



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:35 PM GMT

PDB ID : 4GDF
Title : A Crystal Structure of SV40 Large T Antigen
Authors : Chang, Y.P.; Xu, M.; Chen, X.S.
Deposited on : 2012-07-31
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

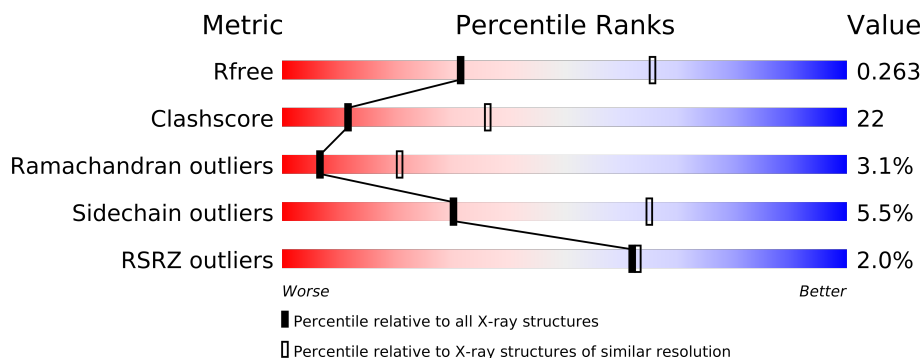
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	497	
1	B	497	
1	E	497	
1	F	497	
2	C	32	
2	G	32	
3	D	32	
3	H	32	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18835 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Large T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			4035	2601	675	733	26			
1	B	497	Total	C	N	O	S	0	0	0
			4035	2601	675	733	26			
1	E	497	Total	C	N	O	S	0	0	0
			4035	2601	675	733	26			
1	F	497	Total	C	N	O	S	0	0	0
			4035	2601	675	733	26			

- Molecule 2 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	32	Total	C	N	O	P	0	0	0
			657	312	126	188	31			
2	G	32	Total	C	N	O	P	0	0	0
			657	312	126	188	31			

- Molecule 3 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	32	Total	C	N	O	P	0	0	0
			649	310	116	192	31			
3	H	32	Total	C	N	O	P	0	0	0
			649	310	116	192	31			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total 1	Zn 1	0	0
4	E	1	Total 1	Zn 1	0	0

- Molecule 5 is water.

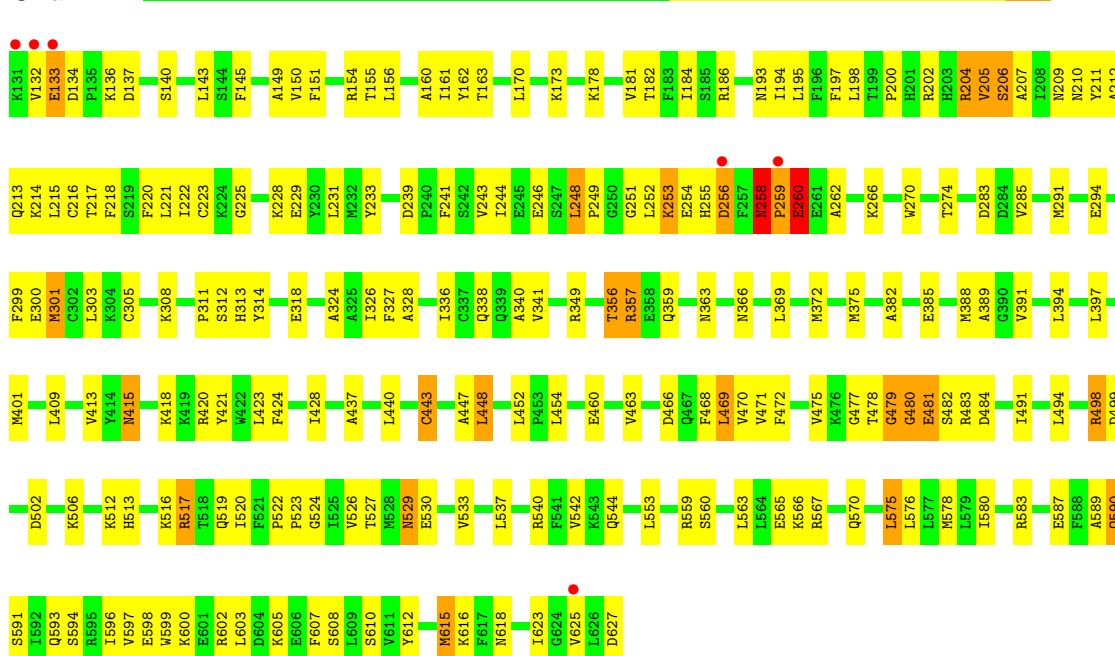
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total 18	O 18	0	0
5	B	12	Total 12	O 12	0	0
5	C	9	Total 9	O 9	0	0
5	D	6	Total 6	O 6	0	0
5	E	14	Total 14	O 14	0	0
5	F	7	Total 7	O 7	0	0
5	G	6	Total 6	O 6	0	0
5	H	7	Total 7	O 7	0	0

3 Residue-property plots

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

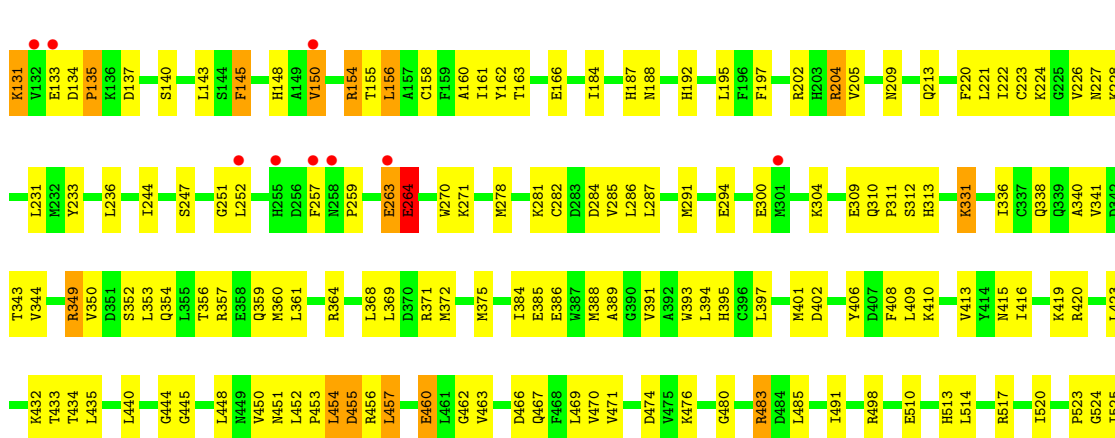
• Molecule 1: Large T antigen

Chain A:



• Molecule 1: Large T antigen

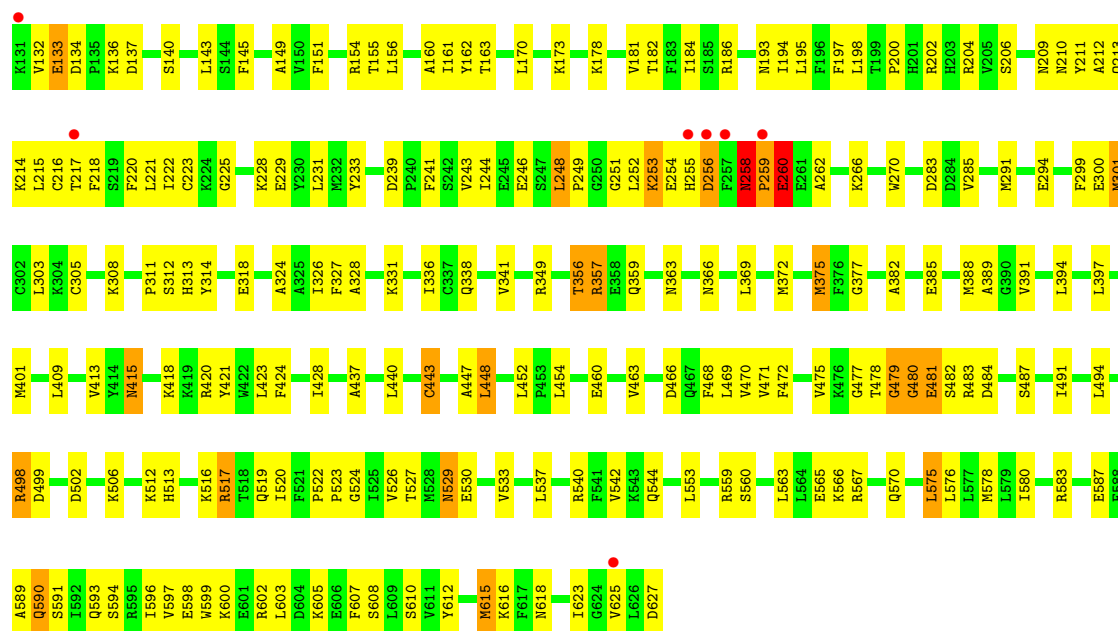
Chain B:





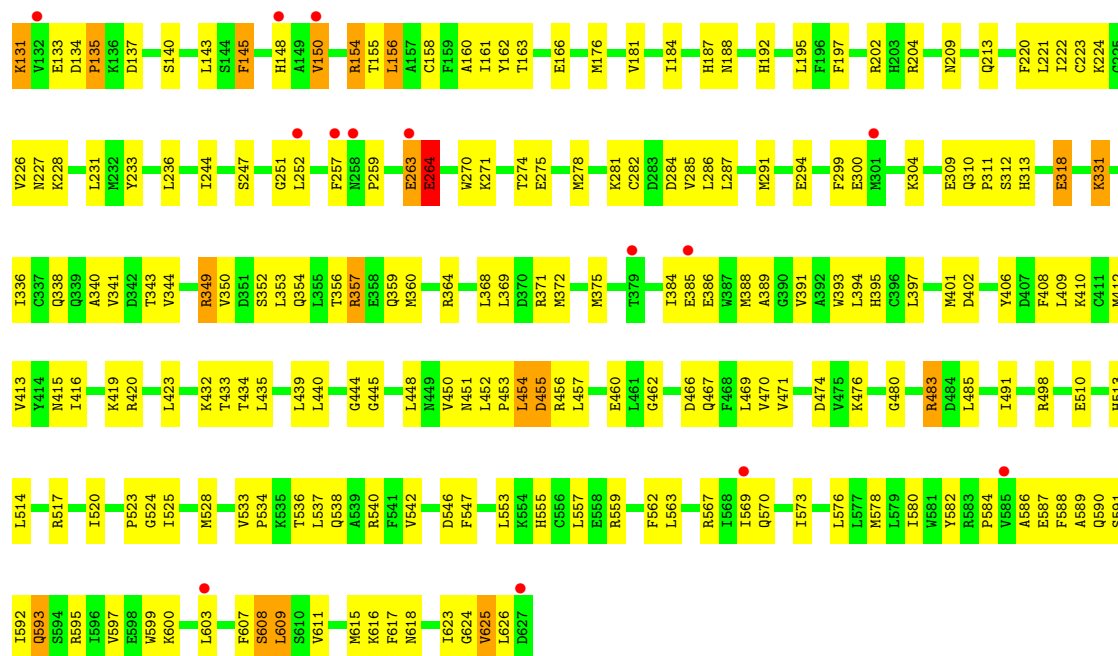
• Molecule 1: Large T antigen

Chain E:



• Molecule 1: Large T antigen

Chain F:



• Molecule 2: DNA (32-MER)

Chain C: 

• Molecule 2: DNA (32-MER)

Chain G: 

• Molecule 3: DNA (32-MER)

Chain D: 

• Molecule 3: DNA (32-MER)

Chain H: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.63Å 128.31Å 166.12Å 90.00° 89.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.37 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 86.4 (48.37-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.255 0.238 , 0.263	Depositor DCC
R_{free} test set	3317 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 24.5	EDS
Estimated twinning fraction	0.460 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 70152 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18835	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.47	0/4124	0.63	3/5562 (0.1%)
1	B	0.45	0/4124	0.62	0/5562
1	E	0.47	0/4124	0.63	3/5562 (0.1%)
1	F	0.45	0/4124	0.62	0/5562
2	C	0.54	0/738	1.00	5/1138 (0.4%)
2	G	0.55	0/738	1.02	5/1138 (0.4%)
3	D	0.54	0/726	0.95	1/1118 (0.1%)
3	H	0.55	0/726	0.96	1/1118 (0.1%)
All	All	0.48	0/19424	0.70	18/26760 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
2	C	0	2
2	G	0	2
3	D	0	3
3	H	0	3
All	All	0	12

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	DA	O4'-C1'-N9	-12.03	99.58	108.00
2	C	3	DT	N1-C1'-C2'	10.90	133.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	DT	N1-C1'-C2'	10.71	132.94	112.60
2	C	1	DA	O4'-C1'-N9	-10.46	100.68	108.00
3	D	31	DG	N9-C1'-C2'	8.13	128.06	112.60
3	H	31	DG	N9-C1'-C2'	7.55	126.95	112.60
2	C	3	DT	O4'-C1'-N1	-6.19	103.67	108.00
1	A	479	GLY	N-CA-C	5.92	127.89	113.10
1	E	479	GLY	N-CA-C	5.90	127.85	113.10
2	G	3	DT	O4'-C1'-N1	-5.87	103.89	108.00
2	G	2	DC	O4'-C1'-N1	-5.71	104.00	108.00
1	A	258	ASN	N-CA-C	-5.68	95.67	111.00
1	A	480	GLY	N-CA-C	5.68	127.30	113.10
1	E	258	ASN	N-CA-C	-5.68	95.67	111.00
1	E	480	GLY	N-CA-C	5.68	127.30	113.10
2	C	1	DA	N9-C1'-C2'	-5.57	102.02	112.60
2	C	2	DC	O4'-C1'-N1	-5.54	104.12	108.00
2	G	1	DA	N9-C1'-C2'	-5.46	102.22	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	309	GLU	Mainchain
2	C	16	DG	Sidechain
2	C	17	DC	Sidechain
3	D	17	DC	Sidechain
3	D	5	DT	Sidechain
3	D	8	DG	Sidechain
1	F	309	GLU	Mainchain
2	G	16	DG	Sidechain
2	G	17	DC	Sidechain
3	H	17	DC	Sidechain
3	H	5	DT	Sidechain
3	H	8	DG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4035	0	4068	179	0
1	B	4035	0	4068	180	0
1	E	4035	0	4068	177	0
1	F	4035	0	4068	182	0
2	C	657	0	360	31	0
2	G	657	0	360	29	0
3	D	649	0	362	26	0
3	H	649	0	362	26	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	18	0	0	0	0
5	B	12	0	0	1	0
5	C	9	0	0	0	0
5	D	6	0	0	0	0
5	E	14	0	0	1	0
5	F	7	0	0	0	0
5	G	6	0	0	0	0
5	H	7	0	0	0	0
All	All	18835	0	17716	798	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (798) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:1:DA:H2'	2:G:2:DC:C5	1.63	1.31
2:C:1:DA:H2'	2:C:2:DC:C5	1.64	1.30
2:G:1:DA:C2'	2:G:2:DC:C5	2.21	1.23
2:C:1:DA:C2'	2:C:2:DC:C5	2.21	1.22
1:F:498:ARG:HD2	1:F:540:ARG:HH21	1.11	1.09
1:B:498:ARG:HD2	1:B:540:ARG:HH21	1.13	1.07
1:E:300:GLU:HG3	1:E:301:MET:HG2	1.36	1.05
1:A:300:GLU:HG3	1:A:301:MET:HG2	1.36	1.05
1:A:198:LEU:HD21	1:A:255:HIS:HB2	1.44	1.00
1:E:198:LEU:HD21	1:E:255:HIS:HB2	1.45	0.99
3:H:31:DG:H2''	3:H:32:DT:H71	1.44	0.97
3:D:31:DG:H2''	3:D:32:DT:H71	1.45	0.95
1:A:529:ASN:HD22	1:A:530:GLU:H	1.15	0.94
1:E:529:ASN:HD22	1:E:530:GLU:H	1.18	0.92
1:F:415:ASN:HD21	1:F:420:ARG:HH11	1.16	0.92
1:F:498:ARG:HD2	1:F:540:ARG:NH2	1.85	0.91

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:498:ARG:HD2	1:B:540:ARG:NH2	1.86	0.90
1:A:428:ILE:H	1:A:428:ILE:HD12	1.35	0.89
1:E:428:ILE:HD12	1:E:428:ILE:H	1.35	0.89
2:G:1:DA:H2'	2:G:2:DC:C4	2.06	0.89
1:B:415:ASN:HD21	1:B:420:ARG:HH11	1.20	0.88
2:C:1:DA:H2'	2:C:2:DC:C4	2.07	0.88
1:A:258:ASN:HB2	1:A:259:PRO:HD3	1.58	0.86
1:E:258:ASN:HB2	1:E:259:PRO:HD3	1.58	0.86
1:A:163:THR:HG22	1:A:221:LEU:HA	1.58	0.86
1:E:163:THR:HG22	1:E:221:LEU:HA	1.59	0.85
1:F:415:ASN:ND2	1:F:420:ARG:HD2	1.92	0.84
1:A:590:GLN:H	1:A:590:GLN:NE2	1.75	0.84
1:E:590:GLN:H	1:E:590:GLN:NE2	1.76	0.83
1:A:423:LEU:HD23	1:A:544:GLN:HG3	1.60	0.82
1:E:423:LEU:HD23	1:E:544:GLN:HG3	1.60	0.82
1:B:415:ASN:ND2	1:B:420:ARG:HD2	1.94	0.81
3:H:3:DC:H1'	3:H:4:DC:H5'	1.62	0.81
3:D:3:DC:H1'	3:D:4:DC:H5'	1.62	0.81
2:G:1:DA:C2'	2:G:2:DC:C6	2.63	0.81
2:C:1:DA:C2'	2:C:2:DC:C6	2.64	0.80
3:H:31:DG:H2''	3:H:32:DT:C7	2.10	0.80
3:D:31:DG:H2''	3:D:32:DT:C7	2.12	0.79
1:B:184:ILE:HG13	1:B:197:PHE:HB3	1.66	0.78
1:E:590:GLN:HA	1:E:593:GLN:HE21	1.49	0.77
1:B:609:LEU:HD23	1:B:609:LEU:H	1.49	0.77
1:F:608:SER:OG	1:F:611:VAL:HG23	1.84	0.77
1:F:609:LEU:HD23	1:F:609:LEU:H	1.49	0.77
1:A:590:GLN:HA	1:A:593:GLN:HE21	1.50	0.77
1:B:608:SER:OG	1:B:611:VAL:HG23	1.84	0.76
1:A:300:GLU:CG	1:A:301:MET:HG2	2.15	0.76
1:A:231:LEU:HD12	1:A:231:LEU:H	1.51	0.76
1:E:231:LEU:HD12	1:E:231:LEU:H	1.51	0.76
1:E:513:HIS:CE1	1:F:513:HIS:HD2	2.03	0.76
1:F:184:ILE:HG13	1:F:197:PHE:HB3	1.68	0.75
1:A:513:HIS:CE1	1:B:513:HIS:HD2	2.04	0.75
1:E:184:ILE:HG13	1:E:197:PHE:HB3	1.69	0.75
2:G:1:DA:H2''	2:G:2:DC:C6	2.22	0.74
1:A:184:ILE:HG13	1:A:197:PHE:HB3	1.69	0.74
2:G:1:DA:C3'	2:G:2:DC:C5	2.70	0.74
2:C:1:DA:H2''	2:C:2:DC:C6	2.23	0.74
1:A:424:PHE:HB2	1:A:527:THR:HG22	1.70	0.74
1:E:565:GLU:HG2	1:F:416:ILE:HG12	1.70	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:1:DA:C3'	2:C:2:DC:C5	2.71	0.73
1:A:565:GLU:HG2	1:B:416:ILE:HG12	1.70	0.73
1:B:448:LEU:HD22	1:B:470:VAL:HG21	1.69	0.73
1:E:424:PHE:HB2	1:E:527:THR:HG22	1.71	0.73
1:E:300:GLU:CG	1:E:301:MET:HG2	2.15	0.72
1:F:448:LEU:HD22	1:F:470:VAL:HG21	1.70	0.72
1:A:440:LEU:HD12	1:A:471:VAL:CG2	2.19	0.72
1:F:389:ALA:HB1	1:F:625:VAL:HG11	1.72	0.72
1:B:389:ALA:HB1	1:B:625:VAL:HG11	1.72	0.71
1:A:253:LYS:HB2	1:A:258:ASN:HB2	1.73	0.71
1:E:513:HIS:HE1	1:F:513:HIS:CD2	2.09	0.71
1:E:466:ASP:H	1:E:519:GLN:HE22	1.38	0.71
1:A:466:ASP:H	1:A:519:GLN:HE22	1.39	0.71
1:E:440:LEU:HD12	1:E:471:VAL:CG2	2.21	0.71
1:E:253:LYS:HB2	1:E:258:ASN:HB2	1.73	0.70
1:A:212:ALA:HB1	1:A:221:LEU:HD11	1.72	0.70
1:E:212:ALA:HB1	1:E:221:LEU:HD11	1.72	0.70
1:B:349:ARG:HD3	1:B:466:ASP:OD2	1.91	0.70
1:F:450:VAL:HG12	1:F:457:LEU:HD12	1.74	0.70
1:A:448:LEU:HD22	1:A:463:VAL:CG2	2.21	0.69
1:B:533:VAL:HG13	1:B:537:LEU:HD23	1.73	0.69
1:B:213:GLN:NE2	1:B:221:LEU:HD23	2.07	0.69
1:A:300:GLU:HG3	1:A:301:MET:CG	2.19	0.69
1:A:259:PRO:O	1:A:260:GLU:HG3	1.93	0.69
1:B:450:VAL:HG12	1:B:457:LEU:HD12	1.75	0.69
1:B:155:THR:HG21	2:C:16:DG:C2'	2.22	0.69
1:B:393:TRP:HE3	1:B:394:LEU:HD22	1.58	0.69
1:F:349:ARG:HD3	1:F:466:ASP:OD2	1.92	0.69
1:E:300:GLU:HG3	1:E:301:MET:CG	2.19	0.69
1:F:393:TRP:HE3	1:F:394:LEU:HD22	1.58	0.69
1:F:563:LEU:HD13	1:F:569:ILE:HD11	1.75	0.69
1:E:448:LEU:HD22	1:E:463:VAL:CG2	2.22	0.68
1:E:259:PRO:O	1:E:260:GLU:HG3	1.93	0.68
3:H:1:DC:H4'	3:H:2:DG:H5'	1.74	0.68
1:A:513:HIS:HE1	1:B:513:HIS:CD2	2.11	0.68
1:B:563:LEU:HD13	1:B:569:ILE:HD11	1.75	0.68
1:F:356:THR:OG1	1:F:359:GLN:HG3	1.93	0.68
1:E:415:ASN:ND2	1:E:420:ARG:HD2	2.09	0.68
1:B:593:GLN:O	1:B:597:VAL:HG23	1.94	0.68
1:F:533:VAL:HG13	1:F:537:LEU:HD23	1.75	0.68
1:F:415:ASN:HD21	1:F:420:ARG:NH1	1.90	0.68
1:F:310:GLN:HG2	1:F:311:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:310:GLN:HG2	1:B:311:PRO:HD2	1.75	0.67
2:G:12:DA:H1'	2:G:13:DA:H5'	1.77	0.67
1:B:356:THR:OG1	1:B:359:GLN:HG3	1.94	0.67
1:A:415:ASN:ND2	1:A:420:ARG:HD2	2.09	0.67
3:D:1:DC:H4'	3:D:2:DG:H5'	1.76	0.67
1:F:213:GLN:NE2	1:F:221:LEU:HD23	2.09	0.67
1:F:593:GLN:O	1:F:597:VAL:HG23	1.95	0.67
1:F:498:ARG:CD	1:F:540:ARG:HH21	1.98	0.66
1:F:155:THR:HG21	2:G:16:DG:C2'	2.24	0.66
1:A:590:GLN:H	1:A:590:GLN:HE21	1.43	0.66
1:E:513:HIS:HE1	1:F:513:HIS:HD2	1.43	0.66
2:C:12:DA:H1'	2:C:13:DA:H5'	1.78	0.66
3:D:14:DG:H1'	3:D:15:DA:H5''	1.75	0.66
1:B:498:ARG:CD	1:B:540:ARG:HH21	1.99	0.66
1:F:453:PRO:HD2	1:F:456:ARG:HB3	1.78	0.66
3:H:14:DG:H1'	3:H:15:DA:H5''	1.77	0.66
1:B:364:ARG:O	1:B:368:LEU:HD23	1.95	0.66
1:E:590:GLN:H	1:E:590:GLN:HE21	1.43	0.65
1:A:300:GLU:HG3	1:A:301:MET:N	2.12	0.65
1:B:453:PRO:HD2	1:B:456:ARG:HB3	1.79	0.65
1:E:300:GLU:HG3	1:E:301:MET:N	2.12	0.65
1:B:156:LEU:HD23	1:B:156:LEU:N	2.11	0.65
1:F:156:LEU:N	1:F:156:LEU:HD23	2.11	0.65
1:B:415:ASN:HD21	1:B:420:ARG:NH1	1.94	0.64
1:F:420:ARG:HB3	1:F:523:PRO:HB3	1.80	0.64
2:C:5:DC:H2''	2:C:6:DT:OP2	1.97	0.64
1:F:364:ARG:O	1:F:368:LEU:HD23	1.97	0.64
2:G:5:DC:H2''	2:G:6:DT:OP2	1.97	0.64
2:G:1:DA:H3'	2:G:2:DC:C5	2.33	0.64
1:F:432:LYS:HG3	1:F:433:THR:N	2.13	0.64
1:F:419:LYS:HA	1:F:542:VAL:HG13	1.81	0.63
1:B:420:ARG:HB3	1:B:523:PRO:HB3	1.80	0.63
1:B:263:GLU:O	1:B:264:GLU:HB2	1.99	0.63
1:F:263:GLU:O	1:F:264:GLU:HB2	1.99	0.63
1:B:457:LEU:HD23	1:B:457:LEU:H	1.64	0.63
1:E:258:ASN:CB	1:E:259:PRO:HD3	2.22	0.63
1:E:415:ASN:HD21	1:E:420:ARG:HD2	1.63	0.63
1:A:506:LYS:HA	1:A:520:ILE:HD13	1.81	0.63
1:A:258:ASN:CB	1:A:259:PRO:HD3	2.22	0.63
1:E:506:LYS:HA	1:E:520:ILE:HD13	1.81	0.63
1:F:166:GLU:CD	1:F:166:GLU:H	2.01	0.63
1:B:432:LYS:HG3	1:B:433:THR:N	2.14	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:457:LEU:H	1:F:457:LEU:HD23	1.64	0.63
1:B:166:GLU:H	1:B:166:GLU:CD	2.02	0.62
1:F:150:VAL:CG1	1:F:224:LYS:HD3	2.30	0.62
1:A:389:ALA:HB1	1:A:625:VAL:HG11	1.80	0.62
1:A:448:LEU:HD22	1:A:463:VAL:HG23	1.81	0.62
1:E:389:ALA:HB1	1:E:625:VAL:HG11	1.80	0.62
1:F:368:LEU:O	1:F:372:MET:HG3	2.00	0.62
1:B:155:THR:HG21	2:C:16:DG:H2''	1.82	0.62
1:F:155:THR:HG21	2:G:16:DG:H2''	1.82	0.62
1:E:254:GLU:O	1:E:260:GLU:HG2	2.00	0.62
1:A:593:GLN:O	1:A:597:VAL:HG23	1.99	0.62
1:A:415:ASN:HD21	1:A:420:ARG:HD2	1.64	0.62
1:B:368:LEU:O	1:B:372:MET:HG3	2.00	0.62
1:E:428:ILE:CD1	1:E:428:ILE:H	2.09	0.62
3:D:14:DG:H2''	3:D:15:DA:H5'	1.82	0.62
1:B:294:GLU:OE2	1:B:304:LYS:NZ	2.31	0.62
1:B:150:VAL:CG1	1:B:224:LYS:HD3	2.30	0.62
1:A:254:GLU:O	1:A:260:GLU:HG2	2.00	0.61
2:C:1:DA:H3'	2:C:2:DC:C5	2.34	0.61
1:B:419:LYS:HA	1:B:542:VAL:HG13	1.83	0.61
1:E:181:VAL:HA	1:E:200:PRO:HD3	1.82	0.61
1:F:434:THR:HG21	1:F:569:ILE:HG22	1.81	0.61
2:G:11:DG:H2''	2:G:12:DA:OP2	2.00	0.61
1:F:498:ARG:HB2	1:F:540:ARG:HE	1.64	0.61
1:B:498:ARG:HB2	1:B:540:ARG:HE	1.64	0.61
1:E:448:LEU:HD22	1:E:463:VAL:HG23	1.82	0.61
1:E:513:HIS:CE1	1:F:513:HIS:CD2	2.86	0.61
1:B:626:LEU:H	1:B:626:LEU:HD12	1.64	0.61
1:A:590:GLN:HA	1:A:593:GLN:HG3	1.82	0.61
1:B:154:ARG:O	1:B:204:ARG:HB3	2.00	0.61
1:F:356:THR:H	1:F:359:GLN:HE21	1.47	0.61
1:A:181:VAL:HA	1:A:200:PRO:HD3	1.83	0.61
1:E:593:GLN:O	1:E:597:VAL:HG23	2.00	0.60
1:F:626:LEU:H	1:F:626:LEU:HD12	1.64	0.60
1:B:158:CYS:SG	1:B:226:VAL:HB	2.40	0.60
1:B:434:THR:HG21	1:B:569:ILE:HG22	1.82	0.60
1:F:294:GLU:OE2	1:F:304:LYS:NZ	2.32	0.60
1:F:483:ARG:N	1:F:483:ARG:HD2	2.15	0.60
1:E:618:ASN:HA	1:E:623:ILE:HD12	1.83	0.60
1:F:158:CYS:SG	1:F:226:VAL:HB	2.41	0.60
2:C:8:DC:H2''	2:C:9:DT:OP2	2.01	0.60
2:G:8:DC:H2''	2:G:9:DT:OP2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:483:ARG:N	1:B:483:ARG:HD2	2.15	0.60
1:E:590:GLN:HA	1:E:593:GLN:HG3	1.83	0.60
1:E:182:THR:HG23	1:E:200:PRO:HG3	1.84	0.60
1:B:356:THR:H	1:B:359:GLN:HE21	1.48	0.60
2:C:11:DG:H2''	2:C:12:DA:OP2	2.02	0.60
1:A:512:LYS:HD2	1:B:514:LEU:O	2.02	0.60
1:A:498:ARG:H	1:A:498:ARG:HD3	1.65	0.60
1:A:618:ASN:HA	1:A:623:ILE:HD12	1.83	0.60
1:E:349:ARG:HD3	1:E:517:ARG:NH2	2.17	0.59
1:B:284:ASP:HB3	1:B:287:LEU:HB3	1.84	0.59
3:H:14:DG:H2''	3:H:15:DA:H5'	1.84	0.59
1:A:182:THR:HG23	1:A:200:PRO:HG3	1.84	0.59
1:A:266:LYS:HD3	1:A:326:ILE:CD1	2.32	0.59
1:E:162:TYR:CD1	1:E:194:ILE:HG12	2.37	0.59
1:B:154:ARG:NH2	1:B:227:ASN:OD1	2.35	0.59
1:B:155:THR:HG21	2:C:16:DG:H2'	1.83	0.59
1:E:498:ARG:HD3	1:E:498:ARG:H	1.66	0.59
1:F:154:ARG:NH2	1:F:227:ASN:OD1	2.36	0.59
1:A:137:ASP:HA	1:A:222:ILE:HD13	1.84	0.59
1:E:482:SER:O	1:E:483:ARG:HD2	2.02	0.59
1:B:590:GLN:HA	1:B:593:GLN:HG3	1.85	0.58
1:E:483:ARG:O	1:E:484:ASP:HB2	2.03	0.58
1:E:137:ASP:HA	1:E:222:ILE:HD13	1.84	0.58
1:A:583:ARG:HB3	1:A:587:GLU:OE1	2.03	0.58
1:F:284:ASP:HB3	1:F:287:LEU:HB3	1.85	0.58
1:A:162:TYR:CD1	1:A:194:ILE:HG12	2.39	0.58
2:C:22:DA:H1'	2:C:23:DG:H5''	1.85	0.58
1:F:580:ILE:O	1:F:600:LYS:HE3	2.04	0.58
1:A:483:ARG:O	1:A:484:ASP:HB2	2.03	0.58
1:B:353:LEU:O	1:B:353:LEU:HD23	2.03	0.58
1:F:372:MET:HG2	1:F:573:ILE:HD12	1.86	0.58
3:D:20:DT:H1'	3:D:21:DT:H5''	1.85	0.58
1:F:356:THR:H	1:F:359:GLN:NE2	2.01	0.58
1:A:349:ARG:HD3	1:A:517:ARG:NH2	2.19	0.58
1:A:482:SER:O	1:A:483:ARG:HD2	2.02	0.58
1:B:372:MET:HG2	1:B:573:ILE:HD12	1.86	0.58
1:B:580:ILE:O	1:B:600:LYS:HE3	2.04	0.58
1:A:140:SER:HA	1:A:143:LEU:HG	1.85	0.57
1:F:204:ARG:HD3	2:G:16:DG:N7	2.19	0.57
1:E:583:ARG:HB3	1:E:587:GLU:OE1	2.04	0.57
1:F:401:MET:HG3	1:F:578:MET:CE	2.33	0.57
1:A:460:GLU:O	1:A:463:VAL:HG22	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:140:SER:HA	1:E:143:LEU:HG	1.85	0.57
1:E:266:LYS:HD3	1:E:326:ILE:CD1	2.34	0.57
1:A:470:VAL:HG12	1:A:471:VAL:N	2.20	0.57
1:F:451:ASN:C	1:F:452:LEU:HD22	2.25	0.57
2:G:22:DA:H1'	2:G:23:DG:H5''	1.86	0.57
1:E:470:VAL:HG12	1:E:471:VAL:N	2.20	0.57
1:F:353:LEU:HD23	1:F:353:LEU:O	2.04	0.57
1:F:590:GLN:HA	1:F:593:GLN:HG3	1.87	0.57
1:B:467:GLN:NE2	1:B:467:GLN:HA	2.20	0.57
1:F:467:GLN:HA	1:F:467:GLN:NE2	2.20	0.57
1:B:401:MET:HG3	1:B:578:MET:CE	2.34	0.57
1:A:529:ASN:HD22	1:A:530:GLU:N	1.95	0.56
1:B:356:THR:H	1:B:359:GLN:NE2	2.03	0.56
3:H:20:DT:H1'	3:H:21:DT:H5''	1.87	0.56
1:A:612:TYR:HA	1:A:615:MET:HG3	1.86	0.56
1:A:590:GLN:N	1:A:590:GLN:NE2	2.51	0.56
1:B:451:ASN:C	1:B:452:LEU:HD22	2.26	0.56
1:E:512:LYS:HD2	1:F:514:LEU:O	2.06	0.56
2:G:1:DA:H3'	2:G:2:DC:H5	1.69	0.56
1:A:428:ILE:H	1:A:428:ILE:CD1	2.09	0.56
1:F:155:THR:HG21	2:G:16:DG:H2'	1.87	0.56
1:E:612:TYR:HA	1:E:615:MET:HG3	1.87	0.56
1:A:213:GLN:HE21	1:A:221:LEU:HD22	1.71	0.56
1:F:209:ASN:O	1:F:213:GLN:HG2	2.06	0.56
1:A:418:LYS:HG2	1:A:502:ASP:OD1	2.06	0.56
1:E:213:GLN:HE21	1:E:221:LEU:HD22	1.71	0.55
1:E:418:LYS:HG2	1:E:502:ASP:OD1	2.06	0.55
1:E:423:LEU:HD23	1:E:544:GLN:CG	2.32	0.55
1:B:209:ASN:O	1:B:213:GLN:HG2	2.06	0.55
1:A:513:HIS:CE1	1:B:513:HIS:CD2	2.87	0.55
1:A:482:SER:C	1:A:483:ARG:HD2	2.27	0.55
3:H:20:DT:H2''	3:H:21:DT:H5'	1.87	0.55
1:E:590:GLN:N	1:E:590:GLN:NE2	2.51	0.55
1:F:590:GLN:HA	1:F:593:GLN:CG	2.37	0.55
1:E:421:TYR:O	1:E:542:VAL:HG12	2.06	0.55
1:A:423:LEU:HD23	1:A:544:GLN:CG	2.32	0.55
1:E:460:GLU:O	1:E:463:VAL:HG22	2.07	0.55
3:D:20:DT:H2''	3:D:21:DT:H5'	1.87	0.55
1:E:482:SER:C	1:E:483:ARG:HD2	2.27	0.55
1:B:590:GLN:HA	1:B:593:GLN:CG	2.37	0.55
1:F:391:VAL:HG13	1:F:578:MET:HB2	1.88	0.55
1:A:580:ILE:CD1	1:A:596:ILE:HD12	2.37	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:162:TYR:HB3	1:B:222:ILE:HB	1.89	0.55
1:E:529:ASN:HD22	1:E:530:GLU:N	1.96	0.54
1:B:440:LEU:HD11	1:B:445:GLY:C	2.27	0.54
1:B:281:LYS:NZ	1:B:371:ARG:HH22	2.05	0.54
1:A:421:TYR:O	1:A:542:VAL:HG12	2.07	0.54
1:E:612:TYR:CE2	1:E:616:LYS:HD2	2.43	0.54
1:E:324:ALA:O	1:E:327:PHE:HB3	2.07	0.54
1:F:419:LYS:HA	1:F:542:VAL:CG1	2.37	0.54
1:F:162:TYR:HB3	1:F:222:ILE:HB	1.90	0.54
1:A:612:TYR:CE2	1:A:616:LYS:HD2	2.43	0.54
1:F:278:MET:SD	1:F:343:THR:HG22	2.48	0.54
2:C:1:DA:H3'	2:C:2:DC:H5	1.70	0.54
1:B:419:LYS:HA	1:B:542:VAL:CG1	2.38	0.54
1:F:434:THR:CG2	1:F:569:ILE:HG22	2.38	0.53
1:F:419:LYS:HB3	1:F:542:VAL:HG11	1.89	0.53
1:F:281:LYS:NZ	1:F:371:ARG:HH22	2.06	0.53
1:F:448:LEU:HD13	1:F:470:VAL:HG23	1.88	0.53
1:B:434:THR:CG2	1:B:569:ILE:HG22	2.38	0.53
1:B:391:VAL:HG13	1:B:578:MET:HB2	1.90	0.53
1:A:470:VAL:O	1:A:524:GLY:HA3	2.09	0.53
1:A:233:TYR:OH	1:A:251:GLY:HA2	2.08	0.53
1:E:580:ILE:CD1	1:E:596:ILE:HD12	2.39	0.53
1:A:440:LEU:HD12	1:A:471:VAL:HG21	1.91	0.53
1:E:533:VAL:HG13	1:E:537:LEU:HD23	1.90	0.53
1:A:324:ALA:O	1:A:327:PHE:HB3	2.08	0.53
1:B:457:LEU:CD2	1:B:457:LEU:H	2.22	0.53
1:B:395:HIS:NE2	1:B:582:TYR:CE2	2.77	0.53
1:E:233:TYR:OH	1:E:251:GLY:HA2	2.09	0.53
1:A:204:ARG:O	1:A:206:SER:N	2.42	0.52
1:F:154:ARG:HG3	1:F:155:THR:N	2.23	0.52
1:A:540:ARG:HH11	1:A:540:ARG:HG2	1.75	0.52
1:A:356:THR:HB	1:A:359:GLN:HG3	1.90	0.52
1:F:467:GLN:HA	1:F:467:GLN:HE21	1.75	0.52
1:A:533:VAL:HG13	1:A:537:LEU:HD23	1.90	0.52
1:F:395:HIS:NE2	1:F:582:TYR:CE2	2.77	0.52
1:A:253:LYS:HB2	1:A:259:PRO:HD3	1.92	0.52
1:F:364:ARG:NE	1:F:368:LEU:HD21	2.25	0.52
1:B:364:ARG:NE	1:B:368:LEU:HD21	2.25	0.52
1:B:467:GLN:HE21	1:B:467:GLN:HA	1.75	0.52
2:C:28:DA:H2''	2:C:29:DG:OP2	2.10	0.52
1:A:156:LEU:HD12	1:A:156:LEU:N	2.24	0.52
1:E:397:LEU:HB3	1:E:401:MET:CE	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:368:LEU:HD12	1:B:573:ILE:HD13	1.92	0.52
2:C:1:DA:C2'	2:C:2:DC:H5	2.14	0.52
1:E:428:ILE:HD12	1:E:428:ILE:N	2.15	0.52
1:E:156:LEU:HD12	1:E:156:LEU:N	2.24	0.52
1:F:156:LEU:O	1:F:202:ARG:HA	2.09	0.52
2:G:1:DA:C3'	2:G:2:DC:H5	2.20	0.51
1:E:253:LYS:HB2	1:E:259:PRO:HD3	1.92	0.51
1:E:389:ALA:HB1	1:E:625:VAL:CG1	2.41	0.51
1:B:419:LYS:HB3	1:B:542:VAL:HG11	1.92	0.51
1:F:440:LEU:HD11	1:F:445:GLY:C	2.30	0.51
2:G:28:DA:H2''	2:G:29:DG:OP2	2.10	0.51
1:A:145:PHE:HB3	1:A:228:LYS:HB2	1.92	0.51
1:E:356:THR:HB	1:E:359:GLN:HG3	1.91	0.51
3:H:14:DG:H1'	3:H:15:DA:C5'	2.40	0.51
1:E:145:PHE:HB3	1:E:228:LYS:HB2	1.92	0.51
1:E:470:VAL:O	1:E:524:GLY:HA3	2.11	0.51
1:F:452:LEU:HB3	1:F:453:PRO:CD	2.41	0.51
1:A:428:ILE:N	1:A:428:ILE:HD12	2.16	0.51
1:B:448:LEU:HD13	1:B:470:VAL:HG23	1.90	0.51
1:A:389:ALA:HB1	1:A:625:VAL:CG1	2.41	0.51
1:F:368:LEU:HD12	1:F:573:ILE:HD13	1.93	0.51
1:B:520:ILE:HG13	1:B:520:ILE:O	2.10	0.51
1:A:299:PHE:CZ	1:A:318:GLU:HB2	2.45	0.51
2:C:1:DA:C3'	2:C:2:DC:H5	2.20	0.51
1:E:299:PHE:CZ	1:E:318:GLU:HB2	2.45	0.51
1:A:239:ASP:HA	1:A:241:PHE:N	2.26	0.51
1:E:472:PHE:HB2	1:E:526:VAL:HG22	1.92	0.51
1:B:278:MET:SD	1:B:343:THR:HG22	2.51	0.51
1:A:397:LEU:HB3	1:A:401:MET:CE	2.41	0.51
1:E:440:LEU:HD12	1:E:471:VAL:HG21	1.93	0.51
1:E:447:ALA:C	1:E:448:LEU:HD23	2.30	0.51
1:F:457:LEU:H	1:F:457:LEU:CD2	2.23	0.51
1:A:447:ALA:C	1:A:448:LEU:HD23	2.30	0.51
1:A:608:SER:C	1:A:610:SER:H	2.13	0.51
1:E:540:ARG:HH11	1:E:540:ARG:HG2	1.76	0.51
1:F:453:PRO:O	1:F:455:ASP:N	2.42	0.51
1:B:154:ARG:HG3	1:B:155:THR:N	2.25	0.51
1:B:589:ALA:O	1:B:593:GLN:HG2	2.11	0.51
1:F:385:GLU:HA	1:F:607:PHE:CE2	2.46	0.51
1:E:608:SER:C	1:E:610:SER:H	2.13	0.51
1:E:563:LEU:HD11	1:E:625:VAL:HG21	1.94	0.50
1:A:498:ARG:CD	1:A:498:ARG:H	2.24	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:576:LEU:HD22	1:B:580:ILE:HD11	1.93	0.50
1:A:472:PHE:HB2	1:A:526:VAL:HG22	1.92	0.50
1:E:239:ASP:HA	1:E:241:PHE:N	2.27	0.50
1:B:452:LEU:HB3	1:B:453:PRO:CD	2.41	0.50
1:F:586:ALA:HA	1:F:593:GLN:OE1	2.10	0.50
1:B:483:ARG:H	1:B:483:ARG:HD2	1.77	0.50
1:A:204:ARG:HD3	1:A:206:SER:OG	2.12	0.50
1:A:170:LEU:O	1:A:173:LYS:HG2	2.10	0.50
1:F:299:PHE:CE1	1:F:318:GLU:HG3	2.46	0.50
1:F:415:ASN:HD21	1:F:420:ARG:HD2	1.76	0.50
1:F:369:LEU:HB3	1:F:595:ARG:NH2	2.26	0.50
1:F:520:ILE:HG13	1:F:520:ILE:O	2.11	0.50
1:F:453:PRO:O	1:F:457:LEU:HD22	2.11	0.50
1:F:356:THR:HG23	1:F:359:GLN:HE21	1.76	0.50
1:B:385:GLU:HA	1:B:607:PHE:CE2	2.47	0.50
1:E:311:PRO:C	1:E:313:HIS:H	2.15	0.50
1:B:448:LEU:CD2	1:B:470:VAL:HG21	2.41	0.50
1:B:453:PRO:O	1:B:455:ASP:N	2.42	0.50
1:A:311:PRO:C	1:A:313:HIS:H	2.15	0.50
1:E:170:LEU:O	1:E:173:LYS:HG2	2.11	0.50
1:B:156:LEU:O	1:B:202:ARG:HA	2.11	0.50
1:A:266:LYS:HD3	1:A:326:ILE:HD12	1.94	0.50
1:F:137:ASP:HA	1:F:222:ILE:HD13	1.94	0.50
1:B:395:HIS:CE1	1:B:616:LYS:HZ2	2.29	0.50
1:A:563:LEU:HD11	1:A:625:VAL:HG21	1.94	0.50
1:B:453:PRO:O	1:B:457:LEU:HD22	2.11	0.50
1:F:576:LEU:HD22	1:F:580:ILE:HD11	1.94	0.50
1:B:435:LEU:HD23	1:B:547:PHE:HZ	1.77	0.50
1:E:590:GLN:HA	1:E:593:GLN:NE2	2.24	0.50
1:E:356:THR:O	1:E:357:ARG:HB2	2.12	0.50
2:G:22:DA:H2''	2:G:23:DG:C5'	2.42	0.49
1:E:498:ARG:CD	1:E:498:ARG:H	2.25	0.49
1:E:204:ARG:HG2	3:H:8:DG:OP2	2.12	0.49
1:F:448:LEU:CD2	1:F:470:VAL:HG21	2.41	0.49
1:F:452:LEU:HB3	1:F:453:PRO:HD2	1.95	0.49
1:B:586:ALA:HA	1:B:593:GLN:OE1	2.10	0.49
1:A:590:GLN:HA	1:A:593:GLN:NE2	2.25	0.49
1:A:356:THR:O	1:A:357:ARG:HB2	2.13	0.49
3:D:20:DT:H2''	3:D:21:DT:C5'	2.42	0.49
1:F:140:SER:HA	1:F:143:LEU:HG	1.94	0.49
1:E:391:VAL:HG13	1:E:578:MET:HG3	1.93	0.49
1:A:391:VAL:HG13	1:A:578:MET:HG3	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:483:ARG:HD2	1:F:483:ARG:H	1.78	0.49
1:B:143:LEU:HD22	1:B:148:HIS:HE1	1.77	0.49
1:E:477:GLY:HA3	1:E:491:ILE:HD12	1.93	0.49
1:F:408:PHE:CZ	1:F:525:ILE:HD11	2.47	0.49
1:E:253:LYS:O	1:E:259:PRO:HG2	2.13	0.49
1:B:386:GLU:O	1:B:389:ALA:HB3	2.12	0.49
1:A:576:LEU:O	1:A:580:ILE:HG12	2.13	0.49
1:A:252:LEU:HD23	1:A:256:ASP:OD2	2.13	0.49
1:F:401:MET:HG3	1:F:578:MET:HE3	1.95	0.49
1:B:140:SER:HA	1:B:143:LEU:HG	1.95	0.49
1:E:291:MET:O	1:E:294:GLU:HB2	2.13	0.49
1:B:270:TRP:CE2	1:B:336:ILE:HG12	2.48	0.49
1:E:338:GLN:O	1:E:341:VAL:HG12	2.12	0.49
1:A:161:ILE:HG12	1:A:223:CYS:CB	2.43	0.49
1:F:540:ARG:HH11	1:F:540:ARG:HG2	1.77	0.49
1:A:253:LYS:O	1:A:259:PRO:HG2	2.13	0.49
1:F:589:ALA:O	1:F:593:GLN:HG2	2.13	0.49
3:H:20:DT:H2''	3:H:21:DT:C5'	2.43	0.49
1:E:229:GLU:HB3	1:E:256:ASP:OD1	2.13	0.48
3:D:19:DA:H1'	3:D:20:DT:H5''	1.94	0.48
3:D:21:DT:H2''	3:D:22:DC:H5'	1.94	0.48
1:A:338:GLN:O	1:A:341:VAL:HG12	2.12	0.48
1:F:415:ASN:ND2	1:F:420:ARG:HH11	1.97	0.48
1:B:452:LEU:HB3	1:B:453:PRO:HD2	1.96	0.48
1:B:356:THR:HG23	1:B:359:GLN:HE21	1.77	0.48
1:E:266:LYS:HD3	1:E:326:ILE:HD12	1.95	0.48
1:B:352:SER:HA	1:B:360:MET:CE	2.44	0.48
1:B:555:HIS:O	1:B:559:ARG:HG2	2.14	0.48
1:F:143:LEU:HD22	1:F:148:HIS:HE1	1.78	0.48
1:A:477:GLY:HA3	1:A:491:ILE:HD12	1.94	0.48
1:F:470:VAL:HG22	1:F:471:VAL:N	2.28	0.48
1:A:470:VAL:HG23	1:A:522:PRO:HB2	1.95	0.48
1:F:386:GLU:O	1:F:389:ALA:HB3	2.13	0.48
3:H:19:DA:H2''	3:H:20:DT:C5'	2.43	0.48
3:H:19:DA:H1'	3:H:20:DT:H5''	1.94	0.48
1:B:369:LEU:HB3	1:B:595:ARG:NH2	2.28	0.48
1:A:291:MET:O	1:A:294:GLU:HB2	2.14	0.48
1:F:419:LYS:CB	1:F:542:VAL:HG11	2.43	0.48
1:B:137:ASP:HA	1:B:222:ILE:HD13	1.95	0.48
1:F:555:HIS:O	1:F:559:ARG:HG2	2.14	0.48
1:E:594:SER:O	1:E:598:GLU:HG3	2.14	0.48
1:E:252:LEU:HD23	1:E:256:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:14:DG:H1'	3:D:15:DA:C5'	2.41	0.48
1:B:263:GLU:O	1:B:264:GLU:CB	2.62	0.48
2:C:22:DA:H2''	2:C:23:DG:C5'	2.44	0.48
1:A:285:VAL:HG13	1:A:341:VAL:HG11	1.95	0.48
1:B:555:HIS:HB3	1:B:559:ARG:HH12	1.79	0.48
1:F:352:SER:HA	1:F:360:MET:CE	2.44	0.48
1:F:435:LEU:HD23	1:F:547:PHE:HZ	1.79	0.48
1:E:567:ARG:HH11	1:E:567:ARG:HG2	1.76	0.48
1:B:145:PHE:HB3	1:B:228:LYS:HB2	1.96	0.48
1:B:415:ASN:HD21	1:B:420:ARG:HD2	1.77	0.48
1:F:263:GLU:O	1:F:264:GLU:CB	2.62	0.48
3:D:19:DA:H2''	3:D:20:DT:C5'	2.43	0.48
1:B:401:MET:HG3	1:B:578:MET:HE3	1.96	0.48
1:F:395:HIS:CE1	1:F:616:LYS:HZ2	2.31	0.48
1:E:305:CYS:SG	1:E:314:TYR:HA	2.54	0.48
1:A:305:CYS:SG	1:A:314:TYR:HA	2.54	0.48
1:F:270:TRP:CE2	1:F:336:ILE:HG12	2.49	0.48
1:B:470:VAL:HG22	1:B:471:VAL:N	2.29	0.48
1:E:161:ILE:HG12	1:E:223:CYS:CB	2.44	0.48
3:H:21:DT:H2''	3:H:22:DC:H5'	1.95	0.48
1:F:592:ILE:C	1:F:592:ILE:HD12	2.34	0.48
1:B:592:ILE:C	1:B:592:ILE:HD12	2.34	0.48
1:E:213:GLN:NE2	1:E:221:LEU:HD22	2.28	0.47
1:A:529:ASN:ND2	1:A:530:GLU:H	1.97	0.47
1:A:229:GLU:HB3	1:A:256:ASP:OD1	2.14	0.47
1:A:231:LEU:CD1	1:A:231:LEU:H	2.24	0.47
1:F:432:LYS:HG3	1:F:433:THR:H	1.79	0.47
1:B:187:HIS:CD2	1:B:236:LEU:HD13	2.50	0.47
1:A:328:ALA:O	1:B:271:LYS:HB2	2.14	0.47
1:E:134:ASP:OD2	1:E:220:PHE:HB3	2.14	0.47
1:A:134:ASP:OD2	1:A:220:PHE:HB3	2.15	0.47
1:F:145:PHE:HB3	1:F:228:LYS:HB2	1.96	0.47
1:F:393:TRP:NE1	1:F:553:LEU:HG	2.29	0.47
1:B:419:LYS:CB	1:B:542:VAL:HG11	2.44	0.47
1:A:594:SER:O	1:A:598:GLU:HG3	2.15	0.47
1:F:555:HIS:HB3	1:F:559:ARG:HH12	1.80	0.47
1:A:163:THR:HG22	1:A:221:LEU:CA	2.38	0.47
3:D:21:DT:H1'	3:D:22:DC:H5''	1.95	0.47
1:E:285:VAL:HG13	1:E:341:VAL:HG11	1.95	0.47
1:F:409:LEU:O	1:F:413:VAL:HG23	2.15	0.47
1:F:131:LYS:N	1:F:131:LYS:HD2	2.29	0.47
1:B:540:ARG:HG2	1:B:540:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:470:VAL:HG23	1:E:522:PRO:HB2	1.96	0.47
1:B:393:TRP:NE1	1:B:553:LEU:HG	2.29	0.47
1:A:303:LEU:H	1:A:303:LEU:HD12	1.79	0.47
1:E:303:LEU:H	1:E:303:LEU:HD12	1.79	0.47
1:A:213:GLN:NE2	1:A:221:LEU:HD22	2.29	0.47
1:F:448:LEU:HD13	1:F:470:VAL:CG2	2.45	0.47
1:F:476:LYS:O	1:F:491:ILE:HG12	2.14	0.47
2:C:17:DC:H2'	2:C:18:DT:H72	1.97	0.47
1:B:131:LYS:HD2	1:B:131:LYS:N	2.29	0.47
1:A:567:ARG:HG2	1:A:567:ARG:HH11	1.77	0.47
1:B:393:TRP:CZ2	1:B:557:LEU:HD11	2.50	0.47
1:B:476:LYS:O	1:B:491:ILE:HG12	2.15	0.47
3:D:19:DA:H2''	3:D:20:DT:H5'	1.97	0.46
3:H:21:DT:H1'	3:H:22:DC:H5''	1.96	0.46
1:B:408:PHE:CZ	1:B:525:ILE:HD11	2.50	0.46
1:A:149:ALA:HA	2:C:21:DG:H3'	1.97	0.46
1:E:151:PHE:O	2:G:22:DA:H2'	2.16	0.46
1:F:406:TYR:CE2	1:F:410:LYS:HE2	2.50	0.46
1:F:385:GLU:HA	1:F:607:PHE:HE2	1.80	0.46
1:E:133:GLU:HA	1:E:133:GLU:OE1	2.16	0.46
1:E:178:LYS:HD3	1:E:211:TYR:CE1	2.50	0.46
1:B:311:PRO:C	1:B:313:HIS:H	2.18	0.46
1:E:576:LEU:O	1:E:580:ILE:HG12	2.16	0.46
2:G:2:DC:H6	2:G:2:DC:O5'	1.99	0.46
1:B:454:LEU:O	1:B:454:LEU:HD13	2.15	0.46
1:F:393:TRP:CZ2	1:F:557:LEU:HD11	2.51	0.46
1:B:281:LYS:HZ2	1:B:371:ARG:HH22	1.62	0.46
1:A:475:VAL:HG12	1:A:491:ILE:HG13	1.96	0.46
1:A:133:GLU:HA	1:A:133:GLU:OE1	2.16	0.46
1:E:163:THR:HG22	1:E:221:LEU:CA	2.39	0.46
1:F:454:LEU:HD13	1:F:454:LEU:O	2.16	0.46
1:F:454:LEU:O	1:F:455:ASP:HB2	2.15	0.46
1:F:434:THR:HG23	1:F:570:GLN:HB3	1.98	0.46
1:F:311:PRO:C	1:F:313:HIS:H	2.18	0.46
1:F:432:LYS:CG	1:F:433:THR:N	2.79	0.46
1:E:560:SER:OG	1:E:625:VAL:HG23	2.16	0.46
1:B:467:GLN:CA	1:B:467:GLN:HE21	2.29	0.46
3:H:19:DA:H2''	3:H:20:DT:H5'	1.97	0.46
1:E:156:LEU:HD22	1:E:225:GLY:HA3	1.98	0.46
1:E:210:ASN:O	1:E:214:LYS:HG2	2.16	0.46
1:B:432:LYS:HG3	1:B:433:THR:H	1.80	0.46
1:F:281:LYS:HZ2	1:F:371:ARG:HH22	1.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:555:HIS:HB3	1:B:559:ARG:NH1	2.30	0.46
1:F:480:GLY:HA3	1:F:485:LEU:HB2	1.98	0.46
1:B:469:LEU:C	1:B:469:LEU:HD12	2.35	0.46
1:A:210:ASN:O	1:A:214:LYS:HG2	2.16	0.46
1:B:434:THR:HG23	1:B:570:GLN:HB3	1.98	0.46
1:F:626:LEU:HD12	1:F:626:LEU:N	2.30	0.46
1:F:340:ALA:O	1:F:343:THR:HB	2.16	0.46
1:B:385:GLU:HA	1:B:607:PHE:HE2	1.80	0.46
1:B:480:GLY:HA3	1:B:485:LEU:HB2	1.98	0.46
2:C:2:DC:O5'	2:C:2:DC:H6	1.99	0.46
1:B:454:LEU:O	1:B:455:ASP:HB2	2.16	0.46
1:E:149:ALA:HA	2:G:21:DG:H3'	1.97	0.46
1:B:626:LEU:N	1:B:626:LEU:HD12	2.30	0.45
1:E:567:ARG:NH1	1:E:567:ARG:HG2	2.31	0.45
1:F:233:TYR:OH	1:F:251:GLY:HA2	2.16	0.45
1:B:394:LEU:HD21	1:B:569:ILE:O	2.15	0.45
1:B:432:LYS:CG	1:B:433:THR:N	2.79	0.45
1:B:588:PHE:HB3	1:B:592:ILE:HD11	1.97	0.45
1:E:529:ASN:ND2	1:E:530:GLU:H	1.98	0.45
1:A:560:SER:OG	1:A:625:VAL:HG23	2.17	0.45
1:E:475:VAL:HG12	1:E:491:ILE:HG13	1.97	0.45
1:B:233:TYR:OH	1:B:251:GLY:HA2	2.17	0.45
2:G:17:DC:H2'	2:G:18:DT:H72	1.98	0.45
1:E:216:CYS:C	1:E:218:PHE:H	2.19	0.45
1:A:211:TYR:O	1:A:215:LEU:HD23	2.16	0.45
1:F:623:ILE:HG22	1:F:624:GLY:N	2.32	0.45
1:B:415:ASN:ND2	1:B:420:ARG:HH11	2.00	0.45
1:E:182:THR:CG2	1:E:200:PRO:HG3	2.47	0.45
1:F:469:LEU:HD12	1:F:469:LEU:C	2.36	0.45
1:A:151:PHE:O	2:C:22:DA:H2'	2.17	0.45
1:F:467:GLN:HE21	1:F:467:GLN:CA	2.30	0.45
1:B:520:ILE:HG12	5:B:801:HOH:O	2.17	0.45
1:F:555:HIS:HB3	1:F:559:ARG:NH1	2.30	0.45
1:A:216:CYS:C	1:A:218:PHE:H	2.19	0.45
1:A:369:LEU:HD12	1:A:372:MET:SD	2.57	0.45
1:E:328:ALA:O	1:F:271:LYS:HB2	2.16	0.45
1:B:406:TYR:CE2	1:B:410:LYS:HE2	2.51	0.45
1:E:590:GLN:CA	1:E:593:GLN:HE21	2.25	0.45
3:H:24:DA:H1'	3:H:25:DG:H5'	1.99	0.45
1:F:291:MET:HA	1:F:291:MET:HE2	1.98	0.45
2:G:1:DA:C3'	2:G:2:DC:C6	2.99	0.45
1:A:156:LEU:HD22	1:A:225:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:186:ARG:HD2	1:E:193:ASN:OD1	2.17	0.45
2:C:19:DC:H2''	2:C:20:DA:C8	2.52	0.45
1:A:448:LEU:HD23	1:A:448:LEU:N	2.31	0.45
1:A:161:ILE:HG12	1:A:223:CYS:HB2	1.99	0.45
1:E:161:ILE:HG12	1:E:223:CYS:HB2	1.99	0.45
1:F:134:ASP:HA	1:F:135:PRO:HD2	1.81	0.45
1:B:291:MET:HA	1:B:291:MET:HE2	1.98	0.45
1:E:258:ASN:N	1:E:259:PRO:CD	2.77	0.45
1:E:448:LEU:N	1:E:448:LEU:HD23	2.31	0.45
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.82	0.45
2:G:22:DA:C2'	2:G:23:DG:H5''	2.47	0.45
1:F:588:PHE:HB3	1:F:592:ILE:HD11	1.98	0.45
1:A:303:LEU:N	1:A:303:LEU:HD12	2.31	0.45
1:A:155:THR:HG21	3:D:8:DG:H2''	1.99	0.45
3:H:12:DC:H2''	3:H:13:DT:H5'	1.98	0.45
1:A:182:THR:CG2	1:A:200:PRO:HG3	2.47	0.44
1:B:623:ILE:HG22	1:B:624:GLY:N	2.32	0.44
1:A:209:ASN:O	1:A:213:GLN:HG2	2.17	0.44
1:B:448:LEU:HD13	1:B:470:VAL:CG2	2.48	0.44
1:F:453:PRO:HD2	1:F:456:ARG:CB	2.47	0.44
1:E:303:LEU:N	1:E:303:LEU:HD12	2.31	0.44
1:A:567:ARG:NH1	1:A:567:ARG:HG2	2.32	0.44
1:A:178:LYS:HD3	1:A:211:TYR:CE1	2.52	0.44
1:B:409:LEU:O	1:B:413:VAL:HG23	2.17	0.44
3:D:24:DA:H1'	3:D:25:DG:H5'	1.99	0.44
1:A:454:LEU:HD23	1:A:454:LEU:N	2.32	0.44
1:B:590:GLN:CD	1:B:590:GLN:H	2.20	0.44
1:E:160:ALA:HA	1:E:195:LEU:O	2.16	0.44
1:B:388:MET:HE1	1:B:603:LEU:HD11	1.99	0.44
1:A:258:ASN:N	1:A:259:PRO:CD	2.77	0.44
1:F:470:VAL:O	1:F:524:GLY:HA3	2.18	0.44
1:B:372:MET:CG	1:B:573:ILE:HD12	2.48	0.44
1:F:372:MET:CG	1:F:573:ILE:HD12	2.48	0.44
1:E:472:PHE:HD1	1:E:526:VAL:HG22	1.83	0.44
1:B:228:LYS:HB3	1:B:231:LEU:HB2	2.00	0.44
1:E:211:TYR:O	1:E:215:LEU:HD23	2.17	0.44
1:A:186:ARG:HD2	1:A:193:ASN:OD1	2.18	0.44
1:B:470:VAL:O	1:B:524:GLY:HA3	2.18	0.44
1:F:386:GLU:HB3	1:F:562:PHE:CE1	2.52	0.44
3:D:12:DC:H2''	3:D:13:DT:H5'	1.99	0.44
1:B:384:ILE:HG13	1:B:384:ILE:O	2.18	0.44
1:B:453:PRO:HD2	1:B:456:ARG:CB	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:570:GLN:O	1:B:570:GLN:HG2	2.17	0.44
1:E:559:ARG:HB2	1:E:623:ILE:O	2.17	0.44
1:F:623:ILE:HG22	1:F:624:GLY:H	1.81	0.44
1:A:590:GLN:HG2	1:A:591:SER:N	2.33	0.44
1:A:590:GLN:CA	1:A:593:GLN:HE21	2.26	0.44
1:E:231:LEU:CD1	1:E:231:LEU:H	2.25	0.44
1:A:559:ARG:HB2	1:A:623:ILE:O	2.16	0.44
1:E:311:PRO:HD2	5:E:802:HOH:O	2.17	0.44
1:B:161:ILE:HG12	1:B:223:CYS:SG	2.57	0.44
1:A:470:VAL:CG1	1:A:471:VAL:N	2.81	0.44
1:B:386:GLU:HB3	1:B:562:PHE:CE1	2.53	0.44
1:F:394:LEU:HD21	1:F:569:ILE:O	2.16	0.44
1:F:570:GLN:HG2	1:F:570:GLN:O	2.18	0.44
1:F:590:GLN:H	1:F:590:GLN:CD	2.20	0.44
1:B:623:ILE:HG22	1:B:624:GLY:H	1.82	0.44
1:E:369:LEU:HD12	1:E:372:MET:SD	2.58	0.44
1:B:163:THR:O	1:B:192:HIS:HB3	2.18	0.44
1:A:394:LEU:HD13	1:A:575:LEU:CD1	2.48	0.44
1:E:454:LEU:HD23	1:E:454:LEU:N	2.33	0.44
2:G:22:DA:H2''	2:G:23:DG:H5'	1.99	0.44
1:A:388:MET:CE	1:A:603:LEU:HD22	2.48	0.44
1:A:388:MET:HE1	1:A:603:LEU:HD22	2.00	0.44
1:B:340:ALA:O	1:B:343:THR:HB	2.18	0.44
1:F:384:ILE:HG13	1:F:384:ILE:O	2.18	0.44
1:F:423:LEU:HD11	1:F:528:MET:HE3	1.99	0.44
1:E:470:VAL:CG1	1:E:471:VAL:N	2.81	0.43
1:B:204:ARG:O	1:B:205:VAL:C	2.54	0.43
1:F:228:LYS:HB3	1:F:231:LEU:HB2	2.00	0.43
1:B:609:LEU:CD2	1:B:609:LEU:H	2.26	0.43
1:F:609:LEU:CD2	1:F:609:LEU:H	2.26	0.43
1:F:388:MET:HE1	1:F:603:LEU:HD11	2.00	0.43
1:B:393:TRP:CE3	1:B:394:LEU:HD22	2.47	0.43
2:C:22:DA:H2''	2:C:23:DG:H5'	2.00	0.43
1:A:472:PHE:HD1	1:A:526:VAL:HG22	1.83	0.43
1:E:209:ASN:O	1:E:213:GLN:HG2	2.18	0.43
1:E:155:THR:HG21	3:H:8:DG:H2''	2.00	0.43
1:B:134:ASP:HA	1:B:135:PRO:HD2	1.82	0.43
1:E:590:GLN:HG2	1:E:591:SER:N	2.33	0.43
1:A:420:ARG:HB2	1:A:523:PRO:HB3	2.00	0.43
3:H:5:DT:O5'	3:H:5:DT:H2'	2.18	0.43
1:F:160:ALA:HA	1:F:195:LEU:O	2.18	0.43
2:C:1:DA:C3'	2:C:2:DC:C6	3.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:7:DG:H1'	3:D:8:DG:C8	2.53	0.43
1:F:393:TRP:CE3	1:F:394:LEU:HD22	2.47	0.43
2:C:22:DA:C2'	2:C:23:DG:H5''	2.49	0.43
1:F:161:ILE:HG12	1:F:223:CYS:SG	2.59	0.43
1:A:252:LEU:HG	1:A:253:LYS:N	2.34	0.43
1:A:437:ALA:O	1:A:440:LEU:HB3	2.19	0.43
1:E:420:ARG:HB2	1:E:523:PRO:HB3	2.00	0.43
1:E:517:ARG:HG2	1:E:517:ARG:HH11	1.84	0.43
1:A:204:ARG:O	1:A:205:VAL:C	2.57	0.43
1:A:248:LEU:HD23	1:A:249:PRO:HD2	2.00	0.43
1:E:437:ALA:O	1:E:440:LEU:HB3	2.19	0.43
1:A:357:ARG:HE	1:A:415:ASN:HB2	1.84	0.43
1:A:248:LEU:HA	1:A:249:PRO:HD2	1.91	0.43
1:A:160:ALA:HA	1:A:195:LEU:O	2.18	0.43
1:A:363:ASN:O	1:A:366:ASN:HB2	2.19	0.43
1:F:282:CYS:O	1:F:344:VAL:HG21	2.19	0.43
1:E:311:PRO:HA	1:E:314:TYR:CZ	2.54	0.42
1:E:599:TRP:O	1:E:602:ARG:HB3	2.19	0.42
1:E:248:LEU:HA	1:E:249:PRO:HD2	1.91	0.42
1:F:163:THR:O	1:F:192:HIS:HB3	2.19	0.42
3:D:5:DT:O5'	3:D:5:DT:H2'	2.18	0.42
1:E:589:ALA:O	1:E:593:GLN:HG3	2.19	0.42
1:A:311:PRO:HA	1:A:314:TYR:CZ	2.54	0.42
3:H:5:DT:H1'	3:H:6:DC:C6	2.53	0.42
3:D:5:DT:H1'	3:D:6:DC:C6	2.53	0.42
1:F:187:HIS:CD2	1:F:236:LEU:HD13	2.55	0.42
1:E:385:GLU:HA	1:E:607:PHE:HZ	1.84	0.42
1:F:615:MET:C	1:F:617:PHE:H	2.22	0.42
1:E:363:ASN:O	1:E:366:ASN:HB2	2.19	0.42
1:A:599:TRP:O	1:A:602:ARG:HB3	2.20	0.42
1:B:563:LEU:HB3	1:B:569:ILE:HG12	2.01	0.42
1:A:136:LYS:O	1:A:137:ASP:HB2	2.19	0.42
1:B:252:LEU:HG	1:B:257:PHE:HB2	2.01	0.42
1:F:563:LEU:HB3	1:F:569:ILE:HG12	2.02	0.42
1:A:155:THR:HG21	3:D:8:DG:C2'	2.50	0.42
1:F:350:VAL:O	1:F:354:GLN:HG3	2.19	0.42
1:E:394:LEU:HD13	1:E:575:LEU:CD1	2.49	0.42
1:A:469:LEU:O	1:A:469:LEU:HD23	2.20	0.42
1:E:300:GLU:CG	1:E:301:MET:N	2.81	0.42
1:A:300:GLU:CG	1:A:301:MET:N	2.81	0.42
3:H:32:DT:H71	3:H:32:DT:OP2	2.19	0.42
1:E:252:LEU:HG	1:E:253:LYS:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:452:LEU:HD22	1:F:452:LEU:N	2.34	0.42
1:E:155:THR:HB	1:E:202:ARG:HB3	2.02	0.42
3:D:12:DC:H1'	3:D:13:DT:H5''	2.02	0.42
1:B:615:MET:C	1:B:617:PHE:H	2.23	0.42
3:H:7:DG:H1'	3:H:8:DG:C8	2.53	0.42
1:A:155:THR:HB	1:A:202:ARG:HB3	2.02	0.42
2:G:19:DC:H2''	2:G:20:DA:C8	2.55	0.42
1:B:395:HIS:NE2	1:B:582:TYR:CZ	2.88	0.42
1:E:608:SER:C	1:E:610:SER:N	2.73	0.42
1:E:270:TRP:CE2	1:E:336:ILE:HG12	2.55	0.42
1:B:331:LYS:N	1:B:331:LYS:HD2	2.35	0.42
1:F:252:LEU:HG	1:F:257:PHE:HB2	2.02	0.42
1:A:443:CYS:HB2	1:A:468:PHE:HD2	1.84	0.42
1:E:216:CYS:O	1:E:217:THR:HB	2.19	0.42
1:A:216:CYS:O	1:A:217:THR:HB	2.20	0.42
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.83	0.42
1:E:248:LEU:HD23	1:E:249:PRO:HD2	2.01	0.42
1:A:385:GLU:HA	1:A:607:PHE:HZ	1.85	0.42
1:A:388:MET:HB3	1:A:615:MET:HE1	2.01	0.42
3:H:12:DC:H1'	3:H:13:DT:H5''	2.02	0.42
1:E:448:LEU:HD21	1:E:470:VAL:HG13	2.02	0.41
1:A:150:VAL:HG12	2:C:22:DA:OP2	2.19	0.41
1:F:576:LEU:O	1:F:580:ILE:HG13	2.20	0.41
1:F:402:ASP:HA	1:F:578:MET:HE3	2.02	0.41
1:F:395:HIS:NE2	1:F:582:TYR:CZ	2.88	0.41
3:H:7:DG:H2''	3:H:8:DG:OP2	2.20	0.41
1:E:388:MET:CE	1:E:603:LEU:HD22	2.50	0.41
1:E:388:MET:HE1	1:E:603:LEU:HD22	2.02	0.41
1:B:423:LEU:HD11	1:B:528:MET:CE	2.49	0.41
1:E:357:ARG:HE	1:E:415:ASN:HB2	1.85	0.41
1:B:402:ASP:HA	1:B:578:MET:HE3	2.02	0.41
1:E:243:VAL:HG12	1:E:244:ILE:N	2.35	0.41
1:E:443:CYS:HB2	1:E:468:PHE:HD2	1.84	0.41
1:A:608:SER:C	1:A:610:SER:N	2.73	0.41
1:B:534:PRO:C	1:B:536:THR:H	2.23	0.41
1:A:589:ALA:O	1:A:593:GLN:HG3	2.20	0.41
1:B:576:LEU:O	1:B:580:ILE:HG13	2.20	0.41
1:A:270:TRP:CE2	1:A:336:ILE:HG12	2.55	0.41
1:B:452:LEU:N	1:B:452:LEU:HD22	2.36	0.41
1:F:567:ARG:HB3	1:F:570:GLN:NE2	2.35	0.41
2:C:6:DT:H2''	2:C:7:DT:OP2	2.20	0.41
1:A:204:ARG:C	1:A:206:SER:N	2.73	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:282:CYS:O	1:B:344:VAL:HG21	2.20	0.41
1:F:331:LYS:HD2	1:F:331:LYS:N	2.36	0.41
1:B:184:ILE:CG1	1:B:197:PHE:HB3	2.44	0.41
1:E:520:ILE:HA	1:E:520:ILE:HD13	1.90	0.41
1:E:136:LYS:O	1:E:137:ASP:HB2	2.20	0.41
1:E:369:LEU:HA	1:E:369:LEU:HD12	1.85	0.41
1:B:534:PRO:C	1:B:536:THR:N	2.73	0.41
1:B:160:ALA:HA	1:B:195:LEU:O	2.20	0.41
1:A:409:LEU:O	1:A:413:VAL:HG23	2.20	0.41
1:A:150:VAL:HG12	2:C:22:DA:P	2.60	0.41
1:A:283:ASP:HA	1:A:341:VAL:CG2	2.50	0.41
1:A:243:VAL:HG12	1:A:244:ILE:N	2.35	0.41
1:F:285:VAL:HG22	1:F:341:VAL:HG21	2.03	0.41
1:B:371:ARG:NH1	1:B:371:ARG:HB2	2.36	0.41
1:E:477:GLY:CA	1:E:491:ILE:HD12	2.50	0.41
1:E:283:ASP:HA	1:E:341:VAL:CG2	2.50	0.41
1:A:207:ALA:HB2	3:D:7:DG:H3'	2.02	0.41
1:E:375:MET:C	1:E:377:GLY:H	2.23	0.41
1:F:188:ASN:OD1	1:F:244:ILE:HD11	2.19	0.41
1:F:534:PRO:C	1:F:536:THR:H	2.23	0.41
1:A:231:LEU:N	1:A:231:LEU:HD12	2.28	0.41
1:B:448:LEU:HD22	1:B:470:VAL:CG2	2.44	0.41
3:D:1:DC:O4'	3:D:1:DC:O2	2.37	0.41
2:G:6:DT:H2''	2:G:7:DT:OP2	2.21	0.41
1:A:596:ILE:O	1:A:600:LYS:HB2	2.20	0.41
1:E:596:ILE:O	1:E:600:LYS:HB2	2.20	0.41
1:E:331:LYS:HD3	1:F:270:TRP:CE2	2.56	0.41
1:F:462:GLY:HA3	1:F:510:GLU:O	2.21	0.41
1:B:285:VAL:HG22	1:B:341:VAL:HG21	2.03	0.41
1:E:409:LEU:O	1:E:413:VAL:HG23	2.20	0.41
1:B:460:GLU:O	1:B:463:VAL:HG23	2.21	0.41
1:F:176:MET:HA	1:F:181:VAL:HG22	2.03	0.41
1:E:477:GLY:O	1:E:487:SER:HA	2.21	0.41
1:A:475:VAL:HG21	1:A:494:LEU:HD11	2.03	0.41
1:E:385:GLU:HA	1:E:607:PHE:CZ	2.55	0.41
1:B:462:GLY:HA3	1:B:510:GLU:O	2.21	0.41
1:B:188:ASN:OD1	1:B:244:ILE:HD11	2.20	0.41
1:B:584:PRO:HB2	1:B:587:GLU:HB2	2.02	0.41
1:B:567:ARG:HB3	1:B:570:GLN:NE2	2.35	0.40
1:E:475:VAL:HG21	1:E:494:LEU:HD11	2.03	0.40
1:A:215:LEU:N	1:A:215:LEU:HD22	2.36	0.40
3:D:7:DG:H2''	3:D:8:DG:OP2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:534:PRO:C	1:F:536:THR:N	2.74	0.40
1:B:350:VAL:O	1:B:354:GLN:HG3	2.21	0.40
1:F:357:ARG:NH1	1:F:412:MET:O	2.52	0.40
3:H:1:DC:O4'	3:H:1:DC:O2	2.37	0.40
1:B:361:LEU:O	1:B:364:ARG:HB3	2.21	0.40
1:E:472:PHE:CD1	1:E:526:VAL:HG22	2.57	0.40
1:A:274:THR:HA	1:A:340:ALA:HB1	2.04	0.40
1:E:231:LEU:HD12	1:E:231:LEU:N	2.29	0.40
1:A:440:LEU:HD12	1:A:471:VAL:HG23	2.00	0.40
1:B:155:THR:HB	1:B:202:ARG:HB3	2.04	0.40
1:F:311:PRO:CG	1:F:312:SER:H	2.34	0.40
1:B:311:PRO:CG	1:B:312:SER:H	2.34	0.40
1:B:371:ARG:O	1:B:375:MET:HB2	2.21	0.40
1:F:371:ARG:O	1:F:375:MET:HB2	2.21	0.40
1:F:408:PHE:CD2	1:F:439:LEU:HD22	2.56	0.40
1:E:215:LEU:N	1:E:215:LEU:HD22	2.36	0.40
1:F:423:LEU:HD11	1:F:528:MET:CE	2.51	0.40
1:A:385:GLU:HA	1:A:607:PHE:CZ	2.56	0.40
1:F:274:THR:O	1:F:275:GLU:C	2.57	0.40
1:E:553:LEU:HA	1:E:553:LEU:HD12	1.93	0.40
1:F:557:LEU:HD23	1:F:563:LEU:HD12	2.02	0.40
1:F:589:ALA:C	1:F:591:SER:H	2.25	0.40
1:E:305:CYS:O	1:E:308:LYS:HG2	2.22	0.40
1:A:305:CYS:O	1:A:308:LYS:HG2	2.22	0.40
1:F:584:PRO:HB2	1:F:587:GLU:HB2	2.03	0.40
1:A:553:LEU:HA	1:A:553:LEU:HD12	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	495/497 (100%)	423 (86%)	52 (10%)	20 (4%)	5 14
1	B	495/497 (100%)	416 (84%)	68 (14%)	11 (2%)	10 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	495/497 (100%)	421 (85%)	55 (11%)	19 (4%)	5	15
1	F	495/497 (100%)	417 (84%)	67 (14%)	11 (2%)	10	32
All	All	1980/1988 (100%)	1677 (85%)	242 (12%)	61 (3%)	7	21

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	357	ARG
1	A	479	GLY
1	A	480	GLY
1	A	481	GLU
1	B	135	PRO
1	B	263	GLU
1	B	455	ASP
1	E	258	ASN
1	E	357	ARG
1	E	479	GLY
1	E	480	GLY
1	E	481	GLU
1	F	135	PRO
1	F	263	GLU
1	F	455	ASP
1	A	205	VAL
1	A	256	ASP
1	A	356	THR
1	B	247	SER
1	B	625	VAL
1	E	256	ASP
1	E	356	THR
1	E	516	LYS
1	F	247	SER
1	F	625	VAL
1	A	133	GLU
1	A	259	PRO
1	A	262	ALA
1	A	382	ALA
1	A	478	THR
1	A	516	LYS
1	B	444	GLY
1	B	474	ASP

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Mol	Chain	Res	Type
1	E	133	GLU
1	E	259	PRO
1	E	262	ALA
1	E	382	ALA
1	E	478	THR
1	F	444	GLY
1	F	474	ASP
1	A	253	LYS
1	A	260	GLU
1	A	312	SER
1	E	253	LYS
1	E	260	GLU
1	E	312	SER
1	B	259	PRO
1	E	246	GLU
1	F	259	PRO
1	A	132	VAL
1	A	246	GLU
1	A	375	MET
1	B	264	GLU
1	B	300	GLU
1	E	132	VAL
1	E	375	MET
1	F	264	GLU
1	F	300	GLU
1	F	150	VAL
1	B	150	VAL

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	446/446 (100%)	422 (95%)	24 (5%)	31	66
1	B	446/446 (100%)	420 (94%)	26 (6%)	28	63
1	E	446/446 (100%)	423 (95%)	23 (5%)	32	68
1	F	446/446 (100%)	421 (94%)	25 (6%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1784/1784 (100%)	1686 (94%)	98 (6%)	30 65

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ARG
1	A	204	ARG
1	A	206	SER
1	A	248	LEU
1	A	258	ASN
1	A	260	GLU
1	A	301	MET
1	A	415	ASN
1	A	443	CYS
1	A	448	LEU
1	A	452	LEU
1	A	469	LEU
1	A	481	GLU
1	A	498	ARG
1	A	499	ASP
1	A	517	ARG
1	A	529	ASN
1	A	566	LYS
1	A	570	GLN
1	A	575	LEU
1	A	590	GLN
1	A	605	LYS
1	A	615	MET
1	A	627	ASP
1	B	131	LYS
1	B	133	GLU
1	B	145	PHE
1	B	154	ARG
1	B	156	LEU
1	B	204	ARG
1	B	220	PHE
1	B	264	GLU
1	B	286	LEU
1	B	331	LYS
1	B	338	GLN
1	B	349	ARG
1	B	357	ARG

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Mol	Chain	Res	Type
1	B	397	LEU
1	B	454	LEU
1	B	457	LEU
1	B	460	GLU
1	B	483	ARG
1	B	517	ARG
1	B	538	GLN
1	B	546	ASP
1	B	593	GLN
1	B	599	TRP
1	B	608	SER
1	B	609	LEU
1	B	618	ASN
1	E	154	ARG
1	E	206	SER
1	E	248	LEU
1	E	258	ASN
1	E	260	GLU
1	E	301	MET
1	E	415	ASN
1	E	443	CYS
1	E	448	LEU
1	E	452	LEU
1	E	469	LEU
1	E	481	GLU
1	E	498	ARG
1	E	499	ASP
1	E	517	ARG
1	E	529	ASN
1	E	566	LYS
1	E	570	GLN
1	E	575	LEU
1	E	590	GLN
1	E	605	LYS
1	E	615	MET
1	E	627	ASP
1	F	131	LYS
1	F	133	GLU
1	F	145	PHE
1	F	154	ARG
1	F	156	LEU
1	F	220	PHE

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Mol	Chain	Res	Type
1	F	264	GLU
1	F	286	LEU
1	F	318	GLU
1	F	331	LYS
1	F	338	GLN
1	F	349	ARG
1	F	357	ARG
1	F	397	LEU
1	F	454	LEU
1	F	460	GLU
1	F	483	ARG
1	F	517	ARG
1	F	538	GLN
1	F	546	ASP
1	F	593	GLN
1	F	599	TRP
1	F	608	SER
1	F	609	LEU
1	F	618	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	209	ASN
1	A	213	GLN
1	A	415	ASN
1	A	508	ASN
1	A	513	HIS
1	A	519	GLN
1	A	529	ASN
1	A	590	GLN
1	A	593	GLN
1	B	209	ASN
1	B	210	ASN
1	B	213	GLN
1	B	267	GLN
1	B	313	HIS
1	B	359	GLN
1	B	415	ASN
1	B	458	ASN
1	B	467	GLN

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Mol	Chain	Res	Type
1	B	492	ASN
1	B	513	HIS
1	B	538	GLN
1	B	570	GLN
1	E	192	HIS
1	E	213	GLN
1	E	415	ASN
1	E	508	ASN
1	E	513	HIS
1	E	519	GLN
1	E	529	ASN
1	E	590	GLN
1	E	593	GLN
1	F	209	ASN
1	F	210	ASN
1	F	213	GLN
1	F	267	GLN
1	F	313	HIS
1	F	338	GLN
1	F	359	GLN
1	F	415	ASN
1	F	458	ASN
1	F	467	GLN
1	F	492	ASN
1	F	513	HIS
1	F	538	GLN
1	F	570	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	497/497 (100%)	-0.13	6 (1%) 75 76	34, 56, 97, 138	0
1	B	497/497 (100%)	0.02	13 (2%) 53 54	29, 59, 107, 126	0
1	E	497/497 (100%)	-0.08	7 (1%) 72 72	33, 56, 96, 138	0
1	F	497/497 (100%)	0.01	14 (2%) 50 52	29, 59, 107, 126	0
2	C	32/32 (100%)	-0.27	1 (3%) 47 47	29, 55, 160, 182	0
2	G	32/32 (100%)	-0.43	1 (3%) 47 47	30, 55, 160, 182	0
3	D	32/32 (100%)	-0.38	0 100 100	30, 48, 107, 139	0
3	H	32/32 (100%)	-0.47	0 100 100	32, 48, 107, 140	0
All	All	2116/2116 (100%)	-0.07	42 (1%) 62 63	29, 58, 106, 182	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	259	PRO	5.3
1	B	257	PHE	5.2
1	B	263	GLU	4.8
1	B	301	MET	4.4
2	C	1	DA	4.3
1	E	131	LYS	4.1
1	A	256	ASP	3.9
1	F	585	VAL	3.7
1	B	258	ASN	3.7
1	F	258	ASN	3.6
1	A	132	VAL	3.2
1	F	150	VAL	3.1
1	E	256	ASP	3.1
1	A	625	VAL	3.1
1	F	263	GLU	3.0
2	G	1	DA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	585	VAL	2.9
1	E	217	THR	2.9
1	B	132	VAL	2.9
1	F	301	MET	2.8
1	A	259	PRO	2.8
1	F	385	GLU	2.8
1	A	133	GLU	2.8
1	B	150	VAL	2.7
1	E	255	HIS	2.6
1	F	132	VAL	2.5
1	A	131	LYS	2.5
1	F	569	ILE	2.4
1	F	252	LEU	2.4
1	F	627	ASP	2.4
1	F	257	PHE	2.3
1	F	148	HIS	2.2
1	F	603	LEU	2.1
1	B	569	ILE	2.1
1	F	379	THR	2.1
1	B	627	ASP	2.1
1	B	619	VAL	2.1
1	B	133	GLU	2.0
1	B	252	LEU	2.0
1	E	625	VAL	2.0
1	B	255	HIS	2.0
1	E	257	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	A	700	1/1	0.16	-0.67	58,58,58,58	0
4	ZN	F	700	1/1	0.14	-0.68	69,69,69,69	0
4	ZN	E	700	1/1	0.14	-0.81	58,58,58,58	0
4	ZN	B	700	1/1	0.13	-0.84	68,68,68,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.