



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 9, 2017 – 08:19 AM EST

PDB ID : 5OGC
EMDB ID: : EMD-3803
Title : Molecular basis of human kinesin-8 function and inhibition
Authors : Locke, J.; Joseph, A.P.; Topf, M.; Moores, C.A.
Deposited on : unknown
Resolution : 4.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

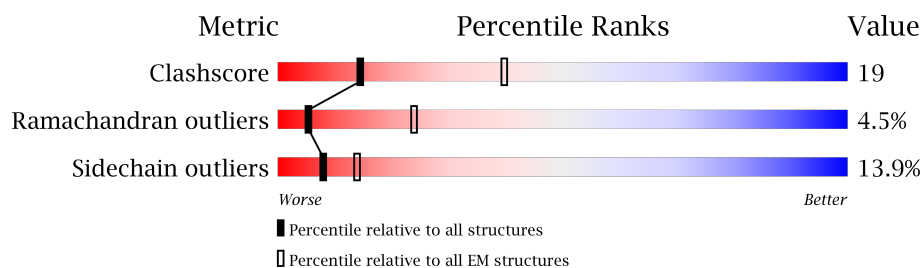
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1-K	377	41% 34% 10% • 13%
1	2-K	377	55% 28% • 13%
2	1-A	451	50% 32% 7% • 9%
2	2-A	451	49% 33% 8% • 9%
3	1-B	445	52% 34% 9% • •
3	2-B	445	52% 34% 9% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GTP	1-A	503	-	-	X	-
7	GTP	2-A	503	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18580 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Kinesin-like protein KIF18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-K	328	Total	C	N	O	S	0	0
			2569	1605	463	489	12		
1	2-K	328	Total	C	N	O	S	0	0
			2569	1605	463	489	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP Q8NI77
K	-1	SER	-	expression tag	UNP Q8NI77
K	0	HIS	-	expression tag	UNP Q8NI77

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		
2	2-A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	LEU	conflict	UNP F2Z4C1
A	265	GLY	ILE	conflict	UNP F2Z4C1
A	358	GLU	GLN	conflict	UNP F2Z4C1

- Molecule 3 is a protein called Tubulin beta chain.

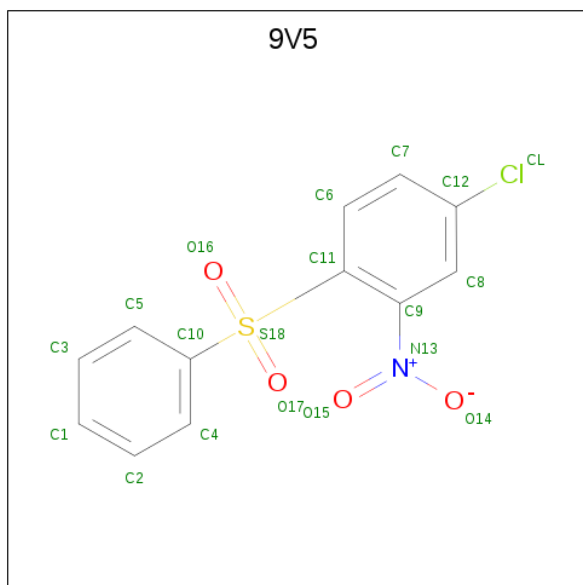
Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2-B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

- Molecule 4 is 4-chloranyl-2-nitro-1-(phenylsulfonyl)benzene (three-letter code: 9V5) (formula: C₁₂H₈ClNO₄S).



Mol	Chain	Residues	Atoms					AltConf	
4	1-K	1	Total	C	Cl	N	O	S	0
			19	12	1	1	4	1	
4	2-K	1	Total	C	Cl	N	O	S	0
			19	12	1	1	4	1	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	2-A	1	Total	Zn	0
			1	1	
5	1-A	1	Total	Zn	0
			1	1	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

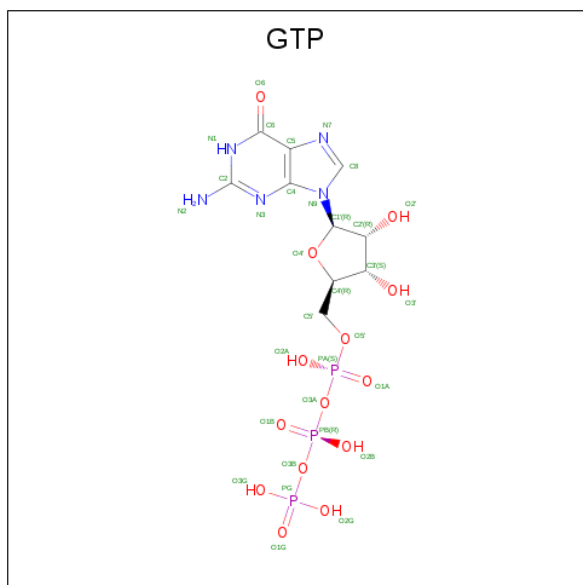
Mol	Chain	Residues	Atoms		AltConf
6	2-A	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

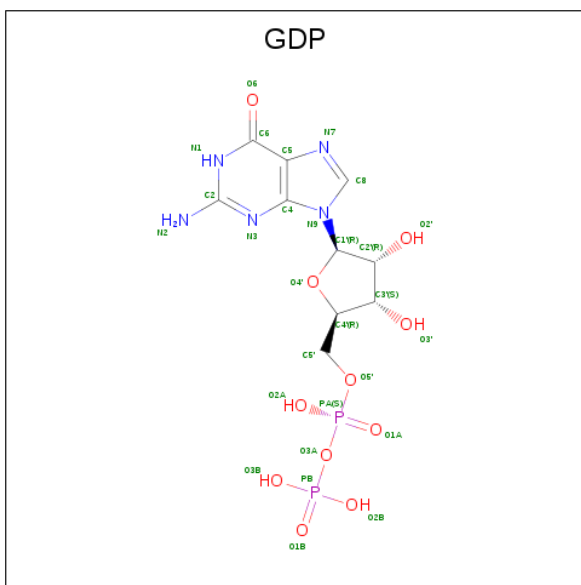
Mol	Chain	Residues	Atoms		AltConf
6	1-A	1	Total	Mg	0
			1	1	

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



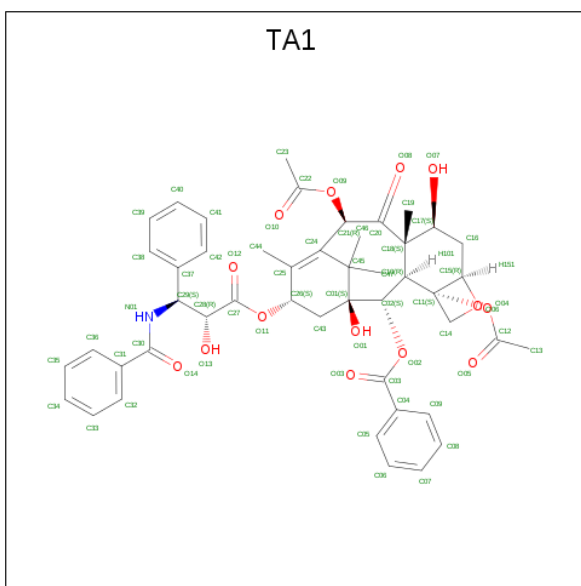
Mol	Chain	Residues	Atoms					AltConf
7	1-A	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	2-A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
8	1-B	1	Total 28	C 10	N 5	O 11	P 2	0
8	2-B	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 9 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).

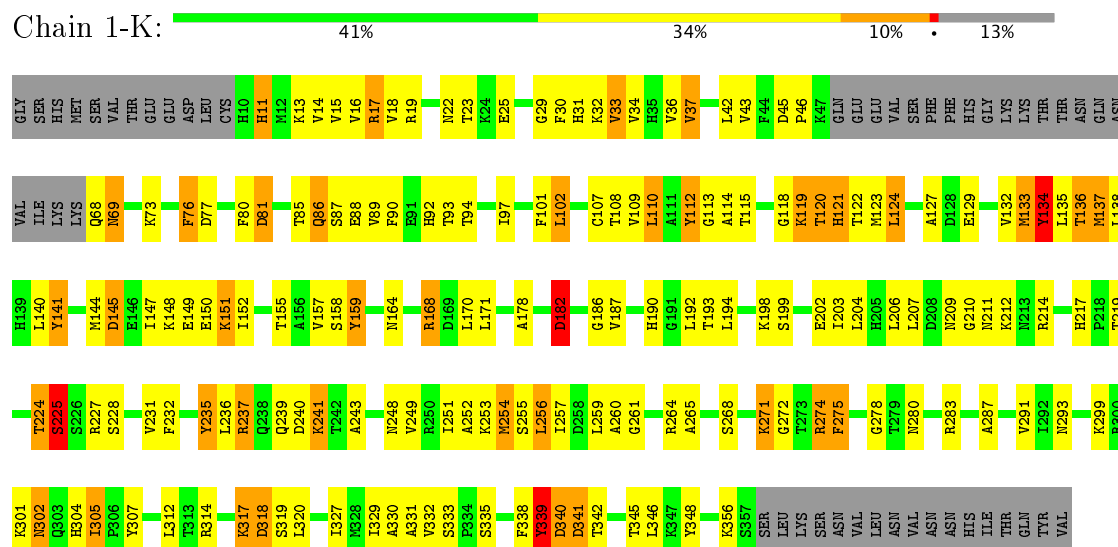


Mol	Chain	Residues	Atoms				AltConf
9	1-B	1	Total 62	C 47	N 1	O 14	0
9	2-B	1	Total 62	C 47	N 1	O 14	0

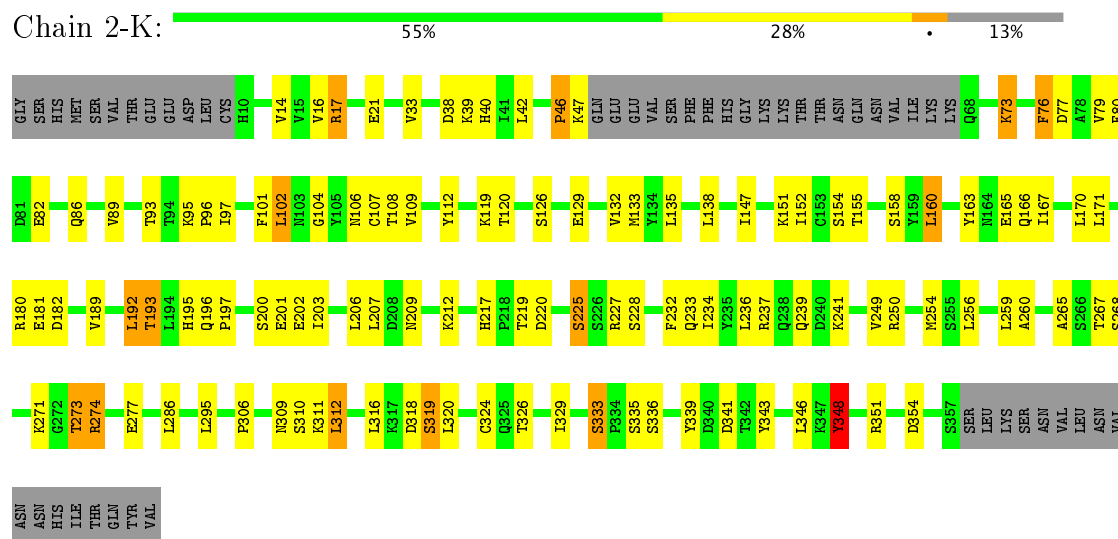
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Kinesin-like protein KIF18A

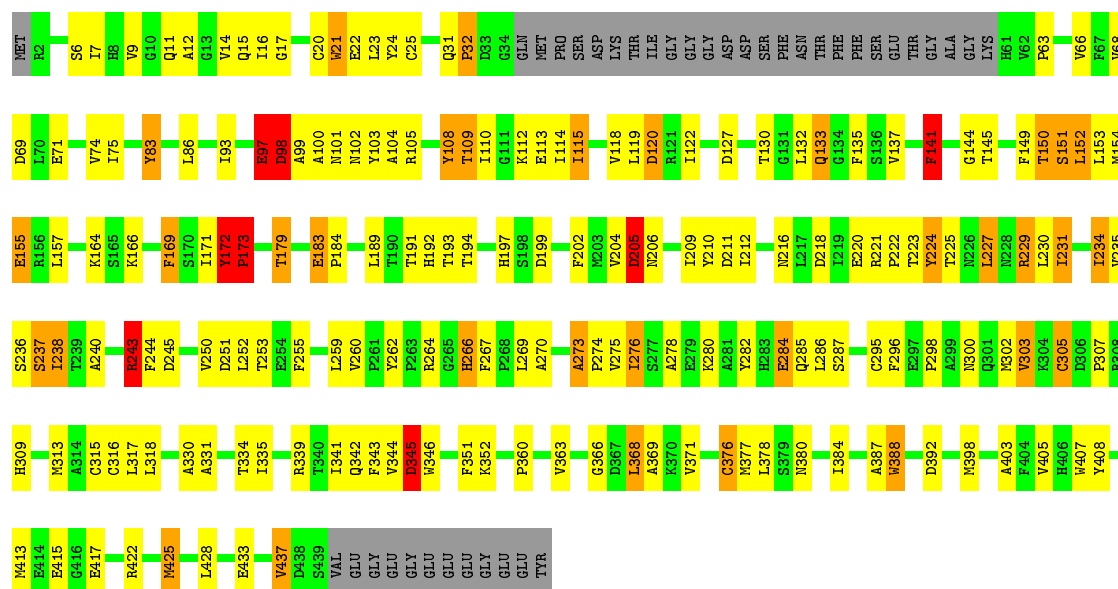


• Molecule 1: Kinesin-like protein KIF18A



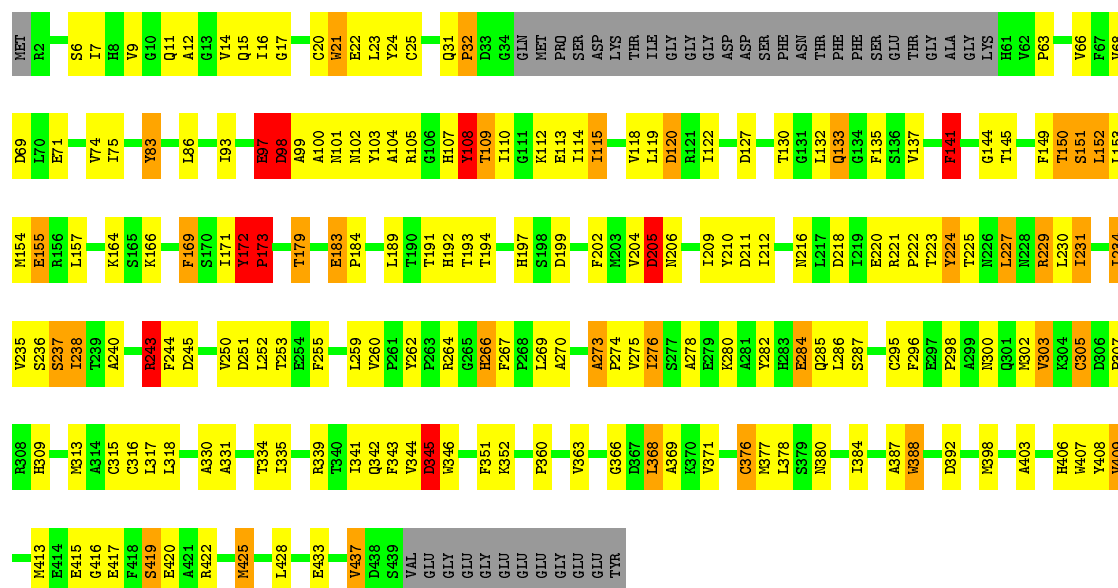
• Molecule 2: Tubulin alpha chain





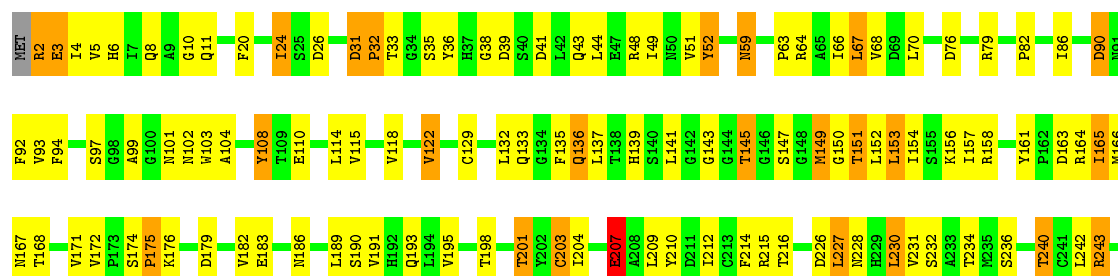
• Molecule 2: Tubulin alpha chain

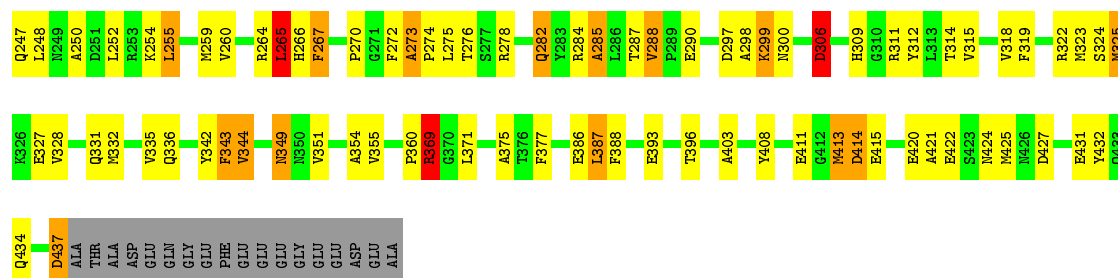
Chain 2-A: 49% 33% 8% 9%



• Molecule 3: Tubulin beta chain

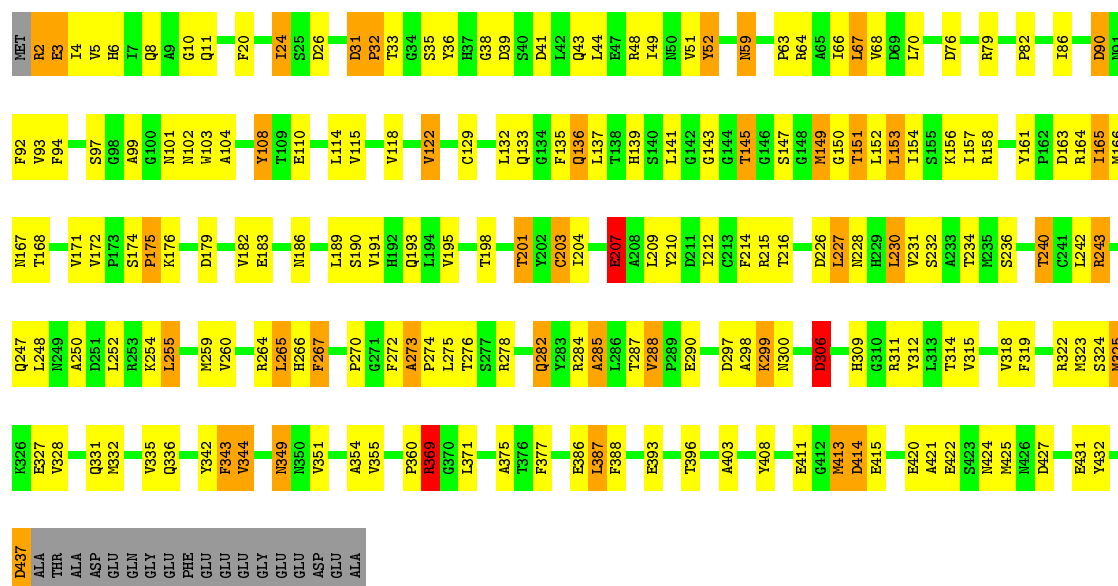
Chain 1-B: 52% 34% 9%





• Molecule 3: Tubulin beta chain

Chain 2-B: 52% 34% 9%



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=81 Å, axial sym=C1	Depositor
Number of segments used	135382	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 9V5, ZN, TA1, MG, GTP

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 > 2$	RMSZ	# $ Z > 2$
1	1-K	0.65	0/2611	1.14	8/3524 (0.2%)
1	2-K	0.32	0/2611	0.49	1/3524 (0.0%)
2	1-A	0.70	0/3300	1.19	10/4482 (0.2%)
2	2-A	0.71	0/3300	1.20	11/4482 (0.2%)
3	1-B	0.74	2/3426 (0.1%)	1.17	8/4642 (0.2%)
3	2-B	0.74	2/3426 (0.1%)	1.17	9/4642 (0.2%)
All	All	0.67	4/18674 (0.0%)	1.10	47/25296 (0.2%)

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	1-K	0	27
1	2-K	1	3
2	1-A	0	27
2	2-A	0	32
3	1-B	0	28
3	2-B	0	28
All	All	1	145

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	431	GLU	CD-OE2	-9.96	1.14	1.25
3	2-B	431	GLU	CD-OE2	-9.96	1.14	1.25
3	1-B	431	GLU	CD-OE1	9.24	1.35	1.25
3	2-B	431	GLU	CD-OE1	9.24	1.35	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	64	ARG	NE-CZ-NH1	11.25	125.93	120.30
3	2-B	64	ARG	NE-CZ-NH1	11.25	125.93	120.30
2	1-A	243	ARG	NE-CZ-NH1	9.74	125.17	120.30
2	2-A	243	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	1-K	340	ASP	CB-CG-OD1	-8.19	110.93	118.30
2	1-A	205	ASP	CB-CG-OD2	-8.12	110.99	118.30
2	2-A	205	ASP	CB-CG-OD2	-8.12	110.99	118.30
3	1-B	64	ARG	NE-CZ-NH2	-7.67	116.46	120.30
3	2-B	64	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	1-K	340	ASP	CB-CG-OD2	-7.23	111.80	118.30
3	1-B	243	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	2-B	243	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	1-B	306	ASP	CB-CG-OD1	-7.04	111.96	118.30
3	2-B	306	ASP	CB-CG-OD1	-7.04	111.96	118.30
3	2-B	264	ARG	NE-CZ-NH1	7.03	123.82	120.30
2	1-A	243	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	2-A	243	ARG	NE-CZ-NH2	-6.76	116.92	120.30
2	1-A	172	TYR	CB-CA-C	6.19	122.77	110.40
2	2-A	172	TYR	CB-CA-C	6.19	122.77	110.40
3	1-B	36	TYR	CB-CG-CD1	-6.05	117.37	121.00
3	2-B	36	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	2-K	348	TYR	CB-CG-CD1	-6.01	117.39	121.00
2	1-A	422	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	2-A	422	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	2-A	108	TYR	CB-CG-CD1	5.93	124.56	121.00
2	1-A	172	TYR	CA-CB-CG	5.92	124.65	113.40
2	2-A	172	TYR	CA-CB-CG	5.92	124.65	113.40
1	1-K	182	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	1-A	405	VAL	CG1-CB-CG2	-5.79	101.63	110.90
2	1-A	305	CYS	CA-CB-SG	-5.69	103.76	114.00
2	2-A	305	CYS	CA-CB-SG	-5.69	103.76	114.00
2	2-A	108	TYR	CB-CG-CD2	-5.69	117.59	121.00
3	1-B	31	ASP	CB-CG-OD1	-5.63	113.24	118.30
3	2-B	31	ASP	CB-CG-OD1	-5.63	113.24	118.30
1	1-K	134	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	1-K	136	THR	CA-CB-CG2	5.53	120.14	112.40
3	1-B	31	ASP	CB-CG-OD2	-5.48	113.37	118.30
3	2-B	31	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	1-K	341	ASP	CB-CG-OD2	-5.43	113.41	118.30
2	1-A	229	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	2-A	229	ARG	NE-CZ-NH2	5.40	123.00	120.30
3	1-B	108	TYR	CB-CG-CD1	-5.35	117.79	121.00
3	2-B	108	TYR	CB-CG-CD1	-5.35	117.79	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-A	83	TYR	CB-CG-CD2	-5.24	117.86	121.00
2	2-A	83	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	1-K	339	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	1-K	81	ASP	CB-CG-OD1	-5.01	113.79	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	2-K	47	LYS	CA

All (145) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1-A	113	GLU	Sidechain
2	1-A	120	ASP	Sidechain
2	1-A	133	GLN	Sidechain
2	1-A	151	SER	Mainchain
2	1-A	166	LYS	Mainchain
2	1-A	17	GLY	Mainchain
2	1-A	179	THR	Mainchain
2	1-A	199	ASP	Sidechain
2	1-A	205	ASP	Sidechain
2	1-A	211	ASP	Sidechain
2	1-A	216	ASN	Sidechain
2	1-A	218	ASP	Sidechain
2	1-A	22	GLU	Sidechain
2	1-A	227	LEU	Mainchain
2	1-A	243	ARG	Sidechain
2	1-A	262	TYR	Sidechain
2	1-A	282	TYR	Sidechain
2	1-A	286	LEU	Mainchain
2	1-A	300	ASN	Sidechain
2	1-A	345	ASP	Sidechain
2	1-A	360	PRO	Mainchain
2	1-A	392	ASP	Mainchain
2	1-A	437	VAL	Mainchain
2	1-A	71	GLU	Sidechain
2	1-A	83	TYR	Sidechain
2	1-A	97	GLU	Sidechain
2	1-A	98	ASP	Sidechain
3	1-B	11	GLN	Sidechain
3	1-B	110	GLU	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	1-B	136	GLN	Sidechain
3	1-B	158	ARG	Sidechain
3	1-B	171	VAL	Mainchain
3	1-B	175	PRO	Mainchain
3	1-B	2	ARG	Mainchain
3	1-B	207	GLU	Sidechain
3	1-B	216	THR	Mainchain
3	1-B	247	GLN	Sidechain
3	1-B	255	LEU	Mainchain
3	1-B	285	ALA	Mainchain
3	1-B	3	GLU	Sidechain
3	1-B	306	ASP	Sidechain
3	1-B	31	ASP	Sidechain
3	1-B	312	TYR	Sidechain
3	1-B	327	GLU	Sidechain
3	1-B	388	PHE	Mainchain
3	1-B	39	ASP	Sidechain
3	1-B	393	GLU	Sidechain
3	1-B	411	GLU	Sidechain
3	1-B	414	ASP	Sidechain
3	1-B	415	GLU	Sidechain
3	1-B	420	GLU	Sidechain
3	1-B	437	ASP	Sidechain
3	1-B	5	VAL	Mainchain
3	1-B	52	TYR	Sidechain
3	1-B	90	ASP	Sidechain
1	1-K	120	THR	Mainchain
1	1-K	141	TYR	Sidechain
1	1-K	145	ASP	Sidechain,Mainchain
1	1-K	149	GLU	Mainchain
1	1-K	150	GLU	Sidechain
1	1-K	168	ARG	Sidechain
1	1-K	182	ASP	Sidechain
1	1-K	186	GLY	Mainchain
1	1-K	202	GLU	Sidechain
1	1-K	225	SER	Mainchain
1	1-K	228	SER	Mainchain
1	1-K	235	TYR	Sidechain
1	1-K	264	ARG	Mainchain
1	1-K	271	LYS	Mainchain
1	1-K	275	PHE	Mainchain
1	1-K	278	GLY	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	1-K	283	ARG	Sidechain
1	1-K	293	ASN	Mainchain
1	1-K	318	ASP	Sidechain
1	1-K	339	TYR	Sidechain
1	1-K	340	ASP	Sidechain
1	1-K	348	TYR	Sidechain
1	1-K	69	ASN	Sidechain
1	1-K	77	ASP	Peptide
1	1-K	81	ASP	Sidechain
1	1-K	86	GLN	Sidechain
2	2-A	108	TYR	Sidechain
2	2-A	113	GLU	Sidechain
2	2-A	120	ASP	Sidechain
2	2-A	133	GLN	Sidechain
2	2-A	151	SER	Mainchain
2	2-A	166	LYS	Mainchain
2	2-A	17	GLY	Mainchain
2	2-A	179	THR	Mainchain
2	2-A	199	ASP	Sidechain
2	2-A	205	ASP	Sidechain
2	2-A	211	ASP	Sidechain
2	2-A	216	ASN	Sidechain
2	2-A	218	ASP	Sidechain
2	2-A	22	GLU	Sidechain
2	2-A	227	LEU	Mainchain
2	2-A	243	ARG	Sidechain
2	2-A	262	TYR	Sidechain
2	2-A	282	TYR	Sidechain
2	2-A	286	LEU	Mainchain
2	2-A	300	ASN	Sidechain
2	2-A	345	ASP	Sidechain
2	2-A	360	PRO	Mainchain
2	2-A	392	ASP	Mainchain
2	2-A	409	VAL	Mainchain
2	2-A	416	GLY	Mainchain
2	2-A	420	GLU	Sidechain,Mainchain
2	2-A	437	VAL	Mainchain
2	2-A	71	GLU	Sidechain
2	2-A	83	TYR	Sidechain
2	2-A	97	GLU	Sidechain
2	2-A	98	ASP	Sidechain
3	2-B	11	GLN	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	2-B	110	GLU	Sidechain
3	2-B	136	GLN	Sidechain
3	2-B	158	ARG	Sidechain
3	2-B	171	VAL	Mainchain
3	2-B	175	PRO	Mainchain
3	2-B	2	ARG	Mainchain
3	2-B	207	GLU	Sidechain
3	2-B	216	THR	Mainchain
3	2-B	247	GLN	Sidechain
3	2-B	255	LEU	Mainchain
3	2-B	285	ALA	Mainchain
3	2-B	3	GLU	Sidechain
3	2-B	306	ASP	Sidechain
3	2-B	31	ASP	Sidechain
3	2-B	312	TYR	Sidechain
3	2-B	327	GLU	Sidechain
3	2-B	388	PHE	Mainchain
3	2-B	39	ASP	Sidechain
3	2-B	393	GLU	Sidechain
3	2-B	411	GLU	Sidechain
3	2-B	414	ASP	Sidechain
3	2-B	415	GLU	Sidechain
3	2-B	420	GLU	Sidechain
3	2-B	437	ASP	Sidechain
3	2-B	5	VAL	Mainchain
3	2-B	52	TYR	Sidechain
3	2-B	90	ASP	Sidechain
1	2-K	181	GLU	Sidechain
1	2-K	343	TYR	Mainchain
1	2-K	348	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-K	2569	0	2587	152	0
1	2-K	2569	0	2587	65	0
2	1-A	3227	0	3143	126	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2-A	3227	0	3143	133	0
3	1-B	3351	0	3229	125	0
3	2-B	3351	0	3229	122	0
4	1-K	19	0	0	0	0
4	2-K	19	0	0	5	0
5	1-A	1	0	0	0	0
5	2-A	1	0	0	0	0
6	1-A	1	0	0	0	0
6	2-A	1	0	0	0	0
7	1-A	32	0	12	10	0
7	2-A	32	0	12	10	0
8	1-B	28	0	12	2	0
8	2-B	28	0	12	2	0
9	1-B	62	0	51	6	0
9	2-B	62	0	51	6	0
All	All	18580	0	18068	707	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 19.

All (707) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:33:VAL:HG13	1:K:34:VAL:H	1.05	1.12
3:B:172:VAL:HG11	3:B:387:LEU:HD21	1.32	1.11
3:B:172:VAL:HG11	3:B:387:LEU:HD21	1.32	1.11
1:K:31:HIS:HE1	1:K:46:PRO:O	1.40	1.02
1:K:291:VAL:HG13	1:K:305:ILE:HD11	1.41	0.97
1:K:31:HIS:CE1	1:K:46:PRO:O	2.18	0.96
1:K:33:VAL:HG23	1:K:339:TYR:HA	1.44	0.96
1:K:19:ARG:HB2	1:K:119:LYS:HG3	1.48	0.94
1:K:33:VAL:HG13	1:K:34:VAL:N	1.85	0.91
1:K:110:LEU:HD23	1:K:257:ILE:HD11	1.55	0.88
2:A:7:ILE:HG22	2:A:66:VAL:HG22	1.56	0.87
2:A:7:ILE:HG22	2:A:66:VAL:HG22	1.56	0.87
1:K:16:VAL:HG22	1:K:330:ALA:HB3	1.56	0.86
3:B:234:THR:HG21	3:B:270:PRO:HB2	1.59	0.85
3:B:234:THR:HG21	3:B:270:PRO:HB2	1.59	0.85
1:K:286:LEU:HD13	2:A:409:VAL:HG21	1.59	0.85
1:K:93:THR:HG21	1:K:329:ILE:HD11	1.56	0.84
1:K:97:ILE:HD11	1:K:327:ILE:HG22	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:152:ILE:HG23	1:K:239:GLN:HB2	1.61	0.83
4:K:401:9V5:S18	4:K:401:9V5:O15	2.38	0.81
3:B:242:LEU:HD22	3:B:250:ALA:H	1.46	0.80
3:B:242:LEU:HD22	3:B:250:ALA:H	1.46	0.80
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.62	0.80
3:B:93:VAL:HG11	3:B:118:VAL:HG22	1.62	0.80
2:A:151:SER:HB3	2:A:193:THR:HG21	1.65	0.78
2:A:151:SER:HB3	2:A:193:THR:HG21	1.65	0.78
2:A:119:LEU:HD23	2:A:122:ILE:HD11	1.65	0.78
2:A:119:LEU:HD23	2:A:122:ILE:HD11	1.65	0.78
3:B:167:ASN:HD21	3:B:252:LEU:HD22	1.49	0.77
3:B:167:ASN:HD21	3:B:252:LEU:HD22	1.49	0.77
3:B:114:LEU:HD23	3:B:149:MET:CE	2.15	0.77
3:B:114:LEU:HD23	3:B:149:MET:CE	2.15	0.77
2:A:12:ALA:HB2	7:A:503:GTP:C8	2.20	0.76
2:A:12:ALA:HB2	7:A:503:GTP:C8	2.20	0.76
1:K:265:ALA:HB2	2:A:108:TYR:CD2	2.21	0.76
2:A:69:ASP:HA	2:A:145:THR:HG21	1.68	0.75
2:A:69:ASP:HA	2:A:145:THR:HG21	1.68	0.75
1:K:42:LEU:HD12	1:K:42:LEU:O	1.86	0.75
1:K:86:GLN:HE21	1:K:132:VAL:H	1.34	0.75
3:B:70:LEU:H	3:B:145:THR:HG21	1.52	0.75
3:B:70:LEU:H	3:B:145:THR:HG21	1.52	0.75
4:K:401:9V5:C10	4:K:401:9V5:O15	2.36	0.74
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.69	0.73
2:A:204:VAL:HG11	2:A:231:ILE:HD12	1.69	0.73
2:A:101:ASN:ND2	7:A:503:GTP:O3G	2.23	0.72
2:A:101:ASN:ND2	7:A:503:GTP:O3G	2.23	0.72
1:K:209:ASN:HA	1:K:212:LYS:HE2	1.70	0.72
2:A:204:VAL:HG13	2:A:209:ILE:HD11	1.72	0.72
2:A:204:VAL:HG13	2:A:209:ILE:HD11	1.72	0.72
1:K:93:THR:HG21	1:K:329:ILE:HD11	1.70	0.72
2:A:7:ILE:HD12	2:A:153:LEU:HD21	1.70	0.71
2:A:7:ILE:HD12	2:A:153:LEU:HD21	1.70	0.71
3:B:66:ILE:CD1	3:B:122:VAL:HG12	2.21	0.71
3:B:66:ILE:CD1	3:B:122:VAL:HG12	2.21	0.71
2:A:243:ARG:NH2	2:A:252:LEU:H	1.88	0.71
2:A:243:ARG:NH2	2:A:252:LEU:H	1.88	0.71
1:K:31:HIS:NE2	1:K:46:PRO:HD2	2.06	0.71
1:K:17:ARG:HD2	1:K:19:ARG:HD2	1.73	0.70
1:K:108:THR:HG21	1:K:320:LEU:CD1	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:118:GLY:H	1:K:121:HIS:HB2	1.57	0.70
3:B:228:ASN:OD1	8:B:600:GDP:N1	2.18	0.70
3:B:228:ASN:OD1	8:B:600:GDP:N1	2.18	0.70
1:K:240:ASP:HB2	1:K:243:ALA:HB3	1.73	0.70
2:A:259:LEU:HD11	2:A:378:LEU:HD13	1.74	0.70
2:A:259:LEU:HD11	2:A:378:LEU:HD13	1.74	0.70
1:K:207:LEU:HD22	4:K:401:9V5:C2	2.22	0.70
2:A:115:ILE:HG13	2:A:152:LEU:HD13	1.73	0.69
2:A:115:ILE:HG13	2:A:152:LEU:HD13	1.73	0.69
3:B:66:ILE:HD13	3:B:122:VAL:HG12	1.73	0.69
3:B:234:THR:HG21	3:B:270:PRO:CB	2.22	0.69
3:B:66:ILE:HD13	3:B:122:VAL:HG12	1.73	0.69
3:B:234:THR:HG21	3:B:270:PRO:CB	2.22	0.69
1:K:155:THR:HG22	1:K:236:LEU:HA	1.76	0.68
1:K:16:VAL:HG23	1:K:76:PHE:CE2	2.28	0.68
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.74	0.68
3:B:273:ALA:HB3	3:B:274:PRO:HD3	1.74	0.68
1:K:32:LYS:N	1:K:32:LYS:HD3	2.09	0.68
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.76	0.67
2:A:273:ALA:HB3	2:A:274:PRO:HD3	1.76	0.67
1:K:33:VAL:CG1	1:K:34:VAL:H	1.92	0.67
2:A:243:ARG:HH21	2:A:252:LEU:H	1.42	0.67
2:A:276:ILE:HG23	2:A:369:ALA:CB	2.25	0.67
1:K:332:VAL:HG12	1:K:342:THR:HG23	1.76	0.67
2:A:243:ARG:HH21	2:A:252:LEU:H	1.42	0.67
2:A:276:ILE:HG23	2:A:369:ALA:CB	2.25	0.67
3:B:250:ALA:HA	3:B:254:LYS:HE2	1.77	0.66
3:B:250:ALA:HA	3:B:254:LYS:HE2	1.77	0.66
1:K:170:LEU:HD23	1:K:210:GLY:HA3	1.78	0.66
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.78	0.65
3:B:209:LEU:HB3	3:B:227:LEU:HD22	1.78	0.65
1:K:115:THR:HA	1:K:261:GLY:HA3	1.78	0.65
1:K:265:ALA:HB2	2:A:108:TYR:CD2	2.30	0.65
1:K:187:VAL:HG21	1:K:314:ARG:HD2	1.79	0.65
1:K:178:ALA:HB3	1:K:190:HIS:NE2	2.12	0.65
1:K:22:ASN:OD1	1:K:23:THR:N	2.29	0.64
1:K:18:VAL:HG22	1:K:332:VAL:CG2	2.28	0.64
3:B:114:LEU:HD23	3:B:149:MET:HE1	1.79	0.64
3:B:114:LEU:HD23	3:B:149:MET:HE1	1.79	0.64
1:K:15:VAL:HG12	1:K:327:ILE:HD11	1.80	0.64
3:B:70:LEU:HD12	3:B:145:THR:HG23	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:70:LEU:HD12	3:B:145:THR:HG23	1.79	0.64
3:B:325:MET:CE	3:B:355:VAL:HG11	2.28	0.63
3:B:325:MET:CE	3:B:355:VAL:HG11	2.28	0.63
1:K:197:PRO:HB3	1:K:203:ILE:HD11	1.80	0.63
1:K:95:LYS:HB3	1:K:96:PRO:HD3	1.80	0.63
1:K:268:SER:HB3	1:K:274:ARG:HD2	1.81	0.63
3:B:325:MET:HE1	3:B:355:VAL:HG11	1.79	0.63
3:B:325:MET:HE1	3:B:355:VAL:HG11	1.79	0.63
3:B:243:ARG:HH21	3:B:252:LEU:H	1.44	0.63
1:K:86:GLN:NE2	1:K:132:VAL:HG23	2.13	0.63
3:B:243:ARG:HH21	3:B:252:LEU:H	1.44	0.63
2:A:237:SER:HB2	2:A:376:CYS:SG	2.39	0.63
2:A:237:SER:HB2	2:A:376:CYS:SG	2.39	0.63
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.81	0.62
1:K:333:SER:HB3	1:K:338:PHE:CG	2.34	0.62
2:A:7:ILE:HD11	2:A:137:VAL:HG22	1.81	0.62
2:A:234:ILE:HG13	2:A:270:ALA:HB1	1.81	0.62
1:K:93:THR:HG23	1:K:327:ILE:HG21	1.80	0.62
1:K:33:VAL:CG2	1:K:339:TYR:HA	2.24	0.62
2:A:234:ILE:HG13	2:A:270:ALA:HB1	1.81	0.62
9:B:601:TA1:H261	9:B:601:TA1:H463	1.80	0.62
9:B:601:TA1:H463	9:B:601:TA1:H261	1.80	0.62
3:B:325:MET:CE	3:B:355:VAL:HG21	2.30	0.62
3:B:325:MET:CE	3:B:355:VAL:HG21	2.30	0.62
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.82	0.62
3:B:115:VAL:HG21	3:B:152:LEU:HD23	1.82	0.62
1:K:14:VAL:HG21	1:K:76:PHE:CD1	2.35	0.62
3:B:20:PHE:CZ	3:B:24:ILE:HD12	2.35	0.61
3:B:332:MET:HE3	3:B:351:VAL:HG11	1.82	0.61
3:B:20:PHE:CZ	3:B:24:ILE:HD12	2.35	0.61
3:B:332:MET:HE3	3:B:351:VAL:HG11	1.82	0.61
1:K:171:LEU:HD13	1:K:206:LEU:HD22	1.83	0.61
1:K:109:VAL:HB	1:K:256:LEU:HG	1.82	0.61
3:B:156:LYS:HE2	3:B:156:LYS:HA	1.82	0.61
3:B:156:LYS:HE2	3:B:156:LYS:HA	1.82	0.61
2:A:184:PRO:HG2	2:A:398:MET:HE1	1.83	0.61
1:K:85:THR:HG23	1:K:87:SER:H	1.65	0.61
2:A:184:PRO:HG2	2:A:398:MET:HE1	1.83	0.61
1:K:163:TYR:O	1:K:166:GLN:HG2	2.01	0.61
2:A:151:SER:CB	2:A:193:THR:HG21	2.30	0.61
3:B:413:MET:HG3	3:B:414:ASP:H	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:151:SER:CB	2:A:193:THR:HG21	2.30	0.61
3:B:413:MET:HG3	3:B:414:ASP:H	1.64	0.61
1:K:348:TYR:CE1	2:A:415:GLU:HG3	2.36	0.61
2:A:7:ILE:HD12	2:A:153:LEU:CD2	2.31	0.60
2:A:7:ILE:HD12	2:A:153:LEU:CD2	2.31	0.60
3:B:259:MET:HA	3:B:314:THR:HG21	1.82	0.60
3:B:259:MET:HA	3:B:314:THR:HG21	1.82	0.60
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.37	0.60
1:K:32:LYS:H	1:K:32:LYS:HD3	1.67	0.60
2:A:118:VAL:HG21	2:A:149:PHE:CZ	2.37	0.60
1:K:333:SER:HB3	1:K:338:PHE:CD2	2.37	0.60
3:B:287:THR:O	3:B:288:VAL:HG23	2.02	0.60
3:B:287:THR:O	3:B:288:VAL:HG23	2.02	0.60
3:B:242:LEU:CD1	3:B:255:LEU:HD11	2.32	0.60
1:K:18:VAL:HG21	1:K:36:VAL:HG21	1.82	0.60
1:K:194:LEU:HD21	1:K:235:TYR:CE2	2.37	0.60
3:B:242:LEU:CD1	3:B:255:LEU:HD11	2.32	0.60
1:K:102:LEU:HD11	1:K:147:ILE:HG21	1.81	0.60
1:K:287:ALA:O	1:K:291:VAL:HG23	2.02	0.60
2:A:223:THR:HB	2:A:225:THR:HG22	1.82	0.60
2:A:223:THR:HB	2:A:225:THR:HG22	1.82	0.60
1:K:31:HIS:HE1	1:K:46:PRO:C	2.06	0.59
1:K:152:ILE:HB	1:K:241:LYS:HE3	1.83	0.59
2:A:276:ILE:HG23	2:A:369:ALA:HB2	1.83	0.59
3:B:115:VAL:HG21	3:B:152:LEU:CD2	2.33	0.59
2:A:276:ILE:HG23	2:A:369:ALA:HB2	1.83	0.59
3:B:115:VAL:HG21	3:B:152:LEU:CD2	2.33	0.59
1:K:259:LEU:HD12	1:K:259:LEU:N	2.18	0.59
1:K:265:ALA:HB2	2:A:108:TYR:HD2	1.65	0.59
2:A:425:MET:HE2	2:A:428:LEU:HD23	1.83	0.58
2:A:425:MET:HE2	2:A:428:LEU:HD23	1.83	0.58
2:A:68:VAL:HG11	2:A:149:PHE:CZ	2.39	0.58
1:K:307:TYR:CE1	1:K:317:LYS:HG3	2.38	0.58
2:A:68:VAL:HG11	2:A:149:PHE:CZ	2.39	0.58
2:A:231:ILE:HA	2:A:234:ILE:HG22	1.86	0.58
2:A:231:ILE:HA	2:A:234:ILE:HG22	1.86	0.58
2:A:115:ILE:CG1	2:A:152:LEU:HD13	2.33	0.58
2:A:115:ILE:CG1	2:A:152:LEU:HD13	2.33	0.58
3:B:250:ALA:HB1	3:B:254:LYS:HB2	1.84	0.58
3:B:250:ALA:HB1	3:B:254:LYS:HB2	1.84	0.58
3:B:93:VAL:HG11	3:B:118:VAL:CG2	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:93:VAL:HG11	3:B:118:VAL:CG2	2.32	0.58
3:B:10:GLY:HA2	3:B:145:THR:HB	1.85	0.57
3:B:10:GLY:HA2	3:B:145:THR:HB	1.85	0.57
2:A:11:GLN:HG3	2:A:74:VAL:HG11	1.87	0.57
2:A:11:GLN:HG3	2:A:74:VAL:HG11	1.87	0.57
3:B:182:VAL:HG23	3:B:186:ASN:HD21	1.69	0.57
3:B:182:VAL:HG23	3:B:186:ASN:HD21	1.69	0.57
3:B:137:LEU:HD22	3:B:154:ILE:HG21	1.87	0.57
3:B:137:LEU:HD22	3:B:154:ILE:HG21	1.87	0.57
1:K:119:LYS:HA	1:K:119:LYS:HE3	1.87	0.57
4:K:401:9V5:O16	4:K:401:9V5:O15	2.23	0.57
2:A:7:ILE:HG22	2:A:66:VAL:CG2	2.33	0.56
3:B:331:GLN:O	3:B:335:VAL:HG23	2.04	0.56
1:K:236:LEU:HD23	1:K:237:ARG:N	2.20	0.56
2:A:7:ILE:HG22	2:A:66:VAL:CG2	2.33	0.56
3:B:331:GLN:O	3:B:335:VAL:HG23	2.04	0.56
2:A:122:ILE:HD12	2:A:157:LEU:HD21	1.86	0.56
2:A:104:ALA:CB	2:A:413:MET:HG3	2.35	0.56
2:A:122:ILE:HD12	2:A:157:LEU:HD21	1.86	0.56
2:A:104:ALA:CB	2:A:413:MET:HG3	2.35	0.56
2:A:250:VAL:HG22	2:A:352:LYS:NZ	2.21	0.56
2:A:250:VAL:HG22	2:A:352:LYS:NZ	2.21	0.56
1:K:170:LEU:HD23	1:K:210:GLY:CA	2.36	0.56
3:B:209:LEU:HG	3:B:230:LEU:HD22	1.86	0.56
3:B:209:LEU:HG	3:B:230:LEU:HD22	1.86	0.56
1:K:203:ILE:O	1:K:207:LEU:HG	2.06	0.56
1:K:158:SER:CB	1:K:192:LEU:HD21	2.36	0.56
2:A:259:LEU:HD11	2:A:378:LEU:CD1	2.35	0.56
2:A:259:LEU:HD11	2:A:378:LEU:CD1	2.35	0.56
1:K:138:LEU:O	1:K:138:LEU:HD23	2.06	0.55
1:K:274:ARG:HE	1:K:275:PHE:HA	1.71	0.55
1:K:351:ARG:HH21	2:A:419:SER:HB3	1.71	0.55
1:K:16:VAL:HB	1:K:79:VAL:HG22	1.88	0.55
1:K:202:GLU:O	1:K:206:LEU:HG	2.05	0.55
3:B:66:ILE:C	3:B:67:LEU:HD23	2.26	0.55
3:B:66:ILE:C	3:B:67:LEU:HD23	2.26	0.55
2:A:169:PHE:CE2	2:A:235:VAL:HG22	2.41	0.55
3:B:132:LEU:HD23	3:B:164:ARG:HG3	1.89	0.55
1:K:101:PHE:CZ	1:K:236:LEU:HB2	2.42	0.55
2:A:169:PHE:CE2	2:A:235:VAL:HG22	2.41	0.55
3:B:132:LEU:HD23	3:B:164:ARG:HG3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:35:SER:HB3	3:B:59:ASN:HA	1.88	0.55
3:B:35:SER:HB3	3:B:59:ASN:HA	1.88	0.55
1:K:171:LEU:HD23	1:K:193:THR:HB	1.89	0.55
3:B:259:MET:HG2	3:B:314:THR:HG21	1.87	0.55
3:B:259:MET:HG2	3:B:314:THR:HG21	1.87	0.55
3:B:204:ILE:HG21	3:B:231:VAL:HG22	1.88	0.55
3:B:204:ILE:HG21	3:B:231:VAL:HG22	1.88	0.55
1:K:209:ASN:HA	1:K:212:LYS:HE3	1.89	0.54
1:K:219:THR:HG23	1:K:271:LYS:HE3	1.89	0.54
1:K:305:ILE:HG23	1:K:307:TYR:CE1	2.42	0.54
3:B:272:PHE:CE1	9:B:601:TA1:H391	2.43	0.54
3:B:360:PRO:HB2	9:B:601:TA1:H281	1.90	0.54
1:K:32:LYS:CD	1:K:32:LYS:H	2.19	0.54
1:K:93:THR:HG21	1:K:329:ILE:CD1	2.35	0.54
3:B:272:PHE:CE1	9:B:601:TA1:H391	2.43	0.54
3:B:360:PRO:HB2	9:B:601:TA1:H281	1.90	0.54
1:K:108:THR:HG21	1:K:320:LEU:HG	1.90	0.54
1:K:33:VAL:HG23	1:K:339:TYR:CA	2.30	0.54
3:B:204:ILE:HD13	3:B:231:VAL:HG22	1.89	0.54
1:K:227:ARG:HA	1:K:260:ALA:HB2	1.90	0.54
1:K:37:VAL:HG21	1:K:43:VAL:HG23	1.89	0.54
3:B:204:ILE:HD13	3:B:231:VAL:HG22	1.89	0.54
2:A:305:CYS:SG	2:A:384:ILE:HD13	2.48	0.54
1:K:187:VAL:HG21	1:K:314:ARG:CD	2.38	0.54
2:A:305:CYS:SG	2:A:384:ILE:HD13	2.48	0.54
3:B:150:GLY:HA2	3:B:153:LEU:HD22	1.90	0.54
3:B:150:GLY:HA2	3:B:153:LEU:HD22	1.90	0.54
2:A:296:PHE:CD2	2:A:341:ILE:HD11	2.43	0.53
3:B:20:PHE:CE1	3:B:24:ILE:HD12	2.43	0.53
2:A:296:PHE:CD2	2:A:341:ILE:HD11	2.43	0.53
3:B:20:PHE:CE1	3:B:24:ILE:HD12	2.43	0.53
2:A:206:ASN:ND2	7:A:503:GTP:O2'	2.41	0.53
2:A:206:ASN:ND2	7:A:503:GTP:O2'	2.41	0.53
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.73	0.53
1:K:112:TYR:HB3	1:K:330:ALA:HA	1.91	0.53
2:A:118:VAL:HG21	2:A:149:PHE:HZ	1.73	0.53
2:A:11:GLN:N	7:A:503:GTP:O2B	2.42	0.53
2:A:7:ILE:CG1	2:A:137:VAL:HG22	2.39	0.53
3:B:137:LEU:HD22	3:B:154:ILE:CG2	2.39	0.53
2:A:11:GLN:N	7:A:503:GTP:O2B	2.42	0.53
2:A:7:ILE:CG1	2:A:137:VAL:HG22	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:137:LEU:HD22	3:B:154:ILE:CG2	2.39	0.53
1:K:119:LYS:N	1:K:119:LYS:HD2	2.22	0.53
3:B:396:THR:HG23	3:B:422:GLU:OE2	2.09	0.53
3:B:6:HIS:CE1	3:B:8:GLN:HG2	2.44	0.53
3:B:396:THR:HG23	3:B:422:GLU:OE2	2.09	0.53
3:B:6:HIS:CE1	3:B:8:GLN:HG2	2.44	0.53
2:A:179:THR:HG21	3:B:248:LEU:CD2	2.37	0.53
3:B:172:VAL:CG1	3:B:387:LEU:HD21	2.23	0.53
2:A:179:THR:HG21	3:B:248:LEU:CD2	2.37	0.53
3:B:172:VAL:CG1	3:B:387:LEU:HD21	2.23	0.53
2:A:151:SER:HB3	2:A:193:THR:CG2	2.38	0.52
2:A:151:SER:HB3	2:A:193:THR:CG2	2.38	0.52
1:K:106:ASN:OD1	1:K:319:SER:HA	2.09	0.52
2:A:316:CYS:HB3	2:A:378:LEU:HD11	1.90	0.52
3:B:122:VAL:HG21	3:B:157:ILE:CD1	2.39	0.52
1:K:108:THR:HG21	1:K:320:LEU:HG	1.91	0.52
1:K:159:TYR:CD2	1:K:170:LEU:HD22	2.44	0.52
1:K:108:THR:HG21	1:K:320:LEU:HD12	1.91	0.52
2:A:316:CYS:HB3	2:A:378:LEU:HD11	1.90	0.52
3:B:122:VAL:HG21	3:B:157:ILE:CD1	2.39	0.52
1:K:108:THR:HG23	1:K:326:THR:HG23	1.91	0.52
1:K:102:LEU:HD11	1:K:147:ILE:HG21	1.90	0.52
2:A:12:ALA:CB	7:A:503:GTP:C8	2.91	0.52
2:A:172:TYR:OH	2:A:387:ALA:HB1	2.09	0.52
2:A:344:VAL:HG11	2:A:346:TRP:CE2	2.45	0.52
3:B:182:VAL:HG23	3:B:186:ASN:ND2	2.24	0.52
1:K:19:ARG:HB2	1:K:119:LYS:CG	2.32	0.52
2:A:12:ALA:CB	7:A:503:GTP:C8	2.91	0.52
2:A:172:TYR:OH	2:A:387:ALA:HB1	2.09	0.52
2:A:344:VAL:HG11	2:A:346:TRP:CE2	2.45	0.52
3:B:182:VAL:HG23	3:B:186:ASN:ND2	2.24	0.52
1:K:123:MET:HG2	1:K:124:LEU:HD22	1.92	0.52
1:K:158:SER:OG	1:K:192:LEU:HD21	2.09	0.52
1:K:133:MET:HA	1:K:136:THR:HG22	1.89	0.52
1:K:32:LYS:N	1:K:32:LYS:CD	2.73	0.52
1:K:152:ILE:HG22	1:K:241:LYS:NZ	2.24	0.52
2:A:24:TYR:CE1	2:A:240:ALA:HB2	2.45	0.52
2:A:15:GLN:NE2	7:A:503:GTP:N7	2.57	0.52
3:B:336:GLN:HE22	3:B:349:ASN:ND2	2.08	0.52
2:A:24:TYR:CE1	2:A:240:ALA:HB2	2.45	0.52
2:A:15:GLN:NE2	7:A:503:GTP:N7	2.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:336:GLN:HE22	3:B:349:ASN:ND2	2.08	0.52
2:A:103:TYR:CD2	2:A:189:LEU:HD13	2.45	0.51
2:A:103:TYR:CD2	2:A:189:LEU:HD13	2.45	0.51
1:K:335:SER:HB3	1:K:338:PHE:HD2	1.76	0.51
2:A:205:ASP:HB3	2:A:303:VAL:HA	1.92	0.51
2:A:317:LEU:HD23	2:A:377:MET:HB3	1.92	0.51
2:A:205:ASP:HB3	2:A:303:VAL:HA	1.92	0.51
2:A:317:LEU:HD23	2:A:377:MET:HB3	1.92	0.51
2:A:204:VAL:CG1	2:A:231:ILE:HD12	2.41	0.51
2:A:204:VAL:CG1	2:A:231:ILE:HD12	2.41	0.51
1:K:90:PHE:CG	1:K:135:LEU:HB3	2.45	0.51
1:K:204:LEU:HA	1:K:207:LEU:HD12	1.93	0.51
1:K:30:PHE:O	1:K:31:HIS:C	2.49	0.51
2:A:296:PHE:CE2	2:A:341:ILE:HD11	2.46	0.51
1:K:113:GLY:HA2	1:K:331:ALA:HB3	1.92	0.51
2:A:296:PHE:CE2	2:A:341:ILE:HD11	2.46	0.51
3:B:141:LEU:HA	3:B:147:SER:HB3	1.93	0.51
3:B:8:GLN:CD	3:B:67:LEU:HD22	2.31	0.51
1:K:171:LEU:HD13	1:K:206:LEU:CD2	2.40	0.51
3:B:141:LEU:HA	3:B:147:SER:HB3	1.93	0.51
3:B:8:GLN:CD	3:B:67:LEU:HD22	2.31	0.51
1:K:86:GLN:HE21	1:K:132:VAL:N	2.07	0.50
1:K:141:TYR:CZ	1:K:199:SER:HA	2.47	0.50
1:K:234:ILE:HB	1:K:254:MET:HB3	1.92	0.50
3:B:108:TYR:CD1	3:B:413:MET:HE1	2.47	0.50
3:B:108:TYR:CD1	3:B:413:MET:HE1	2.47	0.50
1:K:14:VAL:HG23	1:K:14:VAL:O	2.11	0.50
3:B:103:TRP:CE3	3:B:189:LEU:HD13	2.47	0.50
1:K:194:LEU:N	1:K:194:LEU:HD12	2.27	0.50
3:B:103:TRP:CE3	3:B:189:LEU:HD13	2.47	0.50
3:B:179:ASP:HB2	8:B:600:GDP:H3'	1.94	0.50
3:B:179:ASP:HB2	8:B:600:GDP:H3'	1.94	0.50
3:B:168:THR:HB	3:B:201:THR:HG23	1.94	0.49
3:B:168:THR:HB	3:B:201:THR:HG23	1.94	0.49
4:K:401:9V5:O15	4:K:401:9V5:C5	2.60	0.49
2:A:234:ILE:HD13	2:A:234:ILE:C	2.33	0.49
2:A:234:ILE:C	2:A:234:ILE:HD13	2.33	0.49
3:B:204:ILE:HG21	3:B:231:VAL:CG2	2.42	0.49
3:B:274:PRO:O	9:B:601:TA1:H151	2.12	0.49
1:K:193:THR:C	1:K:194:LEU:HD12	2.33	0.49
1:K:253:LYS:HE2	1:K:319:SER:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:204:ILE:HG21	3:B:231:VAL:CG2	2.42	0.49
3:B:274:PRO:O	9:B:601:TA1:H151	2.12	0.49
1:K:17:ARG:NH2	1:K:123:MET:HG3	2.27	0.49
1:K:145:ASP:HA	1:K:148:LYS:HE3	1.93	0.49
2:A:107:HIS:CD2	2:A:108:TYR:CE1	3.00	0.49
1:K:273:THR:O	1:K:277:GLU:HB3	2.13	0.49
3:B:325:MET:HE2	3:B:355:VAL:HG21	1.93	0.49
3:B:325:MET:HE2	3:B:355:VAL:HG21	1.93	0.49
1:K:45:ASP:N	1:K:46:PRO:HD3	2.28	0.48
2:A:114:ILE:O	2:A:118:VAL:HG23	2.13	0.48
2:A:132:LEU:HD23	2:A:132:LEU:H	1.78	0.48
1:K:97:ILE:HD11	1:K:327:ILE:CG2	2.39	0.48
2:A:114:ILE:O	2:A:118:VAL:HG23	2.13	0.48
2:A:132:LEU:HD23	2:A:132:LEU:H	1.78	0.48
3:B:285:ALA:HB1	3:B:290:GLU:HG2	1.95	0.48
3:B:285:ALA:HB1	3:B:290:GLU:HG2	1.95	0.48
3:B:189:LEU:HD23	3:B:421:ALA:CB	2.44	0.48
1:K:18:VAL:HG22	1:K:332:VAL:HG23	1.96	0.48
3:B:189:LEU:HD23	3:B:421:ALA:CB	2.44	0.48
2:A:179:THR:HG21	3:B:248:LEU:HD21	1.96	0.48
3:B:20:PHE:HA	3:B:232:SER:HB2	1.96	0.48
3:B:323:MET:CE	3:B:328:VAL:HG22	2.43	0.48
1:K:133:MET:O	1:K:137:MET:HB2	2.12	0.48
1:K:241:LYS:HA	1:K:241:LYS:NZ	2.28	0.48
2:A:179:THR:HG21	3:B:248:LEU:HD21	1.96	0.48
3:B:20:PHE:HA	3:B:232:SER:HB2	1.96	0.48
3:B:323:MET:CE	3:B:328:VAL:HG22	2.43	0.48
1:K:135:LEU:HD12	1:K:138:LEU:HD12	1.96	0.48
1:K:306:PRO:HB2	1:K:309:ASN:HB2	1.96	0.48
2:A:102:ASN:HB2	2:A:408:TYR:CE1	2.49	0.48
2:A:209:ILE:HG22	2:A:227:LEU:HD22	1.96	0.48
2:A:250:VAL:HG22	2:A:352:LYS:HZ2	1.79	0.48
2:A:388:TRP:CE3	2:A:425:MET:HE3	2.49	0.48
2:A:102:ASN:HB2	2:A:408:TYR:CE1	2.49	0.48
2:A:209:ILE:HG22	2:A:227:LEU:HD22	1.96	0.48
2:A:250:VAL:HG22	2:A:352:LYS:HZ2	1.79	0.48
2:A:388:TRP:CE3	2:A:425:MET:HE3	2.49	0.48
1:K:14:VAL:HG23	1:K:77:ASP:H	1.78	0.48
2:A:209:ILE:CG2	2:A:227:LEU:HD22	2.44	0.48
2:A:209:ILE:CG2	2:A:227:LEU:HD22	2.44	0.48
3:B:102:ASN:HD21	3:B:408:TYR:HA	1.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:102:ASN:HD21	3:B:408:TYR:HA	1.77	0.47
2:A:14:VAL:HG21	2:A:75:ILE:CD1	2.44	0.47
3:B:250:ALA:CA	3:B:254:LYS:HE2	2.43	0.47
3:B:203:CYS:SG	3:B:267:PHE:HB3	2.54	0.47
1:K:17:ARG:HH22	1:K:86:GLN:HE22	1.62	0.47
2:A:14:VAL:HG21	2:A:75:ILE:CD1	2.44	0.47
3:B:250:ALA:CA	3:B:254:LYS:HE2	2.43	0.47
3:B:203:CYS:SG	3:B:267:PHE:HB3	2.54	0.47
1:K:312:LEU:O	1:K:316:LEU:HG	2.14	0.47
1:K:119:LYS:HG2	1:K:333:SER:HB3	1.96	0.47
2:A:7:ILE:HG21	2:A:122:ILE:HG21	1.96	0.47
3:B:274:PRO:HG2	3:B:371:LEU:HD21	1.95	0.47
3:B:104:ALA:HB2	3:B:413:MET:SD	2.55	0.47
1:K:118:GLY:N	1:K:121:HIS:HB2	2.26	0.47
1:K:42:LEU:HD12	1:K:42:LEU:C	2.34	0.47
2:A:7:ILE:HG21	2:A:122:ILE:HG21	1.96	0.47
3:B:274:PRO:HG2	3:B:371:LEU:HD21	1.95	0.47
3:B:104:ALA:HB2	3:B:413:MET:SD	2.55	0.47
1:K:109:VAL:HB	1:K:256:LEU:HD12	1.96	0.47
3:B:204:ILE:CD1	3:B:231:VAL:HG13	2.44	0.47
1:K:178:ALA:HB3	1:K:190:HIS:CD2	2.49	0.47
1:K:22:ASN:HB3	1:K:25:GLU:CD	2.34	0.47
3:B:204:ILE:CD1	3:B:231:VAL:HG13	2.44	0.47
1:K:39:LYS:HE2	1:K:80:PHE:HD1	1.79	0.47
1:K:144:MET:HE2	1:K:155:THR:HG21	1.96	0.47
1:K:253:LYS:HE2	1:K:319:SER:CA	2.45	0.47
2:A:225:THR:O	2:A:229:ARG:HG3	2.15	0.47
2:A:225:THR:O	2:A:229:ARG:HG3	2.15	0.47
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.96	0.47
3:B:191:VAL:HG11	3:B:425:MET:HG3	1.96	0.47
3:B:67:LEU:HD23	3:B:67:LEU:N	2.30	0.47
1:K:25:GLU:HB3	1:K:335:SER:HB2	1.96	0.47
3:B:242:LEU:HD12	3:B:255:LEU:HD11	1.96	0.47
1:K:80:PHE:CZ	1:K:92:HIS:HB2	2.50	0.47
2:A:31:GLN:HB3	2:A:32:PRO:HD2	1.96	0.47
3:B:191:VAL:HG11	3:B:425:MET:HG3	1.96	0.47
3:B:67:LEU:N	3:B:67:LEU:HD23	2.30	0.47
3:B:242:LEU:HD12	3:B:255:LEU:HD11	1.96	0.47
2:A:209:ILE:HG23	2:A:230:LEU:HD23	1.96	0.47
3:B:167:ASN:OD1	3:B:252:LEU:HD13	2.15	0.47
1:K:241:LYS:HA	1:K:241:LYS:CE	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:209:ILE:HG23	2:A:230:LEU:HD23	1.96	0.47
3:B:167:ASN:OD1	3:B:252:LEU:HD13	2.15	0.47
2:A:7:ILE:CD1	2:A:137:VAL:HG22	2.44	0.46
2:A:7:ILE:CD1	2:A:137:VAL:HG22	2.44	0.46
3:B:264:ARG:O	3:B:265:LEU:HB3	2.15	0.46
1:K:127:ALA:HA	1:K:134:TYR:HE2	1.81	0.46
1:K:295:LEU:HD21	1:K:320:LEU:HB3	1.96	0.46
3:B:230:LEU:HD23	3:B:231:VAL:N	2.31	0.46
3:B:325:MET:HA	3:B:325:MET:HE3	1.96	0.46
3:B:230:LEU:HD23	3:B:231:VAL:N	2.31	0.46
3:B:325:MET:HE3	3:B:325:MET:HA	1.96	0.46
2:A:9:VAL:HG11	2:A:150:THR:OG1	2.15	0.46
2:A:9:VAL:HG11	2:A:150:THR:OG1	2.15	0.46
1:K:122:THR:HG22	1:K:129:GLU:HG3	1.96	0.46
1:K:112:TYR:CZ	1:K:345:THR:HG22	2.51	0.46
2:A:343:PHE:CZ	2:A:351:PHE:CE2	3.03	0.46
1:K:304:HIS:HA	3:B:434:GLN:NE2	2.31	0.46
1:K:265:ALA:HB2	2:A:108:TYR:HD2	1.75	0.46
2:A:343:PHE:CZ	2:A:351:PHE:CE2	3.03	0.46
2:A:93:ILE:HG21	2:A:118:VAL:HG22	1.98	0.46
3:B:67:LEU:HD12	3:B:92:PHE:CE1	2.50	0.46
1:K:114:ALA:CB	1:K:338:PHE:HD1	2.29	0.46
2:A:93:ILE:HG21	2:A:118:VAL:HG22	1.98	0.46
3:B:67:LEU:HD12	3:B:92:PHE:CE1	2.50	0.46
1:K:227:ARG:HA	1:K:260:ALA:HB2	1.98	0.46
2:A:264:ARG:HB2	2:A:266:HIS:CD2	2.51	0.46
3:B:299:LYS:HD3	3:B:299:LYS:H	1.81	0.46
3:B:4:ILE:HG21	3:B:136:GLN:HG2	1.97	0.46
2:A:264:ARG:HB2	2:A:266:HIS:CD2	2.51	0.46
3:B:299:LYS:HD3	3:B:299:LYS:H	1.81	0.46
3:B:4:ILE:HG21	3:B:136:GLN:HG2	1.97	0.46
1:K:108:THR:HG21	1:K:320:LEU:CG	2.46	0.45
1:K:189:VAL:HG23	1:K:192:LEU:HD23	1.97	0.45
2:A:331:ALA:O	2:A:335:ILE:HG12	2.16	0.45
1:K:237:ARG:HG2	1:K:249:VAL:CG2	2.46	0.45
1:K:335:SER:HB3	1:K:338:PHE:CD2	2.51	0.45
2:A:331:ALA:O	2:A:335:ILE:HG12	2.16	0.45
1:K:101:PHE:CZ	1:K:236:LEU:HB2	2.52	0.45
3:B:276:THR:O	9:B:601:TA1:H192	2.16	0.45
3:B:276:THR:O	9:B:601:TA1:H192	2.16	0.45
1:K:163:TYR:CE1	1:K:277:GLU:HG3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:23:LEU:HD23	2:A:236:SER:HB2	1.99	0.45
2:A:278:ALA:HB2	2:A:368:LEU:O	2.16	0.45
3:B:332:MET:CE	3:B:351:VAL:HG11	2.46	0.45
2:A:23:LEU:HD23	2:A:236:SER:HB2	1.99	0.45
2:A:278:ALA:HB2	2:A:368:LEU:O	2.16	0.45
3:B:332:MET:CE	3:B:351:VAL:HG11	2.46	0.45
2:A:112:LYS:O	2:A:115:ILE:HG22	2.17	0.45
2:A:184:PRO:HG2	2:A:398:MET:CE	2.46	0.45
2:A:112:LYS:O	2:A:115:ILE:HG22	2.17	0.45
2:A:184:PRO:HG2	2:A:398:MET:CE	2.46	0.45
1:K:86:GLN:OE1	1:K:132:VAL:HG23	2.16	0.45
3:B:369:ARG:C	3:B:369:ARG:HD2	2.38	0.45
3:B:315:VAL:HG13	3:B:377:PHE:CE1	2.52	0.45
1:K:80:PHE:CE2	1:K:88:GLU:HG2	2.52	0.45
3:B:369:ARG:HD2	3:B:369:ARG:C	2.38	0.45
3:B:315:VAL:HG13	3:B:377:PHE:CE1	2.52	0.45
2:A:313:MET:HB3	2:A:344:VAL:HG21	1.98	0.45
2:A:313:MET:HB3	2:A:344:VAL:HG21	1.98	0.45
3:B:319:PHE:CD2	3:B:375:ALA:HB2	2.51	0.44
3:B:319:PHE:CD2	3:B:375:ALA:HB2	2.51	0.44
2:A:98:ASP:HB2	2:A:105:ARG:HH21	1.80	0.44
1:K:157:VAL:HG21	1:K:203:ILE:HD12	2.00	0.44
2:A:98:ASP:HB2	2:A:105:ARG:HH21	1.80	0.44
1:K:286:LEU:CD1	2:A:409:VAL:HG21	2.41	0.44
1:K:37:VAL:CG2	1:K:43:VAL:HG23	2.48	0.44
1:K:312:LEU:HD22	1:K:312:LEU:HA	1.82	0.44
3:B:318:VAL:HA	3:B:354:ALA:HB3	1.98	0.44
3:B:318:VAL:HA	3:B:354:ALA:HB3	1.98	0.44
2:A:317:LEU:HD23	2:A:377:MET:CB	2.48	0.44
3:B:67:LEU:HD12	3:B:92:PHE:CD1	2.53	0.44
2:A:317:LEU:HD23	2:A:377:MET:CB	2.48	0.44
3:B:67:LEU:HD12	3:B:92:PHE:CD1	2.53	0.44
2:A:220:GLU:C	2:A:222:PRO:HD3	2.38	0.44
2:A:144:GLY:N	7:A:503:GTP:O3G	2.48	0.44
2:A:220:GLU:C	2:A:222:PRO:HD3	2.38	0.44
2:A:144:GLY:N	7:A:503:GTP:O3G	2.48	0.44
3:B:118:VAL:O	3:B:122:VAL:HG13	2.18	0.44
1:K:113:GLY:CA	1:K:331:ALA:HB3	2.47	0.44
1:K:304:HIS:HA	3:B:434:GLN:HE22	1.83	0.44
3:B:118:VAL:O	3:B:122:VAL:HG13	2.18	0.44
1:K:271:LYS:HG2	1:K:271:LYS:H	1.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:17:ARG:HG3	1:K:89:VAL:CG2	2.48	0.44
2:A:231:ILE:O	2:A:235:VAL:HG23	2.17	0.44
2:A:231:ILE:O	2:A:235:VAL:HG23	2.17	0.44
1:K:97:ILE:HG23	1:K:107:CYS:HB3	2.00	0.44
1:K:31:HIS:CE1	1:K:46:PRO:HB2	2.53	0.43
2:A:115:ILE:O	2:A:115:ILE:HD13	2.18	0.43
2:A:231:ILE:HD13	2:A:231:ILE:N	2.34	0.43
2:A:236:SER:O	2:A:240:ALA:HB3	2.18	0.43
2:A:104:ALA:HB1	2:A:413:MET:HG3	1.99	0.43
3:B:33:THR:HG22	3:B:33:THR:O	2.18	0.43
9:B:601:TA1:C26	9:B:601:TA1:H463	2.46	0.43
1:K:133:MET:HG2	1:K:256:LEU:HD13	1.99	0.43
1:K:307:TYR:CD1	1:K:317:LYS:HG3	2.53	0.43
2:A:115:ILE:O	2:A:115:ILE:HD13	2.18	0.43
2:A:231:ILE:N	2:A:231:ILE:HD13	2.34	0.43
2:A:236:SER:O	2:A:240:ALA:HB3	2.18	0.43
2:A:104:ALA:HB1	2:A:413:MET:HG3	1.99	0.43
3:B:33:THR:O	3:B:33:THR:HG22	2.18	0.43
9:B:601:TA1:H463	9:B:601:TA1:C26	2.46	0.43
2:A:109:THR:HG22	2:A:110:ILE:N	2.34	0.43
3:B:147:SER:O	3:B:151:THR:HB	2.18	0.43
3:B:319:PHE:HA	3:B:375:ALA:HA	2.00	0.43
1:K:13:LYS:HB2	1:K:13:LYS:HE3	1.70	0.43
1:K:151:LYS:HA	1:K:241:LYS:HG2	2.00	0.43
2:A:109:THR:HG22	2:A:110:ILE:N	2.34	0.43
3:B:147:SER:O	3:B:151:THR:HB	2.18	0.43
3:B:319:PHE:HA	3:B:375:ALA:HA	2.00	0.43
1:K:286:LEU:CD2	2:A:406:HIS:HA	2.48	0.43
2:A:238:ILE:HD11	2:A:378:LEU:HD23	1.99	0.43
1:K:265:ALA:CB	2:A:108:TYR:HD2	2.31	0.43
2:A:238:ILE:HD11	2:A:378:LEU:HD23	1.99	0.43
3:B:101:ASN:ND2	3:B:143:GLY:HA2	2.33	0.43
3:B:101:ASN:ND2	3:B:143:GLY:HA2	2.33	0.43
1:K:165:GLU:HG3	1:K:311:LYS:HE3	2.00	0.43
2:A:191:THR:HG21	2:A:425:MET:SD	2.59	0.43
3:B:176:LYS:HE3	3:B:207:GLU:HG3	2.00	0.43
1:K:90:PHE:CD2	1:K:135:LEU:HB3	2.54	0.43
2:A:191:THR:HG21	2:A:425:MET:SD	2.59	0.43
3:B:176:LYS:HE3	3:B:207:GLU:HG3	2.00	0.43
2:A:341:ILE:O	2:A:341:ILE:HG12	2.19	0.43
2:A:341:ILE:O	2:A:341:ILE:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:237:ARG:HG2	1:K:249:VAL:HG21	1.99	0.43
1:K:271:LYS:HG3	1:K:273:THR:HG23	2.00	0.43
2:A:16:ILE:HD12	2:A:171:ILE:HD11	2.01	0.43
2:A:202:PHE:CE1	2:A:378:LEU:HD22	2.53	0.43
2:A:224:TYR:OH	7:A:503:GTP:H2'	2.19	0.43
2:A:407:TRP:HE1	3:B:260:VAL:HG23	1.83	0.43
2:A:16:ILE:HD12	2:A:171:ILE:HD11	2.01	0.43
2:A:202:PHE:CE1	2:A:378:LEU:HD22	2.53	0.43
2:A:224:TYR:OH	7:A:503:GTP:H2'	2.19	0.43
2:A:407:TRP:HE1	3:B:260:VAL:HG23	1.83	0.43
2:A:318:LEU:HB2	2:A:376:CYS:SG	2.59	0.42
3:B:210:TYR:CD1	3:B:227:LEU:HD21	2.53	0.42
1:K:265:ALA:HB2	2:A:108:TYR:CE2	2.54	0.42
2:A:318:LEU:HB2	2:A:376:CYS:SG	2.59	0.42
3:B:210:TYR:CD1	3:B:227:LEU:HD21	2.53	0.42
1:K:46:PRO:HB2	1:K:47:LYS:H	1.66	0.42
1:K:14:VAL:HB	1:K:76:PHE:CE2	2.54	0.42
1:K:113:GLY:HA3	1:K:120:THR:HG22	2.01	0.42
1:K:158:SER:HB2	1:K:192:LEU:HD11	2.00	0.42
1:K:164:ASN:HA	1:K:280:ASN:CG	2.39	0.42
2:A:144:GLY:H	7:A:503:GTP:PG	2.42	0.42
1:K:236:LEU:O	1:K:251:ILE:HA	2.20	0.42
2:A:144:GLY:H	7:A:503:GTP:PG	2.42	0.42
2:A:104:ALA:HB2	2:A:413:MET:HG3	1.99	0.42
2:A:132:LEU:CD2	2:A:164:LYS:HE3	2.50	0.42
2:A:152:LEU:HA	2:A:155:GLU:HB2	1.99	0.42
2:A:269:LEU:HD22	2:A:384:ILE:HD11	2.00	0.42
2:A:104:ALA:HB2	2:A:413:MET:HG3	1.99	0.42
2:A:132:LEU:CD2	2:A:164:LYS:HE3	2.50	0.42
2:A:152:LEU:HA	2:A:155:GLU:HB2	1.99	0.42
2:A:269:LEU:HD22	2:A:384:ILE:HD11	2.00	0.42
3:B:297:ASP:OD2	3:B:299:LYS:HE2	2.20	0.42
3:B:413:MET:CG	3:B:414:ASP:H	2.32	0.42
1:K:107:CYS:O	1:K:254:MET:HA	2.19	0.42
1:K:11:HIS:CE1	1:K:299:LYS:HE3	2.55	0.42
3:B:297:ASP:OD2	3:B:299:LYS:HE2	2.20	0.42
3:B:413:MET:CG	3:B:414:ASP:H	2.32	0.42
1:K:217:HIS:CD2	1:K:225:SER:HA	2.54	0.42
1:K:232:PHE:HB3	1:K:256:LEU:HB3	2.02	0.42
1:K:265:ALA:HB2	2:A:108:TYR:CE2	2.54	0.42
2:A:344:VAL:HG12	2:A:345:ASP:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:172:VAL:HG11	3:B:387:LEU:CD2	2.24	0.42
2:A:344:VAL:HG12	2:A:345:ASP:N	2.34	0.42
3:B:172:VAL:HG11	3:B:387:LEU:CD2	2.24	0.42
1:K:163:TYR:HE1	1:K:277:GLU:HG3	1.84	0.42
1:K:160:LEU:HD13	1:K:167:ILE:HG23	2.02	0.42
2:A:141:PHE:HB3	2:A:173:PRO:HD3	2.02	0.42
3:B:3:GLU:HA	3:B:51:VAL:HA	2.01	0.42
1:K:101:PHE:CD1	1:K:252:ALA:HB3	2.55	0.42
1:K:305:ILE:C	1:K:305:ILE:HD13	2.40	0.42
2:A:141:PHE:HB3	2:A:173:PRO:HD3	2.02	0.42
3:B:3:GLU:HA	3:B:51:VAL:HA	2.01	0.42
2:A:11:GLN:HB3	7:A:503:GTP:O2B	2.20	0.42
2:A:179:THR:HG21	3:B:248:LEU:HD22	2.00	0.42
1:K:94:THR:HG21	1:K:136:THR:HB	2.01	0.42
2:A:11:GLN:HB3	7:A:503:GTP:O2B	2.20	0.42
2:A:179:THR:HG21	3:B:248:LEU:HD22	2.00	0.42
3:B:191:VAL:CG1	3:B:425:MET:HG3	2.50	0.41
3:B:44:LEU:HD12	3:B:49:ILE:HD13	2.01	0.41
1:K:140:LEU:HG	1:K:144:MET:SD	2.60	0.41
1:K:144:MET:O	1:K:148:LYS:HG3	2.20	0.41
3:B:191:VAL:CG1	3:B:425:MET:HG3	2.50	0.41
3:B:44:LEU:HD12	3:B:49:ILE:HD13	2.01	0.41
2:A:21:TRP:HE1	2:A:63:PRO:HB3	1.85	0.41
2:A:99:ALA:H	3:B:2:ARG:HH22	1.68	0.41
3:B:93:VAL:CG1	3:B:118:VAL:HG22	2.42	0.41
3:B:147:SER:HB2	3:B:190:SER:HB3	2.01	0.41
3:B:154:ILE:HG22	3:B:166:MET:CE	2.51	0.41
1:K:151:LYS:HB3	1:K:239:GLN:O	2.20	0.41
1:K:204:LEU:HD13	1:K:207:LEU:HD12	2.01	0.41
2:A:21:TRP:HE1	2:A:63:PRO:HB3	1.85	0.41
2:A:99:ALA:H	3:B:2:ARG:HH22	1.68	0.41
3:B:93:VAL:CG1	3:B:118:VAL:HG22	2.42	0.41
3:B:147:SER:HB2	3:B:190:SER:HB3	2.01	0.41
3:B:154:ILE:HG22	3:B:166:MET:CE	2.51	0.41
3:B:24:ILE:HD11	3:B:52:TYR:CE2	2.56	0.41
3:B:24:ILE:HD11	3:B:52:TYR:CE2	2.56	0.41
2:A:152:LEU:HD12	2:A:153:LEU:N	2.35	0.41
2:A:274:PRO:HB2	2:A:371:VAL:HG21	2.03	0.41
1:K:86:GLN:CG	1:K:129:GLU:HB3	2.50	0.41
1:K:159:TYR:CE2	1:K:170:LEU:HD22	2.55	0.41
2:A:152:LEU:HD12	2:A:153:LEU:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:274:PRO:HB2	2:A:371:VAL:HG21	2.03	0.41
2:A:210:TYR:CD1	2:A:227:LEU:HD21	2.56	0.41
3:B:63:PRO:HD2	3:B:86:ILE:HG12	2.03	0.41
1:K:272:GLY:HA2	1:K:275:PHE:HB2	2.02	0.41
2:A:210:TYR:CD1	2:A:227:LEU:HD21	2.56	0.41
3:B:63:PRO:HD2	3:B:86:ILE:HG12	2.03	0.41
1:K:73:LYS:HG3	1:K:73:LYS:H	1.70	0.41
3:B:154:ILE:HG22	3:B:166:MET:HE1	2.02	0.41
1:K:159:TYR:CD2	1:K:231:VAL:O	2.73	0.41
3:B:154:ILE:HG22	3:B:166:MET:HE1	2.02	0.41
1:K:33:VAL:HG21	1:K:339:TYR:HA	2.01	0.41
3:B:114:LEU:HD23	3:B:149:MET:HE2	1.98	0.41
1:K:232:PHE:O	1:K:255:SER:HA	2.20	0.41
3:B:114:LEU:HD23	3:B:149:MET:HE2	1.98	0.41
2:A:212:ILE:HD11	2:A:302:MET:H	1.86	0.41
3:B:165:ILE:H	3:B:165:ILE:HD13	1.85	0.41
3:B:35:SER:HB3	3:B:59:ASN:CA	2.51	0.41
1:K:217:HIS:NE2	1:K:225:SER:HA	2.36	0.41
2:A:212:ILE:HD11	2:A:302:MET:H	1.86	0.41
3:B:165:ILE:H	3:B:165:ILE:HD13	1.85	0.41
3:B:35:SER:HB3	3:B:59:ASN:CA	2.51	0.41
1:K:152:ILE:HG23	1:K:239:GLN:HB3	2.03	0.41
2:A:315:CYS:HB3	2:A:377:MET:HE2	2.02	0.41
3:B:212:ILE:HG12	3:B:300:ASN:H	1.86	0.41
3:B:236:SER:O	3:B:240:THR:HG23	2.20	0.41
2:A:97:GLU:HB2	2:A:110:ILE:HD11	2.03	0.41
2:A:315:CYS:HB3	2:A:377:MET:HE2	2.02	0.41
3:B:212:ILE:HG12	3:B:300:ASN:H	1.86	0.41
3:B:236:SER:O	3:B:240:THR:HG23	2.20	0.41
2:A:97:GLU:HB2	2:A:110:ILE:HD11	2.03	0.41
2:A:229:ARG:NH1	2:A:363:VAL:HG21	2.36	0.41
1:K:18:VAL:HG22	1:K:332:VAL:HG21	2.03	0.41
2:A:229:ARG:NH1	2:A:363:VAL:HG21	2.36	0.41
1:K:163:TYR:HB2	1:K:228:SER:OG	2.20	0.41
2:A:234:ILE:HD13	2:A:234:ILE:O	2.21	0.40
3:B:76:ASP:HA	3:B:79:ARG:HG2	2.03	0.40
1:K:17:ARG:HE	1:K:17:ARG:HB3	1.72	0.40
1:K:332:VAL:HG11	1:K:346:LEU:HD21	2.03	0.40
2:A:234:ILE:O	2:A:234:ILE:HD13	2.21	0.40
3:B:76:ASP:HA	3:B:79:ARG:HG2	2.03	0.40
1:K:119:LYS:H	1:K:119:LYS:HD2	1.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:196:GLN:HA	1:K:197:PRO:HD3	1.90	0.40
1:K:33:VAL:CG2	1:K:339:TYR:HA	2.51	0.40
2:A:115:ILE:CD1	2:A:119:LEU:HG	2.50	0.40
2:A:9:VAL:HG21	2:A:149:PHE:HD1	1.86	0.40
2:A:295:CYS:HB3	2:A:377:MET:HG2	2.02	0.40
2:A:63:PRO:HD3	2:A:86:LEU:O	2.21	0.40
3:B:133:GLN:HE21	3:B:243:ARG:NH2	2.18	0.40
1:K:17:ARG:NE	1:K:89:VAL:HG21	2.36	0.40
1:K:227:ARG:HA	1:K:260:ALA:CB	2.50	0.40
2:A:115:ILE:CD1	2:A:119:LEU:HG	2.50	0.40
2:A:9:VAL:HG21	2:A:149:PHE:HD1	1.86	0.40
2:A:295:CYS:HB3	2:A:377:MET:HG2	2.02	0.40
2:A:63:PRO:HD3	2:A:86:LEU:O	2.21	0.40
3:B:133:GLN:HE21	3:B:243:ARG:NH2	2.18	0.40
1:K:17:ARG:HG3	1:K:89:VAL:HG22	2.03	0.40
2:A:133:GLN:HB3	2:A:243:ARG:HH12	1.86	0.40
3:B:242:LEU:HD23	3:B:242:LEU:HA	1.90	0.40
3:B:70:LEU:H	3:B:145:THR:CG2	2.29	0.40
1:K:90:PHE:CG	1:K:135:LEU:CB	3.03	0.40
2:A:133:GLN:HB3	2:A:243:ARG:HH12	1.86	0.40
3:B:242:LEU:HA	3:B:242:LEU:HD23	1.90	0.40
3:B:70:LEU:H	3:B:145:THR:CG2	2.29	0.40
1:K:241:LYS:HE3	1:K:241:LYS:HA	2.03	0.40
2:A:155:GLU:HA	2:A:197:HIS:ND1	2.36	0.40
2:A:298:PRO:HB3	2:A:307:PRO:HD2	2.03	0.40
3:B:311:ARG:HD3	3:B:342:TYR:HA	2.04	0.40
1:K:17:ARG:HH21	1:K:123:MET:HG3	1.86	0.40
1:K:152:ILE:HG13	1:K:237:ARG:HH22	1.87	0.40
2:A:155:GLU:HA	2:A:197:HIS:ND1	2.36	0.40
2:A:298:PRO:HB3	2:A:307:PRO:HD2	2.03	0.40
3:B:311:ARG:HD3	3:B:342:TYR:HA	2.04	0.40
1:K:152:ILE:HG22	1:K:241:LYS:HG3	2.03	0.40
1:K:21:GLU:HG2	1:K:335:SER:HB2	2.04	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 PDB entries followed by that with respect to all EM entries.

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	1-K	324/377 (86%)	288 (89%)	28 (9%)	8 (2%)	6	42
1	2-K	324/377 (86%)	292 (90%)	28 (9%)	4 (1%)	15	58
2	1-A	408/451 (90%)	316 (78%)	66 (16%)	26 (6%)	1	23
2	2-A	408/451 (90%)	317 (78%)	65 (16%)	26 (6%)	1	23
3	1-B	424/445 (95%)	338 (80%)	66 (16%)	20 (5%)	3	29
3	2-B	424/445 (95%)	338 (80%)	66 (16%)	20 (5%)	3	29
All	All	2312/2546 (91%)	1889 (82%)	319 (14%)	104 (4%)	5	30

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-K	33	VAL
1	1-K	268	SER
2	1-A	97	GLU
2	1-A	108	TYR
2	1-A	109	THR
2	1-A	141	PHE
2	1-A	183	GLU
2	1-A	245	ASP
2	1-A	266	HIS
2	1-A	280	LYS
2	1-A	284	GLU
2	1-A	285	GLN
2	1-A	437	VAL
3	1-B	82	PRO
3	1-B	97	SER
3	1-B	183	GLU
3	1-B	278	ARG
3	1-B	282	GLN
3	1-B	288	VAL
3	1-B	344	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1-B	369	ARG
3	1-B	403	ALA
2	2-A	97	GLU
2	2-A	109	THR
2	2-A	141	PHE
2	2-A	183	GLU
2	2-A	245	ASP
2	2-A	266	HIS
2	2-A	280	LYS
2	2-A	284	GLU
2	2-A	285	GLN
2	2-A	437	VAL
3	2-B	82	PRO
3	2-B	97	SER
3	2-B	183	GLU
3	2-B	265	LEU
3	2-B	278	ARG
3	2-B	282	GLN
3	2-B	288	VAL
3	2-B	344	VAL
3	2-B	369	ARG
3	2-B	403	ALA
1	1-K	69	ASN
1	1-K	224	THR
2	1-A	100	ALA
2	1-A	251	ASP
2	1-A	342	GLN
3	1-B	38	GLY
3	1-B	175	PRO
3	1-B	265	LEU
3	1-B	266	HIS
1	2-K	46	PRO
2	2-A	100	ALA
2	2-A	108	TYR
2	2-A	251	ASP
2	2-A	342	GLN
3	2-B	38	GLY
3	2-B	175	PRO
3	2-B	266	HIS
2	1-A	309	HIS
2	1-A	330	ALA
2	1-A	339	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1-B	32	PRO
3	1-B	273	ALA
1	2-K	40	HIS
2	2-A	309	HIS
2	2-A	330	ALA
2	2-A	339	ARG
3	2-B	32	PRO
3	2-B	273	ALA
1	1-K	37	VAL
1	1-K	301	LYS
1	1-K	302	ASN
2	1-A	173	PRO
2	1-A	255	PHE
2	1-A	287	SER
2	1-A	366	GLY
3	1-B	43	GLN
3	1-B	99	ALA
3	1-B	298	ALA
1	2-K	220	ASP
2	2-A	173	PRO
2	2-A	255	PHE
2	2-A	287	SER
2	2-A	366	GLY
3	2-B	43	GLN
3	2-B	99	ALA
3	2-B	298	ALA
2	1-A	403	ALA
3	1-B	343	PHE
3	1-B	386	GLU
2	2-A	403	ALA
3	2-B	343	PHE
3	2-B	386	GLU
2	1-A	221	ARG
2	1-A	273	ALA
2	2-A	221	ARG
2	2-A	273	ALA
1	1-K	29	GLY
1	2-K	104	GLY
2	1-A	238	ILE
2	2-A	238	ILE
2	1-A	275	VAL
2	2-A	275	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 PDB entries followed by that with respect to all EM entries.

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	1-K	287/334 (86%)	251 (88%)	36 (12%)	5	28
1	2-K	287/334 (86%)	243 (85%)	44 (15%)	3	21
2	1-A	347/377 (92%)	303 (87%)	44 (13%)	5	27
2	2-A	347/377 (92%)	303 (87%)	44 (13%)	5	27
3	1-B	367/381 (96%)	312 (85%)	55 (15%)	3	22
3	2-B	367/381 (96%)	312 (85%)	55 (15%)	3	22
All	All	2002/2184 (92%)	1724 (86%)	278 (14%)	8	25

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-K	11	HIS
1	1-K	17	ARG
1	1-K	68	GLN
1	1-K	73	LYS
1	1-K	76	PHE
1	1-K	102	LEU
1	1-K	110	LEU
1	1-K	112	TYR
1	1-K	119	LYS
1	1-K	121	HIS
1	1-K	124	LEU
1	1-K	133	MET
1	1-K	134	TYR
1	1-K	137	MET
1	1-K	151	LYS
1	1-K	159	TYR
1	1-K	168	ARG
1	1-K	182	ASP
1	1-K	198	LYS
1	1-K	211	ASN
1	1-K	214	ARG
1	1-K	224	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-K	225	SER
1	1-K	237	ARG
1	1-K	241	LYS
1	1-K	248	ASN
1	1-K	254	MET
1	1-K	256	LEU
1	1-K	274	ARG
1	1-K	302	ASN
1	1-K	305	ILE
1	1-K	312	LEU
1	1-K	317	LYS
1	1-K	318	ASP
1	1-K	341	ASP
1	1-K	356	LYS
2	1-A	6	SER
2	1-A	20	CYS
2	1-A	21	TRP
2	1-A	25	CYS
2	1-A	32	PRO
2	1-A	98	ASP
2	1-A	115	ILE
2	1-A	120	ASP
2	1-A	127	ASP
2	1-A	130	THR
2	1-A	135	PHE
2	1-A	141	PHE
2	1-A	150	THR
2	1-A	152	LEU
2	1-A	154	MET
2	1-A	155	GLU
2	1-A	169	PHE
2	1-A	172	TYR
2	1-A	173	PRO
2	1-A	183	GLU
2	1-A	192	HIS
2	1-A	194	THR
2	1-A	224	TYR
2	1-A	231	ILE
2	1-A	234	ILE
2	1-A	237	SER
2	1-A	243	ARG
2	1-A	244	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1-A	253	THR
2	1-A	260	VAL
2	1-A	267	PHE
2	1-A	276	ILE
2	1-A	284	GLU
2	1-A	303	VAL
2	1-A	334	THR
2	1-A	345	ASP
2	1-A	368	LEU
2	1-A	376	CYS
2	1-A	380	ASN
2	1-A	388	TRP
2	1-A	415	GLU
2	1-A	417	GLU
2	1-A	425	MET
2	1-A	433	GLU
3	1-B	24	ILE
3	1-B	26	ASP
3	1-B	32	PRO
3	1-B	41	ASP
3	1-B	48	ARG
3	1-B	59	ASN
3	1-B	67	LEU
3	1-B	68	VAL
3	1-B	90	ASP
3	1-B	94	PHE
3	1-B	122	VAL
3	1-B	129	CYS
3	1-B	135	PHE
3	1-B	139	HIS
3	1-B	145	THR
3	1-B	149	MET
3	1-B	151	THR
3	1-B	153	LEU
3	1-B	161	TYR
3	1-B	163	ASP
3	1-B	165	ILE
3	1-B	174	SER
3	1-B	193	GLN
3	1-B	195	VAL
3	1-B	198	THR
3	1-B	201	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1-B	203	CYS
3	1-B	207	GLU
3	1-B	214	PHE
3	1-B	215	ARG
3	1-B	226	ASP
3	1-B	227	LEU
3	1-B	230	LEU
3	1-B	240	THR
3	1-B	265	LEU
3	1-B	267	PHE
3	1-B	275	LEU
3	1-B	282	GLN
3	1-B	284	ARG
3	1-B	299	LYS
3	1-B	306	ASP
3	1-B	309	HIS
3	1-B	322	ARG
3	1-B	324	SER
3	1-B	325	MET
3	1-B	343	PHE
3	1-B	344	VAL
3	1-B	349	ASN
3	1-B	369	ARG
3	1-B	387	LEU
3	1-B	413	MET
3	1-B	424	ASN
3	1-B	427	ASP
3	1-B	432	TYR
3	1-B	437	ASP
1	2-K	17	ARG
1	2-K	38	ASP
1	2-K	42	LEU
1	2-K	73	LYS
1	2-K	76	PHE
1	2-K	82	GLU
1	2-K	102	LEU
1	2-K	112	TYR
1	2-K	120	THR
1	2-K	126	SER
1	2-K	129	GLU
1	2-K	133	MET
1	2-K	151	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-K	154	SER
1	2-K	155	THR
1	2-K	158	SER
1	2-K	160	LEU
1	2-K	170	LEU
1	2-K	180	ARG
1	2-K	182	ASP
1	2-K	192	LEU
1	2-K	193	THR
1	2-K	195	HIS
1	2-K	200	SER
1	2-K	201	GLU
1	2-K	219	THR
1	2-K	225	SER
1	2-K	233	GLN
1	2-K	250	ARG
1	2-K	259	LEU
1	2-K	267	THR
1	2-K	273	THR
1	2-K	274	ARG
1	2-K	310	SER
1	2-K	312	LEU
1	2-K	318	ASP
1	2-K	319	SER
1	2-K	324	CYS
1	2-K	333	SER
1	2-K	336	SER
1	2-K	341	ASP
1	2-K	346	LEU
1	2-K	348	TYR
1	2-K	354	ASP
2	2-A	6	SER
2	2-A	20	CYS
2	2-A	21	TRP
2	2-A	25	CYS
2	2-A	32	PRO
2	2-A	98	ASP
2	2-A	115	ILE
2	2-A	120	ASP
2	2-A	127	ASP
2	2-A	130	THR
2	2-A	135	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2-A	141	PHE
2	2-A	150	THR
2	2-A	152	LEU
2	2-A	154	MET
2	2-A	155	GLU
2	2-A	169	PHE
2	2-A	172	TYR
2	2-A	173	PRO
2	2-A	183	GLU
2	2-A	192	HIS
2	2-A	194	THR
2	2-A	224	TYR
2	2-A	231	ILE
2	2-A	234	ILE
2	2-A	237	SER
2	2-A	243	ARG
2	2-A	244	PHE
2	2-A	253	THR
2	2-A	260	VAL
2	2-A	267	PHE
2	2-A	276	ILE
2	2-A	284	GLU
2	2-A	303	VAL
2	2-A	334	THR
2	2-A	345	ASP
2	2-A	368	LEU
2	2-A	376	CYS
2	2-A	380	ASN
2	2-A	388	TRP
2	2-A	417	GLU
2	2-A	419	SER
2	2-A	425	MET
2	2-A	433	GLU
3	2-B	24	ILE
3	2-B	26	ASP
3	2-B	32	PRO
3	2-B	41	ASP
3	2-B	48	ARG
3	2-B	59	ASN
3	2-B	67	LEU
3	2-B	68	VAL
3	2-B	90	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-B	94	PHE
3	2-B	122	VAL
3	2-B	129	CYS
3	2-B	135	PHE
3	2-B	139	HIS
3	2-B	145	THR
3	2-B	149	MET
3	2-B	151	THR
3	2-B	153	LEU
3	2-B	161	TYR
3	2-B	163	ASP
3	2-B	165	ILE
3	2-B	174	SER
3	2-B	193	GLN
3	2-B	195	VAL
3	2-B	198	THR
3	2-B	201	THR
3	2-B	203	CYS
3	2-B	207	GLU
3	2-B	214	PHE
3	2-B	215	ARG
3	2-B	226	ASP
3	2-B	227	LEU
3	2-B	230	LEU
3	2-B	240	THR
3	2-B	265	LEU
3	2-B	267	PHE
3	2-B	275	LEU
3	2-B	282	GLN
3	2-B	284	ARG
3	2-B	299	LYS
3	2-B	306	ASP
3	2-B	309	HIS
3	2-B	322	ARG
3	2-B	324	SER
3	2-B	325	MET
3	2-B	343	PHE
3	2-B	344	VAL
3	2-B	349	ASN
3	2-B	369	ARG
3	2-B	387	LEU
3	2-B	413	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-B	424	ASN
3	2-B	427	ASP
3	2-B	432	TYR
3	2-B	437	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-K	31	HIS
1	1-K	106	ASN
1	1-K	205	HIS
1	1-K	209	ASN
1	1-K	222	ASN
1	1-K	302	ASN
1	1-K	325	GLN
2	1-A	8	HIS
2	1-A	11	GLN
2	1-A	15	GLN
2	1-A	206	ASN
2	1-A	216	ASN
2	1-A	226	ASN
2	1-A	256	GLN
2	1-A	380	ASN
3	1-B	102	ASN
3	1-B	133	GLN
3	1-B	136	GLN
3	1-B	186	ASN
3	1-B	206	ASN
3	1-B	349	ASN
3	1-B	380	ASN
3	1-B	385	GLN
3	1-B	424	ASN
3	1-B	433	GLN
3	1-B	434	GLN
3	1-B	436	GLN
1	2-K	293	ASN
1	2-K	303	GLN
1	2-K	344	ASN
1	2-K	350	ASN
2	2-A	8	HIS
2	2-A	11	GLN
2	2-A	15	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2-A	206	ASN
2	2-A	216	ASN
2	2-A	226	ASN
2	2-A	256	GLN
2	2-A	380	ASN
3	2-B	102	ASN
3	2-B	133	GLN
3	2-B	136	GLN
3	2-B	186	ASN
3	2-B	206	ASN
3	2-B	349	ASN
3	2-B	380	ASN
3	2-B	385	GLN
3	2-B	424	ASN
3	2-B	433	GLN
3	2-B	436	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GTP	1-A	503	6	27,34,34	1.53	2 (7%)	27,54,54	2.16	5 (18%)
8	GDP	1-B	600	-	25,30,30	2.61	8 (32%)	26,47,47	3.64	9 (34%)
9	TA1	1-B	601	-	68,68,68	1.97	20 (29%)	105,105,105	1.33	9 (8%)
4	9V5	1-K	401	-	18,20,20	0.63	0	24,29,29	1.48	3 (12%)
7	GTP	2-A	503	6	27,34,34	1.53	2 (7%)	27,54,54	2.16	5 (18%)
8	GDP	2-B	600	-	25,30,30	2.61	8 (32%)	26,47,47	3.64	9 (34%)
9	TA1	2-B	601	-	68,68,68	1.97	20 (29%)	105,105,105	1.33	9 (8%)
4	9V5	2-K	401	-	18,20,20	2.86	4 (22%)	24,29,29	1.90	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GTP	1-A	503	6	-	0/18/38/38	0/3/3/3
8	GDP	1-B	600	-	-	0/12/32/32	0/3/3/3
9	TA1	1-B	601	-	-	0/41/127/127	0/5/7/7
4	9V5	1-K	401	-	-	1/14/16/16	0/2/2/2
7	GTP	2-A	503	6	-	0/18/38/38	0/3/3/3
8	GDP	2-B	600	-	-	0/12/32/32	0/3/3/3
9	TA1	2-B	601	-	-	0/41/127/127	0/5/7/7
4	9V5	2-K	401	-	-	0/14/16/16	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2-B	601	TA1	C08-C07	-5.12	1.25	1.38
9	1-B	601	TA1	C08-C07	-5.12	1.25	1.38
8	2-B	600	GDP	PB-O2B	-3.54	1.40	1.54
8	1-B	600	GDP	PB-O2B	-3.54	1.40	1.54
9	2-B	601	TA1	C04-C03	-2.31	1.44	1.49
9	1-B	601	TA1	C04-C03	-2.31	1.44	1.49
4	2-K	401	9V5	C11-S18	-2.24	1.75	1.78
9	2-B	601	TA1	C10-C02	2.02	1.62	1.57
9	1-B	601	TA1	C10-C02	2.02	1.62	1.57
8	2-B	600	GDP	O3'-C3'	2.11	1.47	1.43
8	1-B	600	GDP	O3'-C3'	2.11	1.47	1.43
9	2-B	601	TA1	C41-C42	2.12	1.42	1.38
9	1-B	601	TA1	C41-C42	2.12	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2-B	601	TA1	C18-C20	2.17	1.62	1.56
9	1-B	601	TA1	C18-C20	2.17	1.62	1.56
9	2-B	601	TA1	C37-C29	2.18	1.54	1.51
9	1-B	601	TA1	C37-C29	2.18	1.54	1.51
9	2-B	601	TA1	C16-C15	2.20	1.56	1.52
9	1-B	601	TA1	C16-C15	2.20	1.56	1.52
8	2-B	600	GDP	PB-O3B	2.22	1.63	1.54
8	1-B	600	GDP	PB-O3B	2.22	1.63	1.54
9	2-B	601	TA1	C01-C45	2.23	1.66	1.56
9	1-B	601	TA1	C01-C45	2.23	1.66	1.56
9	2-B	601	TA1	C11-C10	2.26	1.61	1.55
9	1-B	601	TA1	C11-C10	2.26	1.61	1.55
8	2-B	600	GDP	C5-C4	2.42	1.45	1.40
8	1-B	600	GDP	C5-C4	2.42	1.45	1.40
9	2-B	601	TA1	C26-C25	2.48	1.56	1.51
9	1-B	601	TA1	C26-C25	2.48	1.56	1.51
9	2-B	601	TA1	C43-C26	2.49	1.58	1.52
9	1-B	601	TA1	C43-C26	2.49	1.58	1.52
9	2-B	601	TA1	C43-C01	2.91	1.60	1.54
9	1-B	601	TA1	C43-C01	2.91	1.60	1.54
9	2-B	601	TA1	C25-C24	2.99	1.39	1.34
9	1-B	601	TA1	C25-C24	2.99	1.39	1.34
9	2-B	601	TA1	C46-C45	3.05	1.60	1.53
9	1-B	601	TA1	C46-C45	3.05	1.60	1.53
4	2-K	401	9V5	O16-S18	3.26	1.50	1.44
8	2-B	600	GDP	C8-N7	3.37	1.41	1.34
8	1-B	600	GDP	C8-N7	3.37	1.41	1.34
4	2-K	401	9V5	O17-S18	3.40	1.50	1.44
9	2-B	601	TA1	O02-C03	3.44	1.41	1.34
9	1-B	601	TA1	O02-C03	3.44	1.41	1.34
9	2-B	601	TA1	C36-C31	3.50	1.45	1.39
9	1-B	601	TA1	C36-C31	3.50	1.45	1.39
9	2-B	601	TA1	C45-C24	3.52	1.61	1.54
9	1-B	601	TA1	C45-C24	3.52	1.61	1.54
7	2-A	503	GTP	PG-O3B	3.84	1.66	1.60
7	1-A	503	GTP	PG-O3B	3.84	1.66	1.60
8	2-B	600	GDP	O6-C6	4.08	1.34	1.24
8	1-B	600	GDP	O6-C6	4.08	1.34	1.24
9	2-B	601	TA1	C18-C10	4.29	1.69	1.57
9	1-B	601	TA1	C18-C10	4.29	1.69	1.57
9	2-B	601	TA1	C05-C04	4.49	1.46	1.39
9	1-B	601	TA1	C05-C04	4.49	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-A	503	GTP	C6-N1	4.78	1.41	1.33
7	1-A	503	GTP	C6-N1	4.78	1.41	1.33
9	2-B	601	TA1	C06-C05	5.84	1.50	1.38
9	1-B	601	TA1	C06-C05	5.84	1.50	1.38
8	2-B	600	GDP	O4'-C1'	6.17	1.49	1.41
8	1-B	600	GDP	O4'-C1'	6.17	1.49	1.41
8	2-B	600	GDP	C2-N1	7.61	1.49	1.35
8	1-B	600	GDP	C2-N1	7.61	1.49	1.35
4	2-K	401	9V5	O15-N13	10.74	1.42	1.22

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	2-B	600	GDP	C6-C5-C4	-11.37	109.54	120.84
8	1-B	600	GDP	C6-C5-C4	-11.37	109.54	120.84
7	2-A	503	GTP	C5-C6-N1	-7.10	113.37	123.48
7	1-A	503	GTP	C5-C6-N1	-7.10	113.37	123.48
8	2-B	600	GDP	N2-C2-N1	-5.89	107.82	117.24
8	1-B	600	GDP	N2-C2-N1	-5.89	107.82	117.24
4	2-K	401	9V5	O17-S18-O16	-5.49	108.24	119.29
8	2-B	600	GDP	C4-C5-N7	-5.06	104.53	109.41
8	1-B	600	GDP	C4-C5-N7	-5.06	104.53	109.41
8	2-B	600	GDP	N3-C2-N1	-4.95	120.24	127.46
8	1-B	600	GDP	N3-C2-N1	-4.95	120.24	127.46
9	2-B	601	TA1	C06-C05-C04	-4.90	114.59	120.35
9	1-B	601	TA1	C06-C05-C04	-4.90	114.59	120.35
9	2-B	601	TA1	C05-C04-C03	-3.96	111.47	120.39
9	1-B	601	TA1	C05-C04-C03	-3.96	111.47	120.39
7	2-A	503	GTP	N3-C2-N1	-3.23	122.74	127.46
7	1-A	503	GTP	N3-C2-N1	-3.23	122.74	127.46
9	2-B	601	TA1	O04-C11-C14	-2.76	101.75	108.14
9	1-B	601	TA1	O04-C11-C14	-2.76	101.75	108.14
7	2-A	503	GTP	C6-C5-C4	-2.41	118.44	120.84
7	1-A	503	GTP	C6-C5-C4	-2.41	118.44	120.84
9	2-B	601	TA1	C08-C09-C04	-2.01	117.98	120.35
9	1-B	601	TA1	C08-C09-C04	-2.01	117.98	120.35
7	2-A	503	GTP	O5'-C5'-C4'	2.00	116.10	109.00
7	1-A	503	GTP	O5'-C5'-C4'	2.00	116.10	109.00
8	2-B	600	GDP	O2'-C2'-C3'	2.29	119.17	111.83
8	1-B	600	GDP	O2'-C2'-C3'	2.29	119.17	111.83
9	2-B	601	TA1	O01-C01-C43	2.48	113.42	106.86
9	1-B	601	TA1	O01-C01-C43	2.48	113.42	106.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2-K	401	9V5	C6-C11-S18	2.50	119.88	116.33
4	1-K	401	9V5	C6-C11-S18	2.61	120.03	116.33
9	2-B	601	TA1	C45-C01-C02	2.65	115.17	111.85
9	1-B	601	TA1	C45-C01-C02	2.65	115.17	111.85
9	2-B	601	TA1	C17-C18-C20	2.84	109.83	102.33
9	1-B	601	TA1	C17-C18-C20	2.84	109.83	102.33
4	1-K	401	9V5	O17-S18-O16	3.04	125.40	119.29
8	2-B	600	GDP	C2'-C3'-C4'	3.41	109.26	102.62
8	1-B	600	GDP	C2'-C3'-C4'	3.41	109.26	102.62
9	2-B	601	TA1	C09-C04-C03	3.53	128.34	120.39
9	1-B	601	TA1	C09-C04-C03	3.53	128.34	120.39
8	2-B	600	GDP	C2-N3-C4	3.59	119.36	115.16
8	1-B	600	GDP	C2-N3-C4	3.59	119.36	115.16
4	1-K	401	9V5	C8-C9-N13	3.62	120.02	115.82
4	2-K	401	9V5	C8-C9-N13	3.86	120.30	115.82
8	2-B	600	GDP	C4'-O4'-C1'	4.04	114.07	109.77
8	1-B	600	GDP	C4'-O4'-C1'	4.04	114.07	109.77
4	2-K	401	9V5	C10-S18-C11	4.40	110.81	105.19
9	2-B	601	TA1	C07-C08-C09	5.24	127.42	120.21
9	1-B	601	TA1	C07-C08-C09	5.24	127.42	120.21
7	2-A	503	GTP	C6-N1-C2	6.00	124.69	116.06
7	1-A	503	GTP	C6-N1-C2	6.00	124.69	116.06
8	2-B	600	GDP	N2-C2-N3	7.68	131.94	117.75
8	1-B	600	GDP	N2-C2-N3	7.68	131.94	117.75

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1-K	401	9V5	C9-C11-S18-C10

There are no ring outliers.

7 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1-A	503	GTP	10	0
8	1-B	600	GDP	2	0
9	1-B	601	TA1	6	0
7	2-A	503	GTP	10	0
8	2-B	600	GDP	2	0
9	2-B	601	TA1	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	2-K	401	9V5	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.