



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:08 am BST

PDB ID : 4ICQ
Title : Structural basis for substrate recognition and reaction mechanism of bacterial aminopeptidase peps
Authors : Ta, M.H.; Kim, K.K.; Lee, S.
Deposited on : 2012-12-11
Resolution : 2.25 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
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

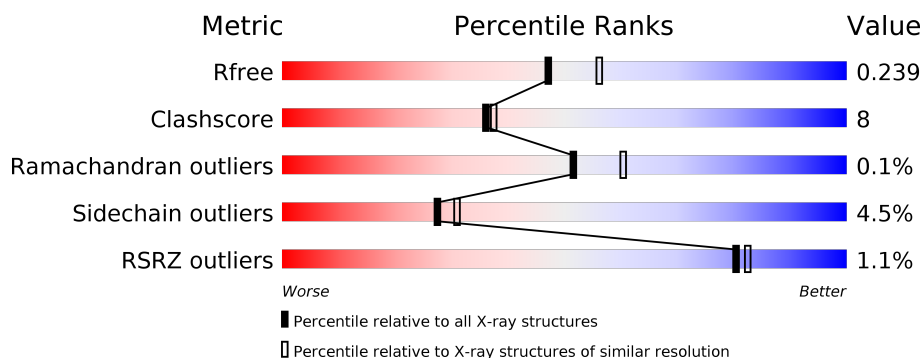
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	413	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 85%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> • </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 85% 15% </div> </div>
1	B	413	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 83%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> • </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 83% 14% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6616 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 Aminopeptidase PepS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3183	2007	541	621	14			
1	B	413	Total	C	N	O	S	0	0	0
			3183	2007	541	621	14			

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	137	Total	O	0	0
			137	137		

- Molecule 1: Aminopeptidase PepS



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.64Å 126.64Å 139.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.90 – 2.25 43.52 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.90-2.25) 99.9 (43.52-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.199 , 0.246 0.196 , 0.239	Depositor DCC
R_{free} test set	2760 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6616	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

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	1.06	2/3248 (0.1%)	0.95	8/4409 (0.2%)
1	B	1.06	6/3248 (0.2%)	0.94	8/4409 (0.2%)
All	All	1.06	8/6496 (0.1%)	0.94	16/8818 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	219	GLY	N-CA	7.34	1.57	1.46
1	B	33	SER	CB-OG	-7.14	1.32	1.42
1	A	166	GLU	CG-CD	6.29	1.61	1.51
1	A	298	GLU	CG-CD	6.13	1.61	1.51
1	B	84	GLU	CG-CD	5.81	1.60	1.51
1	B	178	LYS	CE-NZ	5.68	1.63	1.49
1	B	406	PHE	CE2-CZ	5.06	1.47	1.37
1	B	92	TYR	CD1-CE1	5.03	1.47	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	PRO	C-N-CA	-10.55	100.15	122.30
1	A	315	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	261	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	221	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	39	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	407	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	218	PRO	O-C-N	-6.37	112.36	123.20
1	B	39	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	218	PRO	CA-C-N	5.79	127.79	116.20
1	B	172	LEU	CB-CG-CD2	5.54	120.42	111.00
1	A	235	ALA	C-N-CA	-5.52	110.70	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	70	LYS	CD-CE-NZ	5.27	123.83	111.70
1	B	315	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	306	ASP	CB-CG-OD1	5.13	122.91	118.30
1	B	112	ASN	C-N-CA	-5.01	111.78	122.30

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	3183	0	3109	45	0
1	B	3183	0	3110	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	109	0	0	4	0
3	B	137	0	0	6	0
All	All	6616	0	6219	101	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 (101) 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:B:347:ASN:ND2	1:B:391:MET:HE1	1.50	1.23
1:B:347:ASN:HD22	1:B:391:MET:CE	1.49	1.22
1:A:21:GLY:CA	1:A:249:MET:CE	2.18	1.21
1:A:21:GLY:HA2	1:A:249:MET:CE	1.78	1.11
1:A:21:GLY:HA3	1:A:249:MET:HE3	1.37	1.04
1:A:21:GLY:HA2	1:A:249:MET:HE1	1.45	0.98
1:B:133:MET:HA	1:B:133:MET:HE3	1.44	0.98
1:A:21:GLY:CA	1:A:249:MET:HE1	1.96	0.96
1:B:270:THR:HG21	1:B:387:GLY:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLY:CA	1:A:249:MET:HE3	1.91	0.93
1:B:347:ASN:ND2	1:B:391:MET:CE	2.17	0.91
1:B:161:ASN:HD22	1:B:161:ASN:H	1.14	0.89
1:A:100:ARG:HG3	1:A:133:MET:HE2	1.57	0.86
1:A:150:ALA:HA	1:A:172:LEU:HD13	1.60	0.83
1:A:100:ARG:HG3	1:A:133:MET:CE	2.09	0.82
1:B:35:ASP:HA	1:B:62:THR:HG22	1.60	0.81
1:A:21:GLY:HA3	1:A:249:MET:CE	1.99	0.78
1:B:347:ASN:HD22	1:B:391:MET:HE1	0.66	0.78
1:A:291:GLN:NE2	1:A:315:ARG:NH2	2.37	0.73
1:B:150:ALA:HA	1:B:172:LEU:HD13	1.71	0.72
1:B:161:ASN:HD22	1:B:161:ASN:N	1.86	0.72
1:A:369:GLU:O	3:A:662:HOH:O	2.08	0.72
1:B:391:MET:HE2	1:B:393:ILE:HD11	1.71	0.71
1:B:84:GLU:OE1	3:B:712:HOH:O	2.08	0.71
1:B:186:ASP:CG	1:B:189:LYS:HD3	2.10	0.71
1:B:391:MET:CE	1:B:393:ILE:HD11	2.23	0.67
1:B:331:GLN:HG2	3:B:603:HOH:O	1.95	0.65
1:A:21:GLY:N	1:A:249:MET:HE1	2.11	0.65
1:B:413:ASN:O	3:B:698:HOH:O	2.14	0.63
1:B:270:THR:CG2	1:B:387:GLY:O	2.46	0.63
1:A:181:ARG:HA	3:A:608:HOH:O	2.01	0.61
1:B:133:MET:CE	1:B:133:MET:HA	2.25	0.60
1:A:21:GLY:HA2	1:A:249:MET:HE2	1.76	0.60
1:B:239:ASN:HD21	1:B:243:GLU:H	1.50	0.59
1:B:94:LEU:HD21	1:B:133:MET:HE3	1.85	0.59
1:A:281:GLU:OE1	1:A:299:LYS:HD3	2.02	0.59
1:B:134:ARG:O	1:B:138:GLN:HG3	2.02	0.59
1:B:124:LYS:HA	1:B:311:ASN:HD21	1.68	0.58
1:B:161:ASN:H	1:B:161:ASN:ND2	1.93	0.58
1:B:239:ASN:ND2	1:B:243:GLU:H	2.00	0.58
1:A:21:GLY:N	1:A:249:MET:CE	2.65	0.58
1:B:239:ASN:C	1:B:239:ASN:HD22	2.09	0.56
1:A:18:VAL:HG12	1:A:52:LEU:HD12	1.88	0.55
1:B:131:LYS:HB3	1:B:132:PRO:HD3	1.88	0.55
1:A:107:ASP:OD1	1:A:157:LYS:HE3	2.07	0.55
1:B:186:ASP:OD2	1:B:189:LYS:HD3	2.07	0.54
1:A:239:ASN:O	1:A:241:GLN:N	2.41	0.54
1:B:154:TRP:O	1:B:158:VAL:HG23	2.10	0.52
1:B:94:LEU:HD21	1:B:133:MET:CE	2.40	0.52
1:B:42:ALA:O	1:B:46:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HG3	1:A:133:MET:HE1	1.89	0.51
1:A:239:ASN:C	1:A:241:GLN:H	2.14	0.51
1:A:100:ARG:CG	1:A:133:MET:HE1	2.41	0.50
1:A:154:TRP:CE3	1:A:172:LEU:HD11	2.46	0.50
1:B:22:ILE:HG22	1:B:22:ILE:O	2.11	0.50
1:B:167:GLU:HG2	1:B:171:PHE:CE1	2.47	0.49
1:A:330:SER:HB2	1:A:345:ALA:O	2.12	0.49
1:B:181:ARG:HA	3:B:631:HOH:O	2.12	0.49
1:A:22:ILE:O	1:A:23:ASN:HB3	2.13	0.48
1:A:389:ASN:C	1:A:389:ASN:HD22	2.16	0.48
1:B:124:LYS:HA	1:B:311:ASN:ND2	2.28	0.48
1:B:35:ASP:CA	1:B:62:THR:HG22	2.40	0.48
1:A:100:ARG:CG	1:A:133:MET:CE	2.86	0.48
1:A:389:ASN:HD22	1:A:390:GLN:N	2.12	0.48
1:A:46:VAL:HG21	1:B:66:ILE:HG12	1.96	0.48
1:B:354:ALA:HB3	1:B:375:LEU:HB3	1.96	0.47
1:B:356:ALA:O	1:B:362:GLY:HA3	2.13	0.47
1:A:100:ARG:NH1	3:A:648:HOH:O	2.47	0.47
1:B:178:LYS:HE2	1:B:178:LYS:HB2	1.46	0.47
1:A:366:SER:OG	1:A:369:GLU:HG3	2.16	0.46
1:A:178:LYS:HE2	1:A:178:LYS:HB2	1.68	0.46
1:B:186:ASP:OD1	1:B:189:LYS:HD3	2.16	0.45
1:B:22:ILE:O	1:B:22:ILE:CG2	2.64	0.45
1:A:291:GLN:HE21	1:A:315:ARG:NH2	2.11	0.45
1:A:229:ASN:O	1:A:360:VAL:HG23	2.17	0.45
1:A:150:ALA:HA	1:A:172:LEU:CD1	2.40	0.45
1:A:356:ALA:O	1:A:362:GLY:HA3	2.16	0.45
1:B:319:GLU:HB3	1:B:350:ALA:HB3	1.99	0.44
1:B:410:ASN:ND2	1:B:411:TRP:H	2.14	0.44
1:A:205:LEU:HD21	1:A:405:LEU:HD21	2.01	0.43
1:B:270:THR:HG21	1:B:387:GLY:N	2.34	0.43
1:A:376:ASN:C	1:A:377:ARG:HD2	2.39	0.43
1:B:19:ALA:O	1:B:23:ASN:HA	2.18	0.43
1:B:325:ASP:N	1:B:326:PRO:CD	2.82	0.43
1:B:281:GLU:OE1	1:B:299:LYS:HD2	2.18	0.42
1:B:399:ASP:OD1	1:B:399:ASP:C	2.57	0.42
1:B:375:LEU:HD23	1:B:375:LEU:N	2.35	0.42
1:B:324:PRO:HG3	1:B:411:TRP:NE1	2.35	0.42
1:B:329:ILE:HG22	1:B:345:ALA:HB2	2.02	0.42
1:A:107:ASP:HB3	1:A:110:ALA:HB2	2.01	0.41
1:A:325:ASP:N	1:A:326:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ALA:O	1:A:46:VAL:HG23	2.20	0.41
1:B:194:HIS:ND1	3:B:639:HOH:O	2.37	0.41
1:A:82:VAL:HA	1:A:83:PRO:HD2	1.85	0.41
1:B:347:ASN:ND2	1:B:391:MET:HE2	2.22	0.41
1:A:254:VAL:O	1:A:254:VAL:HG23	2.20	0.40
1:B:22:ILE:HD13	1:B:22:ILE:HA	1.89	0.40
1:B:3:LEU:HA	1:B:4:PRO:HD2	1.97	0.40
1:A:100:ARG:NH2	3:A:647:HOH:O	2.54	0.40
1:B:299:LYS:HD3	3:B:662:HOH:O	2.20	0.40
1:B:391:MET:HE3	1:B:393:ILE:HD11	2.02	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	411/413 (100%)	398 (97%)	12 (3%)	1 (0%)	47	55
1	B	411/413 (100%)	398 (97%)	13 (3%)	0	100	100
All	All	822/826 (100%)	796 (97%)	25 (3%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	ALA

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	335/335 (100%)	320 (96%)	15 (4%)	27	31
1	B	335/335 (100%)	320 (96%)	15 (4%)	27	31
All	All	670/670 (100%)	640 (96%)	30 (4%)	27	31

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	3	LEU
1	A	16	LEU
1	A	28	HIS
1	A	30	LEU
1	A	72	LEU
1	A	128	LEU
1	A	137	THR
1	A	152	LEU
1	A	172	LEU
1	A	189	LYS
1	A	228	LYS
1	A	296	THR
1	A	389	ASN
1	A	405	LEU
1	B	3	LEU
1	B	32	LEU
1	B	39	ARG
1	B	55	HIS
1	B	62	THR
1	B	133	MET
1	B	137	THR
1	B	161	ASN
1	B	172	LEU
1	B	178	LYS
1	B	239	ASN
1	B	270	THR
1	B	288	LYS
1	B	293	VAL
1	B	331	GLN

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	20	ASN
1	A	81	ASN
1	A	291	GLN
1	A	389	ASN
1	B	20	ASN
1	B	81	ASN
1	B	161	ASN
1	B	209	GLN
1	B	239	ASN
1	B	241	GLN
1	B	311	ASN
1	B	347	ASN
1	B	410	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are 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

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	413/413 (100%)	-0.30	5 (1%) 79 81	22, 33, 48, 78	0
1	B	413/413 (100%)	-0.33	4 (0%) 82 84	21, 31, 45, 58	0
All	All	826/826 (100%)	-0.31	9 (1%) 80 82	21, 32, 47, 78	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.0
1	A	2	VAL	3.6
1	A	3	LEU	3.5
1	A	4	PRO	3.4
1	B	161	ASN	2.9
1	B	162	ALA	2.7
1	A	240	ALA	2.3
1	B	240	ALA	2.1
1	B	163	ALA	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. 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	ZN	B	502	1/1	0.98	0.15	32,32,32,32	0
2	ZN	B	501	1/1	0.98	0.14	35,35,35,35	0
2	ZN	A	501	1/1	0.99	0.10	38,38,38,38	0
2	ZN	A	502	1/1	0.99	0.09	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.