



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:57 AM UTC

PDB ID : 7R0I / pdb_00007r0i
Title : STRUCTURAL BASIS OF ION UPTAKE IN COPPER-TRANSPORTING
P1B-TYPE ATPASES
Authors : Salustros, N.; Groenberg, C.; Wang, K.; Gourdon, P.
Deposited on : 2022-02-02
Resolution : 2.70 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

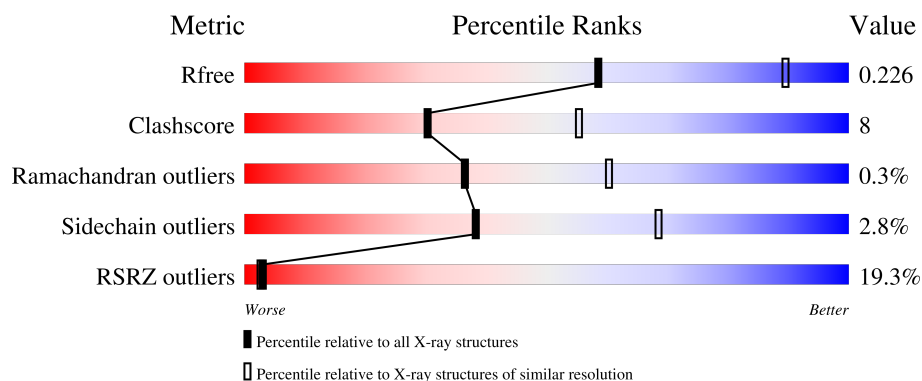
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	658	19% 77% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4931 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 Putative copper-exporting P-type ATPase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			4929	3176	829	909	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLY	-	expression tag	UNP A0A117KM49

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

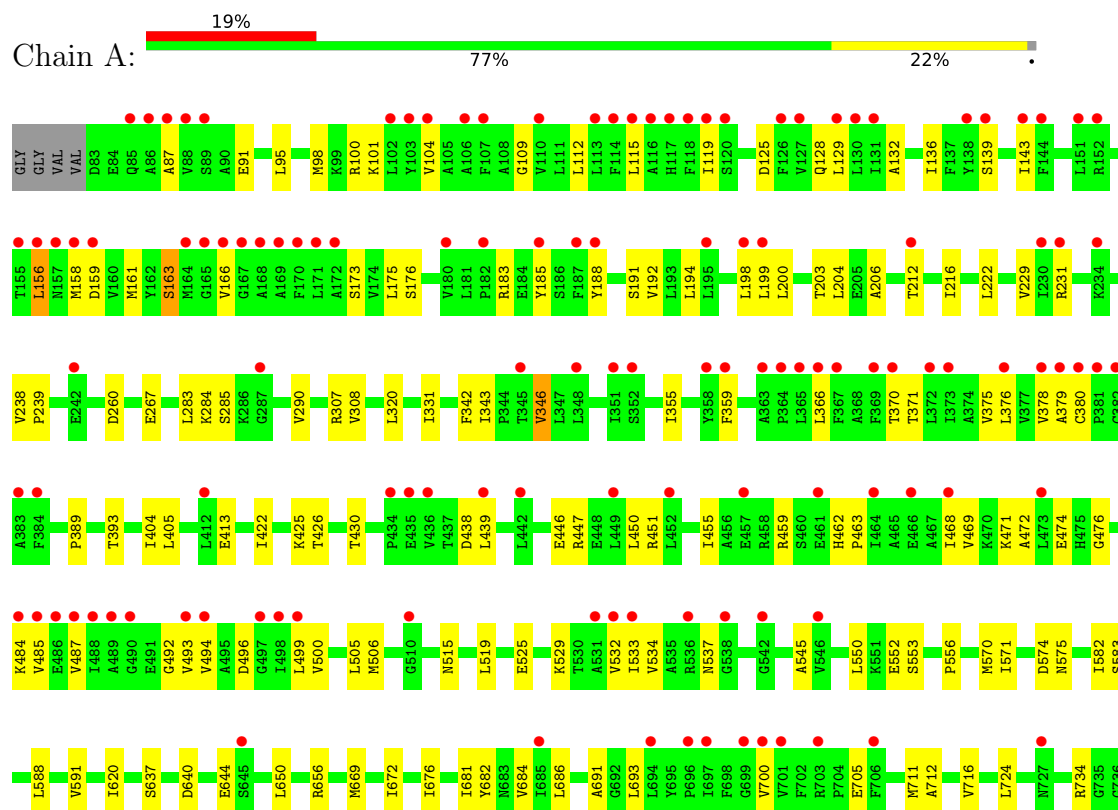
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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: Putative copper-exporting P-type ATPase A



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.53Å 150.10Å 218.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.65 – 2.70 45.65 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.65-2.70) 91.4 (45.65-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.225 , 0.256 (Not available) , 0.226	Depositor DCC
R_{free} test set	1998 reflections (6.83%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4931	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: MG, K

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	0.47	0/5003	0.71	0/6785

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	LEU	Peptide
1	A	346	VAL	Peptide

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	4929	0	5172	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	1	0	0	0	0
All	All	4931	0	5172	85	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 (85) 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:115:LEU:HB3	1:A:128:GLN:HE22	1.50	0.77
1:A:176:SER:HB2	1:A:185:TYR:HB2	1.70	0.72
1:A:260:ASP:HB2	1:A:307:ARG:HB2	1.73	0.71
1:A:163:SER:HA	1:A:166:VAL:HG12	1.73	0.70
1:A:583:SER:HB2	1:A:591:VAL:HG21	1.73	0.69
1:A:425:LYS:NZ	1:A:574:ASP:OD2	2.29	0.64
1:A:484:LYS:HB3	1:A:496:ASP:H	1.63	0.63
1:A:447:ARG:NH2	1:A:476:GLY:O	2.32	0.62
1:A:191:SER:HA	1:A:194:LEU:HB2	1.83	0.60
1:A:438:ASP:OD2	1:A:529:LYS:NZ	2.35	0.60
1:A:156:LEU:HD23	1:A:343:ILE:HG22	1.83	0.60
1:A:378:VAL:HA	1:A:711:MET:HE2	1.84	0.59
1:A:450:LEU:HD21	1:A:472:ALA:HA	1.85	0.58
1:A:355:ILE:O	1:A:359:PHE:HB2	2.03	0.58
1:A:422:ILE:HG21	1:A:571:ILE:HG13	1.87	0.56
1:A:471:LYS:NZ	1:A:474:GLU:OE2	2.37	0.56
1:A:681:ILE:HA	1:A:684:VAL:HG22	1.90	0.54
1:A:200:LEU:HD23	1:A:712:ALA:HB1	1.89	0.54
1:A:95:LEU:HD22	1:A:206:ALA:HB1	1.90	0.54
1:A:101:LYS:HG2	1:A:139:SER:HA	1.90	0.53
1:A:212:THR:O	1:A:216:ILE:HD12	2.09	0.53
1:A:459:ARG:HD2	1:A:485:VAL:HG21	1.90	0.53
1:A:143:ILE:HG21	1:A:198:LEU:HD21	1.89	0.53
1:A:204:LEU:HD11	1:A:716:VAL:HG12	1.90	0.53
1:A:331:ILE:HG21	1:A:669:MET:HE1	1.89	0.53
1:A:583:SER:HA	1:A:588:LEU:HD12	1.91	0.51
1:A:438:ASP:HB2	1:A:545:ALA:HB3	1.92	0.51
1:A:159:ASP:O	1:A:163:SER:OG	2.26	0.51
1:A:413:GLU:HG3	1:A:669:MET:HE2	1.94	0.50
1:A:342:PHE:O	1:A:346:VAL:HG22	2.12	0.49
1:A:125:ASP:OD2	1:A:183:ARG:NH2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:MET:HE3	1:A:533:ILE:HB	1.95	0.49
1:A:430:THR:HG22	1:A:550:LEU:HD23	1.95	0.49
1:A:494:VAL:HG22	1:A:499:LEU:HD21	1.94	0.49
1:A:500:VAL:HG22	1:A:534:VAL:HG12	1.94	0.48
1:A:212:THR:HG22	1:A:393:THR:HG21	1.96	0.48
1:A:136:ILE:HD11	1:A:192:VAL:HG22	1.96	0.47
1:A:682:TYR:CZ	1:A:686:LEU:HD22	2.50	0.47
1:A:462:HIS:CG	1:A:463:PRO:HD2	2.50	0.47
1:A:705:GLU:H	1:A:705:GLU:CD	2.23	0.46
1:A:109:GLY:HA2	1:A:112:LEU:HB2	1.97	0.46
1:A:267:GLU:HG3	1:A:285:SER:HB3	1.98	0.46
1:A:320:LEU:HD22	1:A:405:LEU:HB3	1.97	0.46
1:A:468:ILE:HD12	1:A:469:VAL:N	2.30	0.46
1:A:158:MET:HA	1:A:380:CYS:SG	2.56	0.46
1:A:371:THR:HB	1:A:691:ALA:HA	1.97	0.46
1:A:422:ILE:CG2	1:A:571:ILE:HG13	2.46	0.46
1:A:525:GLU:OE2	1:A:575:ASN:ND2	2.48	0.46
1:A:389:PRO:O	1:A:393:THR:HG23	2.15	0.45
1:A:537:ASN:N	1:A:537:ASN:OD1	2.49	0.45
1:A:499:LEU:HD22	1:A:505:LEU:HD11	1.97	0.45
1:A:672:ILE:O	1:A:676:ILE:HG13	2.17	0.44
1:A:87:ALA:O	1:A:91:GLU:HG3	2.18	0.43
1:A:229:VAL:HG12	1:A:231:ARG:HG3	1.99	0.43
1:A:366:LEU:O	1:A:370:THR:HG23	2.18	0.43
1:A:284:LYS:HE3	1:A:290:VAL:HG12	2.00	0.43
1:A:375:VAL:HG21	1:A:691:ALA:HB2	2.00	0.43
1:A:553:SER:C	1:A:556:PRO:HD2	2.44	0.43
1:A:637:SER:HB2	1:A:644:GLU:HG3	2.00	0.43
1:A:375:VAL:CG2	1:A:691:ALA:HB2	2.49	0.43
1:A:112:LEU:HD21	1:A:132:ALA:HB2	2.01	0.42
1:A:98:MET:HB3	1:A:203:THR:HG22	2.01	0.42
1:A:375:VAL:O	1:A:379:ALA:N	2.52	0.42
1:A:439:LEU:HD23	1:A:439:LEU:HA	1.81	0.42
1:A:446:GLU:N	1:A:446:GLU:OE1	2.53	0.42
1:A:570:MET:HE1	1:A:582:ILE:HB	2.02	0.42
1:A:100:ARG:O	1:A:104:VAL:HG23	2.19	0.42
1:A:112:LEU:HD23	1:A:188:TYR:O	2.20	0.42
1:A:500:VAL:HG13	1:A:532:VAL:HG21	2.00	0.42
1:A:515:ASN:O	1:A:519:LEU:HD22	2.20	0.41
1:A:492:GLY:HA3	1:A:505:LEU:HG	2.01	0.41
1:A:552:GLU:CD	1:A:656:ARG:HH22	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:GLU:HG2	1:A:283:LEU:HD11	2.02	0.41
1:A:468:ILE:HD12	1:A:469:VAL:H	1.85	0.41
1:A:487:VAL:HG13	1:A:493:VAL:HG12	2.03	0.41
1:A:681:ILE:HG13	1:A:682:TYR:N	2.36	0.41
1:A:161:MET:HE2	1:A:379:ALA:HB3	2.01	0.41
1:A:161:MET:HE1	1:A:376:LEU:HD22	2.03	0.40
1:A:199:LEU:HA	1:A:199:LEU:HD23	1.72	0.40
1:A:404:ILE:HA	1:A:650:LEU:HD13	2.02	0.40
1:A:173:SER:HA	1:A:185:TYR:O	2.22	0.40
1:A:238:VAL:HG23	1:A:239:PRO:O	2.22	0.40
1:A:451:ARG:O	1:A:455:ILE:HG12	2.21	0.40
1:A:499:LEU:HD23	1:A:499:LEU:HA	1.63	0.40
1:A:640:ASP:O	1:A:644:GLU:HG2	2.22	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	652/658 (99%)	612 (94%)	38 (6%)	2 (0%)	36	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	700	VAL
1	A	693	LEU

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	361/523 (69%)	351 (97%)	10 (3%)	38	68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ILE
1	A	129	LEU
1	A	156	LEU
1	A	163	SER
1	A	175	LEU
1	A	308	VAL
1	A	426	THR
1	A	620	ILE
1	A	724	LEU
1	A	734	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	128	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

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	654/658 (99%)	1.01	126 (19%) 3 3	47, 86, 146, 171	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	PHE	8.4
1	A	382	CYS	5.8
1	A	531	ALA	5.7
1	A	487	VAL	5.6
1	A	113	LEU	5.5
1	A	461	GLU	5.3
1	A	700	VAL	5.3
1	A	143	ILE	5.1
1	A	489	ALA	5.0
1	A	383	ALA	4.9
1	A	486	GLU	4.9
1	A	701	VAL	4.8
1	A	435	GLU	4.7
1	A	164	MET	4.6
1	A	172	ALA	4.6
1	A	119	ILE	4.6
1	A	116	ALA	4.6
1	A	366	LEU	4.5
1	A	89	SER	4.3
1	A	378	VAL	4.2
1	A	168	ALA	4.2
1	A	86	ALA	4.1
1	A	381	PRO	4.0
1	A	697	ILE	3.9
1	A	485	VAL	3.8
1	A	379	ALA	3.8
1	A	118	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	351	ILE	3.7
1	A	117	HIS	3.7
1	A	199	LEU	3.6
1	A	473	LEU	3.5
1	A	370	THR	3.5
1	A	139	SER	3.4
1	A	466	GLU	3.4
1	A	380	CYS	3.3
1	A	110	VAL	3.3
1	A	497	GLY	3.3
1	A	103	TYR	3.3
1	A	115	LEU	3.3
1	A	156	LEU	3.3
1	A	436	VAL	3.3
1	A	703	ARG	3.3
1	A	102	LEU	3.2
1	A	185	TYR	3.2
1	A	234	LYS	3.2
1	A	439	LEU	3.2
1	A	104	VAL	3.2
1	A	195	LEU	3.1
1	A	352	SER	3.1
1	A	231	ARG	3.1
1	A	165	GLY	3.0
1	A	158	MET	3.0
1	A	287	GLY	3.0
1	A	187	PHE	3.0
1	A	442	LEU	3.0
1	A	493	VAL	2.9
1	A	348	LEU	2.9
1	A	126	PHE	2.9
1	A	449	LEU	2.9
1	A	182	PRO	2.9
1	A	533	ILE	2.9
1	A	155	THR	2.9
1	A	170	PHE	2.8
1	A	498	ILE	2.8
1	A	490	GLY	2.8
1	A	180	VAL	2.8
1	A	88	VAL	2.8
1	A	188	TYR	2.8
1	A	536	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	358	TYR	2.8
1	A	120	SER	2.7
1	A	167	GLY	2.7
1	A	359	PHE	2.7
1	A	230	ILE	2.7
1	A	412	LEU	2.7
1	A	372	LEU	2.7
1	A	127	VAL	2.7
1	A	464	ILE	2.6
1	A	510	GLY	2.6
1	A	151	LEU	2.6
1	A	494	VAL	2.6
1	A	434	PRO	2.6
1	A	131	ILE	2.6
1	A	138	TYR	2.6
1	A	706	PHE	2.6
1	A	129	LEU	2.6
1	A	542	GLY	2.6
1	A	107	PHE	2.6
1	A	367	PHE	2.6
1	A	538	GLY	2.5
1	A	452	LEU	2.5
1	A	369	PHE	2.5
1	A	171	LEU	2.5
1	A	159	ASP	2.5
1	A	364	PRO	2.5
1	A	645	SER	2.4
1	A	532	VAL	2.4
1	A	87	ALA	2.4
1	A	488	ILE	2.4
1	A	85	GLN	2.4
1	A	166	VAL	2.4
1	A	499	LEU	2.4
1	A	457	GLU	2.4
1	A	727	ASN	2.4
1	A	130	LEU	2.3
1	A	699	GLY	2.3
1	A	694	LEU	2.3
1	A	468	ILE	2.3
1	A	212	THR	2.3
1	A	696	PRO	2.3
1	A	376	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	685	ILE	2.2
1	A	242	GLU	2.2
1	A	365	LEU	2.2
1	A	144	PHE	2.2
1	A	106	ALA	2.2
1	A	363	ALA	2.2
1	A	373	ILE	2.2
1	A	546	VAL	2.1
1	A	345	THR	2.1
1	A	157	ASN	2.1
1	A	384	PHE	2.1
1	A	169	ALA	2.1
1	A	484	LYS	2.1
1	A	152	ARG	2.1
1	A	198	LEU	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
3	MG	A	802	1/1	0.77	0.30	83,83,83,83	0
2	K	A	801	1/1	0.93	0.08	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.