Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 03:04 PM JST

PDB ID	:	8Y4C
EMDB ID	:	EMD-38915
Title	:	BA.2.86 S-trimer in complex with Nab XGv280
Authors	:	Zhu, Q.; Liu, P.
Deposited on	:	2024-01-30
Resolution	:	3.75 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:

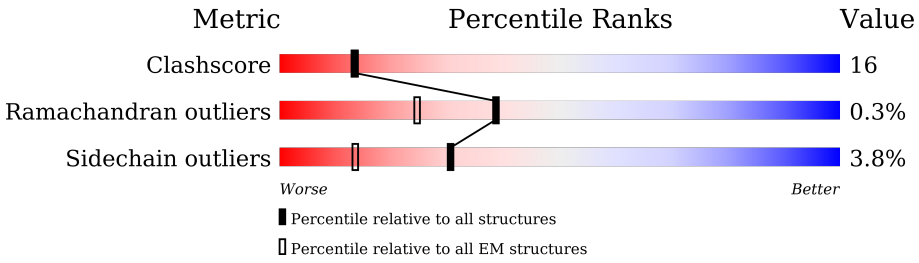
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.75 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1204	60% 26% • 12%
1	B	1204	59% 28% • 12%
1	C	1204	59% 28% • 12%
2	D	126	60% 36% •
2	E	126	58% 38% •
2	H	126	63% 33% •
3	F	111	64% 35% •
3	G	111	62% 37% •
3	L	111	63% 36% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31050 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	A	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
1	B	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
1	C	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		

There are 213 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P0DTC2
A	24	THR	ARG	conflict	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	conflict	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	conflict	UNP P0DTC2
A	216	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
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	conflict	UNP P0DTC2
B	24	THR	ARG	conflict	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	conflict	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	conflict	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
B	339	HIS	GLY	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	376	ALA	THR	conflict	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	conflict	UNP P0DTC2
B	408	SER	ARG	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	446	SER	GLY	conflict	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	conflict	UNP P0DTC2
B	486	PRO	PHE	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	ARG	PRO	conflict	UNP P0DTC2
B	683	ALA	ARG	conflict	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	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	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	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	conflict	UNP P0DTC2
C	24	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	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	conflict	UNP P0DTC2
C	216	PHE	LEU	conflict	UNP P0DTC2
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	conflict	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	376	ALA	THR	conflict	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	conflict	UNP P0DTC2
C	408	SER	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	conflict	UNP P0DTC2
C	486	PRO	PHE	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	ARG	PRO	conflict	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
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	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2

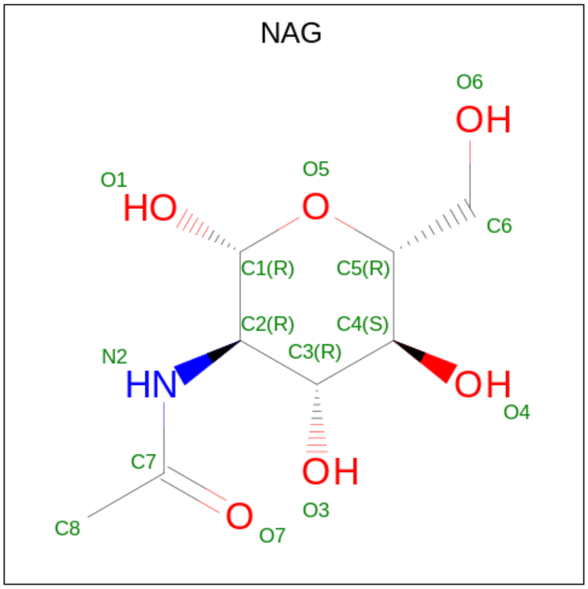
- Molecule 2 is a protein called XGv280 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	126	Total	C	N	O	S	0	0
			969	616	163	188	2		
2	D	126	Total	C	N	O	S	0	0
			969	616	163	188	2		
2	E	126	Total	C	N	O	S	0	0
			969	616	163	188	2		

- Molecule 3 is a protein called XGv280 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	111	Total	C	N	O	S	0	0
			813	505	141	165	2		
3	F	111	Total	C	N	O	S	0	0
			813	505	141	165	2		
3	G	111	Total	C	N	O	S	0	0
			813	505	141	165	2		

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



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

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

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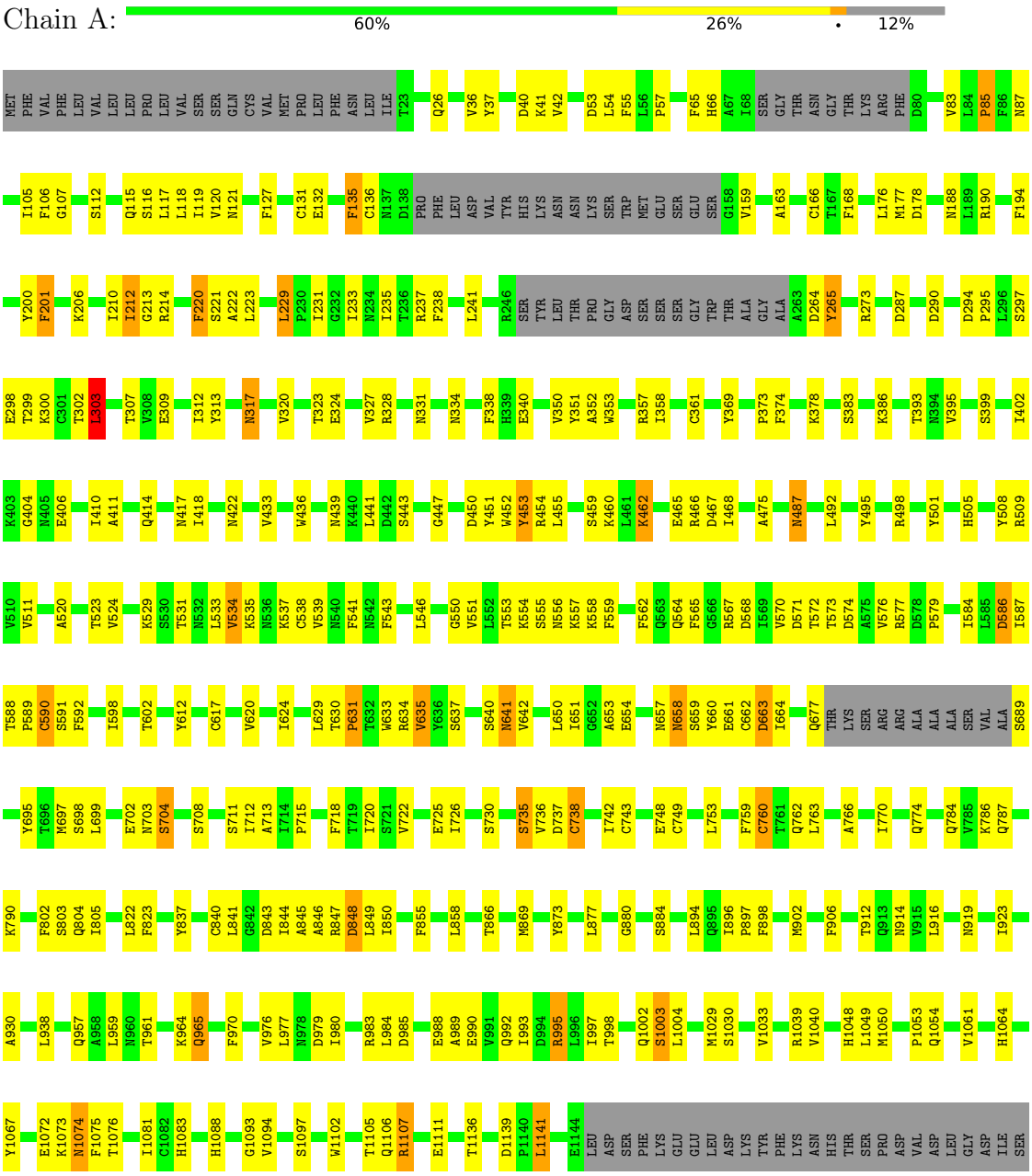
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total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

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.

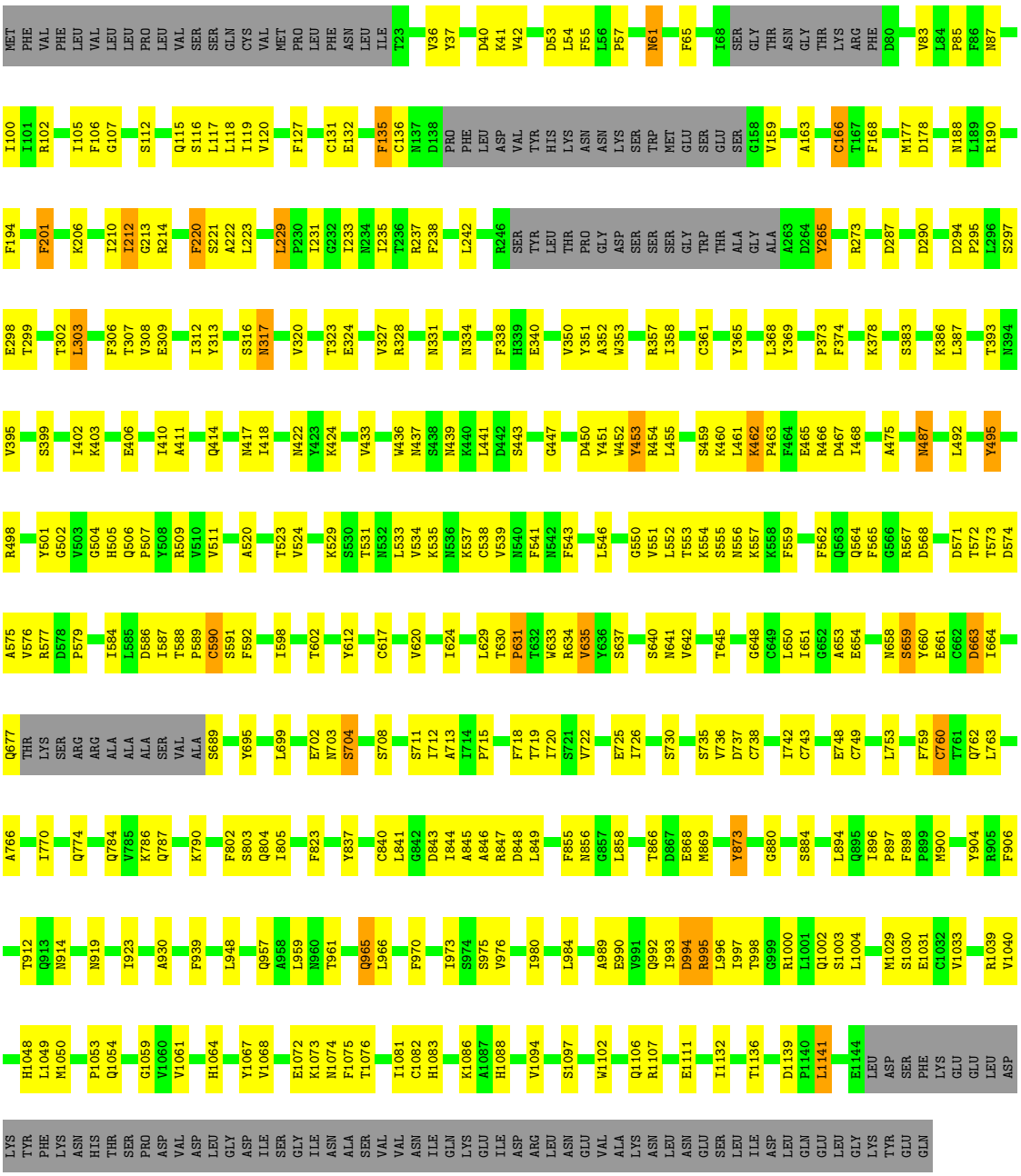
- Molecule 1: Spike glycoprotein

Chain A:



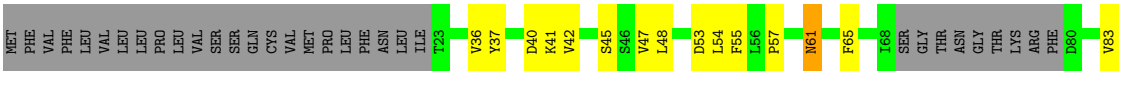
• Molecule 1: Spike glycoprotein

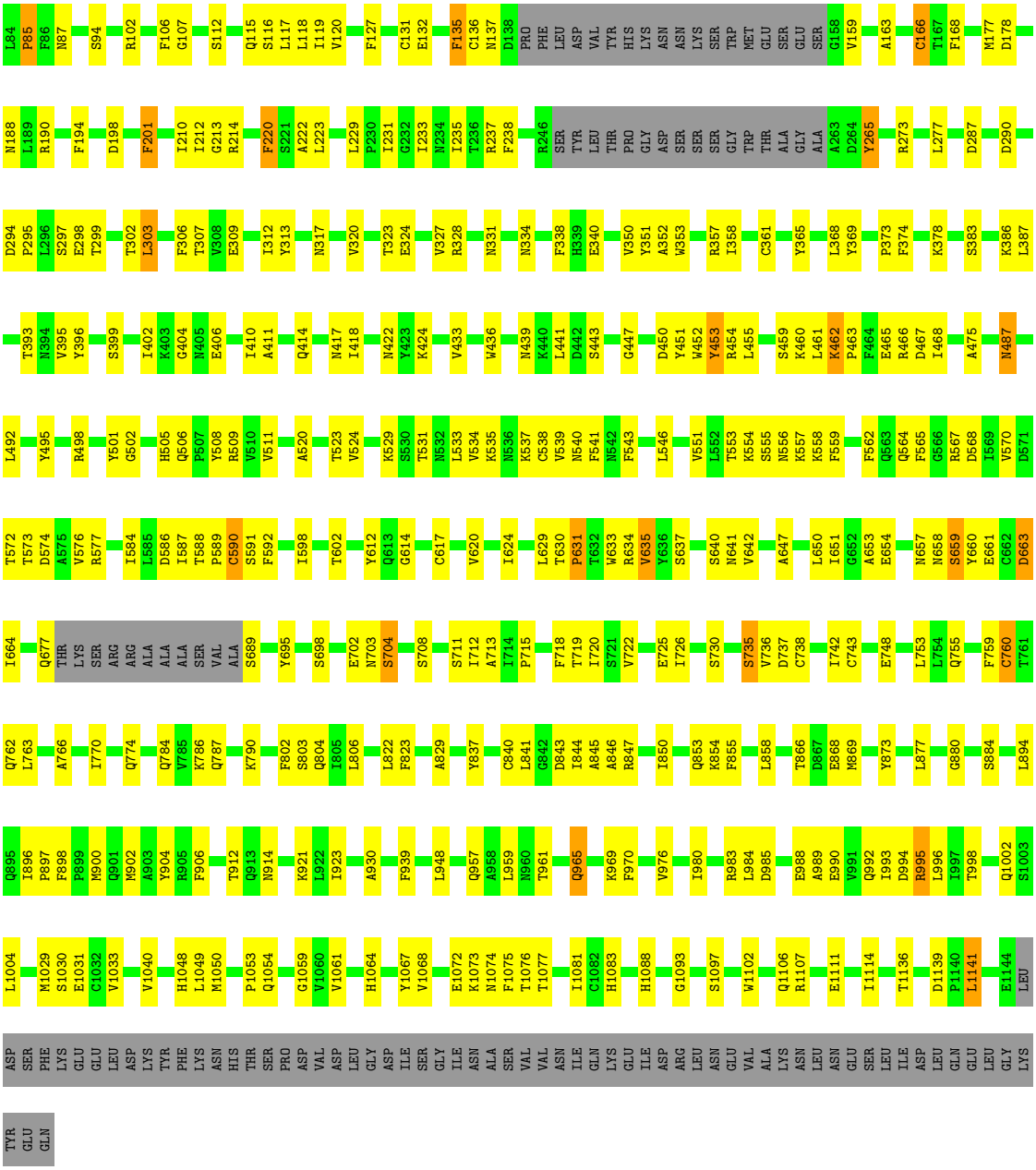
Chain B:



• Molecule 1: Spike glycoprotein

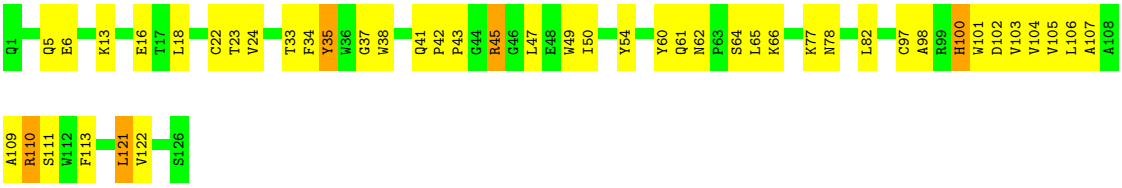
Chain C:





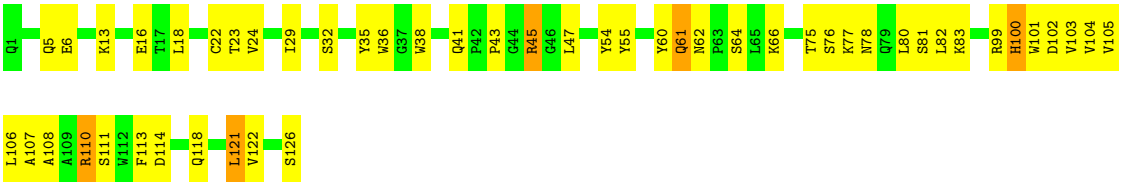
• Molecule 2: XGv280 Heavy chain

Chain H:



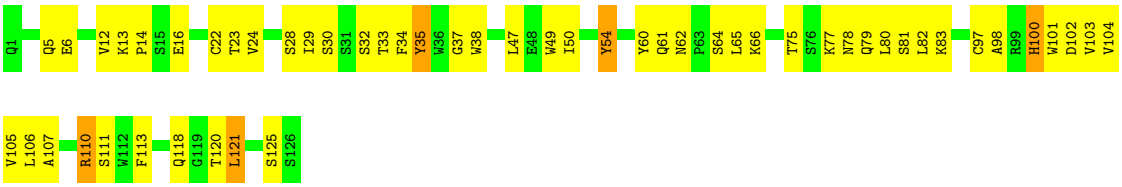
• Molecule 2: XGv280 Heavy chain

Chain D:



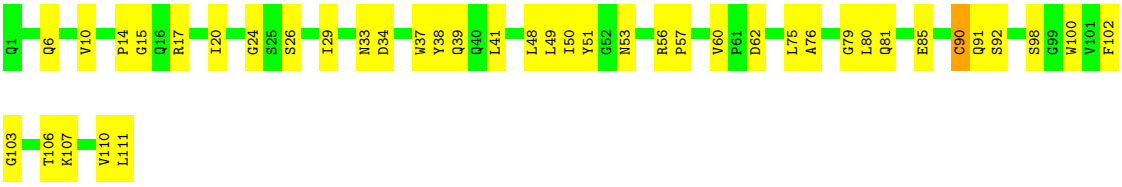
• Molecule 2: XGv280 Heavy chain

Chain E:



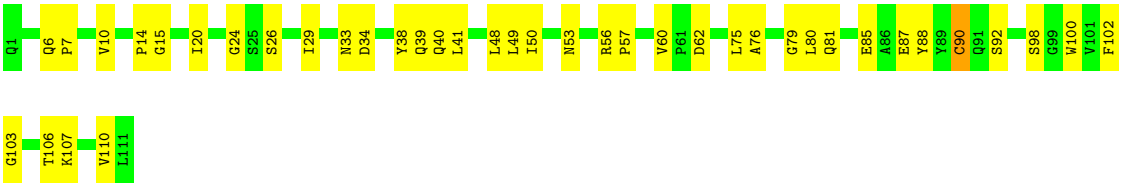
• Molecule 3: XGv280 Light chain

Chain L:



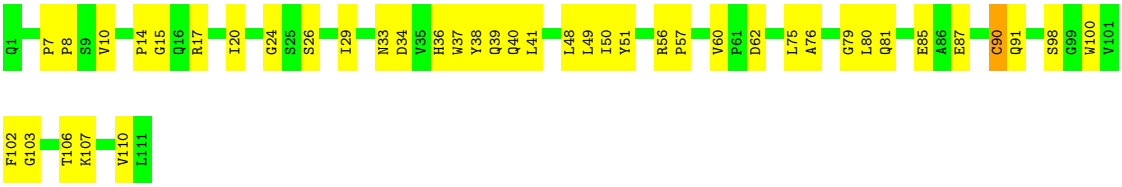
• Molecule 3: XGv280 Light chain

Chain F:



• Molecule 3: XGv280 Light chain

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	60	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0/8516	0.54	3/11591 (0.0%)
1	B	0.34	0/8516	0.54	2/11591 (0.0%)
1	C	0.34	0/8516	0.55	3/11591 (0.0%)
2	D	0.31	0/994	0.60	0/1360
2	E	0.31	0/994	0.61	0/1360
2	H	0.31	0/994	0.60	0/1360
3	F	0.31	0/832	0.51	0/1134
3	G	0.32	0/832	0.53	0/1134
3	L	0.32	0/832	0.53	0/1134
All	All	0.33	0/31026	0.55	8/42255 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	631	PRO	CA-N-CD	-10.88	96.28	111.50
1	B	631	PRO	CA-N-CD	-10.48	96.82	111.50
1	A	631	PRO	CA-N-CD	-9.69	97.93	111.50
1	A	85	PRO	CA-N-CD	-6.28	102.70	111.50
1	C	198	ASP	CB-CG-OD1	5.84	123.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	85	PRO	CA-N-CD	-5.21	104.21	111.50
1	A	303	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	303	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	LEU	Peptide
1	C	303	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8316	0	8100	296	0
1	B	8316	0	8100	304	0
1	C	8316	0	8100	295	0
2	D	969	0	949	43	0
2	E	969	0	949	45	0
2	H	969	0	949	34	0
3	F	813	0	783	27	0
3	G	813	0	783	28	0
3	L	813	0	783	30	0
4	A	252	0	234	1	0
4	B	252	0	234	2	0
4	C	252	0	234	2	0
All	All	31050	0	30198	975	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 16.

All (975) 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:B:856:ASN:HD21	1:B:966:LEU:HD13	1.37	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:CYS:HA	1:B:166:CYS:HB2	1.55	0.86
1:C:131:CYS:HA	1:C:166:CYS:HB2	1.57	0.85
1:C:718:PHE:HB2	1:C:1067:TYR:HE1	1.44	0.82
1:B:718:PHE:HB2	1:B:1067:TYR:HE1	1.44	0.82
1:B:112:SER:HA	1:B:132:GLU:HG2	1.64	0.80
1:A:131:CYS:HA	1:A:166:CYS:HB2	1.65	0.79
1:C:112:SER:HA	1:C:132:GLU:HG2	1.63	0.79
1:C:107:GLY:H	1:C:235:ILE:HG23	1.48	0.79
1:A:844:ILE:HG23	1:C:584:ILE:HG21	1.65	0.78
1:C:383:SER:HB3	1:C:386:LYS:HB2	1.66	0.78
1:A:112:SER:HA	1:A:132:GLU:HG2	1.64	0.77
1:A:383:SER:HB3	1:A:386:LYS:HB2	1.66	0.77
1:A:718:PHE:HB2	1:A:1067:TYR:HE1	1.47	0.77
2:E:6:GLU:N	2:E:6:GLU:OE2	2.18	0.76
1:A:352:ALA:HB2	1:A:468:ILE:HD11	1.67	0.76
3:F:34:ASP:OD1	3:F:53:ASN:ND2	2.19	0.76
1:B:584:ILE:HG21	1:C:844:ILE:HG23	1.68	0.76
1:A:562:PHE:O	1:B:41:LYS:NZ	2.19	0.76
1:A:107:GLY:H	1:A:235:ILE:HG23	1.50	0.75
1:B:352:ALA:HB2	1:B:468:ILE:HD11	1.67	0.75
1:B:383:SER:HB3	1:B:386:LYS:HB2	1.66	0.75
1:B:107:GLY:H	1:B:235:ILE:HG23	1.52	0.75
1:B:562:PHE:O	1:C:41:LYS:NZ	2.19	0.75
1:C:352:ALA:HB2	1:C:468:ILE:HD11	1.67	0.74
2:E:5:GLN:HA	2:E:118:GLN:HE22	1.50	0.74
1:B:802:PHE:O	1:B:804:GLN:N	2.21	0.74
2:E:13:LYS:HE3	2:E:13:LYS:HA	1.70	0.74
2:D:105:VAL:HG23	2:D:106:LEU:HD22	1.70	0.74
1:A:586:ASP:OD2	1:B:844:ILE:N	2.18	0.74
1:C:802:PHE:O	1:C:804:GLN:N	2.21	0.73
1:A:1048:HIS:NE2	1:A:1050:MET:O	2.20	0.73
1:A:970:PHE:O	1:A:995:ARG:NH2	2.22	0.73
1:C:762:GLN:OE1	1:C:762:GLN:N	2.22	0.73
1:B:568:ASP:OD1	1:B:572:THR:OG1	2.04	0.73
1:A:802:PHE:O	1:A:804:GLN:N	2.22	0.72
1:A:65:PHE:HB2	1:A:265:TYR:HB3	1.71	0.72
2:D:5:GLN:HA	2:D:118:GLN:HE22	1.54	0.72
1:C:763:LEU:HD13	1:C:1004:LEU:HD22	1.71	0.72
1:A:210:ILE:O	1:A:213:GLY:N	2.23	0.72
1:B:557:LYS:HG3	1:C:844:ILE:HD13	1.72	0.72
1:B:210:ILE:O	1:B:213:GLY:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:PHE:HE1	1:C:358:ILE:HD13	1.55	0.71
2:D:43:PRO:O	2:D:45:ARG:NH2	2.19	0.71
1:B:970:PHE:O	1:B:995:ARG:NH2	2.22	0.71
1:A:1107:ARG:NH2	1:B:904:TYR:OH	2.23	0.71
1:C:784:GLN:NE2	1:C:1030:SER:OG	2.24	0.71
1:A:784:GLN:NE2	1:A:1030:SER:OG	2.24	0.70
1:A:763:LEU:HD13	1:A:1004:LEU:HD22	1.72	0.70
1:B:533:LEU:HD23	1:B:535:LYS:HE3	1.73	0.70
1:B:763:LEU:HD13	1:B:1004:LEU:HD22	1.72	0.70
1:C:210:ILE:O	1:C:213:GLY:N	2.23	0.70
1:B:338:PHE:HE1	1:B:358:ILE:HD13	1.57	0.70
1:A:565:PHE:HE1	1:A:567:ARG:HH21	1.40	0.70
2:H:105:VAL:HG13	2:H:106:LEU:HD22	1.72	0.69
1:B:462:LYS:HD2	1:B:465:GLU:HB2	1.74	0.69
1:A:41:LYS:NZ	1:C:562:PHE:O	2.20	0.69
1:B:546:LEU:HD22	1:B:565:PHE:HE2	1.56	0.69
1:C:462:LYS:HD2	1:C:465:GLU:HB2	1.74	0.69
1:C:970:PHE:O	1:C:995:ARG:NH2	2.25	0.69
2:E:61:GLN:HE21	2:E:66:LYS:HA	1.58	0.69
1:A:584:ILE:HG21	1:B:844:ILE:HG23	1.74	0.69
4:C:1304:NAG:H2	2:E:105:VAL:HG23	1.75	0.68
1:A:533:LEU:HD23	1:A:535:LYS:HE3	1.74	0.68
1:C:1048:HIS:NE2	1:C:1050:MET:O	2.25	0.68
3:L:34:ASP:OD1	3:L:53:ASN:ND2	2.25	0.68
1:B:565:PHE:HE1	1:B:567:ARG:HH21	1.41	0.68
1:B:1048:HIS:NE2	1:B:1050:MET:O	2.26	0.68
1:C:533:LEU:HD23	1:C:535:LYS:HE3	1.73	0.68
1:B:556:ASN:H	1:C:844:ILE:HD11	1.58	0.68
1:C:914:ASN:ND2	1:C:1111:GLU:OE2	2.26	0.68
1:A:462:LYS:HD2	1:A:465:GLU:HB2	1.74	0.68
1:B:784:GLN:NE2	1:B:1030:SER:OG	2.26	0.67
2:H:101:TRP:HA	2:H:111:SER:HB2	1.76	0.67
1:C:37:TYR:OH	1:C:54:LEU:O	2.11	0.67
1:A:338:PHE:HE1	1:A:358:ILE:HD13	1.58	0.67
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.77	0.67
2:D:111:SER:OG	3:F:100:TRP:NE1	2.28	0.67
2:D:6:GLU:OE1	2:D:6:GLU:N	2.25	0.67
1:A:762:GLN:OE1	1:A:762:GLN:N	2.24	0.67
1:B:1106:GLN:NE2	1:B:1111:GLU:OE1	2.27	0.67
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.77	0.66
1:B:555:SER:HB3	1:C:844:ILE:CG1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:SER:OG	3:G:100:TRP:NE1	2.28	0.66
2:D:62:ASN:ND2	2:D:64:SER:OG	2.28	0.66
1:C:177:MET:O	1:C:190:ARG:NH2	2.28	0.66
1:A:546:LEU:HD22	1:A:565:PHE:HE2	1.61	0.66
1:A:837:TYR:OH	1:C:590:CYS:O	2.09	0.66
1:A:914:ASN:ND2	1:A:1111:GLU:OE2	2.29	0.66
1:A:844:ILE:CG1	1:C:555:SER:HB3	2.25	0.66
2:H:111:SER:OG	3:L:100:TRP:NE1	2.26	0.66
1:A:555:SER:HB3	1:B:844:ILE:CG1	2.26	0.66
1:A:844:ILE:H	1:C:586:ASP:CG	1.99	0.66
1:B:914:ASN:ND2	1:B:1111:GLU:OE2	2.28	0.65
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.77	0.65
1:A:844:ILE:HD13	1:C:557:LYS:HG3	1.78	0.65
1:B:730:SER:HB2	1:B:774:GLN:HB3	1.79	0.65
1:B:586:ASP:HB2	1:C:841:LEU:C	2.17	0.65
1:C:722:VAL:HG12	1:C:930:ALA:HB1	1.79	0.65
1:C:661:GLU:O	1:C:695:TYR:OH	2.14	0.65
1:A:177:MET:O	1:A:190:ARG:NH2	2.30	0.64
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.79	0.64
2:H:62:ASN:ND2	2:H:64:SER:OG	2.30	0.64
1:A:844:ILE:HG21	1:C:557:LYS:HB2	1.78	0.64
1:A:37:TYR:OH	1:A:54:LEU:O	2.11	0.64
1:A:844:ILE:HD11	1:C:556:ASN:H	1.63	0.64
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.16	0.64
1:B:722:VAL:HG12	1:B:930:ALA:HB1	1.78	0.64
1:B:555:SER:HB3	1:C:844:ILE:HG13	1.80	0.64
1:B:661:GLU:O	1:B:695:TYR:OH	2.15	0.64
2:D:22:CYS:HB3	2:D:80:LEU:HB2	1.78	0.64
1:A:722:VAL:HG12	1:A:930:ALA:HB1	1.78	0.64
1:B:866:THR:HG22	1:B:869:MET:HG2	1.77	0.64
1:A:557:LYS:HB2	1:B:844:ILE:HG21	1.80	0.64
1:C:309:GLU:O	1:C:313:TYR:OH	2.12	0.64
1:A:37:TYR:HB3	1:A:223:LEU:HB2	1.80	0.64
1:A:541:PHE:CE2	1:A:587:ILE:HD12	2.33	0.64
1:B:557:LYS:HB2	1:C:844:ILE:HG21	1.79	0.64
1:B:1094:VAL:HG22	1:C:904:TYR:OH	1.97	0.63
1:A:708:SER:HB3	1:A:711:SER:HB3	1.80	0.63
1:B:708:SER:HB3	1:B:711:SER:HB3	1.79	0.63
2:E:16:GLU:N	2:E:16:GLU:OE1	2.32	0.63
2:H:61:GLN:HE21	2:H:66:LYS:HA	1.63	0.63
4:B:1304:NAG:H2	2:D:105:VAL:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:850:ILE:HD12	1:C:850:ILE:H	1.64	0.63
2:D:41:GLN:HG3	2:D:47:LEU:HD23	1.80	0.63
1:A:661:GLU:O	1:A:695:TYR:OH	2.15	0.63
1:C:65:PHE:HB2	1:C:265:TYR:HB3	1.80	0.63
1:C:1093:GLY:HA2	1:C:1107:ARG:HD3	1.81	0.63
2:E:111:SER:HG	3:G:100:TRP:HE1	1.46	0.62
1:A:880:GLY:O	1:A:884:SER:OG	2.16	0.62
1:B:880:GLY:O	1:B:884:SER:OG	2.15	0.62
1:B:37:TYR:OH	1:B:54:LEU:O	2.11	0.62
1:B:586:ASP:CG	1:C:844:ILE:H	2.03	0.62
1:A:590:CYS:O	1:B:837:TYR:OH	2.11	0.62
1:B:177:MET:O	1:B:190:ARG:NH2	2.31	0.62
2:H:50:ILE:HG13	2:H:65:LEU:HD12	1.82	0.62
1:B:309:GLU:O	1:B:313:TYR:OH	2.11	0.61
1:A:1106:GLN:NE2	1:A:1111:GLU:OE1	2.34	0.61
1:A:589:PRO:HG3	1:B:855:PHE:HA	1.81	0.61
1:B:437:ASN:ND2	1:B:439:ASN:OD1	2.33	0.61
3:F:6:GLN:HG2	3:F:7:PRO:HD2	1.83	0.61
1:A:556:ASN:H	1:B:844:ILE:HD11	1.64	0.61
2:E:62:ASN:ND2	2:E:64:SER:OG	2.32	0.61
1:A:557:LYS:HG3	1:B:844:ILE:HD13	1.83	0.61
1:B:298:GLU:HB2	1:B:633:TRP:HZ2	1.66	0.61
1:B:699:LEU:HD21	1:C:869:MET:HB2	1.83	0.61
2:H:111:SER:HG	3:L:100:TRP:HE1	1.45	0.61
1:A:586:ASP:HB2	1:B:841:LEU:C	2.21	0.60
3:L:20:ILE:HD12	3:L:106:THR:HG21	1.82	0.60
2:H:16:GLU:N	2:H:16:GLU:OE1	2.34	0.60
1:B:588:THR:OG1	1:C:841:LEU:HB3	2.01	0.60
2:E:47:LEU:HD12	2:E:47:LEU:H	1.66	0.60
1:A:553:THR:OG1	1:A:554:LYS:N	2.33	0.60
1:C:912:THR:OG1	1:C:914:ASN:OD1	2.18	0.60
3:G:39:GLN:HE22	3:G:41:LEU:HG	1.66	0.60
1:B:843:ASP:O	1:B:845:ALA:N	2.32	0.60
1:C:298:GLU:HB2	1:C:633:TRP:HZ2	1.66	0.60
1:B:590:CYS:O	1:C:837:TYR:OH	2.10	0.60
1:C:657:ASN:O	1:C:658:ASN:ND2	2.34	0.60
1:B:586:ASP:OD2	1:C:844:ILE:N	2.32	0.60
1:B:912:THR:OG1	1:B:914:ASN:OD1	2.20	0.60
1:B:770:ILE:O	1:B:774:GLN:NE2	2.34	0.60
1:C:880:GLY:O	1:C:884:SER:OG	2.16	0.60
1:A:237:ARG:NH1	2:H:35:TYR:OH	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:HB2	1:A:633:TRP:HZ2	1.66	0.60
1:A:557:LYS:HD2	1:B:844:ILE:HB	1.84	0.59
2:H:61:GLN:NE2	2:H:66:LYS:HA	2.18	0.59
1:B:567:ARG:HG3	1:B:568:ASP:H	1.67	0.59
2:D:100:HIS:HB3	2:D:113:PHE:HA	1.84	0.59
2:D:16:GLU:OE1	2:D:16:GLU:N	2.35	0.59
1:C:1106:GLN:NE2	1:C:1111:GLU:OE1	2.36	0.59
1:C:843:ASP:O	1:C:845:ALA:N	2.34	0.58
1:A:617:CYS:HA	1:A:620:VAL:HG12	1.85	0.58
1:A:567:ARG:NH1	1:A:571:ASP:OD1	2.36	0.58
1:B:589:PRO:HG3	1:C:855:PHE:HA	1.85	0.58
1:C:617:CYS:HA	1:C:620:VAL:HG12	1.84	0.58
3:G:107:LYS:HE3	3:G:107:LYS:HA	1.85	0.58
1:B:629:LEU:HG	1:B:634:ARG:HB3	1.85	0.58
1:A:1075:PHE:O	1:A:1076:THR:OG1	2.21	0.58
2:E:100:HIS:HB3	2:E:113:PHE:HA	1.86	0.58
2:H:38:TRP:NE1	2:H:82:LEU:HB2	2.19	0.58
1:A:718:PHE:HB2	1:A:1067:TYR:CE1	2.34	0.57
2:H:100:HIS:HB3	2:H:113:PHE:HA	1.86	0.57
1:A:574:ASP:CG	1:B:847:ARG:HG3	2.25	0.57
1:B:1075:PHE:O	1:B:1076:THR:OG1	2.21	0.57
1:A:844:ILE:HG12	1:C:555:SER:HB3	1.86	0.57
1:B:848:ASP:OD1	1:B:848:ASP:N	2.34	0.57
2:E:24:VAL:O	2:E:78:ASN:ND2	2.37	0.57
1:A:841:LEU:C	1:C:586:ASP:HB2	2.24	0.57
1:B:116:SER:OG	1:B:117:LEU:N	2.36	0.57
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.87	0.57
1:C:718:PHE:HB2	1:C:1067:TYR:CE1	2.34	0.57
1:A:309:GLU:O	1:A:313:TYR:OH	2.12	0.57
1:A:327:VAL:O	1:A:531:THR:OG1	2.17	0.57
2:D:111:SER:HG	3:F:100:TRP:HE1	1.50	0.57
1:C:677:GLN:N	1:C:689:SER:O	2.36	0.57
2:E:6:GLU:HA	2:E:22:CYS:HA	1.85	0.57
1:A:135:PHE:HD1	1:A:136:CYS:N	2.03	0.57
1:A:116:SER:OG	1:A:117:LEU:N	2.37	0.56
1:A:565:PHE:HD1	1:B:42:VAL:HG12	1.69	0.56
1:C:116:SER:OG	1:C:117:LEU:N	2.36	0.56
1:A:617:CYS:HB3	1:A:642:VAL:HG12	1.87	0.56
1:A:844:ILE:HB	1:C:557:LYS:HD2	1.87	0.56
1:B:131:CYS:HA	1:B:166:CYS:CB	2.33	0.56
1:B:919:ASN:O	1:B:923:ILE:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:PHE:HD2	1:C:287:ASP:HA	1.70	0.56
1:A:629:LEU:HG	1:A:634:ARG:HB3	1.88	0.56
1:A:742:ILE:HD11	1:A:753:LEU:HD22	1.87	0.56
1:B:402:ILE:HD13	1:B:410:ILE:HD11	1.88	0.56
1:B:965:GLN:HE22	1:B:1000:ARG:HA	1.71	0.56
3:G:20:ILE:HD12	3:G:106:THR:HG21	1.86	0.56
2:H:5:GLN:O	2:H:23:THR:N	2.37	0.56
3:L:39:GLN:HE22	3:L:41:LEU:HG	1.69	0.56
1:B:327:VAL:O	1:B:531:THR:OG1	2.18	0.56
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.46	0.56
1:A:847:ARG:HG3	1:C:574:ASP:CG	2.26	0.56
1:C:730:SER:HB2	1:C:774:GLN:HB3	1.88	0.56
1:A:1093:GLY:HA2	1:A:1107:ARG:NE	2.21	0.56
1:A:131:CYS:HA	1:A:166:CYS:CB	2.34	0.56
1:A:964:LYS:HD3	1:C:570:VAL:HG23	1.87	0.56
1:B:135:PHE:HD1	1:B:136:CYS:N	2.03	0.56
2:D:6:GLU:HA	2:D:22:CYS:HA	1.88	0.56
1:B:557:LYS:HD2	1:C:844:ILE:HB	1.87	0.55
1:B:574:ASP:CG	1:C:847:ARG:HG3	2.26	0.55
1:A:26:GLN:HG2	2:H:66:LYS:HD3	1.89	0.55
1:A:970:PHE:HB2	1:A:995:ARG:HH12	1.70	0.55
3:F:39:GLN:HE22	3:F:41:LEU:HG	1.71	0.55
1:C:541:PHE:CE2	1:C:587:ILE:HD12	2.40	0.55
1:A:760:CYS:HA	1:A:763:LEU:HD12	1.89	0.55
1:B:565:PHE:HD1	1:C:42:VAL:HG12	1.70	0.55
1:C:629:LEU:HG	1:C:634:ARG:HB3	1.88	0.55
3:G:29:ILE:HG13	3:G:33:ASN:HB2	1.87	0.55
1:A:178:ASP:N	1:A:178:ASP:OD1	2.38	0.55
1:B:718:PHE:HB2	1:B:1067:TYR:CE1	2.35	0.55
2:D:24:VAL:O	2:D:78:ASN:ND2	2.40	0.55
1:C:135:PHE:HD1	1:C:136:CYS:N	2.05	0.55
1:C:439:ASN:O	1:C:443:SER:OG	2.24	0.55
1:C:708:SER:HB3	1:C:711:SER:HB3	1.87	0.55
1:C:760:CYS:HA	1:C:763:LEU:HD12	1.89	0.55
1:A:588:THR:HG23	1:B:840:CYS:HB2	1.87	0.55
1:A:677:GLN:N	1:A:689:SER:O	2.36	0.55
1:A:841:LEU:O	1:C:553:THR:HG22	2.06	0.55
1:A:641:ASN:OD1	1:A:642:VAL:HG13	2.06	0.55
1:C:422:ASN:ND2	1:C:454:ARG:O	2.36	0.55
1:C:178:ASP:N	1:C:178:ASP:OD1	2.39	0.54
1:A:634:ARG:NH1	3:L:26:SER:OG	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:VAL:O	2:H:78:ASN:ND2	2.40	0.54
1:C:220:PHE:CD2	1:C:287:ASP:HA	2.42	0.54
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.36	0.54
1:B:1081:ILE:O	1:B:1088:HIS:N	2.38	0.54
2:D:5:GLN:O	2:D:23:THR:N	2.36	0.54
1:A:439:ASN:O	1:A:443:SER:OG	2.24	0.54
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.39	0.54
1:B:546:LEU:HD22	1:B:565:PHE:CE2	2.40	0.54
1:B:553:THR:HG22	1:C:841:LEU:HD12	1.90	0.54
1:C:1075:PHE:O	1:C:1076:THR:OG1	2.20	0.54
2:E:38:TRP:CD1	2:E:82:LEU:HB2	2.42	0.54
1:B:961:THR:HB	1:C:762:GLN:HE21	1.72	0.54
1:C:634:ARG:NH1	3:G:26:SER:OG	2.40	0.54
1:A:553:THR:HG22	1:B:841:LEU:HD12	1.90	0.54
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.36	0.54
2:E:5:GLN:O	2:E:23:THR:N	2.38	0.54
1:A:87:ASN:OD1	1:A:87:ASN:N	2.41	0.53
1:A:844:ILE:CG2	1:C:557:LYS:HB2	2.39	0.53
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.89	0.53
1:B:307:THR:HA	1:B:602:THR:HG21	1.90	0.53
1:B:557:LYS:HB2	1:C:844:ILE:CG2	2.38	0.53
1:C:629:LEU:O	1:C:634:ARG:NH1	2.36	0.53
1:B:303:LEU:HD23	1:B:303:LEU:O	2.09	0.53
1:B:538:CYS:HA	1:B:551:VAL:HG22	1.90	0.53
2:D:32:SER:O	2:D:54:TYR:OH	2.22	0.53
1:C:131:CYS:HA	1:C:166:CYS:CB	2.34	0.53
1:B:422:ASN:ND2	1:B:454:ARG:O	2.36	0.53
1:B:712:ILE:HD13	1:C:896:ILE:HD12	1.90	0.53
1:B:441:LEU:HD22	1:B:509:ARG:HH12	1.72	0.53
1:B:475:ALA:O	1:B:487:ASN:ND2	2.42	0.53
1:B:677:GLN:N	1:B:689:SER:O	2.36	0.53
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.90	0.53
1:C:538:CYS:HA	1:C:551:VAL:HG22	1.90	0.53
2:D:107:ALA:HB3	2:D:110:ARG:HH21	1.71	0.53
1:A:843:ASP:O	1:A:845:ALA:N	2.36	0.53
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.38	0.53
2:D:13:LYS:NZ	2:D:126:SER:O	2.39	0.53
2:E:107:ALA:HB3	2:E:110:ARG:HH21	1.74	0.53
1:A:546:LEU:HD22	1:A:565:PHE:CE2	2.42	0.53
1:B:65:PHE:HB2	1:B:265:TYR:HB3	1.91	0.53
1:B:220:PHE:CD2	1:B:287:ASP:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:40:GLN:HB3	3:F:87:GLU:HB3	1.91	0.53
1:A:303:LEU:O	1:A:303:LEU:HD23	2.09	0.52
1:A:538:CYS:HA	1:A:551:VAL:HG22	1.90	0.52
1:A:116:SER:N	1:A:131:CYS:O	2.33	0.52
1:A:568:ASP:OD1	1:A:572:THR:N	2.37	0.52
1:C:866:THR:HG22	1:C:869:MET:HG2	1.91	0.52
1:A:441:LEU:HD22	1:A:509:ARG:HH12	1.75	0.52
1:C:475:ALA:O	1:C:487:ASN:ND2	2.42	0.52
2:H:41:GLN:HG3	2:H:47:LEU:HD23	1.91	0.52
1:B:659:SER:O	1:B:659:SER:OG	2.24	0.52
1:C:568:ASP:OD1	1:C:572:THR:N	2.40	0.52
1:A:399:SER:HB3	1:A:511:VAL:HG22	1.92	0.52
3:F:15:GLY:N	3:F:80:LEU:O	2.37	0.52
1:C:85:PRO:HG3	2:E:60:TYR:CE1	2.44	0.52
1:C:965:GLN:HE21	1:C:965:GLN:HA	1.74	0.52
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.91	0.52
1:A:402:ILE:HD13	1:A:410:ILE:HD11	1.91	0.52
1:B:634:ARG:NH1	3:F:26:SER:OG	2.42	0.52
1:A:220:PHE:CD2	1:A:287:ASP:HA	2.45	0.52
1:A:475:ALA:O	1:A:487:ASN:ND2	2.42	0.52
1:A:980:ILE:HD11	1:A:992:GLN:HB2	1.92	0.52
1:B:87:ASN:N	1:B:87:ASN:OD1	2.41	0.52
1:B:399:SER:HB3	1:B:511:VAL:HG22	1.91	0.52
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.91	0.52
1:C:980:ILE:HD11	1:C:992:GLN:HB2	1.92	0.52
1:C:998:THR:O	1:C:1002:GLN:HG2	2.08	0.52
1:A:866:THR:HG22	1:A:869:MET:HG2	1.90	0.52
1:C:299:THR:HA	1:C:302:THR:HG22	1.92	0.52
1:C:402:ILE:HD13	1:C:410:ILE:HD11	1.92	0.52
1:C:1081:ILE:O	1:C:1088:HIS:N	2.40	0.52
1:B:760:CYS:HA	1:B:763:LEU:HD12	1.92	0.52
1:C:399:SER:HB3	1:C:511:VAL:HG22	1.92	0.52
1:C:441:LEU:HD22	1:C:509:ARG:HH12	1.74	0.52
1:C:742:ILE:HD11	1:C:753:LEU:HD22	1.92	0.52
2:E:101:TRP:HA	2:E:111:SER:HB2	1.92	0.52
1:A:1081:ILE:O	1:A:1088:HIS:N	2.38	0.52
2:H:38:TRP:CZ3	2:H:97:CYS:HB3	2.45	0.52
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.41	0.52
1:C:829:ALA:O	1:C:850:ILE:HD11	2.10	0.52
1:A:422:ASN:ND2	1:A:454:ARG:O	2.36	0.51
1:A:567:ARG:HG3	1:A:568:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:SER:HB2	1:A:774:GLN:HB3	1.91	0.51
1:B:454:ARG:NH1	1:B:467:ASP:O	2.43	0.51
1:C:87:ASN:OD1	1:C:87:ASN:N	2.42	0.51
1:C:1083:HIS:CD2	1:C:1136:THR:HA	2.46	0.51
1:B:976:VAL:O	1:B:980:ILE:HG22	2.11	0.51
1:C:501:TYR:HB3	1:C:505:HIS:HB3	1.92	0.51
1:A:983:ARG:HH22	1:A:984:LEU:HD22	1.75	0.51
1:B:897:PRO:HG2	1:B:900:MET:SD	2.50	0.51
2:D:104:VAL:HG13	2:D:105:VAL:HG22	1.92	0.51
1:C:546:LEU:HD22	1:C:565:PHE:CE1	2.46	0.51
1:A:210:ILE:HG22	1:A:214:ARG:HH12	1.76	0.51
1:A:637:SER:HB3	1:A:641:ASN:CG	2.30	0.51
2:H:121:LEU:HD12	2:H:121:LEU:H	1.76	0.51
1:B:439:ASN:O	1:B:443:SER:OG	2.27	0.51
1:B:501:TYR:HB3	1:B:505:HIS:HB3	1.92	0.51
1:C:976:VAL:O	1:C:980:ILE:HG22	2.11	0.51
1:C:983:ARG:HH22	1:C:984:LEU:HD22	1.76	0.51
1:B:36:VAL:HG13	1:B:55:PHE:HE2	1.75	0.51
1:B:83:VAL:HG11	1:B:237:ARG:CZ	2.41	0.51
1:C:327:VAL:O	1:C:531:THR:OG1	2.18	0.51
2:E:61:GLN:NE2	2:E:66:LYS:HA	2.24	0.51
1:A:454:ARG:NH1	1:A:467:ASP:O	2.44	0.51
1:B:551:VAL:HB	1:C:841:LEU:HD22	1.93	0.51
1:A:83:VAL:HG11	1:A:237:ARG:CZ	2.40	0.51
1:C:36:VAL:HG13	1:C:55:PHE:HE2	1.76	0.51
1:A:501:TYR:HB3	1:A:505:HIS:HB3	1.92	0.51
1:B:210:ILE:HG22	1:B:214:ARG:HH12	1.76	0.51
1:B:573:THR:O	1:C:847:ARG:NH2	2.38	0.51
1:C:541:PHE:CZ	1:C:587:ILE:HD12	2.46	0.51
1:A:557:LYS:HB2	1:B:844:ILE:CG2	2.41	0.51
1:B:299:THR:HA	1:B:302:THR:HG22	1.93	0.51
1:B:629:LEU:O	1:B:634:ARG:NH1	2.37	0.51
1:C:735:SER:O	1:C:735:SER:OG	2.25	0.51
1:A:553:THR:HG22	1:B:841:LEU:O	2.11	0.51
1:A:844:ILE:N	1:C:586:ASP:OD1	2.40	0.51
3:L:85:GLU:HB2	3:L:110:VAL:HG23	1.93	0.51
1:B:220:PHE:HD2	1:B:287:ASP:HA	1.75	0.51
3:G:85:GLU:HB2	3:G:110:VAL:HG23	1.92	0.51
1:C:194:PHE:HB3	1:C:201:PHE:HE1	1.76	0.50
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.35	0.50
3:F:90:CYS:O	3:F:103:GLY:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:VAL:HG11	1:C:237:ARG:CZ	2.41	0.50
1:C:543:PHE:HB3	1:C:576:VAL:HG11	1.94	0.50
1:B:629:LEU:HD23	1:B:634:ARG:HD2	1.92	0.50
1:A:299:THR:HA	1:A:302:THR:HG22	1.93	0.50
1:A:713:ALA:HB2	1:A:1074:ASN:HB3	1.94	0.50
1:C:454:ARG:NH1	1:C:467:ASP:O	2.45	0.50
1:A:323:THR:OG1	1:A:324:GLU:N	2.44	0.50
1:A:555:SER:HB3	1:B:844:ILE:HG12	1.93	0.50
1:B:178:ASP:OD1	1:B:178:ASP:N	2.38	0.50
1:B:980:ILE:HD11	1:B:992:GLN:HB2	1.92	0.50
1:A:36:VAL:HG13	1:A:55:PHE:HE2	1.77	0.50
1:A:85:PRO:HG3	2:H:60:TYR:CE1	2.46	0.50
1:C:307:THR:HA	1:C:602:THR:HG21	1.93	0.50
1:A:629:LEU:HD23	1:A:634:ARG:HD2	1.93	0.50
1:A:1083:HIS:CD2	1:A:1136:THR:HA	2.46	0.50
3:L:17:ARG:HH22	3:L:76:ALA:HB1	1.76	0.50
1:B:617:CYS:HB3	1:B:642:VAL:HG12	1.93	0.50
1:B:637:SER:HB3	1:B:641:ASN:CG	2.32	0.50
1:C:629:LEU:HD23	1:C:634:ARG:HD2	1.93	0.50
1:A:660:TYR:HB2	1:A:695:TYR:CZ	2.47	0.50
1:A:965:GLN:NE2	1:A:1003:SER:HB2	2.27	0.50
1:A:976:VAL:O	1:A:980:ILE:HG22	2.11	0.50
3:L:79:GLY:O	3:L:81:GLN:NE2	2.44	0.50
2:E:102:ASP:HB3	2:E:106:LEU:HD23	1.92	0.50
1:A:220:PHE:HD2	1:A:287:ASP:HA	1.76	0.50
1:C:40:ASP:OD1	1:C:42:VAL:HG22	2.12	0.50
1:C:402:ILE:HD11	1:C:418:ILE:HG21	1.94	0.50
1:A:402:ILE:HD11	1:A:418:ILE:HG21	1.93	0.49
1:B:40:ASP:OD1	1:B:42:VAL:HG22	2.12	0.49
1:C:194:PHE:HB3	1:C:201:PHE:CE1	2.47	0.49
1:A:136:CYS:HB2	1:A:159:VAL:O	2.12	0.49
1:B:523:THR:HG22	1:B:524:VAL:HG23	1.95	0.49
1:B:660:TYR:HB2	1:B:695:TYR:CZ	2.48	0.49
2:D:61:GLN:HE21	2:D:66:LYS:HA	1.77	0.49
1:C:897:PRO:HG2	1:C:900:MET:SD	2.51	0.49
1:B:136:CYS:HB2	1:B:159:VAL:O	2.12	0.49
1:A:896:ILE:HD12	1:C:712:ILE:HD13	1.94	0.49
1:C:637:SER:HB3	1:C:641:ASN:CG	2.32	0.49
2:E:81:SER:HB3	2:E:83:LYS:HZ1	1.77	0.49
1:B:115:GLN:HG2	1:B:233:ILE:HG21	1.95	0.49
1:B:984:LEU:HB3	1:B:989:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:THR:OG1	1:B:324:GLU:N	2.45	0.49
1:A:573:THR:O	1:B:847:ARG:NH2	2.37	0.49
1:B:742:ILE:HG13	1:B:743:CYS:SG	2.53	0.49
1:B:402:ILE:HD11	1:B:418:ILE:HG21	1.94	0.49
2:E:6:GLU:HG2	2:E:120:THR:HG23	1.94	0.49
1:B:1083:HIS:CD2	1:B:1136:THR:HA	2.48	0.49
2:E:22:CYS:HB3	2:E:80:LEU:HB2	1.95	0.49
1:A:351:TYR:CE1	1:A:452:TRP:HB2	2.48	0.49
1:C:210:ILE:HG22	1:C:214:ARG:HH12	1.78	0.49
2:E:61:GLN:HE22	2:E:66:LYS:HG3	1.78	0.48
1:A:630:THR:HB	1:A:631:PRO:HD2	1.95	0.48
1:C:323:THR:OG1	1:C:324:GLU:N	2.46	0.48
3:G:17:ARG:HH22	3:G:76:ALA:HB1	1.77	0.48
2:H:47:LEU:HB2	3:L:102:PHE:CG	2.49	0.48
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.96	0.48
1:B:541:PHE:CE2	1:B:587:ILE:HD12	2.48	0.48
1:C:748:GLU:CD	1:C:748:GLU:H	2.15	0.48
1:B:567:ARG:HG3	1:B:568:ASP:N	2.28	0.48
2:E:121:LEU:HD12	2:E:121:LEU:H	1.78	0.48
1:A:117:LEU:HD21	1:A:119:ILE:HD11	1.96	0.48
1:A:369:TYR:HA	1:A:374:PHE:CZ	2.48	0.48
1:C:502:GLY:O	1:C:506:GLN:NE2	2.47	0.48
1:C:617:CYS:HB3	1:C:642:VAL:HG12	1.94	0.48
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.96	0.48
1:A:450:ASP:OD1	1:A:450:ASP:N	2.47	0.48
1:A:459:SER:OG	1:A:460:LYS:N	2.47	0.48
1:A:1094:VAL:HG23	1:A:1107:ARG:NH2	2.29	0.48
1:A:523:THR:HG22	1:A:524:VAL:HG23	1.96	0.48
1:B:748:GLU:CD	1:B:748:GLU:H	2.16	0.48
1:B:1139:ASP:OD1	1:B:1141:LEU:HD12	2.13	0.48
1:C:117:LEU:HD21	1:C:119:ILE:HD11	1.95	0.48
1:A:742:ILE:HG13	1:A:743:CYS:SG	2.54	0.48
1:A:748:GLU:H	1:A:748:GLU:CD	2.16	0.48
1:A:1107:ARG:NE	1:A:1107:ARG:HA	2.29	0.48
1:B:57:PRO:HB3	1:B:273:ARG:NH1	2.29	0.48
1:B:351:TYR:CE1	1:B:452:TRP:HB2	2.48	0.48
1:B:630:THR:HB	1:B:631:PRO:HD2	1.96	0.48
2:D:121:LEU:HD12	2:D:121:LEU:H	1.79	0.48
1:C:136:CYS:HB2	1:C:159:VAL:O	2.14	0.48
1:C:369:TYR:HA	1:C:374:PHE:CZ	2.49	0.48
2:D:99:ARG:HH21	2:D:114:ASP:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:85:GLU:HB2	3:F:110:VAL:HG23	1.96	0.48
1:C:350:VAL:HG22	1:C:422:ASN:HB3	1.96	0.48
1:C:1139:ASP:OD1	1:C:1141:LEU:HD12	2.13	0.48
1:A:897:PRO:HG3	1:C:1077:THR:HG21	1.96	0.48
1:B:450:ASP:OD1	1:B:450:ASP:N	2.46	0.48
1:B:459:SER:OG	1:B:460:LYS:N	2.47	0.48
1:B:654:GLU:OE1	1:B:654:GLU:N	2.47	0.48
1:C:340:GLU:OE1	1:C:340:GLU:N	2.46	0.48
1:A:340:GLU:OE1	1:A:340:GLU:N	2.47	0.47
1:A:965:GLN:HE21	1:A:1003:SER:HB2	1.79	0.47
1:B:957:GLN:O	1:B:961:THR:HG23	2.14	0.47
3:F:10:VAL:HG11	3:F:20:ILE:HD11	1.96	0.47
3:F:79:GLY:O	3:F:81:GLN:NE2	2.47	0.47
1:C:118:LEU:HG	1:C:120:VAL:HG12	1.96	0.47
2:E:77:LYS:HG3	2:E:79:GLN:HB2	1.95	0.47
1:A:194:PHE:HB3	1:A:201:PHE:CE1	2.49	0.47
1:A:307:THR:HA	1:A:602:THR:HG21	1.96	0.47
1:A:985:ASP:OD1	1:A:988:GLU:HB3	2.13	0.47
2:D:35:TYR:CD1	2:D:101:TRP:CD1	3.01	0.47
1:A:40:ASP:OD1	1:A:42:VAL:HG22	2.14	0.47
1:A:406:GLU:HG2	1:A:418:ILE:HG13	1.96	0.47
2:D:36:TRP:HB3	2:D:80:LEU:HD21	1.96	0.47
2:D:102:ASP:OD1	2:D:103:VAL:N	2.47	0.47
3:F:57:PRO:HD2	3:F:60:VAL:HG21	1.96	0.47
1:C:116:SER:N	1:C:131:CYS:O	2.34	0.47
2:E:37:GLY:N	2:E:98:ALA:O	2.40	0.47
2:E:102:ASP:OD1	2:E:104:VAL:HG12	2.15	0.47
1:A:766:ALA:O	1:A:770:ILE:HG23	2.15	0.47
1:A:998:THR:O	1:A:1002:GLN:HG2	2.15	0.47
3:L:91:GLN:HB2	3:L:102:PHE:CD1	2.49	0.47
1:B:543:PHE:HB3	1:B:576:VAL:HG11	1.96	0.47
1:C:57:PRO:HB3	1:C:273:ARG:NH1	2.29	0.47
1:C:331:ASN:HD22	4:C:1307:NAG:C7	2.27	0.47
1:C:902:MET:HE2	1:C:902:MET:HA	1.96	0.47
3:G:39:GLN:HB2	3:G:49:LEU:HD11	1.95	0.47
1:A:588:THR:OG1	1:B:841:LEU:HB3	2.14	0.47
1:B:447:GLY:HA2	1:B:498:ARG:HG2	1.95	0.47
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.79	0.47
1:B:1040:VAL:HG13	1:C:1030:SER:O	2.15	0.47
1:C:985:ASP:OD1	1:C:988:GLU:HB3	2.14	0.47
3:G:79:GLY:O	3:G:81:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PRO:HB3	1:A:273:ARG:NH1	2.30	0.47
1:A:331:ASN:HD22	4:A:1307:NAG:C7	2.27	0.47
1:A:846:ALA:HA	1:C:567:ARG:O	2.14	0.47
1:A:1107:ARG:HA	1:A:1107:ARG:HE	1.80	0.47
1:C:766:ALA:O	1:C:770:ILE:HG23	2.15	0.47
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.50	0.47
1:B:222:ALA:O	1:B:223:LEU:HD22	2.15	0.47
1:B:331:ASN:HD22	4:B:1307:NAG:C7	2.27	0.47
1:B:735:SER:O	1:B:735:SER:OG	2.26	0.47
1:C:135:PHE:HE1	1:C:137:ASN:HB2	1.79	0.47
1:C:229:LEU:HG	1:C:231:ILE:HG12	1.96	0.47
1:C:351:TYR:CE1	1:C:452:TRP:HB2	2.48	0.47
1:C:459:SER:OG	1:C:460:LYS:N	2.47	0.47
1:C:738:CYS:HB3	1:C:760:CYS:HB2	1.69	0.47
1:C:866:THR:HG23	1:C:868:GLU:H	1.80	0.47
3:G:15:GLY:N	3:G:80:LEU:O	2.43	0.47
1:A:654:GLU:N	1:A:654:GLU:OE1	2.47	0.47
1:B:194:PHE:HB3	1:B:201:PHE:CE1	2.50	0.47
1:B:369:TYR:HA	1:B:374:PHE:CZ	2.50	0.47
1:B:998:THR:O	1:B:1002:GLN:HG2	2.14	0.47
1:C:450:ASP:N	1:C:450:ASP:OD1	2.47	0.47
1:C:660:TYR:HB2	1:C:695:TYR:CZ	2.49	0.47
1:A:222:ALA:O	1:A:223:LEU:HD22	2.15	0.47
1:A:1030:SER:O	1:C:1040:VAL:HG13	2.15	0.47
1:A:1139:ASP:OD1	1:A:1141:LEU:HD12	2.15	0.47
3:L:15:GLY:N	3:L:80:LEU:O	2.45	0.47
1:B:340:GLU:N	1:B:340:GLU:OE1	2.47	0.47
2:D:35:TYR:CD1	2:D:101:TRP:HD1	2.33	0.47
1:A:634:ARG:HG2	1:A:635:VAL:H	1.80	0.47
3:L:90:CYS:O	3:L:103:GLY:N	2.40	0.47
1:B:117:LEU:HD23	1:B:118:LEU:N	2.30	0.47
1:C:417:ASN:HD22	1:C:455:LEU:HD23	1.80	0.47
1:C:654:GLU:N	1:C:654:GLU:OE1	2.47	0.47
1:C:957:GLN:O	1:C:961:THR:HG23	2.16	0.47
2:H:6:GLU:HA	2:H:22:CYS:HA	1.97	0.46
2:H:43:PRO:O	2:H:45:ARG:NH2	2.48	0.46
1:B:970:PHE:C	1:B:995:ARG:HH12	2.19	0.46
1:A:334:ASN:CG	1:A:361:CYS:HA	2.36	0.46
1:A:558:LYS:HA	1:A:558:LYS:HD3	1.67	0.46
1:A:574:ASP:OD2	1:B:843:ASP:HB3	2.15	0.46
1:A:790:LYS:HZ2	1:C:702:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.79	0.46
3:L:10:VAL:HG11	3:L:20:ILE:HD11	1.97	0.46
3:L:80:LEU:HD22	3:L:110:VAL:HG13	1.96	0.46
1:B:742:ILE:HD11	1:B:753:LEU:HD22	1.97	0.46
1:A:612:TYR:HE2	1:A:651:ILE:HG21	1.80	0.46
1:A:738:CYS:O	1:A:742:ILE:HG12	2.15	0.46
1:C:406:GLU:HG2	1:C:418:ILE:HG13	1.96	0.46
1:A:417:ASN:HD22	1:A:455:LEU:HD23	1.80	0.46
1:A:737:ASP:OD1	1:A:737:ASP:N	2.49	0.46
3:L:57:PRO:HD2	3:L:60:VAL:HG21	1.97	0.46
1:B:334:ASN:CG	1:B:361:CYS:HA	2.35	0.46
3:F:39:GLN:HB2	3:F:49:LEU:HD11	1.97	0.46
1:C:338:PHE:CE1	1:C:358:ILE:HD13	2.44	0.46
1:C:641:ASN:OD1	1:C:642:VAL:HG13	2.16	0.46
1:A:702:GLU:CD	1:B:790:LYS:HZ2	2.19	0.46
1:B:168:PHE:HZ	1:B:229:LEU:HB2	1.81	0.46
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.97	0.46
1:B:966:LEU:HD11	1:B:1000:ARG:HH21	1.80	0.46
1:C:568:ASP:OD2	1:C:570:VAL:HG12	2.16	0.46
2:E:50:ILE:HG13	2:E:65:LEU:HD12	1.97	0.46
1:A:447:GLY:HA2	1:A:498:ARG:HG2	1.98	0.46
3:L:17:ARG:NH2	3:L:76:ALA:HB1	2.31	0.46
1:B:117:LEU:HD21	1:B:119:ILE:HD11	1.97	0.46
1:B:617:CYS:HA	1:B:620:VAL:HG12	1.97	0.46
1:B:703:ASN:OD1	1:B:704:SER:N	2.49	0.46
1:B:990:GLU:HA	1:B:993:ILE:HG12	1.98	0.46
1:C:168:PHE:HZ	1:C:229:LEU:HB2	1.80	0.46
1:C:334:ASN:CG	1:C:361:CYS:HA	2.35	0.46
1:A:115:GLN:HG2	1:A:233:ILE:HG21	1.97	0.46
1:A:320:VAL:N	1:A:591:SER:OG	2.49	0.46
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.98	0.46
1:A:589:PRO:O	1:B:837:TYR:HE1	1.99	0.46
1:B:541:PHE:CZ	1:B:587:ILE:HD12	2.51	0.46
1:B:1107:ARG:NH1	1:C:904:TYR:CZ	2.83	0.46
3:F:75:LEU:HD12	3:F:76:ALA:H	1.81	0.46
1:C:94:SER:HB2	1:C:265:TYR:H	1.81	0.46
1:C:117:LEU:HD23	1:C:118:LEU:N	2.30	0.46
1:C:990:GLU:HA	1:C:993:ILE:HG12	1.98	0.46
2:E:49:TRP:HZ2	2:E:60:TYR:HB3	1.80	0.46
1:A:121:ASN:HD21	1:A:176:LEU:H	1.62	0.46
1:A:168:PHE:HZ	1:A:229:LEU:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:SER:HB3	1:B:844:ILE:HG13	1.97	0.46
1:C:461:LEU:HD23	1:C:461:LEU:HA	1.84	0.46
1:C:612:TYR:HE2	1:C:651:ILE:HG21	1.81	0.46
1:A:194:PHE:HB3	1:A:201:PHE:HE1	1.80	0.46
2:H:38:TRP:CD1	2:H:82:LEU:HB2	2.50	0.46
1:B:116:SER:N	1:B:131:CYS:O	2.35	0.46
1:C:568:ASP:OD1	1:C:572:THR:OG1	2.20	0.46
1:B:320:VAL:N	1:B:591:SER:OG	2.49	0.46
1:B:634:ARG:HG2	1:B:635:VAL:H	1.81	0.45
1:C:369:TYR:HA	1:C:374:PHE:HZ	1.81	0.45
1:C:984:LEU:HB3	1:C:989:ALA:HB2	1.96	0.45
3:G:57:PRO:HD2	3:G:60:VAL:HG21	1.97	0.45
1:A:984:LEU:HB3	1:A:989:ALA:HB2	1.98	0.45
1:A:1029:MET:HA	1:A:1033:VAL:HG23	1.98	0.45
1:B:502:GLY:O	1:B:506:GLN:NE2	2.46	0.45
1:B:629:LEU:HD22	3:F:24:GLY:O	2.16	0.45
3:F:50:ILE:HD13	3:F:56:ARG:HB3	1.98	0.45
1:C:357:ARG:HG3	1:C:396:TYR:CE1	2.50	0.45
1:A:369:TYR:HA	1:A:374:PHE:HZ	1.80	0.45
1:A:840:CYS:O	1:C:586:ASP:HB3	2.17	0.45
2:H:37:GLY:N	2:H:98:ALA:O	2.42	0.45
1:B:194:PHE:HB3	1:B:201:PHE:HE1	1.81	0.45
1:B:866:THR:HG23	1:B:868:GLU:H	1.80	0.45
2:D:61:GLN:NE2	2:D:66:LYS:HG3	2.30	0.45
2:D:81:SER:HB3	2:D:83:LYS:HZ1	1.82	0.45
1:C:523:THR:HG22	1:C:524:VAL:HG23	1.97	0.45
1:C:786:LYS:HG3	1:C:787:GLN:HG3	1.99	0.45
1:A:312:ILE:HG13	1:A:598:ILE:HG22	1.97	0.45
1:A:990:GLU:HA	1:A:993:ILE:HG12	1.99	0.45
1:B:612:TYR:HE2	1:B:651:ILE:HG21	1.82	0.45
1:B:1094:VAL:HG13	1:C:900:MET:HE1	1.97	0.45
1:C:365:TYR:CZ	1:C:387:LEU:HB3	2.52	0.45
1:C:634:ARG:HG2	1:C:635:VAL:H	1.81	0.45
2:E:105:VAL:CG1	2:E:106:LEU:HD22	2.46	0.45
1:A:553:THR:HG23	1:A:554:LYS:O	2.16	0.45
1:A:841:LEU:N	1:C:588:THR:OG1	2.50	0.45
1:A:896:ILE:CD1	1:C:712:ILE:HD13	2.46	0.45
2:H:109:ALA:HB1	3:L:33:ASN:HD22	1.80	0.45
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.98	0.45
1:B:1097:SER:HB2	1:B:1102:TRP:CD2	2.52	0.45
1:C:447:GLY:HA2	1:C:498:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:LEU:HD22	3:G:24:GLY:O	2.17	0.45
2:E:102:ASP:OD1	2:E:103:VAL:N	2.49	0.45
1:A:847:ARG:NH2	1:C:573:THR:O	2.39	0.45
2:H:24:VAL:HG12	2:H:78:ASN:HD21	1.81	0.45
3:F:14:PRO:HG3	3:F:110:VAL:HG12	1.98	0.45
3:G:10:VAL:HG11	3:G:20:ILE:HD11	1.97	0.45
3:G:17:ARG:NH2	3:G:76:ALA:HB1	2.32	0.45
3:L:39:GLN:HB2	3:L:49:LEU:HD11	1.98	0.45
3:G:50:ILE:HD13	3:G:56:ARG:HB3	1.98	0.45
1:A:117:LEU:HD23	1:A:118:LEU:N	2.32	0.45
1:A:786:LYS:HG3	1:A:787:GLN:HG3	1.99	0.45
1:A:844:ILE:HG13	1:C:555:SER:HB3	1.97	0.45
3:L:37:TRP:CD1	3:L:75:LEU:HD21	2.52	0.45
1:B:403:LYS:HG2	1:B:504:GLY:O	2.16	0.45
1:B:620:VAL:O	1:B:624:ILE:HG13	2.16	0.45
2:D:81:SER:HB3	2:D:83:LYS:NZ	2.32	0.45
1:C:222:ALA:O	1:C:223:LEU:HD22	2.16	0.45
1:C:533:LEU:HD12	1:C:533:LEU:HA	1.77	0.45
1:A:735:SER:O	1:A:735:SER:OG	2.25	0.45
1:B:312:ILE:HG13	1:B:598:ILE:HG22	1.98	0.45
1:B:553:THR:HG23	1:B:554:LYS:O	2.16	0.45
1:A:529:LYS:HD2	1:A:529:LYS:HA	1.76	0.45
1:A:640:SER:HB2	1:A:654:GLU:HG3	1.99	0.45
1:A:713:ALA:HA	1:A:1074:ASN:HA	1.99	0.45
1:A:770:ILE:O	1:A:774:GLN:HG2	2.16	0.45
3:L:50:ILE:HD13	3:L:56:ARG:HB3	1.98	0.45
1:B:586:ASP:C	1:B:587:ILE:HG12	2.38	0.45
1:B:713:ALA:HA	1:B:1074:ASN:HA	1.98	0.45
2:E:24:VAL:HG12	2:E:78:ASN:HD21	1.81	0.45
2:E:35:TYR:CD1	2:E:101:TRP:CD1	3.05	0.45
1:A:105:ILE:HD11	1:A:241:LEU:HD21	1.98	0.44
1:B:702:GLU:CD	1:C:790:LYS:HZ2	2.20	0.44
2:D:76:SER:OG	2:D:77:LYS:NZ	2.36	0.44
1:C:630:THR:HB	1:C:631:PRO:HD2	1.98	0.44
1:C:742:ILE:HG13	1:C:743:CYS:SG	2.57	0.44
1:A:553:THR:CG2	1:B:841:LEU:HD12	2.47	0.44
1:A:703:ASN:OD1	1:A:704:SER:N	2.50	0.44
1:A:894:LEU:HD13	1:C:715:PRO:HD3	2.00	0.44
3:L:14:PRO:HG3	3:L:110:VAL:HG12	1.98	0.44
1:B:568:ASP:HA	1:C:846:ALA:HB1	1.99	0.44
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.50	0.44
1:A:118:LEU:HG	1:A:120:VAL:HG12	2.00	0.44
1:A:715:PRO:HD3	1:B:894:LEU:HD13	2.00	0.44
2:D:101:TRP:HA	2:D:111:SER:HB2	1.99	0.44
1:C:320:VAL:N	1:C:591:SER:OG	2.50	0.44
1:C:452:TRP:HB3	1:C:492:LEU:HD13	1.99	0.44
1:C:1097:SER:HB2	1:C:1102:TRP:HA	1.98	0.44
1:A:919:ASN:O	1:A:923:ILE:HG22	2.18	0.44
1:A:957:GLN:O	1:A:961:THR:HG23	2.17	0.44
2:H:41:GLN:NE2	2:H:42:PRO:O	2.51	0.44
1:B:575:ALA:HB2	1:B:586:ASP:OD2	2.17	0.44
1:B:641:ASN:OD1	1:B:642:VAL:HG13	2.16	0.44
2:E:81:SER:HB3	2:E:83:LYS:NZ	2.32	0.44
1:A:328:ARG:HG2	1:A:579:PRO:HD2	1.99	0.44
1:A:629:LEU:HD22	3:L:24:GLY:O	2.17	0.44
1:B:704:SER:HB2	1:C:790:LYS:HG2	1.98	0.44
1:C:45:SER:O	1:C:47:VAL:HG23	2.18	0.44
1:C:312:ILE:HG13	1:C:598:ILE:HG22	2.00	0.44
1:C:393:THR:HG21	1:C:520:ALA:HB3	1.98	0.44
1:C:703:ASN:OD1	1:C:704:SER:N	2.50	0.44
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.51	0.44
3:G:40:GLN:HB3	3:G:87:GLU:HB3	2.00	0.44
1:A:567:ARG:O	1:B:846:ALA:HA	2.18	0.44
1:A:586:ASP:HB2	1:B:841:LEU:HA	2.00	0.44
2:H:102:ASP:OD1	2:H:104:VAL:HG12	2.17	0.44
3:F:29:ILE:HG13	3:F:33:ASN:HB2	2.00	0.44
2:E:38:TRP:CH2	2:E:97:CYS:HB3	2.52	0.44
1:A:657:ASN:C	1:A:658:ASN:HD22	2.21	0.44
1:A:843:ASP:N	1:C:586:ASP:OD1	2.51	0.44
2:H:49:TRP:HZ2	2:H:60:TYR:HB3	1.81	0.44
1:B:85:PRO:HG3	2:D:60:TYR:CE1	2.52	0.44
1:B:589:PRO:O	1:C:837:TYR:HE1	2.01	0.44
1:B:786:LYS:HG3	1:B:787:GLN:HG3	1.99	0.44
1:C:135:PHE:CE1	1:C:137:ASN:HB2	2.52	0.44
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.82	0.44
3:G:87:GLU:OE2	3:G:107:LYS:HD2	2.18	0.44
1:A:373:PRO:HD2	1:A:436:TRP:CE3	2.53	0.44
1:A:1097:SER:HB2	1:A:1102:TRP:HA	2.00	0.44
1:C:303:LEU:O	1:C:303:LEU:HD23	2.18	0.44
1:C:719:THR:HG22	1:C:1068:VAL:O	2.18	0.44
1:A:452:TRP:HB3	1:A:492:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:29:ILE:HD12	3:L:92:SER:HB3	2.00	0.44
1:B:53:ASP:OD2	1:B:54:LEU:N	2.46	0.44
1:B:766:ALA:O	1:B:770:ILE:HG23	2.17	0.44
3:G:38:TYR:HE1	3:G:48:LEU:HG	1.83	0.44
1:B:105:ILE:HG12	1:B:118:LEU:HD13	2.00	0.43
1:B:328:ARG:HG2	1:B:579:PRO:HD2	2.00	0.43
1:B:369:TYR:HA	1:B:374:PHE:HZ	1.82	0.43
1:B:451:TYR:HB2	1:B:495:TYR:HB3	1.99	0.43
2:D:38:TRP:CG	2:D:82:LEU:HD22	2.52	0.43
1:C:294:ASP:OD1	1:C:295:PRO:HD2	2.18	0.43
1:A:106:PHE:HD2	1:A:235:ILE:HG21	1.82	0.43
1:A:559:PHE:HB3	1:A:577:ARG:NH2	2.33	0.43
1:A:564:GLN:OE1	1:A:577:ARG:HD2	2.18	0.43
1:A:959:LEU:HA	1:A:959:LEU:HD23	1.81	0.43
1:B:896:ILE:HD12	1:B:896:ILE:HA	1.89	0.43
1:C:1029:MET:HA	1:C:1033:VAL:HG23	2.00	0.43
2:E:35:TYR:CG	2:E:101:TRP:HD1	2.36	0.43
1:B:959:LEU:HA	1:B:959:LEU:HD23	1.79	0.43
1:C:659:SER:O	1:C:659:SER:OG	2.25	0.43
1:C:713:ALA:HA	1:C:1074:ASN:HA	2.00	0.43
1:C:1114:ILE:HD13	1:C:1114:ILE:HA	1.87	0.43
1:A:663:ASP:HB2	1:A:664:ILE:HD12	1.99	0.43
1:A:1039:ARG:NE	1:B:1031:GLU:OE2	2.38	0.43
1:A:1094:VAL:HG23	1:A:1107:ARG:HH21	1.83	0.43
1:C:451:TYR:HB2	1:C:495:TYR:HB2	2.00	0.43
3:G:48:LEU:HD23	3:G:49:LEU:N	2.33	0.43
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.51	0.43
1:B:290:ASP:O	1:B:297:SER:HB3	2.18	0.43
1:B:533:LEU:HD12	1:B:533:LEU:HA	1.82	0.43
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	1.99	0.43
1:A:294:ASP:OD1	1:A:295:PRO:HD2	2.18	0.43
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.83	0.43
1:A:662:CYS:HB2	1:A:697:MET:SD	2.59	0.43
1:A:704:SER:HB2	1:B:790:LYS:HG2	1.99	0.43
1:A:738:CYS:HB3	1:A:760:CYS:HB2	1.74	0.43
1:A:855:PHE:HA	1:C:589:PRO:HG3	2.00	0.43
1:B:118:LEU:HG	1:B:120:VAL:HG12	2.00	0.43
1:C:770:ILE:O	1:C:774:GLN:HG2	2.19	0.43
1:A:451:TYR:HB2	1:A:495:TYR:HB2	2.00	0.43
1:A:641:ASN:OD1	1:A:642:VAL:N	2.51	0.43
1:A:712:ILE:HD13	1:B:896:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:LEU:HD22	1:C:551:VAL:HB	2.00	0.43
3:L:6:GLN:HE21	3:L:90:CYS:HB3	1.84	0.43
2:D:102:ASP:OD1	2:D:104:VAL:HG12	2.18	0.43
1:B:452:TRP:HB3	1:B:492:LEU:HD13	2.00	0.43
1:B:537:LYS:O	1:B:539:VAL:HG13	2.19	0.43
1:C:229:LEU:HD23	1:C:229:LEU:H	1.84	0.43
1:C:853:GLN:O	1:C:858:LEU:HB2	2.19	0.43
1:A:404:GLY:HA2	1:A:508:TYR:HD2	1.84	0.43
1:A:620:VAL:O	1:A:624:ILE:HG13	2.19	0.43
1:A:650:LEU:HB3	1:A:653:ALA:HB3	1.99	0.43
1:A:992:GLN:HA	1:A:995:ARG:HG2	2.01	0.43
1:B:190:ARG:H	1:B:190:ARG:HG2	1.65	0.43
1:B:640:SER:HB2	1:B:654:GLU:HG3	2.01	0.43
1:B:948:LEU:HD22	1:B:1059:GLY:HA3	2.00	0.43
1:B:993:ILE:HG13	1:B:994:ASP:N	2.34	0.43
1:C:553:THR:HG23	1:C:554:LYS:O	2.18	0.43
1:C:558:LYS:HA	1:C:558:LYS:HD3	1.71	0.43
1:A:320:VAL:HB	1:A:591:SER:CB	2.49	0.43
1:A:802:PHE:HZ	1:A:898:PHE:CZ	2.36	0.43
3:L:48:LEU:HD23	3:L:49:LEU:N	2.33	0.43
1:B:365:TYR:CZ	1:B:387:LEU:HB3	2.54	0.43
1:B:738:CYS:HB3	1:B:760:CYS:HB2	1.82	0.43
3:F:48:LEU:HD23	3:F:49:LEU:N	2.34	0.43
1:C:117:LEU:HD12	1:C:231:ILE:HG21	1.99	0.43
1:C:614:GLY:N	1:C:647:ALA:O	2.37	0.43
3:G:14:PRO:HG3	3:G:110:VAL:HG12	2.00	0.43
1:A:720:ILE:HG13	1:A:923:ILE:HG13	2.00	0.42
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.42
3:L:41:LEU:HD23	3:L:41:LEU:HA	1.86	0.42
1:B:574:ASP:OD2	1:C:843:ASP:HB3	2.19	0.42
1:C:659:SER:HB2	1:C:698:SER:HB3	2.01	0.42
1:C:921:LYS:HD2	1:C:921:LYS:HA	1.91	0.42
1:A:131:CYS:SG	1:A:163:ALA:HA	2.59	0.42
1:A:568:ASP:OD1	1:A:572:THR:OG1	2.21	0.42
1:A:790:LYS:HG2	1:C:704:SER:HB2	2.00	0.42
1:B:713:ALA:HB2	1:B:1074:ASN:HB3	2.01	0.42
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.81	0.42
1:C:992:GLN:HA	1:C:995:ARG:HG2	2.02	0.42
1:A:351:TYR:HB3	1:A:453:TYR:HA	2.01	0.42
1:B:439:ASN:OD1	1:B:507:PRO:HD2	2.19	0.42
2:E:14:PRO:HD3	2:E:125:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:HB2	1:A:300:LYS:HE3	1.71	0.42
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.54	0.42
1:B:303:LEU:HD22	1:B:308:VAL:HG12	2.00	0.42
1:B:358:ILE:HD12	1:B:395:VAL:HG12	2.01	0.42
1:B:663:ASP:HB2	1:B:664:ILE:HD12	2.02	0.42
1:B:1073:LYS:HB2	1:B:1075:PHE:CZ	2.55	0.42
1:C:737:ASP:N	1:C:737:ASP:OD1	2.53	0.42
3:G:91:GLN:HB2	3:G:102:PHE:CD1	2.55	0.42
3:L:29:ILE:HG13	3:L:33:ASN:HB2	2.01	0.42
1:B:100:ILE:O	1:B:242:LEU:HD13	2.19	0.42
1:B:206:LYS:NZ	1:B:221:SER:HB3	2.35	0.42
1:B:294:ASP:OD1	1:B:295:PRO:HD2	2.18	0.42
1:B:417:ASN:HD22	1:B:455:LEU:HD23	1.84	0.42
1:B:641:ASN:OD1	1:B:642:VAL:N	2.52	0.42
1:B:736:VAL:HG22	1:B:858:LEU:CD2	2.50	0.42
2:D:29:ILE:HG23	2:D:75:THR:HG22	2.01	0.42
1:C:61:ASN:N	1:C:61:ASN:OD1	2.52	0.42
2:E:32:SER:O	2:E:54:TYR:OH	2.25	0.42
2:E:33:THR:HG22	2:E:34:PHE:CD2	2.55	0.42
1:A:206:LYS:NZ	1:A:221:SER:HB3	2.34	0.42
1:B:650:LEU:HB3	1:B:653:ALA:HB3	2.00	0.42
1:A:290:ASP:O	1:A:297:SER:HB3	2.20	0.42
1:B:312:ILE:HG13	1:B:598:ILE:CG2	2.49	0.42
1:B:338:PHE:HB3	1:B:368:LEU:HD21	2.01	0.42
1:B:1086:LYS:HE3	1:B:1086:LYS:HB2	1.83	0.42
1:C:287:ASP:HB3	1:C:306:PHE:CZ	2.54	0.42
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.84	0.42
1:C:424:LYS:HG2	1:C:463:PRO:HG3	2.01	0.42
1:C:650:LEU:HB3	1:C:653:ALA:HB3	2.00	0.42
3:G:39:GLN:CB	3:G:49:LEU:HD11	2.50	0.42
1:A:537:LYS:O	1:A:539:VAL:HG13	2.19	0.42
1:A:570:VAL:HG22	1:A:570:VAL:O	2.20	0.42
2:H:107:ALA:HB3	2:H:110:ARG:HH21	1.85	0.42
1:B:212:ILE:HG21	1:B:214:ARG:HD3	2.02	0.42
1:B:378:LYS:HG2	1:B:433:VAL:HG22	2.02	0.42
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.00	0.42
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.85	0.42
1:B:588:THR:HG23	1:C:840:CYS:HB2	2.01	0.42
1:B:737:ASP:OD1	1:B:737:ASP:N	2.53	0.42
1:C:320:VAL:HB	1:C:591:SER:CB	2.50	0.42
1:C:620:VAL:O	1:C:624:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:HD3	1:C:102:ARG:HA	1.86	0.42
1:C:358:ILE:HD12	1:C:395:VAL:HG12	2.02	0.42
1:C:537:LYS:O	1:C:539:VAL:HG13	2.19	0.42
1:C:712:ILE:CG2	1:C:1077:THR:HB	2.49	0.42
1:A:543:PHE:HB3	1:A:576:VAL:HG11	2.01	0.42
2:H:13:LYS:HB2	2:H:16:GLU:OE2	2.19	0.42
1:B:353:TRP:CZ2	1:B:466:ARG:HG2	2.55	0.42
1:B:559:PHE:HB3	1:B:577:ARG:NH2	2.35	0.42
1:B:719:THR:HG22	1:B:1068:VAL:O	2.19	0.42
1:B:856:ASN:ND2	1:B:966:LEU:HD13	2.20	0.42
2:D:66:LYS:HB3	2:D:66:LYS:HE3	1.95	0.42
2:D:113:PHE:O	3:F:38:TYR:OH	2.32	0.42
1:C:559:PHE:HB3	1:C:577:ARG:NH2	2.35	0.42
1:C:634:ARG:CG	1:C:635:VAL:H	2.33	0.42
1:C:641:ASN:OD1	1:C:642:VAL:N	2.52	0.42
1:C:1073:LYS:HB2	1:C:1075:PHE:CZ	2.54	0.42
2:E:38:TRP:NE1	2:E:82:LEU:HB2	2.34	0.42
1:A:411:ALA:HB3	1:A:414:GLN:HG3	2.01	0.41
1:A:640:SER:CB	1:A:654:GLU:HG3	2.50	0.41
1:A:1040:VAL:HG13	1:B:1030:SER:O	2.20	0.41
1:B:53:ASP:HB3	1:B:55:PHE:HE1	1.85	0.41
1:B:550:GLY:HA2	1:B:588:THR:O	2.20	0.41
1:B:996:LEU:HD13	1:B:1000:ARG:HH12	1.85	0.41
3:F:87:GLU:OE1	3:F:107:LYS:HD2	2.20	0.41
1:C:948:LEU:HD22	1:C:1059:GLY:HA3	2.02	0.41
2:E:12:VAL:HG12	2:E:13:LYS:O	2.20	0.41
1:A:188:ASN:OD1	1:A:188:ASN:N	2.53	0.41
1:A:1073:LYS:HB2	1:A:1075:PHE:CZ	2.55	0.41
2:H:33:THR:HG22	2:H:34:PHE:CD1	2.55	0.41
1:B:1082:CYS:HB2	1:B:1132:ILE:HD11	2.02	0.41
2:D:18:LEU:HD11	2:D:122:VAL:HG11	2.01	0.41
1:C:338:PHE:HB3	1:C:368:LEU:HD21	2.01	0.41
1:C:353:TRP:CZ2	1:C:466:ARG:HG2	2.55	0.41
1:A:212:ILE:HG21	1:A:214:ARG:HD3	2.02	0.41
1:A:378:LYS:HG2	1:A:433:VAL:HG22	2.02	0.41
2:H:18:LEU:HD11	2:H:122:VAL:HG11	2.02	0.41
1:B:61:ASN:OD1	1:B:61:ASN:N	2.53	0.41
1:B:338:PHE:CE1	1:B:358:ILE:HD13	2.47	0.41
1:B:634:ARG:CG	1:B:635:VAL:H	2.33	0.41
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.55	0.41
1:B:849:LEU:H	1:B:849:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:41:LEU:HD23	3:F:41:LEU:HA	1.86	0.41
1:C:115:GLN:HG2	1:C:233:ILE:HG21	2.01	0.41
1:C:1074:ASN:OD1	1:C:1074:ASN:N	2.54	0.41
3:G:90:CYS:O	3:G:103:GLY:N	2.44	0.41
1:A:568:ASP:HB2	1:B:846:ALA:HB1	2.03	0.41
1:B:131:CYS:SG	1:B:163:ALA:HA	2.60	0.41
1:B:351:TYR:HB3	1:B:453:TYR:HA	2.03	0.41
1:C:373:PRO:HD2	1:C:436:TRP:CE3	2.54	0.41
1:A:541:PHE:CZ	1:A:587:ILE:HD12	2.56	0.41
3:L:111:LEU:HD23	3:L:111:LEU:HA	1.77	0.41
1:B:188:ASN:N	1:B:188:ASN:OD1	2.54	0.41
1:B:564:GLN:OE1	1:B:577:ARG:HD2	2.21	0.41
1:B:720:ILE:HG13	1:B:923:ILE:HG13	2.03	0.41
1:B:1029:MET:HA	1:B:1033:VAL:HG23	2.01	0.41
3:F:39:GLN:CB	3:F:49:LEU:HD11	2.50	0.41
1:C:48:LEU:HD13	1:C:48:LEU:HA	1.89	0.41
1:C:328:ARG:HD2	1:C:543:PHE:HE1	1.85	0.41
1:C:663:ASP:HB2	1:C:664:ILE:HD12	2.02	0.41
1:C:736:VAL:HG22	1:C:858:LEU:HD23	2.02	0.41
1:C:822:LEU:HD23	1:C:822:LEU:HA	1.89	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.55	0.41
1:A:659:SER:HB2	1:A:698:SER:HB3	2.02	0.41
1:B:802:PHE:HZ	1:B:898:PHE:CZ	2.38	0.41
2:D:47:LEU:HB2	3:F:102:PHE:CG	2.55	0.41
2:D:101:TRP:CZ3	2:D:108:ALA:HA	2.55	0.41
3:G:36:HIS:HB2	3:G:91:GLN:OE1	2.20	0.41
1:A:317:ASN:OD1	1:A:317:ASN:N	2.53	0.41
1:A:849:LEU:HD22	1:A:849:LEU:H	1.85	0.41
1:B:406:GLU:HG2	1:B:418:ILE:HG13	2.01	0.41
1:B:551:VAL:C	1:B:552:LEU:HD12	2.41	0.41
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.61	0.41
3:F:29:ILE:HD12	3:F:92:SER:HB3	2.03	0.41
1:C:53:ASP:HB3	1:C:55:PHE:HE1	1.84	0.41
1:C:378:LYS:HG2	1:C:433:VAL:HG22	2.02	0.41
3:G:7:PRO:HA	3:G:8:PRO:HD2	1.97	0.41
1:A:201:PHE:HB2	1:A:231:ILE:HG13	2.03	0.41
1:A:660:TYR:O	1:A:698:SER:OG	2.32	0.41
1:B:373:PRO:HD2	1:B:436:TRP:CE3	2.55	0.41
1:B:424:LYS:HG2	1:B:463:PRO:HG3	2.02	0.41
1:B:567:ARG:NH1	1:B:571:ASP:OD1	2.53	0.41
3:F:88:TYR:HB2	3:F:106:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:877:LEU:HD23	1:C:877:LEU:HA	1.89	0.41
1:A:312:ILE:HG13	1:A:598:ILE:CG2	2.51	0.41
1:A:353:TRP:CZ2	1:A:466:ARG:HG2	2.55	0.41
1:A:556:ASN:H	1:B:844:ILE:CD1	2.34	0.41
1:A:736:VAL:HG22	1:A:858:LEU:CD2	2.50	0.41
1:A:846:ALA:HB1	1:C:568:ASP:HB2	2.03	0.41
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.95	0.41
1:A:965:GLN:O	1:A:965:GLN:HG3	2.20	0.41
1:B:85:PRO:HG3	2:D:60:TYR:HE1	1.86	0.41
1:B:102:ARG:HD3	1:B:102:ARG:HA	1.85	0.41
1:B:206:LYS:NZ	1:B:222:ALA:O	2.47	0.41
1:B:220:PHE:HD1	1:B:221:SER:N	2.19	0.41
1:B:338:PHE:CE1	1:B:358:ILE:HG21	2.56	0.41
1:B:645:THR:N	1:B:648:GLY:O	2.46	0.41
2:D:24:VAL:HG12	2:D:78:ASN:HD21	1.85	0.41
1:C:351:TYR:HB3	1:C:453:TYR:HA	2.03	0.41
1:C:640:SER:HB2	1:C:654:GLU:HG3	2.02	0.41
1:A:406:GLU:N	1:A:406:GLU:OE1	2.54	0.41
1:A:843:ASP:HB3	1:C:574:ASP:OD2	2.21	0.41
3:L:38:TYR:HE1	3:L:48:LEU:HG	1.85	0.41
1:B:529:LYS:HD2	1:B:529:LYS:HA	1.76	0.41
1:B:557:LYS:HB2	1:C:844:ILE:CB	2.51	0.41
2:D:6:GLU:OE1	2:D:118:GLN:NE2	2.54	0.41
1:C:290:ASP:O	1:C:297:SER:HB3	2.21	0.41
2:E:29:ILE:HG23	2:E:75:THR:HG22	2.02	0.41
3:G:37:TRP:CD1	3:G:75:LEU:HD21	2.56	0.41
1:A:977:LEU:HD23	1:A:977:LEU:HA	1.89	0.40
1:C:188:ASN:N	1:C:188:ASN:OD1	2.53	0.40
1:C:312:ILE:HG13	1:C:598:ILE:CG2	2.51	0.40
1:C:411:ALA:HB3	1:C:414:GLN:HG3	2.02	0.40
1:C:529:LYS:HA	1:C:529:LYS:HD2	1.76	0.40
1:C:802:PHE:HZ	1:C:898:PHE:CZ	2.38	0.40
1:C:850:ILE:O	1:C:854:LYS:HG2	2.21	0.40
1:A:629:LEU:O	1:A:634:ARG:NH1	2.39	0.40
1:A:634:ARG:CG	1:A:635:VAL:H	2.33	0.40
1:A:902:MET:HG3	1:A:916:LEU:HD13	2.03	0.40
1:A:1093:GLY:HA3	1:A:1105:THR:O	2.22	0.40
1:B:117:LEU:HD12	1:B:231:ILE:HG21	2.04	0.40
1:B:317:ASN:OD1	1:B:317:ASN:N	2.53	0.40
1:B:629:LEU:O	1:B:634:ARG:HD3	2.21	0.40
1:B:966:LEU:O	1:B:975:SER:OG	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:LEU:HD23	1:B:1049:LEU:HA	1.81	0.40
1:A:53:ASP:OD2	1:A:54:LEU:N	2.51	0.40
1:A:629:LEU:O	1:A:634:ARG:HD3	2.21	0.40
1:A:976:VAL:HB	1:A:979:ASP:HB3	2.02	0.40
1:B:287:ASP:HB3	1:B:306:PHE:CZ	2.57	0.40
1:B:436:TRP:CD1	1:B:509:ARG:HB3	2.57	0.40
1:B:762:GLN:OE1	1:B:762:GLN:N	2.45	0.40
1:B:973:ILE:HD13	1:B:973:ILE:HA	1.97	0.40
1:C:168:PHE:CZ	1:C:229:LEU:HD12	2.56	0.40
1:C:190:ARG:H	1:C:190:ARG:HG2	1.66	0.40
1:C:564:GLN:OE1	1:C:577:ARG:HD2	2.22	0.40
1:C:993:ILE:HG13	1:C:994:ASP:N	2.37	0.40
1:C:996:LEU:HD23	1:C:996:LEU:HA	1.82	0.40
2:E:28:SER:OG	2:E:30:SER:OG	2.23	0.40
2:E:38:TRP:O	2:E:50:ILE:HG22	2.21	0.40
1:A:264:ASP:OD1	1:A:265:TYR:HB2	2.22	0.40
1:A:358:ILE:HD12	1:A:395:VAL:HG12	2.03	0.40
1:A:534:VAL:O	1:A:534:VAL:HG12	2.21	0.40
1:A:550:GLY:HA2	1:A:588:THR:O	2.21	0.40
1:A:877:LEU:HD23	1:A:877:LEU:HA	1.90	0.40
1:B:201:PHE:HB2	1:B:231:ILE:HG13	2.04	0.40
1:B:712:ILE:O	1:B:1074:ASN:HA	2.22	0.40
1:C:106:PHE:HD2	1:C:235:ILE:HG21	1.87	0.40
1:C:720:ILE:HG13	1:C:923:ILE:HG13	2.04	0.40
1:A:822:LEU:HD23	1:A:822:LEU:HA	1.88	0.40
1:A:848:ASP:OD2	1:A:850:ILE:HG12	2.20	0.40
2:H:102:ASP:OD1	2:H:103:VAL:N	2.54	0.40
1:C:131:CYS:SG	1:C:163:ALA:HA	2.61	0.40
1:C:712:ILE:O	1:C:1074:ASN:HA	2.22	0.40
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.78	0.40
1:C:984:LEU:HD12	1:C:984:LEU:HA	1.92	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	1053/1204 (88%)	952 (90%)	97 (9%)	4 (0%)	30	63
1	B	1053/1204 (88%)	952 (90%)	97 (9%)	4 (0%)	30	63
1	C	1053/1204 (88%)	952 (90%)	97 (9%)	4 (0%)	30	63
2	D	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
2	E	124/126 (98%)	118 (95%)	6 (5%)	0	100	100
2	H	124/126 (98%)	118 (95%)	6 (5%)	0	100	100
3	F	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
3	G	109/111 (98%)	104 (95%)	5 (5%)	0	100	100
3	L	109/111 (98%)	104 (95%)	5 (5%)	0	100	100
All	All	3858/4323 (89%)	3523 (91%)	323 (8%)	12 (0%)	38	68

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ILE
1	A	635	VAL
1	A	803	SER
1	B	212	ILE
1	B	635	VAL
1	B	803	SER
1	C	212	ILE
1	C	635	VAL
1	C	803	SER
1	A	534	VAL
1	B	534	VAL
1	C	534	VAL

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	925/1053 (88%)	891 (96%)	34 (4%)	29	54
1	B	925/1053 (88%)	893 (96%)	32 (4%)	31	56
1	C	925/1053 (88%)	895 (97%)	30 (3%)	34	58
2	D	108/108 (100%)	102 (94%)	6 (6%)	17	45
2	E	108/108 (100%)	103 (95%)	5 (5%)	23	49
2	H	108/108 (100%)	101 (94%)	7 (6%)	14	41
3	F	89/89 (100%)	86 (97%)	3 (3%)	32	57
3	G	89/89 (100%)	84 (94%)	5 (6%)	17	45
3	L	89/89 (100%)	84 (94%)	5 (6%)	17	45
All	All	3366/3750 (90%)	3239 (96%)	127 (4%)	30	53

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	127	PHE
1	A	135	PHE
1	A	200	TYR
1	A	201	PHE
1	A	220	PHE
1	A	229	LEU
1	A	238	PHE
1	A	265	TYR
1	A	317	ASN
1	A	357	ARG
1	A	453	TYR
1	A	462	LYS
1	A	487	ASN
1	A	586	ASP
1	A	590	CYS
1	A	592	PHE
1	A	641	ASN
1	A	658	ASN
1	A	663	ASP
1	A	704	SER
1	A	735	SER
1	A	738	CYS
1	A	759	PHE
1	A	760	CYS
1	A	823	PHE

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Mol	Chain	Res	Type
1	A	848	ASP
1	A	873	TYR
1	A	965	GLN
1	A	995	ARG
1	A	1003	SER
1	A	1074	ASN
1	A	1107	ARG
1	A	1141	LEU
2	H	35	TYR
2	H	45	ARG
2	H	54	TYR
2	H	77	LYS
2	H	100	HIS
2	H	110	ARG
2	H	121	LEU
3	L	51	TYR
3	L	62	ASP
3	L	90	CYS
3	L	98	SER
3	L	107	LYS
1	B	61	ASN
1	B	127	PHE
1	B	135	PHE
1	B	166	CYS
1	B	201	PHE
1	B	220	PHE
1	B	229	LEU
1	B	238	PHE
1	B	265	TYR
1	B	316	SER
1	B	317	ASN
1	B	357	ARG
1	B	453	TYR
1	B	462	LYS
1	B	487	ASN
1	B	495	TYR
1	B	590	CYS
1	B	592	PHE
1	B	658	ASN
1	B	659	SER
1	B	663	ASP
1	B	704	SER

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Mol	Chain	Res	Type
1	B	759	PHE
1	B	760	CYS
1	B	823	PHE
1	B	873	TYR
1	B	939	PHE
1	B	965	GLN
1	B	994	ASP
1	B	995	ARG
1	B	1003	SER
1	B	1141	LEU
2	D	45	ARG
2	D	55	TYR
2	D	61	GLN
2	D	100	HIS
2	D	110	ARG
2	D	121	LEU
3	F	62	ASP
3	F	90	CYS
3	F	98	SER
1	C	61	ASN
1	C	127	PHE
1	C	135	PHE
1	C	166	CYS
1	C	201	PHE
1	C	220	PHE
1	C	238	PHE
1	C	265	TYR
1	C	277	LEU
1	C	317	ASN
1	C	453	TYR
1	C	462	LYS
1	C	487	ASN
1	C	540	ASN
1	C	590	CYS
1	C	592	PHE
1	C	659	SER
1	C	663	ASP
1	C	704	SER
1	C	735	SER
1	C	755	GLN
1	C	759	PHE
1	C	760	CYS

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Mol	Chain	Res	Type
1	C	823	PHE
1	C	873	TYR
1	C	939	PHE
1	C	965	GLN
1	C	969	LYS
1	C	995	ARG
1	C	1141	LEU
2	E	35	TYR
2	E	54	TYR
2	E	100	HIS
2	E	110	ARG
2	E	121	LEU
3	G	34	ASP
3	G	51	TYR
3	G	62	ASP
3	G	90	CYS
3	G	98	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	784	GLN
1	A	1002	GLN
1	B	774	GLN
1	B	784	GLN
1	B	856	ASN
1	B	965	GLN
2	D	61	GLN
2	D	118	GLN
1	C	239	GLN
1	C	755	GLN
1	C	784	GLN
1	C	965	GLN
2	E	61	GLN
3	G	39	GLN

5.3.3 RNA

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)

54 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	$\#\|Z\| > 2$
4	NAG	A	1307	1	14,14,15	0.18	0	17,19,21	0.39	0
4	NAG	C	1312	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	1311	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	A	1304	1	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	C	1315	1	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	B	1316	1	14,14,15	0.33	0	17,19,21	0.42	0
4	NAG	B	1310	1	14,14,15	0.18	0	17,19,21	0.39	0
4	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.32	0
4	NAG	B	1315	1	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	C	1310	1	14,14,15	0.18	0	17,19,21	0.39	0
4	NAG	B	1317	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	C	1316	1	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	A	1315	1	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	C	1317	1	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	1313	1	14,14,15	0.19	0	17,19,21	0.51	0
4	NAG	C	1305	1	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	C	1313	1	14,14,15	0.19	0	17,19,21	0.56	0
4	NAG	A	1318	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	A	1306	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	C	1309	1	14,14,15	0.21	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1311	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	B	1318	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	A	1316	1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	B	1309	1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	C	1304	1	14,14,15	0.18	0	17,19,21	0.49	0
4	NAG	A	1308	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	A	1305	1	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	1307	1	14,14,15	0.20	0	17,19,21	0.37	0
4	NAG	C	1307	1	14,14,15	0.19	0	17,19,21	0.38	0
4	NAG	B	1314	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	A	1312	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	1304	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	0.37	0
4	NAG	A	1310	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	C	1302	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	B	1308	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	A	1314	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.36	0
4	NAG	C	1306	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	C	1314	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	C	1318	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	B	1312	1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	A	1317	1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	A	1313	1	14,14,15	0.19	0	17,19,21	0.55	0
4	NAG	C	1311	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1309	1	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	A	1302	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	B	1302	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	B	1305	1	14,14,15	0.26	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1316	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1317	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1316	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1317	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1318	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1318	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1316	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1314	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1318	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1317	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	C4-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	A	1310	NAG	C4-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1310	NAG	C4-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	A	1315	NAG	O5-C5-C6-O6
4	B	1315	NAG	O5-C5-C6-O6
4	C	1315	NAG	O5-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	A	1311	NAG	C4-C5-C6-O6
4	B	1311	NAG	C4-C5-C6-O6
4	C	1311	NAG	C4-C5-C6-O6
4	A	1310	NAG	O5-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	C	1310	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	B	1302	NAG	C8-C7-N2-C2
4	B	1302	NAG	O7-C7-N2-C2
4	C	1302	NAG	C8-C7-N2-C2
4	C	1302	NAG	O7-C7-N2-C2
4	A	1301	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	A	1315	NAG	C4-C5-C6-O6
4	B	1315	NAG	C4-C5-C6-O6
4	C	1315	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	B	1316	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1318	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	C	1318	NAG	C4-C5-C6-O6
4	C	1316	NAG	O5-C5-C6-O6
4	A	1311	NAG	O5-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	C	1311	NAG	O5-C5-C6-O6
4	A	1318	NAG	O5-C5-C6-O6
4	A	1318	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1318	NAG	C4-C5-C6-O6
4	B	1318	NAG	O5-C5-C6-O6
4	A	1316	NAG	O5-C5-C6-O6
4	C	1312	NAG	C4-C5-C6-O6
4	C	1312	NAG	O5-C5-C6-O6
4	B	1316	NAG	C4-C5-C6-O6
4	B	1312	NAG	C4-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6
4	C	1316	NAG	C4-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1307	NAG	1	0
4	C	1304	NAG	1	0
4	B	1307	NAG	1	0
4	C	1307	NAG	1	0
4	B	1304	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.