Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 11:13 AM EDT

PDB ID	:	1XO0
Title	:	High resolution structure of the holliday junction intermediate in cre-loxp site-specific recombination
Authors	:	Ghosh, K.; Lau, C.K.; Guo, F.; Segall, A.M.; Van Duyne, G.D.
Deposited on	:	2004-10-05
Resolution	:	2.00 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 (i) 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 (1)) were used in the production of this report:

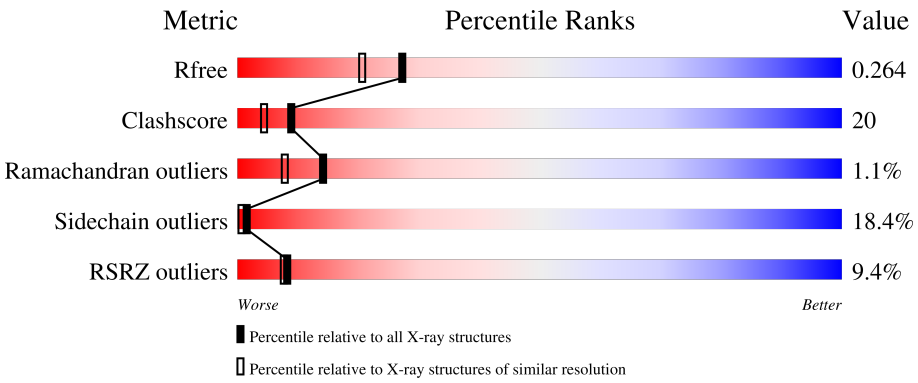
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	C	35	9%, 43%, 54%, ·
2	D	35	3%, 29%, 60%, 11%
3	A	324	10%, 59%, 35%, 6%, ·
3	B	324	9%, 63%, 28%, 6%, · ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7017 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 loxP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	35	715	346	125	210	34	0	0	0

- Molecule 2 is a DNA chain called loxP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	35	713	345	126	208	34	0	0	0

- Molecule 3 is a protein called Recombinase CRE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	322	2548	1584	484	465	15	0	0	0
3	B	322	2548	1584	484	465	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	LYS	ARG	engineered mutation	UNP P06956
B	173	LYS	ARG	engineered mutation	UNP P06956

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	60	60	60	0	0
4	D	88	88	88	0	0
4	A	154	154	154	0	0

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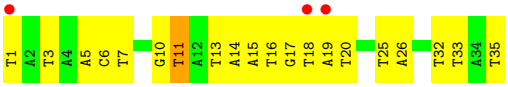
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	191	191	191	0	0

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: loxP

Chain C:

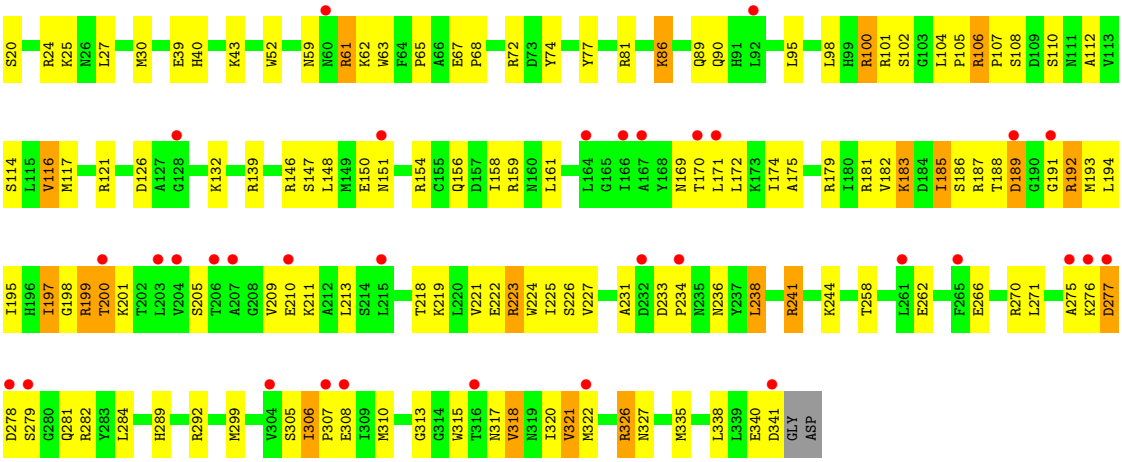


- Molecule 2: loxP

Chain D:

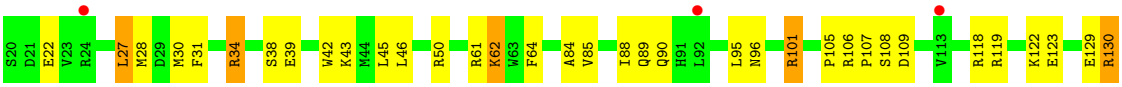
- Molecule 3: Recombinase CRE

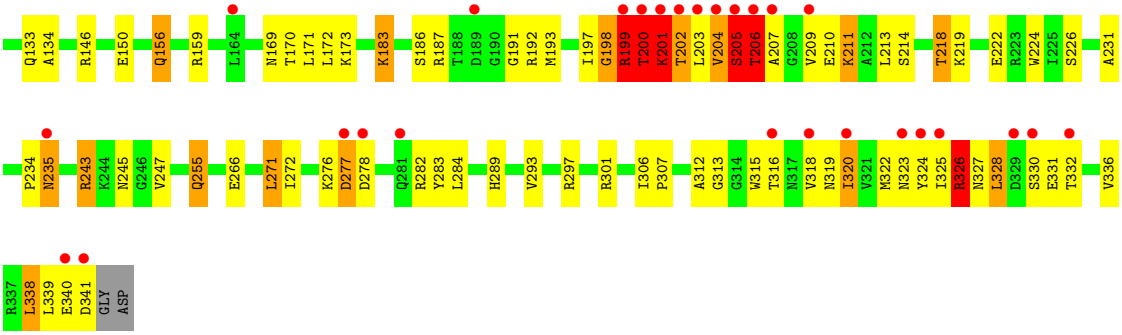
Chain A:



- Molecule 3: Recombinase CRE

Chain B:




Q133 A134 R146 E150 Q156 R159 L164 N169 T170 L171 L172 K173 K183 S186 R187 T188 D189 G190 G191 R192 M193 I197 G198 R199 T200 K201 T202 L203 V204 S205 T206 A207 G208 V209 E210 K211 A212 L213 S214 T218 K219 E222 R223 W224 I225 S226 A231
P234 N235 R243 K244 N245 G246 V247 Q255 E266 L271 I272 K276 D277 D278 Q281 R282 Y283 L284 H289 V293 R297 R301 I306 P307 A312 G313 G314 W315 T316 N317 V318 N319 I320 V321 M322 N323 Y324 I325 R326 N327 L328 D329 S330 E331 T332 V336
R337 L338 L339 E340 D341 GLY ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	107.40Å 123.00Å 180.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 2.00 26.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.00-2.00) 82.9 (26.68-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.99Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.219 , 0.265 0.225 , 0.264	Depositor DCC
R_{free} test set	3452 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 84.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 (i)

5.1 Standard geometry (i)

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	C	1.39	11/801 (1.4%)	1.68	15/1235 (1.2%)
2	D	1.93	11/799 (1.4%)	1.78	15/1231 (1.2%)
3	A	0.40	0/2589	0.57	0/3490
3	B	1.01	6/2589 (0.2%)	1.13	15/3490 (0.4%)
All	All	1.06	28/6778 (0.4%)	1.17	45/9446 (0.5%)

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
3	B	0	3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	DT	O3'-P	42.24	2.11	1.61
3	B	199	ARG	CD-NE	-25.77	1.02	1.46
1	C	1	DT	O3'-P	24.51	1.90	1.61
3	B	202	THR	C-N	22.71	1.86	1.34
3	B	206	THR	C-N	-17.07	0.94	1.34
3	B	198	GLY	C-N	-16.93	0.95	1.34
3	B	199	ARG	CG-CD	-15.43	1.13	1.51
3	B	205	SER	C-N	-12.24	1.05	1.34
2	D	13	DT	O3'-P	-11.57	1.47	1.61
2	D	26	DA	O3'-P	-8.53	1.50	1.61
2	D	33	DT	C5-C7	7.51	1.54	1.50
2	D	11	DT	C5-C7	7.50	1.54	1.50
2	D	32	DT	C5-C7	7.39	1.54	1.50
2	D	23	DT	C5-C7	7.38	1.54	1.50
2	D	13	DT	C5-C7	7.36	1.54	1.50
1	C	3	DT	C5-C7	7.34	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	33	DT	C5-C7	7.31	1.54	1.50
2	D	25	DT	C5-C7	7.30	1.54	1.50
1	C	13	DT	C5-C7	7.30	1.54	1.50
1	C	32	DT	C5-C7	7.27	1.54	1.50
1	C	35	DT	C5-C7	7.23	1.54	1.50
1	C	25	DT	C5-C7	7.20	1.54	1.50
1	C	11	DT	C5-C7	7.19	1.54	1.50
2	D	3	DT	C5-C7	7.16	1.54	1.50
2	D	18	DT	C5-C7	7.11	1.54	1.50
1	C	14	DA	O3'-P	-7.08	1.52	1.61
1	C	3	DT	O3'-P	-6.89	1.52	1.61
1	C	25	DT	O3'-P	-6.24	1.53	1.61

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	DT	O3'-P-O5'	35.94	172.28	104.00
2	D	1	DT	OP1-P-O3'	-30.19	38.78	105.20
2	D	1	DT	P-O3'-C3'	25.10	149.82	119.70
3	B	198	GLY	O-C-N	-24.75	83.10	122.70
3	B	201	LYS	C-N-CA	-21.53	67.88	121.70
3	B	201	LYS	CA-C-N	-21.35	70.23	117.20
3	B	202	THR	C-N-CA	-16.00	81.70	121.70
1	C	1	DT	OP1-P-O3'	-15.77	70.50	105.20
2	D	1	DT	OP2-P-O3'	15.67	139.68	105.20
3	B	199	ARG	CA-CB-CG	-15.13	80.12	113.40
3	B	202	THR	O-C-N	-14.45	99.58	122.70
3	B	202	THR	CA-C-N	-13.78	86.88	117.20
3	B	198	GLY	CA-C-N	13.32	146.51	117.20
3	B	204	VAL	O-C-N	-11.65	104.06	122.70
1	C	1	DT	OP2-P-O3'	-11.35	80.23	105.20
2	D	13	DT	P-O3'-C3'	8.90	130.38	119.70
2	D	34	DA	P-O3'-C3'	-8.40	109.62	119.70
3	B	204	VAL	CA-C-N	8.20	135.25	117.20
3	B	199	ARG	NE-CZ-NH2	7.59	124.10	120.30
3	B	326	ARG	NE-CZ-NH2	7.02	123.81	120.30
2	D	18	DT	O4'-C4'-C3'	-6.25	102.00	104.50
1	C	25	DT	P-O3'-C3'	6.11	127.03	119.70
2	D	1	DT	O3'-P-O5'	6.03	115.45	104.00
3	B	322	MET	CG-SD-CE	5.93	109.68	100.20
3	B	201	LYS	O-C-N	5.71	131.84	122.70
1	C	1	DT	P-O3'-C3'	5.68	126.51	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	25	DT	C4-C5-C6	5.50	121.30	118.00
1	C	3	DT	P-O3'-C3'	5.49	126.29	119.70
1	C	13	DT	C4-C5-C6	5.43	121.26	118.00
2	D	33	DT	C4-C5-C6	5.42	121.25	118.00
3	B	200	THR	N-CA-C	5.41	125.59	111.00
1	C	14	DA	P-O3'-C3'	5.40	126.18	119.70
1	C	33	DT	C4-C5-C6	5.37	121.22	118.00
2	D	32	DT	C4-C5-C6	5.34	121.20	118.00
2	D	11	DT	C4-C5-C6	5.28	121.17	118.00
1	C	11	DT	C4-C5-C6	5.25	121.15	118.00
2	D	3	DT	C4-C5-C6	5.24	121.14	118.00
1	C	32	DT	C4-C5-C6	5.23	121.14	118.00
1	C	3	DT	C4-C5-C6	5.21	121.13	118.00
1	C	25	DT	C4-C5-C6	5.19	121.11	118.00
1	C	35	DT	C4-C5-C6	5.15	121.09	118.00
2	D	23	DT	C4-C5-C6	5.09	121.05	118.00
1	C	11	DT	C6-C5-C7	-5.09	119.85	122.90
2	D	13	DT	C4-C5-C6	5.04	121.03	118.00
2	D	18	DT	C4-C5-C6	5.01	121.00	118.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	198	GLY	Mainchain
3	B	199	ARG	Sidechain
3	B	201	LYS	Mainchain

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	C	715	0	401	29	0
2	D	713	0	400	32	0
3	A	2548	0	2571	88	1
3	B	2548	0	2565	142	1
4	A	154	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	191	0	0	5	0
4	C	60	0	0	1	0
4	D	88	0	0	5	0
All	All	7017	0	5937	253	1

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 20.

All (253) 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:B:202:THR:HG1	3:B:203:LEU:N	0.96	1.43
2:D:24:DA:C5'	3:B:201:LYS:HG2	1.56	1.33
1:C:17:DG:H5"	3:B:202:THR:CB	1.62	1.30
3:B:202:THR:C	3:B:203:LEU:N	1.86	1.28
1:C:17:DG:C5'	3:B:202:THR:HB	1.66	1.26
2:D:24:DA:C5'	3:B:201:LYS:CG	2.22	1.17
3:B:201:LYS:CB	3:B:202:THR:HG23	1.77	1.14
3:B:202:THR:OG1	3:B:203:LEU:N	1.78	1.13
3:B:323:ASN:O	3:B:326:ARG:HB3	1.48	1.12
3:B:202:THR:O	3:B:203:LEU:HA	1.49	1.11
3:B:202:THR:C	3:B:203:LEU:CA	2.19	1.10
1:C:19:DA:H1'	1:C:20:DT:H5"	1.34	1.09
1:C:17:DG:H5"	3:B:202:THR:HB	1.14	1.09
3:B:325:ILE:HG23	3:B:328:LEU:HD23	1.34	1.08
3:B:201:LYS:HB2	3:B:202:THR:HG23	1.13	1.08
1:C:17:DG:C5'	3:B:202:THR:CB	2.25	1.07
1:C:17:DG:H5'	3:B:202:THR:CG2	1.84	1.06
1:C:17:DG:H5'	3:B:202:THR:HG21	1.33	1.04
2:D:24:DA:H5"	3:B:201:LYS:CG	1.88	1.02
2:D:24:DA:H5'	3:B:201:LYS:HG2	1.04	1.01
2:D:24:DA:H5'	3:B:201:LYS:CG	1.86	0.99
3:B:200:THR:HG1	3:B:203:LEU:N	1.60	0.98
2:D:5:DA:H2"	2:D:6:DC:H5"	1.47	0.96
3:B:201:LYS:CB	3:B:202:THR:CG2	2.43	0.96
3:B:199:ARG:HB2	3:B:204:VAL:HA	1.49	0.95
3:B:201:LYS:HB2	3:B:202:THR:CG2	1.97	0.94
2:D:24:DA:H5"	3:B:201:LYS:HG2	1.48	0.91
3:B:202:THR:CA	3:B:203:LEU:N	2.34	0.91
3:B:199:ARG:CA	3:B:203:LEU:O	2.19	0.90
1:C:19:DA:C1'	1:C:20:DT:H5"	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:DA:C4'	3:B:201:LYS:HD2	2.03	0.88
4:D:49:HOH:O	3:A:241:ARG:HD3	1.75	0.87
3:B:133:GLN:OE1	3:B:327:ASN:HB2	1.78	0.84
1:C:17:DG:C5'	3:B:202:THR:CG2	2.52	0.83
2:D:24:DA:H5"	3:B:201:LYS:HG3	1.59	0.83
3:B:320:ILE:O	3:B:323:ASN:HB2	1.79	0.83
2:D:6:DC:H2'	2:D:7:DT:H72	1.62	0.82
3:B:202:THR:C	3:B:203:LEU:HA	1.94	0.81
1:C:19:DA:H1'	1:C:20:DT:C5'	2.08	0.81
2:D:21:DA:H2"	2:D:22:DT:H5"	1.61	0.81
1:C:17:DG:C4'	3:B:202:THR:HB	2.11	0.81
3:A:194:LEU:HG	3:A:210:GLU:OE2	1.82	0.80
3:B:323:ASN:HA	3:B:326:ARG:HB2	1.63	0.80
3:B:306:ILE:HG21	3:B:318:VAL:HG13	1.62	0.79
1:C:5:DA:H2"	1:C:6:DC:H5"	1.66	0.78
3:A:174:ILE:HD12	3:A:258:THR:HB	1.64	0.78
3:A:199:ARG:HD2	3:A:209:VAL:HG21	1.64	0.77
1:C:17:DG:H5"	3:B:202:THR:OG1	1.85	0.77
3:B:199:ARG:CB	3:B:203:LEU:O	2.33	0.76
3:B:200:THR:OG1	3:B:203:LEU:N	2.18	0.76
3:B:199:ARG:HA	3:B:203:LEU:O	1.84	0.75
3:A:317:ASN:ND2	4:A:409:HOH:O	2.18	0.74
3:B:202:THR:CB	3:B:203:LEU:N	2.50	0.74
3:B:325:ILE:HG23	3:B:328:LEU:CD2	2.15	0.74
3:B:323:ASN:O	3:B:326:ARG:CB	2.34	0.74
4:C:73:HOH:O	3:B:156:GLN:HG3	1.86	0.73
3:B:202:THR:O	3:B:203:LEU:CA	2.25	0.73
1:C:17:DG:H2"	1:C:18:DT:H5'	1.71	0.73
3:B:199:ARG:HB2	3:B:203:LEU:O	1.90	0.72
2:D:15:DG:H2"	2:D:16:DC:H5"	1.69	0.71
1:C:17:DG:C5'	3:B:202:THR:HG21	2.13	0.71
3:B:197:ILE:CD1	3:B:211:LYS:HG3	2.22	0.70
3:B:206:THR:HG1	3:B:207:ALA:N	1.90	0.69
2:D:34:DA:H2"	2:D:35:DT:O4'	1.90	0.69
3:B:336:VAL:O	3:B:340:GLU:HG3	1.92	0.69
3:A:193:MET:CE	3:A:218:THR:HG23	2.23	0.69
3:B:146:ARG:O	3:B:150:GLU:HB2	1.92	0.69
1:C:17:DG:H4'	3:B:202:THR:HB	1.74	0.68
2:D:18:DT:H5"	2:D:18:DT:H6	1.59	0.68
1:C:6:DC:H2'	1:C:7:DT:H72	1.74	0.68
3:A:310:MET:SD	3:A:318:VAL:HG13	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:460:HOH:O	3:B:326:ARG:HD2	1.94	0.66
2:D:19:DA:H5"	4:D:99:HOH:O	1.96	0.65
3:B:101:ARG:HG2	3:B:101:ARG:HH11	1.62	0.65
2:D:16:DC:H2"	2:D:17:DA:C8	2.33	0.64
2:D:6:DC:H2'	2:D:7:DT:C7	2.27	0.64
3:A:30:MET:HE1	3:A:101:ARG:HB3	1.79	0.64
3:A:210:GLU:O	3:B:331:GLU:HB2	1.97	0.64
3:A:193:MET:HE3	3:A:218:THR:HG23	1.79	0.64
3:B:106:ARG:O	3:B:109:ASP:HB2	1.98	0.64
1:C:19:DA:C2'	1:C:20:DT:H5"	2.28	0.63
3:B:313:GLY:HA3	3:B:315:TRP:CZ3	2.33	0.63
3:A:185:ILE:HD11	3:A:238:LEU:HG	1.81	0.63
3:A:318:VAL:HG12	3:A:321:VAL:HG11	1.81	0.63
3:B:319:ASN:O	3:B:323:ASN:ND2	2.32	0.63
3:B:205:SER:HG	3:B:206:THR:N	1.94	0.63
2:D:24:DA:O4'	3:B:201:LYS:HD2	1.98	0.63
3:A:158:ILE:HD13	3:A:227:VAL:HG21	1.81	0.62
3:A:188:THR:HB	3:A:194:LEU:HD22	1.80	0.62
3:B:205:SER:OG	3:B:206:THR:N	2.29	0.61
3:B:214:SER:O	3:B:218:THR:HG23	1.99	0.61
3:B:197:ILE:HD13	3:B:211:LYS:HG3	1.80	0.61
3:B:201:LYS:CA	3:B:202:THR:HG23	2.26	0.61
2:D:24:DA:C5'	3:B:201:LYS:CD	2.79	0.61
4:D:91:HOH:O	3:B:243:ARG:HG2	2.00	0.60
3:B:129:GLU:O	3:B:130:ARG:HD3	2.01	0.60
3:A:262:GLU:O	3:A:266:GLU:HG3	2.02	0.60
2:D:5:DA:C2'	2:D:6:DC:H5"	2.27	0.59
3:B:187:ARG:NH2	3:B:222:GLU:OE2	2.36	0.59
3:B:159:ARG:HB2	3:B:224:TRP:CZ3	2.37	0.59
2:D:24:DA:H4'	3:B:201:LYS:HD2	1.84	0.59
3:B:201:LYS:CB	3:B:202:THR:HG22	2.32	0.59
1:C:16:DT:OP2	3:B:320:ILE:HG21	2.03	0.58
2:D:24:DA:C4'	3:B:201:LYS:CD	2.79	0.58
3:A:308:GLU:OE1	3:B:332:THR:HB	2.03	0.58
3:B:62:LYS:HD3	3:B:64:PHE:O	2.04	0.58
3:A:306:ILE:N	3:A:307:PRO:HD2	2.19	0.58
1:C:6:DC:H2'	1:C:7:DT:C7	2.33	0.57
3:A:197:ILE:HG23	3:A:198:GLY:N	2.17	0.57
3:A:81:ARG:NH2	4:A:359:HOH:O	2.30	0.57
3:B:201:LYS:HB3	3:B:202:THR:CG2	2.34	0.57
3:A:30:MET:CE	3:A:101:ARG:HB3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:DT:H1'	2:D:9:DC:H5'	1.88	0.56
3:B:42:TRP:O	3:B:46:LEU:HG	2.06	0.56
3:A:102:SER:HB2	3:A:104:LEU:HD12	1.86	0.56
3:B:183:LYS:HD2	4:B:520:HOH:O	2.07	0.55
1:C:15:DA:N3	3:B:201:LYS:NZ	2.55	0.55
3:A:154:ARG:HH21	3:A:156:GLN:HE21	1.54	0.55
3:B:105:PRO:HD2	4:B:436:HOH:O	2.05	0.55
3:A:154:ARG:NH2	3:A:156:GLN:HE21	2.04	0.55
3:A:100:ARG:NH1	3:A:106:ARG:HD3	2.21	0.55
3:A:182:VAL:HG23	3:A:236:ASN:O	2.06	0.55
3:B:85:VAL:O	3:B:89:GLN:HG3	2.07	0.55
3:A:185:ILE:HG22	3:A:193:MET:HG2	1.88	0.55
3:B:209:VAL:HG22	3:B:210:GLU:H	1.70	0.55
3:A:40:HIS:HE1	4:A:410:HOH:O	1.90	0.55
3:B:187:ARG:HD3	3:B:191:GLY:HA2	1.89	0.55
2:D:18:DT:H6	2:D:18:DT:C5'	2.19	0.55
3:B:306:ILE:N	3:B:307:PRO:HD2	2.22	0.54
3:A:175:ALA:O	3:A:179:ARG:HG3	2.07	0.54
3:B:101:ARG:HH11	3:B:101:ARG:CG	2.20	0.54
3:A:189:ASP:OD1	3:A:189:ASP:C	2.46	0.54
3:B:133:GLN:HE22	3:B:324:TYR:HA	1.73	0.54
3:A:200:THR:HG21	3:A:205:SER:HB2	1.90	0.54
2:D:24:DA:H5'	3:B:201:LYS:CD	2.37	0.54
3:A:340:GLU:O	3:A:341:ASP:HB3	2.07	0.54
3:A:223:ARG:O	3:A:223:ARG:HG3	2.07	0.54
3:B:255:GLN:HG3	4:B:503:HOH:O	2.08	0.54
3:B:201:LYS:HB3	3:B:202:THR:HG22	1.91	0.53
3:B:193:MET:CE	3:B:222:GLU:HG3	2.39	0.53
3:B:315:TRP:HZ2	3:B:324:TYR:CE1	2.27	0.53
3:A:139:ARG:NH1	3:B:339:LEU:HA	2.23	0.53
3:B:85:VAL:HG23	3:B:129:GLU:OE2	2.09	0.53
3:A:59:ASN:O	3:A:61:ARG:HD3	2.08	0.53
3:A:209:VAL:HG12	3:A:210:GLU:N	2.24	0.53
3:A:172:LEU:HD21	3:A:197:ILE:HG21	1.91	0.52
3:B:297:ARG:HG2	3:B:328:LEU:HD22	1.90	0.52
3:A:199:ARG:HD2	3:A:209:VAL:CG2	2.37	0.52
3:A:139:ARG:HH12	3:B:339:LEU:HA	1.74	0.52
3:A:192:ARG:HG3	3:A:192:ARG:NH1	2.25	0.52
3:A:209:VAL:HG12	3:A:210:GLU:H	1.75	0.52
3:A:305:SER:C	3:A:307:PRO:HD2	2.30	0.52
3:A:193:MET:HE2	3:A:218:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:89:GLN:HG3	3:A:117:MET:CE	2.39	0.51
3:B:199:ARG:C	3:B:203:LEU:O	2.49	0.51
4:D:49:HOH:O	3:A:241:ARG:CD	2.44	0.51
4:A:460:HOH:O	3:B:326:ARG:CD	2.57	0.51
3:A:24:ARG:HG3	3:A:24:ARG:HH11	1.75	0.51
2:D:24:DA:C5'	3:B:201:LYS:HD2	2.39	0.51
3:B:202:THR:C	3:B:203:LEU:C	2.69	0.51
3:A:24:ARG:HG3	3:A:24:ARG:NH1	2.26	0.50
3:A:200:THR:O	3:B:130:ARG:NH2	2.44	0.50
3:A:146:ARG:O	3:A:150:GLU:HG3	2.12	0.50
3:A:221:VAL:HG12	3:A:225:ILE:HD11	1.94	0.50
3:A:74:TYR:O	3:A:77:TYR:HB3	2.11	0.50
1:C:19:DA:H2"	1:C:20:DT:C5'	2.40	0.50
3:B:214:SER:O	3:B:218:THR:CG2	2.60	0.49
2:D:24:DA:H4'	3:B:201:LYS:CD	2.42	0.49
3:B:313:GLY:HA3	3:B:315:TRP:CE3	2.47	0.49
3:B:50:ARG:NH2	4:B:529:HOH:O	2.45	0.49
3:B:106:ARG:NH1	3:B:109:ASP:OD2	2.46	0.49
3:A:100:ARG:NH1	3:A:100:ARG:HG3	2.28	0.49
3:B:134:ALA:HA	3:B:283:TYR:CD2	2.48	0.49
3:B:245:ASN:OD1	3:B:247:VAL:HG23	2.12	0.49
3:A:225:ILE:CG2	3:A:231:ALA:HB2	2.42	0.48
3:A:218:THR:O	3:A:222:GLU:HG3	2.14	0.48
3:A:313:GLY:HA3	3:A:315:TRP:CZ3	2.48	0.48
3:B:183:LYS:HB3	3:B:234:PRO:HB2	1.95	0.48
3:B:211:LYS:NZ	3:B:312:ALA:O	2.47	0.48
3:B:272:ILE:HD13	3:B:272:ILE:N	2.28	0.48
3:B:315:TRP:HZ2	3:B:324:TYR:HE1	1.59	0.48
3:B:315:TRP:HD1	3:B:320:ILE:HD13	1.78	0.48
3:B:209:VAL:HG22	3:B:210:GLU:N	2.29	0.47
3:A:89:GLN:HG3	3:A:117:MET:HE2	1.96	0.47
3:A:68:PRO:HB3	3:A:110:SER:CB	2.45	0.47
3:A:187:ARG:NH1	3:A:191:GLY:O	2.47	0.47
3:B:213:LEU:HB2	3:B:218:THR:HG22	1.95	0.47
1:C:19:DA:C2'	1:C:20:DT:C5'	2.92	0.47
3:A:107:PRO:O	3:A:110:SER:HB3	2.15	0.47
3:B:31:PHE:CE2	3:B:34:ARG:NH1	2.83	0.47
3:A:100:ARG:HG3	3:A:100:ARG:HH11	1.79	0.47
3:A:310:MET:HE2	4:A:496:HOH:O	2.13	0.47
3:A:159:ARG:HB2	3:A:224:TRP:CZ3	2.50	0.46
3:A:305:SER:HB2	3:A:307:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:277:ASP:HB3	3:B:284:LEU:HD13	1.96	0.46
3:B:193:MET:HE3	3:B:222:GLU:HG3	1.97	0.46
2:D:3:DT:O2	3:A:244:LYS:NZ	2.49	0.46
1:C:16:DT:OP2	3:B:320:ILE:CG2	2.64	0.46
3:B:172:LEU:HD11	3:B:197:ILE:HD11	1.97	0.46
1:C:11:DT:OP2	3:B:50:ARG:NH1	2.49	0.45
3:B:119:ARG:O	3:B:123:GLU:HG3	2.16	0.45
3:A:195:ILE:HD11	3:A:213:LEU:HD11	1.98	0.45
3:A:326:ARG:HG2	3:A:327:ASN:N	2.32	0.45
2:D:15:DG:O6	3:A:86:LYS:NZ	2.50	0.45
4:D:38:HOH:O	3:A:156:GLN:HB2	2.16	0.45
3:B:170:THR:O	3:B:171:LEU:HB2	2.17	0.45
3:B:271:LEU:HD13	3:B:272:ILE:HD13	1.98	0.45
3:A:183:LYS:HB3	3:A:234:PRO:HB3	1.97	0.45
3:B:101:ARG:CG	3:B:101:ARG:NH1	2.77	0.45
3:B:277:ASP:CB	3:B:284:LEU:HD13	2.47	0.45
3:B:315:TRP:CZ2	3:B:324:TYR:CE1	3.05	0.45
2:D:8:DT:H2"	2:D:9:DC:H5'	1.97	0.44
1:C:17:DG:H2"	1:C:18:DT:C5'	2.45	0.44
4:A:376:HOH:O	3:B:338:LEU:CD1	2.65	0.44
3:B:183:LYS:NZ	3:B:235:ASN:ND2	2.65	0.44
3:A:340:GLU:O	3:A:341:ASP:CB	2.65	0.44
1:C:6:DC:H2'	1:C:7:DT:C5	2.52	0.44
1:C:26:DA:H5'	1:C:26:DA:C8	2.52	0.44
3:B:277:ASP:CG	3:B:278:ASP:H	2.20	0.44
3:A:65:PRO:HG3	3:A:104:LEU:HD22	1.99	0.43
3:A:192:ARG:HH11	3:A:192:ARG:CG	2.31	0.43
3:B:201:LYS:HB3	3:B:201:LYS:HE2	1.81	0.43
3:B:323:ASN:C	3:B:326:ARG:H	2.21	0.43
3:A:104:LEU:HB3	3:A:105:PRO:HD2	2.00	0.43
3:B:84:ALA:O	3:B:88:ILE:HG13	2.18	0.43
2:D:11:DT:H2"	2:D:12:DA:OP2	2.19	0.42
3:B:231:ALA:HB3	4:B:399:HOH:O	2.19	0.42
3:B:27:LEU:HD12	3:B:27:LEU:HA	1.82	0.42
3:B:193:MET:HB2	3:B:218:THR:HB	2.01	0.42
3:B:315:TRP:CZ2	3:B:324:TYR:HE1	2.36	0.42
3:A:72:ARG:HD3	4:A:373:HOH:O	2.19	0.42
3:A:277:ASP:HB2	3:A:284:LEU:HD13	2.02	0.42
3:B:325:ILE:HA	3:B:328:LEU:HB2	2.01	0.42
3:A:112:ALA:O	3:A:116:VAL:HG22	2.19	0.42
3:A:192:ARG:HG3	3:A:192:ARG:HH11	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:DA:C2'	2:D:22:DT:H5"	2.42	0.42
3:A:170:THR:O	3:A:211:LYS:HE3	2.19	0.42
3:A:233:ASP:O	3:A:236:ASN:HB2	2.20	0.42
1:C:10:DG:N7	3:B:43:LYS:NZ	2.49	0.42
3:A:100:ARG:HG3	3:A:106:ARG:HD3	2.02	0.42
3:A:186:SER:OG	3:A:194:LEU:HB3	2.20	0.41
3:A:182:VAL:HG11	3:A:231:ALA:HA	2.00	0.41
3:B:96:ASN:OD1	3:B:107:PRO:HD2	2.20	0.41
3:B:192:ARG:HG2	3:B:213:LEU:O	2.19	0.41
3:A:43:LYS:HA	3:A:43:LYS:HD3	1.94	0.41
3:A:172:LEU:CD1	3:A:197:ILE:HG13	2.50	0.41
3:A:25:LYS:NZ	4:A:468:HOH:O	2.51	0.41
3:A:100:ARG:HG3	3:A:106:ARG:CD	2.50	0.41
3:A:52:TRP:CD1	3:A:63:TRP:HE3	2.38	0.41
3:A:172:LEU:HD11	3:A:197:ILE:HG13	2.03	0.41
3:B:326:ARG:O	3:B:326:ARG:HG2	2.21	0.40
3:B:297:ARG:O	3:B:301:ARG:HG2	2.22	0.40
3:A:227:VAL:HG12	3:A:227:VAL:O	2.20	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	Interatomic distance (Å)	Clash overlap (Å)
3:A:126:ASP:OD2	3:B:199:ARG:NH2[4_566]	2.17	0.03

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	A	320/324 (99%)	301 (94%)	16 (5%)	3 (1%)	17 11
3	B	320/324 (99%)	302 (94%)	14 (4%)	4 (1%)	12 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	640/648 (99%)	603 (94%)	30 (5%)	7 (1%)	14 8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	281	GLN
3	B	200	THR
3	B	201	LYS
3	B	277	ASP
3	A	275	ALA
3	A	278	ASP
3	B	206	THR

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	A	269/270 (100%)	215 (80%)	54 (20%)	1 0
3	B	269/270 (100%)	224 (83%)	45 (17%)	2 1
All	All	538/540 (100%)	439 (82%)	99 (18%)	1 1

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	SER
3	A	27	LEU
3	A	39	GLU
3	A	61	ARG
3	A	62	LYS
3	A	67	GLU
3	A	86	LYS
3	A	90	GLN
3	A	95	LEU
3	A	98	LEU
3	A	100	ARG

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Mol	Chain	Res	Type
3	A	106	ARG
3	A	108	SER
3	A	114	SER
3	A	116	VAL
3	A	121	ARG
3	A	132	LYS
3	A	147	SER
3	A	148	LEU
3	A	151	ASN
3	A	161	LEU
3	A	169	ASN
3	A	171	LEU
3	A	181	ARG
3	A	183	LYS
3	A	185	ILE
3	A	189	ASP
3	A	192	ARG
3	A	197	ILE
3	A	199	ARG
3	A	200	THR
3	A	201	LYS
3	A	219	LYS
3	A	223	ARG
3	A	226	SER
3	A	238	LEU
3	A	241	ARG
3	A	270	ARG
3	A	271	LEU
3	A	276	LYS
3	A	277	ASP
3	A	279	SER
3	A	282	ARG
3	A	289	HIS
3	A	292	ARG
3	A	299	MET
3	A	306	ILE
3	A	318	VAL
3	A	320	ILE
3	A	321	VAL
3	A	322	MET
3	A	326	ARG
3	A	335	MET

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Mol	Chain	Res	Type
3	A	338	LEU
3	B	22	GLU
3	B	27	LEU
3	B	28	MET
3	B	30	MET
3	B	34	ARG
3	B	38	SER
3	B	39	GLU
3	B	45	LEU
3	B	61	ARG
3	B	62	LYS
3	B	90	GLN
3	B	95	LEU
3	B	101	ARG
3	B	108	SER
3	B	118	ARG
3	B	122	LYS
3	B	130	ARG
3	B	156	GLN
3	B	169	ASN
3	B	173	LYS
3	B	183	LYS
3	B	186	SER
3	B	199	ARG
3	B	200	THR
3	B	205	SER
3	B	211	LYS
3	B	218	THR
3	B	219	LYS
3	B	226	SER
3	B	235	ASN
3	B	243	ARG
3	B	255	GLN
3	B	266	GLU
3	B	271	LEU
3	B	276	LYS
3	B	282	ARG
3	B	289	HIS
3	B	293	VAL
3	B	316	THR
3	B	320	ILE
3	B	326	ARG

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Mol	Chain	Res	Type
3	B	328	LEU
3	B	330	SER
3	B	338	LEU
3	B	341	ASP

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

Mol	Chain	Res	Type
3	A	89	GLN
3	A	144	GLN
3	B	90	GLN
3	B	133	GLN
3	B	235	ASN
3	B	311	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)

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

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	B	4
2	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1:DT	O3'	2:DA	P	2.11
1	C	1:DT	O3'	2:DA	P	1.90
1	B	202:THR	C	203:LEU	N	1.86
1	B	205:SER	C	206:THR	N	1.05
1	B	198:GLY	C	199:ARG	N	0.95
1	B	206:THR	C	207:ALA	N	0.94

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	C	35/35 (100%)	0.29	3 (8%)	10	9	25, 39, 75, 90	0
2	D	35/35 (100%)	0.04	1 (2%)	51	50	24, 36, 60, 70	0
3	A	322/324 (99%)	0.64	33 (10%)	6	6	22, 47, 82, 99	0
3	B	322/324 (99%)	0.68	30 (9%)	8	8	19, 35, 83, 99	0
All	All	714/718 (99%)	0.61	67 (9%)	8	8	19, 41, 83, 99	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	203	LEU	13.4
3	B	205	SER	13.3
3	B	204	VAL	12.9
3	B	202	THR	12.6
3	B	200	THR	11.3
3	B	206	THR	8.5
2	D	1	DT	8.2
3	B	201	LYS	8.1
3	B	199	ARG	7.0
1	C	1	DT	6.5
3	A	278	ASP	5.0
3	A	304	VAL	5.0
3	A	166	ILE	4.1
3	B	320	ILE	4.1
3	B	207	ALA	3.8
3	B	340	GLU	3.6
3	A	191	GLY	3.5
3	B	92	LEU	3.5
3	B	324	TYR	3.4
3	B	330	SER	3.3
3	B	323	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	151	ASN	3.1
3	A	277	ASP	3.1
3	B	329	ASP	3.1
3	A	275	ALA	3.0
3	A	167	ALA	3.0
3	B	164	LEU	2.9
3	B	189	ASP	2.9
3	A	207	ALA	2.9
3	A	234	PRO	2.8
3	A	341	ASP	2.8
3	A	276	LYS	2.8
3	B	278	ASP	2.8
3	A	210	GLU	2.8
1	C	18	DT	2.8
3	B	316	THR	2.7
3	A	308	GLU	2.7
1	C	19	DA	2.6
3	A	204	VAL	2.6
3	A	307	PRO	2.6
3	A	316	THR	2.6
3	A	215	LEU	2.6
3	B	341	ASP	2.6
3	A	171	LEU	2.6
3	A	200	THR	2.6
3	A	232	ASP	2.5
3	B	277	ASP	2.5
3	A	92	LEU	2.5
3	B	325	ILE	2.5
3	A	170	THR	2.4
3	B	281	GLN	2.3
3	A	128	GLY	2.3
3	A	206	THR	2.3
3	A	322	MET	2.2
3	B	235	ASN	2.2
3	B	24	ARG	2.2
3	A	279	SER	2.2
3	B	113	VAL	2.2
3	A	189	ASP	2.2
3	A	164	LEU	2.1
3	B	209	VAL	2.1
3	A	265	PHE	2.1
3	A	60	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	318	VAL	2.1
3	B	332	THR	2.1
3	A	203	LEU	2.0
3	A	261	LEU	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.