



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:21 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

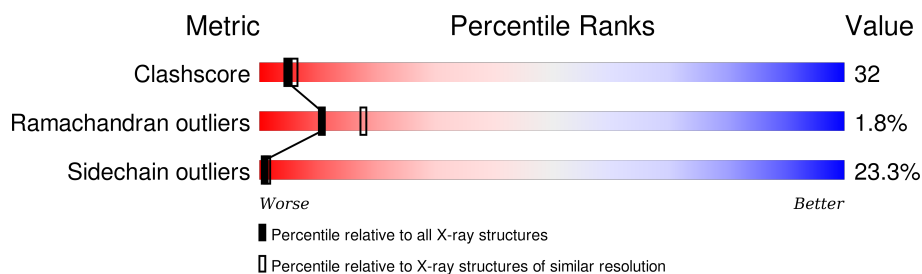
1 Overall quality at a glance

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 ≥ 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.

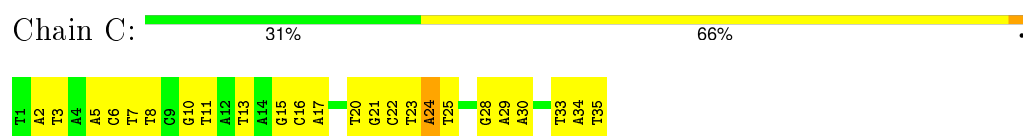
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	126	Total	O	0	0
			126	126		
3	B	150	Total	O	0	0
			150	150		
3	C	31	Total	O	0	0
			31	31		
3	D	54	Total	O	0	0
			54	54		

3 Residue-property plots

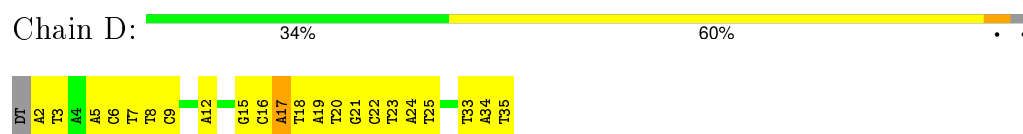
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

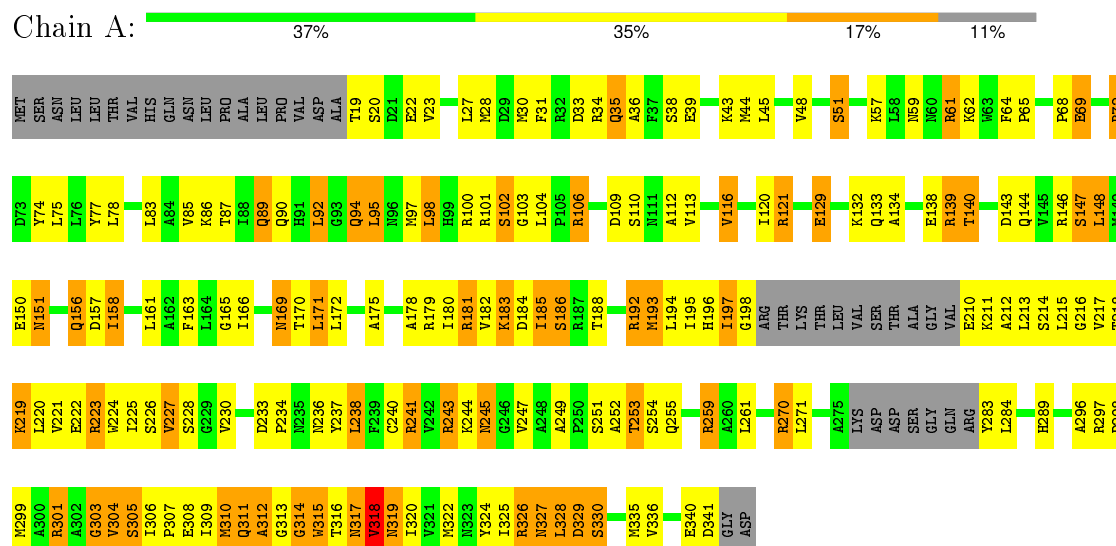
• Molecule 1: DNA 35-MER



• Molecule 1: DNA 35-MER



• Molecule 2: PROTEIN (CRE RECOMBINASE)



• Molecule 2: PROTEIN (CRE RECOMBINASE)



MET	K86	D157	D233	T316
SER	T87	I158	F234	N317
ASN	I88	R159	N235	V318
LEU	Q89	N160	N236	N319
LEU	Q90	L161	Y237	I320
THR	H91	L166	L238	V321
VAL	L92	I167	R241	N322
HIS	L95	Y168	V242	I325
GLN	N96	N169	R243	R326
ASN	N97	T170	R244	ASN
LEU		L171	N245	LEU
PRO	R100	L172	G246	ASP
ALA	R101	R173	V247	SER
LEU	S102	I177	A248	GLU
PRO	G103		A249	THR
VAL	L104	I180	A252	G333
ASP	P105	R181	T253	A334
ALA	R106	V182	S254	N335
T19	F107	K183	Q255	V336
V23	S108	D184	L256	R337
R24	D109	I185	S257	L338
R25	S110	S186	T258	L339
N26	V113	R187	R259	E340
N27	S114	T188	A260	D341
N28	L115	R192	L261	GLY
N30	V116	M193	E266	ASP
R34	M117	L194	L271	
Q35	R118			
S38	I119	I197	D277	
E39	I120	G198	D278	
N42	R121	ARG	S279	
L45	K122	THR	G280	
L46	N124	LYS	Q281	
S51	E129	THR	R282	
K57	R130	LEU	Y283	
N60	A133	VAL	L284	
R61	Q133	SER	A291	
P64	A134	THR	R292	
P65	R139	A207	V293	
A66	T140	G208	D298	
B67	D143	E210	N299	
P68	Q144	A212	A300	
R72	V145	L213	V304	
L78	R146	S214	S305	
Q79	S147	T218	I306	
L83	L148	R219	P307	
	M149	E222	E308	
	E150	R223	I309	
	N151	R224	N310	
	S152	T225	G313	
	D153	S226	G314	
	R154	V227	W315	
	C155			
	Q156			

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	106.90 Å 122.50 Å 180.00 Å 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 ²)	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($^{\circ}$)	Ideal($^{\circ}$)
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
1:C:17:DA:OP2	2:B:316:THR:HG23	1.82	0.79
2:A:243:ARG:CG	2:A:243:ARG:HH11	1.95	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)
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
1:D:21:DG:H2''	1:D:22:DC:H5''	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:193:MET:H	2:B:218:THR:CG2	2.07	0.67
2:B:170:THR:HB	2:B:211:LYS:HG2	1.74	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:67:GLU:HG3	3:B:351:HOH:O	1.95	0.65
2:B:235:ASN:O	2:B:252:ALA:HB1	1.97	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:317:ASN:C	2:A:319:ASN:H	2.03	0.61
2:A:100:ARG:CZ	2:A:106:ARG:HD2	2.31	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:333:GLY:O	2:B:337:ARG:N	2.35	0.59
2:B:313:GLY:HA3	2:B:315:TRP:CE3	2.37	0.59
2:B:159:ARG:HB2	2:B:224:TRP:CE3	2.37	0.59
2:A:270:ARG:HB3	2:A:270:ARG:CZ	2.31	0.59
2:A:245:ASN:N	2:A:245:ASN:HD22	1.99	0.59
2:A:216:GLY:HA3	3:A:430:HOH:O	2.03	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
1:D:18:DT:H5''	3:D:48:HOH:O	2.03	0.58
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:33:DT:H73	3:D:76:HOH:O	2.03	0.58
2:A:64:PHE:CD1	2:A:65:PRO:HA	2.39	0.58
2:A:163:PHE:CE1	2:A:261:LEU:HD22	2.38	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:318:VAL:O	2:B:322:MET:HG2	2.04	0.57
2:B:279:SER:OG	2:B:281:GLN:HG3	2.03	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:309:ILE:O	2:A:309:ILE:HG22	2.04	0.57
2:A:172:LEU:CD2	2:A:197:ILE:HD11	2.35	0.57
2:A:106:ARG:O	2:A:109:ASP:HB2	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
1:D:18:DT:C5'	3:D:48:HOH:O	2.54	0.56
2:A:44:MET:HE3	2:A:44:MET:HA	1.87	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:245:ASN:H	2:A:245:ASN:ND2	2.03	0.55
2:A:181:ARG:HA	2:A:237:TYR:HA	1.88	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
1:D:22:DC:OP1	2:B:101:ARG:NH1	2.37	0.54
2:B:299:MET:O	2:B:304:VAL:HG23	2.07	0.54
1:C:5:DA:C2'	1:C:6:DC:H5"	2.38	0.54
1:C:24:DA:H2'	1:C:25:DT:H72	1.89	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:194:LEU:HD23	2:B:211:LYS:O	2.09	0.53
2:B:181:ARG:NH2	2:B:252:ALA:O	2.41	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:299:MET:HG2	2:B:338:LEU:HD11	1.90	0.52
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: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:B:121:ARG:HH11	2:B:121:ARG:CB	2.19	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: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
1:C:2:DA:C2'	1:C:3:DT:H5'	2.40	0.51
2:B:245:ASN:ND2	2:B:247:VAL:CG2	2.73	0.51
2:A:213:LEU:HD22	2:A:217:VAL:CG1	2.41	0.51
2:A:172:LEU:CD2	2:A:197:ILE:CD1	2.89	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:44:MET:O	2:A:48:VAL:HG23	2.11	0.50
2:A:100:ARG:NH1	2:A:106:ARG:HD2	2.27	0.50
2:A:33:ASP:OD1	2:B:119:ARG:NH1	2.40	0.50
2:A:182:VAL:O	2:A:185:ILE:HG12	2.11	0.50
1:C:28:DG:H2''	1:C:29:DA:O5'	2.12	0.50
2:B:134:ALA:HA	2:B:283:TYR:CD1	2.46	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: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:140:THR:HG21	3:A:423:HOH:O	2.13	0.49
2:B:146:ARG:HA	2:B:161:LEU:HD11	1.93	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:A:210:GLU:O	2:A:211:LYS:HD2	2.13	0.48
2:A:296:ALA:HA	2:A:299:MET:CE	2.42	0.48
2:A:316:THR:CG2	2:A:317:ASN:H	2.18	0.48
2:A:181:ARG:HB3	2:A:181:ARG:HE	1.43	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
1:C:23:DT:H2''	1:C:24:DA:OP2	2.13	0.48
2:B:183:LYS:NZ	3:B:431:HOH:O	2.46	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:306:ILE:N	2:B:307:PRO:HD2	2.29	0.47
2:B:237:TYR:CE2	2:B:255:GLN:HG2	2.49	0.47
2:A:317:ASN:OD1	2:A:317:ASN:N	2.47	0.47
2:B:243:ARG:HE	2:B:243:ARG:HB3	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
1:D:34:DA:H2''	1:D:35:DT:O5'	2.14	0.47
2:B:140:THR:O	2:B:144:GLN:HG3	2.15	0.47
2:A:62:LYS:HZ3	2:A:62:LYS:HB3	1.80	0.47
2:A:44:MET:HB3	2:A:90:GLN:HE22	1.80	0.47
1:D:15:DG:N3	3:D:70:HOH:O	2.35	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
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:B:333:GLY:O	2:B:336:VAL:N	2.49	0.46
2:A:64:PHE:HD1	2:A:65:PRO:HA	1.78	0.46
2:A:182:VAL:HB	2:A:234:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:298:ASP:HA	2:A:301:ARG:HD2	1.98	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:299:MET:C	2:A:304:VAL:HG22	2.37	0.46
2:A:140:THR:CG2	3:A:423:HOH:O	2.64	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:243:ARG:HB2	2:A:245:ASN:ND2	2.31	0.45
2:A:151:ASN:N	2:A:151:ASN:OD1	2.47	0.45
2:B:320:ILE:HD11	3:B:448:HOH:O	2.16	0.45
2:A:301:ARG:C	2:A:303:GLY:N	2.67	0.45
2:A:143:ASP:HA	2:A:146:ARG:NH1	2.30	0.45
1:D:34:DA:H2"	1:D:35:DT:O4'	2.17	0.45
2:A:313:GLY:O	2:A:314:GLY:C	2.53	0.45
2:B:194:LEU:HD23	2:B:211:LYS:C	2.36	0.45
2:A:181:ARG:HG3	2:A:184:ASP:OD1	2.16	0.45
2:A:30:MET:CE	2:A:101:ARG:O	2.64	0.45
1:C:24:DA:H2"	1:C:25:DT:H6	1.81	0.45
2:B:334:ALA:O	2:B:338:LEU:HD12	2.17	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: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: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
1:C:20:DT:H2"	1:C:21:DG:OP2	2.17	0.45
1:D:5:DA:H1'	1:D:6:DC:O4'	2.17	0.45
2:A:106:ARG:H	2:A:106:ARG:HG3	1.61	0.45
2:B:79:GLN:NE2	2:B:124:ASN:OD1	2.50	0.45
2:B:158:ILE:HG21	2:B:223:ARG:HG2	1.99	0.45
2:B:90:GLN:HG2	3:B:371:HOH:O	2.17	0.45
2:A:156:GLN:HE21	2:A:156:GLN:N	2.11	0.44
2:B:186:SER:OG	2:B:187:ARG:N	2.50	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: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:B:34:ARG:HB2	2:B:42:TRP:CE2	2.52	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:309:ILE:HG21	2:B:321:VAL:HG13	1.99	0.44
2:B:158:ILE:CG2	2:B:223:ARG:HG2	2.47	0.44
2:A:310:MET:HE3	2:A:318:VAL:HG13	1.99	0.44
2:A:156:GLN:HG2	2:A:157:ASP:N	2.32	0.44
2:A:296:ALA:HA	2:A:299:MET:HE3	2.00	0.44
2:A:138:GLU:OE2	2:A:301:ARG:NH1	2.51	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:31:PHE:O	2:A:34:ARG:HD3	2.18	0.43
2:A:106:ARG:HH11	2:A:109:ASP:CG	2.22	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:315:TRP:HB3	2:B:320:ILE:CD1	2.48	0.43
2:B:170:THR:C	2:B:171:LEU:HD12	2.38	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:236:ASN:N	2:A:252:ALA:HB2	2.33	0.42
2:A:144:GLN:O	2:A:148:LEU:HD12	2.18	0.42
2:A:100:ARG:C	2:A:102:SER:H	2.22	0.42
1:D:22:DC:H2''	1:D:23:DT:C6	2.55	0.42
2:A:51:SER:OG	2:A:74:TYR:OH	2.37	0.42
2:A:193:MET:H	2:A:193:MET:HG2	1.61	0.42
2:A:271:LEU:HD22	2:A:271:LEU:O	2.20	0.42
2:A:255:GLN:HG2	3:A:447:HOH:O	2.20	0.42
2:A:165:GLY:HA3	2:A:217:VAL:HG22	2.00	0.42
2:A:171:LEU:CD1	2:A:312:ALA:HB1	2.47	0.42
2:A:134:ALA:HB2	2:A:289:HIS:CE1	2.55	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: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:180:ILE:HG22	2:A:238:LEU:HB2	2.01	0.41
2:B:318:VAL:O	2:B:322:MET:CG	2.68	0.41
2:A:72:ARG:HE	2:A:116:VAL:HG13	1.85	0.41
2:A:243:ARG:HB2	2:A:245:ASN:HD21	1.84	0.41
2:A:138:GLU:HG2	2:A:298:ASP:OD1	2.21	0.41
2:B:64:PHE:HA	2:B:65:PRO:C	2.41	0.41
1:C:33:DT:H2"	1:C:34:DA:C8	2.55	0.41
2:A:322:MET:C	2:A:324:TYR:H	2.23	0.41
2:B:317:ASN:HD21	2:B:319:ASN:CB	2.32	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:A:36:ALA:HB1	2:B:118:ARG:HG2	2.02	0.41
2:B:104:LEU:H	2:B:104:LEU:HG	1.57	0.41
2:A:95:LEU:HD12	2:A:95:LEU:HA	1.94	0.41
2:A:35:GLN:HG2	3:A:413:HOH:O	2.21	0.41
2:A:92:LEU:O	2:A:92:LEU:HD22	2.21	0.41
2:A:43:LYS:HD3	2:A:43:LYS:HA	1.81	0.41
2:A:169:ASN:C	2:A:169:ASN:HD22	2.24	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:193:MET:HE3	2:A:218:THR:HA	2.03	0.40
2:A:102:SER:C	2:A:104:LEU:N	2.74	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%)	19	34
All	All	602/686 (88%)	548 (91%)	43 (7%)	11 (2%)	11	18

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%)	1 1

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.