



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:51 pm BST

PDB ID : 6PW2
Title : Structural Basis for Cooperative Binding of EBNA1 to the Epstein-Barr Virus
Dyad Symmetry Minimal Origin of Replication
Authors : Messick, T.E.; Malecka, K.A.; Lieberman, P.M.
Deposited on : 2019-07-22
Resolution : 3.01 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

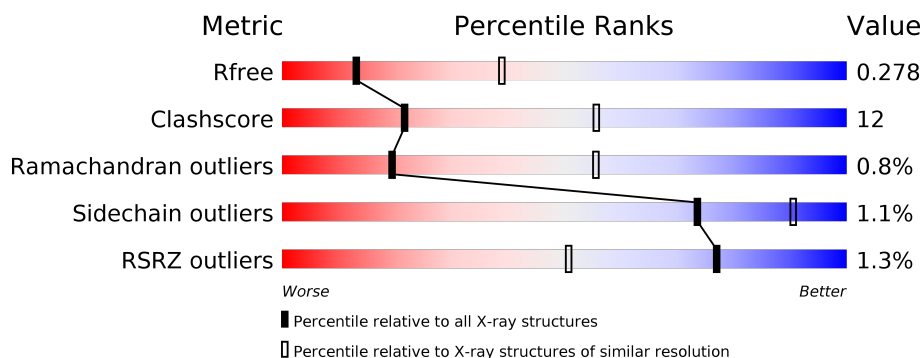
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 on 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	A	147	<div> <div>3%</div> <div>63%</div> <div>34%</div> <div>.</div> </div>
1	B	147	<div> <div>78%</div> <div>22%</div> </div>
1	C	147	<div> <div>3%</div> <div>73%</div> <div>27%</div> <div>.</div> </div>
1	D	147	<div> <div>73%</div> <div>27%</div> </div>
1	I	147	<div> <div>3%</div> <div>69%</div> <div>30%</div> <div>.</div> </div>
1	J	147	<div> <div>76%</div> <div>24%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	147	<div><div><div></div><div></div><div></div></div><div>2%74%25%•</div></div>
1	L	147	<div><div><div></div><div></div><div></div></div><div>%85%14%•</div></div>
2	E	62	<div><div><div></div><div></div><div></div></div><div>48%40%•8%</div></div>
2	G	62	<div><div><div></div><div></div><div></div></div><div>48%29%•21%</div></div>
3	F	62	<div><div><div></div><div></div><div></div></div><div>2%45%37%•15%</div></div>
3	H	62	<div><div><div></div><div></div><div></div></div><div>39%37%•21%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13270 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 protein called Epstein-Barr nuclear antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1125	718	200	200	7			
1	B	147	Total	C	N	O	S	0	0	0
			1125	718	200	200	7			
1	C	147	Total	C	N	O	S	0	0	0
			1125	718	200	200	7			
1	D	147	Total	C	N	O	S	0	0	0
			1125	718	200	200	7			
1	I	147	Total	C	N	O	S	0	0	0
			1125	718	200	200	7			
1	J	147	Total	C	N	O	S	0	0	0
			1125	718	200	200	7			
1	K	147	Total	C	N	O	S	0	0	0
			1125	718	200	200	7			
1	L	147	Total	C	N	O	S	0	0	0
			1125	718	200	200	7			

- Molecule 2 is a DNA chain called DNA (62-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	57	Total	C	N	O	P	0	0	0
			1168	559	206	346	57			
2	G	49	Total	C	N	O	P	0	0	0
			1006	482	178	297	49			

- Molecule 3 is a DNA chain called DNA (62-MER) complementary DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	53	Total	C	N	O	P	0	0	0
			1087	519	201	314	53			
3	H	49	Total	C	N	O	P	0	0	0
			1005	481	185	290	49			

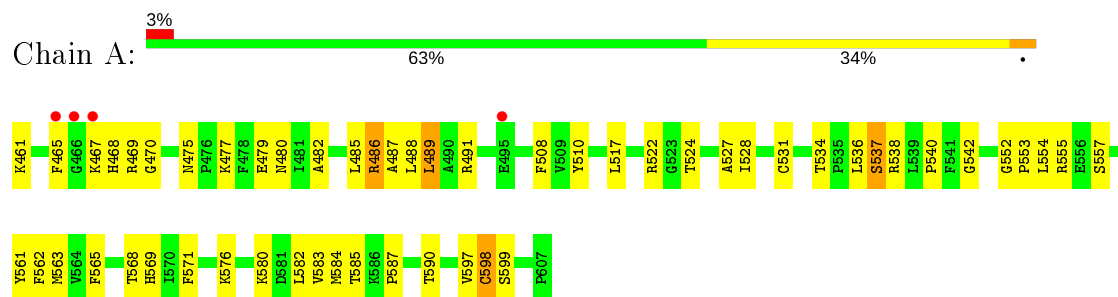
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		
4	J	1	Total	O	0	0
			1	1		
4	K	1	Total	O	0	0
			1	1		

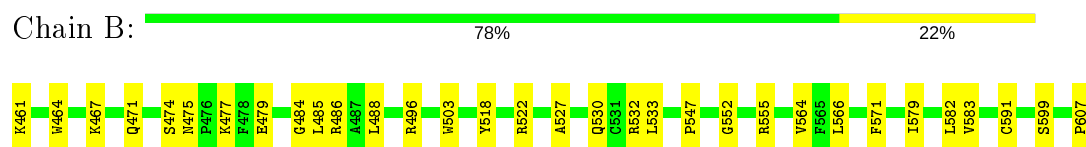
3 Residue-property plots [i](#)

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.

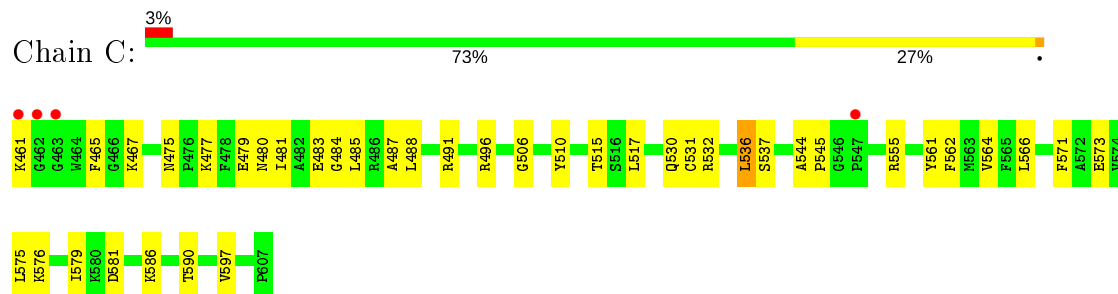
• Molecule 1: Epstein-Barr nuclear antigen 1



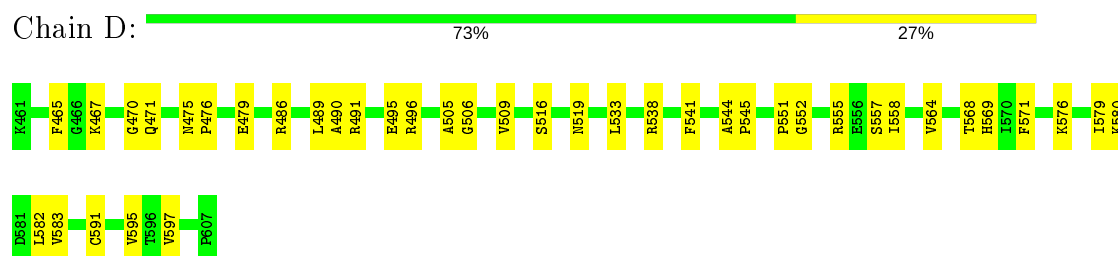
• Molecule 1: Epstein-Barr nuclear antigen 1



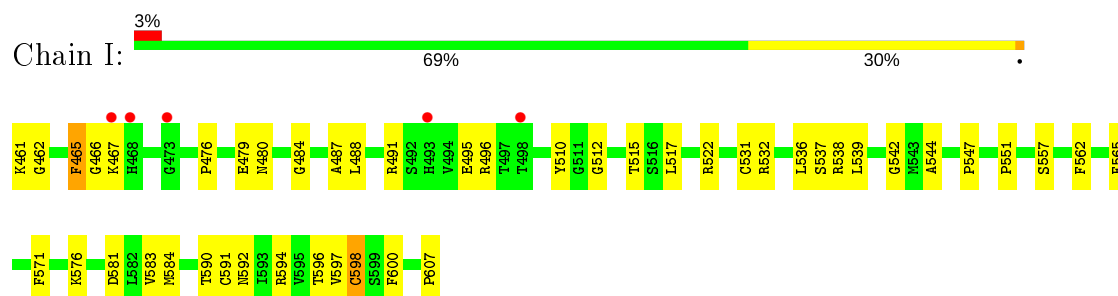
• Molecule 1: Epstein-Barr nuclear antigen 1



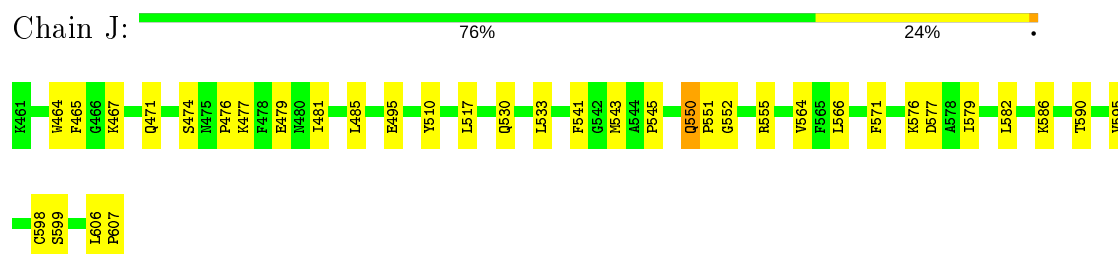
• Molecule 1: Epstein-Barr nuclear antigen 1



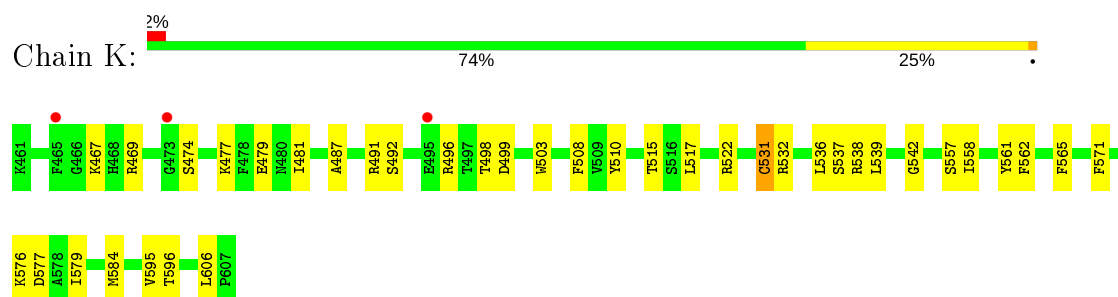
- Molecule 1: Epstein-Barr nuclear antigen 1



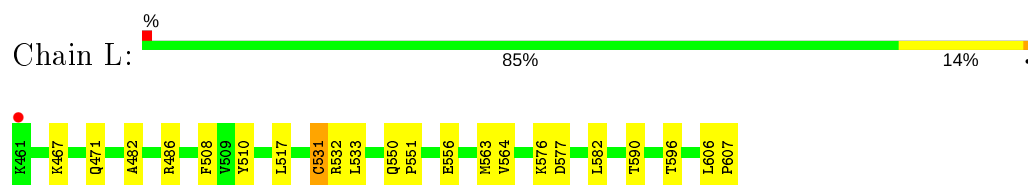
- Molecule 1: Epstein-Barr nuclear antigen 1



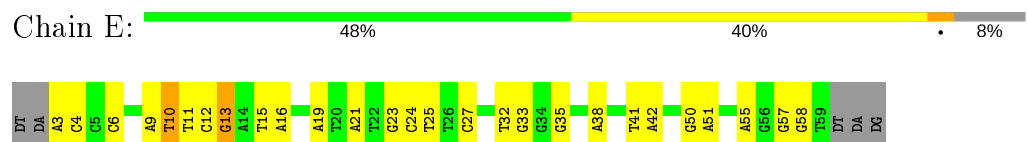
- Molecule 1: Epstein-Barr nuclear antigen 1



- Molecule 1: Epstein-Barr nuclear antigen 1

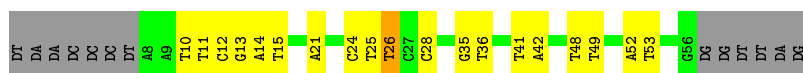


- Molecule 2: DNA (62-MER)

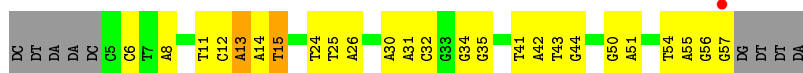


- Molecule 2: DNA (62-MER)

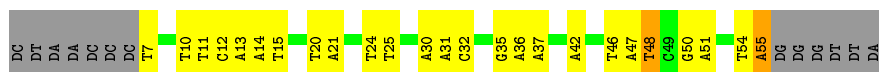




- Molecule 3: DNA (62-MER) complementary DNA strand



- Molecule 3: DNA (62-MER) complementary DNA strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.12Å 283.38Å 63.90Å 90.00° 89.80° 90.00°	Depositor
Resolution (Å)	40.90 – 3.01 47.54 – 3.01	Depositor EDS
% Data completeness (in resolution range)	64.2 (40.90-3.01) 55.2 (47.54-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.277 0.220 , 0.278	Depositor DCC
R_{free} test set	1977 reflections (6.80%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , -19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.397 for l,k,-h 0.428 for -h,-k,l 0.408 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13270	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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	A	0.56	0/1154	0.80	2/1564 (0.1%)
1	B	0.56	0/1154	0.78	0/1564
1	C	0.55	0/1154	0.74	2/1564 (0.1%)
1	D	0.55	0/1154	0.78	1/1564 (0.1%)
1	I	0.63	2/1154 (0.2%)	0.73	0/1564
1	J	0.55	0/1154	0.74	0/1564
1	K	0.61	0/1154	0.73	0/1564
1	L	0.58	0/1154	0.80	1/1564 (0.1%)
2	E	1.05	1/1308 (0.1%)	1.10	2/2017 (0.1%)
2	G	1.11	2/1127 (0.2%)	1.07	2/1738 (0.1%)
3	F	1.08	1/1220 (0.1%)	1.06	2/1880 (0.1%)
3	H	1.04	1/1128 (0.1%)	1.05	1/1738 (0.1%)
All	All	0.78	7/14015 (0.0%)	0.89	13/19885 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	26	DT	C2-O2	-7.80	1.16	1.22
1	I	495	GLU	CB-CG	6.01	1.63	1.52
2	G	26	DT	C1'-N1	6.00	1.57	1.49
3	F	30	DA	N9-C4	5.67	1.41	1.37
2	E	10	DT	C1'-N1	5.33	1.56	1.49
1	I	591	CYS	CB-SG	-5.33	1.73	1.81
3	H	55	DA	N9-C4	5.29	1.41	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	582	LEU	CA-CB-CG	6.17	129.49	115.30
2	E	33	DG	O5'-P-OP2	-5.70	100.57	105.70
2	E	13	DG	O5'-P-OP1	5.51	117.31	110.70
3	F	15	DT	N3-C4-O4	5.50	123.20	119.90
1	L	582	LEU	CA-CB-CG	5.35	127.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	582	LEU	CA-CB-CG	5.27	127.42	115.30
3	F	13	DA	OP1-P-OP2	-5.25	111.73	119.60
1	C	536	LEU	CA-CB-CG	5.13	127.11	115.30
2	G	48	DT	N3-C4-O4	5.12	122.97	119.90
1	C	566	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	489	LEU	CA-CB-CG	5.04	126.88	115.30
3	H	48	DT	N3-C4-O4	5.02	122.91	119.90
2	G	49	DT	N3-C4-O4	5.00	122.90	119.90

There are no chirality outliers.

There are no planarity outliers.

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	A	1125	0	1132	50	0
1	B	1125	0	1132	22	0
1	C	1125	0	1132	35	0
1	D	1125	0	1132	30	0
1	I	1125	0	1132	39	0
1	J	1125	0	1132	27	0
1	K	1125	0	1132	30	0
1	L	1125	0	1132	14	0
2	E	1168	0	647	25	0
2	G	1006	0	557	19	0
3	F	1087	0	598	25	0
3	H	1005	0	554	26	0
4	A	1	0	0	3	0
4	E	1	0	0	1	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
All	All	13270	0	11412	288	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 12.

All (288) 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)
1:A:568:THR:HG21	1:A:571:PHE:HB3	1.41	0.99
1:I:487:ALA:HB1	1:K:584:MET:HG2	1.61	0.82
1:I:584:MET:HG2	1:K:487:ALA:HB1	1.64	0.79
1:C:530:GLN:N	1:C:530:GLN:OE1	2.18	0.77
1:K:467:LYS:HD2	3:H:24:DT:O3'	1.84	0.77
1:A:584:MET:HG2	1:C:487:ALA:HB1	1.69	0.74
2:G:11:DT:H2''	2:G:12:DC:H5''	1.70	0.73
3:H:12:DC:H2''	3:H:13:DA:C8	2.24	0.72
3:F:11:DT:H2''	3:F:12:DC:H5''	1.74	0.70
1:A:542:GLY:N	1:B:607:PRO:OXT	2.25	0.69
1:I:461:LYS:NZ	2:G:26:DT:O2	2.26	0.68
3:H:11:DT:H2''	3:H:12:DC:H5''	1.75	0.67
2:E:11:DT:H2''	2:E:12:DC:H5''	1.76	0.66
1:A:536:LEU:HD12	1:A:562:PHE:HB3	1.77	0.66
1:C:467:LYS:HD2	3:F:25:DT:H5'	1.78	0.65
1:A:568:THR:CG2	1:A:571:PHE:HB3	2.23	0.64
1:C:488:LEU:O	1:C:491:ARG:NE	2.31	0.64
1:I:600:PHE:CD1	1:J:598:CYS:HB3	2.32	0.64
2:E:38:DA:OP2	4:E:101:HOH:O	2.15	0.64
3:H:31:DA:H2'	3:H:32:DC:C6	2.33	0.64
3:H:24:DT:H2'	3:H:25:DT:C6	2.34	0.63
1:K:537:SER:HB3	1:K:561:TYR:CE1	2.33	0.63
1:K:503:TRP:CE2	1:K:606:LEU:HD12	2.34	0.63
1:L:550:GLN:OE1	1:L:551:PRO:HD2	1.99	0.63
1:K:542:GLY:N	1:L:607:PRO:OXT	2.32	0.63
1:K:537:SER:HB3	1:K:561:TYR:HE1	1.62	0.63
1:K:536:LEU:HD12	1:K:562:PHE:HB3	1.80	0.62
1:L:467:LYS:HE3	1:L:471:GLN:O	2.00	0.62
1:I:461:LYS:HD3	1:I:462:GLY:N	2.15	0.61
1:K:539:LEU:HD13	1:L:606:LEU:HD23	1.82	0.61
3:F:6:DC:H5''	3:F:6:DC:H6	1.65	0.61
1:I:542:GLY:N	1:J:607:PRO:OXT	2.33	0.61
1:I:510:TYR:HA	1:I:517:LEU:HD11	1.83	0.61
1:K:477:LYS:O	1:K:481:ILE:HG13	2.00	0.61
1:D:486:ARG:O	1:D:490:ALA:HB2	2.02	0.60
1:I:491:ARG:HD2	1:K:584:MET:HE1	1.82	0.60
3:F:54:DT:H1'	3:F:55:DA:H5'	1.84	0.59
2:G:12:DC:H2''	2:G:13:DG:C8	2.37	0.59
1:C:531:CYS:O	1:C:532:ARG:HD2	2.03	0.59
1:K:517:LEU:HD22	1:K:562:PHE:CE2	2.38	0.59
1:A:569:HIS:CE1	1:A:599:SER:HB2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ARG:HD3	2:E:23:DG:H4'	1.84	0.59
3:F:24:DT:H2'	3:F:25:DT:C6	2.37	0.59
1:A:587:PRO:HG2	2:E:32:DT:H5''	1.85	0.58
3:H:31:DA:H2''	3:H:32:DC:O5'	2.03	0.58
3:F:31:DA:H4'	3:F:32:DC:OP1	2.04	0.57
1:A:531:CYS:HB2	1:A:565:PHE:O	2.04	0.57
1:I:512:GLY:HA2	1:I:592:ASN:HB2	1.85	0.57
1:A:465:PHE:CE2	2:E:25:DT:H1'	2.41	0.56
1:C:576:LYS:HD3	1:C:597:VAL:CG2	2.35	0.56
1:J:477:LYS:HZ1	2:G:12:DC:H2'	1.70	0.56
1:J:552:GLY:O	1:J:555:ARG:HB2	2.04	0.56
1:D:552:GLY:O	1:D:555:ARG:HB2	2.06	0.56
1:J:485:LEU:HD21	1:J:579:ILE:HG12	1.89	0.55
1:J:543:MET:HG2	1:J:550:GLN:HE22	1.72	0.55
1:K:469:ARG:NH1	1:L:556:GLU:OE1	2.39	0.55
1:D:505:ALA:HB2	1:D:569:HIS:ND1	2.22	0.54
1:K:538:ARG:HD3	1:K:557:SER:O	2.07	0.54
1:A:527:ALA:C	1:A:528:ILE:HG13	2.28	0.54
1:D:551:PRO:HB3	1:D:555:ARG:HG2	1.89	0.54
2:G:28:DC:O2	3:H:35:DG:N2	2.41	0.54
1:C:532:ARG:HH22	1:D:551:PRO:HD2	1.73	0.54
2:G:25:DT:H2''	2:G:26:DT:H5'	1.89	0.53
1:I:465:PHE:CZ	2:G:24:DC:H1'	2.43	0.53
1:C:537:SER:HB3	1:C:561:TYR:CE1	2.43	0.53
1:K:510:TYR:HA	1:K:517:LEU:HD11	1.89	0.53
1:J:467:LYS:HE3	1:J:471:GLN:O	2.08	0.53
1:B:518:TYR:O	1:B:522:ARG:HG2	2.08	0.53
2:E:3:DA:H1'	2:E:4:DC:H5'	1.91	0.53
2:E:57:DG:H2''	2:E:58:DG:C8	2.44	0.53
1:I:484:GLY:O	1:I:488:LEU:HD12	2.08	0.53
1:A:568:THR:O	1:A:568:THR:HG23	2.08	0.53
1:A:583:VAL:HG13	1:A:590:THR:O	2.09	0.52
2:G:14:DA:H1'	2:G:15:DT:H5'	1.90	0.52
3:H:11:DT:C2'	3:H:12:DC:H5''	2.38	0.52
3:H:50:DG:H2''	3:H:51:DA:H8	1.75	0.52
1:L:533:LEU:CD2	1:L:564:VAL:HG22	2.40	0.52
1:K:531:CYS:O	1:K:532:ARG:HD3	2.10	0.51
1:L:510:TYR:HA	1:L:517:LEU:HD11	1.93	0.51
2:G:10:DT:H2''	2:G:11:DT:H5''	1.93	0.51
1:I:461:LYS:HZ2	3:H:37:DA:H2	1.59	0.51
1:I:488:LEU:O	1:I:491:ARG:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:581:ASP:HA	1:I:584:MET:HE2	1.92	0.51
3:H:10:DT:H4'	3:H:11:DT:OP1	2.10	0.51
1:K:515:THR:HB	2:G:35:DG:OP2	2.10	0.51
1:K:496:ARG:HG2	1:K:571:PHE:CZ	2.46	0.51
2:G:21:DA:H5''	2:G:21:DA:H8	1.76	0.51
1:I:532:ARG:HH22	1:J:543:MET:HG2	1.76	0.51
1:I:538:ARG:HD2	1:I:557:SER:O	2.11	0.51
1:J:533:LEU:CD2	1:J:564:VAL:HG22	2.41	0.51
2:G:11:DT:C2'	2:G:12:DC:H5''	2.40	0.50
3:H:50:DG:H2''	3:H:51:DA:C8	2.46	0.50
1:D:509:VAL:HG22	1:D:595:VAL:HG13	1.94	0.50
1:I:480:ASN:ND2	3:H:32:DC:OP2	2.44	0.50
1:K:517:LEU:HD22	1:K:562:PHE:HE2	1.75	0.50
1:I:496:ARG:HG2	1:I:571:PHE:CE1	2.47	0.50
1:C:586:LYS:HD2	1:C:590:THR:HG21	1.92	0.50
1:L:576:LYS:HE2	1:L:577:ASP:OD1	2.12	0.50
1:A:510:TYR:HA	1:A:517:LEU:HD11	1.94	0.50
1:A:576:LYS:HD3	1:A:597:VAL:HG23	1.94	0.50
1:D:538:ARG:HH21	1:D:558:ILE:HA	1.77	0.50
3:H:30:DA:H2''	3:H:31:DA:C8	2.47	0.50
1:A:540:PRO:HB2	1:B:532:ARG:HB3	1.93	0.50
1:D:516:SER:HA	1:D:519:ASN:HD22	1.77	0.49
1:A:480:ASN:ND2	3:F:32:DC:OP2	2.45	0.49
1:I:544:ALA:HB2	1:I:551:PRO:HD3	1.94	0.49
1:A:537:SER:HB3	1:A:561:TYR:CE1	2.47	0.49
1:D:583:VAL:HG13	1:D:591:CYS:HA	1.95	0.49
1:L:508:PHE:HB3	1:L:596:THR:HG23	1.94	0.49
1:B:533:LEU:CD2	1:B:564:VAL:HG22	2.42	0.49
3:F:50:DG:H2''	3:F:51:DA:C8	2.47	0.49
1:D:576:LYS:HD3	1:D:597:VAL:HG23	1.94	0.49
1:D:538:ARG:NE	1:D:557:SER:O	2.46	0.48
2:E:15:DT:H2''	2:E:16:DA:C8	2.48	0.48
3:H:47:DA:H2''	3:H:48:DT:H71	1.95	0.48
1:I:536:LEU:HD12	1:I:562:PHE:HB3	1.95	0.48
1:I:496:ARG:HG2	1:I:571:PHE:CD1	2.48	0.48
1:I:598:CYS:HA	1:J:599:SER:O	2.13	0.48
1:J:533:LEU:HD23	1:J:564:VAL:HG22	1.95	0.48
1:K:496:ARG:HG2	1:K:571:PHE:CE1	2.48	0.48
1:J:590:THR:OG1	2:G:13:DG:OP1	2.25	0.48
1:I:461:LYS:CE	2:G:26:DT:O2	2.62	0.48
1:L:533:LEU:HD23	1:L:564:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:11:DT:C3'	3:H:12:DC:H5''	2.42	0.48
3:F:11:DT:C2'	3:F:12:DC:H5''	2.44	0.48
1:B:475:ASN:O	1:B:477:LYS:N	2.47	0.48
1:C:475:ASN:O	1:C:479:GLU:HG3	2.13	0.48
1:D:496:ARG:HG2	1:D:571:PHE:CE1	2.49	0.48
1:A:536:LEU:HB2	2:E:23:DG:P	2.54	0.48
1:B:530:GLN:OE1	1:B:530:GLN:N	2.47	0.48
1:C:506:GLY:HA2	1:C:564:VAL:O	2.14	0.47
1:D:506:GLY:HA2	1:D:564:VAL:O	2.13	0.47
1:J:579:ILE:HG22	1:J:595:VAL:HG21	1.95	0.47
1:K:579:ILE:HB	1:K:595:VAL:HG21	1.95	0.47
1:L:576:LYS:HG2	1:L:577:ASP:N	2.29	0.47
1:J:550:GLN:OE1	1:J:551:PRO:HD2	2.13	0.47
2:E:27:DC:H42	3:F:35:DG:H1	1.60	0.47
1:C:517:LEU:HD22	1:C:562:PHE:CE2	2.50	0.47
1:D:467:LYS:HE3	1:D:471:GLN:O	2.14	0.47
3:F:54:DT:C2	3:F:55:DA:H8	2.33	0.47
1:D:479:GLU:O	1:D:479:GLU:HG2	2.15	0.47
3:F:41:DT:H2''	3:F:42:DA:C8	2.50	0.47
1:I:531:CYS:HB2	1:I:565:PHE:O	2.14	0.47
1:L:531:CYS:O	1:L:532:ARG:HD3	2.14	0.47
1:A:576:LYS:O	1:A:580:LYS:HG3	2.15	0.47
1:J:495:GLU:N	1:J:495:GLU:OE1	2.47	0.47
1:A:461:LYS:HA	1:A:461:LYS:HD3	1.70	0.47
1:C:575:LEU:O	1:C:579:ILE:HG13	2.15	0.47
1:A:489:LEU:N	4:A:701:HOH:O	2.48	0.47
1:J:476:PRO:HA	1:J:479:GLU:OE1	2.15	0.47
1:A:538:ARG:HD3	1:A:557:SER:O	2.15	0.46
1:A:540:PRO:HA	1:A:555:ARG:O	2.15	0.46
1:B:583:VAL:CG1	1:B:591:CYS:HA	2.45	0.46
1:A:488:LEU:O	1:A:491:ARG:NE	2.48	0.46
1:A:508:PHE:HD1	1:A:563:MET:HE3	1.79	0.46
1:A:475:ASN:O	1:A:479:GLU:HG2	2.15	0.46
1:D:533:LEU:CD2	1:D:564:VAL:HG22	2.45	0.46
1:C:573:GLU:OE2	1:C:576:LYS:NZ	2.47	0.46
2:E:12:DC:H2''	2:E:13:DG:C8	2.51	0.46
2:G:52:DA:H2''	2:G:53:DT:H5'	1.96	0.46
1:D:533:LEU:HD23	1:D:564:VAL:HG22	1.97	0.46
1:B:467:LYS:HE3	1:B:471:GLN:O	2.16	0.46
2:E:6:DC:H42	3:F:55:DA:N6	2.14	0.46
1:I:531:CYS:O	1:I:532:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:ARG:NH2	1:D:551:PRO:HD2	2.30	0.46
1:I:576:LYS:HD3	1:I:597:VAL:HG23	1.98	0.46
3:F:12:DC:H2"	3:F:13:DA:C8	2.51	0.45
1:A:584:MET:HE1	1:C:488:LEU:HA	1.99	0.45
1:D:541:PHE:HD2	1:D:555:ARG:HG3	1.80	0.45
2:E:11:DT:C2'	2:E:12:DC:H5"	2.44	0.45
1:C:536:LEU:HD12	1:C:562:PHE:HB3	1.99	0.45
1:J:481:ILE:HG12	1:J:586:LYS:NZ	2.32	0.45
3:H:54:DT:N3	3:H:55:DA:N7	2.64	0.45
1:A:576:LYS:CD	1:A:597:VAL:HG23	2.46	0.45
1:A:569:HIS:HE1	1:A:599:SER:HB2	1.78	0.45
1:J:530:GLN:N	1:J:530:GLN:OE1	2.48	0.45
1:A:485:LEU:HA	1:A:485:LEU:HD23	1.84	0.45
1:D:579:ILE:HG22	1:D:595:VAL:HG21	1.98	0.45
1:D:576:LYS:HE3	1:D:580:LYS:CD	2.47	0.45
1:B:464:TRP:HB2	2:E:19:DA:H5'	1.99	0.45
1:J:606:LEU:HD23	1:J:606:LEU:HA	1.72	0.45
3:F:14:DA:H1'	3:F:15:DT:H5'	1.98	0.44
1:J:576:LYS:HG2	1:J:577:ASP:N	2.30	0.44
1:L:563:MET:HG3	1:L:564:VAL:H	1.83	0.44
1:B:474:SER:HB2	1:B:479:GLU:OE1	2.17	0.44
2:E:57:DG:H2"	2:E:58:DG:H8	1.80	0.44
1:D:576:LYS:HE3	1:D:580:LYS:HD2	2.00	0.44
1:J:566:LEU:HD22	1:J:571:PHE:CD2	2.51	0.44
1:A:522:ARG:HA	1:A:522:ARG:HD2	1.77	0.44
1:I:465:PHE:HE1	1:I:467:LYS:O	2.01	0.44
1:I:583:VAL:HG13	1:I:590:THR:HG22	1.99	0.44
1:K:531:CYS:HB2	1:K:565:PHE:O	2.16	0.44
1:A:584:MET:HE1	1:C:491:ARG:HD3	2.00	0.44
3:F:25:DT:H2"	3:F:26:DA:H5'	1.99	0.44
1:K:474:SER:HB3	1:K:479:GLU:OE2	2.18	0.44
1:A:517:LEU:HA	1:A:517:LEU:HD23	1.82	0.44
1:C:484:GLY:O	1:C:488:LEU:HD13	2.17	0.44
1:D:495:GLU:O	1:D:568:THR:HG21	2.18	0.44
3:F:56:DG:H1'	3:F:57:DG:OP1	2.17	0.44
1:C:480:ASN:HA	1:C:483:GLU:HB3	2.00	0.43
1:I:461:LYS:HD3	1:I:462:GLY:H	1.82	0.43
1:K:522:ARG:HD2	1:K:522:ARG:HA	1.72	0.43
1:B:485:LEU:HG	1:B:582:LEU:HD13	2.00	0.43
1:B:485:LEU:HD21	1:B:579:ILE:HG12	2.00	0.43
1:B:461:LYS:HE2	2:E:15:DT:O2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:LEU:HA	1:C:485:LEU:HD23	1.61	0.43
3:F:31:DA:H2''	3:F:32:DC:O5'	2.18	0.43
1:I:479:GLU:HG2	1:I:479:GLU:H	1.65	0.43
1:D:496:ARG:HG2	1:D:571:PHE:CD1	2.53	0.43
3:F:43:DT:H2''	3:F:44:DG:O5'	2.18	0.43
1:K:576:LYS:HG2	1:K:577:ASP:N	2.31	0.43
1:A:485:LEU:C	1:A:487:ALA:H	2.22	0.43
1:C:465:PHE:CD2	3:F:25:DT:H1'	2.53	0.43
2:E:55:DA:C2	3:F:8:DA:C2	3.07	0.43
1:I:515:THR:HB	3:H:35:DG:OP2	2.18	0.43
1:J:510:TYR:HA	1:J:517:LEU:HD11	1.99	0.43
1:A:485:LEU:O	1:A:487:ALA:N	2.52	0.43
3:H:47:DA:C2'	3:H:48:DT:H71	2.49	0.43
1:C:544:ALA:HA	1:C:545:PRO:HD3	1.88	0.43
1:C:576:LYS:HD3	1:C:597:VAL:HG23	2.00	0.43
1:A:524:THR:HG23	1:A:528:ILE:HD12	2.01	0.43
1:C:477:LYS:O	1:C:481:ILE:HG13	2.19	0.43
2:E:21:DA:H8	2:E:21:DA:H5''	1.82	0.43
2:G:21:DA:C2	3:H:42:DA:C2	3.07	0.43
1:A:585:THR:HG22	1:C:488:LEU:HD11	2.00	0.43
1:C:510:TYR:HA	1:C:517:LEU:HD11	2.01	0.43
3:H:20:DT:H2''	3:H:21:DA:C8	2.54	0.43
1:A:552:GLY:O	1:A:554:LEU:N	2.52	0.43
3:H:14:DA:H1'	3:H:15:DT:H5'	2.01	0.43
1:J:464:TRP:C	1:J:465:PHE:HD1	2.21	0.43
1:A:598:CYS:HA	1:B:599:SER:O	2.18	0.42
1:B:496:ARG:HG3	1:B:571:PHE:CG	2.54	0.42
2:E:50:DG:H2''	2:E:51:DA:C8	2.53	0.42
3:F:55:DA:H2''	3:F:56:DG:H5'	2.01	0.42
1:I:576:LYS:HB2	1:I:597:VAL:HG22	2.01	0.42
1:C:496:ARG:HG2	1:C:571:PHE:CD1	2.55	0.42
1:K:498:THR:HG22	1:K:499:ASP:H	1.83	0.42
1:A:467:LYS:HD3	1:A:467:LYS:HA	1.93	0.42
1:C:488:LEU:HD23	1:C:581:ASP:HB2	2.00	0.42
1:C:517:LEU:HD23	1:C:517:LEU:HA	1.82	0.42
1:C:555:ARG:HG3	1:D:470:GLY:O	2.20	0.42
3:F:41:DT:H2''	3:F:42:DA:H8	1.84	0.42
3:H:46:DT:H2''	3:H:47:DA:C8	2.55	0.42
1:K:467:LYS:NZ	3:H:25:DT:H5'	2.34	0.41
1:B:503:TRP:CH2	1:B:532:ARG:HG2	2.55	0.41
2:E:24:DC:H2'	2:E:25:DT:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:25:DT:O4	3:H:36:DA:N6	2.53	0.41
2:G:35:DG:H1'	2:G:36:DT:H5'	2.02	0.41
1:B:484:GLY:O	1:B:488:LEU:HD12	2.20	0.41
1:I:522:ARG:HD2	1:I:522:ARG:HA	1.86	0.41
1:A:486:ARG:C	4:A:701:HOH:O	2.59	0.41
1:B:496:ARG:HB2	1:B:496:ARG:NH1	2.35	0.41
1:C:515:THR:HB	2:E:35:DG:OP2	2.21	0.41
1:A:477:LYS:NZ	3:F:34:DG:N7	2.57	0.41
1:I:584:MET:HE1	1:K:491:ARG:HD3	2.01	0.41
1:D:538:ARG:NH2	1:D:558:ILE:HA	2.36	0.41
1:A:489:LEU:HB2	4:A:701:HOH:O	2.19	0.41
1:D:475:ASN:HB2	1:D:476:PRO:HD2	2.02	0.41
1:A:469:ARG:HH22	3:F:42:DA:C1'	2.33	0.41
1:C:576:LYS:HB3	1:C:576:LYS:HE2	1.72	0.41
1:J:485:LEU:HG	1:J:582:LEU:HG	2.01	0.41
1:B:552:GLY:H	1:B:555:ARG:HD3	1.86	0.41
1:K:538:ARG:NH1	1:K:558:ILE:HA	2.36	0.41
1:A:488:LEU:HD12	1:A:488:LEU:HA	1.92	0.41
1:I:607:PRO:HG2	1:J:541:PHE:HA	2.03	0.41
1:A:470:GLY:O	1:B:555:ARG:HA	2.21	0.41
1:B:566:LEU:HD22	1:B:571:PHE:CE2	2.56	0.41
1:D:465:PHE:O	1:D:467:LYS:HG2	2.21	0.41
2:E:41:DT:H1'	2:E:42:DA:C8	2.56	0.41
1:L:482:ALA:O	1:L:486:ARG:HG3	2.20	0.41
1:A:482:ALA:O	1:A:486:ARG:HG2	2.21	0.40
1:B:486:ARG:NH1	1:B:527:ALA:HA	2.36	0.40
2:E:9:DA:H2"	2:E:10:DT:H5'	2.02	0.40
1:I:465:PHE:CD1	1:I:466:GLY:N	2.89	0.40
1:C:515:THR:HG21	2:E:35:DG:C8	2.56	0.40
1:D:509:VAL:HG13	1:D:595:VAL:HG22	2.03	0.40
1:I:476:PRO:HA	1:I:479:GLU:OE2	2.21	0.40
1:I:539:LEU:HD13	1:J:606:LEU:HD23	2.03	0.40
1:A:584:MET:HB3	1:A:584:MET:HE3	1.86	0.40
2:G:41:DT:H1'	2:G:42:DA:C8	2.56	0.40
1:A:534:THR:HG23	1:A:534:THR:H	1.69	0.40
1:D:544:ALA:HA	1:D:545:PRO:HD3	1.91	0.40
1:C:517:LEU:HD22	1:C:562:PHE:HE2	1.85	0.40
2:E:21:DA:C8	2:E:21:DA:H5"	2.56	0.40
3:H:7:DT:H6	3:H:7:DT:H2'	1.69	0.40
1:I:596:THR:OG1	1:I:597:VAL:N	2.55	0.40
1:J:474:SER:OG	1:J:479:GLU:OE2	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:508:PHE:HB3	1:K:596:THR:CG2	2.52	0.40

There are no symmetry-related clashes.

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	
1	A	145/147 (99%)	136 (94%)	6 (4%)	3 (2%)	7	31
1	B	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	22	59
1	C	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
1	D	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
1	I	145/147 (99%)	133 (92%)	10 (7%)	2 (1%)	11	41
1	J	145/147 (99%)	133 (92%)	10 (7%)	2 (1%)	11	41
1	K	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
1	L	145/147 (99%)	136 (94%)	8 (6%)	1 (1%)	22	59
All	All	1160/1176 (99%)	1089 (94%)	62 (5%)	9 (1%)	19	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	HIS
1	B	547	PRO
1	I	465	PHE
1	J	545	PRO
1	L	590	THR
1	A	486	ARG
1	A	553	PRO
1	J	550	GLN
1	I	547	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/120 (100%)	118 (98%)	2 (2%)	60	85
1	B	120/120 (100%)	120 (100%)	0	100	100
1	C	120/120 (100%)	119 (99%)	1 (1%)	81	93
1	D	120/120 (100%)	118 (98%)	2 (2%)	60	85
1	I	120/120 (100%)	117 (98%)	3 (2%)	47	78
1	J	120/120 (100%)	120 (100%)	0	100	100
1	K	120/120 (100%)	118 (98%)	2 (2%)	60	85
1	L	120/120 (100%)	119 (99%)	1 (1%)	81	93
All	All	960/960 (100%)	949 (99%)	11 (1%)	73	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	537	SER
1	A	598	CYS
1	C	461	LYS
1	D	489	LEU
1	D	491	ARG
1	I	537	SER
1	I	594	ARG
1	I	598	CYS
1	K	492	SER
1	K	531	CYS
1	L	531	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	569	HIS
1	D	519	ASN
1	L	569	HIS

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

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	A	147/147 (100%)	-0.20	4 (2%) 54 26	28, 56, 101, 133	0
1	B	147/147 (100%)	-0.43	0 100 100	26, 52, 87, 117	0
1	C	147/147 (100%)	-0.09	4 (2%) 54 26	26, 56, 100, 123	0
1	D	147/147 (100%)	-0.40	0 100 100	27, 52, 88, 136	0
1	I	147/147 (100%)	-0.20	5 (3%) 45 19	28, 54, 104, 113	0
1	J	147/147 (100%)	-0.42	0 100 100	27, 53, 88, 154	0
1	K	147/147 (100%)	-0.16	3 (2%) 65 36	30, 54, 105, 131	0
1	L	147/147 (100%)	-0.38	1 (0%) 87 68	26, 51, 89, 127	0
2	E	57/62 (91%)	-0.57	0 100 100	44, 85, 170, 199	0
2	G	49/62 (79%)	-0.63	0 100 100	51, 78, 129, 156	0
3	F	53/62 (85%)	-0.44	1 (1%) 66 37	47, 83, 167, 196	0
3	H	49/62 (79%)	-0.62	0 100 100	41, 82, 138, 161	0
All	All	1384/1424 (97%)	-0.33	18 (1%) 77 51	26, 57, 113, 199	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	461	LYS	4.7
1	I	468	HIS	3.2
1	I	473	GLY	3.0
1	C	463	GLY	2.9
1	C	547	PRO	2.9
1	C	462	GLY	2.8
1	A	495	GLU	2.8
1	K	473	GLY	2.6
1	A	467	LYS	2.4
3	F	57	DG	2.4
1	K	495	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	465	PHE	2.2
1	A	466	GLY	2.1
1	I	493	HIS	2.1
1	K	465	PHE	2.1
1	I	498	THR	2.1
1	I	467	LYS	2.0
1	L	461	LYS	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 carbohydrates 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.