



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:13 PM GMT

PDB ID : 1WP8
Title : crystal structure of Hendra Virus fusion core
Authors : Xu, Y.; Liu, Y.; Lou, Z.; Su, N.; Bai, Z.; Gao, G.F.; Rao, Z.
Deposited on : 2004-08-31
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

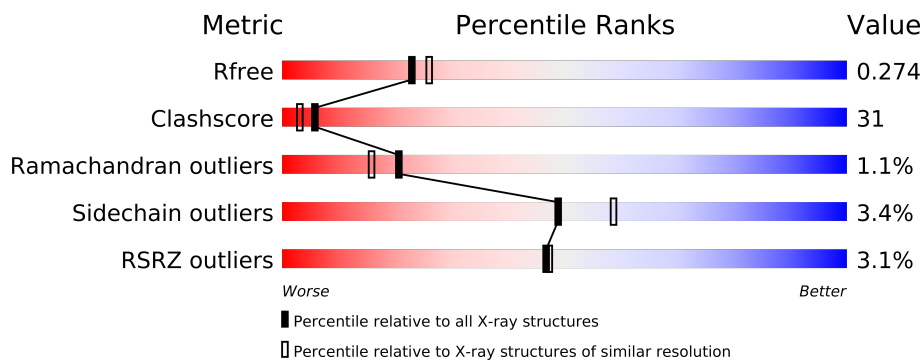
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	89	
1	B	89	
1	C	89	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1670 atoms, of which 0 are hydrogen and 0 are deuterium.

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 fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	64	Total	C	N	O	S	0	0	0
			499	309	82	107	1			
1	B	64	Total	C	N	O	S	0	0	0
			497	309	81	106	1			
1	C	63	Total	C	N	O	S	0	0	0
			491	303	81	106	1			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	-	LINKER	UNP Q8QU00
A	446	GLY	-	LINKER	UNP Q8QU00
A	447	SER	-	LINKER	UNP Q8QU00
A	448	GLY	-	LINKER	UNP Q8QU00
A	449	GLY	-	LINKER	UNP Q8QU00
A	450	SER	-	LINKER	UNP Q8QU00
A	451	GLY	-	LINKER	UNP Q8QU00
A	452	GLY	-	LINKER	UNP Q8QU00
A	486	HIS	-	EXPRESSION TAG	UNP Q8QU00
A	487	HIS	-	EXPRESSION TAG	UNP Q8QU00
A	488	HIS	-	EXPRESSION TAG	UNP Q8QU00
A	489	HIS	-	EXPRESSION TAG	UNP Q8QU00
A	490	HIS	-	EXPRESSION TAG	UNP Q8QU00
A	491	HIS	-	EXPRESSION TAG	UNP Q8QU00
B	445	GLY	-	LINKER	UNP Q8QU00
B	446	GLY	-	LINKER	UNP Q8QU00
B	447	SER	-	LINKER	UNP Q8QU00
B	448	GLY	-	LINKER	UNP Q8QU00
B	449	GLY	-	LINKER	UNP Q8QU00
B	450	SER	-	LINKER	UNP Q8QU00
B	451	GLY	-	LINKER	UNP Q8QU00
B	452	GLY	-	LINKER	UNP Q8QU00
B	486	HIS	-	EXPRESSION TAG	UNP Q8QU00

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Chain	Residue	Modelled	Actual	Comment	Reference
B	487	HIS	-	EXPRESSION TAG	UNP Q8QU00
B	488	HIS	-	EXPRESSION TAG	UNP Q8QU00
B	489	HIS	-	EXPRESSION TAG	UNP Q8QU00
B	490	HIS	-	EXPRESSION TAG	UNP Q8QU00
B	491	HIS	-	EXPRESSION TAG	UNP Q8QU00
C	445	GLY	-	LINKER	UNP Q8QU00
C	446	GLY	-	LINKER	UNP Q8QU00
C	447	SER	-	LINKER	UNP Q8QU00
C	448	GLY	-	LINKER	UNP Q8QU00
C	449	GLY	-	LINKER	UNP Q8QU00
C	450	SER	-	LINKER	UNP Q8QU00
C	451	GLY	-	LINKER	UNP Q8QU00
C	452	GLY	-	LINKER	UNP Q8QU00
C	486	HIS	-	EXPRESSION TAG	UNP Q8QU00
C	487	HIS	-	EXPRESSION TAG	UNP Q8QU00
C	488	HIS	-	EXPRESSION TAG	UNP Q8QU00
C	489	HIS	-	EXPRESSION TAG	UNP Q8QU00
C	490	HIS	-	EXPRESSION TAG	UNP Q8QU00
C	491	HIS	-	EXPRESSION TAG	UNP Q8QU00

- Molecule 2 is water.

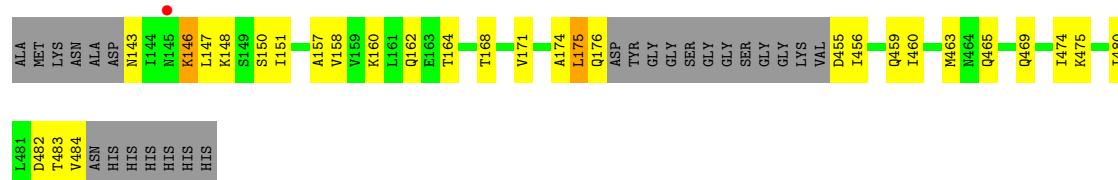
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	B	65	Total O 65 65	0	0
2	C	60	Total O 60 60	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: fusion

Chain A: 



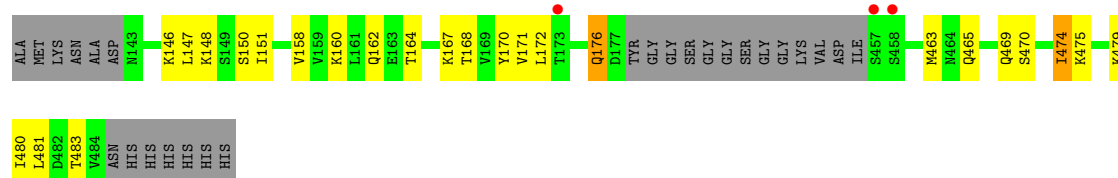
- Molecule 1: fusion

Chain B: 



- Molecule 1: fusion

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	32.19Å 31.90Å 53.87Å 86.33° 86.16° 67.98°	Depositor
Resolution (Å)	35.00 – 2.20 29.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.20) 94.1 (29.81-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.274 0.212 , 0.274	Depositor DCC
R_{free} test set	504 reflections (5.61%)	DCC
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.9	EDS
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 9875 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1670	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.56 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.4554e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.34	0/499	0.51	0/670
1	B	0.34	0/497	0.49	0/668
1	C	0.35	0/491	0.54	0/659
All	All	0.34	0/1487	0.52	0/1997

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	499	0	515	38	0
1	B	497	0	516	32	0
1	C	491	0	504	32	0
2	A	58	0	0	12	0
2	B	65	0	0	15	0
2	C	60	0	0	11	0
All	All	1670	0	1535	95	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (95) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:151:ILE:HD13	1:C:151:ILE:HD11	1.37	1.07
1:A:146:LYS:HG2	1:A:484:VAL:HG22	1.43	0.98
1:A:146:LYS:HB2	1:A:146:LYS:HZ3	1.39	0.88
1:A:146:LYS:HE2	1:A:484:VAL:HA	1.56	0.88
1:C:164:THR:HA	2:C:549:HOH:O	1.76	0.86
1:A:147:LEU:O	1:A:151:ILE:HG12	1.78	0.82
1:B:151:ILE:HB	2:B:512:HOH:O	1.80	0.82
1:A:168:THR:HA	2:A:519:HOH:O	1.82	0.79
1:A:474:ILE:HG12	2:C:538:HOH:O	1.84	0.77
1:C:158:VAL:O	1:C:162:GLN:HG3	1.85	0.76
1:B:146:LYS:HB3	2:B:501:HOH:O	1.89	0.72
1:A:455:ASP:O	1:A:459:GLN:HG2	1.90	0.71
1:C:150:SER:HB2	1:C:480:ILE:HG22	1.75	0.69
1:A:174:ALA:O	1:A:176:GLN:N	2.26	0.67
1:A:463:MET:SD	2:A:545:HOH:O	2.53	0.67
1:C:463:MET:HG2	2:C:549:HOH:O	1.94	0.66
1:A:143:ASN:HA	1:A:146:LYS:NZ	2.13	0.64
1:B:151:ILE:CD1	1:C:151:ILE:HD11	2.21	0.64
1:B:474:ILE:HA	2:B:538:HOH:O	1.98	0.63
1:B:480:ILE:HG12	2:B:547:HOH:O	1.97	0.63
1:B:172:LEU:HD13	1:C:171:VAL:HG21	1.81	0.62
1:B:148:LYS:HG3	1:C:481:LEU:HD11	1.81	0.61
1:B:154:THR:HA	2:B:538:HOH:O	1.99	0.61
1:B:154:THR:HG22	2:B:536:HOH:O	2.00	0.61
1:B:167:LYS:O	1:B:171:VAL:HG23	2.01	0.60
1:A:143:ASN:HA	1:A:146:LYS:HZ1	1.67	0.59
1:B:459:GLN:HA	2:B:543:HOH:O	2.00	0.59
1:C:167:LYS:HA	1:C:170:TYR:CD1	2.36	0.59
1:A:158:VAL:O	1:A:162:GLN:HG3	2.03	0.58
1:B:474:ILE:O	1:B:478:GLN:HG3	2.03	0.58
1:A:175:LEU:O	1:A:176:GLN:HG3	2.03	0.58
1:C:475:LYS:HD3	2:C:508:HOH:O	2.04	0.58
1:A:146:LYS:HD2	1:A:483:THR:HB	1.86	0.58
2:A:521:HOH:O	1:C:162:GLN:HG2	2.04	0.56
1:B:454:VAL:HG12	1:B:455:ASP:OD2	2.05	0.56
1:B:461:SER:O	1:B:465:GLN:HG3	2.05	0.56
1:A:147:LEU:HD21	2:C:525:HOH:O	2.06	0.56
1:A:146:LYS:HG2	1:A:484:VAL:CG2	2.26	0.55
1:B:468:GLN:HA	1:B:471:LYS:HE2	1.87	0.55
1:B:468:GLN:HA	1:B:471:LYS:CE	2.36	0.55
1:C:463:MET:HA	2:C:549:HOH:O	2.07	0.54
1:B:167:LYS:HD2	2:B:543:HOH:O	2.06	0.54
1:C:465:GLN:O	1:C:469:GLN:HG3	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:168:THR:O	1:C:171:VAL:HG22	2.08	0.54
1:C:146:LYS:NZ	1:C:483:THR:HB	2.23	0.53
1:B:158:VAL:O	1:B:162:GLN:HG3	2.09	0.53
1:A:475:LYS:HE3	2:A:501:HOH:O	2.11	0.51
1:C:147:LEU:O	1:C:151:ILE:HG12	2.09	0.51
1:B:146:LYS:HB2	2:B:542:HOH:O	2.10	0.51
1:A:456:ILE:HB	1:C:176:GLN:NE2	2.26	0.51
1:A:150:SER:HB2	1:A:480:ILE:HG22	1.91	0.51
1:A:465:GLN:HG3	1:A:469:GLN:HE21	1.76	0.51
1:A:459:GLN:O	1:A:463:MET:HG3	2.11	0.50
1:B:454:VAL:HG12	1:B:455:ASP:N	2.26	0.50
1:C:160:LYS:HB3	1:C:470:SER:HB2	1.93	0.50
1:A:455:ASP:HB2	2:A:506:HOH:O	2.11	0.50
1:C:171:VAL:HG23	1:C:172:LEU:N	2.27	0.50
1:B:155:ASN:HA	2:B:536:HOH:O	2.12	0.48
1:A:456:ILE:O	1:A:460:ILE:HG13	2.13	0.48
1:A:146:LYS:HD2	1:A:483:THR:CB	2.44	0.48
1:A:463:MET:HB2	2:A:531:HOH:O	2.13	0.47
1:A:150:SER:HB2	1:A:480:ILE:CG2	2.45	0.47
2:A:546:HOH:O	1:C:158:VAL:HG21	2.14	0.46
1:A:146:LYS:CB	1:A:146:LYS:HZ3	2.21	0.46
1:B:480:ILE:HG13	2:B:500:HOH:O	2.15	0.46
1:A:175:LEU:C	1:A:176:GLN:HG3	2.37	0.45
1:C:481:LEU:HD13	2:C:550:HOH:O	2.15	0.45
1:C:172:LEU:HB2	2:C:544:HOH:O	2.15	0.45
1:A:474:ILE:HD13	2:A:546:HOH:O	2.17	0.45
1:C:146:LYS:HD3	1:C:483:THR:OG1	2.16	0.45
1:B:146:LYS:HD3	1:B:483:THR:HG22	1.99	0.44
1:B:484:VAL:HG22	2:B:542:HOH:O	2.17	0.44
1:B:454:VAL:HA	2:B:522:HOH:O	2.17	0.44
1:A:146:LYS:HB2	1:A:146:LYS:NZ	2.20	0.44
1:C:483:THR:HG21	2:C:546:HOH:O	2.18	0.44
1:A:150:SER:HB3	2:A:532:HOH:O	2.18	0.44
1:B:150:SER:HB3	1:B:480:ILE:CG2	2.48	0.43
1:A:164:THR:O	2:A:545:HOH:O	2.21	0.43
1:A:160:LYS:HA	1:A:160:LYS:HD3	1.68	0.43
2:B:494:HOH:O	1:C:481:LEU:HD23	2.17	0.43
1:C:474:ILE:CG2	1:C:475:LYS:N	2.81	0.43
1:C:479:LYS:HZ3	1:C:479:LYS:HB3	1.82	0.43
1:A:146:LYS:CE	1:A:484:VAL:HA	2.39	0.43
1:B:156:GLU:OE1	1:B:156:GLU:HA	2.18	0.42
1:A:157:ALA:HB3	2:A:546:HOH:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:LYS:HD2	1:B:484:VAL:HB	2.02	0.41
1:A:171:VAL:HB	2:A:519:HOH:O	2.20	0.41
1:B:483:THR:HG22	1:B:483:THR:O	2.20	0.41
1:C:146:LYS:HZ2	1:C:483:THR:HB	1.85	0.41
1:C:160:LYS:HE3	2:C:505:HOH:O	2.21	0.41
1:A:174:ALA:C	1:A:176:GLN:H	2.17	0.41
2:B:512:HOH:O	1:C:481:LEU:HD11	2.20	0.41
1:B:169:VAL:HG22	1:C:463:MET:HE2	2.03	0.40
1:C:148:LYS:HB2	2:C:525:HOH:O	2.21	0.40
1:B:160:LYS:HE3	1:B:469:GLN:OE1	2.21	0.40

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	60/89 (67%)	59 (98%)	0	1 (2%)	14	8
1	B	60/89 (67%)	58 (97%)	1 (2%)	1 (2%)	14	8
1	C	59/89 (66%)	59 (100%)	0	0	100	100
All	All	179/267 (67%)	176 (98%)	1 (1%)	2 (1%)	21	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
1	B	456	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	60/77 (78%)	58 (97%)	2 (3%)	50	60
1	B	60/77 (78%)	58 (97%)	2 (3%)	50	60
1	C	59/77 (77%)	57 (97%)	2 (3%)	49	59
All	All	179/231 (78%)	173 (97%)	6 (3%)	49	59

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	LYS
1	A	482	ASP
1	B	455	ASP
1	B	457	SER
1	C	176	GLN
1	C	474	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	176	GLN
1	A	469	GLN
1	B	478	GLN
1	C	176	GLN
1	C	464	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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, 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	64/89 (71%)	-0.14	1 (1%) 68 69	14, 23, 43, 48	0
1	B	64/89 (71%)	0.12	2 (3%) 47 47	12, 25, 37, 54	0
1	C	63/89 (70%)	0.00	3 (4%) 29 29	13, 24, 37, 54	0
All	All	191/267 (71%)	-0.01	6 (3%) 47 47	12, 24, 39, 54	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	454	VAL	2.6
1	C	457	SER	2.5
1	C	173	THR	2.3
1	C	458	SER	2.3
1	B	143	ASN	2.2
1	A	145	ASN	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.