



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:22 AM UTC

PDB ID : 8W9Q / pdb_00008w9q
EMDB ID : EMD-37379
Title : Structure of partial Banna virus
Authors : Li, Z.; Cao, S.
Deposited on : 2023-09-05
Resolution : 5.70 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

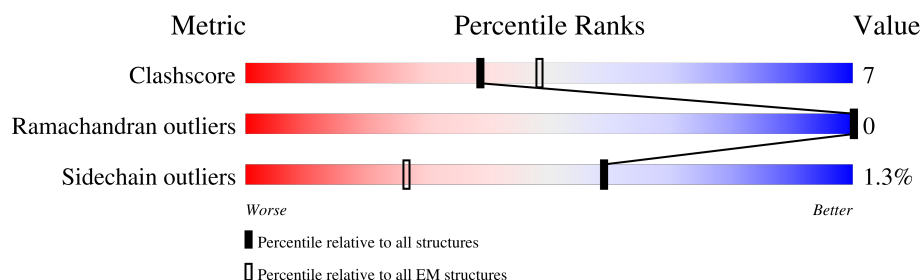
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	955	69% 9% 21%
1	B	955	83% 11% 6%
2	C	302	85% 14% .
2	D	302	85% 14% .
2	E	302	81% 17% .
2	F	302	89% 9% .
2	G	302	82% 17% .
2	H	302	87% 11% ..
2	I	302	87% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	302	 87% 12% .
2	K	302	 86% 12% .
2	L	302	 85% 13% .
2	M	302	 86% 13% .
2	N	302	 83% 16% .
2	O	302	 85% 14% .
3	P	249	 81% 18% .
3	Q	249	 79% 20% .
4	R	628	 75% 21% .
4	S	628	 78% 21% .
4	T	628	 76% 23%
5	r	283	 . . 95%
5	s	283	 . . 95%
5	t	283	 . . 95%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 61697 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 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	751	Total	C	N	O	S	0	0
			6045	3848	1025	1145	27		
1	B	902	Total	C	N	O	S	0	0
			7210	4578	1221	1384	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	LYS	ARG	conflict	UNP Q9INH3
B	97	LYS	ARG	conflict	UNP Q9INH3

- Molecule 2 is a protein called VP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	299	Total	C	N	O	S	0	0
			2288	1449	397	435	7		
2	D	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	E	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	F	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	G	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	H	299	Total	C	N	O	S	0	0
			2288	1449	397	435	7		
2	I	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	J	299	Total	C	N	O	S	0	0
			2288	1449	397	435	7		
2	K	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	L	297	Total	C	N	O	S	0	0
			2270	1438	392	433	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	N	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	O	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	136	ARG	GLN	conflict	UNP W0G587
C	185	LEU	MET	conflict	UNP W0G587
C	266	SER	ALA	conflict	UNP W0G587
D	136	ARG	GLN	conflict	UNP W0G587
D	185	LEU	MET	conflict	UNP W0G587
D	266	SER	ALA	conflict	UNP W0G587
E	136	ARG	GLN	conflict	UNP W0G587
E	185	LEU	MET	conflict	UNP W0G587
E	266	SER	ALA	conflict	UNP W0G587
F	136	ARG	GLN	conflict	UNP W0G587
F	185	LEU	MET	conflict	UNP W0G587
F	266	SER	ALA	conflict	UNP W0G587
G	136	ARG	GLN	conflict	UNP W0G587
G	185	LEU	MET	conflict	UNP W0G587
G	266	SER	ALA	conflict	UNP W0G587
H	136	ARG	GLN	conflict	UNP W0G587
H	185	LEU	MET	conflict	UNP W0G587
H	266	SER	ALA	conflict	UNP W0G587
I	136	ARG	GLN	conflict	UNP W0G587
I	185	LEU	MET	conflict	UNP W0G587
I	266	SER	ALA	conflict	UNP W0G587
J	136	ARG	GLN	conflict	UNP W0G587
J	185	LEU	MET	conflict	UNP W0G587
J	266	SER	ALA	conflict	UNP W0G587
K	136	ARG	GLN	conflict	UNP W0G587
K	185	LEU	MET	conflict	UNP W0G587
K	266	SER	ALA	conflict	UNP W0G587
L	136	ARG	GLN	conflict	UNP W0G587
L	185	LEU	MET	conflict	UNP W0G587
L	266	SER	ALA	conflict	UNP W0G587
M	136	ARG	GLN	conflict	UNP W0G587
M	185	LEU	MET	conflict	UNP W0G587

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	266	SER	ALA	conflict	UNP W0G587
N	136	ARG	GLN	conflict	UNP W0G587
N	185	LEU	MET	conflict	UNP W0G587
N	266	SER	ALA	conflict	UNP W0G587
O	136	ARG	GLN	conflict	UNP W0G587
O	185	LEU	MET	conflict	UNP W0G587
O	266	SER	ALA	conflict	UNP W0G587

- Molecule 3 is a protein called VP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	249	Total	C	N	O	S	0	0
			2014	1276	353	377	8		
3	Q	246	Total	C	N	O	S	0	0
			1986	1258	347	373	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	79	VAL	ILE	conflict	UNP A0A2H4QDD3
Q	79	VAL	ILE	conflict	UNP A0A2H4QDD3

- Molecule 4 is a protein called VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	601	Total	C	N	O	S	0	0
			4706	2969	814	907	16		
4	S	622	Total	C	N	O	S	0	0
			4858	3060	841	941	16		
4	T	627	Total	C	N	O	S	0	0
			4900	3088	848	948	16		

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	15	ASN	SER	conflict	UNP B4Y048
R	61	LEU	ILE	conflict	UNP B4Y048
R	62	ASN	ILE	conflict	UNP B4Y048
R	65	ALA	THR	conflict	UNP B4Y048
R	80	ASN	LYS	conflict	UNP B4Y048
R	94	ILE	VAL	conflict	UNP B4Y048
R	130	VAL	ILE	conflict	UNP B4Y048

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	154	VAL	ILE	conflict	UNP B4Y048
R	235	ALA	SER	conflict	UNP B4Y048
R	271	VAL	THR	conflict	UNP B4Y048
R	278	ILE	VAL	conflict	UNP B4Y048
R	307	LEU	MET	conflict	UNP B4Y048
R	322	ASN	THR	conflict	UNP B4Y048
R	369	ALA	VAL	conflict	UNP B4Y048
R	436	ASP	GLU	conflict	UNP B4Y048
R	439	GLN	LYS	conflict	UNP B4Y048
R	444	THR	ALA	conflict	UNP B4Y048
R	470	LYS	ARG	conflict	UNP B4Y048
R	500	THR	ALA	conflict	UNP B4Y048
R	524	VAL	ILE	conflict	UNP B4Y048
R	537	ASN	ASP	conflict	UNP B4Y048
R	539	SER	ASP	conflict	UNP B4Y048
R	543	SER	LEU	conflict	UNP B4Y048
R	545	ASN	LYS	conflict	UNP B4Y048
R	547	ARG	LYS	conflict	UNP B4Y048
R	575	ALA	THR	conflict	UNP B4Y048
R	628	PRO	SER	conflict	UNP B4Y048
S	15	ASN	SER	conflict	UNP B4Y048
S	61	LEU	ILE	conflict	UNP B4Y048
S	62	ASN	ILE	conflict	UNP B4Y048
S	65	ALA	THR	conflict	UNP B4Y048
S	80	ASN	LYS	conflict	UNP B4Y048
S	94	ILE	VAL	conflict	UNP B4Y048
S	130	VAL	ILE	conflict	UNP B4Y048
S	154	VAL	ILE	conflict	UNP B4Y048
S	235	ALA	SER	conflict	UNP B4Y048
S	271	VAL	THR	conflict	UNP B4Y048
S	278	ILE	VAL	conflict	UNP B4Y048
S	307	LEU	MET	conflict	UNP B4Y048
S	322	ASN	THR	conflict	UNP B4Y048
S	369	ALA	VAL	conflict	UNP B4Y048
S	436	ASP	GLU	conflict	UNP B4Y048
S	439	GLN	LYS	conflict	UNP B4Y048
S	444	THR	ALA	conflict	UNP B4Y048
S	470	LYS	ARG	conflict	UNP B4Y048
S	500	THR	ALA	conflict	UNP B4Y048
S	524	VAL	ILE	conflict	UNP B4Y048
S	537	ASN	ASP	conflict	UNP B4Y048
S	539	SER	ASP	conflict	UNP B4Y048

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	543	SER	LEU	conflict	UNP B4Y048
S	545	ASN	LYS	conflict	UNP B4Y048
S	547	ARG	LYS	conflict	UNP B4Y048
S	575	ALA	THR	conflict	UNP B4Y048
S	628	PRO	SER	conflict	UNP B4Y048
T	15	ASN	SER	conflict	UNP B4Y048
T	61	LEU	ILE	conflict	UNP B4Y048
T	62	ASN	ILE	conflict	UNP B4Y048
T	65	ALA	THR	conflict	UNP B4Y048
T	80	ASN	LYS	conflict	UNP B4Y048
T	94	ILE	VAL	conflict	UNP B4Y048
T	130	VAL	ILE	conflict	UNP B4Y048
T	154	VAL	ILE	conflict	UNP B4Y048
T	235	ALA	SER	conflict	UNP B4Y048
T	271	VAL	THR	conflict	UNP B4Y048
T	278	ILE	VAL	conflict	UNP B4Y048
T	307	LEU	MET	conflict	UNP B4Y048
T	322	ASN	THR	conflict	UNP B4Y048
T	369	ALA	VAL	conflict	UNP B4Y048
T	436	ASP	GLU	conflict	UNP B4Y048
T	439	GLN	LYS	conflict	UNP B4Y048
T	444	THR	ALA	conflict	UNP B4Y048
T	470	LYS	ARG	conflict	UNP B4Y048
T	500	THR	ALA	conflict	UNP B4Y048
T	524	VAL	ILE	conflict	UNP B4Y048
T	537	ASN	ASP	conflict	UNP B4Y048
T	539	SER	ASP	conflict	UNP B4Y048
T	543	SER	LEU	conflict	UNP B4Y048
T	545	ASN	LYS	conflict	UNP B4Y048
T	547	ARG	LYS	conflict	UNP B4Y048
T	575	ALA	THR	conflict	UNP B4Y048
T	628	PRO	SER	conflict	UNP B4Y048

- Molecule 5 is a protein called VP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	r	15	Total	C	N	O	0	0
			117	73	20	24		
5	s	15	Total	C	N	O	0	0
			117	73	20	24		
5	t	15	Total	C	N	O	0	0
			117	73	20	24		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	150	TYR	HIS	conflict	UNP Q9YWN5
r	156	LEU	GLN	conflict	UNP Q9YWN5
r	184	THR	ALA	conflict	UNP Q9YWN5
r	191	ASN	ASP	conflict	UNP Q9YWN5
s	150	TYR	HIS	conflict	UNP Q9YWN5
s	156	LEU	GLN	conflict	UNP Q9YWN5
s	184	THR	ALA	conflict	UNP Q9YWN5
s	191	ASN	ASP	conflict	UNP Q9YWN5
t	150	TYR	HIS	conflict	UNP Q9YWN5
t	156	LEU	GLN	conflict	UNP Q9YWN5
t	184	THR	ALA	conflict	UNP Q9YWN5
t	191	ASN	ASP	conflict	UNP Q9YWN5

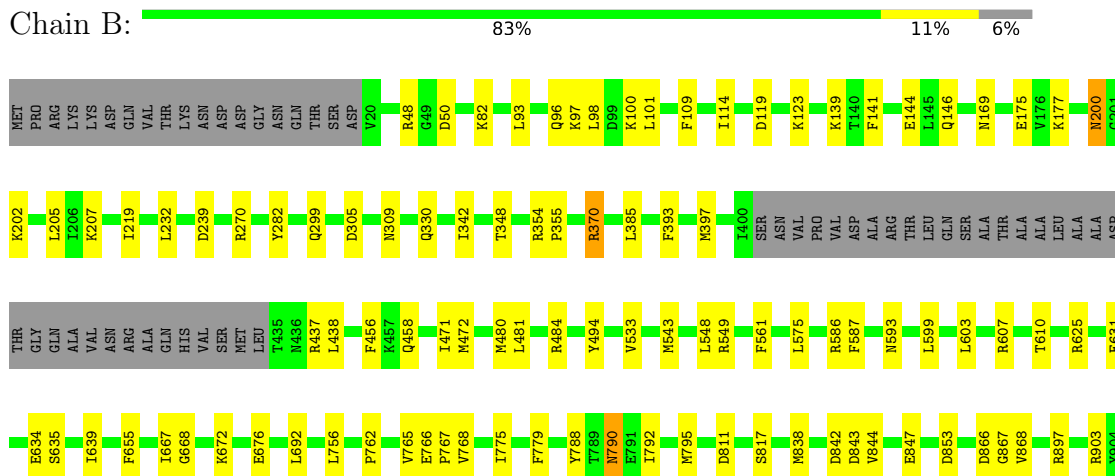
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: VP2



• Molecule 1: VP2





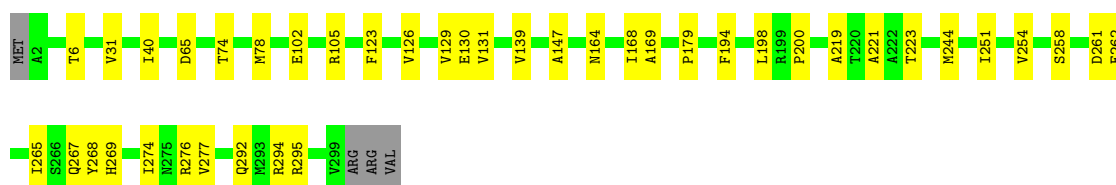
- Molecule 2: VP8

Chain C: 85% 14% .



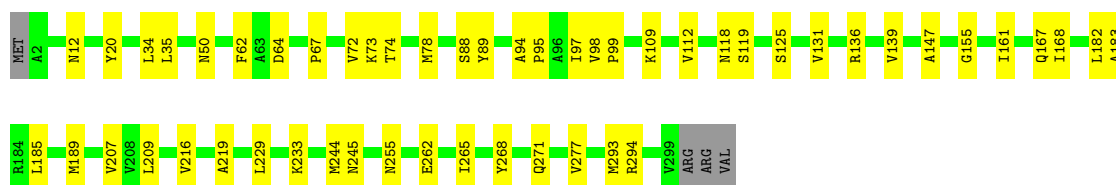
- Molecule 2: VP8

Chain D: 85% 14% .



- Molecule 2: VP8

Chain E: 81% 17% .



- Molecule 2: VP8

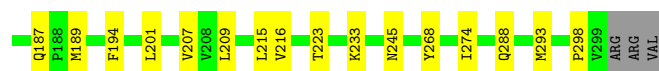
Chain F: 89% 9% .



- Molecule 2: VP8

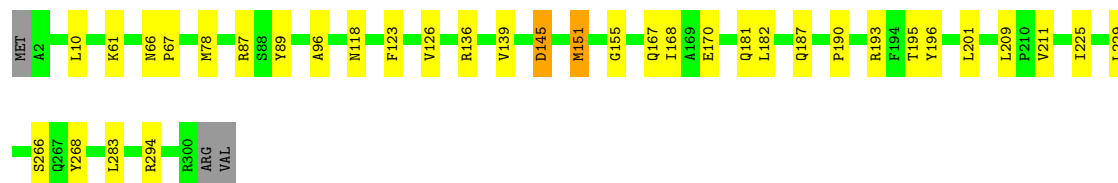
Chain G: 82% 17% .





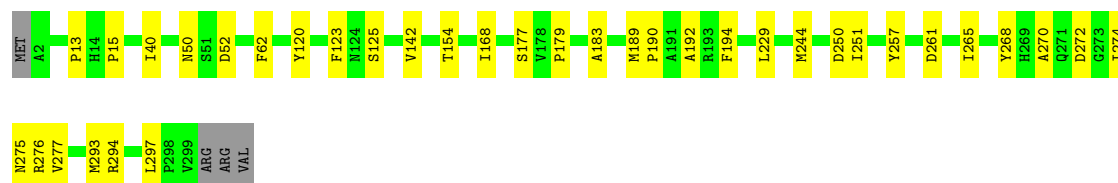
• Molecule 2: VP8

Chain H: 87% 11% ..



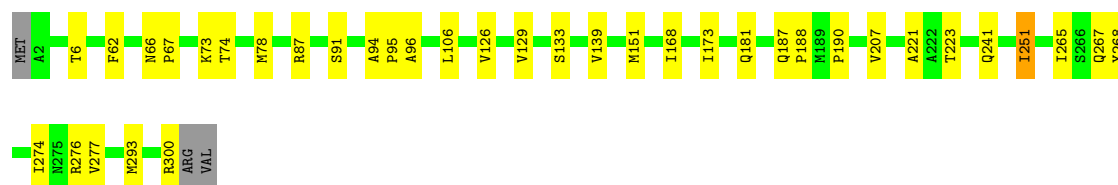
• Molecule 2: VP8

Chain I: 87% 12% .



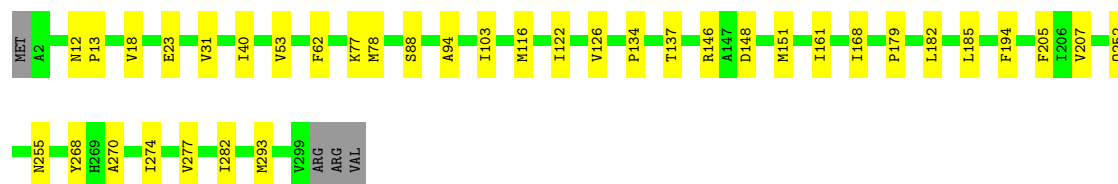
• Molecule 2: VP8

Chain J: 87% 12% .



• Molecule 2: VP8

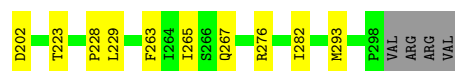
Chain K: 86% 12% .



• Molecule 2: VP8

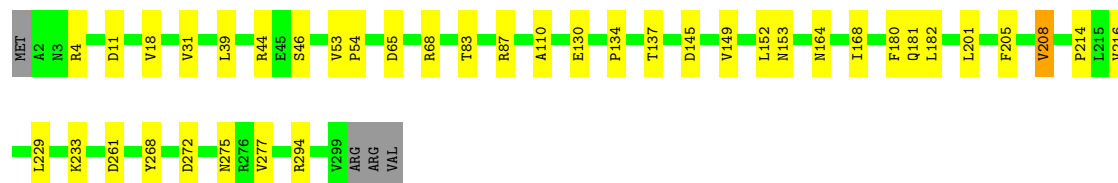
Chain L: 85% 13% .





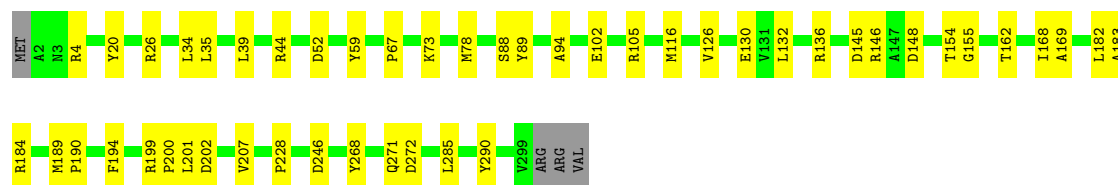
• Molecule 2: VP8

Chain M: 86% 13%



• Molecule 2: VP8

Chain N: 83% 16%



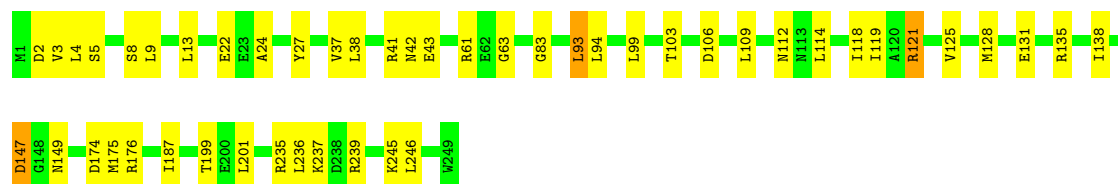
• Molecule 2: VP8

Chain O: 85% 14%



• Molecule 3: VP10

Chain P: 81% 18%



• Molecule 3: VP10

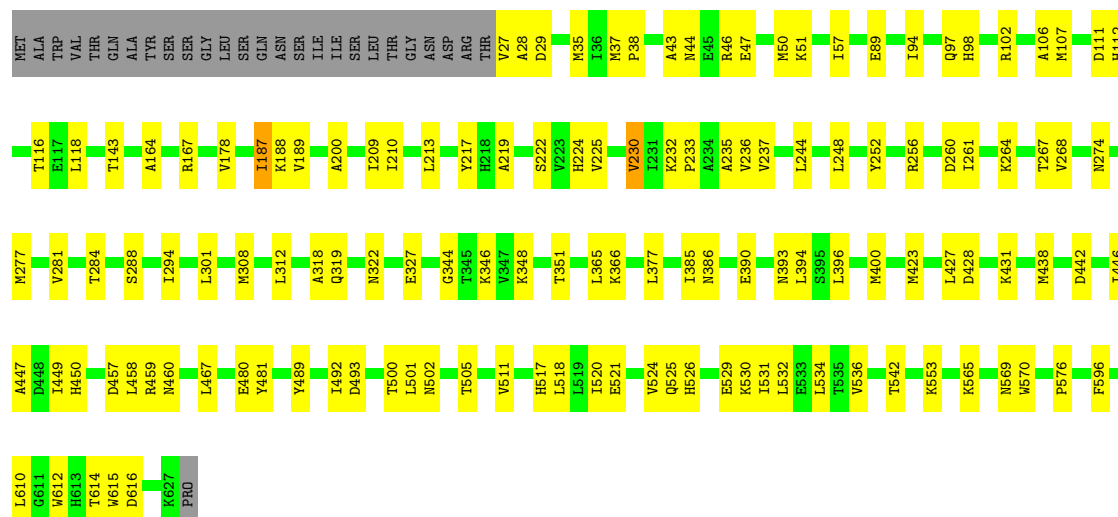
Chain Q: 79% 20%





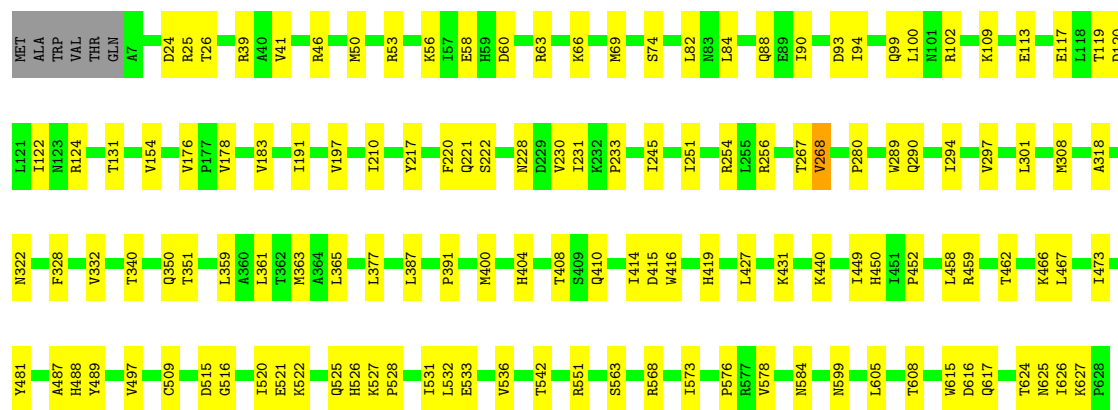
• Molecule 4: VP4

Chain R: 75% 21%



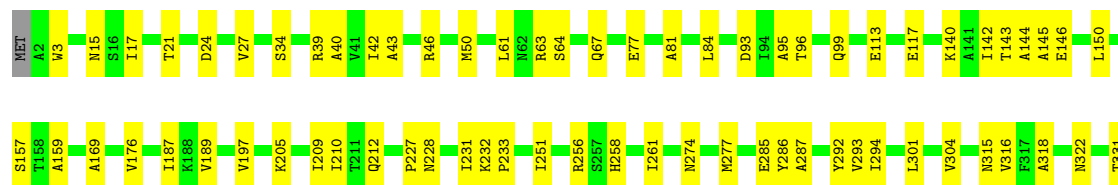
• Molecule 4: VP4

Chain S: 78% 21%



• Molecule 4: VP4

Chain T: 76% 23%





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13225	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/6179	0.25	0/8387
1	B	0.18	0/7361	0.29	0/9987
2	C	0.16	0/2333	0.27	0/3179
2	D	0.14	0/2322	0.26	0/3165
2	E	0.15	0/2322	0.25	0/3165
2	F	0.16	0/2322	0.27	0/3165
2	G	0.16	0/2322	0.28	0/3165
2	H	0.15	0/2333	0.25	0/3179
2	I	0.15	0/2322	0.29	0/3165
2	J	0.16	0/2333	0.27	0/3179
2	K	0.15	0/2322	0.25	0/3165
2	L	0.15	0/2315	0.27	0/3155
2	M	0.15	0/2322	0.27	0/3165
2	N	0.15	0/2322	0.27	0/3165
2	O	0.15	0/2322	0.26	0/3165
3	P	0.15	0/2050	0.24	0/2772
3	Q	0.15	0/2020	0.26	0/2730
4	R	0.15	0/4799	0.29	0/6515
4	S	0.14	0/4953	0.29	0/6725
4	T	0.15	0/4997	0.28	0/6787
5	r	0.11	0/116	0.14	0/154
5	s	0.13	0/116	0.23	0/154
5	t	0.12	0/116	0.26	0/154
All	All	0.15	0/62919	0.27	0/85542

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6045	0	5960	68	0
1	B	7210	0	7136	83	0
2	C	2288	0	2283	34	0
2	D	2277	0	2270	26	0
2	E	2277	0	2270	35	0
2	F	2277	0	2270	21	0
2	G	2277	0	2270	36	0
2	H	2288	0	2283	30	0
2	I	2277	0	2270	29	0
2	J	2288	0	2283	28	0
2	K	2277	0	2270	33	0
2	L	2270	0	2261	28	0
2	M	2277	0	2270	33	0
2	N	2277	0	2270	35	0
2	O	2277	0	2270	31	0
3	P	2014	0	2036	31	0
3	Q	1986	0	2008	37	0
4	R	4706	0	4649	108	0
4	S	4858	0	4796	100	0
4	T	4900	0	4835	125	0
5	r	117	0	130	3	0
5	s	117	0	130	9	0
5	t	117	0	130	3	0
All	All	61697	0	61350	899	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 7.

All (899) 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)
4:S:74:SER:HB3	5:s:5:THR:HG22	1.35	1.07
4:T:210:ILE:CG2	4:T:212:GLN:HG2	1.85	1.05
4:S:74:SER:HB3	5:s:5:THR:CG2	1.86	1.04
2:I:168:ILE:HG12	2:I:268:TYR:CD2	1.93	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:258:HIS:CE1	4:T:356:GLN:HE22	1.79	0.99
2:H:182:LEU:HB3	2:H:196:TYR:CE2	1.97	0.99
4:T:517:HIS:CD2	4:T:519:LEU:HD23	1.97	0.99
4:T:81:ALA:HB1	4:T:527:LYS:CE	1.93	0.98
4:T:99:GLN:HE22	4:T:187:ILE:HD13	1.27	0.98
4:R:438:MET:HE2	4:R:447:ALA:HA	1.42	0.98
2:E:119:SER:HB2	2:E:229:LEU:HD23	1.43	0.98
2:M:268:TYR:CD1	2:M:277:VAL:HG21	1.99	0.97
4:S:233:PRO:CG	4:S:404:HIS:HD2	1.76	0.97
3:P:235:ARG:O	3:P:239:ARG:HG3	1.64	0.96
4:T:81:ALA:HB1	4:T:527:LYS:HE3	1.44	0.96
4:T:210:ILE:HG23	4:T:212:GLN:HG2	1.47	0.96
2:O:268:TYR:CD1	2:O:277:VAL:HG11	2.00	0.96
2:C:183:ALA:HB3	2:C:189:MET:CE	1.95	0.95
2:K:18:VAL:HG21	3:Q:127:LYS:HG2	1.45	0.95
1:B:438:LEU:HD13	1:B:655:PHE:HD1	1.32	0.95
2:I:168:ILE:HG12	2:I:268:TYR:HD2	1.29	0.95
2:D:168:ILE:HD13	2:D:269:HIS:CD2	2.01	0.95
4:T:258:HIS:HE1	4:T:356:GLN:HE22	1.07	0.92
1:B:438:LEU:HD13	1:B:655:PHE:CD1	2.05	0.90
1:B:370:ARG:HG3	1:B:370:ARG:HH11	1.37	0.89
1:B:169:ASN:HD21	1:B:668:GLY:HA3	1.39	0.88
2:C:183:ALA:HB3	2:C:189:MET:HE1	1.55	0.88
4:R:438:MET:CE	4:R:447:ALA:HA	2.05	0.86
2:H:182:LEU:HB3	2:H:196:TYR:HE2	1.41	0.85
4:S:233:PRO:HG2	4:S:404:HIS:CD2	2.13	0.83
3:P:112:ASN:OD1	3:P:147:ASP:HB3	1.78	0.83
2:H:193:ARG:HB2	2:H:196:TYR:HE1	1.42	0.83
4:T:21:THR:HG22	4:T:27:VAL:HB	1.61	0.82
4:T:517:HIS:HD2	4:T:519:LEU:HD23	1.39	0.82
4:R:256:ARG:CZ	4:R:459:ARG:HH21	1.92	0.81
4:S:233:PRO:HG2	4:S:404:HIS:HD2	1.43	0.81
4:R:50:MET:SD	4:S:50:MET:HE1	2.21	0.81
4:S:233:PRO:CG	4:S:404:HIS:CD2	2.62	0.81
4:T:258:HIS:HE1	4:T:356:GLN:NE2	1.79	0.80
2:M:268:TYR:HD1	2:M:277:VAL:HG21	1.45	0.80
4:T:15:ASN:HD22	4:T:371:MET:HG2	1.45	0.80
2:M:168:ILE:HD12	2:M:268:TYR:HE2	1.46	0.80
2:D:251:ILE:O	2:D:254:VAL:HG12	1.82	0.80
2:H:168:ILE:HG21	2:H:268:TYR:CD2	2.17	0.79
2:K:182:LEU:HD12	2:K:207:VAL:HG22	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:368:ALA:HA	4:T:371:MET:HE3	1.65	0.79
2:C:168:ILE:HG23	2:C:268:TYR:CE2	2.18	0.78
2:M:272:ASP:OD2	2:M:275:ASN:HB3	1.83	0.78
2:J:168:ILE:HD12	2:J:268:TYR:CE2	2.19	0.78
4:T:81:ALA:CB	4:T:527:LYS:HE3	2.13	0.78
2:N:199:ARG:NH2	2:N:201:LEU:HD23	1.98	0.78
2:J:168:ILE:HD12	2:J:268:TYR:HE2	1.46	0.77
2:C:168:ILE:HD13	2:C:269:HIS:CD2	2.19	0.77
2:K:168:ILE:HG21	2:K:268:TYR:CD2	2.20	0.77
4:R:44:ASN:HB3	4:R:47:GLU:HB2	1.65	0.76
3:Q:241:THR:HG23	3:Q:243:TYR:H	1.51	0.76
2:N:136:ARG:HE	2:N:155:GLY:HA2	1.50	0.76
4:S:322:ASN:OD1	4:S:322:ASN:O	2.04	0.76
1:B:438:LEU:CD1	1:B:655:PHE:CD1	2.68	0.76
1:A:720:ILE:HD11	1:A:753:LEU:HD12	1.68	0.76
2:E:268:TYR:CD1	2:E:277:VAL:HG21	2.21	0.76
4:R:553:LYS:HD2	4:R:596:PHE:HB3	1.67	0.75
4:S:536:VAL:HG12	4:S:542:THR:HB	1.68	0.75
2:J:274:ILE:O	2:J:277:VAL:HG12	1.86	0.75
2:L:223:THR:HG21	2:L:265:ILE:HD11	1.66	0.75
4:T:457:ASP:OD2	4:T:458:LEU:N	2.20	0.74
2:J:168:ILE:HG21	2:J:268:TYR:CD2	2.22	0.74
2:L:81:ALA:O	2:L:85:VAL:HG23	1.88	0.74
2:I:168:ILE:CG1	2:I:268:TYR:CD2	2.70	0.74
4:T:256:ARG:NH2	4:T:485:PRO:O	2.20	0.74
4:R:189:VAL:HG22	4:R:209:ILE:HD11	1.70	0.74
4:T:534:LEU:HD12	4:T:542:THR:HG21	1.68	0.74
4:R:50:MET:CE	4:T:46:ARG:NH2	2.51	0.74
1:B:169:ASN:ND2	1:B:668:GLY:HA3	2.02	0.73
1:B:437:ARG:HD2	1:B:472:MET:HE3	1.68	0.73
4:S:361:LEU:HD13	4:S:400:MET:SD	2.28	0.73
4:S:74:SER:HB3	5:s:5:THR:HG23	1.69	0.73
3:P:63:GLY:HA2	4:T:286:TYR:OH	1.89	0.73
4:R:438:MET:HE1	4:R:450:HIS:HB2	1.70	0.73
4:T:210:ILE:HG21	4:T:212:GLN:HG2	1.70	0.73
4:R:294:ILE:HG23	4:R:351:THR:HG21	1.71	0.73
2:C:183:ALA:HB3	2:C:189:MET:HE2	1.72	0.72
2:H:181:GLN:NE2	2:H:190:PRO:O	2.22	0.72
2:C:168:ILE:HG21	2:C:268:TYR:CD2	2.24	0.71
2:F:262:GLU:OE1	2:G:175:LYS:NZ	2.23	0.71
4:T:143:THR:HB	4:T:146:GLU:HG2	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:244:GLY:O	3:Q:245:LYS:HG3	1.90	0.71
1:B:868:VAL:HG21	1:B:905:GLU:HG2	1.73	0.70
2:G:168:ILE:HG21	2:G:268:TYR:CD2	2.26	0.70
4:T:64:SER:OG	4:T:67:GLN:HB2	1.91	0.70
4:R:236:VAL:HG13	4:R:237:VAL:HG13	1.74	0.70
2:N:183:ALA:HB3	2:N:189:MET:HE2	1.74	0.70
1:B:458:GLN:HG3	1:B:639:ILE:O	1.92	0.70
2:O:251:ILE:HG22	2:O:252:GLN:N	2.07	0.69
4:R:51:LYS:HE2	4:R:386:ASN:CG	2.17	0.69
2:N:199:ARG:HH22	2:N:201:LEU:HD23	1.57	0.69
4:R:457:ASP:HB3	4:R:460:ASN:HB2	1.75	0.68
4:R:189:VAL:CG2	4:R:209:ILE:HD11	2.23	0.68
2:I:15:PRO:HA	2:I:276:ARG:HH21	1.57	0.68
1:B:561:PHE:HB3	1:B:610:THR:HG23	1.74	0.68
4:R:517:HIS:ND1	4:R:615:TRP:CZ3	2.62	0.68
2:H:182:LEU:HB3	2:H:196:TYR:CD2	2.28	0.68
2:C:151:MET:HE3	2:C:161:ILE:HD12	1.74	0.68
4:S:63:ARG:NH2	4:S:176:VAL:O	2.27	0.67
4:S:74:SER:HB2	5:s:8:ARG:HH21	1.60	0.67
2:J:66:ASN:OD1	2:J:67:PRO:HD2	1.94	0.67
2:H:167:GLN:HG2	2:H:201:LEU:HD12	1.76	0.67
4:R:187:ILE:CG2	4:R:209:ILE:HG12	2.25	0.67
4:R:423:MET:HE3	4:R:427:LEU:HD11	1.74	0.67
2:K:168:ILE:HG21	2:K:268:TYR:CE2	2.30	0.67
2:K:179:PRO:HG3	2:K:194:PHE:CE2	2.30	0.67
4:S:294:ILE:HG23	4:S:351:THR:HG21	1.76	0.67
4:T:142:ILE:HD12	4:T:146:GLU:HB2	1.76	0.67
2:H:193:ARG:HB2	2:H:196:TYR:CE1	2.28	0.67
1:A:749:TYR:CE2	1:A:753:LEU:HD11	2.30	0.67
4:S:233:PRO:HG3	4:S:404:HIS:HD2	1.57	0.66
4:S:489:TYR:HA	4:S:536:VAL:HG23	1.76	0.66
2:M:168:ILE:HD12	2:M:268:TYR:CE2	2.29	0.66
4:R:189:VAL:HG22	4:R:209:ILE:CD1	2.25	0.66
4:R:256:ARG:CZ	4:R:459:ARG:NH2	2.58	0.66
2:C:271:GLN:OE1	2:C:271:GLN:N	2.25	0.66
4:S:69:MET:HE3	4:T:470:LYS:HD3	1.78	0.66
2:I:13:PRO:HG2	2:I:270:ALA:HB2	1.78	0.66
2:L:78:MET:HE1	2:L:109:LYS:HD3	1.76	0.66
2:F:168:ILE:HG21	2:F:268:TYR:CD2	2.30	0.66
2:L:64:ASP:OD1	2:L:109:LYS:CE	2.43	0.66
1:A:801:VAL:HG12	1:A:822:ILE:CD1	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:205:LYS:HE2	4:T:446:ILE:HG12	1.77	0.65
3:Q:86:ILE:HB	3:Q:89:ILE:HD11	1.77	0.65
4:S:221:GLN:NE2	4:S:350:GLN:OE1	2.30	0.65
2:K:116:MET:HE2	2:K:282:ILE:HG12	1.79	0.64
2:C:168:ILE:CG2	2:C:268:TYR:CE2	2.81	0.64
2:D:274:ILE:O	2:D:277:VAL:HG12	1.97	0.64
2:J:168:ILE:HG23	2:J:268:TYR:CE2	2.33	0.64
2:D:267:GLN:HE21	2:D:276:ARG:HD3	1.63	0.63
2:E:161:ILE:HD11	2:E:209:LEU:HD22	1.80	0.63
4:T:46:ARG:HG3	4:T:46:ARG:HH11	1.64	0.63
2:O:168:ILE:HG12	2:O:268:TYR:CD2	2.33	0.63
4:S:391:PRO:HD2	4:S:400:MET:HE1	1.81	0.63
2:J:139:VAL:HG22	2:J:151:MET:HG2	1.80	0.63
2:M:168:ILE:HG21	2:M:268:TYR:CD2	2.34	0.63
4:R:46:ARG:HH12	4:R:50:MET:HB2	1.61	0.63
2:C:168:ILE:HG12	2:C:268:TYR:CD2	2.34	0.63
2:I:229:LEU:HD11	2:K:40:ILE:CD1	2.29	0.62
2:E:119:SER:HB2	2:E:229:LEU:CD2	2.26	0.62
1:B:299:GLN:HG3	1:B:929:MET:HE1	1.80	0.62
3:P:118:ILE:H	3:P:118:ILE:HD12	1.64	0.62
2:E:118:ASN:HB3	2:E:229:LEU:HG	1.81	0.62
2:K:168:ILE:CG2	2:K:268:TYR:CE2	2.82	0.62
2:L:78:MET:HE1	2:L:109:LYS:CD	2.29	0.62
4:R:501:LEU:HD13	5:t:9:ALA:HB3	1.81	0.62
1:A:605:ALA:O	1:A:609:LYS:HG2	2.00	0.62
2:L:184:ARG:HD3	2:L:202:ASP:HB3	1.82	0.62
1:B:370:ARG:HG3	1:B:370:ARG:NH1	2.08	0.62
1:B:587:PHE:O	1:B:593:ASN:ND2	2.32	0.62
4:T:96:THR:HG22	4:T:209:ILE:HG22	1.82	0.62
3:P:41:ARG:NH1	3:P:201:LEU:O	2.31	0.61
1:A:730:ILE:HD12	1:A:734:MET:HE2	1.82	0.61
4:R:489:TYR:HA	4:R:536:VAL:HG23	1.82	0.61
4:S:74:SER:CB	5:s:5:THR:HG22	2.21	0.61
2:F:22:ASP:OD1	2:F:22:ASP:N	2.33	0.61
2:C:168:ILE:HG12	2:C:268:TYR:HD2	1.66	0.61
4:R:480:GLU:HB3	4:R:553:LYS:NZ	2.16	0.61
4:R:500:THR:HG21	4:R:505:THR:HG21	1.82	0.61
2:O:223:THR:HG21	2:O:265:ILE:CD1	2.31	0.61
2:G:78:MET:HE3	2:G:106:LEU:HB3	1.81	0.61
1:A:810:ARG:HB2	1:A:895:GLU:HB2	1.83	0.60
2:I:168:ILE:HG13	2:I:268:TYR:CE2	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:78:MET:HE3	2:J:106:LEU:HB3	1.83	0.60
2:J:181:GLN:NE2	2:J:190:PRO:O	2.33	0.60
2:D:102:GLU:OE2	2:D:105:ARG:NH2	2.32	0.60
2:H:136:ARG:HD2	2:H:155:GLY:HA3	1.81	0.60
4:T:251:ILE:HG12	4:T:408:THR:HG21	1.83	0.60
2:K:182:LEU:HD12	2:K:207:VAL:CG2	2.30	0.60
2:J:168:ILE:CG2	2:J:268:TYR:CD2	2.85	0.59
2:C:168:ILE:CG2	2:C:268:TYR:CD2	2.84	0.59
2:C:184:ARG:HD3	2:C:202:ASP:HB3	1.84	0.59
2:I:229:LEU:HD11	2:K:40:ILE:HD13	1.84	0.59
4:T:99:GLN:NE2	4:T:187:ILE:HD13	2.07	0.59
1:B:897:ARG:HH12	1:B:903:ARG:HD3	1.67	0.59
2:L:85:VAL:HG12	2:L:89:TYR:CE1	2.36	0.59
2:L:145:ASP:OD1	2:L:146:ARG:N	2.34	0.59
2:L:146:ARG:NH1	2:L:148:ASP:OD1	2.34	0.59
1:B:385:LEU:HD12	1:B:635:SER:OG	2.03	0.59
1:B:494:TYR:OH	1:B:533:VAL:O	2.20	0.59
1:A:791:GLU:HG2	1:A:818:LEU:HD12	1.84	0.59
4:R:438:MET:HE2	4:R:447:ALA:CA	2.27	0.59
4:T:493:ASP:OD1	4:T:533:GLU:HG2	2.02	0.59
2:L:223:THR:HG21	2:L:265:ILE:CD1	2.33	0.59
1:A:460:ARG:NH1	1:A:490:SER:CB	2.65	0.58
4:T:517:HIS:CD2	4:T:519:LEU:CD2	2.82	0.58
1:B:232:LEU:HD23	1:B:775:ILE:CG2	2.33	0.58
2:G:115:ASP:OD1	2:G:115:ASP:N	2.37	0.58
3:Q:57:ASP:OD1	3:Q:204:ARG:HG2	2.02	0.58
2:H:168:ILE:HG21	2:H:268:TYR:CE2	2.38	0.58
2:I:274:ILE:O	2:I:277:VAL:HG12	2.03	0.58
4:S:60:ASP:HB2	4:T:61:LEU:HD21	1.85	0.58
2:O:145:ASP:OD1	2:O:146:ARG:N	2.36	0.58
2:G:26:ARG:HD2	2:G:116:MET:HG3	1.85	0.58
3:P:93:LEU:HD21	3:P:109:LEU:HD13	1.86	0.58
4:S:497:VAL:HG22	4:S:528:PRO:HA	1.85	0.58
2:N:168:ILE:HG21	2:N:268:TYR:CD2	2.38	0.58
3:Q:244:GLY:O	3:Q:245:LYS:CG	2.50	0.58
4:R:51:LYS:HE2	4:R:386:ASN:OD1	2.03	0.58
4:T:117:GLU:HB3	4:T:227:PRO:HG3	1.85	0.58
1:A:801:VAL:HG12	1:A:822:ILE:HD11	1.85	0.57
4:R:525:GLN:HB3	4:R:526:HIS:ND1	2.18	0.57
4:R:390:GLU:HG2	4:R:400:MET:HE1	1.86	0.57
4:T:496:VAL:HG22	4:T:566:VAL:HG22	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:565:LYS:NZ	5:t:4:GLU:OE1	2.37	0.57
4:T:322:ASN:OD1	4:T:322:ASN:O	2.23	0.57
2:L:229:LEU:O	2:N:44:ARG:NH1	2.38	0.57
3:Q:226:ARG:O	3:Q:229:SER:OG	2.20	0.57
1:B:330:GLN:HB3	1:B:767:PRO:HB3	1.86	0.57
1:B:239:ASP:OD1	1:B:239:ASP:N	2.36	0.57
2:O:251:ILE:CG2	2:O:252:GLN:N	2.68	0.57
3:P:118:ILE:HG23	3:P:121:ARG:HH12	1.70	0.57
4:T:455:PHE:O	4:T:461:THR:OG1	2.22	0.57
1:B:561:PHE:HB3	1:B:610:THR:CG2	2.34	0.56
2:H:145:ASP:OD1	2:H:145:ASP:N	2.34	0.56
2:J:187:GLN:HG3	2:J:188:PRO:HD2	1.87	0.56
3:P:174:ASP:OD2	3:P:176:ARG:NH1	2.38	0.56
2:H:168:ILE:CG2	2:H:268:TYR:CE2	2.88	0.56
4:R:505:THR:OG1	4:R:525:GLN:OE1	2.20	0.56
2:G:131:VAL:HG11	2:G:139:VAL:HG11	1.87	0.56
4:R:614:THR:OG1	4:R:616:ASP:OD1	2.23	0.56
2:I:168:ILE:CG1	2:I:268:TYR:CE2	2.88	0.56
4:R:517:HIS:ND1	4:R:615:TRP:CH2	2.74	0.56
1:B:667:ILE:HD12	1:B:672:LYS:CD	2.35	0.56
4:R:57:ILE:HD11	4:S:58:GLU:HG3	1.88	0.56
4:R:442:ASP:HB2	4:R:446:ILE:HD12	1.87	0.56
4:R:500:THR:HG22	4:R:502:ASN:H	1.71	0.56
1:A:239:ASP:OD1	1:A:239:ASP:N	2.34	0.56
2:E:136:ARG:HH12	2:E:155:GLY:HA2	1.69	0.56
2:O:223:THR:HG21	2:O:265:ILE:HD11	1.88	0.56
4:R:230:VAL:HG12	4:R:248:LEU:HD23	1.88	0.56
4:S:533:GLU:N	4:S:533:GLU:OE1	2.39	0.56
1:B:842:ASP:OD1	1:B:843:ASP:N	2.38	0.56
2:D:258:SER:OG	2:D:262:GLU:OE2	2.24	0.56
2:G:245:ASN:ND2	2:H:170:GLU:OE1	2.38	0.56
2:N:20:TYR:O	2:N:89:TYR:OH	2.22	0.56
4:T:538:ASP:O	4:T:578:VAL:HG12	2.06	0.56
2:N:146:ARG:NH1	2:N:148:ASP:OD1	2.39	0.55
4:S:122:ILE:HG23	4:S:245:ILE:HD12	1.89	0.55
2:J:241:GLN:HB2	2:K:122:ILE:HD13	1.88	0.55
2:K:12:ASN:O	2:K:255:ASN:ND2	2.39	0.55
2:N:169:ALA:HB3	2:N:200:PRO:HG2	1.89	0.55
4:R:565:LYS:NZ	5:r:4:GLU:OE1	2.37	0.55
4:S:459:ARG:HA	4:S:568:ARG:HH12	1.72	0.55
1:A:737:ILE:O	1:A:740:ILE:HG22	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:132:LEU:HB2	2:G:162:THR:HB	1.88	0.55
1:B:438:LEU:CD1	1:B:655:PHE:CE1	2.89	0.55
2:F:168:ILE:HG23	2:F:268:TYR:CE2	2.42	0.55
4:T:315:ASN:HD22	4:T:331:THR:HG21	1.71	0.55
2:G:62:PHE:CZ	2:G:293:MET:SD	3.00	0.55
2:G:134:PRO:HG2	2:G:159:ALA:HB1	1.89	0.55
2:K:268:TYR:CD1	2:K:277:VAL:HG21	2.42	0.55
2:N:26:ARG:HD2	2:N:116:MET:HG2	1.88	0.55
3:P:2:ASP:OD1	3:P:3:VAL:N	2.39	0.55
4:T:501:LEU:HD21	5:s:6:GLU:HG2	1.88	0.55
2:M:134:PRO:O	2:M:137:THR:OG1	2.24	0.55
4:S:93:ASP:OD1	4:S:93:ASP:N	2.37	0.55
1:B:838:MET:SD	1:B:844:VAL:HG21	2.47	0.55
1:B:667:ILE:HD12	1:B:672:LYS:HD2	1.89	0.55
4:T:205:LYS:CE	4:T:446:ILE:HG23	2.37	0.55
4:S:509:CYS:HB2	4:S:520:ILE:HG12	1.90	0.54
1:A:730:ILE:HD12	1:A:734:MET:CE	2.38	0.54
4:S:473:ILE:HD11	4:S:599:ASN:HD22	1.71	0.54
4:T:365:LEU:HD22	4:T:377:LEU:HD23	1.89	0.54
4:T:498:VAL:HG22	4:T:564:VAL:HG22	1.89	0.54
1:A:784:SER:HB3	1:A:919:PRO:HA	1.88	0.54
1:B:561:PHE:CB	1:B:610:THR:HG23	2.37	0.54
2:I:250:ASP:OD1	2:I:250:ASP:O	2.26	0.54
1:B:393:PHE:O	1:B:397:MET:HG2	2.07	0.54
2:E:50:ASN:OD1	2:F:68:ARG:NH2	2.41	0.54
1:A:536:TYR:OH	1:A:572:GLU:OE1	2.24	0.54
4:R:502:ASN:O	5:r:11:LYS:NZ	2.41	0.54
4:S:41:VAL:HG21	4:S:387:LEU:HD13	1.90	0.54
1:A:928:TYR:CE1	1:A:929:MET:HE2	2.43	0.54
1:B:766:GLU:HG2	1:B:768:VAL:HG12	1.90	0.54
4:T:316:VAL:O	4:T:331:THR:HG23	2.08	0.54
2:C:136:ARG:CZ	2:C:155:GLY:HA2	2.38	0.53
2:N:136:ARG:NH2	2:N:154:THR:O	2.41	0.53
4:R:98:HIS:CE1	4:R:102:ARG:HD2	2.43	0.53
4:R:274:ASN:N	4:R:274:ASN:OD1	2.41	0.53
2:E:125:SER:HB2	2:E:265:ILE:HG13	1.90	0.53
4:R:209:ILE:HD12	4:R:210:ILE:O	2.09	0.53
1:B:811:ASP:OD2	1:B:913:ARG:NH2	2.42	0.53
2:C:201:LEU:HD21	2:G:201:LEU:HD13	1.91	0.53
2:D:251:ILE:O	2:D:254:VAL:CG1	2.56	0.53
1:A:680:GLU:HG3	1:A:733:THR:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LEU:O	1:B:603:LEU:HG	2.07	0.53
2:I:125:SER:HB2	2:I:265:ILE:HG13	1.89	0.53
2:O:116:MET:HE2	2:O:282:ILE:HG12	1.90	0.53
4:R:89:GLU:OE2	4:R:89:GLU:N	2.33	0.53
4:R:489:TYR:CE1	4:R:576:PRO:HB2	2.42	0.53
1:B:928:TYR:CE2	1:B:929:MET:HE2	2.44	0.53
2:L:26:ARG:HG2	2:L:282:ILE:HD11	1.91	0.53
2:E:12:ASN:O	2:E:255:ASN:ND2	2.41	0.53
4:S:616:ASP:N	4:S:616:ASP:OD2	2.33	0.53
4:T:24:ASP:OD1	4:T:24:ASP:N	2.42	0.53
4:S:230:VAL:O	4:S:233:PRO:HD2	2.08	0.53
4:T:205:LYS:HE2	4:T:446:ILE:CG1	2.39	0.53
1:A:498:LEU:HA	1:A:501:MET:HE2	1.90	0.53
1:B:109:PHE:CB	1:B:123:LYS:HG2	2.38	0.53
4:R:520:ILE:HD11	4:R:531:ILE:HG22	1.90	0.53
2:E:118:ASN:CB	2:E:229:LEU:HG	2.38	0.53
2:D:223:THR:HG21	2:D:265:ILE:HD11	1.91	0.53
2:G:56:VAL:O	2:G:60:SER:OG	2.24	0.53
2:O:251:ILE:HG22	2:O:252:GLN:H	1.74	0.53
4:S:74:SER:CB	5:s:5:THR:CG2	2.75	0.53
2:D:130:GLU:HG3	2:D:164:ASN:HB3	1.91	0.52
2:H:123:PHE:HE2	2:H:225:ILE:HB	1.74	0.52
2:H:195:THR:C	2:H:196:TYR:HD1	2.17	0.52
2:I:62:PHE:CZ	2:I:293:MET:SD	3.02	0.52
2:L:68:ARG:HD2	2:L:71:ARG:HD2	1.90	0.52
4:R:143:THR:HG21	4:R:394:LEU:HD12	1.91	0.52
2:D:31:VAL:HG12	2:D:78:MET:HE1	1.92	0.52
3:Q:130:CYS:SG	3:Q:134:LYS:HE3	2.50	0.52
4:R:457:ASP:OD1	4:R:458:LEU:N	2.42	0.52
4:T:600:ILE:HG13	4:T:602:PRO:HD3	1.91	0.52
2:E:168:ILE:HG21	2:E:268:TYR:CD2	2.44	0.52
2:H:66:ASN:OD1	2:H:67:PRO:HD2	2.10	0.52
2:I:244:MET:SD	2:J:173:ILE:HD11	2.50	0.52
2:E:183:ALA:HB3	2:E:189:MET:HE2	1.91	0.52
2:F:145:ASP:OD1	2:F:146:ARG:N	2.43	0.52
2:M:46:SER:HB3	2:M:54:PRO:HG2	1.92	0.52
4:T:487:ALA:C	4:T:578:VAL:HG22	2.34	0.52
1:B:144:GLU:OE2	1:B:146:GLN:HG2	2.09	0.52
4:R:351:THR:HG22	4:R:385:ILE:CG2	2.40	0.52
2:N:126:VAL:O	2:N:126:VAL:HG13	2.10	0.52
4:T:391:PRO:HD2	4:T:400:MET:HE1	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:31:VAL:HG22	2:M:110:ALA:HB3	1.91	0.52
2:O:251:ILE:CG2	2:O:252:GLN:H	2.23	0.52
4:R:46:ARG:NH1	4:R:50:MET:HB2	2.25	0.52
4:T:487:ALA:O	4:T:578:VAL:HG22	2.10	0.52
2:F:100:GLN:HG2	3:P:131:GLU:OE1	2.10	0.52
2:G:274:ILE:H	2:G:274:ILE:HD12	1.74	0.52
1:A:397:MET:HG2	1:A:448:ALA:HB1	1.92	0.52
1:B:175:GLU:OE1	1:B:177:LYS:NZ	2.43	0.52
2:K:126:VAL:O	2:K:126:VAL:HG13	2.10	0.52
2:M:168:ILE:HG23	2:M:268:TYR:CE2	2.45	0.51
2:O:130:GLU:HG3	2:O:164:ASN:HB3	1.91	0.51
4:T:43:ALA:HA	4:T:277:MET:HE1	1.92	0.51
2:I:294:ARG:NH1	2:I:297:LEU:O	2.43	0.51
2:M:145:ASP:OD1	2:M:145:ASP:N	2.38	0.51
4:T:205:LYS:HE2	4:T:446:ILE:HG23	1.93	0.51
4:R:232:LYS:HB2	4:R:233:PRO:HD3	1.92	0.51
4:R:346:LYS:HZ1	4:R:348:LYS:HE2	1.76	0.51
4:S:82:LEU:HD23	4:S:84:LEU:HD21	1.92	0.51
4:T:294:ILE:HG23	4:T:351:THR:HG21	1.93	0.51
4:T:518:LEU:HD23	4:T:520:ILE:HD11	1.93	0.51
2:G:51:SER:OG	2:G:53:VAL:HG23	2.10	0.51
2:L:199:ARG:NH2	2:L:202:ASP:OD1	2.36	0.51
2:N:4:ARG:HH11	2:N:130:GLU:HG3	1.74	0.51
2:G:64:ASP:OD1	2:G:109:LYS:NZ	2.40	0.51
2:N:199:ARG:HG3	2:N:202:ASP:HB2	1.93	0.51
2:O:235:LEU:HD12	2:O:288:GLN:HE21	1.76	0.51
4:T:143:THR:HG22	4:T:145:ALA:H	1.76	0.51
4:T:205:LYS:HE2	4:T:446:ILE:CG2	2.41	0.51
4:R:284:THR:O	4:R:288:SER:OG	2.27	0.51
1:A:460:ARG:HH11	1:A:490:SER:HB3	1.76	0.51
1:A:452:LEU:HA	1:A:455:MET:HG2	1.93	0.51
1:B:575:LEU:HD23	1:B:607:ARG:HD2	1.93	0.51
2:G:61:LYS:O	2:G:109:LYS:NZ	2.43	0.51
2:H:126:VAL:HG13	2:H:126:VAL:O	2.11	0.51
2:I:179:PRO:HD3	2:I:194:PHE:CZ	2.45	0.51
2:O:6:THR:OG1	2:O:129:VAL:O	2.26	0.51
4:S:527:LYS:HG3	4:S:528:PRO:HD2	1.93	0.51
1:A:463:MET:SD	1:A:465:TYR:CE1	3.04	0.51
2:L:44:ARG:NH1	2:M:229:LEU:O	2.43	0.51
2:O:20:TYR:O	2:O:89:TYR:OH	2.27	0.51
1:A:460:ARG:NH1	1:A:490:SER:HB2	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:268:TYR:CE1	2:K:277:VAL:HG21	2.46	0.50
3:P:24:ALA:O	3:P:83:GLY:HA3	2.10	0.50
4:S:440:LYS:NZ	4:S:440:LYS:HB3	2.26	0.50
4:S:608:THR:O	4:S:608:THR:HG22	2.11	0.50
4:T:514:ILE:HG13	4:T:549:HIS:NE2	2.26	0.50
2:C:168:ILE:HD13	2:C:269:HIS:CG	2.46	0.50
2:N:228:PRO:HG2	2:N:285:LEU:HD22	1.92	0.50
2:E:95:PRO:HB2	2:E:97:ILE:HG23	1.93	0.50
2:K:252:GLN:H	2:K:252:GLN:CD	2.18	0.50
2:N:168:ILE:HG23	2:N:268:TYR:CE2	2.46	0.50
4:S:290:GLN:N	4:S:290:GLN:OE1	2.45	0.50
2:C:126:VAL:O	2:C:126:VAL:HG13	2.10	0.50
4:R:517:HIS:CE1	4:R:615:TRP:CZ3	3.00	0.50
1:A:338:LEU:HD13	1:A:945:ILE:HD13	1.93	0.50
1:A:801:VAL:HG12	1:A:822:ILE:HD13	1.92	0.50
1:A:953:THR:HG22	1:B:141:PHE:HB2	1.93	0.50
2:E:34:LEU:HD22	2:E:112:VAL:HG11	1.94	0.50
2:L:134:PRO:HG2	2:L:159:ALA:HB1	1.92	0.50
2:M:233:LYS:HE3	2:M:261:ASP:OD1	2.12	0.50
2:O:189:MET:HE3	2:O:208:VAL:HG23	1.92	0.50
4:R:264:LYS:HG2	4:R:427:LEU:HD13	1.92	0.50
4:R:467:LEU:HD21	4:R:481:TYR:HD1	1.77	0.50
4:R:521:GLU:HB2	4:R:610:LEU:HD11	1.93	0.50
4:S:88:GLN:HG2	4:S:573:ILE:HB	1.92	0.50
4:S:626:ILE:HD12	4:S:627:LYS:H	1.77	0.50
2:C:11:ASP:C	2:C:11:ASP:OD1	2.54	0.50
2:F:126:VAL:O	2:F:126:VAL:HG13	2.11	0.50
1:A:387:GLU:N	1:A:387:GLU:OE1	2.44	0.50
2:D:179:PRO:HG3	2:D:194:PHE:CE2	2.47	0.50
2:E:136:ARG:NH1	2:E:155:GLY:HA2	2.27	0.50
2:K:23:GLU:OE2	3:Q:209:LYS:NZ	2.45	0.50
2:N:246:ASP:OD2	2:N:290:TYR:OH	2.30	0.50
3:Q:25:ILE:HG21	3:Q:89:ILE:HD13	1.94	0.50
4:R:319:GLN:O	4:R:322:ASN:ND2	2.45	0.50
2:J:168:ILE:CG2	2:J:268:TYR:CE2	2.95	0.49
2:L:183:ALA:HB2	2:L:190:PRO:HD3	1.93	0.49
4:T:96:THR:CG2	4:T:209:ILE:HG22	2.41	0.49
2:D:126:VAL:O	2:D:126:VAL:HG13	2.12	0.49
2:L:187:GLN:OE1	2:L:187:GLN:N	2.44	0.49
3:Q:204:ARG:HG3	3:Q:204:ARG:HH11	1.77	0.49
1:B:305:ASP:C	1:B:305:ASP:OD1	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:272:ASP:CG	2:M:275:ASN:HB3	2.37	0.49
2:O:168:ILE:HG12	2:O:268:TYR:HD2	1.75	0.49
3:Q:244:GLY:C	3:Q:245:LYS:HG3	2.37	0.49
4:R:281:VAL:HG23	4:R:344:GLY:HA2	1.94	0.49
4:T:95:ALA:O	4:T:99:GLN:HG2	2.12	0.49
2:I:50:ASN:OD1	2:M:68:ARG:NH1	2.45	0.49
2:M:4:ARG:HG3	2:M:4:ARG:HH11	1.76	0.49
4:T:520:ILE:HD12	4:T:520:ILE:H	1.77	0.49
4:T:527:LYS:HD2	4:T:528:PRO:HD2	1.95	0.49
1:A:880:ASP:OD1	1:A:880:ASP:N	2.43	0.49
1:B:200:ASN:OD1	1:B:200:ASN:N	2.39	0.49
1:B:543:MET:HE1	1:B:625:ARG:HG2	1.94	0.49
4:T:511:VAL:CG1	4:T:552:LEU:HD23	2.42	0.49
2:L:179:PRO:HB2	2:L:192:ALA:HB1	1.92	0.49
3:Q:95:ARG:HG3	3:Q:95:ARG:HH11	1.77	0.49
4:S:466:LYS:NZ	4:S:563:SER:HB2	2.28	0.49
4:S:520:ILE:HD12	4:S:522:LYS:NZ	2.28	0.49
4:T:17:ILE:HD12	4:T:368:ALA:HB2	1.95	0.49
2:J:87:ARG:NH1	3:P:38:LEU:O	2.46	0.49
3:P:114:LEU:HD13	3:P:119:ILE:HD11	1.94	0.49
4:R:27:VAL:HG12	4:R:28:ALA:N	2.27	0.49
1:B:232:LEU:HD23	1:B:775:ILE:HG21	1.94	0.49
2:C:136:ARG:NH2	2:C:155:GLY:HA2	2.28	0.49
2:L:64:ASP:OD1	2:L:109:LYS:HE3	2.11	0.49
4:S:268:VAL:HG21	4:S:427:LEU:HD22	1.94	0.49
1:B:205:LEU:C	1:B:205:LEU:HD12	2.38	0.48
1:B:866:ASP:OD1	1:B:867:GLY:N	2.45	0.48
4:S:46:ARG:HH12	4:S:50:MET:HB2	1.78	0.48
4:S:531:ILE:HG22	4:S:532:LEU:HB2	1.95	0.48
2:N:102:GLU:OE2	2:N:105:ARG:NH1	2.46	0.48
4:R:112:HIS:O	4:R:116:THR:HG23	2.13	0.48
4:T:551:ARG:C	4:T:552:LEU:HD12	2.38	0.48
2:C:175:LYS:NZ	2:E:262:GLU:OE1	2.46	0.48
2:G:151:MET:HB2	2:G:151:MET:HE3	1.80	0.48
4:S:131:THR:HG21	4:S:154:VAL:HG21	1.94	0.48
4:S:254:ARG:HG2	4:S:254:ARG:HH11	1.78	0.48
4:T:143:THR:HG22	4:T:144:ALA:N	2.27	0.48
2:G:126:VAL:HG13	2:G:126:VAL:O	2.14	0.48
2:N:268:TYR:CD2	2:N:268:TYR:O	2.66	0.48
3:Q:195:LEU:HD11	3:Q:212:LYS:HD2	1.96	0.48
4:T:538:ASP:O	4:T:578:VAL:CG1	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:178:VAL:HG22	4:S:222:SER:HB3	1.94	0.48
3:P:118:ILE:HG23	3:P:121:ARG:NH1	2.29	0.48
2:E:182:LEU:HD12	2:E:207:VAL:HG22	1.96	0.48
2:M:168:ILE:CG2	2:M:268:TYR:CE2	2.97	0.48
2:O:146:ARG:NH1	2:O:148:ASP:OD1	2.46	0.48
3:P:13:LEU:HB3	3:P:246:LEU:HD21	1.96	0.48
4:R:37:MET:SD	4:R:38:PRO:HD2	2.53	0.48
4:R:493:ASP:HB3	4:R:530:LYS:HZ1	1.78	0.48
4:S:415:ASP:C	4:S:415:ASP:OD2	2.56	0.48
4:T:210:ILE:CG2	4:T:212:GLN:CG	2.77	0.48
1:B:48:ARG:HG3	1:B:50:ASP:H	1.78	0.48
2:C:170:GLU:OE2	2:E:245:ASN:ND2	2.47	0.48
2:F:70:LEU:C	2:F:70:LEU:HD12	2.38	0.48
2:G:62:PHE:CE2	2:G:293:MET:SD	3.07	0.48
4:R:50:MET:HE3	4:T:46:ARG:HH22	1.79	0.48
4:S:119:THR:HG22	4:S:551:ARG:HH11	1.79	0.48
1:A:319:MET:HE1	1:A:778:ARG:HD3	1.94	0.48
1:B:114:ILE:HG23	1:B:119:ASP:HB2	1.96	0.48
2:K:146:ARG:NH1	2:K:148:ASP:OD1	2.45	0.48
2:K:182:LEU:HD21	2:K:205:PHE:HB3	1.96	0.48
2:M:130:GLU:HG3	2:M:164:ASN:HB3	1.95	0.48
4:R:98:HIS:NE2	4:R:102:ARG:HD2	2.28	0.48
4:S:120:ASP:O	4:S:124:ARG:HG2	2.14	0.48
4:S:466:LYS:HZ3	4:S:563:SER:HB2	1.79	0.48
1:B:437:ARG:HD2	1:B:472:MET:CE	2.40	0.47
1:B:672:LYS:O	1:B:676:GLU:HG3	2.13	0.47
2:J:62:PHE:CZ	2:J:293:MET:SD	3.07	0.47
4:R:106:ALA:HB1	4:R:178:VAL:CG1	2.43	0.47
4:R:501:LEU:HD11	5:t:6:GLU:HA	1.96	0.47
4:S:359:LEU:O	4:S:363:MET:HG3	2.13	0.47
1:B:817:SER:HB3	2:G:105:ARG:HG3	1.94	0.47
2:H:182:LEU:CB	2:H:196:TYR:CE2	2.85	0.47
3:Q:33:PRO:HA	3:Q:61:ARG:HD2	1.96	0.47
4:T:277:MET:SD	4:T:292:TYR:CE2	3.06	0.47
1:A:397:MET:HE2	1:A:397:MET:HB3	1.76	0.47
2:K:88:SER:HA	2:K:94:ALA:HB3	1.96	0.47
3:P:4:LEU:HD22	3:P:187:ILE:HD12	1.97	0.47
4:T:356:GLN:HG3	4:T:416:TRP:CZ2	2.49	0.47
1:B:232:LEU:HD23	1:B:775:ILE:HG23	1.94	0.47
1:B:548:LEU:HD23	1:B:548:LEU:HA	1.78	0.47
2:C:235:LEU:HD13	2:C:292:GLN:NE2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:293:MET:HE2	2:L:293:MET:HB3	1.76	0.47
1:A:792:ILE:HG22	1:A:916:ILE:HG22	1.97	0.47
2:C:20:TYR:O	2:C:89:TYR:OH	2.26	0.47
3:P:125:VAL:HA	3:P:128:MET:HG3	1.95	0.47
4:R:526:HIS:HB3	5:r:8:ARG:HE	1.80	0.47
4:S:113:GLU:O	4:S:117:GLU:HG3	2.15	0.47
4:S:467:LEU:HD11	4:S:481:TYR:HB2	1.96	0.47
1:A:437:ARG:HA	1:A:437:ARG:HD3	1.79	0.47
1:A:837:MET:HE1	1:B:354:ARG:HD3	1.97	0.47
2:K:168:ILE:HG23	2:K:268:TYR:CE2	2.49	0.47
2:L:223:THR:CG2	2:L:265:ILE:HD11	2.42	0.47
2:O:72:VAL:CG1	2:O:74:THR:HG23	2.45	0.47
4:R:46:ARG:NE	4:S:387:LEU:HD21	2.30	0.47
4:S:449:ILE:HG22	4:S:450:HIS:CD2	2.50	0.47
1:A:507:ASN:OD1	1:A:588:ARG:NH1	2.48	0.47
2:C:131:VAL:HG11	2:C:139:VAL:HG11	1.96	0.47
2:C:145:ASP:OD1	2:C:146:ARG:N	2.48	0.47
2:C:149:VAL:HG13	2:C:149:VAL:O	2.15	0.47
2:N:168:ILE:HD12	2:N:268:TYR:HE2	1.79	0.47
3:P:175:MET:HG2	3:P:245:LYS:HB2	1.97	0.47
4:R:256:ARG:NH2	4:R:459:ARG:HH21	2.12	0.47
2:H:89:TYR:HB2	2:H:283:LEU:HD13	1.97	0.47
2:H:139:VAL:HG22	2:H:151:MET:HG2	1.97	0.47
3:Q:151:ASN:O	3:Q:155:ILE:HG13	2.15	0.47
1:B:139:LYS:HB2	1:B:139:LYS:HE2	1.73	0.47
2:E:64:ASP:CG	2:E:109:LYS:HZ1	2.21	0.47
2:G:233:LYS:HE2	2:G:233:LYS:HB3	1.56	0.47
3:P:22:GLU:OE2	3:P:27:TYR:OH	2.25	0.47
4:R:164:ALA:HA	4:R:167:ARG:HH21	1.80	0.47
4:T:285:GLU:CG	4:T:287:ALA:O	2.63	0.47
4:T:480:GLU:HB3	4:T:553:LYS:HE2	1.96	0.47
1:A:374:GLN:OE1	1:B:146:GLN:NE2	2.48	0.46
1:A:928:TYR:HE1	1:A:929:MET:HE2	1.80	0.46
2:G:168:ILE:HG23	2:G:268:TYR:CE2	2.51	0.46
2:O:131:VAL:HG11	2:O:139:VAL:HG11	1.97	0.46
2:E:20:TYR:O	2:E:89:TYR:OH	2.23	0.46
2:K:62:PHE:HZ	2:K:293:MET:HE2	1.79	0.46
2:K:179:PRO:HD3	2:K:194:PHE:CZ	2.50	0.46
1:A:451:VAL:HG13	1:A:621:VAL:HG22	1.96	0.46
1:B:790:ASN:OD1	1:B:790:ASN:N	2.48	0.46
2:M:180:PHE:HE2	2:M:182:LEU:HD12	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:100:LEU:HD22	4:S:267:THR:HG22	1.96	0.46
1:A:207:LYS:NZ	1:A:921:CYS:SG	2.89	0.46
1:B:370:ARG:NH1	1:B:370:ARG:CG	2.75	0.46
3:Q:65:ARG:HH12	3:Q:248:GLY:HA3	1.81	0.46
1:B:342:ILE:HG23	1:B:355:PRO:HG2	1.98	0.46
2:D:223:THR:HG21	2:D:265:ILE:CD1	2.45	0.46
2:F:168:ILE:CG2	2:F:268:TYR:CE2	2.97	0.46
2:O:223:THR:CG2	2:O:265:ILE:HD11	2.46	0.46
4:T:228:ASN:O	4:T:231:ILE:HG22	2.15	0.46
1:A:311:VAL:HG22	1:A:936:VAL:HG22	1.96	0.46
2:O:125:SER:HB2	2:O:265:ILE:HG13	1.98	0.46
2:K:31:VAL:HG12	2:K:78:MET:HE1	1.98	0.46
2:N:35:LEU:HD12	2:N:78:MET:HE1	1.96	0.46
4:S:66:LYS:HE3	4:S:66:LYS:HB3	1.57	0.46
4:T:599:ASN:N	4:T:599:ASN:OD1	2.48	0.46
2:C:72:VAL:O	2:C:72:VAL:HG12	2.16	0.46
2:G:184:ARG:HB2	2:G:187:GLN:HG3	1.96	0.46
2:J:94:ALA:HB2	2:J:251:ILE:HD13	1.98	0.46
2:L:169:ALA:HB3	2:L:200:PRO:HG2	1.98	0.46
3:P:22:GLU:HG3	3:P:94:LEU:HB3	1.97	0.46
3:Q:92:MET:HE3	3:Q:92:MET:HB3	1.81	0.46
4:R:94:ILE:HB	4:R:97:GLN:HG3	1.98	0.46
4:R:268:VAL:HG12	4:R:431:LYS:HB2	1.97	0.46
4:R:322:ASN:OD1	4:R:327:GLU:O	2.33	0.46
1:A:222:VAL:HG21	2:K:53:VAL:HG13	1.97	0.46
1:A:830:ILE:HD13	1:A:838:MET:HE1	1.98	0.46
1:B:907:LYS:HB2	1:B:907:LYS:HE3	1.65	0.46
2:E:62:PHE:CE2	2:E:293:MET:SD	3.08	0.46
2:E:185:LEU:HD23	2:E:185:LEU:HA	1.81	0.46
2:N:132:LEU:HB2	2:N:162:THR:HB	1.97	0.46
2:O:31:VAL:HG22	2:O:110:ALA:HB3	1.98	0.46
4:S:256:ARG:HB3	4:S:459:ARG:HH12	1.81	0.46
4:T:489:TYR:CE1	4:T:576:PRO:HB2	2.51	0.46
2:D:126:VAL:HG23	2:D:221:ALA:HB2	1.97	0.46
2:N:184:ARG:NE	2:N:202:ASP:OD1	2.49	0.46
2:O:223:THR:HG21	2:O:265:ILE:HD12	1.97	0.46
3:Q:92:MET:HB2	3:Q:246:LEU:HD13	1.98	0.46
4:R:213:LEU:HD11	4:R:217:TYR:CE1	2.51	0.46
2:H:10:LEU:HD23	2:H:266:SER:HA	1.97	0.45
2:J:67:PRO:HB3	2:J:73:LYS:HD3	1.96	0.45
4:S:431:LYS:NZ	4:S:452:PRO:O	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:s:7:LEU:HD12	5:s:10:LEU:HD11	1.97	0.45
2:I:179:PRO:HB2	2:I:192:ALA:HB1	1.97	0.45
3:Q:111:THR:OG1	3:Q:147:ASP:OD1	2.32	0.45
4:S:525:GLN:HG3	4:S:526:HIS:ND1	2.32	0.45
1:B:692:LEU:HD23	1:B:756:LEU:HD12	1.98	0.45
4:R:187:ILE:HG21	4:R:209:ILE:HG12	1.97	0.45
4:S:617:GLN:HB3	4:S:626:ILE:HD11	1.98	0.45
2:D:169:ALA:HB3	2:D:200:PRO:HG2	1.98	0.45
2:G:168:ILE:CG2	2:G:268:TYR:CE2	2.99	0.45
2:J:91:SER:HB3	2:J:251:ILE:HD12	1.97	0.45
4:S:56:LYS:NZ	4:T:169:ALA:O	2.50	0.45
2:N:116:MET:SD	2:N:228:PRO:HG3	2.56	0.45
3:P:106:ASP:OD1	3:P:106:ASP:O	2.34	0.45
3:P:135:ARG:HA	3:P:138:ILE:HD12	1.99	0.45
4:R:377:LEU:HD12	4:R:377:LEU:HA	1.82	0.45
1:B:456:PHE:HB3	1:B:458:GLN:NE2	2.31	0.45
2:D:168:ILE:CD1	2:D:269:HIS:CD2	2.88	0.45
2:E:168:ILE:HG23	2:E:268:TYR:CE2	2.52	0.45
2:F:64:ASP:OD1	2:F:109:LYS:NZ	2.44	0.45
4:T:285:GLU:HG3	4:T:287:ALA:O	2.17	0.45
1:B:631:GLU:H	1:B:631:GLU:CD	2.25	0.45
2:F:252:GLN:OE1	2:F:252:GLN:N	2.30	0.45
2:K:168:ILE:HD12	2:K:268:TYR:HE2	1.81	0.45
2:D:65:ASP:OD1	2:D:65:ASP:O	2.34	0.45
2:D:123:PHE:HB3	2:D:261:ASP:OD1	2.16	0.45
2:D:294:ARG:HA	2:D:294:ARG:HD3	1.72	0.45
2:F:41:ASP:OD1	2:F:41:ASP:N	2.50	0.45
2:N:272:ASP:OD1	2:N:272:ASP:N	2.49	0.45
3:Q:70:LEU:HD23	3:Q:70:LEU:HA	1.80	0.45
4:S:220:PHE:CE1	4:S:297:VAL:HG21	2.52	0.45
4:T:301:LEU:HD23	4:T:318:ALA:HA	1.98	0.45
4:T:492:ILE:HD11	4:T:568:ARG:HG2	1.98	0.45
1:B:348:THR:OG1	1:B:549:ARG:NH2	2.44	0.45
2:D:244:MET:HE3	2:D:244:MET:HB2	1.80	0.45
2:H:151:MET:HE2	2:H:209:LEU:HD13	1.97	0.45
2:J:96:ALA:O	3:P:61:ARG:NH1	2.47	0.45
2:N:145:ASP:OD1	2:N:146:ARG:N	2.49	0.45
4:R:492:ILE:HD12	4:R:570:TRP:CZ2	2.51	0.45
1:B:792:ILE:HG22	1:B:916:ILE:HG22	1.99	0.45
4:R:50:MET:CE	4:T:46:ARG:HH22	2.27	0.45
4:T:232:LYS:HB2	4:T:233:PRO:HD3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:261:ILE:HD11	4:T:424:HIS:CD2	2.52	0.45
1:A:495:ARG:HG3	1:A:518:ILE:HG13	1.99	0.44
1:A:569:LYS:NZ	1:A:569:LYS:HB2	2.32	0.44
2:K:185:LEU:HD23	2:K:185:LEU:HA	1.87	0.44
4:T:293:VAL:HG22	4:T:304:VAL:HG22	1.99	0.44
4:T:361:LEU:HD13	4:T:400:MET:HE2	1.99	0.44
4:T:520:ILE:HD12	4:T:520:ILE:N	2.31	0.44
2:C:179:PRO:HG3	2:C:194:PHE:CE2	2.52	0.44
2:L:85:VAL:CG1	2:L:89:TYR:CE1	3.00	0.44
2:L:150:THR:O	2:L:150:THR:HG23	2.16	0.44
3:Q:246:LEU:HD12	3:Q:246:LEU:HA	1.89	0.44
4:R:301:LEU:HD23	4:R:318:ALA:HA	1.97	0.44
4:T:81:ALA:HB1	4:T:527:LYS:CD	2.44	0.44
1:A:678:LEU:HD23	1:A:678:LEU:HA	1.87	0.44
2:E:167:GLN:N	2:E:167:GLN:OE1	2.50	0.44
2:O:258:SER:OG	2:O:262:GLU:OE2	2.35	0.44
3:Q:24:ALA:O	3:Q:83:GLY:HA3	2.17	0.44
2:J:95:PRO:HB3	3:P:37:VAL:HG11	1.99	0.44
2:M:201:LEU:HD23	2:M:201:LEU:HA	1.87	0.44
2:O:250:ASP:OD1	2:O:250:ASP:N	2.51	0.44
4:R:50:MET:HE3	4:T:46:ARG:NH2	2.28	0.44
4:R:178:VAL:HG22	4:R:222:SER:HB3	1.99	0.44
4:T:27:VAL:O	4:T:27:VAL:HG13	2.18	0.44
1:A:822:ILE:HG22	3:Q:182:GLN:HG3	1.99	0.44
1:B:109:PHE:HB2	1:B:123:LYS:HG2	1.99	0.44
2:D:6:THR:HG23	2:D:129:VAL:O	2.18	0.44
2:N:39:LEU:HD23	2:N:39:LEU:HA	1.84	0.44
2:O:56:VAL:O	2:O:60:SER:OG	2.30	0.44
3:P:112:ASN:HB2	4:S:26:THR:HG21	1.99	0.44
4:R:308:MET:HE2	4:R:308:MET:HB3	1.73	0.44
4:R:524:VAL:HG11	4:R:529:GLU:HG3	2.00	0.44
4:T:81:ALA:HB1	4:T:527:LYS:HE2	1.93	0.44
2:K:134:PRO:O	2:K:137:THR:OG1	2.33	0.44
2:K:268:TYR:CD1	2:K:277:VAL:CG2	3.00	0.44
2:E:64:ASP:OD1	2:E:109:LYS:NZ	2.41	0.44
2:L:13:PRO:HB2	2:L:276:ARG:HH12	1.82	0.44
4:R:312:LEU:HD22	4:R:366:LYS:HB2	2.00	0.44
4:S:515:ASP:OD2	4:S:515:ASP:N	2.46	0.44
1:A:687:ASP:HB3	1:A:730:ILE:HD13	2.00	0.44
2:D:131:VAL:HG11	2:D:139:VAL:HG11	2.00	0.44
2:G:168:ILE:CG2	2:G:268:TYR:CD2	3.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:178:VAL:HG22	2:G:215:LEU:HD13	1.98	0.44
2:J:267:GLN:OE1	2:J:276:ARG:NH1	2.50	0.44
4:S:99:GLN:O	4:S:217:TYR:OH	2.33	0.44
4:T:205:LYS:HE3	4:T:446:ILE:HG23	1.99	0.44
1:A:461:ILE:HD12	1:A:461:ILE:HA	1.81	0.44
2:E:67:PRO:HB3	2:E:73:LYS:HE3	1.99	0.44
2:I:272:ASP:OD1	2:I:275:ASN:HB2	2.17	0.44
2:K:151:MET:HE2	2:K:161:ILE:HD12	1.99	0.44
3:Q:198:SER:OG	3:Q:199:THR:N	2.51	0.44
4:S:328:PHE:CE2	4:S:340:THR:HG21	2.53	0.44
4:T:63:ARG:NH1	4:T:176:VAL:HG23	2.33	0.44
4:T:274:ASN:OD1	4:T:274:ASN:N	2.50	0.44
2:G:62:PHE:HZ	2:G:293:MET:SD	2.41	0.43
3:P:236:LEU:HD12	3:P:239:ARG:HD2	2.00	0.43
4:R:520:ILE:CD1	4:R:531:ILE:HG22	2.48	0.43
4:T:457:ASP:O	4:T:461:THR:OG1	2.35	0.43
2:H:168:ILE:HG23	2:H:268:TYR:CE2	2.53	0.43
2:N:59:TYR:CD1	2:N:67:PRO:HG3	2.54	0.43
2:O:44:ARG:CZ	2:O:44:ARG:HB3	2.48	0.43
1:A:202:LYS:HD2	1:A:282:TYR:CE2	2.53	0.43
1:B:853:ASP:O	1:B:853:ASP:CG	2.61	0.43
2:F:152:LEU:HD22	2:F:154:THR:HG23	2.00	0.43
2:G:150:THR:HG23	2:G:216:VAL:HG22	1.99	0.43
2:L:263:PHE:O	2:L:267:GLN:HG2	2.18	0.43
2:M:18:VAL:HG21	4:T:3:TRP:HH2	1.82	0.43
4:R:188:LYS:O	4:R:209:ILE:HG13	2.17	0.43
2:M:68:ARG:HE	2:M:68:ARG:HB3	1.67	0.43
4:R:118:LEU:HD22	4:R:252:TYR:CD2	2.54	0.43
4:R:187:ILE:HG22	4:R:209:ILE:HG12	2.00	0.43
4:S:516:GLY:H	4:S:615:TRP:CD1	2.36	0.43
4:T:430:ARG:HA	4:T:430:ARG:HD2	1.83	0.43
1:B:305:ASP:OD2	1:B:309:ASN:HB2	2.19	0.43
2:M:39:LEU:HD12	2:M:39:LEU:HA	1.91	0.43
4:T:157:SER:C	4:T:159:ALA:H	2.26	0.43
1:A:463:MET:HE1	1:A:650:GLU:CB	2.48	0.43
3:P:99:LEU:O	3:P:103:THR:HG22	2.19	0.43
3:P:149:ASN:ND2	4:S:24:ASP:OD2	2.41	0.43
4:R:111:ASP:OD1	4:R:224:HIS:ND1	2.49	0.43
4:R:235:ALA:HB2	4:R:244:LEU:HD13	2.01	0.43
4:S:332:VAL:HG21	4:S:419:HIS:NE2	2.33	0.43
1:A:197:GLN:HG3	1:A:204:ALA:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ARG:HH11	1:A:490:SER:CB	2.29	0.43
2:H:87:ARG:NH1	3:Q:38:LEU:O	2.51	0.43
2:I:251:ILE:HD12	2:I:251:ILE:HA	1.83	0.43
4:S:365:LEU:HD22	4:S:377:LEU:HD23	2.00	0.43
4:T:492:ILE:HD13	4:T:570:TRP:CE2	2.53	0.43
1:B:100:LYS:HB2	1:B:100:LYS:HE2	1.78	0.43
2:D:168:ILE:HG21	2:D:268:TYR:CD2	2.53	0.43
2:E:147:ALA:HB3	2:E:219:ALA:HB3	2.00	0.43
4:R:260:ASP:OD2	4:R:459:ARG:HD2	2.18	0.43
4:S:410:GLN:NE2	4:S:584:ASN:H	2.16	0.43
4:S:414:ILE:HD11	4:S:416:TRP:CZ2	2.54	0.43
1:A:430:HIS:HA	1:A:433:MET:HE3	2.01	0.43
2:C:134:PRO:HG2	2:C:159:ALA:HB1	2.01	0.43
2:I:52:ASP:OD1	2:I:52:ASP:N	2.51	0.43
2:I:183:ALA:HB2	2:I:190:PRO:HD3	2.01	0.43
4:R:536:VAL:HG12	4:R:542:THR:HB	2.01	0.43
4:S:74:SER:H	5:s:5:THR:CG2	2.31	0.43
4:S:90:ILE:HD12	4:S:462:THR:OG1	2.18	0.43
4:T:43:ALA:CA	4:T:277:MET:HE1	2.48	0.43
1:A:319:MET:HE3	1:A:319:MET:HA	2.01	0.43
1:B:270:ARG:HG3	1:B:270:ARG:HH11	1.84	0.43
2:D:147:ALA:HB3	2:D:219:ALA:HB3	2.00	0.43
2:F:168:ILE:CG2	2:F:268:TYR:CD2	3.01	0.43
2:M:44:ARG:HA	2:M:44:ARG:HD2	1.89	0.43
4:R:365:LEU:HD22	4:R:377:LEU:HD12	2.01	0.43
4:S:69:MET:HE2	4:S:102:ARG:HH12	1.84	0.43
4:R:393:ASN:HB3	4:R:396:LEU:HB2	2.01	0.42
4:T:93:ASP:OD1	4:T:93:ASP:N	2.51	0.42
4:T:140:LYS:HD3	4:T:140:LYS:HA	1.86	0.42
4:T:479:TYR:HH	4:T:561:SER:HG	1.66	0.42
4:T:519:LEU:HD13	4:T:519:LEU:HA	1.90	0.42
2:N:182:LEU:HD12	2:N:207:VAL:HG22	2.01	0.42
4:T:392:ASP:OD1	4:T:392:ASP:N	2.52	0.42
4:T:506:LYS:HB2	4:T:506:LYS:HE2	1.86	0.42
1:A:366:GLY:HA2	1:A:943:VAL:HG23	2.01	0.42
1:A:727:LYS:H	1:A:727:LYS:HG2	1.70	0.42
2:E:35:LEU:HD12	2:E:78:MET:HE1	1.99	0.42
2:F:233:LYS:HE3	2:F:233:LYS:HB3	1.84	0.42
1:A:953:THR:HG23	1:B:139:LYS:O	2.19	0.42
2:C:6:THR:HG23	2:C:129:VAL:O	2.19	0.42
2:C:89:TYR:HB2	2:C:283:LEU:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:252:GLN:H	2:F:252:GLN:CD	2.21	0.42
2:M:152:LEU:HD13	2:M:214:PRO:HG3	2.01	0.42
3:Q:99:LEU:HD12	3:Q:99:LEU:HA	1.91	0.42
4:S:228:ASN:O	4:S:231:ILE:HG22	2.18	0.42
4:T:77:GLU:OE1	4:T:77:GLU:HA	2.19	0.42
4:T:431:LYS:HG3	4:T:451:ILE:HD11	2.02	0.42
4:T:445:VAL:O	4:T:449:ILE:HG13	2.20	0.42
1:B:93:LEU:HD23	1:B:93:LEU:HA	1.87	0.42
1:B:437:ARG:O	1:B:437:ARG:HG2	2.18	0.42
1:B:762:PRO:O	1:B:765:VAL:HG23	2.20	0.42
2:E:131:VAL:HG11	2:E:139:VAL:HG11	2.02	0.42
3:P:9:LEU:HD12	3:P:9:LEU:HA	1.87	0.42
4:R:261:ILE:HD13	4:R:261:ILE:HA	1.85	0.42
4:S:25:ARG:HG3	4:S:25:ARG:HH11	1.84	0.42
1:A:837:MET:HG2	1:B:954:ARG:HB2	2.01	0.42
2:G:151:MET:HE3	2:G:209:LEU:HD13	2.00	0.42
2:I:189:MET:HA	2:I:190:PRO:HD3	1.95	0.42
2:L:118:ASN:OD1	2:L:228:PRO:HA	2.20	0.42
2:M:137:THR:HG22	2:M:153:ASN:HA	2.02	0.42
4:R:502:ASN:HB2	4:R:505:THR:HG23	2.01	0.42
4:S:109:LYS:O	4:S:113:GLU:HG2	2.20	0.42
4:S:197:VAL:HG12	4:S:197:VAL:O	2.20	0.42
4:T:511:VAL:O	4:T:517:HIS:HA	2.19	0.42
1:A:374:GLN:NE2	1:A:551:PRO:HD3	2.34	0.42
1:A:463:MET:SD	1:A:465:TYR:HE1	2.41	0.42
2:H:182:LEU:CB	2:H:196:TYR:HE2	2.22	0.42
2:I:294:ARG:HD3	2:I:294:ARG:HA	1.88	0.42
2:J:300:ARG:CD	3:Q:46:ASN:HD21	2.32	0.42
2:N:88:SER:HA	2:N:94:ALA:HB3	2.02	0.42
4:T:616:ASP:OD1	4:T:617:GLN:N	2.53	0.42
1:A:825:ASN:ND2	3:Q:183:ASP:HA	2.34	0.42
2:D:274:ILE:O	2:D:277:VAL:CG1	2.68	0.42
2:G:179:PRO:HG3	2:G:194:PHE:CZ	2.54	0.42
2:I:120:TYR:CD1	2:I:120:TYR:C	2.98	0.42
3:Q:93:LEU:HG	3:Q:246:LEU:HD11	2.02	0.42
4:R:107:MET:HE2	4:R:458:LEU:HD13	2.01	0.42
4:T:42:ILE:HG22	4:T:277:MET:HE2	2.02	0.42
2:G:183:ALA:HB3	2:G:189:MET:SD	2.60	0.42
2:H:96:ALA:O	3:Q:59:VAL:HG11	2.20	0.42
2:K:13:PRO:HG2	2:K:270:ALA:HB2	2.01	0.42
2:M:294:ARG:HA	2:M:294:ARG:HD3	1.70	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:237:LYS:HB2	3:P:237:LYS:HE3	1.82	0.42
3:Q:152:ASP:OD1	3:Q:152:ASP:N	2.52	0.42
4:R:35:MET:HE3	4:T:40:ALA:HB2	2.01	0.42
4:T:483:ILE:HG23	4:T:494:TYR:CZ	2.55	0.42
1:A:559:ASN:ND2	1:A:563:ILE:O	2.50	0.42
2:F:151:MET:HE3	2:F:161:ILE:HD12	2.02	0.42
2:G:298:PRO:HG2	2:H:118:ASN:O	2.20	0.42
4:R:534:LEU:HD23	4:R:534:LEU:HA	1.90	0.42
4:S:131:THR:CG2	4:S:154:VAL:HG21	2.50	0.42
1:A:749:TYR:O	1:A:753:LEU:HG	2.19	0.41
2:C:184:ARG:CD	2:C:202:ASP:HB3	2.48	0.41
2:H:136:ARG:H	2:H:136:ARG:HG2	1.70	0.41
2:H:294:ARG:HH12	3:Q:42:ASN:HD21	1.68	0.41
2:J:6:THR:OG1	2:J:129:VAL:O	2.33	0.41
2:J:223:THR:HG21	2:J:265:ILE:HD11	2.01	0.41
2:M:53:VAL:N	2:M:54:PRO:HD2	2.35	0.41
2:M:182:LEU:HD21	2:M:205:PHE:HB3	2.02	0.41
4:R:428:ASP:OD1	4:R:428:ASP:N	2.53	0.41
4:S:39:ARG:HD3	4:T:39:ARG:NH2	2.34	0.41
4:S:94:ILE:HD13	4:S:449:ILE:HD12	2.02	0.41
4:S:280:PRO:HG3	4:S:289:TRP:CE2	2.55	0.41
4:T:210:ILE:HG23	4:T:212:GLN:H	1.84	0.41
1:B:779:PHE:O	1:B:788:TYR:OH	2.37	0.41
2:M:11:ASP:OD2	2:N:194:PHE:HD2	2.02	0.41
2:O:126:VAL:HG12	2:O:144:SER:O	2.20	0.41
3:Q:188:VAL:HG23	3:Q:212:LYS:HA	2.02	0.41
1:B:480:MET:HA	1:B:484:ARG:HG2	2.02	0.41
2:D:40:ILE:HD13	2:D:295:ARG:HH21	1.84	0.41
2:E:98:VAL:HA	2:E:99:PRO:HD3	1.92	0.41
2:F:205:PHE:C	2:F:206:ILE:HD13	2.45	0.41
4:R:489:TYR:CZ	4:R:576:PRO:HB2	2.55	0.41
4:S:459:ARG:HB2	4:S:488:HIS:NE2	2.35	0.41
2:I:123:PHE:HD1	2:I:261:ASP:OD1	2.03	0.41
2:I:272:ASP:O	2:I:276:ARG:HG3	2.19	0.41
2:M:83:THR:O	2:M:87:ARG:HG3	2.20	0.41
4:R:219:ALA:HB1	4:R:274:ASN:HB3	2.02	0.41
4:S:458:LEU:HD12	4:S:458:LEU:HA	1.84	0.41
1:B:766:GLU:CG	1:B:768:VAL:HG12	2.49	0.41
2:E:72:VAL:HG12	2:E:74:THR:HG23	2.02	0.41
2:J:126:VAL:HA	2:J:221:ALA:HB3	2.01	0.41
4:S:50:MET:O	4:S:53:ARG:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:614:THR:HG22	4:T:615:TRP:H	1.85	0.41
2:I:62:PHE:CE2	2:I:293:MET:SD	3.13	0.41
2:J:62:PHE:CE2	2:J:293:MET:SD	3.14	0.41
4:R:511:VAL:HG21	4:R:532:LEU:HD22	2.02	0.41
4:S:449:ILE:HG22	4:S:450:HIS:HD2	1.85	0.41
4:S:489:TYR:CE1	4:S:576:PRO:HB2	2.55	0.41
4:S:605:LEU:HD13	4:S:624:THR:OG1	2.21	0.41
4:S:624:THR:HG23	4:S:625:ASN:N	2.35	0.41
4:T:46:ARG:HG3	4:T:46:ARG:NH1	2.30	0.41
4:T:113:GLU:OE1	4:T:113:GLU:C	2.63	0.41
4:T:359:LEU:O	4:T:363:MET:HG3	2.20	0.41
4:T:511:VAL:HG21	4:T:532:LEU:HD22	2.02	0.41
1:A:494:TYR:OH	1:A:533:VAL:O	2.33	0.41
1:B:82:LYS:HE3	1:B:82:LYS:HB3	1.74	0.41
1:B:98:LEU:HD22	1:B:101:LEU:HB3	2.02	0.41
1:B:202:LYS:HE3	1:B:282:TYR:CE1	2.55	0.41
2:K:77:LYS:HE2	2:K:77:LYS:HB3	1.80	0.41
4:R:449:ILE:C	4:R:449:ILE:HD12	2.45	0.41
4:T:516:GLY:HA3	4:T:613:HIS:O	2.20	0.41
1:A:204:ALA:HB3	1:A:925:LEU:HD22	2.03	0.41
1:B:481:LEU:HD23	1:B:481:LEU:HA	1.90	0.41
2:C:40:ILE:HD11	2:C:292:GLN:HA	2.03	0.41
2:N:271:GLN:HG2	2:N:272:ASP:OD1	2.21	0.41
2:O:241:GLN:H	2:O:241:GLN:HG2	1.72	0.41
4:R:27:VAL:CG1	4:R:28:ALA:N	2.84	0.41
4:R:43:ALA:HB2	4:R:277:MET:HE1	2.03	0.41
1:B:96:GLN:O	1:B:97:LYS:NZ	2.48	0.41
1:B:586:ARG:HG3	1:B:586:ARG:NH1	2.36	0.41
2:J:74:THR:HG21	3:P:43:GLU:HB2	2.03	0.41
2:K:179:PRO:HG3	2:K:194:PHE:CD2	2.55	0.41
2:M:181:GLN:HB2	2:M:208:VAL:HG22	2.03	0.41
2:N:268:TYR:O	2:N:268:TYR:HD2	2.04	0.41
3:Q:65:ARG:HD2	3:Q:87:PRO:O	2.21	0.41
4:R:200:ALA:HB1	4:S:624:THR:HG21	2.03	0.41
4:R:493:ASP:HB2	4:R:569:ASN:OD1	2.21	0.41
4:S:487:ALA:C	4:S:578:VAL:HG12	2.46	0.41
1:A:624:TYR:CZ	1:A:670:ILE:HD11	2.56	0.41
2:M:65:ASP:N	2:M:65:ASP:OD1	2.53	0.41
4:T:534:LEU:CD1	4:T:542:THR:HG21	2.46	0.41
4:T:626:ILE:HD12	4:T:626:ILE:HA	1.89	0.41
1:B:207:LYS:HG3	1:B:922:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:756:LEU:HD12	1:B:756:LEU:HA	1.97	0.40
2:G:160:ASN:C	2:G:161:ILE:HD13	2.46	0.40
2:I:244:MET:HE1	2:I:257:TYR:O	2.21	0.40
2:N:183:ALA:HB2	2:N:190:PRO:HD3	2.02	0.40
2:O:111:THR:O	2:O:111:THR:HG23	2.21	0.40
1:B:593:ASN:OD1	1:B:593:ASN:N	2.54	0.40
2:F:26:ARG:HG2	2:F:116:MET:HE3	2.03	0.40
2:G:126:VAL:HG11	2:G:147:ALA:HB2	2.03	0.40
2:N:168:ILE:CG2	2:N:268:TYR:CD2	3.04	0.40
2:O:168:ILE:HG13	2:O:268:TYR:CE2	2.55	0.40
4:S:521:GLU:OE1	4:S:521:GLU:C	2.65	0.40
4:T:27:VAL:HG22	4:T:34:SER:HB2	2.04	0.40
4:T:428:ASP:OD1	4:T:429:SER:N	2.54	0.40
1:A:438:LEU:HD22	1:A:438:LEU:H	1.87	0.40
2:E:233:LYS:HB3	2:E:233:LYS:HE2	1.71	0.40
2:E:271:GLN:OE1	2:E:271:GLN:HA	2.21	0.40
2:G:33:GLU:OE2	2:G:288:GLN:NE2	2.54	0.40
3:Q:174:ASP:OD1	3:Q:175:MET:N	2.54	0.40
4:R:492:ILE:HD12	4:R:570:TRP:CE2	2.57	0.40
4:S:210:ILE:HD12	4:S:210:ILE:HA	1.84	0.40
1:A:350:PRO:HA	1:A:545:VAL:HG11	2.02	0.40
2:C:172:VAL:HG23	2:C:200:PRO:HG3	2.04	0.40
2:E:294:ARG:HA	2:E:294:ARG:HD3	1.93	0.40
2:F:244:MET:SD	2:G:173:ILE:HD11	2.62	0.40
2:H:61:LYS:HD2	2:H:61:LYS:HA	1.71	0.40
4:R:518:LEU:HB2	4:R:612:TRP:HE3	1.86	0.40
4:S:46:ARG:NH1	4:S:50:MET:HB2	2.36	0.40
4:S:301:LEU:HD23	4:S:318:ALA:HA	2.04	0.40
1:A:300:SER:HA	1:A:313:ILE:O	2.21	0.40
1:A:395:LYS:HE2	1:A:395:LYS:HB3	1.73	0.40
2:E:88:SER:HA	2:E:94:ALA:HB3	2.04	0.40
3:Q:20:PRO:HA	3:Q:97:SER:HA	2.04	0.40
4:S:251:ILE:HG12	4:S:408:THR:HG21	2.02	0.40
4:T:499:ASP:CG	4:T:526:HIS:HD1	2.30	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	A	747/955 (78%)	737 (99%)	10 (1%)	0	100	100
1	B	898/955 (94%)	880 (98%)	18 (2%)	0	100	100
2	C	297/302 (98%)	293 (99%)	4 (1%)	0	100	100
2	D	296/302 (98%)	287 (97%)	9 (3%)	0	100	100
2	E	296/302 (98%)	290 (98%)	6 (2%)	0	100	100
2	F	296/302 (98%)	290 (98%)	6 (2%)	0	100	100
2	G	296/302 (98%)	290 (98%)	6 (2%)	0	100	100
2	H	297/302 (98%)	292 (98%)	5 (2%)	0	100	100
2	I	296/302 (98%)	286 (97%)	10 (3%)	0	100	100
2	J	297/302 (98%)	291 (98%)	6 (2%)	0	100	100
2	K	296/302 (98%)	293 (99%)	3 (1%)	0	100	100
2	L	295/302 (98%)	286 (97%)	9 (3%)	0	100	100
2	M	296/302 (98%)	291 (98%)	5 (2%)	0	100	100
2	N	296/302 (98%)	289 (98%)	7 (2%)	0	100	100
2	O	296/302 (98%)	291 (98%)	5 (2%)	0	100	100
3	P	247/249 (99%)	245 (99%)	2 (1%)	0	100	100
3	Q	242/249 (97%)	233 (96%)	9 (4%)	0	100	100
4	R	599/628 (95%)	593 (99%)	6 (1%)	0	100	100
4	S	620/628 (99%)	609 (98%)	11 (2%)	0	100	100
4	T	625/628 (100%)	609 (97%)	16 (3%)	0	100	100
5	r	13/283 (5%)	13 (100%)	0	0	100	100
5	s	13/283 (5%)	13 (100%)	0	0	100	100
5	t	13/283 (5%)	13 (100%)	0	0	100	100
All	All	7867/9067 (87%)	7714 (98%)	153 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	673/846 (80%)	670 (100%)	3 (0%)	84	83
1	B	803/846 (95%)	795 (99%)	8 (1%)	68	77
2	C	249/252 (99%)	245 (98%)	4 (2%)	55	69
2	D	248/252 (98%)	245 (99%)	3 (1%)	63	74
2	E	248/252 (98%)	246 (99%)	2 (1%)	73	79
2	F	248/252 (98%)	242 (98%)	6 (2%)	43	63
2	G	248/252 (98%)	245 (99%)	3 (1%)	63	74
2	H	249/252 (99%)	243 (98%)	6 (2%)	43	63
2	I	248/252 (98%)	244 (98%)	4 (2%)	55	69
2	J	249/252 (99%)	246 (99%)	3 (1%)	63	74
2	K	248/252 (98%)	246 (99%)	2 (1%)	73	79
2	L	247/252 (98%)	244 (99%)	3 (1%)	63	74
2	M	248/252 (98%)	245 (99%)	3 (1%)	63	74
2	N	248/252 (98%)	245 (99%)	3 (1%)	63	74
2	O	248/252 (98%)	246 (99%)	2 (1%)	73	79
3	P	225/225 (100%)	218 (97%)	7 (3%)	35	56
3	Q	223/225 (99%)	220 (99%)	3 (1%)	61	73
4	R	509/532 (96%)	504 (99%)	5 (1%)	68	77
4	S	527/532 (99%)	523 (99%)	4 (1%)	73	79
4	T	531/532 (100%)	520 (98%)	11 (2%)	47	65
5	r	14/245 (6%)	14 (100%)	0	100	100
5	s	14/245 (6%)	14 (100%)	0	100	100
5	t	14/245 (6%)	14 (100%)	0	100	100
All	All	6759/7749 (87%)	6674 (99%)	85 (1%)	59	73

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	877	ILE
1	A	880	ASP
1	A	927	ASP
1	B	200	ASN
1	B	219	ILE
1	B	370	ARG
1	B	471	ILE
1	B	634	GLU
1	B	790	ASN
1	B	795	MET
1	B	847	GLU
2	C	85	VAL
2	C	98	VAL
2	C	103	ILE
2	C	297	LEU
2	D	74	THR
2	D	198	LEU
2	D	292	GLN
2	E	216	VAL
2	E	244	MET
2	F	66	ASN
2	F	85	VAL
2	F	161	ILE
2	F	251	ILE
2	F	274	ILE
2	F	277	VAL
2	G	27	GLN
2	G	207	VAL
2	G	223	THR
2	H	78	MET
2	H	145	ASP
2	H	151	MET
2	H	187	GLN
2	H	211	VAL
2	H	229	LEU
2	I	40	ILE
2	I	142	VAL
2	I	154	THR
2	I	177	SER
2	J	133	SER
2	J	207	VAL
2	J	251	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	103	ILE
2	K	274	ILE
2	L	97	ILE
2	L	101	VAL
2	L	138	THR
2	M	149	VAL
2	M	208	VAL
2	M	216	VAL
2	N	34	LEU
2	N	52	ASP
2	N	73	LYS
2	O	39	LEU
2	O	132	LEU
3	P	5	SER
3	P	8	SER
3	P	42	ASN
3	P	93	LEU
3	P	121	ARG
3	P	147	ASP
3	P	199	THR
3	Q	171	ILE
3	Q	195	LEU
3	Q	230	GLU
4	R	29	ASP
4	R	187	ILE
4	R	225	VAL
4	R	230	VAL
4	R	267	THR
4	S	183	VAL
4	S	191	ILE
4	S	268	VAL
4	S	308	MET
4	T	50	MET
4	T	84	LEU
4	T	150	LEU
4	T	189	VAL
4	T	197	VAL
4	T	370	SER
4	T	408	THR
4	T	451	ILE
4	T	473	ILE
4	T	534	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	T	571	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	330	GLN
1	A	373	ASN
1	A	374	GLN
1	A	589	ASN
1	A	932	GLN
1	B	128	GLN
1	B	146	GLN
1	B	299	GLN
1	B	309	ASN
1	B	373	ASN
1	B	559	ASN
1	B	562	ASN
1	B	717	ASN
1	B	825	ASN
1	B	932	GLN
2	C	93	ASN
2	C	181	GLN
2	D	181	GLN
2	D	267	GLN
2	E	69	HIS
2	E	93	ASN
2	E	255	ASN
2	G	66	ASN
2	G	167	GLN
2	G	288	GLN
2	I	19	ASN
2	I	164	ASN
2	I	267	GLN
2	I	288	GLN
2	I	292	GLN
2	J	80	ASN
2	J	124	ASN
2	J	269	HIS
2	K	80	ASN
2	K	292	GLN
2	L	267	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	288	GLN
2	M	50	ASN
2	M	100	GLN
2	M	187	GLN
2	N	181	GLN
2	N	252	GLN
2	N	255	ASN
2	O	19	ASN
2	O	57	GLN
2	O	100	GLN
3	P	68	ASN
3	P	160	ASN
3	P	165	GLN
3	Q	42	ASN
3	Q	46	ASN
3	Q	68	ASN
3	Q	169	ASN
3	Q	182	GLN
4	R	128	ASN
4	R	282	ASN
4	R	298	GLN
4	R	339	ASN
4	R	488	HIS
4	S	62	ASN
4	S	98	HIS
4	S	99	GLN
4	S	128	ASN
4	S	133	ASN
4	S	138	ASN
4	S	139	GLN
4	S	247	ASN
4	S	249	GLN
4	S	295	HIS
4	S	322	ASN
4	S	393	ASN
4	S	404	HIS
4	S	584	ASN
4	S	617	GLN
4	T	14	GLN
4	T	97	GLN
4	T	99	GLN
4	T	101	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	T	139	GLN
4	T	221	GLN
4	T	258	HIS
4	T	295	HIS
4	T	315	ASN
4	T	319	GLN
4	T	397	GLN
4	T	464	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37379. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.