



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:32 PM UTC

PDB ID : 3US2 / pdb_00003us2
Title : Structure of p63 DNA Binding Domain in Complex with a 19 Base Pair A/T Rich Response Element Containing Two Half Sites with a Single Base Pair Overlap
Authors : Chen, C.; Herzberg, O.
Deposited on : 2011-11-22
Resolution : 4.20 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:

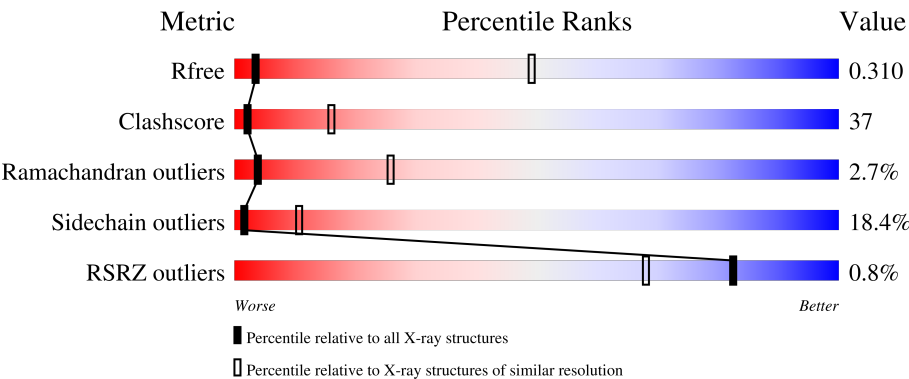
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	203	38%44%11%• 5%
1	B	203	38%35%14%• 10%
1	C	203	33%42%18%• 5%
1	D	203	% 35%38%14%• 10%
1	G	203	% 36%45%11%• 5%

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Mol	Chain	Length	Quality of chain
1	H	203	38%36%13%•10%
1	I	203	% 39%43%11%•5%
1	J	203	% 36%37%14%•10%
2	E	19	58%37%5%
2	K	19	47%53%
3	F	19	32%68%
3	L	19	32%68%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13210 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 Tumor protein 63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1497	938	263	284	12			
1	B	182	Total	C	N	O	S	0	0	0
			1417	891	250	264	12			
1	C	193	Total	C	N	O	S	0	0	0
			1497	938	263	284	12			
1	D	182	Total	C	N	O	S	0	0	0
			1417	891	250	264	12			
1	G	193	Total	C	N	O	S	0	0	0
			1497	938	263	284	12			
1	H	182	Total	C	N	O	S	0	0	0
			1417	891	250	264	12			
1	I	193	Total	C	N	O	S	0	0	0
			1497	938	263	284	12			
1	J	182	Total	C	N	O	S	0	0	0
			1417	891	250	264	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	expression tag	UNP Q9H3D4
A	122	SER	-	expression tag	UNP Q9H3D4
A	123	HIS	-	expression tag	UNP Q9H3D4
A	124	MET	-	expression tag	UNP Q9H3D4
A	125	ALA	-	expression tag	UNP Q9H3D4
A	126	SER	-	expression tag	UNP Q9H3D4
B	121	GLY	-	expression tag	UNP Q9H3D4
B	122	SER	-	expression tag	UNP Q9H3D4
B	123	HIS	-	expression tag	UNP Q9H3D4
B	124	MET	-	expression tag	UNP Q9H3D4
B	125	ALA	-	expression tag	UNP Q9H3D4
B	126	SER	-	expression tag	UNP Q9H3D4
C	121	GLY	-	expression tag	UNP Q9H3D4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	122	SER	-	expression tag	UNP Q9H3D4
C	123	HIS	-	expression tag	UNP Q9H3D4
C	124	MET	-	expression tag	UNP Q9H3D4
C	125	ALA	-	expression tag	UNP Q9H3D4
C	126	SER	-	expression tag	UNP Q9H3D4
D	121	GLY	-	expression tag	UNP Q9H3D4
D	122	SER	-	expression tag	UNP Q9H3D4
D	123	HIS	-	expression tag	UNP Q9H3D4
D	124	MET	-	expression tag	UNP Q9H3D4
D	125	ALA	-	expression tag	UNP Q9H3D4
D	126	SER	-	expression tag	UNP Q9H3D4
G	121	GLY	-	expression tag	UNP Q9H3D4
G	122	SER	-	expression tag	UNP Q9H3D4
G	123	HIS	-	expression tag	UNP Q9H3D4
G	124	MET	-	expression tag	UNP Q9H3D4
G	125	ALA	-	expression tag	UNP Q9H3D4
G	126	SER	-	expression tag	UNP Q9H3D4
H	121	GLY	-	expression tag	UNP Q9H3D4
H	122	SER	-	expression tag	UNP Q9H3D4
H	123	HIS	-	expression tag	UNP Q9H3D4
H	124	MET	-	expression tag	UNP Q9H3D4
H	125	ALA	-	expression tag	UNP Q9H3D4
H	126	SER	-	expression tag	UNP Q9H3D4
I	121	GLY	-	expression tag	UNP Q9H3D4
I	122	SER	-	expression tag	UNP Q9H3D4
I	123	HIS	-	expression tag	UNP Q9H3D4
I	124	MET	-	expression tag	UNP Q9H3D4
I	125	ALA	-	expression tag	UNP Q9H3D4
I	126	SER	-	expression tag	UNP Q9H3D4
J	121	GLY	-	expression tag	UNP Q9H3D4
J	122	SER	-	expression tag	UNP Q9H3D4
J	123	HIS	-	expression tag	UNP Q9H3D4
J	124	MET	-	expression tag	UNP Q9H3D4
J	125	ALA	-	expression tag	UNP Q9H3D4
J	126	SER	-	expression tag	UNP Q9H3D4

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*AP*AP*A
P*CP*AP*TP*GP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	19	Total	C	N	O	P	0	0	0
			387	188	70	111	18			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	19	Total	C	N	O	P	0	0	0
			387	188	70	111	18			

- Molecule 3 is a DNA chain called 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*TP*AP*A
P*CP*AP*TP*GP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	19	Total	C	N	O	P	0	0	0
			386	188	67	113	18			
3	L	19	Total	C	N	O	P	0	0	0
			386	188	67	113	18			

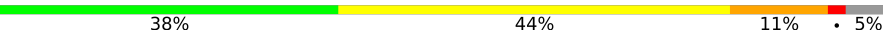
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

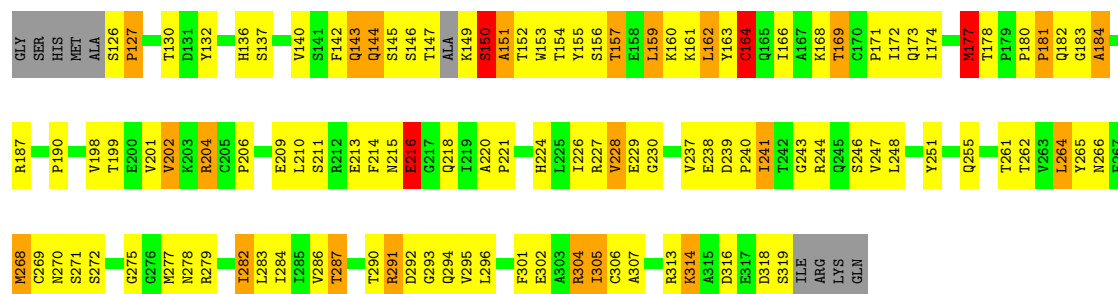
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	G	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		

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.

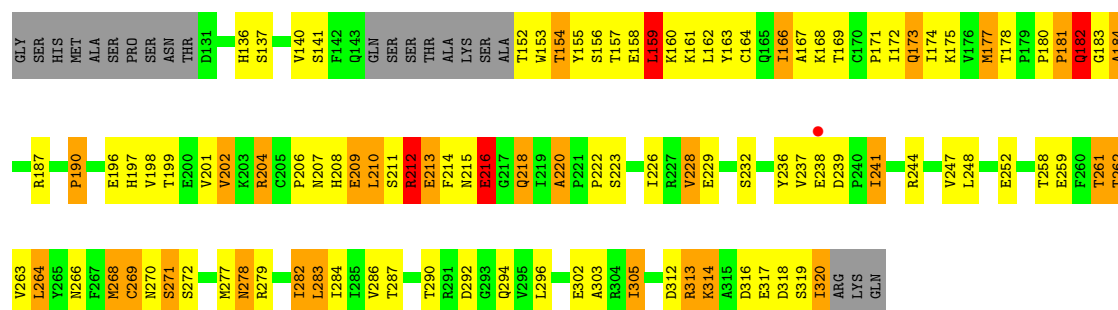
• Molecule 1: Tumor protein 63

Chain A: 

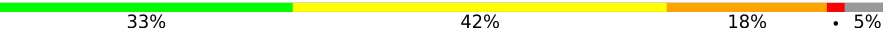


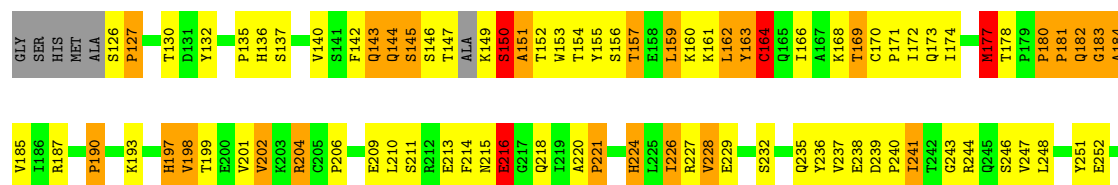
• Molecule 1: Tumor protein 63

Chain B: 



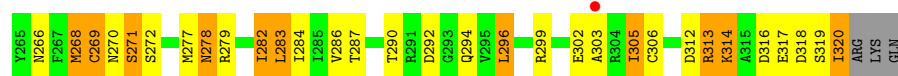
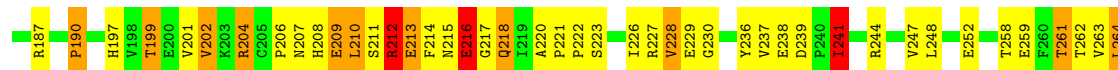
• Molecule 1: Tumor protein 63

Chain C: 

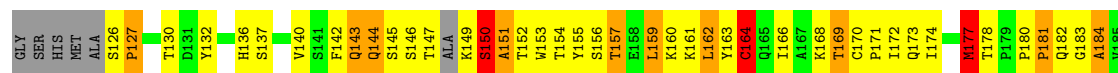




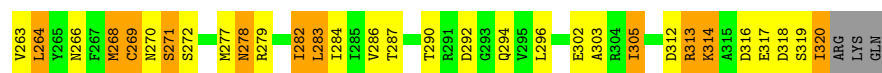
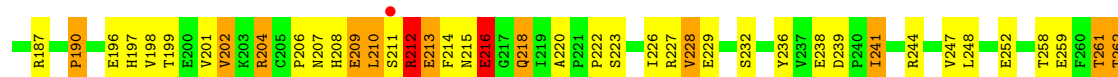
• Molecule 1: Tumor protein 63



• Molecule 1: Tumor protein 63

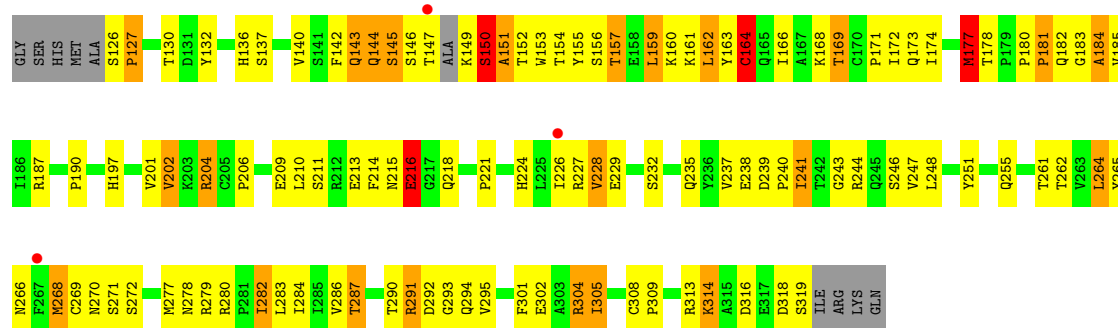


• Molecule 1: Tumor protein 63

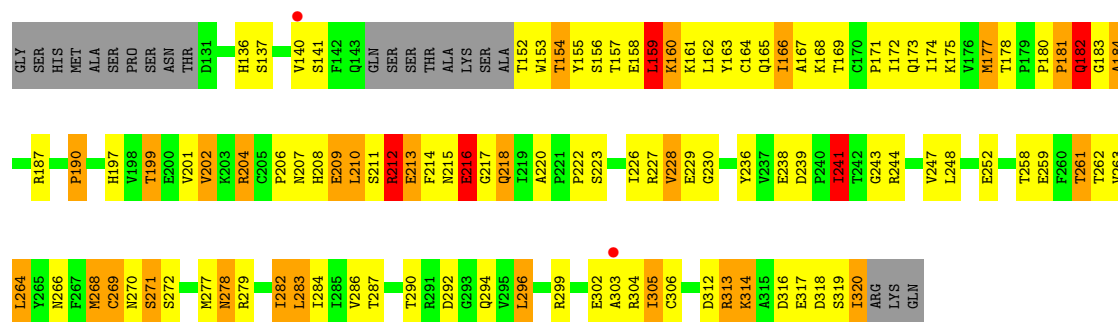


• Molecule 1: Tumor protein 63





• Molecule 1: Tumor protein 63



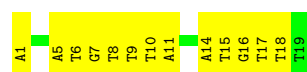
• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*AP*AP*AP*CP*AP*TP*GP*TP*T
P*T)-3'



• Molecule 2: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*AP*AP*AP*CP*AP*TP*GP*TP*T
P*T)-3'

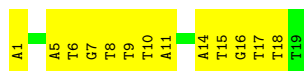


• Molecule 3: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*TP*AP*AP*CP*AP*TP*GP*TP*T
P*T)-3'



- Molecule 3: 5'-D(*AP*AP*AP*CP*AP*TP*GP*TP*TP*TP*AP*AP*CP*AP*TP*GP*TP*TP*T)-3'

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.74Å 180.54Å 98.17Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	59.87 – 4.20 59.87 – 4.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (59.87-4.20) 96.7 (59.87-4.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.326 , 0.334 0.342 , 0.310	Depositor DCC
R_{free} test set	744 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	125.2	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 321.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.309 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13210	wwPDB-VP
Average B, all atoms (Å ²)	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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:
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	1.01	1/1532 (0.1%)	1.31	16/2083 (0.8%)
1	B	0.93	0/1451	1.15	9/1974 (0.5%)
1	C	1.80	24/1532 (1.6%)	1.43	17/2083 (0.8%)
1	D	1.00	6/1451 (0.4%)	1.16	8/1974 (0.4%)
1	G	1.12	3/1532 (0.2%)	1.31	16/2083 (0.8%)
1	H	0.97	0/1451	1.16	7/1974 (0.4%)
1	I	0.83	1/1532 (0.1%)	1.29	15/2083 (0.7%)
1	J	1.12	6/1451 (0.4%)	1.17	7/1974 (0.4%)
2	E	1.02	0/434	1.08	2/668 (0.3%)
2	K	0.61	0/434	1.03	0/668
3	F	1.06	0/432	0.93	0/665
3	L	0.67	0/432	0.86	0/665
All	All	1.10	41/13664 (0.3%)	1.22	97/18894 (0.5%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	241	ILE	CA-CB	-14.38	1.34	1.54
1	D	241	ILE	CA-CB	-11.46	1.38	1.54
1	D	199	THR	CA-CB	-8.74	1.38	1.53
1	J	241	ILE	CB-CG1	8.72	1.71	1.53
1	D	241	ILE	CG1-CD1	8.49	1.84	1.51
1	J	199	THR	CA-CB	-8.07	1.39	1.53
1	C	251	TYR	CA-CB	7.88	1.65	1.53
1	J	199	THR	CB-OG1	7.83	1.56	1.43
1	D	199	THR	CB-OG1	7.75	1.56	1.43
1	C	221	PRO	CA-C	7.62	1.59	1.52
1	J	241	ILE	CG1-CD1	7.42	1.80	1.51
1	G	251	TYR	CA-CB	7.17	1.64	1.53
1	A	251	TYR	CA-CB	7.02	1.64	1.53
1	D	241	ILE	CB-CG1	6.99	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	251	TYR	CA-CB	6.77	1.64	1.53
1	C	252	GLU	C-O	6.63	1.33	1.24
1	C	226	ILE	N-CA	6.48	1.54	1.46
1	C	296	LEU	N-CA	6.27	1.54	1.46
1	C	193	LYS	C-O	6.23	1.31	1.24
1	C	183	GLY	C-N	6.16	1.42	1.33
1	C	190	PRO	C-O	6.15	1.30	1.23
1	J	199	THR	CB-CG2	-6.14	1.32	1.52
1	C	226	ILE	C-O	6.12	1.31	1.24
1	C	224	HIS	CG-ND1	-6.10	1.31	1.38
1	C	198	VAL	N-CA	6.09	1.53	1.46
1	C	170	CYS	CA-C	5.91	1.59	1.52
1	D	199	THR	CB-CG2	-5.86	1.33	1.52
1	C	197	HIS	CA-C	-5.83	1.45	1.52
1	C	135	PRO	N-CA	5.76	1.54	1.47
1	C	299	ARG	C-O	-5.74	1.16	1.23
1	C	280	ARG	C-N	5.44	1.40	1.33
1	C	163	TYR	N-CA	5.39	1.52	1.46
1	C	303	ALA	CA-C	5.33	1.58	1.52
1	C	268	MET	CA-C	5.30	1.61	1.52
1	C	236	TYR	CA-CB	5.14	1.61	1.53
1	C	185	VAL	N-CA	5.12	1.51	1.46
1	C	269	CYS	CB-SG	-5.12	1.64	1.81
1	G	224	HIS	CE1-NE2	-5.08	1.27	1.32
1	C	180	PRO	CA-C	5.08	1.56	1.52
1	G	170	CYS	CA-C	5.06	1.58	1.52
1	C	220	ALA	C-N	5.04	1.39	1.33

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	268	MET	N-CA-C	7.85	122.44	113.02
1	C	268	MET	N-CA-C	7.80	122.38	113.02
1	A	268	MET	N-CA-C	7.78	122.35	113.02
1	C	150	SER	N-CA-C	-7.78	103.37	112.86
1	I	268	MET	N-CA-C	7.59	122.13	113.02
1	I	132	TYR	CA-C-N	7.46	127.83	119.32
1	I	132	TYR	C-N-CA	7.46	127.83	119.32
1	C	132	TYR	CA-C-N	7.41	127.76	119.32
1	C	132	TYR	C-N-CA	7.41	127.76	119.32
1	G	132	TYR	CA-C-N	7.29	127.63	119.32
1	G	132	TYR	C-N-CA	7.29	127.63	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	GLY	N-CA-C	7.20	125.67	115.30
1	I	150	SER	N-CA-C	-7.11	104.18	112.86
1	A	132	TYR	CA-C-N	7.03	127.33	119.32
1	A	132	TYR	C-N-CA	7.03	127.33	119.32
1	G	150	SER	N-CA-C	-6.96	104.37	112.86
1	A	150	SER	N-CA-C	-6.95	104.38	112.86
1	C	255	GLN	N-CA-C	-6.86	101.28	110.55
1	I	293	GLY	N-CA-C	6.80	125.10	115.30
1	B	182	GLN	N-CA-C	6.80	121.83	112.04
1	A	293	GLY	N-CA-C	6.63	124.85	115.30
1	D	182	GLN	N-CA-C	6.62	121.68	111.56
1	H	182	GLN	N-CA-C	6.57	121.50	112.04
1	J	182	GLN	N-CA-C	6.55	121.47	112.04
1	G	293	GLY	N-CA-C	6.45	124.58	115.30
1	C	157	THR	N-CA-C	-6.39	104.32	111.28
1	J	218	GLN	N-CA-C	6.38	119.91	109.06
1	H	218	GLN	N-CA-C	6.38	119.90	109.06
1	D	218	GLN	N-CA-C	6.37	119.88	109.06
1	C	164	CYS	N-CA-C	6.32	118.92	108.99
1	G	157	THR	N-CA-C	-6.29	104.42	111.28
1	C	261	THR	N-CA-C	-6.29	98.96	108.96
1	B	197	HIS	N-CA-C	6.19	121.59	113.30
1	B	218	GLN	N-CA-C	6.17	119.56	109.06
1	I	164	CYS	N-CA-C	6.14	118.63	108.99
1	I	255	GLN	N-CA-C	-6.04	102.40	110.55
1	A	157	THR	N-CA-C	-6.02	104.71	111.28
1	A	255	GLN	N-CA-C	-5.99	102.46	110.55
1	C	177	MET	N-CA-C	-5.98	106.60	114.31
1	G	255	GLN	N-CA-C	-5.98	102.48	110.55
1	I	157	THR	N-CA-C	-5.93	104.81	111.28
1	H	197	HIS	N-CA-C	5.91	121.40	113.72
1	A	164	CYS	N-CA-C	5.90	118.26	108.99
1	G	164	CYS	N-CA-C	5.90	118.26	108.99
1	J	197	HIS	N-CA-C	5.86	121.16	113.30
1	G	241	ILE	CB-CA-C	-5.79	101.79	111.29
1	A	261	THR	N-CA-C	-5.77	99.78	108.96
1	D	197	HIS	N-CA-C	5.77	121.22	113.72
1	A	241	ILE	CB-CA-C	-5.74	101.88	111.29
1	I	241	ILE	CB-CA-C	-5.72	101.91	111.29
1	G	261	THR	N-CA-C	-5.69	99.91	108.96
1	I	261	THR	N-CA-C	-5.67	99.94	108.96
1	A	177	MET	N-CA-C	-5.60	107.08	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	169	THR	N-CA-C	5.55	118.68	109.46
2	E	9	DT	N1-C1'-C2'	-5.53	105.20	113.50
1	A	216	GLU	N-CA-C	5.51	117.75	111.02
1	C	241	ILE	CB-CA-C	-5.51	102.25	111.29
1	C	275	GLY	N-CA-C	-5.50	107.67	115.43
1	I	216	GLU	N-CA-C	5.48	117.71	111.02
1	C	145	SER	N-CA-C	5.45	119.40	112.87
1	J	268	MET	N-CA-C	5.44	120.19	111.81
1	H	159	LEU	N-CA-C	-5.43	105.46	113.61
1	J	261	THR	N-CA-C	-5.42	98.93	108.20
1	G	177	MET	N-CA-C	-5.41	107.33	114.31
1	A	169	THR	N-CA-C	5.38	118.39	109.46
1	I	177	MET	N-CA-C	-5.38	107.37	114.31
1	A	237	VAL	N-CA-C	5.37	116.40	108.45
1	D	261	THR	N-CA-C	-5.37	99.03	108.20
1	B	159	LEU	N-CA-C	-5.36	105.57	113.61
1	C	237	VAL	N-CA-C	5.35	116.37	108.45
1	J	159	LEU	N-CA-C	-5.34	105.59	113.61
1	B	173	GLN	N-CA-C	5.34	117.45	108.96
1	C	216	GLU	N-CA-C	5.34	117.53	111.02
1	G	169	THR	N-CA-C	5.33	118.31	109.46
1	D	268	MET	N-CA-C	5.33	120.02	111.81
1	D	159	LEU	N-CA-C	-5.32	105.63	113.61
1	G	216	GLU	N-CA-C	5.32	117.51	111.02
1	C	169	THR	N-CA-C	5.31	118.27	109.46
1	H	173	GLN	N-CA-C	5.29	117.37	108.96
1	H	268	MET	N-CA-C	5.28	119.94	111.81
1	I	145	SER	N-CA-C	5.27	119.19	112.87
1	D	237	VAL	N-CA-C	5.26	116.29	108.46
1	B	261	THR	N-CA-C	-5.25	99.23	108.20
1	I	237	VAL	N-CA-C	5.24	116.21	108.45
1	C	182	GLN	N-CA-C	5.21	120.67	110.56
1	G	237	VAL	N-CA-C	5.20	116.14	108.45
1	A	145	SER	N-CA-C	5.17	119.07	112.87
1	G	145	SER	N-CA-C	5.17	119.07	112.87
1	J	160	LYS	N-CA-C	-5.15	104.53	111.54
1	B	220	ALA	N-CA-C	5.14	117.60	110.20
1	H	261	THR	N-CA-C	-5.12	99.44	108.20
1	B	268	MET	N-CA-C	5.09	119.64	111.81
1	G	275	GLY	N-CA-C	-5.08	108.27	115.43
1	D	173	GLN	N-CA-C	5.08	117.03	108.96
1	A	275	GLY	N-CA-C	-5.06	108.30	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	9	DT	O4'-C1'-N1	5.05	115.97	108.40
1	B	237	VAL	N-CA-C	5.01	115.92	108.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1497	0	1456	128	0
1	B	1417	0	1377	121	0
1	C	1497	0	1456	123	0
1	D	1417	0	1377	95	9
1	G	1497	0	1456	126	0
1	H	1417	0	1377	118	0
1	I	1497	0	1456	123	0
1	J	1417	0	1377	100	9
2	E	387	0	218	16	0
2	K	387	0	218	17	0
3	F	386	0	219	25	0
3	L	386	0	219	23	0
4	A	1	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
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
All	All	13210	0	12206	943	10

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 37.

All (943) 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:J:241:ILE:CD1	1:J:241:ILE:CG1	1.80	1.58
1:D:241:ILE:CD1	1:D:241:ILE:CG1	1.84	1.52
1:B:196:GLU:HA	1:G:169:THR:CG2	1.69	1.23
1:A:169:THR:CG2	1:H:196:GLU:HA	1.72	1.18
1:B:137:SER:CB	1:B:177:MET:HG3	1.76	1.15
1:B:196:GLU:CA	1:G:169:THR:HG21	1.76	1.15
1:H:137:SER:CB	1:H:177:MET:HG3	1.75	1.15
1:D:137:SER:CB	1:D:177:MET:HG3	1.75	1.14
1:J:137:SER:CB	1:J:177:MET:HG3	1.75	1.14
1:B:290:THR:HG22	1:B:294:GLN:H	1.13	1.13
1:A:169:THR:HG21	1:H:196:GLU:CA	1.82	1.09
1:H:290:THR:HG22	1:H:294:GLN:H	1.14	1.08
1:G:290:THR:HG22	1:G:294:GLN:H	1.20	1.07
1:I:290:THR:HG22	1:I:294:GLN:H	1.20	1.06
1:A:172:ILE:HD12	1:A:265:TYR:HD2	1.22	1.04
1:C:172:ILE:HD12	1:C:265:TYR:HD2	1.20	1.03
1:D:290:THR:HG22	1:D:294:GLN:H	1.16	1.02
1:J:290:THR:HG22	1:J:294:GLN:H	1.17	1.02
1:A:290:THR:HG22	1:A:294:GLN:H	1.18	1.01
1:B:137:SER:HB2	1:B:177:MET:CG	1.90	1.01
1:J:137:SER:HB2	1:J:177:MET:CG	1.89	1.01
1:J:239:ASP:OD1	1:J:241:ILE:HG13	1.58	1.01
1:A:169:THR:HG21	1:H:196:GLU:HA	1.03	1.01
1:C:240:PRO:HG2	1:C:241:ILE:HD12	1.42	1.01
1:H:137:SER:HB2	1:H:177:MET:CG	1.89	1.01
1:D:137:SER:HB2	1:D:177:MET:CG	1.89	1.00
1:G:172:ILE:HD12	1:G:265:TYR:HD2	1.22	1.00
1:B:196:GLU:HA	1:G:169:THR:HG21	1.00	0.99
1:C:290:THR:HG22	1:C:294:GLN:H	1.21	0.99
1:I:172:ILE:HD12	1:I:265:TYR:HD2	1.23	0.99
2:K:9:DT:H1'	2:K:10:DA:H5'	1.44	0.99
1:H:168:LYS:HE2	1:I:168:LYS:HE2	1.45	0.99
1:I:240:PRO:HG2	1:I:241:ILE:HD12	1.45	0.99
2:E:9:DT:H1'	2:E:10:DA:H5'	1.44	0.98
1:D:239:ASP:OD1	1:D:241:ILE:HG13	1.63	0.98
1:G:240:PRO:HG2	1:G:241:ILE:HD12	1.46	0.98
1:A:240:PRO:HG2	1:A:241:ILE:HD12	1.46	0.98
1:B:168:LYS:HE2	1:C:168:LYS:HE2	1.44	0.97
1:H:204:ARG:HD2	1:H:268:MET:HB2	1.46	0.97
1:B:137:SER:HB2	1:B:177:MET:HG3	0.97	0.96
1:D:204:ARG:HD2	1:D:268:MET:HB2	1.47	0.95
1:J:137:SER:HB2	1:J:177:MET:HG3	0.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:204:ARG:HD2	1:J:268:MET:HB2	1.46	0.95
2:K:9:DT:H2"	2:K:10:DA:OP2	1.66	0.95
2:E:9:DT:H2"	2:E:10:DA:OP2	1.68	0.94
1:D:137:SER:HB2	1:D:177:MET:HG3	0.96	0.93
1:H:137:SER:HB2	1:H:177:MET:HG3	0.96	0.93
1:B:204:ARG:HD2	1:B:268:MET:HB2	1.47	0.93
1:B:239:ASP:OD1	1:B:241:ILE:HG13	1.68	0.93
1:I:144:GLN:CD	1:I:144:GLN:H	1.74	0.92
1:H:239:ASP:OD1	1:H:241:ILE:HG13	1.70	0.92
1:B:213:GLU:HB2	1:C:145:SER:O	1.71	0.91
1:A:177:MET:HE3	1:A:177:MET:HA	1.52	0.91
1:B:290:THR:HG22	1:B:294:GLN:N	1.86	0.90
1:H:290:THR:HG22	1:H:294:GLN:N	1.86	0.89
1:D:290:THR:HG22	1:D:294:GLN:N	1.88	0.89
1:G:177:MET:HE3	1:G:177:MET:HA	1.55	0.89
1:A:144:GLN:CD	1:A:144:GLN:H	1.77	0.89
1:G:144:GLN:H	1:G:144:GLN:CD	1.77	0.88
1:H:213:GLU:HB2	1:I:145:SER:O	1.72	0.88
1:B:213:GLU:CB	1:C:145:SER:O	2.21	0.88
1:C:177:MET:HE3	1:C:177:MET:HA	1.52	0.88
1:J:290:THR:HG22	1:J:294:GLN:N	1.89	0.88
1:C:172:ILE:HD12	1:C:265:TYR:CD2	2.10	0.87
1:I:177:MET:HA	1:I:177:MET:HE3	1.54	0.87
1:C:144:GLN:CD	1:C:144:GLN:H	1.82	0.86
1:H:213:GLU:CB	1:I:145:SER:O	2.24	0.85
1:A:204:ARG:HD2	1:A:268:MET:HB2	1.60	0.84
1:G:204:ARG:HD2	1:G:268:MET:HB2	1.60	0.83
1:A:172:ILE:HD12	1:A:265:TYR:CD2	2.11	0.83
1:G:172:ILE:HD12	1:G:265:TYR:CD2	2.12	0.83
1:G:137:SER:HB2	1:G:177:MET:HB2	1.61	0.83
1:I:204:ARG:HD2	1:I:268:MET:HB2	1.58	0.82
1:C:137:SER:HB2	1:C:177:MET:HB2	1.60	0.82
1:H:168:LYS:HE2	1:I:168:LYS:CE	2.10	0.82
1:I:137:SER:HB2	1:I:177:MET:HB2	1.60	0.82
1:I:172:ILE:HD12	1:I:265:TYR:CD2	2.13	0.82
1:A:169:THR:HB	1:A:229:GLU:OE2	1.80	0.82
1:I:143:GLN:HA	1:I:144:GLN:NE2	1.95	0.81
1:A:137:SER:HB2	1:A:177:MET:HB2	1.61	0.81
1:B:168:LYS:HE2	1:C:168:LYS:CE	2.09	0.81
1:H:175:LYS:HD3	1:H:259:GLU:O	1.80	0.81
1:G:169:THR:HB	1:G:229:GLU:OE2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:THR:CG2	1:H:294:GLN:H	1.94	0.81
1:A:290:THR:HG22	1:A:294:GLN:N	1.95	0.80
1:B:175:LYS:HD3	1:B:259:GLU:O	1.81	0.80
1:D:271:SER:O	1:D:279:ARG:HA	1.81	0.80
1:B:290:THR:CG2	1:B:294:GLN:H	1.93	0.80
1:I:290:THR:HG22	1:I:294:GLN:N	1.96	0.80
1:C:169:THR:HB	1:C:229:GLU:OE2	1.82	0.80
1:C:204:ARG:HD2	1:C:268:MET:HB2	1.63	0.80
1:B:199:THR:HG21	1:G:230:GLY:CA	2.12	0.79
1:B:271:SER:O	1:B:279:ARG:HA	1.83	0.79
1:I:169:THR:HB	1:I:229:GLU:OE2	1.83	0.79
1:C:290:THR:HG22	1:C:294:GLN:N	1.98	0.79
1:G:143:GLN:HA	1:G:144:GLN:NE2	1.98	0.78
1:H:271:SER:O	1:H:279:ARG:HA	1.83	0.78
1:D:175:LYS:HD3	1:D:259:GLU:O	1.84	0.78
1:H:277:MET:SD	1:H:282:ILE:HG21	2.24	0.78
1:J:175:LYS:HD3	1:J:259:GLU:O	1.84	0.78
1:J:212:ARG:HH11	1:J:216:GLU:HG2	1.49	0.78
1:I:144:GLN:H	1:I:144:GLN:NE2	1.82	0.77
1:B:212:ARG:HH11	1:B:216:GLU:HG2	1.47	0.77
1:B:277:MET:SD	1:B:282:ILE:HG21	2.23	0.77
1:G:290:THR:HG22	1:G:294:GLN:N	1.96	0.77
1:H:212:ARG:HH11	1:H:216:GLU:HG2	1.48	0.77
1:A:143:GLN:HA	1:A:144:GLN:NE2	1.99	0.77
1:I:227:ARG:NH1	1:I:268:MET:HE2	2.00	0.77
1:J:271:SER:O	1:J:279:ARG:HA	1.84	0.76
1:C:227:ARG:NH1	1:C:268:MET:HE2	2.00	0.76
1:G:144:GLN:H	1:G:144:GLN:NE2	1.84	0.76
1:A:290:THR:CG2	1:A:294:GLN:H	1.99	0.76
1:A:227:ARG:NH1	1:A:268:MET:HE2	2.01	0.76
1:G:227:ARG:NH1	1:G:268:MET:HE2	2.01	0.75
1:J:277:MET:SD	1:J:282:ILE:HG21	2.27	0.75
1:C:277:MET:SD	1:C:282:ILE:HG21	2.26	0.75
1:D:216:GLU:OE1	1:D:216:GLU:HA	1.87	0.74
1:H:168:LYS:CE	1:I:168:LYS:HE2	2.17	0.74
1:C:143:GLN:HA	1:C:144:GLN:NE2	2.02	0.74
1:D:212:ARG:HH11	1:D:216:GLU:HG2	1.50	0.74
3:F:5:DA:H2''	3:F:6:DT:C5'	2.18	0.74
1:J:290:THR:CG2	1:J:294:GLN:H	1.97	0.74
1:B:136:HIS:CE1	1:B:180:PRO:HA	2.22	0.74
1:D:277:MET:SD	1:D:282:ILE:HG21	2.28	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:TYR:CE2	1:G:313:ARG:HA	2.23	0.74
1:B:168:LYS:CE	1:C:168:LYS:HE2	2.17	0.74
1:I:204:ARG:NH2	1:I:215:ASN:HD21	1.86	0.74
1:D:136:HIS:CE1	1:D:180:PRO:HA	2.23	0.74
1:D:290:THR:CG2	1:D:294:GLN:H	1.95	0.73
3:L:5:DA:H2''	3:L:6:DT:C5'	2.17	0.73
1:A:144:GLN:H	1:A:144:GLN:NE2	1.84	0.73
1:J:136:HIS:CE1	1:J:180:PRO:HA	2.24	0.73
1:A:216:GLU:OE1	1:G:216:GLU:OE1	2.06	0.73
1:H:136:HIS:CE1	1:H:180:PRO:HA	2.23	0.73
1:G:290:THR:CG2	1:G:294:GLN:H	2.00	0.73
1:H:220:ALA:HB2	1:H:236:TYR:CZ	2.24	0.72
1:B:216:GLU:OE1	1:B:216:GLU:HA	1.88	0.72
1:I:163:TYR:CE2	1:I:313:ARG:HA	2.24	0.72
1:A:230:GLY:CA	1:H:199:THR:HG21	2.20	0.72
1:H:216:GLU:HA	1:H:216:GLU:OE1	1.88	0.72
1:A:163:TYR:CE2	1:A:313:ARG:HA	2.24	0.72
1:G:277:MET:SD	1:G:282:ILE:HG21	2.30	0.72
1:J:216:GLU:OE1	1:J:216:GLU:HA	1.88	0.72
1:I:290:THR:CG2	1:I:294:GLN:H	2.00	0.71
1:D:226:ILE:HD11	1:D:284:ILE:HD12	1.73	0.71
1:C:144:GLN:H	1:C:144:GLN:NE2	1.89	0.71
1:J:220:ALA:HB2	1:J:236:TYR:CZ	2.26	0.71
1:A:204:ARG:NH2	1:A:215:ASN:HD21	1.89	0.71
1:B:272:SER:HA	1:B:279:ARG:H	1.56	0.70
1:D:169:THR:HB	1:D:229:GLU:OE2	1.92	0.70
1:A:277:MET:SD	1:A:282:ILE:HG21	2.32	0.70
1:C:290:THR:CG2	1:C:294:GLN:H	2.02	0.70
1:I:227:ARG:CZ	1:I:268:MET:HE2	2.22	0.70
1:B:220:ALA:HB2	1:B:236:TYR:CZ	2.26	0.70
1:D:272:SER:HA	1:D:279:ARG:H	1.56	0.69
1:J:269:CYS:O	1:J:305:ILE:HD11	1.92	0.69
1:H:272:SER:HA	1:H:279:ARG:H	1.57	0.69
1:J:226:ILE:HD11	1:J:284:ILE:HD12	1.74	0.69
1:C:163:TYR:CE2	1:C:313:ARG:HA	2.28	0.69
1:D:220:ALA:HB2	1:D:236:TYR:CZ	2.27	0.69
1:G:204:ARG:NH2	1:G:215:ASN:HD21	1.91	0.69
1:H:220:ALA:HB2	1:H:236:TYR:CE1	2.28	0.69
1:H:269:CYS:O	1:H:305:ILE:HD11	1.93	0.69
1:J:169:THR:HB	1:J:229:GLU:OE2	1.92	0.69
1:I:277:MET:SD	1:I:282:ILE:HG21	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:272:SER:HA	1:J:279:ARG:H	1.58	0.69
1:A:272:SER:HA	1:A:279:ARG:H	1.58	0.69
3:L:9:DT:H1'	3:L:10:DT:H5'	1.73	0.69
1:B:220:ALA:HB2	1:B:236:TYR:CE1	2.29	0.68
1:I:272:SER:HA	1:I:279:ARG:H	1.58	0.68
1:J:220:ALA:HB2	1:J:236:TYR:CE1	2.29	0.68
1:D:269:CYS:O	1:D:305:ILE:HD11	1.93	0.68
3:L:7:DG:H2''	3:L:8:DT:H5'	1.76	0.67
1:B:269:CYS:O	1:B:305:ILE:HD11	1.93	0.67
1:G:227:ARG:CZ	1:G:268:MET:HE2	2.25	0.67
1:B:169:THR:HB	1:B:229:GLU:OE2	1.94	0.67
1:G:272:SER:HA	1:G:279:ARG:H	1.59	0.67
1:B:196:GLU:N	1:G:169:THR:HG21	2.09	0.67
1:A:227:ARG:CZ	1:A:268:MET:HE2	2.24	0.67
1:B:213:GLU:HB3	1:C:145:SER:O	1.95	0.67
1:C:204:ARG:NH2	1:C:215:ASN:HD21	1.93	0.67
1:A:169:THR:CG2	1:H:196:GLU:CA	2.58	0.67
1:C:272:SER:HA	1:C:279:ARG:H	1.60	0.67
1:D:220:ALA:HB2	1:D:236:TYR:CE1	2.29	0.67
3:F:9:DT:H1'	3:F:10:DT:H5'	1.76	0.67
1:H:269:CYS:O	1:H:305:ILE:CD1	2.43	0.67
3:L:5:DA:H2''	3:L:6:DT:H5'	1.76	0.67
3:L:10:DT:H1'	3:L:11:DA:H5'	1.77	0.67
1:H:169:THR:HB	1:H:229:GLU:OE2	1.95	0.66
1:B:226:ILE:HD11	1:B:284:ILE:HD12	1.76	0.66
1:B:269:CYS:O	1:B:305:ILE:CD1	2.44	0.66
1:J:269:CYS:O	1:J:305:ILE:CD1	2.43	0.66
1:B:232:SER:HB2	1:C:232:SER:HB3	1.78	0.66
1:D:269:CYS:O	1:D:305:ILE:CD1	2.44	0.66
1:A:177:MET:HA	1:A:177:MET:CE	2.25	0.66
3:F:5:DA:H2''	3:F:6:DT:H5'	1.77	0.66
1:J:163:TYR:CE2	1:J:313:ARG:HA	2.32	0.65
1:B:196:GLU:HA	1:G:169:THR:HG22	1.76	0.65
1:H:226:ILE:HD11	1:H:284:ILE:HD12	1.76	0.65
1:I:204:ARG:HD2	1:I:268:MET:CB	2.26	0.65
1:I:290:THR:HG23	1:I:292:ASP:H	1.62	0.65
1:A:290:THR:CG2	1:A:294:GLN:HB3	2.27	0.65
1:B:164:CYS:O	1:B:305:ILE:HA	1.97	0.65
1:B:183:GLY:O	1:B:184:ALA:O	2.15	0.65
3:F:7:DG:H2''	3:F:8:DT:H5'	1.78	0.64
3:F:10:DT:H1'	3:F:11:DA:H5'	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:CYS:O	1:D:305:ILE:HA	1.98	0.64
1:D:183:GLY:O	1:D:184:ALA:O	2.16	0.64
1:D:313:ARG:O	1:D:317:GLU:HG3	1.98	0.64
1:H:313:ARG:O	1:H:317:GLU:HG3	1.96	0.64
1:G:154:THR:HG23	1:G:163:TYR:HB2	1.80	0.64
1:H:164:CYS:O	1:H:305:ILE:HA	1.97	0.64
1:H:258:THR:HG22	1:H:259:GLU:H	1.63	0.64
1:C:177:MET:HA	1:C:177:MET:CE	2.26	0.64
1:I:161:LYS:HG3	1:I:302:GLU:HB3	1.78	0.64
1:I:218:GLN:NE2	1:I:218:GLN:HA	2.13	0.64
1:J:164:CYS:O	1:J:305:ILE:HA	1.98	0.64
1:A:204:ARG:HD2	1:A:268:MET:CB	2.27	0.64
1:A:271:SER:O	1:A:279:ARG:HA	1.98	0.64
1:B:313:ARG:O	1:B:317:GLU:HG3	1.98	0.64
1:C:227:ARG:CZ	1:C:268:MET:HE2	2.27	0.64
1:H:232:SER:HB2	1:I:232:SER:HB3	1.79	0.64
1:C:161:LYS:HG3	1:C:302:GLU:HB3	1.79	0.64
1:C:290:THR:CG2	1:C:294:GLN:HB3	2.28	0.64
1:D:258:THR:HG22	1:D:259:GLU:H	1.62	0.64
3:F:5:DA:H2"	3:F:6:DT:H5"	1.80	0.63
1:B:199:THR:CG2	1:G:230:GLY:CA	2.76	0.63
1:D:163:TYR:CE2	1:D:313:ARG:HA	2.32	0.63
1:A:282:ILE:HG13	1:A:283:LEU:N	2.14	0.63
1:H:183:GLY:O	1:H:184:ALA:O	2.16	0.63
1:B:163:TYR:CE2	1:B:313:ARG:HA	2.34	0.63
1:G:204:ARG:HD2	1:G:268:MET:CB	2.27	0.63
1:A:161:LYS:HG3	1:A:302:GLU:HB3	1.81	0.63
1:B:258:THR:HG22	1:B:259:GLU:H	1.63	0.63
1:G:161:LYS:HG3	1:G:302:GLU:HB3	1.81	0.63
1:G:290:THR:CG2	1:G:294:GLN:HB3	2.28	0.63
1:G:290:THR:HG23	1:G:292:ASP:H	1.64	0.63
1:C:218:GLN:HA	1:C:218:GLN:NE2	2.12	0.63
1:G:155:TYR:CE2	1:G:157:THR:HA	2.34	0.63
1:G:177:MET:HA	1:G:177:MET:CE	2.28	0.63
1:J:313:ARG:O	1:J:317:GLU:HG3	1.99	0.63
1:A:290:THR:HG23	1:A:292:ASP:H	1.64	0.62
1:D:211:SER:O	1:D:212:ARG:C	2.42	0.62
1:A:154:THR:HG23	1:A:163:TYR:HB2	1.80	0.62
1:A:155:TYR:CE2	1:A:157:THR:HA	2.35	0.62
1:I:271:SER:O	1:I:279:ARG:HA	1.99	0.62
1:I:154:THR:HG23	1:I:163:TYR:HB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:5:DA:H2''	3:L:6:DT:H5''	1.80	0.62
1:J:141:SER:O	1:J:173:GLN:HB2	1.98	0.62
1:D:141:SER:O	1:D:173:GLN:HB2	1.99	0.62
1:G:182:GLN:NE2	1:G:182:GLN:HA	2.15	0.62
1:G:271:SER:O	1:G:279:ARG:HA	2.00	0.62
1:J:211:SER:O	1:J:212:ARG:C	2.43	0.62
1:C:221:PRO:HB2	1:C:224:HIS:CD2	2.35	0.62
1:I:270:ASN:HA	1:I:305:ILE:HG12	1.82	0.62
1:J:183:GLY:O	1:J:184:ALA:O	2.17	0.62
1:C:282:ILE:HG13	1:C:283:LEU:N	2.14	0.62
1:H:211:SER:O	1:H:212:ARG:C	2.42	0.62
1:A:182:GLN:HA	1:A:182:GLN:NE2	2.14	0.61
1:A:169:THR:HG22	1:H:196:GLU:HA	1.79	0.61
1:C:283:LEU:HB3	1:C:302:GLU:HA	1.82	0.61
1:I:156:SER:OG	1:I:159:LEU:HB2	2.01	0.61
1:J:258:THR:HG22	1:J:259:GLU:H	1.63	0.61
1:G:244:ARG:HG2	1:G:244:ARG:HH11	1.65	0.61
1:H:156:SER:HA	1:H:313:ARG:NH2	2.15	0.61
1:H:163:TYR:CE2	1:H:313:ARG:HA	2.34	0.61
1:C:204:ARG:HD2	1:C:268:MET:CB	2.30	0.61
1:H:213:GLU:HB3	1:I:145:SER:O	2.00	0.61
1:B:232:SER:CB	1:C:232:SER:HB3	2.31	0.61
1:G:282:ILE:HG13	1:G:283:LEU:N	2.15	0.61
1:I:282:ILE:HG13	1:I:283:LEU:N	2.15	0.61
1:A:218:GLN:NE2	1:A:218:GLN:HA	2.16	0.61
1:I:155:TYR:CE2	1:I:157:THR:HA	2.36	0.61
1:I:290:THR:CG2	1:I:294:GLN:HB3	2.31	0.61
1:C:155:TYR:CE2	1:C:157:THR:HA	2.36	0.61
1:J:156:SER:HA	1:J:313:ARG:NH2	2.16	0.61
1:B:196:GLU:CA	1:G:169:THR:CG2	2.53	0.61
1:C:154:THR:HG23	1:C:163:TYR:HB2	1.83	0.61
1:C:156:SER:OG	1:C:159:LEU:HB2	2.01	0.61
1:D:156:SER:HA	1:D:313:ARG:NH2	2.15	0.60
1:G:166:ILE:HA	1:G:305:ILE:CD1	2.31	0.60
1:B:156:SER:HA	1:B:313:ARG:NH2	2.15	0.60
1:B:211:SER:O	1:B:212:ARG:C	2.43	0.60
1:C:271:SER:O	1:C:279:ARG:HA	2.02	0.60
1:H:232:SER:CB	1:I:232:SER:HB3	2.31	0.60
1:I:182:GLN:HA	1:I:182:GLN:NE2	2.15	0.60
1:J:290:THR:CG2	1:J:294:GLN:HB3	2.32	0.60
1:H:141:SER:O	1:H:173:GLN:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:OG	1:A:159:LEU:HB2	2.02	0.59
1:B:290:THR:CG2	1:B:294:GLN:HB3	2.32	0.59
1:C:187:ARG:CZ	1:C:248:LEU:HD21	2.32	0.59
1:C:290:THR:HG23	1:C:292:ASP:H	1.65	0.59
1:H:283:LEU:HB3	1:H:302:GLU:HA	1.84	0.59
3:L:14:DA:H2''	3:L:15:DT:C5'	2.31	0.59
1:A:270:ASN:HA	1:A:305:ILE:HG12	1.84	0.59
1:I:177:MET:HA	1:I:177:MET:CE	2.29	0.59
1:A:221:PRO:HB2	1:A:224:HIS:CD2	2.37	0.59
1:G:218:GLN:HA	1:G:218:GLN:NE2	2.16	0.59
3:F:14:DA:H2''	3:F:15:DT:C5'	2.32	0.59
1:G:221:PRO:HB2	1:G:224:HIS:CD2	2.38	0.59
1:D:140:VAL:HG12	1:D:174:ILE:HD13	1.85	0.59
2:E:19:DT:H2''	3:L:1:DA:N1	2.17	0.59
1:H:290:THR:CG2	1:H:294:GLN:HB3	2.32	0.59
1:B:168:LYS:HE2	1:C:168:LYS:NZ	2.18	0.59
1:I:187:ARG:CZ	1:I:248:LEU:HD21	2.32	0.59
1:J:155:TYR:CE2	1:J:157:THR:HA	2.37	0.59
1:A:283:LEU:HB3	1:A:302:GLU:HA	1.83	0.59
1:D:180:PRO:O	1:D:181:PRO:O	2.21	0.59
1:H:187:ARG:CZ	1:H:248:LEU:HD21	2.32	0.59
1:I:283:LEU:HB3	1:I:302:GLU:HA	1.85	0.59
1:C:228:VAL:HG12	1:C:247:VAL:HG21	1.85	0.59
1:B:141:SER:O	1:B:173:GLN:HB2	2.01	0.59
1:D:290:THR:CG2	1:D:294:GLN:HB3	2.33	0.59
1:H:155:TYR:CE2	1:H:157:THR:HA	2.38	0.58
3:F:1:DA:N1	2:K:19:DT:H2''	2.18	0.58
1:G:156:SER:OG	1:G:159:LEU:HB2	2.04	0.58
1:B:283:LEU:HB3	1:B:302:GLU:HA	1.85	0.58
1:D:155:TYR:CE2	1:D:157:THR:HA	2.38	0.58
1:G:270:ASN:HA	1:G:305:ILE:HG12	1.85	0.58
1:G:283:LEU:HB3	1:G:302:GLU:HA	1.83	0.58
1:I:210:LEU:O	1:I:211:SER:C	2.46	0.58
1:B:155:TYR:CE2	1:B:157:THR:HA	2.39	0.58
1:B:180:PRO:O	1:B:181:PRO:O	2.22	0.58
1:C:210:LEU:O	1:C:211:SER:C	2.46	0.58
1:B:278:ASN:O	1:B:279:ARG:HG2	2.04	0.58
1:H:140:VAL:HG12	1:H:174:ILE:HD13	1.84	0.58
1:I:221:PRO:HB2	1:I:224:HIS:CD2	2.39	0.58
1:J:187:ARG:CZ	1:J:248:LEU:HD21	2.33	0.58
1:J:187:ARG:HB3	1:J:287:THR:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:312:ASP:O	1:J:316:ASP:HB2	2.03	0.58
1:D:312:ASP:O	1:D:316:ASP:HB2	2.03	0.58
1:A:166:ILE:HA	1:A:305:ILE:CD1	2.34	0.58
1:A:169:THR:HG21	1:H:196:GLU:N	2.18	0.58
1:C:146:SER:O	1:C:147:THR:HG23	2.04	0.58
1:A:154:THR:CG2	1:A:163:TYR:HB2	2.34	0.57
1:I:244:ARG:HG2	1:I:244:ARG:HH11	1.68	0.57
1:C:180:PRO:O	1:C:181:PRO:O	2.23	0.57
1:D:187:ARG:CZ	1:D:248:LEU:HD21	2.34	0.57
1:H:278:ASN:O	1:H:279:ARG:HG2	2.04	0.57
1:H:187:ARG:HB2	1:H:248:LEU:HD22	1.86	0.57
1:A:290:THR:HG21	1:A:294:GLN:HB3	1.85	0.57
1:B:199:THR:CG2	1:G:230:GLY:HA3	2.35	0.57
1:G:154:THR:CG2	1:G:163:TYR:HB2	2.34	0.57
1:G:210:LEU:O	1:G:211:SER:C	2.47	0.57
1:H:168:LYS:HE2	1:I:168:LYS:NZ	2.19	0.57
1:A:210:LEU:O	1:A:211:SER:C	2.48	0.57
1:B:140:VAL:HG12	1:B:174:ILE:HD13	1.85	0.57
1:B:187:ARG:CZ	1:B:248:LEU:HD21	2.34	0.57
1:B:199:THR:HG21	1:G:230:GLY:HA3	1.86	0.57
1:B:312:ASP:O	1:B:316:ASP:HB2	2.04	0.57
1:G:180:PRO:O	1:G:181:PRO:O	2.22	0.57
1:I:166:ILE:HG13	1:I:305:ILE:HD11	1.86	0.57
1:I:304:ARG:HG3	1:I:304:ARG:HH11	1.70	0.57
1:C:304:ARG:HH11	1:C:304:ARG:HG3	1.70	0.57
1:J:283:LEU:HB3	1:J:302:GLU:HA	1.86	0.57
1:C:226:ILE:HD11	1:C:284:ILE:HD12	1.87	0.57
1:D:278:ASN:O	1:D:279:ARG:HG2	2.04	0.57
1:G:304:ARG:HG3	1:G:304:ARG:HH11	1.70	0.57
1:G:290:THR:HG21	1:G:294:GLN:HB3	1.87	0.57
1:I:154:THR:CG2	1:I:163:TYR:HB2	2.35	0.57
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.68	0.57
1:D:187:ARG:HB3	1:D:287:THR:HG23	1.87	0.57
1:J:140:VAL:HG12	1:J:174:ILE:HD13	1.87	0.57
2:E:9:DT:C2'	2:E:10:DA:OP2	2.49	0.56
1:H:312:ASP:O	1:H:316:ASP:HB2	2.04	0.56
1:A:146:SER:O	1:A:147:THR:HG23	2.05	0.56
1:G:228:VAL:HG12	1:G:247:VAL:HG21	1.88	0.56
1:J:180:PRO:O	1:J:181:PRO:O	2.22	0.56
1:G:166:ILE:HG13	1:G:305:ILE:HD11	1.88	0.56
1:I:166:ILE:HA	1:I:305:ILE:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:THR:HG21	1:H:294:GLN:HB3	1.88	0.56
1:G:146:SER:O	1:G:147:THR:HG23	2.05	0.56
1:A:228:VAL:HG12	1:A:247:VAL:HG21	1.88	0.56
1:D:204:ARG:HD2	1:D:268:MET:CB	2.30	0.56
1:B:290:THR:HG21	1:B:294:GLN:HB3	1.88	0.56
1:I:228:VAL:HG12	1:I:247:VAL:HG21	1.87	0.56
1:C:270:ASN:HA	1:C:305:ILE:HG12	1.86	0.56
1:J:290:THR:HG21	1:J:294:GLN:HB3	1.88	0.55
1:G:187:ARG:CZ	1:G:248:LEU:HD21	2.36	0.55
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.70	0.55
1:B:187:ARG:HB2	1:B:248:LEU:HD22	1.87	0.55
1:G:244:ARG:HG2	1:G:244:ARG:NH1	2.21	0.55
1:H:180:PRO:O	1:H:181:PRO:O	2.24	0.55
1:H:182:GLN:HE21	1:H:182:GLN:HA	1.72	0.55
1:I:146:SER:O	1:I:147:THR:HG23	2.07	0.55
1:I:270:ASN:ND2	2:K:7:DG:H5''	2.21	0.55
1:J:204:ARG:HD2	1:J:268:MET:CB	2.30	0.55
1:A:187:ARG:CZ	1:A:248:LEU:HD21	2.36	0.55
1:C:290:THR:HG21	1:C:294:GLN:HB3	1.87	0.55
1:I:144:GLN:CD	1:I:144:GLN:N	2.57	0.55
1:J:278:ASN:O	1:J:279:ARG:HG2	2.07	0.55
1:C:182:GLN:HA	1:C:182:GLN:NE2	2.22	0.55
1:J:182:GLN:HA	1:J:182:GLN:HE21	1.72	0.55
1:C:291:ARG:NH1	1:C:291:ARG:HG3	2.21	0.55
1:D:283:LEU:HB3	1:D:302:GLU:HA	1.88	0.55
1:A:180:PRO:O	1:A:181:PRO:O	2.24	0.55
3:F:16:DG:H2''	3:F:17:DT:H5'	1.89	0.55
1:A:155:TYR:HE2	1:A:157:THR:HA	1.72	0.54
1:J:187:ARG:HB2	1:J:248:LEU:HD22	1.90	0.54
1:A:166:ILE:HG13	1:A:305:ILE:HD11	1.88	0.54
1:B:187:ARG:HB3	1:B:287:THR:HG23	1.88	0.54
1:G:143:GLN:N	1:G:173:GLN:OE1	2.40	0.54
1:I:190:PRO:C	1:I:202:VAL:HG21	2.33	0.54
1:A:143:GLN:N	1:A:173:GLN:OE1	2.40	0.54
1:C:190:PRO:C	1:C:202:VAL:HG21	2.32	0.54
1:C:244:ARG:HH11	1:C:244:ARG:HG2	1.71	0.54
1:I:142:PHE:CE1	1:I:172:ILE:HG12	2.42	0.54
1:I:226:ILE:HD11	1:I:284:ILE:HD12	1.88	0.54
1:D:258:THR:HG22	1:D:259:GLU:N	2.22	0.54
1:G:226:ILE:HD11	1:G:284:ILE:HD12	1.90	0.54
1:I:180:PRO:O	1:I:181:PRO:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:GLY:O	1:B:184:ALA:C	2.50	0.54
1:H:258:THR:HG22	1:H:259:GLU:N	2.23	0.54
1:H:290:THR:HG23	1:H:292:ASP:H	1.73	0.54
1:I:143:GLN:N	1:I:173:GLN:OE1	2.40	0.54
1:I:244:ARG:HG2	1:I:244:ARG:NH1	2.23	0.54
1:I:290:THR:HG21	1:I:294:GLN:HB3	1.89	0.54
1:C:143:GLN:N	1:C:173:GLN:OE1	2.40	0.54
1:I:201:VAL:HG12	1:I:202:VAL:N	2.22	0.54
1:J:258:THR:HG22	1:J:259:GLU:N	2.23	0.54
3:L:16:DG:H2''	3:L:17:DT:H5'	1.89	0.54
1:C:154:THR:CG2	1:C:163:TYR:HB2	2.37	0.54
1:H:161:LYS:HD3	1:H:163:TYR:CZ	2.43	0.54
1:B:258:THR:HG22	1:B:259:GLU:N	2.23	0.53
1:C:162:LEU:HD12	1:C:301:PHE:HE2	1.73	0.53
1:D:213:GLU:O	1:D:214:PHE:HB2	2.08	0.53
1:D:290:THR:HG21	1:D:294:GLN:HB3	1.89	0.53
2:E:19:DT:H71	2:K:19:DT:H71	1.89	0.53
1:D:182:GLN:HE21	1:D:182:GLN:HA	1.73	0.53
1:J:152:THR:HG23	1:J:153:TRP:HD1	1.73	0.53
3:L:14:DA:H2''	3:L:15:DT:H5'	1.90	0.53
1:C:187:ARG:HB3	1:C:287:THR:HG23	1.90	0.53
1:D:187:ARG:HB2	1:D:248:LEU:HD22	1.89	0.53
1:D:214:PHE:O	1:D:218:GLN:HG3	2.09	0.53
1:G:155:TYR:HE2	1:G:157:THR:HA	1.71	0.53
1:G:190:PRO:C	1:G:202:VAL:HG21	2.33	0.53
1:J:270:ASN:C	1:J:272:SER:H	2.16	0.53
1:B:290:THR:HG23	1:B:292:ASP:H	1.73	0.53
1:G:142:PHE:CE1	1:G:172:ILE:HG12	2.42	0.53
1:H:187:ARG:HB3	1:H:287:THR:HG23	1.90	0.53
1:H:270:ASN:C	1:H:272:SER:H	2.16	0.53
1:A:142:PHE:CE1	1:A:172:ILE:HG12	2.43	0.53
1:B:161:LYS:HD3	1:B:163:TYR:CZ	2.43	0.53
1:H:213:GLU:O	1:H:214:PHE:HB2	2.09	0.53
1:I:155:TYR:HE2	1:I:157:THR:HA	1.73	0.53
1:A:230:GLY:CA	1:H:199:THR:CG2	2.86	0.53
1:C:155:TYR:HE2	1:C:157:THR:HA	1.73	0.53
1:C:166:ILE:HA	1:C:305:ILE:CD1	2.39	0.53
1:J:213:GLU:O	1:J:214:PHE:HB2	2.08	0.53
1:D:215:ASN:O	1:D:216:GLU:C	2.52	0.53
1:D:161:LYS:HD3	1:D:163:TYR:CZ	2.44	0.53
2:E:2:DA:H2''	2:E:3:DA:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ILE:HD11	1:A:284:ILE:HD12	1.90	0.53
1:B:213:GLU:O	1:B:214:PHE:HB2	2.09	0.53
1:H:204:ARG:HD2	1:H:268:MET:CB	2.29	0.53
1:J:214:PHE:O	1:J:218:GLN:HG3	2.09	0.53
3:L:14:DA:H2''	3:L:15:DT:H5''	1.90	0.53
1:A:183:GLY:O	1:A:184:ALA:C	2.51	0.52
1:B:215:ASN:O	1:B:216:GLU:C	2.52	0.52
2:E:9:DT:H2'	2:E:9:DT:O5'	2.08	0.52
1:A:201:VAL:HG12	1:A:202:VAL:N	2.23	0.52
1:B:204:ARG:HD2	1:B:268:MET:CB	2.31	0.52
1:G:201:VAL:HG12	1:G:202:VAL:N	2.25	0.52
1:H:183:GLY:O	1:H:184:ALA:C	2.51	0.52
1:A:190:PRO:C	1:A:202:VAL:HG21	2.34	0.52
1:A:209:GLU:HG2	1:A:209:GLU:O	2.08	0.52
1:B:270:ASN:C	1:B:272:SER:H	2.17	0.52
1:B:318:ASP:C	1:B:320:ILE:H	2.18	0.52
1:C:166:ILE:HG13	1:C:305:ILE:HD11	1.91	0.52
1:H:152:THR:HG23	1:H:153:TRP:HD1	1.74	0.52
2:K:2:DA:H2''	2:K:3:DA:C8	2.43	0.52
3:L:5:DA:C2'	3:L:6:DT:H5''	2.39	0.52
1:B:214:PHE:O	1:B:218:GLN:HG3	2.09	0.52
1:D:169:THR:HA	1:D:266:ASN:ND2	2.25	0.52
1:I:183:GLY:O	1:I:184:ALA:C	2.53	0.52
1:I:209:GLU:O	1:I:209:GLU:HG2	2.09	0.52
1:J:161:LYS:HD3	1:J:163:TYR:CZ	2.45	0.52
1:G:149:LYS:C	1:G:151:ALA:N	2.67	0.52
1:G:183:GLY:O	1:G:184:ALA:C	2.51	0.52
1:H:214:PHE:O	1:H:218:GLN:HG3	2.10	0.52
1:C:143:GLN:HB3	1:C:173:GLN:NE2	2.24	0.52
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.23	0.52
1:C:142:PHE:CE1	1:C:172:ILE:HG12	2.45	0.52
3:F:10:DT:H2''	3:F:11:DA:OP2	2.10	0.52
1:J:215:ASN:O	1:J:216:GLU:C	2.53	0.52
1:B:199:THR:CG2	1:G:230:GLY:HA2	2.39	0.52
3:L:10:DT:H2''	3:L:11:DA:OP2	2.09	0.52
1:A:187:ARG:HB3	1:A:287:THR:HG23	1.90	0.51
1:D:270:ASN:C	1:D:272:SER:H	2.17	0.51
3:F:14:DA:H2''	3:F:15:DT:H5''	1.92	0.51
1:C:270:ASN:ND2	2:E:7:DG:H5''	2.25	0.51
1:D:152:THR:HG23	1:D:153:TRP:HD1	1.75	0.51
1:D:183:GLY:O	1:D:184:ALA:C	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:DA:C6	2:E:3:DA:C6	2.99	0.51
1:I:136:HIS:CE1	1:I:180:PRO:HA	2.45	0.51
1:I:187:ARG:HB3	1:I:287:THR:HG23	1.91	0.51
1:B:152:THR:HG23	1:B:153:TRP:HD1	1.75	0.51
1:I:150:SER:O	1:I:152:THR:N	2.42	0.51
1:G:239:ASP:O	1:G:243:GLY:N	2.44	0.51
3:F:14:DA:H2''	3:F:15:DT:H5'	1.91	0.51
1:H:172:ILE:HG22	1:H:263:VAL:HB	1.93	0.51
1:C:140:VAL:HG12	1:C:174:ILE:HD13	1.92	0.51
3:F:5:DA:C2'	3:F:6:DT:H5''	2.39	0.51
1:J:290:THR:HG23	1:J:292:ASP:H	1.76	0.51
1:C:209:GLU:O	1:C:209:GLU:HG2	2.09	0.51
1:J:156:SER:OG	1:J:159:LEU:HB2	2.11	0.51
1:D:318:ASP:C	1:D:320:ILE:H	2.19	0.51
1:I:291:ARG:NH1	1:I:291:ARG:HG3	2.26	0.51
1:A:153:TRP:HB3	1:A:164:CYS:HB2	1.93	0.51
1:A:209:GLU:C	1:A:210:LEU:HD12	2.36	0.51
1:G:166:ILE:HA	1:G:305:ILE:HD11	1.92	0.51
1:A:230:GLY:HA3	1:H:199:THR:HG21	1.92	0.51
1:C:190:PRO:O	1:C:202:VAL:HG21	2.11	0.51
1:D:204:ARG:NH1	1:D:208:HIS:HB3	2.26	0.51
1:H:215:ASN:O	1:H:216:GLU:C	2.53	0.51
1:I:140:VAL:HG12	1:I:174:ILE:HD13	1.93	0.51
1:B:196:GLU:HG2	1:G:169:THR:HG22	1.93	0.50
1:C:277:MET:O	1:C:278:ASN:C	2.54	0.50
1:G:187:ARG:HB3	1:G:287:THR:HG23	1.92	0.50
1:I:209:GLU:C	1:I:210:LEU:HD12	2.36	0.50
1:J:183:GLY:O	1:J:184:ALA:C	2.54	0.50
1:A:144:GLN:CD	1:A:144:GLN:N	2.59	0.50
1:B:182:GLN:HA	1:B:182:GLN:HE21	1.75	0.50
1:I:187:ARG:HB2	1:I:248:LEU:CD2	2.41	0.50
1:J:190:PRO:C	1:J:202:VAL:HG21	2.37	0.50
1:B:171:PRO:HA	1:B:264:LEU:HD12	1.93	0.50
1:C:244:ARG:HG2	1:C:244:ARG:NH1	2.24	0.50
1:G:209:GLU:O	1:G:209:GLU:HG2	2.10	0.50
1:H:318:ASP:C	1:H:320:ILE:H	2.19	0.50
1:J:171:PRO:HA	1:J:264:LEU:HD12	1.93	0.50
1:A:150:SER:O	1:A:152:THR:N	2.43	0.50
1:B:204:ARG:NH1	1:B:208:HIS:HB3	2.26	0.50
1:C:150:SER:O	1:C:152:THR:N	2.43	0.50
1:C:291:ARG:HG3	1:C:291:ARG:HH11	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:TRP:HB3	1:H:164:CYS:HB2	1.93	0.50
1:G:162:LEU:HD12	1:G:301:PHE:HE2	1.76	0.50
1:G:187:ARG:HB2	1:G:248:LEU:CD2	2.42	0.50
1:H:171:PRO:HA	1:H:264:LEU:HD12	1.92	0.50
1:J:204:ARG:NH1	1:J:208:HIS:HB3	2.26	0.50
1:A:291:ARG:NH1	1:A:291:ARG:HG3	2.26	0.50
1:C:136:HIS:CE1	1:C:180:PRO:HA	2.47	0.50
1:D:156:SER:OG	1:D:159:LEU:HB2	2.12	0.50
1:I:162:LEU:HD12	1:I:301:PHE:HE2	1.77	0.50
1:C:187:ARG:NH1	1:C:248:LEU:HD21	2.27	0.50
1:D:171:PRO:HA	1:D:264:LEU:HD12	1.93	0.50
3:F:8:DT:H2'	3:F:9:DT:H72	1.94	0.50
1:G:206:PRO:HD2	1:H:207:ASN:OD1	2.12	0.50
1:I:149:LYS:C	1:I:151:ALA:N	2.68	0.50
1:J:169:THR:HA	1:J:266:ASN:ND2	2.27	0.50
2:K:2:DA:C6	2:K:3:DA:C6	2.99	0.50
1:A:162:LEU:HD12	1:A:301:PHE:HE2	1.77	0.50
1:B:175:LYS:CD	1:B:259:GLU:O	2.57	0.50
1:I:187:ARG:NH1	1:I:248:LEU:HD21	2.27	0.50
1:C:162:LEU:HD12	1:C:301:PHE:CE2	2.47	0.50
1:H:156:SER:OG	1:H:159:LEU:HB2	2.12	0.50
1:D:290:THR:HG23	1:D:292:ASP:H	1.76	0.49
3:F:17:DT:C6	3:F:18:DT:H72	2.47	0.49
1:B:277:MET:O	1:B:278:ASN:C	2.55	0.49
1:C:240:PRO:HG2	1:C:241:ILE:CD1	2.28	0.49
1:G:164:CYS:O	1:G:305:ILE:HA	2.13	0.49
1:G:209:GLU:C	1:G:210:LEU:HD12	2.37	0.49
2:K:9:DT:H2'	2:K:9:DT:O5'	2.12	0.49
1:B:153:TRP:HB3	1:B:164:CYS:HB2	1.93	0.49
1:J:172:ILE:HG22	1:J:263:VAL:HB	1.94	0.49
1:J:277:MET:O	1:J:278:ASN:C	2.55	0.49
1:H:169:THR:HA	1:H:266:ASN:ND2	2.28	0.49
1:I:164:CYS:O	1:I:305:ILE:HA	2.12	0.49
1:G:240:PRO:HG2	1:G:241:ILE:CD1	2.32	0.49
1:H:187:ARG:NH1	1:H:248:LEU:HD21	2.27	0.49
1:A:240:PRO:HG2	1:A:241:ILE:CD1	2.31	0.49
1:C:153:TRP:HB3	1:C:164:CYS:HB2	1.94	0.49
1:C:187:ARG:HB2	1:C:248:LEU:CD2	2.42	0.49
1:G:140:VAL:HG12	1:G:174:ILE:HD13	1.95	0.49
1:I:143:GLN:HB3	1:I:173:GLN:OE1	2.13	0.49
1:I:314:LYS:HE3	1:I:318:ASP:OD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:HG12	1:A:174:ILE:HD13	1.94	0.49
1:A:164:CYS:O	1:A:305:ILE:HA	2.13	0.49
1:B:172:ILE:HG22	1:B:263:VAL:HB	1.93	0.49
1:G:314:LYS:HE3	1:G:318:ASP:OD2	2.12	0.49
1:A:187:ARG:HB2	1:A:248:LEU:CD2	2.43	0.49
1:D:201:VAL:HG12	1:D:202:VAL:N	2.27	0.49
1:I:143:GLN:HB3	1:I:173:GLN:NE2	2.28	0.49
1:J:201:VAL:HG12	1:J:202:VAL:N	2.27	0.49
1:B:156:SER:OG	1:B:159:LEU:HB2	2.13	0.49
1:C:209:GLU:C	1:C:210:LEU:HD12	2.38	0.49
1:H:204:ARG:NH1	1:H:208:HIS:HB3	2.27	0.49
1:B:169:THR:HA	1:B:266:ASN:ND2	2.28	0.48
1:B:190:PRO:C	1:B:202:VAL:HG21	2.38	0.48
1:B:199:THR:HG21	1:G:230:GLY:HA2	1.89	0.48
1:C:143:GLN:CB	1:C:173:GLN:HE22	2.27	0.48
1:C:171:PRO:HA	1:C:264:LEU:HD12	1.95	0.48
1:D:277:MET:O	1:D:278:ASN:C	2.56	0.48
1:G:291:ARG:NH1	1:G:291:ARG:HG3	2.28	0.48
1:H:272:SER:HA	1:H:279:ARG:N	2.27	0.48
1:H:314:LYS:C	1:H:314:LYS:HD2	2.39	0.48
3:L:8:DT:H2'	3:L:9:DT:H72	1.94	0.48
1:A:241:ILE:HD12	1:A:241:ILE:N	2.29	0.48
1:C:206:PRO:HD2	1:D:207:ASN:OD1	2.13	0.48
1:G:190:PRO:O	1:G:202:VAL:HG21	2.14	0.48
1:A:241:ILE:HD12	1:A:241:ILE:H	1.78	0.48
1:C:143:GLN:HB3	1:C:173:GLN:HE22	1.77	0.48
1:B:168:LYS:CD	1:C:168:LYS:HE2	2.44	0.48
1:B:187:ARG:NH1	1:B:248:LEU:HD21	2.28	0.48
1:C:314:LYS:HE3	1:C:318:ASP:OD2	2.13	0.48
1:D:153:TRP:HB3	1:D:164:CYS:HB2	1.94	0.48
1:G:166:ILE:HA	1:G:305:ILE:HD12	1.95	0.48
1:I:241:ILE:HD12	1:I:241:ILE:N	2.28	0.48
1:C:241:ILE:HD12	1:C:241:ILE:H	1.79	0.48
1:D:190:PRO:C	1:D:202:VAL:HG21	2.38	0.48
1:H:201:VAL:HG12	1:H:202:VAL:N	2.28	0.48
1:A:230:GLY:HA3	1:H:199:THR:CG2	2.43	0.48
1:G:270:ASN:ND2	2:K:16:DG:H5''	2.28	0.48
1:H:168:LYS:CD	1:I:168:LYS:HE2	2.43	0.48
1:J:153:TRP:HB3	1:J:164:CYS:HB2	1.95	0.48
1:A:270:ASN:ND2	2:E:16:DG:H5''	2.29	0.47
1:D:187:ARG:NH1	1:D:248:LEU:HD21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:239:ASP:O	1:I:243:GLY:N	2.47	0.47
1:B:201:VAL:HG12	1:B:202:VAL:N	2.29	0.47
1:C:241:ILE:HD12	1:C:241:ILE:N	2.29	0.47
1:G:241:ILE:HD12	1:G:241:ILE:H	1.79	0.47
1:I:169:THR:HA	1:I:266:ASN:ND2	2.30	0.47
1:I:272:SER:HA	1:I:279:ARG:N	2.28	0.47
1:J:318:ASP:C	1:J:320:ILE:H	2.22	0.47
1:D:172:ILE:HG22	1:D:263:VAL:HB	1.96	0.47
1:G:169:THR:HA	1:G:266:ASN:ND2	2.29	0.47
1:A:149:LYS:C	1:A:151:ALA:N	2.69	0.47
1:A:314:LYS:HE3	1:A:318:ASP:OD2	2.13	0.47
1:C:149:LYS:C	1:C:151:ALA:N	2.72	0.47
1:A:143:GLN:HB3	1:A:173:GLN:NE2	2.30	0.47
1:D:216:GLU:OE1	1:D:216:GLU:CA	2.60	0.47
1:G:153:TRP:HB3	1:G:164:CYS:HB2	1.95	0.47
1:J:187:ARG:NH1	1:J:248:LEU:HD21	2.29	0.47
1:A:277:MET:O	1:A:278:ASN:C	2.57	0.47
1:C:143:GLN:HB3	1:C:173:GLN:OE1	2.14	0.47
1:G:150:SER:O	1:G:152:THR:N	2.45	0.47
1:G:162:LEU:HD12	1:G:301:PHE:CE2	2.50	0.47
1:G:239:ASP:O	1:G:243:GLY:HA2	2.14	0.47
1:G:277:MET:O	1:G:278:ASN:C	2.58	0.47
1:I:241:ILE:HD12	1:I:241:ILE:H	1.78	0.47
1:A:206:PRO:HD2	1:B:207:ASN:OD1	2.14	0.47
1:C:140:VAL:HG12	1:C:174:ILE:CD1	2.45	0.47
1:D:209:GLU:O	1:D:222:PRO:HB2	2.15	0.47
1:G:136:HIS:CE1	1:G:180:PRO:HA	2.50	0.47
1:I:153:TRP:HB3	1:I:164:CYS:HB2	1.96	0.47
1:I:206:PRO:HD2	1:J:207:ASN:OD1	2.14	0.47
1:J:209:GLU:O	1:J:222:PRO:HB2	2.15	0.47
1:G:143:GLN:HB3	1:G:173:GLN:NE2	2.30	0.47
1:A:126:SER:HA	1:A:127:PRO:HD2	1.71	0.47
1:A:166:ILE:HA	1:A:305:ILE:HD11	1.96	0.47
1:A:169:THR:HA	1:A:266:ASN:ND2	2.30	0.47
1:D:228:VAL:HG12	1:D:247:VAL:HG21	1.97	0.47
1:H:244:ARG:HH11	1:H:244:ARG:HG2	1.80	0.47
1:J:272:SER:HA	1:J:279:ARG:N	2.28	0.47
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.79	0.47
1:C:150:SER:C	1:C:152:THR:H	2.22	0.47
1:I:201:VAL:CG1	1:I:202:VAL:N	2.78	0.47
1:J:228:VAL:HG12	1:J:247:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:O	1:A:202:VAL:HG21	2.15	0.46
1:I:291:ARG:HG3	1:I:291:ARG:HH11	1.80	0.46
1:J:216:GLU:OE1	1:J:216:GLU:CA	2.61	0.46
1:H:190:PRO:C	1:H:202:VAL:HG21	2.39	0.46
1:A:166:ILE:HA	1:A:305:ILE:HD12	1.98	0.46
1:B:228:VAL:HG12	1:B:247:VAL:HG21	1.98	0.46
1:C:156:SER:O	1:C:160:LYS:N	2.48	0.46
1:H:228:VAL:HG12	1:H:247:VAL:HG21	1.98	0.46
1:C:239:ASP:O	1:C:243:GLY:N	2.46	0.46
1:A:143:GLN:HB3	1:A:173:GLN:OE1	2.14	0.46
1:A:154:THR:OG1	1:A:313:ARG:NH1	2.49	0.46
1:A:201:VAL:CG1	1:A:202:VAL:N	2.78	0.46
1:C:201:VAL:HG12	1:C:202:VAL:N	2.31	0.46
1:G:241:ILE:HD12	1:G:241:ILE:N	2.30	0.46
1:I:209:GLU:O	1:I:209:GLU:CG	2.64	0.46
3:L:16:DG:C8	3:L:17:DT:H72	2.50	0.46
1:A:136:HIS:CE1	1:A:180:PRO:HA	2.51	0.46
1:B:180:PRO:C	1:B:181:PRO:O	2.59	0.46
3:F:10:DT:H6	3:F:10:DT:H2'	1.63	0.46
1:H:277:MET:O	1:H:278:ASN:C	2.58	0.46
1:J:314:LYS:C	1:J:314:LYS:HD2	2.40	0.46
1:D:175:LYS:CD	1:D:259:GLU:O	2.60	0.46
1:G:126:SER:HA	1:G:127:PRO:HD2	1.71	0.46
1:H:161:LYS:HE3	1:H:302:GLU:OE2	2.16	0.46
1:J:155:TYR:OH	1:J:160:LYS:HA	2.16	0.46
1:J:175:LYS:CD	1:J:259:GLU:O	2.60	0.46
1:J:190:PRO:HG2	1:J:202:VAL:CG2	2.46	0.46
1:A:187:ARG:NH1	1:A:248:LEU:HD21	2.30	0.45
1:A:230:GLY:HA2	1:H:199:THR:HG21	1.96	0.45
1:D:314:LYS:HD2	1:D:314:LYS:C	2.41	0.45
1:H:244:ARG:HG2	1:H:244:ARG:NH1	2.32	0.45
1:I:143:GLN:HB3	1:I:173:GLN:HE22	1.80	0.45
1:J:161:LYS:HE3	1:J:302:GLU:OE2	2.16	0.45
1:C:183:GLY:O	1:C:184:ALA:C	2.59	0.45
1:G:272:SER:HA	1:G:279:ARG:N	2.29	0.45
1:I:140:VAL:HG12	1:I:174:ILE:CD1	2.46	0.45
1:I:162:LEU:HD12	1:I:301:PHE:CE2	2.51	0.45
1:D:272:SER:HA	1:D:279:ARG:N	2.26	0.45
1:G:143:GLN:HB3	1:G:173:GLN:OE1	2.16	0.45
1:G:171:PRO:HA	1:G:264:LEU:HD12	1.98	0.45
1:H:209:GLU:O	1:H:222:PRO:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:240:PRO:HG2	1:I:241:ILE:CD1	2.31	0.45
1:A:140:VAL:HG12	1:A:174:ILE:CD1	2.47	0.45
1:A:162:LEU:HD12	1:A:301:PHE:CE2	2.50	0.45
1:B:314:LYS:HD2	1:B:314:LYS:C	2.41	0.45
3:F:16:DG:C8	3:F:17:DT:H72	2.51	0.45
1:G:213:GLU:O	1:G:214:PHE:HB2	2.17	0.45
1:I:190:PRO:O	1:I:202:VAL:HG21	2.16	0.45
1:J:244:ARG:HG2	1:J:244:ARG:HH11	1.81	0.45
1:B:209:GLU:O	1:B:222:PRO:HB2	2.16	0.45
1:C:235:GLN:O	1:C:235:GLN:HG3	2.15	0.45
1:G:143:GLN:HB3	1:G:173:GLN:HE22	1.82	0.45
1:I:150:SER:C	1:I:152:THR:H	2.24	0.45
2:E:3:DA:H1'	2:E:4:DC:H5'	1.98	0.45
1:G:154:THR:OG1	1:G:313:ARG:NH1	2.49	0.45
1:I:156:SER:O	1:I:160:LYS:N	2.49	0.45
2:E:16:DG:C2	3:F:5:DA:C2	3.04	0.45
1:H:166:ILE:C	1:H:168:LYS:H	2.25	0.45
1:I:277:MET:O	1:I:278:ASN:C	2.58	0.45
1:A:171:PRO:HA	1:A:264:LEU:HD12	1.98	0.45
1:C:143:GLN:HB3	1:C:173:GLN:CD	2.42	0.45
1:A:169:THR:HG22	1:H:196:GLU:HG2	1.99	0.45
1:A:209:GLU:O	1:A:209:GLU:CG	2.64	0.45
1:A:218:GLN:NE2	1:A:218:GLN:CA	2.78	0.45
1:B:190:PRO:HG2	1:B:202:VAL:CG2	2.47	0.45
1:C:163:TYR:N	1:C:163:TYR:CD1	2.85	0.45
1:D:155:TYR:OH	1:D:160:LYS:HA	2.16	0.45
1:H:140:VAL:HG12	1:H:174:ILE:CD1	2.46	0.45
3:L:17:DT:C6	3:L:18:DT:H72	2.51	0.45
1:A:182:GLN:NE2	1:A:182:GLN:CA	2.77	0.45
1:C:126:SER:HA	1:C:127:PRO:HD2	1.73	0.45
1:D:206:PRO:O	1:D:210:LEU:HD12	2.16	0.45
1:I:166:ILE:HA	1:I:305:ILE:HD12	1.98	0.45
1:J:182:GLN:HA	1:J:182:GLN:NE2	2.32	0.45
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.81	0.44
1:D:180:PRO:C	1:D:181:PRO:O	2.58	0.44
1:H:158:GLU:H	1:H:158:GLU:CD	2.25	0.44
1:I:166:ILE:HA	1:I:305:ILE:HD11	1.99	0.44
1:J:180:PRO:C	1:J:181:PRO:O	2.59	0.44
1:B:232:SER:HB2	1:C:232:SER:CB	2.47	0.44
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.32	0.44
1:C:213:GLU:O	1:C:214:PHE:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:LYS:HE3	1:D:302:GLU:OE2	2.17	0.44
1:D:190:PRO:HG2	1:D:202:VAL:CG2	2.46	0.44
1:G:201:VAL:CG1	1:G:202:VAL:N	2.80	0.44
1:H:155:TYR:OH	1:H:160:LYS:HA	2.18	0.44
1:H:190:PRO:HG2	1:H:202:VAL:CG2	2.47	0.44
1:I:171:PRO:HA	1:I:264:LEU:HD12	1.98	0.44
1:G:140:VAL:HG12	1:G:174:ILE:CD1	2.47	0.44
1:A:239:ASP:O	1:A:243:GLY:N	2.46	0.44
1:B:140:VAL:HG12	1:B:174:ILE:CD1	2.47	0.44
1:H:282:ILE:HG13	1:H:283:LEU:N	2.32	0.44
1:J:201:VAL:CG1	1:J:202:VAL:N	2.81	0.44
1:J:244:ARG:HG2	1:J:244:ARG:NH1	2.32	0.44
2:K:16:DG:C2	3:L:5:DA:C2	3.05	0.44
1:D:244:ARG:HG2	1:D:244:ARG:HH11	1.82	0.44
1:D:244:ARG:HG2	1:D:244:ARG:NH1	2.33	0.44
2:E:16:DG:N2	3:F:5:DA:N3	2.65	0.44
1:G:187:ARG:NH1	1:G:248:LEU:HD21	2.32	0.44
1:J:284:ILE:HG12	1:J:303:ALA:HB2	1.99	0.44
1:A:143:GLN:HB3	1:A:173:GLN:HE22	1.82	0.44
1:B:272:SER:HA	1:B:279:ARG:N	2.27	0.44
1:C:209:GLU:O	1:C:209:GLU:CG	2.66	0.44
1:D:201:VAL:CG1	1:D:202:VAL:N	2.81	0.44
1:D:284:ILE:HG12	1:D:303:ALA:HB2	2.00	0.44
1:G:264:LEU:HD12	1:G:264:LEU:HA	1.74	0.44
1:H:262:THR:HG21	1:I:216:GLU:HB2	1.99	0.44
1:I:163:TYR:N	1:I:163:TYR:CD1	2.86	0.44
1:J:206:PRO:O	1:J:210:LEU:HD12	2.18	0.44
1:J:252:GLU:O	1:J:261:THR:CG2	2.65	0.44
1:B:155:TYR:OH	1:B:160:LYS:HA	2.17	0.43
1:C:144:GLN:CD	1:C:144:GLN:N	2.64	0.43
1:C:239:ASP:O	1:C:243:GLY:HA2	2.18	0.43
1:G:209:GLU:O	1:G:209:GLU:CG	2.65	0.43
1:I:143:GLN:CB	1:I:173:GLN:HE22	2.31	0.43
1:A:239:ASP:O	1:A:243:GLY:HA2	2.17	0.43
1:A:264:LEU:HD12	1:A:264:LEU:HA	1.74	0.43
1:B:166:ILE:C	1:B:168:LYS:H	2.25	0.43
1:H:180:PRO:C	1:H:181:PRO:O	2.60	0.43
1:H:187:ARG:HB2	1:H:248:LEU:CD2	2.47	0.43
1:A:153:TRP:CB	1:A:164:CYS:HB2	2.48	0.43
1:C:169:THR:HA	1:C:266:ASN:ND2	2.33	0.43
1:B:161:LYS:HE3	1:B:302:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:175:LYS:CD	1:H:259:GLU:O	2.57	0.43
1:H:232:SER:HB2	1:I:232:SER:CB	2.47	0.43
1:I:182:GLN:NE2	1:I:182:GLN:CA	2.79	0.43
1:A:213:GLU:O	1:A:214:PHE:HB2	2.18	0.43
1:B:213:GLU:HB2	1:C:145:SER:C	2.42	0.43
1:D:140:VAL:HG12	1:D:174:ILE:CD1	2.47	0.43
1:G:144:GLN:CD	1:G:144:GLN:N	2.59	0.43
1:G:163:TYR:CD1	1:G:163:TYR:N	2.86	0.43
1:I:187:ARG:HB2	1:I:248:LEU:HD22	2.01	0.43
1:J:166:ILE:C	1:J:168:LYS:H	2.26	0.43
1:B:187:ARG:HB2	1:B:248:LEU:CD2	2.49	0.43
1:C:308:CYS:O	1:C:309:PRO:C	2.61	0.43
1:G:308:CYS:O	1:G:309:PRO:C	2.61	0.43
1:H:182:GLN:HA	1:H:182:GLN:NE2	2.32	0.43
1:C:164:CYS:O	1:C:305:ILE:HA	2.19	0.43
1:C:166:ILE:HA	1:C:305:ILE:HD11	1.99	0.43
1:D:158:GLU:CD	1:D:158:GLU:H	2.26	0.43
1:A:163:TYR:N	1:A:163:TYR:CD1	2.86	0.43
1:D:166:ILE:C	1:D:168:LYS:H	2.27	0.43
1:G:291:ARG:HG3	1:G:291:ARG:HH11	1.81	0.43
1:H:284:ILE:HG12	1:H:303:ALA:HB2	2.01	0.43
1:I:143:GLN:HB3	1:I:173:GLN:CD	2.44	0.43
1:G:182:GLN:NE2	1:G:182:GLN:CA	2.78	0.43
1:I:218:GLN:NE2	1:I:218:GLN:CA	2.75	0.43
1:J:161:LYS:HG3	1:J:302:GLU:HB3	2.01	0.43
2:E:9:DT:C2'	2:E:9:DT:O5'	2.67	0.43
1:I:308:CYS:O	1:I:309:PRO:C	2.61	0.43
3:L:16:DG:H1'	3:L:17:DT:H5''	2.00	0.43
1:C:153:TRP:CB	1:C:164:CYS:HB2	2.49	0.42
1:H:212:ARG:HD2	1:H:216:GLU:OE2	2.19	0.42
1:I:154:THR:OG1	1:I:313:ARG:NH1	2.51	0.42
1:B:155:TYR:HE2	1:B:157:THR:HA	1.84	0.42
1:H:201:VAL:CG1	1:H:202:VAL:N	2.82	0.42
1:J:140:VAL:HG22	1:J:299:ARG:CB	2.49	0.42
1:J:154:THR:HG23	1:J:163:TYR:HB2	2.01	0.42
1:J:158:GLU:H	1:J:158:GLU:CD	2.28	0.42
1:A:220:ALA:HA	1:A:221:PRO:HD3	1.90	0.42
1:B:158:GLU:CD	1:B:158:GLU:H	2.27	0.42
1:B:218:GLN:HE21	1:C:264:LEU:CD2	2.32	0.42
1:H:216:GLU:OE1	1:H:216:GLU:CA	2.62	0.42
2:K:3:DA:H1'	2:K:4:DC:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLY:HA2	1:H:199:THR:CG2	2.48	0.42
3:F:7:DG:H2'	3:F:8:DT:H71	2.00	0.42
1:I:213:GLU:O	1:I:214:PHE:HB2	2.19	0.42
1:A:150:SER:C	1:A:152:THR:H	2.26	0.42
1:D:182:GLN:HA	1:D:182:GLN:NE2	2.34	0.42
1:G:156:SER:O	1:G:160:LYS:N	2.52	0.42
1:J:212:ARG:HD2	1:J:216:GLU:OE2	2.20	0.42
1:A:143:GLN:HB3	1:A:173:GLN:CD	2.45	0.42
1:C:291:ARG:HH11	1:C:291:ARG:CG	2.32	0.42
1:D:187:ARG:HB2	1:D:248:LEU:CD2	2.49	0.42
3:L:10:DT:H1'	3:L:11:DA:C5'	2.48	0.42
1:B:154:THR:HG23	1:B:163:TYR:HB2	2.02	0.42
1:J:155:TYR:HE2	1:J:157:THR:HA	1.83	0.42
1:A:143:GLN:CB	1:A:173:GLN:HE22	2.33	0.42
1:A:161:LYS:HB3	1:A:163:TYR:HE1	1.85	0.42
3:F:1:DA:C2	2:K:19:DT:H2''	2.55	0.42
1:G:187:ARG:HB2	1:G:248:LEU:HD22	2.02	0.42
1:G:239:ASP:O	1:G:243:GLY:CA	2.68	0.42
1:A:272:SER:HA	1:A:279:ARG:N	2.28	0.42
1:B:284:ILE:HG12	1:B:303:ALA:HB2	2.01	0.42
1:C:182:GLN:NE2	1:C:182:GLN:CA	2.83	0.42
1:D:179:PRO:HA	1:D:180:PRO:HD2	1.92	0.42
1:G:228:VAL:HG21	1:G:249:VAL:HG21	2.02	0.42
1:J:270:ASN:C	1:J:272:SER:N	2.78	0.42
1:C:304:ARG:HG3	1:C:304:ARG:NH1	2.35	0.42
3:F:16:DG:H1'	3:F:17:DT:H5''	2.02	0.42
1:H:172:ILE:CG2	1:H:263:VAL:HB	2.50	0.42
1:H:218:GLN:HE21	1:I:264:LEU:CD2	2.32	0.42
1:I:161:LYS:HB3	1:I:163:TYR:HE1	1.84	0.42
1:J:140:VAL:HG12	1:J:174:ILE:CD1	2.49	0.42
1:J:290:THR:HB	1:J:296:LEU:HD21	2.02	0.42
1:G:143:GLN:CB	1:G:173:GLN:HE22	2.32	0.41
1:H:252:GLU:O	1:H:261:THR:CG2	2.68	0.41
1:I:239:ASP:O	1:I:243:GLY:HA2	2.19	0.41
1:B:161:LYS:HD3	1:B:163:TYR:OH	2.21	0.41
1:B:172:ILE:CG2	1:B:263:VAL:HB	2.50	0.41
1:B:201:VAL:CG1	1:B:202:VAL:N	2.83	0.41
1:B:206:PRO:O	1:B:210:LEU:HD12	2.20	0.41
1:B:282:ILE:HG13	1:B:283:LEU:N	2.33	0.41
1:J:204:ARG:CG	1:J:268:MET:O	2.68	0.41
1:J:227:ARG:HA	1:J:236:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:282:ILE:HG13	1:J:283:LEU:N	2.34	0.41
2:K:16:DG:N2	3:L:5:DA:N3	2.67	0.41
1:A:270:ASN:O	1:A:277:MET:HE3	2.21	0.41
1:D:161:LYS:HG3	1:D:302:GLU:HB3	2.01	0.41
1:H:211:SER:O	1:H:213:GLU:N	2.53	0.41
1:B:216:GLU:OE1	1:B:216:GLU:CA	2.63	0.41
1:B:270:ASN:C	1:B:272:SER:N	2.78	0.41
1:C:197:HIS:CD2	1:C:280:ARG:HH11	2.38	0.41
1:D:154:THR:HG23	1:D:163:TYR:HB2	2.02	0.41
1:G:197:HIS:CD2	1:G:280:ARG:HH11	2.38	0.41
3:L:17:DT:H5'	3:L:17:DT:H6	1.86	0.41
1:A:156:SER:O	1:A:160:LYS:N	2.53	0.41
1:A:290:THR:HG22	1:A:294:GLN:HB3	2.02	0.41
1:B:262:THR:HG21	1:C:216:GLU:HB2	2.02	0.41
1:D:252:GLU:O	1:D:261:THR:CG2	2.69	0.41
1:G:196:GLU:HG3	1:G:197:HIS:CE1	2.56	0.41
1:C:154:THR:OG1	1:C:313:ARG:NH1	2.52	0.41
1:C:290:THR:HB	1:C:296:LEU:HD21	2.03	0.41
1:D:220:ALA:HA	1:D:221:PRO:HD3	1.86	0.41
3:F:17:DT:H5'	3:F:17:DT:H6	1.85	0.41
1:G:198:VAL:HG23	1:G:199:THR:N	2.34	0.41
1:A:198:VAL:O	1:A:244:ARG:NH2	2.54	0.41
1:B:182:GLN:HA	1:B:182:GLN:NE2	2.36	0.41
1:G:161:LYS:HB3	1:G:163:TYR:HE1	1.85	0.41
1:G:290:THR:HG22	1:G:294:GLN:HB3	2.02	0.41
1:H:166:ILE:C	1:H:168:LYS:N	2.79	0.41
1:B:212:ARG:HD2	1:B:216:GLU:OE2	2.21	0.41
1:C:187:ARG:HB2	1:C:248:LEU:HD22	2.02	0.41
1:I:197:HIS:CD2	1:I:280:ARG:HH11	2.39	0.41
1:J:264:LEU:HD12	1:J:264:LEU:HA	1.78	0.41
1:A:306:CYS:HB2	1:A:307:ALA:H	1.67	0.41
1:B:166:ILE:C	1:B:168:LYS:N	2.79	0.41
1:B:211:SER:O	1:B:213:GLU:N	2.54	0.41
1:D:140:VAL:HG22	1:D:299:ARG:CB	2.50	0.41
3:F:8:DT:C2'	3:F:9:DT:H72	2.50	0.41
1:G:270:ASN:O	1:G:277:MET:HE3	2.21	0.41
1:H:206:PRO:O	1:H:210:LEU:HD12	2.21	0.41
1:I:270:ASN:HD22	2:K:7:DG:H5''	1.85	0.41
1:A:166:ILE:C	1:A:168:LYS:H	2.29	0.41
1:A:304:ARG:HG3	1:A:304:ARG:NH1	2.35	0.41
1:B:252:GLU:O	1:B:261:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:PRO:HD3	1:C:275:GLY:O	2.21	0.41
1:C:218:GLN:HA	1:C:218:GLN:HE21	1.85	0.41
2:E:19:DT:H71	2:K:19:DT:C7	2.51	0.41
1:G:143:GLN:HB3	1:G:173:GLN:CD	2.46	0.41
1:H:154:THR:HG23	1:H:163:TYR:HB2	2.03	0.41
1:J:187:ARG:HB2	1:J:248:LEU:CD2	2.50	0.41
3:L:8:DT:C2'	3:L:9:DT:H72	2.51	0.41
1:A:290:THR:HB	1:A:296:LEU:HD21	2.03	0.40
1:D:155:TYR:HE2	1:D:157:THR:HA	1.83	0.40
1:D:227:ARG:HA	1:D:236:TYR:HE2	1.86	0.40
1:H:227:ARG:HA	1:H:236:TYR:HE2	1.86	0.40
1:I:235:GLN:O	1:I:235:GLN:HG3	2.21	0.40
1:J:239:ASP:O	1:J:243:GLY:N	2.53	0.40
2:K:2:DA:C5	2:K:3:DA:C6	3.09	0.40
2:K:11:DA:H2''	2:K:12:DA:C8	2.56	0.40
1:B:198:VAL:O	1:B:244:ARG:NH2	2.54	0.40
1:C:272:SER:HA	1:C:279:ARG:N	2.30	0.40
1:G:290:THR:HB	1:G:296:LEU:HD21	2.03	0.40
1:I:183:GLY:O	1:I:185:VAL:HG13	2.21	0.40
1:A:198:VAL:HG23	1:A:199:THR:N	2.36	0.40
2:E:9:DT:H2'	2:E:9:DT:H6	1.50	0.40
1:G:166:ILE:C	1:G:168:LYS:H	2.30	0.40
1:I:278:ASN:O	1:I:279:ARG:HG2	2.21	0.40
1:J:304:ARG:HH11	1:J:304:ARG:HG3	1.86	0.40
3:L:7:DG:C8	3:L:8:DT:H72	2.56	0.40
1:A:161:LYS:HB3	1:A:163:TYR:CE1	2.57	0.40
1:A:187:ARG:HB2	1:A:248:LEU:HD22	2.03	0.40
1:C:198:VAL:HG23	1:C:199:THR:N	2.36	0.40
1:D:290:THR:HB	1:D:296:LEU:HD21	2.02	0.40
1:H:198:VAL:O	1:H:244:ARG:NH2	2.55	0.40
1:I:126:SER:HA	1:I:127:PRO:HD2	1.70	0.40
1:I:153:TRP:CE3	1:I:154:THR:N	2.89	0.40
1:J:165:GLN:HA	1:J:306:CYS:O	2.21	0.40
1:J:166:ILE:C	1:J:168:LYS:N	2.80	0.40
1:C:264:LEU:HD12	1:C:264:LEU:HA	1.76	0.40
1:D:165:GLN:HA	1:D:306:CYS:O	2.21	0.40
1:D:211:SER:O	1:D:213:GLU:N	2.53	0.40
3:F:10:DT:H1'	3:F:11:DA:C5'	2.49	0.40
1:G:150:SER:C	1:G:152:THR:H	2.28	0.40
1:I:270:ASN:C	1:I:272:SER:H	2.30	0.40

All (10) 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:D:241:ILE:CD1	1:J:199:THR:CG2[3_545]	1.74	0.46
1:D:199:THR:CG2	1:J:241:ILE:CD1[3_545]	1.76	0.44
1:D:199:THR:OG1	1:J:241:ILE:CG2[3_545]	1.89	0.31
1:D:241:ILE:CG2	1:J:199:THR:OG1[3_545]	1.96	0.24
1:D:199:THR:CG2	1:J:241:ILE:CB[3_545]	2.08	0.12
1:D:199:THR:CG2	1:J:241:ILE:CG1[3_545]	2.09	0.11
1:D:241:ILE:CG1	1:J:199:THR:CG2[3_545]	2.10	0.10
1:J:217:GLY:O	1:J:230:GLY:CA[2_456]	2.13	0.07
1:D:217:GLY:O	1:D:230:GLY:CA[2_656]	2.14	0.06
1:D:241:ILE:CB	1:J:199:THR:CG2[3_545]	2.19	0.01

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	189/203 (93%)	167 (88%)	18 (10%)	4 (2%)	5	30
1	B	178/203 (88%)	151 (85%)	21 (12%)	6 (3%)	3	21
1	C	189/203 (93%)	167 (88%)	18 (10%)	4 (2%)	5	30
1	D	178/203 (88%)	152 (85%)	20 (11%)	6 (3%)	3	21
1	G	189/203 (93%)	167 (88%)	18 (10%)	4 (2%)	5	30
1	H	178/203 (88%)	152 (85%)	20 (11%)	6 (3%)	3	21
1	I	189/203 (93%)	166 (88%)	19 (10%)	4 (2%)	5	30
1	J	178/203 (88%)	151 (85%)	21 (12%)	6 (3%)	3	21
All	All	1468/1624 (90%)	1273 (87%)	155 (11%)	40 (3%)	4	26

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ALA

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Mol	Chain	Res	Type
1	A	181	PRO
1	B	181	PRO
1	B	184	ALA
1	B	216	GLU
1	C	151	ALA
1	C	181	PRO
1	D	181	PRO
1	D	184	ALA
1	D	216	GLU
1	G	151	ALA
1	G	181	PRO
1	H	181	PRO
1	H	184	ALA
1	H	216	GLU
1	I	151	ALA
1	I	181	PRO
1	J	181	PRO
1	J	184	ALA
1	J	216	GLU
1	A	127	PRO
1	A	184	ALA
1	B	167	ALA
1	B	319	SER
1	C	127	PRO
1	C	184	ALA
1	D	167	ALA
1	G	127	PRO
1	G	184	ALA
1	H	167	ALA
1	H	319	SER
1	I	127	PRO
1	I	184	ALA
1	J	167	ALA
1	D	319	SER
1	J	319	SER
1	B	212	ARG
1	D	212	ARG
1	H	212	ARG
1	J	212	ARG

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	167/179 (93%)	139 (83%)	28 (17%)	2	12
1	B	157/179 (88%)	125 (80%)	32 (20%)	1	8
1	C	167/179 (93%)	139 (83%)	28 (17%)	2	12
1	D	157/179 (88%)	125 (80%)	32 (20%)	1	8
1	G	167/179 (93%)	139 (83%)	28 (17%)	2	12
1	H	157/179 (88%)	126 (80%)	31 (20%)	1	9
1	I	167/179 (93%)	139 (83%)	28 (17%)	2	12
1	J	157/179 (88%)	125 (80%)	32 (20%)	1	8
All	All	1296/1432 (90%)	1057 (82%)	239 (18%)	1	11

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	THR
1	A	143	GLN
1	A	144	GLN
1	A	150	SER
1	A	159	LEU
1	A	162	LEU
1	A	164	CYS
1	A	177	MET
1	A	178	THR
1	A	202	VAL
1	A	204	ARG
1	A	216	GLU
1	A	228	VAL
1	A	238	GLU
1	A	246	SER
1	A	262	THR
1	A	264	LEU
1	A	269	CYS
1	A	282	ILE

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Mol	Chain	Res	Type
1	A	286	VAL
1	A	287	THR
1	A	291	ARG
1	A	295	VAL
1	A	304	ARG
1	A	305	ILE
1	A	314	LYS
1	A	316	ASP
1	A	319	SER
1	B	154	THR
1	B	159	LEU
1	B	162	LEU
1	B	166	ILE
1	B	177	MET
1	B	178	THR
1	B	182	GLN
1	B	190	PRO
1	B	202	VAL
1	B	204	ARG
1	B	209	GLU
1	B	210	LEU
1	B	212	ARG
1	B	213	GLU
1	B	216	GLU
1	B	223	SER
1	B	228	VAL
1	B	238	GLU
1	B	241	ILE
1	B	262	THR
1	B	264	LEU
1	B	269	CYS
1	B	271	SER
1	B	278	ASN
1	B	282	ILE
1	B	283	LEU
1	B	286	VAL
1	B	296	LEU
1	B	305	ILE
1	B	313	ARG
1	B	314	LYS
1	B	320	ILE
1	C	130	THR

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Mol	Chain	Res	Type
1	C	143	GLN
1	C	144	GLN
1	C	150	SER
1	C	159	LEU
1	C	162	LEU
1	C	164	CYS
1	C	177	MET
1	C	178	THR
1	C	202	VAL
1	C	204	ARG
1	C	216	GLU
1	C	228	VAL
1	C	238	GLU
1	C	246	SER
1	C	262	THR
1	C	264	LEU
1	C	269	CYS
1	C	282	ILE
1	C	286	VAL
1	C	287	THR
1	C	291	ARG
1	C	295	VAL
1	C	304	ARG
1	C	305	ILE
1	C	314	LYS
1	C	316	ASP
1	C	319	SER
1	D	154	THR
1	D	159	LEU
1	D	162	LEU
1	D	166	ILE
1	D	177	MET
1	D	178	THR
1	D	182	GLN
1	D	190	PRO
1	D	202	VAL
1	D	204	ARG
1	D	209	GLU
1	D	210	LEU
1	D	212	ARG
1	D	213	GLU
1	D	216	GLU

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Mol	Chain	Res	Type
1	D	223	SER
1	D	228	VAL
1	D	238	GLU
1	D	241	ILE
1	D	262	THR
1	D	264	LEU
1	D	269	CYS
1	D	271	SER
1	D	278	ASN
1	D	282	ILE
1	D	283	LEU
1	D	286	VAL
1	D	296	LEU
1	D	305	ILE
1	D	313	ARG
1	D	314	LYS
1	D	320	ILE
1	G	130	THR
1	G	143	GLN
1	G	144	GLN
1	G	150	SER
1	G	159	LEU
1	G	162	LEU
1	G	164	CYS
1	G	177	MET
1	G	178	THR
1	G	202	VAL
1	G	204	ARG
1	G	216	GLU
1	G	228	VAL
1	G	238	GLU
1	G	246	SER
1	G	262	THR
1	G	264	LEU
1	G	269	CYS
1	G	282	ILE
1	G	286	VAL
1	G	287	THR
1	G	291	ARG
1	G	295	VAL
1	G	304	ARG
1	G	305	ILE

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Mol	Chain	Res	Type
1	G	314	LYS
1	G	316	ASP
1	G	319	SER
1	H	154	THR
1	H	159	LEU
1	H	162	LEU
1	H	177	MET
1	H	178	THR
1	H	182	GLN
1	H	190	PRO
1	H	202	VAL
1	H	204	ARG
1	H	209	GLU
1	H	210	LEU
1	H	212	ARG
1	H	213	GLU
1	H	216	GLU
1	H	223	SER
1	H	228	VAL
1	H	238	GLU
1	H	241	ILE
1	H	262	THR
1	H	264	LEU
1	H	269	CYS
1	H	271	SER
1	H	278	ASN
1	H	282	ILE
1	H	283	LEU
1	H	286	VAL
1	H	296	LEU
1	H	305	ILE
1	H	313	ARG
1	H	314	LYS
1	H	320	ILE
1	I	130	THR
1	I	143	GLN
1	I	144	GLN
1	I	150	SER
1	I	159	LEU
1	I	162	LEU
1	I	164	CYS
1	I	177	MET

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Mol	Chain	Res	Type
1	I	178	THR
1	I	202	VAL
1	I	204	ARG
1	I	216	GLU
1	I	228	VAL
1	I	238	GLU
1	I	246	SER
1	I	262	THR
1	I	264	LEU
1	I	269	CYS
1	I	282	ILE
1	I	286	VAL
1	I	287	THR
1	I	291	ARG
1	I	295	VAL
1	I	304	ARG
1	I	305	ILE
1	I	314	LYS
1	I	316	ASP
1	I	319	SER
1	J	154	THR
1	J	159	LEU
1	J	162	LEU
1	J	166	ILE
1	J	177	MET
1	J	178	THR
1	J	182	GLN
1	J	190	PRO
1	J	202	VAL
1	J	204	ARG
1	J	209	GLU
1	J	210	LEU
1	J	212	ARG
1	J	213	GLU
1	J	216	GLU
1	J	223	SER
1	J	228	VAL
1	J	238	GLU
1	J	241	ILE
1	J	262	THR
1	J	264	LEU
1	J	269	CYS

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Mol	Chain	Res	Type
1	J	271	SER
1	J	278	ASN
1	J	282	ILE
1	J	283	LEU
1	J	286	VAL
1	J	296	LEU
1	J	305	ILE
1	J	313	ARG
1	J	314	LYS
1	J	320	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	144	GLN
1	A	182	GLN
1	A	197	HIS
1	A	215	ASN
1	A	224	HIS
1	A	245	GLN
1	A	266	ASN
1	B	173	GLN
1	B	182	GLN
1	B	197	HIS
1	B	218	GLN
1	B	266	ASN
1	B	270	ASN
1	C	143	GLN
1	C	144	GLN
1	C	182	GLN
1	C	197	HIS
1	C	215	ASN
1	C	224	HIS
1	C	245	GLN
1	C	266	ASN
1	D	173	GLN
1	D	182	GLN
1	D	218	GLN
1	D	266	ASN
1	D	270	ASN
1	G	143	GLN

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Mol	Chain	Res	Type
1	G	144	GLN
1	G	182	GLN
1	G	197	HIS
1	G	215	ASN
1	G	224	HIS
1	G	245	GLN
1	G	266	ASN
1	H	173	GLN
1	H	182	GLN
1	H	218	GLN
1	H	266	ASN
1	H	270	ASN
1	I	143	GLN
1	I	144	GLN
1	I	182	GLN
1	I	197	HIS
1	I	215	ASN
1	I	224	HIS
1	I	245	GLN
1	I	266	ASN
1	J	173	GLN
1	J	182	GLN
1	J	218	GLN
1	J	266	ASN
1	J	270	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	193/203 (95%)	-0.59	0 100 100	172, 190, 209, 220	0
1	B	182/203 (89%)	-0.48	1 (0%) 87 75	204, 241, 275, 284	0
1	C	193/203 (95%)	-0.60	0 100 100	96, 126, 152, 159	0
1	D	182/203 (89%)	-0.50	3 (1%) 70 54	257, 296, 335, 343	0
1	G	193/203 (95%)	-0.59	2 (1%) 79 63	198, 221, 240, 247	0
1	H	182/203 (89%)	-0.64	1 (0%) 87 75	173, 183, 189, 195	0
1	I	193/203 (95%)	-0.46	3 (1%) 70 54	323, 339, 351, 355	0
1	J	182/203 (89%)	-0.65	2 (1%) 78 62	204, 214, 220, 223	0
2	E	19/19 (100%)	-0.53	0 100 100	150, 159, 172, 177	0
2	K	19/19 (100%)	-0.39	0 100 100	231, 235, 244, 244	0
3	F	19/19 (100%)	-0.51	0 100 100	150, 162, 171, 173	0
3	L	19/19 (100%)	-0.42	0 100 100	229, 236, 244, 247	0
All	All	1576/1700 (92%)	-0.56	12 (0%) 82 68	96, 215, 341, 355	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	140	VAL	5.3
1	J	303	ALA	3.1
1	B	238	GLU	2.9
1	D	174	ILE	2.8
1	I	147	THR	2.8
1	D	303	ALA	2.6
1	I	267	PHE	2.5
1	D	140	VAL	2.5
1	H	211	SER	2.3
1	I	226	ILE	2.1
1	G	186	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	188	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ZN	A	901	1/1	0.99	0.04	206,206,206,206	0
4	ZN	B	901	1/1	0.99	0.04	215,215,215,215	0
4	ZN	D	901	1/1	0.99	0.03	276,276,276,276	0
4	ZN	J	901	1/1	0.99	0.02	211,211,211,211	0
4	ZN	G	901	1/1	1.00	0.03	205,205,205,205	0
4	ZN	H	901	1/1	1.00	0.04	187,187,187,187	0
4	ZN	I	901	1/1	1.00	0.02	332,332,332,332	0
4	ZN	C	901	1/1	1.00	0.02	139,139,139,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.