



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:42 PM GMT

PDB ID : 3RSM
Title : Crystal structure of S108C mutant of PMM/PGM
Authors : Akella, A.; Anbanandam, A.; Kelm, A.; Wei, Y.; Mehra-Chaudhary, R.;
Beamer, L.; Van Doren, S.
Deposited on : 2011-05-02
Resolution : 2.10 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

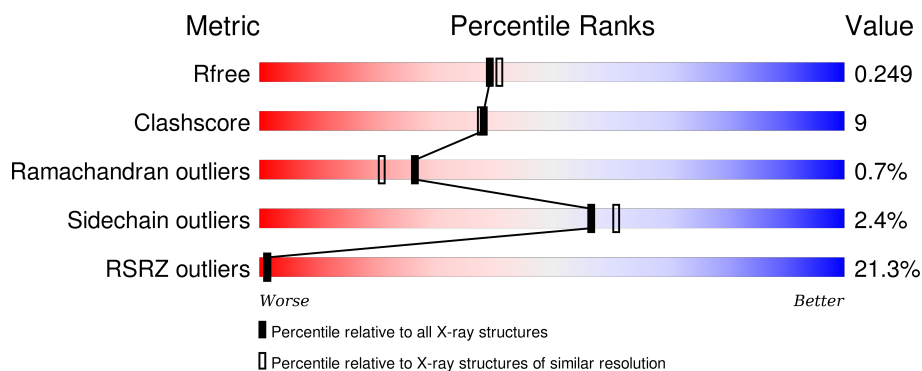
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 $\leq 5\%$. 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	463	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	464	-	-	X	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3401 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 Phosphomannomutase/phosphoglucomutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	5	0
			3279	2081	561	622	15			

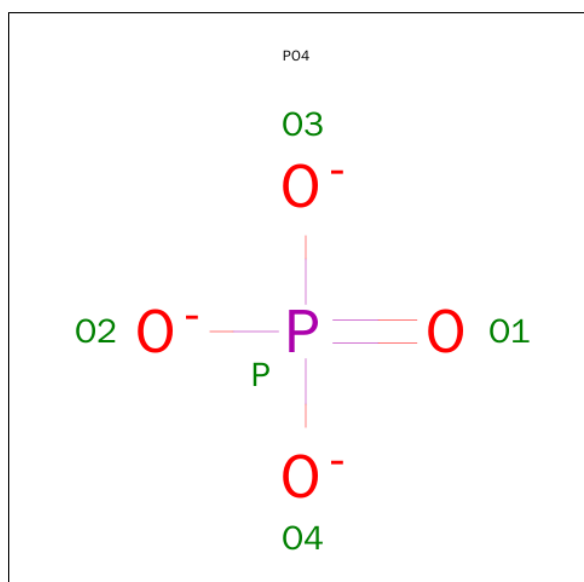
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	VAL	ALA	CONFLICT	UNP P26276
A	108	CYS	SER	ENGINEERED MUTATION	UNP P26276

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

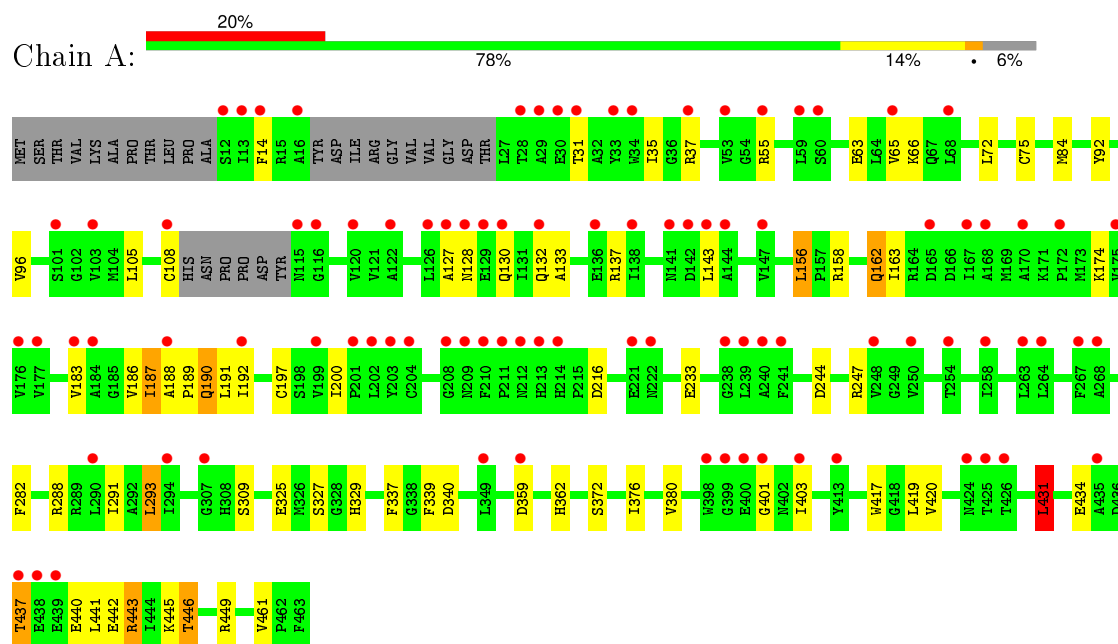


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		

- Molecule 1: Phosphomannomutase/phosphoglucomutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.03Å 72.81Å 93.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.84 – 2.10 32.40 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.84-2.10) 99.8 (32.40-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.213 , 0.253 0.212 , 0.249	Depositor DCC
R_{free} test set	1456 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.2	EDS
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 28729 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3401	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, PO4

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	0.59	0/3352	0.68	2/4551 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	293	LEU	CA-CB-CG	6.18	129.52	115.30
1	A	431	LEU	CA-CB-CG	5.01	126.81	115.30

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	3279	0	3227	59	0
2	A	1	0	0	0	0
3	A	5	0	0	3	0
4	A	116	0	0	1	0
All	All	3401	0	3227	59	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 (59) 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:325[B]:GLU:OE2	4:A:553:HOH:O	1.93	0.86
1:A:190:GLN:HE21	1:A:190:GLN:H	1.30	0.79
1:A:359:ASP:OD1	1:A:362:HIS:HD2	1.66	0.78
1:A:449:ARG:HG3	1:A:461:VAL:HG21	1.71	0.71
1:A:247[B]:ARG:HE	1:A:329:HIS:CE1	2.08	0.71
1:A:329:HIS:HD2	1:A:340:ASP:OD1	1.74	0.71
1:A:247[B]:ARG:NE	3:A:464:PO4:O4	2.26	0.69
1:A:359:ASP:OD1	1:A:362:HIS:CD2	2.48	0.67
1:A:133:ALA:O	1:A:137:ARG:HG3	1.98	0.63
1:A:325[B]:GLU:HG2	1:A:327:SER:H	1.65	0.60
1:A:420:VAL:HB	1:A:431:LEU:HD13	1.81	0.60
1:A:437:THR:HG23	1:A:440:GLU:H	1.68	0.58
1:A:247[B]:ARG:NE	1:A:329:HIS:CE1	2.74	0.55
1:A:401:GLY:O	1:A:403:ILE:HD12	2.09	0.52
1:A:31:THR:HG22	1:A:35:ILE:HD12	1.91	0.51
1:A:376:ILE:HB	1:A:431:LEU:HB2	1.91	0.51
1:A:200:ILE:CD1	1:A:233[A]:GLU:HG2	2.40	0.51
1:A:55[A]:ARG:HH11	1:A:65:VAL:HG21	1.75	0.51
1:A:92:TYR:OH	1:A:162:GLN:NE2	2.43	0.49
1:A:127:ALA:HB2	1:A:309:SER:OG	2.12	0.49
1:A:37:ARG:HG2	1:A:143:LEU:HD13	1.96	0.48
1:A:65:VAL:HG13	1:A:105:LEU:HD22	1.95	0.48
1:A:288:ARG:HG2	1:A:417:TRP:HD1	1.79	0.48
1:A:55[B]:ARG:HH12	1:A:84:MET:HE3	1.79	0.47
1:A:329:HIS:CD2	1:A:340:ASP:OD1	2.63	0.47
1:A:55[B]:ARG:HH12	1:A:84:MET:CE	2.28	0.47
1:A:442:GLU:O	1:A:446:THR:HB	2.15	0.47
1:A:282:PHE:HZ	1:A:291:ILE:HG12	1.80	0.46
1:A:372:SER:HB3	1:A:434:GLU:HG3	1.97	0.46
1:A:325[B]:GLU:CD	1:A:327:SER:OG	2.54	0.46
1:A:216:ASP:OD1	1:A:247[A]:ARG:NH2	2.49	0.46
1:A:288:ARG:HG2	1:A:417:TRP:CD1	2.51	0.46
1:A:92:TYR:OH	1:A:158:ARG:HG2	2.15	0.46
1:A:247[B]:ARG:CZ	3:A:464:PO4:O4	2.63	0.46
1:A:443:ARG:O	1:A:446:THR:HG22	2.15	0.45
1:A:127:ALA:O	1:A:130:GLN:HB2	2.17	0.45
1:A:437:THR:HG23	1:A:440:GLU:CB	2.47	0.45
1:A:156:LEU:HD12	1:A:187:ILE:HD13	1.98	0.45
1:A:437:THR:HG23	1:A:440:GLU:HB2	1.97	0.44
1:A:247[B]:ARG:HE	1:A:329:HIS:HE1	1.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:O	1:A:75:CYS:HB2	2.18	0.44
1:A:420:VAL:HB	1:A:431:LEU:CD1	2.45	0.44
1:A:419:LEU:O	1:A:431:LEU:HA	2.17	0.44
1:A:174:LYS:HE3	1:A:233[A]:GLU:HG3	2.00	0.44
1:A:183:VAL:O	1:A:186:VAL:HG22	2.17	0.43
1:A:437:THR:CG2	1:A:440:GLU:HB2	2.49	0.43
1:A:108:CYS:CB	3:A:464:PO4:O1	2.67	0.43
1:A:192:ILE:O	1:A:197:CYS:HB2	2.19	0.43
1:A:14:PHE:HB3	1:A:132:GLN:HE22	1.84	0.43
1:A:63:GLU:O	1:A:66:LYS:HB2	2.19	0.42
1:A:183:VAL:HG12	1:A:244:ASP:HA	2.02	0.42
1:A:55[A]:ARG:NH1	1:A:65:VAL:HG21	2.35	0.41
1:A:188:ALA:HB3	1:A:189:PRO:HD3	2.02	0.41
1:A:55[B]:ARG:HB3	1:A:65:VAL:HG11	2.02	0.41
1:A:96:VAL:HG13	1:A:158:ARG:CZ	2.51	0.41
1:A:163:ILE:HG21	1:A:191:LEU:HD21	2.02	0.41
1:A:441:LEU:O	1:A:445:LYS:HB2	2.21	0.40
1:A:337:PHE:HB2	1:A:339:PHE:CE2	2.56	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	435/463 (94%)	412 (95%)	20 (5%)	3 (1%)	26 21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	VAL
1	A	128	ASN
1	A	187	ILE

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	340/382 (89%)	332 (98%)	8 (2%)	57 61

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	LEU
1	A	162	GLN
1	A	190	GLN
1	A	293	LEU
1	A	431	LEU
1	A	437	THR
1	A	443	ARG
1	A	446	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	132	GLN
1	A	162	GLN
1	A	181	ASN
1	A	190	GLN
1	A	212	ASN
1	A	329	HIS
1	A	362	HIS
1	A	377	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	PO4	A	464	2	4,4,4	0.42	0	6,6,6	0.29	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	PO4	A	464	2	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	464	PO4	3	0

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	436/463 (94%)	1.18	93 (21%) 1 1	30, 54, 92, 142	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	ILE	8.9
1	A	28	THR	8.1
1	A	12	SER	7.3
1	A	212	ASN	6.7
1	A	14	PHE	6.3
1	A	115	ASN	6.2
1	A	399	GLY	5.3
1	A	138	ILE	5.2
1	A	144	ALA	5.0
1	A	425	THR	5.0
1	A	142	ASP	5.0
1	A	143	LEU	4.8
1	A	34	TRP	4.8
1	A	168	ALA	4.7
1	A	239	LEU	4.6
1	A	177	VAL	4.4
1	A	400	GLU	4.3
1	A	108	CYS	4.2
1	A	116	GLY	4.1
1	A	128	ASN	4.1
1	A	31	THR	4.0
1	A	59	LEU	3.9
1	A	263	LEU	3.9
1	A	248	VAL	3.9
1	A	250	VAL	3.8
1	A	211	PRO	3.7
1	A	210	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	214	HIS	3.6
1	A	413	TYR	3.5
1	A	424	ASN	3.5
1	A	209	ASN	3.4
1	A	258	ILE	3.4
1	A	37	ARG	3.4
1	A	241	PHE	3.3
1	A	240	ALA	3.2
1	A	60	SER	3.2
1	A	438	GLU	3.1
1	A	53	VAL	3.1
1	A	192	ILE	3.1
1	A	188	ALA	3.0
1	A	254	THR	3.0
1	A	238	GLY	3.0
1	A	129	GLU	2.9
1	A	176	VAL	2.9
1	A	33	TYR	2.9
1	A	199	VAL	2.8
1	A	184	ALA	2.8
1	A	55[A]	ARG	2.8
1	A	147	VAL	2.7
1	A	127	ALA	2.7
1	A	398	TRP	2.6
1	A	203	TYR	2.6
1	A	167	ILE	2.6
1	A	290	LEU	2.5
1	A	221	GLU	2.5
1	A	222	ASN	2.5
1	A	141	ASN	2.5
1	A	201	PRO	2.5
1	A	16	ALA	2.4
1	A	208	GLY	2.4
1	A	359	ASP	2.4
1	A	122	ALA	2.4
1	A	307	GLY	2.4
1	A	435	ALA	2.4
1	A	426	THR	2.4
1	A	349	LEU	2.4
1	A	30	GLU	2.4
1	A	65	VAL	2.3
1	A	132	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	120	VAL	2.3
1	A	136	GLU	2.3
1	A	437	THR	2.2
1	A	204	CYS	2.2
1	A	403	ILE	2.2
1	A	401	GLY	2.2
1	A	172	PRO	2.2
1	A	29	ALA	2.2
1	A	68	LEU	2.2
1	A	126	LEU	2.2
1	A	183	VAL	2.2
1	A	294	ILE	2.2
1	A	213	HIS	2.1
1	A	439	GLU	2.1
1	A	103	VAL	2.1
1	A	130	GLN	2.1
1	A	165	ASP	2.1
1	A	268	ALA	2.1
1	A	202	LEU	2.1
1	A	264	LEU	2.1
1	A	101	SER	2.1
1	A	267	PHE	2.1
1	A	170	ALA	2.0
1	A	175	VAL	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	A	464	5/5	0.87	0.33	2.40	54,55,56,57	5
2	ZN	A	500	1/1	0.98	0.06	-2.45	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.