Full wwPDB EM Validation Report ⓘ

Aug 4, 2024 – 12:20 AM JST

PDB ID	:	8XUT
EMDB ID	:	EMD-38683
Title	:	XBB.1.5 Spike Trimer in complex with heparan sulfate
Authors	:	Yue, C.; Liu, P.; Mao, X.
Deposited on	:	2024-01-14
Resolution	:	3.20 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:

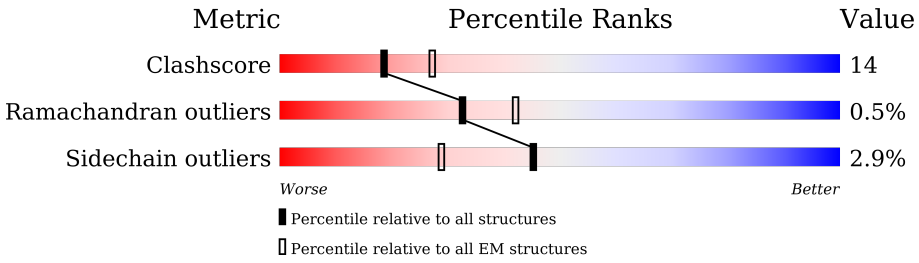
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1269	54% 27% • 18%
1	B	1269	55% 25% • 18%
1	C	1269	58% 23% • 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25149 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	B	1042	Total	C	N	O	S	0	0
			8154	5216	1359	1542	37		
1	A	1042	Total	C	N	O	S	0	0
			8154	5216	1359	1542	37		
1	C	1042	Total	C	N	O	S	0	0
			8154	5216	1359	1542	37		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ILE	THR	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	83	ALA	VAL	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	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
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	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	490	SER	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	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
A	22	ILE	THR	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	83	ALA	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	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	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	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	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	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
C	22	ILE	THR	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	83	ALA	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
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C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	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	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	PRO	VAL	variant	UNP P0DTC2

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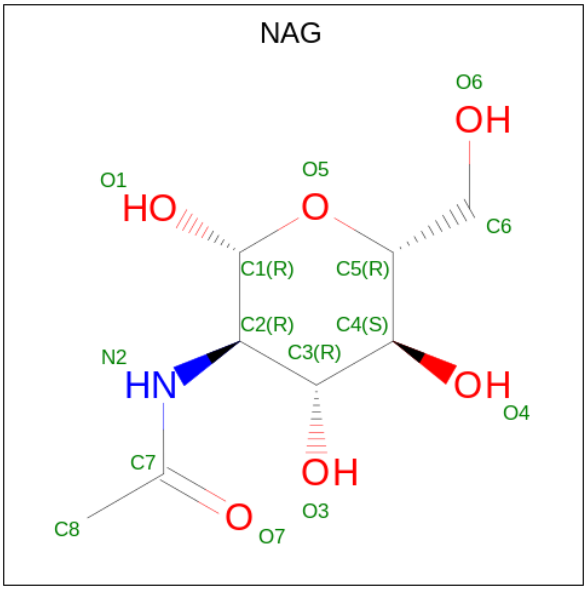
Chain	Residue	Modelled	Actual	Comment	Reference
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	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	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

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

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

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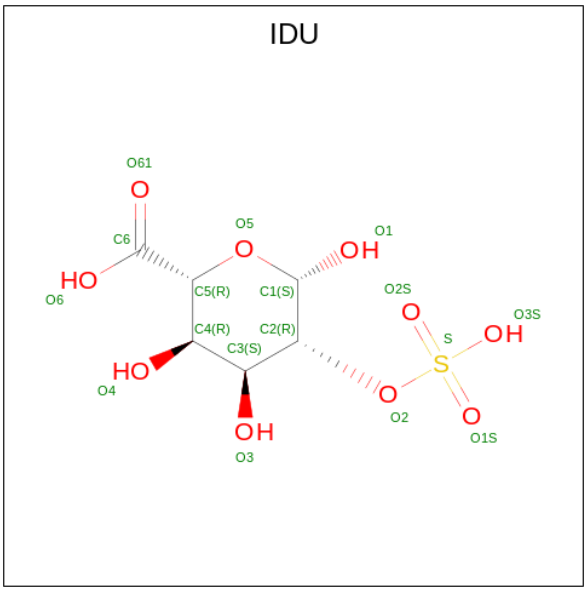
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	

- 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).



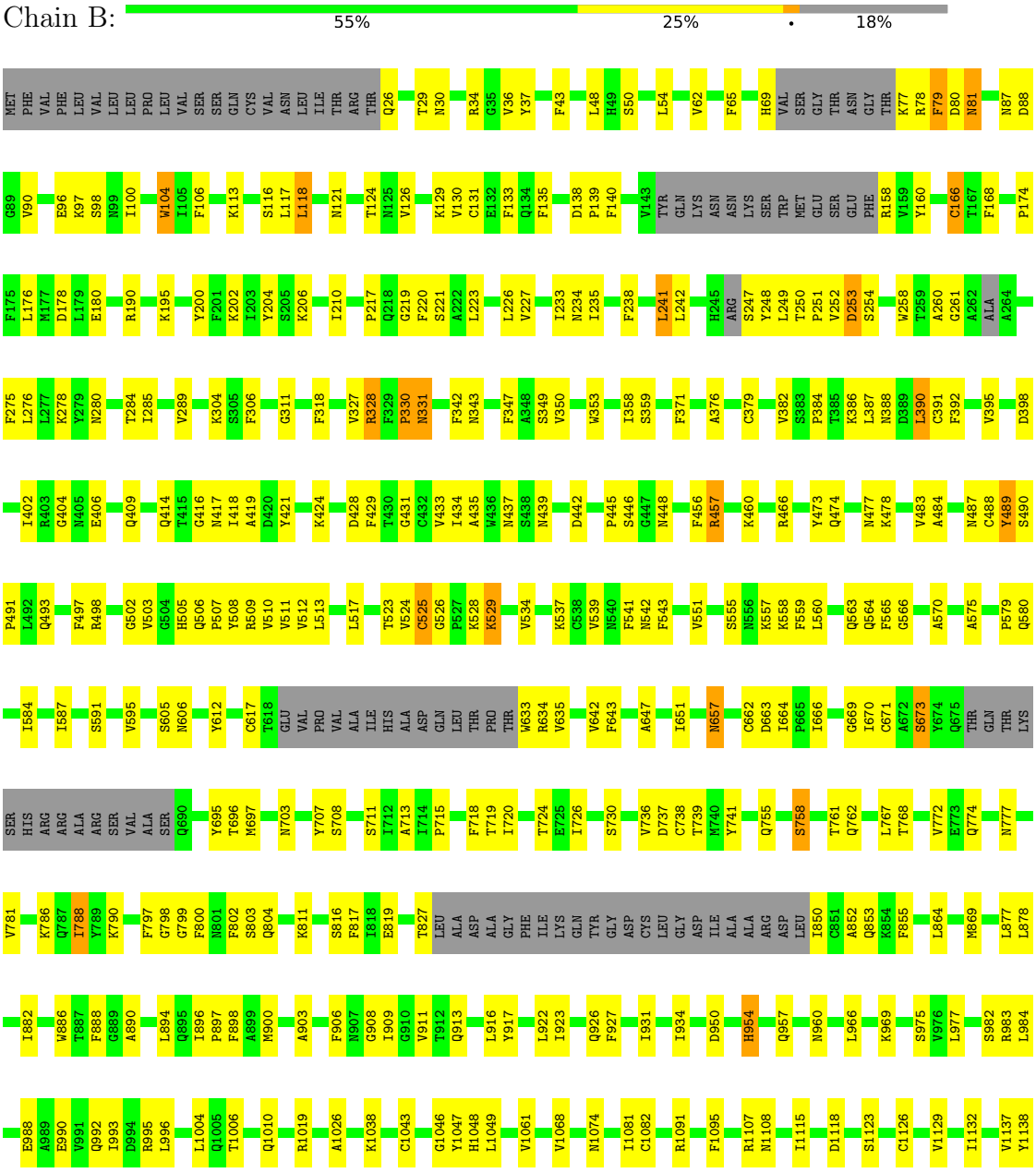
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	S	0
			15	6	8	1	

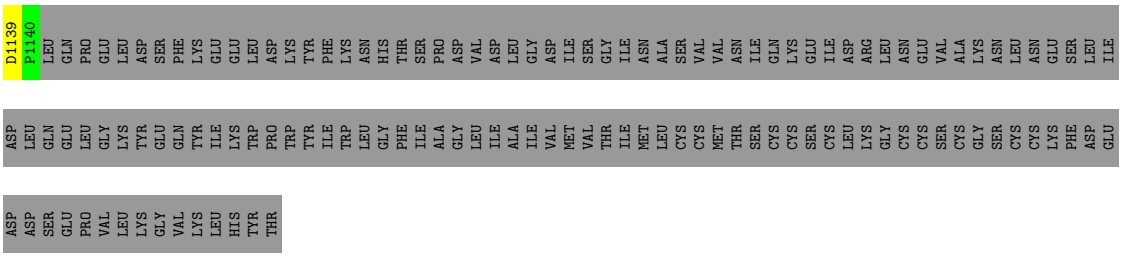
3 Residue-property plots (i)

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

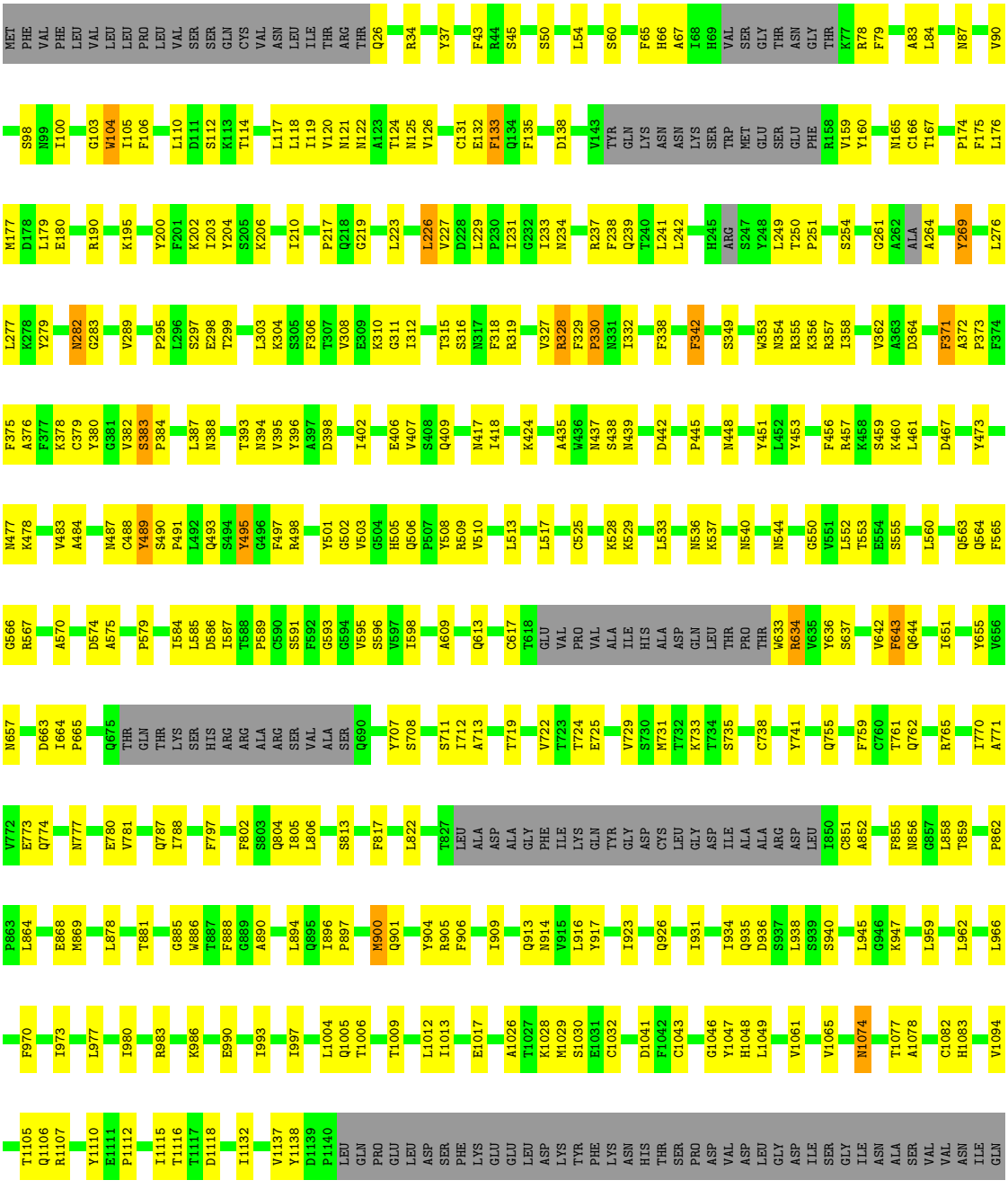
Chain B:

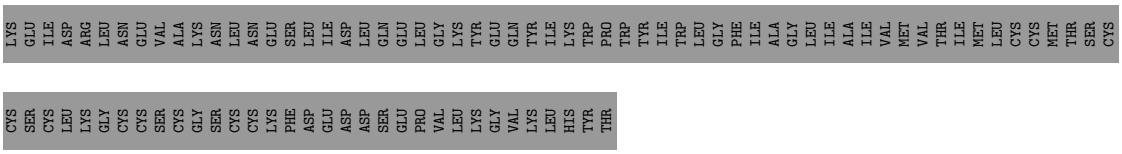




• Molecule 1: Spike glycoprotein

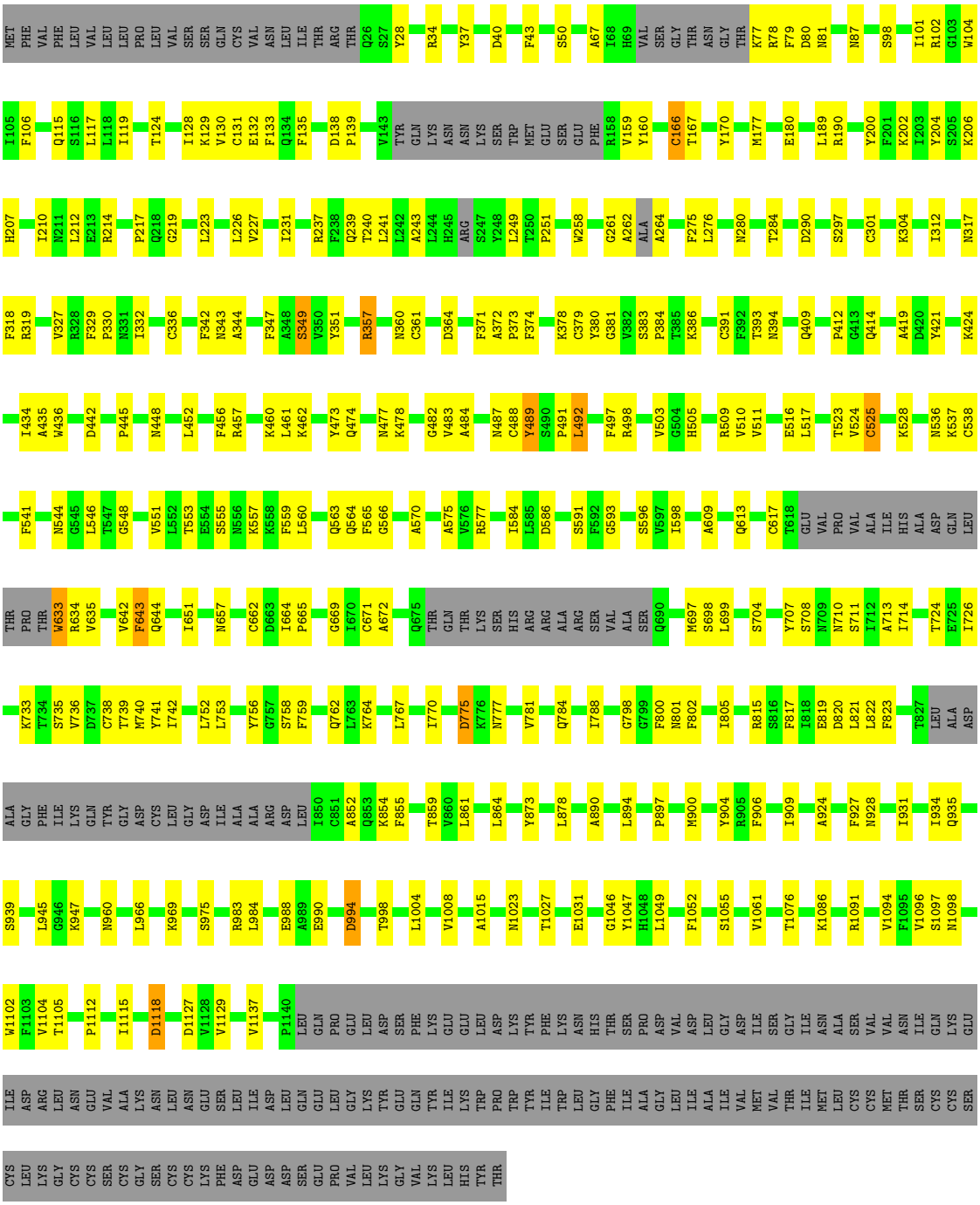
Chain A:





• Molecule 1: Spike glycoprotein

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	257757	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 ($e^-/Å^2$)	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	0.33	0/8345	0.51	0/11349
1	B	0.32	0/8345	0.50	0/11349
1	C	0.30	0/8345	0.49	0/11349
All	All	0.32	0/25035	0.50	0/34047

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	B	158	ARG	Sidechain
1	B	328	ARG	Sidechain

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	A	8154	0	7959	274	0
1	B	8154	0	7959	271	0
1	C	8154	0	7959	235	0
2	A	224	0	208	2	0
2	B	224	0	208	5	0
2	C	224	0	208	4	0
3	A	15	0	4	0	0
All	All	25149	0	24505	718	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 14.

All (718) 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:A:277:LEU:HD11	1:A:279:TYR:CE1	1.76	1.20
1:A:126:VAL:HG21	1:A:175:PHE:HE2	0.99	1.12
1:A:126:VAL:HG21	1:A:175:PHE:CE2	1.86	1.10
1:B:121:ASN:HD22	1:B:176:LEU:HD23	1.07	1.07
1:B:121:ASN:HD22	1:B:176:LEU:CD2	1.72	1.02
1:A:342:PHE:HD1	1:A:371:PHE:HE1	1.09	0.98
1:C:738:CYS:SG	1:C:753:LEU:HD21	2.06	0.95
1:B:121:ASN:ND2	1:B:176:LEU:CD2	2.31	0.92
1:A:460:LYS:HD3	1:A:461:LEU:H	1.32	0.92
1:A:342:PHE:CD1	1:A:371:PHE:HE1	1.90	0.90
1:B:121:ASN:ND2	1:B:176:LEU:HD23	1.86	0.90
1:A:342:PHE:HD1	1:A:371:PHE:CE1	1.89	0.90
1:B:984:LEU:HD12	1:B:988:GLU:CG	2.03	0.89
1:A:126:VAL:CG2	1:A:175:PHE:HE2	1.87	0.85
1:A:277:LEU:CD1	1:A:279:TYR:CE1	2.58	0.85
1:A:477:ASN:O	1:A:478:LYS:HG3	1.77	0.84
1:B:477:ASN:O	1:B:478:LYS:HG3	1.79	0.82
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.60	0.82
1:B:560:LEU:H	1:B:563:GLN:HB3	1.46	0.80
1:C:477:ASN:O	1:C:478:LYS:HG3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:MET:CE	1:B:697:MET:HA	2.11	0.80
1:B:131:CYS:HA	1:B:166:CYS:HB3	1.63	0.79
1:A:330:PRO:HD3	1:A:544:ASN:HD21	1.47	0.79
1:B:984:LEU:HD12	1:B:988:GLU:HG3	1.65	0.77
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.66	0.77
1:B:984:LEU:HD12	1:B:988:GLU:HG2	1.65	0.77
1:C:448:ASN:HB2	1:C:497:PHE:HB2	1.69	0.75
1:B:909:ILE:HD11	1:B:1047:TYR:HB3	1.68	0.75
1:B:456:PHE:H	1:B:491:PRO:HB3	1.51	0.75
1:B:121:ASN:ND2	1:B:176:LEU:HD22	2.00	0.73
1:B:697:MET:HA	1:B:697:MET:HE2	1.70	0.73
1:B:708:SER:HB3	1:B:711:SER:HB3	1.70	0.73
1:A:780:GLU:OE1	1:A:780:GLU:N	2.19	0.73
1:B:206:LYS:HE2	1:B:221:SER:HB2	1.72	0.72
1:C:821:LEU:HD11	1:C:939:SER:HB2	1.72	0.72
1:A:566:GLY:HA3	1:A:575:ALA:HB3	1.72	0.71
1:C:115:GLN:HA	1:C:132:GLU:HG2	1.72	0.71
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.72	0.71
1:C:442:ASP:O	1:C:448:ASN:ND2	2.24	0.71
1:C:724:THR:HG22	1:C:934:ILE:HD11	1.72	0.71
1:B:448:ASN:HB2	1:B:497:PHE:HB2	1.71	0.70
1:B:570:ALA:HB2	1:A:852:ALA:HB1	1.73	0.70
1:B:852:ALA:HB1	1:C:570:ALA:HB2	1.74	0.70
1:A:112:SER:HA	1:A:132:GLU:HG2	1.73	0.70
1:A:442:ASP:O	1:A:448:ASN:ND2	2.25	0.70
1:B:100:ILE:HG22	1:B:242:LEU:HD12	1.73	0.69
1:A:277:LEU:HD11	1:A:279:TYR:HE1	1.47	0.69
1:B:124:THR:HB	2:B:1302:NAG:H62	1.75	0.69
1:B:419:ALA:O	1:B:424:LYS:NZ	2.26	0.69
1:C:189:LEU:HD22	1:C:210:ILE:HG12	1.75	0.69
1:A:456:PHE:H	1:A:491:PRO:HB3	1.57	0.68
1:A:318:PHE:HB3	1:A:593:GLY:HA3	1.75	0.68
1:B:580:GLN:HB3	2:B:1306:NAG:H82	1.76	0.68
1:A:806:LEU:HD23	1:A:878:LEU:HD23	1.76	0.67
1:B:878:LEU:O	1:B:882:ILE:HD12	1.94	0.67
1:A:118:LEU:HD21	1:A:120:VAL:HG23	1.74	0.67
1:C:81:ASN:HB3	1:C:138:ASP:HB2	1.76	0.67
1:A:354:ASN:O	1:A:356:LYS:NZ	2.27	0.67
1:C:67:ALA:HA	1:C:264:ALA:HB2	1.76	0.67
1:B:402:ILE:HG21	1:B:418:ILE:HD11	1.77	0.67
1:A:379:CYS:HB3	1:A:384:PRO:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:PRO:HB2	1:C:332:ILE:HG12	1.77	0.67
1:A:735:SER:HG	1:A:859:THR:HG1	1.43	0.66
1:A:1094:VAL:N	1:A:1105:THR:O	2.27	0.66
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.77	0.66
1:A:435:ALA:HB2	1:A:510:VAL:HG13	1.77	0.66
1:A:643:PHE:HD1	1:A:644:GLN:H	1.40	0.66
1:A:490:SER:O	1:A:493:GLN:NE2	2.29	0.66
1:C:330:PRO:HD3	1:C:544:ASN:HD21	1.61	0.66
1:B:1126:CYS:HB2	1:B:1132:ILE:HG21	1.78	0.66
1:C:139:PRO:HB3	1:C:159:VAL:HA	1.77	0.66
1:C:924:ALA:O	1:C:928:ASN:ND2	2.29	0.66
1:A:448:ASN:HB2	1:A:497:PHE:HB2	1.78	0.65
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.77	0.65
1:C:419:ALA:O	1:C:424:LYS:NZ	2.30	0.65
1:A:100:ILE:HG22	1:A:242:LEU:HD12	1.79	0.65
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.79	0.65
1:B:703:ASN:HD22	1:A:787:GLN:HE21	1.44	0.65
1:A:591:SER:OG	1:A:634:ARG:NH2	2.30	0.65
1:B:984:LEU:HD22	1:C:381:GLY:O	1.97	0.65
1:B:566:GLY:HA3	1:B:575:ALA:HB3	1.80	0.64
1:B:917:TYR:HB3	1:C:1129:VAL:HG23	1.80	0.64
1:B:289:VAL:HG23	1:B:306:PHE:HE1	1.63	0.64
1:C:516:GLU:OE2	1:C:516:GLU:N	2.31	0.64
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.78	0.63
1:A:457:ARG:HH12	1:A:461:LEU:HD13	1.62	0.63
1:A:78:ARG:HE	1:A:261:GLY:HA3	1.63	0.63
1:C:710:ASN:ND2	1:C:1076:THR:OG1	2.31	0.63
1:B:560:LEU:HB2	1:B:563:GLN:HB2	1.80	0.63
1:C:212:LEU:HD12	1:C:214:ARG:H	1.63	0.63
1:B:98:SER:HA	1:B:180:GLU:H	1.63	0.63
1:A:731:MET:H	1:A:774:GLN:HE21	1.47	0.63
1:A:457:ARG:HH22	1:A:461:LEU:HB2	1.64	0.63
1:A:574:ASP:O	1:A:587:ILE:N	2.30	0.62
1:C:102:ARG:HE	1:C:243:ALA:HB3	1.64	0.62
1:A:358:ILE:HB	1:A:395:VAL:HG23	1.80	0.62
1:C:492:LEU:HD12	1:C:492:LEU:O	1.98	0.62
1:B:353:TRP:CZ2	1:B:466:ARG:HD2	2.33	0.62
1:C:34:ARG:NH1	1:C:219:GLY:O	2.32	0.62
1:B:404:GLY:HA2	1:B:508:TYR:HE1	1.64	0.62
1:A:118:LEU:HD23	1:A:119:ILE:N	2.14	0.62
1:A:383:SER:N	1:C:983:ARG:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:H	1:A:563:GLN:HB3	1.63	0.62
1:A:555:SER:HB2	1:A:584:ILE:HB	1.81	0.62
1:A:249:LEU:HG	1:A:251:PRO:HD2	1.81	0.62
1:B:376:ALA:HB3	1:B:435:ALA:HB3	1.82	0.62
1:B:755:GLN:OE1	1:C:969:LYS:HB2	2.00	0.62
1:B:1123:SER:OG	1:A:914:ASN:ND2	2.32	0.62
1:A:357:ARG:NH1	1:A:396:TYR:OH	2.33	0.61
1:A:1046:GLY:HA2	1:C:890:ALA:HA	1.82	0.61
1:A:104:TRP:O	1:A:105:ILE:HD13	2.01	0.61
1:A:460:LYS:HD3	1:A:461:LEU:N	2.09	0.61
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.26	0.61
1:B:29:THR:HG23	1:B:62:VAL:HG23	1.83	0.61
1:B:909:ILE:HG23	1:B:911:VAL:HG23	1.83	0.61
1:A:34:ARG:HH22	1:A:217:PRO:HB2	1.66	0.60
1:B:442:ASP:O	1:B:448:ASN:ND2	2.34	0.60
1:B:409:GLN:O	1:B:414:GLN:NE2	2.34	0.60
1:B:673:SER:HB3	1:B:695:TYR:HE2	1.66	0.60
1:B:897:PRO:HA	1:C:707:TYR:CE1	2.37	0.60
1:B:433:VAL:HG22	1:B:512:VAL:HG23	1.83	0.60
1:A:643:PHE:HE2	1:A:655:TYR:CG	2.20	0.60
1:C:159:VAL:HG13	1:C:160:TYR:HD1	1.67	0.60
1:B:247:SER:O	1:B:248:TYR:HB3	2.02	0.60
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.33	0.60
1:C:477:ASN:O	1:C:478:LYS:CG	2.49	0.59
1:B:289:VAL:HG23	1:B:306:PHE:CE1	2.37	0.59
1:B:992:GLN:HE21	1:B:995:ARG:HH21	1.49	0.59
1:C:204:TYR:HB3	1:C:223:LEU:HG	1.82	0.59
1:A:237:ARG:NH1	1:A:239:GLN:OE1	2.35	0.59
1:C:200:TYR:HB3	1:C:202:LYS:HE2	1.85	0.59
1:C:566:GLY:HA3	1:C:575:ALA:HB3	1.84	0.59
1:A:1041:ASP:OD1	1:A:1041:ASP:O	2.19	0.59
1:B:473:TYR:O	1:B:474:GLN:NE2	2.35	0.59
1:A:316:SER:O	1:A:595:VAL:HG12	2.02	0.59
1:B:1107:ARG:HD2	1:A:904:TYR:CE2	2.38	0.59
1:B:558:LYS:HG3	1:A:282:ASN:HA	1.84	0.59
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.85	0.58
1:B:406:GLU:HB3	1:B:418:ILE:HD12	1.85	0.58
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.36	0.58
1:A:1115:ILE:HG22	1:A:1137:VAL:HG23	1.85	0.58
1:C:318:PHE:HZ	1:C:635:VAL:HA	1.68	0.58
1:C:735:SER:HG	1:C:859:THR:HG1	1.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:PRO:HA	1:C:707:TYR:HE1	1.66	0.58
1:A:477:ASN:O	1:A:478:LYS:CG	2.47	0.58
1:C:523:THR:HG22	1:C:524:VAL:HG13	1.85	0.58
1:B:78:ARG:HH11	1:B:261:GLY:HA3	1.68	0.58
1:A:729:VAL:O	1:A:777:ASN:ND2	2.36	0.58
1:C:966:LEU:O	1:C:975:SER:OG	2.20	0.58
1:B:663:ASP:OD1	1:B:663:ASP:N	2.35	0.58
1:A:315:THR:HG22	1:A:316:SER:H	1.68	0.58
1:A:457:ARG:NE	1:A:459:SER:O	2.37	0.58
1:B:502:GLY:O	1:B:506:GLN:NE2	2.36	0.57
1:B:724:THR:HG23	1:B:934:ILE:HD11	1.86	0.57
1:B:903:ALA:HB1	1:B:913:GLN:HG3	1.85	0.57
1:C:391:CYS:SG	1:C:544:ASN:ND2	2.75	0.57
1:C:564:GLN:HB2	1:C:577:ARG:HG2	1.86	0.57
1:B:139:PRO:HB2	1:B:241:LEU:HD21	1.86	0.57
1:A:617:CYS:N	1:A:644:GLN:OE1	2.37	0.57
1:A:896:ILE:HD11	1:A:900:MET:HG2	1.87	0.57
1:B:477:ASN:O	1:B:478:LYS:CG	2.48	0.57
1:B:439:ASN:ND2	1:B:506:GLN:OE1	2.37	0.57
1:A:564:GLN:HG2	1:A:565:PHE:HD1	1.69	0.57
1:A:990:GLU:HA	1:A:993:ILE:HG22	1.86	0.57
1:A:37:TYR:HB3	1:A:223:LEU:HD23	1.86	0.57
1:A:724:THR:CG2	1:A:725:GLU:N	2.68	0.57
1:C:98:SER:HA	1:C:180:GLU:H	1.69	0.57
1:C:379:CYS:HB3	1:C:384:PRO:HG3	1.87	0.57
1:C:726:ILE:HD11	1:C:947:LYS:HB3	1.87	0.57
1:A:731:MET:HG2	1:A:774:GLN:NE2	2.20	0.57
1:C:770:ILE:HD12	1:C:1015:ALA:HB2	1.87	0.57
1:B:328:ARG:HD2	1:B:580:GLN:HG3	1.86	0.57
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.38	0.56
1:C:190:ARG:HH11	1:C:207:HIS:HD2	1.52	0.56
1:B:117:LEU:HA	1:B:130:VAL:HA	1.87	0.56
1:A:226:LEU:HG	1:A:227:VAL:HG12	1.86	0.56
1:A:973:ILE:HD11	1:A:980:ILE:HG13	1.86	0.56
1:B:69:HIS:HB2	1:B:77:LYS:HD2	1.88	0.56
1:C:261:GLY:O	1:C:262:ALA:C	2.43	0.56
1:B:758:SER:O	1:B:758:SER:OG	2.21	0.56
1:B:738:CYS:SG	1:B:739:THR:N	2.79	0.56
1:A:445:PRO:O	1:A:498:ARG:NH1	2.39	0.56
1:B:555:SER:HB2	1:B:584:ILE:HB	1.88	0.56
1:A:708:SER:HB3	1:A:711:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ASN:HB3	1:C:371:PHE:HZ	1.69	0.56
1:A:250:THR:O	1:A:254:SER:OG	2.20	0.56
1:C:133:PHE:HB2	1:C:135:PHE:CZ	2.40	0.56
1:A:550:GLY:HA3	1:A:589:PRO:HA	1.88	0.55
1:C:212:LEU:HD21	1:C:217:PRO:HB3	1.88	0.55
1:C:473:TYR:O	1:C:474:GLN:NE2	2.39	0.55
1:C:817:PHE:CE2	1:C:935:GLN:HG3	2.41	0.55
1:B:435:ALA:HB2	1:B:510:VAL:HG13	1.87	0.55
1:B:445:PRO:O	1:B:498:ARG:NH1	2.40	0.55
1:A:712:ILE:HD13	1:A:1094:VAL:HG11	1.89	0.55
1:B:210:ILE:HD13	1:B:217:PRO:HG3	1.88	0.55
1:B:487:ASN:HA	1:B:489:TYR:CE1	2.41	0.55
1:C:708:SER:HB3	1:C:711:SER:HB3	1.88	0.55
1:C:726:ILE:HG22	1:C:1061:VAL:HG13	1.89	0.55
1:C:456:PHE:H	1:C:491:PRO:HB3	1.71	0.55
1:B:327:VAL:HB	1:B:528:LYS:HD2	1.88	0.55
1:A:904:TYR:HE1	1:A:913:GLN:HE22	1.53	0.55
1:C:553:THR:HB	1:C:586:ASP:HB3	1.88	0.55
1:B:720:ILE:H	1:B:926:GLN:NE2	2.05	0.54
1:A:282:ASN:N	1:A:282:ASN:OD1	2.40	0.54
1:C:758:SER:O	1:C:758:SER:OG	2.21	0.54
1:B:488:CYS:O	1:B:489:TYR:C	2.46	0.54
1:A:206:LYS:HB2	1:A:223:LEU:HD12	1.90	0.54
1:A:719:THR:HA	1:A:926:GLN:HE22	1.72	0.54
1:B:416:GLY:H	1:B:419:ALA:HB3	1.71	0.54
1:A:289:VAL:HB	1:A:306:PHE:CE1	2.42	0.54
1:B:353:TRP:CH2	1:B:466:ARG:HA	2.43	0.54
1:B:647:ALA:HA	1:A:862:PRO:HG3	1.89	0.54
1:A:707:TYR:HE1	1:C:897:PRO:HA	1.72	0.54
1:A:741:TYR:CD2	1:A:1004:LEU:HD22	2.42	0.54
1:A:1116:THR:HG22	1:A:1118:ASP:H	1.73	0.54
1:C:124:THR:HB	2:C:1302:NAG:H62	1.90	0.54
1:C:318:PHE:HB2	1:C:593:GLY:HA3	1.89	0.54
1:C:360:ASN:H	1:C:523:THR:HG23	1.73	0.54
1:B:755:GLN:HG3	1:C:969:LYS:O	2.07	0.53
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.38	0.53
1:A:311:GLY:HA2	1:A:664:ILE:HG23	1.91	0.53
1:C:393:THR:OG1	1:C:516:GLU:O	2.20	0.53
1:B:78:ARG:HD2	1:B:261:GLY:HA3	1.91	0.53
1:B:318:PHE:HZ	1:B:635:VAL:HA	1.72	0.53
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:CYS:HB2	1:B:697:MET:SD	2.49	0.53
1:B:707:TYR:HE1	1:A:897:PRO:HA	1.73	0.53
1:B:1043:CYS:HB3	1:B:1048:HIS:CD2	2.43	0.53
1:A:310:LYS:HE2	1:A:664:ILE:HD11	1.90	0.53
1:A:731:MET:H	1:A:774:GLN:NE2	2.07	0.53
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.74	0.53
1:B:206:LYS:HE2	1:B:221:SER:CB	2.38	0.53
1:B:890:ALA:HA	1:C:1046:GLY:HA2	1.90	0.53
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.38	0.53
1:A:67:ALA:HA	1:A:264:ALA:HB2	1.91	0.53
1:C:617:CYS:HA	1:C:633:TRP:HB2	1.91	0.53
1:B:386:LYS:O	1:B:390:LEU:HD21	2.09	0.53
1:A:200:TYR:O	1:A:202:LYS:HG3	2.08	0.53
1:A:553:THR:HB	1:A:586:ASP:HB2	1.91	0.53
1:A:851:CYS:O	1:A:855:PHE:CE2	2.62	0.53
1:C:487:ASN:HA	1:C:489:TYR:CE2	2.44	0.53
1:C:591:SER:O	1:C:634:ARG:NH2	2.32	0.53
1:C:596:SER:HB2	1:C:613:GLN:HE22	1.74	0.53
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.34	0.53
1:B:249:LEU:HG	1:B:251:PRO:HG2	1.91	0.52
1:C:374:PHE:HD1	1:C:436:TRP:HB3	1.74	0.52
1:B:523:THR:HG22	1:B:524:VAL:HG12	1.90	0.52
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.91	0.52
1:B:226:LEU:HG	1:B:227:VAL:HG13	1.92	0.52
1:A:175:PHE:HE1	1:A:203:ILE:HD11	1.75	0.52
1:B:984:LEU:CD1	1:B:988:GLU:HG3	2.36	0.52
1:A:1026:ALA:O	1:A:1030:SER:OG	2.21	0.52
1:C:456:PHE:HB3	1:C:473:TYR:HE2	1.73	0.52
1:B:1006:THR:HG21	1:A:762:GLN:HE22	1.73	0.52
1:C:488:CYS:O	1:C:489:TYR:C	2.48	0.52
1:B:804:GLN:HA	1:B:817:PHE:CD2	2.44	0.52
1:B:437:ASN:HA	1:B:508:TYR:HD2	1.73	0.52
1:C:37:TYR:HB3	1:C:223:LEU:HB3	1.92	0.52
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.75	0.52
1:B:1107:ARG:HG2	1:A:904:TYR:HE2	1.75	0.52
1:C:357:ARG:NE	1:C:357:ARG:O	2.43	0.52
1:C:435:ALA:HB2	1:C:510:VAL:HG13	1.92	0.52
1:A:644:GLN:HE21	2:A:1309:NAG:H82	1.75	0.51
1:A:103:GLY:HA3	1:A:241:LEU:HB2	1.91	0.51
1:C:40:ASP:N	1:C:40:ASP:OD1	2.41	0.51
1:C:931:ILE:O	1:C:934:ILE:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:NH1	1:B:219:GLY:O	2.44	0.51
1:C:767:LEU:HD21	1:C:1008:VAL:HG22	1.91	0.51
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.76	0.51
1:A:79:PHE:CE2	1:A:138:ASP:HB2	2.46	0.51
1:C:822:LEU:HD23	1:C:945:LEU:HD11	1.93	0.51
1:C:909:ILE:HG21	1:C:1047:TYR:HB3	1.90	0.51
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.44	0.51
1:A:312:ILE:HG23	1:A:596:SER:OG	2.11	0.51
1:A:487:ASN:HA	1:A:489:TYR:CE2	2.46	0.51
1:A:574:ASP:HA	1:A:587:ILE:HB	1.93	0.51
1:C:312:ILE:HG23	1:C:596:SER:OG	2.11	0.51
1:A:78:ARG:HH21	1:A:261:GLY:HA3	1.77	0.50
1:A:724:THR:HG22	1:A:725:GLU:N	2.25	0.50
1:C:364:ASP:N	1:C:364:ASP:OD1	2.44	0.50
1:B:982:SER:HA	1:C:386:LYS:HE2	1.93	0.50
1:A:488:CYS:O	1:A:489:TYR:C	2.49	0.50
1:C:421:TYR:HD1	1:C:460:LYS:HA	1.76	0.50
1:B:280:ASN:OD1	1:B:284:THR:N	2.45	0.50
1:B:43:PHE:N	1:C:565:PHE:O	2.41	0.50
1:A:175:PHE:H	1:A:175:PHE:HD2	1.60	0.50
1:A:502:GLY:O	1:A:506:GLN:NE2	2.45	0.50
1:B:96:GLU:O	1:B:190:ARG:NH2	2.36	0.50
1:B:204:TYR:HB3	1:B:223:LEU:HG	1.94	0.50
1:B:911:VAL:HG22	1:B:1108:ASN:HB2	1.92	0.50
1:A:437:ASN:HB3	1:A:508:TYR:CZ	2.47	0.50
1:C:301:CYS:O	1:C:304:LYS:NZ	2.44	0.50
1:B:87:ASN:N	1:B:87:ASN:OD1	2.45	0.50
1:B:877:LEU:HD23	1:B:888:PHE:HE2	1.77	0.50
1:A:328:ARG:CG	1:A:579:PRO:HD2	2.42	0.50
1:A:394:ASN:OD1	1:A:394:ASN:N	2.45	0.50
1:C:327:VAL:HG21	1:C:528:LYS:HD3	1.93	0.50
1:A:761:THR:O	1:A:765:ARG:HB2	2.12	0.50
1:A:909:ILE:HG21	1:A:1047:TYR:HB3	1.93	0.50
1:A:393:THR:OG1	1:A:394:ASN:OD1	2.28	0.49
1:A:642:VAL:HG22	1:A:651:ILE:HG22	1.93	0.49
1:A:822:LEU:HD21	1:A:938:LEU:HD21	1.94	0.49
1:A:916:LEU:HD12	1:A:923:ILE:HG13	1.93	0.49
1:A:1006:THR:HG21	1:C:762:GLN:HE22	1.76	0.49
1:B:250:THR:N	1:B:251:PRO:HD2	2.27	0.49
1:B:708:SER:HB3	1:B:711:SER:CB	2.41	0.49
1:A:589:PRO:HD2	1:C:855:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:TYR:CD2	1:B:1004:LEU:HD22	2.48	0.49
1:A:104:TRP:C	1:A:105:ILE:HD13	2.33	0.49
1:A:327:VAL:HG11	1:A:528:LYS:HG2	1.93	0.49
1:C:815:ARG:HB2	1:C:819:GLU:HB2	1.94	0.49
1:B:565:PHE:O	1:A:43:PHE:HB3	2.13	0.49
1:C:79:PHE:HB2	1:C:258:TRP:CE3	2.47	0.49
1:B:505:HIS:CE1	1:A:503:VAL:HG11	2.48	0.49
1:B:737:ASP:OD2	1:C:317:ASN:ND2	2.46	0.49
1:B:781:VAL:HG22	1:B:1026:ALA:HB2	1.95	0.49
1:A:977:LEU:O	1:A:980:ILE:HG22	2.13	0.49
1:C:190:ARG:HD2	1:C:207:HIS:CD2	2.48	0.49
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.94	0.49
1:B:311:GLY:HA2	1:B:664:ILE:HG22	1.95	0.49
1:B:741:TYR:CE1	1:B:966:LEU:HD11	2.48	0.49
1:A:643:PHE:HD1	1:A:644:GLN:N	2.08	0.49
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.95	0.49
1:B:330:PRO:O	1:B:331:ASN:HB2	2.12	0.49
1:B:724:THR:CG2	1:B:934:ILE:HD11	2.42	0.49
1:A:724:THR:HG23	1:A:1061:VAL:HG13	1.95	0.49
1:B:343:ASN:HB3	1:B:371:PHE:HZ	1.78	0.48
1:B:797:PHE:O	1:B:799:GLY:N	2.46	0.48
1:A:665:PRO:HB3	1:C:864:LEU:HD11	1.95	0.48
1:A:780:GLU:H	1:A:780:GLU:CD	2.10	0.48
1:C:104:TRP:HB2	1:C:119:ILE:HB	1.94	0.48
1:B:249:LEU:HB3	1:B:252:VAL:HG22	1.96	0.48
1:B:1139:ASP:OD1	1:B:1139:ASP:N	2.39	0.48
1:A:409:GLN:OE1	1:A:417:ASN:N	2.46	0.48
1:C:560:LEU:H	1:C:563:GLN:HB3	1.78	0.48
1:B:138:ASP:OD1	1:B:138:ASP:N	2.47	0.48
1:B:1126:CYS:HB3	1:B:1132:ILE:HD13	1.95	0.48
1:A:881:THR:HA	1:A:885:GLY:O	2.13	0.48
1:B:48:LEU:HB3	1:B:276:LEU:HD11	1.95	0.48
1:B:715:PRO:HD3	1:A:894:LEU:HD13	1.96	0.48
1:A:822:LEU:HD22	1:A:945:LEU:HD11	1.95	0.48
1:C:372:ALA:N	1:C:373:PRO:HD2	2.28	0.48
1:B:977:LEU:HD21	1:B:996:LEU:HD22	1.95	0.48
1:B:343:ASN:HB3	1:B:371:PHE:CZ	2.48	0.48
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	1.96	0.48
1:A:330:PRO:CD	1:A:544:ASN:HD21	2.22	0.48
1:A:713:ALA:HB3	1:C:894:LEU:HB3	1.95	0.48
1:C:735:SER:HB3	1:C:861:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:HA	1:B:223:LEU:HB3	1.95	0.48
1:A:233:ILE:HG12	1:A:234:ASN:H	1.79	0.48
1:C:738:CYS:SG	1:C:753:LEU:CD2	2.94	0.48
1:B:657:ASN:OD1	2:B:1310:NAG:N2	2.47	0.48
1:A:487:ASN:HA	1:A:489:TYR:CZ	2.49	0.48
1:A:560:LEU:HB2	1:A:563:GLN:HB2	1.96	0.48
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.96	0.48
1:C:378:LYS:HD3	1:C:380:TYR:CZ	2.48	0.48
1:B:736:VAL:HG22	1:B:767:LEU:HD12	1.96	0.48
1:A:98:SER:HA	1:A:179:LEU:HB2	1.95	0.48
1:A:372:ALA:N	1:A:373:PRO:HD2	2.29	0.48
1:A:856:ASN:HD22	1:A:966:LEU:HD12	1.79	0.48
1:A:858:LEU:HD22	1:A:959:LEU:HD22	1.95	0.48
1:B:80:ASP:HA	1:B:260:ALA:HA	1.95	0.47
1:B:617:CYS:SG	1:B:635:VAL:HG21	2.54	0.47
1:B:864:LEU:HD22	1:C:665:PRO:HB3	1.96	0.47
1:A:537:LYS:HA	1:A:537:LYS:HD3	1.58	0.47
1:A:552:LEU:HD12	1:A:585:LEU:HB3	1.96	0.47
1:C:798:GLY:C	1:C:800:PHE:H	2.17	0.47
1:B:50:SER:HA	1:B:276:LEU:HA	1.96	0.47
1:B:1081:ILE:HG13	1:B:1095:PHE:CD2	2.49	0.47
1:C:318:PHE:CZ	1:C:635:VAL:HA	2.48	0.47
1:B:200:TYR:O	1:B:202:LYS:HG3	2.13	0.47
1:B:421:TYR:O	1:B:457:ARG:NH1	2.35	0.47
1:A:175:PHE:N	1:A:175:PHE:CD2	2.82	0.47
1:A:733:LYS:HD2	1:A:771:ALA:HB1	1.95	0.47
1:C:280:ASN:OD1	1:C:284:THR:N	2.46	0.47
1:A:125:ASN:HA	1:A:174:PRO:HD3	1.95	0.47
1:C:671:CYS:SG	1:C:697:MET:HE3	2.54	0.47
1:C:714:ILE:HD11	1:C:1094:VAL:HG21	1.97	0.47
1:B:252:VAL:O	1:B:253:ASP:C	2.53	0.47
1:A:114:THR:O	1:A:132:GLU:HG3	2.14	0.47
1:C:131:CYS:HB3	1:C:166:CYS:HB3	1.74	0.47
1:C:742:ILE:HD11	1:C:1004:LEU:HD12	1.95	0.47
1:B:90:VAL:HG21	1:B:238:PHE:CZ	2.49	0.47
1:B:483:VAL:O	1:B:484:ALA:C	2.53	0.47
1:A:50:SER:HA	1:A:276:LEU:HA	1.95	0.47
1:A:663:ASP:OD1	1:A:663:ASP:N	2.47	0.47
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.49	0.47
1:C:330:PRO:HD3	1:C:544:ASN:ND2	2.30	0.47
1:C:777:ASN:O	1:C:781:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ILE:HD13	1:B:235:ILE:HD11	1.96	0.47
1:A:277:LEU:C	1:A:277:LEU:HD12	2.35	0.47
1:C:664:ILE:O	1:C:664:ILE:HG13	2.14	0.47
1:B:797:PHE:O	1:B:800:PHE:HD1	1.98	0.47
1:A:1094:VAL:HG22	1:C:904:TYR:OH	2.15	0.47
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.50	0.47
1:B:113:LYS:HB3	1:B:113:LYS:HE3	1.78	0.47
1:C:560:LEU:HB2	1:C:563:GLN:HB2	1.97	0.47
1:B:106:PHE:HB3	1:B:235:ILE:HD12	1.96	0.46
1:B:328:ARG:HG2	1:B:579:PRO:HD2	1.98	0.46
1:B:730:SER:HB2	1:B:774:GLN:HG3	1.98	0.46
1:A:118:LEU:HD23	1:A:118:LEU:C	2.36	0.46
1:A:467:ASP:N	1:A:467:ASP:OD1	2.47	0.46
1:C:474:GLN:HE22	1:C:482:GLY:H	1.62	0.46
1:C:665:PRO:HA	1:C:671:CYS:SG	2.55	0.46
1:B:517:LEU:HD12	1:A:983:ARG:HD3	1.96	0.46
1:C:434:ILE:HB	1:C:511:VAL:HG23	1.97	0.46
1:B:79:PHE:HB2	1:B:258:TRP:HB3	1.96	0.46
1:A:713:ALA:HA	1:A:1074:ASN:HA	1.97	0.46
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.97	0.46
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.50	0.46
1:A:1082:CYS:HB2	1:A:1132:ILE:HG12	1.97	0.46
1:B:129:LYS:HB3	1:B:131:CYS:SG	2.55	0.46
1:B:983:ARG:HD3	1:C:517:LEU:HD12	1.97	0.46
1:C:330:PRO:CD	1:C:544:ASN:HD21	2.27	0.46
1:A:50:SER:HB2	1:A:276:LEU:HD12	1.96	0.46
1:A:781:VAL:O	1:A:1029:MET:HG2	2.16	0.46
1:B:36:VAL:HG11	1:B:220:PHE:HZ	1.81	0.46
1:B:442:ASP:HB2	1:B:509:ARG:HH21	1.80	0.46
1:B:605:SER:OG	1:B:606:ASN:N	2.49	0.46
1:B:950:ASP:O	1:B:954:HIS:HB2	2.15	0.46
1:A:402:ILE:HD11	1:A:510:VAL:HG21	1.96	0.46
1:C:249:LEU:HG	1:C:251:PRO:HD2	1.97	0.46
1:A:970:PHE:HE1	1:C:756:TYR:HA	1.81	0.46
1:A:1009:THR:O	1:A:1013:ILE:HD12	2.15	0.46
1:C:190:ARG:HH11	1:C:207:HIS:CD2	2.32	0.46
1:A:210:ILE:HG21	1:A:217:PRO:HG2	1.97	0.46
1:C:77:LYS:HG3	1:C:78:ARG:HG2	1.97	0.46
1:B:894:LEU:HB3	1:C:713:ALA:HB3	1.96	0.46
1:B:969:LYS:HZ3	1:B:975:SER:H	1.63	0.46
1:B:1046:GLY:HA2	1:A:890:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HB3	1:A:231:ILE:HD11	1.98	0.46
1:B:897:PRO:HB2	1:B:900:MET:HG2	1.97	0.46
1:B:931:ILE:O	1:B:934:ILE:HG22	2.16	0.46
1:A:993:ILE:O	1:A:997:ILE:HG12	2.15	0.46
1:B:54:LEU:HD12	1:B:195:LYS:HD3	1.98	0.45
1:B:797:PHE:CD2	1:B:802:PHE:HD2	2.35	0.45
1:A:533:LEU:HD22	1:A:585:LEU:HD11	1.97	0.45
1:A:596:SER:HB2	1:A:613:GLN:HE22	1.81	0.45
1:C:445:PRO:O	1:C:498:ARG:NH1	2.49	0.45
1:B:121:ASN:HD21	1:B:176:LEU:H	1.64	0.45
1:A:78:ARG:HB3	1:A:261:GLY:C	2.37	0.45
1:B:26:GLN:HG3	1:B:65:PHE:HA	1.99	0.45
1:B:786:LYS:HB2	1:B:786:LYS:HE2	1.77	0.45
1:B:864:LEU:O	1:C:669:GLY:N	2.43	0.45
1:A:456:PHE:HB3	1:A:473:TYR:HE2	1.81	0.45
1:B:81:ASN:N	1:B:81:ASN:OD1	2.48	0.45
1:B:327:VAL:HG13	1:B:542:ASN:HB3	1.98	0.45
1:A:1110:TYR:CZ	1:A:1112:PRO:HG3	2.52	0.45
1:C:343:ASN:HB3	1:C:371:PHE:CZ	2.50	0.45
1:C:598:ILE:HD12	1:C:664:ILE:HD12	1.97	0.45
1:C:642:VAL:HG12	1:C:651:ILE:HG22	1.99	0.45
1:B:118:LEU:N	1:B:129:LYS:O	2.49	0.45
1:B:384:PRO:HA	1:B:387:LEU:HD13	1.99	0.45
1:B:398:ASP:HB3	1:B:512:VAL:HG12	1.99	0.45
1:B:439:ASN:HA	1:B:507:PRO:HG2	1.98	0.45
1:A:43:PHE:HE1	1:A:283:GLY:HA3	1.82	0.45
1:A:175:PHE:CE1	1:A:203:ILE:HD11	2.51	0.45
1:A:804:GLN:HA	1:A:817:PHE:CD2	2.51	0.45
1:B:490:SER:O	1:B:493:GLN:NE2	2.49	0.45
1:B:541:PHE:CZ	1:B:587:ILE:HD13	2.51	0.45
1:A:176:LEU:HD12	1:A:190:ARG:HH11	1.82	0.45
1:C:87:ASN:OD1	1:C:87:ASN:N	2.48	0.45
1:C:736:VAL:HG11	1:C:1004:LEU:HD21	1.98	0.45
1:C:752:LEU:HD11	1:C:990:GLU:OE2	2.15	0.45
1:B:34:ARG:HH22	1:B:217:PRO:HB2	1.82	0.45
1:B:755:GLN:OE1	1:C:969:LYS:CB	2.64	0.45
1:B:850:ILE:O	1:B:853:GLN:HG2	2.17	0.45
1:A:79:PHE:HE2	1:A:138:ASP:HB2	1.79	0.45
1:B:777:ASN:HD21	1:B:1019:ARG:HA	1.81	0.45
1:A:87:ASN:OD1	1:A:87:ASN:N	2.47	0.45
1:A:896:ILE:HD12	1:A:897:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG21	1:A:387:LEU:HD11	1.98	0.45
1:A:550:GLY:CA	1:A:589:PRO:HA	2.46	0.45
1:B:104:TRP:CZ3	1:B:238:PHE:HD2	2.35	0.45
1:B:388:ASN:OD1	1:B:526:GLY:HA3	2.17	0.45
1:B:788:ILE:HD11	1:C:699:LEU:HB3	1.99	0.45
1:A:797:PHE:HD2	1:A:802:PHE:HD2	1.65	0.45
1:A:817:PHE:N	1:A:817:PHE:CD1	2.82	0.45
1:C:591:SER:H	1:C:634:ARG:HH12	1.64	0.45
1:C:664:ILE:HD11	1:C:672:ALA:HB3	1.98	0.45
1:C:394:ASN:OD1	1:C:394:ASN:O	2.35	0.44
1:A:26:GLN:OE1	1:A:66:HIS:NE2	2.50	0.44
1:A:591:SER:HG	1:A:634:ARG:NH2	2.16	0.44
1:B:328:ARG:HB3	1:B:543:PHE:CE1	2.53	0.44
1:A:565:PHE:O	1:C:43:PHE:N	2.46	0.44
1:C:452:LEU:HD11	1:C:492:LEU:HB2	1.98	0.44
1:B:719:THR:HA	1:B:926:GLN:HE22	1.83	0.44
1:B:811:LYS:H	1:B:811:LYS:HG2	1.53	0.44
1:A:353:TRP:HH2	1:A:418:ILE:HD11	1.81	0.44
1:A:505:HIS:HE2	1:C:503:VAL:HG11	1.82	0.44
1:A:858:LEU:HD21	1:A:962:LEU:HD23	1.98	0.44
1:B:882:ILE:HG23	1:B:898:PHE:CD2	2.52	0.44
1:C:34:ARG:HA	1:C:34:ARG:HD3	1.74	0.44
1:C:101:ILE:HD11	1:C:240:THR:OG1	2.18	0.44
1:C:662:CYS:HB2	1:C:671:CYS:HB3	1.69	0.44
1:B:434:ILE:HB	1:B:511:VAL:HG23	1.99	0.44
1:B:803:SER:OG	1:B:804:GLN:NE2	2.49	0.44
1:C:237:ARG:HG2	1:C:239:GLN:NE2	2.33	0.44
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.18	0.44
1:B:29:THR:OG1	1:B:30:ASN:N	2.50	0.44
1:B:534:VAL:HG21	1:B:539:VAL:HG11	2.00	0.44
1:B:1129:VAL:HG22	1:A:917:TYR:HB3	1.99	0.44
1:A:328:ARG:HG3	1:A:579:PRO:HD2	2.00	0.44
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.18	0.44
1:C:409:GLN:O	1:C:414:GLN:NE2	2.50	0.44
1:B:391:CYS:HA	1:B:525:CYS:HB3	2.00	0.44
1:B:635:VAL:HG12	1:B:635:VAL:O	2.18	0.44
1:B:1010:GLN:OE1	1:B:1010:GLN:HA	2.18	0.44
1:A:1028:LYS:HB2	1:A:1028:LYS:HE3	1.62	0.44
1:C:994:ASP:O	1:C:998:THR:HG23	2.18	0.44
1:B:347:PHE:CD1	1:B:509:ARG:HD2	2.53	0.44
1:B:379:CYS:HB2	1:B:384:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:SER:H	1:B:634:ARG:HH12	1.66	0.44
1:B:922:LEU:HD11	2:B:1312:NAG:H3	1.99	0.44
1:A:886:TRP:HZ3	1:A:901:GLN:HG3	1.83	0.44
1:C:80:ASP:HB2	1:C:262:ALA:H	1.83	0.44
1:C:546:LEU:HD21	1:C:565:PHE:HZ	1.83	0.44
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.53	0.44
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.50	0.44
1:B:669:GLY:N	1:A:864:LEU:O	2.46	0.43
1:C:1115:ILE:HG22	1:C:1137:VAL:HG23	2.00	0.43
1:B:133:PHE:HB2	1:B:135:PHE:CZ	2.53	0.43
1:B:666:ILE:HB	1:B:670:ILE:O	2.18	0.43
1:B:708:SER:HA	2:B:1311:NAG:H82	1.99	0.43
1:B:896:ILE:HD12	1:B:897:PRO:HD2	1.99	0.43
1:B:990:GLU:HA	1:B:993:ILE:HG22	2.00	0.43
1:A:110:LEU:HD12	1:A:135:PHE:HD2	1.83	0.43
1:A:517:LEU:HD12	1:C:983:ARG:NH1	2.33	0.43
1:C:80:ASP:H	1:C:262:ALA:HB2	1.83	0.43
1:C:698:SER:O	1:C:698:SER:OG	2.34	0.43
1:A:319:ARG:HH12	1:C:740:MET:HB2	1.82	0.43
1:A:536:ASN:O	1:A:537:LYS:HD3	2.18	0.43
1:C:591:SER:N	1:C:634:ARG:HH12	2.16	0.43
1:B:421:TYR:CD1	1:B:460:LYS:HD2	2.54	0.43
1:A:54:LEU:HB2	1:A:195:LYS:HE3	2.01	0.43
1:B:126:VAL:HB	1:B:174:PRO:HA	2.01	0.43
1:B:869:MET:H	1:B:869:MET:HG2	1.57	0.43
1:A:98:SER:HA	1:A:180:GLU:H	1.83	0.43
1:A:276:LEU:HD11	1:A:304:LYS:HD3	2.00	0.43
1:A:936:ASP:O	1:A:940:SER:N	2.51	0.43
1:C:34:ARG:HH21	1:C:217:PRO:HG2	1.84	0.43
1:C:318:PHE:O	1:C:319:ARG:HG3	2.19	0.43
1:C:708:SER:HA	2:C:1311:NAG:H82	1.99	0.43
1:C:969:LYS:NZ	1:C:975:SER:H	2.16	0.43
1:A:166:CYS:HB2	1:A:167:THR:H	1.60	0.43
1:C:206:LYS:HB2	1:C:223:LEU:HD13	2.01	0.43
1:C:240:THR:O	1:C:241:LEU:HD22	2.17	0.43
1:C:801:ASN:N	1:C:928:ASN:OD1	2.41	0.43
1:C:1098:ASN:OD1	1:C:1098:ASN:N	2.52	0.43
1:B:416:GLY:N	1:B:419:ALA:HB3	2.33	0.43
1:B:528:LYS:HD3	1:B:529:LYS:N	2.34	0.43
1:B:595:VAL:HG22	1:B:612:TYR:CE1	2.53	0.43
1:A:83:ALA:HA	1:A:237:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LYS:HD3	1:A:380:TYR:CZ	2.54	0.43
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.83	0.43
1:A:570:ALA:HB2	1:C:852:ALA:HB1	2.01	0.43
1:C:457:ARG:HH22	1:C:461:LEU:HB2	1.82	0.43
1:C:477:ASN:C	1:C:478:LYS:HG3	2.38	0.43
1:B:278:LYS:HB2	1:B:306:PHE:CE2	2.53	0.43
1:B:342:PHE:HE1	1:B:511:VAL:HG21	1.83	0.43
1:B:392:PHE:HD1	1:B:517:LEU:HD21	1.84	0.43
1:A:355:ARG:CZ	1:A:396:TYR:HB3	2.49	0.43
1:C:378:LYS:HD3	1:C:380:TYR:CE2	2.54	0.43
1:B:353:TRP:HD1	1:B:398:ASP:OD1	2.02	0.43
1:B:719:THR:O	1:B:1068:VAL:HG22	2.19	0.43
1:B:737:ASP:OD1	1:B:737:ASP:N	2.51	0.43
1:A:289:VAL:HB	1:A:306:PHE:HE1	1.84	0.43
1:C:487:ASN:HA	1:C:489:TYR:CZ	2.54	0.43
1:C:739:THR:HG22	1:C:753:LEU:HD23	2.01	0.43
1:C:800:PHE:HD2	1:C:927:PHE:CD2	2.37	0.43
1:C:819:GLU:OE1	1:C:1055:SER:HB2	2.19	0.43
1:B:720:ILE:HD12	1:B:923:ILE:HG23	2.00	0.42
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.37	0.42
1:A:552:LEU:HD12	1:A:585:LEU:HD22	2.01	0.42
1:C:129:LYS:HA	1:C:129:LYS:HE2	2.01	0.42
1:B:233:ILE:HG12	1:B:234:ASN:H	1.83	0.42
1:A:121:ASN:OD1	1:A:175:PHE:HD2	2.02	0.42
1:A:505:HIS:NE2	1:C:503:VAL:HG11	2.33	0.42
1:A:1107:ARG:HD3	1:C:904:TYR:CD2	2.54	0.42
1:C:117:LEU:HA	1:C:130:VAL:HA	2.01	0.42
1:C:643:PHE:HD1	1:C:644:GLN:H	1.66	0.42
1:A:34:ARG:NH1	1:A:217:PRO:O	2.52	0.42
1:A:396:TYR:O	1:A:513:LEU:HA	2.20	0.42
1:A:707:TYR:CE1	1:C:897:PRO:HA	2.53	0.42
1:A:986:LYS:HA	1:A:986:LYS:HD3	1.88	0.42
1:C:81:ASN:OD1	1:C:81:ASN:N	2.53	0.42
1:B:382:VAL:HG13	1:A:983:ARG:HH11	1.85	0.42
1:A:357:ARG:NE	1:C:231:ILE:O	2.52	0.42
1:A:1106:GLN:H	1:A:1106:GLN:HG3	1.56	0.42
1:C:128:ILE:HG12	1:C:170:TYR:CD1	2.55	0.42
1:A:931:ILE:O	1:A:934:ILE:HG22	2.20	0.42
1:C:81:ASN:HB3	1:C:138:ASP:CB	2.49	0.42
1:C:131:CYS:HB2	1:C:133:PHE:CZ	2.54	0.42
1:C:878:LEU:HD11	1:C:1052:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:LYS:HD3	1:B:424:LYS:HA	1.86	0.42
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.54	0.42
1:A:328:ARG:HG2	1:A:579:PRO:HD2	2.01	0.42
1:A:376:ALA:HB3	1:A:435:ALA:HB3	2.00	0.42
1:A:617:CYS:HA	1:A:633:TRP:N	2.35	0.42
1:C:34:ARG:NH2	1:C:217:PRO:HG2	2.34	0.42
1:C:854:LYS:HE3	1:C:854:LYS:HB3	1.90	0.42
1:B:178:ASP:OD1	1:B:178:ASP:N	2.53	0.42
1:B:768:THR:O	1:B:772:VAL:HG13	2.19	0.42
1:A:118:LEU:CD2	1:A:120:VAL:HG23	2.46	0.42
1:B:497:PHE:CE2	1:B:507:PRO:HB3	2.55	0.42
1:A:126:VAL:HB	1:A:174:PRO:HA	2.02	0.42
1:A:159:VAL:HG23	1:A:160:TYR:H	1.83	0.42
1:A:438:SER:HB3	1:A:509:ARG:HG2	2.02	0.42
1:A:536:ASN:O	1:A:537:LYS:CD	2.68	0.42
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.19	0.42
1:B:707:TYR:CE1	1:A:897:PRO:HA	2.53	0.42
1:A:34:ARG:NH1	1:A:219:GLY:O	2.52	0.42
1:A:122:ASN:O	1:A:124:THR:N	2.52	0.42
1:A:295:PRO:HA	1:A:298:GLU:HB3	2.02	0.42
1:C:50:SER:HA	1:C:276:LEU:HA	2.02	0.42
1:C:159:VAL:HG13	1:C:160:TYR:CD1	2.51	0.42
1:C:258:TRP:CD1	1:C:258:TRP:N	2.88	0.42
1:B:247:SER:O	1:B:248:TYR:CB	2.68	0.42
1:B:477:ASN:C	1:B:478:LYS:HG3	2.39	0.42
1:A:131:CYS:HB2	1:A:133:PHE:CZ	2.54	0.42
1:A:299:THR:HG22	1:A:308:VAL:HG11	2.02	0.42
1:A:332:ILE:HG23	1:A:362:VAL:HG23	2.01	0.42
1:A:349:SER:HB2	1:A:451:TYR:CD1	2.54	0.42
1:A:355:ARG:HD3	1:A:398:ASP:OD1	2.20	0.42
1:A:804:GLN:HG3	1:A:931:ILE:HG23	2.02	0.42
1:C:557:LYS:HE2	1:C:557:LYS:HB3	1.88	0.41
1:C:726:ILE:HG22	1:C:1061:VAL:HG22	2.01	0.41
1:B:992:GLN:NE2	1:B:995:ARG:HH21	2.17	0.41
1:C:541:PHE:CZ	1:C:548:GLY:HA3	2.56	0.41
1:C:1094:VAL:HG23	1:C:1096:VAL:HG23	2.01	0.41
1:B:140:PHE:HA	1:B:241:LEU:HD11	2.02	0.41
1:B:715:PRO:HD3	1:A:894:LEU:CD1	2.50	0.41
1:B:816:SER:OG	1:B:819:GLU:HG3	2.20	0.41
1:B:983:ARG:O	1:C:383:SER:N	2.53	0.41
1:A:565:PHE:HD2	1:A:567:ARG:HH21	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:SER:OG	1:A:868:GLU:OE2	2.30	0.41
1:C:28:TYR:CE2	2:C:1301:NAG:H62	2.56	0.41
1:B:133:PHE:HB3	1:B:160:TYR:HB3	2.02	0.41
1:B:428:ASP:OD1	1:B:429:PHE:N	2.53	0.41
1:B:557:LYS:HB3	1:B:557:LYS:HE2	1.83	0.41
1:B:560:LEU:N	1:B:563:GLN:HB3	2.26	0.41
1:B:713:ALA:HA	1:B:1074:ASN:HA	2.01	0.41
1:B:827:THR:O	1:B:827:THR:OG1	2.37	0.41
1:A:869:MET:H	1:A:869:MET:HG2	1.70	0.41
1:C:537:LYS:C	1:C:551:VAL:HG12	2.41	0.41
1:C:697:MET:HA	1:C:697:MET:CE	2.50	0.41
1:B:359:SER:HA	1:B:523:THR:HG23	2.02	0.41
1:B:446:SER:O	1:B:498:ARG:NH2	2.53	0.41
1:B:633:TRP:O	1:B:634:ARG:HG3	2.20	0.41
1:B:761:THR:CG2	1:B:762:GLN:N	2.83	0.41
1:B:121:ASN:OD1	1:B:174:PRO:HB3	2.21	0.41
1:B:537:LYS:C	1:B:551:VAL:HG12	2.40	0.41
1:B:790:LYS:HE2	1:C:704:SER:HB3	2.01	0.41
1:A:269:TYR:CD1	1:A:269:TYR:N	2.88	0.41
1:C:177:MET:H	1:C:190:ARG:HH12	1.68	0.41
1:B:43:PHE:CE2	1:C:557:LYS:HD3	2.55	0.41
1:B:877:LEU:HD23	1:B:888:PHE:CE2	2.55	0.41
1:A:356:LYS:HE2	1:A:356:LYS:HB2	1.77	0.41
1:A:364:ASP:N	1:A:364:ASP:OD1	2.54	0.41
1:A:1083:HIS:CG	1:A:1137:VAL:HG12	2.55	0.41
1:C:1023:ASN:O	1:C:1027:THR:HG23	2.21	0.41
1:C:1086:LYS:HA	1:C:1086:LYS:HD2	1.90	0.41
1:B:804:GLN:HA	1:B:817:PHE:HD2	1.86	0.41
1:A:65:PHE:CZ	1:A:84:LEU:HD21	2.55	0.41
1:A:644:GLN:HG3	2:A:1309:NAG:HN2	1.86	0.41
1:C:349:SER:HB3	1:C:351:TYR:CD1	2.56	0.41
1:C:726:ILE:CD1	1:C:947:LYS:HB3	2.49	0.41
1:B:304:LYS:HE3	1:B:304:LYS:HB3	1.89	0.41
1:B:349:SER:OG	1:B:350:VAL:N	2.54	0.41
1:B:487:ASN:HA	1:B:489:TYR:CZ	2.55	0.41
1:B:503:VAL:HG11	1:C:505:HIS:NE2	2.36	0.41
1:B:642:VAL:HG22	1:B:651:ILE:HG22	2.03	0.41
1:B:916:LEU:HD12	1:B:923:ILE:HG13	2.02	0.41
1:A:138:ASP:OD1	1:A:138:ASP:N	2.53	0.41
1:A:394:ASN:ND2	1:C:200:TYR:OH	2.53	0.41
1:A:424:LYS:HD3	1:A:424:LYS:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ASP:O	1:C:297:SER:OG	2.28	0.41
1:C:483:VAL:O	1:C:484:ALA:C	2.58	0.41
1:C:559:PHE:HD1	1:C:563:GLN:HG3	1.85	0.41
1:B:431:GLY:HA3	1:B:513:LEU:O	2.21	0.41
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	2.02	0.41
1:B:969:LYS:O	1:A:755:GLN:HB3	2.21	0.41
1:C:424:LYS:HD3	1:C:424:LYS:HA	1.94	0.41
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.86	0.41
1:C:817:PHE:CZ	1:C:821:LEU:HD12	2.56	0.41
1:B:558:LYS:O	1:B:559:PHE:HB2	2.21	0.40
1:B:564:GLN:HG2	1:B:565:PHE:HD1	1.86	0.40
1:B:664:ILE:O	1:B:671:CYS:HB3	2.21	0.40
1:B:1006:THR:HG23	1:A:1005:GLN:HE22	1.86	0.40
1:B:1095:PHE:HD1	1:B:1095:PHE:HA	1.80	0.40
1:A:135:PHE:HE1	1:A:159:VAL:HB	1.86	0.40
1:A:204:TYR:HB2	1:A:223:LEU:HD21	2.03	0.40
1:A:483:VAL:O	1:A:484:ALA:C	2.59	0.40
1:C:304:LYS:HA	1:C:304:LYS:HD3	1.93	0.40
1:C:336:CYS:HB2	1:C:361:CYS:HB2	1.95	0.40
1:C:555:SER:HB2	1:C:584:ILE:HB	2.04	0.40
1:C:559:PHE:CD1	1:C:563:GLN:HG3	2.56	0.40
1:C:726:ILE:C	1:C:726:ILE:HD12	2.41	0.40
1:B:390:LEU:O	1:B:525:CYS:HB3	2.20	0.40
1:B:695:TYR:HD1	1:B:696:THR:O	2.04	0.40
1:A:797:PHE:HE2	1:A:806:LEU:HD11	1.87	0.40
1:C:347:PHE:CD2	1:C:509:ARG:HD2	2.56	0.40
1:C:380:TYR:HE2	1:C:412:PRO:HD3	1.87	0.40
1:C:714:ILE:HD12	1:C:1096:VAL:HG21	2.02	0.40
1:C:764:LYS:HB3	1:C:764:LYS:HE3	1.87	0.40
1:C:984:LEU:HD22	1:C:988:GLU:HG3	2.03	0.40
1:B:220:PHE:HE2	1:B:285:ILE:HG22	1.86	0.40
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.40	0.40
1:B:456:PHE:CE1	1:A:372:ALA:HB1	2.56	0.40
1:B:957:GLN:HA	1:B:960:ASN:HB3	2.03	0.40
1:A:375:PHE:CE2	1:A:407:VAL:HG11	2.57	0.40
1:A:375:PHE:HE2	1:A:407:VAL:HG11	1.86	0.40
1:A:636:TYR:HB3	1:A:637:SER:H	1.69	0.40
1:C:28:TYR:CD2	2:C:1301:NAG:H62	2.57	0.40
1:C:167:THR:O	1:C:167:THR:OG1	2.39	0.40
1:B:409:GLN:OE1	1:B:417:ASN:N	2.55	0.40
1:A:105:ILE:HB	1:A:239:GLN:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:TYR:CE1	1:C:966:LEU:HD11	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	A	1026/1269 (81%)	911 (89%)	109 (11%)	6 (1%)	25	64
1	B	1026/1269 (81%)	923 (90%)	96 (9%)	7 (1%)	22	61
1	C	1026/1269 (81%)	936 (91%)	87 (8%)	3 (0%)	41	74
All	All	3078/3807 (81%)	2770 (90%)	292 (10%)	16 (0%)	32	67

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	ASN
1	B	253	ASP
1	B	788	ILE
1	B	798	GLY
1	A	788	ILE
1	C	788	ILE
1	B	330	PRO
1	B	489	TYR
1	A	177	MET
1	A	738	CYS
1	C	489	TYR
1	B	254	SER
1	A	330	PRO
1	A	489	TYR
1	A	888	PHE
1	C	166	CYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	908/1109 (82%)	877 (97%)	31 (3%)	37 70
1	B	908/1109 (82%)	883 (97%)	25 (3%)	43 74
1	C	908/1109 (82%)	884 (97%)	24 (3%)	46 76
All	All	2724/3327 (82%)	2644 (97%)	80 (3%)	45 74

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	79	PHE
1	B	81	ASN
1	B	88	ASP
1	B	97	LYS
1	B	104	TRP
1	B	116	SER
1	B	118	LEU
1	B	166	CYS
1	B	168	PHE
1	B	241	LEU
1	B	275	PHE
1	B	390	LEU
1	B	457	ARG
1	B	525	CYS
1	B	529	LYS
1	B	643	PHE
1	B	657	ASN
1	B	673	SER
1	B	718	PHE
1	B	758	SER
1	B	855	PHE
1	B	886	TRP
1	B	954	HIS
1	B	1082	CYS
1	B	1138	TYR
1	A	45	SER

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Mol	Chain	Res	Type
1	A	60	SER
1	A	104	TRP
1	A	133	PHE
1	A	165	ASN
1	A	226	LEU
1	A	269	TYR
1	A	282	ASN
1	A	297	SER
1	A	303	LEU
1	A	338	PHE
1	A	342	PHE
1	A	371	PHE
1	A	383	SER
1	A	388	ASN
1	A	453	TYR
1	A	495	TYR
1	A	501	TYR
1	A	525	CYS
1	A	529	LYS
1	A	540	ASN
1	A	634	ARG
1	A	643	PHE
1	A	657	ASN
1	A	759	PHE
1	A	773	GLU
1	A	900	MET
1	A	947	LYS
1	A	1017	GLU
1	A	1074	ASN
1	A	1138	TYR
1	C	275	PHE
1	C	342	PHE
1	C	349	SER
1	C	357	ARG
1	C	462	LYS
1	C	492	LEU
1	C	525	CYS
1	C	536	ASN
1	C	538	CYS
1	C	633	TRP
1	C	643	PHE
1	C	657	ASN

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Mol	Chain	Res	Type
1	C	759	PHE
1	C	775	ASP
1	C	784	GLN
1	C	820	ASP
1	C	823	PHE
1	C	873	TYR
1	C	900	MET
1	C	960	ASN
1	C	994	ASP
1	C	1104	VAL
1	C	1118	ASP
1	C	1127	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	ASN
1	B	317	ASN
1	B	439	ASN
1	B	774	GLN
1	B	804	GLN
1	B	926	GLN
1	B	955	ASN
1	B	957	GLN
1	B	1005	GLN
1	B	1011	GLN
1	B	1106	GLN
1	A	211	ASN
1	A	354	ASN
1	A	360	ASN
1	A	439	ASN
1	A	544	ASN
1	A	762	GLN
1	A	774	GLN
1	A	787	GLN
1	A	907	ASN
1	A	913	GLN
1	A	914	ASN
1	A	926	GLN
1	A	1010	GLN
1	A	1011	GLN
1	A	1048	HIS

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Mol	Chain	Res	Type
1	A	1135	ASN
1	C	207	HIS
1	C	239	GLN
1	C	339	HIS
1	C	544	ASN
1	C	613	GLN
1	C	710	ASN
1	C	751	ASN
1	C	755	GLN
1	C	762	GLN
1	C	774	GLN
1	C	777	ASN
1	C	872	GLN
1	C	901	GLN
1	C	926	GLN
1	C	1011	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

49 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	C	1305	1	14,14,15	0.49	0	17,19,21	0.43	0
2	NAG	B	1306	1	14,14,15	0.33	0	17,19,21	0.40	0
2	NAG	C	1303	1	14,14,15	0.39	0	17,19,21	0.50	0
2	NAG	A	1316	1	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	A	1305	1	14,14,15	0.40	0	17,19,21	0.39	0
2	NAG	C	1302	1	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	A	1313	1	14,14,15	0.23	0	17,19,21	0.48	0
2	NAG	C	1311	1	14,14,15	0.41	0	17,19,21	0.49	0
2	NAG	C	1316	1	14,14,15	0.23	0	17,19,21	0.45	0
3	IDU	A	1317	-	15,15,17	0.92	1 (6%)	15,22,26	1.17	1 (6%)
2	NAG	B	1315	1	14,14,15	0.21	0	17,19,21	0.47	0
2	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	B	1314	1	14,14,15	0.38	0	17,19,21	0.64	0
2	NAG	B	1304	1	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	C	1313	1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	A	1311	1	14,14,15	0.41	0	17,19,21	0.48	0
2	NAG	C	1312	1	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	C	1306	1	14,14,15	0.32	0	17,19,21	0.43	0
2	NAG	C	1315	1	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.42	0
2	NAG	A	1312	1	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	A	1315	1	14,14,15	0.20	0	17,19,21	0.49	0
2	NAG	B	1316	1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	B	1308	1	14,14,15	0.18	0	17,19,21	0.43	0
2	NAG	A	1314	1	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	C	1314	1	14,14,15	0.24	0	17,19,21	0.51	0
2	NAG	A	1304	1	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	B	1309	1	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	B	1313	1	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	B	1310	1	14,14,15	0.34	0	17,19,21	0.50	0
2	NAG	A	1303	1	14,14,15	0.38	0	17,19,21	0.38	0
2	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	C	1308	1	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	C	1309	1	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	B	1312	1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	B	1303	1	14,14,15	1.03	1 (7%)	17,19,21	1.29	1 (5%)
2	NAG	C	1307	1	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	C	1301	1	14,14,15	0.31	0	17,19,21	0.47	0
2	NAG	C	1304	1	14,14,15	0.24	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1310	1	14,14,15	0.39	0	17,19,21	0.35	0
2	NAG	A	1306	1	14,14,15	0.27	0	17,19,21	0.45	0
2	NAG	B	1302	1	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	B	1311	1	14,14,15	0.39	0	17,19,21	0.41	0
2	NAG	A	1307	1	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.48	0
2	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.42	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	C	1305	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1316	1	-	0/6/23/26	0/1/1/1
3	IDU	A	1317	-	-	4/9/22/29	1/1/1/1
2	NAG	B	1315	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1314	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1315	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1315	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1316	1	-	0/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1303	NAG	O5-C1	3.72	1.49	1.43
3	A	1317	IDU	O6-C6	-2.88	1.21	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1303	NAG	C1-O5-C5	5.07	119.06	112.19
3	A	1317	IDU	O6-C6-C5	2.26	119.49	113.03

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1317	IDU	C1-C2-O2-S
3	A	1317	IDU	C3-C2-O2-S
2	C	1307	NAG	C4-C5-C6-O6
2	B	1307	NAG	C4-C5-C6-O6
2	B	1315	NAG	O5-C5-C6-O6
2	C	1314	NAG	O5-C5-C6-O6
2	B	1304	NAG	O5-C5-C6-O6
2	A	1315	NAG	O5-C5-C6-O6
2	C	1315	NAG	O5-C5-C6-O6
2	A	1307	NAG	C4-C5-C6-O6
2	C	1307	NAG	O5-C5-C6-O6
2	C	1313	NAG	O5-C5-C6-O6
2	A	1308	NAG	C4-C5-C6-O6
2	B	1303	NAG	O5-C5-C6-O6
2	B	1315	NAG	C4-C5-C6-O6
2	B	1307	NAG	O5-C5-C6-O6
2	A	1307	NAG	O5-C5-C6-O6
2	C	1314	NAG	C4-C5-C6-O6
2	B	1306	NAG	O5-C5-C6-O6
2	A	1306	NAG	O5-C5-C6-O6
2	B	1304	NAG	C4-C5-C6-O6
2	C	1315	NAG	C4-C5-C6-O6
2	A	1311	NAG	C8-C7-N2-C2
2	A	1315	NAG	C4-C5-C6-O6
2	A	1306	NAG	C4-C5-C6-O6
2	B	1306	NAG	C4-C5-C6-O6
2	C	1313	NAG	C4-C5-C6-O6
2	B	1305	NAG	C8-C7-N2-C2
2	B	1305	NAG	O7-C7-N2-C2
2	A	1305	NAG	C8-C7-N2-C2
2	A	1305	NAG	O7-C7-N2-C2
2	A	1311	NAG	O7-C7-N2-C2
2	C	1305	NAG	C8-C7-N2-C2
2	C	1305	NAG	O7-C7-N2-C2
2	C	1311	NAG	C8-C7-N2-C2
2	A	1308	NAG	O5-C5-C6-O6
2	C	1304	NAG	O5-C5-C6-O6
2	B	1313	NAG	O5-C5-C6-O6
2	C	1306	NAG	C4-C5-C6-O6
2	C	1304	NAG	C4-C5-C6-O6
2	B	1313	NAG	C4-C5-C6-O6
2	A	1316	NAG	O5-C5-C6-O6
2	B	1303	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	1311	NAG	O7-C7-N2-C2
2	B	1310	NAG	C4-C5-C6-O6
2	A	1316	NAG	C4-C5-C6-O6
2	C	1306	NAG	O5-C5-C6-O6
2	C	1302	NAG	C4-C5-C6-O6
2	A	1311	NAG	O5-C5-C6-O6
2	C	1303	NAG	O5-C5-C6-O6
2	B	1310	NAG	O5-C5-C6-O6
2	C	1309	NAG	C4-C5-C6-O6
2	A	1309	NAG	C4-C5-C6-O6
2	C	1302	NAG	O5-C5-C6-O6
2	A	1309	NAG	O5-C5-C6-O6
2	B	1306	NAG	C1-C2-N2-C7
2	C	1309	NAG	O5-C5-C6-O6
2	B	1305	NAG	C4-C5-C6-O6
3	A	1317	IDU	O5-C5-C6-O61
2	B	1314	NAG	C3-C2-N2-C7
2	A	1314	NAG	C3-C2-N2-C7
2	C	1314	NAG	C3-C2-N2-C7
2	C	1305	NAG	C4-C5-C6-O6
3	A	1317	IDU	C4-C5-C6-O61

All (1) ring outliers are listed below:

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

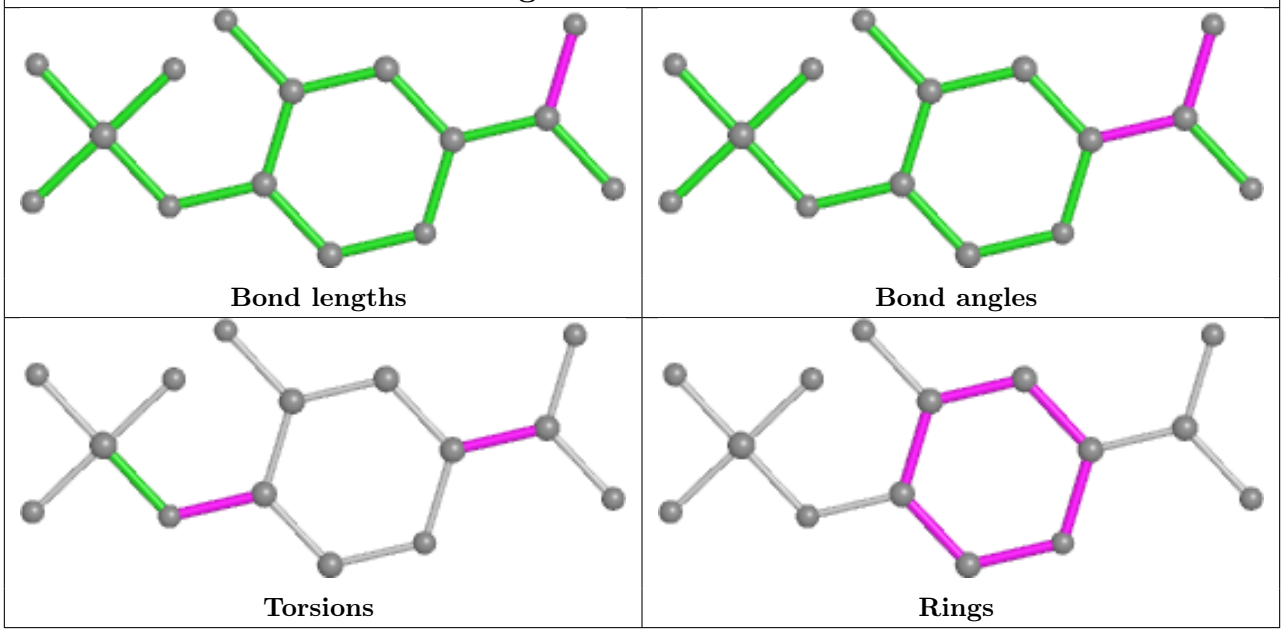
9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1306	NAG	1	0
2	C	1302	NAG	1	0
2	C	1311	NAG	1	0
2	B	1310	NAG	1	0
2	A	1309	NAG	2	0
2	B	1312	NAG	1	0
2	C	1301	NAG	2	0
2	B	1302	NAG	1	0
2	B	1311	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 then 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.

Ligand IDU A 1317



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.