



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:51 PM UTC

PDB ID : 4U04 / pdb_00004u04
Title : Structure of a eukaryotic fic domain containing protein
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Deposited on : 2014-07-11
Resolution : 2.48 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

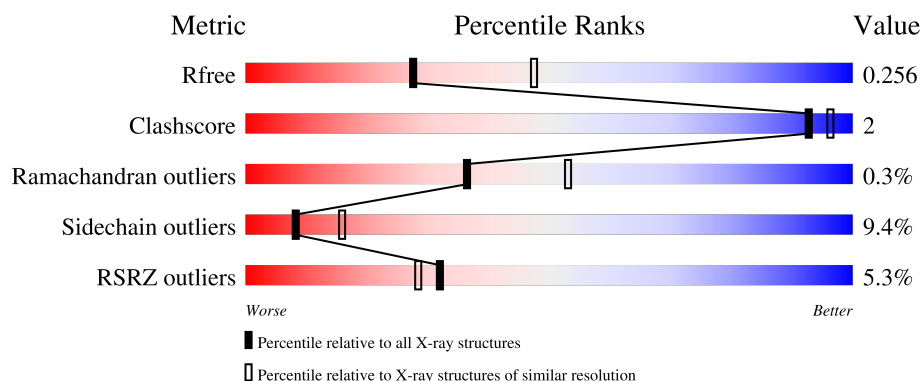
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	344	3% 82% 9% 8%
1	B	344	7% 82% 11% 6%

2 Entry composition [i](#)

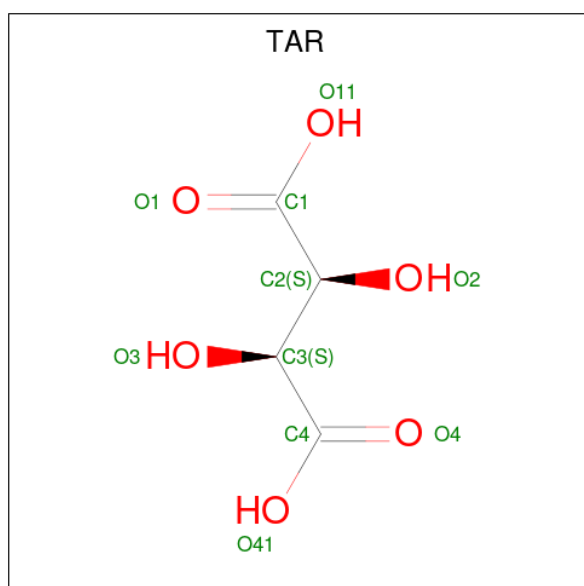
There are 4 unique types of molecules in this entry. The entry contains 5184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosine monophosphate-protein transferase FICD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2459	1573	420	457	9			
1	B	324	Total	C	N	O	S	0	0	0
			2531	1614	441	466	10			

- Molecule 2 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		

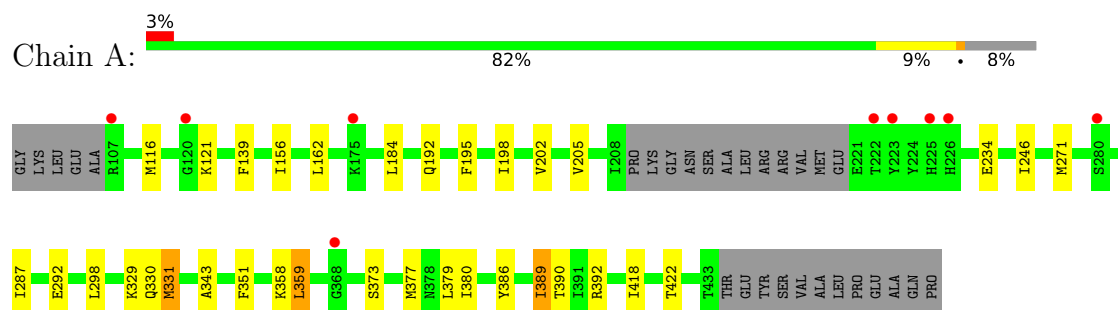
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	60	Total	O	0	0
			60	60		

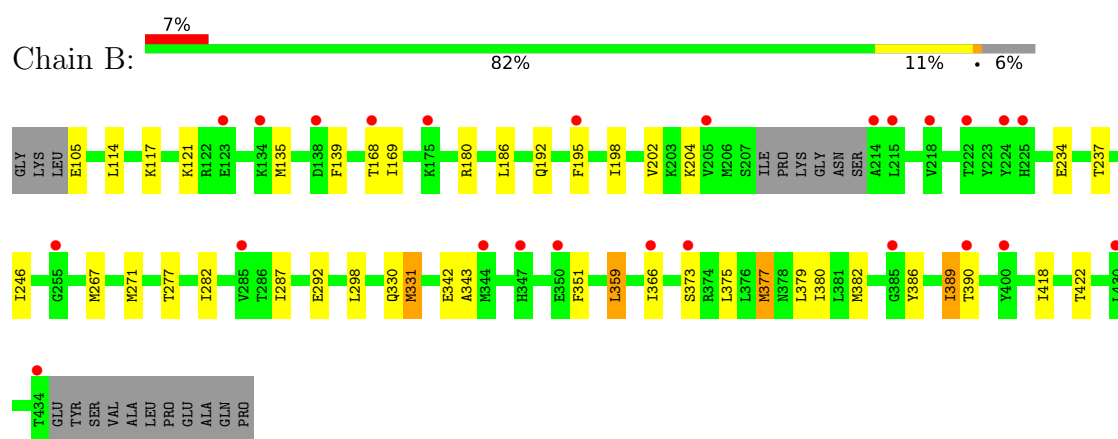
3 Residue-property plots [i](#)

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: Adenosine monophosphate-protein transferase FICD



• Molecule 1: Adenosine monophosphate-protein transferase FICD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.19Å 76.81Å 93.19Å 90.00° 108.05° 90.00°	Depositor
Resolution (Å)	43.81 – 2.48 43.81 – 2.48	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.81-2.48) 97.7 (43.81-2.48)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.218 , 0.245 0.234 , 0.256	Depositor DCC
R_{free} test set	1688 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5184	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAR, PG4

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	0.84	2/2514 (0.1%)	1.18	4/3421 (0.1%)
1	B	0.84	3/2586 (0.1%)	1.17	2/3516 (0.1%)
All	All	0.84	5/5100 (0.1%)	1.17	6/6937 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	MET	SD-CE	-9.51	1.55	1.79
1	A	331	MET	SD-CE	-7.93	1.59	1.79
1	B	331	MET	SD-CE	-7.84	1.59	1.79
1	B	377	MET	SD-CE	-7.25	1.61	1.79
1	B	382	MET	SD-CE	-5.67	1.65	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	195	PHE	CA-CB-CG	5.89	119.69	113.80
1	B	195	PHE	CA-CB-CG	5.82	119.62	113.80
1	B	139	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	392	ARG	CA-C-N	5.14	127.42	120.38
1	A	392	ARG	C-N-CA	5.14	127.42	120.38

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	2459	0	2341	7	0
1	B	2531	0	2429	8	0
2	A	10	0	4	0	0
3	A	13	0	18	1	0
3	B	13	0	18	0	0
4	A	98	0	0	0	0
4	B	60	0	0	0	0
All	All	5184	0	4810	15	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 (15) 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:202:VAL:HG21	1:A:386:TYR:CE2	2.41	0.56
1:A:418:ILE:O	1:A:422:THR:HG23	2.12	0.50
1:B:389:ILE:HG12	1:B:422:THR:HG22	1.94	0.49
1:A:389:ILE:HG12	1:A:422:THR:HG22	1.94	0.49
1:B:202:VAL:HG21	1:B:386:TYR:CE2	2.49	0.47
1:A:358:LYS:HE3	3:A:502:PG4:H71	1.97	0.47
1:B:377:MET:CE	1:B:418:ILE:HG23	2.46	0.46
1:B:418:ILE:O	1:B:422:THR:HG23	2.18	0.44
1:A:198:ILE:O	1:A:202:VAL:HG23	2.18	0.44
1:A:359:LEU:HD12	1:A:373:SER:HB3	2.00	0.43
1:A:343:ALA:HB1	1:A:351:PHE:CE1	2.54	0.43
1:B:343:ALA:HB1	1:B:351:PHE:CE1	2.54	0.42
1:B:359:LEU:HD12	1:B:373:SER:HB3	2.01	0.42
1:B:198:ILE:O	1:B:202:VAL:HG23	2.21	0.41
1:B:267:MET:HE1	1:B:375:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	311/344 (90%)	306 (98%)	4 (1%)	1 (0%)	36	53
1	B	320/344 (93%)	315 (98%)	4 (1%)	1 (0%)	36	53
All	All	631/688 (92%)	621 (98%)	8 (1%)	2 (0%)	36	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	LYS
1	A	121	LYS

5.3.2 Protein sidechains

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	249/302 (82%)	229 (92%)	20 (8%)	11	21
1	B	259/302 (86%)	231 (89%)	28 (11%)	6	11
All	All	508/604 (84%)	460 (91%)	48 (9%)	8	16

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	MET
1	A	156	ILE
1	A	162	LEU
1	A	184	LEU

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Mol	Chain	Res	Type
1	A	192	GLN
1	A	205	VAL
1	A	234	GLU
1	A	246	ILE
1	A	271	MET
1	A	287	ILE
1	A	292	GLU
1	A	298	LEU
1	A	329	LYS
1	A	330	GLN
1	A	331	MET
1	A	359	LEU
1	A	379	LEU
1	A	380	ILE
1	A	389	ILE
1	A	390	THR
1	B	105	GLU
1	B	114	LEU
1	B	117	LYS
1	B	135	MET
1	B	168	THR
1	B	169	ILE
1	B	180	ARG
1	B	186	LEU
1	B	192	GLN
1	B	204	LYS
1	B	234	GLU
1	B	237	THR
1	B	246	ILE
1	B	271	MET
1	B	277	THR
1	B	282	ILE
1	B	287	ILE
1	B	292	GLU
1	B	298	LEU
1	B	330	GLN
1	B	331	MET
1	B	342	GLU
1	B	359	LEU
1	B	366	ILE
1	B	379	LEU
1	B	380	ILE

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Mol	Chain	Res	Type
1	B	389	ILE
1	B	390	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS
1	A	319	HIS
1	B	245	HIS
1	B	275	ASN
1	B	319	HIS
1	B	401	HIS

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](#)

3 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	PG4	A	502	-	12,12,12	0.58	0	11,11,11	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PG4	B	501	-	12,12,12	0.51	0	11,11,11	0.21	0
2	TAR	A	501	-	9,9,9	1.11	0	12,12,12	1.23	2 (16%)

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	PG4	A	502	-	-	8/10/10/10	-
3	PG4	B	501	-	-	5/10/10/10	-
2	TAR	A	501	-	-	7/12/12/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	TAR	O11-C1-C2	2.43	120.05	113.31
2	A	501	TAR	O41-C4-C3	2.09	119.13	113.31

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	TAR	O3-C3-C4-O4
2	A	501	TAR	O3-C3-C4-O41
3	B	501	PG4	O3-C5-C6-O4
3	A	502	PG4	O1-C1-C2-O2
3	B	501	PG4	O1-C1-C2-O2
2	A	501	TAR	C2-C3-C4-O4
3	A	502	PG4	O4-C7-C8-O5
2	A	501	TAR	C2-C3-C4-O41
3	B	501	PG4	C5-C6-O4-C7
3	A	502	PG4	C3-C4-O3-C5
3	B	501	PG4	C8-C7-O4-C6
3	A	502	PG4	O2-C3-C4-O3
3	A	502	PG4	C1-C2-O2-C3
2	A	501	TAR	C1-C2-C3-O3
3	A	502	PG4	C5-C6-O4-C7
2	A	501	TAR	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	B	501	PG4	O2-C3-C4-O3
2	A	501	TAR	C1-C2-C3-C4
3	A	502	PG4	C4-C3-O2-C2
3	A	502	PG4	O3-C5-C6-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	315/344 (91%)	0.37	9 (2%) 53 50	37, 70, 115, 129	0
1	B	324/344 (94%)	0.65	25 (7%) 19 17	57, 84, 128, 182	0
All	All	639/688 (92%)	0.51	34 (5%) 32 28	37, 77, 124, 182	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	ALA	3.8
1	B	168	THR	3.8
1	B	390	THR	3.7
1	A	368	GLY	3.6
1	B	434	THR	3.2
1	B	195	PHE	3.2
1	A	223	TYR	3.0
1	B	218	VAL	2.8
1	B	175	LYS	2.7
1	B	385	GLY	2.7
1	B	255	GLY	2.6
1	A	120	GLY	2.6
1	B	224	TYR	2.6
1	A	107	ARG	2.5
1	B	138	ASP	2.5
1	A	222	THR	2.5
1	B	400	TYR	2.5
1	B	222	THR	2.4
1	A	226	HIS	2.4
1	B	215	LEU	2.3
1	A	175	LYS	2.3
1	B	350	GLU	2.3
1	B	123	GLU	2.3
1	A	225	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	366	ILE	2.2
1	A	280	SER	2.2
1	B	430	LEU	2.2
1	B	205	VAL	2.1
1	B	285	VAL	2.1
1	B	225	HIS	2.1
1	B	347	HIS	2.1
1	B	373	SER	2.0
1	B	134	LYS	2.0
1	B	344	MET	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
2	TAR	A	501	10/10	0.65	0.17	112,116,119,120	0
3	PG4	B	501	13/13	0.82	0.17	88,94,99,100	0
3	PG4	A	502	13/13	0.87	0.13	68,82,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.