Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:03 PM GMT

PDB ID	:	1RWL
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

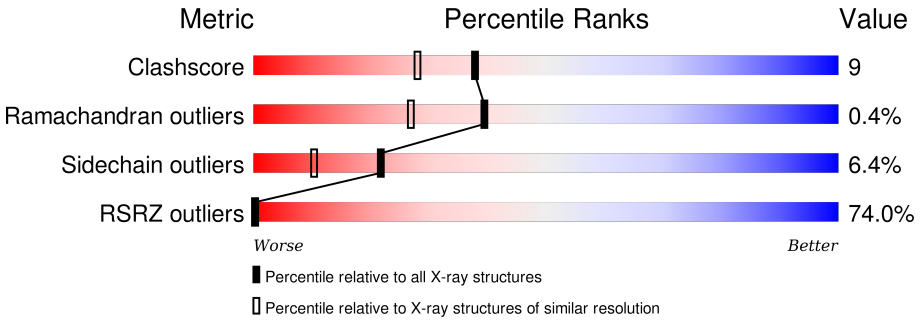
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	70%, 72%, 19%, 6%

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 (three-letter code: CD) (formula: Cd).

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

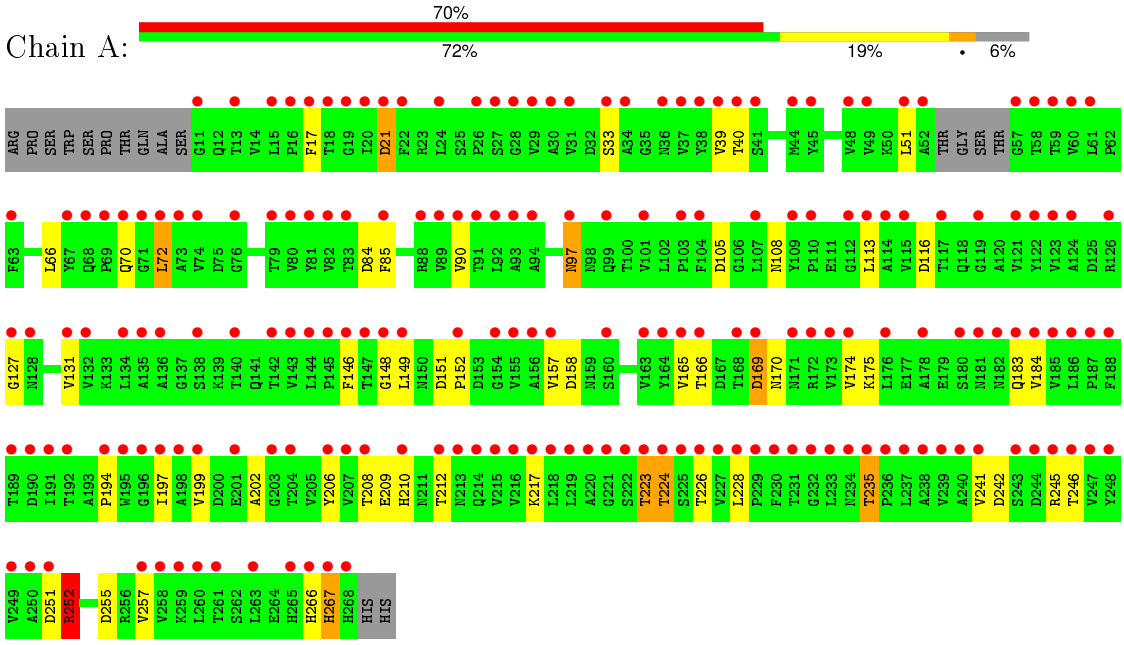
- Molecule 3 is water.

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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 (i)

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 23.64 – 1.64	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-1.90) 24.3 (23.64-1.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.262 0.557 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	1.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.62 , 1058.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 17368 reflections	Xtriage
F_o,F_c correlation	0.53	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.78	0/1905	0.96	6/2614 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	252	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	255	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	105	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	242	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	21	ASP	CB-CG-OD2	5.19	122.97	118.30

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	1871	0	1815	34	0
2	A	4	0	0	0	0
3	A	70	0	0	2	0
All	All	1945	0	1815	34	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 (34) 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: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:97:ASN:HD22	1:A:97:ASN:C	1.96	0.68
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:266:HIS:CD2	1:A:267:HIS:HD1	2.25	0.54
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:97:ASN:ND2	1:A:97:ASN:C	2.66	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:17:PHE:CE1	1:A:51:LEU:HB2	2.51	0.44
1:A:209:GLU:CB	1:A:212:THR:HG22	2.48	0.43
1:A:148:GLY:O	1:A:170:ASN:ND2	2.51	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
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%)	39 27

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%)	189 (94%)	13 (6%)	22 10

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	33	SER
1	A	72	LEU
1	A	84	ASP
1	A	97	ASN
1	A	113	LEU
1	A	169	ASP
1	A	223	THR
1	A	224	THR
1	A	226	THR

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Mol	Chain	Res	Type
1	A	235	THR
1	A	245	ARG
1	A	252	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) 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	214	GLN
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 carbohydrates 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, 95^{th} 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%)	3.25	188 (74%)	0	0	23, 35, 47, 52	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	THR	8.3
1	A	231	THR	6.9
1	A	72	LEU	6.7
1	A	176	LEU	6.7
1	A	20	ILE	6.5
1	A	147	THR	6.4
1	A	155	VAL	6.3
1	A	197	ILE	6.2
1	A	212	THR	6.2
1	A	31	VAL	6.2
1	A	29	VAL	6.1
1	A	17	PHE	6.0
1	A	227	VAL	6.0
1	A	19	GLY	6.0
1	A	219	LEU	6.0
1	A	263	LEU	5.8
1	A	93	ALA	5.7
1	A	223	THR	5.7
1	A	266	HIS	5.6
1	A	144	LEU	5.6
1	A	22	PHE	5.6
1	A	71	GLY	5.6
1	A	104	PHE	5.6
1	A	166	THR	5.5
1	A	218	LEU	5.5
1	A	229	PRO	5.5
1	A	132	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	198	ALA	5.5
1	A	239	VAL	5.5
1	A	163	VAL	5.3
1	A	11	GLY	5.2
1	A	156	ALA	5.1
1	A	113	LEU	5.0
1	A	117	THR	5.0
1	A	187	PRO	5.0
1	A	18	THR	5.0
1	A	28	GLY	5.0
1	A	123	VAL	5.0
1	A	267	HIS	5.0
1	A	199	VAL	5.0
1	A	51	LEU	4.9
1	A	260	LEU	4.9
1	A	121	VAL	4.9
1	A	40	THR	4.8
1	A	195	TRP	4.8
1	A	85	PHE	4.8
1	A	145	PRO	4.8
1	A	196	GLY	4.8
1	A	238	ALA	4.8
1	A	186	LEU	4.7
1	A	183	GLN	4.7
1	A	74	VAL	4.7
1	A	109	TYR	4.7
1	A	33	SER	4.7
1	A	250	ALA	4.7
1	A	82	VAL	4.6
1	A	63	PHE	4.6
1	A	225	SER	4.6
1	A	27	SER	4.5
1	A	190	ASP	4.5
1	A	173	VAL	4.5
1	A	188	PHE	4.5
1	A	89	VAL	4.5
1	A	268	HIS	4.4
1	A	157	VAL	4.4
1	A	58	THR	4.4
1	A	226	THR	4.3
1	A	15	LEU	4.3
1	A	189	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	16	PRO	4.2
1	A	44	MET	4.2
1	A	216	VAL	4.2
1	A	240	ALA	4.1
1	A	228	LEU	4.1
1	A	265	HIS	4.0
1	A	184	VAL	4.0
1	A	215	VAL	4.0
1	A	92	LEU	4.0
1	A	48	VAL	3.9
1	A	233	LEU	3.8
1	A	236	PRO	3.8
1	A	222	SER	3.8
1	A	207	VAL	3.8
1	A	91	THR	3.8
1	A	140	THR	3.8
1	A	21	ASP	3.8
1	A	174	VAL	3.8
1	A	124	ALA	3.7
1	A	126	ARG	3.7
1	A	67	TYR	3.7
1	A	214	GLN	3.7
1	A	94	ALA	3.7
1	A	107	LEU	3.7
1	A	201	GLU	3.7
1	A	247	VAL	3.7
1	A	206	TYR	3.7
1	A	230	PHE	3.7
1	A	119	GLY	3.6
1	A	146	PHE	3.6
1	A	30	ALA	3.6
1	A	154	GLY	3.6
1	A	39	VAL	3.6
1	A	203	GLY	3.5
1	A	83	THR	3.5
1	A	131	VAL	3.5
1	A	185	VAL	3.5
1	A	208	THR	3.5
1	A	45	TYR	3.4
1	A	213	ASN	3.4
1	A	149	LEU	3.4
1	A	257	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	128	ASN	3.4
1	A	249	VAL	3.4
1	A	59	THR	3.3
1	A	248	TYR	3.3
1	A	73	ALA	3.3
1	A	69	PRO	3.3
1	A	192	THR	3.3
1	A	178	ALA	3.3
1	A	152	PRO	3.2
1	A	165	VAL	3.2
1	A	245	ARG	3.2
1	A	24	LEU	3.2
1	A	79	THR	3.2
1	A	261	THR	3.2
1	A	52	ALA	3.2
1	A	234	ASN	3.2
1	A	26	PRO	3.2
1	A	34	ALA	3.2
1	A	90	VAL	3.1
1	A	101	VAL	3.1
1	A	135	ALA	3.1
1	A	237	LEU	3.1
1	A	221	GLY	3.1
1	A	180	SER	3.1
1	A	88	ARG	3.1
1	A	244	ASP	3.1
1	A	191	ILE	3.0
1	A	122	TYR	3.0
1	A	97	ASN	3.0
1	A	148	GLY	3.0
1	A	220	ALA	3.0
1	A	143	VAL	3.0
1	A	112	GLY	2.9
1	A	81	TYR	2.9
1	A	142	THR	2.8
1	A	169	ASP	2.8
1	A	103	PRO	2.8
1	A	99	GLN	2.8
1	A	114	ALA	2.8
1	A	60	VAL	2.8
1	A	172	ARG	2.8
1	A	258	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	259	LYS	2.7
1	A	115	VAL	2.7
1	A	194	PRO	2.6
1	A	246	THR	2.6
1	A	138	SER	2.6
1	A	70	GLN	2.5
1	A	160	SER	2.5
1	A	168	THR	2.5
1	A	38	TYR	2.5
1	A	61	LEU	2.5
1	A	241	VAL	2.4
1	A	134	LEU	2.4
1	A	68	GLN	2.4
1	A	182	ASN	2.4
1	A	36	ASN	2.3
1	A	49	VAL	2.3
1	A	80	VAL	2.3
1	A	57	GLY	2.3
1	A	127	GLY	2.3
1	A	181	ASN	2.3
1	A	110	PRO	2.3
1	A	251	ASP	2.3
1	A	164	TYR	2.3
1	A	37	VAL	2.2
1	A	210	HIS	2.2
1	A	235	THR	2.2
1	A	136	ALA	2.2
1	A	171	ASN	2.1
1	A	204	THR	2.1
1	A	13	THR	2.1
1	A	41	SER	2.1
1	A	232	GLY	2.0
1	A	217	LYS	2.0
1	A	243	SER	2.0
1	A	76	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	CD	A	501	1/1	0.99	0.14	-	31,31,31,31	0
2	CD	A	502	1/1	0.99	0.08	-	39,39,39,39	0
2	CD	A	503	1/1	0.82	0.11	-	49,49,49,49	1
2	CD	A	504	1/1	0.93	0.10	-	31,31,31,31	1

6.5 Other polymers (i)

There are no such residues in this entry.