



Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 12:49 AM JST

PDB ID : 8XUS
EMDB ID : EMD-38682
Title : JN.1 Spike Trimer in complex with heparan sulfate
Authors : Yue, C.; Liu, P.
Deposited on : 2024-01-14
Resolution : 3.18 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

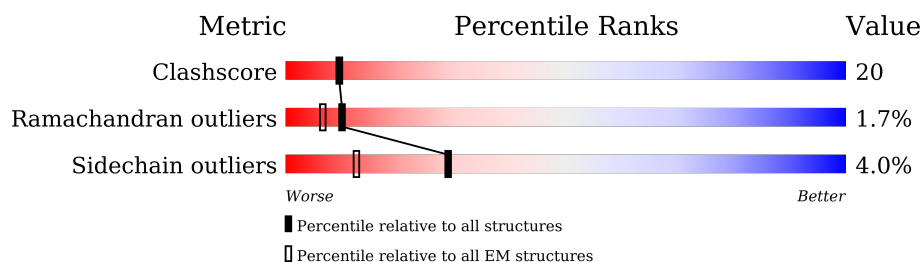
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1206	
1	B	1206	
1	C	1206	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25713 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	1063	Total	C	N	O	S	0	0
			8314	5319	1383	1574	38		
1	A	1063	Total	C	N	O	S	0	0
			8314	5319	1383	1574	38		
1	B	1063	Total	C	N	O	S	0	0
			8314	5319	1383	1574	38		

There are 222 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	16	MET	-	insertion	UNP P0DTC2
C	17	PRO	-	insertion	UNP P0DTC2
C	18	LEU	-	insertion	UNP P0DTC2
C	19	PHE	-	insertion	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	24	THR	ARG	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	455	SER	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	16	MET	-	insertion	UNP P0DTC2
A	17	PRO	-	insertion	UNP P0DTC2
A	18	LEU	-	insertion	UNP P0DTC2
A	19	PHE	-	insertion	UNP P0DTC2
A	22	ILE	THR	variant	UNP P0DTC2
A	24	THR	ARG	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	variant	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	HIS	VAL	conflict	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	455	SER	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	554	LYS	GLU	conflict	UNP P0DTC2
A	570	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2

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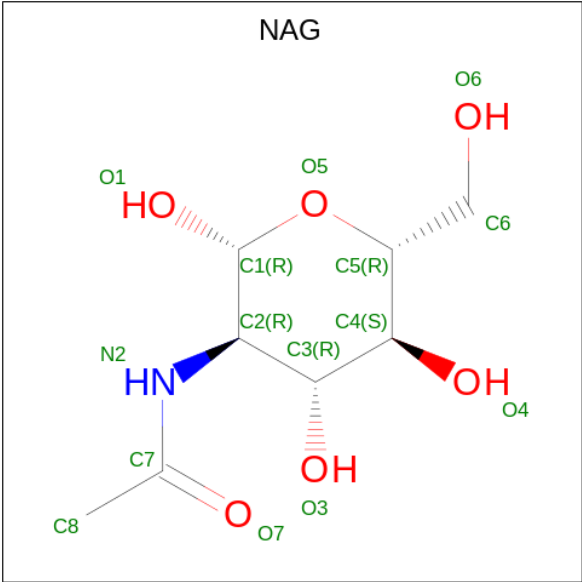
Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	insertion	UNP P0DTC2
B	17	PRO	-	insertion	UNP P0DTC2
B	18	LEU	-	insertion	UNP P0DTC2
B	19	PHE	-	insertion	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	24	THR	ARG	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
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B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
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B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	455	SER	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	conflict	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	

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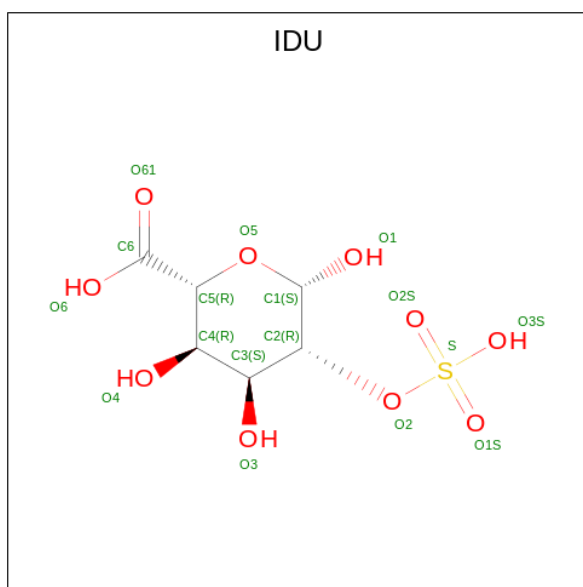
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is 2-O-sulfo-beta-L-altropyranuronic acid (three-letter code: IDU) (formula: $C_6H_{10}O_{10}S$) (labeled as "Ligand of Interest" by depositor).

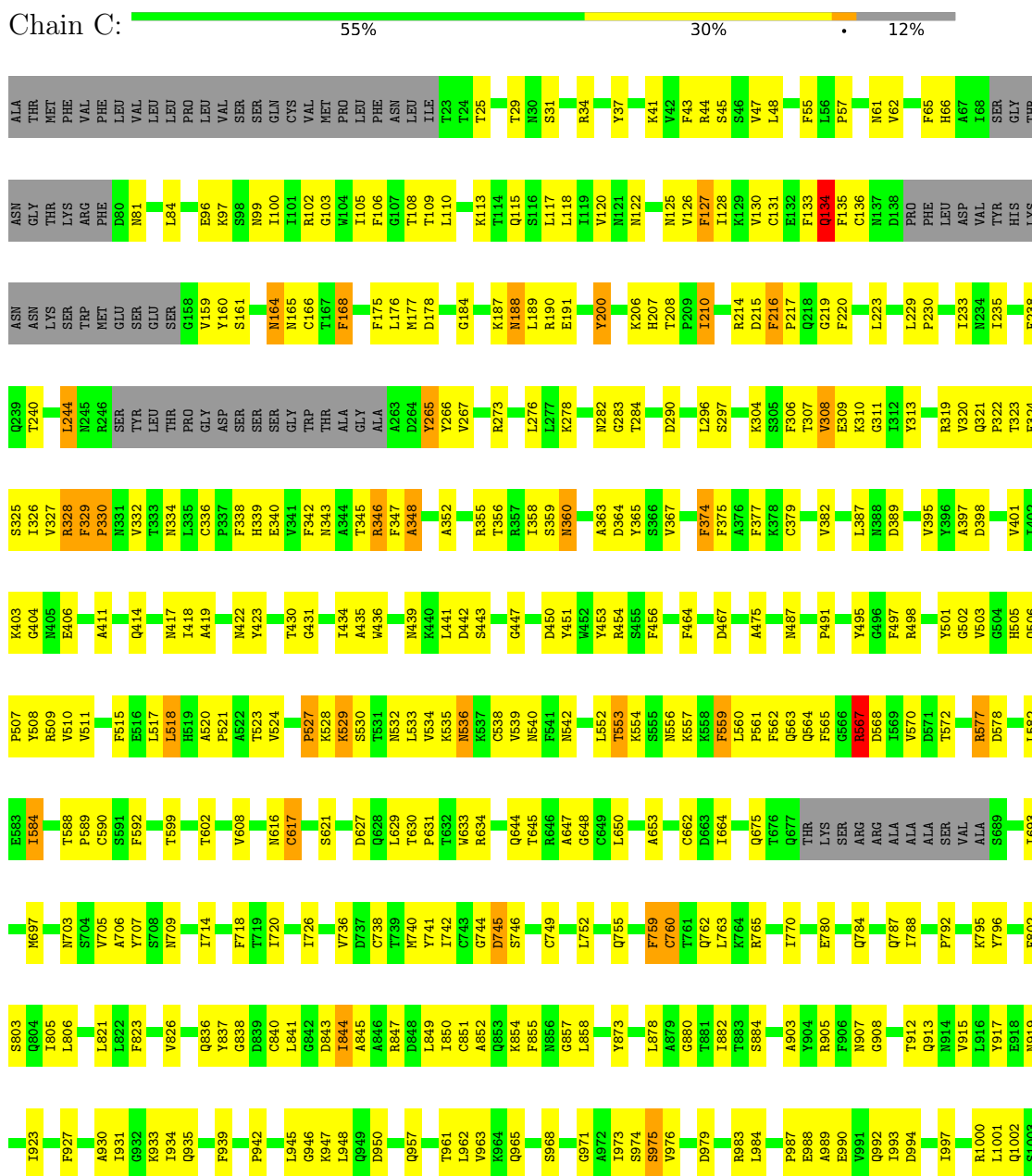


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
3	B	1	15	6	8	1	0

3 Residue-property plots

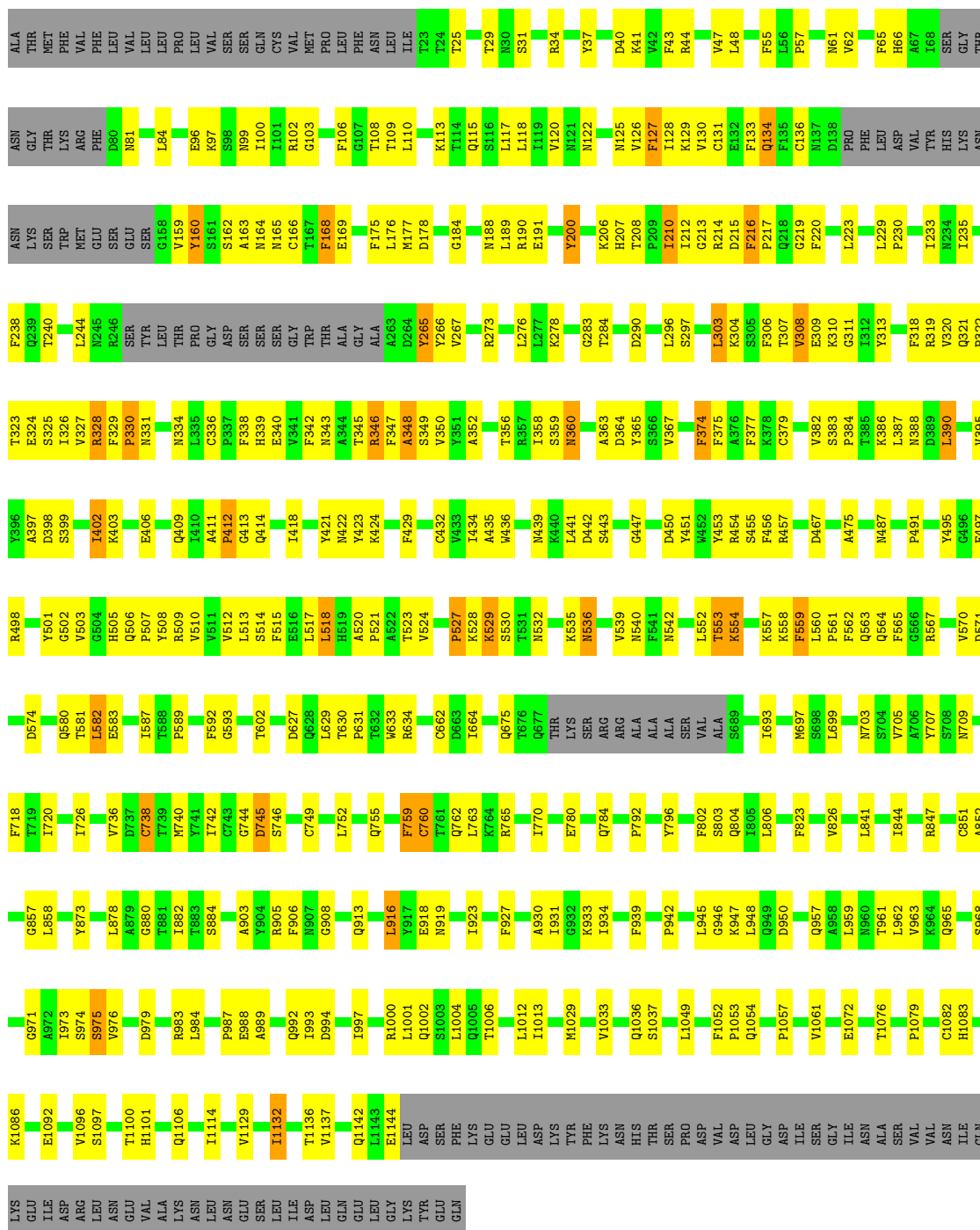
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

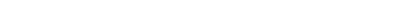
- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein

Chain A:  56% 29% 1% 14%



Chain B:  57% 29% • 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	301841	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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, IDU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/8514	0.60	0/11588
1	B	0.45	0/8514	0.60	0/11588
1	C	0.44	0/8514	0.60	0/11588
All	All	0.44	0/25542	0.60	0/34764

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	A	0	2
1	B	0	3
1	C	0	4
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	A	346	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	328	ARG	Sidechain
1	B	346	ARG	Sidechain
1	C	328	ARG	Sidechain
1	C	346	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	567	ARG	Sidechain
1	C	577	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8314	0	8094	383	0
1	B	8314	0	8094	363	0
1	C	8314	0	8094	396	0
2	A	252	0	234	6	0
2	B	252	0	234	5	0
2	C	252	0	234	10	0
3	B	15	0	4	1	0
All	All	25713	0	24988	993	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 20.

All (993) 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:C:430:THR:CG2	1:C:517:LEU:HD12	1.63	1.26
1:C:503:VAL:CG2	1:A:505:HIS:CE1	2.20	1.25
1:C:759:PHE:HZ	1:A:1002:GLN:CG	1.49	1.24
1:A:503:VAL:CG2	1:B:505:HIS:CE1	2.21	1.23
1:A:759:PHE:HZ	1:B:1002:GLN:CG	1.56	1.17
1:C:1002:GLN:HG3	1:B:759:PHE:HZ	1.07	1.16
1:C:759:PHE:CZ	1:A:1002:GLN:HG3	1.80	1.16
1:C:503:VAL:HG21	1:A:505:HIS:CE1	1.78	1.15
1:C:1002:GLN:HG3	1:B:759:PHE:CZ	1.81	1.15
1:C:430:THR:HG21	1:C:517:LEU:HD12	1.25	1.15
1:A:759:PHE:CZ	1:B:1002:GLN:HG3	1.82	1.14
1:C:505:HIS:CE1	1:B:503:VAL:CG2	2.29	1.14
1:C:503:VAL:HG21	1:A:505:HIS:HE1	1.00	1.13
1:C:505:HIS:HE1	1:B:503:VAL:HG21	1.06	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:PHE:HZ	1:B:1002:GLN:HG3	1.05	1.13
1:A:503:VAL:HG21	1:B:505:HIS:CE1	1.78	1.13
1:A:841:LEU:HB2	1:B:553:THR:HG21	1.22	1.12
1:C:1002:GLN:CG	1:B:759:PHE:HZ	1.63	1.12
1:C:326:ILE:HD11	1:C:534:VAL:HG23	1.19	1.11
1:C:759:PHE:HZ	1:A:1002:GLN:HG3	1.02	1.11
1:C:755:GLN:OE1	1:A:971:GLY:HA2	1.51	1.10
1:C:553:THR:HG21	1:B:841:LEU:HB2	1.13	1.09
1:C:759:PHE:CZ	1:A:1002:GLN:CG	2.33	1.09
1:A:503:VAL:HG21	1:B:505:HIS:HE1	0.97	1.09
1:C:971:GLY:HA2	1:B:755:GLN:OE1	1.51	1.08
1:A:759:PHE:CZ	1:B:1002:GLN:CG	2.38	1.07
1:A:755:GLN:OE1	1:B:971:GLY:HA2	1.54	1.07
1:C:983:ARG:CD	1:A:517:LEU:HD13	1.85	1.06
1:C:505:HIS:HE1	1:B:503:VAL:CG2	1.65	1.06
1:A:503:VAL:CG2	1:B:505:HIS:HE1	1.64	1.06
1:A:841:LEU:HB2	1:B:553:THR:CG2	1.88	1.03
1:C:505:HIS:CE1	1:B:503:VAL:HG21	1.92	1.03
1:A:903:ALA:HB1	1:A:913:GLN:HB3	1.42	1.02
1:C:1083:HIS:ND1	1:C:1137:VAL:HG22	1.74	1.02
1:B:1083:HIS:ND1	1:B:1137:VAL:HG22	1.74	1.02
1:C:553:THR:CG2	1:B:841:LEU:HB2	1.90	1.02
1:C:1002:GLN:CG	1:B:759:PHE:CZ	2.40	1.02
1:A:1083:HIS:ND1	1:A:1137:VAL:HG22	1.74	1.01
1:A:983:ARG:CD	1:B:517:LEU:HD13	1.90	1.00
1:C:1083:HIS:CG	1:C:1137:VAL:HG22	1.97	1.00
1:B:1083:HIS:CG	1:B:1137:VAL:HG22	1.97	0.99
1:C:503:VAL:CG2	1:A:505:HIS:HE1	1.64	0.99
1:A:1083:HIS:CG	1:A:1137:VAL:HG22	1.97	0.98
1:C:326:ILE:HD13	1:C:533:LEU:HA	1.47	0.95
1:C:983:ARG:HD3	1:A:517:LEU:HD13	1.45	0.95
1:C:841:LEU:HB2	1:A:553:THR:HG21	1.48	0.94
1:A:983:ARG:HD3	1:B:517:LEU:HD13	1.50	0.93
1:C:382:VAL:HG11	1:C:387:LEU:HD13	1.50	0.92
1:A:503:VAL:HG23	1:B:505:HIS:CE1	2.06	0.90
1:C:505:HIS:CE1	1:B:503:VAL:HG23	2.04	0.89
1:C:62:VAL:HG11	1:C:216:PHE:HE2	1.36	0.88
1:A:62:VAL:HG11	1:A:216:PHE:HE2	1.36	0.88
1:B:300:LYS:HG2	1:B:308:VAL:HG23	1.55	0.87
1:B:559:PHE:HB2	1:B:584:ILE:HD11	1.56	0.87
1:C:503:VAL:HG23	1:A:505:HIS:CE1	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:PRO:HG2	1:B:540:ASN:HD21	1.40	0.86
1:C:326:ILE:HD11	1:C:534:VAL:CG2	2.06	0.86
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.06	0.86
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.58	0.85
1:C:553:THR:HG21	1:B:841:LEU:CB	2.02	0.85
1:A:841:LEU:CB	1:B:553:THR:HG21	2.04	0.85
1:A:322:PRO:HG2	1:A:540:ASN:HD21	1.40	0.85
1:C:322:PRO:HG2	1:C:540:ASN:HD21	1.40	0.85
1:A:326:ILE:HD12	1:A:532:ASN:O	1.76	0.84
1:B:326:ILE:CG2	1:B:532:ASN:O	2.26	0.84
1:B:326:ILE:HD12	1:B:532:ASN:O	1.76	0.84
1:B:557:LYS:HD3	1:B:559:PHE:HE1	1.43	0.83
1:C:1082:CYS:HB2	1:C:1132:ILE:HG13	1.58	0.83
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.61	0.83
1:A:326:ILE:CG2	1:A:532:ASN:O	2.26	0.83
1:C:759:PHE:CZ	1:A:1002:GLN:HG2	2.14	0.82
1:B:326:ILE:HG23	1:B:532:ASN:O	1.80	0.82
1:C:983:ARG:HD2	1:A:517:LEU:HD13	1.60	0.81
1:A:983:ARG:HD2	1:B:517:LEU:HD13	1.63	0.81
1:A:326:ILE:HG23	1:A:532:ASN:O	1.80	0.81
1:B:325:SER:HA	1:B:539:VAL:HG13	1.63	0.81
1:B:1082:CYS:HB2	1:B:1132:ILE:HG13	1.61	0.81
1:A:325:SER:HA	1:A:539:VAL:HG13	1.63	0.81
1:C:326:ILE:HD13	1:C:533:LEU:CA	2.11	0.80
1:C:325:SER:HA	1:C:539:VAL:HG13	1.63	0.80
1:A:1082:CYS:HB2	1:A:1132:ILE:HG13	1.62	0.80
1:C:838:GLY:HA3	2:A:1309:NAG:H81	1.62	0.79
1:B:1083:HIS:ND1	1:B:1137:VAL:CG2	2.46	0.79
1:C:328:ARG:HG3	1:C:530:SER:HB2	1.66	0.78
1:A:328:ARG:HG3	1:A:530:SER:HB2	1.65	0.78
1:B:328:ARG:HG3	1:B:530:SER:HB2	1.66	0.78
1:C:1083:HIS:ND1	1:C:1137:VAL:CG2	2.46	0.77
1:A:1083:HIS:ND1	1:A:1137:VAL:CG2	2.46	0.77
1:C:178:ASP:HA	1:C:188:ASN:HD21	1.49	0.77
1:A:503:VAL:HG23	1:B:505:HIS:NE2	1.99	0.77
1:C:329:PHE:HB3	1:C:330:PRO:HD3	1.66	0.76
1:A:322:PRO:HG2	1:A:540:ASN:ND2	2.01	0.76
1:C:310:LYS:HG2	1:C:664:ILE:HD11	1.68	0.76
1:C:802:PHE:H	2:C:1313:NAG:H82	1.49	0.76
1:C:322:PRO:HG2	1:C:540:ASN:ND2	2.01	0.76
1:A:310:LYS:HG2	1:A:664:ILE:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ASN:O	1:C:422:ASN:ND2	2.20	0.75
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.68	0.75
1:B:322:PRO:HG2	1:B:540:ASN:ND2	2.01	0.75
1:C:788:ILE:HD11	1:A:699:LEU:HB2	1.67	0.75
1:A:62:VAL:HG11	1:A:216:PHE:CE2	2.21	0.75
1:C:503:VAL:HG23	1:A:505:HIS:NE2	2.02	0.75
1:C:707:TYR:HD1	1:B:792:PRO:HG3	1.52	0.75
1:C:62:VAL:HG11	1:C:216:PHE:CE2	2.21	0.75
2:C:1311:NAG:H62	1:B:796:TYR:CD2	2.22	0.75
1:A:37:TYR:HA	1:A:223:LEU:HB2	1.69	0.74
1:A:759:PHE:CZ	1:B:1002:GLN:HG2	2.22	0.73
1:A:43:PHE:HA	1:B:563:GLN:OE1	1.88	0.73
1:A:557:LYS:HD3	1:A:559:PHE:HE1	1.52	0.73
1:C:983:ARG:HD2	1:A:517:LEU:CD1	2.18	0.73
1:C:430:THR:HG22	1:C:517:LEU:HD12	1.64	0.73
1:C:365:TYR:CE2	1:C:387:LEU:HG	2.24	0.73
1:B:577:ARG:HG2	1:B:584:ILE:HG12	1.71	0.73
1:C:430:THR:CG2	1:C:517:LEU:CD1	2.57	0.72
1:C:330:PRO:HG2	1:C:332:VAL:HG22	1.71	0.72
1:C:503:VAL:CB	1:A:505:HIS:CE1	2.72	0.72
1:C:983:ARG:CD	1:A:517:LEU:CD1	2.67	0.72
1:B:65:PHE:HB2	1:B:265:TYR:HB3	1.72	0.71
1:A:65:PHE:HB2	1:A:265:TYR:HB3	1.72	0.71
1:C:65:PHE:HB2	1:C:265:TYR:HB3	1.72	0.71
1:C:971:GLY:CA	1:B:755:GLN:OE1	2.36	0.71
1:B:44:ARG:HB3	1:B:47:VAL:HG11	1.72	0.71
1:C:1083:HIS:CE1	1:C:1137:VAL:HG22	2.26	0.71
1:A:852:ALA:HB1	1:B:570:VAL:HG22	1.72	0.71
1:A:106:PHE:HD1	1:A:235:ILE:HD13	1.56	0.71
1:B:1083:HIS:CE1	1:B:1137:VAL:HG22	2.26	0.71
1:A:503:VAL:CG2	1:B:505:HIS:NE2	2.53	0.71
1:C:44:ARG:HB3	1:C:47:VAL:HG11	1.72	0.70
1:A:1083:HIS:CE1	1:A:1137:VAL:HG22	2.26	0.70
1:B:96:GLU:OE1	1:B:100:ILE:N	2.24	0.70
1:C:43:PHE:HA	1:A:563:GLN:OE1	1.91	0.70
1:C:96:GLU:OE1	1:C:100:ILE:N	2.24	0.70
1:A:44:ARG:HB3	1:A:47:VAL:HG11	1.72	0.70
1:C:503:VAL:CG2	1:A:505:HIS:NE2	2.53	0.70
1:C:987:PRO:HD2	1:C:988:GLU:OE2	1.92	0.70
1:A:96:GLU:OE1	1:A:100:ILE:N	2.24	0.70
1:B:106:PHE:HD1	1:B:235:ILE:HD13	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:903:ALA:HB1	1:C:913:GLN:HB3	1.72	0.70
1:C:106:PHE:HD1	1:C:235:ILE:HD13	1.56	0.69
1:C:326:ILE:CD1	1:C:534:VAL:HG23	2.11	0.69
1:C:505:HIS:NE2	1:B:503:VAL:HG23	2.08	0.69
1:A:987:PRO:HD2	1:A:988:GLU:OE2	1.92	0.69
1:B:327:VAL:HG11	1:B:528:LYS:CE	2.23	0.69
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.75	0.69
1:B:903:ALA:HB1	1:B:913:GLN:HB3	1.75	0.69
1:C:229:LEU:HD23	1:C:229:LEU:H	1.58	0.68
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.75	0.68
1:C:454:ARG:NH1	1:C:467:ASP:O	2.27	0.68
1:A:43:PHE:CA	1:B:563:GLN:OE1	2.42	0.68
1:B:128:ILE:HD11	1:B:175:PHE:HZ	1.59	0.68
1:C:456:PHE:HB2	1:C:491:PRO:HA	1.75	0.68
1:C:1129:VAL:HG13	1:B:917:TYR:HB3	1.76	0.68
1:C:326:ILE:CD1	1:C:534:VAL:N	2.57	0.68
1:A:454:ARG:NH1	1:A:467:ASP:O	2.27	0.68
1:A:456:PHE:HB2	1:A:491:PRO:HA	1.75	0.68
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.75	0.68
1:A:983:ARG:HD2	1:B:517:LEU:CD1	2.24	0.68
1:C:326:ILE:CD1	1:C:533:LEU:C	2.62	0.67
1:A:327:VAL:HG11	1:A:528:LYS:CE	2.23	0.67
1:B:456:PHE:HB2	1:B:491:PRO:HA	1.75	0.67
1:A:229:LEU:HD23	1:A:229:LEU:H	1.58	0.67
1:C:327:VAL:HG11	1:C:528:LYS:CE	2.23	0.67
1:A:350:VAL:HG21	1:A:418:ILE:HG23	1.74	0.67
1:B:129:LYS:HD2	1:B:160:TYR:CE2	2.30	0.67
1:B:454:ARG:NH1	1:B:467:ASP:O	2.27	0.67
1:C:852:ALA:HB1	1:A:570:VAL:HG22	1.77	0.66
1:A:852:ALA:HB1	1:B:570:VAL:CG2	2.26	0.66
1:B:115:GLN:HE21	1:B:233:ILE:HB	1.61	0.65
1:B:327:VAL:HG11	1:B:528:LYS:HE3	1.78	0.65
1:B:375:PHE:CD1	1:B:508:TYR:OH	2.41	0.65
1:A:379:CYS:HA	1:A:432:CYS:HA	1.79	0.65
1:A:327:VAL:HG11	1:A:528:LYS:HE3	1.78	0.65
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.30	0.65
1:A:375:PHE:CD1	1:A:508:TYR:OH	2.41	0.65
1:C:115:GLN:HE21	1:C:233:ILE:HB	1.61	0.65
1:C:327:VAL:HG11	1:C:528:LYS:HE3	1.78	0.65
1:C:128:ILE:HD11	1:C:175:PHE:HZ	1.62	0.65
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:VAL:HB	1:A:505:HIS:CE1	2.32	0.64
1:A:128:ILE:HD11	1:A:175:PHE:HZ	1.62	0.64
1:A:796:TYR:CD2	2:B:1311:NAG:H62	2.33	0.64
1:C:206:LYS:HB3	1:C:223:LEU:HD13	1.80	0.64
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.30	0.64
1:C:406:GLU:OE1	1:C:406:GLU:N	2.30	0.64
1:C:557:LYS:HG3	1:B:844:ILE:O	1.98	0.64
1:C:917:TYR:HB3	1:A:1129:VAL:HG13	1.80	0.64
1:C:326:ILE:CG2	1:C:532:ASN:O	2.45	0.64
1:A:983:ARG:CD	1:B:517:LEU:CD1	2.74	0.64
1:A:200:TYR:HA	1:A:230:PRO:HA	1.80	0.64
1:C:759:PHE:CE2	1:A:1002:GLN:HG2	2.33	0.64
1:C:1079:PRO:HB3	1:B:917:TYR:CE1	2.33	0.64
1:A:118:LEU:HD11	1:A:159:VAL:HB	1.80	0.64
1:C:311:GLY:HA2	1:C:664:ILE:HD12	1.81	0.63
1:A:303:LEU:HD21	1:A:308:VAL:HG12	1.79	0.63
1:C:200:TYR:HA	1:C:230:PRO:HA	1.80	0.63
1:C:852:ALA:HB1	1:A:570:VAL:CG2	2.28	0.63
1:A:503:VAL:CB	1:B:505:HIS:CE1	2.80	0.63
1:C:787:GLN:OE1	1:A:703:ASN:ND2	2.29	0.63
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.81	0.63
1:C:326:ILE:HD11	1:C:533:LEU:C	2.18	0.63
1:B:311:GLY:HA2	1:B:664:ILE:HD12	1.81	0.63
1:A:792:PRO:HG3	1:B:707:TYR:HD1	1.64	0.63
1:C:556:ASN:H	1:B:844:ILE:HG23	1.64	0.63
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.81	0.63
1:B:39:PRO:HG3	1:B:55:PHE:HZ	1.64	0.63
1:C:788:ILE:CD1	1:A:699:LEU:HB2	2.28	0.63
1:B:134:GLN:HG2	1:B:162:SER:HB2	1.80	0.63
1:B:300:LYS:HG2	1:B:308:VAL:CG2	2.29	0.62
1:C:796:TYR:CD2	2:A:1311:NAG:H62	2.34	0.62
1:A:398:ASP:HB2	1:A:512:VAL:HG12	1.81	0.62
1:C:821:LEU:HD11	1:C:935:GLN:HG3	1.82	0.62
1:C:136:CYS:HB2	1:C:159:VAL:HA	1.81	0.62
1:B:1100:THR:HB	2:B:1315:NAG:HN2	1.64	0.62
1:A:311:GLY:HA2	1:A:664:ILE:HD12	1.81	0.62
1:C:189:LEU:HD23	1:C:210:ILE:HA	1.81	0.62
1:A:441:LEU:HD22	1:A:509:ARG:HH12	1.65	0.62
1:A:1100:THR:HB	2:A:1315:NAG:HN2	1.65	0.62
1:C:917:TYR:CE1	1:A:1079:PRO:HB3	2.35	0.62
1:B:326:ILE:HG21	1:B:532:ASN:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1002:GLN:HG2	1:B:759:PHE:CE2	2.34	0.61
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.28	0.61
1:C:276:LEU:HD11	1:C:304:LYS:HA	1.81	0.61
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.82	0.61
1:A:276:LEU:HD11	1:A:304:LYS:HA	1.82	0.61
1:B:441:LEU:HD22	1:B:509:ARG:HH12	1.65	0.61
1:C:1013:ILE:HD13	1:B:1012:LEU:HB3	1.83	0.61
1:B:323:THR:OG1	1:B:324:GLU:N	2.34	0.61
1:C:441:LEU:HD22	1:C:509:ARG:HH12	1.65	0.60
1:C:1002:GLN:HG2	1:B:759:PHE:CZ	2.32	0.60
1:A:759:PHE:CE2	1:B:1002:GLN:HG2	2.35	0.60
1:B:662:CYS:HB2	1:B:697:MET:HE3	1.82	0.60
1:C:326:ILE:HG23	1:C:532:ASN:O	2.01	0.60
1:C:375:PHE:CD1	1:C:508:TYR:OH	2.42	0.60
1:C:557:LYS:HD3	1:C:559:PHE:HE1	1.65	0.60
1:C:645:THR:HG23	1:C:647:ALA:H	1.65	0.60
1:C:323:THR:OG1	1:C:324:GLU:N	2.34	0.60
1:C:564:GLN:O	1:C:565:PHE:C	2.40	0.60
1:A:34:ARG:NH1	1:A:191:GLU:OE2	2.34	0.60
1:A:323:THR:OG1	1:A:324:GLU:N	2.34	0.60
1:A:356:THR:OG1	1:A:397:ALA:HB3	2.02	0.60
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.36	0.60
1:A:513:LEU:HG	1:A:515:PHE:CE1	2.37	0.60
1:C:1002:GLN:CG	1:B:759:PHE:CE2	2.84	0.60
1:A:318:PHE:CE1	1:A:593:GLY:HA3	2.37	0.60
1:B:350:VAL:HG21	1:B:418:ILE:HG23	1.84	0.60
1:C:282:ASN:OD1	1:A:558:LYS:HG3	2.02	0.59
1:B:412:PRO:HG3	1:B:429:PHE:HB3	1.84	0.59
1:B:564:GLN:O	1:B:565:PHE:C	2.40	0.59
1:A:567:ARG:HD3	1:A:571:ASP:HA	1.84	0.59
1:A:213:GLY:O	1:A:214:ARG:HG3	2.02	0.59
1:A:564:GLN:O	1:A:565:PHE:C	2.40	0.59
1:C:627:ASP:HA	1:C:634:ARG:HH22	1.68	0.59
1:A:513:LEU:HG	1:A:515:PHE:HE1	1.67	0.59
1:A:206:LYS:HB3	1:A:223:LEU:HD13	1.83	0.59
1:C:359:SER:HA	1:C:524:VAL:HG23	1.85	0.59
1:C:841:LEU:CB	1:A:553:THR:HG21	2.29	0.59
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.28	0.59
1:B:131:CYS:HB3	1:B:133:PHE:CE2	2.38	0.59
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.34	0.59
1:B:326:ILE:H	1:B:539:VAL:HG11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:THR:OG1	1:B:397:ALA:HB3	2.03	0.58
1:B:213:GLY:O	1:B:214:ARG:HG3	2.02	0.58
1:B:334:ASN:ND2	1:B:360:ASN:O	2.35	0.58
1:B:567:ARG:HD3	1:B:571:ASP:HA	1.84	0.58
1:A:326:ILE:H	1:A:539:VAL:HG11	1.68	0.58
1:A:382:VAL:HG23	1:A:517:LEU:HD11	1.84	0.58
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.85	0.58
1:C:334:ASN:ND2	1:C:360:ASN:O	2.35	0.58
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.28	0.58
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.84	0.58
1:C:792:PRO:HG3	1:A:707:TYR:HD1	1.68	0.58
1:C:844:ILE:O	1:A:557:LYS:HG3	2.03	0.58
1:C:976:VAL:HG12	1:C:979:ASP:H	1.69	0.58
1:A:326:ILE:HG21	1:A:532:ASN:O	2.00	0.58
1:A:976:VAL:HG12	1:A:979:ASP:H	1.69	0.58
1:B:81:ASN:ND2	1:B:240:THR:O	2.25	0.58
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.39	0.58
1:C:326:ILE:H	1:C:539:VAL:HG11	1.68	0.58
1:B:62:VAL:HG11	1:B:216:PHE:HE2	1.68	0.58
1:C:742:ILE:HG23	1:C:1000:ARG:HB2	1.86	0.58
1:A:1142:GLN:N	1:A:1142:GLN:OE1	2.36	0.58
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.85	0.58
1:C:336:CYS:HB2	1:C:338:PHE:CE2	2.39	0.57
1:B:976:VAL:HG12	1:B:979:ASP:H	1.69	0.57
1:A:43:PHE:CB	1:B:563:GLN:OE1	2.53	0.57
1:A:847:ARG:HB2	1:A:851:CYS:CB	2.34	0.57
1:A:102:ARG:HH21	1:A:122:ASN:CA	2.18	0.57
1:B:382:VAL:HG23	1:B:517:LEU:HD11	1.86	0.57
1:C:447:GLY:HA2	1:C:498:ARG:HG2	1.87	0.57
1:C:805:ILE:HB	1:C:878:LEU:HD21	1.85	0.57
1:C:1142:GLN:OE1	1:C:1142:GLN:N	2.36	0.57
1:A:1012:LEU:HB3	1:B:1013:ILE:HD13	1.86	0.57
1:B:965:GLN:O	1:B:968:SER:OG	2.22	0.57
1:A:336:CYS:HB2	1:A:338:PHE:CE2	2.39	0.56
1:A:557:LYS:HD3	1:A:559:PHE:CE1	2.36	0.56
1:A:1144:GLU:N	1:A:1144:GLU:OE2	2.38	0.56
1:B:1142:GLN:N	1:B:1142:GLN:OE1	2.36	0.56
1:C:847:ARG:HB2	1:C:851:CYS:HB2	1.85	0.56
1:A:81:ASN:ND2	1:A:240:THR:O	2.25	0.56
1:A:136:CYS:HB2	1:A:159:VAL:HA	1.86	0.56
1:A:213:GLY:O	1:A:214:ARG:CG	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLY:HA2	1:A:498:ARG:HG2	1.87	0.56
1:B:1144:GLU:OE2	1:B:1144:GLU:N	2.38	0.56
1:C:215:ASP:O	1:C:216:PHE:C	2.44	0.56
1:A:322:PRO:CG	1:A:540:ASN:HD21	2.16	0.56
1:B:39:PRO:HG2	1:B:51:THR:HG21	1.87	0.56
1:C:505:HIS:NE2	1:B:503:VAL:CG2	2.68	0.56
1:A:334:ASN:ND2	1:A:360:ASN:O	2.35	0.56
1:B:102:ARG:HH21	1:B:122:ASN:CA	2.18	0.56
1:B:447:GLY:HA2	1:B:498:ARG:HG2	1.87	0.56
1:C:43:PHE:CA	1:A:563:GLN:OE1	2.53	0.56
1:B:336:CYS:HB2	1:B:338:PHE:CE2	2.39	0.56
1:C:503:VAL:HB	1:A:505:HIS:NE2	2.20	0.56
1:C:736:VAL:HG22	1:C:858:LEU:HD22	1.87	0.56
1:C:1144:GLU:N	1:C:1144:GLU:OE2	2.38	0.56
1:B:429:PHE:HE1	1:B:514:SER:HB2	1.71	0.56
1:C:102:ARG:HH21	1:C:122:ASN:CA	2.18	0.56
1:C:178:ASP:N	1:C:178:ASP:OD1	2.39	0.56
1:A:736:VAL:HG22	1:A:858:LEU:HD22	1.87	0.56
1:B:359:SER:HA	1:B:524:VAL:HG23	1.87	0.56
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.72	0.55
1:C:1002:GLN:NE2	1:B:759:PHE:CZ	2.74	0.55
1:A:359:SER:HA	1:A:524:VAL:HG23	1.87	0.55
1:C:102:ARG:HH21	1:C:122:ASN:HA	1.71	0.55
1:C:563:GLN:OE1	1:B:43:PHE:HA	2.06	0.55
1:B:213:GLY:O	1:B:214:ARG:CG	2.54	0.55
1:B:215:ASP:O	1:B:216:PHE:C	2.44	0.55
1:C:836:GLN:HG2	1:C:840:CYS:SG	2.47	0.55
1:C:852:ALA:CB	1:A:570:VAL:HG22	2.36	0.55
1:A:215:ASP:O	1:A:216:PHE:C	2.44	0.55
1:A:384:PRO:HA	1:A:387:LEU:HB2	1.87	0.55
1:B:847:ARG:HB2	1:B:851:CYS:HB2	1.88	0.55
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.34	0.55
1:C:102:ARG:HH12	1:C:176:LEU:HD12	1.72	0.55
1:C:358:ILE:HB	1:C:395:VAL:HB	1.89	0.55
1:C:130:VAL:HG23	1:C:168:PHE:HB3	1.87	0.55
1:A:102:ARG:HH12	1:A:176:LEU:HD12	1.72	0.55
1:A:453:TYR:CD1	1:A:495:TYR:HD1	2.24	0.55
1:A:852:ALA:CB	1:B:570:VAL:HG22	2.36	0.55
1:B:453:TYR:CD1	1:B:495:TYR:HD1	2.24	0.55
1:A:581:THR:C	1:A:583:GLU:H	2.10	0.55
1:C:41:LYS:O	1:A:563:GLN:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ASP:N	1:A:178:ASP:OD1	2.39	0.55
1:B:102:ARG:HH12	1:B:176:LEU:HD12	1.72	0.55
1:A:189:LEU:HG	1:A:208:THR:O	2.07	0.54
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.88	0.54
1:A:102:ARG:HH21	1:A:122:ASN:HA	1.71	0.54
1:A:880:GLY:O	1:A:884:SER:OG	2.23	0.54
1:B:570:VAL:HG23	1:B:570:VAL:O	2.08	0.54
1:C:37:TYR:HA	1:C:223:LEU:HB2	1.88	0.54
1:C:326:ILE:HD11	1:C:534:VAL:N	2.21	0.54
1:C:707:TYR:CD1	1:B:792:PRO:HG3	2.39	0.54
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.90	0.54
1:A:326:ILE:H	1:A:539:VAL:CG1	2.21	0.54
1:A:403:LYS:HD2	1:A:505:HIS:HA	1.89	0.54
1:B:826:VAL:HB	1:B:1057:PRO:HG2	1.90	0.54
1:C:1012:LEU:HB3	1:A:1013:ILE:HD13	1.88	0.54
1:A:570:VAL:O	1:A:570:VAL:HG23	2.08	0.54
1:B:975:SER:O	1:B:975:SER:OG	2.25	0.54
1:C:505:HIS:CE1	1:B:503:VAL:CB	2.91	0.54
1:A:43:PHE:HB2	1:B:563:GLN:OE1	2.08	0.54
1:A:503:VAL:HB	1:B:505:HIS:CE1	2.43	0.54
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.36	0.54
1:C:418:ILE:H	1:C:418:ILE:HD12	1.72	0.54
1:B:736:VAL:HG22	1:B:858:LEU:HD22	1.88	0.54
1:C:720:ILE:HD12	1:C:923:ILE:HD11	1.90	0.54
1:A:742:ILE:HG23	1:A:1000:ARG:HB2	1.88	0.54
1:B:102:ARG:HH21	1:B:122:ASN:HA	1.71	0.54
1:B:475:ALA:HB3	1:B:487:ASN:HB3	1.90	0.54
1:C:62:VAL:CG1	1:C:216:PHE:HE2	2.15	0.54
1:C:453:TYR:CD1	1:C:495:TYR:HD1	2.24	0.54
1:A:560:LEU:O	1:A:562:PHE:N	2.41	0.54
1:B:326:ILE:H	1:B:539:VAL:CG1	2.21	0.54
1:C:326:ILE:H	1:C:539:VAL:CG1	2.21	0.54
1:C:1100:THR:HB	2:C:1315:NAG:HN2	1.73	0.54
1:A:752:LEU:HD12	1:A:993:ILE:HG21	1.90	0.54
1:C:560:LEU:O	1:C:562:PHE:N	2.41	0.53
1:C:975:SER:O	1:C:975:SER:OG	2.25	0.53
1:C:1002:GLN:NE2	1:B:759:PHE:HZ	2.05	0.53
1:A:57:PRO:HG3	1:A:273:ARG:HD2	1.90	0.53
1:A:759:PHE:CE2	1:B:1002:GLN:CG	2.90	0.53
1:B:559:PHE:HB2	1:B:584:ILE:CD1	2.35	0.53
1:C:475:ALA:HB3	1:C:487:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1002:GLN:HE21	1:B:759:PHE:HZ	1.55	0.53
1:A:117:LEU:HD12	1:A:118:LEU:N	2.24	0.53
1:A:429:PHE:HE1	1:A:514:SER:HB2	1.74	0.53
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.90	0.53
1:B:200:TYR:HA	1:B:230:PRO:HA	1.91	0.53
1:B:560:LEU:O	1:B:562:PHE:N	2.41	0.53
1:B:720:ILE:HD12	1:B:923:ILE:HD11	1.90	0.53
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.90	0.53
1:C:375:PHE:CG	1:C:508:TYR:CZ	2.97	0.53
1:C:880:GLY:O	1:C:884:SER:OG	2.23	0.53
1:A:62:VAL:CG1	1:A:216:PHE:HE2	2.15	0.53
1:B:752:LEU:HD12	1:B:993:ILE:HG21	1.90	0.53
1:C:403:LYS:HG2	1:C:505:HIS:HA	1.90	0.53
1:A:129:LYS:HD3	1:A:133:PHE:CZ	2.43	0.53
1:A:965:GLN:O	1:A:968:SER:OG	2.22	0.53
1:A:975:SER:O	1:A:975:SER:OG	2.25	0.53
1:B:129:LYS:HA	1:B:168:PHE:O	2.09	0.53
1:B:439:ASN:O	1:B:443:SER:OG	2.25	0.53
1:B:945:LEU:HD12	1:B:948:LEU:HD12	1.90	0.53
1:C:957:GLN:OE1	1:B:765:ARG:HD3	2.08	0.53
1:B:178:ASP:OD1	1:B:178:ASP:N	2.39	0.53
1:C:765:ARG:HD3	1:A:957:GLN:OE1	2.08	0.53
1:B:847:ARG:HB2	1:B:851:CYS:CB	2.39	0.53
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.90	0.53
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.90	0.53
1:B:375:PHE:CG	1:B:508:TYR:CZ	2.97	0.53
1:C:858:LEU:HD12	1:C:963:VAL:HG12	1.91	0.53
1:C:965:GLN:O	1:C:968:SER:OG	2.22	0.53
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.44	0.53
1:A:720:ILE:HD12	1:A:923:ILE:HD11	1.90	0.53
1:B:880:GLY:O	1:B:884:SER:OG	2.23	0.53
1:C:752:LEU:HD12	1:C:993:ILE:HG21	1.90	0.52
1:B:403:LYS:HD2	1:B:505:HIS:HA	1.90	0.52
1:A:858:LEU:HD12	1:A:963:VAL:HG12	1.91	0.52
1:B:420:ASP:HB3	1:B:460:LYS:HD2	1.91	0.52
1:B:1083:HIS:HB2	1:B:1137:VAL:HG13	1.91	0.52
1:C:993:ILE:O	1:C:997:ILE:HG12	2.10	0.52
1:B:752:LEU:HD12	1:B:993:ILE:CG2	2.40	0.52
1:B:858:LEU:HD12	1:B:963:VAL:HG12	1.91	0.52
1:B:993:ILE:O	1:B:997:ILE:HG12	2.10	0.52
1:C:133:PHE:CD2	1:C:160:TYR:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:GLU:HB2	1:C:223:LEU:HD11	1.91	0.52
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.91	0.52
1:A:945:LEU:HD12	1:A:948:LEU:HD12	1.91	0.52
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.92	0.52
1:C:803:SER:HB3	2:C:1313:NAG:HN2	1.74	0.52
1:A:375:PHE:CG	1:A:508:TYR:CZ	2.97	0.52
1:A:475:ALA:HB3	1:A:487:ASN:HB3	1.90	0.52
1:B:108:THR:C	1:B:110:LEU:H	2.13	0.52
1:B:912:THR:O	1:B:915:VAL:HG12	2.10	0.52
1:B:559:PHE:CB	1:B:584:ILE:HD11	2.36	0.52
1:B:397:ALA:HA	1:B:512:VAL:O	2.09	0.52
1:C:117:LEU:HD12	1:C:118:LEU:N	2.24	0.52
1:C:755:GLN:OE1	1:A:971:GLY:CA	2.41	0.52
1:A:755:GLN:OE1	1:B:971:GLY:CA	2.42	0.52
1:A:752:LEU:HD12	1:A:993:ILE:CG2	2.40	0.52
1:C:1083:HIS:HB2	1:C:1137:VAL:HG13	1.91	0.51
1:A:108:THR:C	1:A:110:LEU:H	2.13	0.51
1:B:229:LEU:H	1:B:229:LEU:HD23	1.75	0.51
1:B:364:ASP:OD1	1:B:364:ASP:N	2.43	0.51
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.92	0.51
1:A:115:GLN:HE21	1:A:233:ILE:HB	1.76	0.51
1:A:993:ILE:O	1:A:997:ILE:HG12	2.10	0.51
1:C:847:ARG:HB2	1:C:851:CYS:CB	2.41	0.51
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.34	0.51
1:A:1083:HIS:HB2	1:A:1137:VAL:HG13	1.91	0.51
1:B:347:PHE:HD2	1:B:399:SER:HB2	1.75	0.51
1:C:752:LEU:HD12	1:C:993:ILE:CG2	2.40	0.51
1:C:912:THR:O	1:C:915:VAL:HG12	2.11	0.51
1:B:931:ILE:O	1:B:934:ILE:HG22	2.09	0.51
1:A:307:THR:HA	1:A:602:THR:HG21	1.93	0.51
1:B:322:PRO:CG	1:B:540:ASN:ND2	2.74	0.51
1:C:364:ASP:N	1:C:364:ASP:OD1	2.43	0.51
1:C:854:LYS:HE2	1:A:592:PHE:CD2	2.46	0.51
1:C:1006:THR:HG21	1:B:762:GLN:OE1	2.10	0.51
1:B:631:PRO:HB3	1:B:633:TRP:CZ2	2.45	0.51
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.43	0.51
1:B:805:ILE:HB	1:B:878:LEU:HD21	1.93	0.51
1:A:31:SER:HB3	1:A:62:VAL:CG2	2.41	0.50
1:B:559:PHE:HD2	1:B:577:ARG:HD2	1.77	0.50
1:C:631:PRO:HB3	1:C:633:TRP:CZ2	2.46	0.50
1:C:759:PHE:CE2	1:A:1002:GLN:CG	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:836:GLN:O	1:C:837:TYR:C	2.50	0.50
1:B:382:VAL:CG2	1:B:517:LEU:HD11	2.41	0.50
1:B:557:LYS:HD3	1:B:559:PHE:CE1	2.34	0.50
1:C:276:LEU:CD1	1:C:304:LYS:HA	2.42	0.50
1:C:854:LYS:HE2	1:A:592:PHE:HD2	1.75	0.50
1:A:387:LEU:HD11	1:A:515:PHE:CE2	2.47	0.50
1:C:563:GLN:OE1	1:B:43:PHE:CA	2.60	0.50
1:C:675:GLN:HG3	1:C:693:ILE:HD11	1.94	0.50
1:A:177:MET:H	1:A:207:HIS:CE1	2.30	0.50
1:A:765:ARG:HD3	1:B:957:GLN:OE1	2.11	0.50
1:B:189:LEU:HG	1:B:208:THR:O	2.12	0.50
1:B:27:SER:O	1:B:64:TRP:N	2.45	0.50
1:B:581:THR:C	1:B:583:GLU:H	2.14	0.50
1:A:290:ASP:O	1:A:297:SER:HB3	2.12	0.50
1:C:187:LYS:O	1:C:188:ASN:C	2.50	0.50
1:C:403:LYS:HB3	1:C:406:GLU:OE1	2.12	0.50
1:B:113:LYS:HD2	1:B:113:LYS:O	2.12	0.50
1:B:317:ASN:HB2	1:B:592:PHE:CE1	2.46	0.50
1:C:31:SER:HB3	1:C:62:VAL:CG2	2.41	0.50
1:C:762:GLN:OE1	1:A:1006:THR:HG21	2.12	0.50
1:A:382:VAL:CG2	1:A:517:LEU:HD11	2.41	0.50
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.12	0.50
1:B:215:ASP:HB2	1:B:266:TYR:OH	2.12	0.50
1:C:503:VAL:CB	1:A:505:HIS:NE2	2.75	0.49
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.12	0.49
1:A:364:ASP:OD1	1:A:364:ASP:N	2.43	0.49
1:A:762:GLN:OE1	1:B:1006:THR:HG21	2.12	0.49
1:C:177:MET:H	1:C:207:HIS:CE1	2.30	0.49
1:C:215:ASP:HB2	1:C:266:TYR:OH	2.12	0.49
1:C:290:ASP:O	1:C:297:SER:HB3	2.11	0.49
1:A:360:ASN:H	1:A:523:THR:HB	1.78	0.49
1:B:675:GLN:HG3	1:B:693:ILE:HD11	1.94	0.49
1:C:113:LYS:HD2	1:C:113:LYS:O	2.12	0.49
1:A:276:LEU:CD1	1:A:304:LYS:HA	2.42	0.49
1:A:322:PRO:CG	1:A:540:ASN:ND2	2.74	0.49
1:C:946:GLY:O	1:C:950:ASP:HB2	2.13	0.49
1:A:44:ARG:HB3	1:A:47:VAL:CG1	2.41	0.49
1:B:384:PRO:HA	1:B:387:LEU:HB2	1.94	0.49
1:B:821:LEU:HD11	1:B:935:GLN:HG3	1.94	0.49
1:C:570:VAL:HG23	1:C:572:THR:HG23	1.94	0.49
1:A:113:LYS:HD2	1:A:113:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:PRO:HB3	1:A:633:TRP:CZ2	2.47	0.49
1:A:844:ILE:O	1:B:557:LYS:HG3	2.12	0.49
1:B:131:CYS:SG	1:B:163:ALA:O	2.71	0.49
1:B:946:GLY:O	1:B:950:ASP:HB2	2.13	0.49
1:C:108:THR:C	1:C:110:LEU:H	2.13	0.49
1:C:131:CYS:HB3	1:C:133:PHE:CE2	2.47	0.49
1:A:41:LYS:O	1:B:563:GLN:HA	2.12	0.49
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.53	0.49
1:C:189:LEU:HG	1:C:208:THR:O	2.12	0.49
1:A:191:GLU:HB2	1:A:223:LEU:HD11	1.93	0.49
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.48	0.49
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.93	0.49
1:C:360:ASN:H	1:C:523:THR:HB	1.77	0.49
1:A:131:CYS:HB3	1:A:133:PHE:CE2	2.48	0.49
1:A:946:GLY:O	1:A:950:ASP:HB2	2.13	0.49
1:B:177:MET:H	1:B:207:HIS:CE1	2.30	0.49
1:C:44:ARG:HB3	1:C:47:VAL:CG1	2.41	0.48
1:C:307:THR:HA	1:C:602:THR:HG21	1.95	0.48
1:C:326:ILE:HD13	1:C:533:LEU:C	2.31	0.48
1:C:971:GLY:HA2	1:B:755:GLN:CD	2.31	0.48
1:A:497:PHE:HA	1:A:501:TYR:HE2	1.78	0.48
1:A:675:GLN:HG3	1:A:693:ILE:HD11	1.94	0.48
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.48	0.48
1:B:360:ASN:H	1:B:523:THR:HB	1.77	0.48
1:B:588:THR:HG23	1:B:589:PRO:HD2	1.95	0.48
1:C:578:ASP:O	1:C:582:LEU:N	2.45	0.48
1:C:749:CYS:SG	1:C:997:ILE:HD11	2.53	0.48
1:A:740:MET:HG3	1:B:592:PHE:CZ	2.48	0.48
1:A:973:ILE:HG22	1:A:992:GLN:HG3	1.95	0.48
1:B:556:ASN:O	1:B:557:LYS:C	2.51	0.48
1:B:927:PHE:HZ	1:B:1052:PHE:HE2	1.60	0.48
1:C:568:ASP:HA	1:B:846:ALA:HB1	1.95	0.48
1:C:588:THR:HG22	1:C:589:PRO:O	2.13	0.48
1:C:588:THR:OG1	1:B:841:LEU:HB3	2.13	0.48
1:A:296:LEU:HD11	1:A:308:VAL:HG21	1.95	0.48
1:B:126:VAL:HG11	1:B:175:PHE:CE1	2.49	0.48
1:B:214:ARG:O	1:B:217:PRO:HG3	2.13	0.48
1:B:555:SER:HB3	1:B:584:ILE:HG22	1.95	0.48
1:C:760:CYS:HA	1:C:763:LEU:HG	1.96	0.48
1:A:215:ASP:HB2	1:A:266:TYR:OH	2.12	0.48
1:A:374:PHE:CZ	1:A:434:ILE:HG23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:PHE:HZ	1:A:1052:PHE:HE2	1.61	0.48
1:A:1106:GLN:OE1	1:A:1106:GLN:N	2.47	0.48
1:B:497:PHE:HA	1:B:501:TYR:HE2	1.78	0.48
1:C:214:ARG:O	1:C:217:PRO:HG3	2.13	0.48
1:B:760:CYS:HA	1:B:763:LEU:HG	1.95	0.48
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.12	0.48
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.95	0.48
1:A:106:PHE:CD1	1:A:235:ILE:HG21	2.49	0.48
1:A:802:PHE:O	1:A:804:GLN:N	2.47	0.48
1:C:431:GLY:HA2	1:C:515:PHE:HD2	1.77	0.48
1:B:44:ARG:HB3	1:B:47:VAL:CG1	2.41	0.48
1:B:106:PHE:CD1	1:B:235:ILE:HG21	2.49	0.48
1:B:191:GLU:HB2	1:B:223:LEU:HD11	1.95	0.48
1:C:126:VAL:HG11	1:C:175:PHE:CE1	2.49	0.48
1:A:331:ASN:HB3	1:A:580:GLN:HG2	1.94	0.48
1:B:322:PRO:CG	1:B:540:ASN:HD21	2.16	0.48
1:C:131:CYS:HA	1:C:166:CYS:HA	1.96	0.48
1:A:126:VAL:HG11	1:A:175:PHE:CE1	2.49	0.48
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.53	0.48
1:B:973:ILE:HG22	1:B:992:GLN:HG3	1.95	0.48
1:C:81:ASN:ND2	1:C:240:THR:O	2.25	0.48
1:C:296:LEU:HD11	1:C:308:VAL:HG21	1.95	0.48
1:C:497:PHE:HA	1:C:501:TYR:HE2	1.78	0.48
1:C:843:ASP:O	1:C:845:ALA:N	2.47	0.48
1:C:439:ASN:O	1:C:443:SER:OG	2.25	0.47
1:B:878:LEU:HD13	1:B:1053:PRO:HD2	1.96	0.47
1:C:31:SER:HB3	1:C:62:VAL:HG21	1.96	0.47
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.48	0.47
1:A:439:ASN:O	1:A:443:SER:OG	2.25	0.47
1:C:106:PHE:HB3	1:C:235:ILE:HG23	1.97	0.47
1:C:557:LYS:HB3	1:C:559:PHE:HD1	1.79	0.47
1:C:973:ILE:HG22	1:C:992:GLN:HG3	1.95	0.47
1:A:760:CYS:HA	1:A:763:LEU:HG	1.96	0.47
1:B:213:GLY:C	1:B:214:ARG:HG3	2.35	0.47
1:B:726:ILE:HG23	1:B:1061:VAL:HG22	1.96	0.47
1:C:103:GLY:HA3	1:C:120:VAL:HA	1.96	0.47
1:C:927:PHE:HZ	1:C:1052:PHE:HE2	1.60	0.47
1:C:1002:GLN:CD	1:B:759:PHE:HZ	2.15	0.47
1:A:520:ALA:O	1:A:521:PRO:C	2.53	0.47
1:A:726:ILE:HG23	1:A:1061:VAL:HG22	1.96	0.47
1:B:342:PHE:CZ	1:B:511:VAL:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LEU:HB2	1:C:238:PHE:HD2	1.79	0.47
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.93	0.47
1:A:1101:HIS:CD2	2:A:1315:NAG:H3	2.49	0.47
1:B:84:LEU:HB2	1:B:238:PHE:HD2	1.79	0.47
1:B:383:SER:HB3	1:B:386:LYS:HG2	1.95	0.47
1:C:322:PRO:CG	1:C:540:ASN:HD21	2.16	0.47
1:C:726:ILE:HG23	1:C:1061:VAL:HG22	1.96	0.47
1:C:850:ILE:O	1:C:854:LYS:HG2	2.15	0.47
1:C:931:ILE:O	1:C:934:ILE:HG22	2.15	0.47
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.96	0.47
1:C:106:PHE:CD1	1:C:235:ILE:HG21	2.49	0.47
1:C:356:THR:OG1	1:C:397:ALA:HB3	2.15	0.47
1:A:213:GLY:C	1:A:214:ARG:HG3	2.34	0.47
1:A:931:ILE:O	1:A:934:ILE:HG22	2.15	0.47
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.47
1:B:206:LYS:HB3	1:B:223:LEU:HD13	1.97	0.47
1:B:216:PHE:O	1:B:217:PRO:C	2.52	0.47
1:B:1132:ILE:HD12	1:B:1132:ILE:HA	1.78	0.47
1:C:823:PHE:CD1	1:C:1057:PRO:HG3	2.50	0.47
1:A:106:PHE:HB3	1:A:235:ILE:HG23	1.97	0.47
1:A:214:ARG:O	1:A:217:PRO:HG3	2.13	0.47
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.50	0.47
1:C:177:MET:HB2	1:C:207:HIS:ND1	2.30	0.47
1:C:322:PRO:CG	1:C:540:ASN:ND2	2.74	0.47
1:C:577:ARG:HG2	1:C:584:ILE:HD13	1.97	0.47
1:C:631:PRO:HA	1:C:633:TRP:CZ3	2.50	0.47
1:C:741:TYR:CD2	1:C:1004:LEU:HD22	2.50	0.47
1:A:31:SER:HB3	1:A:62:VAL:HG21	1.96	0.47
1:A:627:ASP:HA	1:A:634:ARG:HH22	1.80	0.47
1:A:823:PHE:CD1	1:A:1057:PRO:HG3	2.50	0.47
1:B:823:PHE:CD1	1:B:1057:PRO:HG3	2.50	0.47
1:A:878:LEU:HD13	1:A:1053:PRO:HD2	1.96	0.46
1:C:175:PHE:CD1	1:C:175:PHE:N	2.82	0.46
1:C:355:ARG:NE	1:C:398:ASP:OD2	2.48	0.46
1:C:742:ILE:HG22	1:C:997:ILE:CD1	2.45	0.46
1:C:983:ARG:HD3	1:A:517:LEU:CD1	2.30	0.46
1:C:1132:ILE:HA	1:C:1132:ILE:HD12	1.77	0.46
1:A:216:PHE:O	1:A:217:PRO:C	2.52	0.46
1:B:204:TYR:CE2	1:B:225:PRO:HG3	2.50	0.46
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.97	0.46
1:C:25:THR:HG23	1:C:66:HIS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:LEU:HD13	1:C:1053:PRO:HD2	1.96	0.46
1:A:84:LEU:HB2	1:A:238:PHE:HD2	1.79	0.46
1:A:318:PHE:HD2	1:A:629:LEU:HD11	1.81	0.46
1:B:103:GLY:HA3	1:B:120:VAL:HA	1.96	0.46
1:B:559:PHE:CD1	1:B:584:ILE:HD13	2.50	0.46
1:B:718:PHE:HE1	1:B:919:ASN:ND2	2.14	0.46
1:C:755:GLN:CD	1:A:971:GLY:HA2	2.30	0.46
1:A:718:PHE:HE1	1:A:919:ASN:ND2	2.14	0.46
1:B:177:MET:HB2	1:B:207:HIS:ND1	2.31	0.46
1:C:176:LEU:HD22	1:C:190:ARG:HD2	1.98	0.46
1:C:645:THR:HG23	1:C:647:ALA:N	2.31	0.46
1:C:650:LEU:HD23	1:C:653:ALA:HB3	1.98	0.46
1:B:129:LYS:HE2	1:B:169:GLU:HG3	1.98	0.46
1:B:307:THR:HA	1:B:602:THR:HG21	1.96	0.46
1:C:563:GLN:HA	1:B:41:LYS:O	2.16	0.46
1:B:25:THR:HG23	1:B:66:HIS:HB2	1.98	0.46
1:B:454:ARG:HH22	1:B:467:ASP:HB3	1.81	0.46
1:A:133:PHE:CD2	1:A:160:TYR:HA	2.51	0.46
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.81	0.46
1:C:1083:HIS:CE1	1:C:1137:VAL:CG2	2.96	0.46
1:A:175:PHE:CD1	1:A:175:PHE:N	2.82	0.46
1:A:347:PHE:HD2	1:A:399:SER:HB2	1.81	0.46
1:B:627:ASP:HA	1:B:634:ARG:HH22	1.80	0.46
1:B:1092:GLU:N	1:B:1092:GLU:OE2	2.49	0.46
1:C:592:PHE:CD1	1:B:740:MET:HE2	2.51	0.46
1:C:763:LEU:HD13	1:C:1004:LEU:HG	1.98	0.46
1:A:342:PHE:CE2	1:A:436:TRP:CZ3	3.04	0.46
1:C:454:ARG:HH22	1:C:467:ASP:HB3	1.81	0.46
1:C:718:PHE:HE1	1:C:919:ASN:ND2	2.14	0.46
1:A:25:THR:HG23	1:A:66:HIS:HB2	1.98	0.46
1:A:177:MET:HB2	1:A:207:HIS:ND1	2.31	0.46
1:A:439:ASN:OD1	1:A:507:PRO:HD2	2.17	0.46
1:A:631:PRO:HA	1:A:633:TRP:CZ3	2.50	0.46
1:B:575:ALA:HA	1:B:585:LEU:O	2.16	0.46
1:C:423:TYR:OH	1:C:464:PHE:HE1	1.98	0.45
1:A:454:ARG:HH22	1:A:467:ASP:HB3	1.81	0.45
1:B:528:LYS:O	1:B:529:LYS:HB3	2.16	0.45
1:C:105:ILE:HD13	1:C:159:VAL:HG11	1.98	0.45
1:C:439:ASN:OD1	1:C:507:PRO:HD2	2.17	0.45
1:C:528:LYS:O	1:C:529:LYS:HB3	2.16	0.45
1:C:617:CYS:O	1:C:621:SER:N	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:PHE:CZ	1:B:1002:GLN:NE2	2.84	0.45
1:A:1092:GLU:OE2	1:A:1092:GLU:N	2.49	0.45
1:B:106:PHE:HB3	1:B:235:ILE:HG23	1.97	0.45
1:B:162:SER:O	1:B:163:ALA:C	2.54	0.45
1:B:631:PRO:HA	1:B:633:TRP:CZ3	2.51	0.45
1:B:763:LEU:HD13	1:B:1004:LEU:HG	1.98	0.45
1:B:1101:HIS:CD2	2:B:1315:NAG:H3	2.51	0.45
1:C:644:GLN:NE2	1:C:648:GLY:O	2.49	0.45
1:A:528:LYS:O	1:A:529:LYS:HB3	2.16	0.45
1:A:763:LEU:HD13	1:A:1004:LEU:HG	1.98	0.45
1:B:106:PHE:CE2	1:B:238:PHE:HD1	2.34	0.45
1:B:878:LEU:O	1:B:882:ILE:HG12	2.17	0.45
1:C:164:ASN:HB2	2:C:1302:NAG:HN2	1.81	0.45
1:C:343:ASN:OD1	1:C:343:ASN:N	2.50	0.45
1:A:1101:HIS:CG	2:A:1315:NAG:H5	2.52	0.45
1:B:327:VAL:HG11	1:B:528:LYS:CG	2.47	0.45
1:C:1092:GLU:OE2	1:C:1092:GLU:N	2.49	0.45
1:A:176:LEU:HD22	1:A:190:ARG:HD2	1.98	0.45
1:B:520:ALA:O	1:B:521:PRO:C	2.53	0.45
1:B:705:VAL:HG12	1:B:707:TYR:H	1.82	0.45
1:A:131:CYS:HA	1:A:166:CYS:HA	1.99	0.45
1:A:210:ILE:H	1:A:210:ILE:HG13	1.56	0.45
1:A:501:TYR:HB3	1:A:505:HIS:HB2	1.98	0.45
1:A:742:ILE:HD13	1:A:1001:LEU:HD13	1.99	0.45
1:B:363:ALA:O	1:B:527:PRO:HD3	2.17	0.45
1:B:878:LEU:HD12	1:B:878:LEU:HA	1.75	0.45
1:C:505:HIS:CE1	1:B:503:VAL:HB	2.52	0.45
1:C:520:ALA:O	1:C:521:PRO:C	2.53	0.45
1:C:742:ILE:HG22	1:C:997:ILE:HD12	1.99	0.45
1:A:303:LEU:H	1:A:303:LEU:HG	1.67	0.45
1:B:97:LYS:HE2	1:B:184:GLY:HA3	1.99	0.45
1:B:342:PHE:CE2	1:B:436:TRP:CZ3	3.04	0.45
1:A:188:ASN:OD1	1:A:188:ASN:N	2.50	0.45
1:A:343:ASN:N	1:A:343:ASN:OD1	2.50	0.45
1:A:390:LEU:HD13	1:A:390:LEU:HA	1.83	0.45
1:A:503:VAL:HB	1:B:505:HIS:NE2	2.31	0.45
1:B:343:ASN:OD1	1:B:343:ASN:N	2.50	0.45
1:C:41:LYS:HB3	1:A:562:PHE:O	2.17	0.45
1:C:97:LYS:HE2	1:C:184:GLY:HA3	1.98	0.45
1:C:125:ASN:HB2	2:C:1301:NAG:H62	1.99	0.45
1:C:321:GLN:NE2	1:C:630:THR:OG1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.98	0.45
1:C:741:TYR:CE2	1:C:1004:LEU:HB2	2.51	0.45
1:C:878:LEU:O	1:C:882:ILE:HG12	2.17	0.45
1:A:129:LYS:HD3	1:A:133:PHE:HZ	1.82	0.45
1:A:327:VAL:HG11	1:A:528:LYS:CG	2.47	0.45
1:A:705:VAL:HG12	1:A:707:TYR:H	1.82	0.45
1:A:744:GLY:O	1:A:746:SER:N	2.50	0.45
1:A:759:PHE:HZ	1:B:1002:GLN:NE2	2.15	0.45
1:C:106:PHE:CE2	1:C:238:PHE:HD1	2.34	0.45
1:C:278:LYS:HB2	1:C:306:PHE:CE1	2.52	0.45
1:C:363:ALA:O	1:C:527:PRO:HD3	2.17	0.45
1:A:106:PHE:CE2	1:A:238:PHE:HD1	2.34	0.45
1:A:363:ALA:O	1:A:527:PRO:HD3	2.17	0.45
1:B:175:PHE:CD1	1:B:175:PHE:N	2.82	0.45
1:C:342:PHE:CE2	1:C:436:TRP:CZ3	3.04	0.44
1:C:1013:ILE:CD1	1:B:1012:LEU:HD13	2.47	0.44
1:B:176:LEU:HD22	1:B:190:ARG:HD2	1.98	0.44
1:C:907:ASN:HB2	1:C:913:GLN:HG2	1.99	0.44
1:B:276:LEU:HD22	1:B:301:CYS:HA	1.99	0.44
1:C:44:ARG:O	1:C:283:GLY:HA2	2.18	0.44
1:C:216:PHE:O	1:C:217:PRO:C	2.52	0.44
1:C:326:ILE:HG12	1:C:532:ASN:O	2.18	0.44
1:A:321:GLN:NE2	1:A:630:THR:OG1	2.49	0.44
1:B:501:TYR:HB3	1:B:505:HIS:HB2	1.98	0.44
1:C:327:VAL:HG11	1:C:528:LYS:CG	2.47	0.44
1:C:780:GLU:O	1:C:784:GLN:NE2	2.49	0.44
1:C:858:LEU:HD13	1:C:962:LEU:HD13	2.00	0.44
1:A:348:ALA:HB1	1:A:352:ALA:O	2.18	0.44
1:B:188:ASN:N	1:B:188:ASN:OD1	2.50	0.44
1:B:450:ASP:OD1	1:B:450:ASP:N	2.50	0.44
1:C:244:LEU:HD23	1:C:244:LEU:HA	1.87	0.44
1:C:567:ARG:HB3	1:C:568:ASP:H	1.67	0.44
1:A:278:LYS:HB2	1:A:306:PHE:CE1	2.52	0.44
1:A:309:GLU:HG2	1:A:313:TYR:OH	2.18	0.44
1:B:34:ARG:NH2	1:B:217:PRO:O	2.51	0.44
1:A:97:LYS:HE2	1:A:184:GLY:HA3	1.98	0.44
1:A:402:ILE:HD11	1:A:510:VAL:HG21	2.00	0.44
1:C:375:PHE:CG	1:C:508:TYR:OH	2.68	0.44
1:C:1002:GLN:HG3	1:B:759:PHE:CE2	2.44	0.44
1:A:125:ASN:HB2	2:A:1301:NAG:H62	1.99	0.44
1:A:742:ILE:HG22	1:A:997:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ALA:HA	1:A:933:LYS:HG2	2.00	0.44
1:B:125:ASN:HB2	2:B:1301:NAG:H62	1.99	0.44
1:B:439:ASN:OD1	1:B:507:PRO:HD2	2.17	0.44
1:B:1101:HIS:CG	2:B:1315:NAG:H5	2.53	0.44
1:C:930:ALA:HA	1:C:933:LYS:HG2	2.00	0.44
1:A:878:LEU:O	1:A:882:ILE:HG12	2.17	0.44
1:B:348:ALA:HB1	1:B:352:ALA:O	2.18	0.44
1:C:348:ALA:HB1	1:C:352:ALA:O	2.18	0.44
1:B:195:LYS:HE2	1:B:195:LYS:HB2	1.79	0.44
1:B:358:ILE:HB	1:B:395:VAL:HB	2.00	0.44
1:B:930:ALA:HA	1:B:933:LYS:HG2	2.00	0.44
1:C:322:PRO:CB	1:C:540:ASN:ND2	2.81	0.43
1:C:339:HIS:O	1:C:340:GLU:C	2.53	0.43
1:C:450:ASP:N	1:C:450:ASP:OD1	2.51	0.43
1:C:562:PHE:O	1:B:41:LYS:HD3	2.17	0.43
1:C:705:VAL:C	1:C:707:TYR:H	2.21	0.43
1:A:44:ARG:O	1:A:283:GLY:HA2	2.18	0.43
1:A:581:THR:O	1:A:583:GLU:N	2.50	0.43
1:A:792:PRO:HG3	1:B:707:TYR:CD1	2.50	0.43
1:B:419:ALA:HA	1:B:423:TYR:O	2.18	0.43
1:C:34:ARG:NH2	1:C:217:PRO:O	2.51	0.43
1:C:1001:LEU:HD12	1:C:1001:LEU:HA	1.77	0.43
1:C:1078:ALA:C	1:B:900:MET:HE1	2.39	0.43
1:A:806:LEU:HD23	1:A:878:LEU:HD23	1.99	0.43
1:B:339:HIS:O	1:B:340:GLU:C	2.53	0.43
1:A:413:GLY:HA2	1:A:424:LYS:HD2	1.98	0.43
1:A:857:GLY:O	1:A:858:LEU:HD23	2.18	0.43
3:B:1317:IDU:O1S	3:B:1317:IDU:O3	2.22	0.43
1:A:454:ARG:HH12	1:A:467:ASP:HB3	1.84	0.43
1:C:401:VAL:HG21	1:C:451:TYR:CE2	2.54	0.43
1:A:554:LYS:HZ2	1:A:554:LYS:HA	1.84	0.43
1:B:322:PRO:CB	1:B:540:ASN:ND2	2.81	0.43
1:B:358:ILE:HG22	1:B:524:VAL:HG21	2.00	0.43
1:C:309:GLU:HG2	1:C:313:TYR:OH	2.18	0.43
1:C:742:ILE:HD13	1:C:1001:LEU:HD13	2.00	0.43
1:C:744:GLY:O	1:C:745:ASP:C	2.57	0.43
1:A:108:THR:O	1:A:110:LEU:N	2.50	0.43
1:A:212:ILE:HG13	1:A:212:ILE:O	2.18	0.43
1:A:339:HIS:O	1:A:340:GLU:C	2.53	0.43
1:A:858:LEU:HD13	1:A:962:LEU:HD13	2.00	0.43
1:A:947:LYS:HE3	1:A:947:LYS:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ILE:HG22	1:C:524:VAL:HG21	2.00	0.43
1:C:557:LYS:CD	1:C:559:PHE:HE1	2.32	0.43
1:A:908:GLY:HA3	1:A:1036:GLN:HE22	1.84	0.43
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.51	0.43
1:B:278:LYS:HB2	1:B:306:PHE:CE1	2.52	0.43
1:B:789:TYR:CE2	1:B:888:PHE:HD2	2.36	0.43
1:C:34:ARG:NH2	1:C:219:GLY:O	2.52	0.43
1:C:382:VAL:HG22	1:C:517:LEU:HD11	2.01	0.43
1:A:164:ASN:O	1:A:166:CYS:N	2.52	0.43
1:B:418:ILE:O	1:B:422:ASN:HB2	2.19	0.43
1:B:454:ARG:HH12	1:B:467:ASP:HB3	1.84	0.43
1:C:118:LEU:HD11	1:C:159:VAL:HB	2.00	0.43
2:C:1311:NAG:H62	1:B:796:TYR:CG	2.54	0.43
1:A:744:GLY:O	1:A:745:ASP:C	2.57	0.43
1:A:841:LEU:HB3	1:B:588:THR:OG1	2.19	0.43
1:A:1083:HIS:CE1	1:A:1137:VAL:CG2	2.96	0.43
1:B:44:ARG:O	1:B:283:GLY:HA2	2.18	0.43
1:B:455:SER:OG	1:B:456:PHE:CD1	2.71	0.43
1:B:908:GLY:HA3	1:B:1036:GLN:HE22	1.84	0.43
1:C:1029:MET:O	1:C:1033:VAL:HB	2.19	0.43
1:A:322:PRO:CB	1:A:540:ASN:ND2	2.81	0.43
1:A:742:ILE:HG22	1:A:997:ILE:HD12	1.99	0.43
1:C:134:GLN:HE21	1:C:135:PHE:H	1.67	0.42
1:A:34:ARG:NH2	1:A:217:PRO:O	2.51	0.42
1:A:34:ARG:NH2	1:A:219:GLY:O	2.52	0.42
1:A:320:VAL:HG22	1:A:629:LEU:HD12	2.01	0.42
1:A:340:GLU:O	1:A:342:PHE:N	2.52	0.42
1:B:303:LEU:H	1:B:303:LEU:HG	1.73	0.42
1:B:375:PHE:CG	1:B:508:TYR:OH	2.68	0.42
1:B:388:ASN:HB3	1:B:527:PRO:HD2	2.00	0.42
1:C:327:VAL:HG13	1:C:542:ASN:HB3	2.01	0.42
1:C:434:ILE:HB	1:C:511:VAL:HG22	2.01	0.42
1:C:744:GLY:O	1:C:746:SER:N	2.52	0.42
1:A:130:VAL:HG23	1:A:168:PHE:HB3	2.00	0.42
1:A:503:VAL:CB	1:B:505:HIS:NE2	2.82	0.42
1:A:847:ARG:HB2	1:A:851:CYS:HB3	2.00	0.42
1:B:299:THR:O	1:B:302:THR:HG22	2.18	0.42
1:B:309:GLU:HG2	1:B:313:TYR:OH	2.19	0.42
1:B:340:GLU:O	1:B:342:PHE:N	2.52	0.42
1:C:62:VAL:HG13	1:C:267:VAL:O	2.20	0.42
1:C:759:PHE:CZ	1:A:1002:GLN:NE2	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:GLY:HA3	1:C:1036:GLN:HE22	1.84	0.42
1:A:99:ASN:HD21	1:A:102:ARG:HH11	1.68	0.42
1:A:423:TYR:OH	1:A:512:VAL:HG11	2.19	0.42
1:A:780:GLU:O	1:A:784:GLN:NE2	2.49	0.42
1:A:984:LEU:HB3	1:A:989:ALA:HB2	2.02	0.42
1:B:34:ARG:NH2	1:B:219:GLY:O	2.52	0.42
1:B:387:LEU:HD11	1:B:515:PHE:CE2	2.55	0.42
1:B:1029:MET:O	1:B:1033:VAL:HB	2.19	0.42
1:C:454:ARG:HH12	1:C:467:ASP:HB3	1.84	0.42
1:A:847:ARG:HB2	1:A:851:CYS:HB2	2.00	0.42
1:A:878:LEU:HA	1:A:878:LEU:HD12	1.75	0.42
1:B:858:LEU:HD13	1:B:962:LEU:HD13	2.00	0.42
1:C:99:ASN:HD21	1:C:102:ARG:HH11	1.68	0.42
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.53	0.42
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.73	0.42
1:A:326:ILE:CD1	1:A:532:ASN:O	2.59	0.42
1:A:1114:ILE:HD13	1:A:1114:ILE:HA	1.93	0.42
1:B:320:VAL:HG22	1:B:629:LEU:HD12	2.02	0.42
1:A:574:ASP:O	1:A:587:ILE:N	2.50	0.42
1:A:983:ARG:HD3	1:B:517:LEU:CD1	2.37	0.42
1:B:364:ASP:O	1:B:367:VAL:HG12	2.20	0.42
1:C:379:CYS:HB3	1:C:382:VAL:O	2.19	0.42
1:C:403:LYS:N	1:C:495:TYR:OH	2.51	0.42
1:A:358:ILE:HB	1:A:395:VAL:HB	2.02	0.42
1:C:1101:HIS:CD2	2:C:1315:NAG:H3	2.54	0.42
1:C:984:LEU:HB3	1:C:989:ALA:HB2	2.02	0.42
1:A:738:CYS:O	1:A:742:ILE:HG13	2.19	0.42
1:A:878:LEU:HD11	1:A:1052:PHE:HB3	2.02	0.42
1:B:327:VAL:HG13	1:B:542:ASN:HB3	2.01	0.42
1:B:375:PHE:CG	1:B:508:TYR:CE1	3.08	0.42
1:B:502:GLY:O	1:B:506:GLN:HG2	2.20	0.42
1:C:97:LYS:O	1:C:97:LYS:NZ	2.52	0.42
1:C:419:ALA:HA	1:C:423:TYR:O	2.19	0.42
1:A:129:LYS:HB3	1:A:169:GLU:HG3	2.01	0.42
1:A:387:LEU:HD11	1:A:515:PHE:CZ	2.55	0.42
1:B:559:PHE:CG	1:B:584:ILE:CD1	3.03	0.42
1:B:984:LEU:HB3	1:B:989:ALA:HB2	2.02	0.42
1:C:187:LYS:H	1:C:210:ILE:CG1	2.33	0.41
1:C:340:GLU:O	1:C:342:PHE:N	2.52	0.41
1:C:347:PHE:CE1	1:C:509:ARG:NH1	2.88	0.41
1:C:527:PRO:O	1:C:528:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:ARG:HE	1:B:42:VAL:HG11	1.85	0.41
1:C:616:ASN:HA	1:C:644:GLN:HE22	1.85	0.41
1:C:742:ILE:CD1	1:C:1001:LEU:HD13	2.49	0.41
1:A:62:VAL:HG13	1:A:267:VAL:O	2.20	0.41
1:A:97:LYS:O	1:A:97:LYS:NZ	2.52	0.41
1:A:130:VAL:CG1	1:A:233:ILE:HD13	2.50	0.41
1:A:318:PHE:CD2	1:A:629:LEU:HD11	2.55	0.41
1:A:375:PHE:CG	1:A:508:TYR:OH	2.68	0.41
1:B:878:LEU:HD11	1:B:1052:PHE:HB3	2.02	0.41
1:C:320:VAL:HG22	1:C:629:LEU:HD12	2.02	0.41
1:C:740:MET:HG2	1:C:857:GLY:HA3	2.01	0.41
1:C:806:LEU:HD21	1:C:882:ILE:HD11	2.02	0.41
1:C:878:LEU:HD11	1:C:1052:PHE:HB3	2.02	0.41
1:C:974:SER:OG	1:C:975:SER:N	2.53	0.41
1:A:1029:MET:O	1:A:1033:VAL:HB	2.19	0.41
1:B:99:ASN:HD21	1:B:102:ARG:HH11	1.68	0.41
1:B:974:SER:OG	1:B:975:SER:N	2.53	0.41
1:C:502:GLY:O	1:C:506:GLN:HG2	2.20	0.41
1:C:703:ASN:HB2	1:B:787:GLN:HB3	2.02	0.41
1:C:1101:HIS:HB2	2:C:1315:NAG:H5	2.02	0.41
1:A:327:VAL:HG13	1:A:542:ASN:HB3	2.01	0.41
1:A:347:PHE:CE1	1:A:509:ARG:NH1	2.88	0.41
1:A:450:ASP:OD1	1:A:450:ASP:N	2.50	0.41
1:A:455:SER:OG	1:A:456:PHE:CD1	2.71	0.41
1:B:108:THR:O	1:B:110:LEU:N	2.50	0.41
1:B:527:PRO:O	1:B:528:LYS:HB3	2.20	0.41
1:B:581:THR:O	1:B:583:GLU:N	2.53	0.41
1:A:527:PRO:O	1:A:528:LYS:HB3	2.20	0.41
1:B:322:PRO:HB2	1:B:540:ASN:ND2	2.36	0.41
1:B:347:PHE:CE1	1:B:509:ARG:NH1	2.88	0.41
1:C:629:LEU:HD23	1:C:631:PRO:HG2	2.03	0.41
1:A:581:THR:C	1:A:583:GLU:N	2.74	0.41
1:B:402:ILE:HD11	1:B:510:VAL:HG21	2.01	0.41
1:B:629:LEU:HD23	1:B:631:PRO:HG2	2.03	0.41
1:C:878:LEU:HA	1:C:878:LEU:HD12	1.75	0.41
1:A:388:ASN:HB3	1:A:527:PRO:HD2	2.02	0.41
1:C:322:PRO:HB2	1:C:540:ASN:ND2	2.36	0.41
1:A:502:GLY:O	1:A:506:GLN:HG2	2.20	0.41
1:A:518:LEU:HD12	1:A:518:LEU:HA	1.83	0.41
1:A:697:MET:H	1:A:697:MET:HG2	1.72	0.41
1:A:974:SER:OG	1:A:975:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:LEU:HD12	1:A:1001:LEU:HA	1.77	0.41
1:C:375:PHE:CG	1:C:508:TYR:CE1	3.08	0.41
1:C:588:THR:HG23	1:C:589:PRO:HD2	2.03	0.41
1:C:947:LYS:HE3	1:C:947:LYS:HB2	1.83	0.41
1:A:134:GLN:HG2	1:A:162:SER:HB2	2.02	0.41
1:A:345:THR:OG1	1:A:346:ARG:N	2.54	0.41
1:A:375:PHE:CG	1:A:508:TYR:CE1	3.08	0.41
1:A:1012:LEU:HB3	1:B:1013:ILE:CD1	2.51	0.41
1:B:390:LEU:HA	1:B:390:LEU:HD13	1.87	0.41
1:B:411:ALA:HB3	1:B:414:GLN:CG	2.49	0.41
1:B:780:GLU:O	1:B:784:GLN:NE2	2.49	0.41
1:C:120:VAL:HG13	1:C:127:PHE:HB3	2.02	0.41
1:C:364:ASP:O	1:C:367:VAL:HG12	2.20	0.41
1:C:435:ALA:HB2	1:C:510:VAL:HG22	2.03	0.41
1:C:759:PHE:HZ	1:A:1002:GLN:NE2	2.19	0.41
1:C:795:LYS:HB3	2:C:1313:NAG:H83	2.03	0.41
1:C:1012:LEU:HB3	1:A:1013:ILE:CD1	2.50	0.41
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.54	0.41
1:A:40:ASP:CG	1:A:41:LYS:H	2.24	0.41
1:A:120:VAL:HG13	1:A:127:PHE:HB3	2.02	0.41
1:A:364:ASP:O	1:A:367:VAL:HG12	2.20	0.41
1:A:383:SER:HB3	1:A:386:LYS:HG2	2.02	0.41
1:A:435:ALA:HB2	1:A:510:VAL:HG22	2.03	0.41
1:A:961:THR:O	1:A:965:GLN:HG2	2.21	0.41
1:B:131:CYS:HB3	1:B:133:PHE:CZ	2.56	0.41
1:B:321:GLN:NE2	1:B:630:THR:OG1	2.49	0.41
1:B:435:ALA:HB2	1:B:510:VAL:HG22	2.03	0.41
1:B:802:PHE:HB3	1:B:805:ILE:HG12	2.02	0.41
1:B:961:THR:O	1:B:965:GLN:HG2	2.21	0.41
1:B:1083:HIS:CE1	1:B:1137:VAL:CG2	2.96	0.41
1:C:535:LYS:O	1:C:536:ASN:CB	2.69	0.41
1:C:714:ILE:HB	1:C:1075:PHE:CE2	2.56	0.41
1:C:759:PHE:HZ	1:A:1002:GLN:CD	2.16	0.41
1:C:961:THR:O	1:C:965:GLN:HG2	2.21	0.41
1:A:365:TYR:CE2	1:A:387:LEU:HG	2.56	0.41
1:A:406:GLU:HA	1:A:409:GLN:HB3	2.03	0.41
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.03	0.41
1:C:345:THR:OG1	1:C:346:ARG:N	2.54	0.40
1:A:535:LYS:O	1:A:536:ASN:CB	2.69	0.40
1:B:40:ASP:CG	1:B:41:LYS:H	2.24	0.40
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1079:PRO:HD2	1:C:1131:GLY:O	2.22	0.40
1:A:358:ILE:HG22	1:A:524:VAL:HG21	2.02	0.40
1:A:857:GLY:C	1:A:858:LEU:HD23	2.42	0.40
1:A:913:GLN:H	1:A:913:GLN:HG3	1.74	0.40
1:B:345:THR:OG1	1:B:346:ARG:N	2.54	0.40
1:B:420:ASP:O	1:B:461:LEU:HB2	2.20	0.40
1:C:168:PHE:CZ	1:C:229:LEU:HB2	2.57	0.40
1:C:411:ALA:HB3	1:C:414:GLN:CG	2.51	0.40
1:C:599:THR:HB	1:C:608:VAL:HG12	2.04	0.40
1:A:759:PHE:HZ	1:B:1002:GLN:CD	2.17	0.40
1:A:959:LEU:O	1:A:963:VAL:HG13	2.22	0.40
1:A:1086:LYS:HE3	1:A:1086:LYS:HB2	1.88	0.40
1:B:231:ILE:HG22	1:B:233:ILE:HG23	2.03	0.40
1:B:599:THR:HB	1:B:608:VAL:HG12	2.04	0.40
1:C:48:LEU:HA	1:C:48:LEU:HD23	1.73	0.40
1:C:374:PHE:CZ	1:C:434:ILE:HG23	2.56	0.40
1:C:375:PHE:CD2	1:C:508:TYR:CZ	3.09	0.40
1:A:206:LYS:HB3	1:A:223:LEU:CD1	2.51	0.40
1:A:349:SER:OG	1:A:451:TYR:HA	2.22	0.40
1:A:554:LYS:HA	1:A:554:LYS:NZ	2.36	0.40
1:A:806:LEU:HD21	1:A:882:ILE:HD11	2.02	0.40
1:B:110:LEU:HD13	1:B:110:LEU:HA	1.94	0.40
1:B:326:ILE:CD1	1:B:532:ASN:O	2.59	0.40
1:B:375:PHE:CD2	1:B:508:TYR:CZ	3.09	0.40
1:B:437:ASN:OD1	1:B:439:ASN:ND2	2.54	0.40
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.86	0.40
1:C:25:THR:O	1:C:65:PHE:HA	2.21	0.40
1:C:518:LEU:HD12	1:C:518:LEU:HA	1.83	0.40
1:C:806:LEU:HD23	1:C:878:LEU:HD23	2.03	0.40
1:C:855:PHE:HD1	1:A:589:PRO:HG3	1.86	0.40
1:C:990:GLU:O	1:C:993:ILE:HG22	2.22	0.40
1:B:25:THR:O	1:B:65:PHE:HA	2.21	0.40
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.87	0.40
1:B:716:THR:HA	1:B:1110:TYR:HB3	2.04	0.40
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.54	0.40
1:B:1083:HIS:CD2	1:B:1137:VAL:H	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1053/1206 (87%)	944 (90%)	91 (9%)	18 (2%)	7	33
1	B	1053/1206 (87%)	944 (90%)	92 (9%)	17 (2%)	8	35
1	C	1053/1206 (87%)	942 (90%)	91 (9%)	20 (2%)	6	31
All	All	3159/3618 (87%)	2830 (90%)	274 (9%)	55 (2%)	10	33

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	329	PHE
1	C	348	ALA
1	C	527	PRO
1	C	536	ASN
1	C	745	ASP
1	A	348	ALA
1	A	527	PRO
1	A	536	ASN
1	A	745	ASP
1	B	348	ALA
1	B	527	PRO
1	B	536	ASN
1	C	109	THR
1	C	559	PHE
1	C	590	CYS
1	A	109	THR
1	A	559	PHE
1	A	803	SER
1	B	109	THR
1	B	213	GLY
1	B	590	CYS
1	C	161	SER
1	C	165	ASN
1	C	188	ASN

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Mol	Chain	Res	Type
1	C	244	LEU
1	C	518	LEU
1	A	165	ASN
1	A	244	LEU
1	A	518	LEU
1	B	244	LEU
1	B	518	LEU
1	B	593	GLY
1	C	529	LYS
1	C	561	PRO
1	A	529	LYS
1	A	561	PRO
1	A	582	LEU
1	B	529	LYS
1	B	557	LYS
1	B	561	PRO
1	C	330	PRO
1	C	706	ALA
1	A	402	ILE
1	B	402	ILE
1	B	582	LEU
1	C	134	GLN
1	C	844	ILE
1	A	163	ALA
1	A	330	PRO
1	B	164	ASN
1	A	412	PRO
1	B	330	PRO
1	C	942	PRO
1	A	942	PRO
1	B	942	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	925/1054 (88%)	887 (96%)	38 (4%)	26	56
1	B	925/1054 (88%)	892 (96%)	33 (4%)	30	59
1	C	925/1054 (88%)	885 (96%)	40 (4%)	25	54
All	All	2775/3162 (88%)	2664 (96%)	111 (4%)	29	56

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	THR
1	C	45	SER
1	C	55	PHE
1	C	61	ASN
1	C	127	PHE
1	C	134	GLN
1	C	164	ASN
1	C	168	PHE
1	C	200	TYR
1	C	210	ILE
1	C	216	PHE
1	C	220	PHE
1	C	265	TYR
1	C	284	THR
1	C	308	VAL
1	C	319	ARG
1	C	360	ASN
1	C	374	PHE
1	C	377	PHE
1	C	389	ASP
1	C	538	CYS
1	C	552	LEU
1	C	553	THR
1	C	554	LYS
1	C	567	ARG
1	C	584	ILE
1	C	617	CYS
1	C	709	ASN
1	C	738	CYS
1	C	759	PHE
1	C	760	CYS

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Mol	Chain	Res	Type
1	C	849	LEU
1	C	873	TYR
1	C	939	PHE
1	C	975	SER
1	C	994	ASP
1	C	1037	SER
1	C	1096	VAL
1	C	1132	ILE
1	C	1136	THR
1	A	29	THR
1	A	55	PHE
1	A	61	ASN
1	A	127	PHE
1	A	134	GLN
1	A	160	TYR
1	A	168	PHE
1	A	200	TYR
1	A	210	ILE
1	A	216	PHE
1	A	220	PHE
1	A	265	TYR
1	A	284	THR
1	A	303	LEU
1	A	308	VAL
1	A	319	ARG
1	A	360	ASN
1	A	374	PHE
1	A	377	PHE
1	A	390	LEU
1	A	552	LEU
1	A	553	THR
1	A	554	LYS
1	A	582	LEU
1	A	709	ASN
1	A	738	CYS
1	A	759	PHE
1	A	760	CYS
1	A	873	TYR
1	A	916	LEU
1	A	918	GLU
1	A	939	PHE
1	A	975	SER

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Mol	Chain	Res	Type
1	A	994	ASP
1	A	1037	SER
1	A	1096	VAL
1	A	1132	ILE
1	A	1136	THR
1	B	45	SER
1	B	127	PHE
1	B	134	GLN
1	B	168	PHE
1	B	200	TYR
1	B	216	PHE
1	B	220	PHE
1	B	265	TYR
1	B	284	THR
1	B	302	THR
1	B	303	LEU
1	B	360	ASN
1	B	374	PHE
1	B	377	PHE
1	B	390	LEU
1	B	538	CYS
1	B	552	LEU
1	B	553	THR
1	B	554	LYS
1	B	572	THR
1	B	709	ASN
1	B	759	PHE
1	B	760	CYS
1	B	786	LYS
1	B	873	TYR
1	B	939	PHE
1	B	975	SER
1	B	983	ARG
1	B	994	ASP
1	B	1037	SER
1	B	1096	VAL
1	B	1132	ILE
1	B	1136	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	207	HIS
1	C	394	ASN
1	C	505	HIS
1	C	540	ASN
1	C	556	ASN
1	C	804	GLN
1	C	965	GLN
1	C	1101	HIS
1	A	164	ASN
1	A	207	HIS
1	A	540	ASN
1	A	580	GLN
1	A	965	GLN
1	A	1101	HIS
1	B	207	HIS
1	B	394	ASN
1	B	540	ASN
1	B	556	ASN
1	B	804	GLN
1	B	935	GLN
1	B	965	GLN
1	B	1101	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

55 ligands 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
2	NAG	A	1301	1	14,14,15	0.40	0	17,19,21	0.76	0
2	NAG	C	1314	1	14,14,15	0.40	0	17,19,21	0.36	0
2	NAG	C	1317	1	14,14,15	0.40	0	17,19,21	0.81	0
2	NAG	B	1304	1	14,14,15	0.38	0	17,19,21	0.54	0
2	NAG	B	1306	1	14,14,15	0.41	0	17,19,21	0.70	0
2	NAG	B	1309	1	14,14,15	0.39	0	17,19,21	0.38	0
2	NAG	A	1310	1	14,14,15	0.39	0	17,19,21	0.61	0
2	NAG	A	1317	1	14,14,15	0.41	0	17,19,21	0.81	0
2	NAG	A	1318	1	14,14,15	0.38	0	17,19,21	0.48	0
2	NAG	B	1312	1	14,14,15	0.40	0	17,19,21	0.81	0
2	NAG	B	1319	1	14,14,15	0.38	0	17,19,21	0.45	0
3	IDU	B	1317	-	15,15,17	0.89	1 (6%)	15,22,26	1.03	1 (6%)
2	NAG	A	1306	1	14,14,15	0.41	0	17,19,21	0.71	0
2	NAG	B	1302	1	14,14,15	0.39	0	17,19,21	0.66	1 (5%)
2	NAG	B	1305	1	14,14,15	0.42	0	17,19,21	0.70	1 (5%)
2	NAG	B	1316	1	14,14,15	0.39	0	17,19,21	0.64	0
2	NAG	B	1318	1	14,14,15	0.38	0	17,19,21	0.49	0
2	NAG	B	1313	1	14,14,15	0.41	0	17,19,21	0.81	0
2	NAG	C	1306	1	14,14,15	0.39	0	17,19,21	0.35	0
2	NAG	C	1304	1	14,14,15	0.37	0	17,19,21	0.55	0
2	NAG	B	1307	1	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
2	NAG	A	1305	1	14,14,15	0.41	0	17,19,21	0.69	1 (5%)
2	NAG	A	1309	1	14,14,15	0.40	0	17,19,21	0.52	0
2	NAG	A	1314	1	14,14,15	0.41	0	17,19,21	0.44	0
2	NAG	A	1302	1	14,14,15	0.37	0	17,19,21	0.97	1 (5%)
2	NAG	B	1315	1	14,14,15	0.39	0	17,19,21	0.39	0
2	NAG	C	1308	1	14,14,15	0.39	0	17,19,21	0.70	0
2	NAG	A	1316	1	14,14,15	0.39	0	17,19,21	0.64	0
2	NAG	C	1316	1	14,14,15	0.39	0	17,19,21	0.64	0
2	NAG	C	1310	1	14,14,15	0.38	0	17,19,21	0.61	0
2	NAG	C	1318	1	14,14,15	0.37	0	17,19,21	0.48	0
2	NAG	A	1311	1	14,14,15	0.37	0	17,19,21	0.54	0
2	NAG	A	1315	1	14,14,15	0.40	0	17,19,21	0.38	0
2	NAG	B	1301	1	14,14,15	0.38	0	17,19,21	0.77	0
2	NAG	B	1314	1	14,14,15	0.39	0	17,19,21	0.36	0
2	NAG	C	1303	1	14,14,15	0.39	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1311	1	14,14,15	0.38	0	17,19,21	0.54	0
2	NAG	C	1313	1	14,14,15	0.38	0	17,19,21	0.45	0
2	NAG	C	1307	1	14,14,15	0.39	0	17,19,21	0.74	1 (5%)
2	NAG	C	1309	1	14,14,15	0.40	0	17,19,21	0.36	0
2	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	0.69	0
2	NAG	B	1303	1	14,14,15	0.39	0	17,19,21	0.74	0
2	NAG	C	1315	1	14,14,15	0.40	0	17,19,21	0.41	0
2	NAG	A	1304	1	14,14,15	0.35	0	17,19,21	0.55	0
2	NAG	B	1311	1	14,14,15	0.38	0	17,19,21	0.54	0
2	NAG	C	1301	1	14,14,15	0.40	0	17,19,21	0.77	0
2	NAG	A	1312	1	14,14,15	0.39	0	17,19,21	0.81	0
2	NAG	C	1312	1	14,14,15	0.39	0	17,19,21	0.81	0
2	NAG	A	1303	1	14,14,15	0.39	0	17,19,21	0.74	0
2	NAG	C	1305	1	14,14,15	0.42	0	17,19,21	0.70	1 (5%)
2	NAG	A	1313	1	14,14,15	0.40	0	17,19,21	0.81	0
2	NAG	A	1307	1	14,14,15	0.38	0	17,19,21	0.75	1 (5%)
2	NAG	B	1308	1	14,14,15	0.39	0	17,19,21	0.69	0
2	NAG	C	1302	1	14,14,15	0.39	0	17,19,21	0.75	1 (5%)
2	NAG	B	1310	1	14,14,15	0.39	0	17,19,21	0.62	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
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1314	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1317	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1317	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1319	1	-	0/6/23/26	0/1/1/1
3	IDU	B	1317	-	-	3/9/22/29	1/1/1/1
2	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1314	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1315	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1318	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1315	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1315	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1317	IDU	O6-C6	-2.89	1.21	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1302	NAG	C2-N2-C7	3.53	127.92	122.90
2	C	1302	NAG	C2-N2-C7	2.59	126.60	122.90
3	B	1317	IDU	O6-C6-C5	2.36	119.77	113.03
2	C	1307	NAG	C1-O5-C5	2.28	115.28	112.19
2	A	1307	NAG	C1-O5-C5	2.27	115.27	112.19
2	B	1307	NAG	C1-O5-C5	2.26	115.25	112.19
2	B	1305	NAG	C1-O5-C5	2.18	115.15	112.19
2	C	1305	NAG	C1-O5-C5	2.16	115.11	112.19
2	A	1305	NAG	C1-O5-C5	2.14	115.09	112.19
2	B	1302	NAG	C2-N2-C7	2.13	125.93	122.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1317	IDU	C3-C2-O2-S
3	B	1317	IDU	O5-C5-C6-O61
2	C	1315	NAG	C8-C7-N2-C2
2	C	1315	NAG	O7-C7-N2-C2
2	A	1315	NAG	C8-C7-N2-C2
2	A	1315	NAG	O7-C7-N2-C2
2	B	1315	NAG	C8-C7-N2-C2
2	B	1315	NAG	O7-C7-N2-C2
2	B	1309	NAG	O5-C5-C6-O6
2	C	1309	NAG	O5-C5-C6-O6
2	C	1315	NAG	O5-C5-C6-O6
2	A	1309	NAG	O5-C5-C6-O6
2	A	1315	NAG	O5-C5-C6-O6
2	B	1315	NAG	O5-C5-C6-O6
2	C	1310	NAG	C1-C2-N2-C7
2	A	1310	NAG	C1-C2-N2-C7
2	B	1310	NAG	C1-C2-N2-C7
2	C	1302	NAG	C3-C2-N2-C7
2	A	1302	NAG	C3-C2-N2-C7
2	B	1302	NAG	C3-C2-N2-C7
3	B	1317	IDU	O5-C5-C6-O6

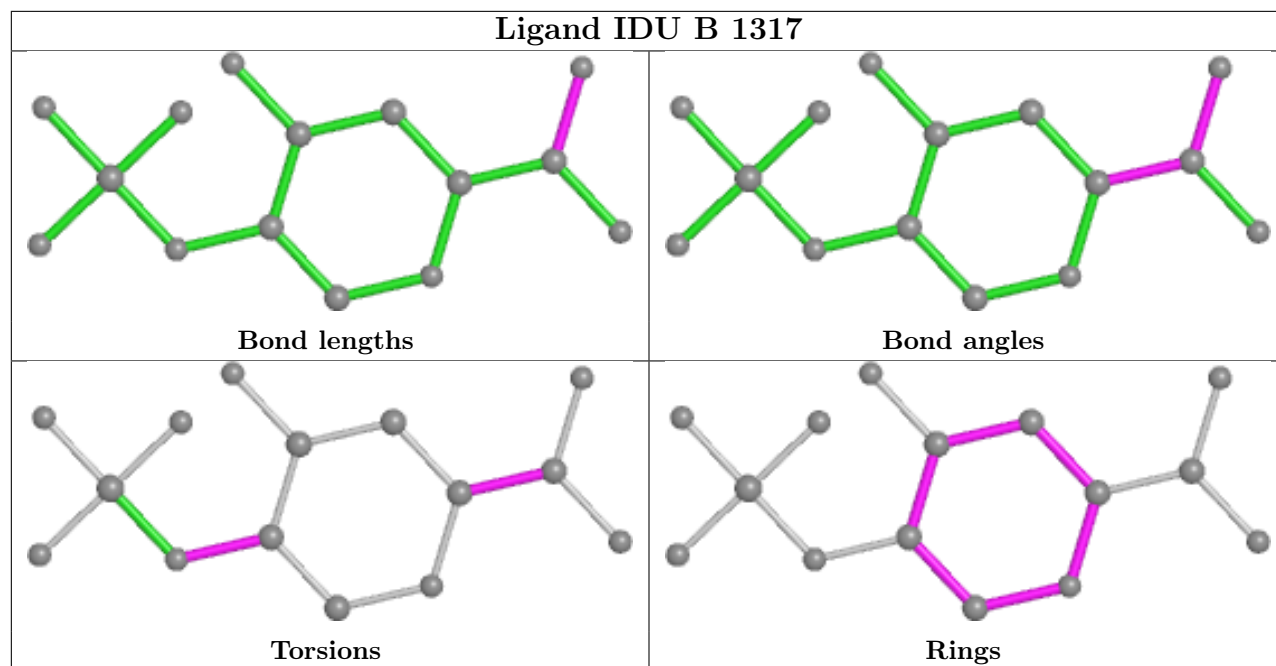
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1317	IDU	C1-C2-C3-C4-C5-O5

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAG	1	0
3	B	1317	IDU	1	0
2	A	1309	NAG	1	0
2	B	1315	NAG	3	0
2	A	1311	NAG	1	0
2	A	1315	NAG	3	0
2	B	1301	NAG	1	0
2	C	1311	NAG	2	0
2	C	1313	NAG	3	0
2	C	1315	NAG	3	0
2	B	1311	NAG	1	0
2	C	1301	NAG	1	0
2	C	1302	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.