



Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 04:58 AM UTC

PDB ID : 9C1J / pdb_00009c1j
EMDB ID : EMD-45121
Title : Rhesus rotavirus (reversed structure at 2.72 Angstrom resolution)
Authors : Jenni, S.; Herrmann, T.; De Sautu, M.; Harrison, S.C.
Deposited on : 2024-05-29
Resolution : 2.72 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

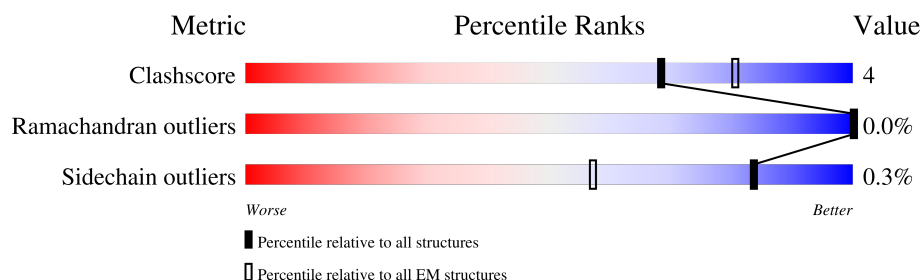
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.72 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	75% 10% 15%
1	1	326	69% 12% 19%
1	P	326	72% 9% 19%
1	Q	326	73% 10% 17%
1	R	326	73% 12% 15%
1	S	326	67% 13% 19%
1	T	326	76% 8% 15%
1	U	326	69% 16% 15%
1	V	326	72% 12% 15%

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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	

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Mol	Chain	Length	Quality of chain
4	M	397	 92%8%
4	N	397	 92%8%
4	O	397	 92%8%
4	f	397	 88%11%
4	g	397	 92%8%
4	h	397	 90%10%
4	i	397	 92%8%
4	j	397	 91%9%
4	k	397	 93%6%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 239272 atoms, of which 118354 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	276	Total	C	H	N	O	S	0	0
			4312	1389	2124	348	435	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
			4312	1389	2124	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		

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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	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		
2	3	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		
2	4	275	Total	C	H	N	O	S	0	0
			4291	1382	2107	368	427	7		

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

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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.

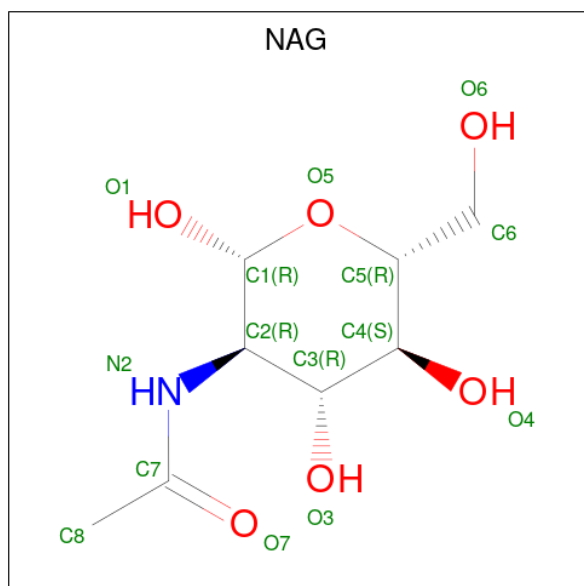
Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	397	Total	C	H	N	O	S	0	0
			6275	2005	3111	551	593	15		
4	D	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	E	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	F	396	Total	C	H	N	O	S	0	0
			6253	1999	3098	549	592	15		
4	G	396	Total	C	H	N	O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

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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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
5	0	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	1	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	P	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	Q	1	Total	C	H	N	O	0
			28	8	14	1	5	

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Mol	Chain	Residues	Atoms					AltConf
5	R	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	S	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	T	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	U	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	V	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	W	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	X	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	Y	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	Z	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	t	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	u	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	v	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	w	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	x	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	y	1	Total	C	H	N	O	0
			28	8	14	1	5	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	0	4	Total	Ca	0
			4	4	
6	1	4	Total	Ca	0
			4	4	
6	P	4	Total	Ca	0
			4	4	
6	Q	4	Total	Ca	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
6	R	4	Total 4	Ca 4	0
6	S	4	Total 4	Ca 4	0
6	T	4	Total 4	Ca 4	0
6	U	4	Total 4	Ca 4	0
6	V	4	Total 4	Ca 4	0
6	W	4	Total 4	Ca 4	0
6	X	4	Total 4	Ca 4	0
6	Y	4	Total 4	Ca 4	0
6	Z	4	Total 4	Ca 4	0
6	t	4	Total 4	Ca 4	0
6	u	4	Total 4	Ca 4	0
6	v	4	Total 4	Ca 4	0
6	w	4	Total 4	Ca 4	0
6	x	4	Total 4	Ca 4	0
6	y	4	Total 4	Ca 4	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	C	2	Total 2	Zn 2	0
7	D	1	Total 1	Zn 1	0
7	E	1	Total 1	Zn 1	0
7	F	2	Total 2	Zn 2	0

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Mol	Chain	Residues	Atoms		AltConf
7	G	1	Total 1	Zn 1	0
7	H	1	Total 1	Zn 1	0
7	I	2	Total 2	Zn 2	0
7	J	1	Total 1	Zn 1	0
7	K	1	Total 1	Zn 1	0
7	L	2	Total 2	Zn 2	0
7	M	1	Total 1	Zn 1	0
7	N	1	Total 1	Zn 1	0
7	O	2	Total 2	Zn 2	0
7	f	2	Total 2	Zn 2	0
7	g	1	Total 1	Zn 1	0
7	h	1	Total 1	Zn 1	0
7	i	2	Total 2	Zn 2	0
7	j	1	Total 1	Zn 1	0
7	k	1	Total 1	Zn 1	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
8	C	1	Total 1	Cl 1	0
8	F	1	Total 1	Cl 1	0
8	J	1	Total 1	Cl 1	0
8	M	1	Total 1	Cl 1	0

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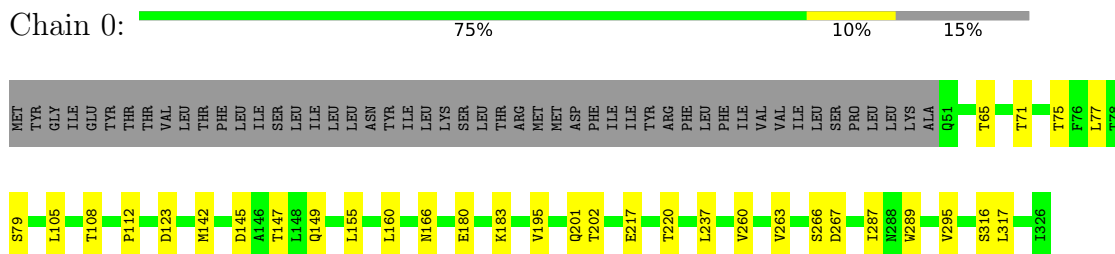
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Mol	Chain	Residues	Atoms		AltConf
8	O	1	Total 1	Cl 1	0
8	f	1	Total 1	Cl 1	0
8	j	1	Total 1	Cl 1	0

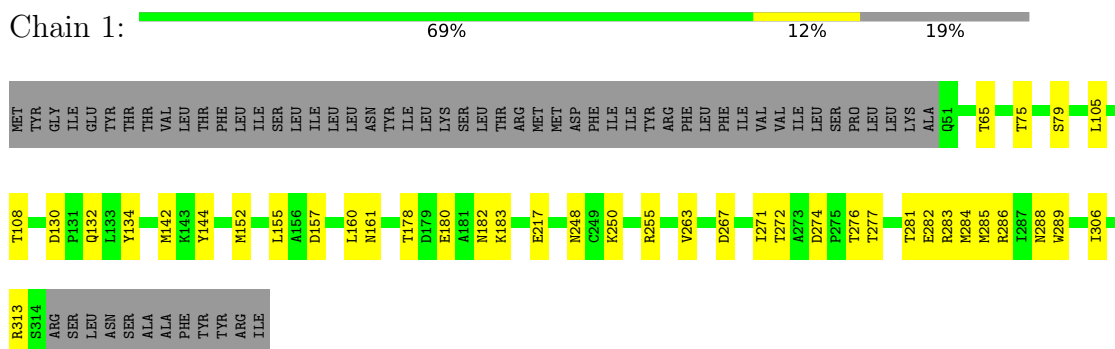
3 Residue-property plots

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

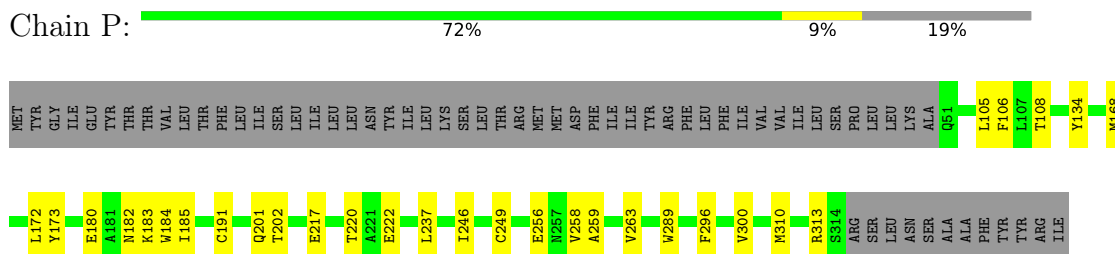
- Molecule 1: Outer capsid glycoprotein VP7



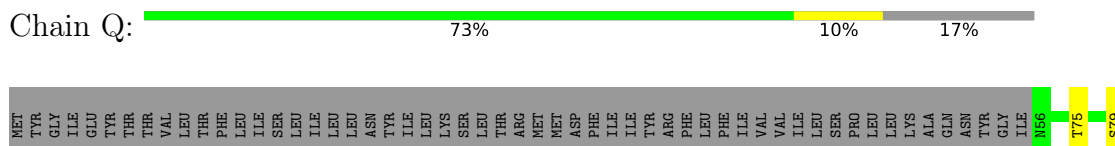
- Molecule 1: Outer capsid glycoprotein VP7



- Molecule 1: Outer capsid glycoprotein VP7



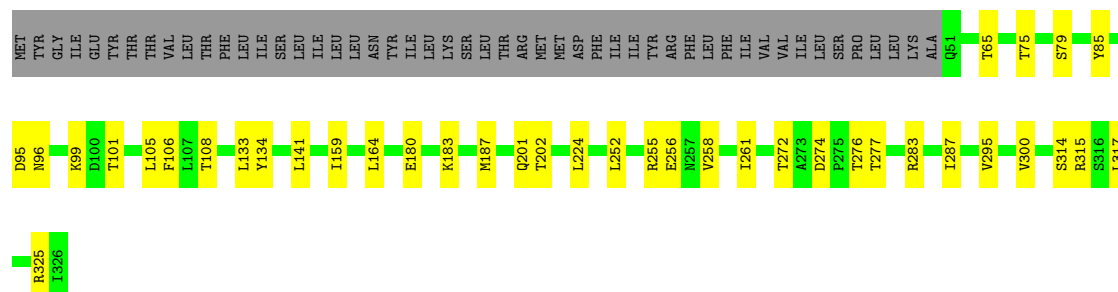
- Molecule 1: Outer capsid glycoprotein VP7





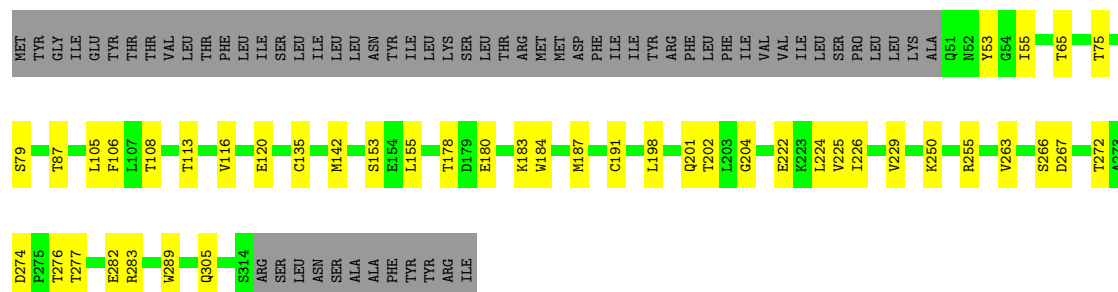
• Molecule 1: Outer capsid glycoprotein VP7

Chain R: 73% 12% 15%



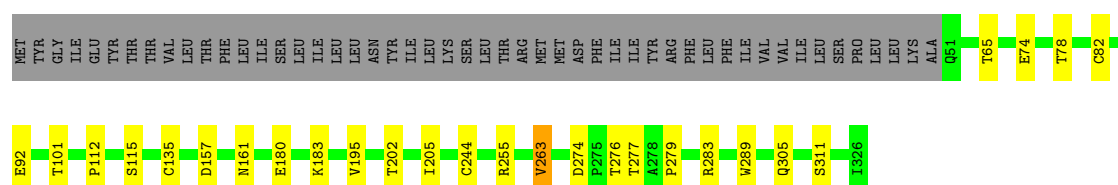
• Molecule 1: Outer capsid glycoprotein VP7

Chain S: 67% 13% 19%



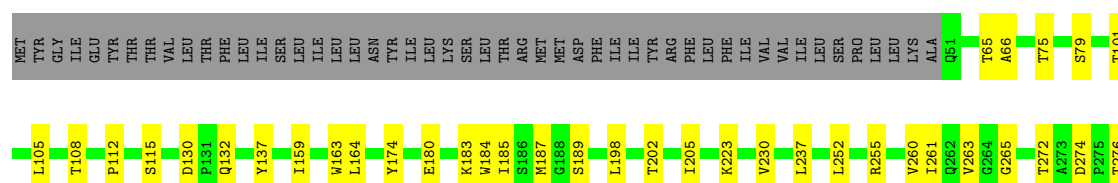
• Molecule 1: Outer capsid glycoprotein VP7

Chain T: 76% 8% 15%



• Molecule 1: Outer capsid glycoprotein VP7

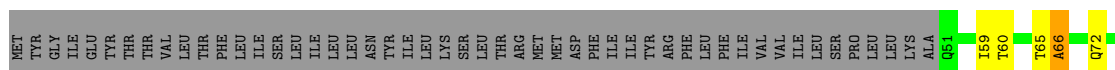
Chain U: 69% 16% 15%





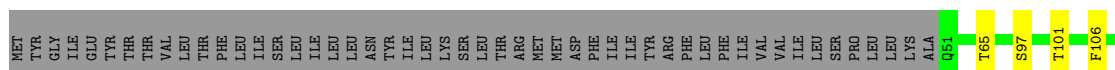
- Molecule 1: Outer capsid glycoprotein VP7

Chain V: 72% 12% 15%



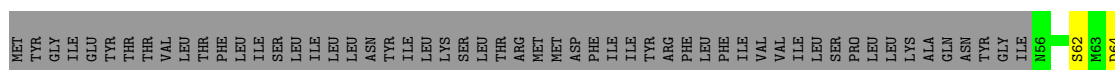
- Molecule 1: Outer capsid glycoprotein VP7

Chain W: 79% 5% 15%



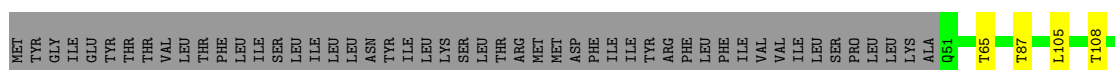
- Molecule 1: Outer capsid glycoprotein VP7

Chain X: 77% 6% 17%



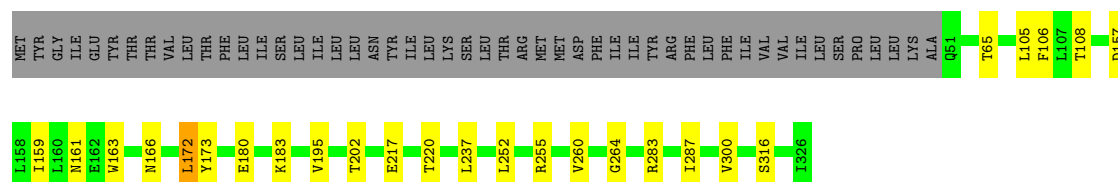
- Molecule 1: Outer capsid glycoprotein VP7

Chain Y: 74% 11% 15%



- Molecule 1: Outer capsid glycoprotein VP7

Chain Z: 77% 8% 15%



• Molecule 1: Outer capsid glycoprotein VP7



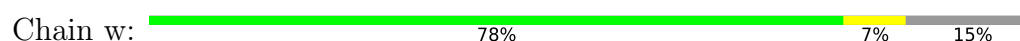
• Molecule 1: Outer capsid glycoprotein VP7



• Molecule 1: Outer capsid glycoprotein VP7

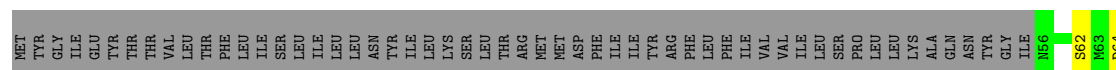


• Molecule 1: Outer capsid glycoprotein VP7

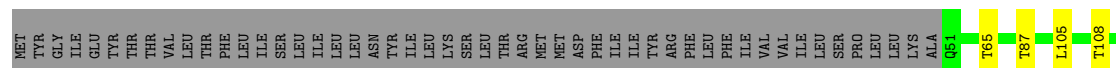
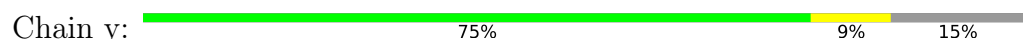




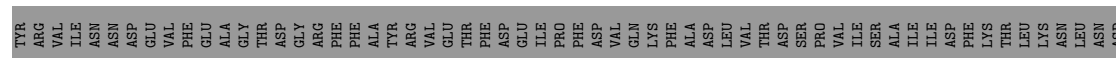
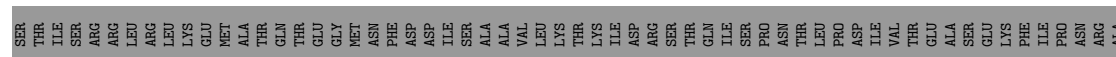
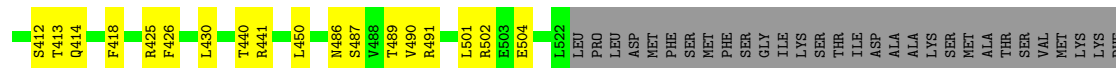
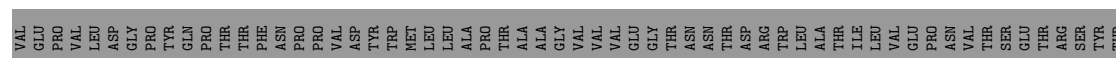
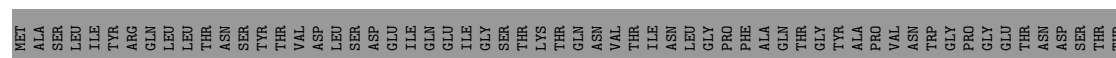
• Molecule 1: Outer capsid glycoprotein VP7

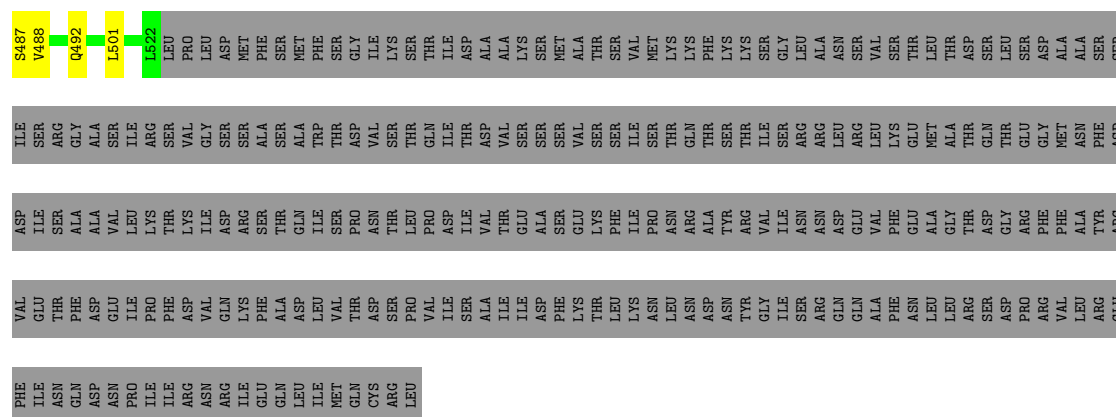


• Molecule 1: Outer capsid glycoprotein VP7

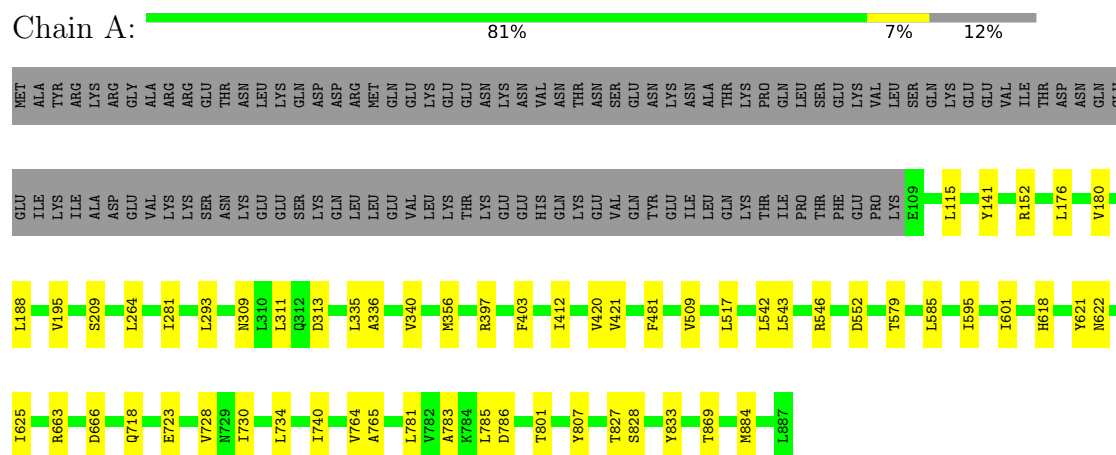


• Molecule 2: Outer capsid protein VP4

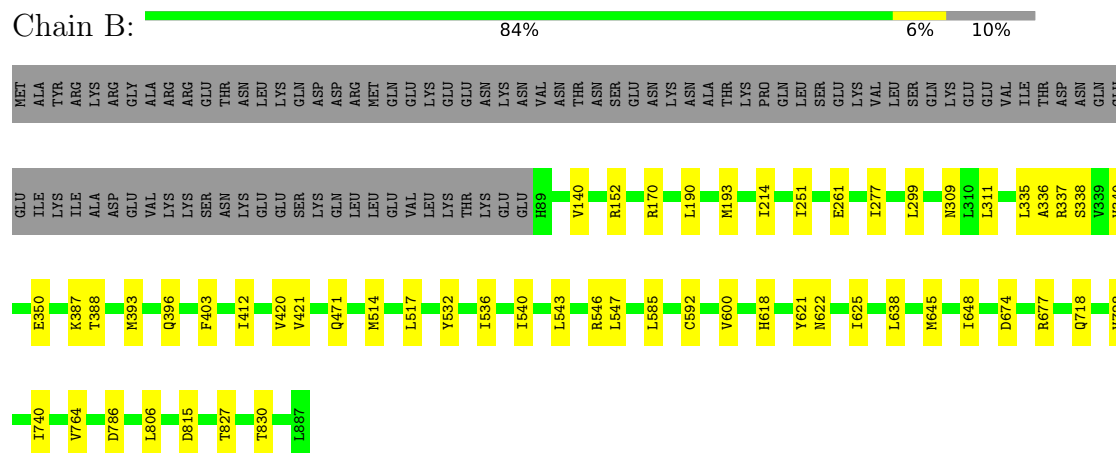




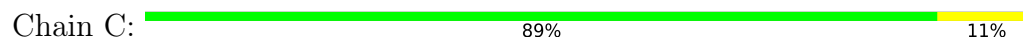
- Molecule 3: Inner capsid protein VP2

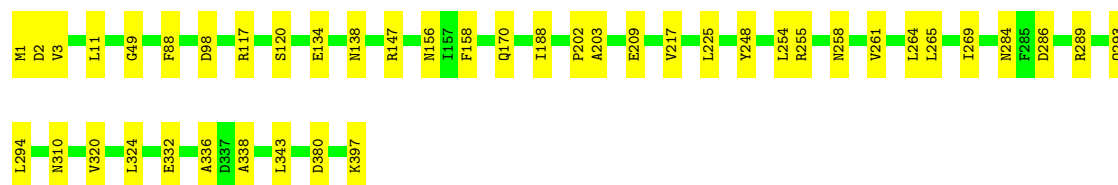


- Molecule 3: Inner capsid protein VP2



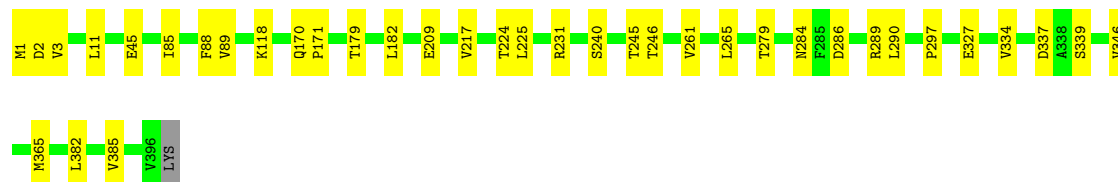
- Molecule 4: Intermediate capsid protein VP6





- Molecule 4: Intermediate capsid protein VP6

Chain D: 90% 9%



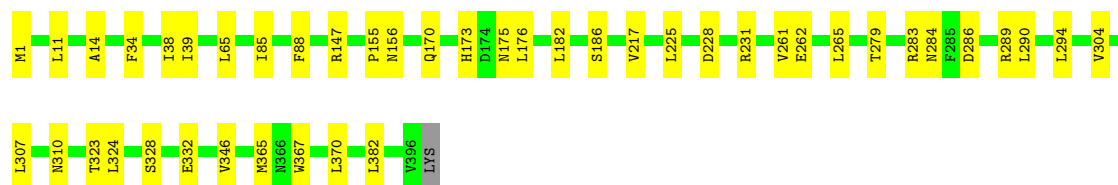
- Molecule 4: Intermediate capsid protein VP6

Chain E: 89% 11%



- Molecule 4: Intermediate capsid protein VP6

Chain F: 89% 11%



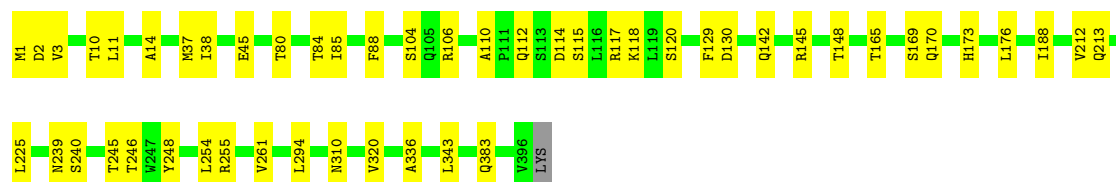
- Molecule 4: Intermediate capsid protein VP6

Chain G: 91% 9%



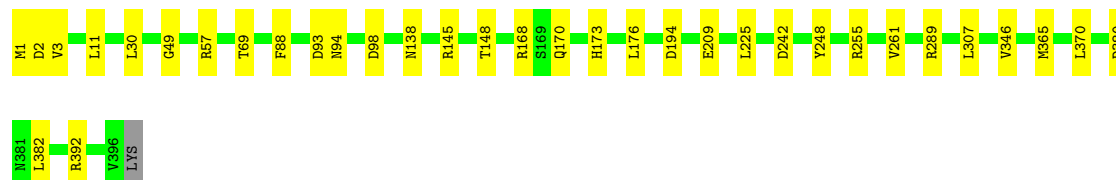
- Molecule 4: Intermediate capsid protein VP6

Chain H: 87% 13%



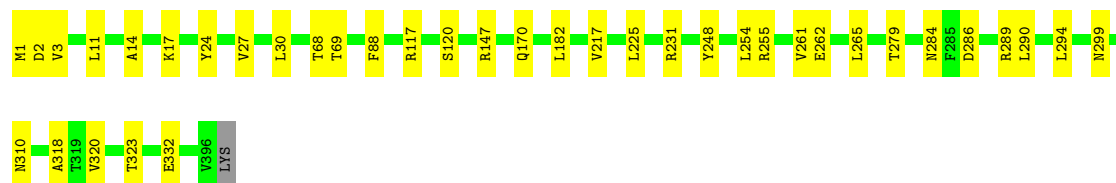
• Molecule 4: Intermediate capsid protein VP6

Chain I: 91% 9%



• Molecule 4: Intermediate capsid protein VP6

Chain J: 90% 10%



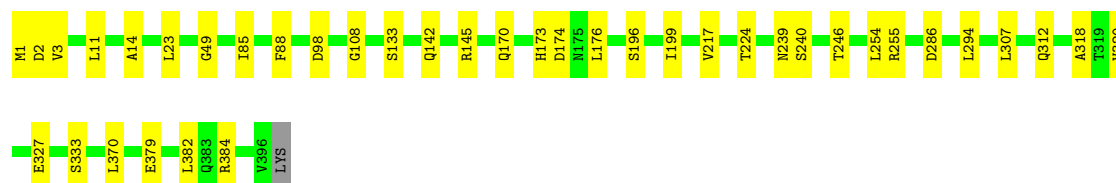
• Molecule 4: Intermediate capsid protein VP6

Chain K: 92% 8%



• Molecule 4: Intermediate capsid protein VP6

Chain L: 90% 10%



• Molecule 4: Intermediate capsid protein VP6

Chain M: 92% 8%



V396
LYS

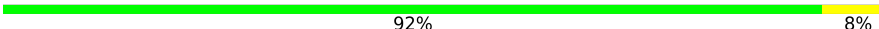
• Molecule 4: Intermediate capsid protein VP6

Chain N:  92% 8%

M1 L11 K17 V27 Q36 T69 F88 R117 S120 R145 H173 L176 Q189 V217 L225 Y248 R255 V261 E262 L265 N284 F285 D286 R289 L290 L294 N299 V320 L370 N373 Y374 S375 L382

V396
LYS

• Molecule 4: Intermediate capsid protein VP6

Chain O:  92% 8%

M1 D2 V3 L11 T22 Q47 T48 G49 N58 T68 L73 I85 F88 V89 D98 R117 S120 N138 T148 R168 S169 Q170 P171 A172 H173 D174 N175 L182 D194 V217 R231 V261 L264 L269 D286 L290

V396
LYS

• Molecule 4: Intermediate capsid protein VP6

Chain f:  88% 11%

M1 L11 A14 I18 Q36 I39 L65 F88 D93 Q105 Q142 R147 P155 H173 L176 L182 S186 V217 L225 R231 V261 E262 L265 T279 R283 N284 F285 D286 R289 L290 L294 V304 L307
N310 V320 L324 S328 E332 V346 P359 N365 W367 L370 L382 Q383 R394 R392 V396
LYS

• Molecule 4: Intermediate capsid protein VP6

Chain g:  92% 8%

M1 L4 L11 Y24 I31 E45 L66 G67 T68 F88 A110 F111 Q112 L116 R117 K118 L119 S120 Q142 R145 N156 A172 H173 D174 V217 L225 Y248 V261 D286 L307 N310 L324 A338 E352 L370

L382
V396
LYS

• Molecule 4: Intermediate capsid protein VP6

Chain h:  90% 10%

M1 D2 V3 T10 L11 A14 N37 I38 T84 I85 F88 D93 S104 Q105 R106 A110 P111 Q112 S113 D114 S115 L116 R117 S120 S169 Q170 H173 L176 I188 V212 L225 N239 T245 T246 Y247 Y248 L254 R255 V261 L294



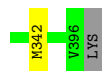
• Molecule 4: Intermediate capsid protein VP6

Chain i: 92% 8%



• Molecule 4: Intermediate capsid protein VP6

Chain j: 91% 9%



• Molecule 4: Intermediate capsid protein VP6

Chain k: 93% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1510279	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: CL, ZN, NAG, FME, CA

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	0.11	0/2234	0.29	0/3051
1	1	0.11	0/2128	0.28	0/2908
1	P	0.11	0/2128	0.27	0/2908
1	Q	0.10	0/2192	0.27	0/2994
1	R	0.11	0/2234	0.28	0/3051
1	S	0.11	0/2128	0.29	0/2908
1	T	0.11	0/2234	0.27	0/3051
1	U	0.11	0/2234	0.30	0/3051
1	V	0.12	0/2234	0.30	0/3051
1	W	0.11	0/2234	0.26	0/3051
1	X	0.11	0/2192	0.27	0/2994
1	Y	0.10	0/2234	0.26	0/3051
1	Z	0.12	0/2234	0.30	0/3051
1	t	0.11	0/2234	0.29	0/3051
1	u	0.11	0/2234	0.28	0/3051
1	v	0.11	0/2234	0.28	0/3051
1	w	0.11	0/2234	0.26	0/3051
1	x	0.11	0/2192	0.28	0/2994
1	y	0.10	0/2234	0.26	0/3051
2	2	0.11	0/2232	0.27	0/3032
2	3	0.10	0/2232	0.26	0/3032
2	4	0.10	0/2232	0.27	0/3032
3	A	0.12	0/6477	0.26	0/8788
3	B	0.12	0/6655	0.28	0/9029
4	C	0.13	0/3224	0.30	0/4387
4	D	0.13	0/3215	0.29	0/4376
4	E	0.12	0/3215	0.29	0/4376
4	F	0.12	0/3215	0.29	0/4376
4	G	0.12	0/3215	0.29	0/4376
4	H	0.12	0/3215	0.29	0/4376
4	I	0.12	0/3215	0.29	0/4376
4	J	0.13	0/3215	0.30	0/4376

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	K	0.12	0/3215	0.28	0/4376
4	L	0.13	0/3215	0.28	0/4376
4	M	0.13	0/3215	0.29	0/4376
4	N	0.12	0/3215	0.29	0/4376
4	O	0.13	0/3215	0.29	0/4376
4	f	0.12	0/3215	0.29	0/4376
4	g	0.13	0/3215	0.29	0/4376
4	h	0.12	0/3215	0.29	0/4376
4	i	0.12	0/3215	0.29	0/4376
4	j	0.12	0/3215	0.30	0/4376
4	k	0.12	0/3215	0.28	0/4376
All	All	0.12	0/122924	0.28	0/167437

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	2188	2124	2124	20	0
1	1	2085	2023	2023	25	0
1	P	2085	2023	2023	19	0
1	Q	2147	2087	2087	20	0
1	R	2188	2124	2124	30	0
1	S	2085	2023	2023	26	0
1	T	2188	2124	2124	17	0
1	U	2188	2124	2124	33	0
1	V	2188	2124	2124	27	0
1	W	2188	2124	2124	13	0
1	X	2147	2087	2087	11	0
1	Y	2188	2124	2124	22	0
1	Z	2188	2124	2124	19	0
1	t	2188	2124	2124	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	u	2188	2124	2124	30	0
1	v	2188	2124	2124	23	0
1	w	2188	2124	2124	14	0
1	x	2147	2087	2087	16	0
1	y	2188	2124	2124	18	0
2	2	2184	2107	2107	36	0
2	3	2184	2107	2107	28	0
2	4	2184	2107	2107	25	0
3	A	6362	6387	6387	40	0
3	B	6535	6563	6563	32	0
4	C	3164	3111	3111	25	0
4	D	3155	3098	3098	23	0
4	E	3155	3098	3098	28	0
4	F	3155	3098	3098	28	0
4	G	3155	3098	3098	26	0
4	H	3155	3098	3098	32	0
4	I	3155	3098	3098	21	0
4	J	3155	3098	3098	25	0
4	K	3155	3098	3098	20	0
4	L	3155	3098	3098	23	0
4	M	3155	3098	3098	20	0
4	N	3155	3098	3098	20	0
4	O	3155	3098	3098	16	0
4	f	3155	3098	3098	28	0
4	g	3155	3098	3098	23	0
4	h	3155	3098	3098	24	0
4	i	3155	3098	3098	20	0
4	j	3155	3098	3098	23	0
4	k	3155	3098	3098	15	0
5	0	14	14	13	0	0
5	1	14	14	13	0	0
5	P	14	14	13	0	0
5	Q	14	14	13	0	0
5	R	14	14	13	0	0
5	S	14	14	13	0	0
5	T	14	14	13	0	0
5	U	14	14	13	0	0
5	V	14	14	13	0	0
5	W	14	14	13	0	0
5	X	14	14	13	0	0
5	Y	14	14	13	0	0
5	Z	14	14	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	t	14	14	13	0	0
5	u	14	14	13	0	0
5	v	14	14	13	0	0
5	w	14	14	13	0	0
5	x	14	14	13	0	0
5	y	14	14	13	0	0
6	0	4	0	0	0	0
6	1	4	0	0	0	0
6	P	4	0	0	0	0
6	Q	4	0	0	0	0
6	R	4	0	0	0	0
6	S	4	0	0	0	0
6	T	4	0	0	0	0
6	U	4	0	0	0	0
6	V	4	0	0	0	0
6	W	4	0	0	0	0
6	X	4	0	0	0	0
6	Y	4	0	0	0	0
6	Z	4	0	0	0	0
6	t	4	0	0	0	0
6	u	4	0	0	0	0
6	v	4	0	0	0	0
6	w	4	0	0	0	0
6	x	4	0	0	0	0
6	y	4	0	0	0	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	2	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	I	2	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	2	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	2	0	0	0	0
7	f	2	0	0	0	0
7	g	1	0	0	0	0
7	h	1	0	0	0	0
7	i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	j	1	0	0	0	0
7	k	1	0	0	0	0
8	C	1	0	0	0	0
8	F	1	0	0	0	0
8	J	1	0	0	0	0
8	M	1	0	0	0	0
8	O	1	0	0	0	0
8	f	1	0	0	0	0
8	j	1	0	0	0	0
All	All	120918	118354	118335	886	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 (886) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:272:THR:HG21	1:y:277:THR:HG23	1.51	0.90
1:Y:272:THR:HG21	1:Y:277:THR:HG23	1.54	0.86
2:4:374:ASN:ND2	1:Q:203:LEU:O	2.11	0.84
4:H:145:ARG:NH1	4:f:142:GLN:O	2.10	0.83
1:R:75:THR:O	1:R:79:SER:OG	1.96	0.83
1:v:75:THR:O	1:v:79:SER:OG	1.97	0.82
1:1:271:ILE:HD13	1:1:284:MET:HE1	1.62	0.82
1:Q:75:THR:O	1:Q:79:SER:OG	1.97	0.81
1:x:75:THR:O	1:x:79:SER:OG	1.98	0.81
1:S:75:THR:O	1:S:79:SER:OG	2.00	0.80
1:V:75:THR:O	1:V:79:SER:OG	1.98	0.80
1:0:217:GLU:OE2	1:0:220:THR:OG1	2.00	0.79
1:X:75:THR:O	1:X:79:SER:OG	1.99	0.79
4:C:338:ALA:O	4:E:328:SER:OG	1.99	0.79
4:D:225:LEU:HD11	4:D:261:VAL:HG21	1.63	0.79
1:U:272:THR:HG21	1:U:277:THR:HG23	1.64	0.78
4:E:255:ARG:NH2	1:R:65:THR:O	2.16	0.78
1:U:75:THR:O	1:U:79:SER:OG	2.02	0.77
1:U:255:ARG:O	1:U:283:ARG:NH1	2.17	0.77
1:u:255:ARG:O	1:u:283:ARG:NH1	2.17	0.77
4:K:142:GLN:OE1	4:L:145:ARG:NH1	2.18	0.77
4:L:224:THR:OG1	4:L:327:GLU:OE2	2.02	0.77
1:S:87:THR:OG1	1:S:120:GLU:OE2	2.03	0.77
4:C:209:GLU:OE2	4:C:289:ARG:NH1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:546:ARG:NH2	3:A:595:ILE:O	2.19	0.76
1:U:105:LEU:O	1:U:108:THR:OG1	2.03	0.76
1:u:272:THR:HG21	1:u:277:THR:HG23	1.68	0.76
4:J:310:ASN:OD1	1:Y:305:GLN:NE2	2.19	0.76
4:I:49:GLY:N	4:I:98:ASP:OD2	2.18	0.75
1:Q:105:LEU:O	1:Q:108:THR:OG1	2.05	0.75
1:T:112:PRO:O	1:T:115:SER:OG	2.05	0.75
1:R:255:ARG:O	1:R:283:ARG:NH1	2.20	0.75
1:T:274:ASP:OD2	1:T:276:THR:OG1	2.04	0.75
1:R:274:ASP:OD2	1:R:276:THR:OG1	2.04	0.74
4:i:49:GLY:N	4:i:98:ASP:OD2	2.20	0.74
1:x:80:THR:HG21	1:x:324:TYR:CE2	2.23	0.74
2:3:491:ARG:NH2	2:4:492:GLN:OE1	2.21	0.74
1:U:112:PRO:O	1:U:115:SER:OG	2.03	0.74
1:V:105:LEU:O	1:V:108:THR:OG1	2.05	0.74
2:3:331:GLY:N	2:3:336:ASP:OD2	2.21	0.73
4:O:47:GLN:OE1	4:O:58:ASN:ND2	2.21	0.73
1:Y:105:LEU:O	1:Y:108:THR:OG1	2.07	0.73
1:l:105:LEU:O	1:l:108:THR:OG1	2.06	0.73
1:v:105:LEU:O	1:v:108:THR:OG1	2.07	0.73
2:4:382:GLY:N	2:4:400:GLY:O	2.22	0.73
1:u:105:LEU:O	1:u:108:THR:OG1	2.05	0.73
4:j:310:ASN:OD1	1:y:305:GLN:NE2	2.21	0.72
1:S:105:LEU:O	1:S:108:THR:OG1	2.07	0.72
3:B:261:GLU:OE1	4:N:69:THR:OG1	2.06	0.72
1:y:105:LEU:O	1:y:108:THR:OG1	2.07	0.72
4:F:155:PRO:O	4:F:186:SER:OG	2.08	0.72
1:X:62:SER:OG	1:X:64:ASP:OD1	2.07	0.72
1:U:272:THR:HG21	1:U:277:THR:O	1.90	0.71
1:u:112:PRO:O	1:u:115:SER:OG	2.08	0.71
3:B:335:LEU:O	3:B:338:SER:OG	2.09	0.71
1:t:255:ARG:O	1:t:283:ARG:NH1	2.23	0.71
1:0:180:GLU:O	1:0:183:LYS:NZ	2.23	0.71
1:t:274:ASP:OD2	1:t:276:THR:OG1	2.08	0.70
1:x:62:SER:OG	1:x:64:ASP:OD1	2.06	0.70
4:L:49:GLY:N	4:L:98:ASP:OD2	2.24	0.70
1:P:105:LEU:O	1:P:108:THR:OG1	2.07	0.70
1:Y:180:GLU:O	1:Y:183:LYS:NZ	2.24	0.70
1:S:178:THR:OG1	1:S:250:LYS:NZ	2.25	0.70
4:f:155:PRO:O	4:f:186:SER:OG	2.10	0.70
1:v:277:THR:HG22	1:v:279:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:65:THR:O	4:N:255:ARG:NH1	2.24	0.70
1:u:75:THR:O	1:u:79:SER:OG	2.03	0.69
1:u:272:THR:HG21	1:u:277:THR:O	1.91	0.69
3:B:674:ASP:OD1	3:B:677:ARG:NH2	2.26	0.69
4:k:310:ASN:OD1	1:w:305:GLN:NE2	2.26	0.69
2:3:255:VAL:HG22	2:3:265:MET:SD	2.32	0.69
4:g:142:GLN:O	4:i:145:ARG:NH1	2.26	0.68
2:2:490:VAL:HG13	2:3:488:VAL:HG11	1.75	0.68
2:3:501:LEU:HD21	2:4:501:LEU:HD22	1.73	0.68
2:2:377:SER:OG	2:2:404:LEU:O	2.07	0.68
4:E:228:ASP:O	4:E:323:THR:OG1	2.11	0.68
1:Z:105:LEU:O	1:Z:108:THR:OG1	2.10	0.68
1:S:274:ASP:OD2	1:S:276:THR:OG1	2.10	0.68
1:V:277:THR:HG22	1:V:279:PRO:HD3	1.76	0.68
2:4:420:SER:N	2:4:486:ASN:OD1	2.27	0.68
4:K:117:ARG:O	4:K:120:SER:OG	2.11	0.67
1:w:262:GLN:NE2	1:w:264:GLY:O	2.26	0.67
2:2:354:ASP:O	2:2:414:GLN:NE2	2.28	0.67
4:F:328:SER:OG	4:G:338:ALA:O	2.13	0.67
4:I:138:ASN:OD1	4:I:148:THR:OG1	2.06	0.67
1:t:112:PRO:O	1:t:115:SER:OG	2.09	0.67
4:k:117:ARG:O	4:k:120:SER:OG	2.13	0.67
1:y:272:THR:HG21	1:y:277:THR:O	1.95	0.67
3:A:412:ILE:CG2	3:A:543:LEU:HD22	2.24	0.66
4:D:209:GLU:OE2	4:D:289:ARG:NH1	2.28	0.66
1:U:174:TYR:CD2	1:U:198:LEU:HD11	2.30	0.66
1:P:217:GLU:OE2	1:P:220:THR:OG1	2.14	0.66
1:T:255:ARG:O	1:T:283:ARG:NH1	2.29	0.66
1:Y:265:GLY:O	1:Y:286:ARG:NH1	2.28	0.66
1:Y:272:THR:HG21	1:Y:277:THR:O	1.95	0.66
4:C:49:GLY:N	4:C:98:ASP:OD2	2.29	0.66
1:y:180:GLU:O	1:y:183:LYS:NZ	2.29	0.66
1:u:174:TYR:CD2	1:u:198:LEU:HD11	2.31	0.65
1:Q:319:SER:O	1:x:324:TYR:OH	2.14	0.65
4:D:279:THR:OG1	4:E:156:ASN:ND2	2.29	0.65
4:j:255:ARG:NH1	1:y:65:THR:O	2.30	0.65
1:v:274:ASP:OD2	1:v:276:THR:OG1	2.13	0.65
4:C:117:ARG:O	4:C:120:SER:OG	2.14	0.65
4:C:134:GLU:OE2	4:C:138:ASN:ND2	2.30	0.65
2:2:491:ARG:NH2	2:3:492:GLN:OE1	2.30	0.65
4:J:68:THR:HG22	4:J:69:THR:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:277:THR:HG22	1:t:279:PRO:HD3	1.78	0.65
4:D:225:LEU:HD11	4:D:261:VAL:CG2	2.27	0.65
4:G:142:GLN:O	4:I:145:ARG:NH1	2.30	0.65
4:J:262:GLU:OE2	4:J:289:ARG:NH2	2.30	0.65
1:T:180:GLU:O	1:T:183:LYS:NZ	2.29	0.65
3:B:546:ARG:NH1	3:B:592:CYS:O	2.30	0.64
1:W:262:GLN:NE2	1:W:264:GLY:O	2.29	0.64
2:3:368:VAL:HB	2:3:411:LEU:HD21	1.79	0.64
1:T:277:THR:HG22	1:T:279:PRO:HD3	1.78	0.64
4:D:224:THR:OG1	4:D:327:GLU:OE2	2.14	0.64
4:k:255:ARG:NH1	1:w:65:THR:O	2.30	0.64
1:u:265:GLY:O	1:u:286:ARG:NH1	2.31	0.64
2:3:346:LYS:N	2:3:349:SER:OG	2.31	0.64
3:A:786:ASP:OD2	3:A:828:SER:OG	2.15	0.64
1:Y:255:ARG:O	1:Y:283:ARG:NH1	2.31	0.64
4:H:310:ASN:OD1	1:T:305:GLN:NE2	2.31	0.63
4:h:117:ARG:O	4:h:120:SER:OG	2.16	0.63
4:j:68:THR:HG22	4:j:69:THR:H	1.63	0.63
4:j:262:GLU:OE2	4:j:289:ARG:NH2	2.31	0.63
4:I:255:ARG:NH1	1:X:65:THR:O	2.31	0.63
1:P:202:THR:O	1:P:202:THR:HG22	1.98	0.63
1:y:255:ARG:O	1:y:283:ARG:NH1	2.31	0.63
2:2:425:ARG:NH2	2:4:487:SER:OG	2.31	0.63
1:U:265:GLY:O	1:U:286:ARG:NH1	2.31	0.63
1:X:180:GLU:O	1:X:183:LYS:NZ	2.31	0.63
4:h:310:ASN:OD1	1:t:305:GLN:NE2	2.32	0.63
1:V:315:ARG:HB3	1:V:325:ARG:HE	1.64	0.62
1:R:164:LEU:HB2	1:R:252:LEU:HD21	1.80	0.62
2:2:382:GLY:N	2:2:400:GLY:O	2.32	0.62
1:v:77:LEU:HD13	1:v:112:PRO:HG3	1.81	0.62
1:1:65:THR:O	4:L:255:ARG:NH2	2.32	0.62
1:1:130:ASP:OD1	1:1:132:GLN:NE2	2.31	0.62
1:t:180:GLU:O	1:t:183:LYS:NZ	2.32	0.62
4:E:294:LEU:HD11	4:E:318:ALA:HB1	1.81	0.62
1:R:201:GLN:O	1:R:202:THR:OG1	2.17	0.62
4:f:11:LEU:HD21	4:f:88:PHE:HB3	1.82	0.62
1:y:265:GLY:O	1:y:286:ARG:NH1	2.33	0.62
2:2:255:VAL:HG22	2:2:265:MET:CE	2.30	0.61
1:S:201:GLN:N	1:S:201:GLN:OE1	2.32	0.61
1:x:112:PRO:O	1:x:115:SER:OG	2.11	0.61
4:g:117:ARG:O	4:g:120:SER:OG	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:265:LEU:HD22	4:C:284:ASN:OD1	2.00	0.61
4:J:147:ARG:NH1	4:J:332:GLU:OE2	2.33	0.61
1:Y:278:ALA:O	1:Y:280:GLN:NE2	2.34	0.61
4:i:255:ARG:NH1	1:x:65:THR:O	2.34	0.61
1:1:134:TYR:O	1:1:313:ARG:NH1	2.34	0.60
4:L:307:LEU:HD11	4:M:248:TYR:CD1	2.36	0.60
1:W:265:GLY:O	1:W:286:ARG:NH1	2.34	0.60
4:J:11:LEU:HD21	4:J:88:PHE:HB3	1.83	0.60
4:K:194:ASP:OD1	4:K:197:CYS:N	2.34	0.60
1:y:278:ALA:O	1:y:280:GLN:NE2	2.34	0.60
4:F:11:LEU:HD21	4:F:88:PHE:HB3	1.84	0.60
4:H:117:ARG:O	4:H:120:SER:OG	2.19	0.60
1:1:263:VAL:HG12	1:1:289:TRP:CD1	2.37	0.60
3:B:532:TYR:CE2	3:B:536:ILE:HD11	2.37	0.60
4:E:294:LEU:HD12	4:E:320:VAL:HG13	1.84	0.60
4:N:225:LEU:HD21	4:N:261:VAL:HG21	1.82	0.59
1:Q:205:ILE:HG22	1:R:101:THR:HG22	1.84	0.59
4:I:209:GLU:OE2	4:I:289:ARG:NE	2.36	0.59
1:Q:180:GLU:O	1:Q:183:LYS:NZ	2.36	0.59
1:w:265:GLY:O	1:w:286:ARG:NH1	2.34	0.59
1:W:101:THR:HG22	1:Y:205:ILE:HG22	1.84	0.59
1:Z:255:ARG:O	1:Z:283:ARG:NH1	2.36	0.59
1:x:80:THR:HG21	1:x:324:TYR:HE2	1.65	0.59
3:A:601:ILE:HD11	3:A:869:THR:CG2	2.31	0.59
3:B:412:ILE:HG22	3:B:543:LEU:HD22	1.83	0.59
4:f:217:VAL:HG22	4:f:286:ASP:HB3	1.83	0.59
4:F:310:ASN:OD1	1:U:305:GLN:NE2	2.36	0.59
4:G:24:TYR:CZ	4:G:68:THR:HG23	2.38	0.59
2:4:432:VAL:HG11	2:4:448:TYR:HB3	1.85	0.58
1:P:106:PHE:CE2	1:P:300:VAL:HG22	2.38	0.58
1:V:77:LEU:HD13	1:V:112:PRO:HG3	1.85	0.58
2:2:487:SER:OG	2:3:354:ASP:OD2	2.12	0.58
1:V:274:ASP:OD2	1:V:276:THR:OG1	2.17	0.58
1:R:325:ARG:NH2	1:Z:316:SER:OG	2.36	0.58
3:A:420:VAL:HG23	3:A:421:VAL:HG23	1.86	0.58
4:J:255:ARG:NH1	1:Y:65:THR:O	2.37	0.58
1:P:201:GLN:N	1:P:201:GLN:OE1	2.36	0.58
4:i:11:LEU:HD21	4:i:88:PHE:HB3	1.86	0.58
4:C:225:LEU:HD22	4:C:261:VAL:HG21	1.86	0.58
4:D:45:GLU:O	4:D:118:LYS:NZ	2.37	0.58
2:2:259:THR:HG22	2:2:260:SER:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:117:ARG:O	4:M:120:SER:OG	2.22	0.57
1:Q:274:ASP:OD2	1:Q:276:THR:OG1	2.21	0.57
4:N:11:LEU:HD21	4:N:88:PHE:HB3	1.86	0.57
1:P:180:GLU:O	1:P:183:LYS:NZ	2.35	0.57
4:j:117:ARG:O	4:j:120:SER:OG	2.22	0.57
1:O:75:THR:O	1:O:79:SER:OG	2.20	0.57
1:O:266:SER:OG	1:O:267:ASP:N	2.37	0.57
4:G:11:LEU:HD21	4:G:88:PHE:HB3	1.85	0.57
4:O:117:ARG:O	4:O:120:SER:OG	2.21	0.57
1:R:272:THR:HG21	1:R:277:THR:O	2.04	0.57
4:O:217:VAL:HG22	4:O:286:ASP:HB3	1.86	0.57
1:1:274:ASP:OD1	1:1:276:THR:OG1	2.22	0.57
4:C:255:ARG:NH1	1:S:65:THR:O	2.36	0.57
1:R:180:GLU:O	1:R:183:LYS:NZ	2.36	0.57
4:h:255:ARG:NH1	1:t:65:THR:O	2.37	0.57
4:j:147:ARG:NH1	4:j:332:GLU:OE2	2.37	0.57
1:R:256:GLU:OE1	1:R:314:SER:OG	2.22	0.57
4:i:307:LEU:HD11	4:j:248:TYR:CD1	2.39	0.57
4:j:11:LEU:HD21	4:j:88:PHE:HB3	1.85	0.57
1:O:105:LEU:O	1:O:108:THR:OG1	2.18	0.57
3:B:190:LEU:HD23	3:B:193:MET:HE3	1.85	0.57
4:F:262:GLU:OE1	4:F:289:ARG:NH1	2.38	0.57
4:I:307:LEU:HD11	4:J:248:TYR:CD1	2.40	0.57
4:E:117:ARG:O	4:E:120:SER:OG	2.23	0.57
2:3:490:VAL:HG13	2:4:488:VAL:HG11	1.86	0.56
4:F:217:VAL:HG22	4:F:286:ASP:HB3	1.87	0.56
3:B:471:GLN:HB3	4:H:80:THR:HG21	1.87	0.56
4:O:11:LEU:HD21	4:O:88:PHE:HB3	1.88	0.56
4:F:307:LEU:HD11	4:G:248:TYR:CD1	2.40	0.56
4:H:254:LEU:O	4:H:320:VAL:HG12	2.05	0.56
4:K:310:ASN:OD1	1:W:305:GLN:NE2	2.38	0.56
1:x:180:GLU:O	1:x:183:LYS:NZ	2.38	0.56
3:A:601:ILE:HD11	3:A:869:THR:HG21	1.87	0.56
4:G:117:ARG:O	4:G:120:SER:OG	2.23	0.56
4:g:11:LEU:HD21	4:g:88:PHE:HB3	1.87	0.56
4:j:261:VAL:HG22	4:j:290:LEU:HD23	1.88	0.56
4:G:68:THR:O	4:G:68:THR:HG22	2.05	0.56
4:L:11:LEU:HD21	4:L:88:PHE:HB3	1.86	0.56
4:O:138:ASN:OD1	4:O:148:THR:OG1	2.10	0.56
4:G:110:ALA:O	4:G:112:GLN:NE2	2.39	0.56
4:C:147:ARG:NH1	4:C:332:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:166:ASN:OD1	1:Y:315:ARG:NH2	2.36	0.56
3:B:140:VAL:HG11	3:B:152:ARG:HD2	1.88	0.56
4:J:225:LEU:HD22	4:J:261:VAL:HG21	1.87	0.56
1:Z:217:GLU:OE2	1:Z:220:THR:OG1	2.22	0.55
2:2:255:VAL:HG22	2:2:265:MET:HE1	1.87	0.55
1:Y:121:TYR:OH	1:Y:141:LEU:O	2.24	0.55
4:f:307:LEU:HD11	4:g:248:TYR:CD1	2.41	0.55
1:1:272:THR:HG21	1:1:277:THR:O	2.05	0.55
2:3:501:LEU:HD21	2:4:501:LEU:CD2	2.37	0.55
4:M:255:ARG:NH1	1:Z:65:THR:O	2.38	0.55
1:R:105:LEU:O	1:R:108:THR:OG1	2.25	0.55
4:j:217:VAL:HG22	4:j:286:ASP:HB3	1.87	0.55
3:A:311:LEU:O	3:A:618:HIS:NE2	2.35	0.55
4:H:188:ILE:HD13	4:H:212:VAL:HG21	1.89	0.55
4:I:11:LEU:HD21	4:I:88:PHE:HB3	1.89	0.55
1:w:316:SER:OG	1:w:318:ASN:O	2.18	0.55
1:V:172:LEU:HD22	1:V:173:TYR:CE1	2.42	0.55
4:f:370:LEU:HD21	4:f:382:LEU:HD13	1.89	0.55
1:Y:184:TRP:CZ3	1:Y:237:LEU:HD21	2.42	0.54
2:2:354:ASP:OD2	2:4:487:SER:OG	2.16	0.54
1:Q:203:LEU:O	1:Q:209:THR:HG23	2.07	0.54
1:Q:285:MET:HE1	1:Q:306:ILE:HG23	1.89	0.54
4:K:255:ARG:NH1	1:W:65:THR:O	2.39	0.54
4:i:168:ARG:NH2	4:i:194:ASP:OD1	2.39	0.54
3:A:403:PHE:HB3	3:A:585:LEU:HD12	1.90	0.54
1:S:272:THR:HG21	1:S:277:THR:O	2.06	0.54
1:w:191:CYS:SG	1:w:193:ILE:HD11	2.48	0.54
2:2:278:ALA:HB2	2:2:299:ALA:HB2	1.89	0.54
1:P:134:TYR:O	1:P:313:ARG:NH1	2.41	0.54
1:X:191:CYS:N	1:X:222:GLU:O	2.37	0.54
4:i:138:ASN:OD1	4:i:148:THR:OG1	2.08	0.54
4:D:337:ASP:OD2	4:D:339:SER:OG	2.26	0.54
4:G:307:LEU:HD11	4:H:248:TYR:CD1	2.43	0.54
4:J:217:VAL:HG22	4:J:286:ASP:HB3	1.89	0.54
2:4:403:SER:OG	2:4:433:GLU:OE2	2.23	0.54
3:A:663:ARG:NH1	3:B:350:GLU:OE2	2.40	0.54
1:U:185:ILE:HG22	1:U:187:MET:HE2	1.88	0.54
4:g:217:VAL:HG22	4:g:286:ASP:HB3	1.90	0.54
4:G:11:LEU:HD21	4:G:88:PHE:CB	2.38	0.54
4:J:68:THR:O	4:J:69:THR:OG1	2.18	0.54
1:1:160:LEU:HD13	1:1:284:MET:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:786:ASP:OD2	3:B:830:THR:OG1	2.20	0.53
4:D:11:LEU:HD21	4:D:88:PHE:HB3	1.90	0.53
4:f:11:LEU:HD21	4:f:88:PHE:CB	2.38	0.53
4:h:188:ILE:HD13	4:h:212:VAL:HG21	1.91	0.53
1:v:180:GLU:O	1:v:183:LYS:NZ	2.40	0.53
1:0:71:THR:OG1	4:N:299:ASN:ND2	2.41	0.53
4:g:310:ASN:OD1	1:v:305:GLN:NE2	2.41	0.53
2:4:368:VAL:HB	2:4:411:LEU:HD11	1.90	0.53
4:H:11:LEU:HD21	4:H:88:PHE:HB3	1.90	0.53
1:U:252:LEU:HD11	1:W:317:LEU:HD21	1.89	0.53
1:X:267:ASP:OD1	1:X:286:ARG:NE	2.38	0.53
1:t:265:GLY:O	1:t:286:ARG:NH1	2.40	0.53
1:w:157:ASP:OD1	1:w:161:ASN:ND2	2.41	0.53
4:K:145:ARG:NH1	4:L:142:GLN:O	2.41	0.53
4:M:11:LEU:HD21	4:M:88:PHE:HB3	1.91	0.53
4:g:45:GLU:O	4:g:118:LYS:NZ	2.41	0.53
1:1:267:ASP:OD1	1:1:286:ARG:NE	2.40	0.53
1:u:252:LEU:HD11	1:w:317:LEU:HD21	1.90	0.53
2:4:375:LEU:HD21	2:4:428:PHE:CZ	2.44	0.53
1:W:180:GLU:O	1:W:183:LYS:NZ	2.42	0.53
1:W:191:CYS:SG	1:W:193:ILE:HD11	2.49	0.53
4:f:328:SER:OG	4:g:338:ALA:O	2.25	0.53
4:k:194:ASP:OD1	4:k:197:CYS:N	2.41	0.53
2:3:325:ASP:OD1	2:3:325:ASP:N	2.42	0.53
4:H:142:GLN:HB2	4:H:148:THR:HG21	1.90	0.53
2:2:491:ARG:NH2	2:3:495:GLU:OE1	2.43	0.52
2:2:501:LEU:HD12	2:3:502:ARG:HD3	1.91	0.52
4:J:11:LEU:HD21	4:J:88:PHE:CB	2.39	0.52
4:f:105:GLN:NE2	4:f:359:PRO:O	2.42	0.52
4:g:68:THR:O	4:g:68:THR:HG22	2.07	0.52
4:h:11:LEU:HD21	4:h:88:PHE:HB3	1.90	0.52
1:y:121:TYR:OH	1:y:141:LEU:O	2.26	0.52
2:2:402:VAL:HG22	2:2:450:LEU:HD13	1.91	0.52
4:C:217:VAL:HG22	4:C:286:ASP:HB3	1.91	0.52
4:N:117:ARG:O	4:N:120:SER:OG	2.25	0.52
4:f:265:LEU:HD22	4:f:284:ASN:ND2	2.24	0.52
3:B:309:ASN:O	3:B:622:ASN:ND2	2.39	0.52
4:E:11:LEU:HD21	4:E:88:PHE:HB3	1.91	0.52
4:G:24:TYR:OH	4:G:68:THR:HG23	2.09	0.52
1:U:65:THR:OG1	1:U:66:ALA:N	2.43	0.52
4:g:307:LEU:HD11	4:h:248:TYR:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:45:GLU:O	4:G:118:LYS:NZ	2.42	0.52
4:g:24:TYR:CZ	4:g:68:THR:HG23	2.45	0.52
4:j:225:LEU:HD22	4:j:261:VAL:HG21	1.91	0.52
1:t:202:THR:HG22	1:t:202:THR:O	2.09	0.52
4:H:255:ARG:NH1	1:T:65:THR:O	2.42	0.52
4:k:11:LEU:HD21	4:k:88:PHE:HB3	1.91	0.52
4:D:279:THR:HG1	4:E:156:ASN:HD21	1.58	0.52
4:E:11:LEU:HD21	4:E:88:PHE:CB	2.39	0.52
1:Y:166:ASN:ND2	1:Y:325:ARG:O	2.43	0.52
4:H:142:GLN:OE1	4:H:383:GLN:NE2	2.41	0.52
1:Z:264:GLY:N	1:Z:287:ILE:O	2.42	0.52
2:3:296:PHE:N	2:3:343:GLU:OE1	2.39	0.52
4:L:217:VAL:HG22	4:L:286:ASP:HB3	1.91	0.52
4:M:93:ASP:OD1	4:M:392:ARG:NE	2.41	0.52
4:i:248:TYR:CD1	4:k:307:LEU:HD11	2.45	0.52
1:R:201:GLN:N	1:R:201:GLN:OE1	2.43	0.52
1:w:180:GLU:O	1:w:183:LYS:NZ	2.42	0.52
3:B:621:TYR:CZ	3:B:625:ILE:HD11	2.45	0.52
4:E:245:THR:OG1	4:E:246:THR:N	2.43	0.52
1:U:180:GLU:O	1:U:183:LYS:NZ	2.43	0.52
1:0:142:MET:HE2	1:0:155:LEU:HD23	1.90	0.51
4:I:242:ASP:N	4:I:242:ASP:OD1	2.44	0.51
4:J:117:ARG:O	4:J:120:SER:OG	2.27	0.51
1:t:288:ASN:ND2	1:v:153:SER:OG	2.42	0.51
4:F:370:LEU:HD21	4:F:382:LEU:HD13	1.92	0.51
4:J:261:VAL:HG22	4:J:290:LEU:HD23	1.92	0.51
4:K:114:ASP:OD1	4:K:117:ARG:NH2	2.42	0.51
4:M:168:ARG:NH2	4:M:194:ASP:OD1	2.40	0.51
4:M:261:VAL:HG22	4:M:290:LEU:HD23	1.92	0.51
1:S:198:LEU:HD22	1:S:202:THR:O	2.09	0.51
1:U:184:TRP:CZ3	1:U:237:LEU:HD21	2.45	0.51
1:v:72:GLN:NE2	1:v:304:ASN:OD1	2.42	0.51
4:J:225:LEU:CD2	4:J:261:VAL:HG21	2.40	0.51
4:K:11:LEU:HD21	4:K:88:PHE:HB3	1.93	0.51
4:N:17:LYS:HB3	4:N:27:VAL:HG12	1.91	0.51
4:M:225:LEU:CD2	4:M:261:VAL:HG21	2.40	0.51
1:R:159:ILE:CG2	1:R:258:VAL:HG11	2.39	0.51
1:T:202:THR:HG22	1:T:202:THR:O	2.11	0.51
4:g:11:LEU:HD21	4:g:88:PHE:CB	2.39	0.51
4:h:93:ASP:OD1	4:h:392:ARG:NE	2.40	0.51
1:R:134:TYR:O	1:R:315:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:263:VAL:HG12	1:T:289:TRP:CG	2.45	0.51
4:f:304:VAL:HA	4:f:307:LEU:HD12	1.93	0.51
4:f:346:VAL:HG11	4:f:365:MET:HE2	1.91	0.51
4:i:11:LEU:HD21	4:i:88:PHE:CB	2.40	0.51
1:u:184:TRP:CZ3	1:u:237:LEU:HD21	2.46	0.51
1:1:281:THR:HB	1:1:284:MET:HE3	1.92	0.51
3:A:336:ALA:O	3:A:340:VAL:HG23	2.11	0.51
1:R:317:LEU:HD21	1:Z:252:LEU:CD1	2.41	0.51
4:h:110:ALA:O	4:h:112:GLN:NE2	2.44	0.51
1:u:65:THR:OG1	1:u:66:ALA:N	2.44	0.51
2:2:375:LEU:HD11	2:2:426:PHE:CD1	2.46	0.51
1:1:178:THR:OG1	1:1:250:LYS:NZ	2.44	0.51
2:2:418:PHE:O	2:2:486:ASN:N	2.43	0.51
4:C:380:ASP:OD2	4:N:145:ARG:NH2	2.43	0.51
4:F:11:LEU:HD21	4:F:88:PHE:CB	2.41	0.50
1:U:274:ASP:OD2	1:U:277:THR:HG22	2.11	0.50
4:E:135:TYR:CE1	4:E:342:MET:HE3	2.46	0.50
4:H:14:ALA:HB1	4:H:85:ILE:HD11	1.93	0.50
1:Y:217:GLU:N	1:Y:217:GLU:OE1	2.42	0.50
1:x:133:LEU:HD13	1:x:258:VAL:HG21	1.92	0.50
1:Q:262:GLN:NE2	1:Q:266:SER:O	2.44	0.50
2:4:278:ALA:HB2	2:4:299:ALA:HB2	1.92	0.50
3:A:403:PHE:CB	3:A:585:LEU:HD12	2.42	0.50
4:H:255:ARG:NH2	1:T:65:THR:O	2.44	0.50
4:J:279:THR:OG1	4:K:156:ASN:ND2	2.43	0.50
4:K:93:ASP:OD1	4:K:392:ARG:NE	2.40	0.50
1:V:129:VAL:O	1:V:129:VAL:HG12	2.12	0.50
4:f:262:GLU:OE1	4:f:289:ARG:NH1	2.44	0.50
1:y:217:GLU:OE1	1:y:217:GLU:N	2.41	0.50
3:A:621:TYR:CZ	3:A:625:ILE:HD11	2.46	0.50
4:M:265:LEU:HD22	4:M:284:ASN:ND2	2.27	0.50
4:N:217:VAL:HG22	4:N:286:ASP:HB3	1.94	0.50
4:h:11:LEU:HD21	4:h:88:PHE:CB	2.42	0.50
4:i:242:ASP:OD1	4:i:242:ASP:N	2.44	0.50
1:y:202:THR:O	1:y:202:THR:HG22	2.11	0.50
1:0:201:GLN:O	1:0:202:THR:OG1	2.19	0.50
2:2:278:ALA:CB	2:2:299:ALA:HB2	2.41	0.50
3:B:740:ILE:HD12	3:B:764:VAL:HG21	1.93	0.50
4:F:265:LEU:HD22	4:F:284:ASN:ND2	2.26	0.50
1:v:129:VAL:HG12	1:v:129:VAL:O	2.12	0.50
4:D:11:LEU:HD21	4:D:88:PHE:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:225:LEU:HD13	4:F:324:LEU:CD1	2.42	0.50
1:R:133:LEU:HD13	1:R:258:VAL:HG21	1.93	0.50
1:S:198:LEU:HD23	1:S:204:GLY:HA2	1.93	0.50
1:T:157:ASP:OD1	1:T:161:ASN:ND2	2.45	0.50
2:2:360:GLN:OE1	2:2:363:ARG:NH1	2.45	0.50
4:F:304:VAL:HA	4:F:307:LEU:HD12	1.94	0.50
4:I:93:ASP:OD1	4:I:392:ARG:NE	2.44	0.50
4:I:225:LEU:HD22	4:I:261:VAL:HG21	1.94	0.50
4:M:2:ASP:OD1	4:M:3:VAL:N	2.44	0.50
3:A:188:LEU:HD22	3:A:264:LEU:HD21	1.92	0.50
3:B:718:GLN:HA	3:B:827:THR:HG22	1.94	0.50
3:A:152:ARG:NH1	3:A:723:GLU:OE1	2.45	0.49
4:C:397:LYS:NZ	4:E:151:THR:OG1	2.40	0.49
1:t:136:ASP:OD1	1:t:315:ARG:NE	2.45	0.49
4:F:279:THR:OG1	4:G:156:ASN:ND2	2.45	0.49
1:R:272:THR:HG21	1:R:277:THR:HG23	1.93	0.49
4:g:110:ALA:O	4:g:112:GLN:NE2	2.45	0.49
4:j:225:LEU:CD2	4:j:261:VAL:HG21	2.41	0.49
4:E:217:VAL:HG22	4:E:286:ASP:HB3	1.93	0.49
4:E:265:LEU:HD22	4:E:284:ASN:ND2	2.27	0.49
4:H:110:ALA:O	4:H:112:GLN:NE2	2.45	0.49
4:H:173:HIS:HA	4:H:176:LEU:HD21	1.94	0.49
4:h:14:ALA:HB1	4:h:85:ILE:HD11	1.95	0.49
1:x:191:CYS:N	1:x:222:GLU:O	2.42	0.49
1:R:315:ARG:NH2	1:Z:166:ASN:OD1	2.45	0.49
4:i:225:LEU:HD22	4:i:261:VAL:HG21	1.94	0.49
4:j:11:LEU:HD21	4:j:88:PHE:CB	2.42	0.49
3:A:397:ARG:NH2	3:A:579:THR:OG1	2.44	0.49
4:H:225:LEU:HD22	4:H:261:VAL:HG21	1.95	0.49
1:u:205:ILE:HG22	1:v:101:THR:HG22	1.95	0.49
2:4:331:GLY:N	2:4:336:ASP:OD2	2.45	0.49
3:B:815:ASP:OD1	3:B:815:ASP:N	2.44	0.49
4:C:11:LEU:HD21	4:C:88:PHE:HB3	1.94	0.49
4:C:254:LEU:O	4:C:320:VAL:HG12	2.13	0.49
4:F:228:ASP:O	4:F:323:THR:OG1	2.27	0.49
4:H:11:LEU:HD21	4:H:88:PHE:CB	2.42	0.49
4:L:11:LEU:HD21	4:L:88:PHE:CB	2.42	0.49
4:i:93:ASP:OD1	4:i:392:ARG:NE	2.44	0.49
1:u:274:ASP:OD2	1:u:277:THR:HG22	2.13	0.49
2:2:357:ASP:OD1	2:2:359:SER:N	2.44	0.49
4:H:104:SER:OG	4:H:106:ARG:O	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:294:LEU:HD12	4:N:320:VAL:HG13	1.94	0.49
1:X:251:LYS:NZ	1:X:271:ILE:O	2.46	0.49
4:f:225:LEU:HD13	4:f:324:LEU:CD1	2.43	0.49
4:g:24:TYR:OH	4:g:68:THR:HG23	2.13	0.49
3:B:311:LEU:O	3:B:618:HIS:NE2	2.44	0.49
3:B:337:ARG:NH1	3:B:388:THR:OG1	2.45	0.49
4:G:217:VAL:HG22	4:G:286:ASP:HB3	1.95	0.49
4:I:11:LEU:HD21	4:I:88:PHE:CB	2.43	0.49
4:I:168:ARG:NH2	4:I:194:ASP:OD1	2.41	0.49
1:y:184:TRP:CZ3	1:y:237:LEU:HD21	2.47	0.49
3:B:336:ALA:O	3:B:340:VAL:HG23	2.12	0.49
4:D:334:VAL:HG23	4:D:382:LEU:HD23	1.95	0.49
4:E:240:SER:OG	4:E:242:ASP:OD1	2.30	0.49
4:G:225:LEU:HD22	4:G:261:VAL:HG21	1.95	0.49
4:j:14:ALA:HA	4:j:30:LEU:HD21	1.93	0.49
4:k:114:ASP:OD1	4:k:117:ARG:NH2	2.46	0.49
1:l:285:MET:HE1	1:l:306:ILE:HG23	1.95	0.48
4:E:135:TYR:CZ	4:E:342:MET:HE3	2.48	0.48
4:N:11:LEU:HD21	4:N:88:PHE:CB	2.43	0.48
1:U:163:TRP:O	1:W:317:LEU:HD22	2.13	0.48
1:V:59:ILE:HD11	1:t:53:TYR:O	2.13	0.48
1:V:315:ARG:CB	1:V:325:ARG:HE	2.23	0.48
1:u:185:ILE:HG22	1:u:187:MET:HE2	1.93	0.48
2:4:251:ASN:ND2	2:4:308:ASP:OD2	2.46	0.48
4:h:225:LEU:HD22	4:h:261:VAL:HG21	1.93	0.48
1:y:87:THR:HG23	1:y:120:GLU:OE2	2.12	0.48
2:2:323:MET:SD	2:2:323:MET:N	2.82	0.48
4:F:225:LEU:HD22	4:F:261:VAL:HG21	1.95	0.48
1:X:133:LEU:HD13	1:X:258:VAL:HG21	1.94	0.48
1:t:101:THR:HG22	1:v:205:ILE:HG22	1.95	0.48
4:E:57:ARG:NH1	4:E:94:ASN:OD1	2.45	0.48
4:L:370:LEU:HD21	4:L:382:LEU:HD13	1.95	0.48
4:E:2:ASP:OD1	4:E:3:VAL:N	2.47	0.48
1:T:263:VAL:HG12	1:T:289:TRP:CD1	2.47	0.48
1:Z:202:THR:O	1:Z:202:THR:HG22	2.13	0.48
4:j:68:THR:O	4:j:69:THR:OG1	2.20	0.48
4:L:174:ASP:OD1	4:L:312:GLN:NE2	2.47	0.48
1:U:263:VAL:HG12	1:U:289:TRP:CD1	2.49	0.48
4:h:104:SER:OG	4:h:106:ARG:O	2.31	0.48
4:N:225:LEU:CD2	4:N:261:VAL:HG21	2.44	0.48
1:Q:271:ILE:C	1:Q:271:ILE:HD12	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:180:GLU:O	1:1:183:LYS:NZ	2.42	0.48
3:A:195:VAL:HG21	3:A:209:SER:HA	1.94	0.48
4:H:45:GLU:O	4:H:118:LYS:NZ	2.44	0.48
4:J:294:LEU:HD11	4:J:318:ALA:HB1	1.96	0.48
1:S:202:THR:O	1:S:202:THR:HG22	2.14	0.48
1:x:251:LYS:NZ	1:x:271:ILE:O	2.46	0.48
4:i:209:GLU:OE2	4:i:289:ARG:NE	2.47	0.48
4:k:11:LEU:HD21	4:k:88:PHE:CB	2.44	0.48
2:3:490:VAL:CG1	2:4:488:VAL:HG11	2.44	0.47
4:K:173:HIS:HA	4:K:176:LEU:HD21	1.96	0.47
1:S:142:MET:HE3	1:S:155:LEU:HD23	1.96	0.47
4:h:38:ILE:HD11	4:h:84:THR:HG21	1.95	0.47
1:x:162:GLU:OE2	1:x:313:ARG:NE	2.47	0.47
1:0:263:VAL:HG12	1:0:289:TRP:CD1	2.49	0.47
4:H:294:LEU:HD23	4:H:320:VAL:HG13	1.96	0.47
4:O:2:ASP:OD1	4:O:3:VAL:N	2.47	0.47
4:h:173:HIS:HA	4:h:176:LEU:HD21	1.96	0.47
2:2:490:VAL:CG1	2:3:488:VAL:HG11	2.43	0.47
4:F:170:GLN:NE2	4:F:175:ASN:O	2.41	0.47
1:R:95:ASP:OD1	1:R:96:ASN:N	2.47	0.47
4:M:11:LEU:HD21	4:M:88:PHE:CB	2.44	0.47
1:U:205:ILE:HG22	1:V:101:THR:HG22	1.95	0.47
4:j:299:ASN:ND2	4:k:244:ALA:O	2.46	0.47
2:2:357:ASP:OD1	2:2:358:ASP:N	2.47	0.47
2:3:252:GLU:O	2:3:269:ARG:NH1	2.47	0.47
4:F:346:VAL:HG11	4:F:365:MET:HE2	1.95	0.47
4:L:254:LEU:O	4:L:320:VAL:HG12	2.14	0.47
4:k:108:GLY:O	4:k:384:ARG:NE	2.41	0.47
2:3:279:SER:OG	2:3:452:ALA:O	2.32	0.47
3:A:309:ASN:O	3:A:622:ASN:ND2	2.44	0.47
3:B:214:ILE:HG21	3:B:251:ILE:HG21	1.95	0.47
4:E:170:GLN:NE2	4:E:175:ASN:O	2.41	0.47
4:E:254:LEU:O	4:E:320:VAL:HG12	2.14	0.47
4:F:283:ARG:NH1	4:G:352:GLU:OE1	2.48	0.47
1:Z:157:ASP:OD1	1:Z:161:ASN:ND2	2.45	0.47
1:1:263:VAL:HG12	1:1:289:TRP:CG	2.49	0.47
3:A:517:LEU:CD1	3:A:543:LEU:HD23	2.45	0.47
4:C:11:LEU:HD21	4:C:88:PHE:CB	2.45	0.47
4:C:294:LEU:HD12	4:C:320:VAL:HG13	1.96	0.47
4:D:265:LEU:HD22	4:D:284:ASN:ND2	2.30	0.47
4:E:199:ILE:HD13	4:E:310:ASN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:173:HIS:HA	4:I:176:LEU:HD21	1.95	0.47
4:M:38:ILE:HD11	4:M:84:THR:HG21	1.97	0.47
1:P:185:ILE:HD12	1:P:249:CYS:HB2	1.97	0.47
1:R:141:LEU:HD23	1:R:261:ILE:HB	1.96	0.47
1:U:164:LEU:HD22	1:U:324:TYR:CZ	2.49	0.47
4:f:279:THR:OG1	4:g:156:ASN:ND2	2.47	0.47
4:h:254:LEU:O	4:h:320:VAL:HG12	2.15	0.47
4:F:39:ILE:HD11	4:F:65:LEU:HD11	1.97	0.47
1:S:263:VAL:HG12	1:S:289:TRP:CD1	2.50	0.47
3:A:728:VAL:HG23	3:A:807:TYR:O	2.15	0.47
4:J:14:ALA:HA	4:J:30:LEU:HD21	1.97	0.47
3:A:740:ILE:HD12	3:A:764:VAL:HG21	1.96	0.47
4:f:261:VAL:HG22	4:f:290:LEU:HD23	1.97	0.47
4:H:11:LEU:HG	4:H:37:MET:HE1	1.98	0.46
1:Q:255:ARG:O	1:Q:283:ARG:NH1	2.48	0.46
4:f:294:LEU:HD23	4:f:320:VAL:HG13	1.98	0.46
1:y:182:ASN:ND2	1:y:248:ASN:OD1	2.43	0.46
3:B:277:ILE:CD1	3:B:299:LEU:HD11	2.46	0.46
4:O:168:ARG:NH2	4:O:194:ASP:OD1	2.43	0.46
1:t:82:CYS:N	1:t:135:CYS:SG	2.89	0.46
1:u:163:TRP:O	1:w:317:LEU:HD22	2.15	0.46
2:2:502:ARG:HD2	2:4:501:LEU:HD12	1.95	0.46
1:P:184:TRP:CZ3	1:P:237:LEU:HD21	2.49	0.46
1:T:101:THR:HG22	1:V:205:ILE:HG22	1.97	0.46
1:X:80:THR:HG21	1:X:324:TYR:HD2	1.81	0.46
4:f:173:HIS:HA	4:f:176:LEU:HD21	1.98	0.46
1:O:160:LEU:HD21	1:O:260:VAL:HG23	1.97	0.46
2:3:489:THR:HG21	2:4:300:ASN:OD1	2.16	0.46
3:A:412:ILE:HG23	3:A:543:LEU:HD22	1.98	0.46
1:R:106:PHE:CE2	1:R:300:VAL:HG22	2.50	0.46
2:2:345:ILE:HG23	2:2:430:LEU:HD13	1.98	0.46
2:2:489:THR:HG22	2:3:298:PRO:HB2	1.96	0.46
4:D:85:ILE:O	4:D:89:VAL:HG23	2.15	0.46
4:F:173:HIS:HA	4:F:176:LEU:HD21	1.98	0.46
4:F:261:VAL:HG22	4:F:290:LEU:HD23	1.97	0.46
1:T:205:ILE:HG22	1:U:101:THR:HG22	1.97	0.46
1:V:59:ILE:HD11	1:t:53:TYR:C	2.41	0.46
1:O:263:VAL:HG12	1:O:289:TRP:CG	2.49	0.46
4:C:225:LEU:HD13	4:C:324:LEU:HD13	1.98	0.46
4:G:370:LEU:HD21	4:G:382:LEU:HD13	1.97	0.46
1:Q:288:ASN:ND2	1:S:153:SER:OG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:367:TRP:CZ3	4:f:370:LEU:HD23	2.51	0.46
3:A:313:ASP:OD1	3:A:621:TYR:OH	2.27	0.46
4:E:231:ARG:O	4:E:236:ARG:NH2	2.45	0.46
3:B:190:LEU:HD23	3:B:193:MET:CE	2.45	0.46
4:H:38:ILE:HD11	4:H:84:THR:HG21	1.97	0.46
1:Q:199:ASN:OD1	1:Q:199:ASN:N	2.49	0.46
1:R:287:ILE:HD11	1:R:295:VAL:HG13	1.97	0.46
1:U:317:LEU:HD13	1:U:319:SER:H	1.81	0.46
2:4:278:ALA:CB	2:4:299:ALA:HB2	2.46	0.46
4:O:11:LEU:HD21	4:O:88:PHE:CB	2.45	0.46
1:Y:87:THR:HG23	1:Y:120:GLU:OE2	2.16	0.46
2:3:354:ASP:OD1	2:3:425:ARG:NE	2.43	0.45
4:D:245:THR:HG22	4:D:246:THR:H	1.81	0.45
4:G:225:LEU:CD2	4:G:261:VAL:HG21	2.46	0.45
4:J:2:ASP:OD1	4:J:3:VAL:N	2.49	0.45
4:K:108:GLY:O	4:K:384:ARG:NE	2.41	0.45
1:Z:180:GLU:O	1:Z:183:LYS:NZ	2.49	0.45
4:g:145:ARG:NH2	4:i:380:ASP:OD1	2.47	0.45
2:4:253:ASP:OD1	2:4:269:ARG:NH2	2.50	0.45
4:F:225:LEU:HD13	4:F:324:LEU:HD13	1.98	0.45
4:G:242:ASP:OD1	4:G:242:ASP:N	2.42	0.45
1:w:74:GLU:O	1:w:78:THR:HG22	2.17	0.45
2:2:412:SER:OG	2:2:413:THR:N	2.49	0.45
4:C:258:ASN:ND2	4:C:293:GLN:OE1	2.49	0.45
4:D:346:VAL:HG11	4:D:365:MET:HE2	1.98	0.45
1:u:191:CYS:N	1:u:222:GLU:O	2.46	0.45
3:A:412:ILE:HG22	3:A:543:LEU:HD22	1.95	0.45
3:B:514:MET:HE2	3:B:547:LEU:HD22	1.97	0.45
3:B:645:MET:HA	3:B:648:ILE:HD12	1.98	0.45
4:M:217:VAL:HG22	4:M:286:ASP:HB3	1.98	0.45
1:Y:224:LEU:HD12	1:Y:225:VAL:N	2.31	0.45
4:f:310:ASN:OD1	1:u:305:GLN:NE2	2.50	0.45
1:w:193:ILE:HD12	1:w:193:ILE:N	2.31	0.45
4:D:170:GLN:HB2	4:D:171:PRO:HD2	1.99	0.45
4:D:217:VAL:HG22	4:D:286:ASP:HB3	1.99	0.45
4:F:147:ARG:NH1	4:F:332:GLU:OE2	2.49	0.45
1:S:266:SER:OG	1:S:267:ASP:N	2.49	0.45
1:V:190:SER:OG	1:V:243:THR:HG21	2.16	0.45
1:W:97:SER:O	1:W:101:THR:HG23	2.16	0.45
4:k:273:TYR:OH	4:k:281:ILE:O	2.33	0.45
4:K:11:LEU:HD21	4:K:88:PHE:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:294:LEU:HD11	4:L:318:ALA:HB1	1.98	0.45
4:H:114:ASP:OD1	4:H:115:SER:N	2.49	0.45
4:K:380:ASP:OD1	4:L:145:ARG:NH2	2.50	0.45
4:L:333:SER:OG	4:L:379:GLU:OE2	2.29	0.45
4:i:370:LEU:HD21	4:i:382:LEU:HD13	1.98	0.45
1:1:255:ARG:O	1:1:283:ARG:NH1	2.49	0.45
2:4:252:GLU:OE1	2:4:254:ILE:HD11	2.17	0.45
3:B:728:VAL:CG2	3:B:806:LEU:HD11	2.47	0.45
1:V:263:VAL:HG12	1:V:289:TRP:CD1	2.52	0.45
4:E:261:VAL:HG23	4:E:290:LEU:HD23	1.99	0.45
4:J:254:LEU:O	4:J:320:VAL:HG12	2.17	0.45
1:P:296:PHE:O	1:P:300:VAL:HG23	2.17	0.45
1:X:164:LEU:HB2	1:X:252:LEU:HD11	1.99	0.44
1:Y:182:ASN:ND2	1:Y:248:ASN:OD1	2.45	0.44
4:j:265:LEU:HD22	4:j:284:ASN:ND2	2.32	0.44
4:G:4:LEU:HD22	4:G:116:LEU:HD13	1.98	0.44
4:L:2:ASP:OD1	4:L:3:VAL:N	2.50	0.44
4:M:225:LEU:HD21	4:M:261:VAL:HG21	2.00	0.44
2:2:345:ILE:HG21	2:2:430:LEU:HD22	1.98	0.44
4:F:367:TRP:CE3	4:F:370:LEU:HD23	2.53	0.44
1:W:193:ILE:N	1:W:193:ILE:HD12	2.32	0.44
1:t:74:GLU:O	1:t:78:THR:HG22	2.17	0.44
1:u:164:LEU:HD22	1:u:324:TYR:CZ	2.52	0.44
1:v:263:VAL:HG12	1:v:289:TRP:CD1	2.53	0.44
1:1:142:MET:HE2	1:1:155:LEU:HD23	1.99	0.44
2:3:455:PRO:O	2:3:462:TYR:OH	2.32	0.44
3:A:481:PHE:HD2	4:G:69:THR:HG23	1.82	0.44
4:C:310:ASN:OD1	1:S:305:GLN:NE2	2.50	0.44
4:D:182:LEU:HD22	4:D:231:ARG:NE	2.33	0.44
4:I:248:TYR:CD1	4:K:307:LEU:HD11	2.52	0.44
1:Q:296:PHE:O	1:Q:300:VAL:HG23	2.17	0.44
1:T:74:GLU:O	1:T:78:THR:HG22	2.18	0.44
1:Z:195:VAL:HG12	1:Z:237:LEU:CD2	2.48	0.44
4:j:2:ASP:OD1	4:j:3:VAL:N	2.50	0.44
2:2:320:VAL:HG11	2:2:345:ILE:HD11	1.99	0.44
2:4:345:ILE:CG2	2:4:430:LEU:HD13	2.48	0.44
4:C:248:TYR:CD1	4:E:307:LEU:HD11	2.53	0.44
4:H:169:SER:HA	4:H:176:LEU:HD23	2.00	0.44
1:R:164:LEU:CB	1:R:252:LEU:HD21	2.47	0.44
4:f:225:LEU:HD13	4:f:324:LEU:HD13	1.99	0.44
2:2:504:GLU:OE2	2:3:502:ARG:NH2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:182:ASN:ND2	1:P:249:CYS:O	2.45	0.44
4:f:367:TRP:CE3	4:f:370:LEU:HD23	2.52	0.44
4:g:172:ALA:HB3	4:g:174:ASP:OD1	2.17	0.44
4:C:202:PRO:O	4:C:203:ALA:HB3	2.17	0.44
4:K:2:ASP:OD1	4:K:3:VAL:N	2.51	0.44
1:Q:185:ILE:HD12	1:Q:226:ILE:HG12	2.00	0.44
1:R:85:TYR:OH	1:R:99:LYS:NZ	2.46	0.44
1:S:187:MET:HE2	1:S:224:LEU:HD13	1.99	0.44
1:X:285:MET:HE1	1:X:306:ILE:HG23	1.99	0.44
4:h:255:ARG:NH2	1:t:65:THR:O	2.51	0.44
1:u:189:SER:O	1:u:223:LYS:NZ	2.47	0.44
3:A:734:LEU:HD21	3:A:833:TYR:CG	2.53	0.44
4:H:336:ALA:HB2	4:H:343:LEU:HD22	1.99	0.44
1:P:256:GLU:O	1:P:310:MET:HE3	2.17	0.44
4:h:11:LEU:HG	4:h:37:MET:HE1	1.98	0.44
1:u:62:SER:OG	1:u:64:ASP:OD1	2.36	0.44
1:v:141:LEU:HD23	1:v:261:ILE:HB	2.00	0.44
1:y:224:LEU:HD12	1:y:225:VAL:N	2.33	0.44
1:1:157:ASP:OD1	1:1:161:ASN:ND2	2.47	0.44
2:3:346:LYS:O	2:3:349:SER:OG	2.28	0.44
4:h:114:ASP:OD1	4:h:115:SER:N	2.51	0.44
1:v:130:ASP:CA	1:v:187:MET:HE3	2.48	0.44
1:x:285:MET:HE1	1:x:306:ILE:HG23	2.00	0.44
1:0:195:VAL:HG22	1:0:237:LEU:CD2	2.48	0.43
4:C:264:LEU:CD2	4:C:269:ILE:HD13	2.48	0.43
1:U:202:THR:O	1:U:202:THR:HG22	2.18	0.43
1:V:141:LEU:HD23	1:V:261:ILE:HB	2.00	0.43
4:j:24:TYR:CZ	4:j:68:THR:HG23	2.52	0.43
2:4:378:VAL:HG22	2:4:379:ILE:N	2.33	0.43
4:L:108:GLY:O	4:L:384:ARG:NE	2.43	0.43
1:Q:112:PRO:O	1:Q:115:SER:OG	2.34	0.43
4:g:370:LEU:HD21	4:g:382:LEU:HD13	2.00	0.43
1:u:130:ASP:OD2	1:u:132:GLN:NE2	2.51	0.43
1:u:202:THR:O	1:u:202:THR:HG22	2.18	0.43
3:A:718:GLN:HA	3:A:827:THR:HG22	2.00	0.43
1:P:172:LEU:HD23	1:P:173:TYR:CZ	2.52	0.43
1:U:261:ILE:HG12	1:U:285:MET:HE2	1.99	0.43
1:U:276:THR:HG22	1:V:285:MET:HE3	1.99	0.43
1:t:133:LEU:HD13	1:t:258:VAL:HG21	2.00	0.43
1:u:180:GLU:O	1:u:183:LYS:NZ	2.52	0.43
4:F:34:PHE:CE2	4:F:38:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:265:LEU:HD22	4:N:284:ASN:ND2	2.33	0.43
4:N:370:LEU:HD21	4:N:382:LEU:HD13	2.00	0.43
1:S:113:THR:HG22	1:S:113:THR:O	2.18	0.43
1:U:230:VAL:HG22	1:V:300:VAL:HG13	2.01	0.43
4:k:173:HIS:HA	4:k:176:LEU:HD21	2.01	0.43
1:u:276:THR:HG22	1:v:285:MET:HE3	1.99	0.43
1:1:217:GLU:OE1	1:1:217:GLU:N	2.45	0.43
2:2:345:ILE:CG2	2:2:430:LEU:HD13	2.49	0.43
4:I:370:LEU:HD21	4:I:382:LEU:HD13	1.99	0.43
4:J:24:TYR:CZ	4:J:68:THR:HG23	2.53	0.43
1:R:317:LEU:HD21	1:Z:252:LEU:HD12	2.00	0.43
1:V:130:ASP:CA	1:V:187:MET:HE3	2.49	0.43
1:W:192:THR:C	1:W:193:ILE:HD12	2.44	0.43
4:g:4:LEU:HD22	4:g:116:LEU:HD13	1.99	0.43
4:H:2:ASP:OD1	4:H:3:VAL:N	2.51	0.43
4:I:57:ARG:NH1	4:I:94:ASN:OD1	2.50	0.43
4:L:196:SER:HB2	4:L:199:ILE:HG22	2.01	0.43
4:N:373:ASN:O	4:N:375:SER:N	2.52	0.43
1:S:191:CYS:N	1:S:222:GLU:O	2.52	0.43
4:f:39:ILE:HD11	4:f:65:LEU:HD11	2.01	0.43
1:t:77:LEU:HD23	1:t:112:PRO:HG3	2.00	0.43
1:v:271:ILE:HG12	1:v:284:MET:HE1	2.01	0.43
3:A:728:VAL:HG22	3:A:730:ILE:HG13	2.01	0.43
3:B:170:ARG:NE	3:B:638:LEU:O	2.50	0.43
3:B:393:MET:O	3:B:396:GLN:NE2	2.49	0.43
4:D:382:LEU:HA	4:D:385:VAL:HG22	2.01	0.43
4:G:225:LEU:HD13	4:G:324:LEU:CD1	2.48	0.43
4:I:346:VAL:HG11	4:I:365:MET:HE2	2.00	0.43
4:L:14:ALA:HB1	4:L:85:ILE:HD11	1.99	0.43
4:M:294:LEU:HD11	4:M:318:ALA:HB1	2.00	0.43
1:Y:193:ILE:N	1:Y:193:ILE:HD12	2.34	0.43
4:i:172:ALA:HB3	4:i:174:ASP:OD2	2.19	0.43
1:0:145:ASP:OD2	1:0:147:THR:OG1	2.35	0.43
3:A:176:LEU:O	3:A:180:VAL:HG23	2.18	0.43
4:f:283:ARG:NH1	4:g:352:GLU:OE1	2.52	0.43
1:1:281:THR:HG22	1:1:282:GLU:N	2.34	0.43
4:J:225:LEU:HD12	4:J:323:THR:O	2.18	0.43
4:O:182:LEU:HD22	4:O:231:ARG:NE	2.34	0.43
1:Y:168:MET:HE2	1:Y:246:ILE:HG12	2.01	0.43
4:h:239:ASN:HA	4:h:246:THR:HG22	2.01	0.43
3:B:517:LEU:HB2	3:B:540:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:103:GLU:OE1	4:K:350:ARG:NH2	2.48	0.42
3:A:356:MET:HG2	3:A:542:LEU:HD22	2.01	0.42
1:V:133:LEU:O	1:V:255:ARG:NH2	2.52	0.42
1:Y:263:VAL:HG12	1:Y:289:TRP:CD1	2.54	0.42
1:Z:106:PHE:CZ	1:Z:300:VAL:HG22	2.54	0.42
3:B:340:VAL:HG11	3:B:387:LYS:HA	2.01	0.42
4:G:145:ARG:NH2	4:I:380:ASP:OD1	2.50	0.42
4:H:225:LEU:CD2	4:H:261:VAL:HG21	2.49	0.42
4:N:173:HIS:HA	4:N:176:LEU:HD21	2.01	0.42
1:P:191:CYS:N	1:P:222:GLU:O	2.51	0.42
1:U:137:TYR:HD1	1:U:310:MET:HE2	1.84	0.42
3:A:281:ILE:HD13	3:A:293:LEU:HD13	2.01	0.42
3:A:801:THR:O	3:A:801:THR:HG22	2.17	0.42
4:F:367:TRP:CZ3	4:F:370:LEU:HD23	2.54	0.42
4:K:188:ILE:HD13	4:K:212:VAL:HG21	2.01	0.42
1:R:317:LEU:HD22	1:Z:163:TRP:O	2.19	0.42
4:h:169:SER:HA	4:h:176:LEU:HD23	2.02	0.42
1:u:159:ILE:HD11	1:u:260:VAL:CG2	2.50	0.42
1:O:77:LEU:HD23	1:O:112:PRO:HG3	2.01	0.42
4:H:239:ASN:ND2	4:H:240:SER:O	2.53	0.42
4:J:299:ASN:ND2	4:K:244:ALA:O	2.49	0.42
4:N:261:VAL:HG22	4:N:290:LEU:HD23	2.00	0.42
1:Q:187:MET:HG3	1:Q:224:LEU:HD13	2.02	0.42
1:S:180:GLU:O	1:S:183:LYS:NZ	2.48	0.42
4:j:209:GLU:OE1	4:j:291:SER:OG	2.33	0.42
1:v:190:SER:OG	1:v:243:THR:HG21	2.19	0.42
1:y:112:PRO:O	1:y:115:SER:OG	2.36	0.42
1:O:149:GLN:NE2	1:1:288:ASN:OD1	2.51	0.42
3:A:764:VAL:HG22	3:A:765:ALA:N	2.35	0.42
4:h:294:LEU:HD23	4:h:320:VAL:HG13	2.00	0.42
2:2:252:GLU:O	2:2:269:ARG:NH1	2.53	0.42
4:F:182:LEU:HD22	4:F:231:ARG:CD	2.49	0.42
4:H:10:THR:HB	4:H:37:MET:HE3	2.00	0.42
4:M:173:HIS:HA	4:M:176:LEU:HD21	2.01	0.42
4:O:172:ALA:HB3	4:O:174:ASP:OD1	2.19	0.42
1:R:187:MET:CG	1:R:224:LEU:HD13	2.49	0.42
4:i:346:VAL:HG11	4:i:365:MET:HE2	2.01	0.42
4:j:254:LEU:O	4:j:320:VAL:HG12	2.20	0.42
2:4:351:VAL:HG21	2:4:404:LEU:HD21	2.02	0.42
3:A:481:PHE:CZ	3:A:509:VAL:HG11	2.55	0.42
4:G:2:ASP:OD1	4:G:3:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:106:PHE:CD2	1:S:116:VAL:HG11	2.55	0.42
4:g:31:ILE:HD12	4:g:66:LEU:HD23	2.01	0.42
4:i:173:HIS:HA	4:i:176:LEU:HD21	2.01	0.42
1:x:267:ASP:OD1	1:x:286:ARG:NE	2.47	0.42
1:0:287:ILE:HD11	1:0:295:VAL:HG13	2.01	0.41
3:B:403:PHE:CB	3:B:585:LEU:HD12	2.50	0.41
4:G:172:ALA:HB3	4:G:174:ASP:OD1	2.20	0.41
4:M:225:LEU:HD22	4:M:261:VAL:HG21	2.01	0.41
1:U:230:VAL:HG21	1:V:105:LEU:HD13	2.03	0.41
1:V:72:GLN:NE2	1:V:304:ASN:OD1	2.52	0.41
1:V:271:ILE:HG12	1:V:284:MET:HE1	2.02	0.41
4:i:225:LEU:CD2	4:i:261:VAL:HG21	2.49	0.41
1:1:182:ASN:ND2	1:1:248:ASN:OD1	2.51	0.41
2:2:440:THR:HG22	2:2:441:ARG:HG2	2.01	0.41
4:I:225:LEU:CD2	4:I:261:VAL:HG21	2.51	0.41
4:O:261:VAL:HG13	4:O:290:LEU:HD23	2.02	0.41
1:V:149:GLN:HA	1:V:152:MET:HE3	2.01	0.41
4:f:14:ALA:HB1	4:f:18:ILE:HD12	2.03	0.41
4:f:93:ASP:OD1	4:f:392:ARG:NE	2.45	0.41
4:i:69:THR:O	4:i:69:THR:HG22	2.20	0.41
4:k:188:ILE:HD13	4:k:212:VAL:HG21	2.01	0.41
1:u:230:VAL:HG22	1:v:300:VAL:HG13	2.02	0.41
1:x:124:ILE:O	1:x:128:SER:OG	2.36	0.41
2:3:447:LEU:H	2:3:447:LEU:HD23	1.85	0.41
3:A:666:ASP:OD1	3:A:666:ASP:N	2.53	0.41
4:I:69:THR:O	4:I:69:THR:HG22	2.20	0.41
4:O:170:GLN:NE2	4:O:175:ASN:O	2.48	0.41
4:f:147:ARG:NH1	4:f:332:GLU:OE2	2.53	0.41
1:w:263:VAL:HG12	1:w:289:TRP:CD1	2.56	0.41
3:A:552:ASP:HB3	3:A:884:MET:HE2	2.01	0.41
4:E:273:TYR:OH	4:E:281:ILE:O	2.29	0.41
4:M:63:PHE:CD1	4:M:84:THR:HG23	2.55	0.41
4:M:255:ARG:NH2	1:Z:65:THR:O	2.53	0.41
4:L:23:LEU:HD11	4:N:36:GLN:HB2	2.02	0.41
4:j:182:LEU:HD22	4:j:231:ARG:CD	2.50	0.41
1:v:112:PRO:O	1:v:115:SER:OG	2.36	0.41
4:D:261:VAL:HG22	4:D:290:LEU:HD23	2.03	0.41
4:K:38:ILE:HD11	4:K:84:THR:HG21	2.02	0.41
1:P:259:ALA:HB2	1:P:310:MET:SD	2.60	0.41
1:S:184:TRP:CH2	1:S:229:VAL:HG21	2.55	0.41
1:V:65:THR:O	1:V:66:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:245:THR:OG1	4:h:246:THR:N	2.53	0.41
4:L:173:HIS:HA	4:L:176:LEU:HD21	2.02	0.41
1:Z:159:ILE:HD11	1:Z:260:VAL:CG2	2.50	0.41
4:h:2:ASP:OD1	4:h:3:VAL:N	2.53	0.41
1:1:75:THR:O	1:1:79:SER:OG	2.26	0.41
2:2:307:ARG:NH1	2:2:359:SER:OG	2.51	0.41
2:2:317:THR:HB	2:2:354:ASP:OD1	2.21	0.41
4:M:307:LEU:HD11	4:N:248:TYR:CD1	2.56	0.41
4:O:49:GLY:N	4:O:98:ASP:OD2	2.44	0.41
1:P:263:VAL:HG12	1:P:289:TRP:CD1	2.55	0.41
1:Y:201:GLN:O	1:Y:202:THR:OG1	2.35	0.41
1:0:316:SER:O	1:0:317:LEU:HG	2.20	0.41
1:1:65:THR:O	4:L:255:ARG:NH1	2.53	0.41
1:1:144:TYR:CD1	1:1:152:MET:HE1	2.56	0.41
3:A:115:LEU:HD23	3:A:335:LEU:HB2	2.03	0.41
3:A:764:VAL:HG22	3:A:765:ALA:H	1.85	0.41
4:C:158:PHE:CZ	4:C:188:ILE:HD11	2.55	0.41
4:D:297:PRO:HB3	4:E:246:THR:HG21	2.02	0.41
4:G:310:ASN:OD1	1:V:305:GLN:NE2	2.53	0.41
4:H:245:THR:OG1	4:H:246:THR:N	2.54	0.41
4:J:182:LEU:HD22	4:J:231:ARG:CD	2.51	0.41
4:L:239:ASN:ND2	4:L:240:SER:O	2.52	0.41
1:Q:263:VAL:HG12	1:Q:289:TRP:CD1	2.55	0.41
1:R:159:ILE:HG23	1:R:258:VAL:HG11	2.03	0.41
1:S:282:GLU:OE1	1:S:282:GLU:N	2.52	0.41
1:U:321:ALA:N	1:U:326:ILE:O	2.53	0.41
1:W:106:PHE:CD2	1:W:116:VAL:HG11	2.55	0.41
4:f:182:LEU:HD22	4:f:231:ARG:CD	2.51	0.41
4:g:225:LEU:HD22	4:g:261:VAL:HG21	2.03	0.41
4:k:2:ASP:OD1	4:k:3:VAL:N	2.54	0.41
1:u:261:ILE:HG12	1:u:285:MET:HE2	2.03	0.41
1:u:317:LEU:HD13	1:u:319:SER:HB2	2.03	0.41
2:3:282:VAL:O	2:3:292:SER:N	2.54	0.41
3:A:141:TYR:N	3:A:723:GLU:O	2.53	0.41
3:A:783:ALA:HB3	3:A:785:LEU:HD13	2.02	0.41
4:C:2:ASP:OD1	4:C:3:VAL:N	2.54	0.41
1:U:159:ILE:HD11	1:U:260:VAL:CG2	2.51	0.41
4:k:38:ILE:HD11	4:k:84:THR:HG21	2.03	0.41
1:v:65:THR:O	1:v:66:ALA:HB3	2.21	0.41
3:B:600:VAL:HG23	3:B:600:VAL:O	2.20	0.40
4:D:2:ASP:OD1	4:D:3:VAL:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:17:LYS:HB3	4:J:27:VAL:HG12	2.02	0.40
4:N:262:GLU:OE1	4:N:289:ARG:NH2	2.49	0.40
1:T:82:CYS:N	1:T:135:CYS:SG	2.93	0.40
1:v:95:ASP:OD1	1:v:96:ASN:N	2.54	0.40
4:E:188:ILE:HD13	4:E:212:VAL:HG21	2.03	0.40
1:P:185:ILE:HD12	1:P:249:CYS:CB	2.51	0.40
1:U:296:PHE:O	1:U:300:VAL:HG23	2.22	0.40
1:Z:172:LEU:HD22	1:Z:173:TYR:CE1	2.56	0.40
4:j:342:MET:HA	4:j:342:MET:HE3	2.04	0.40
3:A:781:LEU:HD13	3:A:807:TYR:CD2	2.56	0.40
3:B:420:VAL:HG23	3:B:421:VAL:HG23	2.02	0.40
4:D:240:SER:N	4:D:245:THR:O	2.50	0.40
4:I:2:ASP:OD1	4:I:3:VAL:N	2.54	0.40
4:O:22:THR:HG22	4:O:73:LEU:HD12	2.03	0.40
1:P:168:MET:HE3	1:P:246:ILE:HG12	2.03	0.40
1:S:225:VAL:C	1:S:226:ILE:HD13	2.46	0.40
1:T:195:VAL:HG21	1:U:297:TYR:HE2	1.86	0.40
4:h:10:THR:HB	4:h:37:MET:HE3	2.01	0.40
1:u:274:ASP:OD2	1:u:276:THR:OG1	2.33	0.40
1:x:263:VAL:HG12	1:x:289:TRP:CD1	2.56	0.40
1:0:123:ASP:OD1	1:0:123:ASP:N	2.53	0.40
4:C:336:ALA:HB2	4:C:343:LEU:HD22	2.03	0.40
4:F:14:ALA:HB1	4:F:85:ILE:HD11	2.03	0.40
4:H:165:THR:OG1	1:V:60:THR:HG23	2.21	0.40
4:J:265:LEU:HD22	4:J:284:ASN:ND2	2.36	0.40
4:O:264:LEU:HD11	4:O:269:ILE:HD13	2.03	0.40
1:P:258:VAL:C	1:P:310:MET:HE1	2.47	0.40
1:S:255:ARG:O	1:S:283:ARG:NH1	2.54	0.40
1:U:130:ASP:OD2	1:U:132:GLN:NE2	2.55	0.40
1:t:195:VAL:HG21	1:u:297:TYR:HE2	1.85	0.40
1:y:166:ASN:ND2	1:y:325:ARG:O	2.54	0.40
2:2:325:ASP:OD2	2:2:341:ARG:NH2	2.55	0.40
2:3:351:VAL:HG21	2:3:404:LEU:HD21	2.03	0.40
4:H:129:PHE:O	4:H:130:ASP:C	2.65	0.40
4:O:85:ILE:O	4:O:89:VAL:HG23	2.22	0.40
1:Q:271:ILE:HG12	1:Q:284:MET:HE1	2.02	0.40
1:R:317:LEU:HD21	1:Z:252:LEU:HD11	2.03	0.40
1:S:53:TYR:O	1:S:55:ILE:N	2.46	0.40
1:U:189:SER:O	1:U:223:LYS:NZ	2.52	0.40
4:g:225:LEU:HD13	4:g:324:LEU:CD1	2.52	0.40
1:v:157:ASP:OD1	1:v:161:ASN:ND2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:133:LEU:HD13	1:w:258:VAL:HG21	2.03	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%)	255 (97%)	7 (3%)	0	100	100
1	P	262/326 (80%)	259 (99%)	3 (1%)	0	100	100
1	Q	269/326 (82%)	268 (100%)	1 (0%)	0	100	100
1	R	274/326 (84%)	270 (98%)	4 (2%)	0	100	100
1	S	262/326 (80%)	257 (98%)	5 (2%)	0	100	100
1	T	274/326 (84%)	273 (100%)	1 (0%)	0	100	100
1	U	274/326 (84%)	264 (96%)	10 (4%)	0	100	100
1	V	274/326 (84%)	264 (96%)	9 (3%)	1 (0%)	30	52
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%)	270 (98%)	4 (2%)	0	100	100
1	Z	274/326 (84%)	263 (96%)	11 (4%)	0	100	100
1	t	274/326 (84%)	268 (98%)	6 (2%)	0	100	100
1	u	274/326 (84%)	265 (97%)	9 (3%)	0	100	100
1	v	274/326 (84%)	263 (96%)	10 (4%)	1 (0%)	30	52
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%)	270 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	273/776 (35%)	265 (97%)	8 (3%)	0	100	100
2	3	273/776 (35%)	264 (97%)	9 (3%)	0	100	100
2	4	273/776 (35%)	265 (97%)	8 (3%)	0	100	100
3	A	777/887 (88%)	765 (98%)	12 (2%)	0	100	100
3	B	797/887 (90%)	787 (99%)	10 (1%)	0	100	100
4	C	395/397 (100%)	385 (98%)	10 (2%)	0	100	100
4	D	394/397 (99%)	385 (98%)	9 (2%)	0	100	100
4	E	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	F	394/397 (99%)	382 (97%)	12 (3%)	0	100	100
4	G	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
4	H	394/397 (99%)	386 (98%)	8 (2%)	0	100	100
4	I	394/397 (99%)	386 (98%)	8 (2%)	0	100	100
4	J	394/397 (99%)	382 (97%)	12 (3%)	0	100	100
4	K	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	L	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	M	394/397 (99%)	382 (97%)	12 (3%)	0	100	100
4	N	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	O	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	f	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	g	394/397 (99%)	383 (97%)	11 (3%)	0	100	100
4	h	394/397 (99%)	387 (98%)	7 (2%)	0	100	100
4	i	394/397 (99%)	388 (98%)	6 (2%)	0	100	100
4	j	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
4	k	394/397 (99%)	384 (98%)	10 (2%)	0	100	100
All	All	15035/17839 (84%)	14702 (98%)	331 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	v	66	ALA
1	V	66	ALA

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%)	247 (100%)	0	100	100
1	1	237/295 (80%)	237 (100%)	0	100	100
1	P	237/295 (80%)	237 (100%)	0	100	100
1	Q	243/295 (82%)	243 (100%)	0	100	100
1	R	247/295 (84%)	247 (100%)	0	100	100
1	S	237/295 (80%)	236 (100%)	1 (0%)	84	92
1	T	247/295 (84%)	243 (98%)	4 (2%)	55	78
1	U	247/295 (84%)	246 (100%)	1 (0%)	84	92
1	V	247/295 (84%)	246 (100%)	1 (0%)	84	92
1	W	247/295 (84%)	246 (100%)	1 (0%)	84	92
1	X	243/295 (82%)	243 (100%)	0	100	100
1	Y	247/295 (84%)	247 (100%)	0	100	100
1	Z	247/295 (84%)	246 (100%)	1 (0%)	84	92
1	t	247/295 (84%)	244 (99%)	3 (1%)	63	82
1	u	247/295 (84%)	245 (99%)	2 (1%)	73	87
1	v	247/295 (84%)	247 (100%)	0	100	100
1	w	247/295 (84%)	246 (100%)	1 (0%)	84	92
1	x	243/295 (82%)	243 (100%)	0	100	100
1	y	247/295 (84%)	247 (100%)	0	100	100
2	2	241/688 (35%)	240 (100%)	1 (0%)	84	92
2	3	241/688 (35%)	241 (100%)	0	100	100
2	4	241/688 (35%)	241 (100%)	0	100	100
3	A	715/818 (87%)	715 (100%)	0	100	100
3	B	735/818 (90%)	735 (100%)	0	100	100
4	C	349/349 (100%)	347 (99%)	2 (1%)	78	90
4	D	348/349 (100%)	347 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	348/349 (100%)	347 (100%)	1 (0%)	86	93
4	F	348/349 (100%)	346 (99%)	2 (1%)	78	90
4	G	348/349 (100%)	348 (100%)	0	100	100
4	H	348/349 (100%)	346 (99%)	2 (1%)	78	90
4	I	348/349 (100%)	346 (99%)	2 (1%)	78	90
4	J	348/349 (100%)	347 (100%)	1 (0%)	86	93
4	K	348/349 (100%)	348 (100%)	0	100	100
4	L	348/349 (100%)	345 (99%)	3 (1%)	70	86
4	M	348/349 (100%)	345 (99%)	3 (1%)	70	86
4	N	348/349 (100%)	347 (100%)	1 (0%)	86	93
4	O	348/349 (100%)	347 (100%)	1 (0%)	86	93
4	f	348/349 (100%)	346 (99%)	2 (1%)	78	90
4	g	348/349 (100%)	348 (100%)	0	100	100
4	h	348/349 (100%)	345 (99%)	3 (1%)	70	86
4	i	348/349 (100%)	346 (99%)	2 (1%)	78	90
4	j	348/349 (100%)	347 (100%)	1 (0%)	86	93
4	k	348/349 (100%)	347 (100%)	1 (0%)	86	93
All	All	13437/15936 (84%)	13393 (100%)	44 (0%)	84	93

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	338	VAL
4	C	156	ASN
4	C	170	GLN
4	D	179	THR
4	E	264	LEU
4	F	156	ASN
4	F	294	LEU
4	H	170	GLN
4	H	213	GLN
4	I	30	LEU
4	I	170	GLN
4	J	170	GLN
4	L	133	SER
4	L	170	GLN

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Mol	Chain	Res	Type
4	L	246	THR
4	M	36	GLN
4	M	170	GLN
4	M	179	THR
4	N	189	GLN
4	O	68	THR
1	S	135	CYS
1	T	92	GLU
1	T	244	CYS
1	T	263	VAL
1	T	311	SER
1	U	326	ILE
1	V	209	THR
1	W	209	THR
1	Z	172	LEU
4	f	36	GLN
4	f	384	ARG
4	h	170	GLN
4	h	377	SER
4	h	384	ARG
4	i	30	LEU
4	i	170	GLN
4	j	170	GLN
4	k	170	GLN
1	t	92	GLU
1	t	227	THR
1	t	326	ILE
1	u	210	THR
1	u	317	LEU
1	w	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	104	GLN
1	0	305	GLN
1	1	176	GLN
2	2	324	ASN
2	2	348	ASN
2	2	405	HIS
2	4	324	ASN
2	4	348	ASN

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Mol	Chain	Res	Type
2	4	405	HIS
3	A	266	HIS
3	A	316	ASN
3	A	423	ASN
3	A	484	ASN
3	A	497	ASN
3	A	503	ASN
3	A	642	GLN
3	A	756	ASN
3	A	760	ASN
3	A	792	GLN
3	A	847	HIS
3	A	885	ASN
3	B	137	GLN
3	B	175	ASN
3	B	240	GLN
3	B	257	HIS
3	B	279	ASN
3	B	460	GLN
3	B	609	HIS
3	B	657	GLN
3	B	695	ASN
3	B	733	ASN
3	B	756	ASN
3	B	792	GLN
3	B	852	ASN
3	B	885	ASN
4	C	140	ASN
4	C	206	GLN
4	D	36	GLN
4	D	58	ASN
4	D	128	ASN
4	D	142	GLN
4	D	206	GLN
4	D	258	ASN
4	D	345	ASN
4	E	36	GLN
4	E	72	ASN
4	E	146	GLN
4	E	156	ASN
4	E	257	ASN
4	F	140	ASN

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Mol	Chain	Res	Type
4	F	167	ASN
4	F	175	ASN
4	F	206	GLN
4	F	310	ASN
4	G	47	GLN
4	G	58	ASN
4	G	128	ASN
4	G	140	ASN
4	G	206	GLN
4	G	268	GLN
4	G	383	GLN
4	H	44	ASN
4	H	142	GLN
4	H	204	ASN
4	H	206	GLN
4	H	383	GLN
4	I	32	GLN
4	I	146	GLN
4	I	204	ASN
4	I	206	GLN
4	J	128	ASN
4	J	140	ASN
4	J	156	ASN
4	J	170	GLN
4	J	175	ASN
4	J	204	ASN
4	J	206	GLN
4	J	257	ASN
4	K	32	GLN
4	K	140	ASN
4	L	140	ASN
4	L	200	ASN
4	L	204	ASN
4	L	206	GLN
4	L	345	ASN
4	L	373	ASN
4	M	32	GLN
4	M	47	GLN
4	M	140	ASN
4	M	206	GLN
4	M	345	ASN
4	M	383	GLN

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Mol	Chain	Res	Type
4	N	183	ASN
4	N	204	ASN
4	N	257	ASN
4	N	258	ASN
4	O	140	ASN
4	O	206	GLN
4	O	345	ASN
4	O	383	GLN
1	P	176	GLN
1	P	280	GLN
1	R	308	GLN
1	S	280	GLN
1	S	305	GLN
1	T	138	ASN
1	T	166	ASN
1	T	305	GLN
1	U	72	GLN
1	U	262	GLN
1	U	280	GLN
1	U	305	GLN
1	U	308	GLN
1	V	176	GLN
1	V	280	GLN
1	V	305	GLN
1	W	305	GLN
1	X	149	GLN
1	Y	52	ASN
1	Y	56	ASN
1	Y	72	GLN
1	Y	176	GLN
1	Y	305	GLN
1	Z	132	GLN
1	Z	288	ASN
4	f	140	ASN
4	f	156	ASN
4	f	167	ASN
4	f	175	ASN
4	f	206	GLN
4	g	36	GLN
4	g	47	GLN
4	g	58	ASN
4	g	105	GLN

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Mol	Chain	Res	Type
4	g	128	ASN
4	g	140	ASN
4	g	213	GLN
4	g	268	GLN
4	g	310	ASN
4	g	383	GLN
4	h	44	ASN
4	h	47	GLN
4	h	72	ASN
4	h	204	ASN
4	h	206	GLN
4	i	32	GLN
4	i	33	GLN
4	i	142	GLN
4	i	146	GLN
4	i	204	ASN
4	j	128	ASN
4	j	140	ASN
4	j	142	GLN
4	j	170	GLN
4	j	204	ASN
4	j	206	GLN
4	j	257	ASN
4	k	32	GLN
4	k	128	ASN
4	k	140	ASN
1	t	52	ASN
1	t	138	ASN
1	t	201	GLN
1	t	305	GLN
1	u	280	GLN
1	u	305	GLN
1	u	308	GLN
1	v	176	GLN
1	v	235	HIS
1	v	305	GLN
1	w	104	GLN
1	w	305	GLN
1	x	149	GLN
1	x	176	GLN
1	y	176	GLN
1	y	305	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	F	1	4	8,9,10	0.37	0	8,9,11	1.04	1 (12%)
4	FME	E	1	4	8,9,10	0.38	0	8,9,11	1.08	1 (12%)
4	FME	D	1	4	8,9,10	0.38	0	8,9,11	1.05	1 (12%)
4	FME	K	1	4	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
4	FME	J	1	4	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
4	FME	k	1	4	8,9,10	0.37	0	8,9,11	1.09	1 (12%)
4	FME	H	1	4	8,9,10	0.38	0	8,9,11	1.02	1 (12%)
4	FME	I	1	4	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
4	FME	L	1	4	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
4	FME	j	1	4	8,9,10	0.38	0	8,9,11	1.04	1 (12%)
4	FME	f	1	4	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
4	FME	g	1	4	8,9,10	0.38	0	8,9,11	1.07	1 (12%)
4	FME	h	1	4	8,9,10	0.38	0	8,9,11	1.06	1 (12%)
4	FME	M	1	4	8,9,10	0.38	0	8,9,11	1.04	1 (12%)
4	FME	N	1	4	8,9,10	0.38	0	8,9,11	1.03	1 (12%)
4	FME	i	1	4	8,9,10	0.38	0	8,9,11	1.00	1 (12%)
4	FME	C	1	4	8,9,10	0.38	0	8,9,11	1.07	1 (12%)
4	FME	G	1	4	8,9,10	0.38	0	8,9,11	1.04	1 (12%)
4	FME	O	1	4	8,9,10	0.38	0	8,9,11	1.05	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	F	1	4	-	1/7/9/11	-
4	FME	E	1	4	-	1/7/9/11	-
4	FME	D	1	4	-	1/7/9/11	-
4	FME	K	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	H	1	4	-	1/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-
4	FME	L	1	4	-	1/7/9/11	-
4	FME	j	1	4	-	1/7/9/11	-
4	FME	f	1	4	-	1/7/9/11	-
4	FME	g	1	4	-	1/7/9/11	-
4	FME	h	1	4	-	1/7/9/11	-
4	FME	M	1	4	-	1/7/9/11	-
4	FME	N	1	4	-	1/7/9/11	-
4	FME	i	1	4	-	1/7/9/11	-
4	FME	C	1	4	-	1/7/9/11	-
4	FME	G	1	4	-	1/7/9/11	-
4	FME	O	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	k	1	FME	CA-N-CN	2.47	126.63	122.82
4	C	1	FME	CA-N-CN	2.40	126.51	122.82
4	E	1	FME	CA-N-CN	2.40	126.51	122.82
4	g	1	FME	CA-N-CN	2.38	126.48	122.82
4	I	1	FME	CA-N-CN	2.38	126.48	122.82
4	h	1	FME	CA-N-CN	2.36	126.44	122.82
4	J	1	FME	CA-N-CN	2.35	126.44	122.82
4	f	1	FME	CA-N-CN	2.35	126.43	122.82
4	D	1	FME	CA-N-CN	2.33	126.40	122.82
4	O	1	FME	CA-N-CN	2.32	126.38	122.82
4	F	1	FME	CA-N-CN	2.31	126.38	122.82
4	M	1	FME	CA-N-CN	2.31	126.37	122.82
4	G	1	FME	CA-N-CN	2.29	126.34	122.82
4	j	1	FME	CA-N-CN	2.29	126.34	122.82
4	N	1	FME	CA-N-CN	2.27	126.31	122.82
4	K	1	FME	CA-N-CN	2.26	126.30	122.82
4	H	1	FME	CA-N-CN	2.25	126.28	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1	FME	CA-N-CN	2.25	126.28	122.82
4	i	1	FME	CA-N-CN	2.16	126.15	122.82

There are no chirality outliers.

All (19) 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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 109 are monoatomic - leaving 19 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	$\# Z > 2$
5	NAG	S	401	1	14,14,15	0.70	0	17,19,21	0.95	0
5	NAG	R	401	1	14,14,15	0.70	0	17,19,21	0.88	0
5	NAG	Y	401	1	14,14,15	0.70	0	17,19,21	0.94	0
5	NAG	W	401	1	14,14,15	0.71	0	17,19,21	0.88	0
5	NAG	x	401	1	14,14,15	0.71	0	17,19,21	0.84	0
5	NAG	Z	401	1	14,14,15	0.70	0	17,19,21	0.92	0
5	NAG	y	401	1	14,14,15	0.70	0	17,19,21	0.91	0
5	NAG	t	401	1	14,14,15	0.71	0	17,19,21	0.87	0
5	NAG	T	401	1	14,14,15	0.71	0	17,19,21	0.92	0
5	NAG	u	401	1	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
5	NAG	Q	401	1	14,14,15	0.69	0	17,19,21	0.98	0
5	NAG	0	401	1	14,14,15	0.70	0	17,19,21	0.98	0
5	NAG	w	401	1	14,14,15	0.71	0	17,19,21	0.87	0
5	NAG	v	401	1	14,14,15	0.71	0	17,19,21	0.88	0
5	NAG	X	401	1	14,14,15	0.70	0	17,19,21	0.84	0
5	NAG	U	401	1	14,14,15	0.70	0	17,19,21	0.90	0
5	NAG	P	401	1	14,14,15	0.71	0	17,19,21	0.84	0
5	NAG	l	401	1	14,14,15	0.73	0	17,19,21	0.92	0
5	NAG	V	401	1	14,14,15	0.69	0	17,19,21	0.93	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
5	NAG	S	401	1	-	4/6/23/26	0/1/1/1
5	NAG	R	401	1	-	4/6/23/26	0/1/1/1
5	NAG	Y	401	1	-	2/6/23/26	0/1/1/1
5	NAG	W	401	1	-	2/6/23/26	0/1/1/1
5	NAG	x	401	1	-	4/6/23/26	0/1/1/1
5	NAG	Z	401	1	-	3/6/23/26	0/1/1/1
5	NAG	y	401	1	-	3/6/23/26	0/1/1/1
5	NAG	t	401	1	-	2/6/23/26	0/1/1/1
5	NAG	T	401	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	u	401	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	401	1	-	2/6/23/26	0/1/1/1
5	NAG	0	401	1	-	2/6/23/26	0/1/1/1
5	NAG	w	401	1	-	2/6/23/26	0/1/1/1
5	NAG	v	401	1	-	4/6/23/26	0/1/1/1
5	NAG	X	401	1	-	2/6/23/26	0/1/1/1
5	NAG	U	401	1	-	4/6/23/26	0/1/1/1
5	NAG	P	401	1	-	2/6/23/26	0/1/1/1
5	NAG	1	401	1	-	2/6/23/26	0/1/1/1
5	NAG	V	401	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	u	401	NAG	O5-C1-C2	-2.06	108.11	111.29

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	v	401	NAG	O5-C5-C6-O6
5	T	401	NAG	O5-C5-C6-O6
5	R	401	NAG	O5-C5-C6-O6
5	v	401	NAG	C4-C5-C6-O6
5	T	401	NAG	C4-C5-C6-O6
5	R	401	NAG	C4-C5-C6-O6
5	V	401	NAG	O5-C5-C6-O6
5	V	401	NAG	C4-C5-C6-O6
5	S	401	NAG	C4-C5-C6-O6
5	S	401	NAG	O5-C5-C6-O6
5	0	401	NAG	C1-C2-N2-C7
5	P	401	NAG	C1-C2-N2-C7
5	Q	401	NAG	C1-C2-N2-C7
5	R	401	NAG	C1-C2-N2-C7
5	S	401	NAG	C1-C2-N2-C7
5	T	401	NAG	C1-C2-N2-C7
5	U	401	NAG	C1-C2-N2-C7
5	V	401	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	W	401	NAG	C1-C2-N2-C7
5	Y	401	NAG	C1-C2-N2-C7
5	Z	401	NAG	C1-C2-N2-C7
5	t	401	NAG	C1-C2-N2-C7
5	u	401	NAG	C1-C2-N2-C7
5	v	401	NAG	C1-C2-N2-C7
5	w	401	NAG	C1-C2-N2-C7
5	x	401	NAG	C1-C2-N2-C7
5	y	401	NAG	C1-C2-N2-C7
5	x	401	NAG	C4-C5-C6-O6
5	0	401	NAG	C3-C2-N2-C7
5	1	401	NAG	C3-C2-N2-C7
5	S	401	NAG	C3-C2-N2-C7
5	T	401	NAG	C3-C2-N2-C7
5	V	401	NAG	C3-C2-N2-C7
5	W	401	NAG	C3-C2-N2-C7
5	X	401	NAG	C3-C2-N2-C7
5	Y	401	NAG	C3-C2-N2-C7
5	Z	401	NAG	C3-C2-N2-C7
5	w	401	NAG	C3-C2-N2-C7
5	x	401	NAG	C3-C2-N2-C7
5	y	401	NAG	C3-C2-N2-C7
5	Z	401	NAG	C4-C5-C6-O6
5	U	401	NAG	C4-C5-C6-O6
5	1	401	NAG	C1-C2-N2-C7
5	X	401	NAG	C1-C2-N2-C7
5	x	401	NAG	O5-C5-C6-O6
5	y	401	NAG	C4-C5-C6-O6
5	P	401	NAG	C3-C2-N2-C7
5	Q	401	NAG	C3-C2-N2-C7
5	R	401	NAG	C3-C2-N2-C7
5	U	401	NAG	C3-C2-N2-C7
5	t	401	NAG	C3-C2-N2-C7
5	u	401	NAG	C3-C2-N2-C7
5	v	401	NAG	C3-C2-N2-C7
5	U	401	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45121. 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.