



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:47 AM UTC

PDB ID : 6CWU / pdb_00006cwu
Title : Protein Tyrosine Phosphatase 1B F135Y mutant
Authors : Hjortness, M.; Zwart, P.; Sankaran, B.; Fox, J.M.
Deposited on : 2018-03-31
Resolution : 2.08 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

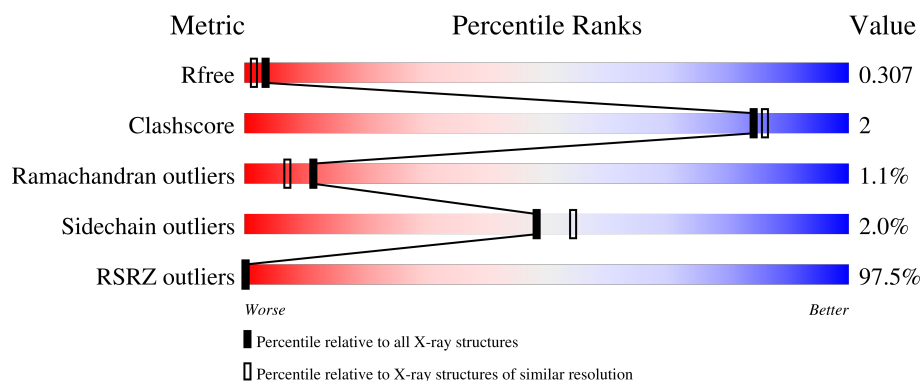
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	329	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2709 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 Tyrosine-protein phosphatase non-receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	11	0
			2356	1498	402	436	20			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	TYR	PHE	engineered mutation	UNP P18031
A	322	LEU	-	expression tag	UNP P18031
A	323	GLU	-	expression tag	UNP P18031
A	324	HIS	-	expression tag	UNP P18031
A	325	HIS	-	expression tag	UNP P18031
A	326	HIS	-	expression tag	UNP P18031
A	327	HIS	-	expression tag	UNP P18031
A	328	HIS	-	expression tag	UNP P18031
A	329	HIS	-	expression tag	UNP P18031

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

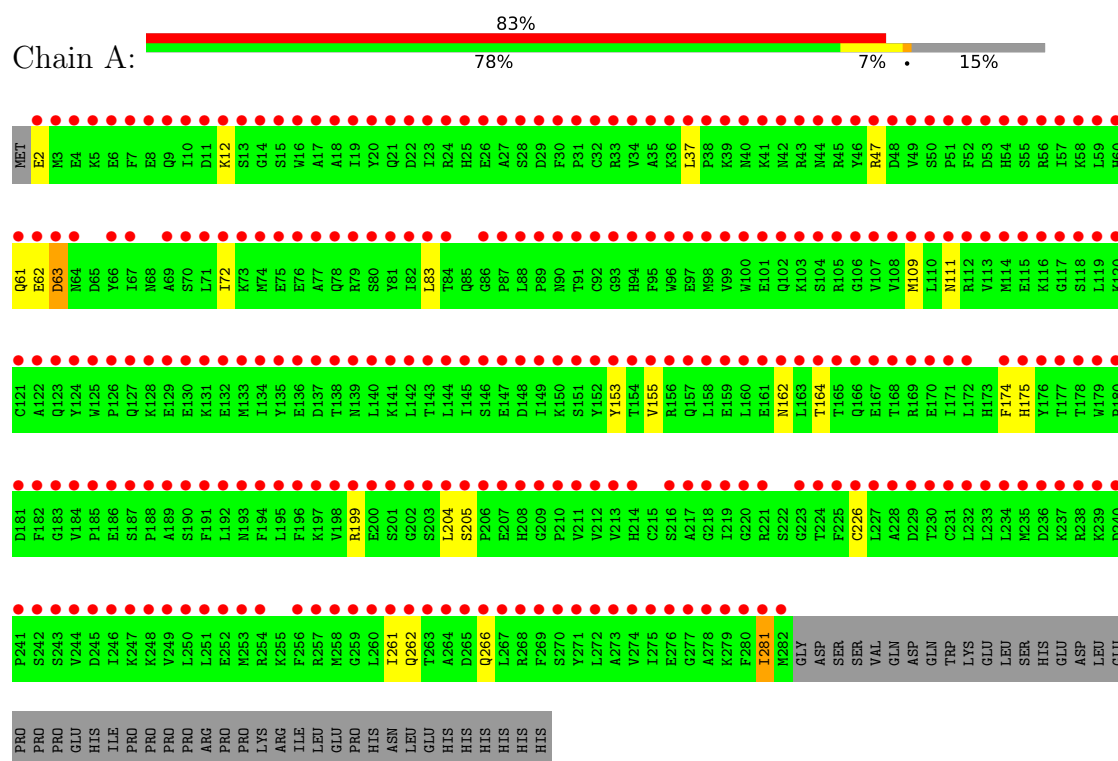
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	352	Total	O	0	0
			352	352		

3 Residue-property plots

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: Tyrosine-protein phosphatase non-receptor type 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.20Å 89.20Å 105.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.25 – 2.08 77.25 – 2.08	Depositor EDS
% Data completeness (in resolution range)	96.0 (77.25-2.08) 96.0 (77.25-2.08)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.08Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.255 , 0.291 0.259 , 0.307	Depositor DCC
R_{free} test set	1362 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	2.9	Xtriage
Anisotropy	6.996	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	2709	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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

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	0.44	0/2440	0.71	3/3284 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	281	ILE	N-CA-C	5.27	111.85	106.21
1	A	205	SER	CA-C-N	5.15	125.45	119.47
1	A	205	SER	C-N-CA	5.15	125.45	119.47

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	2356	0	2354	11	0
2	A	1	0	0	0	0
3	A	352	0	0	0	0
All	All	2709	0	2354	11	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 2.

All (11) 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:262:GLN:H	1:A:266:GLN:NE2	1.97	0.63
1:A:83:LEU:HD11	1:A:226[A]:CYS:SG	2.49	0.53
1:A:162:ASN:OD1	1:A:164:THR:HG22	2.13	0.49
1:A:111:ASN:O	1:A:175:HIS:HE1	1.96	0.48
1:A:281:ILE:O	1:A:281:ILE:HG23	2.13	0.48
1:A:62:GLU:O	1:A:63:ASP:CB	2.63	0.45
1:A:262:GLN:H	1:A:266:GLN:HE22	1.66	0.43
1:A:199:ARG:HG2	1:A:204:LEU:HD12	2.01	0.43
1:A:109:MET:HE2	1:A:111:ASN:O	2.19	0.42
1:A:153:TYR:CE2	1:A:155:VAL:HG23	2.56	0.41
1:A:155:VAL:HG22	1:A:174:PHE:CD1	2.55	0.41

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	289/329 (88%)	275 (95%)	11 (4%)	3 (1%)	12 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	61	GLN
1	A	261	ILE

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	266/302 (88%)	261 (98%)	5 (2%)	50 56

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	12	LYS
1	A	37	LEU
1	A	47	ARG
1	A	72	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	A	193	ASN
1	A	266	GLN

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

Of 1 ligands modelled in this entry, 1 is 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	281/329 (85%)	5.23	274 (97%) 0 0	20, 40, 76, 118	12 (4%)

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	PHE	15.1
1	A	281	ILE	14.5
1	A	282[A]	MET	14.0
1	A	63	ASP	12.4
1	A	5	LYS	12.2
1	A	7	PHE	11.3
1	A	164	THR	10.9
1	A	12	LYS	10.4
1	A	25	HIS	10.3
1	A	4	GLU	10.0
1	A	62	GLU	9.7
1	A	41	LYS	9.5
1	A	165	THR	9.2
1	A	2	GLU	9.1
1	A	13	SER	9.0
1	A	47	ARG	8.8
1	A	239	LYS	8.8
1	A	61	GLN	8.7
1	A	16	TRP	8.7
1	A	19	ILE	8.5
1	A	10	ILE	8.5
1	A	279	LYS	8.4
1	A	3[A]	MET	8.3
1	A	196	PHE	8.3
1	A	42	ASN	8.2
1	A	272	LEU	8.1
1	A	150	LYS	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	15	SER	7.9
1	A	140	LEU	7.8
1	A	135	TYR	7.8
1	A	17	ALA	7.7
1	A	149	ILE	7.6
1	A	136	GLU	7.5
1	A	233	LEU	7.5
1	A	18	ALA	7.4
1	A	276	GLU	7.4
1	A	247	LYS	7.4
1	A	275	ILE	7.3
1	A	11	ASP	7.3
1	A	186	GLU	7.3
1	A	9[A]	GLN	7.3
1	A	204	LEU	7.3
1	A	162	ASN	7.3
1	A	33[A]	ARG	7.2
1	A	14	GLY	7.2
1	A	155	VAL	7.2
1	A	6	GLU	7.0
1	A	139	ASN	7.0
1	A	151	SER	7.0
1	A	24	ARG	7.0
1	A	152	TYR	7.0
1	A	73	LYS	7.0
1	A	131	LYS	7.0
1	A	160	LEU	7.0
1	A	37	LEU	6.9
1	A	163	LEU	6.9
1	A	138	THR	6.9
1	A	34	VAL	6.8
1	A	153	TYR	6.8
1	A	182	PHE	6.7
1	A	242	SER	6.7
1	A	240	ASP	6.7
1	A	168	THR	6.7
1	A	191	PHE	6.7
1	A	166	GLN	6.7
1	A	23	ILE	6.6
1	A	237	LYS	6.6
1	A	271	TYR	6.6
1	A	195	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	26	GLU	6.6
1	A	60	HIS	6.5
1	A	206	PRO	6.5
1	A	137	ASP	6.5
1	A	128	LYS	6.4
1	A	180	PRO	6.4
1	A	20	TYR	6.4
1	A	145	ILE	6.4
1	A	8	GLU	6.3
1	A	75	GLU	6.3
1	A	118	SER	6.3
1	A	107	VAL	6.3
1	A	127	GLN	6.2
1	A	157	GLN	6.2
1	A	148	ASP	6.2
1	A	124	TYR	6.2
1	A	232	LEU	6.2
1	A	244	VAL	6.2
1	A	77	ALA	6.1
1	A	246	ILE	6.1
1	A	218	GLY	6.1
1	A	248	LYS	6.1
1	A	122	ALA	6.1
1	A	141	LYS	6.1
1	A	189	ALA	6.1
1	A	179	TRP	6.0
1	A	197	LYS	6.0
1	A	243	SER	6.0
1	A	241	PRO	6.0
1	A	184	VAL	5.9
1	A	278	ALA	5.8
1	A	134	ILE	5.8
1	A	236	ASP	5.8
1	A	263	THR	5.8
1	A	36	LYS	5.8
1	A	90[A]	ASN	5.7
1	A	234	LEU	5.7
1	A	78	GLN	5.7
1	A	260	LEU	5.6
1	A	142	LEU	5.6
1	A	144	LEU	5.6
1	A	100	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	5.6
1	A	274	VAL	5.6
1	A	46	TYR	5.5
1	A	192	LEU	5.5
1	A	59	LEU	5.5
1	A	106	GLY	5.4
1	A	188	PRO	5.4
1	A	22[A]	ASP	5.4
1	A	265	ASP	5.4
1	A	119	LEU	5.4
1	A	183	GLY	5.4
1	A	273	ALA	5.3
1	A	211	VAL	5.3
1	A	177	THR	5.3
1	A	48	ASP	5.3
1	A	57	ILE	5.3
1	A	245	ASP	5.2
1	A	185	PRO	5.2
1	A	43	ARG	5.2
1	A	187	SER	5.1
1	A	87	PRO	5.1
1	A	110	LEU	5.0
1	A	181	ASP	4.9
1	A	270	SER	4.9
1	A	31	PRO	4.9
1	A	202	GLY	4.9
1	A	251	LEU	4.9
1	A	207	GLU	4.9
1	A	203	SER	4.9
1	A	167[A]	GLU	4.8
1	A	125	TRP	4.8
1	A	249	VAL	4.8
1	A	29[A]	ASP	4.8
1	A	267	LEU	4.7
1	A	86	GLY	4.7
1	A	82	ILE	4.7
1	A	205	SER	4.6
1	A	108	VAL	4.6
1	A	96	TRP	4.6
1	A	120	LYS	4.6
1	A	21[A]	GLN	4.6
1	A	269	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	66	TYR	4.5
1	A	193	ASN	4.5
1	A	190	SER	4.4
1	A	133	MET	4.4
1	A	259	GLY	4.4
1	A	170	GLU	4.4
1	A	256	PHE	4.4
1	A	228	ALA	4.4
1	A	238	ARG	4.3
1	A	38	PRO	4.3
1	A	212	VAL	4.3
1	A	147	GLU	4.3
1	A	171	ILE	4.3
1	A	176	TYR	4.3
1	A	89	PRO	4.3
1	A	250	LEU	4.3
1	A	44	ASN	4.3
1	A	262	GLN	4.3
1	A	45	ARG	4.2
1	A	227	LEU	4.2
1	A	28	SER	4.2
1	A	161	GLU	4.2
1	A	121	CYS	4.1
1	A	58	LYS	4.1
1	A	35	ALA	4.1
1	A	112	ARG	4.1
1	A	268	ARG	4.1
1	A	194	PHE	4.1
1	A	219	ILE	4.1
1	A	261	ILE	4.1
1	A	178	THR	4.1
1	A	266	GLN	4.1
1	A	217	ALA	4.0
1	A	30	PHE	4.0
1	A	95	PHE	4.0
1	A	146	SER	4.0
1	A	88	LEU	4.0
1	A	67	ILE	4.0
1	A	72	ILE	4.0
1	A	169	ARG	4.0
1	A	116	LYS	3.9
1	A	49	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	83	LEU	3.9
1	A	208	HIS	3.9
1	A	53	ASP	3.9
1	A	71	LEU	3.9
1	A	159	GLU	3.9
1	A	258	MET	3.9
1	A	213	VAL	3.8
1	A	123	GLN	3.8
1	A	158	LEU	3.8
1	A	175	HIS	3.8
1	A	154	THR	3.8
1	A	114	MET	3.8
1	A	111	ASN	3.7
1	A	174	PHE	3.7
1	A	79	ARG	3.7
1	A	80	SER	3.7
1	A	69	ALA	3.7
1	A	223	GLY	3.6
1	A	198	VAL	3.6
1	A	74	MET	3.6
1	A	216	SER	3.6
1	A	199	ARG	3.6
1	A	200	GLU	3.5
1	A	99	VAL	3.4
1	A	52	PHE	3.4
1	A	94	HIS	3.4
1	A	235[A]	MET	3.4
1	A	54	HIS	3.3
1	A	132	GLU	3.3
1	A	143	THR	3.3
1	A	50	SER	3.3
1	A	129	GLU	3.3
1	A	113	VAL	3.3
1	A	39	LYS	3.3
1	A	277	GLY	3.3
1	A	126	PRO	3.2
1	A	156	ARG	3.2
1	A	230	THR	3.2
1	A	81	TYR	3.2
1	A	32	CYS	3.2
1	A	264	ALA	3.1
1	A	105	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	109	MET	3.1
1	A	103	LYS	3.1
1	A	172	LEU	3.1
1	A	40	ASN	3.0
1	A	210	PRO	3.0
1	A	221	ARG	3.0
1	A	117	GLY	3.0
1	A	224	THR	2.9
1	A	93	GLY	2.9
1	A	226[A]	CYS	2.9
1	A	231	CYS	2.9
1	A	220	GLY	2.9
1	A	102	GLN	2.8
1	A	91	THR	2.8
1	A	56	ARG	2.7
1	A	51	PRO	2.7
1	A	254	ARG	2.7
1	A	130	GLU	2.7
1	A	225	PHE	2.7
1	A	84	THR	2.7
1	A	101	GLU	2.7
1	A	252	GLU	2.7
1	A	214	HIS	2.7
1	A	253	MET	2.7
1	A	97	GLU	2.6
1	A	76	GLU	2.5
1	A	104	SER	2.5
1	A	115	GLU	2.5
1	A	92	CYS	2.5
1	A	257	ARG	2.5
1	A	55	SER	2.5
1	A	98	MET	2.4
1	A	229	ASP	2.4
1	A	70	SER	2.3
1	A	201	SER	2.3
1	A	209	GLY	2.1
1	A	64	ASN	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 [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	MG	A	401	1/1	0.77	0.18	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.