



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 PM UTC

PDB ID : 4KIS / pdb_00004kis
Title : Crystal Structure of a LSR-DNA Complex
Authors : Rutherford, K.; Yuan, P.; Perry, K.; Van Duyne, G.D.
Deposited on : 2013-05-02
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

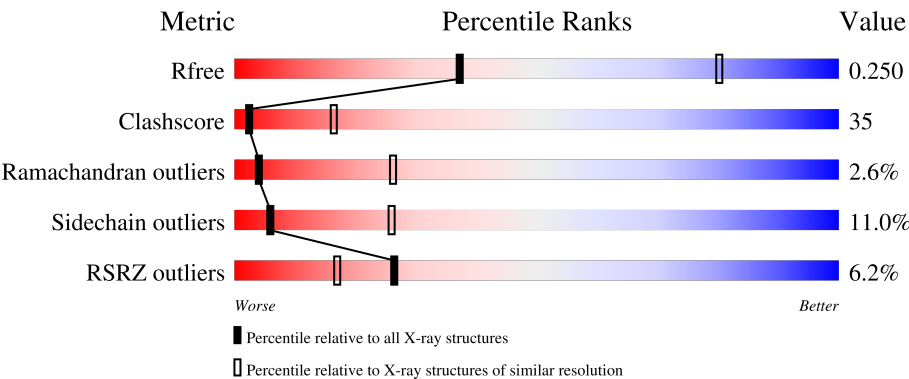
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



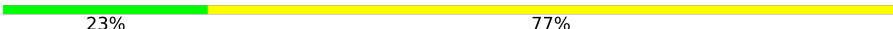
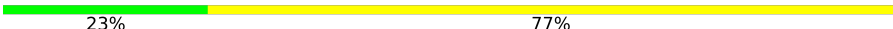
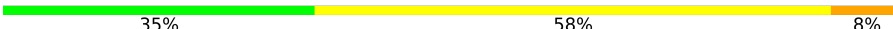
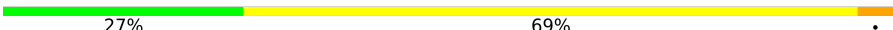
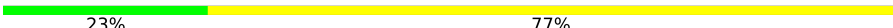
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	328	4% 38%48%9%
1	B	328	5% 38%41%13%7%
1	C	328	9% 33%50%10%6%
1	D	328	9% 39%39%8%12%
2	E	26	23%77%

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Mol	Chain	Length	Quality of chain
2	G	26	 58%42%
2	I	26	 23%77%
2	K	26	 23%77%
3	F	26	 35%58%8%
3	H	26	 27%69%.
3	J	26	 23%77%
3	L	26	 19%73%8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14347 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 Putative integrase [Bacteriophage A118].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2651	1683	464	493	11			
1	B	305	Total	C	N	O	S	0	0	0
			2557	1630	439	477	11			
1	C	309	Total	C	N	O	S	0	0	0
			2589	1646	448	484	11			
1	D	287	Total	C	N	O	S	0	0	0
			2289	1454	413	413	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	LEU	-	expression tag	UNP Q928V6
A	454	GLU	-	expression tag	UNP Q928V6
A	455	HIS	-	expression tag	UNP Q928V6
A	456	HIS	-	expression tag	UNP Q928V6
A	457	HIS	-	expression tag	UNP Q928V6
A	458	HIS	-	expression tag	UNP Q928V6
A	459	HIS	-	expression tag	UNP Q928V6
A	460	HIS	-	expression tag	UNP Q928V6
B	453	LEU	-	expression tag	UNP Q928V6
B	454	GLU	-	expression tag	UNP Q928V6
B	455	HIS	-	expression tag	UNP Q928V6
B	456	HIS	-	expression tag	UNP Q928V6
B	457	HIS	-	expression tag	UNP Q928V6
B	458	HIS	-	expression tag	UNP Q928V6
B	459	HIS	-	expression tag	UNP Q928V6
B	460	HIS	-	expression tag	UNP Q928V6
C	453	LEU	-	expression tag	UNP Q928V6
C	454	GLU	-	expression tag	UNP Q928V6
C	455	HIS	-	expression tag	UNP Q928V6
C	456	HIS	-	expression tag	UNP Q928V6
C	457	HIS	-	expression tag	UNP Q928V6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	458	HIS	-	expression tag	UNP Q928V6
C	459	HIS	-	expression tag	UNP Q928V6
C	460	HIS	-	expression tag	UNP Q928V6
D	453	LEU	-	expression tag	UNP Q928V6
D	454	GLU	-	expression tag	UNP Q928V6
D	455	HIS	-	expression tag	UNP Q928V6
D	456	HIS	-	expression tag	UNP Q928V6
D	457	HIS	-	expression tag	UNP Q928V6
D	458	HIS	-	expression tag	UNP Q928V6
D	459	HIS	-	expression tag	UNP Q928V6
D	460	HIS	-	expression tag	UNP Q928V6

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	26	Total	C	N	O	P	0	0	0
			522	254	76	167	25			
2	G	26	Total	C	N	O	P	0	0	0
			522	254	76	167	25			
2	I	26	Total	C	N	O	P	0	0	0
			522	254	76	167	25			
2	K	26	Total	C	N	O	P	0	0	0
			522	254	76	167	25			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	26	Total	C	N	O	P	0	0	0
			538	255	117	141	25			
3	H	26	Total	C	N	O	P	0	0	0
			538	255	117	141	25			
3	J	26	Total	C	N	O	P	0	0	0
			538	255	117	141	25			
3	L	26	Total	C	N	O	P	0	0	0
			538	255	117	141	25			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Zn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Zn 1	0	0
4	C	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Ca 2	0	0
5	E	1	Total 1	Ca 1	0	0
5	B	2	Total 2	Ca 2	0	0
5	C	1	Total 1	Ca 1	0	0
5	D	1	Total 1	Ca 1	0	0

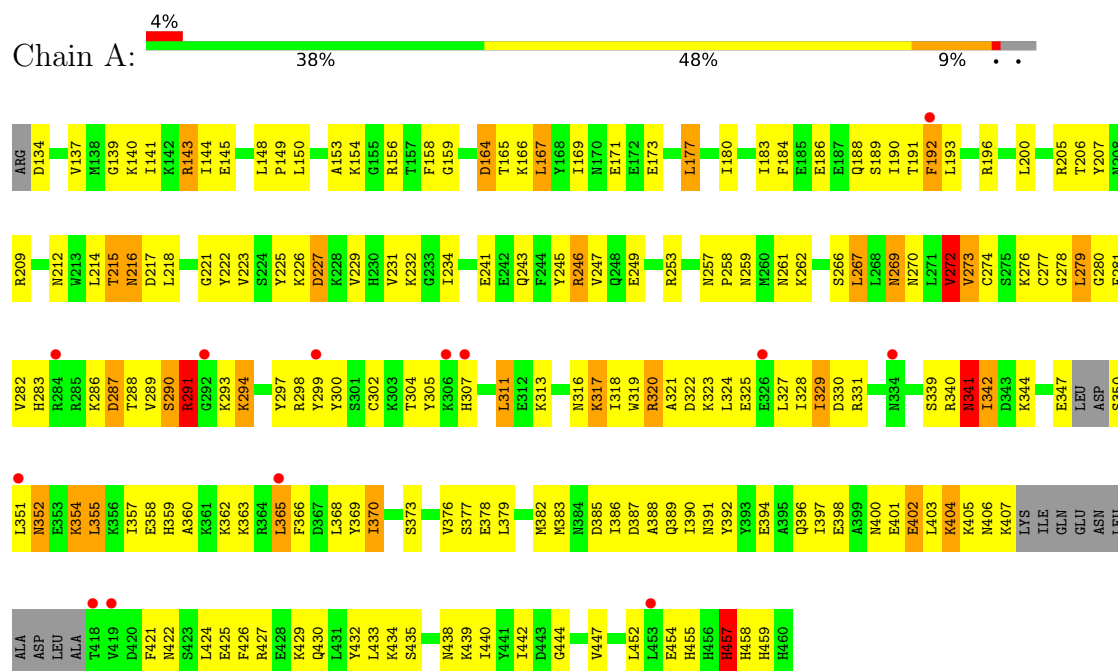
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	2	Total 2	O 2	0	0
6	F	1	Total 1	O 1	0	0
6	G	2	Total 2	O 2	0	0
6	H	1	Total 1	O 1	0	0
6	I	1	Total 1	O 1	0	0
6	J	1	Total 1	O 1	0	0

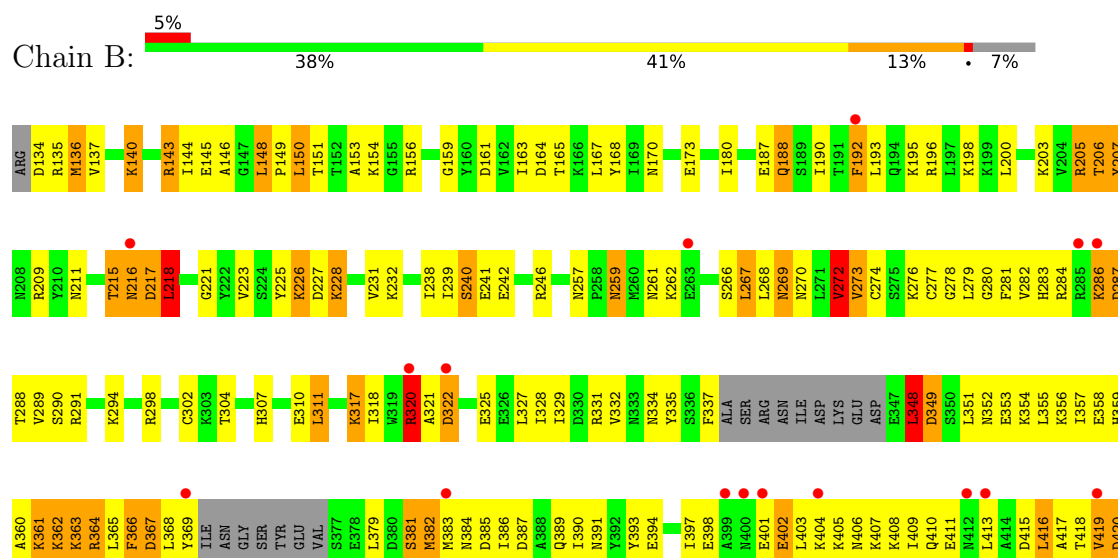
3 Residue-property plots

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

• Molecule 1: Putative integrase [Bacteriophage A118]

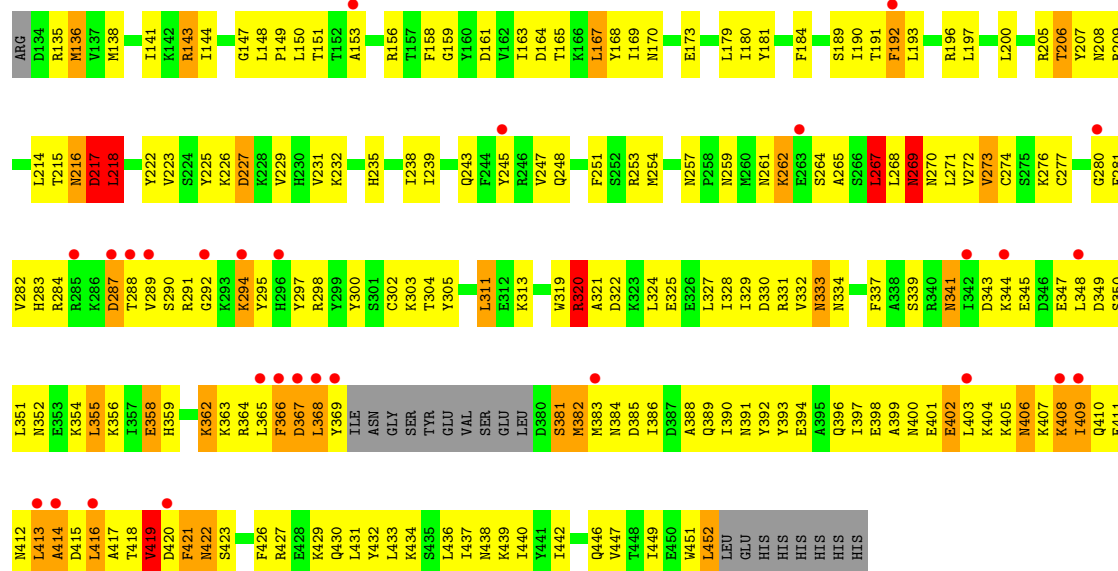


• Molecule 1: Putative integrase [Bacteriophage A118]

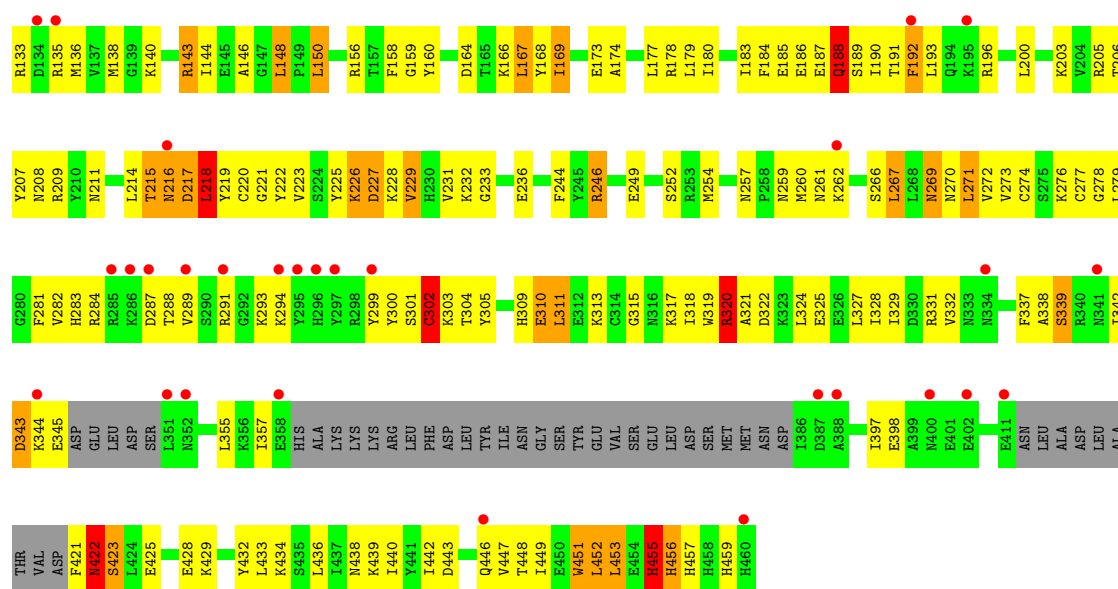




• Molecule 1: Putative integrase [Bacteriophage A118]



• Molecule 1: Putative integrase [Bacteriophage A118]

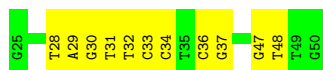


• Molecule 2: DNA (26-MER)





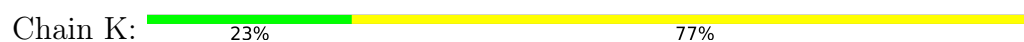
• Molecule 2: DNA (26-MER)



• Molecule 2: DNA (26-MER)



• Molecule 2: DNA (26-MER)



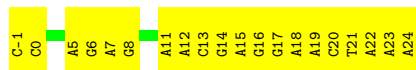
• Molecule 3: DNA (26-MER)



• Molecule 3: DNA (26-MER)



• Molecule 3: DNA (26-MER)



• Molecule 3: DNA (26-MER)



C-1
C0
A1
A2
A5
G6
A7
G8
A9
A10
A11
A12
C13
G14
A15
G16
G17
A18
A19
C20
T21
A22
A23
A24

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	290.75 Å 290.75 Å 290.75 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 3.20 49.86 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.86-3.20) 98.3 (49.86-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.12 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.236 , 0.256 0.219 , 0.250	Depositor DCC
R_{free} test set	3353 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	92.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.002 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14347	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN

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	0.55	0/2702	1.10	20/3620 (0.6%)
1	B	0.59	0/2601	1.12	21/3485 (0.6%)
1	C	0.47	0/2634	1.05	19/3530 (0.5%)
1	D	0.53	0/2333	1.13	23/3136 (0.7%)
2	E	0.42	0/579	0.90	0/892
2	G	0.42	0/579	0.89	0/892
2	I	0.35	0/579	0.80	0/892
2	K	0.41	0/579	0.86	0/892
3	F	0.37	0/609	0.68	0/938
3	H	0.42	0/609	0.72	0/938
3	J	0.32	0/609	0.59	0/938
3	L	0.38	0/609	0.68	0/938
All	All	0.49	0/15022	1.00	83/21091 (0.4%)

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	B	0	1
1	D	0	1
3	F	0	2
3	H	0	1
3	L	0	2
All	All	0	7

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	LEU	N-CA-C	-11.93	98.44	113.23
1	B	218	LEU	N-CA-C	-11.63	97.57	112.23
1	C	419	VAL	N-CA-C	-11.36	99.25	113.22
1	B	420	ASP	N-CA-C	-10.56	100.39	113.38
1	B	348	LEU	N-CA-C	-9.98	100.52	112.89
1	D	148	LEU	CA-C-N	9.24	129.33	119.90
1	D	148	LEU	C-N-CA	9.24	129.33	119.90
1	A	342	ILE	N-CA-C	9.03	121.98	108.80
1	B	228	LYS	N-CA-C	-8.06	103.58	113.41
1	D	216	ASN	N-CA-C	8.06	120.97	111.71
1	D	218	LEU	N-CA-C	-7.99	102.17	112.23
1	A	404	LYS	N-CA-C	-7.78	104.68	114.56
1	C	416	LEU	N-CA-C	-7.69	101.76	112.45
1	A	221	GLY	N-CA-C	7.65	123.58	114.48
1	A	222	TYR	N-CA-C	7.37	121.42	110.52
1	D	451	TRP	N-CA-C	7.21	126.16	110.80
1	C	381	SER	N-CA-C	-7.20	104.47	113.18
1	A	388	ALA	N-CA-C	-7.06	103.93	112.54
1	A	148	LEU	CA-C-N	7.05	127.02	119.76
1	A	148	LEU	C-N-CA	7.05	127.02	119.76
1	B	161	ASP	N-CA-C	-6.75	99.31	110.17
1	A	355	LEU	N-CA-C	-6.74	103.96	111.71
1	C	366	PHE	N-CA-C	-6.73	103.95	111.28
1	D	169	ILE	N-CA-C	6.65	119.21	109.63
1	C	341	ASN	N-CA-C	-6.65	98.78	109.96
1	D	455	HIS	N-CA-C	-6.60	99.78	110.20
1	A	457	HIS	N-CA-C	6.48	118.23	110.19
1	D	457	HIS	N-CA-C	-6.48	105.34	113.18
1	D	398	GLU	N-CA-C	-6.40	105.63	113.50
1	B	135	ARG	N-CA-C	-6.39	104.58	112.38
1	D	320	ARG	N-CA-C	-6.33	100.47	109.96
1	A	291	ARG	CB-CA-C	-6.29	109.33	116.63
1	C	216	ASN	N-CA-C	6.21	120.42	112.34
1	C	320	ARG	N-CA-C	-6.21	99.89	109.76
1	B	221	GLY	N-CA-C	6.18	123.98	115.27
1	C	319	TRP	N-CA-C	6.16	118.73	110.35
1	A	169	ILE	N-CA-C	6.15	118.31	109.51
1	A	354	LYS	N-CA-C	-6.13	105.96	113.50
1	B	148	LEU	CA-C-N	6.13	126.07	119.76
1	B	148	LEU	C-N-CA	6.13	126.07	119.76
1	B	241	GLU	N-CA-C	-6.03	105.64	112.87
1	C	409	ILE	N-CA-C	-5.99	105.23	111.58
1	D	319	TRP	N-CA-C	5.99	118.69	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ARG	N-CA-C	-5.93	104.39	111.69
1	A	272	VAL	N-CA-C	5.82	116.68	108.36
1	B	216	ASN	N-CA-C	5.81	117.29	111.07
1	A	164	ASP	CB-CA-C	-5.80	109.34	117.23
1	B	425	GLU	N-CA-C	-5.80	103.00	110.19
1	C	138	MET	N-CA-C	-5.78	105.50	112.54
1	A	317	LYS	N-CA-C	5.77	117.99	110.43
1	A	341	ASN	N-CA-C	-5.76	98.53	110.80
1	D	221	GLY	N-CA-C	5.74	123.27	115.00
1	D	343	ASP	N-CA-C	5.70	117.17	111.07
1	C	408	LYS	N-CA-C	-5.69	105.44	112.38
1	B	361	LYS	N-CA-C	-5.68	106.19	113.23
1	B	203	LYS	N-CA-C	-5.67	100.57	109.25
1	D	220	CYS	N-CA-C	-5.67	106.26	112.72
1	C	135	ARG	N-CA-C	-5.62	105.24	111.71
1	D	246	ARG	N-CA-C	-5.58	105.28	111.36
1	D	397	ILE	N-CA-C	-5.55	107.86	113.47
1	D	138	MET	N-CA-C	-5.53	106.37	113.01
1	C	165	THR	N-CA-C	-5.50	107.21	114.31
1	C	333	ASN	N-CA-C	-5.50	106.65	113.19
1	D	422	ASN	N-CA-C	-5.49	106.28	112.87
1	A	352	ASN	N-CA-C	-5.49	107.23	114.31
1	A	246	ARG	N-CA-C	-5.48	104.95	111.69
1	A	215	THR	N-CA-C	-5.48	101.80	109.69
1	C	413	LEU	N-CA-C	-5.43	105.34	112.72
1	B	145	GLU	N-CA-C	-5.40	105.79	112.38
1	D	203	LYS	N-CA-C	-5.38	102.32	110.28
1	C	161	ASP	N-CA-C	-5.38	101.77	110.32
1	B	320	ARG	N-CA-C	-5.35	101.25	109.76
1	C	414	ALA	N-CA-C	-5.34	105.53	111.36
1	D	229	VAL	N-CA-C	5.32	115.71	107.78
1	D	302	CYS	N-CA-C	-5.26	103.59	110.53
1	B	363	LYS	N-CA-C	-5.26	104.97	111.33
1	D	310	GLU	N-CA-C	5.22	116.98	111.28
1	B	358	GLU	N-CA-C	-5.21	105.29	111.69
1	B	272	VAL	N-CA-C	5.19	115.78	108.36
1	B	381	SER	N-CA-C	-5.17	105.72	112.23
1	D	208	ASN	N-CA-C	5.12	117.59	111.71
1	A	290	SER	N-CA-C	-5.09	99.68	108.69
1	C	248	GLN	N-CA-C	-5.02	105.94	111.71

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	168	TYR	Sidechain
1	D	168	TYR	Sidechain
3	F	-1	DC	Sidechain
3	F	16	DG	Sidechain
3	H	-1	DC	Sidechain
3	L	-1	DC	Sidechain
3	L	24	DA	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	2651	0	2628	190	0
1	B	2557	0	2565	187	0
1	C	2589	0	2594	224	0
1	D	2289	0	2170	162	0
2	E	522	0	302	46	0
2	G	522	0	302	17	0
2	I	522	0	302	35	0
2	K	522	0	302	32	0
3	F	538	0	289	28	0
3	H	538	0	289	27	0
3	J	538	0	289	24	0
3	L	538	0	289	33	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	1	0	0	0	0
6	J	1	0	0	0	0
All	All	14347	0	12321	934	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 35.

All (934) 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)
1:C:415:ASP:HA	1:C:418:THR:HG23	1.36	1.08
3:J:18:DA:H2''	3:J:19:DA:H5''	1.37	1.07
2:E:30:DG:H2''	2:E:31:DT:H5''	1.37	1.02
2:K:25:DG:H2''	2:K:26:DT:H5'	1.39	1.01
2:I:44:DC:H2''	2:I:45:DT:H5''	1.43	1.00
1:A:304:THR:HA	1:A:311:LEU:HD13	1.47	0.97
3:H:23:DA:H2''	3:H:24:DA:H5''	1.42	0.97
2:E:44:DC:H2''	2:E:45:DT:H5'	1.47	0.97
1:B:304:THR:HA	1:B:311:LEU:HD13	1.47	0.96
3:J:23:DA:H2''	3:J:24:DA:H5''	1.43	0.96
1:A:257:ASN:HD22	1:A:434:LYS:HE3	1.27	0.95
1:A:369:TYR:HA	1:A:373:SER:CB	1.96	0.94
3:F:15:DA:H2''	3:F:16:DG:C5'	1.98	0.93
2:E:34:DC:H2''	2:E:35:DT:H5'	1.49	0.92
2:G:31:DT:H2''	2:G:32:DT:H5'	1.48	0.92
2:E:34:DC:H2''	2:E:35:DT:C5'	1.98	0.92
2:G:47:DG:H2''	2:G:48:DT:H71	1.52	0.92
1:A:391:ASN:HA	1:A:394:GLU:HG2	1.52	0.92
3:F:18:DA:H2''	3:F:19:DA:H5''	1.54	0.90
1:C:273:VAL:HA	1:C:280:GLY:HA2	1.54	0.90
3:J:18:DA:C2'	3:J:19:DA:H5''	2.02	0.90
1:B:257:ASN:ND2	1:B:434:LYS:HE3	1.87	0.89
2:E:33:DC:H2''	2:E:34:DC:O5'	1.72	0.89
3:F:15:DA:H2''	3:F:16:DG:H5'	1.55	0.88
3:J:18:DA:H2''	3:J:19:DA:C5'	2.04	0.87
1:D:133:ARG:HD2	3:L:2:DA:H5''	1.54	0.87
2:E:47:DG:H2''	2:E:48:DT:H71	1.57	0.87
2:E:43:DT:H2''	2:E:44:DC:H5'	1.54	0.86
1:A:362:LYS:HE3	1:A:383:MET:HE3	1.57	0.86
2:K:47:DG:H2''	2:K:48:DT:H72	1.57	0.86
1:A:354:LYS:HA	1:A:357:ILE:HG12	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ARG:HD2	3:L:2:DA:C5'	2.06	0.85
2:K:33:DC:H2''	2:K:34:DC:O5'	1.75	0.84
2:E:30:DG:H2''	2:E:31:DT:C5'	2.08	0.83
1:B:362:LYS:HB2	1:B:362:LYS:HZ2	1.44	0.83
2:K:44:DC:H2''	2:K:45:DT:H5'	1.59	0.83
1:A:257:ASN:ND2	1:A:434:LYS:HE3	1.92	0.83
1:B:365:LEU:HD11	1:B:382:MET:HE3	1.61	0.83
1:A:368:LEU:O	1:A:373:SER:HB3	1.79	0.82
1:C:347:GLU:O	1:C:351:LEU:HD23	1.79	0.82
2:E:30:DG:C2'	2:E:31:DT:H5''	2.10	0.81
2:G:28:DT:H2''	2:G:29:DA:H5'	1.62	0.81
1:B:366:PHE:C	1:B:366:PHE:CD2	2.58	0.81
3:H:23:DA:C2'	3:H:24:DA:H5''	2.10	0.81
1:C:295:TYR:HB3	1:C:297:TYR:HE2	1.44	0.81
1:D:257:ASN:HD22	1:D:434:LYS:HE3	1.43	0.81
1:D:452:LEU:O	1:D:453:LEU:HB2	1.81	0.81
1:C:289:VAL:HG13	1:C:294:LYS:HG2	1.61	0.81
1:B:418:THR:O	1:B:420:ASP:N	2.15	0.80
1:B:366:PHE:C	1:B:366:PHE:HD2	1.89	0.80
3:J:23:DA:C2'	3:J:24:DA:H5''	2.11	0.80
3:L:18:DA:H2''	3:L:19:DA:C5'	2.10	0.80
1:C:304:THR:HA	1:C:311:LEU:CD1	2.12	0.80
2:E:26:DT:H2''	2:E:27:DT:H5''	1.62	0.80
1:C:415:ASP:HA	1:C:418:THR:CG2	2.11	0.80
1:A:386:ILE:O	1:A:390:ILE:HG12	1.81	0.79
1:C:257:ASN:HD22	1:C:434:LYS:HE3	1.47	0.79
1:C:404:LYS:O	1:C:408:LYS:HG2	1.82	0.79
1:C:269:ASN:O	1:C:271:LEU:HD13	1.81	0.79
1:A:289:VAL:HG22	1:A:294:LYS:HA	1.65	0.79
1:C:399:ALA:O	1:C:403:LEU:HG	1.83	0.79
3:F:7:DA:H2''	3:F:8:DG:H5'	1.63	0.78
1:B:366:PHE:CZ	1:C:245:TYR:HE2	2.01	0.78
1:B:327:LEU:C	1:B:327:LEU:HD23	2.08	0.78
3:F:18:DA:H2''	3:F:19:DA:C5'	2.15	0.77
1:C:406:ASN:HD22	1:C:407:LYS:N	1.83	0.77
1:B:355:LEU:HD23	1:B:393:TYR:HB2	1.65	0.77
1:A:159:GLY:HA2	1:A:173:GLU:HB2	1.67	0.77
1:C:289:VAL:CG1	1:C:294:LYS:HG2	2.15	0.77
1:D:269:ASN:O	1:D:271:LEU:HD13	1.86	0.76
1:A:421:PHE:HA	1:A:424:LEU:HD12	1.67	0.76
3:J:7:DA:H2''	3:J:8:DG:H5'	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:HG22	1:A:216:ASN:N	2.01	0.76
2:I:44:DC:C2'	2:I:45:DT:H5''	2.15	0.76
3:L:18:DA:H2''	3:L:19:DA:H5''	1.66	0.76
1:D:446:GLN:O	1:D:446:GLN:HG3	1.85	0.75
3:F:23:DA:H2''	3:F:24:DA:H5''	1.68	0.75
1:C:413:LEU:HD13	1:C:416:LEU:HD22	1.66	0.75
3:F:18:DA:C2'	3:F:19:DA:H5''	2.15	0.75
1:C:402:GLU:HG3	1:C:403:LEU:N	1.99	0.75
1:B:320:ARG:HD2	1:B:322:ASP:OD1	1.87	0.75
1:A:358:GLU:HG3	1:A:386:ILE:HB	1.67	0.74
1:D:257:ASN:ND2	1:D:434:LYS:HE3	2.01	0.74
3:F:15:DA:H2''	3:F:16:DG:H5''	1.67	0.74
1:A:339:SER:O	1:A:340:ARG:HB3	1.86	0.74
1:B:360:ALA:HA	1:B:363:LYS:HE3	1.70	0.74
1:B:302:CYS:SG	1:B:304:THR:HG23	2.28	0.74
1:C:272:VAL:HG13	1:C:442:ILE:HD13	1.71	0.73
1:C:390:ILE:O	1:C:394:GLU:HG3	1.88	0.73
1:D:190:ILE:O	1:D:193:LEU:HB3	1.89	0.73
1:A:304:THR:HA	1:A:311:LEU:CD1	2.17	0.73
1:A:351:LEU:O	1:A:397:ILE:HD11	1.87	0.73
3:J:-1:DC:H2''	3:J:0:DC:H5'	1.69	0.73
1:C:394:GLU:O	1:C:398:GLU:HG3	1.89	0.72
2:K:29:DA:H2''	2:K:30:DG:H5'	1.70	0.72
1:B:387:ASP:O	1:B:390:ILE:HG22	1.90	0.72
1:B:416:LEU:HD13	1:B:417:ALA:N	2.03	0.72
1:C:144:ILE:HG23	1:C:223:VAL:HG12	1.71	0.72
3:L:23:DA:H2''	3:L:24:DA:H5''	1.72	0.72
3:J:12:DA:H1'	3:J:13:DC:H5''	1.70	0.72
1:C:191:THR:OG1	2:I:37:DG:H3'	1.90	0.71
3:L:18:DA:C2'	3:L:19:DA:H5''	2.20	0.71
1:A:438:ASN:HB2	1:A:452:LEU:HD13	1.73	0.71
2:E:44:DC:H2''	2:E:45:DT:C5'	2.18	0.71
1:C:148:LEU:O	1:C:223:VAL:HG11	1.91	0.71
1:C:268:LEU:HD13	1:C:325:GLU:HG2	1.71	0.71
1:D:425:GLU:HB2	1:D:428:GLU:HG3	1.71	0.71
1:C:383:MET:HA	1:C:383:MET:HE3	1.72	0.71
1:D:159:GLY:HA2	1:D:173:GLU:HB2	1.73	0.71
3:F:23:DA:C2'	3:F:24:DA:H5''	2.21	0.71
3:F:15:DA:C2'	3:F:16:DG:H5''	2.21	0.70
1:A:359:HIS:O	1:A:363:LYS:HG3	1.92	0.70
2:K:25:DG:H2''	2:K:26:DT:C5'	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:31:DT:H6	2:E:31:DT:H5'	1.57	0.70
1:B:452:LEU:O	1:B:452:LEU:HD12	1.92	0.69
1:A:140:LYS:HE3	2:E:48:DT:O2	1.93	0.69
1:C:291:ARG:HG2	1:C:292:GLY:H	1.58	0.69
1:A:143:ARG:NH2	1:A:165:THR:OG1	2.26	0.69
1:C:295:TYR:HB3	1:C:297:TYR:CE2	2.27	0.69
1:B:381:SER:HA	1:B:384:ASN:HD22	1.58	0.69
1:C:253:ARG:NH1	1:C:431:LEU:HD22	2.07	0.69
3:H:12:DA:H1'	3:H:13:DC:H5''	1.75	0.69
3:H:18:DA:H2''	3:H:19:DA:C5'	2.23	0.68
1:B:257:ASN:HD22	1:B:434:LYS:HE3	1.58	0.68
1:C:364:ARG:O	1:C:368:LEU:HG	1.93	0.68
2:I:26:DT:H2''	2:I:27:DT:H5''	1.75	0.68
1:D:136:MET:HE3	3:L:1:DA:C2	2.28	0.68
2:G:47:DG:H2''	2:G:48:DT:C7	2.24	0.68
1:B:356:LYS:HA	1:B:359:HIS:HB2	1.75	0.68
2:E:26:DT:H2''	2:E:27:DT:C5'	2.24	0.68
1:B:307:HIS:O	1:B:311:LEU:HD12	1.94	0.68
2:E:34:DC:H2''	2:E:35:DT:H5''	1.73	0.68
1:A:404:LYS:O	1:A:407:LYS:HG3	1.94	0.67
3:L:23:DA:C2'	3:L:24:DA:H5''	2.24	0.67
1:A:289:VAL:HG13	1:A:293:LYS:O	1.94	0.67
1:B:266:SER:O	1:B:269:ASN:HB3	1.94	0.67
2:I:44:DC:H2''	2:I:45:DT:C5'	2.21	0.67
1:D:218:LEU:C	1:D:218:LEU:HD23	2.18	0.67
1:D:254:MET:HE3	2:K:38:DT:H3'	1.76	0.67
2:E:26:DT:C2'	2:E:27:DT:H5''	2.24	0.67
1:A:288:THR:HG23	3:F:21:DT:H73	1.75	0.67
1:B:403:LEU:HD23	1:B:403:LEU:O	1.95	0.67
3:L:-1:DC:H2''	3:L:0:DC:H5'	1.77	0.67
3:L:7:DA:H2''	3:L:8:DG:H5'	1.77	0.67
1:B:416:LEU:O	1:B:416:LEU:HD22	1.96	0.66
3:H:7:DA:H2''	3:H:8:DG:H5'	1.76	0.66
3:H:0:DC:H6	3:H:0:DC:H5'	1.61	0.66
3:L:23:DA:H2''	3:L:24:DA:O4'	1.95	0.66
1:A:391:ASN:HA	1:A:394:GLU:CG	2.25	0.66
2:E:25:DG:H2''	2:E:26:DT:C5'	2.24	0.66
1:B:419:VAL:HG23	1:B:432:TYR:OH	1.96	0.66
2:G:31:DT:C2'	2:G:32:DT:H5'	2.23	0.66
1:C:388:ALA:HA	1:C:391:ASN:HD22	1.60	0.66
2:G:30:DG:H2''	2:G:31:DT:H5'	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD23	1:A:218:LEU:C	2.21	0.65
1:A:196:ARG:O	1:A:200:LEU:HD13	1.95	0.65
1:A:215:THR:O	1:A:216:ASN:HB3	1.96	0.65
1:C:344:LYS:HG3	1:C:404:LYS:CE	2.26	0.65
1:B:288:THR:HG22	1:B:289:VAL:N	2.12	0.65
1:D:338:ALA:O	1:D:339:SER:HB3	1.95	0.65
1:B:325:GLU:O	1:B:329:ILE:HG13	1.97	0.65
1:C:257:ASN:ND2	1:C:434:LYS:HE3	2.11	0.65
1:A:298:ARG:HH12	1:A:321:ALA:HB1	1.62	0.64
1:A:369:TYR:HA	1:A:373:SER:HB2	1.76	0.64
1:B:153:ALA:HB3	1:B:156:ARG:HD2	1.78	0.64
2:E:25:DG:H2''	2:E:26:DT:H5''	1.78	0.64
1:B:281:PHE:CZ	1:B:442:ILE:HG21	2.33	0.64
1:A:298:ARG:NH1	1:A:321:ALA:HB1	2.12	0.64
1:C:386:ILE:O	1:C:390:ILE:HG13	1.96	0.64
1:C:401:GLU:O	1:C:405:LYS:HG2	1.97	0.64
1:A:327:LEU:HD23	1:A:327:LEU:C	2.23	0.64
1:B:438:ASN:O	1:B:439:LYS:HD2	1.98	0.63
1:C:227:ASP:OD2	1:C:227:ASP:C	2.40	0.63
1:C:304:THR:HA	1:C:311:LEU:HD13	1.80	0.63
1:C:363:LYS:O	1:C:367:ASP:HB2	1.98	0.63
1:D:422:ASN:HA	1:D:429:LYS:HE3	1.79	0.63
1:C:158:PHE:CE1	1:C:173:GLU:HB3	2.33	0.63
1:D:343:ASP:O	1:D:345:GLU:N	2.32	0.63
3:J:11:DA:H2''	3:J:12:DA:OP2	1.98	0.63
2:K:47:DG:H2''	2:K:48:DT:C7	2.27	0.63
1:A:191:THR:OG1	2:E:37:DG:H3'	1.98	0.63
1:B:148:LEU:N	1:B:148:LEU:HD12	2.14	0.63
1:B:348:LEU:HD13	1:B:352:ASN:HD21	1.63	0.63
1:B:401:GLU:C	1:B:403:LEU:H	2.06	0.63
1:D:309:HIS:HB2	1:D:310:GLU:OE1	1.98	0.63
1:A:144:ILE:HG23	1:A:223:VAL:CG1	2.29	0.62
1:A:360:ALA:HA	1:A:363:LYS:HD2	1.79	0.62
1:B:386:ILE:O	1:B:390:ILE:HB	2.00	0.62
1:C:267:LEU:HD22	1:C:268:LEU:HD12	1.81	0.62
1:B:269:ASN:ND2	1:B:434:LYS:HZ3	1.98	0.62
1:C:344:LYS:HZ2	1:C:348:LEU:HD12	1.63	0.62
1:B:180:ILE:HG23	1:B:193:LEU:HD21	1.81	0.62
2:I:34:DC:H2''	2:I:35:DT:O5'	2.00	0.62
1:D:325:GLU:O	1:D:329:ILE:HG13	1.99	0.62
1:B:366:PHE:HD2	1:B:366:PHE:O	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:DC:H42	3:J:8:DG:H1	1.48	0.62
1:C:150:LEU:C	1:C:150:LEU:HD23	2.25	0.62
2:I:29:DA:H1'	2:I:30:DG:C8	2.34	0.62
1:D:140:LYS:HE3	2:K:48:DT:O2	2.00	0.62
3:L:-1:DC:H2''	3:L:0:DC:OP2	2.00	0.62
2:K:30:DG:H2'	2:K:31:DT:H72	1.82	0.62
1:C:148:LEU:N	1:C:148:LEU:HD12	2.14	0.62
1:A:144:ILE:HG23	1:A:223:VAL:HG12	1.82	0.61
1:B:144:ILE:HG23	1:B:223:VAL:HG12	1.82	0.61
1:B:269:ASN:ND2	1:B:434:LYS:NZ	2.48	0.61
2:G:33:DC:H2''	2:G:34:DC:O5'	1.99	0.61
1:A:191:THR:HG1	2:E:37:DG:H3'	1.65	0.61
1:B:381:SER:HA	1:B:384:ASN:ND2	2.16	0.61
1:A:243:GLN:O	1:A:247:VAL:HG23	2.00	0.61
1:D:190:ILE:HB	1:D:207:TYR:CE1	2.36	0.61
1:B:405:LYS:O	1:B:409:ILE:HG13	2.00	0.61
2:I:47:DG:H2''	2:I:48:DT:H72	1.83	0.61
1:A:171:GLU:OE1	1:A:171:GLU:HA	2.01	0.61
1:A:369:TYR:HD1	1:A:370:ILE:HD13	1.66	0.60
1:C:167:LEU:H	1:C:167:LEU:HD12	1.65	0.60
1:C:332:VAL:C	1:C:334:ASN:H	2.09	0.60
1:A:215:THR:HG22	1:A:216:ASN:H	1.65	0.60
1:B:136:MET:HE3	3:H:1:DA:C2	2.37	0.60
1:D:274:CYS:SG	1:D:276:LYS:O	2.60	0.60
1:B:170:ASN:CG	1:B:173:GLU:HG3	2.27	0.60
1:B:217:ASP:OD2	1:B:217:ASP:C	2.45	0.60
1:D:455:HIS:O	1:D:456:HIS:HB2	2.02	0.60
2:K:42:DC:H2''	2:K:43:DT:OP2	2.01	0.60
1:B:238:ILE:O	1:B:239:ILE:HD13	2.02	0.59
1:A:369:TYR:HA	1:A:373:SER:HB3	1.81	0.59
1:A:427:ARG:O	1:A:430:GLN:HG3	2.02	0.59
1:B:366:PHE:O	1:B:369:TYR:HB2	2.02	0.59
1:A:153:ALA:HB3	1:A:156:ARG:HD2	1.83	0.59
1:C:344:LYS:NZ	1:C:400:ASN:HB3	2.18	0.59
1:A:226:LYS:O	1:A:226:LYS:HG2	2.02	0.59
1:D:180:ILE:HG22	1:D:214:LEU:HD21	1.85	0.59
1:C:407:LYS:HA	1:C:410:GLN:HB3	1.84	0.59
1:A:340:ARG:O	1:A:341:ASN:HB3	2.03	0.59
1:B:192:PHE:O	1:B:196:ARG:HG3	2.03	0.59
1:D:160:TYR:HE2	1:D:218:LEU:HD21	1.68	0.59
3:L:12:DA:H1'	3:L:13:DC:H5''	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LEU:HA	1:B:406:ASN:OD1	2.02	0.58
1:B:416:LEU:HD22	1:B:416:LEU:C	2.28	0.58
3:H:18:DA:H2''	3:H:19:DA:H5''	1.84	0.58
3:F:-1:DC:H2''	3:F:0:DC:OP2	2.00	0.58
2:I:33:DC:H4'	2:I:33:DC:OP1	2.03	0.58
2:K:30:DG:H2''	2:K:31:DT:C6	2.38	0.58
1:B:355:LEU:HD23	1:B:393:TYR:CB	2.33	0.58
1:D:133:ARG:HD2	3:L:2:DA:H5'	1.82	0.58
1:B:416:LEU:O	1:B:419:VAL:HG12	2.03	0.58
1:A:358:GLU:OE2	1:A:386:ILE:HG22	2.04	0.58
2:E:39:DT:H1'	2:E:40:DT:H5''	1.85	0.58
2:E:43:DT:H2''	2:E:44:DC:C5'	2.29	0.58
1:C:148:LEU:HB3	1:C:149:PRO:HD2	1.86	0.58
3:L:1:DA:H2''	3:L:2:DA:OP2	2.03	0.58
1:D:143:ARG:O	1:D:146:ALA:HB3	2.03	0.58
3:L:23:DA:C3'	3:L:24:DA:H5''	2.34	0.58
1:B:226:LYS:O	1:B:226:LYS:HG2	2.03	0.58
1:C:231:VAL:HG22	1:C:232:LYS:N	2.18	0.58
1:C:329:ILE:O	1:C:333:ASN:ND2	2.37	0.58
1:D:305:TYR:CE1	1:D:313:LYS:HD3	2.39	0.57
1:D:451:TRP:O	1:D:452:LEU:CB	2.51	0.57
3:J:23:DA:C3'	3:J:24:DA:H5''	2.33	0.57
1:A:158:PHE:CD2	1:A:177:LEU:HD11	2.39	0.57
3:F:23:DA:C3'	3:F:24:DA:H5''	2.34	0.57
1:A:286:LYS:HE2	2:E:30:DG:O6	2.04	0.57
1:B:238:ILE:O	1:B:238:ILE:HG22	2.04	0.57
1:B:390:ILE:CG2	1:B:391:ASN:N	2.67	0.57
2:I:28:DT:H2''	2:I:29:DA:C8	2.40	0.57
1:C:351:LEU:HB3	1:C:397:ILE:CG1	2.34	0.57
1:C:358:GLU:CG	1:C:390:ILE:HG12	2.34	0.57
1:D:453:LEU:HD13	1:D:453:LEU:O	2.03	0.57
2:K:33:DC:H4'	2:K:33:DC:OP1	2.02	0.57
1:A:269:ASN:ND2	1:A:434:LYS:NZ	2.53	0.57
1:B:421:PHE:CE2	1:B:429:LYS:HD3	2.39	0.57
1:D:338:ALA:O	1:D:339:SER:CB	2.53	0.57
1:B:349:ASP:HA	1:B:352:ASN:HD22	1.69	0.57
2:G:30:DG:H2''	2:G:31:DT:C5'	2.35	0.57
2:I:27:DT:H2'	2:I:28:DT:H71	1.85	0.57
1:A:405:LYS:O	1:D:276:LYS:HE3	2.05	0.57
1:B:360:ALA:HA	1:B:363:LYS:CE	2.34	0.57
1:C:393:TYR:O	1:C:397:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:TYR:HB3	1:A:229:VAL:HB	1.86	0.57
1:A:150:LEU:C	1:A:150:LEU:HD23	2.30	0.56
3:J:22:DA:H2''	3:J:23:DA:OP2	2.04	0.56
1:C:413:LEU:O	1:C:416:LEU:HB3	2.05	0.56
1:B:140:LYS:HE3	2:G:48:DT:O2	2.05	0.56
1:B:273:VAL:HA	1:B:280:GLY:HA2	1.87	0.56
1:B:353:GLU:HG3	1:B:354:LYS:N	2.19	0.56
3:H:12:DA:H2''	3:H:13:DC:OP2	2.05	0.56
1:C:268:LEU:HB2	1:C:300:TYR:HE2	1.70	0.56
1:C:351:LEU:HB3	1:C:397:ILE:HG12	1.87	0.56
1:D:288:THR:HG23	3:L:21:DT:C7	2.35	0.56
1:D:303:LYS:HE2	3:L:15:DA:OP2	2.05	0.56
1:D:317:LYS:C	1:D:318:ILE:HD12	2.30	0.56
1:B:420:ASP:O	1:B:422:ASN:N	2.38	0.56
1:D:133:ARG:HD3	3:L:1:DA:H4'	1.86	0.56
1:A:276:LYS:O	1:A:277:CYS:SG	2.64	0.56
1:D:288:THR:HG22	1:D:289:VAL:N	2.21	0.56
1:D:455:HIS:O	1:D:456:HIS:CB	2.52	0.56
1:A:317:LYS:C	1:A:318:ILE:HD12	2.31	0.56
3:H:18:DA:H2''	3:H:19:DA:H5'	1.88	0.56
2:K:40:DT:H2''	2:K:41:DT:H5'	1.88	0.56
3:F:23:DA:H2''	3:F:24:DA:O4'	2.06	0.56
1:B:286:LYS:HE2	2:G:30:DG:O6	2.06	0.56
1:B:359:HIS:O	1:B:363:LYS:HG3	2.05	0.56
1:A:189:SER:HB3	1:A:192:PHE:HB2	1.88	0.56
1:B:196:ARG:NH2	1:D:164:ASP:OD1	2.38	0.56
2:K:47:DG:C2'	2:K:48:DT:H72	2.34	0.56
1:C:437:ILE:HG22	1:C:438:ASN:N	2.20	0.56
2:I:25:DG:H2''	2:I:26:DT:H5'	1.88	0.56
2:I:26:DT:C2'	2:I:27:DT:H5''	2.34	0.56
2:I:30:DG:H2''	2:I:31:DT:H5'	1.87	0.56
1:D:160:TYR:CE2	1:D:218:LEU:HD21	2.41	0.56
1:A:227:ASP:OD2	1:A:227:ASP:C	2.48	0.55
1:C:362:LYS:HA	1:C:383:MET:HE1	1.86	0.55
3:H:23:DA:H2''	3:H:24:DA:C5'	2.26	0.55
1:A:320:ARG:HB3	1:A:323:LYS:HG2	1.87	0.55
2:E:47:DG:H2''	2:E:48:DT:C7	2.31	0.55
1:A:325:GLU:O	1:A:329:ILE:HD12	2.05	0.55
1:A:454:GLU:HG2	1:D:337:PHE:CD1	2.40	0.55
2:G:36:DC:H1'	2:G:37:DG:C8	2.41	0.55
1:C:207:TYR:C	1:C:207:TYR:CD2	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:LYS:HG3	1:C:411:GLU:OE2	2.06	0.55
3:L:5:DA:H1'	3:L:6:DG:C8	2.41	0.55
1:A:289:VAL:HG22	1:A:294:LYS:CA	2.34	0.55
1:A:298:ARG:NH1	1:A:321:ALA:CB	2.70	0.55
1:A:354:LYS:HA	1:A:357:ILE:CG1	2.35	0.55
1:A:158:PHE:HD2	1:A:177:LEU:HD11	1.70	0.55
1:A:324:LEU:O	1:A:328:ILE:HG12	2.07	0.55
2:E:44:DC:H1'	2:E:45:DT:H5''	1.87	0.55
1:B:276:LYS:O	1:B:277:CYS:SG	2.65	0.55
1:B:368:LEU:HD22	1:B:379:LEU:HD12	1.89	0.55
1:C:287:ASP:OD2	1:C:287:ASP:N	2.40	0.55
1:C:328:ILE:O	1:C:332:VAL:HG23	2.06	0.55
1:D:254:MET:HE3	2:K:38:DT:C3'	2.37	0.55
1:A:190:ILE:HB	1:A:207:TYR:CE1	2.42	0.55
1:B:274:CYS:SG	1:B:276:LYS:O	2.65	0.55
1:B:409:ILE:O	1:B:413:LEU:HG	2.06	0.55
1:B:427:ARG:O	1:B:430:GLN:HG3	2.07	0.55
1:A:289:VAL:HG13	1:A:293:LYS:C	2.31	0.55
1:C:168:TYR:HE2	1:D:179:LEU:HD13	1.71	0.55
1:D:328:ILE:CD1	1:D:440:ILE:HD13	2.37	0.55
1:B:164:ASP:OD1	1:C:196:ARG:NH2	2.41	0.54
1:B:420:ASP:O	1:B:421:PHE:C	2.49	0.54
1:C:190:ILE:HB	1:C:207:TYR:CE1	2.42	0.54
2:K:27:DT:H2''	2:K:28:DT:H5'	1.89	0.54
2:K:29:DA:H2''	2:K:30:DG:C5'	2.36	0.54
1:A:341:ASN:HB2	1:D:447:VAL:HG22	1.89	0.54
1:C:367:ASP:O	1:C:369:TYR:N	2.41	0.54
1:D:318:ILE:HG22	1:D:318:ILE:O	2.07	0.54
1:A:321:ALA:O	1:A:325:GLU:HG3	2.08	0.54
2:E:28:DT:H2''	2:E:29:DA:H5'	1.89	0.54
1:B:282:VAL:HG12	1:B:283:HIS:N	2.22	0.54
1:B:352:ASN:HB3	1:B:356:LYS:NZ	2.22	0.54
1:A:217:ASP:N	1:A:217:ASP:OD2	2.39	0.54
1:C:153:ALA:HB3	1:C:156:ARG:HD2	1.88	0.54
1:C:388:ALA:HA	1:C:391:ASN:ND2	2.23	0.54
2:I:26:DT:H2''	2:I:27:DT:C5'	2.38	0.54
1:A:180:ILE:HG22	1:A:214:LEU:HD21	1.90	0.54
1:C:216:ASN:OD1	1:C:218:LEU:HB3	2.07	0.54
1:D:305:TYR:OH	1:D:315:GLY:HA2	2.08	0.54
1:B:287:ASP:N	1:B:287:ASP:OD2	2.39	0.54
1:B:391:ASN:HA	1:B:394:GLU:CD	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:CG2	1:A:216:ASN:N	2.69	0.54
1:B:148:LEU:HB3	1:B:149:PRO:HD2	1.90	0.54
1:D:144:ILE:HG23	1:D:223:VAL:HG12	1.90	0.54
1:A:340:ARG:O	1:A:340:ARG:HG2	2.08	0.54
1:B:418:THR:HG23	1:B:419:VAL:H	1.71	0.54
3:H:18:DA:C2'	3:H:19:DA:H5''	2.37	0.54
1:A:167:LEU:HD12	1:A:167:LEU:H	1.72	0.54
1:C:168:TYR:CE2	1:D:179:LEU:HD13	2.43	0.54
1:B:453:LEU:C	1:B:453:LEU:HD13	2.32	0.53
1:C:136:MET:SD	2:I:50:DG:C2	3.01	0.53
1:A:288:THR:HG22	1:A:289:VAL:N	2.23	0.53
1:A:403:LEU:N	1:A:403:LEU:HD22	2.23	0.53
1:C:251:PHE:HD2	1:C:254:MET:HE2	1.72	0.53
1:C:288:THR:HG23	3:J:21:DT:C7	2.38	0.53
1:D:187:GLU:O	1:D:188:GLN:C	2.52	0.53
3:F:12:DA:H1'	3:F:13:DC:H5''	1.90	0.53
1:D:225:TYR:HB3	1:D:229:VAL:HB	1.90	0.53
1:B:290:SER:O	1:B:291:ARG:HB2	2.08	0.53
1:C:305:TYR:CE1	1:C:313:LYS:HD3	2.44	0.53
1:D:226:LYS:NZ	1:D:228:LYS:HE3	2.24	0.53
3:L:18:DA:H2''	3:L:19:DA:H5'	1.87	0.53
1:A:289:VAL:CG2	1:A:294:LYS:HG2	2.38	0.53
1:B:163:ILE:HG21	1:C:179:LEU:HD22	1.90	0.53
1:B:368:LEU:O	1:B:369:TYR:C	2.51	0.53
1:B:411:GLU:O	1:B:415:ASP:HB2	2.09	0.53
1:D:246:ARG:O	1:D:249:GLU:HB3	2.07	0.53
1:A:458:HIS:O	1:A:459:HIS:HD2	1.90	0.53
1:B:418:THR:HG23	1:B:419:VAL:N	2.23	0.53
1:A:323:LYS:O	1:A:324:LEU:C	2.51	0.53
1:D:355:LEU:C	1:D:357:ILE:H	2.16	0.53
1:B:366:PHE:CZ	1:C:245:TYR:CE2	2.91	0.52
1:D:259:ASN:O	1:D:261:ASN:N	2.42	0.52
1:C:438:ASN:O	1:C:439:LYS:HD2	2.10	0.52
1:A:342:ILE:HD12	1:A:347:GLU:HB3	1.92	0.52
1:B:196:ARG:O	1:B:200:LEU:HD13	2.10	0.52
1:B:426:PHE:O	1:B:429:LYS:HB2	2.09	0.52
1:C:355:LEU:HD23	1:C:393:TYR:CB	2.39	0.52
1:C:382:MET:HE2	1:C:382:MET:HA	1.91	0.52
1:C:442:ILE:HG13	1:C:447:VAL:HG12	1.91	0.52
1:A:246:ARG:O	1:A:249:GLU:HB3	2.09	0.52
1:A:289:VAL:HG22	1:A:294:LYS:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLU:HB3	1:A:390:ILE:HD11	1.92	0.52
1:C:352:ASN:HB3	1:C:356:LYS:HE3	1.91	0.52
1:C:243:GLN:O	1:C:247:VAL:HG23	2.08	0.52
1:D:187:GLU:O	1:D:189:SER:N	2.42	0.52
1:D:304:THR:HA	1:D:311:LEU:CD1	2.40	0.52
1:C:302:CYS:SG	1:C:304:THR:HG23	2.49	0.52
1:C:427:ARG:HG3	1:C:427:ARG:HH11	1.75	0.52
1:D:191:THR:OG1	2:K:38:DT:OP2	2.20	0.52
1:D:310:GLU:OE1	1:D:310:GLU:N	2.42	0.52
2:K:27:DT:H2''	2:K:28:DT:C5'	2.38	0.52
1:C:320:ARG:HG2	1:C:320:ARG:HH11	1.75	0.52
2:K:31:DT:OP2	2:K:31:DT:H2'	2.10	0.52
1:B:402:GLU:CD	1:B:402:GLU:C	2.77	0.52
2:E:39:DT:H2''	2:E:40:DT:H5'	1.92	0.52
1:D:196:ARG:O	1:D:200:LEU:HD12	2.10	0.52
1:D:216:ASN:O	1:D:217:ASP:HB3	2.09	0.52
1:D:225:TYR:O	1:D:226:LYS:C	2.53	0.52
1:A:273:VAL:HA	1:A:280:GLY:HA2	1.93	0.51
1:C:268:LEU:HD12	1:C:268:LEU:N	2.25	0.51
1:A:258:PRO:HD2	1:A:270:ASN:OD1	2.10	0.51
1:A:344:LYS:O	1:A:347:GLU:HG2	2.10	0.51
1:B:363:LYS:O	1:B:367:ASP:HB2	2.10	0.51
1:C:225:TYR:O	1:C:226:LYS:C	2.53	0.51
1:B:269:ASN:O	1:B:270:ASN:HB2	2.10	0.51
1:D:276:LYS:O	1:D:277:CYS:SG	2.68	0.51
1:D:328:ILE:HD11	1:D:440:ILE:HD13	1.90	0.51
1:A:341:ASN:C	1:A:341:ASN:OD1	2.52	0.51
1:A:396:GLN:O	1:A:400:ASN:HB2	2.10	0.51
3:H:-1:DC:H2''	3:H:0:DC:H5'	1.92	0.51
1:A:438:ASN:O	1:A:439:LYS:HD2	2.11	0.51
1:B:288:THR:HG22	1:B:289:VAL:H	1.76	0.51
1:C:397:ILE:O	1:C:401:GLU:HG3	2.11	0.51
1:C:421:PHE:O	1:C:423:SER:N	2.44	0.51
1:D:136:MET:HE3	3:L:1:DA:H2	1.75	0.51
1:B:356:LYS:HA	1:B:359:HIS:CB	2.41	0.51
1:C:392:TYR:O	1:C:396:GLN:HG3	2.11	0.51
1:A:320:ARG:HD2	1:A:322:ASP:OD1	2.10	0.51
1:B:362:LYS:HZ2	1:B:362:LYS:CB	2.21	0.51
1:A:144:ILE:HG22	1:A:229:VAL:HG11	1.92	0.51
1:A:339:SER:HB3	1:A:455:HIS:CD2	2.46	0.51
2:G:28:DT:H2''	2:G:29:DA:C5'	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:LYS:O	1:C:363:LYS:HG3	2.11	0.51
1:D:422:ASN:HA	1:D:429:LYS:CE	2.41	0.51
1:A:368:LEU:C	1:A:373:SER:HB3	2.36	0.50
1:C:347:GLU:CD	1:C:400:ASN:ND2	2.69	0.50
1:D:442:ILE:HG22	1:D:442:ILE:O	2.11	0.50
1:A:288:THR:HG23	3:F:21:DT:C7	2.41	0.50
2:E:31:DT:H2''	2:E:32:DT:O5'	2.11	0.50
1:C:355:LEU:HD23	1:C:393:TYR:HB2	1.93	0.50
1:C:365:LEU:HD21	1:C:382:MET:HB3	1.92	0.50
1:D:148:LEU:HD12	1:D:148:LEU:N	2.25	0.50
1:D:267:LEU:HD22	1:D:433:LEU:HD12	1.92	0.50
1:C:437:ILE:CG2	1:C:438:ASN:N	2.74	0.50
1:C:283:HIS:HD2	1:C:300:TYR:HE1	1.59	0.50
1:C:362:LYS:HA	1:C:383:MET:CE	2.40	0.50
1:A:231:VAL:HG22	1:A:232:LYS:N	2.27	0.50
1:A:290:SER:O	1:A:291:ARG:HB2	2.12	0.50
1:B:277:CYS:O	1:B:279:LEU:N	2.44	0.50
1:B:353:GLU:O	1:B:357:ILE:HG13	2.11	0.50
1:C:288:THR:HG22	1:C:289:VAL:N	2.26	0.50
1:B:298:ARG:NH1	1:B:321:ALA:HB1	2.27	0.50
1:C:269:ASN:HD21	1:C:434:LYS:NZ	2.10	0.50
1:C:332:VAL:C	1:C:334:ASN:N	2.68	0.50
3:J:16:DG:H2''	3:J:17:DG:OP2	2.11	0.50
1:D:227:ASP:C	1:D:227:ASP:OD2	2.54	0.50
1:D:320:ARG:NH1	2:K:28:DT:OP2	2.44	0.50
1:B:379:LEU:HA	1:B:382:MET:HB2	1.94	0.50
1:C:382:MET:HA	1:C:382:MET:CE	2.41	0.50
1:C:412:ASN:C	1:C:414:ALA:H	2.19	0.50
1:C:426:PHE:O	1:C:429:LYS:HB2	2.11	0.50
2:E:27:DT:H2'	2:E:28:DT:H72	1.93	0.50
1:B:154:LYS:HG3	2:G:47:DG:OP1	2.12	0.50
1:D:266:SER:O	1:D:269:ASN:HB3	2.12	0.50
1:A:189:SER:CB	1:A:192:PHE:HB2	2.42	0.50
1:D:183:ILE:HG22	1:D:184:PHE:N	2.25	0.50
1:D:287:ASP:OD2	1:D:287:ASP:N	2.44	0.49
1:A:406:ASN:O	1:A:407:LYS:C	2.55	0.49
3:F:0:DC:H6	3:F:0:DC:H5'	1.76	0.49
1:D:231:VAL:HG22	1:D:232:LYS:N	2.27	0.49
1:A:281:PHE:CD2	1:A:302:CYS:HA	2.48	0.49
1:A:392:TYR:C	1:A:392:TYR:CD2	2.90	0.49
1:B:211:ASN:O	1:B:215:THR:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:HB3	1:B:156:ARG:CD	2.42	0.49
1:B:421:PHE:O	1:B:423:SER:N	2.45	0.49
2:I:45:DT:H2''	2:I:46:DC:C6	2.48	0.49
1:D:148:LEU:O	1:D:223:VAL:HG11	2.12	0.49
1:A:305:TYR:CE1	1:A:313:LYS:HD3	2.47	0.49
1:A:339:SER:HB3	1:A:455:HIS:NE2	2.27	0.49
1:B:307:HIS:HB2	1:B:311:LEU:HD11	1.94	0.49
1:C:216:ASN:C	1:C:218:LEU:H	2.21	0.49
1:A:266:SER:O	1:A:267:LEU:C	2.56	0.49
1:A:269:ASN:ND2	1:A:434:LYS:HZ1	2.09	0.49
1:B:360:ALA:HA	1:B:363:LYS:CD	2.42	0.49
3:L:19:DA:H2''	3:L:20:DC:O5'	2.13	0.49
1:A:154:LYS:HG3	2:E:47:DG:OP1	2.13	0.49
3:J:12:DA:H2''	3:J:13:DC:C5'	2.43	0.49
1:D:282:VAL:HG12	1:D:283:HIS:N	2.27	0.49
1:B:206:THR:O	1:B:207:TYR:C	2.55	0.49
1:B:327:LEU:HD23	1:B:328:ILE:N	2.27	0.49
1:C:206:THR:HG23	1:C:209:ARG:HB2	1.94	0.49
1:C:238:ILE:HG22	1:C:239:ILE:CD1	2.41	0.49
1:A:307:HIS:HB2	1:A:311:LEU:HD11	1.95	0.48
1:C:190:ILE:HG13	1:C:207:TYR:CZ	2.48	0.48
1:C:238:ILE:HG22	1:C:239:ILE:HD13	1.94	0.48
1:D:140:LYS:O	1:D:143:ARG:HB3	2.13	0.48
1:A:166:LYS:HG2	1:A:234:ILE:HD11	1.94	0.48
1:A:340:ARG:HG3	1:A:340:ARG:HH11	1.77	0.48
1:B:143:ARG:NH2	1:B:165:THR:OG1	2.46	0.48
1:A:297:TYR:OH	2:E:27:DT:H5'	2.13	0.48
1:B:360:ALA:CA	1:B:363:LYS:HE3	2.42	0.48
1:B:362:LYS:HB2	1:B:362:LYS:NZ	2.22	0.48
1:D:259:ASN:C	1:D:261:ASN:N	2.71	0.48
1:D:288:THR:HG23	3:L:21:DT:H73	1.95	0.48
1:C:144:ILE:HG23	1:C:223:VAL:CG1	2.40	0.48
1:D:302:CYS:SG	1:D:304:THR:HG23	2.53	0.48
1:A:164:ASP:OD2	1:A:166:LYS:NZ	2.46	0.48
1:A:305:TYR:HE1	1:A:313:LYS:HD3	1.78	0.48
1:A:457:HIS:CB	1:D:331:ARG:CZ	2.91	0.48
1:B:331:ARG:NH1	1:B:447:VAL:HG23	2.29	0.48
1:D:222:TYR:N	1:D:222:TYR:CD2	2.82	0.48
2:E:25:DG:H2''	2:E:26:DT:H5'	1.93	0.48
2:E:28:DT:H2''	2:E:29:DA:C5'	2.43	0.48
1:B:281:PHE:CE2	1:B:302:CYS:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LEU:C	1:B:355:LEU:HD13	2.38	0.48
1:B:418:THR:OG1	1:B:420:ASP:OD1	2.30	0.48
3:F:0:DC:H2''	3:F:1:DA:H5'	1.95	0.48
2:K:44:DC:C2'	2:K:45:DT:H5'	2.37	0.48
1:A:394:GLU:O	1:A:398:GLU:HG2	2.14	0.48
1:B:150:LEU:HD23	1:B:150:LEU:C	2.39	0.48
1:B:240:SER:C	1:B:242:GLU:N	2.70	0.48
1:C:348:LEU:HD23	1:C:348:LEU:O	2.13	0.48
1:C:362:LYS:HG2	1:C:386:ILE:HG21	1.95	0.48
2:E:40:DT:H5'	2:E:40:DT:H6	1.77	0.48
1:B:442:ILE:O	1:B:442:ILE:HG22	2.13	0.48
1:C:341:ASN:C	1:C:343:ASP:H	2.21	0.48
1:C:348:LEU:HD23	1:C:348:LEU:C	2.39	0.48
1:D:158:PHE:CD2	1:D:177:LEU:HD13	2.48	0.48
1:D:277:CYS:O	1:D:279:LEU:N	2.46	0.48
1:A:281:PHE:CE2	1:A:302:CYS:HB2	2.49	0.48
1:C:259:ASN:C	1:C:261:ASN:N	2.71	0.48
1:D:185:GLU:CD	1:D:246:ARG:HH21	2.21	0.48
1:D:283:HIS:HB2	1:D:300:TYR:CE2	2.48	0.48
1:D:305:TYR:OH	1:D:315:GLY:CA	2.61	0.48
2:K:50:DG:H1	3:L:0:DC:H42	1.61	0.48
1:B:205:ARG:HD3	1:B:209:ARG:NH1	2.29	0.47
1:B:446:GLN:HG3	1:B:446:GLN:O	2.14	0.47
3:H:0:DC:H2''	3:H:1:DA:H5'	1.95	0.47
1:C:180:ILE:HG22	1:C:214:LEU:HD21	1.96	0.47
1:C:282:VAL:HG12	1:C:283:HIS:N	2.28	0.47
1:C:390:ILE:HG22	1:C:394:GLU:OE1	2.14	0.47
2:I:42:DC:N4	3:J:8:DG:H1	2.12	0.47
1:D:183:ILE:O	1:D:186:GLU:N	2.44	0.47
1:A:328:ILE:HD12	1:A:440:ILE:HD13	1.96	0.47
3:H:23:DA:H2''	3:H:24:DA:O4'	2.14	0.47
1:D:177:LEU:HD21	1:D:219:TYR:CE1	2.49	0.47
1:D:271:LEU:CD1	1:D:271:LEU:N	2.77	0.47
1:B:328:ILE:HD12	1:B:440:ILE:HD13	1.96	0.47
3:H:23:DA:C3'	3:H:24:DA:H5''	2.43	0.47
1:C:218:LEU:O	1:C:218:LEU:HG	2.10	0.47
1:D:216:ASN:C	1:D:218:LEU:H	2.21	0.47
1:D:318:ILE:HD12	1:D:318:ILE:N	2.29	0.47
1:A:272:VAL:HB	1:A:281:PHE:HB2	1.95	0.47
2:E:40:DT:H5'	2:E:40:DT:C6	2.49	0.47
3:H:16:DG:H2''	3:H:17:DG:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:TYR:OH	2:I:26:DT:H71	2.15	0.47
1:C:259:ASN:C	1:C:261:ASN:H	2.21	0.47
1:D:192:PHE:O	1:D:196:ARG:HG3	2.14	0.47
1:D:317:LYS:HG2	1:D:318:ILE:N	2.28	0.47
1:D:343:ASP:C	1:D:345:GLU:H	2.22	0.47
1:C:269:ASN:HD21	1:C:434:LYS:HZ3	1.62	0.47
1:C:344:LYS:HZ1	1:C:400:ASN:HB3	1.79	0.47
1:C:402:GLU:C	1:C:404:LYS:H	2.23	0.47
1:D:143:ARG:HH21	1:D:148:LEU:HB3	1.79	0.47
1:A:191:THR:OG1	2:E:38:DT:OP2	2.23	0.47
1:B:267:LEU:CD2	1:B:433:LEU:HD12	2.45	0.47
1:C:225:TYR:HB3	1:C:229:VAL:HB	1.96	0.47
1:C:402:GLU:C	1:C:404:LYS:N	2.71	0.47
1:D:164:ASP:OD2	1:D:166:LYS:NZ	2.46	0.47
1:D:269:ASN:OD1	1:D:269:ASN:C	2.58	0.47
1:D:269:ASN:OD1	1:D:270:ASN:ND2	2.41	0.47
2:K:40:DT:H2''	2:K:41:DT:C5'	2.45	0.47
1:A:274:CYS:SG	1:A:276:LYS:O	2.73	0.47
1:C:405:LYS:O	1:C:409:ILE:HG12	2.15	0.47
1:C:446:GLN:O	1:C:446:GLN:HG3	2.14	0.47
1:D:328:ILE:HD13	1:D:449:ILE:HD11	1.96	0.47
1:D:329:ILE:HA	1:D:332:VAL:HG12	1.96	0.47
1:A:188:GLN:OE1	1:A:253:ARG:NH2	2.45	0.47
1:B:266:SER:OG	3:H:16:DG:OP1	2.31	0.47
1:A:342:ILE:O	1:D:448:THR:HA	2.15	0.47
1:B:404:LYS:O	1:B:408:LYS:HG3	2.15	0.47
2:K:44:DC:H1'	2:K:45:DT:H5''	1.96	0.47
1:A:358:GLU:HB3	1:A:390:ILE:CD1	2.45	0.46
2:E:34:DC:C2'	2:E:35:DT:H5'	2.35	0.46
1:B:421:PHE:O	1:B:424:LEU:N	2.36	0.46
3:H:19:DA:H2''	3:H:20:DC:C5'	2.46	0.46
1:C:148:LEU:N	1:C:148:LEU:CD1	2.78	0.46
1:C:218:LEU:HA	1:C:222:TYR:O	2.16	0.46
1:D:324:LEU:O	1:D:327:LEU:HB3	2.14	0.46
1:B:407:LYS:O	1:B:411:GLU:HG3	2.16	0.46
1:C:231:VAL:CG2	1:C:232:LYS:N	2.77	0.46
1:C:355:LEU:HD13	1:C:359:HIS:NE2	2.30	0.46
1:C:407:LYS:HD3	1:C:410:GLN:HB3	1.97	0.46
1:D:144:ILE:C	1:D:146:ALA:N	2.72	0.46
1:D:269:ASN:ND2	1:D:434:LYS:NZ	2.63	0.46
1:A:457:HIS:HB2	1:D:331:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:DT:H2''	2:E:33:DC:O5'	2.16	0.46
1:C:397:ILE:HG22	1:C:401:GLU:OE2	2.14	0.46
1:A:397:ILE:HG22	1:A:398:GLU:N	2.30	0.46
3:F:15:DA:C2'	3:F:16:DG:C5'	2.78	0.46
1:B:317:LYS:CG	1:B:318:ILE:N	2.79	0.46
1:C:288:THR:HG23	3:J:21:DT:H73	1.96	0.46
2:I:42:DC:H2''	2:I:43:DT:OP2	2.15	0.46
1:D:135:ARG:HG3	1:D:135:ARG:HH11	1.81	0.46
1:A:190:ILE:O	1:A:193:LEU:HB3	2.16	0.46
1:A:432:TYR:HD2	1:A:433:LEU:HD23	1.81	0.46
1:B:328:ILE:CD1	1:B:440:ILE:HD13	2.45	0.46
1:C:143:ARG:NH1	2:I:48:DT:H4'	2.31	0.46
1:C:189:SER:HB3	1:C:192:PHE:HB2	1.98	0.46
1:D:299:TYR:HD1	1:D:320:ARG:HA	1.81	0.46
1:A:289:VAL:HG21	1:A:294:LYS:HG2	1.98	0.46
1:A:379:LEU:C	1:A:379:LEU:HD13	2.41	0.46
1:B:401:GLU:C	1:B:403:LEU:N	2.73	0.46
3:J:12:DA:H2''	3:J:13:DC:H5'	1.98	0.46
1:A:365:LEU:HD21	1:A:379:LEU:HD22	1.98	0.46
1:C:141:ILE:HG23	1:C:229:VAL:HG21	1.97	0.46
2:K:27:DT:H2''	2:K:28:DT:O5'	2.16	0.46
1:A:183:ILE:O	1:A:186:GLU:HB2	2.15	0.46
1:B:205:ARG:HG2	1:B:209:ARG:HD3	1.98	0.46
1:B:288:THR:CG2	1:B:289:VAL:N	2.79	0.45
1:D:332:VAL:CG2	1:D:432:TYR:HE2	2.29	0.45
1:A:317:LYS:CG	1:A:318:ILE:N	2.79	0.45
1:B:207:TYR:C	1:B:207:TYR:CD2	2.94	0.45
1:C:410:GLN:C	1:C:412:ASN:H	2.24	0.45
1:C:147:GLY:C	1:C:148:LEU:HD12	2.41	0.45
1:C:167:LEU:CD1	1:C:235:HIS:HB3	2.46	0.45
1:C:264:SER:O	1:C:265:ALA:C	2.59	0.45
1:C:438:ASN:HB2	1:C:452:LEU:HB3	1.99	0.45
1:A:266:SER:O	1:A:269:ASN:HB3	2.17	0.45
1:A:180:ILE:HG23	1:A:193:LEU:HD21	1.97	0.45
1:A:318:ILE:HD12	1:A:318:ILE:N	2.32	0.45
1:C:297:TYR:OH	2:I:27:DT:H5'	2.15	0.45
1:C:337:PHE:HD1	1:C:339:SER:H	1.65	0.45
3:L:10:DA:H2''	3:L:11:DA:OP2	2.17	0.45
1:A:150:LEU:HD23	1:A:150:LEU:O	2.17	0.45
1:A:184:PHE:CE2	1:A:247:VAL:HG13	2.51	0.45
1:B:391:ASN:HA	1:B:394:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LYS:HG3	1:C:404:LYS:NZ	2.31	0.45
1:D:160:TYR:HB3	1:D:167:LEU:HB2	1.99	0.45
1:A:243:GLN:O	1:A:243:GLN:HG2	2.16	0.45
1:A:427:ARG:HG3	1:A:427:ARG:HH11	1.81	0.45
1:B:416:LEU:HA	1:B:419:VAL:HB	1.99	0.45
1:C:385:ASP:O	1:C:389:GLN:HG3	2.17	0.45
1:D:438:ASN:HB2	1:D:452:LEU:CD1	2.47	0.45
3:L:6:DG:H2''	3:L:7:DA:C8	2.52	0.45
1:A:287:ASP:OD2	1:A:287:ASP:N	2.49	0.45
2:E:29:DA:H2''	2:E:30:DG:H8	1.82	0.45
1:C:305:TYR:HE1	1:C:313:LYS:HD3	1.81	0.45
1:C:332:VAL:HG22	1:C:451:TRP:CH2	2.52	0.45
1:C:452:LEU:CD2	1:C:452:LEU:N	2.80	0.45
1:B:238:ILE:O	1:B:238:ILE:CG2	2.64	0.45
1:B:268:LEU:N	1:B:268:LEU:CD1	2.80	0.45
1:B:268:LEU:N	1:B:268:LEU:HD12	2.32	0.45
1:C:280:GLY:O	1:C:303:LYS:HG3	2.17	0.45
1:D:259:ASN:C	1:D:261:ASN:H	2.23	0.45
1:A:378:GLU:O	1:A:382:MET:HG3	2.17	0.45
2:E:39:DT:H2''	2:E:40:DT:C5'	2.46	0.45
1:B:144:ILE:C	1:B:146:ALA:N	2.73	0.45
1:B:195:LYS:O	1:B:198:LYS:HB3	2.16	0.45
1:B:386:ILE:HD12	1:B:386:ILE:N	2.32	0.45
1:C:164:ASP:OD1	1:D:196:ARG:NH2	2.49	0.45
1:C:406:ASN:HD22	1:C:407:LYS:H	1.61	0.45
1:D:284:ARG:HG3	1:D:284:ARG:HH11	1.82	0.45
1:A:269:ASN:HB2	3:F:16:DG:OP1	2.16	0.44
1:B:259:ASN:C	1:B:261:ASN:N	2.73	0.44
1:C:283:HIS:HD2	1:C:300:TYR:CE1	2.35	0.44
1:C:331:ARG:HD2	1:C:449:ILE:CD1	2.47	0.44
2:I:30:DG:H1'	2:I:31:DT:C5'	2.47	0.44
1:A:134:ASP:O	1:A:137:VAL:HB	2.18	0.44
1:A:369:TYR:CA	1:A:373:SER:HB3	2.46	0.44
2:E:44:DC:C2'	2:E:45:DT:C5'	2.92	0.44
1:B:277:CYS:O	1:B:279:LEU:HG	2.17	0.44
3:J:14:DG:H2''	3:J:15:DA:N7	2.33	0.44
1:B:259:ASN:O	1:B:261:ASN:N	2.50	0.44
1:A:150:LEU:C	1:A:150:LEU:CD2	2.90	0.44
1:C:226:LYS:HG3	1:C:226:LYS:O	2.16	0.44
1:C:332:VAL:HG22	1:C:451:TRP:HH2	1.82	0.44
1:C:350:SER:O	1:C:354:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:20:DC:H2''	3:J:21:DT:OP2	2.16	0.44
1:D:133:ARG:NH1	3:L:2:DA:OP1	2.49	0.44
1:A:366:PHE:O	1:A:369:TYR:HB3	2.18	0.44
1:B:357:ILE:O	1:B:361:LYS:HG3	2.17	0.44
1:C:267:LEU:CD2	1:C:433:LEU:HD12	2.47	0.44
1:D:436:LEU:HG	1:D:451:TRP:CZ3	2.53	0.44
1:A:137:VAL:C	1:A:139:GLY:N	2.75	0.44
1:A:207:TYR:C	1:A:207:TYR:CD2	2.96	0.44
1:A:344:LYS:HD2	1:A:347:GLU:OE1	2.17	0.44
1:B:383:MET:O	1:B:387:ASP:CG	2.60	0.44
3:H:5:DA:C2	3:H:6:DG:C6	3.05	0.44
3:H:10:DA:H2''	3:H:11:DA:OP2	2.17	0.44
1:C:216:ASN:O	1:C:218:LEU:N	2.49	0.44
1:D:332:VAL:HG22	1:D:332:VAL:O	2.18	0.44
1:D:355:LEU:C	1:D:357:ILE:N	2.76	0.44
1:A:355:LEU:HD12	1:A:397:ILE:HG12	1.97	0.44
1:A:407:LYS:HD2	1:D:276:LYS:NZ	2.32	0.44
1:B:418:THR:C	1:B:420:ASP:N	2.76	0.44
1:C:167:LEU:HD12	1:C:167:LEU:N	2.30	0.44
1:D:249:GLU:O	1:D:252:SER:HB3	2.17	0.44
1:A:299:TYR:HA	1:A:319:TRP:O	2.18	0.44
3:H:1:DA:H2''	3:H:2:DA:OP2	2.18	0.44
3:H:19:DA:H2''	3:H:20:DC:O5'	2.18	0.44
1:A:216:ASN:O	1:A:216:ASN:OD1	2.36	0.44
1:B:134:ASP:C	1:B:136:MET:N	2.74	0.44
1:B:150:LEU:C	1:B:150:LEU:CD2	2.91	0.44
1:B:281:PHE:CD2	1:B:302:CYS:HA	2.53	0.44
1:C:180:ILE:CG2	1:C:214:LEU:HD21	2.48	0.44
1:C:438:ASN:O	1:C:439:LYS:CD	2.66	0.44
1:D:143:ARG:NH1	2:K:48:DT:H4'	2.33	0.44
1:D:156:ARG:HD3	3:L:6:DG:H1'	1.99	0.44
1:D:313:LYS:NZ	2:K:30:DG:OP1	2.48	0.44
1:A:426:PHE:O	1:A:429:LYS:HB2	2.18	0.43
1:B:159:GLY:HA2	1:B:173:GLU:HB2	1.99	0.43
1:B:362:LYS:CB	1:B:362:LYS:NZ	2.81	0.43
1:B:416:LEU:HD13	1:B:416:LEU:C	2.43	0.43
1:C:406:ASN:HD22	1:C:406:ASN:C	2.16	0.43
1:D:446:GLN:O	1:D:446:GLN:CG	2.61	0.43
1:A:158:PHE:CD2	1:A:177:LEU:CD1	3.01	0.43
1:C:159:GLY:HA2	1:C:173:GLU:HB2	1.98	0.43
1:C:274:CYS:HB2	1:C:281:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ARG:HD2	1:C:449:ILE:HD12	1.99	0.43
1:C:432:TYR:CZ	1:C:436:LEU:HD22	2.54	0.43
1:D:186:GLU:O	1:D:188:GLN:HG2	2.18	0.43
1:D:231:VAL:CG2	1:D:232:LYS:N	2.81	0.43
1:D:281:PHE:CD1	1:D:301:SER:C	2.96	0.43
1:D:304:THR:HA	1:D:311:LEU:HD13	1.99	0.43
1:B:190:ILE:HB	1:B:207:TYR:CE1	2.53	0.43
1:C:226:LYS:HB3	3:J:5:DA:OP2	2.19	0.43
1:A:317:LYS:HG2	1:A:318:ILE:N	2.33	0.43
1:B:298:ARG:HB2	1:B:321:ALA:HB3	2.00	0.43
1:B:320:ARG:HD2	1:B:322:ASP:CG	2.42	0.43
1:C:163:ILE:HG21	1:D:179:LEU:HD22	2.00	0.43
1:C:298:ARG:HB2	1:C:321:ALA:HB3	2.01	0.43
1:A:278:GLY:C	1:A:279:LEU:O	2.60	0.43
1:B:187:GLU:C	1:B:188:GLN:CG	2.91	0.43
1:B:284:ARG:HH11	1:B:284:ARG:HG3	1.84	0.43
1:B:418:THR:O	1:B:419:VAL:C	2.61	0.43
1:C:388:ALA:O	1:C:391:ASN:HB2	2.18	0.43
2:I:30:DG:H2"	2:I:31:DT:OP2	2.17	0.43
1:A:212:ASN:O	1:A:215:THR:O	2.36	0.43
1:A:370:ILE:HD13	1:A:370:ILE:N	2.34	0.43
1:C:344:LYS:HG3	1:C:404:LYS:HE3	2.00	0.43
1:D:272:VAL:HB	1:D:281:PHE:HB2	1.99	0.43
1:D:436:LEU:HG	1:D:451:TRP:HZ3	1.83	0.43
1:A:200:LEU:HD12	1:A:200:LEU:N	2.32	0.43
1:B:282:VAL:CG1	1:B:283:HIS:N	2.82	0.43
1:B:419:VAL:O	1:B:419:VAL:HG13	2.18	0.43
1:C:136:MET:SD	2:I:50:DG:N3	2.91	0.43
1:C:217:ASP:O	1:C:222:TYR:HB2	2.19	0.43
1:D:207:TYR:C	1:D:207:TYR:CD2	2.96	0.43
1:A:180:ILE:CG2	1:A:214:LEU:HD21	2.49	0.43
1:B:276:LYS:O	1:B:277:CYS:CB	2.65	0.43
1:D:226:LYS:O	1:D:226:LYS:CG	2.66	0.43
1:D:284:ARG:HG3	1:D:284:ARG:NH1	2.34	0.43
1:D:438:ASN:O	1:D:439:LYS:HD2	2.19	0.43
1:C:190:ILE:CD1	1:C:214:LEU:HD12	2.49	0.43
1:A:327:LEU:C	1:A:327:LEU:CD2	2.92	0.43
1:A:386:ILE:O	1:A:389:GLN:HB3	2.18	0.43
1:B:226:LYS:O	1:B:228:LYS:N	2.52	0.43
1:C:169:ILE:HG22	1:C:170:ASN:N	2.34	0.43
1:C:196:ARG:O	1:C:200:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ASN:C	1:C:406:ASN:ND2	2.77	0.43
1:D:205:ARG:HG2	1:D:209:ARG:HH11	1.84	0.43
2:E:38:DT:H1'	2:E:39:DT:H5''	2.01	0.42
2:G:29:DA:H2''	2:G:30:DG:C8	2.54	0.42
1:C:282:VAL:CG1	1:C:283:HIS:N	2.82	0.42
1:C:417:ALA:C	1:C:419:VAL:H	2.27	0.42
1:B:328:ILE:HD11	1:B:440:ILE:HG21	2.01	0.42
1:B:384:ASN:HA	1:B:387:ASP:HB2	2.02	0.42
1:B:421:PHE:O	1:B:422:ASN:C	2.62	0.42
1:C:345:GLU:O	1:C:349:ASP:HB2	2.19	0.42
1:A:407:LYS:HD2	1:D:276:LYS:HZ1	1.84	0.42
1:B:310:GLU:OE1	1:B:310:GLU:N	2.51	0.42
1:B:351:LEU:CD1	1:B:397:ILE:HG12	2.49	0.42
1:C:400:ASN:C	1:C:402:GLU:N	2.73	0.42
2:K:25:DG:H8	2:K:25:DG:O5'	2.02	0.42
1:A:259:ASN:C	1:A:261:ASN:N	2.76	0.42
1:A:402:GLU:OE2	1:A:402:GLU:N	2.52	0.42
1:C:272:VAL:HA	1:C:440:ILE:O	2.19	0.42
1:D:174:ALA:O	1:D:178:ARG:HG3	2.20	0.42
1:D:206:THR:HG23	1:D:209:ARG:HB2	2.02	0.42
1:A:350:SER:C	1:A:352:ASN:H	2.26	0.42
1:A:421:PHE:CE2	1:A:429:LYS:HD3	2.53	0.42
3:H:0:DC:H5'	3:H:0:DC:C6	2.49	0.42
1:C:337:PHE:C	1:C:339:SER:N	2.76	0.42
2:I:47:DG:H2''	2:I:48:DT:C7	2.50	0.42
1:D:169:ILE:CD1	1:D:236:GLU:HB3	2.49	0.42
1:C:207:TYR:HE1	2:I:38:DT:OP2	2.02	0.42
1:C:321:ALA:O	1:C:322:ASP:C	2.62	0.42
1:D:211:ASN:O	1:D:215:THR:HB	2.18	0.42
1:D:332:VAL:HG21	1:D:432:TYR:HE2	1.84	0.42
1:A:369:TYR:HA	1:A:373:SER:OG	2.20	0.42
3:H:6:DG:H2''	3:H:7:DA:C8	2.55	0.42
1:C:276:LYS:O	1:C:277:CYS:SG	2.78	0.42
1:C:320:ARG:HH11	1:C:320:ARG:CG	2.33	0.42
1:C:324:LEU:O	1:C:327:LEU:HB3	2.19	0.42
1:D:254:MET:CE	2:K:38:DT:H3'	2.45	0.42
1:A:350:SER:C	1:A:352:ASN:N	2.78	0.42
3:F:11:DA:H2''	3:F:12:DA:OP2	2.19	0.42
1:B:335:TYR:CE2	1:B:436:LEU:HD11	2.55	0.42
1:C:295:TYR:CE2	2:I:26:DT:H72	2.54	0.42
1:C:355:LEU:HD23	1:C:393:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:GLU:HG2	1:C:390:ILE:HG12	2.01	0.42
1:D:217:ASP:HB2	1:D:244:PHE:CZ	2.54	0.42
1:D:452:LEU:HB3	1:D:453:LEU:H	1.61	0.42
3:L:13:DC:H5'	3:L:13:DC:H6	1.85	0.42
1:A:141:ILE:O	1:A:145:GLU:HG3	2.20	0.42
1:B:225:TYR:O	1:B:226:LYS:C	2.63	0.42
1:B:385:ASP:O	1:B:389:GLN:HG2	2.19	0.42
1:C:216:ASN:C	1:C:218:LEU:N	2.77	0.42
1:D:421:PHE:C	1:D:423:SER:H	2.27	0.42
3:F:0:DC:H5'	3:F:0:DC:C6	2.55	0.42
1:C:421:PHE:HE2	1:C:429:LYS:HD3	1.84	0.42
1:D:332:VAL:HG21	1:D:432:TYR:CE2	2.55	0.42
1:B:269:ASN:HD21	1:B:434:LYS:HZ3	1.66	0.41
2:G:31:DT:H5'	2:G:31:DT:H6	1.84	0.41
3:H:13:DC:H6	3:H:13:DC:H5'	1.85	0.41
1:C:143:ARG:NH2	1:C:149:PRO:HG2	2.35	0.41
1:C:191:THR:HG1	2:I:37:DG:H3'	1.83	0.41
1:C:206:THR:O	1:C:207:TYR:C	2.62	0.41
1:C:268:LEU:CD1	1:C:325:GLU:HG2	2.43	0.41
1:A:276:LYS:HD2	1:A:316:ASN:HB2	2.02	0.41
1:A:369:TYR:CD1	1:A:370:ILE:HD13	2.50	0.41
1:A:425:GLU:OE2	1:A:425:GLU:HA	2.20	0.41
1:A:435:SER:O	1:A:452:LEU:HD23	2.20	0.41
2:E:28:DT:H1'	2:E:29:DA:H5''	2.03	0.41
1:B:218:LEU:C	1:B:218:LEU:HD23	2.45	0.41
1:C:267:LEU:C	1:C:267:LEU:HD23	2.45	0.41
2:I:33:DC:H2''	2:I:34:DC:O5'	2.19	0.41
1:D:191:THR:OG1	2:K:37:DG:H3'	2.20	0.41
1:B:144:ILE:HD11	1:B:150:LEU:HA	2.01	0.41
1:B:327:LEU:C	1:B:327:LEU:CD2	2.82	0.41
1:C:205:ARG:HD3	1:C:209:ARG:NH1	2.35	0.41
1:C:215:THR:O	1:C:215:THR:HG22	2.20	0.41
2:I:50:DG:H1	3:J:0:DC:H42	1.68	0.41
1:A:289:VAL:HG12	1:A:290:SER:N	2.35	0.41
3:F:6:DG:H2''	3:F:7:DA:C8	2.55	0.41
2:G:29:DA:H2''	2:G:30:DG:H8	1.84	0.41
3:H:12:DA:H1'	3:H:13:DC:C5'	2.48	0.41
1:C:169:ILE:CG2	1:C:170:ASN:N	2.83	0.41
1:C:419:VAL:HG12	1:C:423:SER:OG	2.20	0.41
1:D:321:ALA:O	1:D:322:ASP:C	2.63	0.41
3:F:23:DA:H2''	3:F:24:DA:C5'	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:HD21	1:B:433:LEU:HD12	2.02	0.41
1:C:298:ARG:NH1	1:C:321:ALA:HB1	2.34	0.41
1:D:226:LYS:HZ2	1:D:228:LYS:HE3	1.84	0.41
1:A:328:ILE:CD1	1:A:440:ILE:HD13	2.50	0.41
2:E:31:DT:C5'	2:E:31:DT:H6	2.30	0.41
2:E:31:DT:H2''	2:E:32:DT:C5'	2.50	0.41
1:B:190:ILE:O	1:B:193:LEU:HB3	2.21	0.41
1:B:349:ASP:HA	1:B:352:ASN:ND2	2.33	0.41
1:C:259:ASN:O	1:C:262:LYS:HB2	2.20	0.41
1:A:215:THR:CG2	1:A:216:ASN:H	2.29	0.41
1:A:225:TYR:O	1:A:226:LYS:C	2.63	0.41
1:B:332:VAL:C	1:B:334:ASN:N	2.78	0.41
1:B:386:ILE:O	1:B:386:ILE:HG22	2.21	0.41
2:G:29:DA:H1'	2:G:30:DG:C8	2.56	0.41
1:C:144:ILE:HD11	1:C:150:LEU:HA	2.03	0.41
1:C:362:LYS:HE2	1:C:366:PHE:HE2	1.85	0.41
1:D:455:HIS:O	1:D:456:HIS:CG	2.73	0.41
3:L:6:DG:H2''	3:L:7:DA:H8	1.86	0.41
3:L:16:DG:H2''	3:L:17:DG:OP2	2.20	0.41
1:A:289:VAL:HG22	1:A:294:LYS:HG2	2.03	0.41
1:A:331:ARG:NH1	1:A:447:VAL:HG23	2.36	0.41
2:E:25:DG:C2'	2:E:26:DT:H5''	2.49	0.41
3:F:5:DA:C2	3:F:6:DG:C6	3.09	0.41
1:B:143:ARG:HH21	1:B:148:LEU:HB3	1.85	0.41
1:B:231:VAL:HG22	1:B:232:LYS:N	2.35	0.41
1:B:259:ASN:C	1:B:261:ASN:H	2.28	0.41
1:B:352:ASN:HB3	1:B:356:LYS:HZ3	1.86	0.41
1:A:205:ARG:HD3	1:A:209:ARG:NH1	2.36	0.41
1:A:266:SER:O	1:A:269:ASN:N	2.51	0.41
1:A:391:ASN:CA	1:A:394:GLU:HG2	2.37	0.41
1:B:284:ARG:HG3	1:B:284:ARG:NH1	2.35	0.41
1:B:363:LYS:HG3	1:B:363:LYS:H	1.67	0.41
1:C:170:ASN:OD1	1:C:173:GLU:HG3	2.20	0.41
1:C:253:ARG:CZ	1:C:431:LEU:HD22	2.49	0.41
1:C:267:LEU:CD2	1:C:267:LEU:C	2.94	0.41
1:C:268:LEU:CD1	1:C:268:LEU:H	2.33	0.41
1:C:268:LEU:O	1:C:269:ASN:C	2.62	0.41
1:C:269:ASN:ND2	1:C:434:LYS:NZ	2.69	0.41
1:C:290:SER:O	1:C:291:ARG:HB3	2.21	0.41
1:C:365:LEU:CD2	1:C:382:MET:HB3	2.51	0.41
1:C:427:ARG:O	1:C:430:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:5:DA:H1'	3:J:6:DG:C8	2.56	0.41
1:D:187:GLU:C	1:D:189:SER:N	2.78	0.41
1:D:223:VAL:HG23	1:D:233:GLY:HA3	2.03	0.41
1:D:421:PHE:C	1:D:423:SER:N	2.75	0.41
3:F:12:DA:H2''	3:F:13:DC:C5'	2.51	0.41
1:B:216:ASN:O	1:B:217:ASP:CB	2.68	0.41
1:B:337:PHE:CD2	1:B:337:PHE:N	2.89	0.41
3:J:7:DA:C2'	3:J:8:DG:H5'	2.42	0.41
1:D:216:ASN:C	1:D:218:LEU:N	2.79	0.41
1:D:451:TRP:O	1:D:452:LEU:HB2	2.20	0.41
1:A:241:GLU:HG2	1:A:245:TYR:CE2	2.56	0.40
1:A:376:VAL:HG13	1:A:377:SER:N	2.36	0.40
3:F:-1:DC:H2''	3:F:0:DC:H5'	2.03	0.40
1:B:361:LYS:HA	1:B:364:ARG:HB2	2.02	0.40
1:B:391:ASN:HA	1:B:394:GLU:HG2	2.04	0.40
1:C:184:PHE:CG	1:C:214:LEU:HD13	2.57	0.40
1:C:207:TYR:O	1:C:208:ASN:C	2.63	0.40
1:C:295:TYR:HE2	2:I:26:DT:H72	1.85	0.40
1:C:384:ASN:N	1:C:384:ASN:HD22	2.19	0.40
1:C:413:LEU:CD1	1:C:416:LEU:HD22	2.46	0.40
1:D:226:LYS:O	1:D:226:LYS:HG2	2.20	0.40
1:A:404:LYS:HE2	1:D:443:ASP:OD2	2.22	0.40
1:C:267:LEU:C	1:C:269:ASN:H	2.30	0.40
1:D:267:LEU:CD2	1:D:433:LEU:HD12	2.51	0.40
1:D:288:THR:HG23	3:L:21:DT:H72	2.02	0.40
1:A:282:VAL:HG12	1:A:283:HIS:N	2.37	0.40
3:F:12:DA:H2''	3:F:13:DC:H5'	2.03	0.40
1:B:410:GLN:O	1:B:413:LEU:HB2	2.22	0.40
1:C:284:ARG:HG3	1:C:284:ARG:HH11	1.85	0.40
2:I:27:DT:H2''	2:I:28:DT:O5'	2.21	0.40
2:I:47:DG:C2'	2:I:48:DT:H72	2.50	0.40
1:A:143:ARG:NH1	1:A:149:PRO:O	2.54	0.40
1:A:144:ILE:HG22	1:A:229:VAL:CG1	2.52	0.40
1:A:257:ASN:ND2	1:A:434:LYS:CE	2.76	0.40
1:B:272:VAL:CG1	1:B:442:ILE:HD13	2.50	0.40
1:B:415:ASP:O	1:B:418:THR:CG2	2.70	0.40
1:C:180:ILE:HG22	1:C:181:TYR:N	2.35	0.40
1:D:150:LEU:C	1:D:150:LEU:CD2	2.94	0.40
1:A:300:TYR:CD1	1:A:324:LEU:HD23	2.57	0.40
1:C:193:LEU:HD11	1:C:197:LEU:HD11	2.04	0.40
1:C:427:ARG:HG3	1:C:427:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:LEU:C	1:D:455:HIS:N	2.79	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	
1	A	309/328 (94%)	263 (85%)	43 (14%)	3 (1%)	12	45
1	B	299/328 (91%)	256 (86%)	34 (11%)	9 (3%)	3	23
1	C	305/328 (93%)	251 (82%)	47 (15%)	7 (2%)	5	29
1	D	279/328 (85%)	228 (82%)	39 (14%)	12 (4%)	2	16
All	All	1192/1312 (91%)	998 (84%)	163 (14%)	31 (3%)	4	26

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	B	227	ASP
1	B	278	GLY
1	B	419	VAL
1	B	421	PHE
1	B	422	ASN
1	C	422	ASN
1	D	278	GLY
1	D	339	SER
1	D	344	LYS
1	D	453	LEU
1	A	444	GLY
1	C	269	ASN
1	C	368	LEU

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Mol	Chain	Res	Type
1	D	188	GLN
1	D	227	ASP
1	D	452	LEU
1	D	456	HIS
1	B	207	TYR
1	D	260	MET
1	B	226	LYS
1	C	267	LEU
1	C	270	ASN
1	D	291	ARG
1	A	279	LEU
1	B	317	LYS
1	C	217	ASP
1	C	421	PHE
1	D	226	LYS
1	B	259	ASN
1	D	342	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/302 (96%)	263 (90%)	28 (10%)	8	32
1	B	281/302 (93%)	242 (86%)	39 (14%)	3	17
1	C	284/302 (94%)	254 (89%)	30 (11%)	6	27
1	D	228/302 (76%)	206 (90%)	22 (10%)	8	32
All	All	1084/1208 (90%)	965 (89%)	119 (11%)	6	26

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ARG
1	A	167	LEU
1	A	177	LEU
1	A	192	PHE

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Mol	Chain	Res	Type
1	A	206	THR
1	A	216	ASN
1	A	227	ASP
1	A	262	LYS
1	A	267	LEU
1	A	269	ASN
1	A	272	VAL
1	A	273	VAL
1	A	287	ASP
1	A	291	ARG
1	A	294	LYS
1	A	311	LEU
1	A	320	ARG
1	A	329	ILE
1	A	330	ASP
1	A	365	LEU
1	A	370	ILE
1	A	385	ASP
1	A	387	ASP
1	A	401	GLU
1	A	402	GLU
1	A	422	ASN
1	A	442	ILE
1	A	457	HIS
1	B	136	MET
1	B	137	VAL
1	B	140	LYS
1	B	143	ARG
1	B	150	LEU
1	B	151	THR
1	B	167	LEU
1	B	188	GLN
1	B	192	PHE
1	B	205	ARG
1	B	206	THR
1	B	215	THR
1	B	217	ASP
1	B	218	LEU
1	B	240	SER
1	B	262	LYS
1	B	267	LEU
1	B	269	ASN

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Mol	Chain	Res	Type
1	B	272	VAL
1	B	273	VAL
1	B	286	LYS
1	B	287	ASP
1	B	294	LYS
1	B	311	LEU
1	B	320	ARG
1	B	322	ASP
1	B	348	LEU
1	B	349	ASP
1	B	362	LYS
1	B	364	ARG
1	B	366	PHE
1	B	367	ASP
1	B	382	MET
1	B	398	GLU
1	B	402	GLU
1	B	416	LEU
1	B	442	ILE
1	B	452	LEU
1	B	453	LEU
1	C	136	MET
1	C	143	ARG
1	C	151	THR
1	C	167	LEU
1	C	192	PHE
1	C	206	THR
1	C	217	ASP
1	C	218	LEU
1	C	227	ASP
1	C	262	LYS
1	C	267	LEU
1	C	269	ASN
1	C	273	VAL
1	C	287	ASP
1	C	294	LYS
1	C	311	LEU
1	C	320	ARG
1	C	330	ASP
1	C	355	LEU
1	C	358	GLU
1	C	362	LYS

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Mol	Chain	Res	Type
1	C	367	ASP
1	C	381	SER
1	C	382	MET
1	C	402	GLU
1	C	406	ASN
1	C	419	VAL
1	C	420	ASP
1	C	422	ASN
1	C	452	LEU
1	D	143	ARG
1	D	150	LEU
1	D	167	LEU
1	D	188	GLN
1	D	192	PHE
1	D	215	THR
1	D	217	ASP
1	D	218	LEU
1	D	262	LYS
1	D	267	LEU
1	D	269	ASN
1	D	271	LEU
1	D	273	VAL
1	D	293	LYS
1	D	294	LYS
1	D	302	CYS
1	D	311	LEU
1	D	320	ARG
1	D	422	ASN
1	D	423	SER
1	D	455	HIS
1	D	459	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	211	ASN
1	A	257	ASN
1	A	269	ASN
1	A	270	ASN
1	A	307	HIS
1	A	359	HIS

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Mol	Chain	Res	Type
1	A	384	ASN
1	A	396	GLN
1	A	400	ASN
1	A	406	ASN
1	A	457	HIS
1	A	460	HIS
1	B	208	ASN
1	B	211	ASN
1	B	212	ASN
1	B	257	ASN
1	B	269	ASN
1	B	270	ASN
1	B	334	ASN
1	B	352	ASN
1	B	384	ASN
1	B	396	GLN
1	B	412	ASN
1	C	176	GLN
1	C	261	ASN
1	C	269	ASN
1	C	270	ASN
1	C	333	ASN
1	C	341	ASN
1	C	384	ASN
1	C	391	ASN
1	C	396	GLN
1	C	400	ASN
1	C	406	ASN
1	C	410	GLN
1	D	211	ASN
1	D	230	HIS
1	D	257	ASN
1	D	456	HIS
1	D	458	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/328 (96%)	0.15	13 (4%) 41 25	31, 87, 156, 171	3 (0%)
1	B	305/328 (92%)	0.24	18 (5%) 28 18	21, 81, 149, 167	2 (0%)
1	C	309/328 (94%)	0.50	28 (9%) 15 9	52, 117, 167, 190	0
1	D	287/328 (87%)	0.51	29 (10%) 12 8	42, 91, 166, 184	1 (0%)
2	E	26/26 (100%)	0.00	0 100 100	68, 87, 115, 116	0
2	G	26/26 (100%)	-0.05	0 100 100	64, 82, 99, 109	0
2	I	26/26 (100%)	0.22	0 100 100	89, 116, 157, 165	0
2	K	26/26 (100%)	0.06	0 100 100	77, 93, 118, 121	0
3	F	26/26 (100%)	0.26	0 100 100	69, 96, 128, 135	0
3	H	26/26 (100%)	0.23	0 100 100	69, 85, 108, 111	0
3	J	26/26 (100%)	0.62	0 100 100	96, 120, 174, 188	0
3	L	26/26 (100%)	0.21	0 100 100	72, 96, 123, 131	0
All	All	1424/1520 (93%)	0.32	88 (6%) 26 17	21, 94, 161, 190	6 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	ARG	9.5
1	C	263	GLU	6.3
1	D	192	PHE	5.4
1	C	413	LEU	5.1
1	B	263	GLU	5.1
1	A	419	VAL	5.0
1	B	399	ALA	4.9
1	B	322	ASP	4.6
1	C	366	PHE	4.5
1	C	289	VAL	4.3
1	B	192	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	294	LYS	4.1
1	C	192	PHE	4.0
1	D	460	HIS	4.0
1	D	262	LYS	3.9
1	B	412	ASN	3.4
1	C	288	THR	3.4
1	D	299	TYR	3.4
1	B	286	LYS	3.4
1	C	287	ASP	3.3
1	B	453	LEU	3.3
1	C	367	ASP	3.2
1	B	401	GLU	3.2
1	A	284	ARG	3.1
1	C	414	ALA	3.1
1	D	289	VAL	3.1
1	D	287	ASP	3.0
1	A	418	THR	3.0
1	A	192	PHE	2.9
1	D	402	GLU	2.9
1	C	416	LEU	2.9
1	A	306	LYS	2.9
1	A	351	LEU	2.8
1	D	294	LYS	2.8
1	C	420	ASP	2.7
1	A	334	ASN	2.7
1	A	326	GLU	2.7
1	B	404	LYS	2.6
1	D	341	ASN	2.6
1	D	286	LYS	2.6
1	D	446	GLN	2.6
1	D	358	GLU	2.6
1	A	292	GLY	2.6
1	C	365	LEU	2.6
1	C	344	LYS	2.6
1	C	280	GLY	2.6
1	D	134	ASP	2.6
1	D	344	LYS	2.6
1	C	383	MET	2.5
1	C	245	TYR	2.5
1	D	291	ARG	2.5
1	D	285	ARG	2.5
1	C	342	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	216	ASN	2.5
1	D	351	LEU	2.4
1	B	419	VAL	2.4
1	C	292	GLY	2.4
1	D	135	ARG	2.4
1	A	453	LEU	2.4
1	C	285	ARG	2.4
1	B	216	ASN	2.3
1	D	296	HIS	2.3
1	C	408	LYS	2.3
1	C	409	ILE	2.3
1	D	295	TYR	2.3
1	C	296	HIS	2.3
1	D	400	ASN	2.3
1	D	387	ASP	2.3
1	D	352	ASN	2.3
1	D	411	GLU	2.2
1	D	388	ALA	2.2
1	B	400	ASN	2.2
1	C	348	LEU	2.2
1	C	368	LEU	2.2
1	D	195	LYS	2.2
1	B	320	ARG	2.2
1	A	299	TYR	2.2
1	D	297	TYR	2.2
1	D	334	ASN	2.2
1	B	369	TYR	2.1
1	A	365	LEU	2.1
1	C	153	ALA	2.1
1	B	454	GLU	2.1
1	B	413	LEU	2.1
1	A	307	HIS	2.0
1	B	383	MET	2.0
1	C	403	LEU	2.0
1	C	369	TYR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	A	504	1/1	0.76	0.17	132,132,132,132	0
5	CA	D	502	1/1	0.77	0.20	145,145,145,145	0
5	CA	C	502	1/1	0.79	0.24	145,145,145,145	0
5	CA	E	101	1/1	0.85	0.12	118,118,118,118	0
5	CA	B	502	1/1	0.85	0.24	125,125,125,125	0
5	CA	A	505	1/1	0.89	0.26	160,160,160,160	0
5	CA	B	503	1/1	0.91	0.34	121,121,121,121	0
4	ZN	C	501	1/1	0.98	0.04	144,144,144,144	0
4	ZN	A	502	1/1	0.99	0.03	87,87,87,87	0
4	ZN	A	503	1/1	0.99	0.02	110,110,110,110	0
4	ZN	A	501	1/1	1.00	0.01	106,106,106,106	0
4	ZN	D	501	1/1	1.00	0.02	116,116,116,116	0
4	ZN	B	501	1/1	1.00	0.02	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.