



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:59 AM UTC

PDB ID : 1YXV / pdb_00001yxv
Title : Crystal Structure of Kinase Pim1 in complex with 3,4-Dihydroxy-1-methylqu
inolin-2(1H)-one
Authors : Kumar, A.; Mandiyan, V.; Suzuki, Y.; Zhang, C.; Rice, J.; Tsai, J.; Artis,
D.R.; Ibrahim, P.; Bremer, R.
Deposited on : 2005-02-22
Resolution : 2.00 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
Mogul : 2022.3.0, CSD as543be (2022)
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

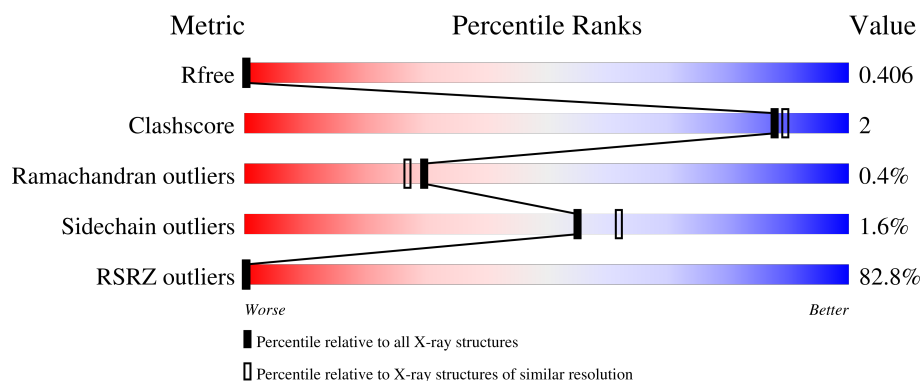
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	293	77% 86% 6% • 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2436 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.

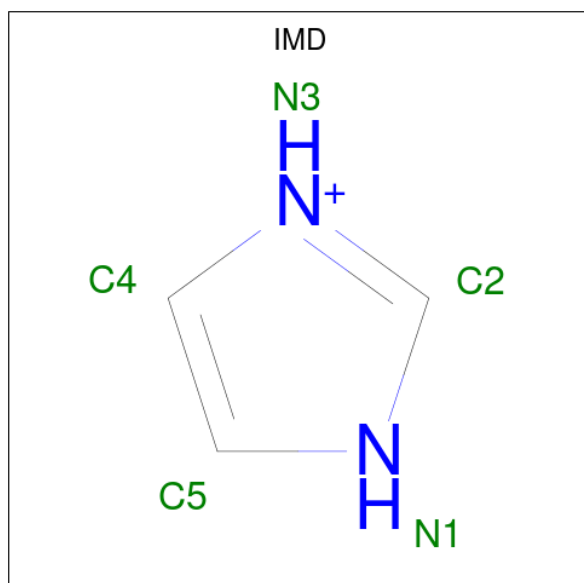
- Molecule 1 is a protein called Proto-oncogene serine/threonine-protein kinase Pim-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	274	2247	1435	393	411	8	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

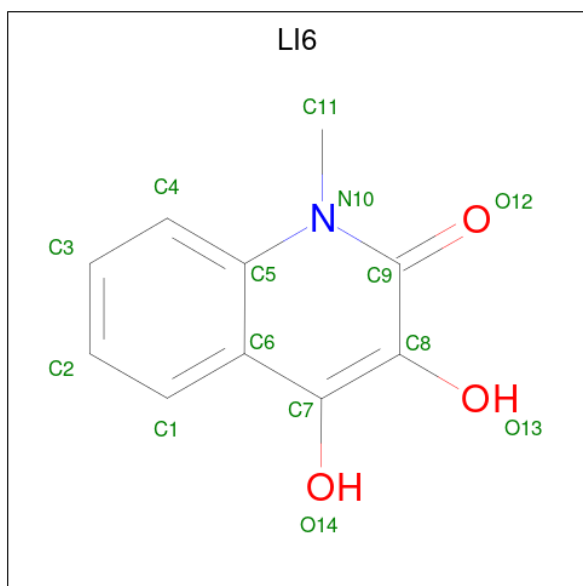
Chain	Residue	Modelled	Actual	Comment	Reference
A	314	VAL	-	expression tag	UNP P11309
A	315	ASP	-	expression tag	UNP P11309
A	316	HIS	-	expression tag	UNP P11309
A	317	HIS	-	expression tag	UNP P11309
A	318	HIS	-	expression tag	UNP P11309
A	319	HIS	-	expression tag	UNP P11309
A	320	HIS	-	expression tag	UNP P11309
A	321	HIS	-	expression tag	UNP P11309

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N		
			5	3	2	0	0

- Molecule 3 is 3,4-DIHYDROXY-1-METHYLQUINOLIN-2(1H)-ONE (CCD ID: LI6) (formula: C₁₀H₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O		
			14	10	1	3	0	0

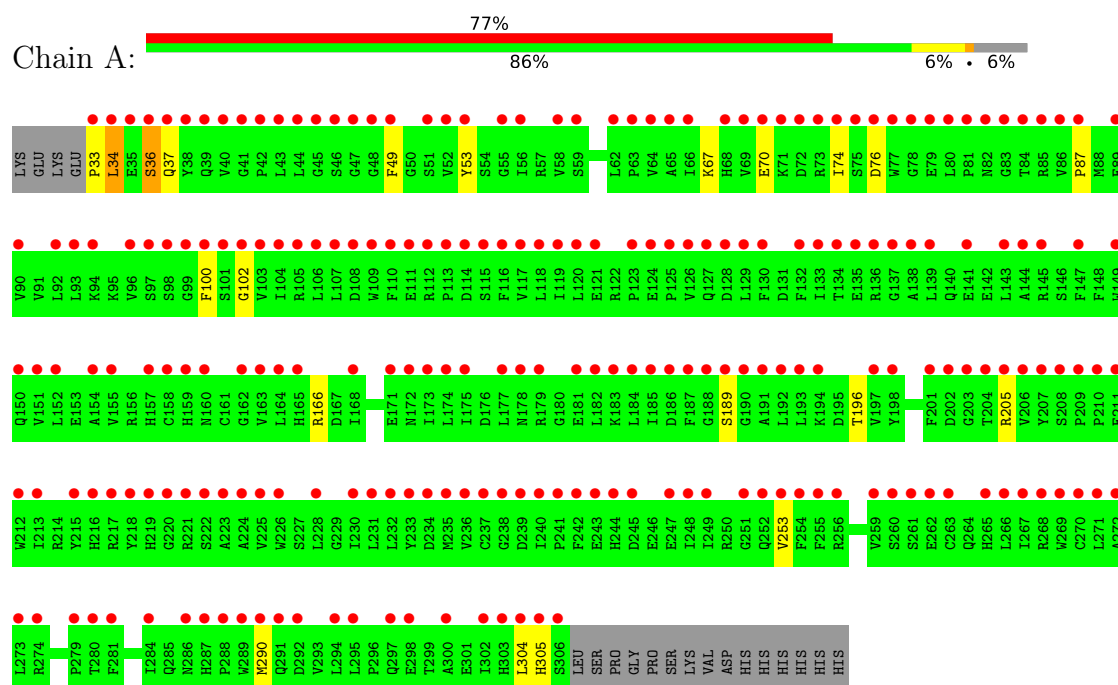
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total	O		
			170	170	0	0

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: Proto-oncogene serine/threonine-protein kinase Pim-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	96.59Å 96.59Å 80.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.51 – 2.00 83.65 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (84.51-2.00) 99.5 (83.65-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.188 , 0.211 0.410 , 0.406	Depositor DCC
R_{free} test set	1495 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	2436	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: IMD, LI6

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	0.57	0/2307	0.86	1/3131 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	SER	N-CA-C	-6.08	106.00	113.41

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	2247	0	2185	9	2
2	A	5	0	5	0	0
3	A	14	0	7	0	0
4	A	170	0	0	2	1
All	All	2436	0	2197	9	2

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 (9) 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:33:PRO:HA	1:A:37:GLN:HE21	1.38	0.89
1:A:166:ARG:HD3	1:A:189:SER:O	2.04	0.57
1:A:33:PRO:O	1:A:34:LEU:CB	2.60	0.49
1:A:100:PHE:CZ	1:A:102:GLY:HA3	2.48	0.49
1:A:253:VAL:HG23	4:A:489:HOH:O	2.15	0.46
1:A:74:ILE:HD13	1:A:87:PRO:HG3	1.97	0.45
1:A:49:PHE:O	1:A:67:LYS:HE2	2.17	0.44
1:A:305:HIS:CG	1:A:305:HIS:O	2.71	0.44
1:A:205:ARG:NH2	4:A:416:HOH:O	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:OE2	1:A:196:THR:OG1[5_665]	1.94	0.26
1:A:53:TYR:OH	4:A:457:HOH:O[5_665]	1.96	0.24

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	274/293 (94%)	265 (97%)	8 (3%)	1 (0%)	30 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	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	247/263 (94%)	243 (98%)	4 (2%)	55 62

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	76	ASP
1	A	290	MET
1	A	304	LEU

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	37	GLN
1	A	291	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 [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	LI6	A	323	-	15,15,15	3.73	4 (26%)	19,22,22	1.50	4 (21%)
2	IMD	A	322	-	5,5,5	0.61	0	5,5,5	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LI6	A	323	-	-	-	0/2/2/2
2	IMD	A	322	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	323	LI6	C8-C7	12.36	1.48	1.36
3	A	323	LI6	C6-C5	5.37	1.49	1.41
3	A	323	LI6	C8-C9	3.41	1.49	1.45
3	A	323	LI6	C9-N10	3.09	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	323	LI6	O12-C9-C8	-3.32	118.43	122.96
3	A	323	LI6	O13-C8-C9	2.98	121.24	116.08
3	A	323	LI6	C11-N10-C9	2.75	119.99	117.34
3	A	323	LI6	O14-C7-C6	2.10	119.85	115.69

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	274/293 (93%)	3.26	227 (82%) 0 0	10, 22, 40, 50	2 (0%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	VAL	8.5
1	A	58	VAL	8.2
1	A	34	LEU	7.1
1	A	64	VAL	6.9
1	A	48	GLY	6.6
1	A	42	PRO	6.6
1	A	76	ASP	6.1
1	A	178	ASN	6.0
1	A	100	PHE	6.0
1	A	74	ILE	5.9
1	A	41	GLY	5.7
1	A	126	VAL	5.7
1	A	306	SER	5.6
1	A	254	PHE	5.5
1	A	155	VAL	5.5
1	A	45	GLY	5.4
1	A	80	LEU	5.4
1	A	98	SER	5.4
1	A	213	ILE	5.4
1	A	249	ILE	5.3
1	A	44	LEU	5.3
1	A	69	VAL	5.3
1	A	116	PHE	5.3
1	A	96	VAL	5.2
1	A	77	TRP	5.2
1	A	204	THR	5.2
1	A	47	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	110	PHE	5.0
1	A	49	PHE	4.9
1	A	81	PRO	4.9
1	A	113	PRO	4.9
1	A	72	ASP	4.9
1	A	38	TYR	4.9
1	A	93	LEU	4.9
1	A	102	GLY	4.8
1	A	52	VAL	4.8
1	A	62	LEU	4.7
1	A	305	HIS	4.6
1	A	164	LEU	4.6
1	A	177	LEU	4.6
1	A	90	VAL	4.6
1	A	56	ILE	4.6
1	A	86	VAL	4.5
1	A	202	ASP	4.5
1	A	151	VAL	4.5
1	A	33	PRO	4.5
1	A	252[A]	GLN	4.5
1	A	83	GLY	4.5
1	A	63	PRO	4.5
1	A	84	THR	4.4
1	A	201	PHE	4.4
1	A	175	ILE	4.4
1	A	215	TYR	4.4
1	A	144	ALA	4.4
1	A	147	PHE	4.3
1	A	190	GLY	4.3
1	A	267	ILE	4.3
1	A	207	TYR	4.3
1	A	223	ALA	4.2
1	A	255	PHE	4.2
1	A	231	LEU	4.2
1	A	99	GLY	4.2
1	A	191	ALA	4.2
1	A	85	ARG	4.2
1	A	304	LEU	4.1
1	A	150	GLN	4.1
1	A	73	ARG	4.1
1	A	188	GLY	4.1
1	A	51	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	273	LEU	4.0
1	A	107	LEU	4.0
1	A	104	ILE	4.0
1	A	133	ILE	4.0
1	A	163	VAL	3.9
1	A	35	GLU	3.9
1	A	271	LEU	3.9
1	A	53	TYR	3.9
1	A	120	LEU	3.9
1	A	186[A]	ASP	3.8
1	A	46	SER	3.8
1	A	75	SER	3.8
1	A	103	VAL	3.8
1	A	182	LEU	3.8
1	A	272	ALA	3.8
1	A	288	PRO	3.8
1	A	189	SER	3.7
1	A	197	VAL	3.7
1	A	125	PRO	3.7
1	A	117	VAL	3.7
1	A	289	TRP	3.7
1	A	187	PHE	3.7
1	A	300	ALA	3.7
1	A	192	LEU	3.6
1	A	114	ASP	3.6
1	A	168	ILE	3.6
1	A	240	ILE	3.6
1	A	212	TRP	3.6
1	A	216	HIS	3.6
1	A	59	SER	3.6
1	A	134	THR	3.6
1	A	87	PRO	3.6
1	A	106	LEU	3.5
1	A	55	GLY	3.5
1	A	109	TRP	3.5
1	A	244	HIS	3.5
1	A	233	TYR	3.5
1	A	291	GLN	3.5
1	A	92	LEU	3.5
1	A	205	ARG	3.4
1	A	37	GLN	3.4
1	A	281	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	111	GLU	3.4
1	A	173	ILE	3.4
1	A	222	SER	3.4
1	A	248	ILE	3.4
1	A	39	GLN	3.4
1	A	101	SER	3.3
1	A	65	ALA	3.3
1	A	226	TRP	3.3
1	A	235	MET	3.3
1	A	152	LEU	3.3
1	A	158	CYS	3.2
1	A	108	ASP	3.2
1	A	127	GLN	3.2
1	A	79	GLU	3.2
1	A	206	VAL	3.2
1	A	174	LEU	3.2
1	A	143	LEU	3.1
1	A	97	SER	3.1
1	A	132	PHE	3.1
1	A	82	ASN	3.1
1	A	171	GLU	3.1
1	A	243	GLU	3.1
1	A	295	LEU	3.1
1	A	124	GLU	3.0
1	A	135	GLU	3.0
1	A	130	PHE	3.0
1	A	239	ASP	3.0
1	A	237	CYS	3.0
1	A	68	HIS	3.0
1	A	66	ILE	3.0
1	A	149	TRP	3.0
1	A	230	ILE	2.9
1	A	179	ARG	2.9
1	A	232	LEU	2.9
1	A	225	VAL	2.9
1	A	236	VAL	2.9
1	A	165	HIS	2.9
1	A	203	GLY	2.9
1	A	266	LEU	2.8
1	A	294	LEU	2.8
1	A	137	GLY	2.8
1	A	162	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	89	GLU	2.8
1	A	247	GLU	2.8
1	A	241	PRO	2.8
1	A	260	SER	2.8
1	A	221	ARG	2.8
1	A	238	GLY	2.8
1	A	118	LEU	2.8
1	A	228	LEU	2.8
1	A	302	ILE	2.8
1	A	105	ARG	2.8
1	A	265	HIS	2.8
1	A	78	GLY	2.8
1	A	269	TRP	2.8
1	A	219	HIS	2.7
1	A	287	HIS	2.7
1	A	154	ALA	2.7
1	A	129	LEU	2.7
1	A	112	ARG	2.7
1	A	280	THR	2.7
1	A	279	PRO	2.7
1	A	36	SER	2.7
1	A	242	PHE	2.7
1	A	172	ASN	2.7
1	A	115	SER	2.7
1	A	185	ILE	2.7
1	A	263	CYS	2.7
1	A	290	MET	2.6
1	A	209	PRO	2.6
1	A	70	GLU	2.6
1	A	71	LYS	2.6
1	A	136	ARG	2.6
1	A	284	ILE	2.6
1	A	138	ALA	2.6
1	A	119	ILE	2.6
1	A	297	GLN	2.5
1	A	259	VAL	2.5
1	A	224	ALA	2.5
1	A	123	PRO	2.5
1	A	210	PRO	2.5
1	A	217	ARG	2.5
1	A	218	TYR	2.5
1	A	139	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	251	GLY	2.5
1	A	160	ASN	2.5
1	A	128	ASP	2.4
1	A	253	VAL	2.4
1	A	256	ARG	2.4
1	A	193	LEU	2.4
1	A	141	GLU	2.4
1	A	181	GLU	2.4
1	A	157	HIS	2.4
1	A	286	ASN	2.3
1	A	268	ARG	2.3
1	A	184	LEU	2.3
1	A	270	CYS	2.3
1	A	292	ASP	2.3
1	A	234	ASP	2.3
1	A	198	TYR	2.3
1	A	211	GLU	2.2
1	A	145	ARG	2.2
1	A	245	ASP	2.2
1	A	208	SER	2.2
1	A	262	GLU	2.2
1	A	298	GLU	2.2
1	A	220	GLY	2.2
1	A	194	LYS	2.1
1	A	159	HIS	2.1
1	A	303	HIS	2.1
1	A	183	LYS	2.1
1	A	121	GLU	2.1
1	A	274	ARG	2.1
1	A	94	LYS	2.0
1	A	261	SER	2.0
1	A	43	LEU	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 ⓘ

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	LI6	A	323	14/14	0.51	0.34	43,45,45,47	0
2	IMD	A	322	5/5	0.78	0.25	43,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.