



Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 01:20 AM UTC

PDB ID : 9C1H / pdb_00009c1h
EMDB ID : EMD-45119
Title : Rhesus rotavirus (upright structure at 2.88 Angstrom resolution)
Authors : Jenni, S.; Herrmann, T.; De Sautu, M.; Harrison, S.C.
Deposited on : 2024-05-29
Resolution : 2.88 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
Mogul : 2022.3.0, CSD as543be (2022)
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

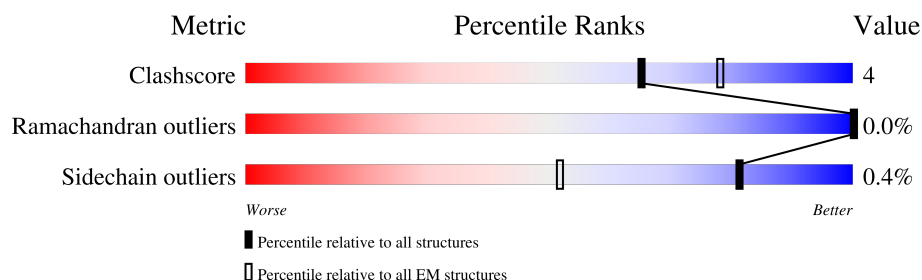
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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	0	326	73% 12% 15%
1	1	326	69% 12% 19%
1	P	326	72% 9% 19%
1	Q	326	74% 9% 17%
1	R	326	73% 8% 18%
1	S	326	72% 9% 19%
1	T	326	77% 7% 15%
1	U	326	71% 13% 15%
1	V	326	74% 10% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	W	326	
1	X	326	
1	Y	326	
1	Z	326	
1	t	326	
1	u	326	
1	v	326	
1	w	326	
1	x	326	
1	y	326	
2	2	776	
2	3	776	
2	4	776	
3	A	887	
3	B	887	
4	C	397	
4	D	397	
4	E	397	
4	F	397	
4	G	397	
4	H	397	
4	I	397	
4	J	397	
4	K	397	
4	L	397	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	M	397	 92% 8%
4	N	397	 91% 9%
4	O	397	 92% 7%
4	f	397	 90% 10%
4	g	397	 92% 8%
4	h	397	 90% 10%
4	i	397	 91% 9%
4	j	397	 88% 11%
4	k	397	 91% 8%
5	a	5	 20% 80%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 258079 atoms, of which 127694 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 Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	1	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	P	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	Q	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	R	266	Total	C	H	N	O	S	0	0
			4161	1338	2056	336	415	16		
1	S	264	Total	C	H	N	O	S	0	0
			4108	1322	2023	329	418	16		
1	T	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	U	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	V	276	Total	C	H	N	O	S	0	0
			4311	1389	2123	348	435	16		
1	W	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	X	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	Y	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	Z	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	t	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	u	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	v	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		
1	w	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	x	271	Total	C	H	N	O	S	0	0
			4234	1363	2087	341	427	16		
1	y	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	16		

- Molecule 2 is a protein called Outer capsid protein VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	750	Total	C	H	N	O	S	0	0
			11654	3715	5753	990	1176	20		
2	3	750	Total	C	H	N	O	S	0	0
			11655	3715	5754	990	1176	20		
2	4	542	Total	C	H	N	O	S	0	0
			8465	2681	4198	726	845	15		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	73	THR	SER	conflict	UNP P12473
2	311	GLU	ASP	conflict	UNP P12473
2	338	VAL	ILE	conflict	UNP P12473
2	421	LEU	PHE	conflict	UNP P12473
2	445	SER	GLY	conflict	UNP P12473
2	446	ARG	GLY	conflict	UNP P12473
2	454	ASN	TYR	conflict	UNP P12473
2	468	PHE	LEU	conflict	UNP P12473
2	519	ASP	TYR	conflict	UNP P12473
2	690	PHE	TYR	conflict	UNP P12473
3	73	THR	SER	conflict	UNP P12473
3	311	GLU	ASP	conflict	UNP P12473
3	338	VAL	ILE	conflict	UNP P12473
3	421	LEU	PHE	conflict	UNP P12473
3	445	SER	GLY	conflict	UNP P12473
3	446	ARG	GLY	conflict	UNP P12473
3	454	ASN	TYR	conflict	UNP P12473
3	468	PHE	LEU	conflict	UNP P12473
3	519	ASP	TYR	conflict	UNP P12473
3	690	PHE	TYR	conflict	UNP P12473
4	73	THR	SER	conflict	UNP P12473
4	311	GLU	ASP	conflict	UNP P12473
4	338	VAL	ILE	conflict	UNP P12473
4	421	LEU	PHE	conflict	UNP P12473

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
4	445	SER	GLY	conflict	UNP P12473
4	446	ARG	GLY	conflict	UNP P12473
4	454	ASN	TYR	conflict	UNP P12473
4	468	PHE	LEU	conflict	UNP P12473
4	519	ASP	TYR	conflict	UNP P12473
4	690	PHE	TYR	conflict	UNP P12473

- Molecule 3 is a protein called Inner capsid protein VP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	779	Total	C	H	N	O	S	0	0
			12749	4041	6387	1098	1187	36		
3	B	799	Total	C	H	N	O	S	0	0
			13098	4154	6563	1126	1219	36		

- Molecule 4 is a protein called Intermediate capsid protein VP6.

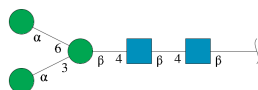
Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	397	Total	C	H	N	O	S	0	0
			6275	2005	3111	551	593	15		
4	D	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	E	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	F	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	G	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	H	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	I	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	J	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	K	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	L	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	M	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	N	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
4	O	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	f	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	g	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	h	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	i	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	j	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0
4	k	396	Total 6253	C 1999	H 3098	N 549	O 592	S 15	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	5	Total	C	H	N	O	0	0
			114	34	53	2	25		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					AltConf
6	0	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	1	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	P	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	Q	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	S	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	T	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	U	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	V	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	X	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	Y	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	Z	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	t	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	u	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	v	1	Total	C	H	N	O	0
			28	8	14	1	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
6	w	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	x	1	Total	C	H	N	O	0
			28	8	14	1	5	
6	y	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	0	4	Total	Ca	0
			4	4	
7	1	4	Total	Ca	0
			4	4	
7	P	4	Total	Ca	0
			4	4	
7	Q	4	Total	Ca	0
			4	4	
7	R	4	Total	Ca	0
			4	4	
7	S	4	Total	Ca	0
			4	4	
7	T	4	Total	Ca	0
			4	4	
7	U	4	Total	Ca	0
			4	4	
7	V	4	Total	Ca	0
			4	4	
7	W	4	Total	Ca	0
			4	4	
7	X	4	Total	Ca	0
			4	4	
7	Y	4	Total	Ca	0
			4	4	
7	Z	4	Total	Ca	0
			4	4	
7	t	4	Total	Ca	0
			4	4	
7	u	4	Total	Ca	0
			4	4	
7	v	4	Total	Ca	0
			4	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
7	w	4	Total 4	Ca 4	0
7	x	4	Total 4	Ca 4	0
7	y	4	Total 4	Ca 4	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	C	2	Total 2	Zn 2	0
8	D	1	Total 1	Zn 1	0
8	E	1	Total 1	Zn 1	0
8	F	2	Total 2	Zn 2	0
8	G	1	Total 1	Zn 1	0
8	H	1	Total 1	Zn 1	0
8	I	2	Total 2	Zn 2	0
8	J	1	Total 1	Zn 1	0
8	K	1	Total 1	Zn 1	0
8	L	2	Total 2	Zn 2	0
8	M	1	Total 1	Zn 1	0
8	N	1	Total 1	Zn 1	0
8	O	2	Total 2	Zn 2	0
8	f	2	Total 2	Zn 2	0
8	g	1	Total 1	Zn 1	0
8	h	1	Total 1	Zn 1	0

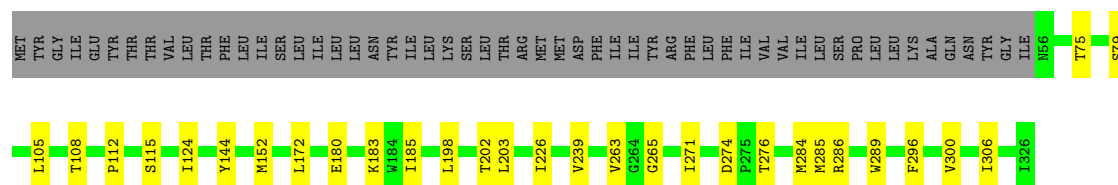
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
8	i	2	Total 2	Zn 2	0
8	j	1	Total 1	Zn 1	0
8	k	1	Total 1	Zn 1	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
9	C	1	Total 1	Cl 1	0
9	F	1	Total 1	Cl 1	0
9	J	1	Total 1	Cl 1	0
9	M	1	Total 1	Cl 1	0
9	O	1	Total 1	Cl 1	0
9	h	1	Total 1	Cl 1	0
9	j	1	Total 1	Cl 1	0



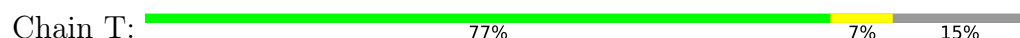
• Molecule 1: Outer capsid glycoprotein VP7



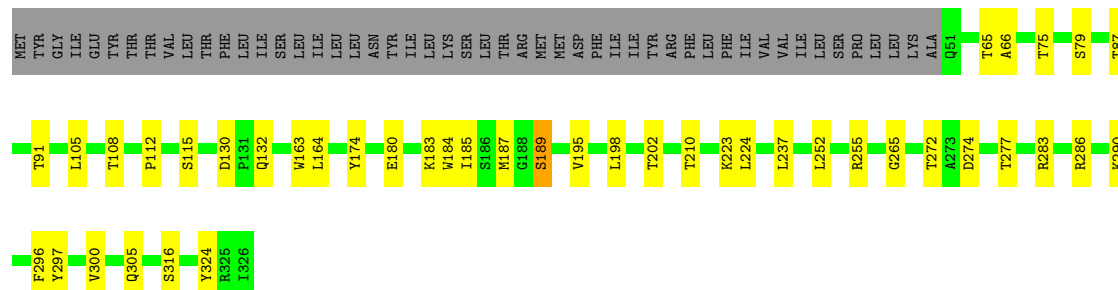
• Molecule 1: Outer capsid glycoprotein VP7



• Molecule 1: Outer capsid glycoprotein VP7

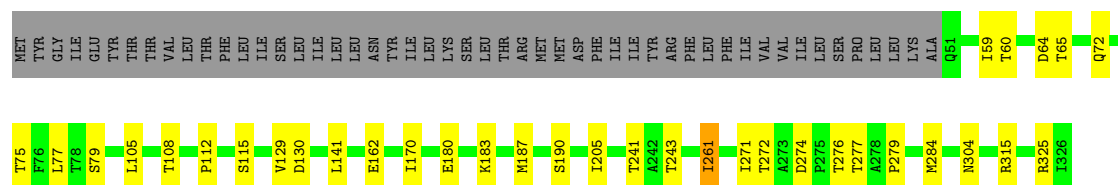


• Molecule 1: Outer capsid glycoprotein VP7



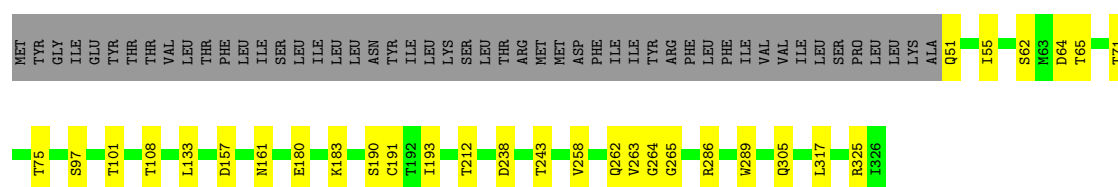
- Molecule 1: Outer capsid glycoprotein VP7

Chain V:  74% 10% 15%



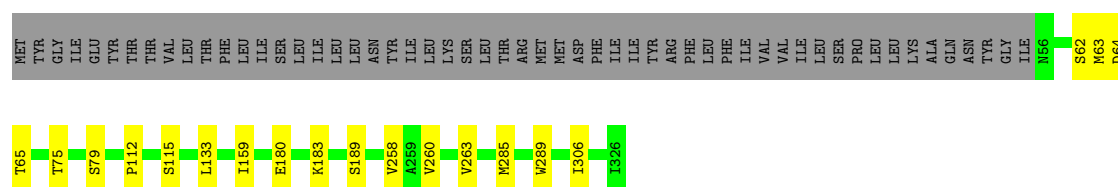
- Molecule 1: Outer capsid glycoprotein VP7

Chain W:  75% 10% 15%



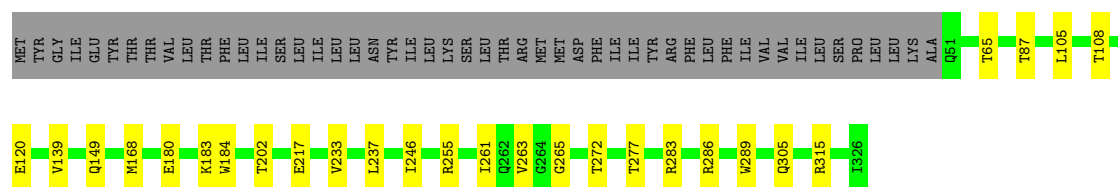
- Molecule 1: Outer capsid glycoprotein VP7

Chain X:  77% 6% 17%



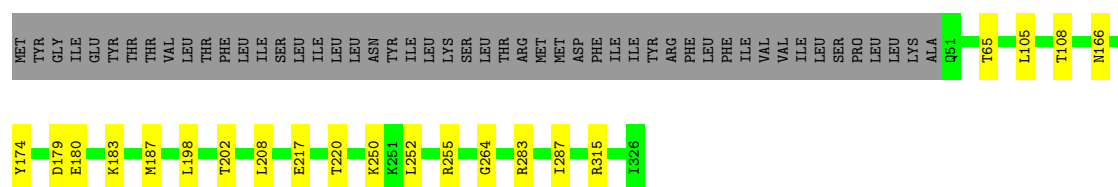
- Molecule 1: Outer capsid glycoprotein VP7

Chain Y:  76% 8% 15%

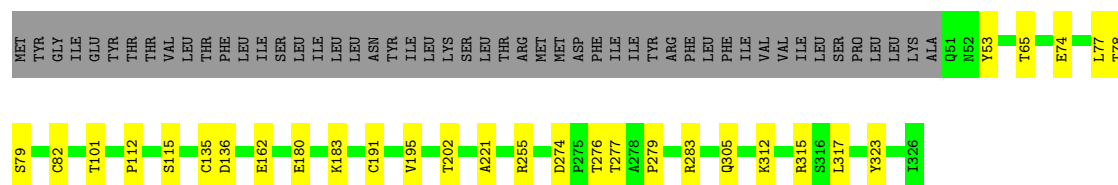


- Molecule 1: Outer capsid glycoprotein VP7

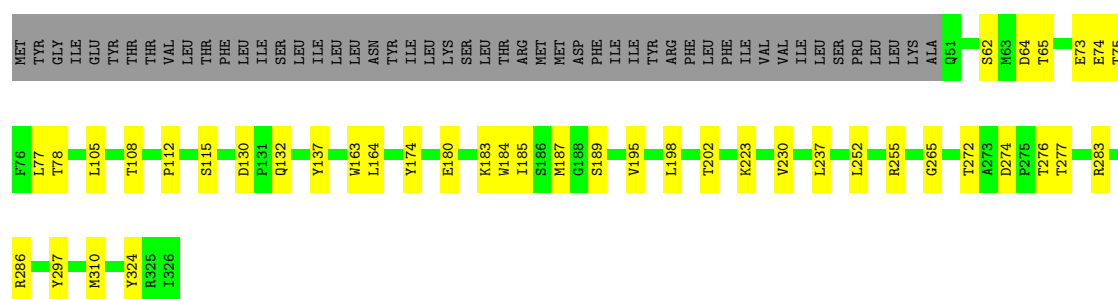
Chain Z:  78% 6% 15%



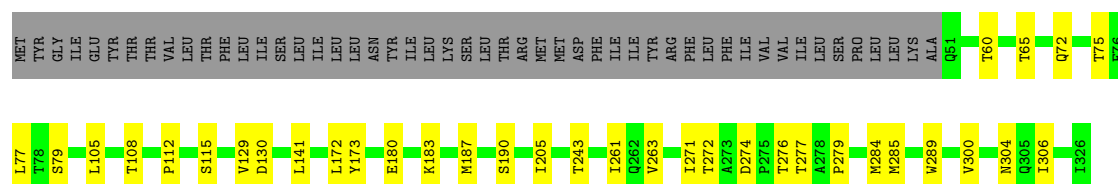
● Molecule 1: Outer capsid glycoprotein VP7

Chain t:  75% 9% 15%

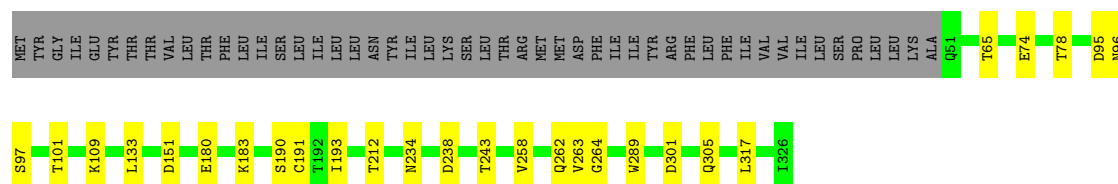
● Molecule 1: Outer capsid glycoprotein VP7

Chain u:  72% 13% 15%

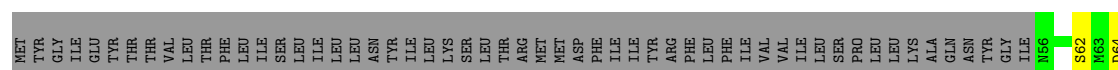
● Molecule 1: Outer capsid glycoprotein VP7

Chain v:  74% 11% 15%

● Molecule 1: Outer capsid glycoprotein VP7

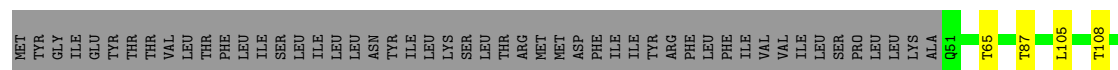
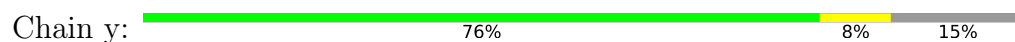
Chain w:  76% 8% 15%

● Molecule 1: Outer capsid glycoprotein VP7

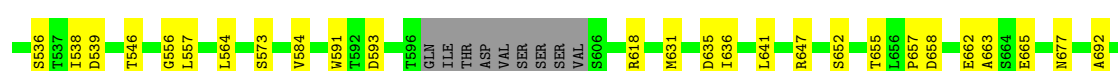
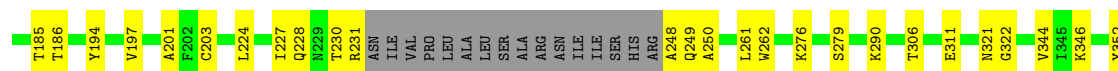
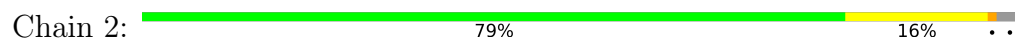
Chain x:  75% 9% 17%



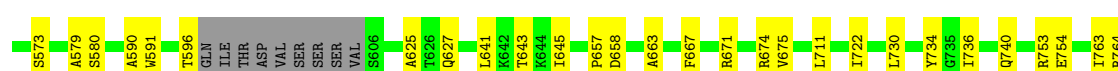
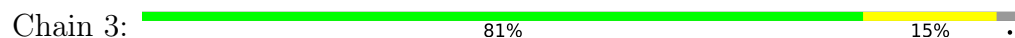
• Molecule 1: Outer capsid glycoprotein VP7



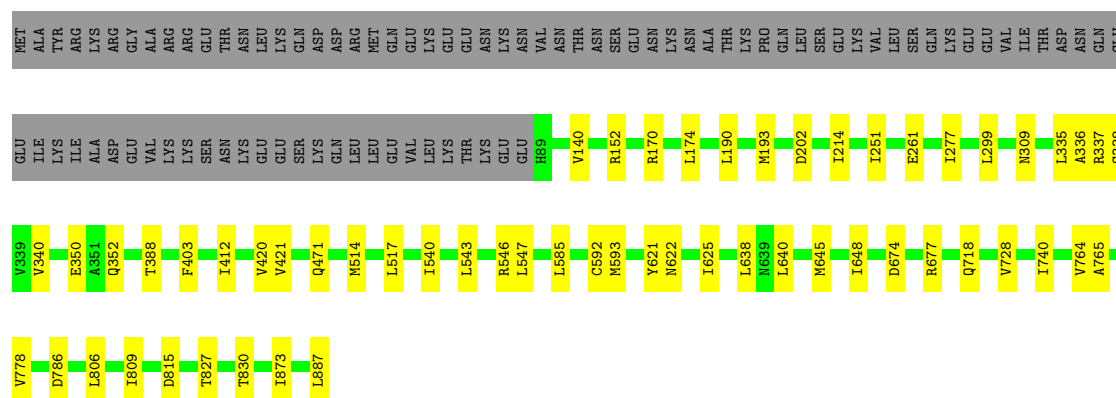
• Molecule 2: Outer capsid protein VP4



• Molecule 2: Outer capsid protein VP4

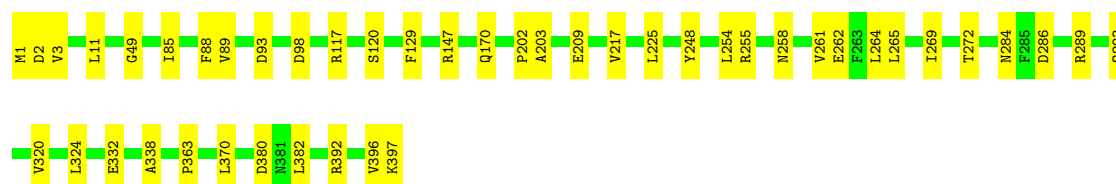


Chain B:  84% 7% 10%



- Molecule 4: Intermediate capsid protein VP6

Chain C:  89% 11%



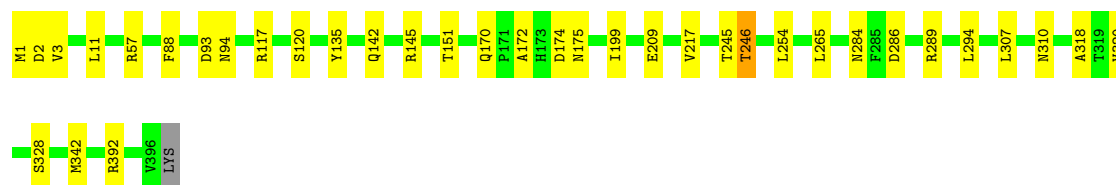
- Molecule 4: Intermediate capsid protein VP6

Chain D:  92% 8%



- Molecule 4: Intermediate capsid protein VP6

Chain E:  91% 9%



- Molecule 4: Intermediate capsid protein VP6

Chain F:  90% 10%





- Molecule 4: Intermediate capsid protein VP6

Chain G: 92% 8%



- Molecule 4: Intermediate capsid protein VP6

Chain H: 90% 10%



- Molecule 4: Intermediate capsid protein VP6

Chain I: 92% 8%



- Molecule 4: Intermediate capsid protein VP6

Chain J: 90% 10%

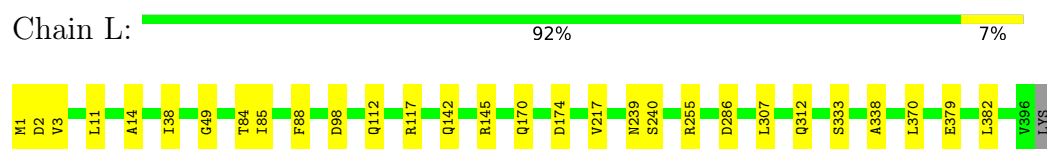


- Molecule 4: Intermediate capsid protein VP6

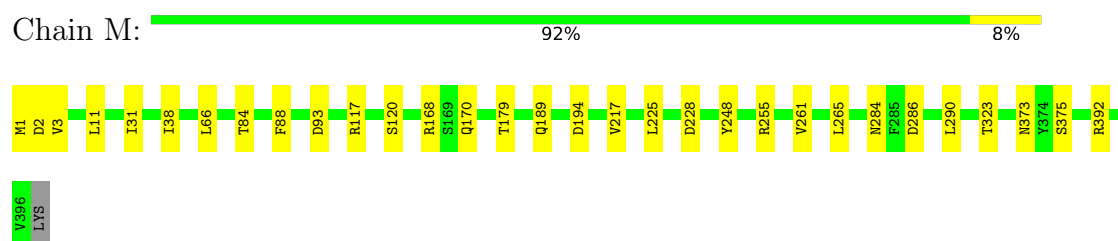
Chain K: 93% 7%



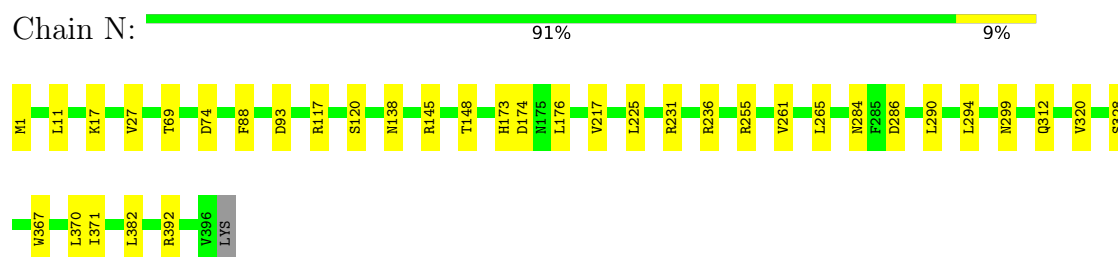
- Molecule 4: Intermediate capsid protein VP6



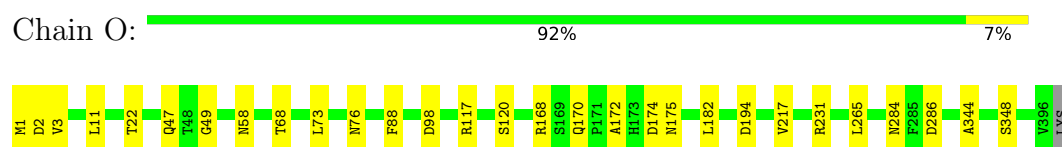
- Molecule 4: Intermediate capsid protein VP6



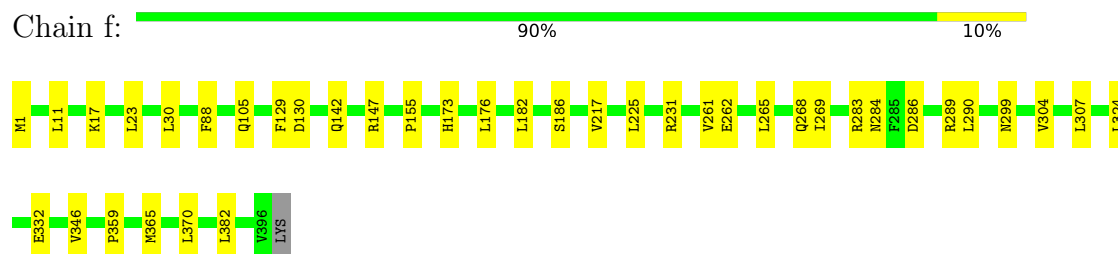
- Molecule 4: Intermediate capsid protein VP6



- Molecule 4: Intermediate capsid protein VP6



- Molecule 4: Intermediate capsid protein VP6

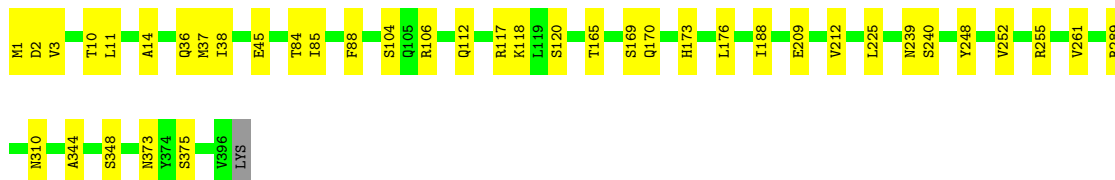


- Molecule 4: Intermediate capsid protein VP6

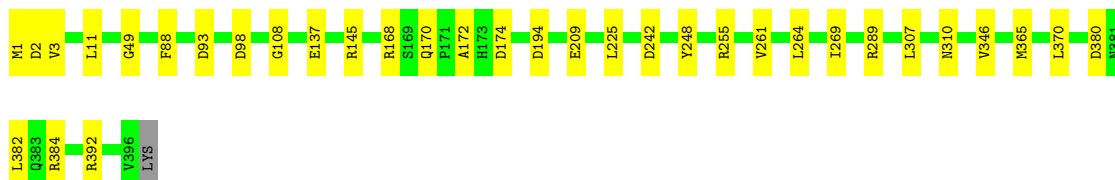
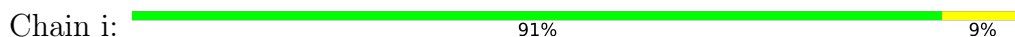




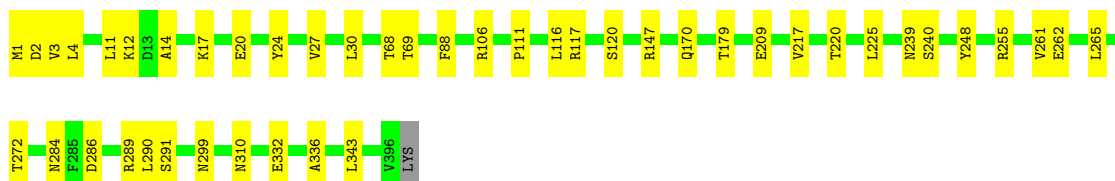
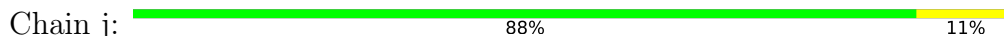
- Molecule 4: Intermediate capsid protein VP6



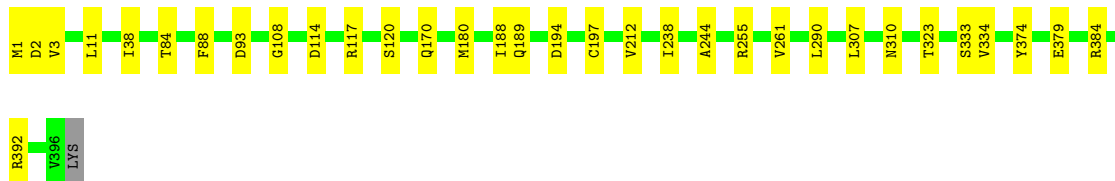
- Molecule 4: Intermediate capsid protein VP6



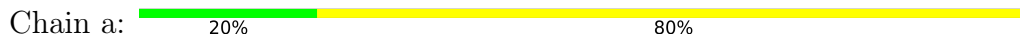
- Molecule 4: Intermediate capsid protein VP6



- Molecule 4: Intermediate capsid protein VP6



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	542965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: ZN, CL, CA, FME, MAN, BMA, NAG

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	0	0.14	0/2234	0.30	0/3051
1	1	0.14	0/2128	0.28	0/2908
1	P	0.14	0/2128	0.28	0/2908
1	Q	0.13	0/2192	0.29	0/2994
1	R	0.14	0/2148	0.28	0/2932
1	S	0.14	0/2128	0.29	0/2908
1	T	0.13	0/2234	0.26	0/3051
1	U	0.13	0/2234	0.29	0/3051
1	V	0.14	0/2234	0.29	0/3051
1	W	0.13	0/2234	0.27	0/3051
1	X	0.13	0/2192	0.27	0/2994
1	Y	0.13	0/2234	0.26	0/3051
1	Z	0.14	0/2234	0.30	0/3051
1	t	0.14	0/2234	0.28	0/3051
1	u	0.14	0/2234	0.30	0/3051
1	v	0.13	0/2234	0.29	0/3051
1	w	0.14	0/2234	0.28	0/3051
1	x	0.13	0/2192	0.28	0/2994
1	y	0.13	0/2234	0.26	0/3051
2	2	0.15	0/6021	0.41	2/8192 (0.0%)
2	3	0.14	0/6021	0.39	0/8192
2	4	0.16	0/4343	0.38	0/5885
3	A	0.16	0/6477	0.27	0/8788
3	B	0.16	0/6655	0.28	0/9029
4	C	0.17	0/3224	0.31	0/4387
4	D	0.16	0/3215	0.30	0/4376
4	E	0.16	0/3215	0.30	0/4376
4	F	0.16	0/3215	0.30	0/4376
4	G	0.16	0/3215	0.29	0/4376
4	H	0.16	0/3215	0.30	0/4376
4	I	0.16	0/3215	0.30	0/4376
4	J	0.16	0/3215	0.31	0/4376

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	K	0.15	0/3215	0.28	0/4376
4	L	0.16	0/3215	0.29	0/4376
4	M	0.16	0/3215	0.29	0/4376
4	N	0.16	0/3215	0.30	0/4376
4	O	0.16	0/3215	0.30	0/4376
4	f	0.16	0/3215	0.30	0/4376
4	g	0.16	0/3215	0.30	0/4376
4	h	0.16	0/3215	0.29	0/4376
4	i	0.16	0/3215	0.29	0/4376
4	j	0.16	0/3215	0.30	0/4376
4	k	0.15	0/3215	0.28	0/4376
All	All	0.15	0/132527	0.30	2/180491 (0.0%)

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
2	2	0	4
2	3	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	483	PRO	CA-N-CD	-6.35	103.11	112.00
2	2	482	THR	N-CA-C	5.11	121.10	109.81

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	480	TYR	Peptide
2	2	481	GLN	Peptide
2	2	482	THR	Peptide
2	2	631	MET	Peptide
2	3	41	ALA	Peptide

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	0	2188	2124	2124	22	0
1	1	2085	2023	2023	24	0
1	P	2085	2023	2023	17	0
1	Q	2147	2087	2087	15	0
1	R	2105	2056	2056	19	0
1	S	2085	2023	2023	16	0
1	T	2188	2124	2124	16	0
1	U	2188	2124	2124	29	0
1	V	2188	2123	2124	25	0
1	W	2188	2124	2124	27	0
1	X	2147	2087	2087	10	0
1	Y	2188	2124	2124	19	0
1	Z	2188	2124	2124	16	0
1	t	2188	2124	2124	21	0
1	u	2188	2124	2124	29	0
1	v	2188	2124	2124	23	0
1	w	2188	2124	2124	18	0
1	x	2147	2087	2087	18	0
1	y	2188	2124	2124	17	0
2	2	5901	5753	5754	97	0
2	3	5901	5754	5754	98	0
2	4	4267	4198	4198	115	0
3	A	6362	6387	6387	36	0
3	B	6535	6563	6563	33	0
4	C	3164	3111	3111	26	0
4	D	3155	3098	3098	17	0
4	E	3155	3098	3098	23	0
4	F	3155	3098	3098	25	0
4	G	3155	3098	3098	25	0
4	H	3155	3098	3098	26	0
4	I	3155	3098	3098	20	0
4	J	3155	3098	3098	28	0
4	K	3155	3098	3098	16	0
4	L	3155	3098	3098	19	0
4	M	3155	3098	3098	19	0
4	N	3155	3098	3098	23	0
4	O	3155	3098	3098	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	f	3155	3098	3098	27	0
4	g	3155	3098	3098	21	0
4	h	3155	3098	3098	24	0
4	i	3155	3098	3098	20	0
4	j	3155	3098	3098	30	0
4	k	3155	3098	3098	18	0
5	a	61	53	52	0	0
6	0	14	14	13	0	0
6	1	14	14	13	0	0
6	P	14	14	13	0	0
6	Q	14	14	13	0	0
6	S	14	14	13	0	0
6	T	14	14	13	0	0
6	U	14	14	13	0	0
6	V	14	14	13	0	0
6	X	14	14	13	0	0
6	Y	14	14	13	0	0
6	Z	14	14	13	0	0
6	t	14	14	13	0	0
6	u	14	14	13	2	0
6	v	14	14	13	0	0
6	w	14	14	13	0	0
6	x	14	14	13	0	0
6	y	14	14	13	0	0
7	0	4	0	0	0	0
7	1	4	0	0	0	0
7	P	4	0	0	0	0
7	Q	4	0	0	0	0
7	R	4	0	0	0	0
7	S	4	0	0	0	0
7	T	4	0	0	0	0
7	U	4	0	0	0	0
7	V	4	0	0	0	0
7	W	4	0	0	0	0
7	X	4	0	0	0	0
7	Y	4	0	0	0	0
7	Z	4	0	0	0	0
7	t	4	0	0	0	0
7	u	4	0	0	0	0
7	v	4	0	0	0	0
7	w	4	0	0	0	0
7	x	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	y	4	0	0	0	0
8	C	2	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	2	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	I	2	0	0	0	0
8	J	1	0	0	0	0
8	K	1	0	0	0	0
8	L	2	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	O	2	0	0	0	0
8	f	2	0	0	0	0
8	g	1	0	0	0	0
8	h	1	0	0	0	0
8	i	2	0	0	0	0
8	j	1	0	0	0	0
8	k	1	0	0	0	0
9	C	1	0	0	0	0
9	F	1	0	0	0	0
9	J	1	0	0	0	0
9	M	1	0	0	0	0
9	O	1	0	0	0	0
9	h	1	0	0	0	0
9	j	1	0	0	0	0
All	All	130385	127694	127678	1041	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 4.

All (1041) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:228:GLN:OE1	2:2:230:THR:OG1	1.78	1.01
2:2:722:ILE:HD11	2:2:752:LEU:HD21	1.51	0.91
2:4:265:MET:HE3	2:4:482:THR:HG21	1.51	0.90
2:3:261:LEU:O	2:4:443:ARG:NH2	2.05	0.90
1:1:271:ILE:HD13	1:1:284:MET:HE1	1.53	0.87
1:Y:272:THR:HG21	1:Y:277:THR:HG23	1.56	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:75:THR:O	1:x:79:SER:OG	1.95	0.84
2:3:568:LEU:HD12	2:3:590:ALA:HB3	1.59	0.84
1:u:105:LEU:O	1:u:108:THR:OG1	1.95	0.83
1:X:75:THR:O	1:X:79:SER:OG	1.96	0.83
2:2:248:ALA:O	2:3:467:ARG:NH1	2.11	0.83
1:Z:179:ASP:OD1	1:Z:250:LYS:NZ	2.11	0.82
1:u:74:GLU:O	1:u:78:THR:OG1	1.96	0.82
2:3:43:THR:O	2:4:443:ARG:NH1	2.11	0.82
1:R:105:LEU:O	1:R:108:THR:OG1	1.97	0.82
1:S:75:THR:O	1:S:79:SER:OG	1.97	0.82
1:V:75:THR:O	1:V:79:SER:OG	1.97	0.82
1:v:75:THR:O	1:v:79:SER:OG	1.96	0.82
1:Q:75:THR:O	1:Q:79:SER:OG	1.97	0.81
2:4:700:GLU:OE1	4:f:268:GLN:NE2	2.13	0.80
1:R:274:ASP:OD2	1:R:276:THR:OG1	1.99	0.80
2:4:728:LYS:NZ	4:f:269:ILE:O	2.13	0.80
2:3:18:LEU:HD21	2:4:19:SER:OG	1.82	0.80
2:4:439:ILE:O	2:4:442:THR:OG1	2.00	0.79
1:y:272:THR:HG21	1:y:277:THR:HG23	1.64	0.79
1:0:217:GLU:OE2	1:0:220:THR:OG1	2.00	0.79
4:G:255:ARG:NH1	1:V:65:THR:O	2.16	0.79
2:3:228:GLN:OE1	2:3:230:THR:OG1	2.01	0.79
3:A:546:ARG:NH2	3:A:595:ILE:O	2.16	0.79
2:4:528:PHE:O	2:4:532:SER:OG	1.98	0.79
4:K:142:GLN:OE1	4:L:145:ARG:NH1	2.16	0.79
1:U:105:LEU:O	1:U:108:THR:OG1	2.02	0.78
4:H:145:ARG:NH1	4:f:142:GLN:O	2.16	0.78
1:U:255:ARG:O	1:U:283:ARG:NH1	2.17	0.78
1:v:105:LEU:O	1:v:108:THR:OG1	2.03	0.77
1:U:272:THR:HG21	1:U:277:THR:HG23	1.65	0.77
4:K:310:ASN:OD1	1:W:305:GLN:NE2	2.17	0.77
1:u:255:ARG:O	1:u:283:ARG:NH1	2.18	0.76
2:3:573:SER:OG	2:4:647:ARG:NH1	2.18	0.76
1:u:272:THR:HG21	1:u:277:THR:HG23	1.68	0.76
1:U:112:PRO:O	1:U:115:SER:OG	2.02	0.76
1:V:274:ASP:OD2	1:V:276:THR:OG1	2.04	0.76
4:O:47:GLN:OE1	4:O:58:ASN:ND2	2.19	0.76
1:P:105:LEU:O	1:P:108:THR:OG1	2.04	0.75
1:Y:105:LEU:O	1:Y:108:THR:OG1	2.05	0.75
1:V:105:LEU:O	1:V:108:THR:OG1	2.04	0.75
2:2:261:LEU:HD11	2:3:40:PHE:CE1	2.22	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:112:PRO:O	1:u:115:SER:OG	2.02	0.75
1:u:62:SER:OG	1:u:65:THR:OG1	1.97	0.75
1:y:272:THR:HG21	1:y:277:THR:O	1.87	0.75
4:I:49:GLY:N	4:I:98:ASP:OD2	2.19	0.74
1:1:134:TYR:O	1:1:313:ARG:NH1	2.20	0.74
2:2:556:GLY:N	2:2:665:GLU:OE2	2.19	0.74
4:i:49:GLY:N	4:i:98:ASP:OD2	2.20	0.74
1:v:274:ASP:OD2	1:v:276:THR:OG1	2.05	0.74
1:T:274:ASP:OD2	1:T:276:THR:OG1	2.04	0.74
1:S:87:THR:OG1	1:S:120:GLU:OE2	2.06	0.73
1:t:274:ASP:OD2	1:t:276:THR:OG1	2.05	0.73
2:4:457:ASN:ND2	2:4:457:ASN:O	2.21	0.73
2:4:416:THR:OG1	2:4:419:VAL:O	2.05	0.73
2:4:503:GLU:N	2:4:503:GLU:OE1	2.20	0.73
2:4:768:GLU:OE2	6:u:401:NAG:O4	2.05	0.73
1:Q:105:LEU:O	1:Q:108:THR:OG1	2.06	0.73
4:L:49:GLY:N	4:L:98:ASP:OD2	2.21	0.73
1:U:75:THR:O	1:U:79:SER:OG	2.06	0.73
1:T:112:PRO:O	1:T:115:SER:OG	2.07	0.73
1:x:80:THR:HG21	1:x:324:TYR:CE2	2.24	0.72
1:y:105:LEU:O	1:y:108:THR:OG1	2.08	0.72
1:0:96:ASN:ND2	2:2:481:GLN:OE1	2.22	0.71
2:2:227:ILE:O	2:2:228:GLN:NE2	2.23	0.71
1:U:272:THR:HG21	1:U:277:THR:O	1.89	0.71
2:4:527:MET:HE1	2:4:549:MET:SD	2.30	0.71
1:R:255:ARG:O	1:R:283:ARG:NH1	2.23	0.71
1:1:105:LEU:O	1:1:108:THR:OG1	2.09	0.71
2:4:271:ILE:HD12	2:4:273:ILE:HD11	1.72	0.71
4:J:310:ASN:OD1	1:Y:305:GLN:NE2	2.24	0.71
1:0:69:ASN:OD1	1:0:70:SER:N	2.24	0.71
2:2:53:GLY:N	2:2:354:ASP:OD2	2.23	0.70
3:B:140:VAL:HG11	3:B:152:ARG:HD2	1.73	0.70
1:Y:272:THR:HG21	1:Y:277:THR:O	1.91	0.70
1:u:272:THR:HG21	1:u:277:THR:O	1.90	0.70
4:C:338:ALA:O	4:E:328:SER:OG	2.08	0.70
1:t:79:SER:OG	1:t:312:LYS:NZ	2.25	0.70
2:3:28:THR:O	2:4:321:ASN:ND2	2.25	0.70
1:W:190:SER:O	1:W:243:THR:OG1	2.06	0.70
4:G:142:GLN:O	4:I:145:ARG:NH1	2.25	0.69
1:R:256:GLU:OE1	1:R:314:SER:OG	2.10	0.69
2:2:532:SER:OG	2:4:562:SER:OG	2.03	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:262:GLU:OE2	4:J:289:ARG:NH2	2.25	0.69
2:4:519:ASP:OD1	2:4:753:ARG:NE	2.26	0.69
1:V:277:THR:HG22	1:V:279:PRO:HD3	1.75	0.69
4:g:142:GLN:O	4:i:145:ARG:NH1	2.26	0.69
1:v:277:THR:HG22	1:v:279:PRO:HD3	1.75	0.69
4:F:328:SER:OG	4:G:338:ALA:O	2.10	0.69
2:4:555:SER:O	2:4:559:ASN:ND2	2.26	0.69
2:2:467:ARG:NH1	2:3:248:ALA:O	2.26	0.68
4:k:310:ASN:OD1	1:w:305:GLN:NE2	2.27	0.68
1:1:130:ASP:OD1	1:1:132:GLN:NE2	2.27	0.68
2:2:652:SER:HG	2:2:655:THR:HG1	1.32	0.68
2:4:649:THR:OG1	2:4:650:GLN:OE1	2.12	0.68
1:Z:105:LEU:O	1:Z:108:THR:OG1	2.11	0.68
1:S:105:LEU:O	1:S:108:THR:OG1	2.10	0.68
1:t:180:GLU:O	1:t:183:LYS:NZ	2.26	0.68
2:2:662:GLU:HG3	2:2:776:LEU:HD12	1.76	0.68
1:R:201:GLN:O	1:R:202:THR:OG1	2.11	0.67
4:j:310:ASN:OD1	1:y:305:GLN:NE2	2.28	0.67
4:f:155:PRO:O	4:f:186:SER:OG	2.13	0.67
1:0:142:MET:HE2	1:0:155:LEU:HD23	1.77	0.67
1:R:77:LEU:HD13	1:Z:166:ASN:ND2	2.10	0.67
3:B:335:LEU:O	3:B:338:SER:OG	2.09	0.67
2:2:496:ARG:CD	1:W:108:THR:HG23	2.26	0.66
2:3:514:MET:HE1	2:3:764:ARG:HB3	1.77	0.66
2:4:692:ALA:O	2:4:701:ILE:N	2.29	0.66
4:M:189:GLN:HG3	4:M:323:THR:HG23	1.76	0.66
1:W:62:SER:OG	1:W:64:ASP:OD1	2.13	0.66
1:S:180:GLU:O	1:S:183:LYS:NZ	2.28	0.66
2:2:76:PRO:O	2:2:169:LYS:NZ	2.29	0.66
1:Z:217:GLU:OE2	1:Z:220:THR:OG1	2.14	0.66
3:B:261:GLU:OE1	4:N:69:THR:OG1	2.11	0.66
1:x:62:SER:OG	1:x:64:ASP:OD1	2.09	0.66
2:3:579:ALA:O	2:3:580:SER:OG	2.14	0.65
3:A:412:ILE:CG2	3:A:543:LEU:HD22	2.25	0.65
2:4:431:THR:HG21	1:Q:203:LEU:HD11	1.78	0.65
3:B:546:ARG:NH1	3:B:592:CYS:O	2.29	0.65
1:R:164:LEU:HB2	1:R:252:LEU:HD21	1.77	0.65
4:j:262:GLU:OE2	4:j:289:ARG:NH2	2.30	0.65
1:1:75:THR:O	1:1:79:SER:OG	2.14	0.65
4:j:68:THR:HG22	4:j:69:THR:H	1.62	0.65
2:3:419:VAL:HG12	2:4:391:VAL:HG11	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:277:THR:HG22	1:T:279:PRO:HD3	1.79	0.64
1:t:112:PRO:O	1:t:115:SER:OG	2.13	0.64
1:0:85:TYR:OH	1:0:99:LYS:NZ	2.30	0.64
1:X:62:SER:OG	1:X:64:ASP:OD1	2.12	0.64
4:E:117:ARG:O	4:E:120:SER:OG	2.16	0.64
4:J:68:THR:HG22	4:J:69:THR:H	1.63	0.64
1:0:65:THR:O	4:N:255:ARG:NH1	2.30	0.64
4:C:397:LYS:NZ	4:E:151:THR:OG1	2.26	0.64
4:f:299:ASN:ND2	4:g:244:ALA:O	2.31	0.64
3:A:601:ILE:HD11	3:A:869:THR:HG21	1.80	0.64
1:S:178:THR:OG1	1:S:250:LYS:NZ	2.31	0.64
1:u:174:TYR:CD2	1:u:198:LEU:HD11	2.32	0.64
1:U:316:SER:OG	1:W:325:ARG:NH2	2.31	0.63
4:C:49:GLY:N	4:C:98:ASP:OD2	2.31	0.63
4:F:155:PRO:O	4:F:186:SER:OG	2.13	0.63
2:2:714:ASP:OD2	2:3:753:ARG:NH1	2.30	0.63
4:K:255:ARG:NH1	1:W:65:THR:O	2.32	0.63
1:T:255:ARG:O	1:T:283:ARG:NH1	2.32	0.63
4:D:45:GLU:O	4:D:118:LYS:NZ	2.31	0.63
1:Y:265:GLY:O	1:Y:286:ARG:NH1	2.31	0.63
1:0:180:GLU:O	1:0:183:LYS:NZ	2.32	0.63
2:4:557:LEU:N	2:4:665:GLU:OE2	2.31	0.62
1:t:255:ARG:O	1:t:283:ARG:NH1	2.32	0.62
1:1:274:ASP:OD1	1:1:276:THR:OG1	2.18	0.62
4:N:174:ASP:OD2	4:N:312:GLN:NE2	2.29	0.62
1:0:170:ILE:O	1:0:171:THR:OG1	2.15	0.62
4:C:93:ASP:OD1	4:C:396:VAL:HG21	1.99	0.62
2:4:305:TYR:OH	2:4:355:TYR:OH	2.14	0.62
4:I:255:ARG:NH1	1:X:65:THR:O	2.33	0.62
2:2:511:GLU:OE1	2:2:647:ARG:NH1	2.32	0.62
1:1:157:ASP:OD1	1:1:161:ASN:ND2	2.32	0.62
1:t:277:THR:HG22	1:t:279:PRO:HD3	1.80	0.62
1:w:180:GLU:O	1:w:183:LYS:NZ	2.31	0.62
4:E:57:ARG:NH1	4:E:94:ASN:OD1	2.32	0.62
4:G:45:GLU:O	4:G:118:LYS:NZ	2.32	0.62
4:O:117:ARG:O	4:O:120:SER:OG	2.17	0.62
2:2:97:ASN:HB3	2:2:197:VAL:HG12	1.81	0.61
1:U:130:ASP:OD2	1:U:132:GLN:NE2	2.33	0.61
1:U:174:TYR:CD2	1:U:198:LEU:HD11	2.34	0.61
4:k:255:ARG:NH1	1:w:65:THR:O	2.33	0.61
4:k:117:ARG:O	4:k:120:SER:OG	2.18	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:265:GLY:O	1:U:286:ARG:NH1	2.33	0.61
2:2:564:LEU:HD21	2:2:591:TRP:CH2	2.36	0.61
4:f:262:GLU:OE1	4:f:289:ARG:NH1	2.33	0.61
1:w:262:GLN:NE2	1:w:264:GLY:O	2.34	0.61
2:2:19:SER:CB	2:2:546:THR:HG21	2.30	0.61
1:W:262:GLN:NE2	1:W:264:GLY:O	2.34	0.61
4:g:255:ARG:NH1	1:v:65:THR:O	2.33	0.61
2:4:526:ASP:OD1	2:4:529:SER:OG	2.16	0.61
1:1:263:VAL:HG12	1:1:289:TRP:CD1	2.36	0.60
3:A:311:LEU:O	3:A:618:HIS:NE2	2.34	0.60
4:J:147:ARG:NH1	4:J:332:GLU:OE2	2.33	0.60
4:i:255:ARG:NH1	1:x:65:THR:O	2.32	0.60
4:G:145:ARG:NH2	4:I:380:ASP:OD1	2.33	0.60
4:M:93:ASP:OD1	4:M:392:ARG:NE	2.34	0.60
1:S:201:GLN:N	1:S:201:GLN:OE1	2.33	0.60
4:h:239:ASN:ND2	4:h:240:SER:O	2.34	0.60
2:2:485:THR:HG22	2:2:485:THR:O	2.01	0.60
2:2:652:SER:OG	2:2:655:THR:OG1	2.11	0.60
2:4:514:MET:HE2	2:4:768:GLU:HG2	1.84	0.60
1:V:77:LEU:HD13	1:V:112:PRO:HG3	1.83	0.60
1:x:112:PRO:O	1:x:115:SER:OG	2.13	0.60
2:2:573:SER:HG	2:3:643:THR:HG1	1.05	0.60
3:A:601:ILE:HD11	3:A:869:THR:CG2	2.32	0.60
1:t:136:ASP:OD1	1:t:315:ARG:NE	2.35	0.60
4:C:262:GLU:HG3	4:C:272:THR:HG22	1.84	0.60
2:2:19:SER:HB2	2:2:546:THR:HG21	1.83	0.60
2:2:129:THR:O	2:2:154:GLN:NE2	2.34	0.60
2:4:722:ILE:HD11	2:4:752:LEU:HD11	1.84	0.60
4:C:265:LEU:HD22	4:C:284:ASN:OD1	2.01	0.60
4:I:174:ASP:OD1	4:I:312:GLN:NE2	2.34	0.60
2:3:25:ILE:O	2:3:28:THR:OG1	2.16	0.60
4:O:344:ALA:O	4:O:348:SER:OG	2.17	0.60
2:3:625:ALA:O	2:3:627:GLN:N	2.34	0.60
4:K:117:ARG:O	4:K:120:SER:OG	2.17	0.60
4:i:307:LEU:HD11	4:j:248:TYR:CD1	2.36	0.60
2:3:346:LYS:NZ	2:3:448:TYR:O	2.28	0.59
3:A:412:ILE:HG22	3:A:543:LEU:HD22	1.83	0.59
4:C:209:GLU:OE2	4:C:289:ARG:NH1	2.35	0.59
2:3:84:LEU:HD21	2:3:201:ALA:HB1	1.85	0.59
2:4:3:SER:OG	2:4:635:ASP:OD1	2.16	0.59
2:4:608:ILE:O	2:4:612:THR:HG23	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:420:VAL:HG23	3:A:421:VAL:HG23	1.85	0.59
3:B:336:ALA:O	3:B:340:VAL:HG23	2.03	0.59
3:B:412:ILE:HG22	3:B:543:LEU:HD22	1.82	0.59
4:O:217:VAL:HG22	4:O:286:ASP:HB3	1.84	0.59
4:j:255:ARG:NH1	1:y:65:THR:O	2.35	0.59
1:Z:255:ARG:O	1:Z:283:ARG:NH1	2.36	0.59
2:2:492:GLN:N	2:2:492:GLN:OE1	2.35	0.59
1:P:201:GLN:N	1:P:201:GLN:OE1	2.35	0.59
1:S:272:THR:HG21	1:S:277:THR:O	2.02	0.59
2:4:772:MET:SD	6:u:401:NAG:O6	2.55	0.59
2:3:457:ASN:O	2:3:457:ASN:ND2	2.36	0.58
1:P:263:VAL:HG12	1:P:289:TRP:CD1	2.37	0.58
1:S:274:ASP:OD2	1:S:276:THR:OG1	2.17	0.58
1:Y:255:ARG:O	1:Y:283:ARG:NH1	2.36	0.58
2:2:457:ASN:O	2:2:457:ASN:ND2	2.36	0.58
2:4:16:VAL:HG11	2:4:550:LYS:HA	1.85	0.58
3:A:403:PHE:HB3	3:A:585:LEU:HD12	1.85	0.58
2:3:100:ASP:OD2	2:3:192:THR:OG1	2.21	0.58
4:F:262:GLU:OE1	4:F:289:ARG:NH1	2.36	0.58
1:w:190:SER:O	1:w:243:THR:OG1	2.16	0.58
2:2:743:ASN:HB2	2:2:751:VAL:HG21	1.86	0.58
1:P:217:GLU:OE2	1:P:220:THR:OG1	2.21	0.58
2:3:19:SER:OG	2:3:546:THR:HG21	2.04	0.58
3:B:309:ASN:O	3:B:622:ASN:ND2	2.36	0.58
1:R:272:THR:HG21	1:R:277:THR:HG23	1.84	0.58
2:2:496:ARG:HD2	1:W:108:THR:HG23	1.86	0.58
2:2:677:ASN:CB	2:2:711:LEU:HD21	2.34	0.58
2:4:325:ASP:OD1	2:4:341:ARG:NH1	2.37	0.58
4:g:117:ARG:O	4:g:120:SER:OG	2.22	0.57
4:j:68:THR:O	4:j:69:THR:OG1	2.18	0.57
1:1:180:GLU:O	1:1:183:LYS:NZ	2.37	0.57
4:J:255:ARG:NH1	1:Y:65:THR:O	2.36	0.57
4:L:307:LEU:HD11	4:M:248:TYR:CD1	2.39	0.57
1:v:77:LEU:HD13	1:v:112:PRO:HG3	1.86	0.57
2:3:224:LEU:HD12	2:3:225:PRO:O	2.04	0.57
2:4:557:LEU:HD21	2:4:624:MET:HE1	1.86	0.57
3:A:786:ASP:OD2	3:A:828:SER:OG	2.21	0.57
4:C:255:ARG:NH1	1:S:65:THR:O	2.36	0.57
2:4:593:ASP:O	2:4:618:ARG:NH2	2.36	0.57
4:G:24:TYR:OH	4:G:68:THR:HG23	2.04	0.57
4:J:217:VAL:HG22	4:J:286:ASP:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:307:LEU:HD11	4:h:248:TYR:CD1	2.40	0.57
2:2:677:ASN:HB3	2:2:711:LEU:HD21	1.87	0.57
2:3:516:GLN:OE1	2:3:516:GLN:N	2.37	0.57
4:I:307:LEU:HD11	4:J:248:TYR:CD1	2.40	0.57
1:U:316:SER:O	1:W:325:ARG:NH2	2.37	0.57
1:U:164:LEU:HD23	1:W:75:THR:HG21	1.87	0.57
2:2:3:SER:OG	2:2:635:ASP:N	2.38	0.56
2:3:27:SER:HG	2:4:352:TYR:HH	1.50	0.56
2:4:290:LYS:NZ	2:4:336:ASP:O	2.38	0.56
4:G:68:THR:O	4:G:68:THR:HG22	2.05	0.56
1:U:189:SER:O	1:U:223:LYS:NZ	2.39	0.56
1:W:71:THR:HG22	1:W:71:THR:O	2.05	0.56
1:x:133:LEU:HD13	1:x:258:VAL:HG21	1.87	0.56
2:3:730:LEU:HD21	2:3:763:ILE:HD11	1.88	0.56
4:H:117:ARG:O	4:H:120:SER:OG	2.23	0.56
4:M:168:ARG:NH2	4:M:194:ASP:OD1	2.38	0.56
1:1:65:THR:O	4:L:255:ARG:NH2	2.37	0.56
2:2:692:ALA:O	2:2:701:ILE:N	2.38	0.56
3:A:663:ARG:NH1	3:B:350:GLU:OE2	2.38	0.56
1:V:72:GLN:NE2	1:V:304:ASN:OD1	2.38	0.56
4:h:117:ARG:O	4:h:120:SER:OG	2.23	0.56
1:y:255:ARG:O	1:y:283:ARG:NH1	2.38	0.56
1:O:105:LEU:O	1:O:108:THR:OG1	2.16	0.56
2:2:346:LYS:NZ	2:2:448:TYR:O	2.23	0.56
3:B:786:ASP:OD2	3:B:830:THR:OG1	2.18	0.56
2:3:530:MET:HE2	2:3:645:ILE:CD1	2.36	0.56
2:3:536:SER:O	2:3:536:SER:OG	2.24	0.56
4:G:24:TYR:CZ	4:G:68:THR:HG23	2.41	0.56
4:I:248:TYR:CD1	4:K:307:LEU:HD11	2.41	0.56
1:O:166:ASN:OD1	1:Y:315:ARG:NH2	2.38	0.55
3:B:471:GLN:HB3	4:H:80:THR:HG21	1.86	0.55
4:i:225:LEU:HD22	4:i:261:VAL:HG21	1.87	0.55
2:4:494:LEU:HD23	1:u:108:THR:HG23	1.87	0.55
1:R:159:ILE:CG2	1:R:258:VAL:HG11	2.35	0.55
1:T:180:GLU:O	1:T:183:LYS:NZ	2.39	0.55
4:E:294:LEU:HD12	4:E:320:VAL:HG13	1.89	0.55
1:P:134:TYR:O	1:P:313:ARG:NH1	2.40	0.55
2:2:84:LEU:HD22	2:2:93:VAL:HB	1.89	0.55
3:B:190:LEU:HD23	3:B:193:MET:HE3	1.89	0.55
1:u:252:LEU:HD11	1:w:317:LEU:HD21	1.87	0.55
2:2:536:SER:O	2:2:536:SER:OG	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:419:VAL:HG12	2:4:391:VAL:CG1	2.37	0.55
1:W:180:GLU:O	1:W:183:LYS:NZ	2.39	0.55
1:X:133:LEU:HD13	1:X:258:VAL:HG21	1.89	0.55
2:2:121:LEU:HD13	2:2:152:TYR:CZ	2.41	0.55
2:2:279:SER:OG	2:2:452:ALA:O	2.13	0.55
4:f:307:LEU:HD11	4:g:248:TYR:CD1	2.41	0.55
4:h:45:GLU:O	4:h:118:LYS:NZ	2.39	0.55
4:N:231:ARG:O	4:N:236:ARG:NH1	2.40	0.55
2:3:49:ASN:ND2	2:4:391:VAL:HG13	2.22	0.54
2:3:382:GLY:N	2:3:400:GLY:O	2.40	0.54
4:J:68:THR:O	4:J:69:THR:OG1	2.17	0.54
4:j:117:ARG:O	4:j:120:SER:OG	2.25	0.54
1:0:95:ASP:OD1	1:0:97:SER:N	2.38	0.54
2:3:56:ASN:ND2	2:3:320:VAL:O	2.40	0.54
4:C:117:ARG:O	4:C:120:SER:OG	2.26	0.54
4:C:147:ARG:NH1	4:C:332:GLU:OE2	2.41	0.54
4:E:294:LEU:HD11	4:E:318:ALA:HB1	1.89	0.54
1:t:74:GLU:O	1:t:78:THR:HG22	2.07	0.54
1:U:252:LEU:HD11	1:W:317:LEU:HD21	1.88	0.54
1:Z:180:GLU:O	1:Z:183:LYS:NZ	2.40	0.54
1:0:75:THR:O	1:0:79:SER:OG	2.13	0.54
2:2:194:TYR:O	2:2:197:VAL:HG22	2.07	0.54
4:I:225:LEU:HD22	4:I:261:VAL:HG21	1.89	0.54
4:K:380:ASP:OD1	4:L:145:ARG:NH2	2.41	0.54
1:U:274:ASP:OD2	1:U:277:THR:HG22	2.08	0.54
2:3:107:LEU:HD11	2:3:138:TRP:HB3	1.90	0.54
2:2:106:ILE:HD12	2:2:130:ILE:HG21	1.90	0.54
3:A:336:ALA:O	3:A:340:VAL:HG23	2.07	0.54
3:A:403:PHE:CB	3:A:585:LEU:HD12	2.38	0.54
4:J:117:ARG:O	4:J:120:SER:OG	2.25	0.54
4:J:225:LEU:HD22	4:J:261:VAL:HG21	1.89	0.54
4:N:225:LEU:HD21	4:N:261:VAL:HG21	1.89	0.54
4:k:114:ASP:OD1	4:k:117:ARG:NH2	2.40	0.54
2:2:143:VAL:HG12	2:2:152:TYR:CD1	2.43	0.54
4:C:225:LEU:HD22	4:C:261:VAL:HG21	1.89	0.54
4:H:255:ARG:NH1	1:T:65:THR:O	2.40	0.54
1:u:184:TRP:CZ3	1:u:237:LEU:HD21	2.42	0.54
1:w:74:GLU:O	1:w:78:THR:HG22	2.07	0.54
1:T:74:GLU:O	1:T:78:THR:HG22	2.08	0.54
1:U:184:TRP:CZ3	1:U:237:LEU:HD21	2.41	0.54
1:x:267:ASP:OD1	1:x:286:ARG:NE	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:722:ILE:HG22	2:4:722:ILE:O	2.08	0.54
4:G:367:TRP:CZ3	4:G:370:LEU:HD22	2.43	0.54
4:M:255:ARG:NH1	1:Z:65:THR:O	2.40	0.54
4:f:147:ARG:NH1	4:f:332:GLU:OE2	2.41	0.54
1:v:180:GLU:O	1:v:183:LYS:NZ	2.41	0.54
2:3:63:PRO:O	2:3:64:VAL:HG12	2.08	0.53
2:3:568:LEU:CD1	2:3:590:ALA:HB3	2.35	0.53
4:F:307:LEU:HD11	4:G:248:TYR:CD1	2.43	0.53
4:J:261:VAL:HG22	4:J:290:LEU:HD23	1.90	0.53
4:g:217:VAL:HG22	4:g:286:ASP:HB3	1.90	0.53
1:x:285:MET:HE1	1:x:306:ILE:HG23	1.90	0.53
2:2:523:LEU:HD12	2:4:568:LEU:CD1	2.38	0.53
2:3:641:LEU:HD13	2:3:663:ALA:CB	2.38	0.53
2:2:368:VAL:HG11	2:2:411:LEU:HD13	1.91	0.53
4:G:117:ARG:O	4:G:120:SER:OG	2.27	0.53
4:j:11:LEU:HD21	4:j:88:PHE:HB3	1.90	0.53
1:u:130:ASP:OD2	1:u:132:GLN:NE2	2.40	0.53
1:u:274:ASP:OD2	1:u:277:THR:HG22	2.07	0.53
1:v:271:ILE:HG12	1:v:284:MET:HE1	1.90	0.53
2:4:263:LYS:NZ	2:4:481:GLN:O	2.42	0.53
1:0:95:ASP:OD1	1:0:96:ASN:N	2.42	0.53
4:i:168:ARG:NH2	4:i:194:ASP:OD1	2.40	0.53
2:3:76:PRO:O	2:3:169:LYS:NZ	2.40	0.53
2:3:667:PHE:O	2:3:671:ARG:NH2	2.41	0.53
2:3:740:GLN:NE2	2:3:754:GLU:OE2	2.41	0.53
2:4:328:PHE:CZ	2:4:442:THR:HG22	2.44	0.53
3:A:195:VAL:HG21	3:A:209:SER:HA	1.90	0.53
4:F:76:ASN:ND2	4:g:74:ASP:OD2	2.41	0.53
2:2:12:ASN:O	2:2:15:THR:OG1	2.27	0.53
4:f:225:LEU:HD13	4:f:324:LEU:CD1	2.39	0.53
1:y:184:TRP:CZ3	1:y:237:LEU:HD21	2.44	0.53
2:2:557:LEU:N	2:2:665:GLU:OE2	2.40	0.53
1:Q:274:ASP:OD2	1:Q:276:THR:OG1	2.24	0.53
1:T:263:VAL:HG12	1:T:289:TRP:CD1	2.44	0.53
1:u:180:GLU:O	1:u:183:LYS:NZ	2.42	0.53
2:4:19:SER:OG	2:4:546:THR:HG21	2.09	0.53
2:4:734:TYR:O	2:4:736:ILE:HG23	2.08	0.52
3:A:152:ARG:NH1	3:A:723:GLU:OE1	2.42	0.52
4:K:194:ASP:OD1	4:K:197:CYS:N	2.43	0.52
1:Y:87:THR:HG23	1:Y:120:GLU:OE2	2.08	0.52
1:v:272:THR:HG21	1:v:277:THR:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:j:217:VAL:HG22	4:j:286:ASP:HB3	1.90	0.52
4:j:261:VAL:HG22	4:j:290:LEU:HD23	1.91	0.52
1:0:201:GLN:O	1:0:202:THR:OG1	2.17	0.52
1:1:272:THR:HG21	1:1:277:THR:O	2.09	0.52
4:g:11:LEU:HD21	4:g:88:PHE:HB3	1.91	0.52
4:i:248:TYR:CD1	4:k:307:LEU:HD11	2.43	0.52
3:B:190:LEU:HD23	3:B:193:MET:CE	2.39	0.52
4:M:261:VAL:HG22	4:M:290:LEU:HD23	1.91	0.52
1:S:106:PHE:CD2	1:S:116:VAL:HG11	2.44	0.52
4:i:209:GLU:OE2	4:i:289:ARG:NE	2.42	0.52
1:1:65:THR:O	4:L:255:ARG:NH1	2.42	0.52
2:4:569:SER:O	2:4:573:SER:OG	2.19	0.52
3:B:740:ILE:HD12	3:B:764:VAL:HG21	1.91	0.52
4:H:104:SER:OG	4:H:106:ARG:O	2.26	0.52
1:1:160:LEU:HD13	1:1:284:MET:HE2	1.91	0.52
2:3:568:LEU:HD22	2:4:523:LEU:HD22	1.92	0.52
2:4:544:MET:O	2:4:548:VAL:HG23	2.10	0.52
1:R:315:ARG:NH2	1:Z:166:ASN:OD1	2.42	0.52
1:Z:264:GLY:N	1:Z:287:ILE:O	2.42	0.52
4:f:261:VAL:HG22	4:f:290:LEU:HD23	1.92	0.52
4:k:194:ASP:OD1	4:k:197:CYS:N	2.42	0.52
4:O:11:LEU:HD21	4:O:88:PHE:HB3	1.92	0.52
1:Z:174:TYR:CD1	1:Z:198:LEU:HD11	2.45	0.52
4:i:242:ASP:OD1	4:i:242:ASP:N	2.43	0.52
4:E:245:THR:OG1	4:E:246:THR:N	2.43	0.52
1:W:157:ASP:OD1	1:W:161:ASN:ND2	2.43	0.52
1:v:129:VAL:HG12	1:v:129:VAL:O	2.10	0.52
2:3:530:MET:HE1	2:3:641:LEU:HD23	1.92	0.52
2:4:389:LEU:HD23	2:4:395:PRO:HD2	1.91	0.52
2:3:580:SER:O	2:3:596:THR:N	2.40	0.51
2:4:584:VAL:O	2:4:584:VAL:HG22	2.10	0.51
4:D:209:GLU:OE2	4:D:289:ARG:NH1	2.43	0.51
4:N:138:ASN:OD1	4:N:148:THR:OG1	2.09	0.51
1:Y:217:GLU:N	1:Y:217:GLU:OE1	2.41	0.51
4:f:182:LEU:HD22	4:f:231:ARG:CD	2.40	0.51
4:h:255:ARG:NH1	1:t:65:THR:O	2.43	0.51
1:t:202:THR:HG22	1:t:202:THR:O	2.11	0.51
1:w:191:CYS:SG	1:w:193:ILE:HD11	2.50	0.51
1:y:202:THR:O	1:y:202:THR:HG22	2.11	0.51
1:P:106:PHE:CE2	1:P:300:VAL:HG22	2.45	0.51
1:S:187:MET:HE2	1:S:224:LEU:HD13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:191:CYS:SG	1:W:193:ILE:HD11	2.50	0.51
2:2:481:GLN:O	2:2:483:PRO:CD	2.58	0.51
2:4:522:LEU:HD11	2:4:749:PRO:HB3	1.92	0.51
4:C:248:TYR:CD1	4:E:307:LEU:HD11	2.45	0.51
4:E:135:TYR:CZ	4:E:342:MET:HE3	2.46	0.51
4:F:265:LEU:HD22	4:F:284:ASN:ND2	2.25	0.51
4:I:242:ASP:OD1	4:I:242:ASP:N	2.44	0.51
4:L:338:ALA:O	4:N:328:SER:OG	2.19	0.51
1:P:160:LEU:O	1:P:283:ARG:NH2	2.43	0.51
2:2:106:ILE:HD12	2:2:130:ILE:CG2	2.41	0.51
4:H:239:ASN:ND2	4:H:240:SER:O	2.43	0.51
4:J:11:LEU:HD21	4:J:88:PHE:HB3	1.93	0.51
4:M:117:ARG:O	4:M:120:SER:OG	2.28	0.51
1:V:272:THR:HG21	1:V:277:THR:O	2.08	0.51
1:V:315:ARG:HB3	1:V:325:ARG:HE	1.75	0.51
2:3:143:VAL:HG12	2:3:152:TYR:CD1	2.46	0.51
4:E:265:LEU:HD22	4:E:284:ASN:ND2	2.25	0.51
1:W:133:LEU:HD13	1:W:258:VAL:HG21	1.92	0.51
2:3:51:GLY:H	2:3:52:PRO:HD3	1.75	0.51
2:3:493:ASP:N	2:3:493:ASP:OD1	2.44	0.51
3:B:815:ASP:OD1	3:B:815:ASP:N	2.44	0.51
4:i:346:VAL:HG11	4:i:365:MET:HE2	1.92	0.51
1:u:185:ILE:HG22	1:u:187:MET:HE2	1.92	0.51
4:D:224:THR:OG1	4:D:327:GLU:OE2	2.29	0.51
4:G:225:LEU:HD22	4:G:261:VAL:HG21	1.93	0.51
4:N:217:VAL:HG22	4:N:286:ASP:HB3	1.91	0.51
4:O:170:GLN:NE2	4:O:175:ASN:O	2.41	0.51
1:V:112:PRO:O	1:V:115:SER:OG	2.25	0.51
2:3:270:ASP:O	2:3:307:ARG:NH1	2.41	0.51
4:F:11:LEU:HD21	4:F:88:PHE:HB3	1.93	0.51
1:T:77:LEU:HD23	1:T:112:PRO:HG3	1.93	0.51
4:i:310:ASN:OD1	1:x:305:GLN:NE2	2.44	0.51
1:Q:112:PRO:O	1:Q:115:SER:OG	2.27	0.50
1:U:180:GLU:O	1:U:183:LYS:NZ	2.43	0.50
2:4:364:ASN:O	2:4:486:ASN:ND2	2.42	0.50
2:4:557:LEU:O	2:4:561:VAL:HG23	2.11	0.50
1:R:201:GLN:N	1:R:201:GLN:OE1	2.44	0.50
4:j:225:LEU:HD22	4:j:261:VAL:HG21	1.93	0.50
2:4:726:THR:HG23	2:4:762:ILE:HG22	1.92	0.50
4:H:11:LEU:HD21	4:H:88:PHE:HB3	1.94	0.50
4:I:297:PRO:HB3	4:J:246:THR:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:294:LEU:HD12	4:N:320:VAL:HG13	1.94	0.50
1:t:101:THR:HG22	1:v:205:ILE:HG22	1.93	0.50
2:2:51:GLY:H	2:2:52:PRO:HD3	1.75	0.50
2:2:107:LEU:HD11	2:2:138:TRP:HB3	1.93	0.50
3:B:621:TYR:CZ	3:B:625:ILE:HD11	2.47	0.50
4:I:11:LEU:HD21	4:I:88:PHE:HB3	1.94	0.50
4:f:217:VAL:HG22	4:f:286:ASP:HB3	1.91	0.50
2:3:674:ARG:NH2	2:3:722:ILE:O	2.43	0.50
4:i:93:ASP:OD1	4:i:392:ARG:NE	2.44	0.50
1:1:285:MET:HE1	1:1:306:ILE:HG23	1.93	0.50
1:T:202:THR:HG22	1:T:202:THR:O	2.11	0.50
4:j:225:LEU:CD2	4:j:261:VAL:HG21	2.41	0.50
2:2:227:ILE:O	2:2:228:GLN:CD	2.54	0.50
4:E:135:TYR:CE1	4:E:342:MET:HE3	2.47	0.50
4:f:225:LEU:HD13	4:f:324:LEU:HD13	1.94	0.50
2:2:57:ASP:OD1	2:2:58:SER:N	2.44	0.50
2:2:69:TYR:OH	2:2:290:LYS:NZ	2.31	0.50
4:C:254:LEU:O	4:C:320:VAL:HG12	2.12	0.50
4:h:188:ILE:HD13	4:h:212:VAL:HG21	1.94	0.50
4:h:310:ASN:OD1	1:t:305:GLN:NE2	2.44	0.50
1:w:263:VAL:HG12	1:w:289:TRP:CD1	2.47	0.50
1:y:217:GLU:OE1	1:y:217:GLU:N	2.40	0.50
2:2:635:ASP:OD1	2:2:636:ILE:N	2.45	0.50
4:I:168:ARG:NH2	4:I:194:ASP:OD1	2.39	0.50
1:S:198:LEU:HD22	1:S:202:THR:O	2.10	0.50
2:3:564:LEU:HD21	2:3:591:TRP:CH2	2.47	0.49
4:f:11:LEU:HD21	4:f:88:PHE:HB3	1.94	0.49
2:3:734:TYR:O	2:3:736:ILE:HG23	2.12	0.49
2:4:473:LEU:HD12	2:4:537:THR:HG22	1.93	0.49
2:2:384:ASP:OD1	2:2:398:THR:OG1	2.15	0.49
4:O:49:GLY:N	4:O:98:ASP:OD2	2.40	0.49
1:O:71:THR:OG1	4:N:299:ASN:ND2	2.45	0.49
4:F:370:LEU:HD21	4:F:382:LEU:HD13	1.94	0.49
4:O:68:THR:O	4:O:68:THR:OG1	2.26	0.49
1:y:87:THR:HG23	1:y:120:GLU:OE2	2.13	0.49
2:2:321:ASN:OD1	2:2:322:GLY:N	2.45	0.49
4:N:265:LEU:HD22	4:N:284:ASN:ND2	2.28	0.49
4:j:147:ARG:NH1	4:j:332:GLU:OE2	2.45	0.49
4:G:307:LEU:HD11	4:H:248:TYR:CD1	2.47	0.49
4:I:346:VAL:HG11	4:I:365:MET:HE2	1.95	0.49
4:M:217:VAL:HG22	4:M:286:ASP:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:180:GLU:O	1:P:183:LYS:NZ	2.43	0.49
1:S:202:THR:O	1:S:202:THR:HG22	2.13	0.49
4:j:24:TYR:CZ	4:j:68:THR:HG23	2.47	0.49
1:t:191:CYS:O	1:t:221:ALA:N	2.46	0.49
2:2:29:LYS:CB	2:3:33:VAL:HG12	2.43	0.49
2:4:12:ASN:O	2:4:15:THR:OG1	2.31	0.49
4:F:17:LYS:HD3	4:F:30:LEU:HD22	1.95	0.49
4:F:304:VAL:HA	4:F:307:LEU:HD12	1.95	0.49
1:1:178:THR:OG1	1:1:250:LYS:NZ	2.45	0.49
2:2:496:ARG:HD3	1:W:108:THR:HG23	1.93	0.49
4:F:333:SER:OG	4:F:379:GLU:OE2	2.27	0.49
4:G:110:ALA:O	4:G:112:GLN:NE2	2.46	0.49
4:M:225:LEU:HD22	4:M:261:VAL:HG21	1.93	0.49
1:Y:202:THR:HG22	1:Y:202:THR:O	2.12	0.49
1:t:77:LEU:HD23	1:t:112:PRO:HG3	1.93	0.49
1:P:296:PHE:O	1:P:300:VAL:HG23	2.13	0.49
1:Q:271:ILE:HG12	1:Q:284:MET:HE1	1.95	0.49
1:v:172:LEU:HD22	1:v:173:TYR:CE1	2.47	0.49
2:4:384:ASP:OD1	2:4:398:THR:HG23	2.14	0.48
4:J:225:LEU:CD2	4:J:261:VAL:HG21	2.43	0.48
1:R:317:LEU:HD21	1:Z:252:LEU:HD12	1.94	0.48
4:h:225:LEU:HD22	4:h:261:VAL:HG21	1.94	0.48
2:2:584:VAL:HG11	2:2:705:VAL:HG22	1.94	0.48
2:4:492:GLN:OE1	2:4:492:GLN:N	2.44	0.48
1:U:65:THR:OG1	1:U:66:ALA:N	2.47	0.48
2:2:482:THR:HG22	2:2:482:THR:O	2.12	0.48
2:3:65:LEU:HD21	2:3:219:TYR:HE2	1.77	0.48
4:h:14:ALA:HB1	4:h:85:ILE:HD11	1.96	0.48
4:j:14:ALA:HA	4:j:30:LEU:HD21	1.93	0.48
2:4:22:ILE:O	2:4:26:GLY:N	2.45	0.48
2:4:636:ILE:O	2:4:640:VAL:HG23	2.12	0.48
3:B:514:MET:HE2	3:B:547:LEU:HD22	1.94	0.48
4:D:85:ILE:O	4:D:89:VAL:HG23	2.14	0.48
4:J:24:TYR:CZ	4:J:68:THR:HG23	2.49	0.48
1:V:64:ASP:OD2	1:V:64:ASP:C	2.57	0.48
4:M:265:LEU:HD22	4:M:284:ASN:ND2	2.29	0.48
1:1:144:TYR:CD1	1:1:152:MET:HE1	2.48	0.48
1:1:271:ILE:CD1	1:1:284:MET:HE1	2.36	0.48
2:2:121:LEU:O	2:2:124:THR:HG22	2.14	0.48
2:2:436:SER:OG	2:2:447:LEU:O	2.29	0.48
4:H:11:LEU:HG	4:H:37:MET:HE1	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:11:LEU:HD21	4:M:88:PHE:HB3	1.95	0.48
4:E:145:ARG:NH2	4:j:111:PRO:O	2.45	0.48
4:H:165:THR:OG1	1:V:60:THR:HG23	2.14	0.48
4:H:255:ARG:NH2	1:T:65:THR:O	2.46	0.48
4:i:137:GLU:OE2	4:j:12:LYS:NZ	2.47	0.48
2:4:412:SER:OG	2:4:425:ARG:NH2	2.47	0.48
4:G:217:VAL:HG22	4:G:286:ASP:HB3	1.96	0.48
1:v:141:LEU:HD23	1:v:261:ILE:HB	1.96	0.48
3:A:740:ILE:HD12	3:A:764:VAL:HG21	1.95	0.48
4:M:2:ASP:OD1	4:M:3:VAL:N	2.47	0.48
1:P:256:GLU:O	1:P:310:MET:HE3	2.14	0.48
1:U:163:TRP:O	1:W:317:LEU:HD22	2.14	0.48
1:1:265:GLY:O	1:1:286:ARG:NH1	2.47	0.48
4:H:38:ILE:HD11	4:H:84:THR:HG21	1.96	0.48
4:M:225:LEU:CD2	4:M:261:VAL:HG21	2.44	0.48
3:B:728:VAL:CG2	3:B:806:LEU:HD11	2.44	0.47
4:L:217:VAL:HG22	4:L:286:ASP:HB3	1.96	0.47
1:Z:202:THR:O	1:Z:202:THR:HG22	2.14	0.47
2:3:279:SER:OG	2:3:452:ALA:O	2.27	0.47
2:4:294:ILE:HG23	2:4:342:TYR:HB2	1.95	0.47
3:A:621:TYR:CZ	3:A:625:ILE:HD11	2.49	0.47
1:x:133:LEU:HD13	1:x:258:VAL:CG2	2.44	0.47
4:F:225:LEU:HD13	4:F:324:LEU:CD1	2.44	0.47
4:K:38:ILE:HD11	4:K:84:THR:HG21	1.97	0.47
1:Q:271:ILE:C	1:Q:271:ILE:HD12	2.38	0.47
4:h:173:HIS:HA	4:h:176:LEU:HD21	1.95	0.47
2:3:365:MET:CE	2:3:470:LEU:HD22	2.44	0.47
3:B:174:LEU:HD22	3:B:640:LEU:CD1	2.44	0.47
1:R:317:LEU:HD21	1:Z:252:LEU:CD1	2.44	0.47
1:X:285:MET:HE1	1:X:306:ILE:HG23	1.96	0.47
2:2:249:GLN:O	2:2:250:ALA:HB3	2.15	0.47
2:3:365:MET:HE3	2:3:470:LEU:HD22	1.97	0.47
1:Q:180:GLU:O	1:Q:183:LYS:NZ	2.48	0.47
1:V:129:VAL:O	1:V:129:VAL:HG12	2.14	0.47
4:f:370:LEU:HD21	4:f:382:LEU:HD13	1.96	0.47
2:3:730:LEU:CD2	2:3:763:ILE:HD11	2.44	0.47
3:A:309:ASN:O	3:A:622:ASN:ND2	2.42	0.47
4:N:225:LEU:CD2	4:N:261:VAL:HG21	2.45	0.47
1:u:164:LEU:HD22	1:u:324:TYR:CZ	2.50	0.47
1:1:142:MET:HE2	1:1:155:LEU:HD23	1.96	0.47
2:2:440:THR:HG22	2:3:230:THR:HG21	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:41:ALA:HB1	2:3:42:GLN:HG2	1.96	0.47
2:3:64:VAL:HG13	2:3:65:LEU:HG	1.97	0.47
4:C:11:LEU:HD21	4:C:88:PHE:HB3	1.96	0.47
4:L:11:LEU:HD21	4:L:88:PHE:HB3	1.95	0.47
1:U:164:LEU:HD22	1:U:324:TYR:CZ	2.50	0.47
4:h:169:SER:HA	4:h:176:LEU:HD23	1.97	0.47
1:u:75:THR:HG23	1:u:137:TYR:HE2	1.80	0.47
1:1:263:VAL:HG12	1:1:289:TRP:CG	2.49	0.47
2:2:593:ASP:O	2:2:618:ARG:NH1	2.47	0.47
4:E:93:ASP:OD1	4:E:392:ARG:NE	2.45	0.47
4:h:11:LEU:HG	4:h:37:MET:HE1	1.96	0.47
1:R:141:LEU:HD23	1:R:261:ILE:HB	1.97	0.47
1:S:191:CYS:N	1:S:222:GLU:O	2.43	0.47
4:j:11:LEU:HD21	4:j:88:PHE:CB	2.45	0.47
2:3:81:TRP:CZ3	2:3:168:MET:HE2	2.50	0.46
4:D:225:LEU:HD22	4:D:261:VAL:HG21	1.97	0.46
2:2:352:TYR:OH	2:3:54:GLU:OE1	2.11	0.46
2:3:81:TRP:NE1	2:3:166:ALA:HB1	2.30	0.46
2:4:273:ILE:HG21	2:4:353:VAL:HG11	1.96	0.46
4:G:225:LEU:CD2	4:G:261:VAL:HG21	2.46	0.46
1:Q:285:MET:HE1	1:Q:306:ILE:HG23	1.97	0.46
2:2:306:THR:HG22	2:2:311:GLU:HG2	1.98	0.46
4:H:14:ALA:HB1	4:H:85:ILE:HD11	1.97	0.46
4:f:225:LEU:HD22	4:f:261:VAL:HG21	1.96	0.46
4:h:11:LEU:HD21	4:h:88:PHE:HB3	1.96	0.46
4:E:170:GLN:NE2	4:E:175:ASN:O	2.40	0.46
4:F:310:ASN:OD1	1:U:305:GLN:NE2	2.49	0.46
4:k:108:GLY:O	4:k:384:ARG:NE	2.40	0.46
1:O:266:SER:OG	1:O:267:ASP:N	2.49	0.46
4:E:254:LEU:O	4:E:320:VAL:HG12	2.15	0.46
1:S:263:VAL:HG12	1:S:289:TRP:CD1	2.50	0.46
1:Y:184:TRP:CZ3	1:Y:237:LEU:HD21	2.50	0.46
4:j:336:ALA:HB2	4:j:343:LEU:HD22	1.98	0.46
1:u:163:TRP:O	1:w:317:LEU:HD22	2.15	0.46
1:y:278:ALA:O	1:y:280:GLN:NE2	2.47	0.46
2:2:230:THR:HG22	2:2:231:ARG:H	1.81	0.46
2:3:32:ASN:OD1	2:3:32:ASN:N	2.48	0.46
1:Q:144:TYR:HA	1:Q:152:MET:HE1	1.97	0.46
4:f:17:LYS:HD3	4:f:30:LEU:HD22	1.97	0.46
4:g:68:THR:O	4:g:68:THR:HG22	2.15	0.46
4:k:333:SER:OG	4:k:379:GLU:OE2	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:159:ILE:HD11	1:x:260:VAL:CG2	2.46	0.46
4:D:265:LEU:HD22	4:D:284:ASN:ND2	2.31	0.46
4:N:17:LYS:HB3	4:N:27:VAL:HG12	1.97	0.46
1:R:262:GLN:NE2	1:R:266:SER:O	2.46	0.46
4:h:104:SER:OG	4:h:106:ARG:O	2.32	0.46
4:h:165:THR:OG1	1:v:60:THR:HG23	2.16	0.46
2:2:39:PRO:O	2:2:40:PHE:C	2.58	0.46
2:2:439:ILE:O	2:3:228:GLN:NE2	2.49	0.46
2:3:75:ASN:N	2:3:75:ASN:OD1	2.49	0.46
2:4:730:LEU:HD22	2:4:763:ILE:HD11	1.98	0.46
4:J:239:ASN:ND2	4:J:240:SER:O	2.49	0.46
4:L:239:ASN:ND2	4:L:240:SER:O	2.47	0.46
1:U:202:THR:O	1:U:202:THR:HG22	2.16	0.46
4:g:11:LEU:HD21	4:g:88:PHE:CB	2.45	0.46
2:4:19:SER:CB	2:4:546:THR:HG21	2.45	0.46
2:4:339:ILE:HD11	2:4:387:PHE:HE2	1.81	0.46
3:B:214:ILE:HG21	3:B:251:ILE:HG21	1.97	0.46
4:h:11:LEU:HD21	4:h:88:PHE:CB	2.46	0.46
4:i:172:ALA:HB3	4:i:174:ASP:OD2	2.16	0.46
1:v:263:VAL:HG12	1:v:289:TRP:CD1	2.51	0.46
1:y:180:GLU:O	1:y:183:LYS:NZ	2.48	0.46
2:3:84:LEU:HD23	2:3:203:CYS:SG	2.56	0.45
2:4:16:VAL:HA	2:4:546:THR:HG23	1.97	0.45
2:4:478:ASP:N	2:4:478:ASP:OD1	2.48	0.45
2:4:581:ILE:HG23	2:4:593:ASP:HB2	1.98	0.45
1:P:185:ILE:HD12	1:P:249:CYS:HB2	1.98	0.45
1:y:265:GLY:O	1:y:286:ARG:NH1	2.49	0.45
2:2:5:ILE:HG23	2:2:6:TYR:N	2.31	0.45
2:2:476:SER:CB	2:3:259:THR:HG23	2.46	0.45
2:3:730:LEU:O	2:3:734:TYR:N	2.44	0.45
2:4:294:ILE:HG23	2:4:342:TYR:CB	2.46	0.45
2:4:570:ASP:OD2	2:4:577:ARG:NH2	2.49	0.45
3:B:277:ILE:CD1	3:B:299:LEU:HD11	2.45	0.45
4:D:334:VAL:HG23	4:D:382:LEU:HD23	1.98	0.45
2:4:398:THR:HG22	2:4:399:GLY:H	1.81	0.45
4:J:225:LEU:HD12	4:J:323:THR:O	2.16	0.45
1:W:263:VAL:HG12	1:W:289:TRP:CD1	2.51	0.45
2:2:107:LEU:HD13	2:2:140:PHE:CE1	2.51	0.45
1:W:265:GLY:O	1:W:286:ARG:NH1	2.49	0.45
4:g:262:GLU:HG3	4:g:272:THR:HG23	1.98	0.45
3:A:728:VAL:HG23	3:A:807:TYR:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:11:LEU:HD21	4:C:88:PHE:CB	2.47	0.45
4:I:173:HIS:HA	4:I:176:LEU:HD21	1.98	0.45
4:f:265:LEU:HD22	4:f:284:ASN:ND2	2.31	0.45
4:h:373:ASN:O	4:h:375:SER:N	2.50	0.45
4:j:239:ASN:ND2	4:j:240:SER:O	2.50	0.45
1:v:130:ASP:CA	1:v:187:MET:HE3	2.46	0.45
4:E:209:GLU:OE2	4:E:289:ARG:NE	2.49	0.45
4:H:142:GLN:HB2	4:H:148:THR:HG21	1.98	0.45
4:L:333:SER:OG	4:L:379:GLU:OE2	2.30	0.45
1:V:59:ILE:HD11	1:t:53:TYR:O	2.16	0.45
4:g:370:LEU:HD21	4:g:382:LEU:HD13	1.98	0.45
1:v:190:SER:OG	1:v:243:THR:HG21	2.17	0.45
2:2:121:LEU:HD13	2:2:152:TYR:OH	2.17	0.45
2:2:185:THR:OG1	2:2:186:THR:N	2.50	0.45
2:4:287:LEU:HD12	2:4:287:LEU:H	1.81	0.45
2:4:364:ASN:ND2	2:4:484:ILE:O	2.42	0.45
4:G:225:LEU:HD13	4:G:324:LEU:CD1	2.46	0.45
4:I:370:LEU:HD21	4:I:382:LEU:HD13	1.99	0.45
1:U:185:ILE:HG22	1:U:187:MET:HE2	1.97	0.45
4:f:304:VAL:HA	4:f:307:LEU:HD12	1.98	0.45
4:g:160:TYR:OH	1:u:64:ASP:OD2	2.21	0.45
2:4:594:VAL:HG11	2:4:611:GLN:OE1	2.17	0.45
4:E:11:LEU:HD21	4:E:88:PHE:CB	2.46	0.45
4:H:11:LEU:HD21	4:H:88:PHE:CB	2.46	0.45
4:N:261:VAL:HG22	4:N:290:LEU:HD23	1.97	0.45
1:P:172:LEU:HD23	1:P:173:TYR:CZ	2.52	0.45
4:i:370:LEU:HD21	4:i:382:LEU:HD13	1.97	0.45
1:t:82:CYS:N	1:t:135:CYS:SG	2.90	0.45
2:2:227:ILE:O	2:2:227:ILE:HG22	2.16	0.45
2:2:371:LEU:HD13	2:2:424:LEU:HD11	1.99	0.45
2:4:368:VAL:O	2:4:538:ILE:N	2.47	0.45
3:A:320:ASN:O	3:A:671:ARG:NH2	2.44	0.45
4:C:93:ASP:OD1	4:C:392:ARG:NE	2.47	0.45
4:C:264:LEU:CD2	4:C:269:ILE:HD13	2.47	0.45
4:E:142:GLN:OE1	4:j:106:ARG:NH2	2.49	0.45
1:V:271:ILE:HG12	1:V:284:MET:HE1	1.99	0.45
1:u:202:THR:O	1:u:202:THR:HG22	2.17	0.45
1:w:109:LYS:NZ	1:w:301:ASP:OD1	2.36	0.45
1:y:168:MET:HE2	1:y:246:ILE:HG12	1.98	0.45
2:2:344:VAL:HG23	2:2:450:LEU:C	2.41	0.45
2:4:557:LEU:HD21	2:4:624:MET:CE	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:202:PRO:O	4:C:203:ALA:HB3	2.17	0.45
4:C:225:LEU:HD13	4:C:324:LEU:HD13	1.99	0.45
4:M:11:LEU:HD21	4:M:88:PHE:CB	2.47	0.45
4:M:228:ASP:OD2	4:N:236:ARG:NH2	2.50	0.45
2:3:276:LYS:HD2	2:3:277:PHE:O	2.16	0.44
3:A:718:GLN:HA	3:A:827:THR:HG22	1.99	0.44
4:F:261:VAL:HG22	4:F:290:LEU:HD23	1.98	0.44
4:O:182:LEU:HD22	4:O:231:ARG:CD	2.47	0.44
4:g:145:ARG:NH2	4:i:380:ASP:OD1	2.50	0.44
4:M:31:ILE:HD12	4:M:66:LEU:HD23	1.99	0.44
4:N:11:LEU:HD21	4:N:88:PHE:HB3	1.98	0.44
1:V:130:ASP:CA	1:V:187:MET:HE3	2.48	0.44
4:h:10:THR:HB	4:h:37:MET:HE3	1.99	0.44
1:x:80:THR:HG21	1:x:324:TYR:HE2	1.74	0.44
3:B:873:ILE:HD11	3:B:887:LEU:CD2	2.48	0.44
1:V:180:GLU:O	1:V:183:LYS:NZ	2.50	0.44
4:f:283:ARG:NH1	4:g:352:GLU:OE1	2.51	0.44
4:h:209:GLU:OE2	4:h:289:ARG:NH1	2.50	0.44
2:4:16:VAL:HG11	2:4:550:LYS:CA	2.47	0.44
4:C:85:ILE:O	4:C:89:VAL:HG23	2.17	0.44
4:L:174:ASP:OD1	4:L:312:GLN:NE2	2.45	0.44
1:R:164:LEU:CB	1:R:252:LEU:HD21	2.47	0.44
1:x:98:TRP:HA	1:x:101:THR:HG22	1.98	0.44
2:2:485:THR:O	2:2:486:ASN:HB2	2.16	0.44
2:2:514:MET:HE1	2:2:764:ARG:HB3	1.99	0.44
2:3:206:TYR:OH	2:3:224:LEU:HD22	2.18	0.44
2:4:508:LEU:O	2:4:647:ARG:NH2	2.50	0.44
2:4:522:LEU:HD11	2:4:749:PRO:CB	2.46	0.44
3:A:281:ILE:HD13	3:A:293:LEU:HD13	1.98	0.44
4:I:11:LEU:HD21	4:I:88:PHE:CB	2.48	0.44
1:U:87:THR:O	1:U:91:THR:HG23	2.18	0.44
4:g:45:GLU:O	4:g:118:LYS:NZ	2.49	0.44
1:w:193:ILE:HD12	1:w:193:ILE:N	2.32	0.44
2:3:185:THR:OG1	2:3:186:THR:N	2.51	0.44
2:3:194:TYR:O	2:3:197:VAL:HG22	2.18	0.44
2:3:480:TYR:CE1	1:Z:208:LEU:HD23	2.52	0.44
4:J:299:ASN:ND2	4:K:244:ALA:O	2.49	0.44
1:P:258:VAL:C	1:P:310:MET:HE1	2.42	0.44
1:T:133:LEU:HD13	1:T:258:VAL:HG21	1.99	0.44
4:h:252:VAL:O	4:h:252:VAL:HG13	2.18	0.44
4:j:2:ASP:OD1	4:j:3:VAL:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:75:ASN:OD1	2:2:75:ASN:N	2.51	0.44
3:A:141:TYR:N	3:A:723:GLU:O	2.47	0.44
3:B:352:GLN:NE2	3:B:593:MET:O	2.48	0.44
4:H:225:LEU:HD22	4:H:261:VAL:HG21	2.00	0.44
1:u:230:VAL:HG22	1:v:300:VAL:HG13	1.98	0.44
3:A:481:PHE:HD1	4:G:69:THR:HG23	1.81	0.44
4:f:105:GLN:NE2	4:f:359:PRO:O	2.51	0.44
2:3:81:TRP:HE1	2:3:166:ALA:HB1	1.83	0.44
3:A:764:VAL:HG22	3:A:765:ALA:H	1.83	0.44
4:F:346:VAL:HG11	4:F:365:MET:HE2	1.99	0.44
4:G:11:LEU:HD21	4:G:88:PHE:HB3	1.98	0.44
4:O:168:ARG:NH2	4:O:194:ASP:OD1	2.44	0.44
1:Q:263:VAL:HG12	1:Q:289:TRP:CD1	2.53	0.44
1:V:141:LEU:HD23	1:V:261:ILE:HB	2.00	0.44
1:W:212:THR:HG23	1:W:238:ASP:OD2	2.18	0.44
2:2:523:LEU:HD12	2:4:568:LEU:HD12	2.00	0.43
2:3:675:VAL:HG11	2:3:711:LEU:HB3	1.99	0.43
2:4:706:GLN:O	2:4:706:GLN:HG2	2.18	0.43
4:C:2:ASP:OD1	4:C:3:VAL:N	2.51	0.43
4:F:182:LEU:HD22	4:F:231:ARG:CD	2.48	0.43
1:0:145:ASP:OD2	1:0:147:THR:OG1	2.36	0.43
2:3:42:GLN:HB3	2:4:329:ASN:O	2.18	0.43
2:4:5:ILE:HG23	2:4:6:TYR:N	2.33	0.43
4:L:370:LEU:HD21	4:L:382:LEU:HD13	2.00	0.43
2:2:63:PRO:O	2:2:64:VAL:HB	2.17	0.43
2:2:84:LEU:HD23	2:2:203:CYS:SG	2.58	0.43
2:2:439:ILE:HD11	2:2:442:THR:HG21	2.01	0.43
2:3:227:ILE:O	2:3:227:ILE:HG22	2.17	0.43
3:A:154:TYR:OH	3:A:723:GLU:OE2	2.34	0.43
4:F:173:HIS:HA	4:F:176:LEU:HD21	2.00	0.43
4:K:145:ARG:NH1	4:L:142:GLN:O	2.50	0.43
4:N:370:LEU:HD21	4:N:382:LEU:HD13	2.00	0.43
1:P:144:TYR:CD1	1:P:152:MET:HE1	2.53	0.43
1:P:259:ALA:HB2	1:P:310:MET:SD	2.59	0.43
4:k:11:LEU:HD21	4:k:88:PHE:HB3	2.00	0.43
1:u:276:THR:HG22	1:v:285:MET:HE3	2.00	0.43
2:3:95:GLY:HA2	2:3:198:ASN:O	2.18	0.43
3:A:764:VAL:HG22	3:A:765:ALA:N	2.33	0.43
3:B:170:ARG:NE	3:B:638:LEU:O	2.49	0.43
3:B:517:LEU:HB2	3:B:540:ILE:HG23	2.00	0.43
4:C:380:ASP:OD2	4:N:145:ARG:NH2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:373:ASN:O	4:H:375:SER:N	2.52	0.43
1:R:182:ASN:ND2	1:R:248:ASN:OD1	2.47	0.43
1:U:195:VAL:HG23	1:U:237:LEU:HD23	2.00	0.43
2:3:489:THR:HB	2:4:431:THR:HG23	2.00	0.43
4:J:11:LEU:HD21	4:J:88:PHE:CB	2.48	0.43
4:N:173:HIS:HA	4:N:176:LEU:HD21	2.01	0.43
1:R:317:LEU:HD11	1:Z:315:ARG:HG3	1.98	0.43
1:w:212:THR:HG23	1:w:238:ASP:OD2	2.18	0.43
2:2:84:LEU:HD21	2:2:201:ALA:HB1	2.01	0.43
2:2:262:TRP:O	2:3:260:SER:N	2.43	0.43
3:B:764:VAL:HG22	3:B:765:ALA:H	1.84	0.43
1:V:162:GLU:OE1	1:t:317:LEU:HD11	2.18	0.43
1:V:190:SER:OG	1:V:243:THR:HG21	2.18	0.43
1:X:180:GLU:O	1:X:183:LYS:NZ	2.51	0.43
4:j:265:LEU:HD22	4:j:284:ASN:ND2	2.34	0.43
4:k:189:GLN:HG3	4:k:323:THR:HG23	2.01	0.43
2:4:324:ASN:OD1	2:4:324:ASN:N	2.52	0.43
2:4:592:THR:O	2:4:592:THR:HG22	2.18	0.43
3:B:420:VAL:HG23	3:B:421:VAL:HG23	2.00	0.43
4:D:261:VAL:HG22	4:D:290:LEU:HD23	2.01	0.43
4:E:199:ILE:HD13	4:E:310:ASN:HA	2.01	0.43
4:E:217:VAL:HG22	4:E:286:ASP:HB3	2.01	0.43
4:H:10:THR:HB	4:H:37:MET:HE3	2.00	0.43
4:J:236:ARG:NH2	1:X:63:MET:SD	2.87	0.43
1:X:263:VAL:HG12	1:X:289:TRP:CD1	2.54	0.43
4:i:11:LEU:HD21	4:i:88:PHE:HB3	2.01	0.43
1:w:151:ASP:CG	1:x:290:LYS:HZ1	2.26	0.43
1:1:281:THR:HG22	1:1:282:GLU:N	2.34	0.43
4:I:299:ASN:ND2	4:J:244:ALA:O	2.47	0.43
4:M:255:ARG:NH2	1:Z:65:THR:O	2.49	0.43
1:X:159:ILE:HD11	1:X:260:VAL:CG2	2.49	0.43
2:4:365:MET:HE1	2:4:424:LEU:HD13	2.01	0.43
4:F:23:LEU:HD11	4:H:36:GLN:HB2	2.01	0.43
4:G:4:LEU:HD22	4:G:116:LEU:HD13	2.00	0.43
4:H:173:HIS:HA	4:H:176:LEU:HD21	2.00	0.43
4:M:38:ILE:HD11	4:M:84:THR:HG21	2.01	0.43
4:N:367:TRP:O	4:N:371:ILE:HG22	2.18	0.43
4:g:242:ASP:OD1	4:g:242:ASP:N	2.49	0.43
4:h:38:ILE:HD11	4:h:84:THR:HG21	2.00	0.43
4:D:240:SER:N	4:D:245:THR:O	2.49	0.43
4:F:11:LEU:HD21	4:F:88:PHE:CB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:11:LEU:HD21	4:G:88:PHE:CB	2.49	0.43
4:G:172:ALA:HB3	4:G:174:ASP:OD1	2.19	0.43
4:H:112:GLN:O	4:H:117:ARG:NH2	2.52	0.43
4:I:4:LEU:HD22	4:I:116:LEU:HD13	2.01	0.43
4:J:279:THR:OG1	4:K:156:ASN:ND2	2.46	0.43
4:N:117:ARG:O	4:N:120:SER:OG	2.35	0.43
1:R:130:ASP:OD2	1:R:132:GLN:NE2	2.51	0.43
1:V:325:ARG:HB2	1:t:323:TYR:CE1	2.54	0.43
1:W:193:ILE:N	1:W:193:ILE:HD12	2.34	0.43
1:Y:168:MET:HE2	1:Y:246:ILE:HG12	2.01	0.43
2:4:265:MET:CE	2:4:482:THR:HG21	2.36	0.42
3:A:272:LEU:HD11	3:A:277:ILE:HG13	2.01	0.42
4:j:4:LEU:HD22	4:j:116:LEU:HD13	2.01	0.42
1:v:72:GLN:NE2	1:v:304:ASN:OD1	2.52	0.42
1:0:123:ASP:OD1	1:0:123:ASP:N	2.52	0.42
2:2:63:PRO:O	2:2:64:VAL:CB	2.67	0.42
2:2:84:LEU:HD21	2:2:201:ALA:CB	2.49	0.42
2:3:41:ALA:HB1	2:3:42:GLN:CG	2.50	0.42
2:3:368:VAL:HG23	2:3:470:LEU:CD1	2.49	0.42
3:B:337:ARG:NH1	3:B:388:THR:OG1	2.52	0.42
4:i:264:LEU:HD21	4:i:269:ILE:HD13	2.01	0.42
1:u:73:GLU:OE2	1:u:77:LEU:HD22	2.19	0.42
2:3:255:VAL:HG23	2:3:255:VAL:O	2.19	0.42
2:4:374:ASN:O	2:4:375:LEU:HD23	2.19	0.42
2:4:642:LYS:NZ	2:4:646:ASP:OD1	2.45	0.42
4:O:11:LEU:HD21	4:O:88:PHE:CB	2.48	0.42
4:O:182:LEU:HD22	4:O:231:ARG:NE	2.34	0.42
2:3:65:LEU:HD21	2:3:219:TYR:CE2	2.54	0.42
2:3:371:LEU:CD2	2:3:424:LEU:HD11	2.50	0.42
2:3:530:MET:HE2	2:3:645:ILE:HD11	2.01	0.42
2:4:273:ILE:HB	2:4:464:VAL:HG22	2.01	0.42
2:4:486:ASN:OD1	2:4:486:ASN:O	2.37	0.42
4:K:11:LEU:HD21	4:K:88:PHE:HB3	2.01	0.42
4:L:14:ALA:HB1	4:L:85:ILE:HD11	2.01	0.42
1:T:195:VAL:HG21	1:U:297:TYR:HE2	1.84	0.42
1:W:265:GLY:O	1:Y:149:GLN:NE2	2.52	0.42
2:2:734:TYR:O	2:2:735:GLY:C	2.62	0.42
2:2:743:ASN:CB	2:2:751:VAL:HG21	2.48	0.42
4:J:68:THR:HG22	4:J:69:THR:N	2.33	0.42
4:f:173:HIS:HA	4:f:176:LEU:HD21	2.00	0.42
4:i:2:ASP:OD1	4:i:3:VAL:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:195:VAL:HG21	1:u:297:TYR:HE2	1.84	0.42
1:0:193:ILE:N	1:0:193:ILE:HD12	2.35	0.42
2:2:400:GLY:N	2:2:436:SER:O	2.53	0.42
2:3:397:MET:HE2	2:3:439:ILE:CG2	2.50	0.42
4:D:245:THR:HG22	4:D:246:THR:H	1.85	0.42
4:L:11:LEU:HD21	4:L:88:PHE:CB	2.50	0.42
4:D:93:ASP:OD1	4:D:392:ARG:NE	2.42	0.42
4:E:11:LEU:HD21	4:E:88:PHE:HB3	2.01	0.42
1:t:162:GLU:OE1	1:t:323:TYR:OH	2.29	0.42
1:v:285:MET:HE2	1:v:306:ILE:HG12	2.00	0.42
1:x:151:ASP:OD1	1:y:290:LYS:NZ	2.44	0.42
1:0:296:PHE:O	1:0:300:VAL:HG23	2.20	0.42
1:1:217:GLU:OE1	1:1:217:GLU:N	2.46	0.42
2:2:523:LEU:HD12	2:4:568:LEU:HD13	2.01	0.42
2:3:273:ILE:HD12	2:3:273:ILE:H	1.84	0.42
2:4:559:ASN:O	2:4:563:THR:HG23	2.19	0.42
2:4:670:ASN:OD1	2:4:670:ASN:N	2.45	0.42
3:A:329:THR:HG23	3:A:395:SER:O	2.20	0.42
4:D:48:THR:HG23	4:D:98:ASP:HB2	2.02	0.42
4:G:225:LEU:HD13	4:G:324:LEU:HD13	2.01	0.42
4:J:2:ASP:OD1	4:J:3:VAL:N	2.53	0.42
4:J:265:LEU:HD22	4:J:284:ASN:ND2	2.35	0.42
4:N:93:ASP:OD1	4:N:392:ARG:NE	2.48	0.42
1:U:187:MET:HG3	1:U:224:LEU:HD13	2.02	0.42
1:U:296:PHE:O	1:U:300:VAL:HG23	2.20	0.42
1:u:265:GLY:O	1:u:286:ARG:NH1	2.53	0.42
1:x:162:GLU:OE2	1:x:313:ARG:NE	2.47	0.42
2:3:538:ILE:O	2:3:539:ASP:HB2	2.20	0.42
2:4:329:ASN:HA	2:4:338:VAL:HG22	2.01	0.42
4:H:169:SER:HA	4:H:176:LEU:HD23	2.02	0.42
4:J:182:LEU:HD22	4:J:231:ARG:CD	2.50	0.42
1:W:97:SER:O	1:W:101:THR:HG23	2.19	0.42
4:i:108:GLY:O	4:i:384:ARG:NE	2.48	0.42
4:j:299:ASN:ND2	4:k:244:ALA:O	2.49	0.42
1:w:133:LEU:HD13	1:w:258:VAL:HG21	2.02	0.42
3:A:137:GLN:O	3:A:138:LEU:HD12	2.19	0.42
1:T:151:ASP:OD1	1:U:290:LYS:NZ	2.52	0.42
1:W:108:THR:HG21	1:Y:233:VAL:CG2	2.50	0.42
4:h:2:ASP:OD1	4:h:3:VAL:N	2.52	0.42
2:3:49:ASN:HD21	2:4:391:VAL:HG13	1.83	0.41
2:4:624:MET:CG	2:4:624:MET:O	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:182:LEU:HD22	4:D:231:ARG:CD	2.50	0.41
4:D:182:LEU:HD22	4:D:231:ARG:NE	2.35	0.41
4:F:217:VAL:HG22	4:F:286:ASP:HB3	2.02	0.41
1:V:325:ARG:NH2	1:t:317:LEU:HD12	2.35	0.41
1:w:97:SER:O	1:w:101:THR:HG23	2.20	0.41
3:A:176:LEU:O	3:A:180:VAL:HG23	2.19	0.41
3:B:674:ASP:OD1	3:B:677:ARG:NH2	2.53	0.41
4:F:76:ASN:OD1	4:g:75:ALA:N	2.53	0.41
4:F:225:LEU:HD13	4:F:324:LEU:HD13	2.02	0.41
4:g:4:LEU:HD22	4:g:116:LEU:HD13	2.01	0.41
1:u:189:SER:O	1:u:223:LYS:NZ	2.51	0.41
2:3:69:TYR:OH	2:3:290:LYS:NZ	2.41	0.41
2:4:516:GLN:OE1	2:4:516:GLN:N	2.42	0.41
2:4:678:ASN:O	2:4:679:ASP:OD1	2.38	0.41
3:A:449:MET:SD	3:A:470:ILE:HD13	2.61	0.41
3:A:728:VAL:HG22	3:A:730:ILE:HG13	2.02	0.41
4:H:142:GLN:OE1	4:H:383:GLN:NE2	2.44	0.41
4:L:112:GLN:O	4:L:117:ARG:NH1	2.52	0.41
1:S:172:LEU:HD23	1:S:173:TYR:CZ	2.55	0.41
1:V:170:ILE:HD11	1:V:241:THR:CG2	2.50	0.41
4:k:188:ILE:HD13	4:k:212:VAL:HG21	2.02	0.41
1:u:137:TYR:HD1	1:u:310:MET:HE2	1.84	0.41
2:2:657:PRO:O	2:2:658:ASP:CG	2.64	0.41
2:3:164:LEU:HD22	2:3:223:GLY:HA2	2.02	0.41
2:3:276:LYS:HD2	2:3:276:LYS:C	2.45	0.41
2:4:505:PHE:O	2:4:644:LYS:HE3	2.20	0.41
2:4:776:LEU:C	2:4:776:LEU:HD23	2.45	0.41
3:B:403:PHE:HB3	3:B:585:LEU:HD12	2.02	0.41
3:B:645:MET:HA	3:B:648:ILE:HD12	2.03	0.41
4:D:382:LEU:HA	4:D:385:VAL:HG22	2.03	0.41
4:H:45:GLU:O	4:H:118:LYS:NZ	2.53	0.41
4:f:225:LEU:CD2	4:f:261:VAL:HG21	2.51	0.41
4:f:346:VAL:HG11	4:f:365:MET:HE2	2.02	0.41
4:k:334:VAL:O	4:k:374:TYR:OH	2.37	0.41
1:u:195:VAL:HG23	1:u:237:LEU:HD23	2.02	0.41
2:2:641:LEU:HD13	2:2:663:ALA:CB	2.49	0.41
2:2:734:TYR:O	2:2:736:ILE:HG23	2.21	0.41
2:3:28:THR:HG22	2:4:352:TYR:HE2	1.85	0.41
2:4:631:MET:HE2	2:4:636:ILE:HD11	2.01	0.41
4:C:370:LEU:HD11	4:C:382:LEU:HD13	2.02	0.41
4:F:39:ILE:HD11	4:F:65:LEU:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:185:ILE:HD12	1:P:249:CYS:CB	2.51	0.41
1:Q:296:PHE:O	1:Q:300:VAL:HG23	2.20	0.41
4:j:262:GLU:HG2	4:j:272:THR:HG22	2.02	0.41
1:u:73:GLU:OE2	1:u:77:LEU:HD13	2.21	0.41
1:0:195:VAL:HG22	1:0:237:LEU:CD2	2.50	0.41
1:1:191:CYS:N	1:1:222:GLU:O	2.51	0.41
4:C:258:ASN:ND2	4:C:293:GLN:OE1	2.53	0.41
4:F:129:PHE:O	4:F:130:ASP:C	2.64	0.41
4:I:264:LEU:HD21	4:I:269:ILE:HD13	2.02	0.41
2:4:579:ALA:HB1	4:G:205:ILE:HG21	2.01	0.41
2:4:697:THR:HG23	2:4:699:ASP:OD1	2.20	0.41
3:A:734:LEU:HD21	3:A:833:TYR:CG	2.55	0.41
3:A:801:THR:O	3:A:801:THR:HG22	2.20	0.41
4:E:2:ASP:OD1	4:E:3:VAL:N	2.54	0.41
1:V:60:THR:HG22	1:V:60:THR:O	2.19	0.41
1:W:108:THR:HG21	1:Y:233:VAL:HG23	2.03	0.41
1:y:112:PRO:O	1:y:115:SER:OG	2.38	0.41
1:y:121:TYR:OH	1:y:141:LEU:O	2.32	0.41
2:2:230:THR:HG22	2:2:231:ARG:N	2.36	0.41
2:2:538:ILE:O	2:2:539:ASP:HB2	2.20	0.41
2:3:42:GLN:OE1	2:4:328:PHE:CD1	2.74	0.41
2:4:265:MET:HE1	1:w:234:ASN:OD1	2.21	0.41
3:A:666:ASP:OD1	3:A:666:ASP:N	2.53	0.41
4:H:188:ILE:HD13	4:H:212:VAL:HG21	2.01	0.41
4:N:74:ASP:OD2	4:O:76:ASN:ND2	2.46	0.41
1:T:101:THR:HG22	1:V:205:ILE:HG22	2.02	0.41
4:f:129:PHE:O	4:f:130:ASP:C	2.64	0.41
4:h:344:ALA:O	4:h:348:SER:OG	2.33	0.41
4:j:17:LYS:HB3	4:j:27:VAL:HG12	2.02	0.41
4:j:68:THR:HG22	4:j:69:THR:N	2.32	0.41
2:2:386:SER:HA	2:2:396:VAL:HG12	2.02	0.41
2:4:662:GLU:OE1	2:4:776:LEU:HD21	2.21	0.41
2:4:733:ASN:OD1	2:4:733:ASN:N	2.53	0.41
4:O:172:ALA:HB3	4:O:174:ASP:OD1	2.21	0.41
1:Y:139:VAL:CG1	1:Y:261:ILE:HD12	2.51	0.41
4:k:261:VAL:HG23	4:k:290:LEU:HD23	2.03	0.41
1:w:95:ASP:OD1	1:w:96:ASN:N	2.54	0.41
2:3:81:TRP:CD1	2:3:166:ALA:HB1	2.56	0.41
2:3:167:VAL:HG22	2:3:168:MET:N	2.36	0.41
2:3:657:PRO:O	2:3:658:ASP:CG	2.64	0.41
2:3:734:TYR:CZ	4:C:363:PRO:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:245:THR:OG1	4:H:246:THR:N	2.54	0.41
4:L:38:ILE:HD11	4:L:84:THR:HG21	2.02	0.41
4:O:2:ASP:OD1	4:O:3:VAL:N	2.54	0.41
4:f:11:LEU:HD21	4:f:88:PHE:CB	2.51	0.41
2:4:530:MET:CE	2:4:641:LEU:HD23	2.52	0.40
2:4:598:ILE:O	2:4:599:THR:HB	2.21	0.40
3:A:624:ARG:HD2	3:A:655:ARG:HB3	2.02	0.40
4:C:217:VAL:HG22	4:C:286:ASP:HB3	2.03	0.40
4:D:9:LYS:NZ	4:D:132:SER:OG	2.47	0.40
4:D:48:THR:HG21	4:D:94:ASN:HB3	2.02	0.40
1:P:184:TRP:CZ3	1:P:237:LEU:HD21	2.55	0.40
1:Q:198:LEU:HD22	1:Q:202:THR:O	2.21	0.40
4:f:23:LEU:HD11	4:h:36:GLN:HB2	2.03	0.40
4:j:220:THR:HG22	4:j:220:THR:O	2.21	0.40
2:4:727:LEU:HD11	2:4:745:LEU:HD22	2.03	0.40
3:B:778:VAL:HG22	3:B:809:ILE:HG23	2.02	0.40
4:E:172:ALA:HB3	4:E:174:ASP:OD2	2.20	0.40
4:J:14:ALA:HA	4:J:30:LEU:HD21	2.03	0.40
4:K:129:PHE:O	4:K:130:ASP:C	2.64	0.40
4:K:273:TYR:OH	4:K:281:ILE:O	2.36	0.40
4:O:265:LEU:HD22	4:O:284:ASN:ND2	2.36	0.40
1:W:51:GLN:O	1:W:55:ILE:N	2.54	0.40
1:X:112:PRO:O	1:X:115:SER:OG	2.36	0.40
4:k:93:ASP:OD1	4:k:392:ARG:NE	2.46	0.40
1:l:53:TYR:O	1:l:55:ILE:N	2.52	0.40
3:B:718:GLN:HA	3:B:827:THR:HG22	2.04	0.40
4:K:93:ASP:OD1	4:K:392:ARG:NE	2.49	0.40
4:L:2:ASP:OD1	4:L:3:VAL:N	2.54	0.40
4:M:373:ASN:O	4:M:375:SER:N	2.54	0.40
4:O:22:THR:HG22	4:O:73:LEU:HD12	2.03	0.40
1:T:82:CYS:N	1:T:135:CYS:SG	2.94	0.40
1:Y:180:GLU:O	1:Y:183:LYS:NZ	2.53	0.40
4:j:209:GLU:OE1	4:j:291:SER:OG	2.34	0.40
4:k:180:MET:HE1	4:k:238:ILE:CD1	2.51	0.40
1:v:130:ASP:HA	1:v:187:MET:HE3	2.02	0.40
4:F:34:PHE:CE2	4:F:38:ILE:HD11	2.57	0.40
4:I:2:ASP:OD1	4:I:3:VAL:N	2.54	0.40
4:J:157:ILE:HD12	4:J:371:ILE:HD11	2.04	0.40
1:Q:185:ILE:HD12	1:Q:226:ILE:HG12	2.03	0.40
4:k:2:ASP:OD1	4:k:3:VAL:N	2.55	0.40
4:k:38:ILE:HD11	4:k:84:THR:HG21	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:263:VAL:HG12	1:x:289:TRP:CD1	2.56	0.40
1:0:316:SER:O	1:0:317:LEU:HG	2.20	0.40
3:B:277:ILE:HD11	3:B:299:LEU:HD11	2.03	0.40
4:G:31:ILE:HD12	4:G:66:LEU:HD23	2.03	0.40
4:K:2:ASP:OD1	4:K:3:VAL:N	2.55	0.40
1:Q:265:GLY:O	1:Q:286:ARG:NH1	2.54	0.40
1:Y:263:VAL:HG12	1:Y:289:TRP:CD1	2.56	0.40
4:g:225:LEU:CD2	4:g:261:VAL:HG21	2.51	0.40
1:v:112:PRO:O	1:v:115:SER:OG	2.38	0.40
1:x:180:GLU:O	1:x:183:LYS:NZ	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	0	274/326 (84%)	266 (97%)	8 (3%)	0	100	100
1	1	262/326 (80%)	254 (97%)	8 (3%)	0	100	100
1	P	262/326 (80%)	254 (97%)	8 (3%)	0	100	100
1	Q	269/326 (82%)	264 (98%)	5 (2%)	0	100	100
1	R	262/326 (80%)	256 (98%)	6 (2%)	0	100	100
1	S	262/326 (80%)	252 (96%)	10 (4%)	0	100	100
1	T	274/326 (84%)	272 (99%)	2 (1%)	0	100	100
1	U	274/326 (84%)	262 (96%)	12 (4%)	0	100	100
1	V	274/326 (84%)	263 (96%)	11 (4%)	0	100	100
1	W	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	X	269/326 (82%)	262 (97%)	7 (3%)	0	100	100
1	Y	274/326 (84%)	264 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	274/326 (84%)	263 (96%)	11 (4%)	0	100	100
1	t	274/326 (84%)	269 (98%)	5 (2%)	0	100	100
1	u	274/326 (84%)	265 (97%)	9 (3%)	0	100	100
1	v	274/326 (84%)	263 (96%)	11 (4%)	0	100	100
1	w	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	x	269/326 (82%)	264 (98%)	5 (2%)	0	100	100
1	y	274/326 (84%)	269 (98%)	5 (2%)	0	100	100
2	2	744/776 (96%)	681 (92%)	59 (8%)	4 (0%)	24	51
2	3	744/776 (96%)	689 (93%)	53 (7%)	2 (0%)	36	62
2	4	538/776 (69%)	500 (93%)	38 (7%)	0	100	100
3	A	777/887 (88%)	766 (99%)	11 (1%)	0	100	100
3	B	797/887 (90%)	782 (98%)	15 (2%)	0	100	100
4	C	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
4	D	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
4	E	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
4	F	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
4	G	394/397 (99%)	380 (96%)	14 (4%)	0	100	100
4	H	394/397 (99%)	385 (98%)	9 (2%)	0	100	100
4	I	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
4	J	394/397 (99%)	385 (98%)	9 (2%)	0	100	100
4	K	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	L	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
4	M	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
4	N	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
4	O	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	f	394/397 (99%)	381 (97%)	13 (3%)	0	100	100
4	g	394/397 (99%)	382 (97%)	12 (3%)	0	100	100
4	h	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
4	i	394/397 (99%)	385 (98%)	9 (2%)	0	100	100
4	j	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
4	k	394/397 (99%)	383 (97%)	11 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	16230/17839 (91%)	15724 (97%)	500 (3%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	64	VAL
2	2	482	THR
2	2	483	PRO
2	3	64	VAL
2	2	486	ASN
2	3	51	GLY

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	0	247/295 (84%)	245 (99%)	2 (1%)	73	89
1	1	237/295 (80%)	237 (100%)	0	100	100
1	P	237/295 (80%)	236 (100%)	1 (0%)	84	94
1	Q	243/295 (82%)	240 (99%)	3 (1%)	63	84
1	R	238/295 (81%)	238 (100%)	0	100	100
1	S	237/295 (80%)	236 (100%)	1 (0%)	84	94
1	T	247/295 (84%)	247 (100%)	0	100	100
1	U	247/295 (84%)	245 (99%)	2 (1%)	73	89
1	V	247/295 (84%)	246 (100%)	1 (0%)	84	94
1	W	247/295 (84%)	247 (100%)	0	100	100
1	X	243/295 (82%)	242 (100%)	1 (0%)	84	94
1	Y	247/295 (84%)	247 (100%)	0	100	100
1	Z	247/295 (84%)	246 (100%)	1 (0%)	84	94
1	t	247/295 (84%)	247 (100%)	0	100	100
1	u	247/295 (84%)	247 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v	247/295 (84%)	247 (100%)	0	100	100
1	w	247/295 (84%)	247 (100%)	0	100	100
1	x	243/295 (82%)	243 (100%)	0	100	100
1	y	247/295 (84%)	247 (100%)	0	100	100
2	2	664/688 (96%)	659 (99%)	5 (1%)	73	89
2	3	664/688 (96%)	663 (100%)	1 (0%)	87	96
2	4	481/688 (70%)	469 (98%)	12 (2%)	42	72
3	A	715/818 (87%)	715 (100%)	0	100	100
3	B	735/818 (90%)	734 (100%)	1 (0%)	88	97
4	C	349/349 (100%)	347 (99%)	2 (1%)	78	92
4	D	348/349 (100%)	345 (99%)	3 (1%)	70	88
4	E	348/349 (100%)	347 (100%)	1 (0%)	86	95
4	F	348/349 (100%)	347 (100%)	1 (0%)	86	95
4	G	348/349 (100%)	348 (100%)	0	100	100
4	H	348/349 (100%)	347 (100%)	1 (0%)	86	95
4	I	348/349 (100%)	347 (100%)	1 (0%)	86	95
4	J	348/349 (100%)	348 (100%)	0	100	100
4	K	348/349 (100%)	347 (100%)	1 (0%)	86	95
4	L	348/349 (100%)	347 (100%)	1 (0%)	86	95
4	M	348/349 (100%)	346 (99%)	2 (1%)	78	92
4	N	348/349 (100%)	348 (100%)	0	100	100
4	O	348/349 (100%)	348 (100%)	0	100	100
4	f	348/349 (100%)	348 (100%)	0	100	100
4	g	348/349 (100%)	347 (100%)	1 (0%)	86	95
4	h	348/349 (100%)	346 (99%)	2 (1%)	78	92
4	i	348/349 (100%)	347 (100%)	1 (0%)	86	95
4	j	348/349 (100%)	345 (99%)	3 (1%)	70	88
4	k	348/349 (100%)	347 (100%)	1 (0%)	86	95
All	All	14514/15936 (91%)	14462 (100%)	52 (0%)	81	94

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	83	LEU
1	0	92	GLU
2	2	106	ILE
2	2	224	LEU
2	2	276	LYS
2	2	697	THR
2	2	774	CYS
2	3	176	THR
2	4	15	THR
2	4	279	SER
2	4	280	SER
2	4	318	CYS
2	4	464	VAL
2	4	505	PHE
2	4	616	SER
2	4	621	LEU
2	4	624	MET
2	4	677	ASN
2	4	712	VAL
2	4	762	ILE
3	B	202	ASP
4	C	129	PHE
4	C	170	GLN
4	D	30	LEU
4	D	170	GLN
4	D	179	THR
4	E	246	THR
4	F	156	ASN
4	H	170	GLN
4	I	30	LEU
4	K	170	GLN
4	L	170	GLN
4	M	170	GLN
4	M	179	THR
1	P	227	THR
1	Q	124	ILE
1	Q	172	LEU
1	Q	239	VAL
1	S	237	LEU
1	U	189	SER
1	U	210	THR
1	V	261	ILE
1	X	189	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Z	187	MET
4	g	133	SER
4	h	112	GLN
4	h	170	GLN
4	i	170	GLN
4	j	20	GLU
4	j	170	GLN
4	j	179	THR
4	k	170	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	104	GLN
1	0	234	ASN
1	0	305	GLN
1	1	262	GLN
2	2	98	ASN
2	2	251	ASN
2	2	364	ASN
2	2	405	HIS
2	2	414	GLN
2	3	677	ASN
2	4	266	GLN
2	4	321	ASN
2	4	477	ASN
2	4	757	ASN
3	A	257	HIS
3	A	266	HIS
3	A	316	ASN
3	A	460	GLN
3	A	484	ASN
3	A	503	ASN
3	A	512	GLN
3	A	708	GLN
3	A	792	GLN
3	A	835	GLN
3	A	885	ASN
3	B	137	GLN
3	B	175	ASN
3	B	257	HIS
3	B	279	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	407	ASN
3	B	657	GLN
3	B	733	ASN
3	B	852	ASN
3	B	885	ASN
4	C	53	ASN
4	C	140	ASN
4	C	142	GLN
4	C	206	GLN
4	C	210	HIS
4	D	36	GLN
4	D	189	GLN
4	D	206	GLN
4	D	266	ASN
4	D	345	ASN
4	E	36	GLN
4	E	47	GLN
4	E	58	ASN
4	E	72	ASN
4	E	146	GLN
4	E	167	ASN
4	E	257	ASN
4	F	140	ASN
4	F	142	GLN
4	F	167	ASN
4	F	250	ASN
4	F	345	ASN
4	G	36	GLN
4	G	47	GLN
4	G	58	ASN
4	G	128	ASN
4	G	140	ASN
4	G	206	GLN
4	G	210	HIS
4	H	44	ASN
4	H	47	GLN
4	H	72	ASN
4	H	128	ASN
4	H	170	GLN
4	H	200	ASN
4	H	204	ASN
4	I	32	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	I	44	ASN
4	I	128	ASN
4	I	131	ASN
4	I	142	GLN
4	I	170	GLN
4	I	204	ASN
4	I	206	GLN
4	J	36	GLN
4	J	44	ASN
4	J	128	ASN
4	J	140	ASN
4	J	206	GLN
4	K	32	GLN
4	K	72	ASN
4	K	140	ASN
4	K	170	GLN
4	K	204	ASN
4	K	206	GLN
4	K	299	ASN
4	L	32	GLN
4	L	105	GLN
4	L	140	ASN
4	L	200	ASN
4	L	204	ASN
4	L	206	GLN
4	M	32	GLN
4	M	140	ASN
4	M	204	ASN
4	M	206	GLN
4	M	257	ASN
4	M	258	ASN
4	N	170	GLN
4	N	183	ASN
4	N	204	ASN
4	O	44	ASN
4	O	140	ASN
4	O	206	GLN
4	O	250	ASN
1	P	72	GLN
1	P	234	ASN
1	Q	149	GLN
1	R	288	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	308	GLN
1	S	280	GLN
1	S	305	GLN
1	T	72	GLN
1	T	138	ASN
1	T	176	GLN
1	T	234	ASN
1	T	308	GLN
1	U	72	GLN
1	U	161	ASN
1	U	262	GLN
1	U	280	GLN
1	U	305	GLN
1	V	176	GLN
1	W	104	GLN
1	W	305	GLN
1	X	304	ASN
1	Y	72	GLN
1	Y	176	GLN
1	Y	305	GLN
1	Z	288	ASN
1	Z	305	GLN
4	f	36	GLN
4	f	140	ASN
4	f	207	GLN
4	f	258	ASN
4	g	36	GLN
4	g	47	GLN
4	g	58	ASN
4	g	128	ASN
4	g	140	ASN
4	g	206	GLN
4	g	239	ASN
4	h	44	ASN
4	h	72	ASN
4	h	204	ASN
4	i	32	GLN
4	i	33	GLN
4	i	128	ASN
4	i	131	ASN
4	i	142	GLN
4	i	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	i	170	GLN
4	i	206	GLN
4	j	36	GLN
4	j	44	ASN
4	j	128	ASN
4	j	140	ASN
4	j	170	GLN
4	j	206	GLN
4	j	257	ASN
4	k	32	GLN
4	k	72	ASN
4	k	107	ASN
4	k	128	ASN
4	k	140	ASN
4	k	206	GLN
1	t	72	GLN
1	t	138	ASN
1	t	161	ASN
1	t	166	ASN
1	t	305	GLN
1	t	308	GLN
1	u	161	ASN
1	u	280	GLN
1	u	305	GLN
1	v	176	GLN
1	v	182	ASN
1	v	235	HIS
1	w	104	GLN
1	w	305	GLN
1	x	262	GLN
1	x	305	GLN
1	y	72	GLN
1	y	176	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

19 non-standard protein/DNA/RNA residues are modelled in this entry.

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
4	FME	g	1	4	8,9,10	0.37	0	8,9,11	0.96	1 (12%)
4	FME	M	1	4	8,9,10	0.37	0	8,9,11	0.95	1 (12%)
4	FME	N	1	4	8,9,10	0.36	0	8,9,11	1.02	1 (12%)
4	FME	k	1	4	8,9,10	0.37	0	8,9,11	1.00	1 (12%)
4	FME	H	1	4	8,9,10	0.38	0	8,9,11	1.00	1 (12%)
4	FME	J	1	4	8,9,10	0.37	0	8,9,11	0.99	1 (12%)
4	FME	K	1	4	8,9,10	0.37	0	8,9,11	1.02	1 (12%)
4	FME	f	1	4	8,9,10	0.37	0	8,9,11	1.01	1 (12%)
4	FME	E	1	4	8,9,10	0.37	0	8,9,11	1.01	1 (12%)
4	FME	I	1	4	8,9,10	0.38	0	8,9,11	0.95	1 (12%)
4	FME	F	1	4	8,9,10	0.37	0	8,9,11	1.02	1 (12%)
4	FME	j	1	4	8,9,10	0.38	0	8,9,11	0.99	1 (12%)
4	FME	L	1	4	8,9,10	0.36	0	8,9,11	1.04	1 (12%)
4	FME	D	1	4	8,9,10	0.36	0	8,9,11	1.07	1 (12%)
4	FME	O	1	4	8,9,10	0.37	0	8,9,11	1.01	1 (12%)
4	FME	G	1	4	8,9,10	0.36	0	8,9,11	1.02	1 (12%)
4	FME	C	1	4	8,9,10	0.37	0	8,9,11	1.03	1 (12%)
4	FME	h	1	4	8,9,10	0.37	0	8,9,11	0.99	1 (12%)
4	FME	i	1	4	8,9,10	0.38	0	8,9,11	0.96	1 (12%)

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
4	FME	g	1	4	-	2/7/9/11	-
4	FME	M	1	4	-	2/7/9/11	-
4	FME	N	1	4	-	1/7/9/11	-
4	FME	k	1	4	-	1/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	H	1	4	-	1/7/9/11	-
4	FME	J	1	4	-	1/7/9/11	-
4	FME	K	1	4	-	1/7/9/11	-
4	FME	f	1	4	-	1/7/9/11	-
4	FME	E	1	4	-	2/7/9/11	-
4	FME	I	1	4	-	2/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	j	1	4	-	2/7/9/11	-
4	FME	L	1	4	-	1/7/9/11	-
4	FME	D	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	G	1	4	-	1/7/9/11	-
4	FME	C	1	4	-	1/7/9/11	-
4	FME	h	1	4	-	1/7/9/11	-
4	FME	i	1	4	-	1/7/9/11	-

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	FME	CA-N-CN	2.46	126.60	122.82
4	C	1	FME	CA-N-CN	2.32	126.38	122.82
4	L	1	FME	CA-N-CN	2.30	126.37	122.82
4	N	1	FME	CA-N-CN	2.29	126.34	122.82
4	K	1	FME	CA-N-CN	2.28	126.32	122.82
4	G	1	FME	CA-N-CN	2.26	126.30	122.82
4	E	1	FME	CA-N-CN	2.26	126.30	122.82
4	O	1	FME	CA-N-CN	2.26	126.30	122.82
4	F	1	FME	CA-N-CN	2.25	126.28	122.82
4	H	1	FME	CA-N-CN	2.22	126.24	122.82
4	f	1	FME	CA-N-CN	2.22	126.23	122.82
4	k	1	FME	CA-N-CN	2.19	126.19	122.82
4	j	1	FME	CA-N-CN	2.18	126.18	122.82
4	h	1	FME	CA-N-CN	2.17	126.16	122.82
4	J	1	FME	CA-N-CN	2.16	126.15	122.82
4	i	1	FME	CA-N-CN	2.10	126.06	122.82
4	g	1	FME	CA-N-CN	2.09	126.03	122.82
4	I	1	FME	CA-N-CN	2.06	125.99	122.82
4	M	1	FME	CA-N-CN	2.05	125.97	122.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	FME	O1-CN-N-CA
4	D	1	FME	O1-CN-N-CA
4	E	1	FME	O1-CN-N-CA
4	F	1	FME	O1-CN-N-CA
4	G	1	FME	O1-CN-N-CA
4	H	1	FME	O1-CN-N-CA
4	I	1	FME	O1-CN-N-CA
4	J	1	FME	O1-CN-N-CA
4	K	1	FME	O1-CN-N-CA
4	L	1	FME	O1-CN-N-CA
4	M	1	FME	O1-CN-N-CA
4	N	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA
4	f	1	FME	O1-CN-N-CA
4	g	1	FME	O1-CN-N-CA
4	h	1	FME	O1-CN-N-CA
4	i	1	FME	O1-CN-N-CA
4	j	1	FME	O1-CN-N-CA
4	k	1	FME	O1-CN-N-CA
4	E	1	FME	N-CA-CB-CG
4	M	1	FME	N-CA-CB-CG
4	j	1	FME	N-CA-CB-CG
4	I	1	FME	N-CA-CB-CG
4	g	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

5 monosaccharides are modelled in this entry.

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
5	NAG	a	1	5,1	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
5	NAG	a	2	5	14,14,15	0.73	0	17,19,21	0.81	0
5	BMA	a	3	5	11,11,12	0.80	0	15,15,17	1.64	1 (6%)
5	MAN	a	4	5	11,11,12	0.75	0	15,15,17	1.01	1 (6%)
5	MAN	a	5	5	11,11,12	0.79	1 (9%)	15,15,17	1.11	1 (6%)

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
5	NAG	a	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	a	2	5	-	0/6/23/26	0/1/1/1
5	BMA	a	3	5	-	2/2/19/22	0/1/1/1
5	MAN	a	4	5	-	1/2/19/22	0/1/1/1
5	MAN	a	5	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	5	MAN	O5-C1	-2.00	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	3	BMA	C1-O5-C5	4.88	118.73	112.19
5	a	5	MAN	C1-O5-C5	2.78	115.91	112.19
5	a	4	MAN	C1-O5-C5	2.64	115.73	112.19
5	a	1	NAG	O5-C1-C2	-2.45	107.50	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	1	NAG	C1-C2-N2-C7
5	a	1	NAG	O5-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
5	a	3	BMA	C4-C5-C6-O6
5	a	3	BMA	O5-C5-C6-O6

Continued on next page...

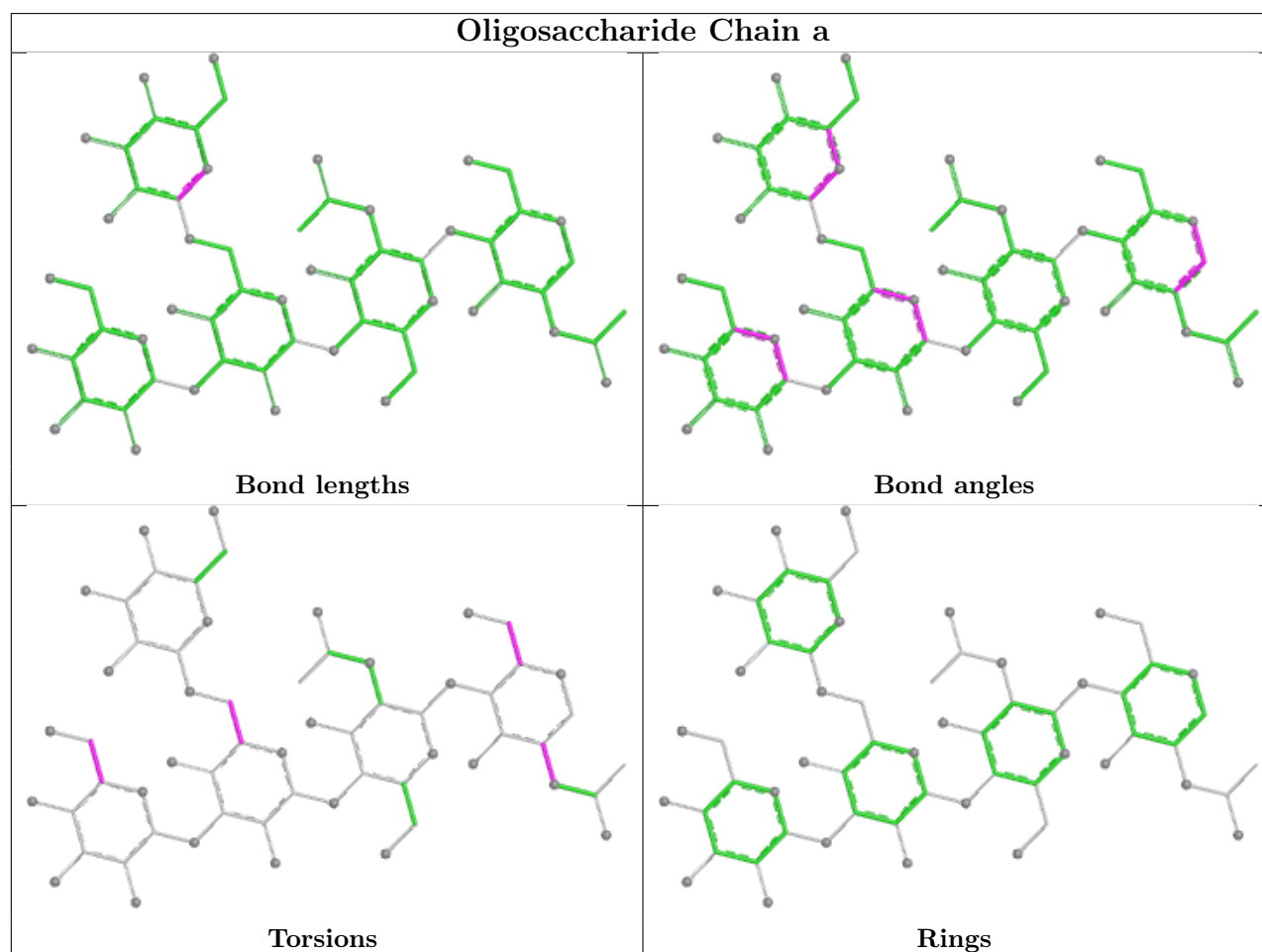
Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	a	1	NAG	C3-C2-N2-C7
5	a	4	MAN	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 126 ligands modelled in this entry, 109 are monoatomic - leaving 17 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	$\# Z > 2$
6	NAG	x	401	1	14,14,15	0.69	0	17,19,21	0.87	0
6	NAG	y	401	1	14,14,15	0.70	0	17,19,21	0.94	0
6	NAG	0	401	1	14,14,15	0.67	0	17,19,21	0.96	1 (5%)
6	NAG	u	401	1	14,14,15	0.71	0	17,19,21	1.36	2 (11%)
6	NAG	w	401	1	14,14,15	0.73	0	17,19,21	1.04	0
6	NAG	S	401	1	14,14,15	0.70	0	17,19,21	0.91	0
6	NAG	Q	401	1	14,14,15	0.71	0	17,19,21	0.88	0
6	NAG	T	401	1	14,14,15	0.71	0	17,19,21	0.91	0
6	NAG	Z	401	1	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
6	NAG	V	401	1	14,14,15	0.72	0	17,19,21	1.05	1 (5%)
6	NAG	v	401	1	14,14,15	0.71	0	17,19,21	0.97	1 (5%)
6	NAG	U	401	1	14,14,15	0.71	0	17,19,21	0.96	0
6	NAG	t	401	1	14,14,15	0.72	0	17,19,21	0.87	0
6	NAG	Y	401	1	14,14,15	0.68	0	17,19,21	1.09	1 (5%)
6	NAG	X	401	1	14,14,15	0.68	0	17,19,21	0.99	1 (5%)
6	NAG	P	401	1	14,14,15	0.72	0	17,19,21	1.02	1 (5%)
6	NAG	1	401	1	14,14,15	0.71	0	17,19,21	0.86	0

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
6	NAG	x	401	1	-	4/6/23/26	0/1/1/1
6	NAG	y	401	1	-	2/6/23/26	0/1/1/1
6	NAG	0	401	1	-	2/6/23/26	0/1/1/1
6	NAG	u	401	1	-	3/6/23/26	0/1/1/1
6	NAG	w	401	1	-	4/6/23/26	0/1/1/1
6	NAG	S	401	1	-	4/6/23/26	0/1/1/1
6	NAG	Q	401	1	-	4/6/23/26	0/1/1/1
6	NAG	T	401	1	-	2/6/23/26	0/1/1/1
6	NAG	Z	401	1	-	4/6/23/26	0/1/1/1
6	NAG	V	401	1	-	4/6/23/26	0/1/1/1
6	NAG	v	401	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	U	401	1	-	2/6/23/26	0/1/1/1
6	NAG	t	401	1	-	4/6/23/26	0/1/1/1
6	NAG	Y	401	1	-	2/6/23/26	0/1/1/1
6	NAG	X	401	1	-	3/6/23/26	0/1/1/1
6	NAG	P	401	1	-	4/6/23/26	0/1/1/1
6	NAG	1	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	u	401	NAG	C2-N2-C7	3.51	127.60	122.90
6	P	401	NAG	O5-C1-C2	-2.56	107.33	111.29
6	u	401	NAG	O5-C1-C2	-2.55	107.34	111.29
6	V	401	NAG	O5-C1-C2	-2.29	107.75	111.29
6	X	401	NAG	O5-C1-C2	-2.24	107.83	111.29
6	Y	401	NAG	C2-N2-C7	2.16	125.79	122.90
6	0	401	NAG	O5-C1-C2	-2.11	108.03	111.29
6	v	401	NAG	O5-C1-C2	-2.03	108.15	111.29
6	Z	401	NAG	O5-C1-C2	-2.02	108.17	111.29

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	0	401	NAG	C1-C2-N2-C7
6	Y	401	NAG	C1-C2-N2-C7
6	u	401	NAG	C3-C2-N2-C7
6	u	401	NAG	O5-C5-C6-O6
6	P	401	NAG	O5-C5-C6-O6
6	u	401	NAG	C4-C5-C6-O6
6	P	401	NAG	C4-C5-C6-O6
6	t	401	NAG	O5-C5-C6-O6
6	x	401	NAG	O5-C5-C6-O6
6	t	401	NAG	C4-C5-C6-O6
6	w	401	NAG	O5-C5-C6-O6
6	w	401	NAG	C4-C5-C6-O6
6	x	401	NAG	C4-C5-C6-O6
6	Q	401	NAG	C4-C5-C6-O6
6	V	401	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	Q	401	NAG	O5-C5-C6-O6
6	Z	401	NAG	C4-C5-C6-O6
6	V	401	NAG	O5-C5-C6-O6
6	1	401	NAG	C1-C2-N2-C7
6	P	401	NAG	C1-C2-N2-C7
6	Q	401	NAG	C1-C2-N2-C7
6	S	401	NAG	C1-C2-N2-C7
6	U	401	NAG	C1-C2-N2-C7
6	V	401	NAG	C1-C2-N2-C7
6	X	401	NAG	C1-C2-N2-C7
6	Z	401	NAG	C1-C2-N2-C7
6	t	401	NAG	C1-C2-N2-C7
6	v	401	NAG	C1-C2-N2-C7
6	x	401	NAG	C1-C2-N2-C7
6	y	401	NAG	C1-C2-N2-C7
6	S	401	NAG	C4-C5-C6-O6
6	0	401	NAG	C3-C2-N2-C7
6	1	401	NAG	C3-C2-N2-C7
6	P	401	NAG	C3-C2-N2-C7
6	Q	401	NAG	C3-C2-N2-C7
6	T	401	NAG	C3-C2-N2-C7
6	U	401	NAG	C3-C2-N2-C7
6	Z	401	NAG	C3-C2-N2-C7
6	t	401	NAG	C3-C2-N2-C7
6	v	401	NAG	C3-C2-N2-C7
6	w	401	NAG	C3-C2-N2-C7
6	x	401	NAG	C3-C2-N2-C7
6	Z	401	NAG	O5-C5-C6-O6
6	X	401	NAG	C4-C5-C6-O6
6	T	401	NAG	C1-C2-N2-C7
6	w	401	NAG	C1-C2-N2-C7
6	S	401	NAG	O5-C5-C6-O6
6	S	401	NAG	C3-C2-N2-C7
6	V	401	NAG	C3-C2-N2-C7
6	X	401	NAG	C3-C2-N2-C7
6	Y	401	NAG	C3-C2-N2-C7
6	y	401	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	u	401	NAG	2	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.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45119. 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.