



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:45 AM UTC

PDB ID : 1XO0 / pdb_00001xo0
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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

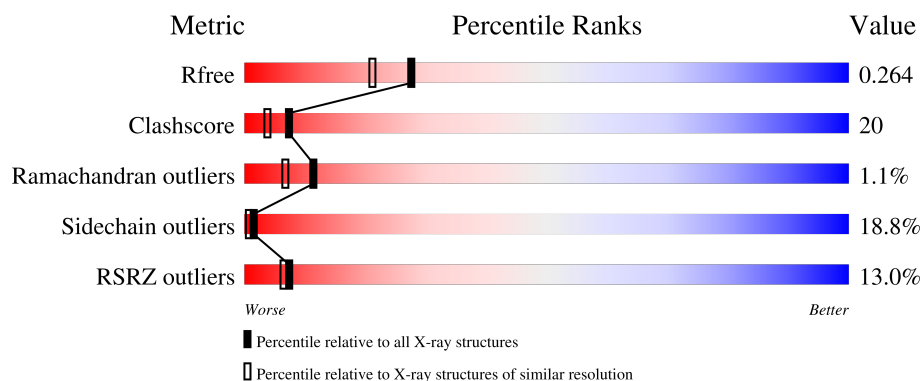
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	C	35	9% 57% 43%
2	D	35	3% 37% 57% 6%
3	A	324	13% 58% 34% 7% .
3	B	324	15% 63% 27% 8% ..

2 Entry composition

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
1	C	35	Total	C	N	O	P	0	0	0
			715	346	125	210	34			

- Molecule 2 is a DNA chain called loxP.

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

- Molecule 3 is a protein called Recombinase CRE.

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

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
4	C	60	Total	O	0	0
			60	60		
4	D	88	Total	O	0	0
			88	88		
4	A	154	Total	O	0	0
			154	154		

Continued on next page...

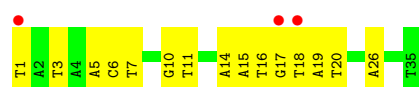
Continued from previous page...

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

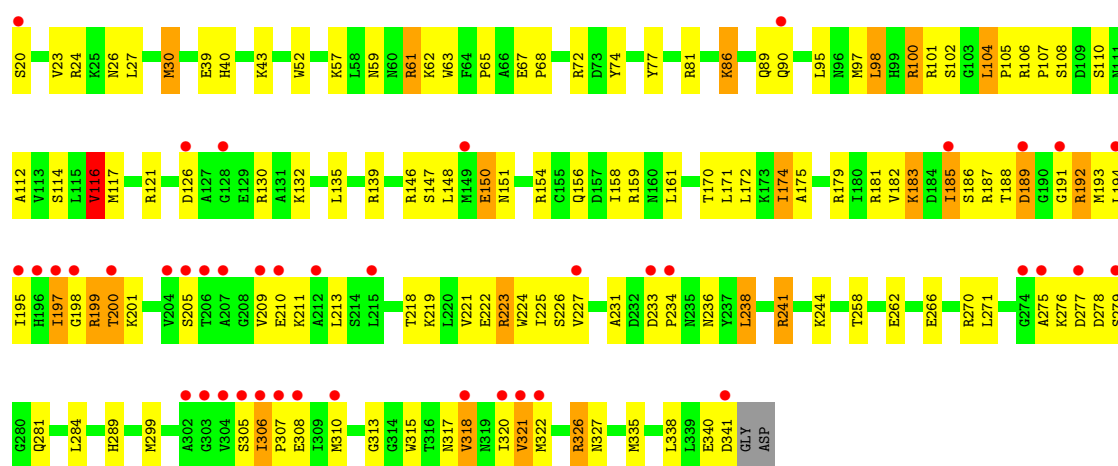
• Molecule 1: loxP



• Molecule 2: loxP

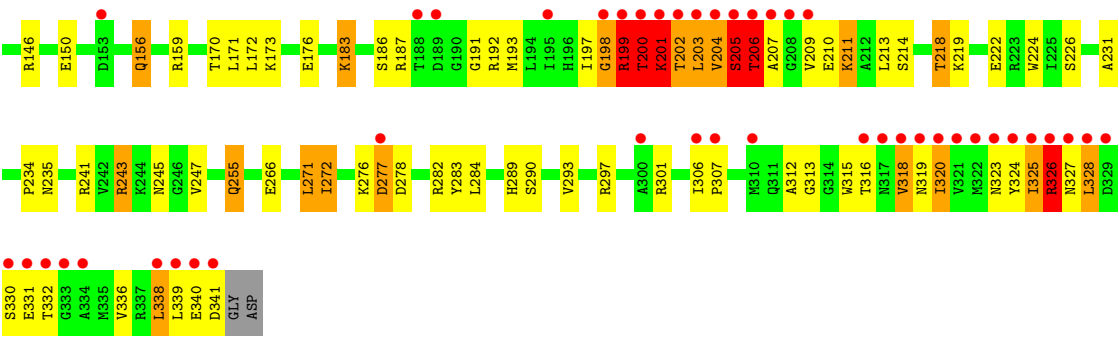


• Molecule 3: Recombinase CRE



• Molecule 3: Recombinase CRE





4 Data and refinement statistics

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 26.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.00-2.00) 82.9 (26.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.36 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

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	C	0.90	3/801 (0.4%)	1.66	3/1235 (0.2%)
2	D	1.36	3/799 (0.4%)	1.36	7/1231 (0.6%)
3	A	0.49	0/2589	0.93	3/3490 (0.1%)
3	B	1.42	8/2589 (0.3%)	1.54	21/3490 (0.6%)
All	All	1.09	14/6778 (0.2%)	1.34	34/9446 (0.4%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	THR	C-N	36.65	1.86	1.33
2	D	1	DT	O3'-P	33.79	2.11	1.61
3	B	199	ARG	CD-NE	-31.15	1.02	1.46
3	B	206	THR	C-N	-27.79	0.94	1.33
3	B	198	GLY	C-N	-27.55	0.95	1.33
3	B	205	SER	C-N	-19.86	1.05	1.33
1	C	1	DT	O3'-P	19.61	1.90	1.61
3	B	199	ARG	CG-CD	-13.03	1.13	1.52
2	D	13	DT	O3'-P	-9.26	1.47	1.61
3	B	206	THR	CA-C	-7.24	1.43	1.52
2	D	26	DA	O3'-P	-6.82	1.50	1.61
3	B	205	SER	CA-C	-6.56	1.44	1.52
1	C	14	DA	O3'-P	-5.66	1.52	1.61
1	C	3	DT	O3'-P	-5.51	1.52	1.61

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	DT	O3'-P-O5'	45.52	172.28	104.00
3	B	198	GLY	O-C-N	-30.46	83.10	122.70
3	B	201	LYS	CA-C-N	-28.10	67.88	121.54
3	B	201	LYS	C-N-CA	-28.10	67.88	121.54
3	B	202	THR	CA-C-N	-27.46	81.70	121.24
3	B	202	THR	C-N-CA	-27.46	81.70	121.24
2	D	1	DT	OP1-P-O3'	-23.07	38.78	108.00
2	D	1	DT	P-O3'-C3'	19.75	149.82	120.20
3	B	202	THR	O-C-N	-17.30	99.58	122.59
3	B	199	ARG	CA-CB-CG	-16.99	80.12	114.10
3	B	204	VAL	O-C-N	-14.81	104.06	122.57
1	C	1	DT	OP1-P-O3'	-12.50	70.50	108.00
2	D	1	DT	OP2-P-O3'	10.56	139.68	108.00
1	C	1	DT	OP2-P-O3'	-9.26	80.23	108.00
2	D	1	DT	O3'-P-O5'	7.63	115.45	104.00
2	D	34	DA	P-O3'-C3'	-7.05	109.62	120.20
3	B	201	LYS	O-C-N	6.95	131.84	122.59
3	B	200	THR	N-CA-C	6.95	125.59	110.80
2	D	13	DT	P-O3'-C3'	6.79	130.38	120.20
3	B	290	SER	N-CA-C	6.74	119.49	111.33
3	A	116	VAL	CB-CA-C	-6.71	102.96	112.22
3	B	22	GLU	N-CA-C	-5.96	104.86	111.36
3	B	206	THR	CA-C-N	5.63	132.28	121.54
3	B	206	THR	C-N-CA	5.63	132.28	121.54
3	B	199	ARG	NE-CZ-NH2	5.44	124.10	119.20
2	D	35	DT	C2'-C3'-O3'	-5.43	103.35	111.50
3	B	206	THR	O-C-N	5.40	129.78	122.59
3	B	134	ALA	N-CA-C	5.25	117.49	110.35
3	A	174	ILE	N-CA-C	5.23	115.95	110.62
3	A	135	LEU	N-CA-C	-5.21	102.14	109.96
3	B	203	LEU	N-CA-C	5.17	117.19	109.59
3	B	325	ILE	N-CA-C	-5.14	106.88	112.80
3	B	326	ARG	NE-CZ-NH2	5.12	123.81	119.20
3	B	102	SER	N-CA-C	-5.00	107.18	113.28

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 ⓘ

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	33	0
3	A	2548	0	2571	90	1
3	B	2548	0	2565	141	1
4	A	154	0	0	7	0
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	255	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 (255) 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
3:B:202:THR:C	3:B:203:LEU:N	1.86	1.33
1:C:17:DG:H5''	3:B:202:THR:CB	1.62	1.30
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:202:THR:C	3:B:203:LEU:CA	2.19	1.14
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
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
3:A:193:MET:HE3	3:A:218:THR:HG23	1.32	1.06
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:202:THR:C	3:B:203:LEU:HA	1.94	0.86
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
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:A:89:GLN:HG3	3:A:117:MET:HE2	1.67	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:30:MET:HE2	3:A:101:ARG:HB3	1.73	0.70
3:B:197:ILE:CD1	3:B:211:LYS:HG3	2.22	0.70
2:D:34:DA:H2''	2:D:35:DT:O4'	1.90	0.69
3:B:206:THR:HG1	3:B:207:ALA:N	1.90	0.69
3:B:336:VAL:O	3:B:340:GLU:HG3	1.92	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
4:A:460:HOH:O	3:B:326:ARG:HD2	1.94	0.66
3:B:205:SER:HG	3:B:206:THR:N	1.91	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:210:GLU:O	3:B:331:GLU:HB2	1.97	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
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:A:193:MET:HE3	3:A:218:THR:CG2	2.20	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
3:B:202:THR:C	3:B:203:LEU:C	2.69	0.60
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:189:ASP:OD1	3:A:189:ASP:C	2.46	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
3:A:26:ASN:O	3:A:30:MET:HE3	2.04	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
2:D:8:DT:H1'	2:D:9:DC:H5'	1.88	0.56
3:A:305:SER:C	3:A:307:PRO:HD2	2.30	0.56
3:B:42:TRP:O	3:B:46:LEU:HG	2.06	0.56
3:B:193:MET:HE3	3:B:222:GLU:HG3	1.88	0.56
3:B:199:ARG:C	3:B:203:LEU:O	2.49	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:202:THR:O	3:B:203:LEU:CA	2.25	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:89:GLN:CG	3:A:117:MET:HE2	2.38	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: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
3:A:89:GLN:HG3	3:A:117:MET:CE	2.39	0.50
3:B:277:ASP:CG	3:B:278:ASP:H	2.20	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:323:ASN:C	3:B:326:ARG:H	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:22:DT:H2'	2:D:23:DT:H71	1.97	0.46
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
3:B:277:ASP:HB3	3:B:284:LEU:HD13	1.96	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:A:193:MET:CE	3:A:218:THR:HG23	2.23	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:201:LYS:HB3	3:B:201:LYS:HE2	1.81	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:A:231:ALA:C	3:A:233:ASP:H	2.28	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:97:MET:O	3:A:98:LEU:C	2.62	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
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: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:297:ARG:O	3:B:301:ARG:HG2	2.22	0.40
3:A:227:VAL:O	3:A:227:VAL:HG12	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%)	14	9
3	B	320/324 (99%)	302 (94%)	14 (4%)	4 (1%)	9	5
All	All	640/648 (99%)	603 (94%)	30 (5%)	7 (1%)	11	7

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%)	214 (80%)	55 (20%)	1	0
3	B	269/270 (100%)	223 (83%)	46 (17%)	2	1
All	All	538/540 (100%)	437 (81%)	101 (19%)	1	1

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	20	SER
3	A	23	VAL
3	A	27	LEU
3	A	30	MET
3	A	39	GLU
3	A	57	LYS
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
3	A	104	LEU
3	A	108	SER
3	A	114	SER
3	A	116	VAL
3	A	121	ARG
3	A	130	ARG
3	A	132	LYS
3	A	147	SER
3	A	148	LEU
3	A	150	GLU
3	A	151	ASN
3	A	161	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	276	LYS
3	A	279	SER
3	A	289	HIS
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
3	A	338	LEU
3	B	22	GLU
3	B	23	VAL
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	95	LEU
3	B	101	ARG
3	B	108	SER
3	B	122	LYS
3	B	130	ARG
3	B	156	GLN
3	B	173	LYS
3	B	176	GLU
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	241	ARG
3	B	243	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	255	GLN
3	B	266	GLU
3	B	271	LEU
3	B	272	ILE
3	B	276	LYS
3	B	282	ARG
3	B	289	HIS
3	B	293	VAL
3	B	316	THR
3	B	318	VAL
3	B	320	ILE
3	B	326	ARG
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	89	GLN
3	A	156	GLN
3	A	269	HIS
3	B	40	HIS
3	B	90	GLN
3	B	94	GLN
3	B	133	GLN
3	B	235	ASN
3	B	255	GLN
3	B	311	GLN
3	B	319	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides 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

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	C	35/35 (100%)	0.28	3 (8%) 16 15	25, 39, 75, 90	0
2	D	35/35 (100%)	0.18	1 (2%) 53 52	24, 36, 60, 70	0
3	A	322/324 (99%)	0.84	42 (13%) 7 6	22, 47, 82, 99	0
3	B	322/324 (99%)	0.62	47 (14%) 6 5	19, 35, 83, 99	0
All	All	714/718 (99%)	0.68	93 (13%) 7 6	19, 41, 83, 99	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	202	THR	11.4
3	B	205	SER	10.4
3	B	200	THR	9.9
3	B	204	VAL	9.1
3	B	203	LEU	8.7
3	B	199	ARG	8.6
2	D	1	DT	8.3
3	B	320	ILE	7.2
3	B	201	LYS	6.9
1	C	1	DT	6.5
3	B	323	ASN	5.3
3	B	20	SER	4.8
3	A	209	VAL	4.8
3	B	198	GLY	4.5
3	A	307	PRO	4.5
3	B	206	THR	4.3
3	B	340	GLU	4.1
3	B	321	VAL	4.0
3	A	306	ILE	3.9
3	B	324	TYR	3.9
3	A	304	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	325	ILE	3.8
3	A	210	GLU	3.8
3	A	189	ASP	3.7
3	B	277	ASP	3.7
3	B	207	ALA	3.7
3	B	307	PRO	3.6
3	A	191	GLY	3.5
3	B	208	GLY	3.4
3	B	326	ARG	3.3
3	B	317	ASN	3.2
3	A	194	LEU	3.2
3	B	331	GLU	3.2
3	A	204	VAL	3.0
3	A	308	GLU	3.0
3	B	341	ASP	3.0
3	A	126	ASP	2.9
3	A	303	GLY	2.9
3	A	341	ASP	2.8
3	B	329	ASP	2.8
3	B	332	THR	2.8
3	B	327	ASN	2.8
3	A	197	ILE	2.8
3	B	319	ASN	2.7
3	A	195	ILE	2.7
3	A	205	SER	2.7
3	A	234	PRO	2.7
3	B	318	VAL	2.7
3	A	215	LEU	2.7
3	B	328	LEU	2.7
3	A	322	MET	2.7
3	A	20	SER	2.7
3	A	275	ALA	2.6
3	B	209	VAL	2.6
1	C	18	DT	2.6
3	B	322	MET	2.6
3	A	227	VAL	2.6
3	A	198	GLY	2.6
3	B	316	THR	2.6
3	A	149	MET	2.5
3	A	90	GLN	2.4
3	A	185	ILE	2.4
3	A	279	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	330	SER	2.4
3	B	334	ALA	2.4
3	A	320	ILE	2.4
3	A	310	MET	2.4
3	B	338	LEU	2.3
3	A	277	ASP	2.3
3	B	189	ASP	2.3
3	A	196	HIS	2.3
3	A	200	THR	2.3
3	A	206	THR	2.3
1	C	17	DG	2.3
3	A	233	ASP	2.3
3	A	318	VAL	2.2
3	B	126	ASP	2.2
3	B	153	ASP	2.2
3	B	188	THR	2.2
3	A	321	VAL	2.2
3	B	310	MET	2.2
3	A	274	GLY	2.2
3	A	212	ALA	2.2
3	A	302	ALA	2.2
3	A	305	SER	2.2
3	B	195	ILE	2.1
3	B	333	GLY	2.1
3	A	207	ALA	2.1
3	B	60	ASN	2.1
3	B	306	ILE	2.1
3	A	128	GLY	2.1
3	B	300	ALA	2.0
3	B	339	LEU	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 oligosaccharides 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.