Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2016 – 02:22 PM EDT

PDB ID	:	5A0M
Title	:	THE CRYSTAL STRUCTURE OF I-SCEI IN COMPLEX WITH ITS TARGET DNA IN THE PRESENCE OF MN
Authors	:	Prieto, J.; Redondo, P.; Merino, N.; Villate, M.; Blanco, F.J.; Molina, R.
Deposited on	:	2015-04-21
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

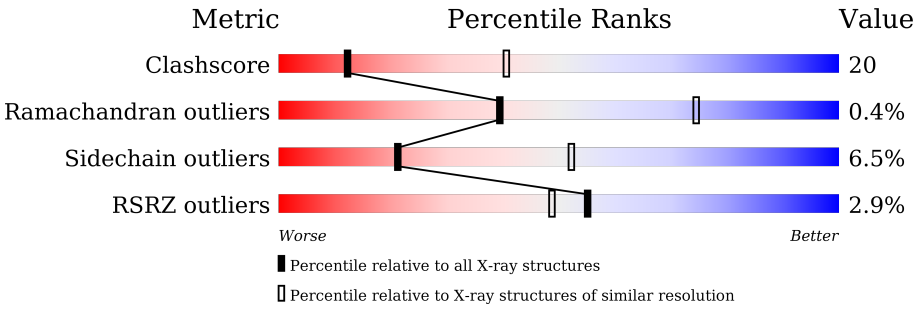
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	235	6% 60% 31% 5%
2	B	235	% 61% 32%
3	C	14	29% 64% 7%
3	E	14	7% 86% 14%
4	D	16	6% 75% 13% 6%
4	H	16	19% 63% 13% 6%
5	I	9	67% 33%

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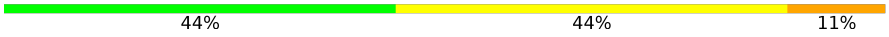
Mol	Chain	Length	Quality of chain
5	L	9	
6	J	11	
6	K	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MN	B	1529	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5761 atoms, of which 13 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called INTRON-ENCODED ENDONUCLEASE I-SCEI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1862	1213	308	330	11			

- Molecule 2 is a protein called INTRON-ENCODED ENDONUCLEASE I-SCEI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1874	1220	309	334	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	P	0	0	0
			268	128	55	73	12			
3	E	14	Total	C	N	O	P	0	0	0
			287	137	58	79	13			

- Molecule 4 is a DNA chain called 5'-D(*GP*GP*TP*AP*TP*TP*AP*CP*CP*CP*TP*GP*TP*TP *AP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	P	0	0	0
			304	147	48	94	15			
4	H	15	Total	C	N	O	P	0	0	0
			301	147	48	92	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	9	Total	C	N	O	P	0	0	0
			182	86	31	56	9			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	L	9	Total C H N O P 194 86 12 31 56 9	0	0	0

- Molecule 6 is a DNA chain called 5'-D(*CP*AP*GP*GP*GP*TP*AP*AP*TP*AP*CP)-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	J	11	Total C N O P 229 108 45 65 11	0	0	0
6	K	11	Total C H N O P 230 108 1 45 65 11	0	0	0

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total Mn 1 1	0	0
7	B	3	Total Mn 3 3	0	0
7	A	3	Total Mn 3 3	0	0
7	D	1	Total Mn 1 1	0	0

- Molecule 8 is water.

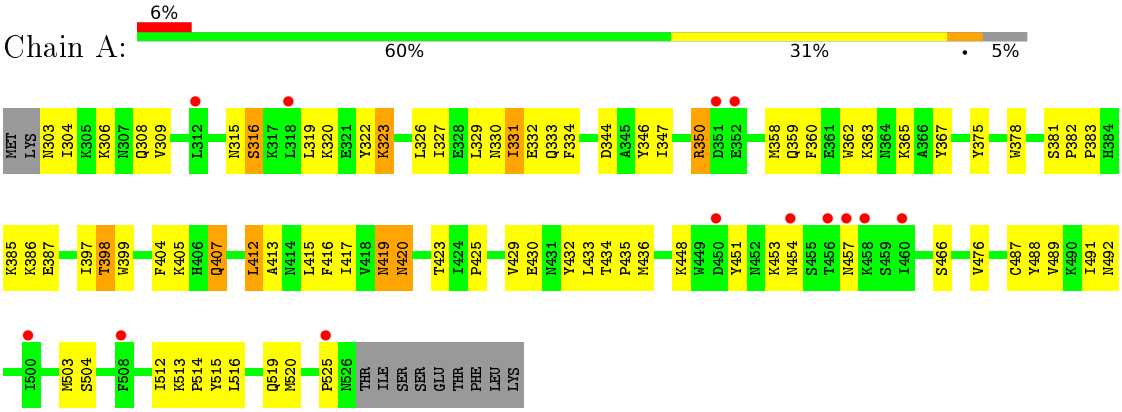
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	8	Total O 8 8	0	0
8	B	5	Total O 5 5	0	0
8	C	1	Total O 1 1	0	0
8	D	2	Total O 2 2	0	0
8	E	2	Total O 2 2	0	0
8	H	1	Total O 1 1	0	0
8	I	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

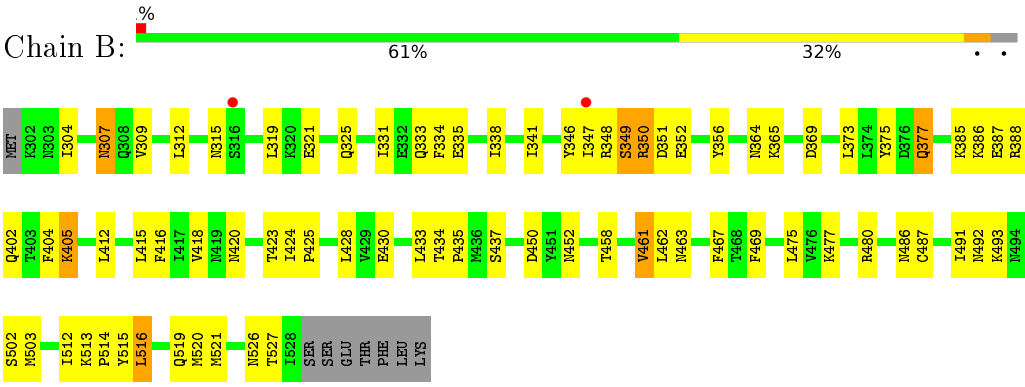
- Molecule 1: INTRON-ENCODED ENDONUCLEASE I-SCEI

Chain A:



- Molecule 2: INTRON-ENCODED ENDONUCLEASE I-SCEI

Chain B:

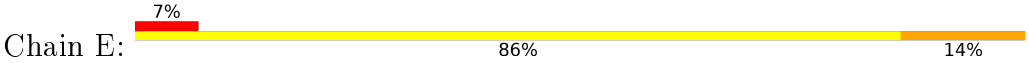


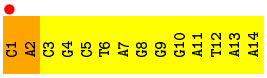
- Molecule 3: 5'-D(*CP*AP*CP*GP*CP*TP*AP*GP*GP*GP*AP*TP*AP*AP)-3'

Chain C:

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

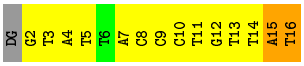
Chain E:





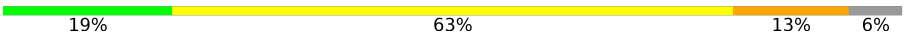
• Molecule 4: 5'-D(*GP*GP*TP*AP*TP*TP*AP*CP*CP*CP*TP*GP*TP*TP *AP*TP)-3'

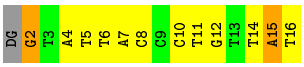
Chain D:



• Molecule 4: 5'-D(*GP*GP*TP*AP*TP*TP*AP*CP*CP*CP*TP*GP*TP*TP *AP*TP)-3'

Chain H:



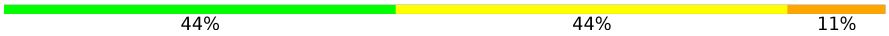


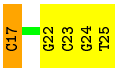
• Molecule 5: 5'-D(*CP*CP*CP*TP*AP*GP*CP*GP*TP)-3'

Chain I:

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

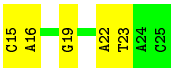
Chain L:





• Molecule 6: 5'-D(*CP*AP*GP*GP*GP*TP*AP*AP*TP*AP*CP)-3'

Chain J:



• Molecule 6: 5'-D(*CP*AP*GP*GP*GP*TP*AP*AP*TP*AP*CP)-3'

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.11Å 80.56Å 130.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.90 – 2.90 42.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.90-2.90) 100.0 (42.90-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.186 , 0.249 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.954	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.057 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5761	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.47	0/1909	0.57	0/2580
2	B	0.50	0/1921	0.60	0/2599
3	C	1.14	1/302 (0.3%)	1.05	0/465
3	E	1.91	10/323 (3.1%)	1.57	5/497 (1.0%)
4	D	0.99	0/338	1.29	3/519 (0.6%)
4	H	1.27	3/335 (0.9%)	1.37	2/515 (0.4%)
5	I	1.35	1/202 (0.5%)	1.21	0/307
5	L	1.10	1/202 (0.5%)	1.10	0/307
6	J	1.21	1/257 (0.4%)	1.07	0/393
6	K	1.18	1/257 (0.4%)	0.99	1/393 (0.3%)
All	All	0.88	18/6046 (0.3%)	0.90	11/8575 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	17	DC	OP3-P	-11.43	1.47	1.61
3	E	2	DA	P-O5'	10.86	1.70	1.59
6	K	15	DC	OP3-P	-10.68	1.48	1.61
6	J	15	DC	OP3-P	-10.63	1.48	1.61
3	E	1	DC	C2-O2	10.31	1.33	1.24
5	L	17	DC	OP3-P	-9.15	1.50	1.61
3	E	2	DA	N9-C4	8.53	1.43	1.37
3	E	2	DA	P-OP1	7.47	1.61	1.49
3	E	2	DA	C2'-C1'	7.21	1.59	1.52
4	H	15	DA	C3'-O3'	-6.78	1.35	1.44
4	H	2	DG	C8-N7	6.66	1.34	1.30
3	E	1	DC	C4'-O4'	6.36	1.51	1.45
3	E	2	DA	P-OP2	6.14	1.59	1.49
4	H	2	DG	N9-C8	-5.82	1.33	1.37
3	E	1	DC	N1-C6	-5.52	1.33	1.37
3	C	12	DT	C3'-O3'	-5.51	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	DC	N3-C4	5.39	1.37	1.33
3	E	2	DA	C8-N7	5.29	1.35	1.31

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	DA	O5'-P-OP1	-18.32	88.72	110.70
3	E	1	DC	O4'-C1'-N1	10.37	115.26	108.00
4	D	16	DT	O4'-C4'-C3'	-9.06	100.57	106.00
3	E	2	DA	OP1-P-OP2	8.49	132.33	119.60
3	E	2	DA	O4'-C1'-N9	6.61	112.63	108.00
4	H	15	DA	O4'-C4'-C3'	-6.49	101.91	104.50
4	H	15	DA	C3'-C2'-C1'	-6.09	95.19	102.50
4	D	15	DA	OP1-P-O3'	5.92	118.21	105.20
4	D	15	DA	O4'-C1'-N9	-5.59	104.09	108.00
6	K	20	DT	N3-C4-O4	5.41	123.14	119.90
3	E	2	DA	O4'-C4'-C3'	-5.05	102.48	104.50

There are no chirality outliers.

There are no planarity outliers.

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	A	1862	0	1876	60	0
2	B	1874	0	1877	73	0
3	C	268	0	147	9	0
3	E	287	0	158	22	1
4	D	304	0	173	24	0
4	H	301	0	174	19	1
5	I	182	0	102	1	0
5	L	182	12	102	12	0
6	J	229	0	124	3	0
6	K	229	1	124	11	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
7	H	1	0	0	0	0
8	A	8	0	0	2	0
8	B	5	0	0	0	0
8	C	1	0	0	0	0
8	D	2	0	0	0	0
8	E	2	0	0	0	0
8	H	1	0	0	0	0
8	I	3	0	0	0	0
All	All	5748	13	4857	201	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 20.

All (201) 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:E:2:DA:H8	3:E:2:DA:H5"	1.11	1.13
3:E:2:DA:C8	3:E:2:DA:H5"	1.85	1.11
3:C:5:DC:H2"	3:C:6:DT:H5"	1.37	1.03
5:L:23:DC:H2"	5:L:24:DG:H5'	1.41	0.98
2:B:480:ARG:NH1	2:B:487:CYS:O	2.00	0.94
4:H:5:DT:H2"	4:H:6:DT:H5'	1.49	0.93
4:D:15:DA:H1'	4:D:16:DT:H5"	1.51	0.91
6:K:20:DT:H2"	6:K:21:DA:C8	2.09	0.88
2:B:402:GLN:HE22	4:H:8:DC:H2'	1.36	0.87
4:D:4:DA:H2"	4:D:5:DT:H5'	1.57	0.84
2:B:461:VAL:HG11	2:B:497:ILE:HD12	1.58	0.83
3:E:2:DA:OP2	3:E:2:DA:H4'	1.79	0.83
3:C:10:DG:H1	5:L:17:DC:H5	1.29	0.80
6:K:20:DT:H2"	6:K:21:DA:N7	1.97	0.79
4:H:10:DC:H2"	4:H:11:DT:H5'	1.65	0.78
2:B:512:ILE:HG13	2:B:516:LEU:HD12	1.66	0.77
3:E:2:DA:H8	3:E:2:DA:C5'	1.95	0.76
2:B:433:LEU:HD12	2:B:437:SER:CB	2.16	0.76
4:D:3:DT:H2"	4:D:4:DA:H5'	1.66	0.76
2:B:402:GLN:NE2	4:H:8:DC:H2'	2.00	0.75
2:B:365:LYS:HE3	2:B:369:ASP:OD2	1.89	0.73
2:B:433:LEU:HD12	2:B:437:SER:HB3	1.74	0.70
1:A:362:TRP:O	1:A:398:THR:HG22	1.91	0.69
4:D:10:DC:H2'	4:D:11:DT:C6	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:DC:C2'	3:C:6:DT:H5"	2.18	0.68
1:A:419:ASN:N	1:A:419:ASN:OD1	2.16	0.68
3:E:2:DA:C8	3:E:2:DA:C5'	2.71	0.68
1:A:316:SER:O	1:A:320:LYS:HG3	1.95	0.66
2:B:462:LEU:HB2	2:B:498:ILE:HB	1.78	0.66
1:A:344:ASP:O	8:A:2004:HOH:O	2.13	0.66
2:B:309:VAL:HA	2:B:312:LEU:HD12	1.77	0.66
2:B:424:ILE:HD11	2:B:467:PHE:CE2	2.31	0.66
2:B:513:LYS:HB3	2:B:514:PRO:HD3	1.78	0.65
1:A:407:GLN:HG2	1:A:407:GLN:O	1.96	0.65
1:A:346:TYR:CZ	6:K:16:DA:H2'	2.31	0.65
4:D:9:DC:H2'	4:D:10:DC:C6	2.31	0.65
2:B:388:ARG:NH2	4:H:12:DG:N7	2.42	0.65
1:A:519:GLN:OE1	1:A:519:GLN:N	2.29	0.64
3:E:3:DC:H1'	3:E:4:DG:C8	2.32	0.64
4:H:10:DC:H2'	4:H:11:DT:C6	2.31	0.64
2:B:493:LYS:HG3	4:H:16:DT:C7	2.27	0.63
1:A:386:LYS:NZ	4:D:11:DT:H71	2.13	0.63
3:E:6:DT:H2'	3:E:7:DA:C8	2.35	0.62
2:B:493:LYS:NZ	3:E:10:DG:O6	2.33	0.61
2:B:364:ASN:HD22	2:B:520:MET:HE3	1.65	0.61
1:A:457:ASN:ND2	8:A:2007:HOH:O	2.32	0.61
4:D:16:DT:H6	4:D:16:DT:H5'	1.65	0.61
4:D:4:DA:H2"	4:D:5:DT:C5'	2.29	0.61
3:E:4:DG:H2"	3:E:5:DC:H5'	1.82	0.61
1:A:334:PHE:CE1	1:A:412:LEU:HD13	2.36	0.60
4:D:2:DG:H2'	4:D:3:DT:C6	2.37	0.60
2:B:461:VAL:CG1	2:B:497:ILE:HD12	2.28	0.60
4:D:16:DT:C6	4:D:16:DT:H5'	2.36	0.60
3:C:7:DA:H4'	3:C:8:DG:OP1	2.02	0.59
2:B:364:ASN:HD22	2:B:520:MET:CE	2.14	0.59
1:A:436:MET:HG3	1:A:515:TYR:CD2	2.37	0.59
2:B:346:TYR:CZ	6:J:16:DA:H2'	2.37	0.59
2:B:404:PHE:HB3	4:H:7:DA:H5"	1.84	0.59
3:E:10:DG:H2"	3:E:11:DA:C8	2.37	0.59
1:A:429:VAL:HG22	1:A:433:LEU:HD22	1.85	0.59
1:A:419:ASN:O	1:A:420:ASN:HB2	2.04	0.58
1:A:448:LYS:HB2	1:A:451:TYR:CZ	2.39	0.58
4:D:4:DA:H1'	4:D:5:DT:H5"	1.84	0.58
1:A:367:TYR:HB2	1:A:520:MET:HE1	1.86	0.58
4:D:14:DT:H2"	4:D:15:DA:N7	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:THR:OG1	2:B:502:SER:HB2	2.03	0.58
2:B:433:LEU:HD12	2:B:437:SER:HB2	1.86	0.58
6:K:19:DG:H2'	6:K:20:DT:H72	1.85	0.58
1:A:363:LYS:NZ	3:C:13:DA:OP2	2.37	0.57
2:B:493:LYS:HG3	4:H:16:DT:H72	1.86	0.57
5:L:24:DG:H2"	5:L:25:DT:H72	1.86	0.56
3:E:8:DG:H2"	3:E:9:DG:H5'	1.86	0.56
1:A:303:ASN:OD1	1:A:304:ILE:N	2.39	0.56
6:K:19:DG:H2"	6:K:20:DT:C6	2.41	0.55
5:L:22:DG:H2"	5:L:23:DC:C6	2.41	0.55
2:B:347:ILE:O	2:B:347:ILE:HG23	2.07	0.55
4:D:3:DT:C2'	4:D:4:DA:H5'	2.35	0.55
1:A:404:PHE:HB3	4:D:7:DA:H5"	1.90	0.54
1:A:416:PHE:O	1:A:423:THR:HB	2.07	0.54
1:A:430:GLU:OE1	1:A:430:GLU:N	2.38	0.54
2:B:377:GLN:NE2	2:B:377:GLN:H	2.06	0.54
2:B:424:ILE:HG21	2:B:475:LEU:HD21	1.90	0.53
1:A:385:LYS:HE2	1:A:397:ILE:HG23	1.90	0.53
2:B:493:LYS:NZ	3:E:10:DG:N7	2.46	0.53
4:D:9:DC:H2'	4:D:10:DC:H6	1.72	0.53
2:B:346:TYR:CZ	2:B:348:ARG:HB3	2.44	0.53
3:E:11:DA:N6	4:H:15:DA:N6	2.56	0.53
1:A:513:LYS:N	1:A:514:PRO:CD	2.72	0.53
2:B:492:ASN:OD1	2:B:493:LYS:HG2	2.08	0.53
2:B:309:VAL:HB	2:B:319:LEU:HD13	1.92	0.52
2:B:331:ILE:O	2:B:335:GLU:HG3	2.10	0.52
2:B:425:PRO:HD2	2:B:428:LEU:HB2	1.91	0.52
2:B:493:LYS:HG3	4:H:16:DT:H73	1.92	0.52
6:K:17:DG:H2"	6:K:18:DG:O5'	2.10	0.52
1:A:385:LYS:NZ	1:A:387:GLU:OE2	2.29	0.51
3:C:2:DA:H61	5:L:25:DT:H3	1.58	0.51
3:C:10:DG:N1	5:L:17:DC:H5	2.05	0.51
1:A:405:LYS:HG2	4:D:7:DA:OP2	2.11	0.51
2:B:477:LYS:O	2:B:477:LYS:HG2	2.11	0.51
4:D:10:DC:H2"	4:D:11:DT:O4'	2.11	0.51
2:B:396:VAL:HG22	3:E:12:DT:H5"	1.93	0.51
1:A:347:ILE:HG23	1:A:347:ILE:O	2.10	0.51
2:B:396:VAL:CG2	3:E:12:DT:H5"	2.41	0.51
1:A:365:LYS:HG3	1:A:399:TRP:CE2	2.46	0.51
2:B:333:GLN:HE21	2:B:375:TYR:HA	1.76	0.50
5:L:24:DG:C2'	5:L:25:DT:H72	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:VAL:HG21	1:A:489:VAL:HG23	1.94	0.50
3:E:4:DG:C2'	3:E:5:DC:H5'	2.41	0.50
2:B:349:SER:HB3	2:B:356:TYR:CE2	2.46	0.50
1:A:319:LEU:O	1:A:322:TYR:HB3	2.11	0.50
2:B:416:PHE:O	2:B:423:THR:HB	2.12	0.50
2:B:519:GLN:OE1	2:B:519:GLN:N	2.39	0.50
2:B:430:GLU:N	2:B:430:GLU:OE1	2.43	0.49
1:A:512:ILE:O	1:A:516:LEU:HD13	2.12	0.49
5:L:25:DT:H6	5:L:25:DT:C5'	2.26	0.49
3:E:11:DA:C6	4:H:15:DA:N6	2.81	0.49
4:H:5:DT:C2'	4:H:6:DT:H5'	2.34	0.48
4:D:12:DG:H2"	4:D:13:DT:O5'	2.13	0.48
2:B:434:THR:HB	2:B:435:PRO:CD	2.44	0.48
3:C:5:DC:H2"	3:C:6:DT:C5'	2.27	0.47
2:B:304:ILE:N	2:B:325:GLN:OE1	2.47	0.47
3:E:8:DG:H2"	3:E:9:DG:C5'	2.43	0.47
3:E:6:DT:C2'	3:E:7:DA:C8	2.97	0.47
1:A:432:TYR:O	1:A:434:THR:HG23	2.14	0.47
1:A:514:PRO:HB2	1:A:515:TYR:CD1	2.50	0.47
2:B:513:LYS:N	2:B:514:PRO:HD2	2.29	0.47
1:A:346:TYR:CE2	6:K:16:DA:H2'	2.50	0.47
1:A:365:LYS:HG3	1:A:399:TRP:CZ2	2.49	0.47
2:B:415:LEU:O	2:B:425:PRO:HG3	2.14	0.47
4:H:14:DT:H2"	4:H:15:DA:C5	2.50	0.47
2:B:334:PHE:CE1	2:B:412:LEU:HD23	2.51	0.46
2:B:338:ILE:HG12	2:B:338:ILE:H	1.59	0.46
4:H:14:DT:H2"	4:H:15:DA:N7	2.31	0.46
2:B:304:ILE:HD13	2:B:321:GLU:HB3	1.97	0.46
2:B:526:ASN:O	2:B:527:THR:CG2	2.64	0.46
2:B:350:ARG:NH2	6:J:19:DG:O6	2.49	0.46
2:B:385:LYS:HE2	2:B:387:GLU:OE2	2.16	0.46
2:B:433:LEU:CD1	2:B:437:SER:CB	2.91	0.46
3:C:8:DG:H2"	3:C:9:DG:OP2	2.16	0.46
1:A:350:ARG:NH2	6:K:19:DG:O6	2.46	0.46
6:J:22:DA:H2"	6:J:23:DT:O5'	2.15	0.45
1:A:365:LYS:CG	1:A:399:TRP:CE2	2.99	0.45
5:L:17:DC:OP2	5:L:17:DC:H4'	2.16	0.45
5:L:24:DG:H2"	5:L:25:DT:C7	2.46	0.45
1:A:315:ASN:O	1:A:320:LYS:HD2	2.16	0.45
1:A:329:LEU:HD23	1:A:378:TRP:CZ2	2.52	0.45
2:B:315:ASN:ND2	4:H:4:DA:H2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:LEU:CD1	2:B:437:SER:HB2	2.46	0.44
1:A:323:LYS:NZ	4:D:7:DA:OP1	2.49	0.44
1:A:346:TYR:HE2	6:K:17:DG:N7	2.15	0.44
2:B:405:LYS:HD3	4:H:7:DA:OP2	2.17	0.44
2:B:341:ILE:HG21	2:B:416:PHE:CD2	2.53	0.44
1:A:491:ILE:HG22	1:A:492:ASN:N	2.31	0.44
1:A:367:TYR:HB2	1:A:520:MET:CE	2.48	0.44
1:A:347:ILE:HD11	1:A:413:ALA:HB2	2.00	0.44
2:B:418:VAL:O	2:B:418:VAL:HG23	2.18	0.43
2:B:424:ILE:HD11	2:B:467:PHE:CZ	2.54	0.43
1:A:381:SER:OG	4:D:8:DC:OP1	2.31	0.43
1:A:453:LYS:O	1:A:454:ASN:HB2	2.18	0.43
2:B:433:LEU:CD1	2:B:437:SER:HB3	2.47	0.43
1:A:320:LYS:HA	1:A:323:LYS:HG3	1.99	0.43
2:B:424:ILE:HA	2:B:425:PRO:HD3	1.91	0.43
5:I:23:DC:H2"	5:I:24:DG:C8	2.53	0.43
1:A:417:ILE:N	1:A:417:ILE:HD13	2.34	0.43
4:D:14:DT:H2"	4:D:15:DA:C5	2.54	0.43
1:A:330:ASN:OD1	1:A:333:GLN:HG3	2.19	0.42
2:B:396:VAL:HG22	3:E:12:DT:C5'	2.49	0.42
1:A:326:LEU:HB3	1:A:378:TRP:CH2	2.54	0.42
1:A:487:CYS:O	1:A:488:TYR:HB3	2.20	0.42
1:A:306:LYS:HA	1:A:309:VAL:HG22	2.00	0.42
2:B:493:LYS:O	2:B:495:LYS:HD2	2.20	0.42
2:B:513:LYS:HB3	2:B:514:PRO:CD	2.47	0.42
5:L:25:DT:H6	5:L:25:DT:O5'	2.02	0.42
1:A:448:LYS:HB2	1:A:451:TYR:CE2	2.54	0.42
2:B:402:GLN:NE2	4:H:8:DC:H6	2.18	0.42
1:A:359:GLN:NE2	6:K:17:DG:O6	2.53	0.42
5:L:23:DC:C2'	5:L:24:DG:H5'	2.30	0.42
1:A:434:THR:HB	1:A:435:PRO:HD2	2.02	0.42
2:B:385:LYS:HE3	2:B:397:ILE:HG21	2.01	0.42
2:B:514:PRO:HB2	2:B:515:TYR:CE2	2.55	0.42
4:D:16:DT:C5'	4:D:16:DT:C6	3.02	0.42
4:D:2:DG:H2'	4:D:3:DT:C5	2.54	0.42
3:E:3:DC:H1'	3:E:4:DG:N7	2.35	0.42
4:H:10:DC:H2"	4:H:11:DT:C5'	2.42	0.41
2:B:386:LYS:HB2	2:B:398:THR:CG2	2.51	0.41
2:B:469:PHE:CE1	2:B:491:ILE:HD13	2.56	0.41
2:B:513:LYS:HD2	2:B:513:LYS:HA	1.83	0.41
1:A:385:LYS:HE2	1:A:397:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:O	1:A:425:PRO:HG3	2.20	0.41
2:B:351:ASP:O	2:B:352:GLU:HB2	2.20	0.41
2:B:364:ASN:ND2	2:B:520:MET:CE	2.82	0.41
1:A:382:PRO:HA	1:A:383:PRO:HD3	1.74	0.41
3:E:13:DA:C2	3:E:14:DA:C4	3.08	0.41
1:A:333:GLN:HB3	1:A:375:TYR:CE1	2.55	0.41
1:A:514:PRO:HB2	1:A:515:TYR:CE1	2.56	0.41
2:B:450:ASP:OD1	2:B:452:ASN:HB2	2.21	0.41
2:B:307:ASN:N	2:B:307:ASN:OD1	2.52	0.41
1:A:358:MET:HE2	1:A:360:PHE:CZ	2.57	0.40
1:A:331:ILE:HA	1:A:331:ILE:HD12	1.84	0.40
4:D:14:DT:O3'	4:D:15:DA:C8	2.74	0.40
6:K:19:DG:H2"	6:K:20:DT:H6	1.86	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)
3:E:1:DC:N4	4:H:2:DG:N7[1_545]	1.86	0.34

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	222/235 (94%)	201 (90%)	20 (9%)	1 (0%)	34 71
2	B	225/235 (96%)	211 (94%)	13 (6%)	1 (0%)	39 74
All	All	447/470 (95%)	412 (92%)	33 (7%)	2 (0%)	39 74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	463	ASN
1	A	525	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
1	A	207/218 (95%)	192 (93%)	15 (7%)	18 46
2	B	207/218 (95%)	195 (94%)	12 (6%)	25 58
All	All	414/436 (95%)	387 (94%)	27 (6%)	21 52

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	A	316	SER
1	A	323	LYS
1	A	327	ILE
1	A	331	ILE
1	A	332	GLU
1	A	350	ARG
1	A	398	THR
1	A	407	GLN
1	A	412	LEU
1	A	419	ASN
1	A	420	ASN
1	A	466	SER
1	A	503	MET
1	A	504	SER
2	B	307	ASN
2	B	349	SER
2	B	350	ARG
2	B	373	LEU
2	B	377	GLN
2	B	405	LYS
2	B	420	ASN

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Mol	Chain	Res	Type
2	B	461	VAL
2	B	486	ASN
2	B	503	MET
2	B	516	LEU
2	B	521	MET

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

Mol	Chain	Res	Type
2	B	364	ASN
2	B	377	GLN
2	B	402	GLN

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 8 ligands modelled in this entry, 8 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

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

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	224/235 (95%)	0.43	13 (5%) 26 20	52, 76, 108, 130	0
2	B	227/235 (96%)	0.07	2 (0%) 85 84	44, 64, 94, 132	0
3	C	13/14 (92%)	-0.01	0 100 100	51, 72, 95, 96	0
3	E	14/14 (100%)	-0.14	1 (7%) 19 13	41, 61, 80, 90	0
4	D	15/16 (93%)	-0.55	0 100 100	57, 63, 83, 92	0
4	H	15/16 (93%)	-0.53	0 100 100	45, 56, 72, 74	0
5	I	9/9 (100%)	-0.60	0 100 100	43, 63, 76, 82	0
5	L	9/9 (100%)	-0.30	0 100 100	58, 79, 98, 116	0
6	J	11/11 (100%)	-0.18	0 100 100	44, 62, 73, 74	0
6	K	11/11 (100%)	-0.32	0 100 100	49, 72, 80, 91	0
All	All	548/570 (96%)	0.15	16 (2%) 55 49	41, 69, 100, 132	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	THR	5.9
1	A	352	GLU	5.1
1	A	454	ASN	4.8
1	A	508	PHE	3.9
1	A	312	LEU	3.8
3	E	1	DC	3.3
1	A	450	ASP	3.2
1	A	458	LYS	2.8
1	A	460	ILE	2.8
1	A	500	ILE	2.5
1	A	351	ASP	2.5
1	A	318	LEU	2.4
1	A	525	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	457	ASN	2.2
2	B	347	ILE	2.1
2	B	316	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
7	MN	B	1529	1/1	0.98	0.20	2.25	57,57,57,57	0
7	MN	A	1527	1/1	0.97	0.19	0.86	63,63,63,63	0
7	MN	A	1528	1/1	0.95	0.20	0.66	56,56,56,56	0
7	MN	B	1531	1/1	0.97	0.20	0.34	52,52,52,52	0
7	MN	B	1530	1/1	0.97	0.18	-0.08	49,49,49,49	0
7	MN	A	1529	1/1	0.96	0.15	-0.80	56,56,56,56	0
7	MN	D	1017	1/1	0.98	0.18	-	64,64,64,64	0
7	MN	H	1017	1/1	0.97	0.24	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.