



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

PDB ID : 1DH3
Title : CRYSTAL STRUCTURE OF A CREB BZIP-CRE COMPLEX REVEALS
THE BASIS FOR CREB FAIMLY SELECTIVE DIMERIZATION AND DNA
BINDING
Authors : Schumacher, M.A.; Goodman, R.H.; Brennan, R.G.
Deposited on : 1999-11-27
Resolution : 3.00 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
<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

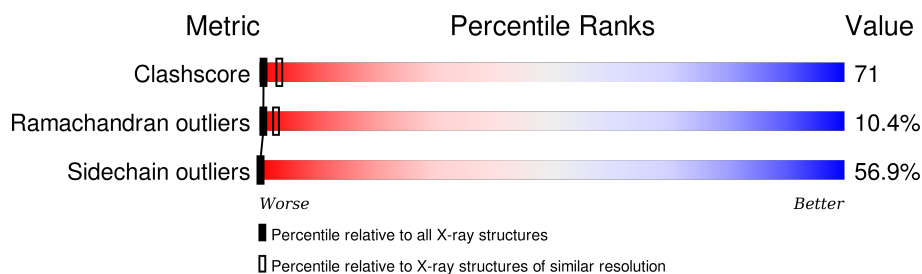
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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. 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	B	21	<div> <div>5%</div> <div>86%</div> <div>10%</div> </div>
1	D	21	<div> <div>5%</div> <div>62%</div> <div>33%</div> </div>
2	A	55	<div> <div>13%</div> <div>27%</div> <div>31%</div> <div>29%</div> </div>
2	C	55	<div> <div>9%</div> <div>27%</div> <div>44%</div> <div>20%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1804 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 (5'-D(*CP*CP*TP*TP*GP*GP*CP*TP*GP*AP*CP*GP*TP*CP*AP*GP*CP*CP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	21	Total	C	N	O	P	0	0	0
			426	203	79	124	20			
1	D	21	Total	C	N	O	P	0	0	0
			426	203	79	124	20			

- Molecule 2 is a protein called TRANSCRIPTION FACTOR CREB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	55	Total	C	N	O	S	0	0	0
			467	289	93	84	1			
2	C	55	Total	C	N	O	S	0	0	0
			467	289	93	84	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	SER	CYS	ENGINEERED	UNP Q01147
A	310	SER	CYS	ENGINEERED	UNP Q01147
A	300	SER	CYS	ENGINEERED	UNP Q01147
C	300	SER	CYS	ENGINEERED	UNP Q01147
C	310	SER	CYS	ENGINEERED	UNP Q01147
C	300	SER	CYS	ENGINEERED	UNP Q01147

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	O 5	0	0
4	B	2	Total 2	O 2	0	0
4	C	9	Total 9	O 9	0	0
4	D	1	Total 1	O 1	0	0

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 (5'-D(*CP*CP*TP*TP*GP*GP*CP*TP*GP*AP*CP*GP*TP*CP*AP*GP*CP*CP*AP*AP*G)-3')

Chain B: 



- Molecule 1: DNA (5'-D(*CP*CP*TP*TP*GP*GP*CP*TP*GP*AP*CP*GP*TP*CP*AP*GP*CP*CP*AP*AP*G)-3')

Chain D: 



- Molecule 2: TRANSCRIPTION FACTOR CREB

Chain A: 



- Molecule 2: TRANSCRIPTION FACTOR CREB

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.61Å 49.32Å 79.25Å 90.00° 122.18° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	98.0 (10.00-3.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.223 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1804	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	B	0.99	0/477	1.43	5/734 (0.7%)
1	D	1.18	2/477 (0.4%)	1.80	16/734 (2.2%)
2	A	1.94	10/469 (2.1%)	1.99	16/619 (2.6%)
2	C	1.92	9/469 (1.9%)	2.08	22/619 (3.6%)
All	All	1.57	21/1892 (1.1%)	1.82	59/2706 (2.2%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	339	LYS	CA-C	12.20	1.84	1.52
2	A	339	LYS	C-O	-10.77	1.02	1.23
2	C	339	LYS	N-CA	10.54	1.67	1.46
2	C	339	LYS	CA-C	10.15	1.79	1.52
2	A	315	VAL	CB-CG1	9.71	1.73	1.52
2	C	339	LYS	C-O	-9.35	1.05	1.23
2	C	297	ALA	CA-CB	-8.44	1.34	1.52
2	A	308	VAL	CB-CG1	-7.19	1.37	1.52
2	C	336	TYR	CD1-CE1	-7.01	1.28	1.39
2	A	327	GLU	CG-CD	6.86	1.62	1.51
2	C	338	HIS	CA-CB	-6.82	1.39	1.53
2	A	338	HIS	C-N	6.57	1.49	1.34
2	A	308	VAL	CA-CB	-6.24	1.41	1.54
2	A	287	GLU	CG-CD	6.09	1.61	1.51
2	C	308	VAL	CB-CG2	-5.50	1.41	1.52
2	A	336	TYR	CD1-CE1	-5.49	1.31	1.39
1	D	-8	DT	C2-N3	-5.39	1.33	1.37
2	A	308	VAL	CB-CG2	-5.37	1.41	1.52
2	C	338	HIS	C-N	5.34	1.46	1.34
1	D	-8	DT	N1-C6	5.32	1.42	1.38
2	C	308	VAL	CB-CG1	-5.12	1.42	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	329	LEU	CA-CB-CG	-11.46	88.95	115.30
1	D	-8	DT	O4'-C1'-N1	11.33	115.93	108.00
1	D	-8	DT	O4'-C1'-C2'	11.16	114.83	105.90
1	D	-1	DC	O4'-C4'-C3'	-10.80	99.52	106.00
2	A	318	LEU	CB-CG-CD1	9.49	127.14	111.00
2	A	289	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	D	8	DA	O4'-C4'-C3'	-8.77	100.74	106.00
1	D	-8	DT	C5-C6-N1	-8.75	118.45	123.70
1	D	-8	DT	C6-N1-C2	8.72	125.66	121.30
2	A	311	LEU	CA-CB-CG	-8.48	95.81	115.30
2	C	286	ARG	N-CA-C	-8.39	88.35	111.00
2	C	311	LEU	CB-CG-CD2	8.16	124.88	111.00
1	D	-8	DT	C2-N1-C1'	-8.16	105.14	118.20
2	C	336	TYR	N-CA-C	8.12	132.93	111.00
2	C	311	LEU	CA-CB-CG	7.89	133.44	115.30
2	C	322	ASN	C-N-CA	-7.78	102.25	121.70
2	A	318	LEU	CA-CB-CG	-7.51	98.03	115.30
2	A	339	LYS	CA-C-O	-7.44	104.47	120.10
1	B	-11	DC	O4'-C4'-C3'	-7.17	101.63	104.50
2	A	335	LEU	CB-CG-CD2	7.09	123.05	111.00
2	C	339	LYS	N-CA-C	-6.95	92.23	111.00
1	D	-8	DT	N1-C1'-C2'	6.91	125.73	112.60
2	C	301	ARG	NE-CZ-NH2	-6.87	116.86	120.30
2	C	336	TYR	CB-CG-CD1	-6.78	116.93	121.00
2	C	307	TYR	C-N-CA	-6.76	104.79	121.70
1	D	9	DA	O4'-C1'-N9	-6.54	103.42	108.00
1	D	-11	DC	P-O3'-C3'	6.41	127.39	119.70
2	C	335	LEU	CB-CA-C	6.30	122.18	110.20
2	C	328	GLU	OE1-CD-OE2	6.29	130.85	123.30
2	A	315	VAL	CB-CA-C	-6.29	99.45	111.40
2	C	310	SER	N-CA-CB	-6.27	101.10	110.50
2	A	325	LEU	CB-CG-CD2	6.23	121.60	111.00
2	C	336	TYR	CA-CB-CG	-6.17	101.68	113.40
2	A	289	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	D	1	DG	O4'-C1'-N9	-6.13	103.71	108.00
2	C	290	LEU	CA-CB-CG	-6.10	101.27	115.30
1	D	-1	DC	C1'-O4'-C4'	-6.09	104.01	110.10
2	A	331	ALA	CB-CA-C	-6.00	101.11	110.10
2	C	334	ASP	CB-CA-C	5.90	122.19	110.40
1	D	-8	DT	C6-N1-C1'	5.86	129.19	120.40
2	C	315	VAL	CB-CA-C	-5.75	100.47	111.40
2	C	336	TYR	CG-CD2-CE2	-5.73	116.72	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	315	VAL	CA-CB-CG2	-5.66	102.40	110.90
2	A	309	LYS	N-CA-CB	5.63	120.73	110.60
2	A	291	MET	CG-SD-CE	-5.51	91.39	100.20
1	B	-11	DC	P-O3'-C3'	5.47	126.27	119.70
1	D	8	DA	C4'-C3'-C2'	-5.40	98.24	103.10
2	C	299	GLU	CB-CA-C	-5.39	99.61	110.40
2	A	327	GLU	OE1-CD-OE2	-5.38	116.84	123.30
2	C	328	GLU	CG-CD-OE1	-5.22	107.85	118.30
1	B	-4	DT	O4'-C1'-N1	5.22	111.66	108.00
2	C	299	GLU	OE1-CD-OE2	5.18	129.51	123.30
2	C	326	ILE	C-N-CA	-5.14	108.84	121.70
1	B	-5	DC	O4'-C4'-C3'	-5.06	102.47	104.50
2	A	290	LEU	CA-CB-CG	-5.05	103.68	115.30
2	A	333	LYS	CD-CE-NZ	5.04	123.30	111.70
1	D	-8	DT	C1'-O4'-C4'	-5.03	105.07	110.10
1	D	7	DC	O4'-C4'-C3'	-5.03	102.49	104.50
1	B	-11	DC	C1'-O4'-C4'	-5.02	105.08	110.10

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	B	426	0	237	54	0
1	D	426	0	237	59	0
2	A	467	0	504	65	0
2	C	467	0	504	65	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	B	2	0	0	0	0
4	C	9	0	0	2	0
4	D	1	0	0	0	0
All	All	1804	0	1482	220	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 71.

All (220) 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:C:339:LYS:CA	2:C:339:LYS:C	1.79	1.49
2:A:339:LYS:CA	2:A:339:LYS:C	1.84	1.44
2:A:289:ARG:HH11	2:A:289:ARG:HG2	1.20	1.02
2:C:317:VAL:HG22	2:C:318:LEU:HD23	1.41	0.99
1:B:9:DA:H1'	1:B:10:DG:H5'	1.46	0.96
1:D:6:DC:H2'	1:D:7:DC:C6	2.09	0.88
1:B:-8:DT:H2'	1:B:-7:DG:C8	2.10	0.86
2:A:329:LEU:CD1	2:C:329:LEU:HD12	2.06	0.85
2:C:315:VAL:HG23	2:C:316:ALA:H	1.42	0.85
1:B:10:DG:H1	1:D:-10:DC:H42	1.25	0.83
2:A:329:LEU:HD13	2:C:329:LEU:HD12	1.61	0.83
1:B:-11:DC:C2'	1:B:-10:DC:H5''	2.09	0.83
1:B:-11:DC:H2''	1:B:-10:DC:H5''	1.61	0.81
1:D:-7:DG:H2''	1:D:-6:DG:C5'	2.11	0.79
2:C:318:LEU:N	2:C:318:LEU:HD23	1.99	0.77
2:A:298:ARG:HB2	2:A:298:ARG:HH11	1.49	0.77
2:A:304:LYS:HD2	4:C:412:HOH:O	1.86	0.76
2:A:339:LYS:CA	2:A:339:LYS:O	2.32	0.75
2:A:286:ARG:HH11	2:A:286:ARG:HG2	1.52	0.75
1:B:7:DC:H2'	1:B:7:DC:OP2	1.88	0.74
2:C:314:ARG:C	2:C:317:VAL:HG13	2.10	0.72
2:C:304:LYS:O	2:C:308:VAL:HG12	1.90	0.72
1:B:2:DT:H2''	1:B:3:DC:H6	1.55	0.71
2:A:287:GLU:O	2:A:290:LEU:HB2	1.89	0.71
2:C:311:LEU:O	2:C:315:VAL:HG22	1.91	0.71
1:B:9:DA:H1'	1:B:10:DG:C5'	2.21	0.71
2:C:313:ASN:O	2:C:316:ALA:N	2.24	0.70
2:A:289:ARG:HG3	2:A:290:LEU:N	2.07	0.70
1:B:10:DG:C8	1:B:10:DG:H5'	2.27	0.70
2:C:288:VAL:HG12	2:C:289:ARG:N	2.05	0.70
2:A:333:LYS:O	2:A:336:TYR:HB3	1.92	0.70
2:C:291:MET:O	2:C:294:ARG:HB2	1.92	0.69
2:C:314:ARG:O	2:C:317:VAL:HG13	1.93	0.69
2:A:332:LEU:N	2:A:332:LEU:HD13	2.07	0.69
2:A:314:ARG:O	2:A:317:VAL:HG12	1.92	0.68
2:A:289:ARG:NH1	2:A:289:ARG:HG2	1.95	0.67
2:A:309:LYS:O	2:A:312:GLU:HB2	1.95	0.67
1:B:10:DG:H1	1:D:-10:DC:N4	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:MET:HA	2:C:294:ARG:HD3	1.77	0.66
1:D:8:DA:H2''	1:D:9:DA:C8	2.30	0.66
1:D:7:DC:H2''	1:D:8:DA:O5'	1.95	0.66
2:A:301:ARG:HH11	2:A:301:ARG:CB	2.09	0.66
2:A:301:ARG:HH11	2:A:301:ARG:CG	2.08	0.66
2:C:339:LYS:N	2:C:339:LYS:C	2.49	0.66
2:C:317:VAL:HG22	2:C:318:LEU:N	2.11	0.65
1:B:5:DG:H2''	1:B:6:DC:O5'	1.96	0.65
1:D:-10:DC:H2'	1:D:-9:DT:C6	2.31	0.65
1:B:3:DC:H2''	1:B:4:DA:H5''	1.79	0.64
1:D:8:DA:H8	1:D:8:DA:H5''	1.62	0.64
1:D:7:DC:H4'	1:D:8:DA:OP1	1.98	0.63
1:B:7:DC:H42	1:D:-7:DG:H22	1.46	0.63
2:C:313:ASN:O	2:C:315:VAL:HG23	1.99	0.62
1:D:-9:DT:H2''	1:D:-8:DT:C6	2.34	0.62
1:D:-7:DG:H2''	1:D:-6:DG:H5'	1.81	0.62
2:C:315:VAL:HG23	2:C:316:ALA:N	2.08	0.62
2:A:326:ILE:HG22	2:A:327:GLU:N	2.13	0.61
2:C:303:LYS:O	2:C:306:GLU:N	2.33	0.61
2:A:285:LYS:O	2:A:288:VAL:HG12	2.01	0.61
2:C:295:GLU:O	2:C:298:ARG:HB2	2.01	0.61
1:D:8:DA:H5''	1:D:8:DA:C8	2.36	0.61
2:A:325:LEU:O	2:A:328:GLU:HB2	2.01	0.61
2:C:331:ALA:HA	2:C:334:ASP:HB3	1.81	0.60
2:C:335:LEU:HD22	2:C:335:LEU:H	1.66	0.60
2:C:314:ARG:CA	2:C:317:VAL:HG13	2.32	0.60
2:A:329:LEU:HD11	2:C:329:LEU:HD12	1.84	0.60
1:B:2:DT:H2''	1:B:3:DC:C6	2.37	0.60
1:B:6:DC:H2''	1:B:7:DC:OP2	1.99	0.60
2:C:330:LYS:HD3	2:C:330:LYS:C	2.21	0.59
2:A:332:LEU:HD12	2:A:335:LEU:HD23	1.85	0.59
2:A:304:LYS:O	2:A:307:TYR:HB3	2.02	0.59
1:D:8:DA:H2''	1:D:9:DA:H8	1.68	0.59
2:A:333:LYS:HG3	2:A:333:LYS:O	1.99	0.59
2:C:331:ALA:O	2:C:334:ASP:HB3	2.03	0.59
1:D:-10:DC:H2'	1:D:-9:DT:C5	2.38	0.58
1:D:-7:DG:H2''	1:D:-6:DG:O5'	2.02	0.58
1:D:-10:DC:C2'	1:D:-9:DT:C6	2.86	0.58
2:C:310:SER:OG	2:C:311:LEU:N	2.36	0.58
1:B:-10:DC:C5'	1:B:-10:DC:H6	2.17	0.58
2:C:317:VAL:CG2	2:C:318:LEU:HD23	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:DG:H8	1:B:10:DG:H5'	1.69	0.58
2:C:322:ASN:O	2:C:326:ILE:HG22	2.04	0.58
1:D:-9:DT:H2''	1:D:-8:DT:H6	1.68	0.58
1:B:-6:DG:H2''	1:B:-5:DC:C5'	2.33	0.58
1:B:-6:DG:H2''	1:B:-5:DC:O5'	2.04	0.57
2:A:335:LEU:HG	2:A:335:LEU:O	2.05	0.57
1:D:-1:DC:H2'	1:D:1:DG:C8	2.39	0.57
2:A:285:LYS:HE2	2:A:285:LYS:N	2.20	0.57
1:B:7:DC:N4	1:D:-7:DG:H22	2.02	0.57
1:D:8:DA:H2''	1:D:9:DA:OP2	2.04	0.57
2:A:313:ASN:O	2:A:316:ALA:N	2.29	0.57
2:A:327:GLU:O	2:A:330:LYS:N	2.38	0.57
2:A:339:LYS:C	2:A:339:LYS:N	2.56	0.56
1:B:-11:DC:H2'	1:B:-10:DC:H5''	1.87	0.56
1:B:6:DC:H1'	1:B:7:DC:C6	2.41	0.56
1:D:1:DG:H3'	2:C:294:ARG:NH1	2.21	0.56
2:A:327:GLU:O	2:A:330:LYS:HB3	2.06	0.56
1:B:-9:DT:H2''	1:B:-8:DT:O4'	2.07	0.55
2:A:332:LEU:H	2:A:332:LEU:HD13	1.71	0.55
1:D:-7:DG:H2'	1:D:-6:DG:C8	2.43	0.54
2:C:327:GLU:O	2:C:330:LYS:HB3	2.07	0.54
1:B:-10:DC:H6	1:B:-10:DC:H5''	1.74	0.53
2:C:336:TYR:C	2:C:338:HIS:H	2.12	0.53
2:C:317:VAL:HG22	2:C:318:LEU:CD2	2.28	0.53
1:B:-5:DC:H42	1:D:5:DG:H1	1.56	0.52
2:A:286:ARG:NH1	2:A:286:ARG:HG2	2.23	0.52
2:A:318:LEU:O	2:A:322:ASN:HB2	2.10	0.52
2:A:301:ARG:HH11	2:A:301:ARG:HG2	1.73	0.52
1:D:6:DC:H2''	1:D:7:DC:O4'	2.09	0.52
1:D:9:DA:OP2	1:D:9:DA:O4'	2.28	0.52
2:C:330:LYS:O	2:C:333:LYS:HB3	2.09	0.52
2:A:339:LYS:O	2:A:339:LYS:N	2.43	0.51
2:A:316:ALA:HA	2:A:319:GLU:HB2	1.92	0.51
2:A:312:GLU:OE2	2:C:307:TYR:OH	2.29	0.51
2:A:314:ARG:HA	2:A:317:VAL:CG1	2.41	0.51
1:D:-6:DG:H2''	1:D:-5:DC:H5'	1.92	0.51
1:D:-2:DA:C5	1:D:-1:DC:C5	2.99	0.50
2:A:312:GLU:O	2:A:315:VAL:HG12	2.12	0.50
1:D:-8:DT:H2''	1:D:-7:DG:N7	2.27	0.50
1:B:10:DG:OP2	1:B:10:DG:H8	1.95	0.50
2:A:315:VAL:CG1	2:A:316:ALA:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:DC:H2''	1:D:8:DA:C8	2.47	0.50
1:B:-6:DG:H1'	1:B:-5:DC:H5'	1.94	0.49
2:A:332:LEU:CD1	2:A:332:LEU:N	2.75	0.49
2:A:307:TYR:CZ	2:A:311:LEU:HD11	2.47	0.49
1:D:1:DG:C8	1:D:2:DT:H71	2.47	0.49
2:A:328:GLU:O	2:A:332:LEU:HD22	2.12	0.49
1:B:-6:DG:H2''	1:B:-5:DC:H5'	1.93	0.49
2:C:326:ILE:C	2:C:326:ILE:HD13	2.33	0.49
1:D:-2:DA:C4	1:D:-1:DC:C6	3.01	0.49
2:A:314:ARG:HA	2:A:317:VAL:HG12	1.95	0.49
2:A:289:ARG:O	2:A:292:LYS:N	2.47	0.48
1:B:9:DA:H2'	1:B:9:DA:OP2	2.12	0.48
2:C:315:VAL:O	2:C:319:GLU:HG2	2.14	0.48
1:D:-9:DT:C1'	1:D:-8:DT:C6	2.96	0.48
2:A:337:SER:O	2:A:338:HIS:HB3	2.14	0.48
1:B:4:DA:H2''	1:B:5:DG:C8	2.50	0.47
1:B:8:DA:H2''	1:B:9:DA:OP2	2.14	0.47
2:A:311:LEU:HA	2:A:311:LEU:HD23	1.52	0.47
1:D:2:DT:OP2	2:C:294:ARG:HD2	2.14	0.47
1:D:1:DG:C3'	2:C:294:ARG:NH1	2.78	0.47
1:D:7:DC:C2'	1:D:8:DA:C8	2.98	0.47
2:C:321:GLN:HG2	2:C:325:LEU:HD22	1.96	0.47
2:C:301:ARG:NH1	4:C:405:HOH:O	2.38	0.47
1:D:1:DG:H3'	2:C:294:ARG:HH11	1.79	0.47
2:C:317:VAL:CG2	2:C:318:LEU:N	2.72	0.47
2:C:302:ARG:O	2:C:305:LYS:HB3	2.14	0.47
2:A:288:VAL:CG1	2:A:289:ARG:N	2.78	0.47
1:D:7:DC:H2'	1:D:8:DA:N7	2.30	0.47
1:B:9:DA:N3	1:B:10:DG:C8	2.82	0.46
1:B:1:DG:H3'	2:A:294:ARG:NH2	2.30	0.46
1:B:9:DA:H4'	1:B:10:DG:O5'	2.14	0.46
1:B:7:DC:H6	1:B:7:DC:OP2	1.98	0.46
2:A:314:ARG:CA	2:A:317:VAL:HG12	2.46	0.46
2:A:317:VAL:CG1	2:A:318:LEU:N	2.78	0.46
2:C:309:LYS:HE3	2:C:309:LYS:HB2	1.62	0.46
2:C:314:ARG:HA	2:C:317:VAL:CG1	2.46	0.46
1:B:4:DA:C2'	1:B:5:DG:C8	2.99	0.46
2:C:303:LYS:O	2:C:306:GLU:HB2	2.16	0.45
2:A:290:LEU:HA	2:A:290:LEU:HD12	1.58	0.45
1:B:9:DA:H61	1:D:-9:DT:H3	1.65	0.45
2:C:335:LEU:N	2:C:335:LEU:HD22	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:320:ASN:HA	2:C:320:ASN:HD22	1.32	0.45
2:A:300:SER:HA	2:A:303:LYS:HG3	1.97	0.45
2:C:294:ARG:O	2:C:297:ALA:HB3	2.17	0.45
2:C:315:VAL:H	2:C:315:VAL:HG22	1.28	0.45
1:D:-4:DT:OP2	2:A:300:SER:HB2	2.17	0.45
1:D:-9:DT:H4'	1:D:-8:DT:O5'	2.16	0.45
1:D:6:DC:H2''	1:D:7:DC:OP1	2.16	0.45
1:D:-7:DG:C2'	1:D:-6:DG:C8	3.00	0.44
2:A:331:ALA:HB3	2:A:332:LEU:H	1.34	0.44
1:D:-4:DT:H2''	1:D:-3:DG:C8	2.52	0.44
1:D:-9:DT:H1'	1:D:-8:DT:C6	2.52	0.44
2:C:309:LYS:O	2:C:312:GLU:HB2	2.18	0.44
2:A:323:LYS:O	2:A:326:ILE:HB	2.17	0.44
1:B:-1:DC:H2'	1:B:1:DG:C8	2.52	0.44
1:D:2:DT:H1'	1:D:3:DC:H5'	1.99	0.44
1:B:9:DA:C1'	1:B:10:DG:H5'	2.33	0.44
1:D:-7:DG:C8	1:D:-7:DG:C5'	3.00	0.44
2:C:286:ARG:O	2:C:289:ARG:HG2	2.18	0.44
1:D:-9:DT:C2'	1:D:-8:DT:C6	3.01	0.44
2:C:337:SER:O	2:C:338:HIS:HB3	2.18	0.44
2:A:312:GLU:HG2	2:C:311:LEU:HD11	2.00	0.44
1:B:1:DG:O5'	1:B:1:DG:H2'	2.18	0.43
1:D:-10:DC:H2''	1:D:-9:DT:C6	2.52	0.43
1:D:-9:DT:C6	1:D:-8:DT:C5	3.06	0.43
2:A:318:LEU:HD23	2:A:318:LEU:HA	1.50	0.43
1:D:6:DC:H4'	1:D:7:DC:OP1	2.19	0.43
2:A:322:ASN:HD21	2:C:321:GLN:HB3	1.83	0.43
2:A:325:LEU:O	2:A:329:LEU:N	2.52	0.43
1:B:-7:DG:H2''	1:B:-6:DG:C8	2.54	0.42
1:B:-5:DC:N4	1:D:5:DG:H1	2.15	0.42
2:C:330:LYS:HD3	2:C:331:ALA:N	2.34	0.42
1:B:1:DG:H3'	2:A:294:ARG:NE	2.35	0.42
1:B:6:DC:C2	1:B:7:DC:C4	3.07	0.42
1:D:-3:DG:H2''	1:D:-2:DA:C8	2.54	0.42
1:D:3:DC:OP2	2:C:286:ARG:NH2	2.53	0.42
1:B:-2:DA:N1	1:D:2:DT:O4	2.53	0.42
1:B:6:DC:H1'	1:B:7:DC:O5'	2.20	0.42
1:D:-11:DC:H2''	1:D:-10:DC:OP1	2.20	0.42
1:B:-11:DC:H2''	1:B:-10:DC:C5'	2.42	0.42
1:D:9:DA:H2''	1:D:10:DG:OP2	2.20	0.42
1:B:-1:DC:H2''	1:B:1:DG:H5'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:DA:C2	1:B:10:DG:C4	3.08	0.41
2:A:301:ARG:CB	2:A:301:ARG:NH1	2.79	0.41
2:C:329:LEU:O	2:C:333:LYS:HB2	2.20	0.41
2:A:308:VAL:O	2:A:312:GLU:HG3	2.21	0.41
2:C:321:GLN:HG2	2:C:325:LEU:CD2	2.50	0.41
2:C:320:ASN:O	2:C:323:LYS:N	2.44	0.41
1:B:9:DA:H3'	1:B:9:DA:OP2	2.20	0.41
2:C:297:ALA:HA	2:C:300:SER:HB3	2.03	0.41
2:A:306:GLU:O	2:A:309:LYS:N	2.53	0.41
2:A:339:LYS:CG	2:A:339:LYS:C	2.89	0.41
1:B:9:DA:C1'	1:B:10:DG:C5'	2.96	0.41
2:C:328:GLU:O	2:C:330:LYS:N	2.54	0.41
1:B:10:DG:C8	1:B:10:DG:C3'	3.04	0.40
1:B:10:DG:N1	1:D:-10:DC:N4	2.49	0.40
1:D:-5:DC:H1'	1:D:-4:DT:H5'	2.04	0.40
2:C:321:GLN:O	2:C:324:THR:HG23	2.21	0.40
1:B:-6:DG:C2'	1:B:-5:DC:C5'	3.00	0.40
2:C:328:GLU:C	2:C:330:LYS:N	2.75	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	
2	A	53/55 (96%)	30 (57%)	16 (30%)	7 (13%)	0	1
2	C	53/55 (96%)	34 (64%)	15 (28%)	4 (8%)	1	6
All	All	106/110 (96%)	64 (60%)	31 (29%)	11 (10%)	1	3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	331	ALA
2	A	332	LEU
2	A	335	LEU
2	C	314	ARG
2	C	338	HIS
2	A	288	VAL
2	A	338	HIS
2	A	286	ARG
2	A	330	LYS
2	C	303	LYS
2	C	321	GLN

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	51/51 (100%)	20 (39%)	31 (61%)	0	0
2	C	51/51 (100%)	24 (47%)	27 (53%)	0	0
All	All	102/102 (100%)	44 (43%)	58 (57%)	0	0

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	285	LYS
2	A	286	ARG
2	A	287	GLU
2	A	288	VAL
2	A	289	ARG
2	A	290	LEU
2	A	291	MET
2	A	292	LYS
2	A	294	ARG
2	A	298	ARG
2	A	299	GLU
2	A	301	ARG
2	A	304	LYS

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Mol	Chain	Res	Type
2	A	306	GLU
2	A	308	VAL
2	A	309	LYS
2	A	310	SER
2	A	313	ASN
2	A	314	ARG
2	A	315	VAL
2	A	320	ASN
2	A	324	THR
2	A	326	ILE
2	A	329	LEU
2	A	330	LYS
2	A	332	LEU
2	A	333	LYS
2	A	334	ASP
2	A	337	SER
2	A	338	HIS
2	A	339	LYS
2	C	285	LYS
2	C	288	VAL
2	C	289	ARG
2	C	290	LEU
2	C	294	ARG
2	C	298	ARG
2	C	302	ARG
2	C	303	LYS
2	C	304	LYS
2	C	307	TYR
2	C	308	VAL
2	C	309	LYS
2	C	311	LEU
2	C	314	ARG
2	C	315	VAL
2	C	317	VAL
2	C	320	ASN
2	C	324	THR
2	C	325	LEU
2	C	326	ILE
2	C	329	LEU
2	C	330	LYS
2	C	333	LYS
2	C	335	LEU

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Mol	Chain	Res	Type
2	C	336	TYR
2	C	337	SER
2	C	339	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	313	ASN
2	C	320	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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