



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:21 PM UTC

PDB ID : 1IAW / pdb_00001iaw
Title : CRYSTAL STRUCTURE OF NAEI COMPLEXED WITH 17MER DNA
Authors : Huai, Q.; Colandene, J.D.; Topal, M.D.; Ke, H.
Deposited on : 2001-03-23
Resolution : 2.40 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

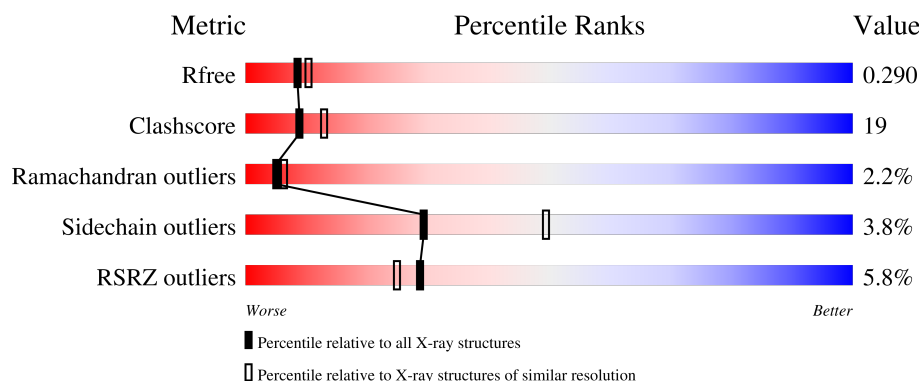
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	17	 6% 65% 29% 6%
1	D	17	 12% 47% 53%
1	E	17	 12% 53% 35% 6% 6%
1	F	17	 12% 59% 24% 12% 6%
2	A	317	 6% 62% 29% 5% 5%

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Mol	Chain	Length	Quality of chain
2	B	317	4% 58% 32% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6195 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(*TP*GP*CP*CP*AP*CP*GP*CP*CP*GP*GP*CP*GP*TP*GP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	16	Total	C	N	O	P	0	0	0
			328	153	63	96	16			
1	D	17	Total	C	N	O	P	0	0	0
			349	163	65	104	17			
1	E	17	Total	C	N	O	P	0	0	0
			349	163	65	104	17			
1	F	17	Total	C	N	O	P	0	0	0
			349	163	65	104	17			

- Molecule 2 is a protein called TYPE II RESTRICTION ENZYME NAEI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	304	Total	C	N	O	S	0	0	0
			2388	1488	452	441	7			
2	B	304	Total	C	N	O	S	0	0	0
			2388	1488	452	441	7			

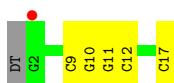
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	O	0	0
			1	1		
3	E	2	Total	O	0	0
			2	2		
3	F	3	Total	O	0	0
			3	3		
3	A	15	Total	O	0	0
			15	15		
3	B	23	Total	O	0	0
			23	23		

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.

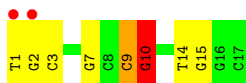
- Molecule 1: 5'-D(*TP*GP*CP*CP*AP*CP*GP*CP*CP*GP*GP*CP*GP*TP*GP*GP*C)-3',



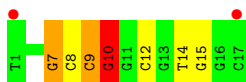
- Molecule 1: 5'-D(*TP*GP*CP*CP*AP*CP*GP*CP*CP*GP*GP*CP*GP*TP*GP*GP*C)-3',



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

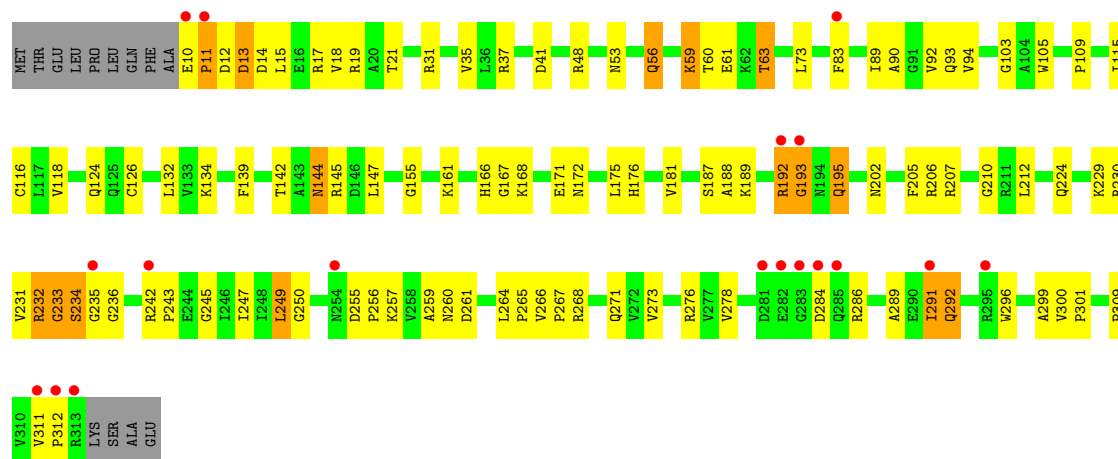


- Molecule 1: 5'-D(*TP*GP*CP*CP*AP*CP*GP*CP*CP*GP*GP*CP*GP*TP*GP*GP*C)-3',

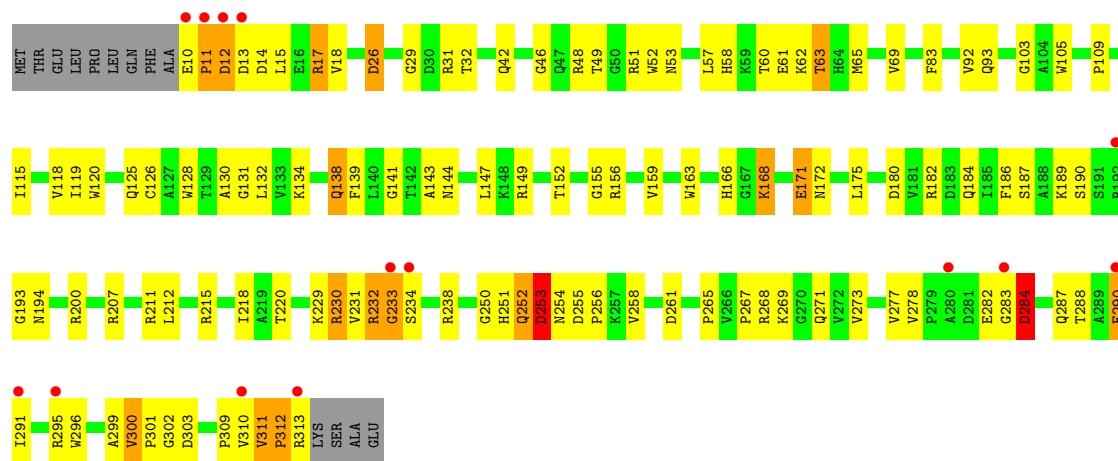


- Molecule 2: TYPE II RESTRICTION ENZYME NAEI





• Molecule 2: TYPE II RESTRICTION ENZYME NAEI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.60Å 65.00Å 258.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.40 99.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	76.2 (99.00-2.40) 76.3 (99.00-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.293 0.241 , 0.290	Depositor DCC
R_{free} test set	3225 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.4	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	0.91	EDS
Total number of atoms	6195	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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	C	0.35	0/367	0.68	0/564
1	D	0.37	0/390	0.69	0/598
1	E	0.40	0/390	0.84	1/598 (0.2%)
1	F	0.39	0/390	0.89	1/598 (0.2%)
2	A	0.46	0/2437	1.04	14/3303 (0.4%)
2	B	0.46	0/2437	1.01	12/3303 (0.4%)
All	All	0.44	0/6411	0.97	28/8964 (0.3%)

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	E	0	2
1	F	0	3
All	All	0	5

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	232	ARG	N-CA-C	9.18	124.59	110.36
2	B	26	ASP	CA-C-N	7.80	127.71	119.05
2	B	26	ASP	C-N-CA	7.80	127.71	119.05
2	A	171	GLU	N-CA-C	7.74	121.19	110.35
2	B	171	GLU	N-CA-C	6.79	120.22	110.10
2	B	32	THR	N-CA-C	-6.45	103.16	111.02
2	A	17	ARG	N-CA-C	-6.44	104.26	111.28
2	B	311	VAL	CA-C-N	6.42	127.86	119.84
2	B	311	VAL	C-N-CA	6.42	127.86	119.84
2	A	311	VAL	CA-C-N	6.07	126.90	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	311	VAL	C-N-CA	6.07	126.90	120.11
1	E	10	DG	N9-C1'-C2'	-5.99	104.51	113.50
2	B	233	GLY	N-CA-C	5.98	127.35	113.18
2	A	312	PRO	N-CA-C	5.82	119.65	111.33
2	A	56	GLN	N-CA-C	-5.70	106.17	113.02
2	A	13	ASP	N-CA-C	5.66	117.31	111.03
2	B	253	ASP	CB-CA-C	-5.59	110.11	116.54
2	A	249	LEU	N-CA-C	5.51	117.72	108.96
2	A	73	LEU	N-CA-C	-5.50	105.28	111.28
2	B	234	SER	N-CA-C	5.41	117.17	111.28
2	B	252	GLN	N-CA-C	5.37	118.03	109.65
2	B	207	ARG	N-CA-C	5.33	119.79	113.28
2	A	268	ARG	N-CA-C	-5.28	103.71	110.53
2	B	277	VAL	N-CA-C	5.20	115.39	108.11
2	A	61	GLU	N-CA-C	-5.10	105.80	112.23
1	F	10	DG	C2'-C3'-O3'	-5.10	103.86	111.50
2	A	59	LYS	N-CA-C	5.02	117.14	111.11
2	A	145	ARG	N-CA-C	-5.01	106.43	112.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	DG	Sidechain
1	E	9	DC	Sidechain
1	F	10	DG	Sidechain
1	F	7	DG	Sidechain
1	F	9	DC	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	328	0	178	8	0
1	D	349	0	190	12	0
1	E	349	0	190	6	0
1	F	349	0	190	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2388	0	2365	102	0
2	B	2388	0	2365	103	0
3	A	15	0	0	2	0
3	B	23	0	0	2	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	3	0	0	0	0
All	All	6195	0	5478	216	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 19.

All (216) 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:B:168:LYS:HD3	2:B:168:LYS:H	1.11	1.15
1:F:10:DG:H21	2:A:63:THR:HG21	1.06	1.12
2:B:300:VAL:HG22	2:B:301:PRO:HD2	1.33	1.10
2:A:192:ARG:HB3	2:A:192:ARG:HH11	1.18	1.03
1:D:9:DC:H2'	2:B:232:ARG:HD2	1.49	0.92
2:A:192:ARG:HD2	2:A:193:GLY:N	1.86	0.90
2:B:83:PHE:H	2:B:93:GLN:HE22	1.22	0.88
1:F:10:DG:N2	2:A:63:THR:HG21	1.90	0.87
2:B:230:ARG:HA	2:B:230:ARG:NH1	1.91	0.85
1:F:10:DG:H21	2:A:63:THR:CG2	1.88	0.85
2:B:11:PRO:HG2	2:B:134:LYS:HE3	1.59	0.84
2:A:11:PRO:HB3	2:A:134:LYS:HG2	1.62	0.82
1:F:7:DG:H2''	1:F:8:DC:H5''	1.62	0.82
2:B:26:ASP:OD2	2:B:29:GLY:HA2	1.82	0.78
2:B:252:GLN:HG3	2:B:253:ASP:OD1	1.82	0.78
2:B:230:ARG:HA	2:B:230:ARG:HH11	1.46	0.78
2:A:249:LEU:HD13	2:A:259:ALA:HB2	1.64	0.78
2:A:192:ARG:HD2	2:A:193:GLY:H	1.47	0.77
2:B:13:ASP:O	2:B:17:ARG:HB2	1.83	0.77
2:A:192:ARG:HB3	2:A:192:ARG:NH1	2.00	0.76
2:A:192:ARG:CD	2:A:193:GLY:H	1.97	0.76
2:B:288:THR:HG21	2:B:295:ARG:CZ	2.15	0.75
2:B:103:GLY:HA2	2:B:105:TRP:CZ3	2.22	0.74
2:B:229:LYS:O	2:B:229:LYS:HD3	1.87	0.74
2:B:48:ARG:HG3	2:B:49:THR:HG23	1.70	0.74
2:A:192:ARG:NH1	2:A:193:GLY:H	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ASP:O	2:B:184:GLN:HG2	1.87	0.73
2:A:192:ARG:HH11	2:A:192:ARG:CB	2.01	0.72
1:F:10:DG:H5'	2:B:60:THR:HG21	1.70	0.72
2:B:11:PRO:CG	2:B:134:LYS:HE3	2.20	0.72
2:A:11:PRO:HD3	2:A:134:LYS:HZ2	1.55	0.71
2:B:138:GLN:H	2:B:138:GLN:HE21	1.38	0.71
2:B:10:GLU:HG3	2:B:11:PRO:HD2	1.71	0.70
2:B:278:VAL:HG13	2:B:299:ALA:HB2	1.73	0.70
2:A:212:LEU:HD13	2:A:271:GLN:NE2	2.06	0.70
2:B:250:GLY:O	2:B:267:PRO:HG2	1.92	0.70
1:F:14:DT:H2''	1:F:15:DG:N7	2.07	0.69
2:B:300:VAL:CG2	2:B:301:PRO:HD2	2.19	0.69
2:A:250:GLY:O	2:A:267:PRO:HG2	1.93	0.69
2:A:10:GLU:HB3	2:A:13:ASP:HB2	1.78	0.66
2:A:192:ARG:HH11	2:A:193:GLY:H	1.42	0.66
2:A:11:PRO:HA	2:A:134:LYS:HD3	1.78	0.65
2:B:168:LYS:H	2:B:168:LYS:CD	1.93	0.65
1:F:8:DC:H2''	1:F:9:DC:H5''	1.77	0.65
2:A:53:ASN:HB3	2:A:56:GLN:HG3	1.79	0.65
2:B:53:ASN:HD22	2:B:175:LEU:HD13	1.62	0.64
1:D:7:DG:N7	2:A:230:ARG:NH2	2.45	0.64
1:E:14:DT:H2''	1:E:15:DG:N7	2.13	0.63
2:A:296:TRP:CZ2	2:A:309:PRO:HG3	2.33	0.63
2:A:11:PRO:CD	2:A:134:LYS:HZ2	2.12	0.63
2:A:249:LEU:HD22	2:A:255:ASP:HA	1.79	0.63
2:B:252:GLN:O	2:B:256:PRO:HD3	1.98	0.62
2:A:11:PRO:HD3	2:A:134:LYS:NZ	2.14	0.62
1:E:10:DG:H21	2:B:63:THR:HG21	1.64	0.62
2:A:19:ARG:HD2	3:A:322:HOH:O	2.00	0.62
2:B:296:TRP:CZ2	2:B:309:PRO:HG3	2.34	0.62
2:B:265:PRO:O	2:B:273:VAL:HG21	2.01	0.61
2:A:105:TRP:CE2	2:A:118:VAL:HB	2.36	0.61
2:B:14:ASP:O	2:B:18:VAL:HG23	2.01	0.60
2:B:168:LYS:HD3	2:B:168:LYS:N	1.97	0.60
2:A:291:ILE:HG21	2:A:309:PRO:HB2	1.82	0.60
2:B:105:TRP:CE2	2:B:118:VAL:HB	2.37	0.59
2:A:278:VAL:HG13	2:A:299:ALA:HB2	1.85	0.59
2:B:282:GLU:C	2:B:284:ASP:H	2.11	0.58
1:D:8:DC:OP1	2:B:215:ARG:HD2	2.04	0.58
2:A:187:SER:O	2:A:189:LYS:HG2	2.02	0.58
1:D:17:DC:H4'	2:B:193:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:DC:C4'	2:A:192:ARG:HE	2.16	0.58
2:A:15:LEU:HA	2:A:115:ILE:HD13	1.86	0.58
2:B:10:GLU:C	2:B:12:ASP:H	2.11	0.58
2:B:282:GLU:O	2:B:284:ASP:N	2.30	0.58
2:A:247:ILE:HA	3:A:327:HOH:O	2.04	0.57
1:F:8:DC:C2'	1:F:9:DC:H5''	2.34	0.57
2:A:192:ARG:NH1	2:A:193:GLY:N	2.52	0.57
2:B:48:ARG:HG3	2:B:49:THR:CG2	2.33	0.57
2:A:105:TRP:CZ2	2:A:118:VAL:HB	2.40	0.57
2:B:51:ARG:NH1	2:B:57:LEU:HD23	2.20	0.56
2:B:254:ASN:O	2:B:258:VAL:HG23	2.04	0.56
2:A:10:GLU:HG3	2:A:11:PRO:HD2	1.88	0.56
2:A:10:GLU:O	2:A:14:ASP:HB2	2.05	0.56
1:D:9:DC:H2''	1:D:10:DG:C8	2.41	0.56
1:C:12:DC:H5	2:A:234:SER:CB	2.18	0.56
2:B:212:LEU:HD23	2:B:273:VAL:HG22	1.88	0.55
2:A:261:ASP:HB2	2:A:289:ALA:HB2	1.88	0.55
2:B:255:ASP:HB2	2:B:256:PRO:HD3	1.89	0.55
2:B:65:MET:O	2:B:69:VAL:HG23	2.06	0.54
1:C:12:DC:H5	2:A:234:SER:HB3	1.72	0.54
2:A:212:LEU:HD23	2:A:273:VAL:HG22	1.89	0.54
2:B:143:ALA:HB1	2:B:147:LEU:HA	1.90	0.54
2:A:192:ARG:HH11	2:A:193:GLY:N	2.05	0.53
2:A:212:LEU:HD22	2:A:267:PRO:HB3	1.90	0.53
1:D:16:DG:H2''	1:D:17:DC:C5	2.43	0.53
2:B:103:GLY:HA2	2:B:105:TRP:CH2	2.43	0.52
2:A:31:ARG:O	2:A:35:VAL:HG23	2.09	0.52
2:B:10:GLU:HG3	3:B:329:HOH:O	2.09	0.52
2:B:252:GLN:O	2:B:255:ASP:HB2	2.10	0.52
1:E:2:DG:H2''	1:E:3:DC:OP2	2.10	0.52
2:B:163:TRP:O	2:B:166:HIS:HD2	1.92	0.52
1:D:2:DG:H2''	1:D:3:DC:OP2	2.10	0.52
2:A:245:GLY:O	2:A:276:ARG:HA	2.10	0.52
2:A:109:PRO:HD3	2:A:147:LEU:O	2.10	0.52
2:B:15:LEU:C	2:B:15:LEU:HD23	2.35	0.52
2:A:103:GLY:HA2	2:A:105:TRP:CZ3	2.45	0.52
2:B:296:TRP:CE2	2:B:309:PRO:HG3	2.45	0.52
2:A:212:LEU:HD13	2:A:271:GLN:HE22	1.74	0.51
2:B:138:GLN:H	2:B:138:GLN:NE2	2.05	0.51
2:A:92:VAL:HG11	2:A:115:ILE:HD12	1.93	0.51
2:A:192:ARG:CZ	2:A:193:GLY:H	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:DC:H2''	1:F:9:DC:C5'	2.41	0.50
2:A:126:CYS:O	2:A:168:LYS:HB2	2.11	0.50
2:A:291:ILE:HD12	2:A:309:PRO:HG2	1.93	0.50
1:D:7:DG:OP2	2:A:224:GLN:HB2	2.11	0.50
2:A:166:HIS:ND1	2:A:167:GLY:O	2.41	0.50
2:A:181:VAL:HG13	2:A:207:ARG:HB3	1.93	0.50
2:A:265:PRO:O	2:A:273:VAL:HG21	2.11	0.50
2:B:229:LYS:HD3	2:B:229:LYS:C	2.36	0.50
1:D:17:DC:H5''	2:B:194:ASN:ND2	2.27	0.49
2:A:291:ILE:HG22	2:A:292:GLN:N	2.26	0.49
2:B:14:ASP:HB3	2:B:115:ILE:HD11	1.93	0.49
2:A:124:GLN:NE2	2:A:175:LEU:HD11	2.27	0.49
2:B:282:GLU:C	2:B:284:ASP:N	2.71	0.49
1:C:11:DG:O6	2:A:229:LYS:HE3	2.12	0.48
2:B:49:THR:OG1	2:B:51:ARG:HG3	2.13	0.48
2:B:109:PRO:HD3	2:B:147:LEU:O	2.12	0.48
2:A:15:LEU:HD23	2:A:15:LEU:C	2.38	0.48
2:B:156:ARG:O	2:B:159:VAL:HG23	2.12	0.48
2:A:195:GLN:HE21	2:A:195:GLN:HB2	1.50	0.48
1:D:10:DG:OP2	2:B:238:ARG:NH1	2.46	0.48
1:F:9:DC:H1'	2:B:60:THR:HG22	1.96	0.48
1:E:7:DG:O6	2:A:144:ASN:ND2	2.36	0.48
2:A:11:PRO:HB3	2:A:134:LYS:NZ	2.28	0.48
2:A:296:TRP:CE2	2:A:309:PRO:HG3	2.49	0.48
2:B:92:VAL:HG11	2:B:115:ILE:HD12	1.96	0.47
2:B:10:GLU:CG	2:B:11:PRO:HD2	2.41	0.47
2:B:119:ILE:HG22	2:B:120:TRP:N	2.30	0.47
2:B:288:THR:HG21	2:B:295:ARG:NH2	2.29	0.47
2:A:37:ARG:NH2	2:A:41:ASP:OD2	2.44	0.47
2:A:48:ARG:CZ	2:B:42:GLN:HG3	2.45	0.47
2:B:138:GLN:HE21	2:B:138:GLN:N	2.09	0.47
1:E:9:DC:H5'	2:A:59:LYS:HD3	1.97	0.46
2:B:267:PRO:HB2	2:B:271:GLN:HB2	1.97	0.46
1:D:6:DC:C5	2:A:230:ARG:NH2	2.84	0.46
2:A:21:THR:OG1	2:A:90:ALA:HB2	2.16	0.46
2:B:163:TRP:O	2:B:166:HIS:CD2	2.68	0.46
2:B:186:PHE:HA	2:B:200:ARG:HD2	1.97	0.46
2:A:89:ILE:HD12	2:A:94:VAL:HG21	1.97	0.46
2:B:58:HIS:HB3	3:B:340:HOH:O	2.16	0.46
2:B:250:GLY:H	2:B:255:ASP:CG	2.23	0.46
2:B:15:LEU:HA	2:B:115:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:TRP:HZ3	2:B:130:ALA:HB2	1.80	0.46
2:A:202:ASN:O	2:A:206:ARG:HG3	2.16	0.46
2:B:48:ARG:CG	2:B:49:THR:HG23	2.43	0.45
1:F:12:DC:O2	2:A:59:LYS:HE3	2.16	0.45
2:B:218:ILE:HD13	2:B:231:VAL:HG21	1.97	0.45
2:A:229:LYS:O	2:A:229:LYS:HD3	2.16	0.45
2:A:230:ARG:HA	2:A:230:ARG:HH11	1.81	0.45
2:B:61:GLU:O	2:B:62:LYS:C	2.60	0.45
2:A:300:VAL:HG13	2:A:301:PRO:HD2	1.97	0.45
2:A:205:PHE:CE1	2:A:231:VAL:HG22	2.52	0.45
2:B:261:ASP:O	2:B:287:GLN:HB3	2.17	0.45
1:F:12:DC:H1'	2:A:59:LYS:HE3	1.97	0.44
1:C:9:DC:H2'	2:A:232:ARG:HD2	1.98	0.44
2:A:116:CYS:O	2:A:132:LEU:HA	2.17	0.44
2:A:139:PHE:HB3	2:A:155:GLY:CA	2.47	0.44
2:A:255:ASP:N	2:A:256:PRO:HD2	2.33	0.44
2:A:60:THR:O	2:A:63:THR:HB	2.17	0.44
2:A:15:LEU:HD23	2:A:15:LEU:O	2.18	0.43
2:A:229:LYS:C	2:A:231:VAL:H	2.25	0.43
2:A:291:ILE:HG21	2:A:309:PRO:CB	2.48	0.43
2:B:302:GLY:O	2:B:303:ASP:C	2.61	0.43
2:A:267:PRO:HD3	2:A:273:VAL:CG2	2.48	0.43
2:B:14:ASP:HB3	2:B:115:ILE:CD1	2.49	0.43
2:A:161:LYS:HB2	2:A:161:LYS:NZ	2.33	0.43
2:A:11:PRO:HB3	2:A:134:LYS:CG	2.40	0.43
2:A:172:ASN:OD1	2:A:172:ASN:C	2.61	0.43
2:B:52:TRP:CZ2	2:B:182:ARG:HD2	2.54	0.43
1:E:1:DT:H2''	1:E:2:DG:C5	2.54	0.43
2:B:311:VAL:HA	2:B:312:PRO:HD2	1.80	0.43
2:B:251:HIS:CG	2:B:269:LYS:HA	2.54	0.43
2:B:139:PHE:O	2:B:152:THR:HG23	2.19	0.43
2:B:11:PRO:C	2:B:13:ASP:N	2.76	0.42
2:A:83:PHE:H	2:A:93:GLN:HE22	1.66	0.42
2:B:17:ARG:HH11	2:B:17:ARG:HG2	1.84	0.42
1:F:7:DG:N7	2:B:144:ASN:HB2	2.35	0.42
2:A:257:LYS:O	2:A:260:ASN:N	2.52	0.42
2:B:15:LEU:N	2:B:115:ILE:HD11	2.34	0.42
2:B:268:ARG:O	2:B:269:LYS:C	2.63	0.42
2:A:144:ASN:HD22	2:A:144:ASN:HA	1.56	0.42
2:A:234:SER:O	2:A:236:GLY:N	2.52	0.42
2:B:131:GLY:O	2:B:132:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:GLN:NE2	2:B:138:GLN:N	2.67	0.42
2:B:290:GLU:HG2	2:B:291:ILE:N	2.35	0.42
2:A:126:CYS:SG	2:A:176:HIS:NE2	2.93	0.42
2:B:171:GLU:OE2	2:B:211:ARG:NH2	2.53	0.42
2:B:187:SER:O	2:B:189:LYS:HG3	2.20	0.42
2:A:14:ASP:O	2:A:18:VAL:HG23	2.19	0.41
2:B:10:GLU:C	2:B:12:ASP:N	2.78	0.41
2:A:286:ARG:NH1	2:A:300:VAL:HG23	2.35	0.41
2:B:51:ARG:CZ	2:B:57:LEU:HD23	2.50	0.41
2:A:242:ARG:HB3	2:A:243:PRO:CD	2.50	0.41
1:C:12:DC:H41	2:A:235:GLY:H	1.69	0.41
2:B:26:ASP:HB2	2:B:31:ARG:HD3	2.03	0.41
2:A:210:GLY:HA2	2:A:264:LEU:HD22	2.03	0.41
2:B:141:GLY:O	2:B:149:ARG:NH1	2.51	0.41
2:B:13:ASP:HB3	2:B:17:ARG:HE	1.86	0.41
2:B:46:GLY:O	2:B:220:THR:HA	2.20	0.41
1:D:8:DC:C2	1:D:9:DC:C5	3.09	0.41
2:A:187:SER:O	2:A:188:ALA:C	2.63	0.41
1:C:10:DG:H2'	2:A:233:GLY:HA3	2.03	0.40
2:B:152:THR:O	2:B:155:GLY:N	2.54	0.40
2:B:172:ASN:OD1	2:B:172:ASN:C	2.63	0.40
2:B:250:GLY:O	2:B:267:PRO:CG	2.67	0.40
2:B:125:GLN:O	2:B:126:CYS:C	2.64	0.40
1:C:12:DC:C5	2:A:234:SER:HB3	2.55	0.40
1:F:10:DG:N2	2:A:63:THR:CG2	2.68	0.40
2:B:310:VAL:HG13	2:B:310:VAL:O	2.22	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	302/317 (95%)	274 (91%)	21 (7%)	7 (2%)	5	6
2	B	302/317 (95%)	274 (91%)	22 (7%)	6 (2%)	6	7
All	All	604/634 (95%)	548 (91%)	43 (7%)	13 (2%)	5	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	193	GLY
2	A	234	SER
2	A	284	ASP
2	A	233	GLY
2	A	292	GLN
2	A	11	PRO
2	B	232	ARG
2	B	284	ASP
2	A	291	ILE
2	B	11	PRO
2	B	233	GLY
2	B	283	GLY
2	B	312	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	
2	A	252/263 (96%)	245 (97%)	7 (3%)	38	60
2	B	252/263 (96%)	240 (95%)	12 (5%)	23	40
All	All	504/526 (96%)	485 (96%)	19 (4%)	29	49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	12	ASP
2	A	63	THR
2	A	142	THR

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Mol	Chain	Res	Type
2	A	144	ASN
2	A	192	ARG
2	A	195	GLN
2	A	266	VAL
2	B	12	ASP
2	B	17	ARG
2	B	63	THR
2	B	138	GLN
2	B	168	LYS
2	B	190	SER
2	B	230	ARG
2	B	253	ASP
2	B	284	ASP
2	B	290	GLU
2	B	300	VAL
2	B	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	58	HIS
2	A	93	GLN
2	A	102	GLN
2	A	124	GLN
2	A	125	GLN
2	A	144	ASN
2	A	170	GLN
2	A	194	ASN
2	A	195	GLN
2	A	224	GLN
2	A	251	HIS
2	A	254	ASN
2	A	271	GLN
2	A	285	GLN
2	B	47	GLN
2	B	93	GLN
2	B	102	GLN
2	B	114	HIS
2	B	124	GLN
2	B	125	GLN
2	B	138	GLN
2	B	166	HIS

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Mol	Chain	Res	Type
2	B	194	ASN
2	B	251	HIS
2	B	285	GLN
2	B	292	GLN

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 oligosaccharides 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	C	16/17 (94%)	0.28	1 (6%) 26 22	22, 41, 77, 100	0
1	D	17/17 (100%)	0.47	2 (11%) 9 6	29, 42, 87, 98	0
1	E	17/17 (100%)	0.30	2 (11%) 9 6	19, 35, 98, 100	0
1	F	17/17 (100%)	0.09	2 (11%) 9 6	22, 37, 89, 99	0
2	A	304/317 (95%)	0.37	18 (5%) 28 24	16, 35, 68, 94	0
2	B	304/317 (95%)	0.32	14 (4%) 37 33	16, 33, 70, 96	0
All	All	675/702 (96%)	0.34	39 (5%) 29 25	16, 34, 72, 100	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	10	GLU	6.0
2	B	10	GLU	5.3
2	A	11	PRO	4.3
2	B	11	PRO	4.2
2	B	233	GLY	4.2
2	B	291	ILE	3.9
2	A	192	ARG	3.4
1	D	17	DC	3.4
2	A	313	ARG	3.4
1	E	1	DT	3.4
2	B	13	ASP	3.4
2	B	12	ASP	3.2
2	A	311	VAL	3.1
1	D	1	DT	3.1
2	B	313	ARG	3.1
1	E	2	DG	3.0
2	A	285	GLN	2.8
1	F	17	DC	2.8
2	A	291	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	2	DG	2.7
2	A	83	PHE	2.6
2	A	295	ARG	2.5
2	B	280	ALA	2.5
2	B	295	ARG	2.5
2	B	234	SER	2.5
2	B	192	ARG	2.4
2	B	290	GLU	2.4
2	A	312	PRO	2.3
2	A	242	ARG	2.3
2	A	193	GLY	2.3
2	A	235	GLY	2.2
2	B	283	GLY	2.2
2	A	284	ASP	2.2
2	A	282	GLU	2.2
2	A	281	ASP	2.1
1	F	1	DT	2.1
2	A	254	ASN	2.1
2	A	283	GLY	2.1
2	B	310	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.