



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:53 am GMT

PDB ID : 2CRX  
Title : STRUCTURE OF THE HOLLIDAY JUNCTION INTERMEDIATE IN CRE-  
LOXP SITE-SPECIFIC RECOMBINATION  
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Deposited on : 1998-06-19  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

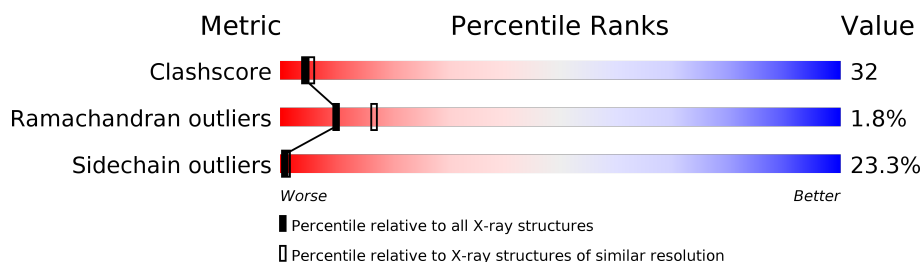
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	35	
1	D	35	
2	A	343	
2	B	343	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6639 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 DNA 35-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	35	Total	C	N	O	P	0	0	0
			711	345	126	207	33			
1	D	34	Total	C	N	O	P	0	0	0
			694	335	124	202	33			

- Molecule 2 is a protein called PROTEIN (CRE RECOMBINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	305	Total	C	N	O	S	0	0	0
			2424	1510	460	439	15			
2	B	309	Total	C	N	O	S	0	0	0
			2449	1524	468	442	15			

- Molecule 3 is water.

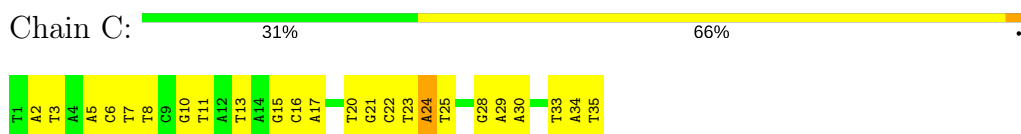
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		
3	B	150	Total	O	0	0
			150	150		
3	C	31	Total	O	0	0
			31	31		
3	D	54	Total	O	0	0
			54	54		

### 3 Residue-property plots

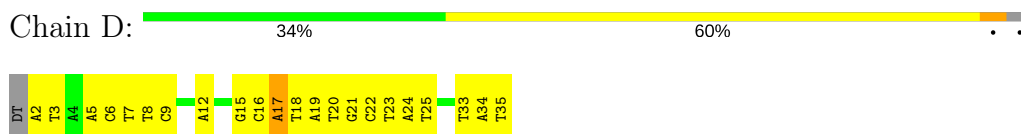
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

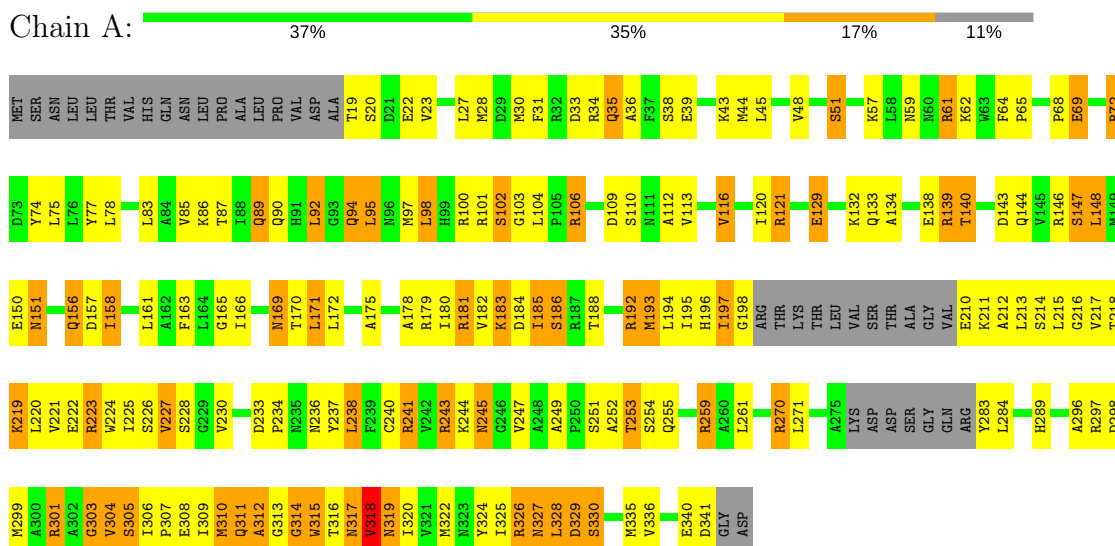
#### • Molecule 1: DNA 35-MER



#### • Molecule 1: DNA 35-MER



#### • Molecule 2: PROTEIN (CRE RECOMBINASE)



#### • Molecule 2: PROTEIN (CRE RECOMBINASE)



MET	K86	D157	D233	T316
SER	T87	I158	F294	N317
ASN	I88	R159	N235	V318
LEU	Q89	N160	N236	N319
LEU	Q90	L161	Y237	I320
THR	H91	L238	L238	V321
VAL	L92	I166		M322
HIS		A167	R241	
GLN	L95	Y168	V242	I325
ASN	N96	N169	R243	R326
LEU	M97	T170	R244	ASN
PRO		L171	N245	LEU
ALA	R100	L172	G246	ASP
LEU	R101	R173	V247	SER
PRO	S102		A248	GLU
VAL	G103	I177	A249	THR
ASP	L104			
ALA	P105	I180	A252	G333
T19	R106	R181	T253	A334
	P107	V182	S254	M335
V23	S108	K183	Q255	V336
R24	D109	D184	Q256	R337
K25	S110	I185	L256	L338
N26		S186	S257	L339
L27	V113	R187	T258	E340
H28	S114	T188	R259	D341
M30	L115		A260	GLY
	V116	R192	L261	ASP
R34	M117	M193	E266	
Q35	R118	L194		
	R119		L271	
	I120	I197		
S38	R121	G198	D277	
E39	K122	ARG	D278	
	E123	THR	S279	
W42	N124	LYS	G280	
		THR	Q281	
L45	E129	LEU	E282	
L46	R130	VAL	Y283	
		SER	L284	
S51	Q133	THR		
K57	A134	A207	A291	
		G208	R292	
N60	R139	V209	V293	
R61	T140	E210		
		K211	D298	
F64	D143	A212	M299	
P65	Q144	L213	A300	
A66	V145	S214		
E67	R146		V304	
P68	S147	T218	S305	
	L148	K219	I306	
R72	M149		P307	
	E150	E222	E308	
L78	N151	R223	I309	
Q79	S152	W224	M310	
	D153	I225		
L83	R154	S226	G313	
	C155	V227	G314	
	Q156		W315	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.90Å 122.50Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.30 – 2.50	Depositor
% Data completeness (in resolution range)	94.4 (27.30-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.198 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6639	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

## 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	0.48	0/796	0.80	0/1225
1	D	0.58	0/777	0.84	1/1195 (0.1%)
2	A	0.38	0/2463	0.64	1/3319 (0.0%)
2	B	0.43	0/2488	0.64	1/3350 (0.0%)
All	All	0.44	0/6524	0.69	3/9089 (0.0%)

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
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	17	DA	C5'-C4'-C3'	-7.04	101.42	114.10
2	B	207	ALA	N-CA-C	-5.78	95.38	111.00
2	A	102	SER	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	24	DA	Sidechain
1	D	24	DA	Sidechain

## 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	711	0	402	23	0
1	D	694	0	389	28	0
2	A	2424	0	2437	219	0
2	B	2449	0	2465	126	0
3	A	126	0	0	18	0
3	B	150	0	0	9	0
3	C	31	0	0	1	0
3	D	54	0	0	5	0
All	All	6639	0	5693	380	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 32.

All (380) 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)
2:A:19:THR:HA	2:A:22:GLU:HG3	1.31	1.10
1:D:19:DA:H2''	1:D:20:DT:H5''	1.32	1.10
2:B:333:GLY:HA2	2:B:336:VAL:HB	1.27	1.05
2:A:132:LYS:HB3	2:A:283:TYR:CE2	1.96	1.00
2:B:333:GLY:O	2:B:334:ALA:C	2.02	0.94
1:D:17:DA:H2''	1:D:18:DT:H6	1.32	0.94
2:A:192:ARG:HA	2:A:218:THR:HG21	1.48	0.93
2:B:193:MET:HB2	2:B:218:THR:HG22	1.52	0.91
2:A:259:ARG:HG3	2:A:259:ARG:HH11	1.37	0.90
2:A:132:LYS:HB3	2:A:283:TYR:HE2	1.36	0.89
1:D:17:DA:H2''	1:D:18:DT:C6	2.09	0.87
2:A:299:MET:HB3	2:A:304:VAL:HG21	1.57	0.87
2:B:188:THR:HG23	2:B:192:ARG:O	1.72	0.87
1:D:19:DA:C2'	1:D:20:DT:H5''	2.05	0.86
2:A:34:ARG:HG2	3:A:413:HOH:O	1.76	0.86
1:D:6:DC:H2'	1:D:7:DT:H72	1.59	0.84
1:D:5:DA:H2''	1:D:6:DC:H5''	1.60	0.84
2:A:316:THR:HG22	2:A:317:ASN:H	1.42	0.83
2:B:313:GLY:HA3	2:B:315:TRP:CZ3	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:306:ILE:HG23	2:A:307:PRO:HD3	1.61	0.82
2:B:333:GLY:HA2	2:B:336:VAL:CB	2.10	0.81
2:B:317:ASN:ND2	2:B:320:ILE:HG13	1.97	0.80
1:D:17:DA:C8	1:D:18:DT:H72	2.18	0.79
2:A:243:ARG:CG	2:A:243:ARG:HH11	1.95	0.79
1:C:17:DA:OP2	2:B:316:THR:HG23	1.82	0.79
2:B:121:ARG:HB2	2:B:121:ARG:HH11	1.46	0.79
2:B:193:MET:H	2:B:218:THR:HG21	1.46	0.78
2:A:221:VAL:O	2:A:225:ILE:HG13	1.84	0.78
2:A:270:ARG:NH1	2:A:270:ARG:HB3	1.99	0.77
2:A:146:ARG:O	2:A:150:GLU:HB2	1.83	0.77
2:A:304:VAL:HG23	2:A:309:ILE:HD11	1.67	0.77
2:A:197:ILE:HG23	2:A:198:GLY:N	1.99	0.77
2:A:243:ARG:HG2	2:A:243:ARG:HH11	1.50	0.76
2:A:62:LYS:NZ	2:A:62:LYS:HB3	2.01	0.76
1:C:5:DA:H2''	1:C:6:DC:H5''	1.68	0.75
2:A:310:MET:HE1	2:A:318:VAL:HG13	1.69	0.75
2:A:69:GLU:HG3	3:A:348:HOH:O	1.85	0.75
1:D:6:DC:H2'	1:D:7:DT:C7	2.16	0.74
2:B:317:ASN:HD22	2:B:320:ILE:HG13	1.49	0.74
2:A:259:ARG:HG3	2:A:259:ARG:NH1	1.99	0.74
2:A:310:MET:CE	2:A:318:VAL:HG13	2.18	0.73
2:A:185:ILE:N	2:A:185:ILE:HD13	2.04	0.73
2:B:129:GLU:O	2:B:130:ARG:HD3	1.88	0.72
2:A:317:ASN:O	2:A:319:ASN:N	2.23	0.72
2:B:119:ARG:O	2:B:123:GLU:HG3	1.89	0.72
2:B:173:ARG:HD2	3:B:461:HOH:O	1.88	0.72
2:A:188:THR:HG21	2:A:194:LEU:HD22	1.72	0.72
1:C:16:DC:H2''	1:C:17:DA:C8	2.25	0.72
1:C:2:DA:H2''	1:C:3:DT:H5'	1.72	0.71
2:A:132:LYS:HB3	2:A:283:TYR:CD2	2.25	0.71
1:D:19:DA:H2''	1:D:20:DT:C5'	2.16	0.71
2:A:223:ARG:O	2:A:227:VAL:HG22	1.91	0.70
2:A:311:GLN:HG3	2:A:312:ALA:N	2.04	0.70
2:B:333:GLY:O	2:B:334:ALA:O	2.09	0.70
2:B:146:ARG:O	2:B:150:GLU:HB2	1.91	0.70
2:B:277:ASP:OD1	2:B:284:LEU:HD13	1.91	0.70
2:A:19:THR:CA	2:A:22:GLU:HG3	2.14	0.70
2:A:186:SER:OG	2:A:194:LEU:HB3	1.93	0.69
2:A:85:VAL:HG23	2:A:129:GLU:OE2	1.92	0.69
2:A:45:LEU:HD11	2:A:98:LEU:HD22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:DG:H2''	1:D:22:DC:H5''	1.72	0.69
2:A:218:THR:O	2:A:222:GLU:HG3	1.92	0.69
1:C:6:DC:H2'	1:C:7:DT:H71	1.72	0.69
2:A:171:LEU:HD13	2:A:312:ALA:HB1	1.75	0.68
2:A:158:ILE:HG12	2:A:223:ARG:HG2	1.76	0.68
2:A:94:GLN:HE21	2:A:94:GLN:HA	1.58	0.68
2:B:214:SER:O	2:B:218:THR:HG23	1.94	0.68
2:A:186:SER:O	2:A:194:LEU:N	2.27	0.68
2:A:297:ARG:O	2:A:301:ARG:HG3	1.93	0.68
2:A:306:ILE:CG2	2:A:307:PRO:HD3	2.23	0.67
2:B:170:THR:HB	2:B:211:LYS:HG2	1.74	0.67
2:B:193:MET:H	2:B:218:THR:CG2	2.07	0.67
2:A:74:TYR:O	2:A:77:TYR:HB3	1.94	0.67
2:A:316:THR:HG22	2:A:317:ASN:N	2.08	0.67
2:B:192:ARG:HG2	2:B:213:LEU:O	1.95	0.66
2:A:106:ARG:HD3	2:A:109:ASP:OD2	1.94	0.66
2:B:334:ALA:HB3	3:B:400:HOH:O	1.96	0.66
2:A:98:LEU:H	2:A:98:LEU:HD23	1.61	0.66
2:B:42:TRP:O	2:B:46:LEU:HG	1.96	0.66
2:A:317:ASN:C	2:A:319:ASN:N	2.48	0.65
2:B:235:ASN:O	2:B:252:ALA:HB1	1.97	0.65
2:B:67:GLU:HG3	3:B:351:HOH:O	1.95	0.65
2:A:156:GLN:HE21	2:A:156:GLN:H	1.44	0.65
2:A:245:ASN:H	2:A:245:ASN:HD22	1.43	0.64
2:A:192:ARG:HA	2:A:218:THR:CG2	2.26	0.64
2:B:113:VAL:O	2:B:116:VAL:HG12	1.97	0.64
2:B:177:ILE:O	2:B:180:ILE:HG13	1.97	0.63
2:A:305:SER:OG	2:A:307:PRO:HD2	1.99	0.63
2:A:193:MET:HE1	2:A:221:VAL:HB	1.81	0.63
1:C:34:DA:H2''	1:C:35:DT:OP2	1.99	0.63
2:A:77:TYR:HD1	2:A:78:LEU:HD23	1.63	0.63
2:A:245:ASN:O	2:A:247:VAL:HG23	1.99	0.63
2:B:60:ASN:O	2:B:61:ARG:HD2	1.99	0.63
2:A:213:LEU:HD22	2:A:217:VAL:HG11	1.81	0.62
2:A:192:ARG:HH11	2:A:215:LEU:HG	1.63	0.62
2:B:317:ASN:HD21	2:B:319:ASN:HB3	1.64	0.62
2:A:139:ARG:HH12	2:B:339:LEU:HA	1.64	0.61
2:A:100:ARG:CZ	2:A:106:ARG:HD2	2.31	0.61
2:A:317:ASN:C	2:A:319:ASN:H	2.03	0.61
2:B:139:ARG:HG2	2:B:139:ARG:HH11	1.65	0.61
2:A:35:GLN:HB2	2:B:119:ARG:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:48:VAL:HG21	2:A:94:GLN:HG3	1.83	0.61
2:A:197:ILE:CG2	2:A:198:GLY:N	2.63	0.61
2:A:172:LEU:HD21	2:A:197:ILE:CD1	2.31	0.60
2:A:301:ARG:C	2:A:303:GLY:H	2.04	0.60
2:A:193:MET:HG2	2:A:218:THR:HG23	1.83	0.60
2:B:139:ARG:HG2	2:B:139:ARG:NH1	2.16	0.60
2:A:188:THR:CG2	2:A:194:LEU:HD22	2.31	0.60
2:B:68:PRO:HB3	2:B:110:SER:OG	2.02	0.59
2:B:315:TRP:HB3	2:B:320:ILE:HD12	1.83	0.59
1:D:16:DC:O4'	3:D:70:HOH:O	2.17	0.59
2:B:159:ARG:HB2	2:B:224:TRP:CE3	2.37	0.59
2:B:313:GLY:HA3	2:B:315:TRP:CE3	2.37	0.59
2:B:333:GLY:O	2:B:337:ARG:N	2.35	0.59
2:A:270:ARG:HB3	2:A:270:ARG:CZ	2.31	0.59
2:A:216:GLY:HA3	3:A:430:HOH:O	2.03	0.59
2:A:245:ASN:N	2:A:245:ASN:HD22	1.99	0.59
2:B:159:ARG:HB2	2:B:224:TRP:CZ3	2.37	0.59
2:A:192:ARG:HD3	2:A:215:LEU:CD2	2.33	0.59
2:A:194:LEU:HD12	2:A:212:ALA:HA	1.85	0.58
2:B:299:MET:HG2	2:B:304:VAL:HG21	1.83	0.58
1:D:18:DT:H5''	3:D:48:HOH:O	2.03	0.58
1:D:33:DT:H73	3:D:76:HOH:O	2.03	0.58
2:A:163:PHE:CE1	2:A:261:LEU:HD22	2.38	0.58
2:A:64:PHE:CD1	2:A:65:PRO:HA	2.39	0.58
2:A:121:ARG:HD3	3:A:437:HOH:O	2.04	0.58
2:A:33:ASP:OD2	2:B:72:ARG:NH1	2.37	0.58
2:A:62:LYS:HZ2	2:A:62:LYS:HB3	1.69	0.58
2:A:306:ILE:HG23	2:A:307:PRO:CD	2.33	0.58
1:C:6:DC:H2'	1:C:7:DT:C7	2.34	0.58
2:A:193:MET:HE2	2:A:218:THR:HG23	1.86	0.57
2:B:187:ARG:NH2	2:B:222:GLU:OE2	2.36	0.57
2:B:279:SER:OG	2:B:281:GLN:HG3	2.03	0.57
2:B:318:VAL:O	2:B:322:MET:HG2	2.04	0.57
2:A:183:LYS:HG3	2:A:234:PRO:O	2.04	0.57
2:A:75:LEU:HD11	2:A:92:LEU:HG	1.86	0.57
2:A:156:GLN:HG2	2:A:157:ASP:H	1.69	0.57
2:B:317:ASN:HD22	2:B:320:ILE:CG1	2.16	0.57
2:A:106:ARG:O	2:A:109:ASP:HB2	2.04	0.57
2:A:172:LEU:CD2	2:A:197:ILE:HD11	2.35	0.57
2:A:309:ILE:O	2:A:309:ILE:HG22	2.04	0.57
2:A:326:ARG:HG3	2:A:327:ASN:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:SER:O	2:A:104:LEU:N	2.38	0.57
2:A:112:ALA:O	2:A:116:VAL:HG22	2.04	0.57
2:A:193:MET:CE	2:A:221:VAL:HB	2.34	0.56
2:A:44:MET:HE3	2:A:44:MET:HA	1.87	0.56
1:D:18:DT:C5'	3:D:48:HOH:O	2.54	0.56
2:A:226:SER:HB2	3:A:466:HOH:O	2.05	0.56
2:A:89:GLN:HG2	3:A:350:HOH:O	2.05	0.56
2:A:106:ARG:NH1	2:A:109:ASP:OD1	2.39	0.56
2:A:147:SER:HB2	3:A:462:HOH:O	2.05	0.55
2:A:170:THR:HB	2:A:211:LYS:HG3	1.88	0.55
2:A:181:ARG:HA	2:A:237:TYR:HA	1.88	0.55
2:A:245:ASN:H	2:A:245:ASN:ND2	2.03	0.55
2:A:307:PRO:O	2:A:310:MET:HB2	2.07	0.55
2:A:197:ILE:HG23	2:A:198:GLY:H	1.70	0.55
2:B:145:VAL:HG13	2:B:149:MET:SD	2.47	0.55
2:A:87:THR:O	2:A:90:GLN:HB3	2.08	0.54
2:A:326:ARG:HG3	2:A:327:ASN:N	2.23	0.54
2:B:299:MET:O	2:B:304:VAL:HG23	2.07	0.54
1:D:22:DC:OP1	2:B:101:ARG:NH1	2.37	0.54
1:C:24:DA:H2'	1:C:25:DT:H72	1.89	0.54
1:C:5:DA:C2'	1:C:6:DC:H5''	2.38	0.54
2:A:30:MET:HE1	2:A:101:ARG:O	2.06	0.54
2:A:77:TYR:CD1	2:A:78:LEU:HD23	2.43	0.54
1:C:24:DA:H2''	1:C:25:DT:C6	2.44	0.53
1:D:8:DT:H2''	1:D:9:DC:H5'	1.89	0.53
2:B:181:ARG:NH2	2:B:252:ALA:O	2.41	0.53
2:B:194:LEU:HD23	2:B:211:LYS:O	2.09	0.53
2:A:178:ALA:HB2	2:A:261:LEU:HD11	1.91	0.53
2:A:102:SER:C	2:A:104:LEU:H	2.12	0.53
1:C:29:DA:H1'	1:C:30:DA:C8	2.44	0.53
2:A:328:LEU:HD13	2:A:329:ASP:H	1.74	0.52
2:B:256:LEU:HD23	2:B:261:LEU:HD21	1.91	0.52
2:A:299:MET:HG2	2:B:338:LEU:HD11	1.90	0.52
2:A:85:VAL:HG11	2:A:121:ARG:HG2	1.90	0.52
2:A:340:GLU:O	2:A:341:ASP:HB3	2.08	0.52
2:A:39:GLU:O	2:A:43:LYS:HG2	2.10	0.52
2:A:224:TRP:O	2:A:228:SER:HB3	2.09	0.52
2:B:30:MET:SD	2:B:101:ARG:HG2	2.49	0.52
2:B:121:ARG:HH11	2:B:121:ARG:CB	2.19	0.52
2:A:94:GLN:O	2:A:98:LEU:HD23	2.10	0.52
2:B:233:ASP:O	2:B:236:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:DT:O4	2:B:259:ARG:HG2	2.09	0.52
2:A:143:ASP:HA	2:A:146:ARG:HH11	1.75	0.52
2:A:172:LEU:HD22	2:A:197:ILE:HD11	1.91	0.51
2:A:62:LYS:HE2	2:A:65:PRO:O	2.10	0.51
2:A:195:ILE:HD11	2:A:213:LEU:HD11	1.92	0.51
2:B:245:ASN:ND2	2:B:247:VAL:CG2	2.73	0.51
1:C:2:DA:C2'	1:C:3:DT:H5'	2.40	0.51
2:A:172:LEU:CD2	2:A:197:ILE:CD1	2.89	0.51
2:A:213:LEU:HD22	2:A:217:VAL:CG1	2.41	0.51
1:D:15:DG:O3'	1:D:16:DC:H5''	2.11	0.51
2:A:193:MET:HE2	2:A:218:THR:O	2.09	0.51
2:A:217:VAL:O	2:A:221:VAL:HG23	2.11	0.51
1:D:25:DT:OP1	2:B:173:ARG:HB3	2.11	0.51
2:A:192:ARG:HD3	2:A:215:LEU:HG	1.92	0.51
2:A:192:ARG:CA	2:A:218:THR:HG21	2.32	0.51
2:A:299:MET:HA	2:B:338:LEU:HD21	1.94	0.51
2:B:78:LEU:HB3	2:B:83:LEU:HD12	1.92	0.51
2:A:146:ARG:HD2	3:A:377:HOH:O	2.11	0.50
2:A:172:LEU:HD21	2:A:197:ILE:HD12	1.93	0.50
2:A:175:ALA:O	2:A:179:ARG:HG3	2.10	0.50
2:A:193:MET:CE	2:A:218:THR:HG23	2.41	0.50
2:A:100:ARG:NH1	2:A:106:ARG:HD2	2.27	0.50
2:A:44:MET:O	2:A:48:VAL:HG23	2.11	0.50
2:A:182:VAL:O	2:A:185:ILE:HG12	2.11	0.50
2:A:33:ASP:OD1	2:B:119:ARG:NH1	2.40	0.50
2:B:134:ALA:HA	2:B:283:TYR:CD1	2.46	0.50
1:C:28:DG:H2''	1:C:29:DA:O5'	2.12	0.50
2:B:92:LEU:O	2:B:92:LEU:HD12	2.12	0.50
1:C:16:DC:H6	3:B:448:HOH:O	1.95	0.49
2:B:172:LEU:HD11	2:B:197:ILE:HD11	1.94	0.49
2:B:309:ILE:HG21	2:B:321:VAL:CG1	2.41	0.49
1:D:17:DA:C2'	1:D:18:DT:C6	2.91	0.49
2:B:279:SER:CB	2:B:281:GLN:HE21	2.25	0.49
2:B:317:ASN:OD1	2:B:318:VAL:N	2.46	0.49
2:B:34:ARG:HB2	2:B:42:TRP:CZ2	2.47	0.49
2:B:235:ASN:O	2:B:252:ALA:CB	2.61	0.49
2:A:140:THR:HG21	3:A:423:HOH:O	2.13	0.49
2:A:217:VAL:O	2:A:220:LEU:HB2	2.12	0.49
2:A:305:SER:O	2:A:308:GLU:HB3	2.12	0.49
2:A:317:ASN:O	2:A:318:VAL:C	2.50	0.49
2:A:210:GLU:O	2:A:211:LYS:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:ARG:HB2	3:B:478:HOH:O	2.11	0.48
2:B:146:ARG:HA	2:B:161:LEU:HD11	1.93	0.48
2:A:296:ALA:HA	2:A:299:MET:CE	2.42	0.48
2:A:181:ARG:HB3	2:A:181:ARG:HE	1.43	0.48
2:A:316:THR:CG2	2:A:317:ASN:H	2.18	0.48
2:A:241:ARG:HD3	3:A:381:HOH:O	2.13	0.48
2:A:328:LEU:HD12	2:A:330:SER:OG	2.14	0.48
2:A:68:PRO:HB3	2:A:110:SER:CB	2.44	0.48
2:B:79:GLN:HA	2:B:88:ILE:HD11	1.95	0.48
2:B:183:LYS:NZ	3:B:431:HOH:O	2.46	0.48
1:C:23:DT:H2''	1:C:24:DA:OP2	2.13	0.48
2:A:316:THR:O	2:A:317:ASN:C	2.51	0.48
2:B:57:LYS:HB2	2:B:57:LYS:HE2	1.41	0.48
2:A:116:VAL:O	2:A:120:ILE:HG13	2.14	0.47
2:A:299:MET:HG2	2:B:338:LEU:CD1	2.44	0.47
2:A:44:MET:CA	2:A:44:MET:HE3	2.43	0.47
2:B:237:TYR:CE2	2:B:255:GLN:HG2	2.49	0.47
2:B:306:ILE:N	2:B:307:PRO:HD2	2.29	0.47
2:A:317:ASN:N	2:A:317:ASN:OD1	2.47	0.47
2:B:243:ARG:HB3	2:B:243:ARG:HE	1.54	0.47
1:D:2:DA:OP2	1:D:2:DA:H3'	2.14	0.47
2:B:336:VAL:O	2:B:340:GLU:HG3	2.14	0.47
2:B:245:ASN:ND2	2:B:247:VAL:HG23	2.30	0.47
1:C:13:DT:H71	2:B:87:THR:HG23	1.95	0.47
2:A:315:TRP:CZ2	2:A:324:TYR:HE2	2.33	0.47
2:B:140:THR:O	2:B:144:GLN:HG3	2.15	0.47
1:D:34:DA:H2''	1:D:35:DT:O5'	2.14	0.47
2:A:44:MET:HB3	2:A:90:GLN:HE22	1.80	0.47
2:A:62:LYS:HZ3	2:A:62:LYS:HB3	1.80	0.47
2:B:106:ARG:HG3	2:B:109:ASP:OD2	2.15	0.47
2:B:106:ARG:O	2:B:109:ASP:HB2	2.14	0.47
1:D:15:DG:N3	3:D:70:HOH:O	2.35	0.47
2:A:219:LYS:HA	2:A:222:GLU:OE1	2.14	0.46
2:A:243:ARG:CG	2:A:243:ARG:NH1	2.64	0.46
3:C:42:HOH:O	2:B:86:LYS:HD2	2.13	0.46
1:C:15:DG:O6	2:B:86:LYS:NZ	2.47	0.46
2:A:226:SER:C	2:A:228:SER:H	2.18	0.46
2:A:336:VAL:O	2:A:340:GLU:HG3	2.15	0.46
2:A:182:VAL:HB	2:A:234:PRO:HA	1.97	0.46
2:A:298:ASP:HA	2:A:301:ARG:HD2	1.98	0.46
2:A:64:PHE:HD1	2:A:65:PRO:HA	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:GLY:O	2:B:336:VAL:N	2.49	0.46
1:C:21:DG:H2''	1:C:22:DC:C6	2.50	0.46
2:A:214:SER:HA	2:B:336:VAL:HG13	1.98	0.46
2:B:241:ARG:HG3	2:B:249:ALA:HB3	1.98	0.46
2:A:113:VAL:HA	2:A:116:VAL:CG2	2.46	0.46
2:A:140:THR:CG2	3:A:423:HOH:O	2.64	0.46
2:A:299:MET:C	2:A:304:VAL:HG22	2.37	0.46
2:B:185:ILE:HD11	2:B:238:LEU:HD22	1.97	0.46
2:A:305:SER:O	2:A:308:GLU:N	2.48	0.46
2:A:151:ASN:N	2:A:151:ASN:OD1	2.47	0.45
2:A:243:ARG:HB2	2:A:245:ASN:ND2	2.31	0.45
2:A:301:ARG:C	2:A:303:GLY:N	2.67	0.45
2:B:320:ILE:HD11	3:B:448:HOH:O	2.16	0.45
2:A:143:ASP:HA	2:A:146:ARG:NH1	2.30	0.45
2:A:313:GLY:O	2:A:314:GLY:C	2.53	0.45
1:D:34:DA:H2''	1:D:35:DT:O4'	2.17	0.45
2:A:30:MET:CE	2:A:101:ARG:O	2.64	0.45
2:A:181:ARG:HG3	2:A:184:ASP:OD1	2.16	0.45
2:B:194:LEU:HD23	2:B:211:LYS:C	2.36	0.45
1:C:24:DA:H2''	1:C:25:DT:H6	1.81	0.45
2:A:270:ARG:HB3	2:A:270:ARG:HH11	1.80	0.45
2:A:78:LEU:HB3	2:A:83:LEU:HD12	1.99	0.45
2:B:291:ALA:HB3	3:B:344:HOH:O	2.17	0.45
2:B:334:ALA:O	2:B:338:LEU:HD12	2.17	0.45
2:A:245:ASN:ND2	2:A:247:VAL:HB	2.32	0.45
2:B:227:VAL:HG12	2:B:227:VAL:O	2.16	0.45
2:B:96:ASN:ND2	2:B:108:SER:HB2	2.32	0.45
1:C:20:DT:H2''	1:C:21:DG:OP2	2.17	0.45
1:D:17:DA:C2'	1:D:18:DT:C7	2.95	0.45
1:D:2:DA:H2''	1:D:3:DT:O5'	2.17	0.45
2:A:106:ARG:HG3	2:A:106:ARG:H	1.61	0.45
2:B:158:ILE:HG21	2:B:223:ARG:HG2	1.99	0.45
2:B:79:GLN:NE2	2:B:124:ASN:OD1	2.50	0.45
2:B:90:GLN:HG2	3:B:371:HOH:O	2.17	0.45
1:D:5:DA:H1'	1:D:6:DC:O4'	2.17	0.45
2:A:156:GLN:HE21	2:A:156:GLN:N	2.11	0.44
2:A:170:THR:HA	2:A:211:LYS:HE2	1.99	0.44
2:A:233:ASP:O	2:A:236:ASN:HB2	2.17	0.44
2:B:186:SER:OG	2:B:187:ARG:N	2.50	0.44
2:A:185:ILE:HA	2:A:194:LEU:O	2.17	0.44
2:A:328:LEU:HD13	3:A:452:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:304:VAL:CG2	2:A:309:ILE:HD11	2.44	0.44
2:B:317:ASN:HB3	2:B:320:ILE:HD11	1.99	0.44
2:A:36:ALA:HB1	2:B:118:ARG:CD	2.48	0.44
2:B:19:THR:OG1	2:B:23:VAL:HG23	2.18	0.44
2:B:34:ARG:HB2	2:B:42:TRP:CE2	2.52	0.44
2:B:158:ILE:CG2	2:B:223:ARG:HG2	2.47	0.44
2:B:309:ILE:HG21	2:B:321:VAL:HG13	1.99	0.44
2:A:156:GLN:HG2	2:A:157:ASP:N	2.32	0.44
2:A:310:MET:HE3	2:A:318:VAL:HG13	1.99	0.44
2:A:138:GLU:OE2	2:A:301:ARG:NH1	2.51	0.44
2:A:296:ALA:HA	2:A:299:MET:HE3	2.00	0.44
2:B:143:ASP:O	2:B:147:SER:HB3	2.17	0.44
2:B:27:LEU:HD22	2:B:102:SER:HB2	1.99	0.44
2:A:196:HIS:HA	2:A:210:GLU:HG2	1.98	0.43
2:A:158:ILE:HG13	3:A:451:HOH:O	2.18	0.43
2:A:106:ARG:HH11	2:A:109:ASP:CG	2.22	0.43
2:A:31:PHE:O	2:A:34:ARG:HD3	2.18	0.43
2:A:156:GLN:NE2	2:A:156:GLN:H	2.12	0.43
2:A:325:ILE:O	2:A:328:LEU:HB2	2.19	0.43
2:B:170:THR:C	2:B:171:LEU:HD12	2.38	0.43
2:B:315:TRP:HB3	2:B:320:ILE:CD1	2.48	0.43
2:B:97:MET:O	2:B:101:ARG:HB2	2.19	0.43
2:B:96:ASN:HD21	2:B:108:SER:HB2	1.82	0.43
2:A:144:GLN:O	2:A:148:LEU:HD12	2.18	0.42
2:A:236:ASN:N	2:A:252:ALA:HB2	2.33	0.42
2:A:100:ARG:C	2:A:102:SER:H	2.22	0.42
2:A:51:SER:OG	2:A:74:TYR:OH	2.37	0.42
1:D:22:DC:H2''	1:D:23:DT:C6	2.55	0.42
2:A:193:MET:H	2:A:193:MET:HG2	1.61	0.42
2:A:255:GLN:HG2	3:A:447:HOH:O	2.20	0.42
2:A:271:LEU:HD22	2:A:271:LEU:O	2.20	0.42
2:A:165:GLY:HA3	2:A:217:VAL:HG22	2.00	0.42
2:A:134:ALA:HB2	2:A:289:HIS:CE1	2.55	0.42
2:A:171:LEU:CD1	2:A:312:ALA:HB1	2.47	0.42
2:A:240:CYS:HB3	3:A:435:HOH:O	2.20	0.42
2:A:305:SER:OG	2:A:308:GLU:HB2	2.19	0.42
2:A:59:ASN:O	2:A:61:ARG:HD3	2.20	0.42
2:B:170:THR:O	2:B:171:LEU:HB2	2.20	0.41
2:A:228:SER:OG	2:A:230:VAL:HG13	2.20	0.41
2:A:182:VAL:HG21	2:A:230:VAL:O	2.20	0.41
1:D:12:DA:H5'	3:A:405:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:180:ILE:HG22	2:A:238:LEU:HB2	2.01	0.41
2:A:193:MET:HG3	2:A:213:LEU:HD12	2.01	0.41
2:A:243:ARG:HH12	2:A:249:ALA:HB2	1.85	0.41
2:B:166:ILE:O	2:B:170:THR:HG23	2.20	0.41
2:A:72:ARG:HE	2:A:116:VAL:HG13	1.85	0.41
2:B:318:VAL:O	2:B:322:MET:CG	2.68	0.41
2:A:138:GLU:HG2	2:A:298:ASP:OD1	2.21	0.41
2:A:243:ARG:HB2	2:A:245:ASN:HD21	1.84	0.41
2:B:64:PHE:HA	2:B:65:PRO:C	2.41	0.41
2:A:322:MET:C	2:A:324:TYR:H	2.23	0.41
1:C:33:DT:H2"	1:C:34:DA:C8	2.55	0.41
2:A:95:LEU:HD12	2:A:95:LEU:HA	1.94	0.41
2:B:104:LEU:H	2:B:104:LEU:HG	1.57	0.41
2:A:36:ALA:HB1	2:B:118:ARG:HG2	2.02	0.41
2:B:257:SER:C	2:B:259:ARG:N	2.74	0.41
2:B:306:ILE:O	2:B:309:ILE:HB	2.21	0.41
2:B:317:ASN:HD21	2:B:319:ASN:CB	2.32	0.41
2:A:169:ASN:C	2:A:169:ASN:HD22	2.24	0.41
2:A:35:GLN:HG2	3:A:413:HOH:O	2.21	0.41
2:A:43:LYS:HD3	2:A:43:LYS:HA	1.81	0.41
2:A:92:LEU:O	2:A:92:LEU:HD22	2.21	0.41
2:B:245:ASN:ND2	2:B:247:VAL:HG21	2.36	0.40
2:B:139:ARG:HH11	2:B:139:ARG:CG	2.30	0.40
2:B:300:ALA:HB2	2:B:325:ILE:HD13	2.03	0.40
2:A:192:ARG:HD3	2:A:215:LEU:CG	2.50	0.40
2:B:168:TYR:OH	2:B:298:ASP:OD2	2.23	0.40
2:A:102:SER:C	2:A:104:LEU:N	2.74	0.40
2:A:193:MET:HE3	2:A:218:THR:HA	2.03	0.40
2:A:28:MET:HE3	3:A:406:HOH:O	2.21	0.40
2:A:139:ARG:CG	2:A:139:ARG:HH11	2.34	0.40
2:A:253:THR:OG1	2:A:254:SER:N	2.53	0.40
2:B:152:SER:OG	2:B:154:ARG:HB2	2.21	0.40
1:C:10:DG:H2"	1:C:11:DT:OP2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	299/343 (87%)	262 (88%)	29 (10%)	8 (3%)	6	9
2	B	303/343 (88%)	286 (94%)	14 (5%)	3 (1%)	18	32
All	All	602/686 (88%)	548 (91%)	43 (7%)	11 (2%)	10	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	334	ALA
2	A	103	GLY
2	A	303	GLY
2	A	312	ALA
2	A	318	VAL
2	B	278	ASP
2	B	340	GLU
2	A	314	GLY
2	A	327	ASN
2	A	192	ARG
2	A	227	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	
2	A	255/287 (89%)	189 (74%)	66 (26%)	0	1
2	B	256/287 (89%)	203 (79%)	53 (21%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	511/574 (89%)	392 (77%)	119 (23%)	<b>1</b> <b>1</b>

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	20	SER
2	A	23	VAL
2	A	27	LEU
2	A	35	GLN
2	A	38	SER
2	A	51	SER
2	A	57	LYS
2	A	61	ARG
2	A	69	GLU
2	A	72	ARG
2	A	86	LYS
2	A	89	GLN
2	A	92	LEU
2	A	94	GLN
2	A	95	LEU
2	A	97	MET
2	A	98	LEU
2	A	106	ARG
2	A	116	VAL
2	A	121	ARG
2	A	129	GLU
2	A	133	GLN
2	A	139	ARG
2	A	140	THR
2	A	147	SER
2	A	148	LEU
2	A	151	ASN
2	A	156	GLN
2	A	158	ILE
2	A	161	LEU
2	A	166	ILE
2	A	169	ASN
2	A	171	LEU
2	A	181	ARG
2	A	183	LYS
2	A	185	ILE
2	A	186	SER

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Mol	Chain	Res	Type
2	A	193	MET
2	A	197	ILE
2	A	219	LYS
2	A	223	ARG
2	A	238	LEU
2	A	241	ARG
2	A	243	ARG
2	A	244	LYS
2	A	245	ASN
2	A	251	SER
2	A	253	THR
2	A	259	ARG
2	A	270	ARG
2	A	284	LEU
2	A	301	ARG
2	A	304	VAL
2	A	305	SER
2	A	310	MET
2	A	311	GLN
2	A	315	TRP
2	A	317	ASN
2	A	318	VAL
2	A	319	ASN
2	A	320	ILE
2	A	326	ARG
2	A	328	LEU
2	A	329	ASP
2	A	330	SER
2	A	335	MET
2	B	19	THR
2	B	25	LYS
2	B	27	LEU
2	B	28	MET
2	B	30	MET
2	B	34	ARG
2	B	35	GLN
2	B	38	SER
2	B	39	GLU
2	B	45	LEU
2	B	51	SER
2	B	57	LYS
2	B	86	LYS

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Mol	Chain	Res	Type
2	B	95	LEU
2	B	97	MET
2	B	100	ARG
2	B	101	ARG
2	B	104	LEU
2	B	106	ARG
2	B	108	SER
2	B	114	SER
2	B	121	ARG
2	B	129	GLU
2	B	130	ARG
2	B	133	GLN
2	B	155	CYS
2	B	156	GLN
2	B	169	ASN
2	B	183	LYS
2	B	186	SER
2	B	188	THR
2	B	192	ARG
2	B	209	VAL
2	B	211	LYS
2	B	219	LYS
2	B	226	SER
2	B	243	ARG
2	B	254	SER
2	B	255	GLN
2	B	266	GLU
2	B	271	LEU
2	B	278	ASP
2	B	293	VAL
2	B	305	SER
2	B	308	GLU
2	B	310	MET
2	B	316	THR
2	B	317	ASN
2	B	319	ASN
2	B	320	ILE
2	B	326	ARG
2	B	337	ARG
2	B	341	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	89	GLN
2	A	90	GLN
2	A	94	GLN
2	A	133	GLN
2	A	144	GLN
2	A	156	GLN
2	A	245	ASN
2	A	311	GLN
2	A	319	ASN
2	B	40	HIS
2	B	60	ASN
2	B	89	GLN
2	B	281	GLN
2	B	289	HIS
2	B	319	ASN

### 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 carbohydrates 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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.