



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:15 PM GMT

PDB ID : 4GCK  
Title : structure of no-dna complex  
Authors : Schumacher, M.A.  
Deposited on : 2012-07-30  
Resolution : 2.05 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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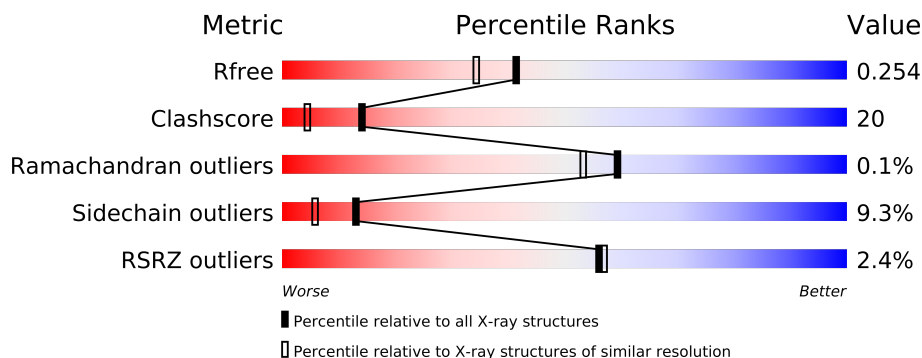
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.05 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	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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  $\geq 3$ , 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	212	
1	B	212	
1	C	212	
1	D	212	
2	W	12	
2	Z	12	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7088 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 Nucleoid occlusion factor SlmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1544	973	279	285	7			
1	B	189	Total	C	N	O	S	0	0	0
			1533	967	275	284	7			
1	C	190	Total	C	N	O	S	0	0	0
			1544	973	279	285	7			
1	D	189	Total	C	N	O	S	0	0	0
			1533	967	275	284	7			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP B5XTG2
A	-12	PRO	-	EXPRESSION TAG	UNP B5XTG2
A	-11	PRO	-	EXPRESSION TAG	UNP B5XTG2
A	-10	GLY	-	EXPRESSION TAG	UNP B5XTG2
A	-9	LYS	-	EXPRESSION TAG	UNP B5XTG2
A	-8	CYS	-	EXPRESSION TAG	UNP B5XTG2
A	-7	LEU	-	EXPRESSION TAG	UNP B5XTG2
A	-6	PHE	-	EXPRESSION TAG	UNP B5XTG2
A	-5	SER	-	EXPRESSION TAG	UNP B5XTG2
A	-4	GLY	-	EXPRESSION TAG	UNP B5XTG2
A	-3	VAL	-	EXPRESSION TAG	UNP B5XTG2
A	-2	PHE	-	EXPRESSION TAG	UNP B5XTG2
A	-1	CYS	-	EXPRESSION TAG	UNP B5XTG2
A	0	ASN	-	EXPRESSION TAG	UNP B5XTG2
B	-13	MET	-	EXPRESSION TAG	UNP B5XTG2
B	-12	PRO	-	EXPRESSION TAG	UNP B5XTG2
B	-11	PRO	-	EXPRESSION TAG	UNP B5XTG2
B	-10	GLY	-	EXPRESSION TAG	UNP B5XTG2
B	-9	LYS	-	EXPRESSION TAG	UNP B5XTG2
B	-8	CYS	-	EXPRESSION TAG	UNP B5XTG2
B	-7	LEU	-	EXPRESSION TAG	UNP B5XTG2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	PHE	-	EXPRESSION TAG	UNP B5XTG2
B	-5	SER	-	EXPRESSION TAG	UNP B5XTG2
B	-4	GLY	-	EXPRESSION TAG	UNP B5XTG2
B	-3	VAL	-	EXPRESSION TAG	UNP B5XTG2
B	-2	PHE	-	EXPRESSION TAG	UNP B5XTG2
B	-1	CYS	-	EXPRESSION TAG	UNP B5XTG2
B	0	ASN	-	EXPRESSION TAG	UNP B5XTG2
C	-13	MET	-	EXPRESSION TAG	UNP B5XTG2
C	-12	PRO	-	EXPRESSION TAG	UNP B5XTG2
C	-11	PRO	-	EXPRESSION TAG	UNP B5XTG2
C	-10	GLY	-	EXPRESSION TAG	UNP B5XTG2
C	-9	LYS	-	EXPRESSION TAG	UNP B5XTG2
C	-8	CYS	-	EXPRESSION TAG	UNP B5XTG2
C	-7	LEU	-	EXPRESSION TAG	UNP B5XTG2
C	-6	PHE	-	EXPRESSION TAG	UNP B5XTG2
C	-5	SER	-	EXPRESSION TAG	UNP B5XTG2
C	-4	GLY	-	EXPRESSION TAG	UNP B5XTG2
C	-3	VAL	-	EXPRESSION TAG	UNP B5XTG2
C	-2	PHE	-	EXPRESSION TAG	UNP B5XTG2
C	-1	CYS	-	EXPRESSION TAG	UNP B5XTG2
C	0	ASN	-	EXPRESSION TAG	UNP B5XTG2
D	-13	MET	-	EXPRESSION TAG	UNP B5XTG2
D	-12	PRO	-	EXPRESSION TAG	UNP B5XTG2
D	-11	PRO	-	EXPRESSION TAG	UNP B5XTG2
D	-10	GLY	-	EXPRESSION TAG	UNP B5XTG2
D	-9	LYS	-	EXPRESSION TAG	UNP B5XTG2
D	-8	CYS	-	EXPRESSION TAG	UNP B5XTG2
D	-7	LEU	-	EXPRESSION TAG	UNP B5XTG2
D	-6	PHE	-	EXPRESSION TAG	UNP B5XTG2
D	-5	SER	-	EXPRESSION TAG	UNP B5XTG2
D	-4	GLY	-	EXPRESSION TAG	UNP B5XTG2
D	-3	VAL	-	EXPRESSION TAG	UNP B5XTG2
D	-2	PHE	-	EXPRESSION TAG	UNP B5XTG2
D	-1	CYS	-	EXPRESSION TAG	UNP B5XTG2
D	0	ASN	-	EXPRESSION TAG	UNP B5XTG2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	12	Total 243	C 117	N 45	O 70	P 11	0	0	0

- Molecule 3 is water.

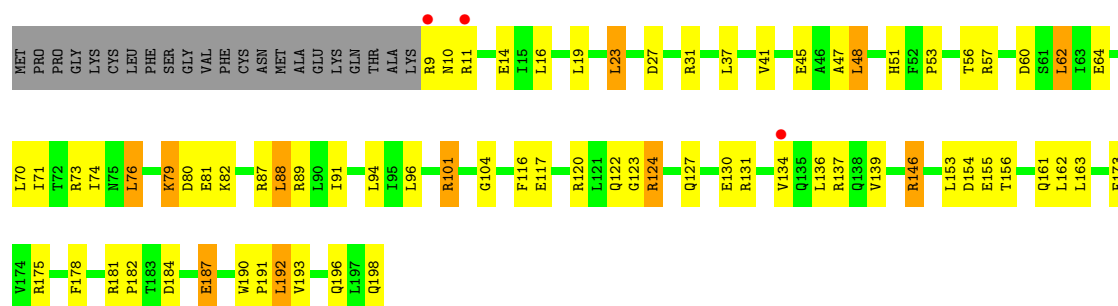
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	80	Total 80	O 80	0	0
3	C	116	Total 116	O 116	0	0
3	D	108	Total 108	O 108	0	0
3	W	21	Total 21	O 21	0	0
3	Z	21	Total 21	O 21	0	0

### 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.

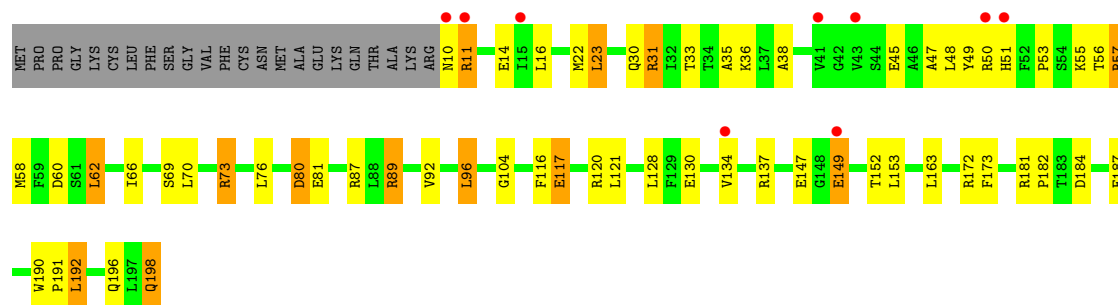
#### • Molecule 1: Nucleoid occlusion factor SlmA

Chain A: 



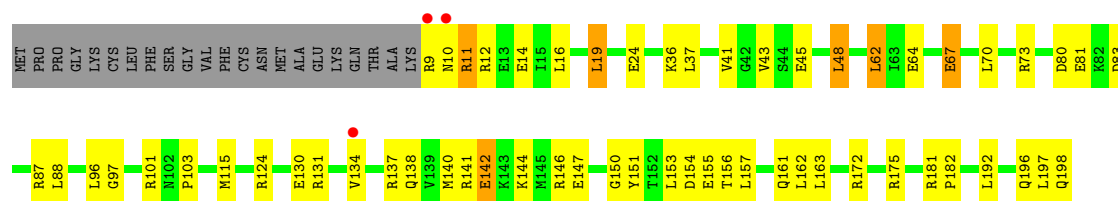
#### • Molecule 1: Nucleoid occlusion factor SlmA

Chain B: 



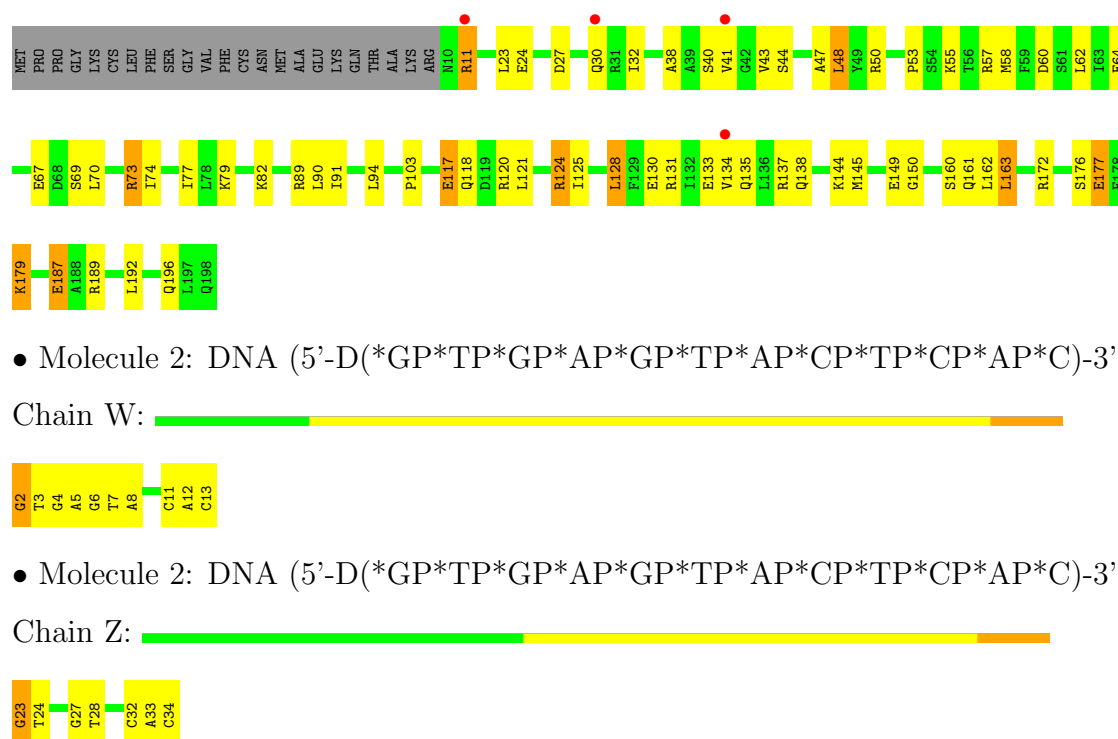
#### • Molecule 1: Nucleoid occlusion factor SlmA

Chain C: 



#### • Molecule 1: Nucleoid occlusion factor SlmA

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.49Å 80.75Å 201.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.00 – 2.05 74.94 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.8 (74.00-2.05) 94.9 (74.94-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.05Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.218 , 0.243 0.228 , 0.254	Depositor DCC
$R_{free}$ test set	7056 reflections (10.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	6 of 70429 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	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 44.95 % 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 1.4170e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities 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	0.54	0/1564	0.73	1/2098 (0.0%)
1	B	0.54	0/1553	0.70	1/2084 (0.0%)
1	C	0.59	0/1564	0.76	2/2098 (0.1%)
1	D	0.55	0/1553	0.72	2/2084 (0.1%)
2	W	0.61	0/272	0.88	0/418
2	Z	0.60	0/272	0.95	1/418 (0.2%)
All	All	0.56	0/6778	0.75	7/9200 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	W	0	1
2	Z	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	ASP	CB-CG-OD1	8.70	126.13	118.30
1	D	89	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	89	ARG	NE-CZ-NH1	-5.91	117.35	120.30
2	Z	32	DC	OP2-P-O3'	5.70	117.73	105.20
1	B	80	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	175	ARG	CB-CA-C	-5.43	99.54	110.40
1	D	89	ARG	NE-CZ-NH1	-5.27	117.67	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	W	2	DG	Sidechain
2	Z	23	DG	Sidechain

## 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	1544	0	1585	72	0
1	B	1533	0	1572	56	0
1	C	1544	0	1585	70	1
1	D	1533	0	1572	60	1
2	W	243	0	137	15	0
2	Z	243	0	137	5	0
3	A	102	0	0	10	0
3	B	80	0	0	1	0
3	C	116	0	0	16	0
3	D	108	0	0	7	0
3	W	21	0	0	0	0
3	Z	21	0	0	0	0
All	All	7088	0	6588	260	1

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 20.

All (260) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:55:LYS:HA	1:B:58:MET:HE3	1.33	1.09
1:D:55:LYS:HA	1:D:58:MET:HE3	1.27	1.08
1:C:161:GLN:HE21	1:C:196:GLN:NE2	1.53	1.03
1:C:161:GLN:NE2	1:C:196:GLN:HE22	1.67	0.92
1:B:81:GLU:O	1:B:87:ARG:HD2	1.74	0.88
1:A:161:GLN:HE21	1:A:196:GLN:HE22	1.17	0.88
1:A:130:GLU:O	1:A:134:VAL:HG23	1.76	0.86
1:C:134:VAL:HG22	1:C:137:ARG:NH2	1.91	0.86
1:D:73:ARG:HG2	1:D:73:ARG:HH11	1.42	0.85
1:A:101:ARG:HH11	1:A:101:ARG:HG2	1.42	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:ASN:O	1:A:14:GLU:HB2	1.77	0.83
1:A:81:GLU:O	1:A:87:ARG:HD2	1.80	0.82
1:D:134:VAL:HG22	1:D:137:ARG:NH2	1.95	0.81
1:C:161:GLN:HE21	1:C:196:GLN:HE22	0.86	0.81
1:B:11:ARG:HA	1:B:14:GLU:HG3	1.63	0.81
1:C:81:GLU:O	1:C:87:ARG:HD2	1.80	0.81
1:C:147:GLU:OE2	3:C:312:HOH:O	1.99	0.80
1:C:142:GLU:HG2	1:C:146:ARG:HE	1.46	0.80
1:C:67:GLU:HG3	3:C:227:HOH:O	1.81	0.80
1:B:53:PRO:HD2	1:B:57:ARG:HG3	1.63	0.78
1:C:24:GLU:HG3	1:C:103:PRO:HB2	1.63	0.78
1:C:196:GLN:HE21	1:D:192:LEU:HB3	1.50	0.77
1:B:117:GLU:OE2	3:B:267:HOH:O	2.03	0.77
1:C:115:MET:CE	1:C:115:MET:HA	2.15	0.77
1:C:64:GLU:HG3	1:C:124:ARG:HH22	1.47	0.76
1:C:67:GLU:OE1	3:C:314:HOH:O	2.03	0.76
1:C:163:LEU:HD23	1:D:172:ARG:HH12	1.50	0.76
1:B:55:LYS:HA	1:B:58:MET:CE	2.15	0.75
1:A:161:GLN:HE21	1:A:196:GLN:NE2	1.85	0.75
1:D:138:GLN:HG2	3:D:266:HOH:O	1.86	0.74
1:A:11:ARG:NH1	2:W:2:DG:H5''	2.03	0.73
1:C:134:VAL:HG13	3:C:265:HOH:O	1.88	0.73
1:D:118:GLN:OE1	1:D:120:ARG:HG2	1.89	0.73
2:W:2:DG:H2'	2:W:3:DT:C7	2.19	0.72
1:B:130:GLU:O	1:B:134:VAL:HG23	1.88	0.72
1:D:161:GLN:HE21	1:D:196:GLN:NE2	1.88	0.72
2:W:5:DA:H1'	2:W:6:DG:H5'	1.71	0.72
1:A:101:ARG:HH11	1:A:101:ARG:CG	2.03	0.72
1:A:73:ARG:HH12	1:A:101:ARG:HH22	1.38	0.71
1:B:134:VAL:HG22	1:B:137:ARG:NH2	2.05	0.71
1:D:53:PRO:HD2	1:D:57:ARG:HG3	1.72	0.71
1:A:187:GLU:HB2	3:A:260:HOH:O	1.90	0.71
1:A:9:ARG:HG3	1:A:9:ARG:HH11	1.57	0.69
1:D:43:VAL:HG23	1:D:44:SER:O	1.93	0.69
1:A:134:VAL:HG21	3:A:246:HOH:O	1.91	0.69
1:D:64:GLU:CG	1:D:124:ARG:HH12	2.06	0.69
1:D:70:LEU:O	1:D:74:ILE:HG12	1.93	0.69
1:C:12:ARG:NH1	3:C:275:HOH:O	2.03	0.69
1:A:146:ARG:HG3	1:A:146:ARG:HH11	1.57	0.68
1:A:70:LEU:O	1:A:74:ILE:HG12	1.92	0.68
1:D:74:ILE:HD12	1:D:91:ILE:HG12	1.76	0.68
1:A:153:LEU:HD11	1:A:198:GLN:HB2	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:64:GLU:HG3	1:C:124:ARG:NH2	2.08	0.68
1:D:64:GLU:HG2	1:D:124:ARG:HH12	1.58	0.68
1:D:11:ARG:HH21	1:D:11:ARG:HG2	1.58	0.67
1:B:57:ARG:HA	1:B:57:ARG:HH11	1.60	0.67
1:A:73:ARG:HH12	1:A:101:ARG:NH2	1.91	0.66
1:C:101:ARG:HB3	3:C:308:HOH:O	1.96	0.65
1:C:130:GLU:O	1:C:134:VAL:HG23	1.96	0.65
1:A:153:LEU:CD1	1:A:198:GLN:HB2	2.26	0.65
1:A:101:ARG:HG2	3:A:229:HOH:O	1.98	0.63
1:C:19:LEU:HD13	1:C:62:LEU:HD22	1.80	0.63
1:D:38:ALA:HB2	1:D:48:LEU:HD22	1.80	0.63
1:B:11:ARG:HG2	1:B:11:ARG:HH21	1.64	0.62
1:C:73:ARG:NH1	1:C:101:ARG:HH22	1.97	0.62
1:C:134:VAL:HG23	3:C:306:HOH:O	1.99	0.62
1:B:181:ARG:HB2	1:B:184:ASP:CG	2.21	0.61
1:C:161:GLN:NE2	1:C:196:GLN:NE2	2.35	0.61
1:C:64:GLU:CG	1:C:124:ARG:HH22	2.15	0.60
1:C:19:LEU:HD13	1:C:62:LEU:CD2	2.32	0.60
1:C:134:VAL:CG2	3:C:306:HOH:O	2.49	0.59
1:D:135:GLN:NE2	3:D:233:HOH:O	2.27	0.59
1:C:115:MET:HE2	1:C:115:MET:HA	1.83	0.59
1:C:138:GLN:HG2	3:C:279:HOH:O	2.01	0.59
1:D:118:GLN:NE2	3:D:251:HOH:O	2.36	0.59
1:A:88:LEU:HD13	1:A:139:VAL:HG11	1.84	0.59
1:D:73:ARG:HG2	1:D:73:ARG:NH1	2.16	0.59
1:D:177:GLU:OE2	1:D:179:LYS:NZ	2.36	0.58
2:W:2:DG:H2'	2:W:3:DT:H72	1.85	0.58
1:C:144:LYS:HE3	1:C:150:GLY:HA3	1.85	0.58
1:B:38:ALA:HB2	1:B:48:LEU:HD22	1.85	0.58
1:A:193:VAL:HA	1:B:196:GLN:HE21	1.69	0.57
2:Z:27:DG:H2''	2:Z:28:DT:H5''	1.84	0.57
1:D:130:GLU:O	1:D:134:VAL:HG23	2.05	0.57
1:A:123:GLY:O	1:A:127:GLN:HG3	2.05	0.56
1:A:64:GLU:HG3	1:A:124:ARG:HH22	1.70	0.56
1:B:69:SER:O	1:B:73:ARG:HG3	2.04	0.56
1:C:154:ASP:OD1	1:C:156:THR:N	2.36	0.55
1:A:74:ILE:CD1	1:A:94:LEU:HD23	2.37	0.55
1:C:134:VAL:HG22	1:C:137:ARG:HH22	1.70	0.55
1:C:10:ASN:O	1:C:14:GLU:HB2	2.06	0.54
1:C:16:LEU:HD22	1:C:62:LEU:HD13	1.88	0.54
1:C:45:GLU:O	1:C:48:LEU:HB2	2.07	0.54
1:A:31:ARG:HB3	1:A:116:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:W:2:DG:H2'	2:W:3:DT:H73	1.90	0.53
1:C:73:ARG:HH12	1:C:101:ARG:NH2	2.05	0.53
1:A:31:ARG:HD2	3:A:276:HOH:O	2.07	0.53
1:A:134:VAL:HG22	1:A:137:ARG:NH2	2.22	0.53
1:B:57:ARG:NH1	1:B:57:ARG:HG2	2.24	0.53
1:D:117:GLU:HB3	1:D:121:LEU:HD12	1.90	0.53
1:C:196:GLN:HG2	1:D:192:LEU:O	2.07	0.53
1:A:74:ILE:HD12	1:A:91:ILE:HG23	1.91	0.53
1:C:115:MET:HE3	1:C:115:MET:HA	1.91	0.53
1:C:144:LYS:CD	1:C:150:GLY:HA3	2.38	0.53
1:D:30:GLN:O	1:D:32:ILE:HD12	2.09	0.53
1:B:190:TRP:HB3	1:B:191:PRO:HD3	1.91	0.53
1:C:153:LEU:HD12	1:C:198:GLN:HB2	1.90	0.53
1:A:60:ASP:OD2	1:A:120:ARG:NH2	2.43	0.52
1:A:153:LEU:HD12	1:A:198:GLN:O	2.09	0.52
1:B:60:ASP:OD1	1:B:120:ARG:NH2	2.43	0.52
1:A:37:LEU:O	1:A:41:VAL:HG23	2.10	0.52
1:B:11:ARG:HB2	1:B:51:HIS:NE2	2.25	0.52
1:C:9:ARG:HG3	1:C:9:ARG:HH11	1.75	0.52
1:A:101:ARG:NH1	1:A:101:ARG:CG	2.69	0.52
1:A:45:GLU:O	1:A:48:LEU:HB2	2.10	0.51
2:Z:23:DG:H2'	2:Z:24:DT:C7	2.40	0.51
1:D:57:ARG:NH2	1:D:60:ASP:OD2	2.43	0.51
1:A:74:ILE:CD1	1:A:91:ILE:HG23	2.40	0.51
1:D:134:VAL:HG22	1:D:137:ARG:HH21	1.73	0.51
1:D:60:ASP:CG	1:D:120:ARG:HH22	2.14	0.51
1:B:49:TYR:CE1	2:W:13:DC:H2'	2.45	0.51
1:A:193:VAL:HA	1:B:196:GLN:NE2	2.25	0.51
1:C:73:ARG:NH1	1:C:101:ARG:NH2	2.59	0.51
1:D:149:GLU:N	1:D:149:GLU:OE2	2.44	0.51
1:B:30:GLN:HA	1:B:116:PHE:CZ	2.46	0.51
1:D:47:ALA:O	1:D:50:ARG:HG2	2.11	0.50
2:Z:23:DG:H2'	2:Z:24:DT:H72	1.92	0.50
1:D:144:LYS:HG2	1:D:150:GLY:HA3	1.93	0.50
1:B:173:PHE:CD1	1:B:182:PRO:HD3	2.46	0.50
1:C:144:LYS:CE	1:C:150:GLY:HA3	2.41	0.50
1:D:67:GLU:HG3	1:D:128:LEU:HG	1.94	0.50
1:C:172:ARG:HH12	1:D:160:SER:HB2	1.77	0.50
1:B:11:ARG:CG	1:B:11:ARG:HH21	2.22	0.50
1:C:115:MET:CE	3:C:281:HOH:O	2.59	0.50
1:C:131:ARG:HD2	3:C:216:HOH:O	2.11	0.50
1:D:73:ARG:CG	1:D:73:ARG:HH11	2.19	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:60:ASP:CG	1:B:120:ARG:HH22	2.15	0.50
1:A:154:ASP:OD1	1:A:156:THR:N	2.44	0.49
1:D:79:LYS:HG3	3:D:224:HOH:O	2.12	0.49
1:D:24:GLU:HG3	1:D:103:PRO:HB2	1.94	0.49
1:D:134:VAL:HG13	3:D:253:HOH:O	2.12	0.49
1:C:153:LEU:CD1	1:C:198:GLN:HB2	2.42	0.49
1:B:35:ALA:HB2	1:B:45:GLU:OE1	2.13	0.49
1:A:79:LYS:HD2	1:A:80:ASP:OD1	2.13	0.49
1:A:192:LEU:HD11	1:B:153:LEU:CD1	2.42	0.49
1:D:77:ILE:HD12	1:D:90:LEU:HB3	1.94	0.49
1:B:45:GLU:OE2	2:W:13:DC:N4	2.37	0.48
1:A:74:ILE:HD13	1:A:94:LEU:HD23	1.95	0.48
1:A:161:GLN:NE2	1:A:196:GLN:HE22	1.98	0.48
1:D:133:GLU:OE1	1:D:163:LEU:HD12	2.13	0.48
1:A:146:ARG:HH11	1:A:146:ARG:CG	2.25	0.48
1:B:11:ARG:HA	1:B:14:GLU:CG	2.41	0.48
1:B:57:ARG:HH11	1:B:57:ARG:HG2	1.79	0.47
1:D:176:SER:O	1:D:179:LYS:HD3	2.14	0.47
1:B:89:ARG:HG3	1:B:190:TRP:CD2	2.50	0.47
1:A:134:VAL:HG13	3:A:302:HOH:O	2.14	0.47
2:Z:23:DG:HO5'	2:Z:23:DG:H8	1.62	0.47
1:A:146:ARG:HB3	3:A:299:HOH:O	2.14	0.47
1:A:11:ARG:HD3	1:A:51:HIS:NE2	2.30	0.47
1:D:11:ARG:NH2	1:D:11:ARG:HG2	2.27	0.46
1:A:9:ARG:CG	1:A:9:ARG:HH11	2.25	0.46
1:B:10:ASN:O	1:B:14:GLU:HG3	2.15	0.46
1:D:74:ILE:CD1	1:D:94:LEU:HD23	2.46	0.46
1:C:73:ARG:HH12	1:C:101:ARG:CZ	2.29	0.46
1:D:64:GLU:HG3	1:D:124:ARG:HH12	1.80	0.46
1:C:192:LEU:O	1:D:196:GLN:HG2	2.16	0.46
1:A:173:PHE:CD1	1:A:178:PHE:HA	2.52	0.45
1:A:196:GLN:HE21	1:B:192:LEU:HB3	1.82	0.45
1:D:73:ARG:NH1	1:D:73:ARG:CG	2.78	0.45
1:D:30:GLN:HB2	3:D:279:HOH:O	2.17	0.45
1:A:73:ARG:NH1	1:A:101:ARG:HH22	2.11	0.45
1:C:172:ARG:NH1	1:D:160:SER:HB2	2.31	0.45
1:C:151:TYR:CE1	1:C:197:LEU:HB3	2.52	0.45
1:B:57:ARG:HH11	1:B:57:ARG:CA	2.28	0.45
1:C:11:ARG:NH1	1:C:43:VAL:CG1	2.80	0.45
1:B:11:ARG:CG	1:B:11:ARG:NH2	2.80	0.44
1:B:181:ARG:HB2	1:B:184:ASP:OD1	2.17	0.44
1:A:56:THR:CG2	1:A:120:ARG:HH22	2.29	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:125:ILE:HD13	1:D:125:ILE:HA	1.85	0.44
2:Z:33:DA:C5	2:Z:34:DC:C4	3.04	0.44
1:C:36:LYS:HE2	3:C:256:HOH:O	2.17	0.44
1:B:47:ALA:O	1:B:50:ARG:HG2	2.17	0.44
1:B:22:MET:HE3	1:B:36:LYS:HG2	1.99	0.44
1:C:146:ARG:NH1	3:C:288:HOH:O	2.28	0.44
1:B:57:ARG:HH11	1:B:57:ARG:CG	2.30	0.44
1:D:64:GLU:HG3	1:D:124:ARG:HH22	1.83	0.44
1:A:64:GLU:CG	1:A:124:ARG:HH22	2.30	0.44
1:D:53:PRO:CD	1:D:57:ARG:HG3	2.45	0.44
2:W:7:DT:H2'	2:W:7:DT:H6	1.67	0.44
1:A:23:LEU:HB3	1:A:104:GLY:CA	2.48	0.44
1:D:74:ILE:CD1	1:D:91:ILE:HG12	2.45	0.43
1:A:79:LYS:O	1:A:82:LYS:HE2	2.18	0.43
1:D:176:SER:C	1:D:177:GLU:HG3	2.38	0.43
1:B:56:THR:HG23	1:B:121:LEU:HD11	1.99	0.43
1:C:115:MET:CA	1:C:115:MET:CE	2.93	0.43
1:D:60:ASP:OD1	1:D:120:ARG:NH2	2.47	0.43
2:W:6:DG:H4'	2:W:7:DT:OP1	2.17	0.43
1:C:141:ARG:HG3	1:C:155:GLU:HG2	2.00	0.43
1:A:53:PRO:CG	1:A:57:ARG:HG3	2.49	0.43
2:W:7:DT:H2''	2:W:8:DA:C8	2.54	0.43
1:D:43:VAL:CG2	1:D:47:ALA:HB3	2.48	0.43
1:D:69:SER:O	1:D:73:ARG:HG3	2.19	0.43
1:C:11:ARG:NH1	1:C:43:VAL:HG11	2.34	0.43
1:B:62:LEU:HA	1:B:62:LEU:HD12	1.82	0.43
1:A:101:ARG:NH1	3:A:244:HOH:O	2.45	0.43
1:D:134:VAL:HG23	3:D:232:HOH:O	2.18	0.43
1:D:74:ILE:HD11	1:D:94:LEU:HD23	2.00	0.43
1:B:31:ARG:HH12	2:W:12:DA:H5''	1.84	0.43
1:A:79:LYS:CE	1:A:80:ASP:OD1	2.67	0.43
1:B:66:ILE:O	1:B:70:LEU:HD23	2.19	0.43
2:W:3:DT:H2''	2:W:4:DG:N7	2.34	0.42
1:B:62:LEU:O	1:B:66:ILE:HG13	2.19	0.42
1:A:190:TRP:HB3	1:A:191:PRO:HD3	2.02	0.42
1:A:9:ARG:NH1	1:A:9:ARG:HG3	2.30	0.42
1:A:9:ARG:NH1	1:A:9:ARG:CG	2.81	0.42
1:D:69:SER:O	1:D:73:ARG:CG	2.68	0.42
1:C:197:LEU:HB2	3:C:287:HOH:O	2.20	0.42
1:B:76:LEU:O	1:B:80:ASP:HB2	2.19	0.42
1:A:19:LEU:HD23	1:A:62:LEU:HD22	2.01	0.42
1:B:23:LEU:HB3	1:B:104:GLY:CA	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:VAL:CG2	3:A:246:HOH:O	2.61	0.42
1:A:134:VAL:CG2	3:A:277:HOH:O	2.68	0.42
1:C:97:GLY:O	1:C:101:ARG:HG2	2.20	0.42
1:C:144:LYS:HG3	1:C:150:GLY:N	2.34	0.42
1:C:83:ASP:O	1:C:87:ARG:HD3	2.19	0.42
2:W:5:DA:C1'	2:W:6:DG:H5'	2.45	0.41
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.93	0.41
1:C:172:ARG:HH12	1:D:160:SER:CB	2.33	0.41
1:A:181:ARG:HB2	1:A:184:ASP:OD2	2.19	0.41
1:A:74:ILE:HD12	1:A:91:ILE:HG12	2.00	0.41
1:B:33:THR:HG22	2:W:11:DC:H3'	2.02	0.41
1:A:181:ARG:HA	1:A:182:PRO:HD3	1.88	0.41
1:A:154:ASP:OD1	1:A:156:THR:HB	2.20	0.41
1:A:74:ILE:HD11	1:A:94:LEU:HD23	2.02	0.41
1:C:140:MET:CE	1:C:162:LEU:HD12	2.50	0.41
1:B:152:THR:HB	1:B:198:GLN:OXT	2.20	0.41
1:C:115:MET:HE1	3:C:281:HOH:O	2.19	0.41
1:A:163:LEU:HD23	1:B:172:ARG:HH12	1.85	0.41
1:B:134:VAL:HG22	1:B:137:ARG:HH22	1.84	0.41
2:W:12:DA:C5	2:W:13:DC:C4	3.09	0.41
1:B:149:GLU:O	1:B:149:GLU:OE1	2.39	0.41
1:A:76:LEU:HA	1:A:76:LEU:HD13	1.75	0.41
1:C:37:LEU:O	1:C:41:VAL:HG23	2.21	0.41
1:C:115:MET:HE3	3:C:281:HOH:O	2.19	0.41
1:C:9:ARG:NH1	1:C:9:ARG:HG3	2.36	0.40
1:C:157:LEU:HD11	1:D:189:ARG:HG2	2.02	0.40
1:C:181:ARG:HA	1:C:182:PRO:HD3	1.88	0.40
1:C:11:ARG:HH11	1:C:43:VAL:HG11	1.86	0.40
1:C:24:GLU:OE1	1:C:103:PRO:HG2	2.21	0.40
1:A:11:ARG:HH12	1:A:47:ALA:HB1	1.85	0.40
1:D:48:LEU:HD12	1:D:48:LEU:HA	1.95	0.40
1:B:73:ARG:HG2	1:B:73:ARG:HH11	1.86	0.40
1:B:16:LEU:HD22	1:B:62:LEU:HD13	2.01	0.40
1:A:16:LEU:HD22	1:A:62:LEU:HD13	2.02	0.40
1:B:92:VAL:HG12	1:B:96:LEU:HD22	2.03	0.40
1:B:50:ARG:HG3	1:B:51:HIS:ND1	2.36	0.40
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.80	0.40
1:A:56:THR:HG22	1:A:120:ARG:HH22	1.87	0.40
1:A:173:PHE:CD1	1:A:182:PRO:HD3	2.57	0.40
1:A:117:GLU:HB3	3:A:204:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:146:ARG:NH2	1:D:187:GLU:OE2[4_555]	2.07	0.13

## 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	188/212 (89%)	186 (99%)	2 (1%)	0	100	100
1	B	187/212 (88%)	181 (97%)	6 (3%)	0	100	100
1	C	188/212 (89%)	184 (98%)	4 (2%)	0	100	100
1	D	187/212 (88%)	181 (97%)	5 (3%)	1 (0%)	38	25
All	All	750/848 (88%)	732 (98%)	17 (2%)	1 (0%)	59	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	41	VAL

### 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	167/185 (90%)	147 (88%)	20 (12%)	7	2
1	B	166/185 (90%)	151 (91%)	15 (9%)	14	6
1	C	167/185 (90%)	158 (95%)	9 (5%)	31	20
1	D	166/185 (90%)	148 (89%)	18 (11%)	9	3
All	All	666/740 (90%)	604 (91%)	62 (9%)	13	6

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	27	ASP
1	A	48	LEU
1	A	62	LEU
1	A	71	ILE
1	A	76	LEU
1	A	79	LYS
1	A	88	LEU
1	A	96	LEU
1	A	101	ARG
1	A	122	GLN
1	A	124	ARG
1	A	131	ARG
1	A	136	LEU
1	A	146	ARG
1	A	155	GLU
1	A	162	LEU
1	A	175	ARG
1	A	187	GLU
1	A	192	LEU
1	B	11	ARG
1	B	23	LEU
1	B	31	ARG
1	B	57	ARG
1	B	62	LEU
1	B	73	ARG
1	B	89	ARG
1	B	96	LEU
1	B	117	GLU
1	B	128	LEU
1	B	147	GLU
1	B	149	GLU
1	B	187	GLU
1	B	192	LEU
1	B	198	GLN
1	C	11	ARG
1	C	19	LEU
1	C	48	LEU
1	C	62	LEU
1	C	67	GLU
1	C	70	LEU
1	C	88	LEU
1	C	96	LEU

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Mol	Chain	Res	Type
1	C	142	GLU
1	D	11	ARG
1	D	23	LEU
1	D	27	ASP
1	D	40	SER
1	D	48	LEU
1	D	62	LEU
1	D	73	ARG
1	D	82	LYS
1	D	117	GLU
1	D	124	ARG
1	D	128	LEU
1	D	131	ARG
1	D	145	MET
1	D	162	LEU
1	D	163	LEU
1	D	177	GLU
1	D	179	LYS
1	D	187	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	196	GLN
1	B	10	ASN
1	B	118	GLN
1	B	196	GLN
1	C	122	GLN
1	C	196	GLN
1	D	17	GLN
1	D	122	GLN
1	D	196	GLN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	190/212 (89%)	0.09	3 (1%) 68 70	22, 33, 54, 88	0
1	B	189/212 (89%)	0.36	9 (4%) 29 28	23, 34, 68, 90	0
1	C	190/212 (89%)	0.15	3 (1%) 68 70	17, 29, 48, 95	0
1	D	189/212 (89%)	0.32	4 (2%) 60 61	21, 32, 65, 76	0
2	W	12/12 (100%)	-0.15	0 100 100	33, 44, 52, 53	0
2	Z	12/12 (100%)	-0.33	0 100 100	34, 40, 50, 50	0
All	All	782/872 (89%)	0.21	19 (2%) 56 57	17, 33, 60, 95	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	VAL	5.6
1	D	41	VAL	4.4
1	A	134	VAL	4.4
1	B	11	ARG	4.3
1	D	134	VAL	3.8
1	A	11	ARG	3.7
1	C	134	VAL	3.5
1	C	9	ARG	3.5
1	B	134	VAL	3.2
1	B	50	ARG	2.7
1	B	43	VAL	2.6
1	A	9	ARG	2.5
1	B	15	ILE	2.4
1	B	10	ASN	2.4
1	B	51	HIS	2.3
1	C	10	ASN	2.2
1	D	11	ARG	2.1
1	B	149	GLU	2.0
1	D	30	GLN	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.