



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:01 PM UTC

PDB ID : 1RWL / pdb_00001rwl
Title : Extracellular domain of Mycobacterium tuberculosis PknD
Authors : Good, M.C.; Greenstein, A.E.; Young, T.A.; Ng, H.L.; Alber, T.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2003-12-16
Resolution : 1.90 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

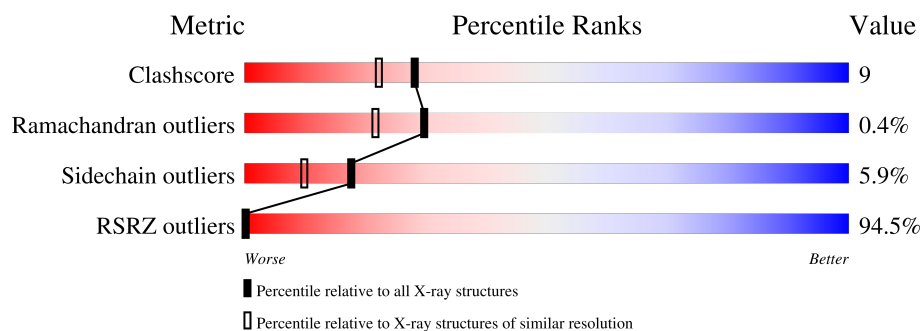
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	270	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1945 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 Serine/threonine-protein kinase pknD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1871	1171	326	373	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	-	cloning artifact	UNP O05871
A	264	GLU	-	cloning artifact	UNP O05871
A	265	HIS	-	expression tag	UNP O05871
A	266	HIS	-	expression tag	UNP O05871
A	267	HIS	-	expression tag	UNP O05871
A	268	HIS	-	expression tag	UNP O05871
A	269	HIS	-	expression tag	UNP O05871
A	270	HIS	-	expression tag	UNP O05871

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cd	0	0
			4	4		

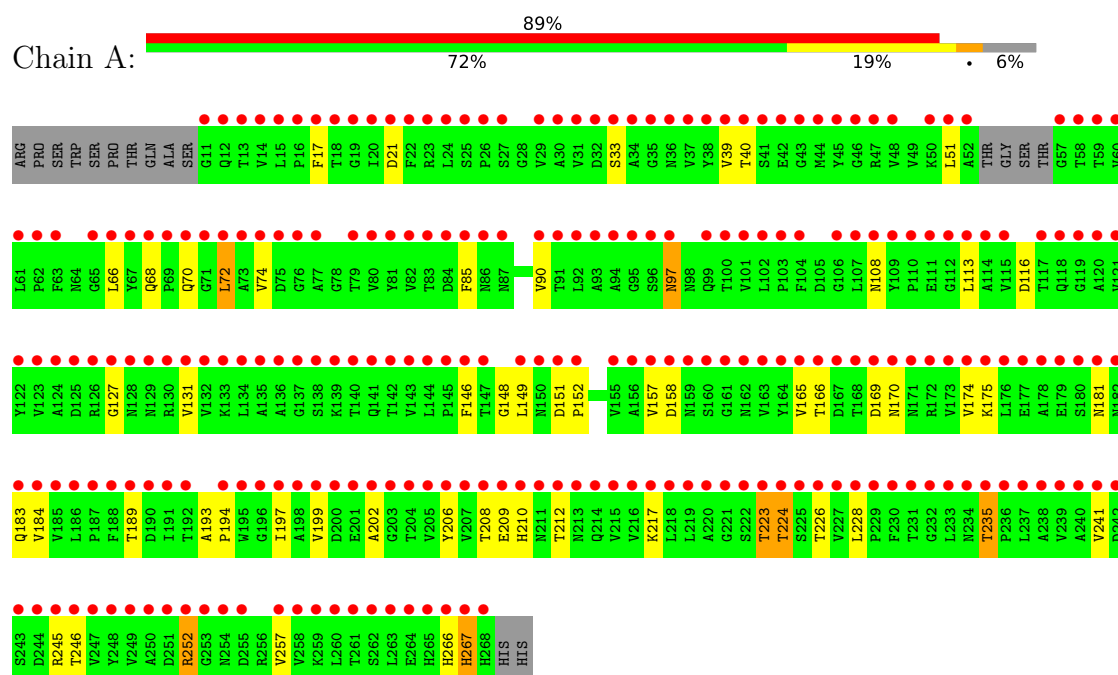
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		

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: Serine/threonine-protein kinase pknD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.94Å 94.58Å 71.77Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-1.90) 34.1 (30.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.262 0.569 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	1.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 273.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.50	EDS
Total number of atoms	1945	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.54% 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: CD

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	1.05	5/1905 (0.3%)	1.03	1/2614 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	GLN	C-O	7.18	1.27	1.23
1	A	193	ALA	CA-CB	-5.99	1.48	1.52
1	A	68	GLN	CA-C	5.72	1.57	1.53
1	A	74	VAL	CA-CB	5.37	1.61	1.54
1	A	189	THR	CA-CB	5.20	1.59	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ALA	O-C-N	5.42	124.02	121.53

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	1871	0	1815	33	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	70	0	0	2	0
All	All	1945	0	1815	33	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 9.

All (33) 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:97:ASN:HD22	1:A:97:ASN:C	1.96	0.73
1:A:174:VAL:CG1	1:A:183:GLN:HG2	2.22	0.70
1:A:202:ALA:O	3:A:554:HOH:O	2.11	0.69
1:A:174:VAL:HG13	1:A:183:GLN:HG2	1.77	0.67
1:A:174:VAL:HG11	1:A:183:GLN:CG	2.31	0.60
1:A:174:VAL:CG1	1:A:183:GLN:CG	2.79	0.60
1:A:158:ASP:HB3	1:A:199:VAL:HG21	1.90	0.53
1:A:66:LEU:HD21	1:A:90:VAL:HG11	1.91	0.53
1:A:151:ASP:HB2	1:A:169:ASP:OD1	2.09	0.52
1:A:131:VAL:HG21	1:A:165:VAL:HG21	1.91	0.52
1:A:70:GLN:HG3	1:A:85:PHE:CE1	2.45	0.52
1:A:175:LYS:HB3	1:A:184:VAL:HG22	1.91	0.51
1:A:266:HIS:CD2	1:A:267:HIS:ND1	2.79	0.50
1:A:116:ASP:HB3	1:A:157:VAL:HG11	1.94	0.49
1:A:197:ILE:HA	1:A:206:TYR:O	2.13	0.48
1:A:151:ASP:OD1	3:A:551:HOH:O	2.20	0.48
1:A:209:GLU:HB3	1:A:212:THR:HG22	1.95	0.47
1:A:108:ASN:HD22	1:A:127:GLY:HA3	1.80	0.47
1:A:146:PHE:CB	1:A:149:LEU:HD11	2.45	0.47
1:A:223:THR:O	1:A:224:THR:HG22	2.15	0.46
1:A:40:THR:HG23	1:A:72:LEU:HG	1.98	0.46
1:A:39:VAL:HG11	1:A:257:VAL:HG21	1.97	0.46
1:A:97:ASN:C	1:A:97:ASN:ND2	2.66	0.45
1:A:17:PHE:CE1	1:A:51:LEU:HB2	2.51	0.44
1:A:148:GLY:O	1:A:170:ASN:ND2	2.51	0.43
1:A:209:GLU:CB	1:A:212:THR:HG22	2.48	0.43
1:A:217:LYS:HB3	1:A:228:LEU:HD11	2.00	0.43
1:A:210:HIS:O	1:A:235:THR:HA	2.19	0.43
1:A:235:THR:O	1:A:252:ARG:HB3	2.19	0.43
1:A:152:PRO:HA	1:A:166:THR:O	2.21	0.41
1:A:241:VAL:HA	1:A:246:THR:O	2.20	0.41
1:A:194:PRO:HA	1:A:208:THR:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:ND2	1:A:127:GLY:HA3	2.36	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	250/270 (93%)	241 (96%)	8 (3%)	1 (0%)	30 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	HIS

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	202/222 (91%)	190 (94%)	12 (6%)	18 10

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	33	SER

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Mol	Chain	Res	Type
1	A	72	LEU
1	A	97	ASN
1	A	113	LEU
1	A	181	ASN
1	A	223	THR
1	A	224	THR
1	A	226	THR
1	A	235	THR
1	A	245	ARG
1	A	252	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	98	ASN
1	A	108	ASN
1	A	182	ASN
1	A	254	ASN

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 4 ligands modelled in this entry, 4 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	254/270 (94%)	4.68	240 (94%) 0 0	23, 35, 47, 52	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	THR	10.6
1	A	250	ALA	10.0
1	A	164	TYR	9.9
1	A	198	ALA	9.6
1	A	231	THR	9.5
1	A	132	VAL	8.8
1	A	93	ALA	8.6
1	A	45	TYR	8.6
1	A	51	LEU	8.5
1	A	185	VAL	8.3
1	A	165	VAL	8.3
1	A	71	GLY	8.2
1	A	11	GLY	8.2
1	A	76	GLY	8.2
1	A	29	VAL	7.9
1	A	14	VAL	7.7
1	A	163	VAL	7.7
1	A	134	LEU	7.7
1	A	31	VAL	7.7
1	A	220	ALA	7.6
1	A	84	ASP	7.6
1	A	213	ASN	7.6
1	A	120	ALA	7.6
1	A	92	LEU	7.5
1	A	90	VAL	7.5
1	A	195	TRP	7.5
1	A	156	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	68	GLN	7.4
1	A	17	PHE	7.3
1	A	146	PHE	7.2
1	A	115	VAL	7.1
1	A	257	VAL	7.1
1	A	241	VAL	7.1
1	A	186	LEU	6.9
1	A	136	ALA	6.9
1	A	65	GLY	6.9
1	A	95	GLY	6.9
1	A	114	ALA	6.9
1	A	162	ASN	6.8
1	A	85	PHE	6.8
1	A	104	PHE	6.8
1	A	251	ASP	6.8
1	A	37	VAL	6.8
1	A	113	LEU	6.7
1	A	44	MET	6.6
1	A	74	VAL	6.6
1	A	217	LYS	6.5
1	A	22	PHE	6.5
1	A	206	TYR	6.3
1	A	102	LEU	6.2
1	A	79	THR	6.2
1	A	144	LEU	6.2
1	A	40	THR	6.2
1	A	39	VAL	6.1
1	A	218	LEU	6.1
1	A	124	ALA	6.0
1	A	211	ASN	6.0
1	A	232	GLY	6.0
1	A	137	GLY	6.0
1	A	210	HIS	6.0
1	A	216	VAL	5.9
1	A	263	LEU	5.9
1	A	204	THR	5.9
1	A	121	VAL	5.9
1	A	222	SER	5.9
1	A	228	LEU	5.8
1	A	21	ASP	5.8
1	A	82	VAL	5.8
1	A	140	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	52	ALA	5.7
1	A	199	VAL	5.7
1	A	172	ARG	5.7
1	A	225	SER	5.7
1	A	246	THR	5.7
1	A	109	TYR	5.6
1	A	96	SER	5.6
1	A	170	ASN	5.6
1	A	63	PHE	5.6
1	A	59	THR	5.5
1	A	123	VAL	5.5
1	A	176	LEU	5.5
1	A	155	VAL	5.5
1	A	258	VAL	5.4
1	A	119	GLY	5.4
1	A	128	ASN	5.4
1	A	73	ALA	5.4
1	A	181	ASN	5.4
1	A	16	PRO	5.3
1	A	192	THR	5.3
1	A	202	ALA	5.3
1	A	36	ASN	5.2
1	A	42	GLU	5.2
1	A	173	VAL	5.2
1	A	117	THR	5.2
1	A	108	ASN	5.1
1	A	62	PRO	5.1
1	A	219	LEU	5.1
1	A	18	THR	5.0
1	A	72	LEU	5.0
1	A	107	LEU	5.0
1	A	188	PHE	5.0
1	A	61	LEU	5.0
1	A	66	LEU	5.0
1	A	81	TYR	5.0
1	A	189	THR	5.0
1	A	25	SER	4.9
1	A	157	VAL	4.9
1	A	260	LEU	4.9
1	A	75	ASP	4.9
1	A	168	THR	4.9
1	A	259	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	183	GLN	4.8
1	A	215	VAL	4.8
1	A	239	VAL	4.8
1	A	236	PRO	4.8
1	A	13	THR	4.7
1	A	254	ASN	4.7
1	A	12	GLN	4.7
1	A	177	GLU	4.7
1	A	174	VAL	4.6
1	A	143	VAL	4.6
1	A	187	PRO	4.6
1	A	24	LEU	4.6
1	A	69	PRO	4.6
1	A	267	HIS	4.5
1	A	100	THR	4.5
1	A	86	ASN	4.5
1	A	265	HIS	4.4
1	A	46	GLY	4.4
1	A	205	VAL	4.4
1	A	238	ALA	4.4
1	A	145	PRO	4.3
1	A	139	LYS	4.3
1	A	266	HIS	4.3
1	A	26	PRO	4.2
1	A	80	VAL	4.2
1	A	101	VAL	4.2
1	A	27	SER	4.2
1	A	57	GLY	4.2
1	A	224	THR	4.2
1	A	221	GLY	4.1
1	A	38	TYR	4.1
1	A	197	ILE	4.1
1	A	227	VAL	4.1
1	A	149	LEU	4.1
1	A	94	ALA	4.0
1	A	133	LYS	4.0
1	A	138	SER	4.0
1	A	233	LEU	4.0
1	A	58	THR	3.9
1	A	203	GLY	3.9
1	A	91	THR	3.9
1	A	223	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	214	GLN	3.9
1	A	60	VAL	3.9
1	A	99	GLN	3.9
1	A	237	LEU	3.9
1	A	229	PRO	3.9
1	A	161	GLY	3.8
1	A	20	ILE	3.8
1	A	255	ASP	3.7
1	A	106	GLY	3.7
1	A	243	SER	3.7
1	A	209	GLU	3.7
1	A	247	VAL	3.7
1	A	180	SER	3.7
1	A	150	ASN	3.7
1	A	184	VAL	3.6
1	A	178	ALA	3.6
1	A	226	THR	3.6
1	A	32	ASP	3.6
1	A	34	ALA	3.5
1	A	130	ARG	3.5
1	A	175	LYS	3.5
1	A	15	LEU	3.5
1	A	249	VAL	3.4
1	A	127	GLY	3.4
1	A	240	ALA	3.4
1	A	242	ASP	3.4
1	A	171	ASN	3.4
1	A	147	THR	3.4
1	A	67	TYR	3.4
1	A	160	SER	3.4
1	A	166	THR	3.4
1	A	159	ASN	3.4
1	A	77	ALA	3.3
1	A	151	ASP	3.3
1	A	126	ARG	3.3
1	A	261	THR	3.3
1	A	131	VAL	3.2
1	A	70	GLN	3.2
1	A	244	ASP	3.2
1	A	97	ASN	3.1
1	A	122	TYR	3.1
1	A	196	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	264	GLU	3.1
1	A	41	SER	3.1
1	A	48	VAL	3.1
1	A	19	GLY	3.1
1	A	179	GLU	3.0
1	A	111	GLU	3.0
1	A	262	SER	3.0
1	A	141	GLN	3.0
1	A	234	ASN	3.0
1	A	248	TYR	3.0
1	A	83	THR	3.0
1	A	118	GLN	2.9
1	A	158	ASP	2.9
1	A	191	ILE	2.9
1	A	43	GLY	2.9
1	A	30	ALA	2.9
1	A	245	ARG	2.9
1	A	190	ASP	2.8
1	A	129	ASN	2.8
1	A	125	ASP	2.8
1	A	135	ALA	2.7
1	A	268	HIS	2.7
1	A	208	THR	2.7
1	A	194	PRO	2.7
1	A	142	THR	2.7
1	A	87	ASN	2.7
1	A	112	GLY	2.6
1	A	235	THR	2.6
1	A	253	GLY	2.6
1	A	207	VAL	2.5
1	A	152	PRO	2.5
1	A	182	ASN	2.4
1	A	167	ASP	2.4
1	A	50	LYS	2.3
1	A	169	ASP	2.3
1	A	47	ARG	2.2
1	A	230	PHE	2.2
1	A	33	SER	2.2
1	A	201	GLU	2.2
1	A	103	PRO	2.2
1	A	110	PRO	2.2
1	A	35	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	23	ARG	2.2
1	A	252	ARG	2.1
1	A	200	ASP	2.1

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	CD	A	503	1/1	0.61	0.25	49,49,49,49	1
2	CD	A	504	1/1	0.76	0.17	31,31,31,31	1
2	CD	A	501	1/1	0.98	0.04	31,31,31,31	0
2	CD	A	502	1/1	0.99	0.05	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.