	4.4
1	B	589	ALA	4.3
1	B	394	SER	4.2
1	A	108	PHE	4.2
1	B	400	LEU	4.1
1	B	402	LEU	4.1
1	B	139	ASP	4.1
1	B	497	ASP	4.1
1	B	554	VAL	4.0
1	B	46	GLY	4.0
1	B	489	GLY	4.0
1	B	238	GLU	4.0
1	B	44	LYS	4.0
1	B	235	PHE	3.9
1	A	228	ILE	3.9
1	B	611	PHE	3.7
1	B	580	VAL	3.7
1	A	402	LEU	3.6
1	A	615	ASP	3.6
1	A	382	GLU	3.5
1	B	236	VAL	3.5
1	B	490	THR	3.5
1	B	492	LEU	3.5
1	A	239	ASP	3.4
1	A	378	ARG	3.4
1	A	110	GLY	3.3
1	A	556	GLN	3.3
1	B	93	ASN	3.2
1	A	374	ASN	3.2
1	A	104	THR	3.2
1	B	395	ALA	3.2
1	A	401	ILE	3.1
1	A	45	ASP	3.1
1	A	496	ASP	3.1
1	A	398	ASN	3.0
1	B	404	VAL	3.0
1	A	349	ASN	2.9
1	A	559	PHE	2.9
1	A	14	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	471	LYS	2.9
1	A	555	TRP	2.9
1	A	400	LEU	2.9
1	A	240	TYR	2.9
1	B	583	VAL	2.9
1	B	639	GLN	2.9
1	B	498	TYR	2.9
1	A	452	PRO	2.8
1	B	290	GLY	2.8
1	A	237	TRP	2.8
1	B	42	LYS	2.8
1	A	106	GLN	2.8
1	B	347	HIS	2.8
1	B	202	GLY	2.8
1	B	493	GLY	2.8
1	A	427	LYS	2.7
1	A	195	GLN	2.7
1	B	115	ASN	2.7
1	B	354	TRP	2.7
1	B	357	VAL	2.6
1	A	188	THR	2.6
1	B	638	GLN	2.6
1	A	639	GLN	2.5
1	A	557	LEU	2.5
1	B	494	THR	2.5
1	B	352	SER	2.5
1	B	43	LYS	2.5
1	B	476	ALA	2.5
1	A	408	ASN	2.4
1	A	551	ASN	2.4
1	B	562	MET	2.4
1	B	116	ASP	2.4
1	A	554	VAL	2.4
1	A	405	LEU	2.4
1	B	399	HIS	2.3
1	B	299	GLY	2.3
1	B	447	MET	2.3
1	A	236	VAL	2.3
1	B	355	THR	2.2
1	A	117	ASP	2.2
1	B	541	PHE	2.2
1	B	556	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	499	LEU	2.2
1	A	232	TYR	2.2
1	A	118	PHE	2.2
1	A	93	ASN	2.2
1	A	375	ARG	2.1
1	B	502	PHE	2.1
1	A	404	VAL	2.1
1	A	262	LYS	2.1
1	B	142	MET	2.1
1	B	114	ASN	2.1
1	A	227	VAL	2.1
1	A	630	GLU	2.0
1	B	68	ASN	2.0
1	A	543	ARG	2.0
1	A	63	THR	2.0
1	A	216	GLU	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(Å ²)	Q<0.9
2	CA	A	703	1/1	0.93	0.07	84,84,84,84	0
2	CA	A	702	1/1	0.96	0.09	75,75,75,75	0
2	CA	A	701	1/1	0.96	0.16	92,92,92,92	0
2	CA	B	703	1/1	0.96	0.05	65,65,65,65	0
2	CA	B	702	1/1	0.98	0.06	78,78,78,78	0
2	CA	B	701	1/1	0.98	0.09	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.