Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 09:41 PM EST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

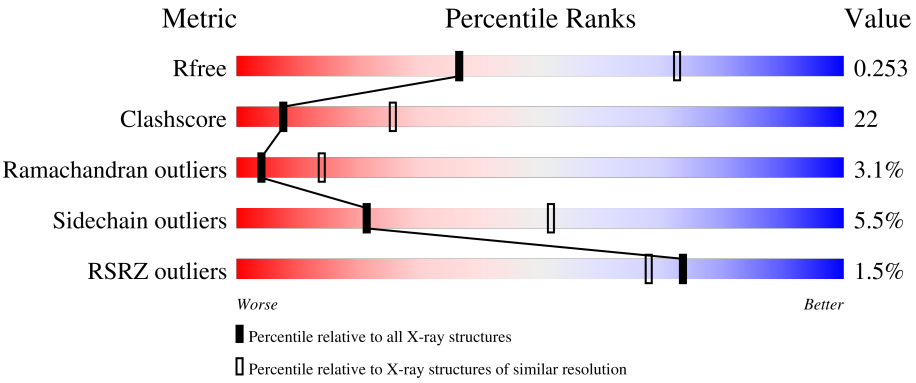
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	58% 37% 5%
1	B	497	60% 36%
1	E	497	58% 37%
1	F	497	59% 38%
2	C	32	3% 34% 53% 12%

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Mol	Chain	Length	Quality of chain
2	G	32	3% 34% 53% 12%
3	D	32	34% 56% 9%
3	H	32	34% 56% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18835 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 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	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

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

- Molecule 5 is water.

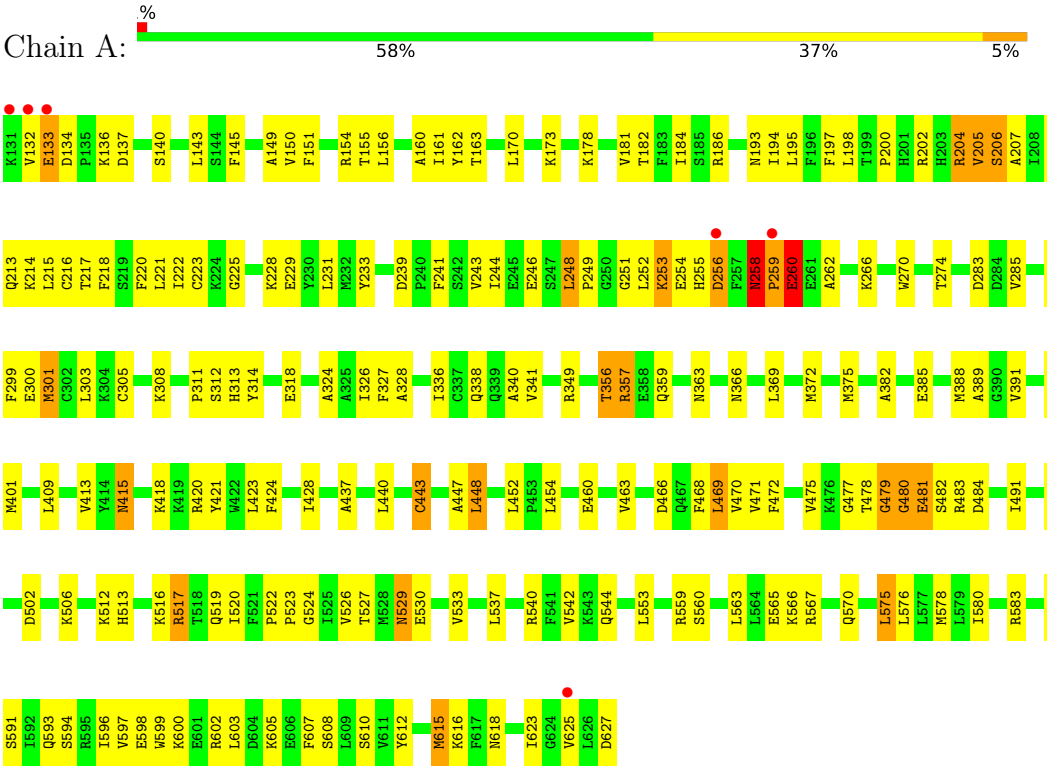
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	12	Total O 12 12	0	0
5	C	9	Total O 9 9	0	0
5	D	6	Total O 6 6	0	0
5	E	14	Total O 14 14	0	0
5	F	7	Total O 7 7	0	0
5	G	6	Total O 6 6	0	0
5	H	7	Total O 7 7	0	0

3 Residue-property plots (i)

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

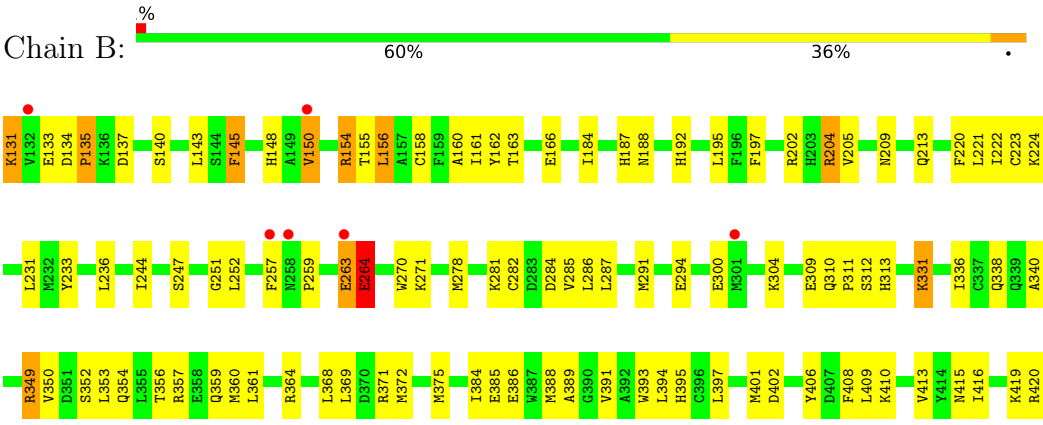
• Molecule 1: Large T antigen

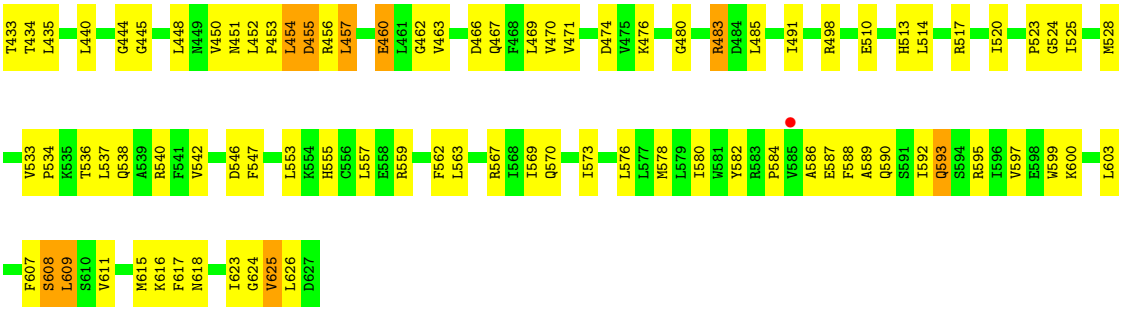
Chain A:



• Molecule 1: Large T antigen

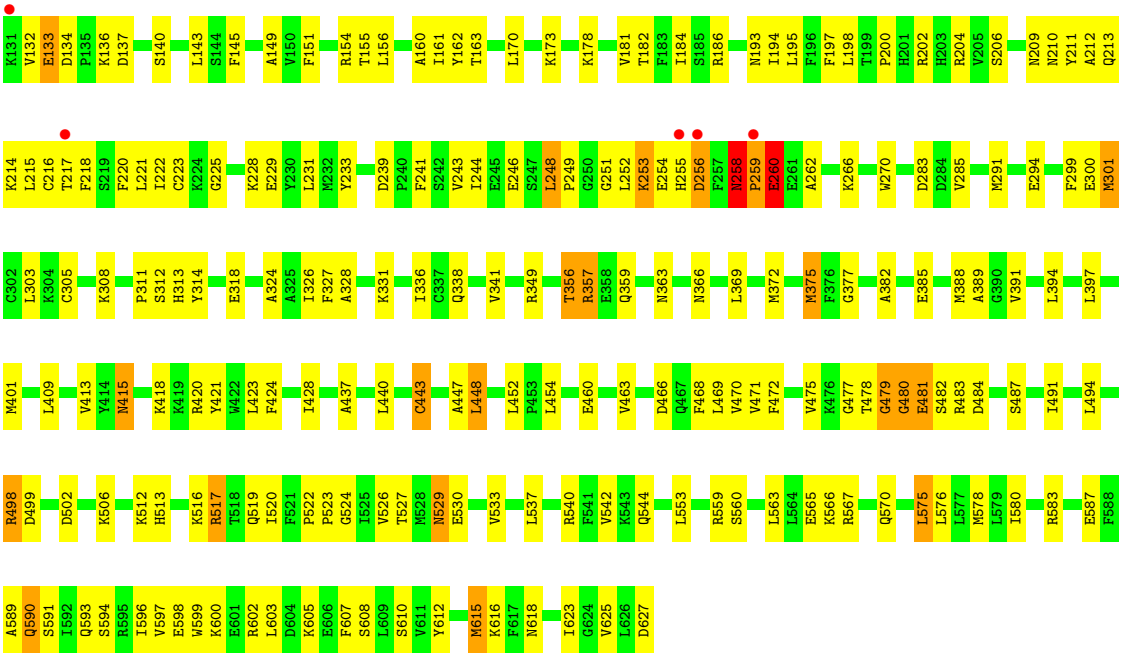
Chain B:





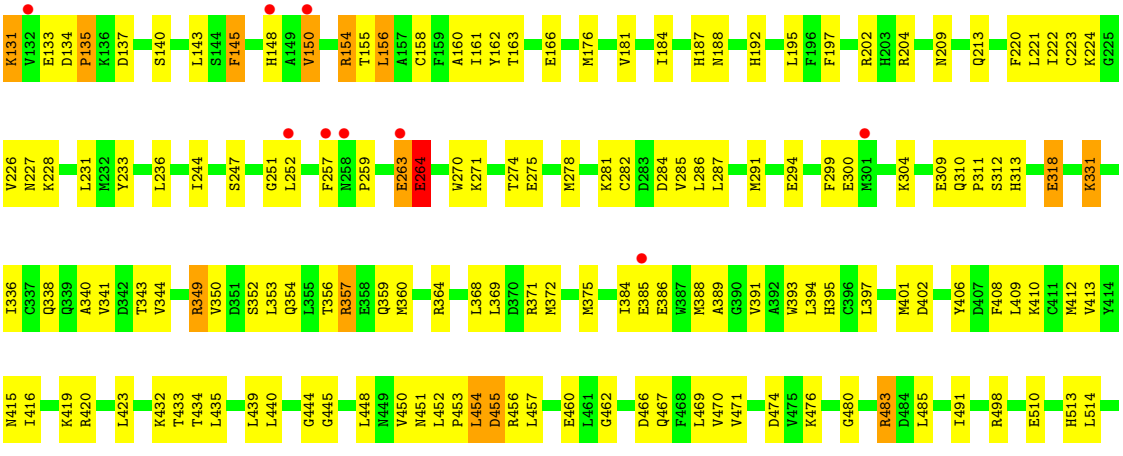
• Molecule 1: Large T antigen

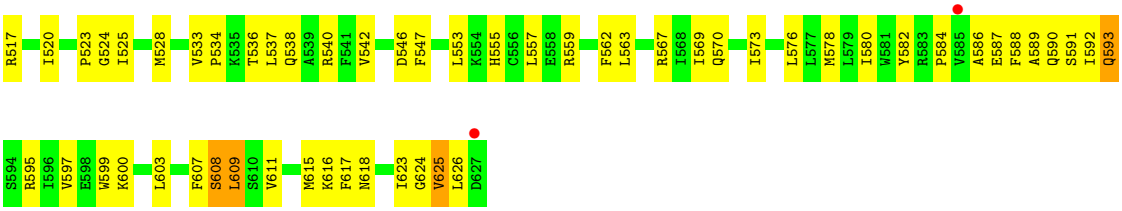
Chain E:



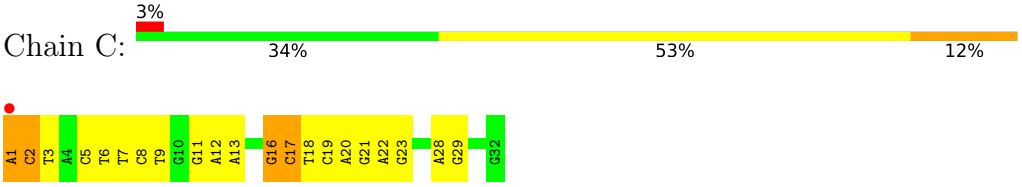
• Molecule 1: Large T antigen

Chain F:

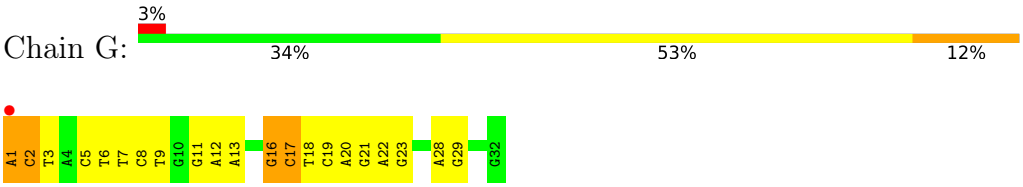




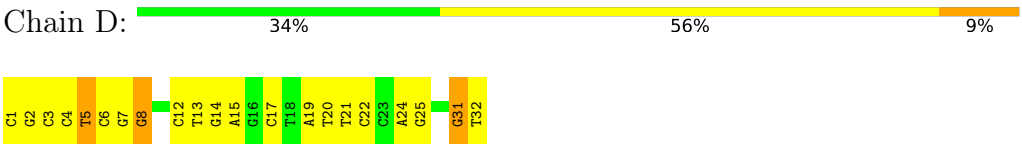
• Molecule 2: DNA (32-MER)



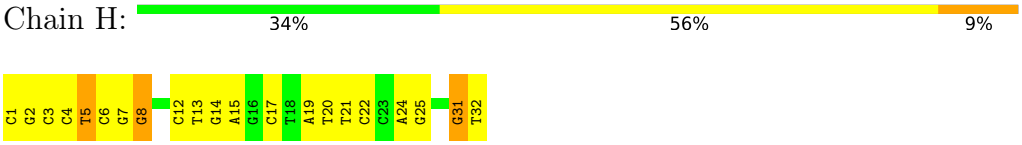
• Molecule 2: DNA (32-MER)



• Molecule 3: DNA (32-MER)



• Molecule 3: DNA (32-MER)



4 Data and refinement statistics (i)

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) 86.5 (48.37-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.255 0.224 , 0.253	Depositor DCC
R_{free} test set	3576 reflections (5.10%)	wwPDB-VP
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 , 26.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.460 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:163:THR:HG22	1:A:221:LEU:HA	1.58	0.86
1:E:258:ASN:HB2	1:E:259:PRO:HD3	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:NE2	1:A:590:GLN:H	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:B:609:LEU:HD23	1:B:609:LEU:H	1.49	0.77
1:E:590:GLN:HA	1:E:593:GLN:HE21	1.49	0.77
1:F:608:SER:OG	1:F:611:VAL:HG23	1.84	0.77
1:F:609:LEU:H	1:F:609:LEU:HD23	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:H	1:A:231:LEU:HD12	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
1:A:184:ILE:HG13	1:A:197:PHE:HB3	1.69	0.74
2:G:1:DA:H2"	2:G:2:DC:C6	2.22	0.74
2:G:1:DA:C3'	2:G:2:DC:C5	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:1:DA:C3'	2:C:2:DC:C5	2.71	0.73
1:E:424:PHE:HB2	1:E:527:THR:HG22	1.71	0.73
1:A:440:LEU:HD12	1:A:471:VAL:CG2	2.19	0.72
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: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:A:466:ASP:H	1:A:519:GLN:HE22	1.39	0.71
1:E:466:ASP:H	1:E:519:GLN:HE22	1.38	0.71
1:E:513:HIS:HE1	1:F:513:HIS:CD2	2.09	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: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:B:450:VAL:HG12	1:B:457:LEU:HD12	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:310:GLN:HG2	1:F:311:PRO:HD2	1.75	0.68
1:F:415:ASN:HD21	1:F:420:ARG:NH1	1.90	0.68
1:B:310:GLN:HG2	1:B:311:PRO:HD2	1.75	0.67
1:A:415:ASN:ND2	1:A:420:ARG:HD2	2.09	0.67
1:B:356:THR:OG1	1:B:359:GLN:HG3	1.94	0.67
2:G:12:DA:H1'	2:G:13:DA:H5'	1.77	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:155:THR:HG21	2:G:16:DG:C2'	2.24	0.66
1:F:498:ARG:CD	1:F:540:ARG:HH21	1.98	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:364:ARG:O	1:B:368:LEU:HD23	1.95	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: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
1:F:432:LYS:HG3	1:F:433:THR:N	2.13	0.64
2:G:1:DA:H3'	2:G:2:DC:C5	2.33	0.64
1:F:419:LYS:HA	1:F:542:VAL:HG13	1.81	0.63
1:B:263:GLU:O	1:B:264:GLU:HB2	1.99	0.63
1:B:420:ARG:HB3	1:B:523:PRO:HB3	1.80	0.63
1:F:263:GLU:O	1:F:264:GLU:HB2	1.99	0.63
1:B:457:LEU:H	1:B:457:LEU:HD23	1.64	0.63
1:A:506:LYS:HA	1:A:520:ILE:HD13	1.81	0.63
1:E:258:ASN:CB	1:E:259:PRO:HD3	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ASN:HD21	1:E:420:ARG:HD2	1.63	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:H	1:F:166:GLU:CD	2.01	0.63
1:B:432:LYS:HG3	1:B:433:THR:N	2.14	0.63
1:F:457:LEU:HD23	1:F:457:LEU:H	1.64	0.63
1:B:166:GLU:CD	1:B:166:GLU:H	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:A:415:ASN:HD21	1:A:420:ARG:HD2	1.64	0.62
1:A:593:GLN:O	1:A:597:VAL:HG23	1.99	0.62
1:B:368:LEU:O	1:B:372:MET:HG3	2.00	0.62
1:E:254:GLU:O	1:E:260:GLU:HG2	2.00	0.62
1:B:150:VAL:CG1	1:B:224:LYS:HD3	2.30	0.62
1:B:294:GLU:OE2	1:B:304:LYS:NZ	2.31	0.62
3:D:14:DG:H2"	3:D:15:DA:H5'	1.82	0.62
1:E:428:ILE:H	1:E:428:ILE:CD1	2.09	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: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:F:498:ARG:HB2	1:F:540:ARG:HE	1.64	0.61
1:B:626:LEU:HD12	1:B:626:LEU:H	1.64	0.61
1:E:513:HIS:CE1	1:F:513:HIS:CD2	2.86	0.61
1:A:590:GLN:HA	1:A:593:GLN:HG3	1.82	0.61
1:A:181:VAL:HA	1:A:200:PRO:HD3	1.83	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:B:158:CYS:SG	1:B:226:VAL:HB	2.40	0.60
1:E:593:GLN:O	1:E:597:VAL:HG23	2.00	0.60
1:F:626:LEU:HD12	1:F:626:LEU:H	1.64	0.60
1:B:434:THR:HG21	1:B:569:ILE:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:GLU:OE2	1:F:304:LYS:NZ	2.32	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
1:F:483:ARG:HD2	1:F:483:ARG:N	2.15	0.60
2:C:8:DC:H2"	2:C:9:DT:OP2	2.01	0.60
1:B:483:ARG:HD2	1:B:483:ARG:N	2.15	0.60
2:G:8:DC:H2"	2:G:9:DT:OP2	2.01	0.60
1:E:182:THR:HG23	1:E:200:PRO:HG3	1.84	0.60
1:E:590:GLN:HA	1:E:593:GLN:HG3	1.83	0.60
1:A:498:ARG:H	1:A:498:ARG:HD3	1.65	0.60
1:A:512:LYS:HD2	1:B:514:LEU:O	2.02	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:618:ASN:HA	1:A:623:ILE:HD12	1.83	0.60
1:B:284:ASP:HB3	1:B:287:LEU:HB3	1.84	0.59
1:E:349:ARG:HD3	1:E:517:ARG:NH2	2.17	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
3:H:14:DG:H2"	3:H:15:DA:H5'	1.84	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:H	1:E:498:ARG:HD3	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:A:583:ARG:HB3	1:A:587:GLU:OE1	2.03	0.58
1:E:137:ASP:HA	1:E:222:ILE:HD13	1.84	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
1:A:483:ARG:O	1:A:484:ASP:HB2	2.03	0.58
1:B:353:LEU:HD23	1:B:353:LEU:O	2.03	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
3:D:20:DT:H1'	3:D:21:DT:H5"	1.85	0.58
1:F:372:MET:HG2	1:F:573:ILE:HD12	1.86	0.58
1:A:349:ARG:HD3	1:A:517:ARG:NH2	2.19	0.58
1:F:356:THR:H	1:F:359:GLN:NE2	2.01	0.58
1:A:482:SER:O	1:A:483:ARG:HD2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:583:ARG:HB3	1:E:587:GLU:OE1	2.04	0.57
1:F:204:ARG:HD3	2:G:16:DG:N7	2.19	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
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:O	1:F:353:LEU:HD23	2.04	0.57
1:B:467:GLN:HA	1:B:467:GLN:NE2	2.20	0.57
1:F:590:GLN:HA	1:F:593:GLN:HG3	1.87	0.57
1:B:401:MET:HG3	1:B:578:MET:CE	2.34	0.57
1:F:467:GLN:NE2	1:F:467:GLN:HA	2.20	0.57
1:A:529:ASN:HD22	1:A:530:GLU:N	1.95	0.56
1:A:612:TYR:HA	1:A:615:MET:HG3	1.86	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:590:GLN:NE2	1:A:590:GLN:N	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
1:A:428:ILE:H	1:A:428:ILE:CD1	2.09	0.56
1:E:612:TYR:HA	1:E:615:MET:HG3	1.87	0.56
1:F:155:THR:HG21	2:G:16:DG:H2'	1.87	0.56
2:G:1:DA:H3'	2:G:2:DC:H5	1.69	0.56
1:A:213:GLN:HE21	1:A:221:LEU:HD22	1.71	0.56
1:A:418:LYS:HG2	1:A:502:ASP:OD1	2.06	0.56
1:F:209:ASN:O	1:F:213:GLN:HG2	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:B:209:ASN:O	1:B:213:GLN:HG2	2.06	0.55
1:E:423:LEU:HD23	1:E:544:GLN:CG	2.32	0.55
1:A:482:SER:C	1:A:483:ARG:HD2	2.27	0.55
1:A:513:HIS:CE1	1:B:513:HIS:CD2	2.87	0.55
3:H:20:DT:H2"	3:H:21:DT:H5'	1.87	0.55
1:E:421:TYR:O	1:E:542:VAL:HG12	2.06	0.55
1:E:590:GLN:NE2	1:E:590:GLN:N	2.51	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:590:GLN:HA	1:F:593:GLN:CG	2.37	0.55
1:A:423:LEU:HD23	1:A:544:GLN:CG	2.32	0.55
3:D:20:DT:H2"	3:D:21:DT:H5'	1.87	0.55
1:E:460:GLU:O	1:E:463:VAL:HG22	2.07	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
1:B:162:TYR:HB3	1:B:222:ILE:HB	1.89	0.55
1:B:281:LYS:NZ	1:B:371:ARG:HH22	2.05	0.54
1:B:440:LEU:HD11	1:B:445:GLY:C	2.27	0.54
1:E:529:ASN:HD22	1:E:530:GLU:N	1.96	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:162:TYR:HB3	1:F:222:ILE:HB	1.90	0.54
1:F:419:LYS:HA	1:F:542:VAL:CG1	2.37	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:281:LYS:NZ	1:F:371:ARG:HH22	2.06	0.53
1:F:419:LYS:HB3	1:F:542:VAL:HG11	1.89	0.53
1:F:434:THR:CG2	1:F:569:ILE:HG22	2.38	0.53
1:B:391:VAL:HG13	1:B:578:MET:HB2	1.90	0.53
1:B:434:THR:CG2	1:B:569:ILE:HG22	2.38	0.53
1:F:448:LEU:HD13	1:F:470:VAL:HG23	1.88	0.53
1:A:233:TYR:OH	1:A:251:GLY:HA2	2.08	0.53
1:A:470:VAL:O	1:A:524:GLY:HA3	2.09	0.53
1:E:580:ILE:CD1	1:E:596:ILE:HD12	2.39	0.53
1:A:324:ALA:O	1:A:327:PHE:HB3	2.08	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:B:395:HIS:NE2	1:B:582:TYR:CE2	2.77	0.53
1:B:457:LEU:H	1:B:457:LEU:CD2	2.22	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:A:540:ARG:HG2	1:A:540:ARG:HH11	1.75	0.52
1:F:154:ARG:HG3	1:F:155:THR:N	2.23	0.52
1:A:356:THR:HB	1:A:359:GLN:HG3	1.90	0.52
1:A:533:VAL:HG13	1:A:537:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:GLN:HA	1:F:467:GLN:HE21	1.75	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:HA	1:B:467:GLN:HE21	1.75	0.52
2:C:28:DA:H2"	2:C:29:DG:OP2	2.10	0.52
1:A:156:LEU:N	1:A:156:LEU:HD12	2.24	0.52
1:E:397:LEU:HB3	1:E:401:MET:CE	2.40	0.52
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:156:LEU:N	1:E:156:LEU:HD12	2.24	0.52
1:E:428:ILE:HD12	1:E:428:ILE:N	2.15	0.52
1:F:156:LEU:O	1:F:202:ARG:HA	2.09	0.52
1:A:145:PHE:HB3	1:A:228:LYS:HB2	1.92	0.51
1:B:419:LYS:HB3	1:B:542:VAL:HG11	1.92	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:F:440:LEU:HD11	1:F:445:GLY:C	2.30	0.51
2:G:1:DA:C3'	2:G:2:DC:H5	2.20	0.51
2:G:28:DA:H2"	2:G:29:DG:OP2	2.10	0.51
1:E:145:PHE:HB3	1:E: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: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:389:ALA:HB1	1:A:625:VAL:CG1	2.41	0.51
1:A:428:ILE:HD12	1:A:428:ILE:N	2.16	0.51
1:B:448:LEU:HD13	1:B:470:VAL:HG23	1.90	0.51
1:B:520:ILE:HG13	1:B:520:ILE:O	2.10	0.51
1:F:368:LEU:HD12	1:F:573:ILE:HD13	1.93	0.51
1:A:299:PHE:CZ	1:A:318:GLU:HB2	2.45	0.51
1:A:239:ASP:HA	1:A:241:PHE:N	2.26	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:397:LEU:HB3	1:A:401:MET:CE	2.41	0.51
1:B:278:MET:SD	1:B:343:THR:HG22	2.51	0.51
1:E:472:PHE:HB2	1:E:526:VAL:HG22	1.92	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:440:LEU:HD12	1:E:471:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:ALA:C	1:E:448:LEU:HD23	2.30	0.51
1:E:540:ARG:HG2	1:E:540:ARG:HH11	1.76	0.51
1:F:457:LEU:H	1:F:457:LEU:CD2	2.23	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:E:608:SER:C	1:E:610:SER:H	2.13	0.51
1:F:385:GLU:HA	1:F:607:PHE:CE2	2.46	0.51
1:F:453:PRO:O	1:F:455:ASP:N	2.42	0.51
1:A:472:PHE:HB2	1:A:526:VAL:HG22	1.92	0.50
1:A:498:ARG:H	1:A:498:ARG:CD	2.24	0.50
1:B:576:LEU:HD22	1:B:580:ILE:HD11	1.93	0.50
1:E:239:ASP:HA	1:E:241:PHE:N	2.27	0.50
1:E:563:LEU:HD11	1:E:625:VAL:HG21	1.94	0.50
1:A:170:LEU:O	1:A:173:LYS:HG2	2.10	0.50
1:A:204:ARG:HD3	1:A:206:SER:OG	2.12	0.50
1:B:452:LEU:HB3	1:B:453:PRO:CD	2.41	0.50
1:B:483:ARG:HD2	1:B:483:ARG:H	1.77	0.50
1:F:299:PHE:CE1	1:F:318:GLU:HG3	2.46	0.50
1:F:586:ALA:HA	1:F:593:GLN:OE1	2.10	0.50
1:F:369:LEU:HB3	1:F:595:ARG:NH2	2.26	0.50
1:F:415:ASN:HD21	1:F:420:ARG:HD2	1.76	0.50
1:F:520:ILE:O	1:F:520:ILE:HG13	2.11	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:F:356:THR:HG23	1:F:359:GLN:HE21	1.76	0.50
1:F:453:PRO:O	1:F:457:LEU:HD22	2.11	0.50
1:A:311:PRO:C	1:A: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:E:170:LEU:O	1:E:173:LYS:HG2	2.11	0.50
1:A:266:LYS:HD3	1:A:326:ILE:HD12	1.94	0.50
1:B:156:LEU:O	1:B:202:ARG:HA	2.11	0.50
1:B:395:HIS:CE1	1:B:616:LYS:HZ2	2.29	0.50
1:F:137:ASP:HA	1:F:222:ILE:HD13	1.94	0.50
1:A:563:LEU:HD11	1:A:625:VAL:HG21	1.94	0.50
1:B:435:LEU:HD23	1:B:547:PHE:HZ	1.77	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:E:356:THR:O	1:E:357:ARG:HB2	2.12	0.50
1:E:590:GLN:HA	1:E:593:GLN:NE2	2.24	0.50
2:G:22:DA:H2"	2:G:23:DG:C5'	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ARG:HG2	3:H:8:DG:OP2	2.12	0.49
1:E:498:ARG:H	1:E:498:ARG:CD	2.25	0.49
1:B:586:ALA:HA	1:B:593:GLN:OE1	2.10	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:A:356:THR:O	1:A:357:ARG:HB2	2.13	0.49
1:A:391:VAL:HG13	1:A:578:MET:HG3	1.94	0.49
1:A:590:GLN:HA	1:A:593:GLN:NE2	2.25	0.49
3:D:20:DT:H2"	3:D:21:DT:C5'	2.42	0.49
1:E:391:VAL:HG13	1:E:578:MET:HG3	1.93	0.49
1:F:140:SER:HA	1:F:143:LEU:HG	1.94	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:F:483:ARG:HD2	1:F:483:ARG:H	1.78	0.49
1:A:576:LEU:O	1:A:580:ILE:HG12	2.13	0.49
1:B:386:GLU:O	1:B:389:ALA:HB3	2.12	0.49
1:E:253:LYS:O	1:E:259:PRO:HG2	2.13	0.49
1:A:161:ILE:HG12	1:A:223:CYS:CB	2.43	0.49
1:A:252:LEU:HD23	1:A:256:ASP:OD2	2.13	0.49
1:B:140:SER:HA	1:B:143:LEU:HG	1.95	0.49
1:B:270:TRP:CE2	1:B:336:ILE:HG12	2.48	0.49
1:E:291:MET:O	1:E:294:GLU:HB2	2.13	0.49
1:E:338:GLN:O	1:E:341:VAL:HG12	2.12	0.49
1:F:401:MET:HG3	1:F:578:MET:HE3	1.95	0.49
1:F:540:ARG:HG2	1:F:540:ARG:HH11	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:A:338:GLN:O	1:A:341:VAL:HG12	2.12	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:E:229:GLU:HB3	1:E:256:ASP:OD1	2.13	0.48
1:B:356:THR:HG23	1:B:359:GLN:HE21	1.77	0.48
1:B:452:LEU:HB3	1:B:453:PRO:HD2	1.96	0.48
1:F:415:ASN:ND2	1:F:420:ARG:HH11	1.97	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:E:266:LYS:HD3	1:E:326:ILE:HD12	1.95	0.48
1:A:477:GLY:HA3	1:A:491:ILE:HD12	1.94	0.48
1:F:143:LEU:HD22	1:F:148:HIS:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:MET:O	1:A:294:GLU:HB2	2.14	0.48
1:A:470:VAL:HG23	1:A:522:PRO:HB2	1.95	0.48
1:B:369:LEU:HB3	1:B:595:ARG:NH2	2.28	0.48
1:F:386:GLU:O	1:F:389:ALA:HB3	2.13	0.48
1:F:470:VAL:HG22	1:F:471:VAL:N	2.28	0.48
3:H:19:DA:H1'	3:H:20:DT:H5"	1.94	0.48
3:H:19:DA:H2"	3:H:20:DT:C5'	2.43	0.48
1:B:137:ASP:HA	1:B:222:ILE:HD13	1.95	0.48
1:E:594:SER:O	1:E:598:GLU:HG3	2.14	0.48
1:F:419:LYS:CB	1:F:542:VAL:HG11	2.43	0.48
1:F:555:HIS:O	1:F:559:ARG:HG2	2.14	0.48
1:A:285:VAL:HG13	1:A:341:VAL:HG11	1.95	0.48
1:B:145:PHE:HB3	1:B:228:LYS:HB2	1.96	0.48
1:B:263:GLU:O	1:B:264:GLU:CB	2.62	0.48
1:B:555:HIS:HB3	1:B:559:ARG:HH12	1.79	0.48
2:C:22:DA:H2"	2:C:23:DG:C5'	2.44	0.48
3:D:14:DG:H1'	3:D:15:DA:C5'	2.41	0.48
1:E:252:LEU:HD23	1:E:256:ASP:OD2	2.14	0.48
1:E:567:ARG:HH11	1:E:567:ARG:HG2	1.76	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:A:305:CYS:SG	1:A:314:TYR:HA	2.54	0.48
1:B:401:MET:HG3	1:B:578:MET:HE3	1.96	0.48
1:B:415:ASN:HD21	1:B:420:ARG:HD2	1.77	0.48
3:D:19:DA:H2"	3:D:20:DT:C5'	2.43	0.48
1:E:305:CYS:SG	1:E:314:TYR:HA	2.54	0.48
1:F:263:GLU:O	1:F:264:GLU:CB	2.62	0.48
1:F:270:TRP:CE2	1:F:336:ILE:HG12	2.49	0.48
1:F:395:HIS:CE1	1:F:616:LYS:HZ2	2.31	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
1:B:592:ILE:C	1:B:592:ILE:HD12	2.34	0.48
1:F:592:ILE:C	1:F:592:ILE:HD12	2.34	0.48
3:H:21:DT:H2"	3:H:22:DC:H5'	1.95	0.48
1:E:213:GLN:NE2	1:E:221:LEU:HD22	2.28	0.47
1:A:134:ASP:OD2	1:A:220:PHE:HB3	2.15	0.47
1:A:229:GLU:HB3	1:A:256:ASP:OD1	2.14	0.47
1:A:231:LEU:H	1:A:231:LEU:CD1	2.24	0.47
1:A:328:ALA:O	1:B:271:LYS:HB2	2.14	0.47
1:A:529:ASN:ND2	1:A:530:GLU:H	1.97	0.47
1:B:187:HIS:CD2	1:B:236:LEU:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:ASP:OD2	1:E:220:PHE:HB3	2.14	0.47
1:F:432:LYS:HG3	1:F:433:THR:H	1.79	0.47
1:F:145:PHE:HB3	1:F:228:LYS:HB2	1.96	0.47
1:A:594:SER:O	1:A:598:GLU:HG3	2.15	0.47
1:B:419:LYS:CB	1:B:542:VAL:HG11	2.44	0.47
1:F:393:TRP:NE1	1:F:553:LEU:HG	2.29	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:131:LYS:N	1:F:131:LYS:HD2	2.29	0.47
1:F:409:LEU:O	1:F:413:VAL:HG23	2.15	0.47
1:A:303:LEU:HD12	1:A:303:LEU:H	1.79	0.47
1:B:393:TRP:NE1	1:B:553:LEU:HG	2.29	0.47
1:B:540:ARG:HH11	1:B:540:ARG:HG2	1.78	0.47
1:E:303:LEU:H	1:E:303:LEU:HD12	1.79	0.47
1:E:470:VAL:HG23	1:E:522:PRO:HB2	1.96	0.47
1:A:213:GLN:NE2	1:A:221:LEU:HD22	2.29	0.47
1:A:567:ARG:HG2	1:A:567:ARG:HH11	1.77	0.47
1:B:131:LYS:HD2	1:B:131:LYS:N	2.29	0.47
2:C:17:DC:H2'	2:C:18:DT:H72	1.97	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
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
1:A:149:ALA:HA	2:C:21:DG:H3'	1.97	0.46
1:B:408:PHE:CZ	1:B:525:ILE:HD11	2.50	0.46
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: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: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:F:385:GLU:HA	1:F:607:PHE:HE2	1.80	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
1:A:133:GLU:OE1	1:A:133:GLU:HA	2.16	0.46
1:A:475:VAL:HG12	1:A:491:ILE:HG13	1.96	0.46
1:B:281:LYS:HZ2	1:B:371:ARG:HH22	1.62	0.46
1:B:454:LEU:HD13	1:B:454:LEU:O	2.15	0.46
1:F:393:TRP:CZ2	1:F:557:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2:DC:O5'	2:G:2:DC:H6	1.99	0.46
1:B:467:GLN:HE21	1:B:467:GLN:CA	2.29	0.46
1:E:156:LEU:HD22	1:E:225:GLY:HA3	1.98	0.46
1:E:163:THR:HG22	1:E:221:LEU:CA	2.39	0.46
1:E:210:ASN:O	1:E:214:LYS:HG2	2.16	0.46
1:E:560:SER:OG	1:E:625:VAL:HG23	2.16	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:F:434:THR:HG23	1:F:570:GLN:HB3	1.98	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
3:H:19:DA:H2"	3:H:20:DT:H5'	1.97	0.46
1:A:210:ASN:O	1:A:214:LYS:HG2	2.16	0.46
1:B:432:LYS:HG3	1:B:433:THR:H	1.80	0.46
1:B:469:LEU:C	1:B:469:LEU:HD12	2.35	0.46
1:B:555:HIS:HB3	1:B:559:ARG:NH1	2.30	0.46
1:F:281:LYS:HZ2	1:F:371:ARG:HH22	1.62	0.46
1:F:480:GLY:HA3	1:F:485:LEU:HB2	1.98	0.46
1:B:385:GLU:HA	1:B:607:PHE:HE2	1.80	0.46
1:B:434:THR:HG23	1:B:570:GLN:HB3	1.98	0.46
1:B:480:GLY:HA3	1:B:485:LEU:HB2	1.98	0.46
1:F:340:ALA:O	1:F:343:THR:HB	2.16	0.46
1:F:626:LEU:HD12	1:F:626:LEU:N	2.30	0.46
1:B:454:LEU:O	1:B:455:ASP:HB2	2.16	0.46
2:C:2:DC:H6	2:C:2:DC:O5'	1.99	0.46
1:E:149:ALA:HA	2:G:21:DG:H3'	1.97	0.46
1:B:626:LEU:HD12	1:B:626:LEU:N	2.30	0.45
1:E:567:ARG:HG2	1:E:567:ARG:NH1	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:A:211:TYR:O	1:A:215:LEU:HD23	2.16	0.45
1:A:560:SER:OG	1:A:625:VAL:HG23	2.17	0.45
1:B:233:TYR:OH	1:B:251:GLY:HA2	2.17	0.45
1:E:216:CYS:C	1:E:218:PHE:H	2.19	0.45
1:E:475:VAL:HG12	1:E:491:ILE:HG13	1.97	0.45
1:E:529:ASN:ND2	1:E:530:GLU:H	1.98	0.45
1:F:623:ILE:HG22	1:F:624:GLY:N	2.32	0.45
2:G:17:DC:H2'	2:G:18:DT:H72	1.98	0.45
1:B:415:ASN:ND2	1:B:420:ARG:HH11	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:406:TYR:CE2	1:B:410:LYS:HE2	2.51	0.45
1:B:520:ILE:HG12	5:B:801:HOH:O	2.17	0.45
1:E:328:ALA:O	1:F:271:LYS:HB2	2.16	0.45
1:F:467:GLN:HE21	1:F:467:GLN:CA	2.30	0.45
1:F:555:HIS:HB3	1:F:559:ARG:NH1	2.30	0.45
1:E:590:GLN:CA	1:E:593:GLN:HE21	2.25	0.45
1:F:291:MET:HA	1:F:291:MET:HE2	1.98	0.45
3:H:24:DA:H1'	3:H:25:DG:H5'	1.99	0.45
1:A:156:LEU:HD22	1:A:225:GLY:HA3	1.99	0.45
2:C:19:DC:H2"	2:C:20:DA:C8	2.52	0.45
1:E:186:ARG:HD2	1:E:193:ASN:OD1	2.17	0.45
2:G:1:DA:C3'	2:G:2:DC:C6	2.99	0.45
1:A:161:ILE:HG12	1:A:223:CYS:HB2	1.99	0.45
1:A:448:LEU:HD23	1:A:448:LEU:N	2.31	0.45
1:B:291:MET:HE2	1:B:291:MET:HA	1.98	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:A:155:THR:HG21	3:D:8:DG:H2"	1.99	0.45
1:A:303:LEU:HD12	1:A:303:LEU:N	2.31	0.45
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.82	0.45
1:E:258:ASN:N	1:E:259:PRO:CD	2.77	0.45
1:E:448:LEU:HD23	1:E:448:LEU:N	2.31	0.45
1:F:588:PHE:HB3	1:F:592:ILE:HD11	1.98	0.45
2:G:22:DA:C2'	2:G:23:DG:H5"	2.47	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:178:LYS:HD3	1:A:211:TYR:CE1	2.52	0.44
1:A:209:ASN:O	1:A:213:GLN:HG2	2.17	0.44
1:A:454:LEU:HD23	1:A:454:LEU:N	2.32	0.44
1:A:567:ARG:HG2	1:A:567:ARG:NH1	2.32	0.44
1:B:409:LEU:O	1:B:413:VAL:HG23	2.17	0.44
1:B:448:LEU:HD13	1:B:470:VAL:CG2	2.48	0.44
3:D:24:DA:H1'	3:D:25:DG:H5'	1.99	0.44
1:E:303:LEU:HD12	1:E:303:LEU:N	2.31	0.44
1:F:453:PRO:HD2	1:F:456:ARG:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:MET:HE1	1:B:603:LEU:HD11	1.99	0.44
1:B:590:GLN:H	1:B:590:GLN:CD	2.20	0.44
1:E:160:ALA:HA	1:E:195:LEU:O	2.16	0.44
1:A:186:ARG:HD2	1:A:193:ASN:OD1	2.18	0.44
1:A:258:ASN:N	1:A:259:PRO:CD	2.77	0.44
1:B:228:LYS:HB3	1:B:231:LEU:HB2	2.00	0.44
1:B:372:MET:CG	1:B:573:ILE:HD12	2.48	0.44
1:E:211:TYR:O	1:E:215:LEU:HD23	2.17	0.44
1:E:472:PHE:HD1	1:E:526:VAL:HG22	1.83	0.44
1:F:372:MET:CG	1:F:573:ILE:HD12	2.48	0.44
1:F:470:VAL:O	1:F:524:GLY:HA3	2.18	0.44
1:B:384:ILE:HG13	1:B:384:ILE:O	2.18	0.44
1:B:470:VAL:O	1:B:524:GLY:HA3	2.18	0.44
3:D:12:DC:H2"	3:D:13:DT:H5'	1.99	0.44
1:F:386:GLU:HB3	1:F:562:PHE:CE1	2.52	0.44
1:B:453:PRO:HD2	1:B:456:ARG:CB	2.48	0.44
1:B:570:GLN:HG2	1:B:570:GLN:O	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:559:ARG:HB2	1:A:623:ILE:O	2.16	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:B:161:ILE:HG12	1:B:223:CYS:SG	2.57	0.44
1:E:231:LEU:H	1:E:231:LEU:CD1	2.25	0.44
1:E:311:PRO:HD2	5:E:802:HOH:O	2.17	0.44
1:A:394:LEU:HD13	1:A:575:LEU:CD1	2.48	0.44
1:A:470:VAL:CG1	1:A:471:VAL:N	2.81	0.44
1:B:163:THR:O	1:B:192:HIS:HB3	2.18	0.44
1:B:386:GLU:HB3	1:B:562:PHE:CE1	2.53	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:E:454:LEU:N	1:E:454:LEU:HD23	2.33	0.44
1:F:394:LEU:HD21	1:F:569:ILE:O	2.16	0.44
1:F:570:GLN:O	1:F:570:GLN:HG2	2.18	0.44
1:F:590:GLN:CD	1:F:590:GLN:H	2.20	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
2:G:22:DA:H2"	2:G:23:DG:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:O	1:B:205:VAL:C	2.54	0.43
1:E:470:VAL:CG1	1:E:471:VAL:N	2.81	0.43
1:F:228:LYS:HB3	1:F:231:LEU:HB2	2.00	0.43
1:B:609:LEU:H	1:B:609:LEU:CD2	2.26	0.43
1:F:388:MET:HE1	1:F:603:LEU:HD11	2.00	0.43
1:F:609:LEU:H	1:F:609:LEU:CD2	2.26	0.43
1:A:472:PHE:HD1	1:A:526:VAL:HG22	1.83	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:E:155:THR:HG21	3:H:8:DG:H2"	2.00	0.43
1:E:209:ASN:O	1:E:213:GLN:HG2	2.18	0.43
1:B:134:ASP:HA	1:B:135:PRO:HD2	1.82	0.43
1:A:420:ARG:HB2	1:A:523:PRO:HB3	2.00	0.43
1:E:590:GLN:HG2	1:E:591:SER:N	2.33	0.43
1:F:160:ALA:HA	1:F:195:LEU:O	2.18	0.43
3:H:5:DT:H2'	3:H:5:DT:O5'	2.18	0.43
2:C:1:DA:C3'	2:C:2:DC:C6	3.01	0.43
3:D:7:DG:H1'	3:D:8:DG:C8	2.53	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:F:393:TRP:CE3	1:F:394:LEU:HD22	2.47	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: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:HH11	1:E:517:ARG:HG2	1.84	0.43
1:A:160:ALA:HA	1:A:195:LEU:O	2.18	0.43
1:A:248:LEU:HA	1:A:249:PRO:HD2	1.91	0.43
1:A:357:ARG:HE	1:A:415:ASN:HB2	1.84	0.43
1:A:363:ASN:O	1:A:366:ASN:HB2	2.19	0.43
1:E:437:ALA:O	1:E:440:LEU:HB3	2.19	0.43
1:F:282:CYS:O	1:F:344:VAL:HG21	2.19	0.43
3:D:5:DT:H2'	3:D:5:DT:O5'	2.18	0.42
1:E:248:LEU:HA	1:E:249:PRO:HD2	1.91	0.42
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:F:163:THR:O	1:F:192:HIS:HB3	2.19	0.42
1:A:311:PRO:HA	1:A:314:TYR:CZ	2.54	0.42
1:A:599:TRP:O	1:A:602:ARG:HB3	2.20	0.42
3:D:5:DT:H1'	3:D:6:DC:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:ASN:O	1:E:366:ASN:HB2	2.19	0.42
1:E:385:GLU:HA	1:E:607:PHE:HZ	1.84	0.42
1:E:589:ALA:O	1:E:593:GLN:HG3	2.19	0.42
1:F:187:HIS:CD2	1:F:236:LEU:HD13	2.55	0.42
1:F:615:MET:C	1:F:617:PHE:H	2.22	0.42
3:H:5:DT:H1'	3:H:6:DC:C6	2.53	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:B:563:LEU:HB3	1:B:569:ILE:HG12	2.01	0.42
1:A:155:THR:HG21	3:D:8:DG:C2'	2.50	0.42
1:A:469:LEU:HD23	1:A:469:LEU:O	2.20	0.42
1:E:394:LEU:HD13	1:E:575:LEU:CD1	2.49	0.42
1:F:350:VAL:O	1:F:354:GLN:HG3	2.19	0.42
1:F:563:LEU:HB3	1:F:569:ILE:HG12	2.02	0.42
1:A:300:GLU:CG	1:A:301:MET:N	2.81	0.42
1:B:615:MET:C	1:B:617:PHE:H	2.23	0.42
3:D:12:DC:H1'	3:D:13:DT:H5"	2.02	0.42
1:E:155:THR:HB	1:E:202:ARG:HB3	2.02	0.42
1:E:252:LEU:HG	1:E:253:LYS:N	2.34	0.42
1:E:300:GLU:CG	1:E:301:MET:N	2.81	0.42
1:F:452:LEU:HD22	1:F:452:LEU:N	2.34	0.42
3:H:32:DT:H71	3:H:32:DT:OP2	2.19	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
3:H:7:DG:H1'	3:H:8:DG:C8	2.53	0.42
1:B:331:LYS:HD2	1:B:331:LYS:N	2.35	0.42
1:B:395:HIS:NE2	1:B:582:TYR:CZ	2.88	0.42
1:E:270:TRP:CE2	1:E:336:ILE:HG12	2.55	0.42
1:E:608:SER:C	1:E:610:SER:N	2.73	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:A:216:CYS:O	1:A:217:THR:HB	2.20	0.42
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.83	0.42
1:A:385:GLU:HA	1:A:607:PHE:HZ	1.85	0.42
1:E:216:CYS:O	1:E:217:THR:HB	2.19	0.42
1:E:248:LEU:HD23	1:E:249:PRO:HD2	2.01	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:A:150:VAL:HG12	2:C:22:DA:OP2	2.19	0.41
1:B:423:LEU:HD11	1:B:528:MET:CE	2.49	0.41
1:E:388:MET:HE1	1:E:603:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:MET:CE	1:E:603:LEU:HD22	2.50	0.41
1:E:448:LEU:HD21	1:E:470:VAL:HG13	2.02	0.41
1:F:395:HIS:NE2	1:F:582:TYR:CZ	2.88	0.41
1:F:402:ASP:HA	1:F:578:MET:HE3	2.02	0.41
1:F:576:LEU:O	1:F:580:ILE:HG13	2.20	0.41
3:H:7:DG:H2"	3:H:8:DG:OP2	2.20	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:357:ARG:HE	1:E:415:ASN:HB2	1.85	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:270:TRP:CE2	1:A:336:ILE:HG12	2.55	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:204:ARG:C	1:A:206:SER:N	2.73	0.41
1:B:282:CYS:O	1:B:344:VAL:HG21	2.20	0.41
1:B:452:LEU:HD22	1:B:452:LEU:N	2.36	0.41
2:C:6:DT:H2"	2:C:7:DT:OP2	2.20	0.41
1:F:331:LYS:HD2	1:F:331:LYS:N	2.36	0.41
1:F:567:ARG:HB3	1:F:570:GLN:NE2	2.35	0.41
1:A:409:LEU:O	1:A:413:VAL:HG23	2.20	0.41
1:B:160:ALA:HA	1:B:195:LEU:O	2.20	0.41
1:B:184:ILE:CG1	1:B:197:PHE:HB3	2.44	0.41
1:B:534:PRO:C	1:B:536:THR:N	2.73	0.41
1:E:136:LYS:O	1:E:137:ASP:HB2	2.20	0.41
1:E:369:LEU:HD12	1:E:369:LEU:HA	1.85	0.41
1:E:520:ILE:HD13	1:E:520:ILE:HA	1.90	0.41
1:A:150:VAL:HG12	2:C:22:DA:P	2.60	0.41
1:A:243:VAL:HG12	1:A:244:ILE:N	2.35	0.41
1:A:283:ASP:HA	1:A:341:VAL:CG2	2.50	0.41
1:F:285:VAL:HG22	1:F:341:VAL:HG21	2.03	0.41
1:A:207:ALA:HB2	3:D:7:DG:H3'	2.02	0.41
1:B:371:ARG:NH1	1:B:371:ARG:HB2	2.36	0.41
1:E:283:ASP:HA	1:E:341:VAL:CG2	2.50	0.41
1:E:375:MET:C	1:E:377:GLY:H	2.23	0.41
1:E:477:GLY:CA	1:E:491:ILE:HD12	2.50	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:HD12	1:A:231:LEU:N	2.28	0.41
1:A:596:ILE:O	1:A:600:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:VAL:HG22	1:B:341:VAL:HG21	2.03	0.41
1:B:448:LEU:HD22	1:B:470:VAL:CG2	2.44	0.41
1:B:460:GLU:O	1:B:463:VAL:HG23	2.21	0.41
3:D:1:DC:O2	3:D:1:DC:O4'	2.37	0.41
1:E:331:LYS:HD3	1:F:270:TRP:CE2	2.56	0.41
1:E:409:LEU:O	1:E:413:VAL:HG23	2.20	0.41
1:E:596:ILE:O	1:E:600:LYS:HB2	2.20	0.41
1:F:176:MET:HA	1:F:181:VAL:HG22	2.03	0.41
1:F:462:GLY:HA3	1:F:510:GLU:O	2.21	0.41
2:G:6:DT:H2"	2:G:7:DT:OP2	2.21	0.41
1:A:475:VAL:HG21	1:A:494:LEU:HD11	2.03	0.41
1:B:188:ASN:OD1	1:B:244:ILE:HD11	2.20	0.41
1:B:462:GLY:HA3	1:B:510:GLU:O	2.21	0.41
1:B:584:PRO:HB2	1:B:587:GLU:HB2	2.02	0.41
1:E:385:GLU:HA	1:E:607:PHE:CZ	2.55	0.41
1:E:477:GLY:O	1:E:487:SER:HA	2.21	0.41
1:A:215:LEU:HD22	1:A:215:LEU:N	2.36	0.40
1:B:350:VAL:O	1:B:354:GLN:HG3	2.21	0.40
1:B:567:ARG:HB3	1:B:570:GLN:NE2	2.35	0.40
3:D:7:DG:H2"	3:D:8:DG:OP2	2.21	0.40
1:E:475:VAL:HG21	1:E:494:LEU:HD11	2.03	0.40
1:F:357:ARG:NH1	1:F:412:MET:O	2.52	0.40
1:F:534:PRO:C	1:F:536:THR:N	2.74	0.40
1:A:274:THR:HA	1:A:340:ALA:HB1	2.04	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
3:H:1:DC:O2	3:H:1:DC:O4'	2.37	0.40
1:A:440:LEU:HD12	1:A:471:VAL:HG23	2.00	0.40
1:E:231:LEU:HD12	1:E:231:LEU:N	2.29	0.40
1:A:385:GLU:HA	1:A:607:PHE:CZ	2.56	0.40
1:B:155:THR:HB	1:B:202:ARG:HB3	2.04	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:E:215:LEU:HD22	1:E:215:LEU:N	2.36	0.40
1:E:553:LEU:HD12	1:E:553:LEU:HA	1.93	0.40
1:F:274:THR:O	1:F:275:GLU:C	2.57	0.40
1:F:311:PRO:CG	1:F:312:SER:H	2.34	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:F:423:LEU:HD11	1:F:528:MET:CE	2.51	0.40
1:A:305:CYS:O	1:A:308:LYS:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:LEU:HD12	1:A:553:LEU:HA	1.93	0.40
1:E:305:CYS:O	1:E:308:LYS:HG2	2.22	0.40
1:F:557:LEU:HD23	1:F:563:LEU:HD12	2.02	0.40
1:F:584:PRO:HB2	1:F:587:GLU:HB2	2.03	0.40
1:F:589:ALA:C	1:F:591:SER:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	495/497 (100%)	423 (86%)	52 (10%)	20 (4%)	3 9
1	B	495/497 (100%)	416 (84%)	68 (14%)	11 (2%)	6 22
1	E	495/497 (100%)	421 (85%)	55 (11%)	19 (4%)	3 10
1	F	495/497 (100%)	417 (84%)	67 (14%)	11 (2%)	6 22
All	All	1980/1988 (100%)	1677 (85%)	242 (12%)	61 (3%)	4 14

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	446/446 (100%)	422 (95%)	24 (5%)	22 53
1	B	446/446 (100%)	420 (94%)	26 (6%)	20 50
1	E	446/446 (100%)	423 (95%)	23 (5%)	23 55
1	F	446/446 (100%)	421 (94%)	25 (6%)	21 51
All	All	1784/1784 (100%)	1686 (94%)	98 (6%)	21 52

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	F	609	LEU
1	F	618	ASN

Sometimes 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
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

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Mol	Chain	Res	Type
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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	497/497 (100%)	-0.19	6 (1%) 79 73	34, 56, 97, 138	0
1	B	497/497 (100%)	-0.06	7 (1%) 75 70	29, 59, 107, 126	0
1	E	497/497 (100%)	-0.15	5 (1%) 82 77	33, 56, 96, 138	0
1	F	497/497 (100%)	-0.07	11 (2%) 62 52	29, 59, 107, 126	0
2	C	32/32 (100%)	-0.30	1 (3%) 49 39	29, 55, 160, 182	0
2	G	32/32 (100%)	-0.46	1 (3%) 49 39	30, 55, 160, 182	0
3	D	32/32 (100%)	-0.41	0 100 100	30, 48, 107, 139	0
3	H	32/32 (100%)	-0.51	0 100 100	32, 48, 107, 140	0
All	All	2116/2116 (100%)	-0.13	31 (1%) 73 68	29, 58, 106, 182	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	259	PRO	4.9
1	B	257	PHE	4.7
1	B	263	GLU	4.4
2	C	1	DA	4.2
1	B	301	MET	3.9
1	E	131	LYS	3.7
1	A	256	ASP	3.6
1	B	258	ASN	3.4
1	F	258	ASN	3.3
1	F	585	VAL	3.2
2	G	1	DA	2.9
1	E	256	ASP	2.8
1	A	132	VAL	2.8
1	F	263	GLU	2.7
1	F	150	VAL	2.7
1	A	625	VAL	2.7

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	F	700	1/1	0.94	0.14	69,69,69,69	0
4	ZN	B	700	1/1	0.95	0.13	68,68,68,68	0
4	ZN	E	700	1/1	0.97	0.14	58,58,58,58	0
4	ZN	A	700	1/1	0.99	0.16	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.