



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 09:33 PM EDT

PDB ID : 4AIL
Title : Crystal Structure of an Evolved Replicating DNA Polymerase
Authors : Wynne, S.A.; Holliger, P.; Leslie, A.G.W.
Deposited on : 2012-02-10
Resolution : 2.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

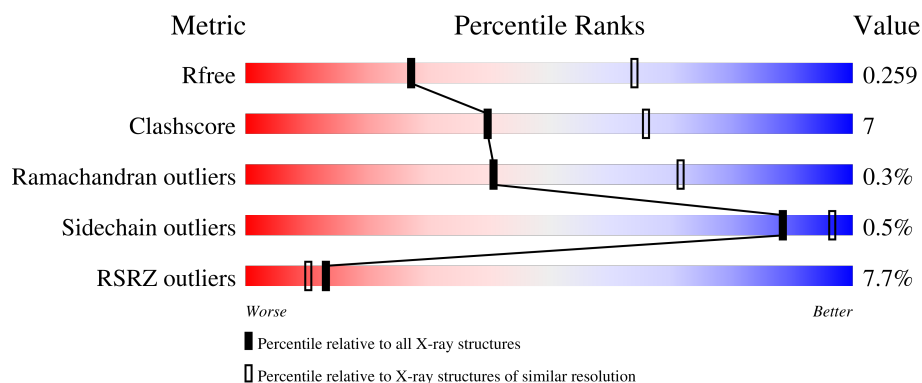
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of 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	11	
2	B	8	
3	C	775	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6553 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 DNA chain called 5'-D(*AP*CP*GP*GP*GP*TP*AP*AP*GP*CP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	8	Total	C	N	O	P	0	0	0
			169	79	35	47	8			

- Molecule 2 is a DNA chain called 5'-D(*TP*GP*CP*TP*TP*AP*CP*DOCP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	P	0	0	0
			160	77	25	50	8			

- Molecule 3 is a protein called DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	750	Total	C	N	O	S	0	0	0
			6145	3985	1021	1125	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	93	GLN	VAL	engineered mutation	UNP P61875
C	141	ALA	ASP	engineered mutation	UNP P61875
C	143	ALA	GLU	engineered mutation	UNP P61875
C	337	ILE	VAL	engineered mutation	UNP P61875
C	399	ASP	GLU	engineered mutation	UNP P61875
C	400	ASP	ASN	engineered mutation	UNP P61875
C	407	ILE	ARG	engineered mutation	UNP P61875
C	546	HIS	TYR	engineered mutation	UNP P61875

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	C	74	Total	O	0	0
			74	74		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	92.85Å 126.77Å 205.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.82 – 2.90 53.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (102.82-2.90) 98.6 (53.96-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0002	Depositor
R, R_{free}	0.227 , 0.259 0.227 , 0.259	Depositor DCC
R_{free} test set	1352 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.2	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	6553	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: DOC

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	0.75	1/190 (0.5%)	0.78	1/290 (0.3%)
2	B	0.84	1/157 (0.6%)	0.88	0/238
3	C	0.27	0/6284	0.47	0/8478
All	All	0.32	2/6631 (0.0%)	0.49	1/9006 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	DT	OP3-P	-10.09	1.49	1.61
1	A	4	DG	OP3-P	-9.83	1.49	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	DA	P-O3'-C3'	5.72	126.56	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	169	0	90	2	0
2	B	160	0	92	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6145	0	6244	91	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	74	0	0	0	0
All	All	6553	0	6426	93	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 7.

All (93) 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)
3:C:687:LEU:HD11	3:C:717:LEU:HD21	1.43	0.98
3:C:651:LEU:HD13	3:C:656:ILE:HD12	1.53	0.90
3:C:416:THR:HG21	3:C:575:LEU:H	1.37	0.87
3:C:464:ILE:HG23	3:C:480:LEU:HD22	1.54	0.87
3:C:264:ILE:HD13	3:C:278:VAL:HG11	1.56	0.86
3:C:5:VAL:HG12	3:C:18:LEU:HD23	1.64	0.79
3:C:684:ALA:HB2	3:C:700:ILE:HD13	1.68	0.76
3:C:386:THR:O	3:C:515:THR:HG21	1.88	0.72
3:C:651:LEU:CD1	3:C:656:ILE:HD12	2.19	0.71
3:C:590:VAL:HG12	3:C:591:THR:HG23	1.76	0.68
3:C:41:LEU:HD13	3:C:80:ILE:HD11	1.77	0.66
3:C:243:ARG:HG2	3:C:248:THR:HG22	1.77	0.65
3:C:341:LEU:O	3:C:341:LEU:HD23	1.98	0.63
3:C:687:LEU:CD1	3:C:717:LEU:HD21	2.26	0.63
3:C:16:ILE:HG21	3:C:120:TYR:CD2	2.33	0.62
3:C:158:ILE:HG23	3:C:299:TRP:CZ3	2.35	0.62
3:C:327:LEU:O	3:C:331:ILE:HG23	2.00	0.62
3:C:641:VAL:HG12	3:C:645:LYS:HE2	1.81	0.62
3:C:209:TYR:HE2	3:C:264:ILE:HD12	1.66	0.61
3:C:606:THR:HG21	3:C:611:ILE:HD12	1.83	0.60
3:C:680:HIS:O	3:C:700:ILE:HD11	2.00	0.60
3:C:644:VAL:HG11	3:C:742:VAL:HG11	1.82	0.60
3:C:129:MET:HE1	3:C:256:ILE:HD11	1.84	0.59
3:C:16:ILE:HG21	3:C:120:TYR:CE2	2.38	0.59
3:C:38:ILE:HG22	3:C:112:TYR:HA	1.85	0.58
3:C:40:ALA:HA	3:C:109:ILE:HG22	1.86	0.58
3:C:159:MET:HE1	3:C:308:VAL:HG12	1.86	0.58
3:C:438:VAL:HG11	3:C:512:GLU:HG2	1.86	0.57
3:C:619:ILE:CD1	3:C:656:ILE:HD13	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:688:ALA:HB2	3:C:694:ILE:HD13	1.85	0.57
3:C:540:ILE:HG23	3:C:545:LEU:HD23	1.87	0.57
3:C:618:GLU:HB3	3:C:660:LYS:HA	1.86	0.57
3:C:666:GLN:HE21	3:C:668:THR:HG22	1.69	0.57
3:C:39:TYR:HB3	3:C:82:VAL:HG11	1.89	0.55
3:C:604:VAL:HG23	3:C:604:VAL:O	2.06	0.54
1:A:4:DG:H22	2:B:8:DOC:C2	2.21	0.54
3:C:529:LEU:HD23	3:C:537:VAL:CG2	2.38	0.54
3:C:260:LEU:HD21	3:C:323:GLY:HA2	1.90	0.54
3:C:158:ILE:HG23	3:C:299:TRP:CH2	2.44	0.53
3:C:331:ILE:HG22	3:C:341:LEU:HD12	1.91	0.52
3:C:651:LEU:HD21	3:C:733:TYR:HB3	1.92	0.52
3:C:73:LYS:HA	3:C:365:ASN:ND2	2.25	0.51
3:C:334:SER:HA	3:C:344:VAL:HG21	1.91	0.51
1:A:5:DG:C2'	1:A:6:DT:H71	2.41	0.51
3:C:243:ARG:CG	3:C:248:THR:HG22	2.40	0.51
3:C:341:LEU:HD23	3:C:341:LEU:C	2.32	0.50
3:C:331:ILE:HG22	3:C:341:LEU:CD1	2.41	0.50
3:C:184:VAL:HG13	3:C:189:GLU:HB2	1.95	0.49
3:C:5:VAL:HG23	3:C:117:ALA:HB1	1.93	0.49
3:C:623:THR:CG2	3:C:644:VAL:HG12	2.43	0.49
3:C:702:TYR:HB2	3:C:715:ALA:HB1	1.94	0.49
3:C:364:ARG:NH2	3:C:452:SER:OG	2.47	0.48
3:C:96:ILE:O	3:C:100:VAL:HG23	2.14	0.48
3:C:420:SER:HB3	3:C:451:PRO:HD3	1.96	0.48
3:C:612:VAL:HG22	3:C:612:VAL:O	2.13	0.48
3:C:331:ILE:C	3:C:331:ILE:HD12	2.34	0.48
3:C:468:MET:O	3:C:471:THR:HG22	2.14	0.47
3:C:628:LEU:HD22	3:C:632:LEU:HD11	1.97	0.47
3:C:101:ARG:HG3	3:C:109:ILE:HD11	1.97	0.46
3:C:519:ARG:HA	3:C:522:ILE:HG22	1.98	0.46
3:C:623:THR:O	3:C:627:VAL:HG23	2.16	0.46
3:C:651:LEU:HD23	3:C:734:ILE:HG13	1.97	0.46
3:C:338:GLY:O	3:C:359:ARG:NH2	2.48	0.45
3:C:630:THR:CG2	3:C:640:ALA:HB2	2.46	0.45
3:C:529:LEU:HD23	3:C:537:VAL:HG22	1.98	0.45
3:C:705:LEU:HD22	3:C:716:ILE:HD12	1.99	0.45
3:C:464:ILE:HG23	3:C:480:LEU:CD2	2.36	0.45
3:C:420:SER:HB3	3:C:451:PRO:CD	2.47	0.45
3:C:258:PHE:CD1	3:C:341:LEU:HD21	2.51	0.45
3:C:37:TYR:OH	3:C:119:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:ILE:HG22	3:C:190:MET:HG3	1.98	0.44
3:C:565:VAL:HA	3:C:568:ILE:HG22	2.00	0.44
3:C:687:LEU:HD11	3:C:717:LEU:CD2	2.30	0.44
3:C:450:ILE:HD12	3:C:498:TYR:CE1	2.53	0.44
3:C:684:ALA:HB2	3:C:700:ILE:CD1	2.44	0.44
3:C:734:ILE:HG23	3:C:739:LEU:HD23	2.00	0.44
3:C:205:ILE:CD1	3:C:327:LEU:HD21	2.48	0.43
3:C:15:VAL:HG22	3:C:32:ARG:HG2	2.00	0.43
3:C:588:PHE:CE2	3:C:745:ILE:HG23	2.54	0.43
3:C:194:PHE:CZ	3:C:198:ILE:HD11	2.53	0.43
3:C:138:LEU:HD12	3:C:163:ALA:O	2.19	0.43
3:C:337:ILE:HD12	3:C:352:LEU:O	2.19	0.42
3:C:637:VAL:O	3:C:641:VAL:HG23	2.18	0.42
3:C:271:PRO:HA	3:C:614:ARG:HD3	2.00	0.42
3:C:274:THR:O	3:C:278:VAL:HG23	2.20	0.42
3:C:103:HIS:CD2	3:C:105:ALA:HB3	2.54	0.42
3:C:416:THR:HG21	3:C:575:LEU:N	2.19	0.42
2:B:6:DA:H5'	3:C:613:ARG:HD2	2.01	0.41
3:C:651:LEU:HD21	3:C:733:TYR:CB	2.51	0.41
3:C:474:PRO:O	3:C:478:ILE:HD13	2.19	0.41
3:C:89:HIS:CG	3:C:90:PRO:HD2	2.56	0.41
3:C:203:PRO:HG2	3:C:206:ILE:HD11	2.03	0.41
3:C:569:ASN:HA	3:C:572:LEU:HD12	2.03	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
3	C	746/775 (96%)	709 (95%)	35 (5%)	2 (0%)	41 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	400	ASP
3	C	430	LYS

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	
3	C	655/679 (96%)	652 (100%)	3 (0%)	88	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	331	ILE
3	C	379	ARG
3	C	517	TRP

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

Mol	Chain	Res	Type
3	C	89	HIS
3	C	103	HIS
3	C	257	HIS
3	C	351	ASN
3	C	546	HIS
3	C	666	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	$\# Z > 2$
2	DOC	B	8	1,2	16,19,20	0.33	0	20,26,29	0.57	0

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	DOC	B	8	1,2	-	0/7/18/19	0/2/2/2

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	8	DOC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	8/11 (72%)	0.17	1 (12%) 3 3	72, 94, 130, 156	0
2	B	7/8 (87%)	-0.38	0 100 100	70, 94, 140, 150	0
3	C	750/775 (96%)	0.38	58 (7%) 13 10	43, 75, 144, 168	0
All	All	765/794 (96%)	0.37	59 (7%) 13 10	43, 75, 144, 168	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	647	VAL	6.5
3	C	685	LYS	5.4
3	C	644	VAL	4.8
3	C	681	VAL	4.6
3	C	689	ALA	4.6
3	C	651	LEU	4.4
3	C	733	TYR	4.4
3	C	672	HIS	4.3
3	C	732	TYR	3.9
3	C	705	LEU	3.8
3	C	656	ILE	3.8
3	C	648	ILE	3.7
3	C	721	TYR	3.7
3	C	677	ILE	3.7
3	C	710	PRO	3.6
3	C	657	PRO	3.6
3	C	684	ALA	3.5
3	C	718	ALA	3.4
3	C	700	ILE	3.3
3	C	712	SER	3.3
3	C	701	GLY	3.2
3	C	148	GLU	3.2
3	C	717	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	688	ALA	3.2
3	C	667	ILE	3.2
3	C	654	TYR	3.1
3	C	283	PHE	3.1
3	C	653	ASN	3.1
3	C	687	LEU	3.0
3	C	659	GLU	3.0
3	C	719	GLU	3.0
3	C	728	TYR	2.8
3	C	694	ILE	2.8
3	C	652	ALA	2.7
3	C	674	TYR	2.6
3	C	704	VAL	2.6
3	C	671	LEU	2.6
3	C	734	ILE	2.6
3	C	649	GLN	2.5
3	C	658	PRO	2.5
3	C	686	LYS	2.5
3	C	715	ALA	2.5
3	C	692	VAL	2.4
3	C	646	GLU	2.4
3	C	713	ASN	2.4
3	C	709	GLY	2.3
3	C	158	ILE	2.3
3	C	703	ILE	2.3
3	C	683	VAL	2.3
3	C	307	ARG	2.3
3	C	720	GLU	2.3
3	C	622	GLU	2.2
1	A	4	DG	2.2
3	C	708	ASP	2.2
3	C	682	ALA	2.2
3	C	663	ILE	2.1
3	C	635	GLY	2.1
3	C	642	ARG	2.1
3	C	753	LYS	2.0

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

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	DOC	B	8	18/19	0.94	0.19	73,76,83,84	0

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.