Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:59 PM GMT

PDB ID	:	1Z9C
Title	:	Crystal structure of OhrR bound to the ohrA promoter: Structure of MarR family protein with operator DNA
Authors	:	Hong, M.; Fuangthong, M.; Helmann, J.D.; Brennan, R.G.
Deposited on	:	2005-04-01
Resolution	:	2.64 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:

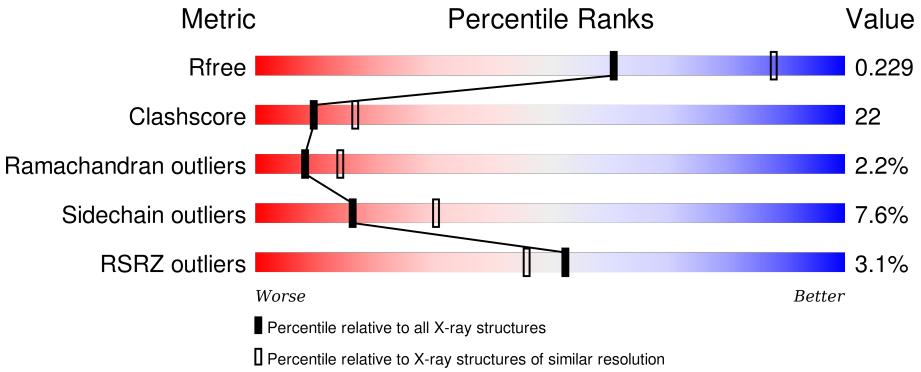
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.64 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}	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	G	29	7% 48% 52%
1	I	29	7% 41% 52%
1	K	29	7% 72% 24%
2	H	29	3% 52% 48%
2	J	29	10% 38% 55%

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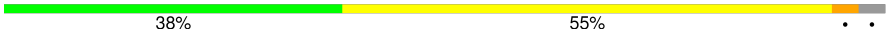
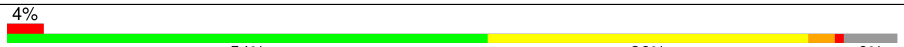
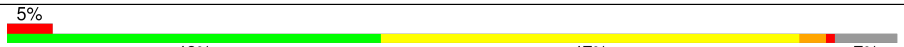
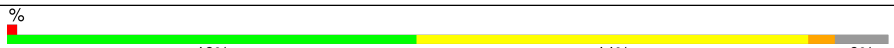
Mol	Chain	Length	Quality of chain
2	L	29	
3	A	147	
3	B	147	
3	C	147	
3	D	147	
3	E	147	
3	F	147	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	29	Total	C	N	O	P	0	0	0
			590	288	99	175	28			
1	I	28	Total	C	N	O	P	0	0	0
			570	278	97	168	27			
1	K	29	Total	C	N	O	P	0	0	0
			590	288	99	175	28			

- Molecule 2 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	29	Total	C	N	O	P	0	0	0
			592	288	105	171	28			
2	J	28	Total	C	N	O	P	0	0	0
			572	278	103	164	27			
2	L	28	Total	C	N	O	P	0	0	0
			572	278	103	164	27			

- Molecule 3 is a protein called Organic hydroperoxide resistance transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	137	Total	C	N	O	S	0	0	0
			1075	688	178	205	4			
3	B	137	Total	C	N	O	S	0	0	0
			1068	684	172	207	5			
3	C	138	Total	C	N	O	S	0	0	0
			1057	677	173	202	5			
3	D	137	Total	C	N	O	S	0	0	0
			1051	670	173	203	5			
3	E	137	Total	C	N	O	S	0	0	0
			1085	693	177	210	5			
3	F	138	Total	C	N	O	S	0	0	0
			1077	690	175	207	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	SER	CYS	ENGINEERED	UNP O34777
B	15	SER	CYS	ENGINEERED	UNP O34777
C	15	SER	CYS	ENGINEERED	UNP O34777
D	15	SER	CYS	ENGINEERED	UNP O34777
E	15	SER	CYS	ENGINEERED	UNP O34777
F	15	SER	CYS	ENGINEERED	UNP O34777

- Molecule 4 is water.

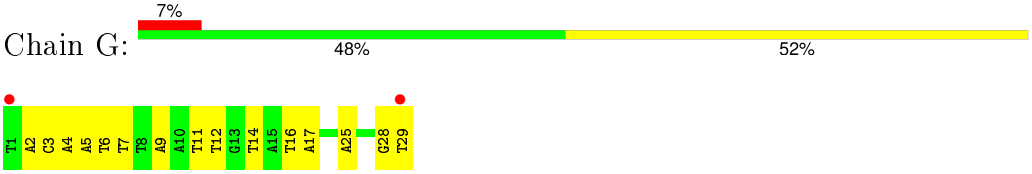
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	16	Total O 16 16	0	0
4	C	16	Total O 16 16	0	0
4	D	14	Total O 14 14	0	0
4	E	21	Total O 21 21	0	0
4	F	22	Total O 22 22	0	0
4	G	13	Total O 13 13	0	0
4	H	11	Total O 11 11	0	0
4	I	7	Total O 7 7	0	0
4	J	8	Total O 8 8	0	0
4	K	11	Total O 11 11	0	0
4	L	10	Total O 10 10	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.

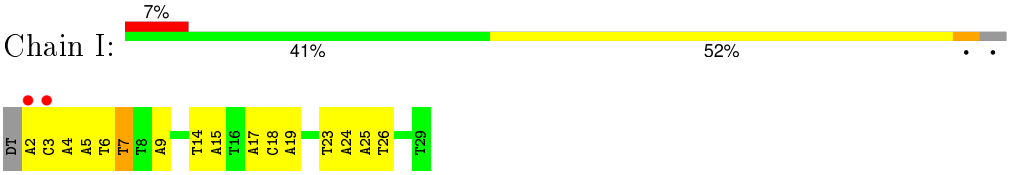
- Molecule 1: DNA (29-MER)

Chain G:



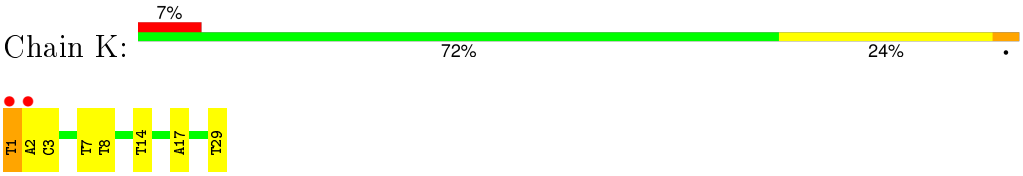
- Molecule 1: DNA (29-MER)

Chain I:



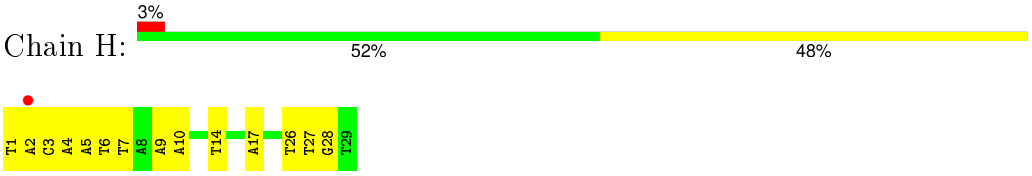
- Molecule 1: DNA (29-MER)

Chain K:



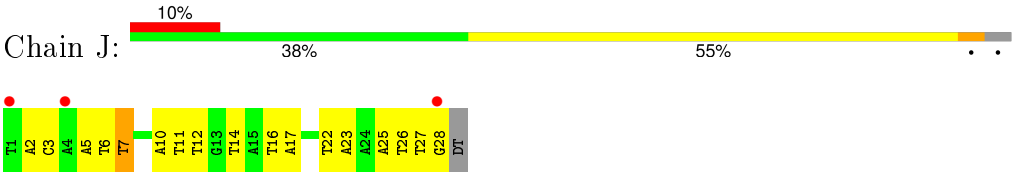
- Molecule 2: DNA (29-MER)

Chain H:



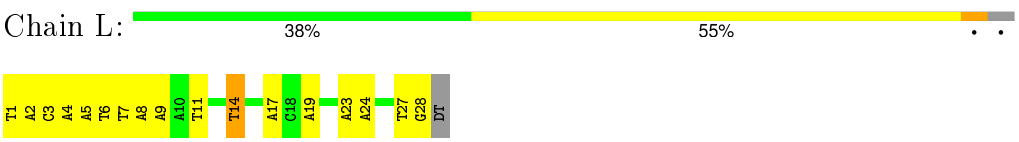
- Molecule 2: DNA (29-MER)

Chain J:



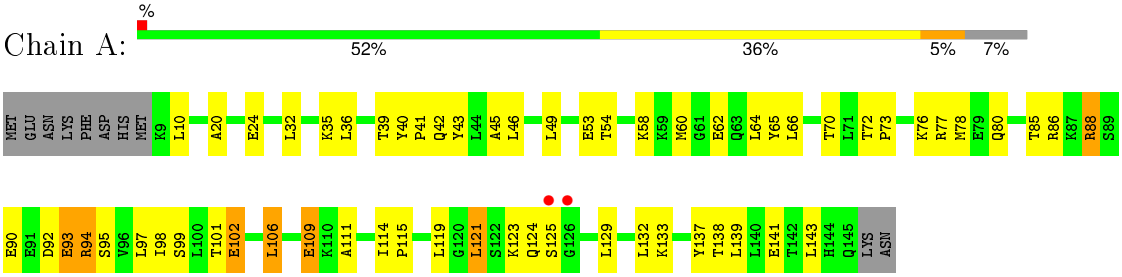
- Molecule 2: DNA (29-MER)

Chain L:



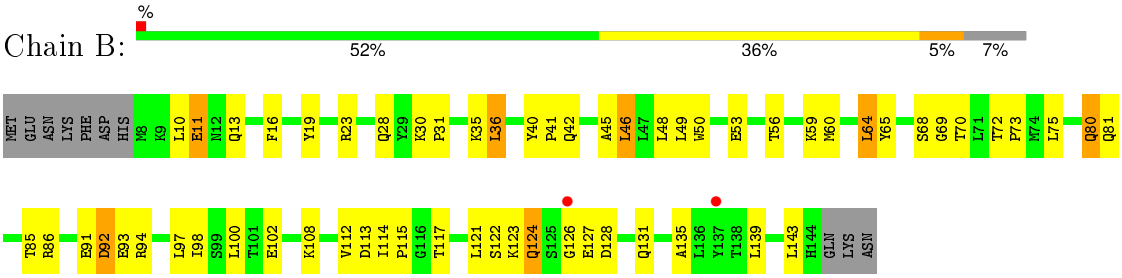
• Molecule 3: Organic hydroperoxide resistance transcriptional regulator

Chain A:



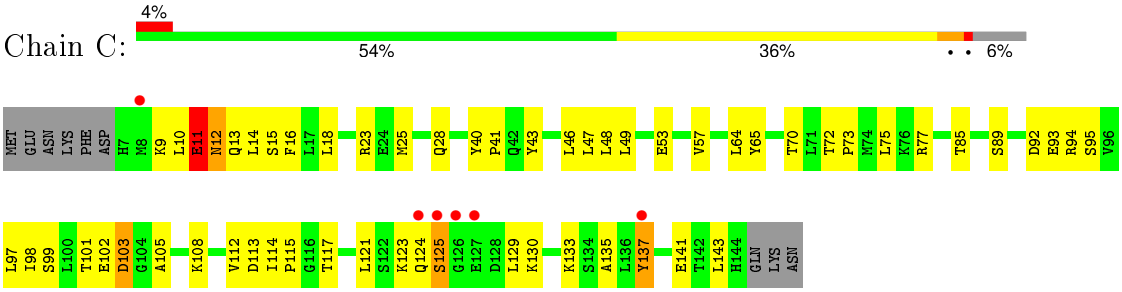
• Molecule 3: Organic hydroperoxide resistance transcriptional regulator

Chain B:



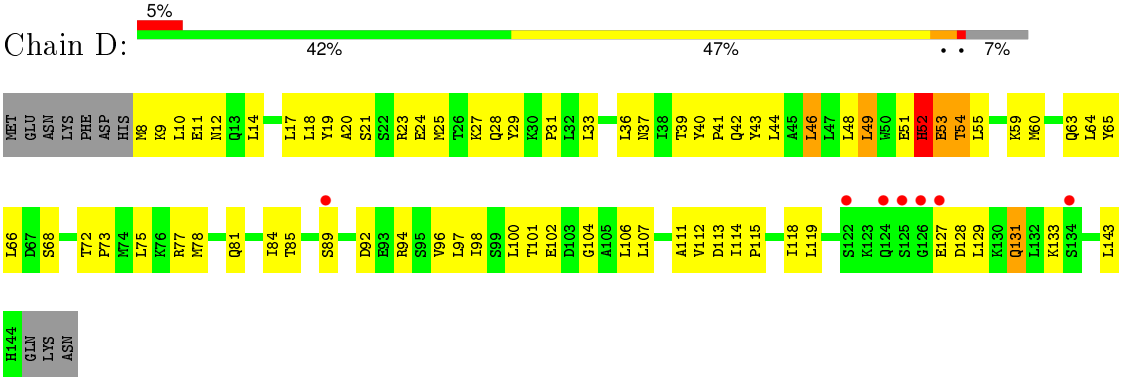
• Molecule 3: Organic hydroperoxide resistance transcriptional regulator

Chain C:



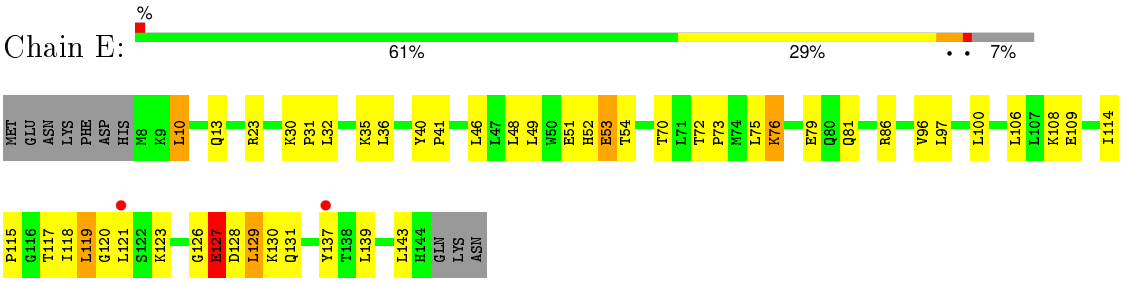
• Molecule 3: Organic hydroperoxide resistance transcriptional regulator

Chain D:



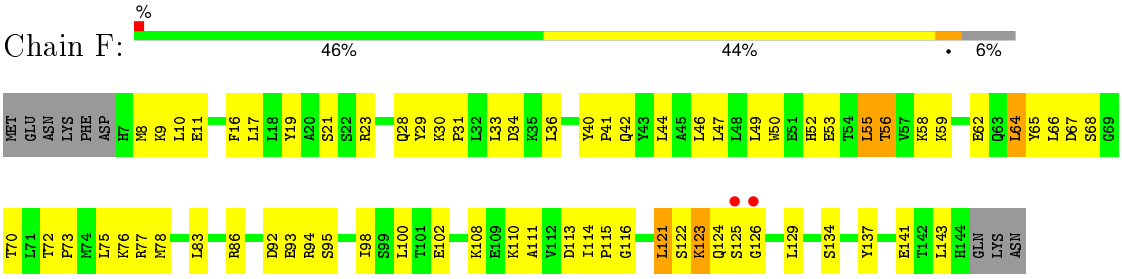
• Molecule 3: Organic hydroperoxide resistance transcriptional regulator

Chain E:



• Molecule 3: Organic hydroperoxide resistance transcriptional regulator

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.90Å 80.96Å 109.34Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	59.65 – 2.64 57.12 – 2.64	Depositor EDS
% Data completeness (in resolution range)	96.0 (59.65-2.64) 91.6 (57.12-2.64)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.277 0.223 , 0.229	Depositor DCC
R_{free} test set	1914 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 38111 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10073	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	G	1.56	2/660 (0.3%)	0.83	0/1017
1	I	1.31	2/638 (0.3%)	0.78	1/983 (0.1%)
1	K	1.53	2/660 (0.3%)	0.92	3/1017 (0.3%)
2	H	1.17	1/664 (0.2%)	0.75	1/1023 (0.1%)
2	J	1.16	2/642 (0.3%)	0.77	1/989 (0.1%)
2	L	1.36	2/642 (0.3%)	0.78	0/989
3	A	0.39	0/1089	0.63	0/1471
3	B	0.40	0/1082	0.67	2/1463 (0.1%)
3	C	0.37	0/1072	0.60	0/1454
3	D	0.34	0/1065	0.62	0/1443
3	E	0.37	0/1099	0.65	0/1483
3	F	0.38	0/1090	0.69	0/1471
All	All	0.88	11/10403 (0.1%)	0.71	8/14803 (0.1%)

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	K	1	0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	14	DT	C5-C7	31.41	1.68	1.50
1	K	14	DT	C5-C7	29.12	1.67	1.50
2	H	14	DT	C5-C7	27.39	1.66	1.50
2	L	14	DT	C5-C7	23.66	1.64	1.50
1	I	7	DT	C5-C7	23.09	1.64	1.50
1	K	7	DT	C5-C7	22.86	1.63	1.50
2	L	7	DT	C5-C7	22.82	1.63	1.50
1	G	7	DT	C5-C7	22.11	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	14	DT	C5-C7	21.37	1.62	1.50
2	J	14	DT	C5-C7	20.75	1.62	1.50
2	J	7	DT	C5-C7	18.40	1.61	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	1	DT	C1'-O4'-C4'	-8.90	101.20	110.10
1	K	1	DT	C4'-C3'-C2'	-6.95	96.85	103.10
1	K	1	DT	C2'-C3'-O3'	-6.12	92.42	112.60
1	I	14	DT	C6-C5-C7	-5.54	119.58	122.90
2	H	14	DT	C6-C5-C7	-5.50	119.60	122.90
3	B	69	GLY	N-CA-C	-5.47	99.43	113.10
3	B	68	SER	N-CA-C	-5.14	97.11	111.00
2	J	14	DT	C6-C5-C7	-5.14	119.82	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	K	1	DT	C3'

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	G	590	0	335	14	0
1	I	570	0	323	17	0
1	K	590	0	335	7	0
2	H	592	0	333	23	0
2	J	572	0	321	20	0
2	L	572	0	321	22	0
3	A	1075	0	1108	51	0
3	B	1068	0	1089	54	0
3	C	1057	0	1060	58	0
3	D	1051	0	1050	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1085	0	1119	50	0
3	F	1077	0	1111	68	0
4	A	25	0	0	2	0
4	B	16	0	0	1	0
4	C	16	0	0	2	0
4	D	14	0	0	1	0
4	E	21	0	0	0	0
4	F	22	0	0	4	0
4	G	13	0	0	0	0
4	H	11	0	0	0	0
4	I	7	0	0	0	0
4	J	8	0	0	0	0
4	K	11	0	0	0	0
4	L	10	0	0	2	0
All	All	10073	0	8505	403	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 22.

All (403) 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:L:19:DA:H5"	3:F:30:LYS:HE3	1.31	1.12
3:E:130:LYS:HD2	3:E:130:LYS:H	1.17	1.10
1:I:17:DA:H2"	1:I:18:DC:H5'	1.37	1.05
2:H:26:DT:H2"	2:H:27:DT:H5'	1.40	1.02
3:C:123:LYS:HB2	3:C:129:LEU:HD22	1.44	0.99
3:B:80:GLN:HE22	3:B:81:GLN:HE21	1.09	0.96
2:L:2:DA:H2"	2:L:3:DC:H5"	1.48	0.95
2:H:2:DA:H2"	2:H:3:DC:H5"	1.47	0.94
3:D:92:ASP:OD1	3:D:94:ARG:HG2	1.66	0.92
3:B:80:GLN:NE2	3:B:81:GLN:HE21	1.68	0.92
3:E:123:LYS:HA	3:E:127:GLU:HB3	1.54	0.89
3:D:128:ASP:HB3	3:E:130:LYS:HE2	1.54	0.89
3:D:9:LYS:HB3	3:D:12:ASN:ND2	1.87	0.88
2:H:2:DA:C2'	2:H:3:DC:H5"	2.05	0.87
2:H:1:DT:H1'	2:H:2:DA:H5'	1.55	0.87
3:C:15:SER:HB3	3:D:25:MET:HE2	1.56	0.86
3:D:114:ILE:HB	3:D:115:PRO:HD3	1.58	0.85
3:A:106:LEU:O	3:A:109:GLU:HG2	1.76	0.84
2:J:5:DA:H2"	2:J:6:DT:H5"	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:59:LYS:O	3:D:63:GLN:HG2	1.78	0.83
3:D:36:LEU:HB3	3:D:107:LEU:HD11	1.61	0.83
3:B:11:GLU:CD	3:B:11:GLU:H	1.81	0.82
3:B:45:ALA:O	3:B:49:LEU:HD23	1.79	0.81
3:D:72:THR:HB	3:D:73:PRO:HD3	1.64	0.79
3:F:29:TYR:HB3	3:F:33:LEU:HD23	1.66	0.78
3:A:70:THR:O	3:A:73:PRO:HD2	1.83	0.77
3:E:130:LYS:HD2	3:E:130:LYS:N	1.99	0.77
3:D:29:TYR:HD2	3:D:33:LEU:HD21	1.49	0.77
3:E:51:GLU:HG2	3:E:52:HIS:CE1	2.20	0.76
3:B:80:GLN:HE22	3:B:81:GLN:NE2	1.83	0.76
3:F:29:TYR:HB3	3:F:33:LEU:CD2	2.16	0.76
3:B:10:LEU:O	3:B:13:GLN:HG2	1.86	0.75
2:J:5:DA:C2'	2:J:6:DT:H5"	2.15	0.75
1:I:2:DA:H5"	1:I:3:DC:C5	2.22	0.75
3:C:12:ASN:HD22	3:C:12:ASN:N	1.82	0.75
1:G:28:DG:H2"	1:G:29:DT:H5'	1.67	0.75
3:B:128:ASP:OD1	3:B:131:GLN:HG3	1.85	0.75
1:G:29:DT:H2'	1:G:29:DT:O2	1.85	0.75
3:F:111:ALA:HA	3:F:114:ILE:HD13	1.68	0.75
3:A:32:LEU:O	3:A:35:LYS:HB2	1.87	0.74
3:D:29:TYR:HB3	3:D:33:LEU:HD23	1.69	0.74
3:B:40:TYR:HB3	3:B:41:PRO:HD3	1.70	0.74
3:E:117:THR:O	3:E:121:LEU:HD13	1.88	0.73
3:E:127:GLU:HB2	3:E:129:LEU:HG	1.69	0.73
3:F:28:GLN:OE1	3:F:121:LEU:HD11	1.89	0.73
2:H:2:DA:C3'	2:H:3:DC:H5"	2.19	0.72
2:L:2:DA:C2'	2:L:3:DC:H5"	2.19	0.72
3:F:56:THR:HG22	3:F:59:LYS:H	1.55	0.72
3:C:130:LYS:HE2	3:C:130:LYS:HA	1.70	0.71
2:H:3:DC:H2"	2:H:4:DA:N7	2.05	0.71
2:H:26:DT:H2"	2:H:27:DT:C5'	2.20	0.71
3:B:56:THR:HG22	3:B:97:LEU:HD23	1.72	0.71
1:I:17:DA:H2"	1:I:18:DC:C5'	2.20	0.70
2:J:2:DA:H2"	2:J:3:DC:H5'	1.73	0.70
3:C:65:TYR:O	3:D:23:ARG:NH2	2.24	0.70
3:F:29:TYR:HD2	3:F:33:LEU:HD21	1.56	0.70
3:A:42:GLN:O	3:A:46:LEU:HD13	1.92	0.69
2:L:19:DA:H5"	3:F:30:LYS:CE	2.17	0.69
3:A:65:TYR:O	3:B:23:ARG:NH2	2.25	0.69
3:A:40:TYR:HB3	3:A:41:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:130:LYS:CD	3:E:130:LYS:H	1.99	0.69
3:C:11:GLU:H	3:C:11:GLU:CD	1.97	0.68
2:L:5:DA:H1'	2:L:6:DT:H5"	1.75	0.68
3:C:11:GLU:C	3:C:12:ASN:HD22	1.97	0.68
3:E:114:ILE:HB	3:E:115:PRO:HD3	1.73	0.68
2:H:9:DA:H2"	2:H:10:DA:H5'	1.76	0.68
3:C:28:GLN:HG3	3:D:143:LEU:HD22	1.76	0.67
3:F:137:TYR:O	3:F:141:GLU:HG3	1.94	0.67
3:E:127:GLU:C	3:E:129:LEU:H	1.96	0.66
3:D:64:LEU:O	3:D:66:LEU:HG	1.96	0.66
3:D:48:LEU:HD12	3:D:64:LEU:HD11	1.78	0.65
3:F:58:LYS:O	3:F:62:GLU:HG3	1.96	0.65
3:E:137:TYR:CZ	3:F:17:LEU:HD11	2.31	0.65
1:G:4:DA:H2"	1:G:5:DA:OP2	1.97	0.65
3:A:92:ASP:OD2	3:A:94:ARG:HB2	1.97	0.65
3:E:23:ARG:NH2	3:F:65:TYR:O	2.30	0.64
2:J:27:DT:H2"	2:J:28:DG:C8	2.32	0.64
3:E:70:THR:O	3:E:73:PRO:HD2	1.96	0.64
3:B:112:VAL:HG13	3:B:113:ASP:N	2.13	0.64
1:K:1:DT:H2'	1:K:2:DA:H5'	1.77	0.64
3:B:91:GLU:O	3:B:91:GLU:HG2	1.97	0.63
3:C:40:TYR:HB3	3:C:41:PRO:HD3	1.79	0.63
2:H:9:DA:H1'	2:H:10:DA:H5"	1.80	0.63
2:J:27:DT:H2"	2:J:28:DG:N7	2.14	0.63
2:L:3:DC:H2"	2:L:4:DA:C8	2.34	0.63
3:A:46:LEU:CD1	3:A:78:MET:HE1	2.29	0.63
3:E:139:LEU:HG	3:E:143:LEU:HD13	1.80	0.63
3:C:101:THR:HG22	3:C:103:ASP:H	1.62	0.63
3:B:60:MET:CE	3:B:98:ILE:HG13	2.27	0.63
3:E:51:GLU:OE2	3:F:9:LYS:HG2	1.99	0.63
3:A:121:LEU:O	3:A:124:GLN:HB3	1.99	0.62
2:J:10:DA:H2'	3:D:72:THR:HG21	1.82	0.62
3:B:30:LYS:HB3	3:B:31:PRO:HD3	1.81	0.62
3:A:76:LYS:HD2	3:A:86:ARG:HH22	1.64	0.61
1:K:8:DT:H3	2:L:23:DA:H2	1.45	0.61
3:D:29:TYR:CD2	3:D:33:LEU:HD21	2.34	0.61
2:J:5:DA:H2"	2:J:6:DT:C5'	2.29	0.61
3:D:48:LEU:HD11	3:D:63:GLN:HB2	1.83	0.61
3:A:36:LEU:HD11	3:A:111:ALA:HB2	1.83	0.61
3:A:88:ARG:HD2	3:A:93:GLU:O	2.02	0.60
2:L:19:DA:C5'	3:F:30:LYS:HE3	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:124:GLN:O	3:F:126:GLY:N	2.35	0.60
3:A:10:LEU:HD22	3:B:48:LEU:HD21	1.84	0.59
3:B:48:LEU:HD11	3:B:64:LEU:HD13	1.83	0.59
1:I:4:DA:H1'	1:I:5:DA:H5'	1.84	0.59
3:E:23:ARG:NH2	3:F:66:LEU:HD23	2.18	0.59
2:L:27:DT:H2"	2:L:28:DG:C8	2.38	0.59
3:C:123:LYS:HG3	3:C:129:LEU:HB2	1.85	0.59
3:F:114:ILE:HB	3:F:115:PRO:HD3	1.85	0.59
2:J:26:DT:H4'	3:C:94:ARG:HH11	1.68	0.58
1:G:29:DT:C2'	1:G:29:DT:O2	2.51	0.58
2:L:27:DT:H2"	2:L:28:DG:N7	2.19	0.58
3:C:23:ARG:NH2	3:D:65:TYR:O	2.37	0.58
1:I:18:DC:H2"	1:I:19:DA:C8	2.39	0.57
3:D:29:TYR:HB3	3:D:33:LEU:CD2	2.34	0.57
3:E:126:GLY:O	3:E:128:ASP:N	2.37	0.57
2:L:2:DA:H2"	2:L:3:DC:C5'	2.31	0.57
3:F:17:LEU:O	3:F:21:SER:HB3	2.05	0.57
3:C:43:TYR:O	3:C:47:LEU:HG	2.05	0.57
3:F:30:LYS:HB3	3:F:31:PRO:HD3	1.87	0.57
3:F:92:ASP:C	3:F:94:ARG:H	2.08	0.57
3:A:46:LEU:HD11	3:A:78:MET:CE	2.34	0.57
3:E:40:TYR:HB3	3:E:41:PRO:HD3	1.87	0.57
3:F:92:ASP:OD2	3:F:94:ARG:HB2	2.05	0.57
1:K:1:DT:H2'	1:K:2:DA:C5'	2.35	0.57
3:A:45:ALA:HB1	3:A:60:MET:CE	2.35	0.57
1:I:23:DT:H2"	1:I:24:DA:C8	2.40	0.56
3:D:128:ASP:HB3	3:E:130:LYS:CE	2.33	0.56
3:E:119:LEU:C	3:E:121:LEU:H	2.09	0.56
1:G:29:DT:O4	2:H:2:DA:N1	2.38	0.56
3:F:29:TYR:CD2	3:F:33:LEU:HD21	2.38	0.56
3:A:66:LEU:HD23	3:B:23:ARG:NH2	2.20	0.56
3:F:10:LEU:HD11	3:F:16:PHE:CD2	2.41	0.56
3:F:11:GLU:HG2	4:F:168:HOH:O	2.06	0.56
3:F:123:LYS:H	3:F:123:LYS:HD3	1.71	0.56
2:H:1:DT:H1'	2:H:2:DA:C5'	2.32	0.56
1:I:24:DA:H2"	1:I:25:DA:OP2	2.06	0.56
3:D:39:THR:OG1	3:D:42:GLN:HG3	2.06	0.56
3:D:112:VAL:HG13	3:D:113:ASP:N	2.21	0.55
3:D:112:VAL:HG13	3:D:113:ASP:H	1.70	0.55
3:E:120:GLY:O	3:E:121:LEU:HD12	2.06	0.55
3:C:70:THR:O	3:C:73:PRO:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:56:THR:HG21	3:F:58:LYS:HG2	1.89	0.55
2:H:9:DA:H2"	2:H:10:DA:C5'	2.37	0.55
3:B:102:GLU:HA	3:B:102:GLU:OE2	2.06	0.55
3:D:43:TYR:O	3:D:46:LEU:HB2	2.07	0.55
3:D:40:TYR:HB3	3:D:41:PRO:HD3	1.88	0.55
3:C:89:SER:HB3	3:C:92:ASP:O	2.06	0.55
3:E:128:ASP:O	3:E:131:GLN:N	2.39	0.55
2:J:10:DA:N7	3:D:68:SER:OG	2.35	0.55
3:C:12:ASN:ND2	3:C:12:ASN:N	2.53	0.55
3:C:10:LEU:O	3:C:12:ASN:N	2.40	0.54
3:B:86:ARG:HG2	3:B:98:ILE:CD1	2.37	0.54
3:C:77:ARG:NH2	4:C:150:HOH:O	2.40	0.54
3:E:10:LEU:HD23	3:F:47:LEU:HD12	1.89	0.54
3:F:33:LEU:N	3:F:33:LEU:HD22	2.22	0.54
3:D:20:ALA:O	3:D:24:GLU:HG2	2.06	0.54
3:C:10:LEU:HD11	3:C:16:PHE:CD2	2.42	0.54
3:D:96:VAL:HG12	3:D:98:ILE:HD12	1.90	0.54
1:G:17:DA:H2'	3:B:70:THR:OG1	2.08	0.54
3:E:30:LYS:HB3	3:E:31:PRO:HD3	1.88	0.54
1:G:25:DA:N3	3:B:94:ARG:HD3	2.22	0.54
1:I:26:DT:H4'	3:D:94:ARG:NE	2.22	0.54
3:D:129:LEU:HD21	3:D:133:LYS:HE3	1.89	0.54
3:C:64:LEU:HD23	3:D:10:LEU:HD21	1.90	0.54
3:D:29:TYR:O	3:D:33:LEU:HD23	2.08	0.54
2:L:14:DT:H5"	4:L:37:HOH:O	2.08	0.53
3:E:108:LYS:HD3	3:F:8:MET:HE2	1.90	0.53
1:I:9:DA:OP1	3:C:95:SER:HB2	2.09	0.53
3:F:102:GLU:HB3	4:F:150:HOH:O	2.09	0.53
3:F:92:ASP:O	3:F:94:ARG:N	2.42	0.53
3:B:92:ASP:O	3:B:94:ARG:N	2.42	0.53
3:E:35:LYS:C	3:E:36:LEU:HD23	2.29	0.53
3:A:123:LYS:C	3:A:125:SER:H	2.10	0.53
1:I:6:DT:H1'	1:I:7:DT:H5'	1.90	0.53
1:G:9:DA:C8	1:G:9:DA:H5'	2.43	0.53
3:F:40:TYR:HB3	3:F:41:PRO:HD3	1.90	0.53
3:C:101:THR:HG22	3:C:102:GLU:N	2.23	0.52
3:D:131:GLN:HB2	3:E:130:LYS:HD3	1.90	0.52
2:J:6:DT:H2"	2:J:7:DT:O5'	2.09	0.52
1:I:15:DA:OP2	3:D:77:ARG:NH1	2.42	0.52
3:D:52:HIS:O	3:D:53:GLU:C	2.47	0.52
3:A:72:THR:HB	3:A:73:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:10:LEU:HD11	3:B:16:PHE:CD2	2.45	0.52
3:C:11:GLU:HB2	4:C:160:HOH:O	2.10	0.52
3:D:84:ILE:HA	3:D:101:THR:HG23	1.92	0.52
3:F:50:TRP:CE2	3:F:108:LYS:HB2	2.44	0.52
2:H:1:DT:C1'	2:H:2:DA:H5'	2.35	0.52
3:A:143:LEU:HD22	3:B:28:GLN:HG3	1.92	0.51
3:F:67:ASP:OD1	3:F:68:SER:O	2.28	0.51
1:K:8:DT:O4	2:L:23:DA:N1	2.43	0.51
3:A:36:LEU:CD1	3:A:111:ALA:HB2	2.41	0.51
3:C:117:THR:O	3:C:121:LEU:HG	2.10	0.51
3:B:45:ALA:O	3:B:49:LEU:CD2	2.55	0.51
3:A:92:ASP:C	3:A:94:ARG:H	2.12	0.51
2:L:23:DA:H2"	2:L:24:DA:H8	1.76	0.51
3:C:85:THR:CG2	3:C:99:SER:HB2	2.40	0.51
3:A:92:ASP:O	3:A:94:ARG:N	2.43	0.51
3:D:19:TYR:O	3:D:23:ARG:HG3	2.11	0.51
3:F:86:ARG:HG2	3:F:98:ILE:CD1	2.40	0.51
3:D:129:LEU:HD11	3:D:133:LYS:HE3	1.94	0.50
3:D:17:LEU:O	3:D:21:SER:HB3	2.11	0.50
3:E:10:LEU:HD21	3:F:44:LEU:HD22	1.93	0.50
3:E:75:LEU:O	3:E:79:GLU:HG3	2.10	0.50
3:F:72:THR:HB	3:F:73:PRO:HD3	1.93	0.50
3:E:127:GLU:C	3:E:129:LEU:N	2.65	0.50
1:I:2:DA:H2'	1:I:3:DC:C2	2.46	0.50
2:L:9:DA:OP2	3:F:58:LYS:HB3	2.11	0.50
1:K:2:DA:H2"	1:K:3:DC:OP2	2.12	0.50
3:D:28:GLN:O	3:D:31:PRO:HD2	2.11	0.50
3:A:86:ARG:HG2	3:A:98:ILE:CD1	2.41	0.50
3:E:123:LYS:HA	3:E:127:GLU:CB	2.36	0.50
3:B:92:ASP:C	3:B:94:ARG:H	2.15	0.50
2:L:6:DT:H6	2:L:6:DT:H5'	1.76	0.50
2:L:17:DA:H2'	3:E:70:THR:OG1	2.12	0.49
3:D:27:LYS:O	3:D:31:PRO:HD3	2.12	0.49
3:D:64:LEU:N	3:D:64:LEU:HD12	2.27	0.49
3:E:48:LEU:HD21	3:F:10:LEU:HD23	1.94	0.49
3:D:9:LYS:HB3	3:D:12:ASN:CG	2.31	0.49
2:L:23:DA:H2"	2:L:24:DA:C8	2.47	0.49
3:F:29:TYR:HB3	3:F:33:LEU:HD21	1.93	0.49
1:G:9:DA:OP1	3:A:95:SER:HB2	2.12	0.49
3:E:49:LEU:HB3	3:E:100:LEU:HG	1.95	0.49
2:J:10:DA:H2"	2:J:11:DT:H5'	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:56:THR:CG2	3:F:58:LYS:HG2	2.43	0.48
3:D:9:LYS:CB	3:D:12:ASN:ND2	2.69	0.48
3:B:72:THR:HB	3:B:73:PRO:HD3	1.95	0.48
3:D:54:THR:OG1	3:D:97:LEU:HG	2.13	0.48
3:C:85:THR:HG22	3:C:99:SER:HB2	1.95	0.48
3:B:64:LEU:O	3:B:65:TYR:HB2	2.12	0.48
3:C:75:LEU:HD13	3:C:98:ILE:HD11	1.95	0.48
3:C:43:TYR:CE1	3:C:47:LEU:HD11	2.48	0.48
1:G:9:DA:H8	1:G:9:DA:H5'	1.78	0.48
3:F:64:LEU:O	3:F:65:TYR:HB2	2.13	0.48
3:A:64:LEU:HD23	3:B:10:LEU:HD21	1.94	0.48
3:A:39:THR:H	3:A:42:GLN:NE2	2.12	0.48
1:G:11:DT:H2"	1:G:12:DT:H5'	1.96	0.48
3:C:137:TYR:O	3:C:141:GLU:HG3	2.13	0.48
3:C:10:LEU:C	3:C:12:ASN:H	2.16	0.48
3:D:11:GLU:CD	3:D:11:GLU:H	2.17	0.47
3:A:54:THR:HG22	3:A:99:SER:OG	2.14	0.47
3:C:143:LEU:HD22	3:D:28:GLN:HG3	1.97	0.47
3:A:46:LEU:HD11	3:A:78:MET:HE3	1.95	0.47
1:G:5:DA:H2"	1:G:6:DT:O5'	2.14	0.47
3:D:102:GLU:O	3:D:106:LEU:HB2	2.14	0.47
3:A:46:LEU:CD1	3:A:78:MET:CE	2.92	0.47
3:F:58:LYS:HG3	3:F:59:LYS:N	2.30	0.47
3:C:89:SER:HB2	3:C:97:LEU:HD21	1.97	0.47
3:C:135:ALA:HA	3:D:127:GLU:OE2	2.14	0.47
3:C:97:LEU:N	3:C:97:LEU:HD22	2.29	0.47
3:D:128:ASP:CB	3:E:130:LYS:HE2	2.36	0.46
2:H:1:DT:H2"	2:H:2:DA:H8	1.80	0.46
3:E:86:ARG:HG3	3:E:96:VAL:HG11	1.95	0.46
3:B:80:GLN:NE2	3:B:81:GLN:NE2	2.49	0.46
3:B:112:VAL:CG1	3:B:113:ASP:N	2.78	0.46
1:I:4:DA:H2"	1:I:5:DA:O5'	2.16	0.46
3:A:132:LEU:HD22	3:B:135:ALA:HB1	1.97	0.46
3:B:122:SER:C	3:B:124:GLN:H	2.18	0.46
3:F:111:ALA:CA	3:F:114:ILE:HD13	2.41	0.46
3:A:66:LEU:HD23	3:B:23:ARG:HH21	1.80	0.46
3:F:52:HIS:HB2	3:F:55:LEU:HD13	1.97	0.46
3:A:133:LYS:O	3:A:137:TYR:HD1	1.98	0.46
3:E:76:LYS:NZ	3:E:76:LYS:HB2	2.30	0.46
3:F:124:GLN:C	3:F:126:GLY:H	2.19	0.46
2:J:22:DT:H2"	2:J:23:DA:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:77:ARG:HB3	4:F:158:HOH:O	2.15	0.46
3:D:60:MET:O	3:D:64:LEU:CD1	2.64	0.46
3:A:77:ARG:NH1	4:A:168:HOH:O	2.49	0.46
2:J:10:DA:H1'	2:J:11:DT:H5"	1.97	0.45
3:C:10:LEU:CD1	3:D:44:LEU:HD22	2.45	0.45
2:J:2:DA:H1'	2:J:3:DC:H5"	1.97	0.45
3:B:50:TRP:HD1	3:B:100:LEU:HD21	1.81	0.45
3:D:46:LEU:O	3:D:49:LEU:N	2.50	0.45
2:L:8:DA:N7	4:L:33:HOH:O	2.36	0.45
3:B:60:MET:O	3:B:64:LEU:HB2	2.16	0.45
3:E:109:GLU:HA	3:E:109:GLU:OE1	2.16	0.45
1:I:17:DA:C2'	1:I:18:DC:H5'	2.26	0.45
3:D:89:SER:HB2	3:D:92:ASP:O	2.16	0.45
3:B:11:GLU:CD	3:B:11:GLU:N	2.59	0.45
3:D:78:MET:O	3:D:81:GLN:HB2	2.17	0.45
3:B:36:LEU:N	3:B:36:LEU:HD23	2.31	0.45
3:B:114:ILE:HB	3:B:115:PRO:HD3	1.97	0.45
3:A:20:ALA:O	3:A:24:GLU:HG2	2.17	0.45
3:F:33:LEU:H	3:F:33:LEU:HD22	1.80	0.45
3:F:122:SER:HB2	3:F:129:LEU:HD11	1.99	0.45
2:H:3:DC:H2"	2:H:4:DA:C8	2.51	0.44
2:J:11:DT:H2'	2:J:12:DT:H71	1.98	0.44
2:L:9:DA:C8	2:L:9:DA:H5'	2.53	0.44
3:F:23:ARG:HH11	3:F:23:ARG:HG3	1.82	0.44
3:C:114:ILE:HB	3:C:115:PRO:HD3	1.99	0.44
2:H:27:DT:H2"	2:H:28:DG:C8	2.52	0.44
3:C:48:LEU:HG	3:D:10:LEU:HD22	1.99	0.44
3:D:48:LEU:CD1	3:D:64:LEU:HD11	2.45	0.44
3:D:29:TYR:C	3:D:33:LEU:HD23	2.36	0.44
3:C:11:GLU:HG2	3:C:12:ASN:ND2	2.33	0.44
3:F:92:ASP:C	3:F:94:ARG:N	2.71	0.44
3:C:72:THR:HB	3:C:73:PRO:HD3	1.98	0.44
3:A:132:LEU:O	3:A:132:LEU:HD12	2.17	0.44
3:C:124:GLN:O	3:C:125:SER:HB3	2.18	0.44
2:J:25:DA:O3'	3:C:93:GLU:HB2	2.18	0.44
3:D:48:LEU:HD11	3:D:63:GLN:CB	2.47	0.44
3:A:40:TYR:O	3:A:43:TYR:HB3	2.17	0.44
3:A:119:LEU:CD1	3:A:123:LYS:HB2	2.48	0.44
3:A:85:THR:CG2	3:A:99:SER:HB2	2.48	0.44
3:D:14:LEU:O	3:D:18:LEU:HG	2.18	0.44
3:C:11:GLU:N	3:C:11:GLU:CD	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:LYS:O	3:C:123:LYS:HE2	2.18	0.44
3:F:30:LYS:HG2	3:F:34:ASP:OD2	2.18	0.43
3:D:63:GLN:HB2	3:D:64:LEU:HD12	2.00	0.43
3:E:120:GLY:C	3:E:121:LEU:HD12	2.38	0.43
3:F:114:ILE:HD12	3:F:114:ILE:N	2.34	0.43
1:G:2:DA:H2"	1:G:3:DC:O5'	2.17	0.43
2:H:17:DA:OP2	3:B:19:TYR:OH	2.33	0.43
2:J:5:DA:H1'	2:J:6:DT:H5"	1.99	0.43
3:B:60:MET:HE1	3:B:98:ILE:HG21	2.01	0.43
3:F:124:GLN:C	3:F:126:GLY:N	2.72	0.43
3:D:43:TYR:HA	3:D:46:LEU:HD23	2.00	0.43
3:A:123:LYS:C	3:A:125:SER:N	2.71	0.43
2:H:5:DA:C2'	2:H:6:DT:H5"	2.48	0.43
2:L:1:DT:H2"	2:L:2:DA:O5'	2.19	0.43
3:C:15:SER:HA	3:C:18:LEU:HD12	2.00	0.43
3:E:48:LEU:HD21	3:F:10:LEU:CD2	2.49	0.43
3:A:138:THR:O	3:A:141:GLU:N	2.51	0.43
1:I:7:DT:H1'	3:C:94:ARG:HH21	1.84	0.43
2:H:5:DA:H2"	2:H:6:DT:H5"	1.99	0.43
3:F:116:GLY:N	4:F:166:HOH:O	2.51	0.43
1:G:16:DT:H5"	4:B:154:HOH:O	2.18	0.43
3:B:56:THR:HG22	3:B:97:LEU:CD2	2.46	0.43
3:A:76:LYS:O	3:A:80:GLN:HG3	2.19	0.43
2:H:5:DA:H1'	2:H:6:DT:H5"	2.01	0.43
3:C:112:VAL:HG13	3:C:113:ASP:N	2.34	0.43
3:C:9:LYS:HA	3:D:51:GLU:OE1	2.18	0.42
3:C:89:SER:CB	3:C:97:LEU:HD21	2.49	0.42
3:B:126:GLY:O	3:B:127:GLU:HB3	2.19	0.42
3:B:139:LEU:O	3:B:143:LEU:HG	2.18	0.42
3:F:42:GLN:HG2	3:F:78:MET:CG	2.48	0.42
3:D:111:ALA:HA	3:D:114:ILE:HG12	2.01	0.42
3:D:60:MET:O	3:D:64:LEU:HD13	2.19	0.42
3:E:72:THR:HB	3:E:73:PRO:HD3	2.01	0.42
3:E:48:LEU:HG	3:F:10:LEU:HD22	2.00	0.42
3:C:129:LEU:O	3:C:133:LYS:HG3	2.19	0.42
3:A:66:LEU:CD2	3:B:23:ARG:NH2	2.82	0.42
3:A:119:LEU:C	3:A:121:LEU:H	2.22	0.42
3:A:86:ARG:HG2	3:A:98:ILE:HG13	2.01	0.42
3:C:130:LYS:HE2	3:C:133:LYS:HE2	2.01	0.42
3:B:60:MET:HE1	3:B:98:ILE:HG13	2.02	0.42
3:D:114:ILE:HB	3:D:115:PRO:CD	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:55:LEU:CD1	3:D:59:LYS:HE3	2.49	0.42
3:B:35:LYS:C	3:B:36:LEU:HD23	2.39	0.42
3:C:13:GLN:NE2	3:C:13:GLN:HA	2.35	0.42
1:K:29:DT:H2'	1:K:29:DT:H6	1.72	0.42
3:A:102:GLU:OE2	3:A:106:LEU:HD13	2.19	0.42
3:E:139:LEU:HG	3:E:143:LEU:CD1	2.48	0.42
3:B:60:MET:HE2	3:B:98:ILE:HG13	2.01	0.42
3:A:123:LYS:HA	3:A:129:LEU:HD11	2.02	0.42
3:C:57:VAL:HG22	3:C:98:ILE:HD11	2.02	0.42
1:K:17:DA:H2'	3:F:70:THR:OG1	2.18	0.42
3:A:58:LYS:HE2	3:A:62:GLU:OE2	2.19	0.42
3:D:118:ILE:O	3:D:119:LEU:C	2.57	0.42
3:D:73:PRO:HG3	4:D:159:HOH:O	2.20	0.42
3:D:96:VAL:HG12	3:D:98:ILE:CD1	2.49	0.42
3:D:100:LEU:HD11	3:D:104:GLY:C	2.40	0.42
3:E:118:ILE:O	3:E:121:LEU:HB2	2.19	0.42
3:D:40:TYR:O	3:D:43:TYR:HB3	2.20	0.42
3:A:114:ILE:HB	3:A:115:PRO:HD3	2.01	0.41
2:H:26:DT:C2'	2:H:27:DT:C5'	2.96	0.41
2:J:5:DA:C1'	2:J:6:DT:H5"	2.49	0.41
3:E:128:ASP:O	3:E:130:LYS:N	2.54	0.41
3:E:137:TYR:CE2	3:F:17:LEU:HD21	2.56	0.41
2:H:6:DT:H2"	2:H:7:DT:O5'	2.20	0.41
3:B:117:THR:O	3:B:121:LEU:HG	2.20	0.41
3:E:52:HIS:O	3:E:54:THR:N	2.53	0.41
3:F:134:SER:HA	3:F:137:TYR:HD1	1.86	0.41
3:E:86:ARG:HG3	3:E:96:VAL:CG1	2.50	0.41
2:J:16:DT:H2"	2:J:17:DA:O5'	2.20	0.41
3:F:19:TYR:CE1	3:F:23:ARG:NH1	2.87	0.41
3:B:128:ASP:CG	3:B:131:GLN:HG3	2.41	0.41
1:I:7:DT:O3'	3:C:94:ARG:NH2	2.54	0.41
3:E:32:LEU:HD12	3:E:118:ILE:HD11	2.03	0.41
3:B:112:VAL:HG13	3:B:113:ASP:H	1.84	0.41
3:A:45:ALA:HB1	3:A:60:MET:HE1	2.02	0.41
3:D:49:LEU:HA	3:D:49:LEU:HD12	1.76	0.41
3:C:89:SER:HA	3:C:97:LEU:CD2	2.50	0.41
1:I:9:DA:H5'	3:C:57:VAL:HB	2.03	0.41
3:D:29:TYR:CB	3:D:33:LEU:HD23	2.46	0.41
3:C:89:SER:HA	3:C:97:LEU:HD23	2.02	0.41
3:B:42:GLN:O	3:B:46:LEU:HD22	2.21	0.41
3:A:101:THR:HB	4:A:156:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:8:MET:HG3	3:D:8:MET:O	2.21	0.41
3:F:92:ASP:OD2	3:F:92:ASP:O	2.39	0.40
3:D:49:LEU:C	3:D:51:GLU:H	2.24	0.40
2:L:11:DT:OP2	3:F:76:LYS:NZ	2.53	0.40
3:F:83:LEU:O	3:F:100:LEU:HD12	2.21	0.40
2:J:2:DA:H2"	2:J:3:DC:C5'	2.46	0.40
3:B:92:ASP:C	3:B:94:ARG:N	2.74	0.40
3:F:50:TRP:CD1	3:F:100:LEU:HD21	2.57	0.40
3:F:28:GLN:HG3	3:F:121:LEU:HD13	2.03	0.40
3:B:50:TRP:CZ2	3:B:108:LYS:HA	2.57	0.40
3:A:138:THR:O	3:A:139:LEU:C	2.59	0.40
3:E:52:HIS:O	3:E:53:GLU:C	2.60	0.40
2:H:5:DA:H2"	2:H:6:DT:C5'	2.52	0.40
3:F:36:LEU:HD22	3:F:110:LYS:HE3	2.03	0.40
3:C:105:ALA:O	3:C:108:LYS:HB3	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
3	A	135/147 (92%)	120 (89%)	13 (10%)	2 (2%)	13 24
3	B	135/147 (92%)	122 (90%)	8 (6%)	5 (4%)	4 5
3	C	136/147 (92%)	119 (88%)	14 (10%)	3 (2%)	8 14
3	D	135/147 (92%)	119 (88%)	14 (10%)	2 (2%)	13 24
3	E	135/147 (92%)	124 (92%)	8 (6%)	3 (2%)	8 14
3	F	136/147 (92%)	123 (90%)	10 (7%)	3 (2%)	8 14
All	All	812/882 (92%)	727 (90%)	67 (8%)	18 (2%)	8 14

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	11	GLU
3	D	53	GLU
3	E	127	GLU
3	F	125	SER
3	A	93	GLU
3	B	92	ASP
3	B	93	GLU
3	B	123	LYS
3	C	125	SER
3	D	52	HIS
3	E	53	GLU
3	E	129	LEU
3	A	53	GLU
3	B	11	GLU
3	B	53	GLU
3	C	53	GLU
3	F	93	GLU
3	F	53	GLU

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	118/135 (87%)	109 (92%)	9 (8%)	16	30
3	B	117/135 (87%)	109 (93%)	8 (7%)	20	37
3	C	113/135 (84%)	105 (93%)	8 (7%)	18	34
3	D	112/135 (83%)	104 (93%)	8 (7%)	18	34
3	E	121/135 (90%)	112 (93%)	9 (7%)	17	32
3	F	118/135 (87%)	107 (91%)	11 (9%)	11	20
All	All	699/810 (86%)	646 (92%)	53 (8%)	16	30

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	49	LEU

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Mol	Chain	Res	Type
3	A	88	ARG
3	A	90	GLU
3	A	94	ARG
3	A	97	LEU
3	A	102	GLU
3	A	106	LEU
3	A	109	GLU
3	A	121	LEU
3	B	36	LEU
3	B	46	LEU
3	B	59	LYS
3	B	64	LEU
3	B	75	LEU
3	B	80	GLN
3	B	85	THR
3	B	124	GLN
3	C	11	GLU
3	C	12	ASN
3	C	14	LEU
3	C	25	MET
3	C	46	LEU
3	C	49	LEU
3	C	103	ASP
3	C	137	TYR
3	D	37	ASN
3	D	46	LEU
3	D	49	LEU
3	D	52	HIS
3	D	54	THR
3	D	75	LEU
3	D	85	THR
3	D	131	GLN
3	E	10	LEU
3	E	13	GLN
3	E	46	LEU
3	E	76	LYS
3	E	81	GLN
3	E	97	LEU
3	E	106	LEU
3	E	119	LEU
3	E	127	GLU
3	F	46	LEU

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Mol	Chain	Res	Type
3	F	49	LEU
3	F	55	LEU
3	F	56	THR
3	F	64	LEU
3	F	75	LEU
3	F	95	SER
3	F	113	ASP
3	F	121	LEU
3	F	123	LYS
3	F	143	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	42	GLN
3	A	80	GLN
3	B	80	GLN
3	C	12	ASN
3	C	13	GLN
3	C	42	GLN
3	C	80	GLN
3	D	12	ASN
3	D	37	ASN
3	D	80	GLN
3	E	12	ASN
3	E	13	GLN
3	E	42	GLN
3	E	52	HIS

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

There are no ligands in this entry.

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	G	29/29 (100%)	0.15	2 (6%) 20 14	18, 45, 114, 148	0
1	I	28/29 (96%)	0.30	2 (7%) 19 13	26, 63, 124, 141	0
1	K	29/29 (100%)	0.11	2 (6%) 20 14	21, 40, 80, 140	0
2	H	29/29 (100%)	0.08	1 (3%) 49 42	17, 45, 109, 150	0
2	J	28/29 (96%)	0.45	3 (10%) 8 5	25, 57, 120, 129	0
2	L	28/29 (96%)	0.02	0 100 100	19, 42, 73, 85	0
3	A	137/147 (93%)	-0.06	2 (1%) 76 71	18, 36, 87, 104	0
3	B	137/147 (93%)	-0.11	2 (1%) 76 71	14, 38, 83, 112	0
3	C	138/147 (93%)	0.01	6 (4%) 39 32	21, 49, 89, 121	0
3	D	137/147 (93%)	0.26	7 (5%) 32 25	29, 53, 100, 129	0
3	E	137/147 (93%)	-0.19	2 (1%) 76 71	14, 36, 97, 115	0
3	F	138/147 (93%)	-0.13	2 (1%) 78 74	17, 35, 78, 102	0
All	All	995/1056 (94%)	-0.00	31 (3%) 52 46	14, 42, 98, 150	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	127	GLU	6.3
1	G	29	DT	4.6
3	D	125	SER	4.6
3	C	125	SER	4.3
3	D	89	SER	4.3
3	F	125	SER	4.3
3	C	126	GLY	4.3
3	D	126	GLY	4.1
1	K	1	DT	3.9
3	D	124	GLN	3.9
3	F	126	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	4	DA	2.8
3	A	125	SER	2.7
3	C	137	TYR	2.7
3	C	8	MET	2.7
2	J	1	DT	2.6
3	A	126	GLY	2.6
1	K	2	DA	2.5
1	I	2	DA	2.4
1	G	1	DT	2.4
3	C	127	GLU	2.4
3	E	137	TYR	2.3
1	I	3	DC	2.3
3	E	121	LEU	2.2
2	H	2	DA	2.2
3	B	126	GLY	2.2
3	D	134	SER	2.1
3	B	137	TYR	2.1
3	D	122	SER	2.1
2	J	28	DG	2.0
3	C	124	GLN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.