



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1ZEB
Title : X-ray structure of alkaline phosphatase from human placenta in complex with 5'-AMP
Authors : Llinas, P.; Stura, E.A.; Menez, A.; Kiss, Z.; Stigbrand, T.; Millan, J.L.; Le Du, M.H.
Deposited on : 2005-04-18
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

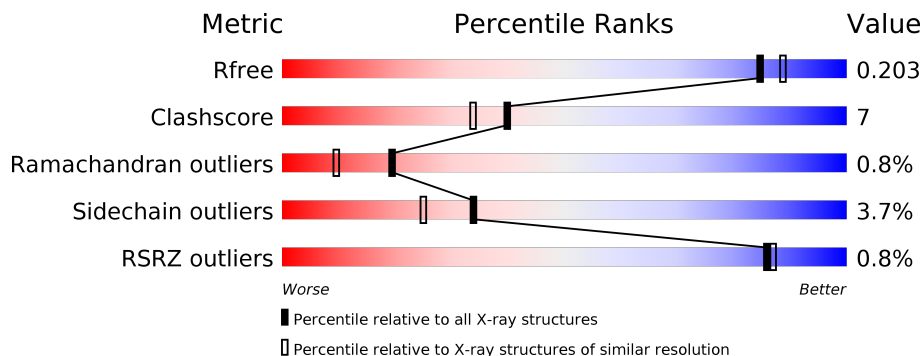
1 Overall quality at a glance

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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	484	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4419 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 Alkaline phosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	480	3677	2297	654	707	1	18	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

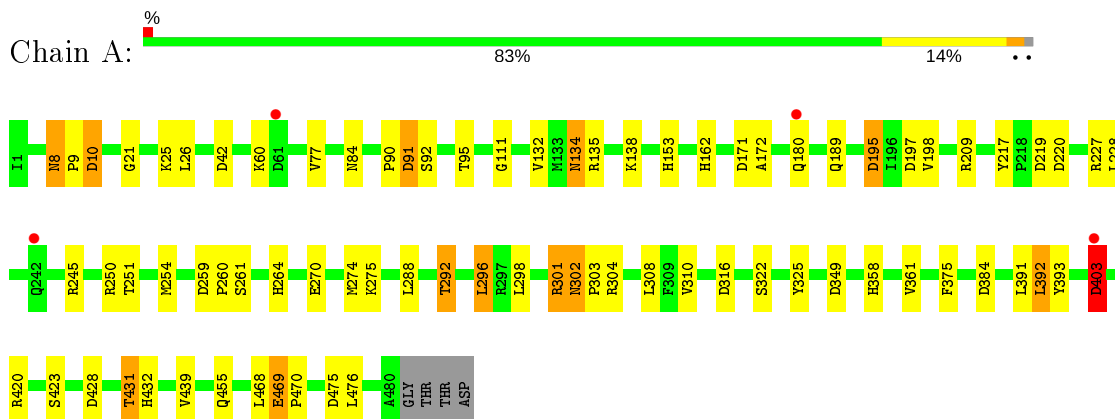
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	710	Total	O	0	0
			710	710		

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: Alkaline phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.02Å 113.89Å 106.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.96 – 1.90 24.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (14.96-1.90) 87.1 (24.96-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.151 , 0.197 0.160 , 0.203	Depositor DCC
R_{free} test set	1871 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtrriage
Anisotropy	0.347	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4419	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: ZN, MG, CA, NAG, SEP

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	0.48	0/3747	0.79	14/5081 (0.3%)

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	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASP	CB-CG-OD2	10.66	127.89	118.30
1	A	349	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	220	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	259	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	301	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	197	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	42	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	195	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	171	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	428	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	219	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	10	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	384	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	403	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	LEU	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	3677	0	3567	53	0
2	A	28	0	26	0	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	710	0	0	8	4
All	All	4419	0	3593	53	4

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 7.

All (53) 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:10:ASP:HB2	6:A:1368:HOH:O	1.64	0.97
1:A:134:ASN:HD21	1:A:138:LYS:NZ	1.79	0.80
1:A:162:HIS:H	1:A:189:GLN:HE22	1.30	0.78
1:A:261:SER:OG	6:A:1504:HOH:O	2.11	0.69
1:A:135:ARG:HH21	1:A:469:GLU:CB	2.08	0.67
1:A:469:GLU:CB	1:A:470:PRO:CD	2.73	0.66
1:A:288:LEU:O	1:A:292:THR:HG23	1.96	0.65
1:A:469:GLU:CA	6:A:1148:HOH:O	2.48	0.61
1:A:251:THR:HG23	6:A:977:HOH:O	2.01	0.58
1:A:111:GLY:O	1:A:162:HIS:HD2	1.87	0.58
1:A:431:THR:HG23	1:A:432:HIS:O	2.05	0.57
1:A:260:PRO:O	1:A:261:SER:CB	2.53	0.56
1:A:153:HIS:HD2	6:A:927:HOH:O	1.90	0.55
1:A:469:GLU:HA	6:A:1148:HOH:O	2.09	0.53
1:A:217:TYR:OH	1:A:275:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASP:OD1	1:A:264:HIS:HE1	1.95	0.50
1:A:8:ASN:HD22	1:A:9:PRO:N	2.11	0.48
1:A:296:LEU:HD13	1:A:308:LEU:HD22	1.95	0.48
1:A:250:ARG:O	1:A:254:MET:HG3	2.14	0.48
1:A:302:ASN:C	1:A:302:ASN:HD22	2.17	0.48
1:A:8:ASN:HD22	1:A:9:PRO:HD2	1.79	0.48
1:A:393:TYR:O	1:A:423:SER:HA	2.13	0.47
1:A:260:PRO:O	1:A:261:SER:OG	2.29	0.47
1:A:469:GLU:CB	1:A:470:PRO:HD2	2.44	0.47
1:A:469:GLU:C	6:A:1148:HOH:O	2.53	0.47
1:A:288:LEU:O	1:A:292:THR:CG2	2.62	0.46
1:A:198:VAL:HG22	1:A:298:LEU:HD23	1.98	0.46
1:A:84:ASN:HD21	1:A:91:ASP:H	1.64	0.45
1:A:8:ASN:HD22	1:A:9:PRO:CD	2.29	0.45
1:A:403:ASP:HB2	6:A:1425:HOH:O	2.15	0.45
1:A:134:ASN:HD21	1:A:138:LYS:HZ2	1.59	0.45
1:A:302:ASN:ND2	1:A:304:ARG:H	2.14	0.45
1:A:8:ASN:C	1:A:8:ASN:HD22	2.20	0.45
1:A:209:ARG:HA	1:A:227:ARG:HB2	1.98	0.45
1:A:302:ASN:HD22	1:A:303:PRO:N	2.15	0.45
1:A:270:GLU:HG3	1:A:274:MET:HA	2.00	0.44
1:A:134:ASN:HD21	1:A:138:LYS:HZ1	1.58	0.44
1:A:308:LEU:HG	1:A:310:VAL:HG23	2.00	0.43
1:A:322:SER:O	1:A:420:ARG:HA	2.18	0.43
1:A:195:ASP:OD1	1:A:264:HIS:CE1	2.71	0.43
1:A:134:ASN:ND2	1:A:138:LYS:HZ2	2.15	0.43
1:A:21:GLY:O	1:A:25:LYS:HG3	2.18	0.43
1:A:135:ARG:HD2	1:A:469:GLU:CB	2.49	0.43
1:A:325:TYR:HA	1:A:375:PHE:CZ	2.54	0.42
1:A:391:LEU:O	1:A:392:LEU:HD13	2.20	0.42
1:A:95:THR:HG22	1:A:455:GLN:HE22	1.85	0.42
1:A:77:VAL:HA	1:A:439:VAL:O	2.20	0.41
1:A:134:ASN:ND2	1:A:138:LYS:NZ	2.56	0.41
1:A:90:PRO:HB2	1:A:95:THR:HG23	2.02	0.41
1:A:358:HIS:CE1	1:A:432:HIS:CD2	3.08	0.41
1:A:134:ASN:HD21	1:A:138:LYS:CE	2.32	0.40
1:A:172:ALA:HB2	1:A:228:LEU:HD13	2.03	0.40
1:A:301:ARG:HH11	1:A:301:ARG:CG	2.34	0.40

All (4) 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)
6:A:1026:HOH:O	6:A:1363:HOH:O[3_655]	2.09	0.11
6:A:1072:HOH:O	6:A:1378:HOH:O[8_555]	2.13	0.07
6:A:1363:HOH:O	6:A:1363:HOH:O[3_655]	2.14	0.06
6:A:1065:HOH:O	6:A:1378:HOH:O[3_655]	2.17	0.03

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	477/484 (99%)	463 (97%)	10 (2%)	4 (1%)	19 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	GLU
1	A	403	ASP
1	A	60	LYS
1	A	361	VAL

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	380/386 (98%)	366 (96%)	14 (4%)	34 25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	26	LEU
1	A	91	ASP
1	A	132	VAL
1	A	134	ASN
1	A	180	GLN
1	A	245	ARG
1	A	292	THR
1	A	296	LEU
1	A	302	ASN
1	A	392	LEU
1	A	431	THR
1	A	475	ASP
1	A	476	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	84	ASN
1	A	127	ASN
1	A	134	ASN
1	A	153	HIS
1	A	162	HIS
1	A	189	GLN
1	A	193	ASN
1	A	235	GLN
1	A	264	HIS
1	A	302	ASN
1	A	445	GLN
1	A	455	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](#)

1 non-standard protein/DNA/RNA residue is 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
1	SEP	A	92	1,3	8,9,10	0.62	0	8,12,14	1.72	3 (37%)

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
1	SEP	A	92	1,3	-	1/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	SEP	O2P-P-OG	-2.31	100.58	106.73
1	A	92	SEP	OG-CB-CA	2.23	110.32	108.14
1	A	92	SEP	O3P-P-O2P	2.06	115.52	107.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	92	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
2	NAG	A	803	1	14,14,15	0.58	0	17,19,21	1.41	3 (17%)
2	NAG	A	801	1	14,14,15	0.59	0	17,19,21	1.11	2 (11%)

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
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	803	NAG	C1-O5-C5	3.57	117.03	112.19
2	A	801	NAG	C1-C2-N2	2.64	114.99	110.49
2	A	801	NAG	O5-C1-C2	-2.50	107.34	111.29
2	A	803	NAG	O5-C1-C2	-2.43	107.45	111.29
2	A	803	NAG	C6-C5-C4	-2.19	107.87	113.00

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 [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	479/484 (98%)	-0.36	4 (0%) 86 87	12, 17, 31, 41	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ASP	3.5
1	A	242	GLN	2.5
1	A	61	ASP	2.1
1	A	180	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	SEP	A	92	10/11	0.98	0.07	12,14,15,15	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	NAG	A	803	14/15	0.88	0.20	26,30,34,36	0
2	NAG	A	801	14/15	0.91	0.12	23,29,33,35	0
4	MG	A	903	1/1	0.98	0.10	10,10,10,10	0
3	ZN	A	901	1/1	0.99	0.04	14,14,14,14	0
3	ZN	A	902	1/1	1.00	0.02	14,14,14,14	0
5	CA	A	904	1/1	1.00	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.