



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:55 PM UTC

PDB ID : 6WXF / pdb_00006wxf
EMDB ID : EMD-21956
Title : Cryo-EM reconstruction of VP5*/VP8* assembly from rhesus rotavirus particles - Intermediate conformation
Authors : Herrmann, T.; Harrison, S.C.; Jenni, S.
Deposited on : 2020-05-10
Resolution : 4.30 Å (reported)
Based on initial models : 1SLQ, 4V7Q

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

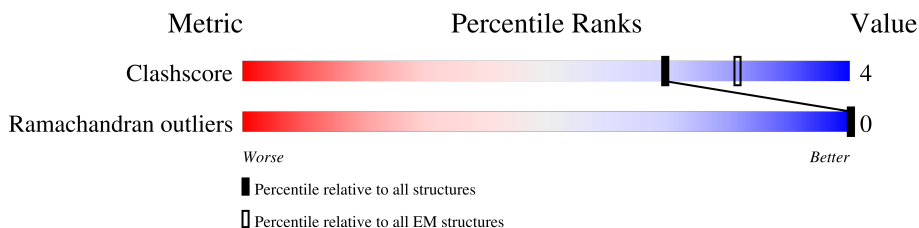
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

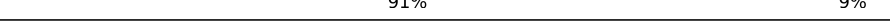
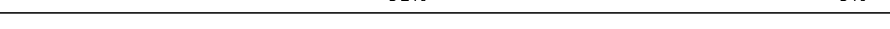
The reported resolution of this entry is 4.30 Å.

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

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	1	776	
1	2	776	
1	3	776	
2	A	397	
2	B	397	
2	C	397	
2	D	397	
2	E	397	
2	F	397	
2	G	397	

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Mol	Chain	Length	Quality of chain
2	H	397	
2	I	397	
2	J	397	
2	K	397	
2	L	397	
2	M	397	
2	N	397	
2	O	397	
2	P	397	
2	Q	397	
2	R	397	
3	a	326	
3	b	326	
3	c	326	
3	d	326	
3	e	326	
3	f	326	
3	g	326	
3	h	326	
3	i	326	
3	j	326	
3	k	326	
3	l	326	
3	m	326	
3	n	326	

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Mol	Chain	Length	Quality of chain
3	o	326	78% 19%
3	p	326	76% 7% 17%
3	q	326	70% 10% 21%
3	r	326	76% 8% 17%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 212266 atoms, of which 105044 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 protein VP4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	511	Total	C	H	N	O	S	0	0
			8009	2543	3973	688	788	17		
1	2	510	Total	C	H	N	O	S	0	0
			7998	2539	3970	686	785	18		
1	3	507	Total	C	H	N	O	S	0	0
			7944	2524	3943	680	779	18		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	567	CYS	SER	engineered mutation	UNP G0YZG6
1	590	CYS	ALA	engineered mutation	UNP G0YZG6
2	567	CYS	SER	engineered mutation	UNP G0YZG6
2	590	CYS	ALA	engineered mutation	UNP G0YZG6
3	567	CYS	SER	engineered mutation	UNP G0YZG6
3	590	CYS	ALA	engineered mutation	UNP G0YZG6

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	B	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	C	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	D	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	E	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	F	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	G	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	I	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	J	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	K	397	Total	C	H	N	O	S	0	0
			6276	2004	3113	551	593	15		
2	L	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	M	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	N	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	O	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	P	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	Q	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		
2	R	397	Total	C	H	N	O	S	0	0
			6275	2004	3112	551	593	15		

- Molecule 3 is a protein called Outer capsid glycoprotein VP7.

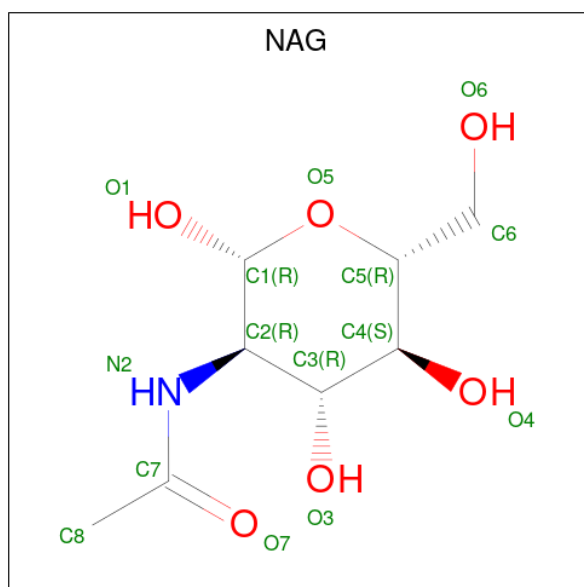
Mol	Chain	Residues	Atoms						AltConf	Trace
3	a	259	Total	C	H	N	O	S	0	0
			4040	1298	1993	324	409	16		
3	b	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	c	261	Total	C	H	N	O	S	0	0
			4073	1308	2010	327	412	16		
3	d	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	e	260	Total	C	H	N	O	S	0	0
			4049	1302	1997	323	411	16		
3	f	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	g	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	h	259	Total	C	H	N	O	S	0	0
			4040	1298	1993	324	409	16		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	i	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	j	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	k	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	l	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	m	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	n	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	o	265	Total	C	H	N	O	S	0	0
			4132	1328	2036	333	419	16		
3	p	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		
3	q	259	Total	C	H	N	O	S	0	0
			4040	1298	1993	324	409	16		
3	r	272	Total	C	H	N	O	S	0	0
			4253	1369	2098	342	428	16		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms					AltConf
4	b	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	c	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	d	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	e	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	f	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	g	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	h	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	i	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	j	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	k	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	l	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	m	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	n	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	o	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	p	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	q	1	Total	C	H	N	O	0
			28	8	14	1	5	
4	r	1	Total	C	H	N	O	0
			28	8	14	1	5	

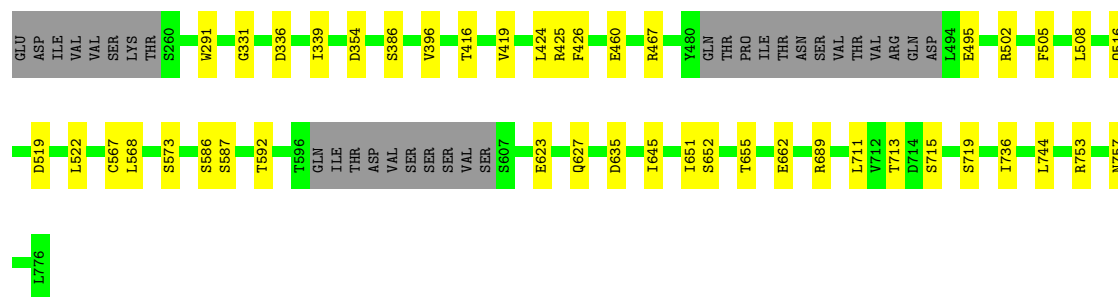
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	a	3	Total	Ca	0
			3	3	
5	b	3	Total	Ca	0
			3	3	

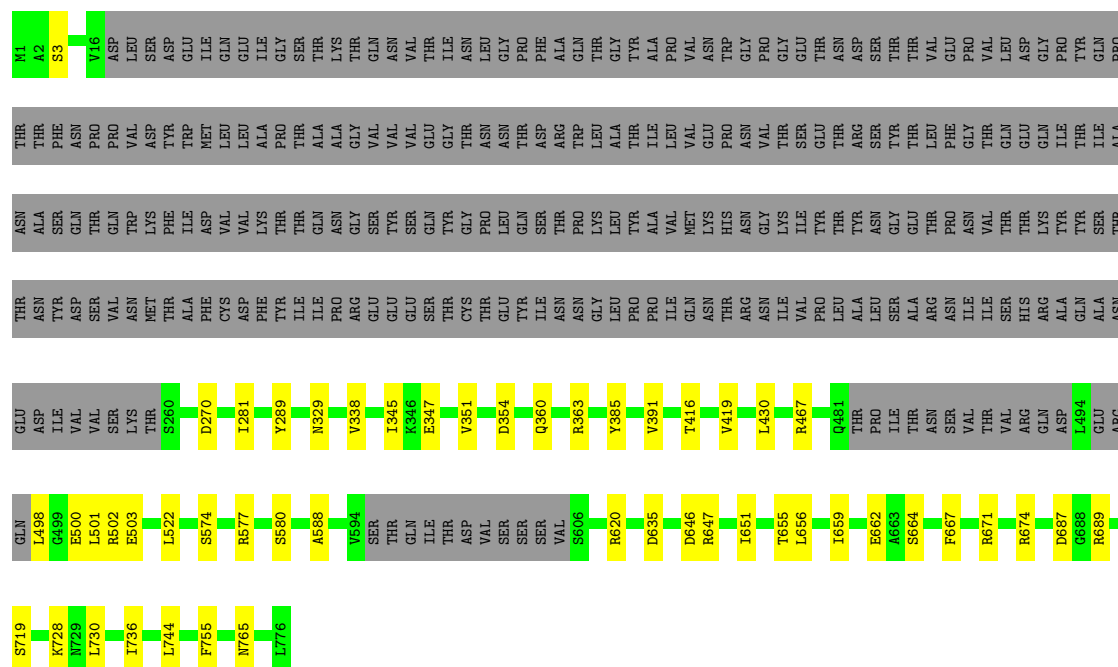
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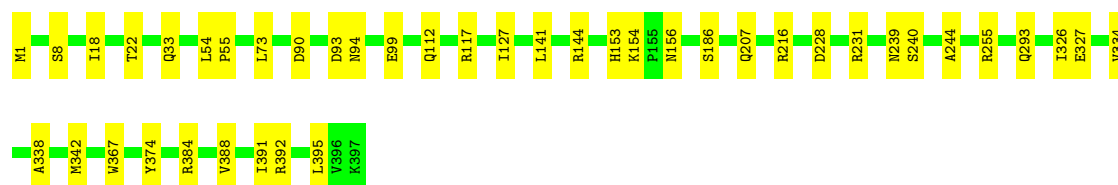
Mol	Chain	Residues	Atoms		AltConf
5	c	3	Total 3	Ca 3	0
5	d	3	Total 3	Ca 3	0
5	e	3	Total 3	Ca 3	0
5	f	3	Total 3	Ca 3	0
5	g	3	Total 3	Ca 3	0
5	h	3	Total 3	Ca 3	0
5	i	3	Total 3	Ca 3	0
5	j	3	Total 3	Ca 3	0
5	k	3	Total 3	Ca 3	0
5	l	3	Total 3	Ca 3	0
5	m	3	Total 3	Ca 3	0
5	n	3	Total 3	Ca 3	0
5	o	3	Total 3	Ca 3	0
5	p	3	Total 3	Ca 3	0
5	q	3	Total 3	Ca 3	0
5	r	3	Total 3	Ca 3	0



- Molecule 1: Outer capsid protein VP4



- Molecule 2: Intermediate capsid protein VP6

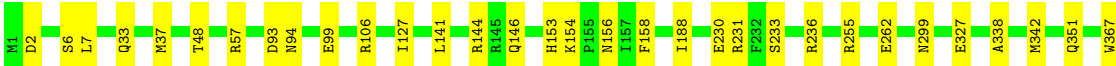


- Molecule 2: Intermediate capsid protein VP6



K397

- Molecule 2: Intermediate capsid protein VP6

Chain C:  91% 9%



- Molecule 2: Intermediate capsid protein VP6

Chain D:  91% 9%



- Molecule 2: Intermediate capsid protein VP6

Chain E:  91% 9%



- Molecule 2: Intermediate capsid protein VP6

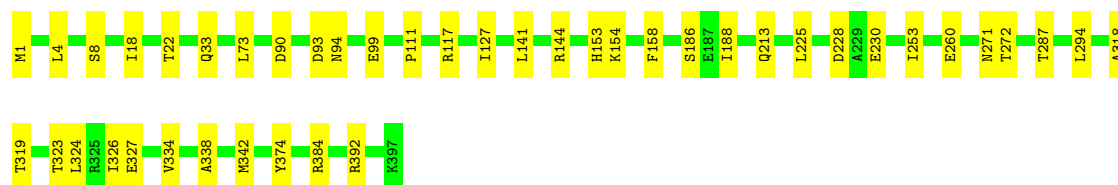
Chain F:  92% 8%



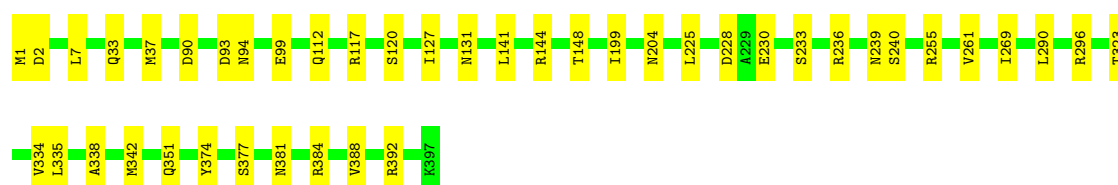
- Molecule 2: Intermediate capsid protein VP6

Chain G:  93% 7%

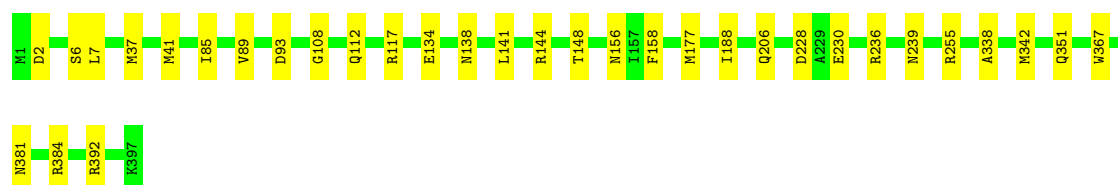

● Molecule 2: Intermediate capsid protein VP6

Chain H:  89% 11%

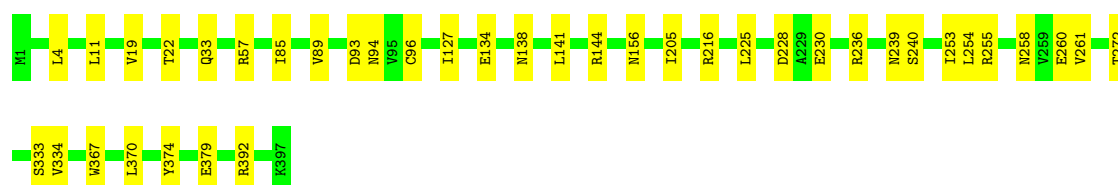
● Molecule 2: Intermediate capsid protein VP6

Chain I:  89% 11%

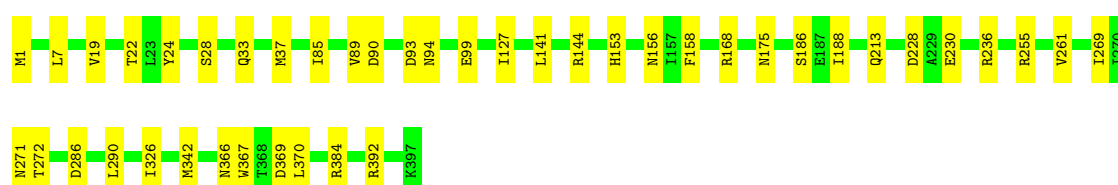
● Molecule 2: Intermediate capsid protein VP6

Chain J:  92% 8%

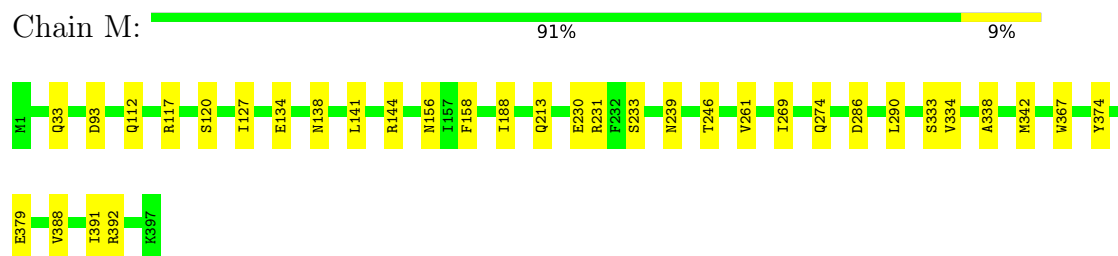
● Molecule 2: Intermediate capsid protein VP6

Chain K:  90% 10%

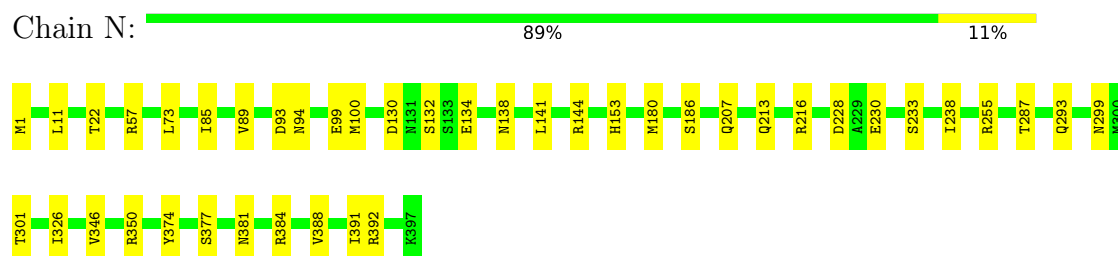
● Molecule 2: Intermediate capsid protein VP6

Chain L:  89% 11%

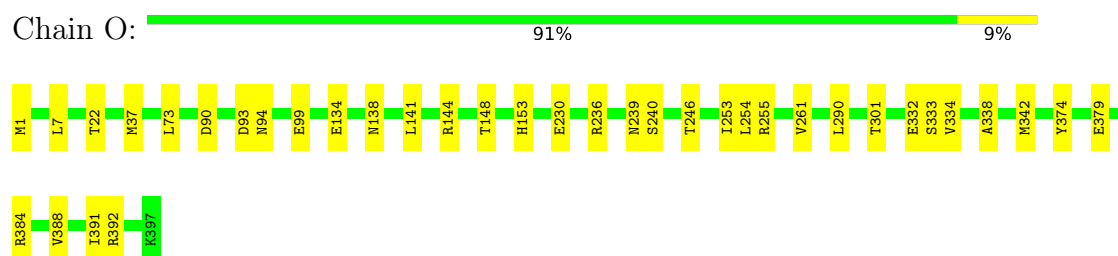
- Molecule 2: Intermediate capsid protein VP6



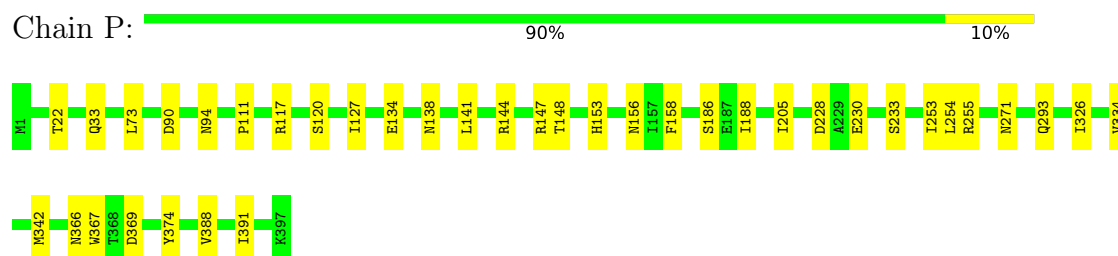
- Molecule 2: Intermediate capsid protein VP6



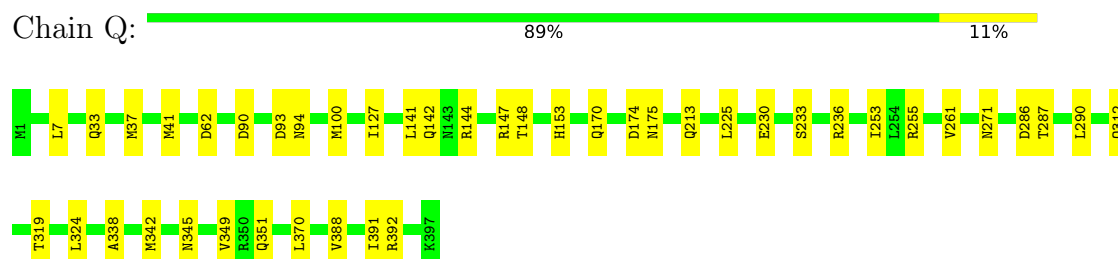
- Molecule 2: Intermediate capsid protein VP6



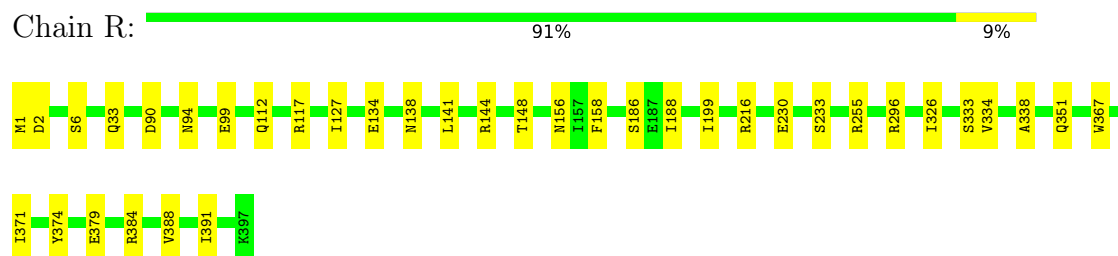
- Molecule 2: Intermediate capsid protein VP6



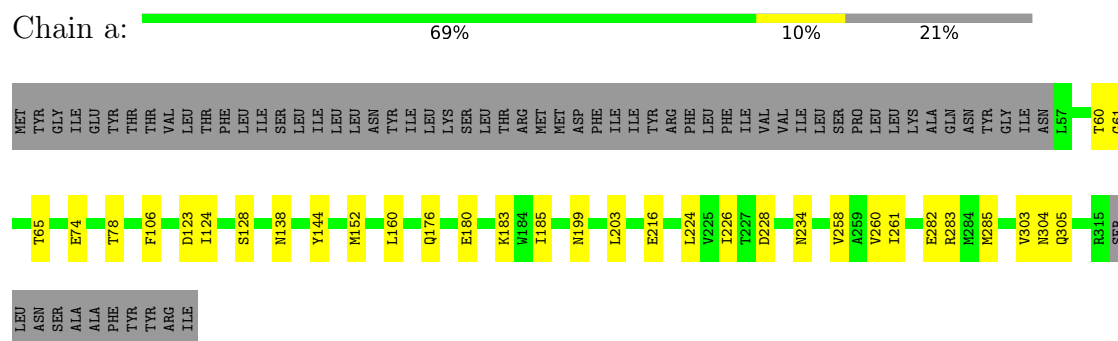
- Molecule 2: Intermediate capsid protein VP6



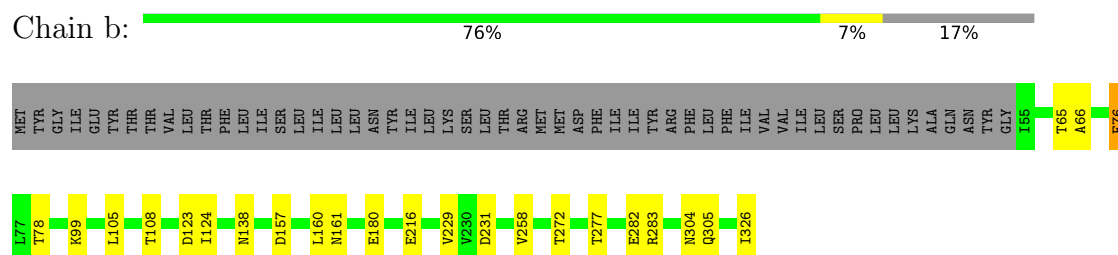
- Molecule 2: Intermediate capsid protein VP6



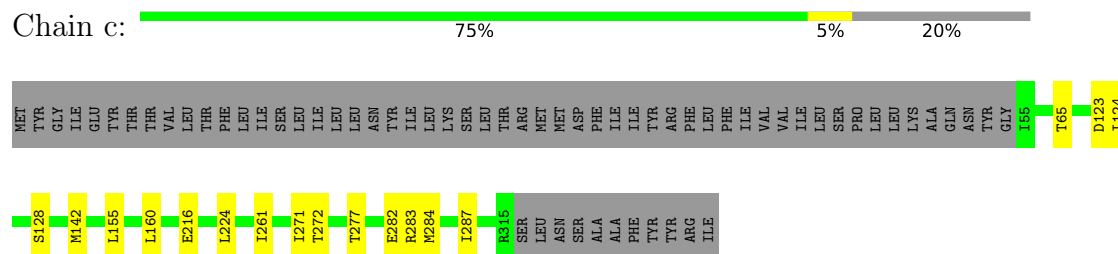
- Molecule 3: Outer capsid glycoprotein VP7



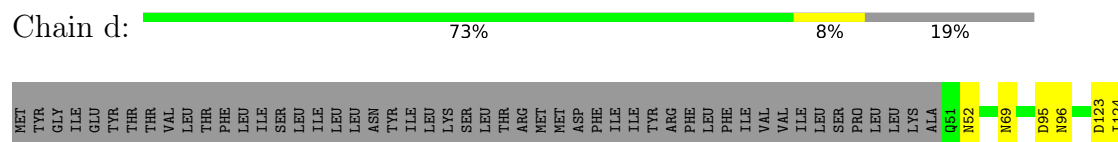
- Molecule 3: Outer capsid glycoprotein VP7



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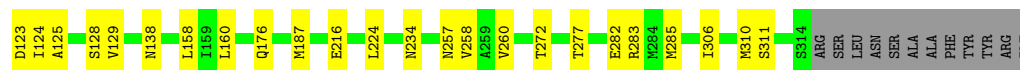
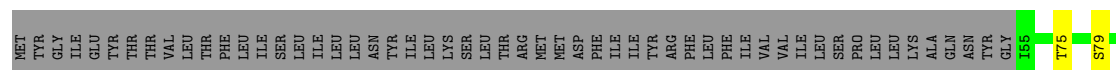


- Molecule 3: Outer capsid glycoprotein VP7

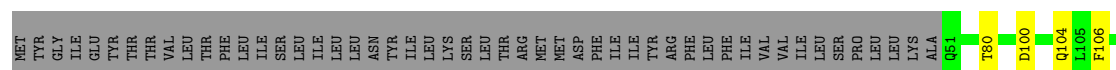




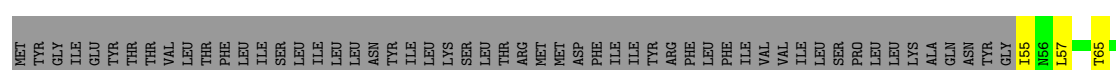
• Molecule 3: Outer capsid glycoprotein VP7



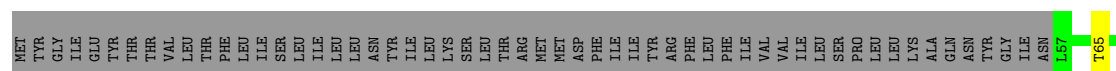
• Molecule 3: Outer capsid glycoprotein VP7



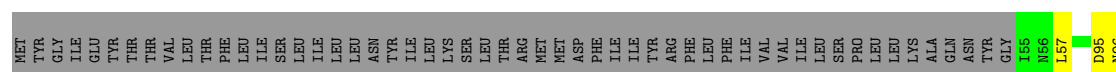
• Molecule 3: Outer capsid glycoprotein VP7



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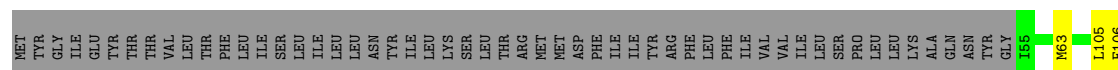
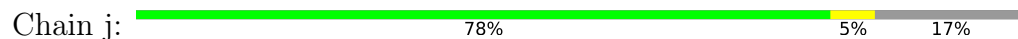


• Molecule 3: Outer capsid glycoprotein VP7

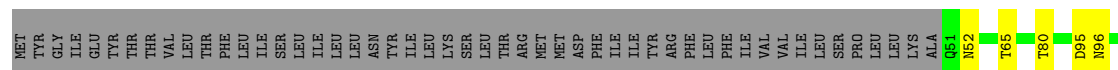




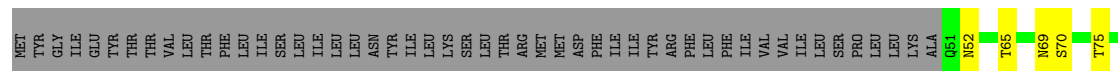
- Molecule 3: Outer capsid glycoprotein VP7



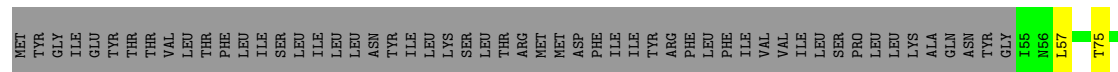
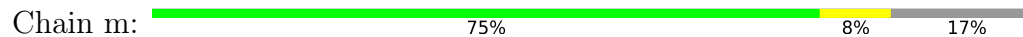
- Molecule 3: Outer capsid glycoprotein VP7



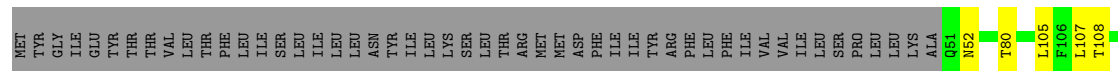
- Molecule 3: Outer capsid glycoprotein VP7



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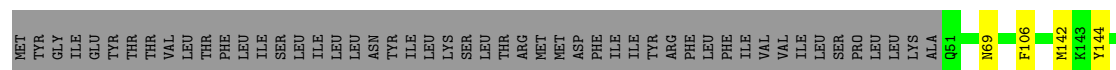
- Molecule 3: Outer capsid glycoprotein VP7





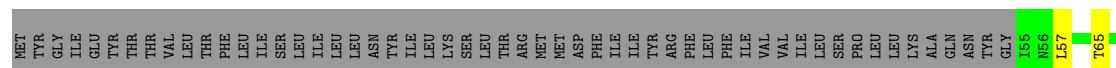
- Molecule 3: Outer capsid glycoprotein VP7

Chain o:
78% 19%



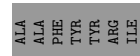
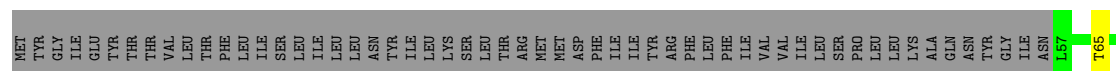
- Molecule 3: Outer capsid glycoprotein VP7

Chain p:
76% 7% 17%



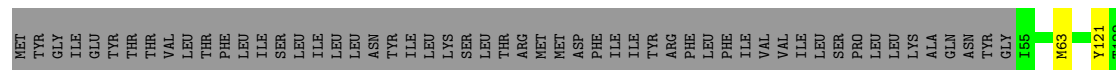
- Molecule 3: Outer capsid glycoprotein VP7

Chain q:
70% 10% 21%



- Molecule 3: Outer capsid glycoprotein VP7

Chain r:
76% 8% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82008	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	40605	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	1	0.20	0/4109	0.42	0/5561
1	2	0.21	0/4101	0.44	0/5549
1	3	0.20	0/4073	0.42	0/5510
2	A	0.19	0/3233	0.40	0/4397
2	B	0.19	0/3233	0.42	0/4397
2	C	0.19	0/3233	0.41	0/4397
2	D	0.19	0/3233	0.41	0/4397
2	E	0.18	0/3233	0.41	0/4397
2	F	0.19	0/3233	0.40	0/4397
2	G	0.19	0/3233	0.41	0/4397
2	H	0.19	0/3233	0.40	0/4397
2	I	0.19	0/3233	0.40	0/4397
2	J	0.19	0/3233	0.42	0/4397
2	K	0.19	0/3233	0.41	0/4397
2	L	0.18	0/3233	0.41	0/4397
2	M	0.19	0/3233	0.41	0/4397
2	N	0.19	0/3233	0.41	0/4397
2	O	0.19	0/3233	0.43	0/4397
2	P	0.18	0/3233	0.40	0/4397
2	Q	0.19	0/3233	0.40	0/4397
2	R	0.20	0/3233	0.42	0/4397
3	a	0.17	0/2089	0.39	0/2854
3	b	0.18	0/2200	0.42	0/3005
3	c	0.17	0/2105	0.38	0/2876
3	d	0.16	0/2139	0.38	0/2922
3	e	0.17	0/2094	0.40	0/2862
3	f	0.17	0/2139	0.39	0/2922
3	g	0.17	0/2200	0.39	0/3005
3	h	0.17	0/2089	0.39	0/2854
3	i	0.16	0/2200	0.38	0/3005
3	j	0.16	0/2200	0.38	0/3005
3	k	0.17	0/2139	0.39	0/2922

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	l	0.17	0/2139	0.39	0/2922
3	m	0.16	0/2200	0.38	0/3005
3	n	0.17	0/2139	0.40	0/2922
3	o	0.16	0/2139	0.38	0/2922
3	p	0.18	0/2200	0.38	0/3005
3	q	0.17	0/2089	0.38	0/2854
3	r	0.17	0/2200	0.39	0/3005
All	All	0.18	0/109177	0.40	0/148633

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
3	b	0	2
3	e	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	537	THR	Peptide
1	1	589	SER	Peptide
3	b	66	ALA	Peptide
3	b	76	PHE	Peptide
3	e	311	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	4036	3973	3971	37	0
1	2	4028	3970	3968	30	0
1	3	4001	3943	3941	35	0
2	A	3163	3112	3112	28	0
2	B	3163	3112	3112	24	0
2	C	3163	3112	3112	28	0
2	D	3163	3112	3112	22	0
2	E	3163	3112	3112	21	0
2	F	3163	3113	3112	20	0
2	G	3163	3112	3112	19	0
2	H	3163	3112	3112	27	0
2	I	3163	3112	3112	30	0
2	J	3163	3112	3112	24	0
2	K	3163	3113	3112	26	0
2	L	3163	3112	3112	28	0
2	M	3163	3112	3112	23	0
2	N	3163	3112	3112	27	0
2	O	3163	3112	3112	27	0
2	P	3163	3112	3112	26	0
2	Q	3163	3112	3112	31	0
2	R	3163	3112	3112	24	0
3	a	2047	1993	1993	21	0
3	b	2155	2098	2097	16	0
3	c	2063	2010	2010	10	0
3	d	2096	2036	2036	16	0
3	e	2052	1997	1997	17	0
3	f	2096	2036	2036	17	0
3	g	2155	2098	2098	23	0
3	h	2047	1993	1992	17	0
3	i	2155	2098	2098	23	0
3	j	2155	2098	2098	11	0
3	k	2096	2036	2036	21	0
3	l	2096	2036	2036	16	0
3	m	2155	2098	2098	20	0
3	n	2096	2036	2036	18	0
3	o	2096	2036	2036	8	0
3	p	2155	2098	2098	15	0
3	q	2047	1993	1992	20	0
3	r	2155	2098	2098	16	0
4	a	14	14	13	0	0
4	b	14	14	13	0	0
4	c	14	14	13	0	0
4	d	14	14	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	e	14	14	13	0	0
4	f	14	14	13	0	0
4	g	14	14	13	0	0
4	h	14	14	13	0	0
4	i	14	14	13	0	0
4	j	14	14	13	0	0
4	k	14	14	13	0	0
4	l	14	14	13	0	0
4	m	14	14	13	0	0
4	n	14	14	13	0	0
4	o	14	14	13	0	0
4	p	14	14	13	0	0
4	q	14	14	13	0	0
4	r	14	14	13	0	0
5	a	3	0	0	0	0
5	b	3	0	0	0	0
5	c	3	0	0	0	0
5	d	3	0	0	0	0
5	e	3	0	0	0	0
5	f	3	0	0	0	0
5	g	3	0	0	0	0
5	h	3	0	0	0	0
5	i	3	0	0	0	0
5	j	3	0	0	0	0
5	k	3	0	0	0	0
5	l	3	0	0	0	0
5	m	3	0	0	0	0
5	n	3	0	0	0	0
5	o	3	0	0	0	0
5	p	3	0	0	0	0
5	q	3	0	0	0	0
5	r	3	0	0	0	0
All	All	107222	105044	105015	768	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 (768) 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)
1:3:501:LEU:HD13	1:3:659:ILE:HD11	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:141:LEU:O	2:R:144:ARG:C	2.29	0.75
1:1:557:LEU:HD21	1:1:624:MET:HE1	1.69	0.74
2:L:141:LEU:O	2:L:144:ARG:C	2.30	0.74
2:B:255:ARG:NH1	3:a:65:THR:O	2.20	0.74
2:D:141:LEU:O	2:D:144:ARG:O	2.07	0.73
3:c:272:THR:OG1	3:c:277:THR:OG1	2.08	0.72
3:g:326:ILE:HG21	3:k:80:THR:HG21	1.70	0.72
2:G:255:ARG:NH1	3:h:65:THR:O	2.23	0.71
2:R:255:ARG:NH1	3:p:65:THR:O	2.23	0.71
2:I:239:ASN:ND2	2:I:240:SER:O	2.23	0.71
2:K:255:ARG:NH1	3:l:65:THR:O	2.23	0.71
2:D:239:ASN:ND2	2:D:240:SER:O	2.24	0.71
2:G:334:VAL:O	2:G:374:TYR:OH	2.07	0.71
2:F:141:LEU:O	2:F:144:ARG:C	2.34	0.70
2:A:334:VAL:O	2:A:374:TYR:OH	2.09	0.70
3:l:160:LEU:O	3:l:283:ARG:NH2	2.25	0.70
1:1:627:GLN:NE2	1:2:522:LEU:O	2.24	0.70
2:I:255:ARG:NH1	3:g:65:THR:O	2.25	0.70
2:R:141:LEU:O	2:R:144:ARG:O	2.10	0.69
2:F:141:LEU:O	2:F:144:ARG:O	2.10	0.69
2:A:255:ARG:NH1	3:c:65:THR:O	2.25	0.69
2:K:141:LEU:O	2:K:144:ARG:O	2.11	0.69
2:O:141:LEU:O	2:O:144:ARG:O	2.11	0.69
2:J:342:MET:SD	2:J:342:MET:N	2.66	0.68
2:L:141:LEU:O	2:L:144:ARG:O	2.11	0.68
2:E:239:ASN:ND2	2:E:240:SER:O	2.25	0.68
1:1:593:ASP:OD2	1:1:618:ARG:NH2	2.27	0.68
3:e:272:THR:HG1	3:e:277:THR:HG1	1.39	0.68
2:A:216:ARG:NH2	2:A:374:TYR:O	2.27	0.67
2:K:239:ASN:ND2	2:K:240:SER:O	2.25	0.67
2:M:246:THR:O	2:O:301:THR:OG1	2.12	0.67
2:P:230:GLU:O	2:P:233:SER:OG	2.11	0.67
1:3:270:ASP:OD1	1:3:467:ARG:NH1	2.26	0.67
2:K:228:ASP:OD2	2:L:236:ARG:NH2	2.28	0.67
3:m:75:THR:O	3:m:79:SER:OG	2.11	0.67
2:A:239:ASN:OD1	2:C:255:ARG:NH2	2.27	0.67
2:C:141:LEU:O	2:C:144:ARG:O	2.12	0.67
3:n:52:ASN:ND2	3:p:57:LEU:O	2.28	0.67
2:P:111:PRO:O	2:P:117:ARG:NH1	2.27	0.67
3:h:272:THR:OG1	3:h:277:THR:OG1	2.07	0.67
2:G:111:PRO:O	2:G:117:ARG:NH1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:342:MET:SD	2:M:342:MET:N	2.68	0.66
2:R:334:VAL:O	2:R:374:TYR:OH	2.11	0.66
3:d:267:ASP:OD2	3:d:280:GLN:NE2	2.28	0.66
2:P:147:ARG:NH1	2:P:148:THR:O	2.29	0.66
2:O:141:LEU:O	2:O:144:ARG:C	2.37	0.66
2:K:216:ARG:NH2	2:K:374:TYR:O	2.29	0.66
3:g:160:LEU:O	3:g:283:ARG:NH2	2.29	0.66
3:i:272:THR:OG1	3:i:277:THR:OG1	2.13	0.66
3:e:272:THR:OG1	3:e:277:THR:OG1	2.12	0.66
3:e:160:LEU:O	3:e:283:ARG:NH2	2.28	0.66
2:J:141:LEU:O	2:J:144:ARG:C	2.39	0.66
2:N:141:LEU:O	2:N:144:ARG:O	2.14	0.66
3:r:272:THR:HG1	3:r:277:THR:HG1	1.44	0.66
1:1:535:LYS:NZ	1:1:649:THR:O	2.29	0.65
2:F:93:ASP:OD1	2:F:392:ARG:NE	2.29	0.65
2:F:134:GLU:O	2:F:138:ASN:ND2	2.29	0.65
2:Q:342:MET:SD	2:Q:342:MET:N	2.69	0.65
2:F:342:MET:SD	2:F:342:MET:N	2.68	0.65
2:J:236:ARG:NH2	2:L:228:ASP:OD2	2.29	0.65
3:h:157:ASP:OD1	3:h:161:ASN:ND2	2.29	0.65
2:J:112:GLN:OE1	2:J:117:ARG:NH2	2.29	0.65
3:d:52:ASN:ND2	3:i:57:LEU:O	2.29	0.65
3:f:160:LEU:O	3:f:283:ARG:NH2	2.29	0.65
2:D:156:ASN:O	2:D:367:TRP:NE1	2.30	0.65
1:2:3:SER:N	1:2:635:ASP:OD1	2.30	0.65
2:M:213:GLN:NE2	2:M:286:ASP:OD2	2.29	0.65
3:b:326:ILE:HG21	3:f:80:THR:HG21	1.79	0.65
2:E:112:GLN:OE1	2:E:117:ARG:NH2	2.30	0.65
2:H:228:ASP:OD2	2:I:236:ARG:NH2	2.30	0.65
2:B:93:ASP:OD1	2:B:392:ARG:NE	2.30	0.64
2:D:141:LEU:O	2:D:144:ARG:C	2.40	0.64
2:L:213:GLN:NE2	2:L:286:ASP:OD2	2.30	0.64
3:i:160:LEU:O	3:i:283:ARG:NH2	2.30	0.64
2:G:216:ARG:NH2	2:G:374:TYR:O	2.29	0.64
3:b:272:THR:OG1	3:b:277:THR:OG1	2.15	0.64
3:e:176:GLN:NE2	3:e:234:ASN:OD1	2.31	0.64
3:m:313:ARG:NH2	3:m:316:SER:O	2.30	0.64
3:q:75:THR:O	3:q:79:SER:OG	2.10	0.64
3:p:306:ILE:HG22	3:p:310:MET:HE2	1.79	0.64
3:r:160:LEU:O	3:r:283:ARG:NH2	2.31	0.64
1:1:477:ASN:ND2	1:1:479:ASP:OD2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:MET:SD	2:C:342:MET:N	2.71	0.64
1:3:674:ARG:NH1	1:3:719:SER:O	2.31	0.64
2:M:112:GLN:OE1	2:M:117:ARG:NH2	2.30	0.64
3:l:52:ASN:ND2	3:m:57:LEU:O	2.31	0.64
3:e:306:ILE:HG22	3:e:310:MET:HE2	1.79	0.64
3:g:57:LEU:O	3:k:52:ASN:ND2	2.31	0.64
2:G:141:LEU:O	2:G:144:ARG:C	2.41	0.63
3:h:306:ILE:HG22	3:h:310:MET:HE2	1.79	0.63
3:r:306:ILE:HG22	3:r:310:MET:HE2	1.80	0.63
1:l:511:GLU:OE1	1:l:647:ARG:NH1	2.31	0.63
3:n:199:ASN:ND2	3:n:201:GLN:OE1	2.30	0.63
2:J:255:ARG:NH1	3:k:65:THR:O	2.32	0.63
3:q:165:CYS:SG	3:q:247:ARG:NH1	2.71	0.63
2:N:301:THR:OG1	2:O:246:THR:O	2.12	0.63
1:2:689:ARG:NH2	2:C:262:GLU:OE1	2.32	0.63
2:B:141:LEU:O	2:B:144:ARG:C	2.42	0.63
3:b:105:LEU:O	3:b:108:THR:OG1	2.14	0.63
2:Q:141:LEU:O	2:Q:144:ARG:O	2.17	0.62
2:A:33:GLN:NE2	2:A:127:ILE:O	2.31	0.62
2:H:342:MET:SD	2:H:342:MET:N	2.72	0.62
2:A:244:ALA:O	2:C:299:ASN:ND2	2.31	0.62
2:C:255:ARG:NH1	3:b:65:THR:O	2.32	0.62
2:H:271:ASN:ND2	2:I:351:GLN:OE1	2.33	0.62
2:H:141:LEU:O	2:H:144:ARG:O	2.17	0.62
2:K:141:LEU:O	2:K:144:ARG:C	2.42	0.62
2:P:228:ASP:OD2	2:Q:236:ARG:NH2	2.32	0.62
3:g:55:ILE:N	3:k:52:ASN:O	2.32	0.62
3:i:165:CYS:SG	3:i:247:ARG:NH1	2.73	0.62
3:i:211:ASP:O	3:i:214:THR:OG1	2.15	0.62
2:I:117:ARG:O	2:I:120:SER:OG	2.17	0.62
2:P:141:LEU:O	2:P:144:ARG:O	2.18	0.62
2:H:213:GLN:OE1	2:H:287:THR:OG1	2.13	0.62
2:N:141:LEU:O	2:N:144:ARG:C	2.43	0.62
1:2:711:LEU:O	1:2:715:SER:OG	2.16	0.62
2:N:186:SER:OG	2:N:326:ILE:O	2.17	0.62
2:G:141:LEU:O	2:G:144:ARG:O	2.17	0.62
2:I:230:GLU:O	2:I:233:SER:OG	2.10	0.62
1:3:736:ILE:HD11	1:3:744:LEU:HD12	1.82	0.61
2:A:342:MET:SD	2:A:342:MET:N	2.72	0.61
1:2:623:GLU:OE2	1:2:719:SER:OG	2.17	0.61
2:L:93:ASP:OD1	2:L:392:ARG:NE	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:138:ASN:OD1	2:O:148:THR:OG1	2.17	0.61
2:A:141:LEU:O	2:A:144:ARG:C	2.43	0.61
1:1:438:SER:OG	1:1:445:SER:OG	2.12	0.61
1:3:728:LYS:NZ	2:M:269:ILE:O	2.32	0.61
2:P:334:VAL:O	2:P:374:TYR:OH	2.16	0.61
2:J:138:ASN:OD1	2:J:148:THR:OG1	2.18	0.61
2:Q:93:ASP:OD1	2:Q:392:ARG:NE	2.33	0.61
1:3:765:ASN:ND2	2:M:274:GLN:OE1	2.34	0.61
1:2:652:SER:OG	1:2:655:THR:OG1	2.18	0.61
2:I:342:MET:SD	2:I:342:MET:N	2.74	0.61
1:3:416:THR:OG1	1:3:419:VAL:O	2.18	0.61
2:B:57:ARG:NH1	2:B:94:ASN:OD1	2.34	0.61
2:C:141:LEU:O	2:C:144:ARG:C	2.43	0.61
2:M:334:VAL:O	2:M:374:TYR:OH	2.14	0.61
2:A:112:GLN:OE1	2:A:117:ARG:NH2	2.34	0.60
2:I:141:LEU:O	2:I:144:ARG:C	2.44	0.60
2:J:141:LEU:O	2:J:144:ARG:O	2.20	0.60
2:H:153:HIS:ND1	2:I:338:ALA:O	2.34	0.60
2:B:230:GLU:OE2	2:C:231:ARG:NH2	2.34	0.60
3:b:160:LEU:O	3:b:283:ARG:NH2	2.35	0.60
1:3:580:SER:O	2:K:258:ASN:ND2	2.32	0.60
2:D:342:MET:SD	2:D:342:MET:N	2.75	0.60
3:k:105:LEU:O	3:k:108:THR:OG1	2.17	0.60
2:P:255:ARG:NH1	3:q:65:THR:O	2.35	0.60
3:n:157:ASP:OD1	3:n:161:ASN:ND2	2.34	0.60
1:1:416:THR:OG1	1:1:419:VAL:O	2.20	0.60
2:P:141:LEU:O	2:P:144:ARG:C	2.44	0.60
2:L:342:MET:SD	2:L:342:MET:N	2.75	0.60
2:O:93:ASP:OD1	2:O:392:ARG:NE	2.34	0.60
2:Q:255:ARG:NH1	3:r:63:MET:O	2.35	0.59
3:n:121:TYR:OH	3:n:141:LEU:O	2.18	0.59
3:h:165:CYS:SG	3:h:247:ARG:NH1	2.75	0.59
3:h:177:GLN:NE2	3:h:229:VAL:O	2.35	0.59
2:E:90:ASP:O	2:E:94:ASN:ND2	2.35	0.59
2:J:93:ASP:OD1	2:J:392:ARG:NE	2.36	0.59
3:q:160:LEU:O	3:q:283:ARG:NH2	2.35	0.59
2:E:141:LEU:O	2:E:144:ARG:O	2.20	0.59
3:p:176:GLN:NE2	3:p:234:ASN:OD1	2.36	0.59
2:B:141:LEU:O	2:B:144:ARG:O	2.20	0.59
2:F:216:ARG:NH2	2:F:374:TYR:O	2.36	0.59
3:n:160:LEU:O	3:n:283:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:160:LEU:O	3:k:283:ARG:NH2	2.35	0.58
2:P:90:ASP:O	2:P:94:ASN:ND2	2.36	0.58
2:B:271:ASN:ND2	2:C:351:GLN:OE1	2.37	0.58
2:L:255:ARG:NH1	3:j:63:MET:O	2.36	0.58
2:N:216:ARG:NH2	2:N:374:TYR:O	2.36	0.58
2:Q:170:GLN:NE2	2:Q:175:ASN:O	2.36	0.58
1:3:687:ASP:OD2	1:3:689:ARG:NE	2.36	0.58
2:I:141:LEU:O	2:I:144:ARG:O	2.22	0.58
2:A:90:ASP:OD1	2:A:94:ASN:ND2	2.36	0.58
2:G:230:GLU:O	2:G:233:SER:OG	2.13	0.58
3:k:272:THR:HG1	3:k:277:THR:HG1	1.51	0.58
2:A:99:GLU:OE2	2:A:384:ARG:NH1	2.37	0.58
2:M:117:ARG:O	2:M:120:SER:OG	2.16	0.57
3:k:165:CYS:SG	3:k:247:ARG:NH1	2.77	0.57
3:l:75:THR:O	3:l:79:SER:OG	2.10	0.57
2:I:93:ASP:OD1	2:I:392:ARG:NE	2.34	0.57
2:N:93:ASP:OD1	2:N:392:ARG:NE	2.37	0.57
2:O:334:VAL:O	2:O:374:TYR:OH	2.21	0.57
2:M:141:LEU:O	2:M:144:ARG:O	2.22	0.57
3:c:128:SER:HB2	3:c:224:LEU:HD22	1.86	0.57
2:G:342:MET:N	2:G:342:MET:SD	2.78	0.57
2:E:156:ASN:O	2:E:367:TRP:NE1	2.37	0.57
1:1:323:MET:SD	1:1:323:MET:N	2.78	0.57
2:N:213:GLN:OE1	2:N:287:THR:OG1	2.12	0.57
3:i:183:LYS:NZ	3:i:228:ASP:OD2	2.38	0.57
2:N:57:ARG:NH1	2:N:94:ASN:OD1	2.37	0.57
2:P:342:MET:SD	2:P:342:MET:N	2.78	0.57
2:L:186:SER:OG	2:L:326:ILE:O	2.23	0.57
1:1:375:LEU:O	3:m:208:LEU:HD21	2.05	0.56
3:a:176:GLN:NE2	3:a:234:ASN:OD1	2.37	0.56
2:J:255:ARG:NH2	2:K:239:ASN:OD1	2.39	0.56
2:K:260:GLU:OE2	2:K:272:THR:OG1	2.23	0.56
2:O:134:GLU:O	2:O:138:ASN:ND2	2.39	0.56
2:H:141:LEU:O	2:H:144:ARG:C	2.48	0.56
3:a:183:LYS:NZ	3:a:228:ASP:OD2	2.39	0.56
2:Q:225:LEU:HD13	2:Q:324:LEU:HD12	1.88	0.56
3:g:272:THR:OG1	3:g:277:THR:OG1	2.23	0.56
2:H:1:MET:HE1	2:H:384:ARG:HG3	1.88	0.56
3:l:272:THR:OG1	3:l:277:THR:OG1	2.24	0.56
3:n:183:LYS:NZ	3:n:228:ASP:OD2	2.39	0.56
3:r:176:GLN:NE2	3:r:234:ASN:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:213:GLN:NE2	2:Q:286:ASP:OD2	2.38	0.56
2:C:144:ARG:NE	2:C:146:GLN:OE1	2.39	0.55
2:E:93:ASP:OD1	2:E:392:ARG:NE	2.39	0.55
2:F:230:GLU:O	2:F:233:SER:OG	2.12	0.55
2:M:231:ARG:NH2	2:O:230:GLU:OE2	2.39	0.55
3:i:313:ARG:NH2	3:i:316:SER:O	2.39	0.55
2:K:57:ARG:NH1	2:K:94:ASN:OD1	2.40	0.55
1:3:667:PHE:O	1:3:671:ARG:NH2	2.40	0.55
2:D:93:ASP:OD1	2:D:392:ARG:NE	2.39	0.55
2:D:134:GLU:O	2:D:138:ASN:ND2	2.39	0.55
2:B:154:LYS:N	2:B:327:GLU:O	2.40	0.55
1:1:587:SER:OG	1:2:757:ASN:OD1	2.25	0.55
3:n:306:ILE:HG22	3:n:310:MET:HE2	1.88	0.55
3:p:160:LEU:O	3:p:283:ARG:NH2	2.39	0.55
2:F:334:VAL:O	2:F:374:TYR:OH	2.18	0.55
2:O:99:GLU:OE2	2:O:384:ARG:NH1	2.40	0.55
2:G:236:ARG:NH2	2:I:228:ASP:OD2	2.39	0.55
2:Q:141:LEU:O	2:Q:144:ARG:C	2.49	0.55
1:2:495:GLU:OE1	1:2:655:THR:OG1	2.14	0.55
2:C:106:ARG:NH2	2:Q:142:GLN:OE1	2.39	0.55
2:K:334:VAL:O	2:K:374:TYR:OH	2.24	0.55
3:h:272:THR:HG1	3:h:277:THR:HG1	1.51	0.54
1:1:516:GLN:NE2	1:3:588:ALA:O	2.40	0.54
2:L:99:GLU:OE2	2:L:384:ARG:NH1	2.39	0.54
2:P:33:GLN:NE2	2:P:127:ILE:O	2.40	0.54
1:1:623:GLU:OE2	1:1:673:TYR:OH	2.23	0.54
1:3:574:SER:O	1:3:577:ARG:N	2.41	0.54
2:A:239:ASN:ND2	2:A:240:SER:O	2.40	0.54
2:N:230:GLU:O	2:N:233:SER:OG	2.15	0.54
2:K:93:ASP:OD1	2:K:392:ARG:NE	2.40	0.54
2:R:156:ASN:O	2:R:367:TRP:NE1	2.41	0.54
2:R:388:VAL:HA	2:R:391:ILE:HD12	1.90	0.54
2:P:271:ASN:ND2	2:Q:351:GLN:OE1	2.41	0.54
2:Q:230:GLU:O	2:Q:233:SER:OG	2.15	0.54
3:b:99:LYS:HB3	3:f:172:LEU:HD21	1.88	0.54
3:m:272:THR:OG1	3:m:277:THR:OG1	2.11	0.54
1:1:589:SER:OG	1:2:519:ASP:OD2	2.11	0.54
3:q:272:THR:OG1	3:q:277:THR:OG1	2.22	0.54
2:A:186:SER:OG	2:A:326:ILE:O	2.25	0.54
2:M:33:GLN:NE2	2:M:127:ILE:O	2.41	0.54
3:f:100:ASP:OD2	3:f:104:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:176:GLN:NE2	3:g:234:ASN:OD1	2.41	0.53
3:k:228:ASP:O	3:l:294:GLN:NE2	2.41	0.53
2:G:388:VAL:HA	2:G:391:ILE:HD12	1.90	0.53
2:M:141:LEU:O	2:M:144:ARG:C	2.52	0.53
2:O:230:GLU:OE1	2:O:230:GLU:N	2.42	0.53
2:O:342:MET:SD	2:O:342:MET:N	2.80	0.53
3:j:121:TYR:OH	3:j:141:LEU:O	2.23	0.53
3:l:121:TYR:OH	3:l:141:LEU:O	2.23	0.53
2:C:93:ASP:OD1	2:C:392:ARG:NE	2.41	0.53
2:D:334:VAL:O	2:D:374:TYR:OH	2.21	0.53
2:P:205:ILE:HD11	2:P:293:GLN:OE1	2.08	0.53
3:j:261:ILE:HG12	3:j:285:MET:HE3	1.90	0.53
2:C:158:PHE:CE1	2:C:188:ILE:HD11	2.43	0.53
3:m:267:ASP:OD1	3:m:286:ARG:NE	2.38	0.53
3:o:216:GLU:N	3:o:216:GLU:OE1	2.42	0.53
2:P:153:HIS:ND1	2:Q:338:ALA:O	2.42	0.53
3:n:176:GLN:NE2	3:n:234:ASN:OD1	2.42	0.53
1:1:383:GLY:N	1:1:454:ASN:O	2.40	0.53
2:D:121:GLY:O	2:D:125:LYS:NZ	2.40	0.53
2:M:239:ASN:OD1	2:O:255:ARG:NH1	2.42	0.53
1:2:467:ARG:CD	3:i:209:THR:HG21	2.39	0.53
1:3:351:VAL:HG23	1:3:430:LEU:HD21	1.91	0.53
2:L:230:GLU:OE1	2:L:230:GLU:N	2.42	0.53
2:Q:271:ASN:ND2	2:R:351:GLN:OE1	2.42	0.53
3:m:216:GLU:N	3:m:216:GLU:OE1	2.41	0.53
1:2:627:GLN:NE2	1:3:522:LEU:O	2.42	0.52
2:C:2:ASP:O	2:C:6:SER:OG	2.20	0.52
2:J:134:GLU:O	2:J:138:ASN:ND2	2.42	0.52
2:J:338:ALA:O	2:L:153:HIS:ND1	2.43	0.52
2:C:230:GLU:O	2:C:233:SER:OG	2.16	0.52
2:D:22:THR:HG22	2:D:73:LEU:HD22	1.91	0.52
2:P:230:GLU:N	2:P:230:GLU:OE1	2.42	0.52
3:k:157:ASP:OD1	3:k:161:ASN:ND2	2.43	0.52
3:l:172:LEU:HD21	3:m:99:LYS:HB2	1.92	0.52
2:D:22:THR:CG2	2:D:73:LEU:HD22	2.38	0.52
3:c:282:GLU:OE1	3:c:282:GLU:N	2.43	0.52
3:o:282:GLU:OE1	3:o:282:GLU:N	2.42	0.52
2:A:207:GLN:OE1	2:A:293:GLN:NE2	2.42	0.52
3:b:304:ASN:OD1	3:b:305:GLN:NE2	2.43	0.52
3:k:282:GLU:N	3:k:282:GLU:OE1	2.43	0.52
2:J:177:MET:HE2	2:J:206:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:388:VAL:HA	2:N:391:ILE:HD12	1.91	0.52
3:m:294:GLN:NE2	3:o:228:ASP:O	2.42	0.52
2:H:33:GLN:NE2	2:H:127:ILE:O	2.43	0.52
2:P:156:ASN:O	2:P:367:TRP:NE1	2.42	0.52
2:R:99:GLU:OE2	2:R:384:ARG:NH1	2.43	0.52
1:3:281:ILE:HG21	1:3:385:TYR:OH	2.10	0.52
2:C:230:GLU:N	2:C:230:GLU:OE1	2.43	0.52
2:M:230:GLU:N	2:M:230:GLU:OE1	2.41	0.52
3:b:216:GLU:OE1	3:b:216:GLU:N	2.43	0.52
1:1:300:ASN:ND2	1:1:317:THR:OG1	2.43	0.52
2:A:388:VAL:HA	2:A:391:ILE:HD12	1.92	0.52
3:g:326:ILE:CG2	3:k:80:THR:HG21	2.38	0.52
3:m:183:LYS:NZ	3:m:228:ASP:OD2	2.42	0.52
1:3:498:LEU:HD23	1:3:501:LEU:HD12	1.92	0.52
3:g:105:LEU:O	3:g:108:THR:OG1	2.23	0.52
3:j:160:LEU:O	3:j:283:ARG:NH2	2.43	0.52
2:G:90:ASP:OD1	2:G:94:ASN:ND2	2.43	0.52
3:a:282:GLU:N	3:a:282:GLU:OE1	2.43	0.52
3:i:282:GLU:N	3:i:282:GLU:OE1	2.43	0.52
3:j:216:GLU:N	3:j:216:GLU:OE1	2.43	0.52
2:Q:147:ARG:NH1	2:Q:148:THR:O	2.42	0.51
2:Q:213:GLN:OE1	2:Q:287:THR:OG1	2.12	0.51
3:b:99:LYS:CB	3:f:172:LEU:HD21	2.40	0.51
2:E:388:VAL:HA	2:E:391:ILE:HD12	1.92	0.51
2:O:332:GLU:N	2:O:332:GLU:OE1	2.43	0.51
2:L:33:GLN:NE2	2:L:127:ILE:O	2.43	0.51
2:C:154:LYS:N	2:C:327:GLU:O	2.44	0.51
2:N:100:MET:O	2:N:350:ARG:NH2	2.44	0.51
1:3:289:TYR:OH	1:3:391:VAL:O	2.19	0.51
2:F:366:ASN:ND2	2:F:369:ASP:OD2	2.44	0.51
2:N:1:MET:HE1	2:N:384:ARG:HG3	1.92	0.51
2:Q:33:GLN:NE2	2:Q:127:ILE:O	2.43	0.51
2:H:230:GLU:N	2:H:230:GLU:OE1	2.43	0.51
3:i:176:GLN:NE2	3:i:234:ASN:OD1	2.42	0.51
2:A:228:ASP:OD2	2:B:236:ARG:NH2	2.43	0.51
2:J:381:ASN:OD1	2:J:384:ARG:NH2	2.44	0.51
2:O:22:THR:CG2	2:O:73:LEU:HD22	2.40	0.51
3:l:282:GLU:OE1	3:l:282:GLU:N	2.43	0.51
2:I:90:ASP:O	2:I:94:ASN:ND2	2.44	0.51
3:e:138:ASN:OD1	3:e:257:ASN:ND2	2.44	0.51
2:A:154:LYS:N	2:A:327:GLU:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:33:GLN:NE2	2:C:127:ILE:O	2.44	0.51
3:b:282:GLU:N	3:b:282:GLU:OE1	2.44	0.51
3:l:172:LEU:HD21	3:m:99:LYS:CB	2.41	0.51
1:3:351:VAL:CG2	1:3:430:LEU:HD21	2.41	0.50
3:f:216:GLU:N	3:f:216:GLU:OE1	2.44	0.50
3:k:176:GLN:NE2	3:k:234:ASN:OD1	2.44	0.50
3:r:313:ARG:NH2	3:r:316:SER:O	2.44	0.50
1:2:331:GLY:N	1:2:336:ASP:OD2	2.45	0.50
2:J:351:GLN:OE1	2:L:271:ASN:ND2	2.44	0.50
1:1:375:LEU:HD11	1:1:426:PHE:CD1	2.46	0.50
2:E:141:LEU:O	2:E:144:ARG:C	2.53	0.50
2:N:130:ASP:OD1	2:N:132:SER:OG	2.26	0.50
3:d:282:GLU:N	3:d:282:GLU:OE1	2.45	0.50
2:K:134:GLU:O	2:K:138:ASN:ND2	2.44	0.50
2:M:388:VAL:HA	2:M:391:ILE:HD12	1.93	0.50
3:c:216:GLU:N	3:c:216:GLU:OE1	2.44	0.50
3:g:313:ARG:NH2	3:g:316:SER:O	2.44	0.50
3:h:75:THR:O	3:h:79:SER:OG	2.21	0.50
3:j:123:ASP:OD1	3:j:124:ILE:N	2.44	0.50
3:d:176:GLN:NE2	3:d:234:ASN:OD1	2.43	0.50
3:g:55:ILE:O	3:k:52:ASN:N	2.45	0.50
2:G:230:GLU:OE1	2:G:230:GLU:N	2.45	0.50
3:f:121:TYR:OH	3:f:141:LEU:O	2.29	0.50
3:k:255:ARG:O	3:k:283:ARG:NH2	2.45	0.50
3:r:211:ASP:O	3:r:214:THR:OG1	2.23	0.50
2:I:230:GLU:N	2:I:230:GLU:OE1	2.45	0.50
3:a:144:TYR:CD2	3:a:152:MET:HE1	2.46	0.50
2:B:228:ASP:OD2	2:C:236:ARG:NH1	2.44	0.50
2:K:33:GLN:NE2	2:K:127:ILE:O	2.45	0.50
3:c:123:ASP:OD1	3:c:124:ILE:N	2.43	0.50
3:e:123:ASP:OD1	3:e:124:ILE:N	2.44	0.50
3:m:282:GLU:N	3:m:282:GLU:OE1	2.45	0.50
1:2:467:ARG:HD3	3:i:209:THR:HG21	1.93	0.50
2:D:338:ALA:O	2:F:153:HIS:ND1	2.44	0.50
2:Q:230:GLU:OE1	2:Q:230:GLU:N	2.45	0.50
1:1:586:SER:O	1:1:587:SER:OG	2.28	0.49
2:K:333:SER:OG	2:K:379:GLU:OE2	2.27	0.49
1:3:651:ILE:HG23	1:3:656:LEU:HD13	1.94	0.49
2:A:8:SER:HA	2:A:395:LEU:HD11	1.94	0.49
3:g:316:SER:OG	3:g:317:LEU:N	2.45	0.49
1:2:460:GLU:OE1	1:2:460:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:271:ASN:ND2	2:E:351:GLN:OE1	2.45	0.49
2:G:33:GLN:NE2	2:G:127:ILE:O	2.45	0.49
2:M:230:GLU:O	2:M:233:SER:OG	2.19	0.49
3:j:106:PHE:HE1	3:j:303:VAL:HG21	1.77	0.49
3:p:282:GLU:N	3:p:282:GLU:OE1	2.46	0.49
3:g:282:GLU:N	3:g:282:GLU:OE1	2.46	0.49
3:n:282:GLU:N	3:n:282:GLU:OE1	2.45	0.49
2:J:239:ASN:OD1	2:L:255:ARG:NH1	2.46	0.49
3:i:318:ASN:ND2	3:i:322:PHE:O	2.45	0.49
3:r:282:GLU:N	3:r:282:GLU:OE1	2.45	0.49
3:a:160:LEU:HD23	3:a:258:VAL:HG23	1.94	0.49
2:K:156:ASN:O	2:K:367:TRP:NE1	2.44	0.49
2:K:230:GLU:N	2:K:230:GLU:OE1	2.45	0.49
3:g:138:ASN:HB2	3:g:258:VAL:HG12	1.95	0.49
2:G:153:HIS:ND1	2:H:338:ALA:O	2.44	0.49
3:a:144:TYR:HD2	3:a:152:MET:HE1	1.78	0.49
3:h:182:ASN:ND2	3:h:248:ASN:OD1	2.45	0.49
3:p:261:ILE:HG12	3:p:285:MET:HE3	1.95	0.49
1:2:586:SER:OG	1:2:587:SER:N	2.46	0.49
3:d:216:GLU:OE1	3:d:216:GLU:N	2.46	0.49
1:1:354:ASP:OD1	1:1:425:ARG:NE	2.44	0.48
2:D:8:SER:HA	2:D:395:LEU:HD11	1.95	0.48
1:3:744:LEU:HD11	1:3:755:PHE:CE2	2.48	0.48
2:D:388:VAL:HA	2:D:391:ILE:HD12	1.95	0.48
3:h:282:GLU:N	3:h:282:GLU:OE1	2.44	0.48
3:q:282:GLU:OE1	3:q:282:GLU:N	2.46	0.48
2:J:230:GLU:OE1	2:J:230:GLU:N	2.47	0.48
2:R:134:GLU:O	2:R:138:ASN:ND2	2.44	0.48
3:l:285:MET:HE1	3:l:306:ILE:HG12	1.96	0.48
3:o:106:PHE:HE1	3:o:303:VAL:HG21	1.77	0.48
3:p:216:GLU:N	3:p:216:GLU:OE1	2.46	0.48
2:I:377:SER:O	2:I:381:ASN:ND2	2.45	0.48
3:q:138:ASN:HB2	3:q:258:VAL:HG12	1.95	0.48
2:J:2:ASP:O	2:J:6:SER:OG	2.25	0.48
2:P:22:THR:HG22	2:P:73:LEU:HD22	1.96	0.48
2:R:371:ILE:HD12	2:R:374:TYR:CD1	2.48	0.48
2:F:156:ASN:O	2:F:367:TRP:NE1	2.46	0.48
3:l:69:ASN:OD1	3:l:70:SER:N	2.47	0.48
2:H:294:LEU:HD21	2:H:318:ALA:HB3	1.96	0.48
2:M:156:ASN:O	2:M:367:TRP:NE1	2.45	0.48
3:a:261:ILE:HG12	3:a:285:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:144:TYR:CD2	3:f:152:MET:HE1	2.48	0.48
3:k:216:GLU:N	3:k:216:GLU:OE1	2.46	0.48
2:J:228:ASP:OD2	2:K:236:ARG:NH2	2.45	0.48
3:f:282:GLU:N	3:f:282:GLU:OE1	2.44	0.48
2:O:7:LEU:HD23	2:O:37:MET:SD	2.54	0.48
2:Q:7:LEU:HD23	2:Q:37:MET:SD	2.54	0.48
3:n:138:ASN:HB2	3:n:258:VAL:HG12	1.95	0.48
2:F:341:THR:O	2:F:345:ASN:ND2	2.47	0.48
3:j:105:LEU:O	3:j:108:THR:OG1	2.28	0.48
3:m:180:GLU:N	3:m:180:GLU:OE1	2.47	0.48
3:m:199:ASN:OD1	3:m:203:LEU:N	2.46	0.48
2:N:100:MET:SD	2:N:346:VAL:HG22	2.55	0.47
2:B:153:HIS:ND1	2:C:338:ALA:O	2.47	0.47
3:h:160:LEU:O	3:h:283:ARG:NH2	2.45	0.47
1:2:424:LEU:HD23	1:2:426:PHE:CZ	2.50	0.47
2:H:93:ASP:OD1	2:H:392:ARG:NE	2.43	0.47
2:O:90:ASP:O	2:O:94:ASN:ND2	2.44	0.47
2:R:2:ASP:O	2:R:6:SER:OG	2.26	0.47
2:A:22:THR:CG2	2:A:73:LEU:HD22	2.44	0.47
2:P:22:THR:CG2	2:P:73:LEU:HD22	2.45	0.47
1:2:516:GLN:N	1:2:516:GLN:OE1	2.48	0.47
2:H:90:ASP:O	2:H:94:ASN:ND2	2.46	0.47
2:J:7:LEU:HD23	2:J:37:MET:SD	2.54	0.47
2:M:134:GLU:O	2:M:138:ASN:ND2	2.45	0.47
2:N:99:GLU:OE2	2:N:384:ARG:NH1	2.46	0.47
3:g:274:ASP:OD2	3:g:276:THR:OG1	2.31	0.47
3:l:216:GLU:OE1	3:l:216:GLU:N	2.47	0.47
2:H:225:LEU:HD12	2:H:323:THR:O	2.14	0.47
2:I:99:GLU:OE2	2:I:384:ARG:NH1	2.47	0.47
2:Q:100:MET:CE	2:Q:349:VAL:HG21	2.44	0.47
3:q:261:ILE:CG1	3:q:285:MET:HE3	2.45	0.47
2:E:7:LEU:HD23	2:E:37:MET:SD	2.54	0.47
2:F:299:ASN:ND2	3:d:69:ASN:O	2.48	0.47
2:B:99:GLU:OE2	2:B:384:ARG:NH1	2.46	0.47
2:G:260:GLU:OE1	2:G:261:VAL:N	2.48	0.47
2:O:388:VAL:HA	2:O:391:ILE:HD12	1.97	0.47
3:i:95:ASP:OD1	3:i:96:ASN:N	2.48	0.47
1:1:5:ILE:HD11	1:1:638:ALA:HB1	1.96	0.47
2:G:7:LEU:HD23	2:G:37:MET:SD	2.55	0.47
3:r:158:LEU:HD21	3:r:187:MET:HE2	1.96	0.47
3:r:255:ARG:O	3:r:283:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1:MET:HE1	2:L:384:ARG:HG3	1.97	0.46
2:Q:388:VAL:HA	2:Q:391:ILE:HD12	1.96	0.46
3:n:107:LEU:HD12	3:n:112:PRO:HA	1.97	0.46
2:A:54:LEU:HD23	2:A:55:PRO:HD2	1.96	0.46
2:D:158:PHE:CZ	2:D:188:ILE:HD11	2.50	0.46
2:N:228:ASP:OD2	2:O:236:ARG:NH2	2.48	0.46
2:R:112:GLN:OE1	2:R:117:ARG:NH2	2.48	0.46
3:q:272:THR:HG1	3:q:277:THR:HG1	1.54	0.46
1:1:360:GLN:OE1	1:1:363:ARG:NH1	2.48	0.46
3:e:138:ASN:HB2	3:e:258:VAL:HG12	1.97	0.46
2:H:334:VAL:O	2:H:374:TYR:OH	2.26	0.46
2:K:370:LEU:HD23	2:K:370:LEU:O	2.15	0.46
2:R:216:ARG:NH2	2:R:374:TYR:O	2.49	0.46
3:d:165:CYS:SG	3:d:247:ARG:NH1	2.88	0.46
2:C:57:ARG:NH1	2:C:94:ASN:OD1	2.49	0.46
2:H:18:ILE:HG23	2:H:73:LEU:HD23	1.98	0.46
2:K:225:LEU:HD22	2:K:261:VAL:HG21	1.98	0.46
3:g:286:ARG:NH1	3:i:268:VAL:O	2.48	0.46
2:I:334:VAL:O	2:I:374:TYR:OH	2.25	0.46
1:1:438:SER:OG	1:1:444:VAL:O	2.33	0.46
2:B:388:VAL:HA	2:B:391:ILE:HD12	1.96	0.46
2:D:142:GLN:HG3	2:D:148:THR:HG21	1.96	0.46
2:R:199:ILE:HD13	2:R:296:ARG:CZ	2.45	0.46
3:i:144:TYR:CD2	3:i:152:MET:HE1	2.51	0.46
3:m:219:ALA:HB2	3:m:225:VAL:HG11	1.98	0.46
1:3:3:SER:OG	1:3:635:ASP:OD1	2.16	0.46
2:A:338:ALA:O	2:C:153:HIS:ND1	2.49	0.46
2:E:215:ARG:O	2:E:216:ARG:NH1	2.49	0.46
2:L:168:ARG:NH2	2:L:175:ASN:OD1	2.48	0.46
2:P:388:VAL:HA	2:P:391:ILE:HD12	1.97	0.46
3:a:216:GLU:N	3:a:216:GLU:OE1	2.48	0.46
1:2:645:ILE:HB	1:2:651:ILE:HG21	1.98	0.45
1:3:345:ILE:HG21	1:3:430:LEU:HD22	1.97	0.45
2:H:186:SER:OG	2:H:326:ILE:O	2.33	0.45
3:d:95:ASP:OD1	3:d:96:ASN:N	2.49	0.45
2:C:99:GLU:OE2	2:C:384:ARG:NH1	2.49	0.45
2:E:99:GLU:OE2	2:E:384:ARG:NH1	2.48	0.45
2:F:99:GLU:OE2	2:F:384:ARG:NH1	2.46	0.45
2:L:7:LEU:HD23	2:L:37:MET:SD	2.56	0.45
2:N:134:GLU:O	2:N:138:ASN:ND2	2.49	0.45
2:Q:7:LEU:HD21	2:Q:41:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:216:GLU:N	3:h:216:GLU:OE1	2.49	0.45
2:P:134:GLU:O	2:P:138:ASN:ND2	2.47	0.45
3:b:229:VAL:O	3:b:231:ASP:OD1	2.34	0.45
3:e:282:GLU:OE1	3:e:282:GLU:N	2.49	0.45
1:3:503:GLU:OE1	1:3:503:GLU:N	2.50	0.45
1:3:620:ARG:NH2	1:3:664:SER:O	2.49	0.45
3:a:138:ASN:HB2	3:a:258:VAL:HG12	1.98	0.45
3:g:165:CYS:SG	3:g:247:ARG:NH1	2.89	0.45
3:q:261:ILE:HG12	3:q:285:MET:HE3	1.97	0.45
1:1:444:VAL:O	1:1:445:SER:OG	2.34	0.45
2:H:22:THR:CG2	2:H:73:LEU:HD22	2.46	0.45
2:I:112:GLN:OE1	2:I:117:ARG:NH2	2.49	0.45
2:L:370:LEU:HD23	2:L:370:LEU:O	2.17	0.45
3:k:272:THR:OG1	3:k:277:THR:OG1	2.22	0.45
3:m:160:LEU:O	3:m:283:ARG:NH2	2.49	0.45
3:r:123:ASP:OD1	3:r:124:ILE:N	2.49	0.45
2:L:269:ILE:HD11	2:L:272:THR:HB	1.98	0.45
3:b:123:ASP:OD1	3:b:124:ILE:N	2.49	0.45
3:o:142:MET:HE2	3:o:155:LEU:HD23	1.99	0.45
2:E:166:LEU:HD22	2:E:176:LEU:HD22	1.99	0.45
2:M:93:ASP:OD1	2:M:392:ARG:NE	2.44	0.45
2:O:239:ASN:ND2	2:O:240:SER:O	2.47	0.45
3:a:123:ASP:OD1	3:a:124:ILE:N	2.50	0.45
3:p:185:ILE:HG22	3:p:226:ILE:HG12	1.99	0.45
1:3:730:LEU:CD2	1:3:736:ILE:HD12	2.47	0.45
2:E:228:ASP:OD2	2:F:236:ARG:NH2	2.48	0.45
2:G:215:ARG:O	2:G:216:ARG:NH1	2.50	0.45
2:H:99:GLU:OE2	2:H:384:ARG:NH1	2.46	0.45
2:J:158:PHE:CE1	2:J:188:ILE:HD11	2.51	0.45
2:L:156:ASN:O	2:L:367:TRP:NE1	2.49	0.45
3:a:199:ASN:OD1	3:a:203:LEU:N	2.47	0.45
3:d:262:GLN:NE2	3:d:266:SER:O	2.46	0.45
3:n:180:GLU:OE1	3:n:180:GLU:N	2.48	0.45
1:3:655:THR:HG22	1:3:659:ILE:HD12	1.98	0.45
2:L:90:ASP:O	2:L:94:ASN:ND2	2.47	0.45
3:e:158:LEU:HD21	3:e:187:MET:HE2	1.99	0.45
3:j:294:GLN:NE2	3:l:228:ASP:O	2.49	0.45
3:n:216:GLU:OE1	3:n:216:GLU:N	2.50	0.45
1:2:519:ASP:OD2	1:2:753:ARG:NE	2.50	0.45
1:2:592:THR:OG1	1:2:713:THR:OG1	2.34	0.45
2:A:93:ASP:OD1	2:A:392:ARG:NE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:158:PHE:CE1	2:M:188:ILE:HD11	2.51	0.45
2:N:377:SER:O	2:N:381:ASN:ND2	2.48	0.45
2:P:253:ILE:C	2:P:254:LEU:HD12	2.42	0.45
3:e:285:MET:SD	3:e:285:MET:N	2.90	0.44
3:j:276:THR:HG21	3:k:305:GLN:HB3	1.99	0.44
1:1:672:ALA:HB3	1:1:720:ALA:HB3	1.99	0.44
2:K:4:LEU:HD21	2:K:96:CYS:SG	2.57	0.44
3:g:95:ASP:OD1	3:g:96:ASN:N	2.51	0.44
2:J:7:LEU:HD21	2:J:41:MET:HE3	1.99	0.44
2:L:158:PHE:CZ	2:L:188:ILE:HD11	2.52	0.44
3:f:106:PHE:HE1	3:f:303:VAL:HG21	1.81	0.44
3:g:217:GLU:OE2	3:g:220:THR:OG1	2.34	0.44
3:i:128:SER:HB2	3:i:224:LEU:HD22	2.00	0.44
3:i:182:ASN:OD1	3:i:248:ASN:ND2	2.49	0.44
3:q:121:TYR:OH	3:q:141:LEU:O	2.33	0.44
3:r:304:ASN:OD1	3:r:305:GLN:NE2	2.50	0.44
2:N:230:GLU:N	2:N:230:GLU:OE1	2.51	0.44
3:g:123:ASP:OD1	3:g:124:ILE:N	2.50	0.44
3:q:123:ASP:OD1	3:q:124:ILE:N	2.50	0.44
2:C:388:VAL:HA	2:C:391:ILE:HD12	1.99	0.44
2:D:186:SER:OG	2:D:326:ILE:O	2.36	0.44
2:Q:253:ILE:HD13	2:Q:319:THR:OG1	2.16	0.44
2:Q:261:VAL:HG13	2:Q:290:LEU:HD23	1.99	0.44
3:g:301:ASP:CG	3:i:231:ASP:OD1	2.51	0.44
1:1:527:MET:HE3	1:1:531:PHE:HE2	1.82	0.44
1:1:674:ARG:NH2	1:1:683:GLU:OE2	2.48	0.44
1:3:360:GLN:OE1	1:3:363:ARG:NH1	2.49	0.44
2:B:108:GLY:O	2:B:384:ARG:NE	2.47	0.44
2:C:48:THR:HG21	2:C:94:ASN:HB3	2.00	0.44
2:Q:174:ASP:OD1	2:Q:312:GLN:NE2	2.48	0.44
2:R:158:PHE:CE1	2:R:188:ILE:HD11	2.52	0.44
3:a:160:LEU:HD21	3:a:260:VAL:HG23	2.00	0.44
3:d:123:ASP:OD1	3:d:124:ILE:N	2.51	0.44
2:F:51:ILE:HG23	2:F:54:LEU:HD12	2.00	0.44
2:H:253:ILE:HD13	2:H:319:THR:OG1	2.18	0.44
3:c:142:MET:HE2	3:c:155:LEU:HD23	2.00	0.44
3:d:199:ASN:OD1	3:d:203:LEU:N	2.49	0.44
3:p:165:CYS:SG	3:p:247:ARG:NH1	2.91	0.44
1:2:502:ARG:NE	1:2:662:GLU:OE2	2.51	0.44
2:I:141:LEU:HB3	2:I:148:THR:HG22	2.00	0.44
3:j:180:GLU:OE1	3:j:180:GLU:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:736:ILE:HD11	1:1:740:GLN:HB3	2.00	0.44
2:B:230:GLU:OE1	2:B:230:GLU:N	2.50	0.44
2:F:253:ILE:HD13	2:F:319:THR:OG1	2.18	0.44
2:O:253:ILE:C	2:O:254:LEU:HD12	2.43	0.44
1:1:581:ILE:HD11	1:1:588:ALA:HB1	2.00	0.43
2:E:153:HIS:ND1	2:F:338:ALA:O	2.51	0.43
3:a:304:ASN:OD1	3:a:305:GLN:N	2.51	0.43
3:e:75:THR:O	3:e:79:SER:OG	2.27	0.43
2:A:153:HIS:ND1	2:B:338:ALA:O	2.51	0.43
2:B:62:ASP:N	2:B:62:ASP:OD1	2.51	0.43
2:E:7:LEU:HD21	2:E:41:MET:HE3	2.00	0.43
3:l:81:LEU:HD12	3:l:137:TYR:O	2.18	0.43
2:B:141:LEU:HB3	2:B:148:THR:HG22	1.99	0.43
2:Q:62:ASP:OD1	2:Q:62:ASP:N	2.49	0.43
3:i:149:GLN:HA	3:i:152:MET:HE2	2.00	0.43
1:3:580:SER:HB2	2:K:205:ILE:HD13	2.01	0.43
2:I:261:VAL:HG22	2:I:290:LEU:CD2	2.47	0.43
2:M:333:SER:OG	2:M:379:GLU:OE2	2.20	0.43
3:k:123:ASP:OD1	3:k:124:ILE:N	2.51	0.43
3:p:228:ASP:O	3:q:294:GLN:NE2	2.51	0.43
1:1:331:GLY:N	1:1:336:ASP:OD2	2.51	0.43
2:H:225:LEU:HD13	2:H:324:LEU:HD12	2.00	0.43
2:P:158:PHE:CE1	2:P:188:ILE:HD11	2.53	0.43
2:R:333:SER:OG	2:R:379:GLU:OE2	2.30	0.43
3:h:183:LYS:NZ	3:h:228:ASP:OD2	2.51	0.43
3:p:138:ASN:HB2	3:p:258:VAL:HG12	2.00	0.43
2:D:230:GLU:O	2:D:233:SER:OG	2.29	0.43
1:2:416:THR:OG1	1:2:419:VAL:O	2.33	0.43
2:I:2:ASP:OD2	2:I:131:ASN:ND2	2.52	0.43
3:m:316:SER:OG	3:m:317:LEU:N	2.51	0.43
3:n:187:MET:SD	3:n:247:ARG:NH2	2.92	0.43
3:q:186:SER:OG	3:q:193:ILE:HD11	2.19	0.43
2:A:141:LEU:O	2:A:144:ARG:O	2.37	0.43
2:J:85:ILE:O	2:J:89:VAL:HG23	2.19	0.43
3:n:149:GLN:HA	3:n:152:MET:HE2	2.01	0.43
3:q:81:LEU:HD13	3:q:307:ILE:HD11	2.01	0.43
2:A:231:ARG:NH2	2:C:230:GLU:OE2	2.52	0.43
2:B:1:MET:HE2	2:B:388:VAL:CG1	2.48	0.43
2:C:7:LEU:HD23	2:C:37:MET:SD	2.58	0.43
2:N:255:ARG:NH1	2:O:239:ASN:OD1	2.51	0.43
3:c:160:LEU:O	3:c:283:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:123:ASP:OD1	3:f:124:ILE:N	2.49	0.43
2:C:156:ASN:O	2:C:367:TRP:NE1	2.50	0.42
2:E:130:ASP:OD1	2:E:132:SER:OG	2.33	0.42
2:E:158:PHE:CE1	2:E:188:ILE:HD11	2.54	0.42
2:H:111:PRO:O	2:H:117:ARG:NE	2.51	0.42
2:K:253:ILE:C	2:K:254:LEU:HD12	2.44	0.42
3:d:255:ARG:O	3:d:283:ARG:NE	2.51	0.42
3:e:128:SER:HB3	3:e:224:LEU:HD22	2.01	0.42
3:h:123:ASP:OD1	3:h:124:ILE:N	2.52	0.42
3:q:180:GLU:OE1	3:q:180:GLU:N	2.51	0.42
1:1:700:GLU:OE2	2:I:269:ILE:HG22	2.18	0.42
1:2:354:ASP:OD1	1:2:425:ARG:NE	2.46	0.42
1:3:347:GLU:N	1:3:347:GLU:OE1	2.48	0.42
2:P:117:ARG:O	2:P:120:SER:OG	2.31	0.42
3:g:261:ILE:CG1	3:g:285:MET:HE3	2.49	0.42
3:f:165:CYS:SG	3:f:247:ARG:NH1	2.93	0.42
3:n:105:LEU:O	3:n:108:THR:OG1	2.27	0.42
3:r:121:TYR:OH	3:r:141:LEU:O	2.35	0.42
1:1:270:ASP:O	1:1:307:ARG:NH2	2.52	0.42
2:G:7:LEU:HD21	2:G:41:MET:HE3	2.02	0.42
2:M:338:ALA:O	2:O:153:HIS:ND1	2.51	0.42
2:O:261:VAL:HG13	2:O:290:LEU:HD23	2.01	0.42
1:3:502:ARG:NE	1:3:662:GLU:OE2	2.52	0.42
2:E:251:PRO:HB3	2:E:319:THR:HG21	2.01	0.42
2:H:260:GLU:OE2	2:H:272:THR:OG1	2.35	0.42
2:J:108:GLY:O	2:J:384:ARG:NE	2.50	0.42
2:R:367:TRP:CZ2	2:R:371:ILE:HD13	2.53	0.42
3:q:185:ILE:HG22	3:q:226:ILE:HG12	2.02	0.42
2:B:7:LEU:HD23	2:B:37:MET:SD	2.60	0.42
2:F:225:LEU:HD13	2:F:324:LEU:HD12	2.02	0.42
2:N:11:LEU:HD22	2:N:85:ILE:HG23	2.00	0.42
3:h:128:SER:HB3	3:h:224:LEU:HD22	2.01	0.42
2:P:186:SER:OG	2:P:326:ILE:O	2.37	0.42
3:m:228:ASP:O	3:n:294:GLN:NE2	2.52	0.42
3:p:123:ASP:OD1	3:p:124:ILE:N	2.53	0.42
2:A:1:MET:HE2	2:A:388:VAL:CG1	2.50	0.42
2:L:366:ASN:ND2	2:L:369:ASP:OD2	2.50	0.42
3:b:138:ASN:HB2	3:b:258:VAL:HG12	2.02	0.42
3:h:276:THR:HG21	3:i:305:GLN:HB3	2.02	0.42
2:A:156:ASN:O	2:A:367:TRP:NE1	2.51	0.42
2:R:90:ASP:O	2:R:94:ASN:ND2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:60:THR:HG22	3:a:61:GLY:H	1.85	0.42
3:l:138:ASN:HB2	3:l:258:VAL:HG12	2.02	0.42
3:p:164:LEU:HB2	3:p:252:LEU:HD11	2.02	0.42
1:2:736:ILE:CD1	1:2:744:LEU:HD12	2.50	0.42
2:I:1:MET:HE2	2:I:388:VAL:HG13	2.01	0.42
2:L:24:TYR:O	2:L:28:SER:OG	2.36	0.42
3:g:216:GLU:OE1	3:g:216:GLU:N	2.53	0.42
1:1:374:ASN:O	3:m:210:THR:OG1	2.37	0.41
1:2:386:SER:HA	1:2:396:VAL:HG12	2.02	0.41
1:2:567:CYS:SG	1:2:568:LEU:N	2.93	0.41
2:I:334:VAL:O	2:I:335:LEU:HD23	2.20	0.41
2:J:156:ASN:O	2:J:367:TRP:NE1	2.53	0.41
2:Q:90:ASP:O	2:Q:94:ASN:ND2	2.49	0.41
3:f:157:ASP:OD1	3:f:161:ASN:ND2	2.53	0.41
3:k:177:GLN:NE2	3:k:182:ASN:O	2.52	0.41
1:2:573:SER:OG	1:3:647:ARG:NH1	2.54	0.41
2:N:22:THR:HG23	2:N:73:LEU:HD13	2.02	0.41
2:N:85:ILE:O	2:N:89:VAL:HG23	2.20	0.41
2:G:1:MET:HE1	2:G:384:ARG:HG3	2.02	0.41
2:H:4:LEU:O	2:H:8:SER:OG	2.39	0.41
2:K:19:VAL:O	2:K:22:THR:HG22	2.21	0.41
2:M:261:VAL:HG13	2:M:290:LEU:HD23	2.02	0.41
2:Q:153:HIS:ND1	2:R:338:ALA:O	2.51	0.41
2:Q:370:LEU:O	2:Q:370:LEU:HD23	2.21	0.41
3:d:182:ASN:OD1	3:d:248:ASN:ND2	2.50	0.41
3:i:123:ASP:OD1	3:i:124:ILE:N	2.51	0.41
3:m:211:ASP:O	3:m:214:THR:OG1	2.34	0.41
1:3:500:GLU:N	1:3:500:GLU:OE1	2.53	0.41
2:H:158:PHE:CE1	2:H:188:ILE:HD11	2.55	0.41
2:K:85:ILE:O	2:K:89:VAL:HG23	2.20	0.41
2:R:1:MET:HE2	2:R:388:VAL:CG1	2.50	0.41
2:I:7:LEU:HD23	2:I:37:MET:SD	2.60	0.41
2:L:85:ILE:O	2:L:89:VAL:HG23	2.20	0.41
2:N:153:HIS:ND1	2:O:338:ALA:O	2.54	0.41
2:N:299:ASN:ND2	3:o:69:ASN:O	2.52	0.41
3:d:172:LEU:HD21	3:i:99:LYS:CB	2.51	0.41
2:F:388:VAL:HA	2:F:391:ILE:HD12	2.02	0.41
2:H:154:LYS:N	2:H:327:GLU:O	2.48	0.41
2:N:207:GLN:OE1	2:N:293:GLN:NE2	2.54	0.41
3:a:180:GLU:OE1	3:a:180:GLU:N	2.50	0.41
3:e:306:ILE:CG2	3:e:310:MET:HE2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:667:PHE:O	1:1:671:ARG:NH2	2.53	0.41
1:2:291:TRP:HB2	1:2:339:ILE:HG22	2.01	0.41
1:3:646:ASP:OD1	1:3:646:ASP:N	2.53	0.41
3:e:125:ALA:O	3:e:129:VAL:HG23	2.21	0.41
1:3:329:ASN:HA	1:3:338:VAL:HG23	2.03	0.41
2:L:19:VAL:O	2:L:22:THR:HG22	2.21	0.41
2:N:180:MET:HE1	2:N:238:ILE:CD1	2.50	0.41
2:P:141:LEU:HB3	2:P:148:THR:HG22	2.03	0.41
3:e:160:LEU:HD21	3:e:260:VAL:HG23	2.01	0.41
3:k:95:ASP:OD1	3:k:96:ASN:N	2.54	0.41
1:1:412:SER:OG	1:1:413:THR:N	2.54	0.41
1:2:505:PHE:O	1:2:508:LEU:C	2.64	0.41
1:3:354:ASP:OD1	1:3:354:ASP:N	2.51	0.41
2:B:85:ILE:O	2:B:89:VAL:HG23	2.20	0.41
2:B:134:GLU:O	2:B:138:ASN:ND2	2.50	0.41
2:B:186:SER:OG	2:B:326:ILE:O	2.35	0.41
2:D:1:MET:HE2	2:D:388:VAL:CG1	2.50	0.41
2:E:176:LEU:HD12	2:E:195:TYR:CZ	2.55	0.41
2:O:1:MET:HE2	2:O:388:VAL:HG13	2.03	0.41
3:a:74:GLU:O	3:a:78:THR:HG22	2.21	0.41
3:a:106:PHE:HE1	3:a:303:VAL:HG21	1.85	0.41
3:b:76:PHE:O	3:b:78:THR:N	2.47	0.41
3:c:271:ILE:HD11	3:c:284:MET:SD	2.61	0.41
3:e:216:GLU:N	3:e:216:GLU:OE1	2.54	0.41
3:h:185:ILE:HG22	3:h:226:ILE:HG12	2.03	0.41
3:n:80:THR:HG21	3:p:326:ILE:HG21	2.02	0.41
3:r:234:ASN:OD1	3:r:234:ASN:N	2.52	0.41
1:1:10:LEU:HD11	1:1:624:MET:HE2	2.03	0.41
2:B:253:ILE:C	2:B:254:LEU:HD12	2.46	0.41
2:I:204:ASN:OD1	2:I:204:ASN:N	2.54	0.41
2:I:225:LEU:HD12	2:I:323:THR:O	2.21	0.41
2:O:333:SER:OG	2:O:379:GLU:OE2	2.28	0.41
2:P:366:ASN:ND2	2:P:369:ASP:OD2	2.53	0.41
2:Q:100:MET:HE1	2:Q:349:VAL:HG21	2.03	0.41
2:R:141:LEU:HB3	2:R:148:THR:HG22	2.03	0.41
2:R:186:SER:OG	2:R:326:ILE:O	2.37	0.41
2:R:230:GLU:O	2:R:233:SER:OG	2.36	0.41
3:f:272:THR:OG1	3:f:277:THR:OG1	2.11	0.41
3:o:144:TYR:CD2	3:o:152:MET:HE1	2.56	0.41
1:1:668:ILE:HG23	1:1:773:GLN:OE1	2.21	0.40
1:2:467:ARG:HD2	3:i:209:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:156:ASN:OD1	2:D:156:ASN:N	2.55	0.40
2:E:85:ILE:O	2:E:89:VAL:HG23	2.20	0.40
2:I:261:VAL:HG22	2:I:290:LEU:HD23	2.03	0.40
2:K:11:LEU:HD22	2:K:85:ILE:HG23	2.02	0.40
2:Q:345:ASN:O	2:Q:349:VAL:HG23	2.21	0.40
3:a:160:LEU:O	3:a:283:ARG:NH2	2.54	0.40
3:a:185:ILE:HG22	3:a:226:ILE:HG12	2.04	0.40
3:f:149:GLN:HA	3:f:152:MET:HE2	2.03	0.40
3:q:261:ILE:HG21	3:q:287:ILE:HD12	2.03	0.40
3:b:157:ASP:OD1	3:b:161:ASN:ND2	2.53	0.40
3:d:158:LEU:HD21	3:d:187:MET:HE2	2.04	0.40
3:f:185:ILE:HG22	3:f:226:ILE:HG12	2.02	0.40
3:o:160:LEU:HD21	3:o:260:VAL:HG23	2.02	0.40
3:q:262:GLN:NE2	3:q:266:SER:O	2.50	0.40
1:l:594:VAL:HA	1:l:614:THR:HG21	2.03	0.40
3:a:128:SER:HB3	3:a:224:LEU:HD22	2.02	0.40
3:d:271:ILE:HD11	3:d:284:MET:SD	2.62	0.40
3:f:274:ASP:OD2	3:f:276:THR:OG1	2.39	0.40
3:q:304:ASN:OD1	3:q:305:GLN:N	2.54	0.40
2:A:18:ILE:HG23	2:A:73:LEU:HD23	2.04	0.40
2:I:33:GLN:NE2	2:I:127:ILE:O	2.55	0.40
2:L:261:VAL:HG13	2:L:290:LEU:CD2	2.51	0.40
2:R:33:GLN:NE2	2:R:127:ILE:O	2.55	0.40
3:b:180:GLU:OE1	3:b:180:GLU:N	2.51	0.40
3:c:261:ILE:HG21	3:c:287:ILE:HD12	2.03	0.40
3:r:180:GLU:OE1	3:r:180:GLU:N	2.52	0.40
2:D:154:LYS:N	2:D:327:GLU:O	2.48	0.40
2:I:199:ILE:HD13	2:I:296:ARG:CZ	2.51	0.40
3:r:162:GLU:OE2	3:r:313:ARG:NH1	2.55	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	1	503/776 (65%)	494 (98%)	9 (2%)	0	100	100
1	2	502/776 (65%)	494 (98%)	8 (2%)	0	100	100
1	3	498/776 (64%)	492 (99%)	6 (1%)	0	100	100
2	A	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	B	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	C	327/397 (82%)	325 (99%)	2 (1%)	0	100	100
2	D	350/397 (88%)	348 (99%)	2 (1%)	0	100	100
2	E	366/397 (92%)	364 (100%)	2 (0%)	0	100	100
2	F	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	G	388/397 (98%)	386 (100%)	2 (0%)	0	100	100
2	H	395/397 (100%)	393 (100%)	2 (0%)	0	100	100
2	I	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	J	395/397 (100%)	392 (99%)	3 (1%)	0	100	100
2	K	353/397 (89%)	353 (100%)	0	0	100	100
2	L	303/397 (76%)	301 (99%)	2 (1%)	0	100	100
2	M	351/397 (88%)	348 (99%)	3 (1%)	0	100	100
2	N	276/397 (70%)	274 (99%)	2 (1%)	0	100	100
2	O	337/397 (85%)	336 (100%)	1 (0%)	0	100	100
2	P	381/397 (96%)	379 (100%)	2 (0%)	0	100	100
2	Q	125/397 (32%)	125 (100%)	0	0	100	100
2	R	244/397 (62%)	244 (100%)	0	0	100	100
3	a	214/326 (66%)	214 (100%)	0	0	100	100
3	b	270/326 (83%)	266 (98%)	4 (2%)	0	100	100
3	c	106/326 (32%)	106 (100%)	0	0	100	100
3	d	263/326 (81%)	263 (100%)	0	0	100	100
3	e	258/326 (79%)	258 (100%)	0	0	100	100
3	f	263/326 (81%)	263 (100%)	0	0	100	100
3	g	270/326 (83%)	270 (100%)	0	0	100	100
3	h	257/326 (79%)	257 (100%)	0	0	100	100
3	i	270/326 (83%)	270 (100%)	0	0	100	100
3	j	270/326 (83%)	270 (100%)	0	0	100	100
3	k	227/326 (70%)	227 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	l	183/326 (56%)	183 (100%)	0	0	100	100
3	m	231/326 (71%)	231 (100%)	0	0	100	100
3	n	263/326 (81%)	263 (100%)	0	0	100	100
3	o	263/326 (81%)	263 (100%)	0	0	100	100
3	p	261/326 (80%)	260 (100%)	1 (0%)	0	100	100
3	q	257/326 (79%)	257 (100%)	0	0	100	100
3	r	270/326 (83%)	270 (100%)	0	0	100	100
All	All	12070/15342 (79%)	12009 (100%)	61 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 54 are monoatomic - leaving 18 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
4	NAG	o	503	3	14,14,15	0.22	0	17,19,21	0.52	0
4	NAG	p	401	3	14,14,15	0.31	0	17,19,21	0.50	0
4	NAG	g	401	3	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	q	401	3	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	n	401	3	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	r	503	3	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	k	401	3	14,14,15	0.25	0	17,19,21	0.56	0
4	NAG	e	401	3	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	f	503	3	14,14,15	0.27	0	17,19,21	0.56	0
4	NAG	a	401	3	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	c	503	3	14,14,15	0.23	0	17,19,21	0.53	0
4	NAG	h	401	3	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	d	401	3	14,14,15	0.17	0	17,19,21	0.48	0
4	NAG	i	503	3	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	l	503	3	14,14,15	0.20	0	17,19,21	0.51	0
4	NAG	j	401	3	14,14,15	0.28	0	17,19,21	0.48	0
4	NAG	m	401	3	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	b	401	3	14,14,15	0.31	0	17,19,21	0.47	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
4	NAG	o	503	3	-	0/6/23/26	0/1/1/1
4	NAG	p	401	3	-	0/6/23/26	0/1/1/1
4	NAG	g	401	3	-	1/6/23/26	0/1/1/1
4	NAG	q	401	3	-	0/6/23/26	0/1/1/1
4	NAG	n	401	3	-	2/6/23/26	0/1/1/1
4	NAG	r	503	3	-	0/6/23/26	0/1/1/1
4	NAG	k	401	3	-	0/6/23/26	0/1/1/1
4	NAG	e	401	3	-	0/6/23/26	0/1/1/1
4	NAG	f	503	3	-	2/6/23/26	0/1/1/1
4	NAG	a	401	3	-	2/6/23/26	0/1/1/1
4	NAG	c	503	3	-	0/6/23/26	0/1/1/1
4	NAG	h	401	3	-	0/6/23/26	0/1/1/1
4	NAG	d	401	3	-	0/6/23/26	0/1/1/1
4	NAG	i	503	3	-	0/6/23/26	0/1/1/1
4	NAG	l	503	3	-	0/6/23/26	0/1/1/1
4	NAG	j	401	3	-	0/6/23/26	0/1/1/1
4	NAG	m	401	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	b	401	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	b	401	NAG	O5-C5-C6-O6
4	n	401	NAG	O5-C5-C6-O6
4	b	401	NAG	C4-C5-C6-O6
4	n	401	NAG	C4-C5-C6-O6
4	g	401	NAG	O5-C5-C6-O6
4	a	401	NAG	C4-C5-C6-O6
4	a	401	NAG	O5-C5-C6-O6
4	f	503	NAG	C4-C5-C6-O6
4	f	503	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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-21956. 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.