



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:33 AM GMT

PDB ID : 3GP8
Title : Crystal structure of the binary complex of RecD2 with DNA
Authors : Saikrishnan, K.; Cook, N.; Wigley, D.B.
Deposited on : 2009-03-23
Resolution : 2.50 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>

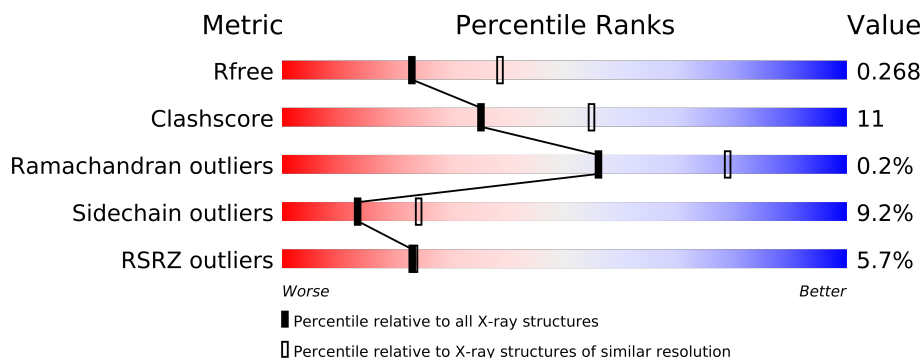
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	574	
2	X	14	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4435 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 Exodeoxyribonuclease V, subunit RecD, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4088	2565	763	750	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	MET	-	EXPRESSION TAG	UNP Q9RT63
A	716	LEU	-	EXPRESSION TAG	UNP Q9RT63
A	717	GLU	-	EXPRESSION TAG	UNP Q9RT63
A	718	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	719	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	720	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	721	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	722	HIS	-	EXPRESSION TAG	UNP Q9RT63
A	723	HIS	-	EXPRESSION TAG	UNP Q9RT63

- Molecule 2 is a DNA chain called 5'-D(*TP*TP*TP*TP*TP*T*TP*TP*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	8	Total	C	N	O	P	0	0	0
			157	80	16	54	7			

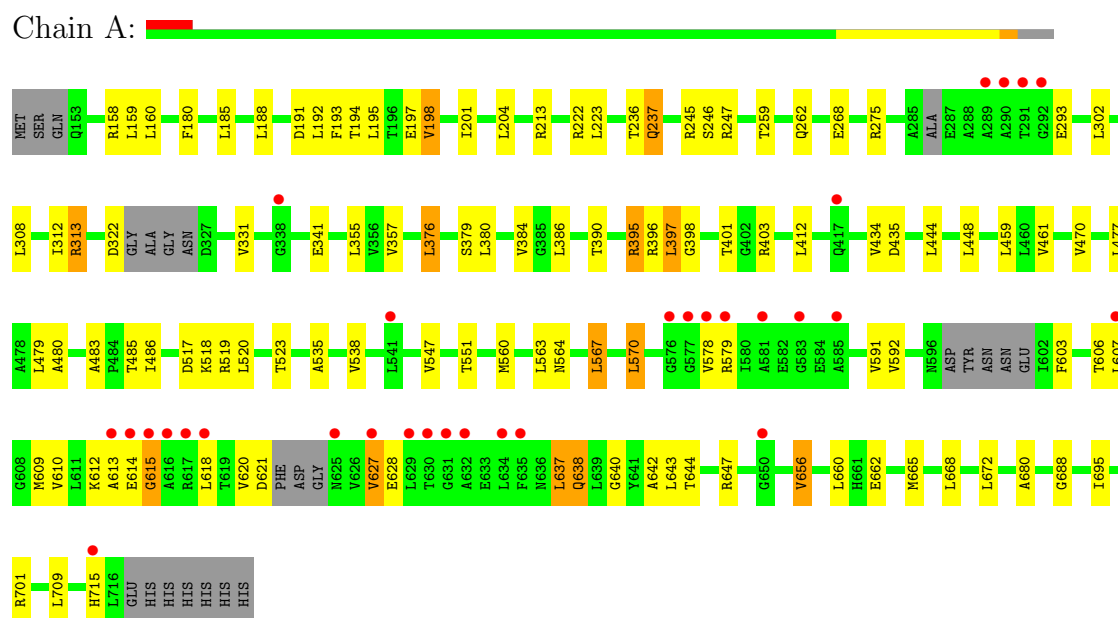
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	186	Total	O	0	0
			186	186		
3	X	4	Total	O	0	0
			4	4		

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: Exodeoxyribonuclease V, subunit RecD, putative



- Molecule 2: 5'-D(*TP*TP*TP*TP*TP*T*TP*TP*TP*TP*TP*TP*TP*T)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.14Å 90.32Å 142.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.18 – 2.50 38.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.18-2.50) 99.0 (38.88-2.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.22 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.268 0.231 , 0.268	Depositor DCC
R_{free} test set	1256 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 24588 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4435	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.42	0/4157	0.60	0/5646
2	X	0.95	0/172	1.74	4/264 (1.5%)
All	All	0.45	0/4329	0.69	4/5910 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	2	DT	C5-C4-O4	-6.01	120.69	124.90
2	X	2	DT	N3-C4-O4	5.52	123.21	119.90
2	X	5	DT	C4-C5-C7	5.52	122.31	119.00
2	X	7	DT	O4'-C1'-N1	-5.33	104.27	108.00

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	4088	0	4121	89	0
2	X	157	0	98	5	0
3	A	186	0	0	1	0
3	X	4	0	0	0	0
All	All	4435	0	4219	90	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 11.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:435:ASP:HA	1:A:461:VAL:HG13	1.46	0.95
1:A:591:VAL:CG1	1:A:637:LEU:HD23	1.97	0.94
1:A:591:VAL:HG11	1:A:637:LEU:HD23	1.50	0.91
1:A:656:VAL:CG1	1:A:680:ALA:HB2	2.02	0.88
1:A:591:VAL:HG11	1:A:637:LEU:CD2	2.07	0.84
1:A:357:VAL:HB	1:A:485:THR:HG22	1.60	0.83
1:A:665:MET:HE1	1:A:668:LEU:HD12	1.58	0.83
1:A:560:MET:CE	1:A:644:THR:HG23	2.08	0.82
1:A:560:MET:HE3	1:A:644:THR:HG23	1.63	0.78
1:A:560:MET:HE2	1:A:644:THR:N	1.98	0.77
1:A:480:ALA:HA	1:A:485:THR:HG21	1.67	0.76
1:A:592:VAL:HG11	1:A:643:LEU:HD21	1.69	0.73
1:A:180:PHE:CZ	1:A:194:THR:CG2	2.79	0.66
1:A:483:ALA:O	1:A:485:THR:HG23	1.95	0.66
1:A:560:MET:CE	1:A:644:THR:H	2.10	0.65
1:A:197:GLU:OE2	1:A:275:ARG:HD2	1.98	0.64
1:A:665:MET:CE	1:A:668:LEU:HD12	2.28	0.62
1:A:560:MET:CE	1:A:644:THR:N	2.63	0.61
1:A:592:VAL:HG12	1:A:607:LEU:HD23	1.83	0.61
1:A:160:LEU:C	1:A:160:LEU:HD23	2.22	0.60
1:A:434:VAL:HG21	1:A:448:LEU:HD21	1.84	0.60
1:A:237:GLN:HB2	2:X:2:DT:O4	2.02	0.60
1:A:578:VAL:HG23	1:A:613:ALA:HB1	1.85	0.59
1:A:357:VAL:HB	1:A:485:THR:CG2	2.32	0.59
1:A:592:VAL:HG13	1:A:640:GLY:HA3	1.86	0.58
1:A:560:MET:HE2	1:A:644:THR:HG23	1.82	0.58
1:A:564:ASN:HD21	1:A:642:ALA:H	1.52	0.58
1:A:198:VAL:HG21	1:A:201:ILE:HD12	1.86	0.57
1:A:313:ARG:HG3	1:A:715:HIS:HB3	1.86	0.56
1:A:672:LEU:HD13	1:A:672:LEU:C	2.27	0.54
1:A:390:THR:HG22	2:X:5:DT:H1'	1.90	0.54
1:A:188:LEU:HD22	1:A:195:LEU:HG	1.90	0.53
1:A:191:ASP:O	1:A:194:THR:HB	2.08	0.53
1:A:610:VAL:HA	1:A:620:VAL:HG22	1.91	0.53
1:A:384:VAL:HG12	1:A:386:LEU:HD12	1.91	0.53
1:A:538:VAL:HG13	1:A:547:VAL:CG1	2.38	0.53
1:A:312:ILE:HD13	1:A:479:LEU:HD21	1.90	0.52
1:A:398:GLY:HA2	1:A:401:THR:HG22	1.91	0.52
1:A:520:LEU:O	1:A:520:LEU:HD23	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:656:VAL:HG13	1:A:680:ALA:HB2	1.88	0.52
1:A:412:LEU:HD11	1:A:448:LEU:HA	1.93	0.51
1:A:560:MET:HE3	1:A:647:ARG:HH11	1.76	0.51
1:A:591:VAL:HG13	1:A:638:GLN:O	2.12	0.50
2:X:3:DT:H72	2:X:4:DT:O4	2.11	0.50
1:A:591:VAL:CG1	1:A:592:VAL:N	2.75	0.49
1:A:563:LEU:O	1:A:567:LEU:HD22	2.12	0.49
1:A:198:VAL:CG2	1:A:201:ILE:HD12	2.42	0.49
1:A:384:VAL:HG12	1:A:386:LEU:CD1	2.42	0.49
1:A:180:PHE:HZ	1:A:194:THR:CG2	2.23	0.49
1:A:386:LEU:HB3	1:A:397:LEU:HD13	1.93	0.49
1:A:665:MET:HE1	1:A:695:ILE:HG21	1.94	0.49
1:A:592:VAL:HG13	1:A:640:GLY:CA	2.43	0.48
1:A:656:VAL:HG11	1:A:680:ALA:HB2	1.92	0.48
1:A:578:VAL:CG2	1:A:613:ALA:HB1	2.44	0.48
1:A:603:PHE:CE2	1:A:606:THR:HG23	2.49	0.48
1:A:376:LEU:HD22	1:A:380:LEU:HD11	1.96	0.48
1:A:259:THR:H	1:A:262:GLN:NE2	2.12	0.48
1:A:610:VAL:HG22	1:A:620:VAL:CG2	2.45	0.47
1:A:647:ARG:HG2	3:A:763:HOH:O	2.15	0.46
1:A:665:MET:CE	1:A:695:ILE:HG21	2.45	0.46
1:A:470:VAL:HB	2:X:5:DT:H73	1.98	0.45
1:A:259:THR:H	1:A:262:GLN:HE21	1.65	0.45
1:A:613:ALA:HB2	1:A:618:LEU:HD23	1.97	0.45
1:A:610:VAL:HG22	1:A:620:VAL:HG22	1.97	0.45
1:A:620:VAL:HG12	1:A:621:ASP:N	2.32	0.45
1:A:246:SER:CB	1:A:293:GLU:OE1	2.65	0.45
1:A:591:VAL:HG12	1:A:637:LEU:HD23	1.89	0.45
1:A:614:GLU:O	1:A:615:GLY:C	2.55	0.45
1:A:401:THR:HG23	1:A:403:ARG:HB2	1.99	0.44
1:A:551:THR:O	1:A:644:THR:HA	2.18	0.44
1:A:180:PHE:CZ	1:A:194:THR:HG22	2.53	0.44
1:A:246:SER:HB3	1:A:293:GLU:OE1	2.18	0.44
1:A:470:VAL:HG11	2:X:4:DT:H1'	1.99	0.43
1:A:609:MET:O	1:A:620:VAL:HG13	2.18	0.43
1:A:486:ILE:HD12	1:A:486:ILE:N	2.33	0.43
1:A:517:ASP:OD1	1:A:518:LYS:N	2.51	0.43
1:A:535:ALA:HB1	1:A:570:LEU:HD12	2.00	0.43
1:A:591:VAL:HG11	1:A:637:LEU:HD22	1.97	0.42
1:A:245:ARG:HH21	1:A:268:GLU:HG3	1.84	0.42
1:A:591:VAL:HG12	1:A:592:VAL:N	2.35	0.42
1:A:627:VAL:HG22	1:A:628:GLU:H	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:398:GLY:CA	1:A:401:THR:HG22	2.49	0.42
1:A:331:VAL:HG23	1:A:331:VAL:O	2.19	0.42
1:A:376:LEU:O	1:A:379:SER:OG	2.29	0.41
1:A:395:ARG:C	1:A:395:ARG:CD	2.89	0.41
1:A:180:PHE:CZ	1:A:194:THR:HG23	2.55	0.41
1:A:401:THR:HG23	1:A:403:ARG:N	2.36	0.41
1:A:660:LEU:O	1:A:688:GLY:HA3	2.21	0.41
1:A:193:PHE:CZ	1:A:222:ARG:HG3	2.55	0.40
1:A:386:LEU:HD22	1:A:401:THR:HG21	2.02	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	541/574 (94%)	519 (96%)	21 (4%)	1 (0%)	56 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	615	GLY

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	403/435 (93%)	366 (91%)	37 (9%)	13 24

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	159	LEU
1	A	185	LEU
1	A	192	LEU
1	A	198	VAL
1	A	204	LEU
1	A	213	ARG
1	A	223	LEU
1	A	236	THR
1	A	237	GLN
1	A	247	ARG
1	A	302	LEU
1	A	308	LEU
1	A	313	ARG
1	A	322	ASP
1	A	341	GLU
1	A	355	LEU
1	A	376	LEU
1	A	395	ARG
1	A	396	ARG
1	A	397	LEU
1	A	444	LEU
1	A	459	LEU
1	A	477	LEU
1	A	519	ARG
1	A	523	THR
1	A	567	LEU
1	A	570	LEU
1	A	579	ARG
1	A	612	LYS
1	A	627	VAL
1	A	637	LEU
1	A	638	GLN
1	A	656	VAL
1	A	662	GLU
1	A	701	ARG
1	A	709	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	262	GLN

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Mol	Chain	Res	Type
1	A	343	GLN
1	A	466	GLN
1	A	502	GLN
1	A	564	ASN
1	A	593	GLN
1	A	638	GLN
1	A	649	GLN
1	A	664	HIS
1	A	671	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	551/574 (95%)	0.35	31 (5%) 24 24	38, 46, 52, 59	1 (0%)
2	X	8/14 (57%)	0.45	1 (12%) 5 4	40, 59, 72, 86	0
All	All	559/588 (95%)	0.35	32 (5%) 23 23	38, 46, 53, 86	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	635	PHE	7.6
1	A	632	ALA	6.6
1	A	613	ALA	6.0
1	A	585	ALA	4.9
1	A	579	ARG	4.9
1	A	578	VAL	4.6
1	A	615	GLY	4.4
1	A	581	ALA	4.1
1	A	614	GLU	3.9
1	A	583	GLY	3.8
1	A	289	ALA	3.8
1	A	634	LEU	3.8
1	A	631	GLY	3.6
1	A	338	GLY	3.6
1	A	577	GLY	3.6
1	A	290	ALA	3.5
1	A	618	LEU	3.4
2	X	8	DT	3.0
1	A	576	GLY	3.0
1	A	291	THR	2.7
1	A	629	LEU	2.7
1	A	625	ASN	2.7
1	A	541	LEU	2.6
1	A	607	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	617	ARG	2.5
1	A	630	THR	2.4
1	A	616	ALA	2.3
1	A	627	VAL	2.3
1	A	292	GLY	2.1
1	A	417	GLN	2.1
1	A	715	HIS	2.0
1	A	650	GLY	2.0

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.