



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 AM UTC

PDB ID : 1N3E / pdb_00001n3e
Title : Crystal structure of I-CreI bound to a palindromic DNA sequence I (palindrome of left side of wildtype DNA target sequence)
Authors : Chevalier, B.; Turmel, M.; Lemieux, C.; Monnat, R.J.; Stoddard, B.L.
Deposited on : 2002-10-28
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

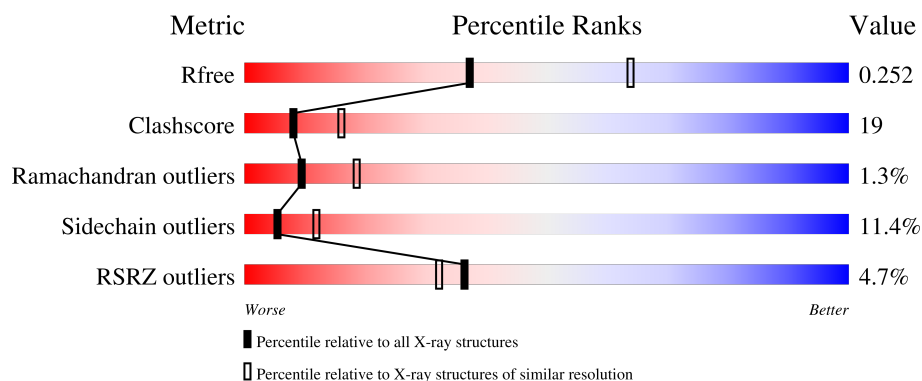
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	14	36% 57% 7%
1	E	14	64% 21% 14%
1	I	14	7% 36% 50% 14%
1	K	14	50% 36% 14%
2	D	10	40% 40% 20%

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Mol	Chain	Length	Quality of chain
2	F	10	60%30%10%
2	J	10	60%20%20%
2	L	10	60%20%10%10%
3	A	163	4% 64%20%8%7%
3	B	163	4% 63%23%6%7%
3	G	163	7% 63%22%7%7%
3	H	163	4% 61%23%9%7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7098 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 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*TP*CP*GP*TP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			
1	E	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			
1	I	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			
1	K	14	Total	C	N	O	P	0	0	0
			284	136	56	79	13			

- Molecule 2 is a DNA chain called 5'-D(P*GP*AP*CP*GP*TP*TP*TP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	P	0	0	0
			206	98	34	64	10			
2	F	10	Total	C	N	O	P	0	0	0
			206	98	34	64	10			
2	J	10	Total	C	N	O	P	0	0	0
			206	98	34	64	10			
2	L	10	Total	C	N	O	P	0	0	0
			206	98	34	64	10			

- Molecule 3 is a protein called DNA endonuclease I-CreI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	151	Total	C	N	O	S	0	0	0
			1223	790	208	224	1			
3	B	151	Total	C	N	O	S	0	0	0
			1223	790	208	224	1			
3	G	151	Total	C	N	O	S	0	0	0
			1223	790	208	224	1			
3	H	151	Total	C	N	O	S	0	0	0
			1226	791	208	226	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	THR	ALA	SEE REMARK 999	UNP P05725
A	110	GLU	TRP	SEE REMARK 999	UNP P05725
A	111	GLN	ARG	SEE REMARK 999	UNP P05725
B	242	THR	ALA	SEE REMARK 999	UNP P05725
B	310	GLU	TRP	SEE REMARK 999	UNP P05725
B	311	GLN	ARG	SEE REMARK 999	UNP P05725
G	542	THR	ALA	SEE REMARK 999	UNP P05725
G	610	GLU	TRP	SEE REMARK 999	UNP P05725
G	611	GLN	ARG	SEE REMARK 999	UNP P05725
H	742	THR	ALA	SEE REMARK 999	UNP P05725
H	810	GLU	TRP	SEE REMARK 999	UNP P05725
H	811	GLN	ARG	SEE REMARK 999	UNP P05725

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	J	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	G	1	Total Na 1 1	0	0
5	H	1	Total Na 1 1	0	0

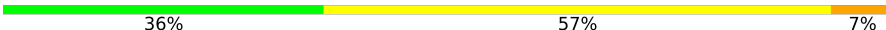
- Molecule 6 is water.

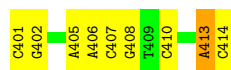
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	18	Total 18	O 18	0	0
6	D	9	Total 9	O 9	0	0
6	E	10	Total 10	O 10	0	0
6	F	13	Total 13	O 13	0	0
6	I	4	Total 4	O 4	0	0
6	J	9	Total 9	O 9	0	0
6	K	14	Total 14	O 14	0	0
6	L	5	Total 5	O 5	0	0
6	A	42	Total 42	O 42	0	0
6	B	38	Total 38	O 38	0	0
6	G	41	Total 41	O 41	0	0
6	H	30	Total 30	O 30	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain C: 



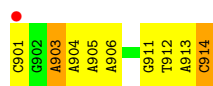
- Molecule 1: 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*TP*CP*GP*TP*AP*C)-3'

Chain E: 



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

Chain I: 



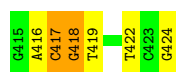
- Molecule 1: 5'-D(*CP*GP*AP*AP*AP*AP*CP*GP*TP*CP*GP*TP*AP*C)-3'

Chain K: 



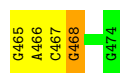
- Molecule 2: 5'-D(P*GP*AP*CP*GP*TP*TP*TP*TP*CP*G)-3'

Chain D: 



- Molecule 2: 5'-D(P*GP*AP*CP*GP*TP*TP*TP*TP*CP*G)-3'

Chain F: 



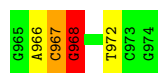
- Molecule 2: 5'-D(P*GP*AP*CP*GP*TP*TP*TP*TP*CP*G)-3'

Chain J: 



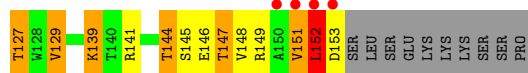
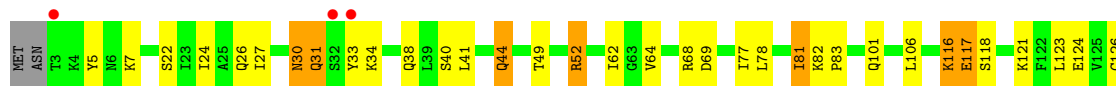
- Molecule 2: 5'-D(P*GP*AP*CP*GP*TP*TP*TP*TP*CP*G)-3'

Chain L: 



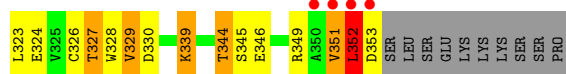
- Molecule 3: DNA endonuclease I-CreI

Chain A: 



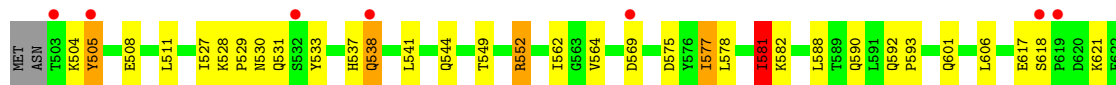
- Molecule 3: DNA endonuclease I-CreI

Chain B: 



- Molecule 3: DNA endonuclease I-CreI

Chain G: 





● Molecule 3: DNA endonuclease I-CreI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.73Å 68.44Å 301.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 2.50 46.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.4 (46.18-2.50) 93.5 (46.18-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.245 0.228 , 0.252	Depositor DCC
R_{free} test set	1598 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7098	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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

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

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	0.37	0/319	0.87	0/490
1	E	0.33	0/319	0.83	1/490 (0.2%)
1	I	0.39	0/319	0.93	0/490
1	K	0.35	0/319	0.83	0/490
2	D	0.40	0/229	1.03	2/350 (0.6%)
2	F	0.44	0/229	1.05	1/350 (0.3%)
2	J	0.47	0/229	1.35	4/350 (1.1%)
2	L	0.41	0/229	1.02	2/350 (0.6%)
3	A	0.55	0/1246	1.14	7/1682 (0.4%)
3	B	0.57	0/1246	1.17	6/1682 (0.4%)
3	G	0.61	0/1246	1.20	8/1682 (0.5%)
3	H	0.56	0/1249	1.10	8/1686 (0.5%)
All	All	0.52	0/7179	1.10	39/10092 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
1	I	0	2
1	K	0	2
2	L	0	1
All	All	0	8

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	544	GLN	OE1-CD-NE2	-10.23	112.37	122.60
2	J	924	DG	C5'-C4'-C3'	-10.16	99.66	114.90
3	A	44	GLN	OE1-CD-NE2	-9.86	112.74	122.60
3	G	538	GLN	OE1-CD-NE2	-9.74	112.86	122.60
3	B	244	GLN	OE1-CD-NE2	-9.09	113.51	122.60
3	B	224	ILE	N-CA-C	8.97	120.67	108.11
2	J	924	DG	C2'-C3'-O3'	7.64	122.96	111.50
3	G	505	TYR	N-CA-C	7.53	120.71	110.55
3	B	351	VAL	N-CA-C	-7.24	102.44	112.50
3	B	281	ILE	N-CA-C	7.13	117.85	110.36
3	H	851	VAL	N-CA-C	-7.11	102.61	112.50
3	A	44	GLN	CG-CD-NE2	7.03	126.95	116.40
3	H	724	ILE	N-CA-C	6.89	118.40	108.48
3	G	581	ILE	N-CA-C	6.81	117.52	110.36
2	J	924	DG	C4'-C3'-O3'	6.74	120.11	110.00
3	G	538	GLN	CG-CD-NE2	6.58	126.27	116.40
3	B	244	GLN	CG-CD-NE2	6.55	126.23	116.40
3	A	24	ILE	N-CA-C	6.49	117.83	108.48
3	G	544	GLN	CG-CD-NE2	6.37	125.96	116.40
2	L	968	DG	N9-C1'-C2'	-6.08	104.37	113.50
3	A	5	TYR	N-CA-C	5.97	119.36	110.52
3	G	645	SER	N-CA-C	-5.92	104.96	111.82
3	H	845	SER	N-CA-C	-5.67	105.25	111.82
2	L	967	DC	N1-C1'-C2'	-5.56	105.15	113.50
3	H	818	SER	CA-C-N	5.56	125.17	119.56
3	H	818	SER	C-N-CA	5.56	125.17	119.56
2	J	918	DG	N9-C1'-C2'	-5.54	105.18	113.50
3	A	49	THR	N-CA-C	5.53	118.07	111.71
3	A	151	VAL	N-CA-C	-5.39	104.22	111.44
2	D	418	DG	N9-C1'-C2'	-5.38	105.42	113.50
3	H	830	ASP	N-CA-C	-5.36	105.52	111.36
3	A	116	LYS	N-CA-C	-5.34	105.51	112.23
2	D	417	DC	N1-C1'-C2'	-5.29	105.56	113.50
3	H	728	LYS	N-CA-C	5.28	117.07	109.04
3	H	816	LYS	N-CA-C	-5.14	105.37	111.69
2	F	468	DG	N9-C1'-C2'	-5.10	105.84	113.50
3	B	228	LYS	N-CA-C	5.08	116.77	109.04
3	G	549	THR	N-CA-C	5.06	117.53	111.71
1	E	464	DC	C2'-C3'-O3'	-5.04	103.94	111.50

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	410	DC	Sidechain
1	C	413	DA	Sidechain
1	E	463	DA	Sidechain
1	I	903	DA	Sidechain
1	I	914	DC	Sidechain
1	K	963	DA	Sidechain
1	K	964	DC	Sidechain
2	L	968	DG	Sidechain

5.2 Too-close contacts [i](#)

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	284	0	157	4	2
1	E	284	0	157	4	0
1	I	284	0	157	13	0
1	K	284	0	157	5	0
2	D	206	0	115	10	0
2	F	206	0	115	5	0
2	J	206	0	115	6	0
2	L	206	0	115	8	0
3	A	1223	0	1257	55	1
3	B	1223	0	1257	40	0
3	G	1223	0	1257	59	0
3	H	1226	0	1259	52	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	42	0	0	4	0
6	B	38	0	0	0	0
6	C	18	0	0	0	1
6	D	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	10	0	0	3	0
6	F	13	0	0	1	0
6	G	41	0	0	2	1
6	H	30	0	0	1	3
6	I	4	0	0	1	0
6	J	9	0	0	0	0
6	K	14	0	0	1	0
6	L	5	0	0	2	0
All	All	7098	0	6118	253	4

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 19.

All (253) 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:D:424:DG:C8	2:J:924:DG:H2''	1.88	1.08
2:D:424:DG:N7	2:J:924:DG:H2''	1.74	1.03
3:G:505:TYR:OH	3:G:562:ILE:HG23	1.59	1.03
1:I:905:DA:H2''	1:I:906:DA:H5'	1.47	0.96
3:G:644:THR:H	3:G:647:THR:CG2	1.80	0.95
3:G:644:THR:HG22	3:G:646:GLU:H	1.32	0.90
3:A:144:THR:H	3:A:147:THR:CG2	1.83	0.89
3:A:144:THR:HG22	3:A:146:GLU:H	1.38	0.87
3:G:644:THR:HG22	3:G:646:GLU:N	1.90	0.86
3:H:844:THR:H	3:H:847:THR:CG2	1.90	0.84
3:B:344:THR:HG22	3:B:346:GLU:H	1.39	0.84
1:E:455:DA:H2''	1:E:456:DA:H5'	1.59	0.84
3:A:118:SER:H	3:A:121:LYS:HE3	1.43	0.84
3:G:623:LEU:CD1	3:G:649:ARG:HG3	2.08	0.83
1:I:912:DT:H5'	1:I:912:DT:H6	1.43	0.82
3:H:844:THR:HG22	3:H:846:GLU:H	1.40	0.82
3:G:649:ARG:O	3:G:652:LEU:HD23	1.80	0.82
3:A:118:SER:OG	3:A:121:LYS:HG3	1.80	0.81
3:A:144:THR:HG22	3:A:146:GLU:N	1.96	0.81
3:H:844:THR:HG22	3:H:846:GLU:N	1.95	0.80
3:G:618:SER:H	3:G:621:LYS:HE3	1.48	0.79
3:H:818:SER:H	3:H:821:LYS:HE3	1.48	0.79
1:K:955:DA:H2''	1:K:956:DA:H5'	1.64	0.79
3:A:149:ARG:C	3:A:151:VAL:H	1.91	0.78
3:B:344:THR:HG22	3:B:346:GLU:N	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:311:GLN:HE21	3:B:321:LYS:CE	1.98	0.77
1:C:405:DA:H2''	1:C:406:DA:H5'	1.66	0.77
3:G:644:THR:H	3:G:647:THR:HG21	1.49	0.76
1:I:911:DG:H2''	1:I:912:DT:H5''	1.68	0.76
6:E:1200:HOH:O	3:A:33:TYR:HD2	1.68	0.75
3:G:530:ASN:HD22	3:G:533:TYR:HE1	1.33	0.74
3:G:505:TYR:HE2	3:G:562:ILE:HA	1.53	0.73
3:H:844:THR:CG2	3:H:846:GLU:H	2.02	0.72
3:A:144:THR:H	3:A:147:THR:HG21	1.52	0.72
3:G:623:LEU:HD11	3:G:649:ARG:HG3	1.71	0.72
3:G:644:THR:CG2	3:G:646:GLU:H	2.03	0.71
3:H:730:ASN:HD22	3:H:733:TYR:HE1	1.36	0.71
3:H:824:GLU:O	3:H:827:THR:HB	1.91	0.70
3:B:344:THR:CG2	3:B:346:GLU:H	2.06	0.69
1:I:912:DT:H6	1:I:912:DT:C5'	2.05	0.68
3:G:624:GLU:O	3:G:627:THR:HB	1.93	0.68
3:A:144:THR:CG2	3:A:146:GLU:H	2.07	0.68
3:G:505:TYR:CE2	3:G:562:ILE:HA	2.28	0.67
3:H:844:THR:H	3:H:847:THR:HG21	1.58	0.66
3:G:644:THR:H	3:G:647:THR:HG23	1.57	0.66
1:I:912:DT:H5'	1:I:912:DT:C6	2.27	0.65
3:G:618:SER:OG	3:G:621:LYS:HG3	1.96	0.65
2:D:424:DG:C8	2:J:924:DG:C2'	2.75	0.65
3:B:262:ILE:HG22	3:B:264:VAL:HG12	1.79	0.65
3:B:311:GLN:HE21	3:B:321:LYS:HE2	1.62	0.65
3:A:52:ARG:NH1	3:A:69:ASP:OD2	2.29	0.65
3:B:311:GLN:NE2	3:B:321:LYS:NZ	2.45	0.65
3:H:844:THR:H	3:H:847:THR:HG23	1.62	0.65
3:H:851:VAL:O	3:H:853:ASP:N	2.30	0.64
3:G:651:VAL:O	3:G:651:VAL:CG1	2.46	0.64
3:B:241:LEU:HD12	3:B:281:ILE:HD11	1.80	0.63
3:G:623:LEU:HD11	3:G:649:ARG:CG	2.28	0.62
3:A:124:GLU:O	3:A:127:THR:HB	1.98	0.62
3:A:144:THR:H	3:A:147:THR:HG23	1.62	0.62
3:G:652:LEU:O	3:G:652:LEU:HG	2.00	0.61
3:G:652:LEU:O	3:G:652:LEU:CG	2.49	0.61
3:B:352:LEU:O	3:B:353:ASP:O	2.19	0.61
3:H:730:ASN:HB3	3:H:733:TYR:CD1	2.35	0.61
3:G:575:ASP:HB2	3:G:577:ILE:CD1	2.31	0.61
6:E:1200:HOH:O	3:A:33:TYR:CD2	2.47	0.60
3:A:144:THR:O	3:A:147:THR:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:505:TYR:OH	3:G:562:ILE:CG2	2.44	0.60
3:G:652:LEU:O	3:G:652:LEU:HD12	2.02	0.60
3:G:644:THR:N	3:G:647:THR:HG23	2.17	0.60
2:D:416:DA:N7	3:A:44:GLN:NE2	2.50	0.60
3:A:151:VAL:O	3:A:153:ASP:N	2.34	0.60
1:I:912:DT:C5'	1:I:912:DT:C6	2.85	0.59
3:H:762:ILE:HG22	3:H:764:VAL:HG12	1.83	0.59
3:A:30:ASN:HB3	3:A:33:TYR:CD1	2.38	0.59
2:F:466:DA:N7	3:B:244:GLN:NE2	2.50	0.59
6:E:1044:HOH:O	3:A:38:GLN:HG3	2.02	0.59
3:B:230:ASN:HB3	3:B:233:TYR:CD1	2.37	0.59
3:H:818:SER:OG	3:H:821:LYS:HG3	2.03	0.58
3:G:651:VAL:O	3:G:651:VAL:HG13	2.03	0.58
1:K:955:DA:C2'	1:K:956:DA:H5'	2.35	0.57
3:A:141:ARG:HD3	6:A:1171:HOH:O	2.05	0.57
3:A:152:LEU:O	3:A:153:ASP:O	2.23	0.56
3:A:117:GLU:HB2	3:A:121:LYS:HZ2	1.69	0.56
3:G:650:ALA:C	3:G:652:LEU:H	2.13	0.56
3:A:118:SER:N	3:A:121:LYS:HE3	2.18	0.56
3:H:776:TYR:O	3:H:777:ILE:HD12	2.06	0.56
3:G:626:CYS:HA	3:G:629:VAL:HG13	1.89	0.55
2:F:467:DC:H2'	2:F:468:DG:H8	1.72	0.55
3:G:562:ILE:HG22	3:G:564:VAL:HG12	1.87	0.55
1:I:911:DG:C2'	1:I:912:DT:H5''	2.33	0.55
3:B:324:GLU:O	3:B:327:THR:HB	2.07	0.55
3:A:123:LEU:CD1	3:A:149:ARG:HG3	2.37	0.55
3:B:311:GLN:NE2	3:B:321:LYS:HZ1	2.03	0.55
3:A:151:VAL:O	3:A:152:LEU:C	2.49	0.55
1:I:912:DT:H2''	1:I:913:DA:C8	2.42	0.54
3:B:351:VAL:O	3:B:353:ASP:N	2.41	0.54
3:H:849:ARG:C	3:H:851:VAL:H	2.15	0.54
3:G:644:THR:N	3:G:647:THR:CG2	2.61	0.54
3:A:144:THR:N	3:A:147:THR:CG2	2.65	0.54
3:G:644:THR:CG2	3:G:645:SER:N	2.70	0.54
3:H:826:CYS:HA	3:H:829:VAL:HG13	1.88	0.54
3:G:644:THR:O	3:G:647:THR:HG23	2.08	0.54
3:H:844:THR:CG2	3:H:845:SER:N	2.70	0.54
3:A:31:GLN:H	3:A:31:GLN:NE2	2.06	0.53
3:H:817:GLU:HB2	3:H:821:LYS:NZ	2.23	0.53
1:E:455:DA:C2'	1:E:456:DA:H5'	2.36	0.53
3:A:62:ILE:HG22	3:A:64:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:704:LYS:O	3:H:704:LYS:HG3	2.06	0.53
2:L:967:DC:H2'	2:L:968:DG:H8	1.74	0.53
3:H:817:GLU:HB2	3:H:821:LYS:HZ2	1.72	0.53
1:I:901:DC:HO5'	1:I:901:DC:H6	1.55	0.53
3:A:40:SER:HB3	6:A:1222:HOH:O	2.08	0.53
3:A:148:VAL:O	3:A:151:VAL:HB	2.09	0.53
3:H:844:THR:N	3:H:847:THR:HG23	2.23	0.53
3:A:81:ILE:HG22	3:A:82:LYS:N	2.23	0.52
3:B:252:ARG:NH1	3:B:269:ASP:OD2	2.43	0.52
3:A:149:ARG:C	3:A:151:VAL:N	2.58	0.52
2:L:967:DC:H2'	2:L:968:DG:C8	2.45	0.52
3:H:741:LEU:HD12	3:H:781:ILE:HD11	1.92	0.52
6:K:1013:HOH:O	3:G:538:GLN:HG3	2.09	0.52
3:B:314:SER:OG	3:B:321:LYS:NZ	2.43	0.52
3:B:323:LEU:HD21	3:B:349:ARG:CD	2.39	0.52
3:G:644:THR:HB	3:G:647:THR:HG22	1.92	0.51
3:G:652:LEU:O	3:G:652:LEU:CD1	2.58	0.51
3:B:349:ARG:O	3:B:352:LEU:HD22	2.10	0.51
3:A:26:GLN:HG3	6:A:1222:HOH:O	2.09	0.51
3:H:737:HIS:CE1	3:H:848:VAL:HG22	2.46	0.51
1:I:905:DA:C2'	1:I:906:DA:H5'	2.31	0.51
3:H:727:ILE:HG21	3:H:848:VAL:HG21	1.92	0.51
3:A:144:THR:N	3:A:147:THR:HG23	2.24	0.51
3:H:722:SER:HB3	3:H:744:GLN:HG2	1.92	0.51
3:G:530:ASN:HB3	3:G:533:TYR:CD1	2.47	0.50
3:H:781:ILE:HG22	3:H:782:LYS:N	2.24	0.50
2:L:966:DA:N7	3:H:744:GLN:NE2	2.59	0.50
3:A:144:THR:HB	3:A:147:THR:HG22	1.92	0.50
2:D:417:DC:H4'	2:D:417:DC:OP1	2.12	0.50
3:A:31:GLN:H	3:A:31:GLN:HE21	1.59	0.50
3:H:730:ASN:HB3	3:H:733:TYR:HD1	1.77	0.49
1:C:405:DA:C2'	1:C:406:DA:H5'	2.37	0.49
1:C:401:DC:H2''	1:C:402:DG:O5'	2.12	0.49
2:D:417:DC:H2'	2:D:418:DG:C8	2.48	0.49
2:L:967:DC:H2''	2:L:968:DG:H5'	1.95	0.49
3:A:41:LEU:HD12	3:A:81:ILE:HD11	1.95	0.49
3:B:230:ASN:HB3	3:B:233:TYR:CE1	2.48	0.49
3:H:818:SER:N	3:H:821:LYS:HE3	2.24	0.49
3:A:144:THR:CG2	3:A:145:SER:N	2.75	0.49
3:B:311:GLN:HG3	3:B:321:LYS:HZ3	1.78	0.49
3:A:40:SER:CB	6:A:1222:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:951:DC:H2''	1:K:952:DG:O5'	2.12	0.48
3:B:344:THR:CG2	3:B:345:SER:N	2.76	0.48
3:B:233:TYR:CE2	3:B:238:GLN:HB2	2.49	0.48
1:K:963:DA:H1'	1:K:964:DC:O4'	2.13	0.48
3:A:30:ASN:HB3	3:A:33:TYR:CE1	2.48	0.48
2:F:465:DG:OP2	6:F:1229:HOH:O	2.18	0.48
3:B:351:VAL:O	3:B:352:LEU:C	2.57	0.48
3:G:530:ASN:ND2	3:G:533:TYR:CE1	2.81	0.48
3:G:552:ARG:NH1	3:G:569:ASP:OD2	2.46	0.48
2:F:467:DC:H2'	2:F:468:DG:C8	2.49	0.48
2:L:967:DC:H1'	6:L:1201:HOH:O	2.13	0.47
3:G:508:GLU:HG3	6:G:1217:HOH:O	2.14	0.47
2:D:417:DC:H2'	2:D:418:DG:H8	1.78	0.47
3:A:52:ARG:NH1	3:A:69:ASP:CG	2.73	0.47
1:I:903:DA:N7	3:H:733:TYR:OH	2.45	0.47
6:G:1155:HOH:O	3:H:707:LYS:HE2	2.15	0.47
2:L:967:DC:H2''	6:L:1201:HOH:O	2.15	0.47
3:G:541:LEU:HD12	3:G:581:ILE:HD11	1.97	0.47
3:G:537:HIS:CE1	3:G:648:VAL:HG22	2.50	0.47
3:H:823:LEU:CD1	3:H:849:ARG:HG3	2.45	0.47
3:H:733:TYR:CE2	3:H:738:GLN:HB2	2.49	0.47
3:A:117:GLU:HB2	3:A:121:LYS:NZ	2.30	0.46
3:B:230:ASN:HB3	3:B:233:TYR:HD1	1.80	0.46
1:I:904:DA:H5'	6:I:1213:HOH:O	2.13	0.46
3:A:27:ILE:HG21	3:A:148:VAL:HG21	1.98	0.46
3:G:588:LEU:O	3:G:592:GLN:HB2	2.16	0.46
3:H:844:THR:HB	3:H:847:THR:CG2	2.45	0.46
3:B:282:LYS:HB3	3:B:283:PRO:CD	2.45	0.46
3:G:537:HIS:ND1	3:G:648:VAL:HG22	2.31	0.46
3:B:326:CYS:HA	3:B:329:VAL:HG13	1.97	0.46
3:A:31:GLN:NE2	3:A:31:GLN:N	2.64	0.46
3:A:139:LYS:HB2	3:A:139:LYS:HE2	1.67	0.46
3:B:323:LEU:HD21	3:B:349:ARG:HG3	1.97	0.46
3:G:618:SER:HG	3:G:621:LYS:HG3	1.81	0.46
2:D:422:DT:H5'	2:D:422:DT:H6	1.80	0.46
3:H:730:ASN:HB3	3:H:733:TYR:CE1	2.52	0.45
3:A:30:ASN:HB3	3:A:33:TYR:HD1	1.80	0.45
3:G:528:LYS:O	3:G:538:GLN:N	2.42	0.45
3:B:244:GLN:HB2	3:B:277:ILE:CD1	2.46	0.45
3:B:307:LYS:HE2	3:B:328:TRP:CH2	2.52	0.45
3:G:623:LEU:HD11	3:G:649:ARG:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:917:DC:H2'	2:J:918:DG:C8	2.51	0.45
3:G:527:ILE:HG21	3:G:648:VAL:HG21	1.99	0.45
3:H:844:THR:HB	3:H:847:THR:HG22	1.99	0.45
3:A:27:ILE:HG21	3:A:148:VAL:CG2	2.46	0.44
3:B:288:LEU:O	3:B:292:GLN:HB2	2.17	0.44
3:B:307:LYS:HE2	3:B:328:TRP:CZ2	2.52	0.44
3:B:323:LEU:CD2	3:B:349:ARG:HG3	2.48	0.44
3:H:839:LYS:HE2	3:H:839:LYS:HB2	1.66	0.44
2:J:917:DC:H2'	2:J:918:DG:H8	1.82	0.44
3:H:792:GLN:HB3	3:H:793:PRO:HD3	1.98	0.44
3:A:22:SER:HB3	3:A:44:GLN:HG2	1.98	0.44
2:D:422:DT:H5'	2:D:422:DT:C6	2.53	0.44
3:G:552:ARG:NH1	3:G:569:ASP:OD1	2.51	0.44
3:B:339:LYS:HE2	3:B:339:LYS:HB2	1.76	0.44
3:G:644:THR:HB	3:G:647:THR:CG2	2.48	0.44
3:H:730:ASN:ND2	3:H:733:TYR:CE1	2.85	0.44
3:B:241:LEU:HD22	3:B:305:VAL:HG13	2.00	0.43
3:G:528:LYS:HA	3:G:529:PRO:HD2	1.88	0.43
3:H:836:ASN:O	6:H:1204:HOH:O	2.21	0.43
3:B:273:VAL:CG1	3:B:274:SER:N	2.82	0.43
3:G:639:LYS:HE2	3:G:639:LYS:HB2	1.61	0.43
3:A:126:CYS:HA	3:A:129:VAL:HG13	2.01	0.43
3:H:817:GLU:CB	3:H:821:LYS:NZ	2.82	0.43
3:G:533:TYR:CZ	3:G:538:GLN:HB2	2.54	0.42
3:A:81:ILE:CG2	3:A:82:LYS:N	2.82	0.42
3:G:530:ASN:ND2	3:G:533:TYR:HE1	2.09	0.42
3:H:749:THR:O	3:H:752:ARG:HB3	2.19	0.42
2:L:972:DT:H5'	2:L:972:DT:H6	1.83	0.42
3:H:737:HIS:ND1	3:H:848:VAL:HG22	2.34	0.42
1:C:413:DA:H1'	1:C:414:DC:O4'	2.19	0.42
3:A:123:LEU:HD11	3:A:149:ARG:CD	2.50	0.42
3:B:228:LYS:HA	3:B:229:PRO:HD2	1.86	0.42
3:G:504:LYS:HA	3:G:590:GLN:HE22	1.85	0.42
3:G:527:ILE:HG21	3:G:648:VAL:CG2	2.50	0.42
3:G:592:GLN:HB3	3:G:593:PRO:HD3	2.01	0.42
3:H:849:ARG:O	3:H:852:LEU:HD22	2.20	0.42
3:A:144:THR:HB	3:A:147:THR:CG2	2.49	0.42
3:A:146:GLU:OE2	3:A:149:ARG:NH2	2.54	0.41
1:K:962:DT:H2''	1:K:963:DA:C8	2.55	0.41
3:H:823:LEU:HD11	3:H:849:ARG:HD3	2.03	0.41
3:A:52:ARG:NH1	3:A:69:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:844:THR:HG23	3:H:845:SER:N	2.34	0.41
3:H:852:LEU:O	3:H:853:ASP:O	2.39	0.41
3:B:222:SER:HB3	3:B:244:GLN:HG2	2.02	0.41
3:A:82:LYS:HB3	3:A:83:PRO:CD	2.51	0.41
3:G:581:ILE:HG22	3:G:582:LYS:N	2.35	0.41
1:I:913:DA:H1'	1:I:914:DC:O4'	2.20	0.41
3:B:352:LEU:C	3:B:353:ASP:O	2.64	0.41
3:G:530:ASN:HB3	3:G:533:TYR:CE1	2.55	0.41
3:H:731:GLN:HA	3:H:736:LYS:HD2	2.03	0.41
3:H:731:GLN:NE2	3:H:731:GLN:H	2.19	0.41
2:D:418:DG:H2''	2:D:419:DT:H5'	2.02	0.40
1:E:453:DA:P	3:A:116:LYS:HE2	2.61	0.40
2:F:467:DC:H2''	2:F:468:DG:H5'	2.02	0.40
3:B:311:GLN:NE2	3:B:321:LYS:CE	2.73	0.40
2:L:966:DA:H2''	2:L:967:DC:O5'	2.21	0.40
2:J:922:DT:H5'	2:J:922:DT:H6	1.86	0.40
3:G:552:ARG:NH1	3:G:569:ASP:CG	2.79	0.40
3:B:330:ASP:OD2	3:B:345:SER:HB3	2.21	0.40
3:G:627:THR:HG22	3:G:628:TRP:CD1	2.56	0.40
1:E:463:DA:H1'	1:E:464:DC:O4'	2.22	0.40
3:H:733:TYR:CZ	3:H:738:GLN:HB2	2.56	0.40
3:H:773:VAL:CG1	3:H:774:SER:N	2.84	0.40
3:H:844:THR:O	3:H:847:THR:HG23	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1216:HOH:O	6:H:1231:HOH:O[3_756]	1.81	0.39
1:C:407:DC:O3'	6:H:1231:HOH:O[3_756]	1.99	0.21
1:C:408:DG:OP1	6:H:1231:HOH:O[3_756]	2.12	0.08
3:A:7:LYS:NZ	6:G:1217:HOH:O[3_656]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	149/163 (91%)	137 (92%)	9 (6%)	3 (2%)	6	10
3	B	149/163 (91%)	141 (95%)	6 (4%)	2 (1%)	9	18
3	G	149/163 (91%)	139 (93%)	9 (6%)	1 (1%)	18	34
3	H	149/163 (91%)	139 (93%)	8 (5%)	2 (1%)	9	18
All	All	596/652 (91%)	556 (93%)	32 (5%)	8 (1%)	9	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	852	LEU
3	A	152	LEU
3	B	352	LEU
3	G	617	GLU
3	B	317	GLU
3	A	117	GLU
3	H	817	GLU
3	A	30	ASN

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	
3	A	136/150 (91%)	121 (89%)	15 (11%)	6	13
3	B	136/150 (91%)	120 (88%)	16 (12%)	5	11
3	G	136/150 (91%)	121 (89%)	15 (11%)	6	13
3	H	137/150 (91%)	121 (88%)	16 (12%)	5	11
All	All	545/600 (91%)	483 (89%)	62 (11%)	5	12

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	31	GLN
3	A	34	LYS
3	A	52	ARG
3	A	68	ARG
3	A	77	ILE
3	A	78	LEU
3	A	81	ILE
3	A	101	GLN
3	A	106	LEU
3	A	127	THR
3	A	129	VAL
3	A	139	LYS
3	A	144	THR
3	A	147	THR
3	A	152	LEU
3	B	231	GLN
3	B	234	LYS
3	B	252	ARG
3	B	268	ARG
3	B	277	ILE
3	B	278	LEU
3	B	281	ILE
3	B	301	GLN
3	B	306	LEU
3	B	316	LYS
3	B	321	LYS
3	B	327	THR
3	B	329	VAL
3	B	339	LYS
3	B	344	THR
3	B	352	LEU
3	G	511	LEU
3	G	531	GLN
3	G	552	ARG
3	G	577	ILE
3	G	578	LEU
3	G	581	ILE
3	G	601	GLN
3	G	606	LEU
3	G	627	THR
3	G	629	VAL
3	G	639	LYS
3	G	644	THR

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Mol	Chain	Res	Type
3	G	647	THR
3	G	651	VAL
3	G	652	LEU
3	H	704	LYS
3	H	726	GLN
3	H	731	GLN
3	H	752	ARG
3	H	768	ARG
3	H	777	ILE
3	H	778	LEU
3	H	781	ILE
3	H	801	GLN
3	H	806	LEU
3	H	827	THR
3	H	829	VAL
3	H	839	LYS
3	H	844	THR
3	H	847	THR
3	H	852	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	30	ASN
3	A	31	GLN
3	B	231	GLN
3	B	311	GLN
3	G	531	GLN
3	G	544	GLN
3	G	599	GLN
3	H	730	ASN
3	H	731	GLN
3	H	737	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are 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 [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	C	14/14 (100%)	-0.33	0 100 100	24, 36, 45, 57	0
1	E	14/14 (100%)	-0.25	0 100 100	25, 45, 52, 55	0
1	I	14/14 (100%)	0.28	1 (7%) 22 19	33, 50, 55, 61	0
1	K	14/14 (100%)	-0.35	0 100 100	30, 40, 48, 50	0
2	D	10/10 (100%)	0.04	0 100 100	29, 48, 60, 61	0
2	F	10/10 (100%)	-0.31	0 100 100	21, 32, 44, 51	0
2	J	10/10 (100%)	-0.07	0 100 100	27, 41, 50, 53	0
2	L	10/10 (100%)	0.30	0 100 100	30, 53, 65, 66	0
3	A	151/163 (92%)	0.13	7 (4%) 37 33	19, 39, 73, 82	0
3	B	151/163 (92%)	0.08	6 (3%) 42 38	17, 31, 65, 76	0
3	G	151/163 (92%)	0.26	12 (7%) 18 16	21, 35, 72, 83	0
3	H	151/163 (92%)	0.39	7 (4%) 37 33	21, 44, 72, 88	0
All	All	700/748 (93%)	0.17	33 (4%) 36 32	17, 39, 71, 88	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	653	ASP	5.5
3	G	505	TYR	5.4
3	G	652	LEU	4.7
3	B	351	VAL	4.5
3	A	153	ASP	4.1
3	B	352	LEU	4.0
3	H	851	VAL	3.9
3	B	353	ASP	3.8
3	H	850	ALA	3.5
3	G	503	THR	3.4
3	H	733	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
3	A	3	THR	3.3
3	A	151	VAL	3.3
3	G	651	VAL	3.1
3	B	350	ALA	3.0
3	H	738	GLN	3.0
3	A	152	LEU	2.9
3	G	650	ALA	2.9
3	A	150	ALA	2.8
3	B	203	THR	2.5
3	G	649	ARG	2.4
3	A	32	SER	2.3
3	G	538	GLN	2.3
3	G	569	ASP	2.3
3	B	232	SER	2.3
3	H	703	THR	2.2
3	H	732	SER	2.2
3	H	852	LEU	2.2
3	A	33	TYR	2.1
3	G	619	PRO	2.1
1	I	901	DC	2.1
3	G	532	SER	2.0
3	G	618	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	H	994	1/1	0.88	0.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	G	995	1/1	0.90	0.19	38,38,38,38	0
5	NA	A	495	1/1	0.93	0.13	34,34,34,34	0
5	NA	B	494	1/1	0.97	0.10	24,24,24,24	0
4	CA	F	491	1/1	0.98	0.03	29,29,29,29	0
4	CA	J	991	1/1	0.98	0.03	29,29,29,29	0
4	CA	C	492	1/1	0.99	0.03	27,27,27,27	0
4	CA	L	992	1/1	0.99	0.03	28,28,28,28	0
4	CA	I	993	1/1	0.99	0.03	30,30,30,30	0
4	CA	D	493	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.