



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:08 PM UTC

PDB ID : 3T2F / pdb_00003t2f
Title : Fructose-1,6-bisphosphate aldolase/phosphatase from *Thermoproteus neutrophilus*, soaked with EDTA and DHAP
Authors : Du, J.; Say, R.; Lue, W.; Fuchs, G.; Einsle, O.
Deposited on : 2011-07-22
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

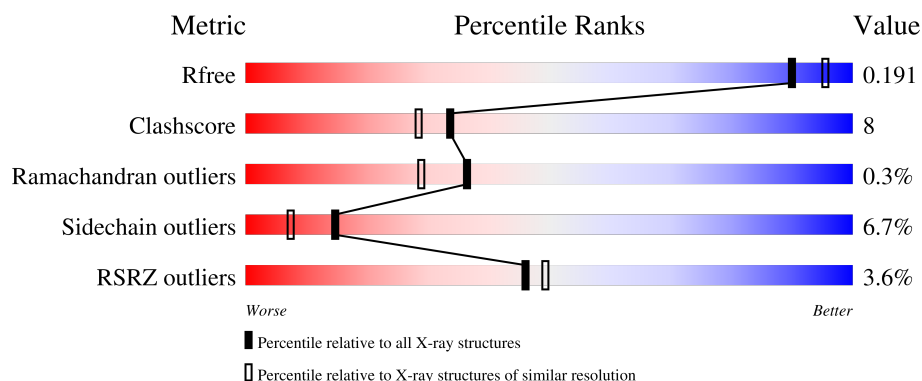
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

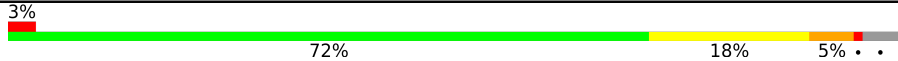
The reported resolution of this entry is 1.90 Å.

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))
R_{free}	180053	7789 (1.90-1.90)
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	407	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3223 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 Fructose-1,6-bisphosphate aldolase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			3061	1973	525	550	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	LEU	-	expression tag	UNP B1YAL1
A	401	GLU	-	expression tag	UNP B1YAL1
A	402	HIS	-	expression tag	UNP B1YAL1
A	403	HIS	-	expression tag	UNP B1YAL1
A	404	HIS	-	expression tag	UNP B1YAL1
A	405	HIS	-	expression tag	UNP B1YAL1
A	406	HIS	-	expression tag	UNP B1YAL1
A	407	HIS	-	expression tag	UNP B1YAL1

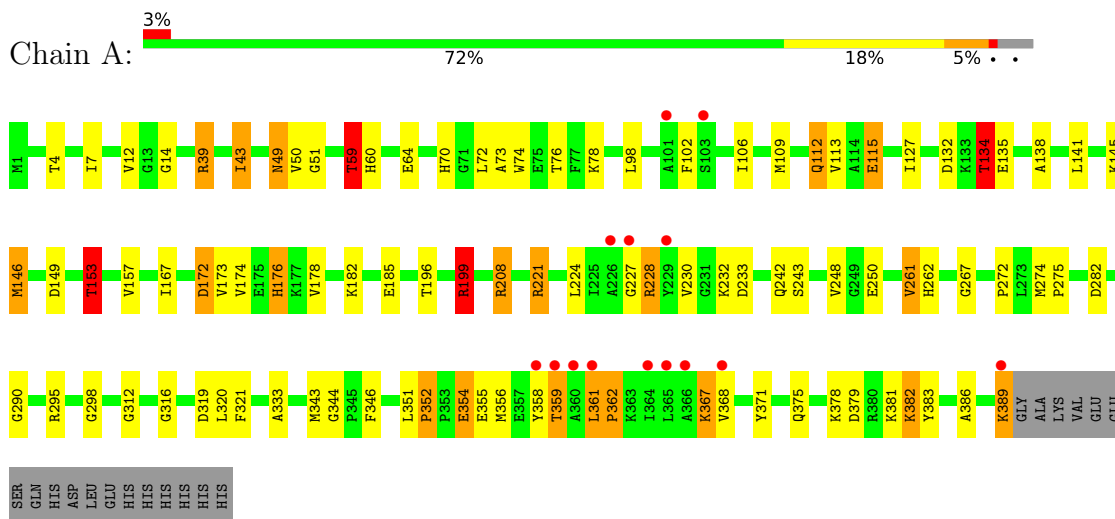
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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	161	Total	O	0	0
			161	161		

- Molecule 1: Fructose-1,6-bisphosphate aldolase/phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.30Å 112.30Å 151.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 1.90 47.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.66-1.90) 100.0 (47.66-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.151 , 0.191 0.151 , 0.191	Depositor DCC
R_{free} test set	1917 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.025 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3223	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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: 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	1.75	41/3141 (1.3%)	1.42	22/4252 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	VAL	CA-CB	7.82	1.64	1.54
1	A	172	ASP	C-O	7.75	1.33	1.24
1	A	141	LEU	CA-C	7.22	1.60	1.52
1	A	321	PHE	N-CA	7.14	1.54	1.46
1	A	316	GLY	N-CA	7.07	1.54	1.44
1	A	352	PRO	CA-C	6.98	1.55	1.51
1	A	333	ALA	CA-CB	6.96	1.64	1.53
1	A	134	THR	C-O	-6.64	1.16	1.23
1	A	319	ASP	N-CA	6.40	1.54	1.46
1	A	298	GLY	N-CA	6.31	1.53	1.44
1	A	72	LEU	CA-C	6.30	1.60	1.52
1	A	149	ASP	N-CA	6.30	1.53	1.45
1	A	12	VAL	CA-CB	6.21	1.62	1.54
1	A	352	PRO	C-O	-6.18	1.19	1.25
1	A	272	PRO	CA-CB	6.05	1.61	1.53
1	A	167	ILE	CA-CB	5.94	1.61	1.54
1	A	14	GLY	N-CA	5.82	1.50	1.44
1	A	76	THR	CA-C	5.75	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	THR	CB-CG2	-5.74	1.33	1.52
1	A	127	ILE	CA-CB	5.58	1.61	1.54
1	A	274	MET	CA-C	5.56	1.59	1.52
1	A	185	GLU	CB-CG	-5.54	1.35	1.52
1	A	261	VAL	N-CA	5.51	1.52	1.46
1	A	295	ARG	CG-CD	5.50	1.69	1.52
1	A	173	VAL	CA-C	5.45	1.58	1.52
1	A	153	THR	C-O	-5.43	1.17	1.23
1	A	282	ASP	CA-C	5.38	1.58	1.52
1	A	320	LEU	CA-C	5.38	1.60	1.52
1	A	115	GLU	N-CA	5.32	1.52	1.45
1	A	267	GLY	N-CA	5.31	1.53	1.45
1	A	178	VAL	CA-CB	-5.30	1.48	1.54
1	A	344	GLY	N-CA	5.26	1.51	1.44
1	A	73	ALA	CA-CB	-5.21	1.45	1.53
1	A	146	MET	N-CA	5.16	1.52	1.46
1	A	232	LYS	CA-C	5.15	1.59	1.53
1	A	49	ASN	CG-OD1	5.14	1.33	1.23
1	A	346	PHE	CA-CB	5.12	1.61	1.53
1	A	7	ILE	CA-C	-5.11	1.46	1.52
1	A	368	VAL	CA-CB	5.07	1.60	1.54
1	A	145	LYS	CE-NZ	5.05	1.64	1.49
1	A	196	THR	C-O	5.02	1.30	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ARG	NE-CZ-NH2	11.10	129.19	119.20
1	A	351	LEU	CA-C-N	9.25	126.41	119.66
1	A	351	LEU	C-N-CA	9.25	126.41	119.66
1	A	199	ARG	NE-CZ-NH1	-7.93	113.57	121.50
1	A	134	THR	CB-CA-C	-7.14	96.68	113.02
1	A	59	THR	OG1-CB-CG2	6.66	122.61	109.30
1	A	185	GLU	CB-CA-C	-6.35	100.24	110.79
1	A	361	LEU	CA-C-N	6.34	127.76	119.84
1	A	361	LEU	C-N-CA	6.34	127.76	119.84
1	A	50	VAL	N-CA-C	-6.18	99.22	108.12
1	A	228	ARG	N-CA-C	5.64	119.02	109.76
1	A	59	THR	CA-CB-OG1	5.58	117.97	109.60
1	A	275	PRO	CB-CA-C	5.34	116.36	111.87
1	A	59	THR	N-CA-CB	-5.30	102.01	111.08
1	A	243	SER	N-CA-C	5.29	118.55	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	VAL	CA-C-N	-5.25	114.87	122.69
1	A	157	VAL	C-N-CA	-5.25	114.87	122.69
1	A	59	THR	CA-CB-CG2	5.24	119.41	110.50
1	A	208	ARG	CG-CD-NE	-5.24	100.47	112.00
1	A	199	ARG	CD-NE-CZ	5.16	131.62	124.40
1	A	233	ASP	N-CA-CB	-5.13	103.31	110.29
1	A	43	ILE	N-CA-C	5.04	115.71	110.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	59	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	227	GLY	Peptide

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	3061	0	3064	47	0
2	A	1	0	0	0	0
3	A	161	0	0	2	0
All	All	3223	0	3064	47	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 8.

All (47) 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:389:LYS:O	1:A:389:LYS:HD3	1.45	1.16
1:A:59:THR:HG21	1:A:312:GLY:O	1.60	1.00
1:A:389:LYS:O	1:A:389:LYS:CD	2.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ALA:O	1:A:389:LYS:HD2	1.82	0.79
1:A:146:MET:O	1:A:153:THR:HG21	1.85	0.75
1:A:379:ASP:HA	1:A:382:LYS:HE2	1.69	0.74
1:A:59:THR:CG2	1:A:312:GLY:O	2.37	0.68
1:A:70:HIS:HD2	1:A:106:ILE:H	1.42	0.66
1:A:153:THR:HB	1:A:250:GLU:HB3	1.80	0.64
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.62	0.64
1:A:172:ASP:OD1	1:A:199:ARG:HD2	1.98	0.62
1:A:134:THR:HG21	1:A:138:ALA:HB2	1.83	0.60
1:A:242:GLN:NE2	1:A:248:VAL:H	2.00	0.58
1:A:74:TRP:CH2	1:A:109:MET:HE2	2.40	0.57
1:A:134:THR:HG22	1:A:135:GLU:H	1.70	0.55
1:A:70:HIS:CD2	1:A:106:ILE:H	2.23	0.55
1:A:356[A]:MET:HE3	1:A:358:TYR:O	2.07	0.55
1:A:379:ASP:HA	1:A:382:LYS:CE	2.36	0.54
1:A:64:GLU:OE1	3:A:541:HOH:O	2.18	0.53
1:A:221:ARG:HH21	1:A:221:ARG:HB3	1.73	0.53
1:A:49:ASN:ND2	1:A:290:GLY:H	2.06	0.52
1:A:367:LYS:HG2	1:A:367:LYS:O	2.09	0.51
1:A:134:THR:HG22	1:A:262:HIS:O	2.11	0.50
1:A:379:ASP:HB2	1:A:383:TYR:CE2	2.46	0.50
1:A:98:LEU:HD21	1:A:228:ARG:NH2	2.27	0.50
1:A:221:ARG:HD2	3:A:519:HOH:O	2.13	0.48
1:A:221:ARG:HB3	1:A:221:ARG:NH2	2.30	0.47
1:A:174:VAL:CG2	1:A:199:ARG:HD3	2.46	0.46
1:A:352:PRO:HB2	1:A:355:GLU:HG3	1.97	0.46
1:A:389:LYS:O	1:A:389:LYS:CG	2.64	0.46
1:A:49:ASN:O	1:A:290:GLY:HA3	2.16	0.45
1:A:371:TYR:CE1	1:A:383:TYR:CE1	3.04	0.45
1:A:51:GLY:HA3	1:A:132:ASP:OD2	2.18	0.43
1:A:134:THR:HG21	1:A:261:VAL:HB	2.00	0.43
1:A:134:THR:CG2	1:A:262:HIS:O	2.66	0.43
1:A:361:LEU:HB3	1:A:362:PRO:CD	2.49	0.43
1:A:359:THR:HG23	1:A:362:PRO:HD2	2.00	0.43
1:A:176:HIS:NE2	1:A:221:ARG:HG3	2.35	0.42
1:A:39:ARG:HD3	1:A:39:ARG:N	2.34	0.42
1:A:102:PHE:HA	1:A:109:MET:HE1	2.01	0.42
1:A:382:LYS:H	1:A:382:LYS:HZ3	1.67	0.42
1:A:4:THR:HB	1:A:60:HIS:CE1	2.55	0.41
1:A:43:ILE:HB	1:A:59:THR:HG23	2.01	0.41
1:A:375:GLN:HE21	1:A:375:GLN:HB2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:HE2	1:A:343:MET:HB3	1.96	0.41
1:A:146:MET:O	1:A:153:THR:CG2	2.63	0.40
1:A:354:GLU:CD	1:A:354:GLU:H	2.25	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	388/407 (95%)	373 (96%)	14 (4%)	1 (0%)	36 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	PRO

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	316/331 (96%)	295 (93%)	21 (7%)	15 8

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	59	THR
1	A	78	LYS
1	A	112	GLN
1	A	115	GLU
1	A	134	THR
1	A	153	THR
1	A	176	HIS
1	A	182	LYS
1	A	199	ARG
1	A	208	ARG
1	A	221	ARG
1	A	224	LEU
1	A	230	VAL
1	A	354	GLU
1	A	359	THR
1	A	367	LYS
1	A	378	LYS
1	A	381	LYS
1	A	382	LYS
1	A	389	LYS

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	49	ASN
1	A	70	HIS
1	A	112	GLN
1	A	242	GLN
1	A	310	HIS
1	A	375	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	389/407 (95%)	-0.36	14 (3%)	46 49	13, 23, 56, 75	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	TYR	4.0
1	A	229	TYR	3.8
1	A	226	ALA	3.0
1	A	361	LEU	2.7
1	A	364	ILE	2.6
1	A	101	ALA	2.6
1	A	360	ALA	2.6
1	A	389	LYS	2.4
1	A	368	VAL	2.4
1	A	359	THR	2.2
1	A	365	LEU	2.2
1	A	366	ALA	2.2
1	A	227	GLY	2.1
1	A	103	SER	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	MG	A	408	1/1	0.99	0.04	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.