



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:43 PM UTC

PDB ID : 2EX5 / pdb_00002ex5
Title : Group I Intron-encoded Homing Endonuclease I-CeuI Complexed With DNA
Authors : Spiegel, P.C.; Stoddard, B.L.
Deposited on : 2005-11-07
Resolution : 2.20 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

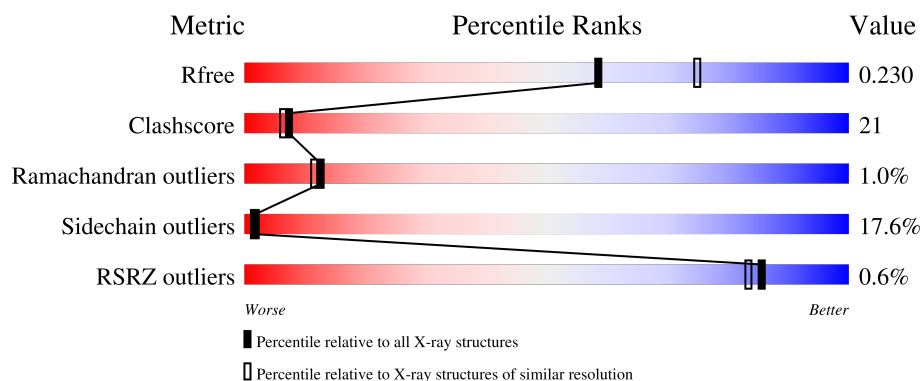
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

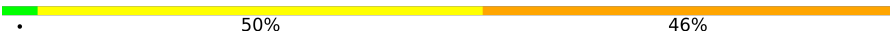
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	X	26	
2	Y	26	
3	A	207	
3	B	207	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4664 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 I-CeuI DNA target site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	26	Total	C	N	O	P	0	0	0
			535	254	106	150	25			

- Molecule 2 is a DNA chain called I-CeuI DNA target site, complementary strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	26	Total	C	N	O	P	0	0	0
			525	252	90	158	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	207	Total	C	N	O	S	0	0	0
			1669	1071	286	311	1			
3	B	207	Total	C	N	O	S	0	0	0
			1669	1071	286	311	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ARG	GLN	engineered mutation	UNP P32761
B	93	ARG	GLN	engineered mutation	UNP P32761

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

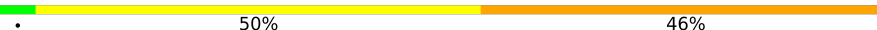
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	27	Total 27	O 27	0	0
5	Y	40	Total 40	O 40	0	0
5	A	118	Total 118	O 118	0	0
5	B	78	Total 78	O 78	0	0

3 Residue-property plots

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: I-CeuI DNA target site

Chain X: 



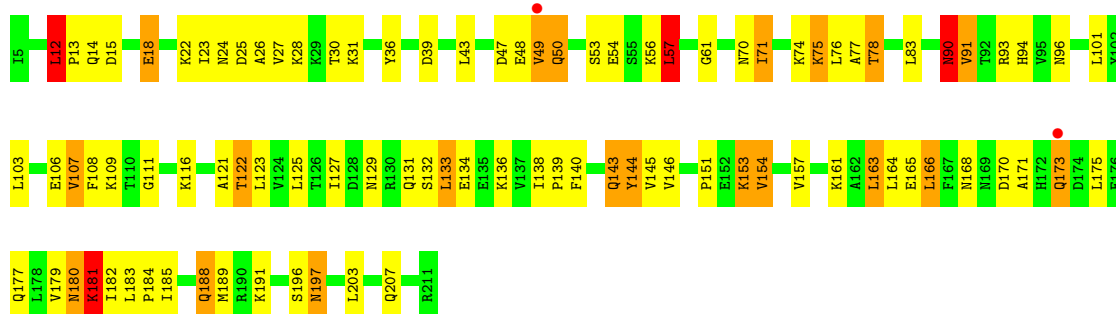
- Molecule 2: I-CeuI DNA target site, complementary strand

Chain Y: 



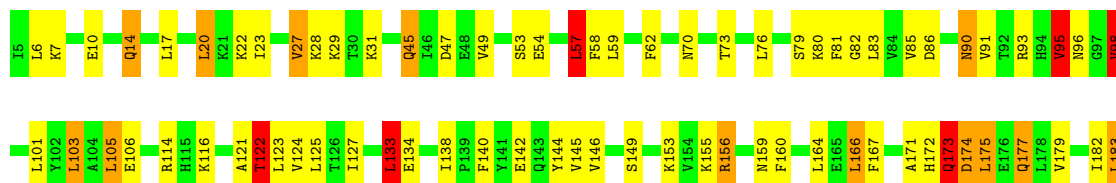
- Molecule 3: DNA endonuclease I-CeuI

Chain A: 



- Molecule 3: DNA endonuclease I-CeuI

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.23Å 69.18Å 169.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.20) 96.2 (20.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.21Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.231 0.218 , 0.230	Depositor DCC
R_{free} test set	3057 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.4	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	0.95	EDS
Total number of atoms	4664	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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

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	X	1.05	0/602	2.25	41/928 (4.4%)
2	Y	1.13	1/586 (0.2%)	2.38	44/902 (4.9%)
3	A	1.77	21/1697 (1.2%)	1.55	17/2283 (0.7%)
3	B	1.52	8/1697 (0.5%)	1.48	16/2283 (0.7%)
All	All	1.53	30/4582 (0.7%)	1.78	118/6396 (1.8%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	145	VAL	CA-CB	8.29	1.64	1.54
3	B	138	ILE	CA-CB	8.03	1.58	1.54
3	A	121	ALA	C-O	7.79	1.29	1.23
3	A	71	ILE	CA-CB	7.68	1.64	1.54
3	B	91	VAL	CA-CB	7.55	1.64	1.54
3	B	86	ASP	N-CA	-7.33	1.39	1.46
3	B	57	LEU	C-O	-7.28	1.15	1.24
3	B	95	VAL	CA-CB	6.96	1.64	1.54
3	A	27	VAL	C-O	6.94	1.32	1.24
3	A	26	ALA	CA-CB	6.93	1.64	1.53
3	A	26	ALA	N-CA	6.80	1.54	1.46
3	A	154	VAL	CA-CB	6.76	1.61	1.54
3	A	30	THR	N-CA	6.08	1.53	1.46
3	A	157	VAL	CA-CB	6.04	1.62	1.54
3	A	49	VAL	CA-CB	6.04	1.63	1.54
3	A	25	ASP	N-CA	5.99	1.53	1.46
3	A	107	VAL	CA-CB	5.99	1.62	1.54
3	B	133	LEU	N-CA	5.78	1.53	1.46
2	Y	716	DG	O3'-P	-5.78	1.52	1.61
3	A	36	TYR	C-O	-5.78	1.17	1.24
3	B	138	ILE	C-O	-5.66	1.19	1.24
3	B	191	LYS	CE-NZ	5.57	1.66	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	90	ASN	CA-C	-5.50	1.45	1.52
3	A	181	LYS	CA-C	5.23	1.58	1.52
3	A	138	ILE	CA-CB	5.22	1.57	1.54
3	A	140	PHE	CG-CD1	5.20	1.49	1.38
3	A	188	GLN	N-CA	5.19	1.52	1.46
3	A	24	ASN	N-CA	5.14	1.52	1.46
3	A	57	LEU	C-O	-5.14	1.18	1.24
3	A	91	VAL	CB-CG1	5.08	1.69	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	723	DA	C5'-C4'-C3'	-11.89	97.07	114.90
2	Y	715	DG	C5'-C4'-O4'	-11.29	92.46	109.40
1	X	614	DA	C5'-C4'-C3'	-10.91	98.54	114.90
1	X	615	DA	P-O5'-C5'	-10.87	103.70	120.00
1	X	605	DA	O3'-P-O5'	9.84	118.77	104.00
2	Y	714	DA	O3'-P-O5'	9.72	118.58	104.00
3	A	134	GLU	N-CA-C	9.44	121.65	111.36
3	B	98	VAL	CB-CA-C	-9.34	97.68	112.16
2	Y	715	DG	P-O5'-C5'	8.94	133.41	120.00
1	X	618	DT	P-O5'-C5'	8.91	133.36	120.00
2	Y	718	DC	P-O5'-C5'	8.51	132.77	120.00
1	X	614	DA	C5'-C4'-O4'	-8.00	97.40	109.40
2	Y	716	DG	C5'-C4'-O4'	8.00	121.40	109.40
2	Y	716	DG	P-O5'-C5'	7.98	131.96	120.00
2	Y	720	DG	P-O3'-C3'	7.93	132.09	120.20
1	X	606	DA	O5'-C5'-C4'	-7.81	99.09	110.80
1	X	601	DC	O4'-C1'-N1	-7.62	96.97	108.40
3	B	177	GLN	N-CA-C	-7.58	104.00	113.55
1	X	607	DC	O4'-C1'-N1	7.51	119.67	108.40
2	Y	708	DT	C6-C5-C7	-7.47	112.80	124.00
2	Y	721	DT	C5'-C4'-C3'	-7.45	103.73	114.90
1	X	625	DG	C5'-C4'-O4'	-7.42	98.27	109.40
1	X	615	DA	C4'-C3'-O3'	-7.40	98.90	110.00
1	X	615	DA	O3'-P-O5'	-7.40	92.90	104.00
3	A	182	ILE	N-CA-C	7.23	117.31	110.30
2	Y	722	DT	P-O3'-C3'	7.22	131.04	120.20
1	X	608	DG	P-O3'-C3'	7.18	130.97	120.20
3	A	122	THR	N-CA-C	7.17	121.09	110.48
3	B	160	PHE	N-CA-C	-7.11	102.95	111.69
1	X	606	DA	O3'-P-O5'	-7.08	93.38	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	107	VAL	N-CA-C	7.02	117.81	110.72
3	B	27	VAL	CB-CA-C	-7.01	100.90	112.26
2	Y	704	DT	C4'-C3'-O3'	-7.00	99.50	110.00
2	Y	723	DA	P-O5'-C5'	-7.00	109.50	120.00
2	Y	714	DA	P-O3'-C3'	6.90	130.54	120.20
3	B	159	ASN	N-CA-C	6.87	119.79	111.82
2	Y	721	DT	C2-N1-C1'	-6.80	109.15	119.35
3	B	95	VAL	CB-CA-C	-6.74	100.23	111.29
2	Y	716	DG	C4'-C3'-O3'	-6.63	100.05	110.00
2	Y	701	DG	C8-N9-C1'	6.59	136.88	127.00
2	Y	705	DC	C6-N1-C1'	6.54	129.50	119.70
1	X	616	DG	P-O5'-C5'	6.49	129.74	120.00
2	Y	723	DA	C5'-C4'-O4'	6.49	119.14	109.40
1	X	624	DA	C4'-C3'-O3'	-6.46	100.31	110.00
2	Y	706	DG	C4'-C3'-O3'	-6.40	100.39	110.00
1	X	604	DT	P-O3'-C3'	6.40	129.80	120.20
2	Y	712	DT	N1-C1'-C2'	6.38	123.08	113.50
3	A	26	ALA	N-CA-C	6.36	117.88	111.07
3	B	134	GLU	N-CA-C	6.31	118.24	111.36
2	Y	714	DA	C4'-C3'-O3'	-6.28	100.58	110.00
1	X	624	DA	O5'-C5'-C4'	-6.21	101.48	110.80
1	X	603	DA	P-O5'-C5'	-6.20	110.70	120.00
1	X	603	DA	C5'-C4'-O4'	-6.19	100.11	109.40
2	Y	705	DC	N1-C1'-C2'	6.16	122.73	113.50
3	B	122	THR	CB-CA-C	6.14	119.88	109.80
2	Y	709	DA	O5'-C5'-C4'	-6.11	101.64	110.80
2	Y	722	DT	C4'-C3'-O3'	-6.04	100.94	110.00
2	Y	717	DA	O3'-P-O5'	6.03	113.05	104.00
1	X	616	DG	O3'-P-O5'	-6.03	94.96	104.00
3	B	173	GLN	N-CA-C	-6.01	104.06	111.40
2	Y	716	DG	C2'-C3'-O3'	5.97	120.45	111.50
1	X	602	DG	C5'-C4'-O4'	5.95	118.32	109.40
2	Y	718	DC	N1-C1'-C2'	5.92	122.39	113.50
3	B	191	LYS	N-CA-C	-5.89	105.86	114.39
3	A	111	GLY	N-CA-C	-5.88	106.05	112.04
1	X	611	DC	N1-C1'-C2'	5.87	122.31	113.50
1	X	603	DA	C5'-C4'-C3'	-5.86	106.11	114.90
2	Y	707	DC	O3'-P-O5'	-5.85	95.22	104.00
1	X	620	DG	C4'-C3'-O3'	-5.82	101.27	110.00
3	B	29	LYS	N-CA-C	5.81	117.41	111.14
1	X	610	DT	C5'-C4'-O4'	5.79	118.08	109.40
2	Y	704	DT	P-O5'-C5'	5.79	128.69	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	612	DC	N1-C1'-C2'	5.79	122.18	113.50
3	A	180	ASN	N-CA-C	5.79	120.35	113.12
3	B	47	ASP	CB-CA-C	5.76	119.49	109.65
2	Y	705	DC	C2-N1-C1'	-5.73	111.10	119.70
2	Y	707	DC	C4'-C3'-O3'	-5.72	101.42	110.00
2	Y	723	DA	C2'-C3'-O3'	5.70	120.05	111.50
3	A	131	GLN	CB-CA-C	-5.69	101.91	110.90
3	A	22	LYS	N-CA-C	-5.68	105.08	111.28
2	Y	720	DG	O5'-C5'-C4'	-5.68	102.28	110.80
1	X	614	DA	N9-C1'-C2'	5.67	122.01	113.50
3	B	140	PHE	N-CA-C	5.64	117.88	111.11
2	Y	722	DT	P-O5'-C5'	5.63	128.44	120.00
3	A	49	VAL	N-CA-C	5.60	116.80	108.46
3	A	12	LEU	CA-C-N	-5.56	114.53	120.03
3	A	12	LEU	C-N-CA	-5.56	114.53	120.03
3	A	131	GLN	CA-CB-CG	5.55	125.20	114.10
1	X	607	DC	C2'-C3'-O3'	-5.55	103.18	111.50
1	X	613	DT	C6-C5-C7	-5.55	115.68	124.00
1	X	601	DC	C2'-C3'-O3'	5.54	119.81	111.50
3	A	53	SER	CA-C-N	5.54	127.64	120.44
3	A	53	SER	C-N-CA	5.54	127.64	120.44
1	X	602	DG	C5'-C4'-C3'	-5.51	106.63	114.90
2	Y	716	DG	O4'-C1'-C2'	-5.49	98.17	106.40
2	Y	704	DT	O4'-C1'-N1	5.48	116.62	108.40
1	X	604	DT	C2'-C3'-O3'	-5.44	103.35	111.50
1	X	614	DA	C5-C6-N6	5.43	131.54	123.40
1	X	603	DA	O4'-C1'-N9	5.42	116.54	108.40
1	X	606	DA	O4'-C1'-C2'	-5.42	98.26	106.40
2	Y	711	DC	P-O3'-C3'	5.42	128.33	120.20
3	A	203	LEU	N-CA-C	5.41	117.17	111.28
1	X	611	DC	C4'-C3'-O3'	-5.37	101.94	110.00
2	Y	701	DG	C4-N9-C1'	-5.35	118.98	127.00
3	B	45	GLN	N-CA-C	-5.32	104.09	111.28
2	Y	711	DC	O3'-P-O5'	-5.29	96.07	104.00
1	X	612	DC	C6-N1-C1'	5.26	127.59	119.70
1	X	602	DG	O5'-C5'-C4'	5.22	118.63	110.80
2	Y	720	DG	P-O5'-C5'	5.18	127.77	120.00
3	A	144	TYR	N-CA-C	5.18	120.25	113.88
1	X	617	DG	O4'-C1'-C2'	-5.17	98.64	106.40
3	B	199	GLY	N-CA-C	-5.16	106.39	112.64
3	B	142	GLU	N-CA-C	-5.14	105.86	111.82
1	X	602	DG	N3-C2-N2	-5.12	112.01	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	704	DT	O4'-C1'-C2'	-5.10	98.75	106.40
2	Y	724	DT	C6-C5-C7	-5.03	116.45	124.00
1	X	625	DG	P-O5'-C5'	-5.03	112.46	120.00
2	Y	716	DG	N1-C2-N2	5.01	123.82	116.30

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	X	535	0	292	20	0
2	Y	525	0	295	30	1
3	A	1669	0	1717	61	0
3	B	1669	0	1717	75	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	X	1	0	0	0	0
5	A	118	0	0	11	0
5	B	78	0	0	10	0
5	X	27	0	0	2	0
5	Y	40	0	0	5	1
All	All	4664	0	4021	170	1

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 21.

All (170) 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)
3:B:22:LYS:HD3	5:B:1213:HOH:O	1.40	1.20
2:Y:721:DT:H2''	2:Y:722:DT:H5'	1.21	1.11
3:B:73:THR:HG22	3:B:85:VAL:HG22	1.40	1.01
2:Y:722:DT:O4	5:Y:1236:HOH:O	1.84	0.95
3:B:53:SER:O	3:B:57:LEU:HD22	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:722:DT:H73	5:Y:1236:HOH:O	1.71	0.91
3:B:156:ARG:HH21	3:B:156:ARG:HG2	1.34	0.90
2:Y:721:DT:H2''	2:Y:722:DT:C5'	2.02	0.90
3:B:174:ASP:OD1	3:B:175:LEU:N	2.08	0.86
3:A:94:HIS:HD2	3:A:96:ASN:H	1.16	0.86
3:A:170:ASP:O	3:A:173:GLN:NE2	2.07	0.86
2:Y:721:DT:C2'	2:Y:722:DT:H5'	2.07	0.83
3:A:163:LEU:CD2	3:A:185:ILE:HG21	2.09	0.81
3:A:170:ASP:C	3:A:173:GLN:HE22	1.88	0.80
3:A:170:ASP:HB3	3:A:173:GLN:NE2	1.96	0.80
3:A:163:LEU:HD21	3:A:185:ILE:CG2	2.12	0.80
3:B:98:VAL:HG13	3:B:123:LEU:HD12	1.64	0.79
1:X:602:DG:H2''	1:X:603:DA:C8	2.18	0.79
3:B:195:GLN:O	3:B:198:GLU:HG2	1.81	0.79
2:Y:723:DA:H2''	2:Y:724:DT:H5''	1.67	0.77
1:X:606:DA:OP2	5:X:1109:HOH:O	2.02	0.77
3:A:127:ILE:HG22	3:A:133:LEU:HD13	1.66	0.77
3:A:71:ILE:HD12	3:A:189:MET:SD	2.25	0.76
3:A:129:ASN:HD22	3:A:132:SER:H	1.33	0.76
3:A:163:LEU:HD21	3:A:185:ILE:HG21	1.64	0.75
3:B:197:ASN:H	3:B:197:ASN:HD22	1.34	0.75
3:A:94:HIS:CD2	3:A:96:ASN:H	2.03	0.74
1:X:601:DC:H2''	1:X:602:DG:O5'	1.87	0.74
3:B:166:LEU:HD22	3:B:182:ILE:HG13	1.71	0.72
3:B:174:ASP:CG	3:B:175:LEU:H	1.97	0.72
2:Y:723:DA:H2''	2:Y:724:DT:C5'	2.21	0.71
1:X:612:DC:OP1	5:X:1042:HOH:O	2.08	0.71
3:A:76:LEU:HD22	3:A:78:THR:HG22	1.73	0.71
3:B:201:PRO:HG3	5:B:1115:HOH:O	1.91	0.70
3:A:196:SER:O	5:A:1204:HOH:O	2.08	0.70
3:B:73:THR:CG2	3:B:85:VAL:HG22	2.20	0.70
3:B:174:ASP:CG	3:B:175:LEU:N	2.49	0.70
3:B:156:ARG:HH21	3:B:156:ARG:CG	1.98	0.70
3:A:49:VAL:HG12	3:A:50:GLN:O	1.91	0.69
3:A:76:LEU:CD2	3:A:78:THR:HG22	2.23	0.69
3:B:179:VAL:HA	3:B:183:LEU:HD23	1.75	0.69
2:Y:706:DG:H4'	3:B:28:LYS:HE3	1.74	0.68
3:B:179:VAL:HG23	3:B:207:GLN:HG2	1.74	0.68
3:B:156:ARG:HG2	3:B:156:ARG:NH2	2.08	0.68
1:X:612:DC:N4	2:Y:715:DG:O6	2.19	0.67
3:A:170:ASP:CA	3:A:173:GLN:HE22	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:179:VAL:CG2	3:B:207:GLN:HG2	2.25	0.66
3:B:175:LEU:O	3:B:179:VAL:HG12	1.96	0.66
3:A:188:GLN:NE2	5:A:1128:HOH:O	2.29	0.65
2:Y:723:DA:C2'	2:Y:724:DT:H5''	2.26	0.65
3:B:156:ARG:CG	3:B:156:ARG:NH2	2.54	0.63
3:B:20:LEU:HD11	3:B:114:ARG:HA	1.80	0.62
3:B:76:LEU:HB3	3:B:79:SER:OG	2.00	0.61
3:B:192:GLN:HE21	3:B:195:GLN:NE2	1.99	0.61
3:A:129:ASN:ND2	3:A:132:SER:H	2.00	0.60
3:B:127:ILE:HG22	3:B:133:LEU:HD13	1.83	0.60
3:A:12:LEU:HD22	3:A:13:PRO:HD2	1.83	0.60
3:B:98:VAL:HG13	3:B:123:LEU:CD1	2.32	0.59
3:B:204:GLU:HA	3:B:207:GLN:HB2	1.84	0.59
1:X:612:DC:N3	2:Y:715:DG:N1	2.42	0.59
3:A:179:VAL:HG13	3:A:207:GLN:HG2	1.86	0.58
2:Y:709:DA:H1'	2:Y:710:DC:H5''	1.85	0.57
1:X:621:DC:H2''	1:X:622:DG:C8	2.39	0.57
3:A:170:ASP:HB3	3:A:173:GLN:CD	2.29	0.57
3:B:6:LEU:HD13	3:B:10:GLU:HG2	1.86	0.56
3:B:105:LEU:HD13	3:B:125:LEU:HD13	1.86	0.56
3:B:95:VAL:O	3:B:98:VAL:HG22	2.05	0.56
3:A:143:GLN:NE2	3:A:144:TYR:CZ	2.73	0.56
3:A:166:LEU:HD22	5:A:1091:HOH:O	2.05	0.56
1:X:616:DG:O6	3:B:116:LYS:CE	2.54	0.55
3:A:170:ASP:O	3:A:173:GLN:CD	2.49	0.55
1:X:602:DG:H2''	1:X:603:DA:H8	1.70	0.55
1:X:614:DA:C8	1:X:614:DA:H5''	2.41	0.55
2:Y:703:DT:H5''	3:B:173:GLN:HE22	1.72	0.55
1:X:602:DG:H4'	1:X:602:DG:OP1	2.07	0.55
3:A:94:HIS:HD2	3:A:96:ASN:N	1.95	0.54
3:B:188:GLN:HG3	5:B:1158:HOH:O	2.07	0.54
3:B:95:VAL:CG2	3:B:121:ALA:HB1	2.37	0.54
5:A:1166:HOH:O	3:B:49:VAL:HG21	2.08	0.54
2:Y:712:DT:H4'	3:B:192:GLN:HG2	1.89	0.54
2:Y:723:DA:H1'	2:Y:724:DT:H5''	1.89	0.53
3:A:90:ASN:ND2	5:A:1032:HOH:O	2.41	0.53
3:A:28:LYS:O	3:A:31:LYS:HE2	2.09	0.53
3:A:161:LYS:O	3:A:165:GLU:HG3	2.09	0.53
3:B:59:LEU:HD13	3:B:103:LEU:HD13	1.91	0.53
3:A:170:ASP:CB	3:A:173:GLN:NE2	2.71	0.52
2:Y:705:DC:H2''	2:Y:706:DG:O5'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:625:DG:H2''	1:X:626:DC:C5	2.44	0.52
3:A:18:GLU:HG3	5:A:1181:HOH:O	2.09	0.52
2:Y:711:DC:H3'	5:Y:1074:HOH:O	2.10	0.51
3:A:163:LEU:HD22	3:A:185:ILE:HG21	1.92	0.51
3:A:75:LYS:CE	5:A:1136:HOH:O	2.58	0.51
3:B:116:LYS:HG3	5:B:1225:HOH:O	2.11	0.51
3:A:170:ASP:HB3	3:A:173:GLN:HE22	1.72	0.51
2:Y:709:DA:H2''	2:Y:710:DC:H5'	1.92	0.51
3:A:170:ASP:CB	3:A:173:GLN:HE22	2.24	0.50
3:B:81:PHE:CE2	3:B:175:LEU:HD23	2.46	0.50
3:B:172:HIS:CD2	3:B:172:HIS:H	2.27	0.50
3:B:105:LEU:HD13	3:B:125:LEU:CD1	2.41	0.50
3:A:163:LEU:HD21	3:A:185:ILE:HG22	1.94	0.50
1:X:619:DA:C2	2:Y:709:DA:C2	2.99	0.50
3:A:57:LEU:HD13	3:A:144:TYR:HD2	1.75	0.50
2:Y:703:DT:OP1	3:B:80:LYS:HB2	2.12	0.49
2:Y:720:DG:N7	3:A:74:LYS:NZ	2.56	0.49
3:B:156:ARG:NH2	5:B:1135:HOH:O	2.43	0.49
3:A:71:ILE:CD1	3:A:189:MET:SD	3.00	0.49
3:B:62:PHE:HZ	3:B:93:ARG:HD3	1.78	0.49
3:B:95:VAL:HG23	3:B:121:ALA:HB1	1.95	0.49
1:X:618:DT:H4'	3:B:195:GLN:HE22	1.78	0.49
3:B:202:ASN:ND2	3:B:205:ALA:H	2.10	0.48
3:B:171:ALA:HB1	3:B:177:GLN:HB3	1.96	0.48
3:A:23:ILE:HD12	3:A:43:LEU:HD22	1.96	0.47
3:A:108:PHE:O	3:A:136:LYS:HE3	2.14	0.47
3:B:14:GLN:HA	3:B:17:LEU:HD12	1.96	0.47
3:A:127:ILE:CG2	3:A:133:LEU:HD13	2.42	0.47
3:A:106:GLU:OE1	3:A:109:LYS:NZ	2.47	0.47
3:B:122:THR:CG2	5:B:1010:HOH:O	2.63	0.47
3:A:75:LYS:HE2	5:A:1136:HOH:O	2.13	0.47
3:A:93:ARG:NH2	5:A:1051:HOH:O	2.22	0.47
3:A:146:VAL:HG13	3:A:154:VAL:HG22	1.96	0.47
2:Y:718:DC:C2'	2:Y:719:DC:H5'	2.45	0.46
3:A:77:ALA:HA	5:A:1066:HOH:O	2.14	0.46
3:B:167:PHE:HD1	3:B:172:HIS:CD2	2.33	0.46
2:Y:703:DT:OP1	3:B:173:GLN:OE1	2.34	0.46
3:A:28:LYS:NZ	5:A:1106:HOH:O	2.49	0.46
3:A:47:ASP:O	3:A:49:VAL:HG23	2.16	0.46
3:B:209:PHE:C	3:B:211:ARG:H	2.24	0.46
3:B:166:LEU:HD23	3:B:171:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:614:DA:H2'	1:X:614:DA:H5'	1.42	0.45
2:Y:704:DT:H3'	5:Y:1151:HOH:O	2.14	0.45
1:X:601:DC:C2'	1:X:602:DG:O5'	2.61	0.45
3:A:23:ILE:HG12	3:A:39:ASP:HB3	1.99	0.45
3:A:180:ASN:O	3:A:184:PRO:HG2	2.17	0.45
3:B:174:ASP:OD1	3:B:174:ASP:C	2.60	0.45
3:B:83:LEU:C	3:B:83:LEU:HD12	2.42	0.45
3:B:188:GLN:HG3	3:B:188:GLN:O	2.16	0.45
3:B:188:GLN:CG	5:B:1158:HOH:O	2.65	0.45
3:B:7:LYS:O	3:B:10:GLU:HB3	2.17	0.44
2:Y:723:DA:H2''	2:Y:724:DT:H5'	1.98	0.44
1:X:617:DG:H1'	1:X:618:DT:H5''	1.99	0.44
2:Y:723:DA:C1'	2:Y:724:DT:H5''	2.47	0.44
2:Y:706:DG:H5''	3:B:28:LYS:HG3	1.99	0.44
3:B:57:LEU:HD13	3:B:144:TYR:HD2	1.82	0.44
2:Y:721:DT:H2'	2:Y:722:DT:C6	2.53	0.44
3:B:155:LYS:HE3	3:B:188:GLN:OE1	2.18	0.43
5:Y:1187:HOH:O	3:A:153:LYS:HE3	2.17	0.43
3:A:90:ASN:C	3:A:90:ASN:HD22	2.26	0.43
3:B:6:LEU:CD1	3:B:10:GLU:O	2.66	0.43
3:B:153:LYS:HG2	5:B:1127:HOH:O	2.18	0.43
3:A:197:ASN:HD22	3:A:197:ASN:H	1.66	0.43
1:X:616:DG:O6	3:B:116:LYS:HE3	2.18	0.43
3:B:22:LYS:CD	5:B:1213:HOH:O	2.23	0.43
3:B:90:ASN:HA	3:B:125:LEU:O	2.17	0.43
3:A:61:GLY:HA3	3:B:58:PHE:O	2.19	0.42
3:A:177:GLN:HE21	3:A:181:LYS:HD2	1.84	0.42
3:B:122:THR:HG22	5:B:1010:HOH:O	2.18	0.42
3:B:198:GLU:O	3:B:199:GLY:C	2.62	0.42
3:B:179:VAL:HG22	3:B:207:GLN:HG2	1.99	0.41
1:X:608:DG:H2''	1:X:609:DG:O5'	2.20	0.41
3:A:171:ALA:HB1	3:A:177:GLN:HB3	2.03	0.41
3:A:146:VAL:O	3:A:146:VAL:CG1	2.66	0.41
1:X:611:DC:H5'	3:A:197:ASN:HB3	2.02	0.41
3:B:82:GLY:HA3	3:B:209:PHE:HE2	1.86	0.41
2:Y:720:DG:H2''	2:Y:721:DT:O5'	2.21	0.41
3:B:73:THR:HG23	3:B:186:TRP:CD1	2.56	0.41
3:B:145:VAL:HG12	3:B:149:SER:HB2	2.03	0.41
3:B:209:PHE:C	3:B:211:ARG:N	2.79	0.40
2:Y:716:DG:O6	3:A:116:LYS:CE	2.69	0.40
3:A:168:ASN:HD22	3:A:168:ASN:HA	1.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:143:GLN:HE21	3:A:143:GLN:C	2.29	0.40

All (1) 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)
2:Y:701:DG:O5'	5:Y:1234:HOH:O[2_674]	1.80	0.40

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	205/207 (99%)	198 (97%)	7 (3%)	0	100	100
3	B	205/207 (99%)	185 (90%)	16 (8%)	4 (2%)	6	4
All	All	410/414 (99%)	383 (93%)	23 (6%)	4 (1%)	12	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	204	GLU
3	B	203	LEU
3	B	96	ASN
3	B	184	PRO

5.3.2 Protein sidechains [i](#)

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	185/185 (100%)	150 (81%)	35 (19%)	1	1
3	B	185/185 (100%)	155 (84%)	30 (16%)	2	2
All	All	370/370 (100%)	305 (82%)	65 (18%)	2	1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	12	LEU
3	A	14	GLN
3	A	15	ASP
3	A	18	GLU
3	A	48	GLU
3	A	50	GLN
3	A	54	GLU
3	A	56	LYS
3	A	57	LEU
3	A	70	ASN
3	A	75	LYS
3	A	78	THR
3	A	83	LEU
3	A	90	ASN
3	A	91	VAL
3	A	101	LEU
3	A	103	LEU
3	A	107	VAL
3	A	122	THR
3	A	123	LEU
3	A	125	LEU
3	A	133	LEU
3	A	139	PRO
3	A	143	GLN
3	A	151	PRO
3	A	153	LYS
3	A	163	LEU
3	A	164	LEU
3	A	166	LEU
3	A	173	GLN
3	A	175	LEU
3	A	181	LYS
3	A	183	LEU
3	A	191	LYS

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Mol	Chain	Res	Type
3	A	197	ASN
3	B	14	GLN
3	B	20	LEU
3	B	23	ILE
3	B	27	VAL
3	B	31	LYS
3	B	45	GLN
3	B	54	GLU
3	B	57	LEU
3	B	70	ASN
3	B	90	ASN
3	B	95	VAL
3	B	98	VAL
3	B	101	LEU
3	B	103	LEU
3	B	105	LEU
3	B	106	GLU
3	B	122	THR
3	B	124	VAL
3	B	133	LEU
3	B	146	VAL
3	B	156	ARG
3	B	164	LEU
3	B	166	LEU
3	B	173	GLN
3	B	174	ASP
3	B	175	LEU
3	B	183	LEU
3	B	192	GLN
3	B	196	SER
3	B	197	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	50	GLN
3	A	70	ASN
3	A	90	ASN
3	A	94	HIS
3	A	129	ASN
3	A	159	ASN
3	A	168	ASN

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Mol	Chain	Res	Type
3	A	173	GLN
3	A	177	GLN
3	A	192	GLN
3	A	193	GLN
3	A	195	GLN
3	A	197	ASN
3	B	70	ASN
3	B	90	ASN
3	B	159	ASN
3	B	168	ASN
3	B	172	HIS
3	B	173	GLN
3	B	180	ASN
3	B	188	GLN
3	B	195	GLN
3	B	197	ASN
3	B	202	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	X	26/26 (100%)	-0.05	0 100 100	38, 48, 71, 86	0
2	Y	26/26 (100%)	-0.12	0 100 100	28, 49, 61, 62	0
3	A	207/207 (100%)	-0.30	2 (0%) 79 77	21, 34, 53, 62	0
3	B	207/207 (100%)	0.09	1 (0%) 87 85	20, 44, 72, 77	0
All	All	466/466 (100%)	-0.10	3 (0%) 85 83	20, 40, 66, 86	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	206	ALA	2.9
3	A	173	GLN	2.4
3	A	49	VAL	2.2

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($\text{\AA}^2$)	Q<0.9
4	CA	B	803	1/1	0.96	0.06	51,51,51,51	0
4	CA	X	802	1/1	0.97	0.04	36,36,36,36	0
4	CA	A	801	1/1	0.98	0.02	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.