Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:34 AM BST

PDB ID	:	5RE1
Title	:	PanDDA analysis group deposition – Endothiapepsin ground state model 58
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Deposited on	:	2020-03-24
Resolution	:	0.97 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:

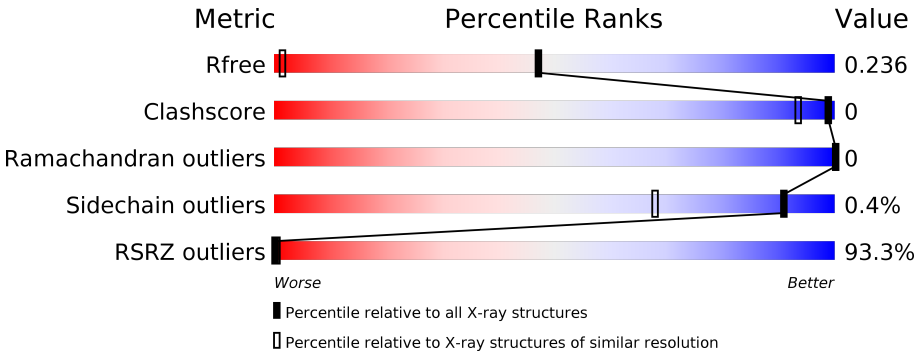
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 0.97 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	1166 (1.06-0.90)
Clashscore	141614	1241 (1.06-0.90)
Ramachandran outliers	138981	1159 (1.06-0.90)
Sidechain outliers	138945	1161 (1.06-0.90)
RSRZ outliers	127900	1132 (1.06-0.90)

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 <=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	419	74% 77% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2578 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 Endothiapepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2462	1566	367	527	2	3	19	0

- Molecule 2 is water.

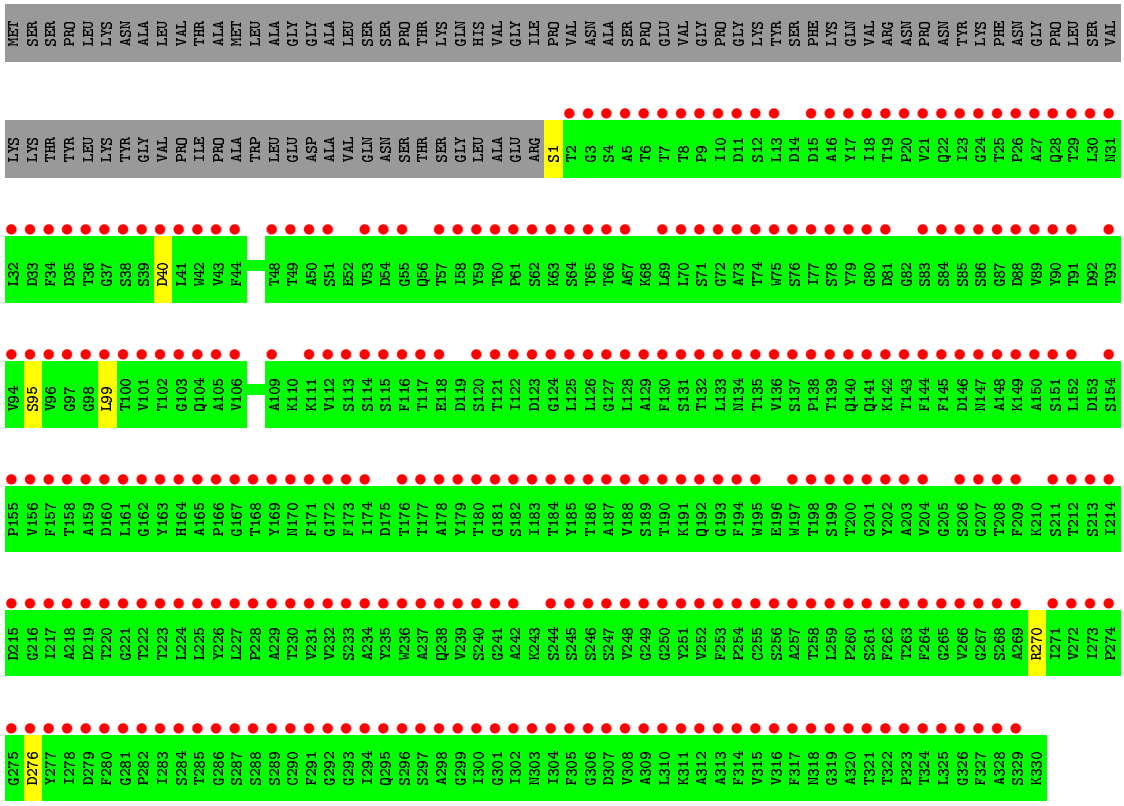
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	116	116	116	0	0

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: Endothiapepsin

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.18Å 72.85Å 52.42Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	49.56 – 0.97 49.51 – 0.97	Depositor EDS
% Data completeness (in resolution range)	91.3 (49.56-0.97) 91.3 (49.51-0.97)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 0.97Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
R, R_{free}	0.244 , 0.244 0.239 , 0.236	Depositor DCC
R_{free} test set	8615 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	9.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2578	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.85	1/2552 (0.0%)	0.89	2/3496 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	SER	CA-CB	-5.02	1.45	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	A	270	ARG	NE-CZ-NH2	-5.37	117.61	120.30

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	2462	0	2329	2	0
2	A	116	0	0	0	0
All	All	2578	0	2329	2	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 0.

All (2) 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:276[B]:ASP:N	1:A:276[B]:ASP:OD1	2.53	0.41
1:A:95:SER:HA	1:A:99:LEU:O	2.20	0.41

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	347/419 (83%)	344 (99%)	3 (1%)	0	100 100

There are no Ramachandran outliers to report.

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	270/336 (80%)	269 (100%)	1 (0%)	91 68

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	330/419 (78%)	3.62	308 (93%)	0	0	7, 10, 17, 23	0

All (308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300[A]	ILE	9.5
1	A	321	THR	8.5
1	A	150	ALA	8.1
1	A	231	VAL	7.6
1	A	259	LEU	7.4
1	A	236	TRP	7.0
1	A	75	TRP	6.8
1	A	248	VAL	6.7
1	A	299[A]	GLY	6.7
1	A	310	LEU	6.0
1	A	271	ILE	6.0
1	A	122	ILE	5.9
1	A	174[A]	ILE	5.8
1	A	322	THR	5.8
1	A	23	ILE	5.8
1	A	294	ILE	5.7
1	A	234	ALA	5.7
1	A	209	PHE	5.6
1	A	264	PHE	5.6
1	A	229	ALA	5.6
1	A	255	CYS	5.4
1	A	34	PHE	5.4
1	A	232	VAL	5.4
1	A	18	ILE	5.4
1	A	197	TRP	5.4
1	A	21	VAL	5.4
1	A	42	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	312	ALA	5.3
1	A	325[A]	LEU	5.3
1	A	128	LEU	5.2
1	A	239	VAL	5.2
1	A	151	SER	5.2
1	A	25	THR	5.2
1	A	258	THR	5.2
1	A	252	VAL	5.2
1	A	298[A]	ALA	5.1
1	A	10	ILE	5.1
1	A	320	ALA	5.0
1	A	32	LEU	5.0
1	A	315	VAL	5.0
1	A	59	TYR	5.0
1	A	273	ILE	5.0
1	A	129	ALA	5.0
1	A	135	THR	5.0
1	A	247	SER	5.0
1	A	41	LEU	4.9
1	A	291	PHE	4.9
1	A	136	VAL	4.9
1	A	144	PHE	4.9
1	A	139	THR	4.8
1	A	157	PHE	4.8
1	A	227	LEU	4.8
1	A	115	SER	4.8
1	A	278	ILE	4.8
1	A	130	PHE	4.8
1	A	192	GLN	4.8
1	A	198	THR	4.7
1	A	317	PHE	4.7
1	A	285	THR	4.7
1	A	165	ALA	4.7
1	A	257	ALA	4.7
1	A	204	VAL	4.7
1	A	183	ILE	4.7
1	A	302	ILE	4.7
1	A	20	PRO	4.6
1	A	195	TRP	4.6
1	A	126	LEU	4.6
1	A	116	PHE	4.6
1	A	327	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	145	PHE	4.5
1	A	58	ILE	4.5
1	A	283	ILE	4.5
1	A	254	PRO	4.5
1	A	253	PHE	4.5
1	A	240[A]	SER	4.4
1	A	137	SER	4.4
1	A	43	VAL	4.4
1	A	208	THR	4.4
1	A	76	SER	4.4
1	A	230	THR	4.4
1	A	304	ILE	4.4
1	A	316	VAL	4.4
1	A	251	TYR	4.4
1	A	224	LEU	4.3
1	A	163	TYR	4.3
1	A	246[A]	SER	4.3
1	A	89	VAL	4.3
1	A	94	VAL	4.3
1	A	226	TYR	4.3
1	A	277	TYR	4.3
1	A	87	GLY	4.3
1	A	282	PRO	4.3
1	A	161	LEU	4.3
1	A	17	TYR	4.3
1	A	7	THR	4.3
1	A	184	THR	4.3
1	A	173	PHE	4.3
1	A	194	PHE	4.3
1	A	80	GLY	4.2
1	A	133	LEU	4.2
1	A	305	PHE	4.2
1	A	112	VAL	4.2
1	A	90	TYR	4.2
1	A	235	TYR	4.2
1	A	158	THR	4.2
1	A	225	LEU	4.1
1	A	266	VAL	4.1
1	A	49	THR	4.1
1	A	77	ILE	4.1
1	A	220	THR	4.1
1	A	222	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	309	ALA	4.1
1	A	202	TYR	4.1
1	A	19	THR	4.1
1	A	214	ILE	4.1
1	A	146	ASP	4.0
1	A	60	THR	4.0
1	A	169	TYR	4.0
1	A	114	SER	4.0
1	A	326	GLY	4.0
1	A	188	VAL	4.0
1	A	51	SER	3.9
1	A	256	SER	3.9
1	A	185	TYR	3.9
1	A	290	CYS	3.9
1	A	16	ALA	3.9
1	A	37	GLY	3.9
1	A	121	THR	3.9
1	A	308	VAL	3.9
1	A	98	GLY	3.9
1	A	217	ILE	3.9
1	A	96	VAL	3.9
1	A	125	LEU	3.9
1	A	24	GLY	3.9
1	A	27	ALA	3.8
1	A	269	ALA	3.8
1	A	280	PHE	3.8
1	A	36	THR	3.8
1	A	57	THR	3.8
1	A	138	PRO	3.8
1	A	30	LEU	3.8
1	A	262	PHE	3.8
1	A	93	THR	3.8
1	A	149[A]	LYS	3.8
1	A	50	ALA	3.8
1	A	313	ALA	3.8
1	A	215[A]	ASP	3.7
1	A	100	THR	3.7
1	A	314	PHE	3.7
1	A	105	ALA	3.7
1	A	101	VAL	3.7
1	A	70	LEU	3.7
1	A	44	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	3.7
1	A	106	VAL	3.7
1	A	103	GLY	3.7
1	A	5	ALA	3.6
1	A	97	GLY	3.6
1	A	69	LEU	3.6
1	A	6	THR	3.6
1	A	81	ASP	3.6
1	A	84	SER	3.6
1	A	73	ALA	3.6
1	A	293	GLY	3.6
1	A	186	THR	3.6
1	A	272	VAL	3.6
1	A	156	VAL	3.5
1	A	159	ALA	3.5
1	A	26	PRO	3.5
1	A	228	PRO	3.5
1	A	242	ALA	3.5
1	A	328	ALA	3.5
1	A	13	LEU	3.5
1	A	143	THR	3.4
1	A	86	SER	3.4
1	A	91	THR	3.4
1	A	276[A]	ASP	3.4
1	A	113	SER	3.4
1	A	203	ALA	3.4
1	A	201	GLY	3.4
1	A	8	THR	3.3
1	A	74	THR	3.3
1	A	199	SER	3.3
1	A	99	LEU	3.3
1	A	297	SER	3.3
1	A	223	THR	3.3
1	A	29	THR	3.3
1	A	324	THR	3.3
1	A	166	PRO	3.3
1	A	233	SER	3.3
1	A	67	ALA	3.2
1	A	237	ALA	3.2
1	A	171	PHE	3.2
1	A	182[A]	SER	3.2
1	A	274	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	152	LEU	3.2
1	A	187	ALA	3.2
1	A	78	SER	3.2
1	A	168	THR	3.2
1	A	127	GLY	3.2
1	A	238	GLN	3.2
1	A	148	ALA	3.1
1	A	132	THR	3.1
1	A	177	THR	3.1
1	A	301	GLY	3.1
1	A	296	SER	3.1
1	A	193	GLY	3.1
1	A	318	ASN	3.1
1	A	2	THR	3.1
1	A	190	THR	3.1
1	A	263	THR	3.1
1	A	164	HIS	3.0
1	A	123	ASP	3.0
1	A	249	GLY	3.0
1	A	65	THR	3.0
1	A	104	GLN	3.0
1	A	124	GLY	3.0
1	A	64	SER	2.9
1	A	22	GLN	2.9
1	A	117	THR	2.9
1	A	218	ALA	2.9
1	A	167	GLY	2.9
1	A	306	GLY	2.9
1	A	66	THR	2.9
1	A	212	THR	2.9
1	A	53	VAL	2.9
1	A	54	ASP	2.9
1	A	9[A]	PRO	2.9
1	A	213	SER	2.8
1	A	221	GLY	2.8
1	A	179	TYR	2.8
1	A	155	PRO	2.8
1	A	102	THR	2.8
1	A	141	GLN	2.8
1	A	160	ASP	2.8
1	A	284	SER	2.8
1	A	292	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	295	GLN	2.8
1	A	120	SER	2.8
1	A	289[A]	SER	2.8
1	A	72	GLY	2.8
1	A	275	GLY	2.8
1	A	319	GLY	2.8
1	A	39	SER	2.7
1	A	48	THR	2.7
1	A	260	PRO	2.7
1	A	176	THR	2.7
1	A	180	THR	2.7
1	A	216	GLY	2.7
1	A	4	SER	2.7
1	A	79	TYR	2.7
1	A	181	GLY	2.7
1	A	200	THR	2.7
1	A	279	ASP	2.6
1	A	265	GLY	2.6
1	A	162	GLY	2.6
1	A	134	ASN	2.6
1	A	323	PRO	2.6
1	A	286	GLY	2.6
1	A	62	SER	2.6
1	A	85	SER	2.6
1	A	288	SER	2.5
1	A	178	ALA	2.5
1	A	38	SER	2.5
1	A	244	SER	2.5
1	A	329	SER	2.5
1	A	303	ASN	2.5
1	A	83	SER	2.5
1	A	287	SER	2.5
1	A	154[A]	SER	2.5
1	A	63	LYS	2.4
1	A	172	GLY	2.4
1	A	71[A]	SER	2.4
1	A	241	GLY	2.4
1	A	61	PRO	2.4
1	A	307	ASP	2.4
1	A	281	GLY	2.4
1	A	31	ASN	2.4
1	A	211	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	40	ASP	2.3
1	A	170	ASN	2.3
1	A	261	SER	2.3
1	A	207	GLY	2.3
1	A	147	ASN	2.3
1	A	12	SER	2.3
1	A	28	GLN	2.3
1	A	55	GLY	2.3
1	A	88	ASP	2.3
1	A	268[A]	SER	2.2
1	A	140	GLN	2.2
1	A	35	ASP	2.2
1	A	118	GLU	2.2
1	A	3	GLY	2.2
1	A	111	LYS	2.2
1	A	15	ASP	2.2
1	A	250	GLY	2.1
1	A	267	GLY	2.1
1	A	131	SER	2.1
1	A	311[A]	LYS	2.1
1	A	11	ASP	2.1
1	A	219	ASP	2.1
1	A	245	SER	2.1
1	A	189	SER	2.1
1	A	206[A]	SER	2.1
1	A	142	LYS	2.1
1	A	191	LYS	2.0
1	A	95	SER	2.0
1	A	33	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.