Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2022 – 01:17 PM EDT

PDB ID	:	5XVO
Title	:	E. fae Cas1-Cas2/prespacer/target ternary complex revealing DNA sampling and half-integration states
Authors	:	Xiao, Y.; Ng, S.; Nam, K.H.; Ke, A.
Deposited on	:	2017-06-28
Resolution	:	3.10 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:

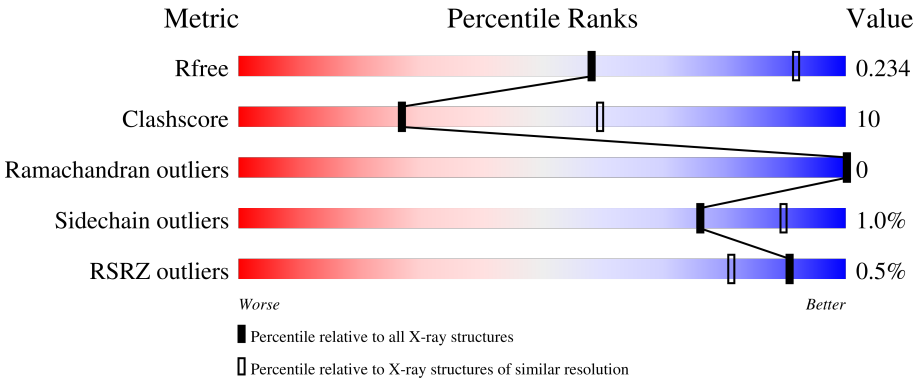
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	288	78% 21%
1	B	288	85% 15%
1	C	288	80% 18% ••
1	D	288	80% 18% •
1	I	288	% 84% 13% •••

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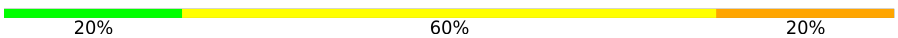
Mol	Chain	Length	Quality of chain
1	J	288	
1	K	288	
1	L	288	
2	E	109	
2	F	109	
2	M	109	
2	N	109	
3	G	28	
3	O	28	
3	P	28	
4	H	5	
5	Q	46	
6	R	69	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 26393 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 protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2358	1515	409	424	10			
1	B	288	Total	C	N	O	S	0	0	0
			2359	1515	409	425	10			
1	C	286	Total	C	N	O	S	0	0	0
			2346	1508	406	422	10			
1	D	287	Total	C	N	O	S	0	0	0
			2351	1510	408	424	9			
1	I	285	Total	C	N	O	S	0	0	0
			2337	1503	404	420	10			
1	J	287	Total	C	N	O	S	0	0	0
			2351	1510	408	424	9			
1	K	285	Total	C	N	O	S	0	0	0
			2337	1503	404	420	10			
1	L	288	Total	C	N	O	S	0	0	0
			2359	1515	409	425	10			

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	106	Total	C	N	O	S	0	0	0
			885	563	160	156	6			
2	F	105	Total	C	N	O	S	0	0	0
			873	554	159	154	6			
2	M	104	Total	C	N	O	S	0	0	0
			862	548	155	153	6			
2	N	105	Total	C	N	O	S	0	0	0
			873	554	159	154	6			

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	25	Total	C	N	O	P	0	2	0
			551	263	94	167	27			
3	O	27	Total	C	N	O	P	0	0	0
			549	261	96	165	27			
3	P	27	Total	C	N	O	P	0	0	0
			549	261	96	165	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	P	0	0	0
			103	48	21	29	5			

- Molecule 5 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	46	Total	C	N	O	P	0	0	0
			938	448	170	274	46			

- Molecule 6 is a DNA chain called DNA (69-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	68	Total	C	N	O	P	0	0	0
			1394	665	247	414	68			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		
7	M	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		

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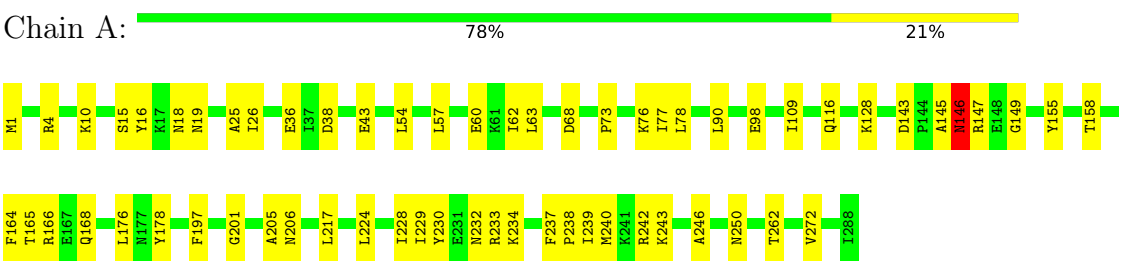
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	2	Total O 2 2	0	0
8	C	1	Total O 1 1	0	0
8	E	1	Total O 1 1	0	0
8	G	1	Total O 1 1	0	0
8	I	1	Total O 1 1	0	0
8	J	1	Total O 1 1	0	0
8	O	1	Total O 1 1	0	0
8	Q	1	Total O 1 1	0	0
8	R	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

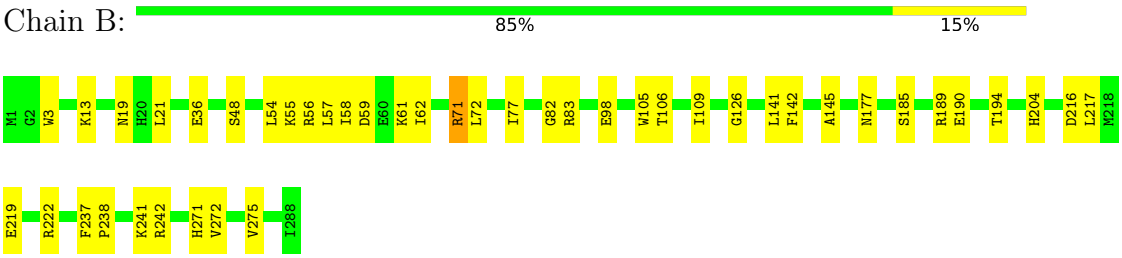
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain A:



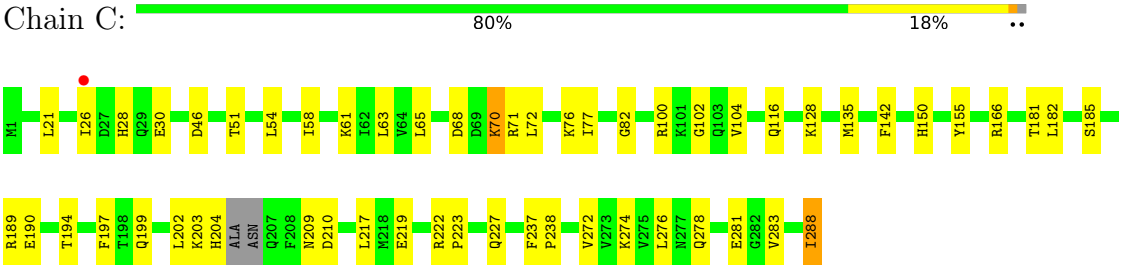
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain B:



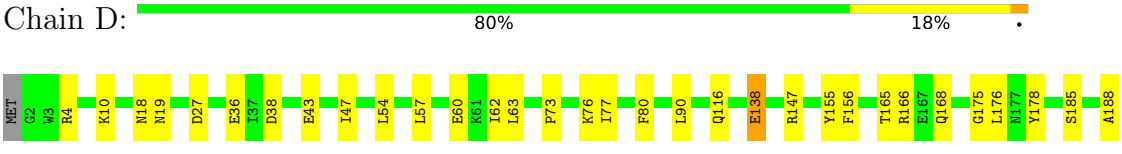
• Molecule 1: CRISPR-associated endonuclease Cas1

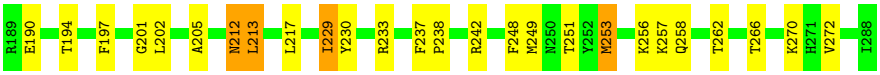
Chain C:



• Molecule 1: CRISPR-associated endonuclease Cas1

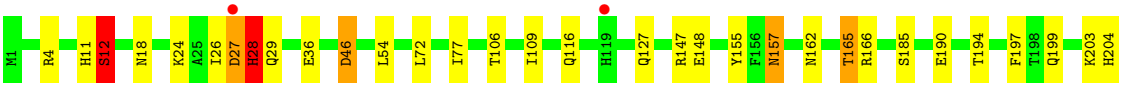
Chain D:

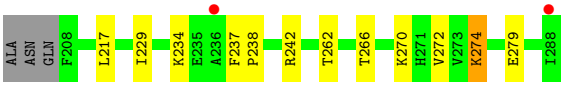




• Molecule 1: CRISPR-associated endonuclease Cas1

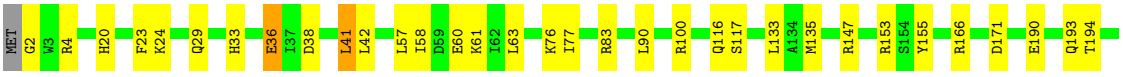
Chain I:





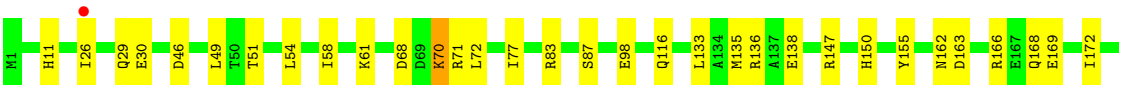
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain J:



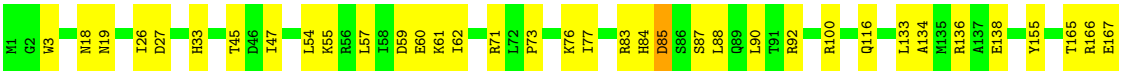
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain K:



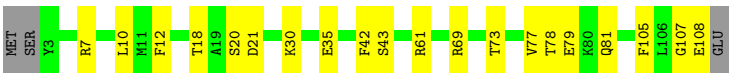
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain L:



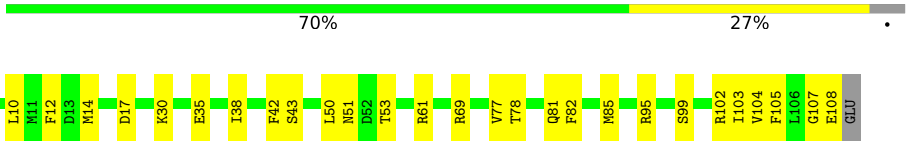
• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain E:



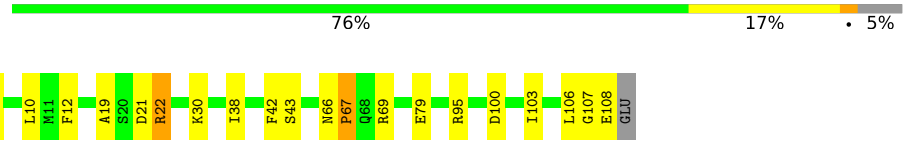
• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain F:



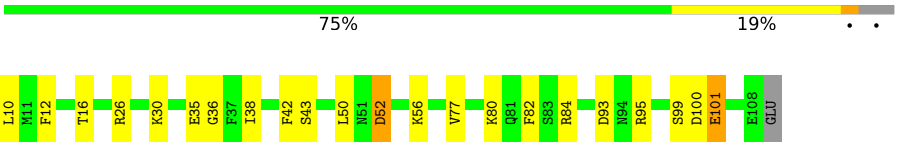
• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain M:



• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain N:



• Molecule 3: DNA (28-MER)

Chain G:

• Molecule 3: DNA (28-MER)

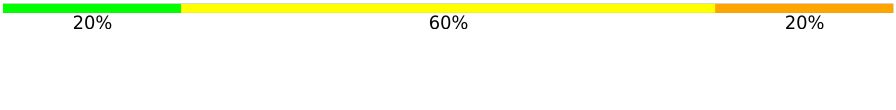
Chain O:

• Molecule 3: DNA (28-MER)

Chain P:

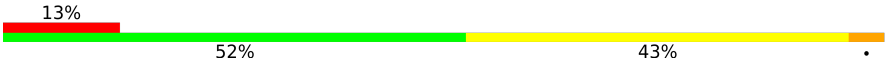
• Molecule 4: DNA (5'-D(P*CP*CP*GP*AP*G)-3')

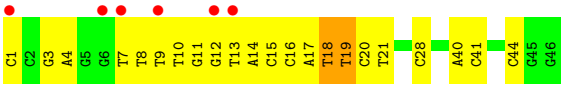
Chain H:



• Molecule 5: DNA (46-MER)

Chain Q:





• Molecule 6: DNA (69-MER)

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.89Å 124.80Å 157.91Å 90.00° 106.50° 90.00°	Depositor
Resolution (Å)	48.95 – 3.10 48.20 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.95-3.10) 97.3 (48.20-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.194 , 0.233 0.200 , 0.234	Depositor DCC
R_{free} test set	4351 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	81.6	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26393	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: MG

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	0.66	0/2406	0.93	7/3247 (0.2%)
1	B	0.65	0/2407	0.86	2/3247 (0.1%)
1	C	0.61	0/2393	0.82	3/3226 (0.1%)
1	D	0.67	2/2399 (0.1%)	0.87	4/3237 (0.1%)
1	I	0.65	0/2384	0.91	12/3214 (0.4%)
1	J	0.61	1/2399 (0.0%)	0.85	6/3237 (0.2%)
1	K	0.62	0/2384	0.86	4/3214 (0.1%)
1	L	0.62	0/2407	0.83	5/3247 (0.2%)
2	E	0.66	0/900	0.87	0/1205
2	F	0.62	0/887	0.84	0/1187
2	M	0.64	0/876	0.90	1/1173 (0.1%)
2	N	0.61	0/887	0.92	1/1187 (0.1%)
3	G	0.59	0/614	0.84	0/943
3	O	0.56	0/613	0.86	1/943 (0.1%)
3	P	0.54	0/613	0.85	0/943
4	H	0.63	0/115	0.95	1/175 (0.6%)
5	Q	0.53	1/1051 (0.1%)	0.90	2/1618 (0.1%)
6	R	0.61	1/1561 (0.1%)	0.90	2/2408 (0.1%)
All	All	0.63	5/27296 (0.0%)	0.87	51/37651 (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	A	0	1
1	D	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	212	ASN	CB-CG	-9.08	1.30	1.51
1	D	212	ASN	CG-OD1	9.01	1.43	1.24
6	R	18	DT	O3'-P	-5.30	1.54	1.61
1	J	36	GLU	CD-OE2	-5.16	1.20	1.25
5	Q	18	DT	O3'-P	-5.05	1.55	1.61

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	146	ASN	N-CA-C	-9.62	85.04	111.00
1	D	212	ASN	CA-CB-CG	-9.30	92.95	113.40
1	A	68	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	I	229	ILE	CG1-CB-CG2	-8.87	91.89	111.40
1	K	70	LYS	N-CA-C	-8.54	87.95	111.00
1	C	70	LYS	N-CA-C	-8.50	88.05	111.00
1	J	41	LEU	CB-CG-CD1	8.07	124.72	111.00
1	L	71	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	71	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	L	71	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	K	49	LEU	CA-CB-CG	6.99	131.38	115.30
1	D	213	LEU	CB-CG-CD1	6.76	122.50	111.00
1	I	46	ASP	CB-CA-C	-6.67	97.07	110.40
1	K	49	LEU	CB-CA-C	-6.52	97.81	110.20
1	C	274	LYS	CB-CG-CD	6.34	128.08	111.60
2	M	67	PRO	N-CA-C	-6.09	96.27	112.10
1	I	165	THR	N-CA-C	5.99	127.19	111.00
1	A	78	LEU	CB-CG-CD1	-5.73	101.25	111.00
1	D	253	MET	CG-SD-CE	-5.72	91.04	100.20
1	I	26	ILE	N-CA-C	-5.72	95.54	111.00
1	L	100	ARG	NE-CZ-NH1	5.65	123.13	120.30
5	Q	19	DT	C4'-C3'-O3'	5.62	123.75	109.70
1	A	146	ASN	CB-CA-C	5.62	121.64	110.40
1	B	71	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	D	229	ILE	CA-CB-CG1	-5.58	100.40	111.00
6	R	21	DT	C4'-C3'-O3'	5.54	123.56	109.70
3	O	14	DC	C5'-C4'-O4'	-5.52	98.82	109.30
1	A	166	ARG	N-CA-CB	-5.46	100.77	110.60
1	I	270	LYS	CB-CA-C	5.44	121.28	110.40
1	A	68	ASP	CB-CG-OD1	5.42	123.18	118.30
1	I	147	ARG	CG-CD-NE	5.38	123.09	111.80
4	H	3	DG	C1'-O4'-C4'	-5.34	104.75	110.10
1	I	46	ASP	N-CA-CB	-5.34	100.99	110.60
1	J	41	LEU	CB-CG-CD2	-5.29	102.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	166	ARG	N-CA-CB	-5.28	101.09	110.60
1	L	222	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	K	166	ARG	N-CA-CB	-5.24	101.17	110.60
1	J	153	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	I	157	ASN	CB-CA-C	5.23	120.86	110.40
1	I	28	HIS	N-CA-C	5.20	125.04	111.00
2	N	52	ASP	CB-CG-OD2	5.20	122.98	118.30
1	I	27	ASP	CB-CG-OD2	5.19	122.97	118.30
1	L	92	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	J	83	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	I	12	SER	CB-CA-C	-5.12	100.36	110.10
1	C	166	ARG	N-CA-CB	-5.11	101.40	110.60
5	Q	28	DC	C1'-O4'-C4'	-5.11	104.99	110.10
1	A	98	GLU	CA-CB-CG	-5.06	102.27	113.40
1	J	100	ARG	NE-CZ-NH1	5.06	122.83	120.30
6	R	21	DT	O4'-C4'-C3'	-5.06	102.48	104.50
1	I	27	ASP	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASN	Peptide
1	D	212	ASN	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2358	0	2386	59	0
1	B	2359	0	2386	37	0
1	C	2346	0	2374	57	0
1	D	2351	0	2374	63	0
1	I	2337	0	2366	35	1
1	J	2351	0	2374	35	0
1	K	2337	0	2366	43	1
1	L	2359	0	2386	53	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	885	0	898	26	0
2	F	873	0	889	31	0
2	M	862	0	876	24	0
2	N	873	0	889	33	0
3	G	551	0	308	13	0
3	O	549	0	305	11	0
3	P	549	0	305	9	0
4	H	103	0	56	7	0
5	Q	938	0	519	21	1
6	R	1394	0	770	28	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
8	A	1	0	0	1	0
8	B	2	0	0	2	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
8	I	1	0	0	0	0
8	J	1	0	0	1	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	4	0	0	0	0
All	All	26393	0	24827	522	2

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 10.

All (522) 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:E:77:VAL:HG13	2:E:81:GLN:OE1	1.23	1.35
2:F:77:VAL:HG13	2:F:81:GLN:OE1	1.24	1.28
2:N:52:ASP:OD2	2:N:56:LYS:NZ	1.69	1.22
1:A:176:LEU:HD21	1:A:229:ILE:HD11	1.27	1.10
1:A:128:LYS:CD	1:A:158:THR:HG21	1.82	1.09
3:G:25[A]:DT:H5"	3:G:25[A]:DT:H6	1.17	1.09
1:I:274:LYS:HE3	1:I:279:GLU:OE1	1.53	1.09
1:C:65:LEU:HD21	1:C:76:LYS:HD3	1.31	1.09
1:D:253:MET:HE1	1:D:256:LYS:C	1.73	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LYS:NZ	1:D:188:ALA:HB3	1.66	1.08
1:A:230:TYR:O	1:A:233:ARG:HG3	1.51	1.08
2:N:52:ASP:CG	2:N:56:LYS:NZ	2.07	1.07
1:A:176:LEU:CD2	1:A:229:ILE:HD11	1.84	1.06
1:B:238:PRO:HA	1:B:241:LYS:HE3	1.07	1.06
1:C:65:LEU:HD23	1:C:76:LYS:CG	1.84	1.06
1:A:128:LYS:HD2	1:A:158:THR:CG2	1.86	1.05
1:D:76:LYS:HZ1	1:D:188:ALA:HB3	1.20	1.04
1:D:76:LYS:HZ1	1:D:188:ALA:CB	1.70	1.04
1:C:65:LEU:HD23	1:C:76:LYS:HG2	1.07	1.03
2:N:52:ASP:OD1	2:N:56:LYS:NZ	1.90	1.03
1:D:253:MET:CE	1:D:256:LYS:C	2.26	1.02
2:E:77:VAL:CG1	2:E:81:GLN:HB2	1.90	1.02
2:F:77:VAL:CG1	2:F:81:GLN:HB2	1.93	0.99
1:B:238:PRO:HA	1:B:241:LYS:CE	1.91	0.99
2:E:105:PHE:CG	2:E:108:GLU:OE1	2.17	0.97
1:B:238:PRO:CA	1:B:241:LYS:HE3	1.93	0.97
1:B:238:PRO:O	1:B:241:LYS:HG2	1.64	0.97
1:I:18:ASN:OD1	1:I:18:ASN:O	1.83	0.95
1:C:104:VAL:HG11	1:C:276:LEU:HD21	1.51	0.92
1:D:253:MET:CE	1:D:257:LYS:N	2.33	0.91
2:N:52:ASP:CG	2:N:56:LYS:HZ2	1.68	0.91
1:A:176:LEU:CD2	1:A:229:ILE:CD1	2.49	0.91
1:B:3:TRP:CH2	1:B:36:GLU:HG2	2.04	0.91
2:E:77:VAL:CG1	2:E:81:GLN:OE1	2.17	0.91
1:L:134:ALA:O	1:L:138:GLU:OE1	1.89	0.91
2:F:77:VAL:CG1	2:F:81:GLN:OE1	2.18	0.90
1:C:65:LEU:CD2	1:C:76:LYS:HG2	2.00	0.90
1:C:76:LYS:HG3	1:D:80:PHE:CZ	2.06	0.90
1:D:253:MET:HE1	1:D:257:LYS:N	1.88	0.89
1:C:65:LEU:CD2	1:C:76:LYS:HD3	2.04	0.88
1:C:76:LYS:HE2	1:D:80:PHE:CE1	2.09	0.88
2:N:43:SER:OG	3:O:15:DC:OP1	1.91	0.87
1:B:126:GLY:HA2	8:B:301:HOH:O	1.73	0.87
1:C:63:LEU:HD11	1:C:76:LYS:HD2	1.57	0.87
2:F:77:VAL:HG12	2:F:81:GLN:HB2	1.54	0.87
3:G:25[A]:DT:H5"	3:G:25[A]:DT:C6	2.08	0.86
2:E:77:VAL:HG12	2:E:81:GLN:HB2	1.55	0.86
2:F:12:PHE:O	2:F:43:SER:OG	1.94	0.86
2:M:19:ALA:HA	2:M:22:ARG:NH2	1.90	0.86
2:E:18:THR:HG22	2:E:20:SER:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:12:PHE:O	2:M:43:SER:OG	1.93	0.85
2:E:12:PHE:O	2:E:43:SER:OG	1.94	0.84
2:E:77:VAL:CG1	2:E:81:GLN:CB	2.56	0.84
1:B:126:GLY:CA	8:B:301:HOH:O	2.26	0.83
2:N:7:ARG:HB3	2:N:77:VAL:HG23	1.59	0.83
1:C:70:LYS:HB3	3:G:25[A]:DT:C4	2.15	0.82
1:I:238:PRO:O	1:I:242:ARG:HG3	1.79	0.82
1:A:230:TYR:CE1	1:A:233:ARG:NH1	2.48	0.82
2:F:77:VAL:CG1	2:F:81:GLN:CB	2.57	0.81
2:N:52:ASP:CG	2:N:56:LYS:HZ3	1.76	0.80
1:K:162:ASN:O	1:K:163:ASP:HB2	1.81	0.80
2:E:105:PHE:CD2	2:E:108:GLU:OE1	2.34	0.80
1:L:88:LEU:O	1:L:88:LEU:HD12	1.81	0.80
1:I:190:GLU:HG3	1:I:266:THR:HA	1.62	0.80
1:A:128:LYS:HD2	1:A:158:THR:HG21	0.90	0.79
1:L:26:ILE:HD12	1:L:27:ASP:HA	1.64	0.79
2:N:38:ILE:HG23	2:N:95:ARG:HH12	1.49	0.78
1:C:65:LEU:CD2	1:C:76:LYS:CG	2.59	0.78
1:K:26:ILE:HG12	3:P:2:DT:O4	1.83	0.78
1:I:24:LYS:HD2	1:I:29:GLN:HG3	1.65	0.78
2:M:66:ASN:OD1	2:M:67:PRO:O	2.01	0.78
1:A:143:ASP:OD1	1:A:145:ALA:O	2.02	0.78
1:C:128:LYS:H	1:C:128:LYS:HD2	1.48	0.78
1:L:166:ARG:HG2	1:L:173:ASN:OD1	1.81	0.78
1:A:4:ARG:NH1	1:A:36:GLU:OE1	2.17	0.77
1:C:65:LEU:HD21	1:C:76:LYS:CD	2.12	0.77
1:D:253:MET:HE2	1:D:256:LYS:HA	1.67	0.77
1:L:251:THR:CG2	1:L:258:GLN:HB3	2.14	0.77
1:C:76:LYS:HE2	1:D:80:PHE:HE1	1.50	0.77
1:J:41:LEU:C	1:J:41:LEU:HD23	2.02	0.77
1:B:106:THR:HG21	1:B:141:LEU:HA	1.66	0.77
1:A:146:ASN:HD22	1:A:149:GLY:HA3	1.48	0.76
1:C:65:LEU:CD2	1:C:76:LYS:CD	2.64	0.76
1:D:253:MET:HE2	1:D:256:LYS:CA	2.15	0.76
1:J:41:LEU:HD23	1:J:42:LEU:N	2.00	0.76
1:I:109:ILE:HD11	1:I:148:GLU:CD	2.07	0.75
1:J:20:HIS:HD2	1:J:33:HIS:HA	1.51	0.75
1:K:133:LEU:HD13	1:K:136:ARG:NH2	2.01	0.75
1:J:58:ILE:HG12	1:J:77:ILE:HD12	1.70	0.74
1:K:26:ILE:CG1	3:P:2:DT:O4	2.37	0.73
1:D:253:MET:HE1	1:D:256:LYS:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ARG:NH1	1:D:36:GLU:OE1	2.22	0.73
2:N:80:LYS:NZ	5:Q:21:DT:OP2	2.22	0.72
1:C:135:MET:HE1	1:C:150:HIS:HB3	1.71	0.72
1:A:176:LEU:HG	1:A:229:ILE:HD13	1.71	0.72
1:K:168:GLN:OE1	1:K:169:GLU:N	2.23	0.72
1:I:274:LYS:CE	1:I:279:GLU:OE1	2.36	0.72
1:C:182:LEU:HD23	3:G:25[B]:DT:C2	2.25	0.71
1:K:58:ILE:O	1:K:61:LYS:HD3	1.90	0.71
1:B:177:ASN:HB3	6:R:4:DC:H5'	1.73	0.71
1:I:203:LYS:O	1:I:204:HIS:HB2	1.91	0.70
4:H:5:DG:O3'	6:R:6:DG:P	2.49	0.70
1:C:100:ARG:HE	1:C:278:GLN:HG2	1.56	0.70
1:A:176:LEU:HG	1:A:229:ILE:CD1	2.22	0.70
2:E:35:GLU:OE1	2:E:61:ARG:NH1	2.23	0.70
1:A:43:GLU:OE2	1:A:242:ARG:NH2	2.26	0.69
1:K:11:HIS:HE1	3:P:2:DT:H2"	1.56	0.69
1:A:90:LEU:HD22	1:A:197:PHE:CE2	2.28	0.69
5:Q:16:DC:H2"	5:Q:17:DA:O5'	1.92	0.68
1:D:43:GLU:OE2	1:D:242:ARG:NH2	2.26	0.68
1:K:135:MET:HE1	1:K:150:HIS:HB3	1.76	0.68
2:N:52:ASP:OD1	2:N:56:LYS:CD	2.42	0.68
6:R:21:DT:H2'	6:R:22:DG:C8	2.29	0.68
1:B:238:PRO:O	1:B:241:LYS:CG	2.39	0.67
1:J:63:LEU:CD1	1:J:76:LYS:HE2	2.24	0.67
1:K:11:HIS:CE1	3:P:2:DT:H2"	2.29	0.67
1:L:3:TRP:CD1	2:N:50:LEU:HD13	2.30	0.67
2:M:19:ALA:HA	2:M:22:ARG:HH22	1.59	0.66
1:I:116:GLN:HB3	1:I:155:TYR:CD2	2.31	0.66
1:J:24:LYS:HG2	1:J:29:GLN:HG2	1.78	0.66
5:Q:19:DT:H4'	5:Q:20:DC:OP1	1.95	0.66
1:K:71:ARG:HD2	3:O:26:DT:H71	1.78	0.66
1:L:76:LYS:HE3	1:L:188:ALA:HB3	1.77	0.66
1:A:146:ASN:ND2	1:A:149:GLY:HA3	2.11	0.66
1:J:63:LEU:HD13	1:J:76:LYS:HE2	1.78	0.66
5:Q:17:DA:H2"	5:Q:18:DT:OP2	1.97	0.65
1:A:201:GLY:H	1:A:205:ALA:HA	1.61	0.65
1:A:63:LEU:CD1	1:A:76:LYS:HE2	2.25	0.65
1:C:76:LYS:HE2	1:D:80:PHE:CZ	2.31	0.65
1:C:281:GLU:HA	1:C:281:GLU:OE1	1.97	0.65
2:N:7:ARG:HB3	2:N:77:VAL:CG2	2.25	0.65
2:F:35:GLU:OE2	2:F:61:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:ILE:HD11	1:I:148:GLU:CG	2.26	0.65
1:A:164:PHE:HA	1:A:168:GLN:NE2	2.11	0.65
1:A:224:LEU:O	1:A:228:ILE:CD1	2.45	0.65
1:A:229:ILE:HG22	1:A:240:MET:HE2	1.78	0.65
1:J:41:LEU:C	1:J:41:LEU:CD2	2.65	0.64
1:A:145:ALA:O	1:A:147:ARG:N	2.29	0.64
1:L:168:GLN:OE1	1:L:168:GLN:HA	1.97	0.64
2:N:42:PHE:O	3:O:16:DT:OP1	2.15	0.64
3:G:25[A]:DT:H6	3:G:25[A]:DT:C5'	2.04	0.64
1:A:176:LEU:CG	1:A:229:ILE:CD1	2.76	0.64
1:J:61:LYS:HD2	1:J:193:GLN:NE2	2.12	0.64
2:N:12:PHE:O	2:N:43:SER:HB3	1.98	0.64
2:E:77:VAL:HG11	2:E:81:GLN:CB	2.28	0.64
1:I:4:ARG:NH1	1:I:36:GLU:OE2	2.31	0.63
1:B:105:TRP:CZ2	1:B:109:ILE:HG13	2.34	0.63
1:A:63:LEU:HD13	1:A:76:LYS:HE2	1.81	0.63
1:A:205:ALA:O	1:A:206:ASN:HB3	1.96	0.63
5:Q:16:DC:C2'	5:Q:17:DA:O5'	2.47	0.63
1:L:26:ILE:HD12	1:L:27:ASP:CA	2.28	0.63
1:K:46:ASP:OD2	3:O:27:DC:N3	2.31	0.63
2:E:7:ARG:NE	2:E:79:GLU:OE1	2.24	0.62
5:Q:9:DT:H2"	5:Q:10:DT:OP2	1.99	0.62
2:N:38:ILE:HG23	2:N:95:ARG:NH1	2.14	0.62
2:N:38:ILE:CG2	2:N:95:ARG:NH1	2.62	0.62
1:C:203:LYS:O	1:C:204:HIS:HB3	1.99	0.62
1:D:76:LYS:NZ	1:D:188:ALA:CB	2.41	0.62
1:K:83:ARG:HD2	1:K:87:SER:CB	2.30	0.62
1:A:1:MET:N	8:A:301:HOH:O	2.32	0.62
2:F:107:GLY:O	2:F:108:GLU:HB3	2.01	0.61
1:J:171:ASP:HB3	1:J:240:MET:CE	2.30	0.61
1:L:165:THR:O	1:L:168:GLN:HB2	2.01	0.61
1:B:238:PRO:C	1:B:241:LYS:HG2	2.21	0.60
2:M:7:ARG:NE	2:M:79:GLU:OE2	2.27	0.60
1:L:251:THR:HG21	1:L:258:GLN:HB3	1.81	0.60
1:C:61:LYS:HE2	1:C:82:GLY:HA3	1.84	0.60
1:A:230:TYR:CZ	1:A:233:ARG:NH1	2.68	0.60
4:H:5:DG:HO3'	6:R:6:DG:P	2.25	0.60
6:R:38:DA:H2"	6:R:39:DA:C8	2.37	0.60
2:E:18:THR:HG22	2:E:20:SER:N	2.15	0.60
1:L:166:ARG:NH1	1:L:177:ASN:OD1	2.35	0.60
2:N:52:ASP:OD1	2:N:56:LYS:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LYS:HG2	1:C:204:HIS:N	2.17	0.59
1:L:251:THR:HG22	1:L:258:GLN:OE1	2.02	0.59
1:B:204:HIS:ND1	1:B:216:ASP:OD1	2.19	0.59
4:H:4:DA:H2'	4:H:5:DG:C8	2.37	0.59
1:J:205:ALA:O	1:J:207:GLN:N	2.35	0.59
2:F:77:VAL:HG11	2:F:81:GLN:CB	2.33	0.59
1:A:145:ALA:O	1:A:146:ASN:C	2.38	0.59
1:K:68:ASP:OD1	1:K:70:LYS:O	2.21	0.59
1:K:133:LEU:CD1	1:K:136:ARG:HH22	2.15	0.59
4:H:5:DG:O3'	6:R:6:DG:OP2	2.21	0.59
1:J:23:PHE:CG	2:M:106:LEU:HD13	2.37	0.59
2:M:5:TYR:CE2	2:M:100:ASP:HB2	2.38	0.59
1:D:165:THR:N	1:D:168:GLN:OE1	2.27	0.59
1:D:253:MET:HE3	1:D:257:LYS:N	2.17	0.59
1:D:251:THR:HG23	1:D:258:GLN:OE1	2.03	0.59
1:C:76:LYS:HG3	1:D:80:PHE:HZ	1.67	0.58
1:L:171:ASP:HB3	1:L:240:MET:CE	2.32	0.58
1:C:288:ILE:OXT	1:C:288:ILE:HG22	2.02	0.58
1:C:102:GLY:HA2	1:C:142:PHE:CE1	2.38	0.58
1:D:63:LEU:CD1	1:D:76:LYS:HD2	2.34	0.58
1:A:176:LEU:CG	1:A:229:ILE:HD13	2.34	0.58
1:C:68:ASP:OD1	1:C:70:LYS:O	2.21	0.58
1:J:58:ILE:HG12	1:J:77:ILE:CD1	2.34	0.58
2:M:108:GLU:OE2	2:M:108:GLU:HA	2.03	0.58
1:L:168:GLN:CB	1:L:173:ASN:ND2	2.67	0.58
1:L:251:THR:HG23	1:L:258:GLN:HB3	1.86	0.58
2:N:84:ARG:NH2	5:Q:21:DT:OP1	2.35	0.57
1:D:76:LYS:HZ2	1:D:188:ALA:HB3	1.63	0.57
2:E:30:LYS:HE3	3:G:6:DA:OP2	2.05	0.57
1:I:11:HIS:HA	1:I:46:ASP:HB3	1.87	0.57
1:C:227:GLN:HE22	1:C:288:ILE:HG21	1.68	0.57
1:L:171:ASP:HB3	1:L:240:MET:HE3	1.86	0.57
3:G:26[B]:DT:O2	3:G:26[B]:DT:O4'	2.19	0.57
1:D:266:THR:HG22	1:D:270:LYS:HE3	1.86	0.56
2:F:38:ILE:CG2	2:F:95:ARG:NH2	2.68	0.56
1:K:266:THR:HG22	1:K:270:LYS:HE3	1.86	0.56
2:E:77:VAL:HG11	2:E:81:GLN:HB3	1.85	0.56
1:L:133:LEU:HD22	1:L:136:ARG:NH2	2.20	0.56
2:M:107:GLY:O	2:M:108:GLU:HB3	2.04	0.56
1:A:164:PHE:HA	1:A:168:GLN:HE22	1.71	0.56
1:C:181:THR:HG22	3:G:25[A]:DT:O4	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LYS:NZ	1:D:185:SER:HA	2.20	0.56
1:C:128:LYS:HD2	1:C:128:LYS:N	2.17	0.56
1:I:72:LEU:HD23	1:I:185:SER:HA	1.88	0.56
1:A:229:ILE:CG2	1:A:240:MET:HE2	2.35	0.56
1:D:10:LYS:NZ	1:D:27:ASP:OD2	2.38	0.56
2:M:95:ARG:HH21	2:M:95:ARG:HB2	1.72	0.55
2:F:77:VAL:HG11	2:F:81:GLN:HB3	1.89	0.55
1:I:12:SER:HB3	1:I:24:LYS:O	2.07	0.55
5:Q:14:DA:H1'	5:Q:15:DC:H5'	1.88	0.55
1:A:201:GLY:N	1:A:205:ALA:HA	2.21	0.55
2:E:42:PHE:O	2:E:43:SER:HB3	2.06	0.55
1:K:133:LEU:CD1	1:K:136:ARG:NH2	2.69	0.55
1:A:176:LEU:HD23	1:A:229:ILE:CD1	2.35	0.54
1:L:84:HIS:CD2	1:L:85:ASP:OD1	2.60	0.54
1:B:61:LYS:HE2	1:B:82:GLY:HA3	1.89	0.54
1:D:202:LEU:HD12	1:D:202:LEU:N	2.21	0.54
2:E:107:GLY:O	2:E:108:GLU:HB3	2.07	0.54
1:B:58:ILE:O	1:B:61:LYS:HD2	2.07	0.54
1:J:171:ASP:HB3	1:J:240:MET:HE1	1.88	0.54
2:E:43:SER:HB2	6:R:-8:DC:H5"	1.88	0.54
1:L:83:ARG:HG2	1:L:85:ASP:H	1.72	0.54
5:Q:19:DT:H1'	5:Q:20:DC:H5'	1.89	0.54
1:C:104:VAL:HG11	1:C:276:LEU:CD2	2.33	0.54
1:C:58:ILE:O	1:C:61:LYS:HD2	2.07	0.54
1:D:253:MET:HE1	1:D:257:LYS:CA	2.37	0.54
2:N:52:ASP:OD1	2:N:56:LYS:CE	2.56	0.54
6:R:3:DT:H5"	6:R:3:DT:C6	2.43	0.54
1:C:28:HIS:CD2	1:C:30:GLU:HG3	2.42	0.54
5:Q:7:DT:H2"	5:Q:8:DT:OP2	2.07	0.54
5:Q:14:DA:H2"	5:Q:15:DC:OP2	2.08	0.54
1:A:224:LEU:O	1:A:228:ILE:HD13	2.07	0.54
1:C:223:PRO:HB2	1:C:288:ILE:HD11	1.90	0.54
6:R:3:DT:O2	6:R:3:DT:H2'	2.07	0.54
1:A:176:LEU:CD2	1:A:229:ILE:HD13	2.36	0.53
2:F:30:LYS:CE	6:R:-17:DA:OP2	2.57	0.53
2:N:38:ILE:CG2	2:N:95:ARG:HH12	2.16	0.53
2:F:42:PHE:O	2:F:43:SER:HB3	2.08	0.53
1:K:83:ARG:HD2	1:K:87:SER:HB2	1.90	0.53
6:R:28:DA:H2"	6:R:29:DA:OP2	2.08	0.53
1:A:224:LEU:O	1:A:228:ILE:HD12	2.08	0.53
6:R:3:DT:OP1	6:R:3:DT:C4'	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:ARG:O	1:I:166:ARG:HG3	2.09	0.52
1:K:172:ILE:HA	1:K:229:ILE:HD11	1.91	0.52
1:L:168:GLN:HB2	1:L:173:ASN:ND2	2.25	0.52
2:M:42:PHE:O	2:M:43:SER:HB3	2.09	0.52
1:A:239:ILE:HG23	1:A:243:LYS:HE3	1.91	0.52
1:I:28:HIS:ND1	1:I:29:GLN:N	2.57	0.52
4:H:5:DG:H3'	6:R:6:DG:OP1	2.08	0.52
5:Q:11:DG:H2"	5:Q:12:DG:OP2	2.09	0.52
1:C:46:ASP:HA	6:R:-20:DC:O4'	2.10	0.52
1:D:90:LEU:HD21	1:D:197:PHE:CE2	2.44	0.52
1:D:253:MET:CE	1:D:256:LYS:CA	2.79	0.51
1:K:230:TYR:O	1:K:233:ARG:NH1	2.43	0.51
1:J:135:MET:HE3	1:J:147:ARG:HH21	1.74	0.51
1:D:230:TYR:O	1:D:233:ARG:NH1	2.43	0.51
5:Q:40:DA:H2'	5:Q:41:DC:C6	2.45	0.51
1:A:232:ASN:OD1	1:A:243:LYS:HD2	2.11	0.51
1:C:104:VAL:HG23	1:C:283:VAL:CG2	2.40	0.51
1:J:90:LEU:HD21	1:J:197:PHE:CE2	2.44	0.51
2:F:77:VAL:HG13	2:F:81:GLN:CD	2.18	0.51
1:C:72:LEU:HD23	1:C:185:SER:HA	1.93	0.51
2:E:105:PHE:CB	2:E:108:GLU:OE1	2.58	0.51
1:K:133:LEU:HD13	1:K:136:ARG:HH21	1.75	0.51
1:D:166:ARG:O	1:D:166:ARG:HG3	2.11	0.51
1:K:219:GLU:OE2	1:K:222:ARG:HD2	2.11	0.51
2:M:95:ARG:HH21	2:M:95:ARG:CB	2.23	0.50
1:C:51:THR:OG1	1:D:47:ILE:HB	2.12	0.50
1:D:217:LEU:HD11	1:D:272:VAL:HG11	1.93	0.50
1:I:165:THR:O	1:I:166:ARG:HB3	2.11	0.50
1:J:217:LEU:HD11	1:J:272:VAL:HG11	1.93	0.50
1:K:72:LEU:HD23	1:K:185:SER:HA	1.92	0.50
1:D:202:LEU:N	1:D:202:LEU:CD1	2.75	0.50
1:D:248:PHE:O	2:F:102:ARG:NH2	2.45	0.50
2:F:38:ILE:HG21	2:F:95:ARG:NH2	2.27	0.50
3:G:26[A]:DT:O4'	3:G:26[A]:DT:O2	2.27	0.50
1:B:238:PRO:HA	1:B:241:LYS:CD	2.41	0.50
1:C:219:GLU:OE2	1:C:222:ARG:HD2	2.12	0.50
1:C:102:GLY:HA2	1:C:142:PHE:HE1	1.75	0.50
1:L:90:LEU:HD21	1:L:197:PHE:CE2	2.47	0.50
2:N:10:LEU:HD23	2:N:10:LEU:C	2.32	0.50
2:N:80:LYS:NZ	5:Q:21:DT:P	2.84	0.50
2:F:30:LYS:HE2	6:R:-17:DA:OP2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:ASP:HB3	1:J:240:MET:HE3	1.95	0.49
1:D:175:GLY:C	1:D:229:ILE:CD1	2.81	0.49
1:J:38:ASP:OD2	1:J:262:THR:HG21	2.11	0.49
1:D:63:LEU:HD11	1:D:76:LYS:HD2	1.94	0.49
2:M:10:LEU:C	2:M:10:LEU:HD23	2.32	0.49
1:D:38:ASP:OD2	1:D:262:THR:HG21	2.12	0.49
3:O:5:DT:H2'	3:O:6:DA:C8	2.48	0.49
1:A:176:LEU:HD21	1:A:229:ILE:CD1	2.15	0.49
1:B:237:PHE:CE2	6:R:3:DT:C4	3.00	0.49
1:I:24:LYS:HD2	1:I:29:GLN:CG	2.39	0.49
1:D:76:LYS:HZ3	1:D:185:SER:HA	1.78	0.49
1:L:83:ARG:HG2	1:L:84:HIS:N	2.27	0.49
2:M:43:SER:HB2	3:P:15:DC:H5"	1.95	0.49
1:I:217:LEU:HD11	1:I:272:VAL:HG11	1.93	0.49
5:Q:19:DT:H1'	5:Q:20:DC:C5'	2.43	0.49
6:R:44:DC:H2"	6:R:45:DG:C8	2.47	0.49
1:C:65:LEU:HD23	1:C:76:LYS:CD	2.36	0.48
2:E:21:ASP:HB3	2:E:69:ARG:HD3	1.93	0.48
1:I:203:LYS:HG2	1:I:204:HIS:N	2.28	0.48
1:L:168:GLN:HB2	1:L:173:ASN:HD21	1.77	0.48
2:E:10:LEU:C	2:E:10:LEU:HD23	2.34	0.48
2:F:43:SER:HB2	3:G:15:DC:H5"	1.96	0.48
3:G:5:DT:H2'	3:G:6:DA:C8	2.48	0.48
1:L:88:LEU:HD12	1:L:88:LEU:C	2.34	0.48
6:R:35:DC:H2"	6:R:36:DC:OP2	2.13	0.48
1:C:217:LEU:HD11	1:C:272:VAL:HG11	1.95	0.48
1:D:54:LEU:HD22	1:D:77:ILE:HD11	1.96	0.48
1:A:217:LEU:HD11	1:A:272:VAL:HG11	1.95	0.48
1:K:217:LEU:HD11	1:K:272:VAL:HG11	1.94	0.48
2:E:77:VAL:HG12	2:E:78:THR:N	2.29	0.48
1:J:4:ARG:NH1	1:J:36:GLU:OE2	2.46	0.48
1:J:20:HIS:HD2	1:J:33:HIS:CA	2.23	0.48
2:F:77:VAL:HG12	2:F:78:THR:N	2.29	0.48
1:I:157:ASN:HB2	1:I:162:ASN:HA	1.96	0.48
1:I:197:PHE:HB2	1:I:199:GLN:OE1	2.14	0.48
5:Q:19:DT:H2"	5:Q:20:DC:H5'	1.96	0.48
1:A:145:ALA:HB1	1:A:147:ARG:NH1	2.28	0.48
1:I:165:THR:O	1:I:166:ARG:CB	2.61	0.48
1:J:77:ILE:O	1:J:77:ILE:HG13	2.13	0.48
1:L:217:LEU:HD11	1:L:272:VAL:HG11	1.96	0.47
2:N:99:SER:OG	2:N:101:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:26:ILE:HG13	3:P:2:DT:O4	2.13	0.47
6:R:30:DT:H2”	6:R:31:DG:C8	2.49	0.47
5:Q:11:DG:N2	6:R:37:DA:C2	2.83	0.47
1:D:76:LYS:HZ1	1:D:188:ALA:HB1	1.68	0.47
1:J:249:MET:HG3	2:M:103:ILE:CD1	2.44	0.47
1:L:26:ILE:HD12	1:L:27:ASP:CB	2.44	0.47
1:B:217:LEU:HD11	1:B:272:VAL:HG11	1.97	0.47
1:B:13:LYS:HG3	1:B:48:SER:OG	2.15	0.47
1:A:233:ARG:HH21	1:A:234:LYS:NZ	2.13	0.47
2:E:77:VAL:HG13	2:E:81:GLN:CD	2.19	0.46
1:A:10:LYS:HE2	1:A:25:ALA:HB1	1.97	0.46
1:K:51:THR:OG1	1:L:47:ILE:HB	2.14	0.46
1:L:26:ILE:HA	1:L:27:ASP:HA	1.61	0.46
1:B:271:HIS:O	1:B:275:VAL:HG13	2.16	0.46
6:R:44:DC:H4’	6:R:44:DC:OP1	2.15	0.46
1:I:203:LYS:O	1:I:204:HIS:CB	2.58	0.46
1:C:197:PHE:HB2	1:C:199:GLN:OE1	2.15	0.46
1:B:106:THR:CG2	1:B:142:PHE:H	2.28	0.46
1:J:249:MET:HG3	2:M:103:ILE:HD11	1.98	0.46
2:N:12:PHE:O	2:N:43:SER:CB	2.64	0.46
1:A:109:ILE:HD12	1:A:109:ILE:HA	1.77	0.46
1:K:71:ARG:NH2	3:O:26:DT:C4	2.84	0.46
3:O:27:DC:H2”	3:O:28:DC:H5”	1.98	0.46
1:C:181:THR:CG2	3:G:25[A]:DT:O4	2.64	0.45
2:N:26:ARG:NH1	3:P:8:DC:OP2	2.46	0.45
1:B:145:ALA:O	5:Q:44:DC:H5”	2.17	0.45
2:F:104:VAL:HG12	2:F:105:PHE:N	2.31	0.45
1:J:2:GLY:N	8:J:301:HOH:O	2.49	0.45
1:K:178:TYR:CE1	1:K:182:LEU:HD11	2.51	0.45
1:B:19:ASN:OD1	1:B:56:ARG:NH2	2.48	0.45
1:K:68:ASP:O	1:K:70:LYS:O	2.34	0.45
6:R:-18:DT:H2’	6:R:-17:DA:C8	2.52	0.45
1:A:54:LEU:HD22	1:A:77:ILE:HD11	1.98	0.45
1:I:190:GLU:O	1:I:194:THR:HG23	2.16	0.45
2:F:4:ARG:HA	2:F:4:ARG:HD2	1.60	0.45
2:F:38:ILE:CG2	2:F:95:ARG:HH22	2.29	0.45
1:C:102:GLY:CA	1:C:142:PHE:CE1	2.99	0.45
1:K:225:VAL:O	1:K:229:ILE:HG22	2.16	0.45
1:A:116:GLN:HB3	1:A:155:TYR:CD1	2.52	0.45
1:L:168:GLN:CB	1:L:173:ASN:HD22	2.29	0.45
1:B:72:LEU:HD23	1:B:185:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:THR:O	1:D:166:ARG:CB	2.64	0.44
2:F:10:LEU:C	2:F:10:LEU:HD23	2.37	0.44
2:N:38:ILE:HG21	2:N:95:ARG:NH1	2.31	0.44
4:H:5:DG:H3'	6:R:6:DG:P	2.57	0.44
1:B:54:LEU:HD22	1:B:77:ILE:HD11	1.99	0.44
1:K:51:THR:HB	1:L:45:THR:HA	1.99	0.44
1:L:61:LYS:HD3	1:L:193:GLN:NE2	2.31	0.44
1:L:83:ARG:CG	1:L:84:HIS:N	2.80	0.44
2:E:73:THR:CG2	2:F:85:MET:SD	3.06	0.44
1:I:11:HIS:CE1	3:O:2:DT:H2"	2.52	0.44
1:D:138:GLU:HB3	1:D:147:ARG:NH1	2.32	0.44
1:K:235:GLU:HB3	1:K:239:ILE:HG23	1.99	0.44
2:M:30:LYS:NZ	3:O:6:DA:OP2	2.49	0.44
1:C:68:ASP:O	1:C:70:LYS:O	2.35	0.44
1:J:57:LEU:O	1:J:60:GLU:O	2.36	0.44
1:L:54:LEU:HD22	1:L:77:ILE:HD11	2.00	0.44
2:N:16:THR:O	2:N:16:THR:HG22	2.18	0.44
6:R:3:DT:O2	6:R:3:DT:C2'	2.63	0.44
1:A:15:SER:OG	1:A:16:TYR:N	2.50	0.44
1:D:4:ARG:NH2	2:F:99:SER:O	2.51	0.44
2:N:80:LYS:HZ1	5:Q:21:DT:P	2.38	0.44
1:D:176:LEU:N	1:D:229:ILE:HD13	2.33	0.43
1:I:27:ASP:C	1:I:27:ASP:OD1	2.55	0.43
1:J:61:LYS:HD2	1:J:193:GLN:CD	2.38	0.43
1:K:190:GLU:O	1:K:194:THR:HG23	2.18	0.43
1:L:57:LEU:O	1:L:60:GLU:O	2.35	0.43
1:C:104:VAL:HG13	1:C:202:LEU:HD13	2.00	0.43
1:D:190:GLU:O	1:D:194:THR:HG23	2.18	0.43
1:J:190:GLU:O	1:J:194:THR:HG23	2.18	0.43
3:P:26:DT:O2	3:P:26:DT:O4'	2.36	0.43
5:Q:3:DG:H1'	5:Q:4:DA:C8	2.53	0.43
1:C:76:LYS:CG	1:D:80:PHE:HZ	2.29	0.43
1:C:102:GLY:CA	1:C:142:PHE:HE1	2.30	0.43
1:L:190:GLU:O	1:L:194:THR:HG23	2.18	0.43
1:A:18:ASN:O	1:A:19:ASN:HB2	2.19	0.43
1:C:237:PHE:HB3	1:C:238:PRO:HD3	2.00	0.43
1:J:271:HIS:O	1:J:275:VAL:HG13	2.18	0.43
1:A:38:ASP:OD2	1:A:262:THR:HG21	2.19	0.43
1:D:57:LEU:O	1:D:60:GLU:O	2.36	0.43
1:J:116:GLN:HB3	1:J:155:TYR:CD1	2.52	0.43
1:L:61:LYS:HE2	1:L:193:GLN:HE22	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:271:HIS:O	1:L:275:VAL:HG13	2.18	0.43
2:N:93:ASP:OD1	2:N:95:ARG:HG3	2.18	0.43
1:L:237:PHE:HB3	1:L:238:PRO:HD3	2.00	0.43
2:M:38:ILE:HD11	2:M:95:ARG:NH2	2.32	0.43
6:R:39:DA:H2"	6:R:40:DA:C8	2.53	0.43
6:R:40:DA:H2"	6:R:41:DC:OP2	2.18	0.43
1:C:116:GLN:HB3	1:C:155:TYR:CD1	2.54	0.43
1:C:54:LEU:HD22	1:C:77:ILE:HD11	2.00	0.43
1:K:203:LYS:HG2	1:K:204:HIS:N	2.34	0.43
1:C:71:ARG:O	1:C:189:ARG:HD3	2.19	0.43
1:J:24:LYS:HG2	1:J:29:GLN:CG	2.47	0.43
1:K:235:GLU:HB3	1:K:239:ILE:CG2	2.48	0.43
1:A:246:ALA:HB1	1:A:250:ASN:OD1	2.19	0.42
1:B:3:TRP:CZ3	1:B:36:GLU:HG2	2.52	0.42
1:B:190:GLU:O	1:B:194:THR:HG23	2.19	0.42
1:J:245:PHE:HB3	2:M:103:ILE:HD13	2.01	0.42
2:M:30:LYS:HE2	3:O:6:DA:OP2	2.19	0.42
3:O:25:DT:O2	3:O:25:DT:O4'	2.35	0.42
1:D:237:PHE:HB3	1:D:238:PRO:HD3	2.00	0.42
6:R:38:DA:N3	6:R:38:DA:H2'	2.33	0.42
1:A:146:ASN:HD22	1:A:149:GLY:CA	2.25	0.42
1:D:116:GLN:HB3	1:D:155:TYR:CD1	2.54	0.42
1:I:29:GLN:N	1:I:29:GLN:OE1	2.52	0.42
1:K:29:GLN:HG2	1:K:30:GLU:N	2.33	0.42
2:M:5:TYR:CD2	2:M:100:ASP:HB2	2.54	0.42
2:N:100:ASP:OD1	2:N:100:ASP:N	2.53	0.42
1:A:57:LEU:HD23	1:A:62:ILE:HD12	2.02	0.42
1:D:249:MET:HG3	2:F:103:ILE:HG12	2.00	0.42
1:D:253:MET:HE2	1:D:256:LYS:C	2.17	0.42
2:M:21:ASP:HB3	2:M:69:ARG:HH21	1.85	0.42
1:B:177:ASN:CB	6:R:4:DC:H5'	2.47	0.42
1:I:106:THR:O	1:I:109:ILE:HG22	2.20	0.42
1:C:190:GLU:O	1:C:194:THR:HG23	2.19	0.42
1:I:54:LEU:HD22	1:I:77:ILE:HD11	2.01	0.42
1:K:54:LEU:HD22	1:K:77:ILE:HD11	2.01	0.42
1:L:73:PRO:HD3	1:L:178:TYR:CE2	2.54	0.42
3:P:5:DT:H2'	3:P:6:DA:C8	2.55	0.42
1:A:57:LEU:O	1:A:60:GLU:O	2.36	0.42
1:D:201:GLY:H	1:D:205:ALA:HA	1.84	0.42
1:K:237:PHE:HB3	1:K:238:PRO:HD3	2.01	0.42
1:L:168:GLN:HB3	1:L:173:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:O	1:A:168:GLN:HG2	2.19	0.42
2:M:5:TYR:HE2	2:M:100:ASP:HB2	1.83	0.42
1:A:73:PRO:HD3	1:A:178:TYR:CE2	2.55	0.42
1:B:219:GLU:OE2	1:B:222:ARG:HD2	2.20	0.42
1:D:57:LEU:HD23	1:D:62:ILE:HD12	2.02	0.42
1:D:155:TYR:HD2	1:D:156:PHE:CD1	2.38	0.42
1:L:26:ILE:HD12	1:L:27:ASP:HB3	2.02	0.42
1:L:55:LYS:NZ	1:L:59:ASP:OD2	2.49	0.42
1:L:116:GLN:HB3	1:L:155:TYR:CD1	2.54	0.42
1:L:171:ASP:HB3	1:L:240:MET:HE1	2.00	0.42
1:A:206:ASN:O	1:B:83:ARG:NH1	2.51	0.41
1:B:55:LYS:NZ	1:B:59:ASP:OD2	2.50	0.41
1:B:109:ILE:HD11	1:B:219:GLU:HG3	2.02	0.41
1:J:237:PHE:HB3	1:J:238:PRO:HD3	2.01	0.41
1:L:166:ARG:HA	1:L:167:GLU:C	2.39	0.41
2:M:95:ARG:HB2	2:M:95:ARG:NH2	2.35	0.41
1:A:90:LEU:HD22	1:A:197:PHE:CD2	2.54	0.41
1:B:71:ARG:O	1:B:189:ARG:HD3	2.20	0.41
1:D:202:LEU:HD11	1:D:213:LEU:CD1	2.50	0.41
1:K:71:ARG:O	1:K:189:ARG:HD3	2.20	0.41
2:E:77:VAL:CG1	2:E:78:THR:N	2.83	0.41
2:F:77:VAL:CG1	2:F:78:THR:N	2.82	0.41
1:K:135:MET:HE2	1:K:147:ARG:HH21	1.85	0.41
1:I:237:PHE:HB3	1:I:238:PRO:HD3	2.01	0.41
1:K:68:ASP:C	1:K:70:LYS:O	2.59	0.41
2:N:30:LYS:HA	2:N:30:LYS:HD3	1.89	0.41
4:H:2:DC:C4	4:H:3:DG:C6	3.09	0.41
1:I:190:GLU:HG2	1:I:266:THR:HG22	2.01	0.41
1:K:116:GLN:HB3	1:K:155:TYR:CD1	2.56	0.41
1:K:209:ASN:OD1	1:K:210:ASP:N	2.54	0.41
1:L:33:HIS:CD2	2:N:36:GLY:HA3	2.56	0.41
1:C:76:LYS:CD	1:D:80:PHE:HZ	2.34	0.41
1:I:262:THR:O	1:I:266:THR:HG23	2.20	0.41
1:A:237:PHE:HB3	1:A:238:PRO:HD3	2.02	0.41
1:L:26:ILE:O	1:L:26:ILE:HG23	2.21	0.41
1:L:166:ARG:HG2	1:L:173:ASN:CG	2.41	0.41
1:A:206:ASN:OD1	1:B:83:ARG:NH1	2.54	0.41
5:Q:13:DT:H2"	5:Q:14:DA:OP2	2.21	0.41
1:B:237:PHE:HB3	1:B:238:PRO:HD3	2.02	0.41
1:B:241:LYS:HG3	1:B:242:ARG:N	2.36	0.41
1:D:73:PRO:HD3	1:D:178:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:LYS:CE	3:G:6:DA:OP2	2.68	0.41
1:I:72:LEU:CD2	1:I:185:SER:HA	2.50	0.41
1:J:24:LYS:HG2	1:J:29:GLN:NE2	2.35	0.41
1:L:26:ILE:HD12	1:L:26:ILE:HA	1.83	0.41
1:B:57:LEU:HD23	1:B:62:ILE:HD12	2.03	0.41
1:C:76:LYS:CG	1:D:80:PHE:CZ	2.89	0.41
1:L:57:LEU:HD23	1:L:62:ILE:HD12	2.02	0.41
1:L:168:GLN:HB3	1:L:173:ASN:ND2	2.34	0.41
2:N:7:ARG:HG2	2:N:82:PHE:CG	2.56	0.41
1:C:209:ASN:OD1	1:C:210:ASP:N	2.54	0.40
1:D:18:ASN:O	1:D:19:ASN:HB2	2.21	0.40
1:D:165:THR:O	1:D:166:ARG:HB3	2.21	0.40
2:F:7:ARG:NH1	2:F:82:PHE:CE2	2.88	0.40
1:I:109:ILE:HD11	1:I:148:GLU:HG3	2.03	0.40
1:D:175:GLY:C	1:D:229:ILE:HD11	2.42	0.40
2:F:12:PHE:CD1	2:F:14:MET:HE3	2.55	0.40
1:J:117:SER:OG	1:J:133:LEU:CD2	2.69	0.40
2:F:69:ARG:HH11	2:F:69:ARG:HG3	1.87	0.40
1:K:176:LEU:HD23	1:K:229:ILE:HG21	2.04	0.40
1:L:18:ASN:O	1:L:19:ASN:HB2	2.21	0.40
2:F:51:ASN:OD1	2:F:53:THR:HB	2.21	0.40

All (2) 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)
1:I:234:LYS:CD	1:L:167:GLU:OE2[2_546]	1.81	0.39
1:K:138:GLU:OE2	5:Q:1:DC:N4[1_655]	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	286/288 (99%)	275 (96%)	11 (4%)	0	100	100
1	B	286/288 (99%)	278 (97%)	8 (3%)	0	100	100
1	C	282/288 (98%)	275 (98%)	7 (2%)	0	100	100
1	D	285/288 (99%)	274 (96%)	11 (4%)	0	100	100
1	I	281/288 (98%)	273 (97%)	8 (3%)	0	100	100
1	J	285/288 (99%)	278 (98%)	7 (2%)	0	100	100
1	K	281/288 (98%)	273 (97%)	8 (3%)	0	100	100
1	L	286/288 (99%)	276 (96%)	10 (4%)	0	100	100
2	E	104/109 (95%)	104 (100%)	0	0	100	100
2	F	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
2	M	102/109 (94%)	102 (100%)	0	0	100	100
2	N	103/109 (94%)	103 (100%)	0	0	100	100
All	All	2684/2740 (98%)	2613 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	255/255 (100%)	253 (99%)	2 (1%)	81	92
1	B	255/255 (100%)	253 (99%)	2 (1%)	81	92
1	C	254/255 (100%)	251 (99%)	3 (1%)	71	88
1	D	254/255 (100%)	253 (100%)	1 (0%)	91	96
1	I	253/255 (99%)	249 (98%)	4 (2%)	62	84
1	J	254/255 (100%)	254 (100%)	0	100	100
1	K	253/255 (99%)	252 (100%)	1 (0%)	91	96
1	L	255/255 (100%)	250 (98%)	5 (2%)	55	80
2	E	96/99 (97%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	95/99 (96%)	93 (98%)	2 (2%)	53 79
2	M	94/99 (95%)	93 (99%)	1 (1%)	73 89
2	N	95/99 (96%)	93 (98%)	2 (2%)	53 79
All	All	2413/2436 (99%)	2390 (99%)	23 (1%)	76 90

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	146	ASN
1	B	21	LEU
1	B	98	GLU
1	C	21	LEU
1	C	26	ILE
1	C	288	ILE
1	D	138	GLU
2	F	17	ASP
2	F	50	LEU
1	I	12	SER
1	I	28	HIS
1	I	127	GLN
1	I	274	LYS
1	K	98	GLU
1	L	85	ASP
1	L	87	SER
1	L	168	GLN
1	L	251	THR
1	L	262	THR
2	M	22	ARG
2	N	35	GLU
2	N	101	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	168	GLN
1	A	212	ASN
1	A	227	GLN
1	B	11	HIS

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Mol	Chain	Res	Type
1	B	227	GLN
1	C	227	GLN
1	D	209	ASN
1	D	227	GLN
1	J	20	HIS
1	J	193	GLN
1	J	212	ASN
1	K	11	HIS
1	L	28	HIS
1	L	84	HIS
1	L	122	GLN
1	L	173	ASN
1	L	193	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	288/288 (100%)	-0.22	0 100 100	58, 86, 116, 140	0
1	B	288/288 (100%)	-0.33	0 100 100	58, 73, 93, 138	0
1	C	286/288 (99%)	-0.26	1 (0%) 94 88	63, 82, 115, 158	0
1	D	287/288 (99%)	-0.23	0 100 100	64, 90, 116, 149	0
1	I	285/288 (98%)	-0.10	4 (1%) 75 56	66, 92, 122, 145	0
1	J	287/288 (99%)	-0.18	0 100 100	63, 90, 117, 143	0
1	K	285/288 (98%)	-0.28	1 (0%) 92 84	71, 89, 117, 151	0
1	L	288/288 (100%)	-0.30	0 100 100	65, 83, 110, 148	0
2	E	106/109 (97%)	-0.25	0 100 100	24, 70, 89, 117	0
2	F	105/109 (96%)	-0.28	0 100 100	24, 73, 95, 108	0
2	M	104/109 (95%)	-0.25	0 100 100	24, 78, 98, 108	0
2	N	105/109 (96%)	-0.24	0 100 100	41, 80, 101, 119	0
3	G	25/28 (89%)	-0.65	0 100 100	61, 70, 81, 104	0
3	O	27/28 (96%)	-0.39	1 (3%) 41 21	69, 96, 136, 165	0
3	P	27/28 (96%)	-0.58	0 100 100	72, 96, 110, 144	0
4	H	5/5 (100%)	-0.35	0 100 100	64, 67, 87, 115	0
5	Q	46/46 (100%)	0.03	6 (13%) 3 1	61, 82, 160, 176	0
6	R	68/69 (98%)	-0.21	3 (4%) 34 17	58, 83, 151, 163	0
All	All	2912/2944 (98%)	-0.24	16 (0%) 91 81	24, 84, 117, 176	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	R	46	DG	3.1
1	K	26	ILE	2.7
5	Q	13	DT	2.7

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Mol	Chain	Res	Type	RSRZ
5	Q	6	DG	2.6
1	I	119	HIS	2.6
1	I	27	ASP	2.6
1	I	236	ALA	2.5
6	R	45	DG	2.4
6	R	42	DC	2.4
1	C	26	ILE	2.3
1	I	288	ILE	2.2
3	O	27	DC	2.2
5	Q	1	DC	2.2
5	Q	7	DT	2.1
5	Q	12	DG	2.1
5	Q	9	DT	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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
7	MG	N	201	1/1	0.95	0.19	60,60,60,60	0
7	MG	E	201	1/1	0.97	0.20	63,63,63,63	0
7	MG	M	201	1/1	0.98	0.24	63,63,63,63	0
7	MG	F	201	1/1	0.98	0.21	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.