Full wwPDB NMR Structure Validation Report (i)

Apr 16, 2023 – 07:23 AM EDT

PDB ID	:	7R7P
BMRB ID	:	30929
Title	:	Immature HIV-1 CACTD-SP1 lattice with Bevirimat (BVM) and Inositol hexakisphosphate (IP6)
Authors	:	Sarkar, S.; Zadrozny, K.K.; Zadorozhnyi, R.; Russell, R.W.; Quinn, C.M.; Kleinpeter, A.; Ablan, S.; Meshkin, H.; Perilla, J.R.; Ganser-Pornillos, B.K.; Pornillos, O.; Freed, E.O.; Gronenborn, A.M.; Polenova, T.
Deposited on	:	2021-06-25

This is a Full wwPDB NMR Structure 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

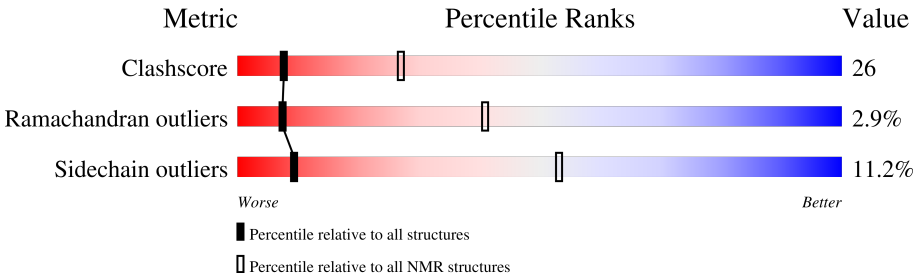
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 9%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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	G	102	51% 43% 6%
1	H	102	54% 44% .
1	I	102	55% 39% 6%
1	J	102	52% 41% 7%
1	K	102	59% 37% .
1	L	102	61% 36% .

2 Ensemble composition and analysis

This entry contains 5 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	G:144-G:245, H:144-H:245, I:144-I:245, J:144-J:245, K:144-K:245, L:144-L:245 (612)	0.49	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 5
2	1, 4
Single-model clusters	2

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9444 atoms, of which 4728 are hydrogens and 0 are deuteriums.

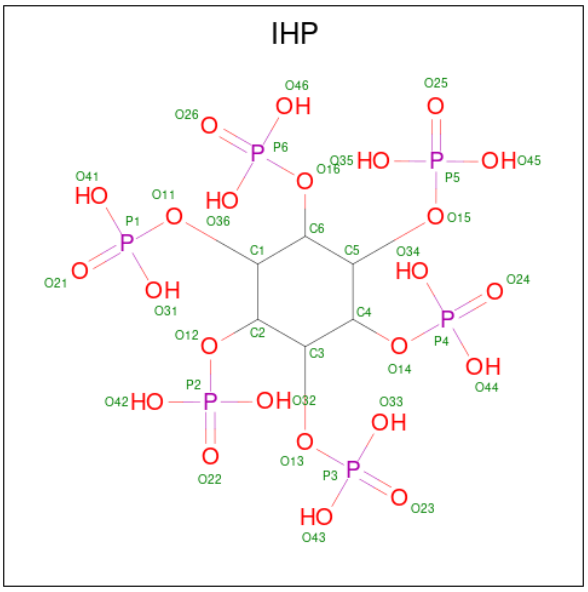
- Molecule 1 is a protein called Gag polyprotein.

Mol	Chain	Residues	Atoms						Trace
1	G	102	Total	C	H	N	O	S	0
			1551	479	778	136	151	7	
1	H	102	Total	C	H	N	O	S	0
			1551	479	778	136	151	7	
1	I	102	Total	C	H	N	O	S	0
			1551	479	778	136	151	7	
1	J	102	Total	C	H	N	O	S	0
			1551	479	778	136	151	7	
1	K	102	Total	C	H	N	O	S	0
			1551	479	778	136	151	7	
1	L	102	Total	C	H	N	O	S	0
			1551	479	778	136	151	7	

There are 18 discrepancies between the modelled and reference sequences:

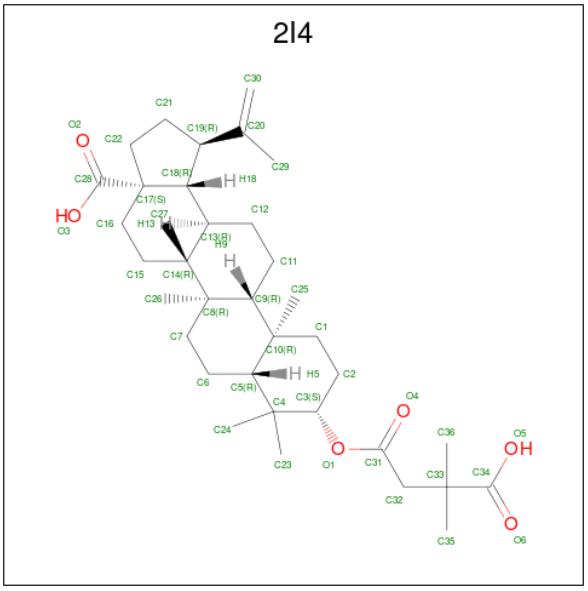
Chain	Residue	Modelled	Actual	Comment	Reference
G	144	GLY	-	expression tag	UNP Q72497
G	145	GLY	-	expression tag	UNP Q72497
G	241	THR	PRO	engineered mutation	UNP Q72497
H	144	GLY	-	expression tag	UNP Q72497
H	145	GLY	-	expression tag	UNP Q72497
H	241	THR	PRO	engineered mutation	UNP Q72497
I	144	GLY	-	expression tag	UNP Q72497
I	145	GLY	-	expression tag	UNP Q72497
I	241	THR	PRO	engineered mutation	UNP Q72497
J	144	GLY	-	expression tag	UNP Q72497
J	145	GLY	-	expression tag	UNP Q72497
J	241	THR	PRO	engineered mutation	UNP Q72497
K	144	GLY	-	expression tag	UNP Q72497
K	145	GLY	-	expression tag	UNP Q72497
K	241	THR	PRO	engineered mutation	UNP Q72497
L	144	GLY	-	expression tag	UNP Q72497
L	145	GLY	-	expression tag	UNP Q72497
L	241	THR	PRO	engineered mutation	UNP Q72497

- Molecule 2 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				
			Total	C	H	O	P
2	G	1	42	6	6	24	6

- Molecule 3 is 3alpha-[(3-carboxy-3-methylbutanoyl)oxy]-8alpha,9beta,10alpha,13alpha,17alpha,19beta-lup-20(29)-en-28-oic acid (three-letter code: 2I4) (formula: $C_{36}H_{56}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			
			Total	C	H	O
3	I	1	96	36	54	6

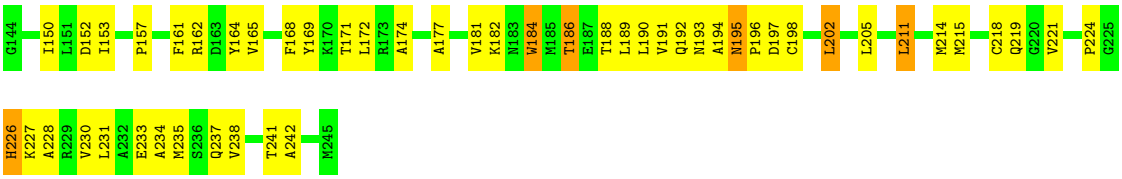
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

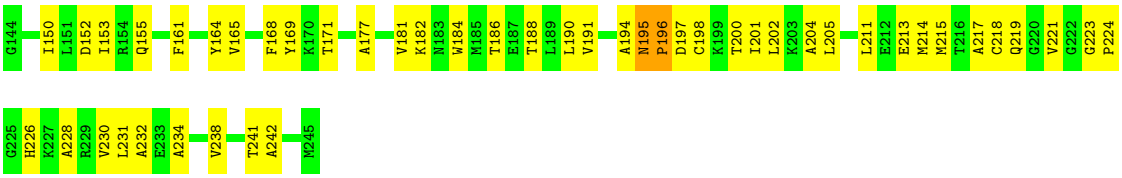
• Molecule 1: Gag polyprotein

Chain G:



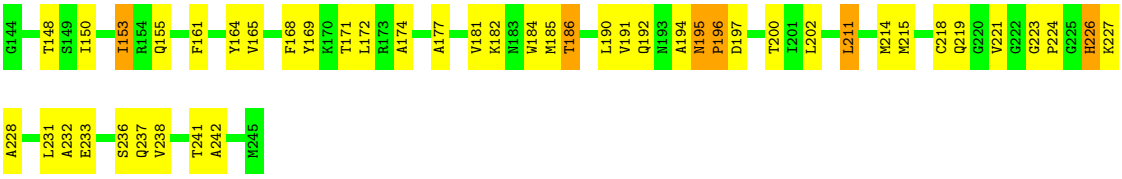
• Molecule 1: Gag polyprotein

Chain H:



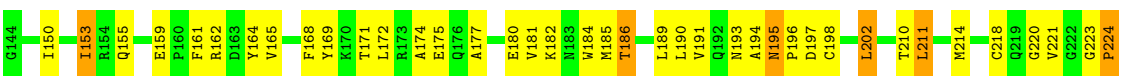
• Molecule 1: Gag polyprotein

Chain I:



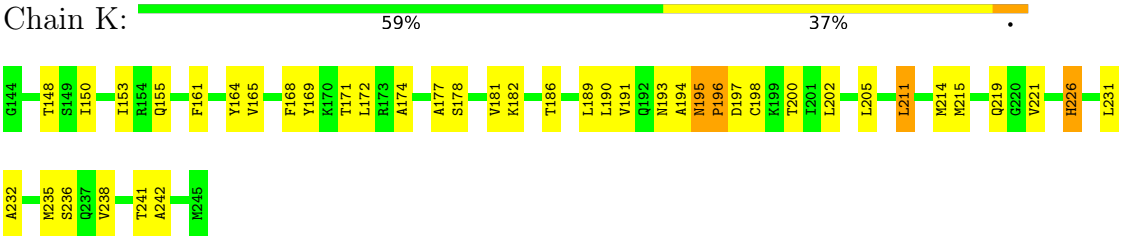
• Molecule 1: Gag polyprotein

Chain J:



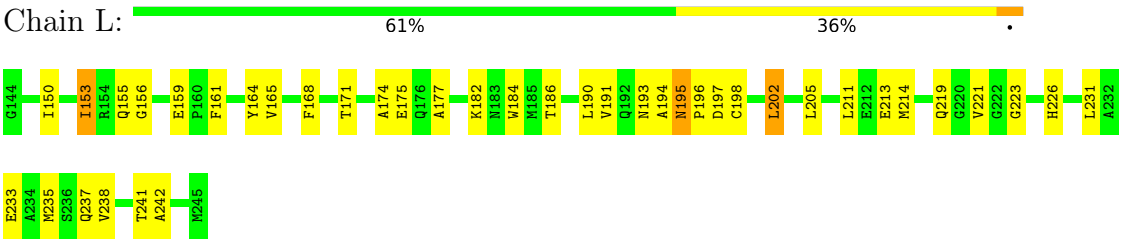
• Molecule 1: Gag polyprotein

Chain K:



• Molecule 1: Gag polyprotein

Chain L:



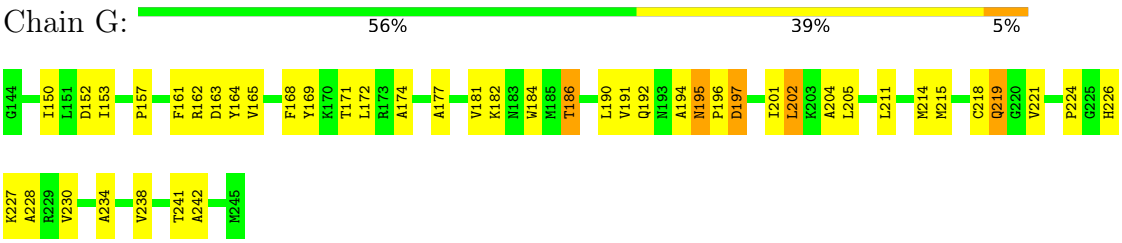
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

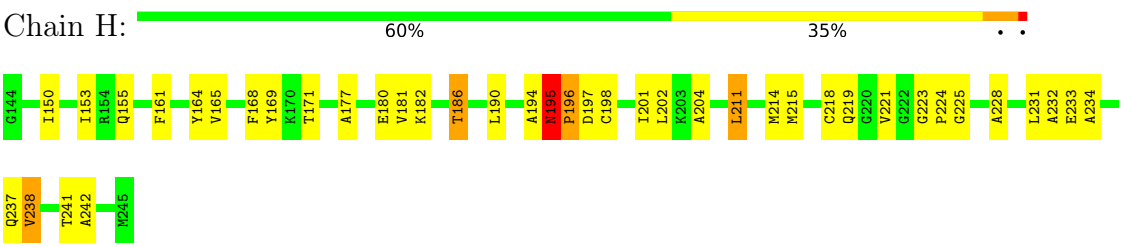
• Molecule 1: Gag polyprotein

Chain G:



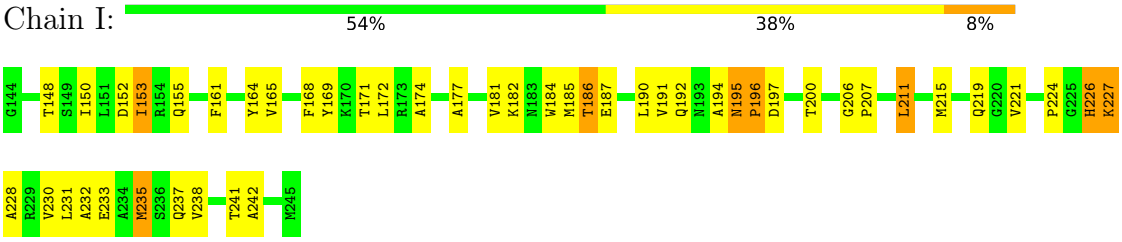
• Molecule 1: Gag polyprotein

Chain H:



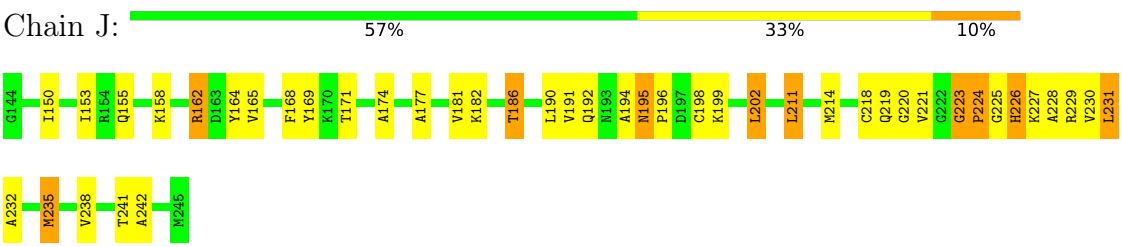
• Molecule 1: Gag polyprotein

Chain I:



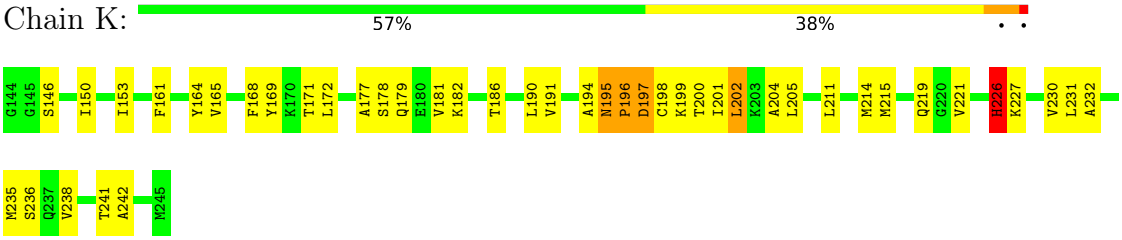
• Molecule 1: Gag polyprotein

Chain J:



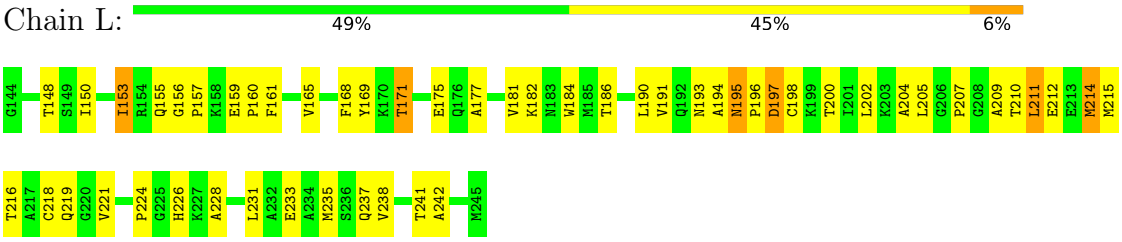
• Molecule 1: Gag polyprotein

Chain K:



• Molecule 1: Gag polyprotein

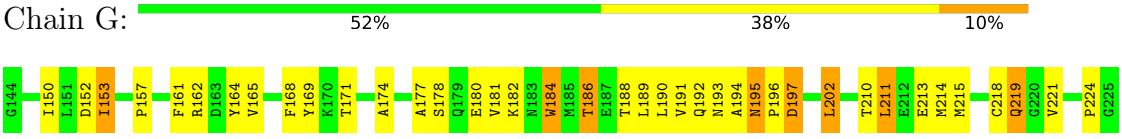
Chain L:



4.2.2 Score per residue for model 2

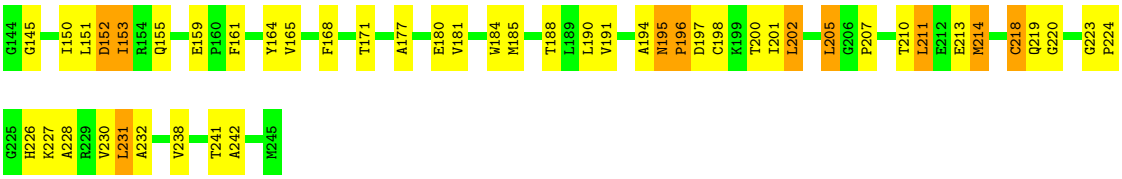
• Molecule 1: Gag polyprotein

Chain G:



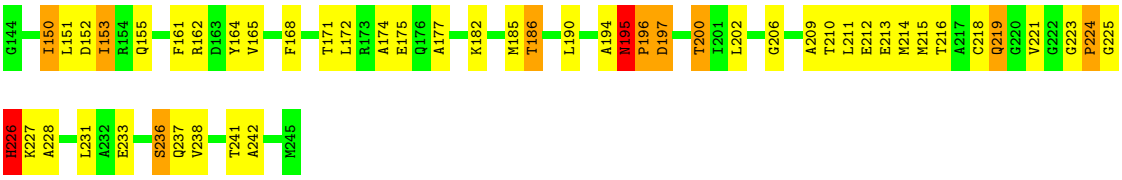
• Molecule 1: Gag polyprotein

Chain H:



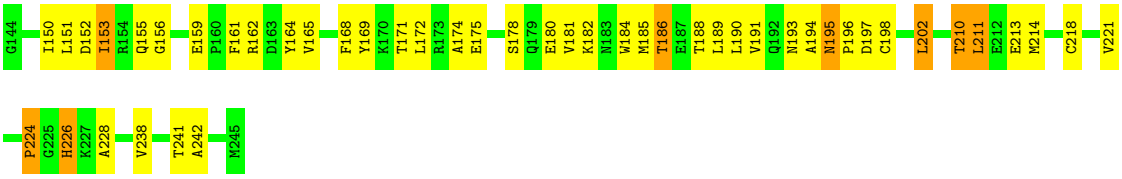
• Molecule 1: Gag polyprotein

Chain I:



• Molecule 1: Gag polyprotein

Chain J:

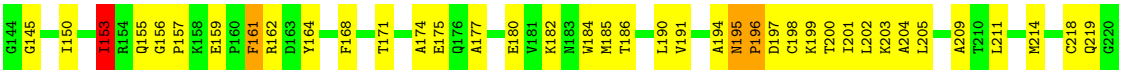


• Molecule 1: Gag polyprotein

Chain K:

• Molecule 1: Gag polyprotein

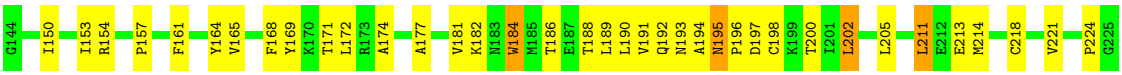
Chain L:



4.2.3 Score per residue for model 3

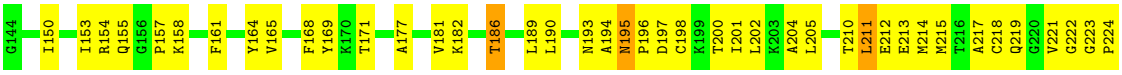
• Molecule 1: Gag polyprotein

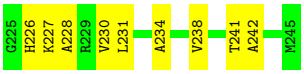
Chain G:



• Molecule 1: Gag polyprotein

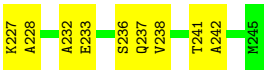
Chain H:





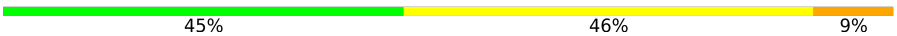
• Molecule 1: Gag polyprotein

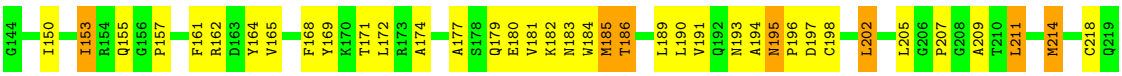
Chain I:



• Molecule 1: Gag polyprotein

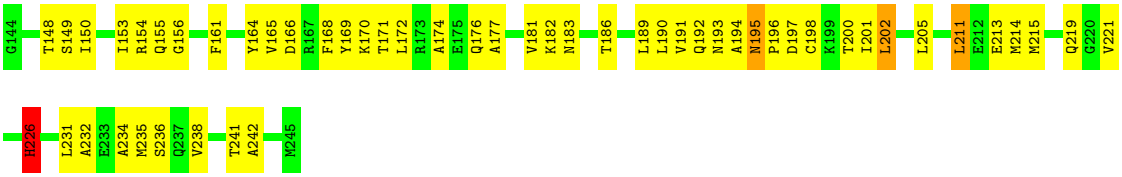
Chain J:





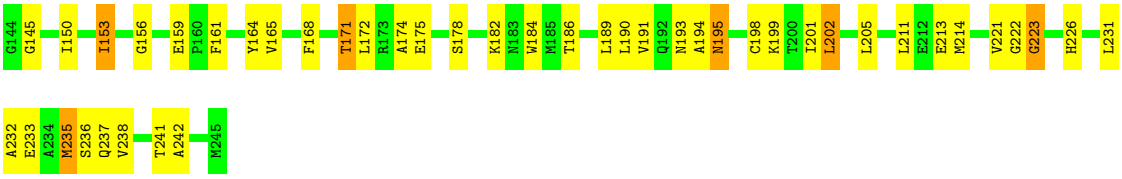
• Molecule 1: Gag polyprotein

Chain K:



• Molecule 1: Gag polyprotein

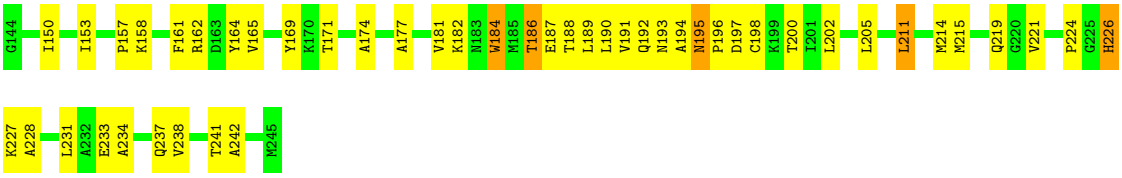
Chain L:



4.2.4 Score per residue for model 4

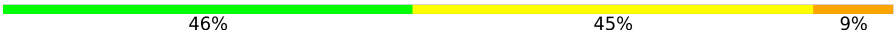
• Molecule 1: Gag polyprotein

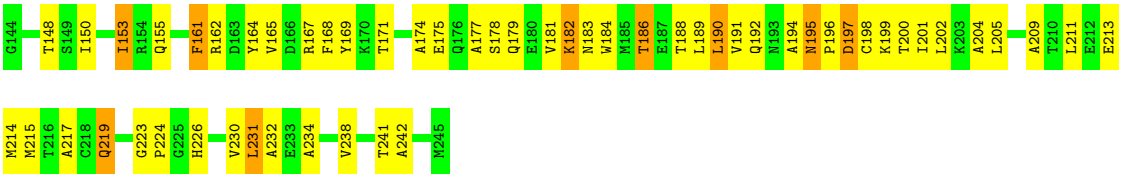
Chain G:



• Molecule 1: Gag polyprotein

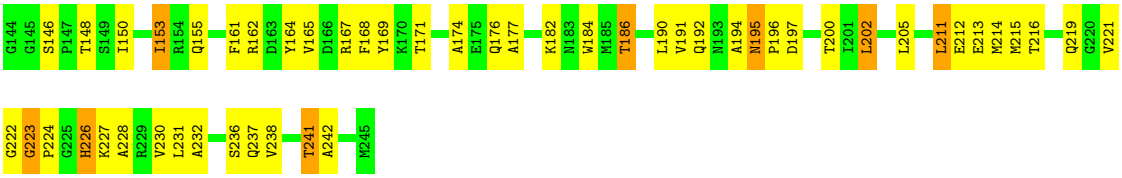
Chain H:





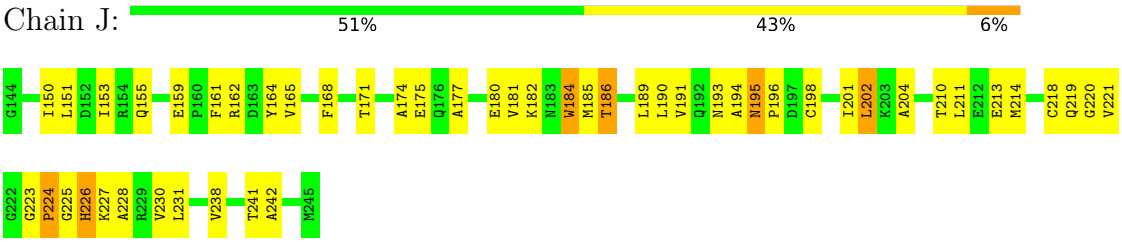
• Molecule 1: Gag polyprotein

Chain I:



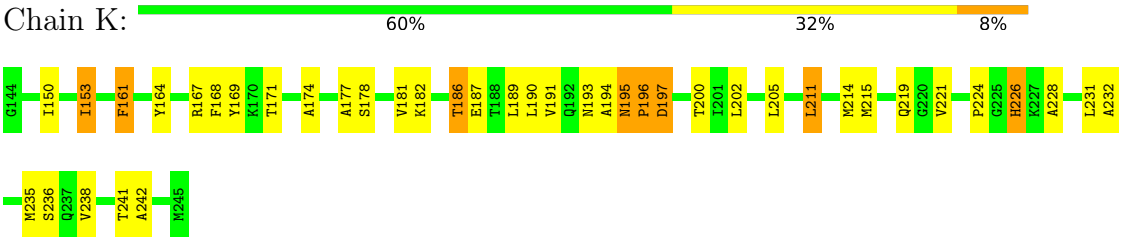
• Molecule 1: Gag polyprotein

Chain J:



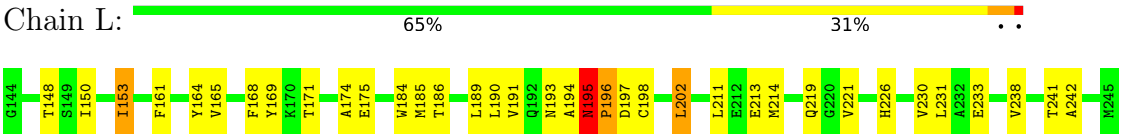
• Molecule 1: Gag polyprotein

Chain K:



• Molecule 1: Gag polyprotein

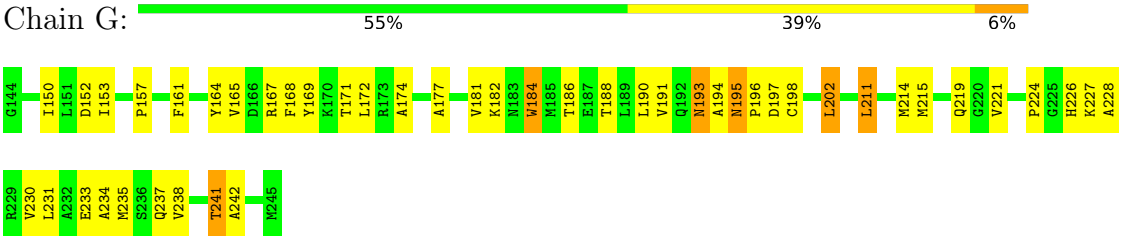
Chain L:



4.2.5 Score per residue for model 5

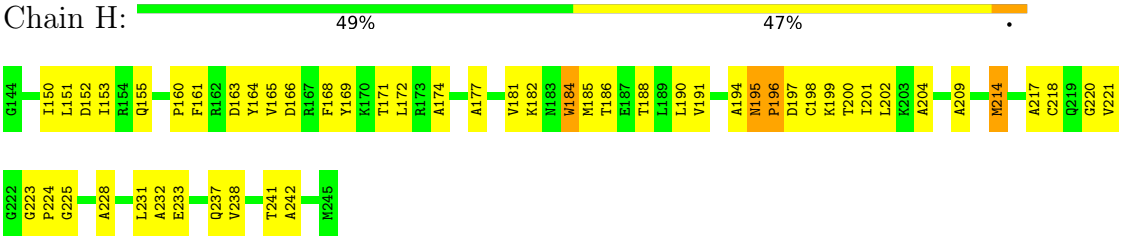
• Molecule 1: Gag polyprotein

Chain G:



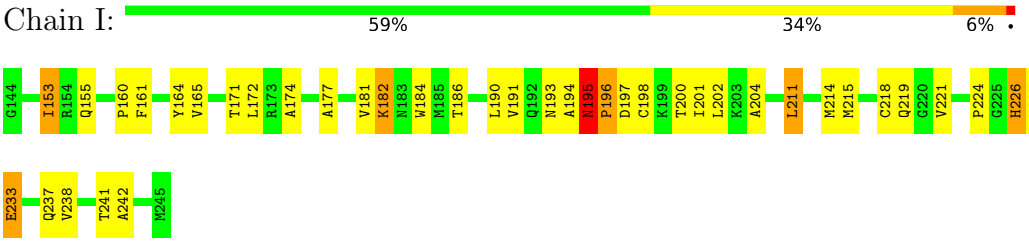
• Molecule 1: Gag polyprotein

Chain H:



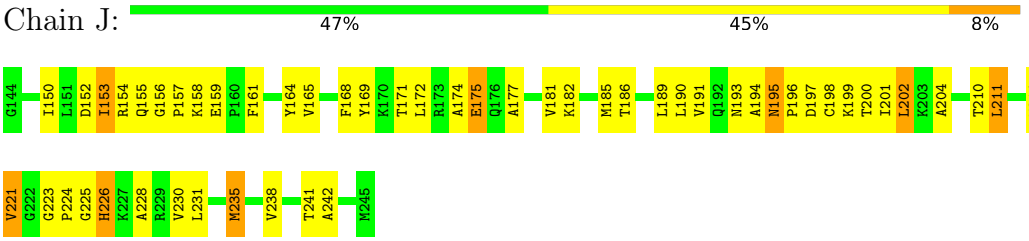
• Molecule 1: Gag polyprotein

Chain I:



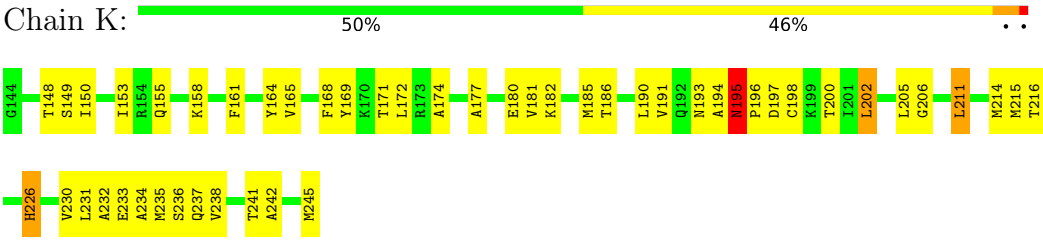
• Molecule 1: Gag polyprotein

Chain J:



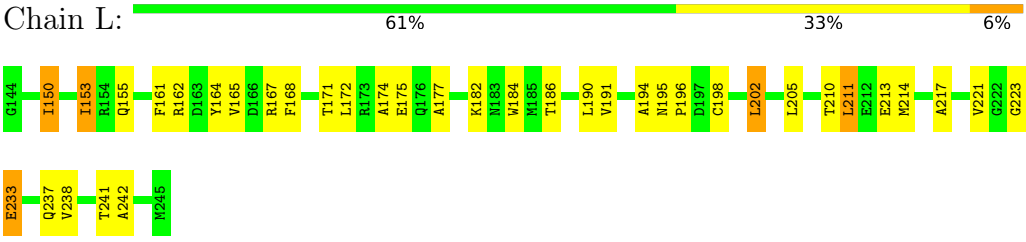
• Molecule 1: Gag polyprotein

Chain K:



• Molecule 1: Gag polyprotein

Chain L:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing.*

Of the 100 calculated structures, 5 were deposited, based on the following criterion: *structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
TALOS-N	structure calculation	
X-PLOR NIH	structure calculation	2.53
X-PLOR NIH	refinement	2.53

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	770
Number of shifts mapped to atoms	770
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, 2I4

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 (average) 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	G	0.91±0.02	0±0/785 (0.0± 0.0%)	0.97±0.02	0±0/1060 (0.0± 0.0%)
1	H	0.83±0.02	0±0/785 (0.0± 0.0%)	0.94±0.01	0±0/1060 (0.0± 0.0%)
1	I	0.89±0.03	0±0/785 (0.0± 0.0%)	0.96±0.03	0±0/1060 (0.0± 0.0%)
1	J	0.87±0.02	0±0/785 (0.0± 0.0%)	0.97±0.01	1±0/1060 (0.1± 0.0%)
1	K	0.88±0.01	0±0/785 (0.0± 0.1%)	0.95±0.01	1±0/1060 (0.1± 0.0%)
1	L	0.85±0.01	0±0/785 (0.0± 0.0%)	0.95±0.01	0±0/1060 (0.0± 0.0%)
All	All	0.87	1/23550 (0.0%)	0.96	10/31800 (0.0%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	K	226	HIS	C-N	-5.09	1.22	1.34	1	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	K	226	HIS	CA-CB-CG	-7.11	101.51	113.60	2	4
1	J	226	HIS	CA-CB-CG	-6.56	102.45	113.60	2	3
1	I	226	HIS	CA-CB-CG	-5.98	103.44	113.60	2	1
1	L	226	HIS	CA-CB-CG	-5.04	105.03	113.60	5	1
1	G	226	HIS	CA-CB-CG	-5.03	105.05	113.60	3	1

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	G	773	778	775	40±1
1	H	773	778	775	45±5
1	I	773	778	775	39±4
1	J	773	778	775	48±4
1	K	773	778	775	45±2
1	L	773	778	775	36±6
3	I	42	54	0	2±1
All	All	23580	23640	23280	1200

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 26.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:234:ALA:HB1	1:H:232:ALA:HB2	0.91	1.42	5	3
1:K:234:ALA:HB1	1:L:232:ALA:HB2	0.88	1.43	5	1
1:L:165:VAL:HG12	1:L:190:LEU:HD11	0.86	1.42	5	1
1:K:221:VAL:HG22	1:K:226:HIS:CE1	0.84	2.07	1	4
1:J:191:VAL:HG22	1:J:202:LEU:HD22	0.83	1.48	5	1
1:H:190:LEU:O	1:H:194:ALA:HB2	0.82	1.73	1	5
1:K:190:LEU:O	1:K:194:ALA:HB2	0.81	1.74	4	5
1:J:238:VAL:O	1:J:242:ALA:HB2	0.81	1.75	2	5
1:G:238:VAL:O	1:G:242:ALA:HB2	0.80	1.75	3	5
1:G:232:ALA:HB2	1:L:234:ALA:HB1	0.80	1.55	2	1
1:J:161:PHE:O	1:J:165:VAL:HG23	0.79	1.78	4	1
1:K:238:VAL:O	1:K:242:ALA:HB2	0.78	1.78	3	5
1:H:238:VAL:O	1:H:242:ALA:HB2	0.78	1.76	3	5
1:H:221:VAL:HG22	1:H:226:HIS:CE1	0.78	2.13	3	1
1:G:190:LEU:O	1:G:194:ALA:HB2	0.77	1.80	4	5
1:G:182:LYS:O	1:G:186:THR:HG23	0.77	1.78	3	2
1:G:191:VAL:HG22	1:G:202:LEU:HD22	0.77	1.54	5	1
1:H:198:CYS:O	1:H:202:LEU:HD12	0.76	1.78	4	5
1:K:230:VAL:HG11	1:L:228:ALA:HB1	0.76	1.54	1	1
1:H:234:ALA:HB1	1:I:232:ALA:HB2	0.75	1.57	4	2
1:K:177:ALA:HB3	1:K:182:LYS:HG3	0.74	1.58	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:J:202:LEU:HD21	1:J:214:MET:SD	0.74	2.21	5	4
1:H:191:VAL:HG12	1:H:202:LEU:HD22	0.74	1.59	4	1
1:G:234:ALA:HB1	1:H:232:ALA:CB	0.73	2.12	5	3
1:G:234:ALA:O	1:G:238:VAL:HG23	0.73	1.82	1	1
1:J:221:VAL:HG22	1:J:226:HIS:NE2	0.72	1.99	3	5
1:I:190:LEU:HD23	1:I:211:LEU:HD21	0.72	1.60	5	1
1:I:221:VAL:HG22	1:I:226:HIS:CE1	0.72	2.19	3	4
1:I:221:VAL:HG22	1:I:226:HIS:NE2	0.72	1.99	4	3
1:I:202:LEU:HD21	1:I:214:MET:SD	0.71	2.25	3	3
1:J:150:ILE:HG21	1:J:185:MET:HG2	0.71	1.61	2	2
1:H:182:LYS:O	1:H:186:THR:HG23	0.71	1.85	5	1
1:H:205:LEU:HD11	1:H:217:ALA:HB3	0.71	1.62	4	2
1:H:202:LEU:HD23	1:H:214:MET:SD	0.71	2.26	4	1
1:G:221:VAL:HG22	1:G:226:HIS:CE1	0.70	2.22	5	5
1:I:238:VAL:O	1:I:242:ALA:HB2	0.70	1.86	5	5
1:L:238:VAL:O	1:L:242:ALA:HB2	0.70	1.86	1	5
1:I:190:LEU:CD2	1:I:211:LEU:HD21	0.69	2.17	4	2
1:J:171:THR:O	1:J:174:ALA:HB3	0.69	1.88	4	5
1:K:150:ILE:HD11	1:K:168:PHE:CD2	0.69	2.23	1	4
1:H:177:ALA:HB1	1:H:181:VAL:CG1	0.68	2.18	5	4
1:J:150:ILE:HD11	1:J:168:PHE:CD2	0.68	2.23	1	5
1:K:198:CYS:SG	1:K:221:VAL:HG21	0.68	2.28	1	4
1:L:190:LEU:O	1:L:194:ALA:HB2	0.68	1.88	2	2
1:I:231:LEU:HD12	1:J:231:LEU:HD22	0.68	1.65	4	1
1:J:182:LYS:O	1:J:186:THR:HG23	0.68	1.89	5	1
1:H:169:TYR:OH	1:H:190:LEU:HD22	0.68	1.89	4	2
1:K:191:VAL:HG22	1:K:202:LEU:HD22	0.67	1.64	5	1
1:J:238:VAL:HG21	1:K:235:MET:HB3	0.67	1.66	4	4
1:I:150:ILE:HG21	1:I:185:MET:HG2	0.67	1.65	1	1
1:J:189:LEU:HD12	1:J:193:ASN:ND2	0.67	2.03	2	1
1:L:205:LEU:HD21	1:L:217:ALA:HB2	0.67	1.67	5	1
1:H:211:LEU:HD22	1:H:214:MET:SD	0.67	2.30	3	3
1:L:194:ALA:O	1:L:198:CYS:HB2	0.67	1.89	5	3
1:K:175:GLU:OE1	1:K:177:ALA:HB2	0.67	1.90	2	1
1:K:150:ILE:HG21	1:K:185:MET:HG2	0.67	1.67	2	1
1:J:190:LEU:O	1:J:194:ALA:HB2	0.66	1.90	4	5
1:K:172:LEU:HD21	1:K:182:LYS:O	0.66	1.90	2	2
1:J:153:ILE:HD11	1:J:171:THR:OG1	0.66	1.90	1	1
1:K:221:VAL:HG22	1:K:226:HIS:ND1	0.66	2.05	2	3
1:J:210:THR:HG23	1:J:213:GLU:H	0.66	1.50	2	2
1:H:205:LEU:HD11	1:H:217:ALA:CB	0.66	2.20	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:I:191:VAL:HG12	1:I:202:LEU:CD2	0.66	2.21	4	1
1:J:150:ILE:HD11	1:J:168:PHE:CG	0.66	2.25	4	3
1:L:148:THR:O	1:L:171:THR:HG22	0.66	1.91	1	1
1:I:190:LEU:O	1:I:194:ALA:HB2	0.66	1.91	5	3
1:H:197:ASP:O	1:H:200:THR:HG22	0.66	1.91	2	2
1:G:232:ALA:CB	1:L:234:ALA:HB1	0.65	2.20	2	1
1:G:189:LEU:O	1:G:193:ASN:OD1	0.65	2.14	4	2
1:J:189:LEU:HD12	1:J:193:ASN:HD21	0.65	1.51	2	1
1:K:202:LEU:HD21	1:K:214:MET:SD	0.65	2.32	5	3
1:I:168:PHE:CE2	1:I:186:THR:HA	0.65	2.26	3	4
1:I:227:LYS:O	1:I:231:LEU:HD12	0.65	1.92	5	2
1:K:211:LEU:HD22	1:K:214:MET:SD	0.65	2.32	3	3
1:L:221:VAL:HG22	1:L:226:HIS:CE1	0.65	2.27	4	5
1:H:202:LEU:HD21	1:H:214:MET:SD	0.64	2.31	1	3
1:L:171:THR:O	1:L:174:ALA:HB3	0.64	1.92	2	3
1:G:202:LEU:HD21	1:G:214:MET:SD	0.64	2.32	3	3
1:L:194:ALA:O	1:L:195:ASN:O	0.64	2.14	4	2
1:I:150:ILE:HD11	1:I:168:PHE:O	0.64	1.91	2	1
1:J:162:ARG:O	1:J:165:VAL:HG12	0.64	1.93	1	2
1:K:221:VAL:HG13	1:K:226:HIS:ND1	0.64	2.07	5	3
1:I:171:THR:O	1:I:174:ALA:HB3	0.64	1.91	1	5
1:I:177:ALA:HB3	1:I:182:LYS:HG3	0.63	1.70	4	3
1:J:164:TYR:CE2	1:J:190:LEU:HD12	0.63	2.28	2	5
1:G:189:LEU:HD12	1:G:193:ASN:ND2	0.63	2.08	2	1
1:I:181:VAL:HG13	1:I:184:TRP:CD1	0.63	2.28	3	1
1:K:161:PHE:CE1	1:K:194:ALA:HB1	0.63	2.27	4	1
1:K:191:VAL:HG12	1:K:202:LEU:CD2	0.63	2.23	4	1
1:I:177:ALA:HB3	1:I:182:LYS:CG	0.63	2.24	1	2
1:I:172:LEU:HD22	1:I:186:THR:HG22	0.63	1.71	5	1
1:J:177:ALA:HB1	1:J:181:VAL:CG1	0.63	2.24	1	4
1:J:150:ILE:HG21	1:J:185:MET:SD	0.63	2.34	5	1
1:L:177:ALA:HB3	1:L:182:LYS:HG2	0.63	1.71	1	1
1:L:198:CYS:O	1:L:202:LEU:HD12	0.63	1.94	4	1
1:H:177:ALA:HB3	1:H:182:LYS:HG2	0.62	1.69	5	1
1:H:224:PRO:O	1:H:228:ALA:HB3	0.62	1.93	1	2
1:J:177:ALA:HB3	1:J:182:LYS:CG	0.62	2.24	4	2
1:I:191:VAL:HG22	1:I:202:LEU:CD2	0.62	2.24	5	1
1:H:164:TYR:CE2	1:H:190:LEU:HD12	0.62	2.30	1	5
1:K:161:PHE:HE1	1:K:194:ALA:HB1	0.62	1.54	4	1
1:K:150:ILE:HG22	1:K:175:GLU:OE2	0.62	1.94	2	1
1:H:150:ILE:HD11	1:H:168:PHE:CD2	0.62	2.30	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:L:150:ILE:HD11	1:L:168:PHE:CG	0.61	2.29	3	2
1:J:224:PRO:O	1:J:228:ALA:HB3	0.61	1.95	3	5
1:K:150:ILE:HD12	1:K:153:ILE:HG13	0.61	1.71	3	3
1:I:202:LEU:HD12	1:I:218:CYS:SG	0.61	2.35	3	1
1:K:197:ASP:O	1:K:200:THR:HG22	0.61	1.96	2	2
1:L:172:LEU:HD21	1:L:182:LYS:HB3	0.61	1.72	5	1
1:I:231:LEU:HD12	1:J:231:LEU:CD2	0.60	2.26	4	1
1:K:171:THR:O	1:K:174:ALA:HB3	0.60	1.96	3	4
1:I:164:TYR:CE2	1:I:190:LEU:HD12	0.60	2.31	4	4
1:G:211:LEU:HD22	1:G:214:MET:SD	0.60	2.37	2	3
3:I:301:2I4:O2	1:L:231:LEU:HD11	0.60	1.96	4	2
1:K:198:CYS:O	1:K:202:LEU:HD12	0.60	1.95	3	1
1:I:222:GLY:O	1:I:223:GLY:O	0.60	2.18	4	1
1:K:191:VAL:CG2	1:K:202:LEU:HD22	0.59	2.27	5	2
1:G:233:GLU:O	1:G:237:GLN:N	0.59	2.35	5	3
1:H:191:VAL:HG12	1:H:202:LEU:CD2	0.59	2.27	4	1
1:J:202:LEU:HD12	1:J:218:CYS:SG	0.59	2.38	1	3
1:K:226:HIS:CD2	1:K:230:VAL:HG23	0.59	2.32	1	2
1:L:150:ILE:HD11	1:L:168:PHE:CD2	0.59	2.32	3	2
1:J:221:VAL:HG22	1:J:226:HIS:CD2	0.59	2.33	5	5
1:J:161:PHE:O	1:J:165:VAL:HG12	0.59	1.97	5	2
1:I:161:PHE:O	1:I:165:VAL:HG23	0.59	1.97	4	1
1:I:182:LYS:O	1:I:186:THR:HG23	0.59	1.97	5	1
1:G:150:ILE:HD12	1:G:153:ILE:HG13	0.59	1.75	5	5
1:H:171:THR:O	1:H:174:ALA:HB3	0.59	1.98	4	2
1:G:171:THR:O	1:G:174:ALA:HB3	0.58	1.98	5	5
1:I:169:TYR:OH	1:I:186:THR:HG23	0.58	1.98	1	2
1:J:150:ILE:HD12	1:J:153:ILE:HG13	0.58	1.73	1	2
1:G:169:TYR:OH	1:G:186:THR:HG23	0.58	1.98	1	3
1:K:177:ALA:HB1	1:K:181:VAL:HB	0.58	1.76	5	3
1:L:172:LEU:HD22	1:L:186:THR:HG22	0.58	1.75	3	1
1:L:189:LEU:O	1:L:193:ASN:OD1	0.58	2.22	4	2
1:K:177:ALA:HB3	1:K:182:LYS:CG	0.58	2.28	5	3
1:G:191:VAL:HG22	1:G:202:LEU:CD2	0.58	2.28	5	1
1:J:150:ILE:HG21	1:J:185:MET:CG	0.58	2.29	2	1
1:G:231:LEU:O	1:G:235:MET:HB2	0.58	1.99	3	1
1:I:233:GLU:O	1:I:237:GLN:N	0.58	2.36	5	4
1:G:198:CYS:O	1:G:202:LEU:HD12	0.57	1.99	3	3
1:J:205:LEU:HB3	1:J:209:ALA:HB2	0.57	1.76	3	1
1:G:228:ALA:HB1	1:L:230:VAL:HG11	0.57	1.76	4	1
1:J:220:GLY:O	1:J:225:GLY:HA3	0.57	1.99	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:177:ALA:HB3	1:G:182:LYS:HG3	0.57	1.75	4	5
1:I:181:VAL:O	1:I:185:MET:HB2	0.57	1.99	1	1
1:K:187:GLU:O	1:K:191:VAL:HG13	0.57	1.99	4	1
1:G:191:VAL:HG12	1:G:202:LEU:CD2	0.57	2.29	4	1
1:L:164:TYR:CE2	1:L:190:LEU:HD12	0.57	2.35	5	3
1:I:231:LEU:CD2	1:J:231:LEU:HD13	0.57	2.30	5	1
1:I:150:ILE:HG21	1:I:185:MET:CG	0.57	2.28	1	1
1:K:150:ILE:HD11	1:K:168:PHE:CG	0.57	2.34	5	4
1:G:164:TYR:CE2	1:G:190:LEU:HD12	0.57	2.35	3	5
1:G:202:LEU:HD12	1:G:218:CYS:SG	0.57	2.40	1	2
1:L:161:PHE:CE1	1:L:202:LEU:HD11	0.56	2.35	5	3
1:J:191:VAL:HG22	1:J:202:LEU:CD2	0.56	2.29	5	1
1:L:182:LYS:O	1:L:186:THR:HG23	0.56	1.99	3	2
1:H:210:THR:HG23	1:H:213:GLU:H	0.56	1.60	2	1
1:L:191:VAL:HG23	1:L:202:LEU:CB	0.56	2.30	3	1
1:L:233:GLU:O	1:L:237:GLN:N	0.56	2.38	1	2
1:G:231:LEU:HD13	1:H:231:LEU:HD21	0.56	1.78	4	1
1:H:150:ILE:HD11	1:H:168:PHE:CG	0.56	2.36	1	5
1:H:177:ALA:HB3	1:H:182:LYS:CG	0.56	2.31	5	1
1:J:172:LEU:HD21	1:J:182:LYS:HB3	0.55	1.77	5	2
1:K:153:ILE:HD11	1:K:171:THR:OG1	0.55	2.01	1	2
1:J:150:ILE:HG12	1:J:172:LEU:HD13	0.55	1.78	2	1
1:J:194:ALA:O	1:J:195:ASN:O	0.55	2.24	5	2
1:G:195:ASN:O	1:G:197:ASP:N	0.55	2.40	5	5
1:J:238:VAL:HG22	1:K:232:ALA:O	0.55	2.02	1	4
1:K:150:ILE:HG21	1:K:185:MET:CG	0.55	2.30	2	1
1:H:189:LEU:O	1:H:193:ASN:OD1	0.55	2.25	3	1
1:K:195:ASN:ND2	1:K:221:VAL:HG11	0.55	2.16	3	1
1:H:150:ILE:HD12	1:H:153:ILE:HG13	0.55	1.76	1	3
1:K:191:VAL:HG12	1:K:202:LEU:HD23	0.55	1.77	4	1
1:K:194:ALA:O	1:K:195:ASN:O	0.55	2.24	2	5
1:L:164:TYR:OH	1:L:193:ASN:OD1	0.55	2.24	4	2
1:G:235:MET:HB3	1:L:238:VAL:HG21	0.55	1.78	5	1
1:L:224:PRO:O	1:L:228:ALA:N	0.55	2.39	1	2
1:K:215:MET:O	1:K:219:GLN:N	0.55	2.39	4	4
1:I:161:PHE:O	1:I:165:VAL:HG12	0.55	2.01	3	4
1:J:191:VAL:HB	1:J:202:LEU:HD22	0.55	1.79	1	1
1:J:201:ILE:O	1:J:204:ALA:HB3	0.55	2.02	5	2
1:H:172:LEU:HD22	1:H:186:THR:HG22	0.55	1.79	5	1
1:I:226:HIS:CD2	1:I:230:VAL:HG21	0.54	2.36	1	1
1:H:177:ALA:HB1	1:H:181:VAL:HB	0.54	1.78	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:172:LEU:CD2	1:H:186:THR:HG22	0.54	2.32	5	1
1:L:150:ILE:O	1:L:153:ILE:HB	0.54	2.02	4	4
1:H:157:PRO:CG	1:I:219:GLN:O	0.54	2.54	3	1
1:G:215:MET:O	1:G:219:GLN:HB2	0.54	2.01	2	3
1:L:190:LEU:CD2	1:L:211:LEU:HD21	0.54	2.32	5	2
1:J:189:LEU:O	1:J:193:ASN:OD1	0.54	2.25	5	3
1:G:177:ALA:HB1	1:G:181:VAL:CG1	0.54	2.32	1	5
1:J:169:TYR:OH	1:J:186:THR:HG23	0.54	2.02	1	2
1:J:150:ILE:O	1:J:153:ILE:HB	0.54	2.02	2	3
1:H:205:LEU:HD13	1:H:213:GLU:HG3	0.54	1.80	3	2
1:L:150:ILE:HD12	1:L:153:ILE:HG13	0.54	1.78	4	2
1:G:164:TYR:OH	1:G:193:ASN:OD1	0.54	2.25	3	2
1:J:154:ARG:HA	1:J:193:ASN:O	0.54	2.02	5	1
1:J:168:PHE:HE2	1:J:186:THR:HG22	0.54	1.62	5	1
1:G:221:VAL:HG22	1:G:226:HIS:NE2	0.54	2.17	3	2
1:I:172:LEU:CD2	1:I:186:THR:HG22	0.54	2.31	5	1
1:H:150:ILE:O	1:H:153:ILE:HB	0.54	2.03	5	3
1:L:209:ALA:HB3	1:L:214:MET:SD	0.54	2.42	2	1
1:L:231:LEU:O	1:L:235:MET:HB2	0.54	2.03	3	1
1:K:164:TYR:CE2	1:K:190:LEU:HD12	0.54	2.38	5	4
1:H:210:THR:HG22	1:H:212:GLU:H	0.53	1.61	3	1
1:I:224:PRO:O	1:I:228:ALA:N	0.53	2.42	5	3
1:I:189:LEU:O	1:I:193:ASN:CG	0.53	2.46	3	1
1:H:214:MET:O	1:H:217:ALA:N	0.53	2.41	5	1
1:L:197:ASP:O	1:L:200:THR:HG22	0.53	2.03	2	1
1:K:153:ILE:HG22	1:K:153:ILE:O	0.53	2.04	1	2
1:H:161:PHE:CG	1:H:218:CYS:SG	0.53	3.01	5	1
1:H:194:ALA:O	1:H:195:ASN:O	0.53	2.27	1	3
1:L:191:VAL:HG23	1:L:202:LEU:HB3	0.53	1.80	3	2
1:J:205:LEU:CB	1:J:209:ALA:HB2	0.53	2.34	3	1
1:L:191:VAL:HG22	1:L:202:LEU:HD22	0.53	1.81	5	1
1:I:191:VAL:HG22	1:I:202:LEU:HD23	0.53	1.80	5	1
1:J:172:LEU:HD12	1:J:175:GLU:HG2	0.53	1.81	5	1
1:I:187:GLU:O	1:I:191:VAL:HG12	0.53	2.03	1	1
1:G:219:GLN:O	1:L:157:PRO:HG3	0.53	2.04	2	1
1:H:209:ALA:HB3	1:H:214:MET:SD	0.53	2.43	5	1
1:L:200:THR:O	1:L:204:ALA:N	0.52	2.42	1	2
1:L:172:LEU:O	1:L:175:GLU:O	0.52	2.26	5	2
1:I:206:GLY:O	1:I:209:ALA:HB2	0.52	2.04	2	1
1:H:155:GLN:HG3	1:H:164:TYR:HB2	0.52	1.82	3	2
1:K:164:TYR:OH	1:K:193:ASN:OD1	0.52	2.25	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:195:ASN:O	1:H:197:ASP:N	0.52	2.42	2	5
1:G:189:LEU:HD12	1:G:193:ASN:HD21	0.52	1.62	2	1
1:J:191:VAL:HG23	1:J:202:LEU:HB3	0.52	1.80	2	2
1:I:224:PRO:O	1:I:228:ALA:HB3	0.52	2.05	3	1
1:L:172:LEU:HD21	1:L:182:LYS:CB	0.52	2.35	5	1
1:L:172:LEU:HD22	1:L:186:THR:CG2	0.52	2.33	5	1
1:K:211:LEU:HD23	1:K:214:MET:SD	0.52	2.45	1	1
1:K:189:LEU:O	1:K:193:ASN:OD1	0.52	2.28	3	2
1:G:157:PRO:HB3	1:H:220:GLY:O	0.52	2.05	2	2
1:K:169:TYR:OH	1:K:186:THR:HG23	0.52	2.04	4	2
1:G:153:ILE:O	1:G:153:ILE:HG22	0.52	2.05	2	4
1:G:161:PHE:O	1:G:165:VAL:HG12	0.52	2.05	5	4
1:J:172:LEU:O	1:J:175:GLU:O	0.52	2.27	2	1
1:I:155:GLN:OE1	1:I:156:GLY:O	0.52	2.27	3	1
1:H:215:MET:O	1:H:219:GLN:CB	0.52	2.59	3	1
1:K:150:ILE:HD12	1:K:153:ILE:HG12	0.52	1.81	5	1
1:G:153:ILE:HD11	1:G:171:THR:OG1	0.51	2.05	4	4
1:K:189:LEU:HD12	1:K:193:ASN:HD21	0.51	1.64	2	1
1:H:177:ALA:HB3	1:H:182:LYS:HG3	0.51	1.81	3	2
1:I:155:GLN:HB2	1:I:164:TYR:CD2	0.51	2.40	2	2
1:H:161:PHE:CE1	1:H:202:LEU:HD11	0.51	2.40	4	3
1:K:153:ILE:HD12	1:K:167:ARG:HG2	0.51	1.82	4	1
1:H:231:LEU:HD21	1:I:231:LEU:HD13	0.51	1.81	2	2
1:I:155:GLN:HB3	1:I:195:ASN:CB	0.51	2.35	3	2
1:J:181:VAL:O	1:J:185:MET:HG3	0.51	2.05	3	1
1:H:238:VAL:HG22	1:I:236:SER:HB3	0.51	1.81	4	1
1:I:195:ASN:O	1:I:197:ASP:N	0.51	2.44	2	5
1:H:191:VAL:HG23	1:H:202:LEU:CB	0.51	2.36	2	1
1:G:161:PHE:O	1:G:165:VAL:HG23	0.51	2.05	4	1
1:K:224:PRO:O	1:K:228:ALA:N	0.51	2.44	4	1
1:L:191:VAL:HG12	1:L:202:LEU:HD22	0.51	1.82	4	1
1:J:231:LEU:O	1:J:235:MET:HB2	0.51	2.04	5	2
1:H:238:VAL:HG13	1:I:236:SER:CB	0.51	2.36	4	2
1:K:195:ASN:O	1:K:197:ASP:N	0.51	2.44	1	5
1:H:152:ASP:O	1:H:152:ASP:CG	0.51	2.49	2	1
1:L:155:GLN:O	1:L:195:ASN:HB2	0.51	2.06	2	1
1:J:164:TYR:OH	1:J:193:ASN:OD1	0.51	2.24	3	3
1:L:198:CYS:O	1:L:201:ILE:HB	0.51	2.06	3	1
1:J:211:LEU:HD22	1:J:214:MET:SD	0.50	2.45	2	2
1:L:155:GLN:HB3	1:L:195:ASN:N	0.50	2.22	1	1
1:I:150:ILE:O	1:I:153:ILE:HB	0.50	2.06	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:J:164:TYR:HE2	1:J:190:LEU:HD12	0.50	1.65	1	3
1:J:194:ALA:O	1:J:198:CYS:HB2	0.50	2.07	5	4
1:K:189:LEU:HD12	1:K:193:ASN:ND2	0.50	2.21	2	1
1:L:150:ILE:CD1	1:L:153:ILE:HG21	0.50	2.35	5	1
1:J:153:ILE:HG21	1:J:168:PHE:CD1	0.50	2.42	1	3
1:L:195:ASN:O	1:L:197:ASP:N	0.50	2.45	2	3
1:I:231:LEU:HD11	3:I:301:2I4:C12	0.50	2.37	4	1
1:G:227:LYS:HE2	1:H:224:PRO:HB3	0.50	1.82	2	3
1:I:177:ALA:HB3	1:I:182:LYS:HG2	0.50	1.83	1	1
1:J:177:ALA:HB1	1:J:181:VAL:HG12	0.50	1.82	4	2
1:L:225:GLY:O	1:L:228:ALA:HB3	0.50	2.07	2	1
1:I:150:ILE:HG21	1:I:185:MET:HB3	0.50	1.84	3	1
1:G:224:PRO:O	1:G:228:ALA:N	0.50	2.42	3	1
1:J:177:ALA:HB3	1:J:182:LYS:HG3	0.50	1.84	1	3
1:J:227:LYS:O	1:J:231:LEU:HD13	0.50	2.07	1	2
1:L:164:TYR:HH	1:L:168:PHE:HD1	0.50	1.49	2	1
1:J:211:LEU:HD22	1:J:214:MET:CE	0.50	2.37	3	1
1:I:224:PRO:O	1:I:228:ALA:CB	0.50	2.60	3	4
1:L:161:PHE:O	1:L:165:VAL:HG12	0.50	2.07	1	2
1:J:153:ILE:O	1:J:153:ILE:HG22	0.50	2.07	5	2
1:H:238:VAL:HG13	1:I:236:SER:HB3	0.50	1.83	4	1
1:J:150:ILE:CD1	1:J:168:PHE:O	0.49	2.60	3	4
1:G:157:PRO:HB2	1:H:222:GLY:C	0.49	2.27	3	1
1:L:205:LEU:HD12	1:L:214:MET:SD	0.49	2.47	2	2
1:H:153:ILE:HG21	1:H:168:PHE:CD1	0.49	2.42	1	4
1:I:153:ILE:CG1	1:I:171:THR:HG21	0.49	2.37	1	2
1:G:168:PHE:CE2	1:G:186:THR:HA	0.49	2.42	3	3
1:L:150:ILE:HD11	1:L:168:PHE:O	0.49	2.06	5	1
1:K:191:VAL:HG23	1:K:202:LEU:HD22	0.49	1.83	1	1
1:K:205:LEU:HD22	1:K:213:GLU:HB3	0.49	1.84	3	1
1:H:224:PRO:O	1:H:228:ALA:CB	0.49	2.61	1	2
1:H:155:GLN:HB3	1:H:195:ASN:N	0.49	2.22	4	2
1:I:227:LYS:HG2	3:I:301:2I4:O4	0.49	2.08	1	1
1:H:164:TYR:HE2	1:H:190:LEU:HD12	0.49	1.67	4	2
1:K:155:GLN:HB3	1:K:195:ASN:N	0.49	2.22	2	2
1:K:238:VAL:HG11	1:L:235:MET:SD	0.49	2.47	3	1
1:L:221:VAL:HA	1:L:226:HIS:CG	0.49	2.42	3	2
1:H:214:MET:O	1:H:218:CYS:SG	0.49	2.71	5	1
1:G:224:PRO:O	1:G:228:ALA:CB	0.49	2.61	1	4
1:I:227:LYS:HB3	3:I:301:2I4:O4	0.49	2.07	2	1
1:K:224:PRO:O	1:K:228:ALA:HB3	0.49	2.08	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:L:198:CYS:HA	1:L:201:ILE:HD12	0.49	1.84	2	1
1:I:155:GLN:OE1	1:I:195:ASN:CB	0.49	2.61	3	1
1:L:161:PHE:CE2	1:L:165:VAL:HG11	0.49	2.42	5	1
1:L:177:ALA:HB1	1:L:181:VAL:CG1	0.49	2.38	1	1
1:L:191:VAL:HA	1:L:202:LEU:HD22	0.49	1.85	1	2
1:I:223:GLY:O	1:I:225:GLY:N	0.49	2.46	2	1
1:H:178:SER:O	1:H:179:GLN:C	0.49	2.51	4	1
1:K:161:PHE:O	1:K:165:VAL:HG12	0.49	2.07	3	4
1:I:150:ILE:CD1	1:I:168:PHE:O	0.49	2.61	4	1
1:G:172:LEU:HD21	1:G:182:LYS:HB3	0.48	1.84	3	3
1:L:155:GLN:CG	1:L:159:GLU:O	0.48	2.61	1	1
1:J:153:ILE:O	1:J:193:ASN:HB3	0.48	2.08	2	1
1:L:161:PHE:O	1:L:165:VAL:HG23	0.48	2.07	4	1
1:J:177:ALA:HB3	1:J:182:LYS:HG2	0.48	1.83	4	2
1:K:186:THR:O	1:K:190:LEU:CB	0.48	2.62	1	5
1:H:184:TRP:CE3	1:H:188:THR:HG21	0.48	2.44	4	3
1:J:211:LEU:HD22	1:J:214:MET:HE1	0.48	1.85	3	1
1:L:202:LEU:HD21	1:L:214:MET:SD	0.48	2.48	3	1
1:G:177:ALA:HB3	1:G:182:LYS:CG	0.48	2.38	4	3
1:G:201:ILE:O	1:G:205:LEU:N	0.48	2.46	1	1
1:H:177:ALA:HB3	1:H:182:LYS:HD2	0.48	1.83	4	1
1:G:165:VAL:O	1:G:169:TYR:HD1	0.48	1.92	4	5
1:L:211:LEU:HD13	1:L:211:LEU:O	0.48	2.09	1	1
1:G:234:ALA:CB	1:H:232:ALA:HB2	0.48	2.32	1	2
1:J:226:HIS:O	1:J:230:VAL:HB	0.48	2.09	3	4
1:K:191:VAL:CB	1:K:202:LEU:HD22	0.48	2.38	1	1
1:K:195:ASN:O	1:K:196:PRO:C	0.48	2.51	3	4
1:H:177:ALA:HB1	1:H:181:VAL:HG11	0.48	1.84	2	2
1:K:168:PHE:CE2	1:K:186:THR:HA	0.48	2.44	2	1
1:I:184:TRP:CD1	1:I:184:TRP:C	0.48	2.85	3	1
1:K:177:ALA:O	1:K:182:LYS:HG3	0.48	2.09	5	2
1:J:169:TYR:N	1:J:169:TYR:CD1	0.48	2.82	2	1
1:K:177:ALA:O	1:K:178:SER:C	0.48	2.51	2	2
1:L:221:VAL:HG13	1:L:226:HIS:ND1	0.48	2.24	4	1
1:L:177:ALA:HB3	1:L:182:LYS:HG3	0.48	1.85	2	1
1:J:150:ILE:HD13	1:J:172:LEU:HB2	0.48	1.85	3	2
1:H:169:TYR:OH	1:H:186:THR:HG23	0.47	2.09	4	3
1:G:184:TRP:CZ3	1:G:188:THR:HG21	0.47	2.43	4	4
1:H:161:PHE:CD2	1:H:165:VAL:HG21	0.47	2.44	4	1
1:J:156:GLY:H	1:J:159:GLU:HB3	0.47	1.69	5	1
1:J:191:VAL:CG2	1:J:202:LEU:HD22	0.47	2.31	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:J:224:PRO:O	1:J:228:ALA:CB	0.47	2.62	5	5
1:J:229:ARG:O	1:J:232:ALA:HB3	0.47	2.08	1	2
1:K:194:ALA:O	1:K:198:CYS:HB2	0.47	2.08	1	2
1:J:191:VAL:CB	1:J:202:LEU:HD22	0.47	2.39	1	1
1:L:162:ARG:O	1:L:165:VAL:HG22	0.47	2.09	5	1
1:H:201:ILE:O	1:H:204:ALA:HB3	0.47	2.09	1	1
1:K:150:ILE:CD1	1:K:168:PHE:O	0.47	2.63	1	2
1:G:164:TYR:HH	1:G:168:PHE:HD1	0.47	1.49	2	2
1:J:178:SER:O	1:J:182:LYS:HB2	0.47	2.09	2	1
1:H:161:PHE:HZ	1:H:202:LEU:HD21	0.47	1.70	4	1
1:I:194:ALA:O	1:I:195:ASN:O	0.47	2.31	5	2
1:I:212:GLU:O	1:I:216:THR:N	0.47	2.48	2	2
1:G:205:LEU:HD22	1:G:213:GLU:HG3	0.47	1.85	3	1
1:K:165:VAL:O	1:K:169:TYR:HD1	0.47	1.92	5	2
1:L:161:PHE:CZ	1:L:202:LEU:HD11	0.47	2.45	2	1
1:G:189:LEU:O	1:G:193:ASN:CG	0.47	2.53	3	2
1:G:205:LEU:CD1	1:G:214:MET:HA	0.47	2.39	3	2
1:L:205:LEU:HD21	1:L:217:ALA:CB	0.47	2.38	5	1
1:K:169:TYR:CD1	1:K:169:TYR:N	0.47	2.81	1	4
1:I:194:ALA:O	1:I:195:ASN:HB3	0.47	2.10	4	3
1:I:227:LYS:O	1:I:231:LEU:HB2	0.47	2.10	4	1
1:L:178:SER:O	1:L:182:LYS:N	0.47	2.48	3	1
1:H:161:PHE:O	1:H:165:VAL:HG12	0.47	2.10	1	4
1:G:177:ALA:HB1	1:G:181:VAL:HG12	0.46	1.86	4	3
1:H:198:CYS:O	1:H:201:ILE:HB	0.46	2.10	4	3
1:H:154:ARG:CG	1:H:193:ASN:HB2	0.46	2.41	3	1
1:H:223:GLY:O	1:H:226:HIS:N	0.46	2.46	2	2
1:L:153:ILE:HG21	1:L:168:PHE:CD1	0.46	2.44	3	3
1:G:187:GLU:O	1:G:191:VAL:HG13	0.46	2.10	4	1
1:H:195:ASN:O	1:H:196:PRO:C	0.46	2.54	1	3
1:I:150:ILE:CD1	1:I:153:ILE:HG21	0.46	2.41	2	1
1:J:150:ILE:HG23	1:J:151:LEU:HD12	0.46	1.87	4	2
1:J:191:VAL:CG1	1:J:202:LEU:HD22	0.46	2.40	4	1
1:L:231:LEU:HD12	1:L:231:LEU:O	0.46	2.10	4	1
1:K:153:ILE:HG21	1:K:168:PHE:CD1	0.46	2.46	1	3
1:I:215:MET:O	1:I:219:GLN:CB	0.46	2.63	3	3
1:K:183:ASN:O	1:K:186:THR:OG1	0.46	2.33	3	1
1:L:171:THR:O	1:L:175:GLU:N	0.46	2.49	4	2
1:I:205:LEU:HD22	1:I:213:GLU:HG3	0.46	1.88	4	1
1:H:150:ILE:HG21	1:H:185:MET:HG2	0.46	1.88	5	1
1:H:202:LEU:HD23	1:H:214:MET:CE	0.46	2.40	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:233:GLU:O	1:H:237:GLN:N	0.46	2.48	5	2
1:J:153:ILE:CG1	1:J:171:THR:HG21	0.46	2.40	4	3
1:G:153:ILE:CG1	1:G:171:THR:HG21	0.46	2.41	3	3
1:H:151:LEU:HD11	1:H:185:MET:SD	0.46	2.50	2	1
1:G:237:GLN:O	1:G:241:THR:N	0.46	2.49	5	2
1:H:184:TRP:CZ3	1:H:188:THR:HG21	0.46	2.46	5	2
1:I:227:LYS:CB	3:I:301:2I4:O4	0.46	2.64	2	1
1:G:150:ILE:HD11	1:G:168:PHE:CD2	0.46	2.46	1	1
1:K:190:LEU:O	1:K:194:ALA:CB	0.46	2.64	3	4
1:G:231:LEU:HD22	1:L:231:LEU:HD11	0.46	1.88	2	1
1:J:194:ALA:O	1:J:195:ASN:HB3	0.46	2.11	2	1
1:K:221:VAL:HA	1:K:226:HIS:HB2	0.46	1.86	2	1
1:J:234:ALA:HB1	1:K:231:LEU:HD23	0.46	1.86	3	1
1:K:172:LEU:HD21	1:K:182:LYS:HB3	0.46	1.87	3	1
1:H:191:VAL:HG22	1:H:202:LEU:HD22	0.46	1.87	5	1
1:J:186:THR:O	1:J:190:LEU:CB	0.46	2.63	5	1
1:G:153:ILE:HG21	1:G:168:PHE:CD1	0.46	2.45	3	3
1:G:219:GLN:O	1:L:157:PRO:CG	0.46	2.64	2	1
1:H:200:THR:O	1:H:204:ALA:N	0.46	2.49	5	3
1:H:161:PHE:CZ	1:H:202:LEU:HD21	0.46	2.46	4	1
1:I:169:TYR:CD1	1:I:169:TYR:N	0.45	2.84	3	2
1:I:153:ILE:HG22	1:I:153:ILE:O	0.45	2.10	5	2
1:I:172:LEU:HD21	1:I:182:LYS:HB3	0.45	1.87	1	1
1:K:177:ALA:HB1	1:K:181:VAL:CB	0.45	2.41	1	1
1:K:238:VAL:O	1:K:238:VAL:HG12	0.45	2.11	3	2
1:L:209:ALA:HB3	1:L:214:MET:CE	0.45	2.41	1	1
1:K:150:ILE:O	1:K:153:ILE:HB	0.45	2.11	2	2
1:H:202:LEU:HD23	1:H:214:MET:HE3	0.45	1.88	5	1
1:L:155:GLN:HB2	1:L:164:TYR:CG	0.45	2.47	5	1
1:H:215:MET:O	1:H:219:GLN:N	0.45	2.49	4	3
1:J:192:GLN:O	1:J:199:LYS:HD3	0.45	2.12	1	1
1:J:182:LYS:O	1:J:186:THR:HB	0.45	2.11	3	1
1:H:205:LEU:HD13	1:H:213:GLU:C	0.45	2.31	4	1
1:H:226:HIS:CD2	1:H:230:VAL:HG21	0.45	2.46	4	1
1:J:156:GLY:N	1:J:159:GLU:HB3	0.45	2.26	2	1
1:J:233:GLU:O	1:J:237:GLN:N	0.45	2.50	3	1
1:H:230:VAL:HG11	1:I:228:ALA:HB1	0.45	1.88	2	1
1:I:227:LYS:CG	3:I:301:2I4:O4	0.45	2.64	4	3
1:H:153:ILE:CG1	1:H:171:THR:HG21	0.45	2.42	5	4
1:L:150:ILE:CD1	1:L:168:PHE:O	0.45	2.65	3	3
1:J:155:GLN:HB2	1:J:164:TYR:CG	0.45	2.46	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:L:150:ILE:HG21	1:L:185:MET:HG2	0.45	1.89	2	1
1:L:211:LEU:HD22	1:L:214:MET:SD	0.45	2.51	3	1
1:I:218:CYS:HA	1:I:221:VAL:HG23	0.45	1.89	2	1
1:L:210:THR:O	1:L:213:GLU:N	0.45	2.50	5	1
1:G:201:ILE:O	1:G:204:ALA:HB3	0.45	2.11	1	1
1:I:168:PHE:CD2	1:I:168:PHE:C	0.45	2.90	2	2
1:J:184:TRP:CE3	1:J:188:THR:HG21	0.45	2.47	2	1
1:L:205:LEU:HD13	1:L:213:GLU:HB3	0.45	1.89	3	1
1:I:191:VAL:HG23	1:I:192:GLN:N	0.45	2.27	4	1
1:K:164:TYR:O	1:K:168:PHE:N	0.45	2.50	4	1
1:I:153:ILE:O	1:I:193:ASN:HB3	0.45	2.12	5	1
1:I:238:VAL:O	1:I:242:ALA:CB	0.45	2.64	5	1
1:L:198:CYS:O	1:L:201:ILE:N	0.45	2.50	3	1
1:H:155:GLN:HB2	1:H:164:TYR:CD2	0.44	2.47	1	2
1:J:168:PHE:CE2	1:J:186:THR:HA	0.44	2.47	3	4
1:J:223:GLY:O	1:J:225:GLY:N	0.44	2.49	1	2
1:L:153:ILE:O	1:L:193:ASN:HB3	0.44	2.12	1	1
1:H:230:VAL:HG12	1:I:228:ALA:HB1	0.44	1.89	3	1
1:I:161:PHE:HB2	1:I:218:CYS:HB3	0.44	1.90	5	2
1:J:195:ASN:O	1:J:198:CYS:N	0.44	2.50	5	2
1:J:161:PHE:HB2	1:J:218:CYS:HB3	0.44	1.88	4	1
1:G:190:LEU:CD2	1:G:211:LEU:HD21	0.44	2.43	5	1
1:J:191:VAL:HG23	1:J:202:LEU:CB	0.44	2.41	2	2
1:H:238:VAL:HG21	1:I:232:ALA:O	0.44	2.12	3	1
1:J:153:ILE:HG12	1:J:171:THR:HG21	0.44	1.88	1	2
1:G:157:PRO:HG2	1:H:221:VAL:O	0.44	2.12	1	1
1:J:169:TYR:OH	1:J:190:LEU:HD22	0.44	2.12	1	1
1:K:231:LEU:O	1:K:235:MET:CB	0.44	2.65	3	4
1:L:161:PHE:HZ	1:L:202:LEU:HD21	0.44	1.73	2	1
1:H:234:ALA:O	1:H:238:VAL:HG22	0.44	2.13	1	1
1:K:199:LYS:HZ2	1:L:216:THR:HG23	0.44	1.73	1	1
1:K:153:ILE:HD11	1:K:171:THR:CB	0.44	2.42	1	2
1:J:155:GLN:NE2	1:J:161:PHE:N	0.44	2.66	2	2
1:J:221:VAL:HG22	1:J:226:HIS:CE1	0.44	2.47	2	1
1:L:150:ILE:HG22	1:L:175:GLU:OE1	0.44	2.13	2	1
1:I:198:CYS:O	1:I:201:ILE:HB	0.44	2.12	3	2
1:I:150:ILE:HD13	1:I:168:PHE:O	0.44	2.12	4	1
1:L:167:ARG:O	1:L:171:THR:N	0.44	2.49	5	1
1:G:226:HIS:O	1:G:227:LYS:C	0.44	2.56	1	2
1:H:224:PRO:O	1:H:225:GLY:C	0.44	2.54	1	2
1:I:181:VAL:HG13	1:I:184:TRP:NE1	0.44	2.27	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:K:155:GLN:OE1	1:K:156:GLY:O	0.44	2.36	3	1
1:K:198:CYS:HA	1:K:201:ILE:HD12	0.44	1.90	3	1
1:G:157:PRO:HB2	1:H:223:GLY:H	0.44	1.73	4	3
1:K:227:LYS:O	1:K:231:LEU:N	0.44	2.51	2	1
1:L:195:ASN:O	1:L:196:PRO:C	0.44	2.56	2	2
1:H:165:VAL:O	1:H:169:TYR:HD1	0.44	1.96	5	2
1:J:157:PRO:HB3	1:K:219:GLN:O	0.44	2.13	3	2
1:G:193:ASN:OD1	1:G:193:ASN:N	0.44	2.51	5	1
1:L:210:THR:HG22	1:L:212:GLU:H	0.43	1.73	1	1
1:J:181:VAL:O	1:J:184:TRP:CD1	0.43	2.71	2	1
1:G:164:TYR:HE2	1:G:190:LEU:HD12	0.43	1.73	3	1
1:H:191:VAL:HG23	1:H:192:GLN:N	0.43	2.27	4	1
1:G:191:VAL:HG13	1:G:192:GLN:N	0.43	2.28	3	3
1:I:177:ALA:HB1	1:I:181:VAL:HG12	0.43	1.88	1	1
1:I:215:MET:O	1:I:219:GLN:HB2	0.43	2.12	1	2
1:L:156:GLY:O	1:L:157:PRO:C	0.43	2.56	1	1
1:K:185:MET:SD	1:K:189:LEU:HD23	0.43	2.53	2	1
1:H:194:ALA:O	1:H:199:LYS:N	0.43	2.51	4	1
1:I:168:PHE:C	1:I:168:PHE:CD2	0.43	2.91	3	1
1:J:238:VAL:HG22	1:K:236:SER:HB2	0.43	1.89	3	2
1:K:166:ASP:O	1:K:170:LYS:N	0.43	2.50	3	1
1:L:159:GLU:O	1:L:160:PRO:C	0.43	2.54	1	1
1:L:214:MET:O	1:L:218:CYS:N	0.43	2.50	1	1
1:H:226:HIS:C	1:H:228:ALA:N	0.43	2.72	3	2
1:G:226:HIS:O	1:G:230:VAL:HB	0.43	2.13	3	1
1:H:224:PRO:HA	1:H:227:LYS:HG2	0.43	1.90	3	1
1:I:164:TYR:OH	1:I:193:ASN:OD1	0.43	2.35	3	1
1:H:160:PRO:O	1:H:164:TYR:N	0.43	2.43	5	1
1:L:165:VAL:HG12	1:L:190:LEU:CD1	0.43	2.30	5	1
1:K:201:ILE:O	1:K:204:ALA:HB3	0.43	2.12	1	1
1:I:155:GLN:NE2	1:I:198:CYS:SG	0.43	2.92	3	1
1:G:158:LYS:HB3	1:H:223:GLY:HA2	0.43	1.90	4	1
1:J:150:ILE:HG22	1:J:175:GLU:OE1	0.43	2.14	5	2
1:K:178:SER:O	1:K:181:VAL:N	0.43	2.51	2	2
1:L:161:PHE:CG	1:L:218:CYS:HB2	0.43	2.48	2	1
1:L:194:ALA:O	1:L:199:LYS:N	0.43	2.52	2	1
1:H:189:LEU:O	1:H:193:ASN:ND2	0.43	2.52	3	1
1:G:197:ASP:OD2	1:H:225:GLY:HA2	0.43	2.13	5	1
1:L:190:LEU:HD23	1:L:211:LEU:HD21	0.43	1.90	5	1
1:L:153:ILE:O	1:L:153:ILE:HG22	0.43	2.13	4	3
1:L:214:MET:O	1:L:218:CYS:SG	0.43	2.77	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:155:GLN:CG	1:H:159:GLU:O	0.43	2.67	2	1
1:L:168:PHE:CE2	1:L:186:THR:HA	0.43	2.49	5	2
1:I:155:GLN:HB2	1:I:164:TYR:CG	0.43	2.49	5	1
1:H:150:ILE:CG2	1:H:151:LEU:HD12	0.43	2.44	2	1
1:H:230:VAL:CG1	1:I:228:ALA:HB1	0.43	2.44	2	1
1:K:147:PRO:C	1:K:148:THR:HG23	0.43	2.34	2	1
1:H:154:ARG:HG2	1:H:193:ASN:HB2	0.43	1.91	3	1
1:I:194:ALA:O	1:I:198:CYS:HB2	0.43	2.14	3	1
1:L:205:LEU:HD13	1:L:213:GLU:CB	0.43	2.44	3	1
1:G:215:MET:O	1:G:219:GLN:CB	0.43	2.67	4	1
1:H:183:ASN:O	1:H:186:THR:HB	0.43	2.13	4	1
1:H:205:LEU:HD22	1:H:213:GLU:HG3	0.43	1.90	4	1
1:J:169:TYR:CE2	1:J:186:THR:HG21	0.43	2.48	5	1
1:J:238:VAL:HG22	1:K:236:SER:HB3	0.43	1.91	5	1
1:H:155:GLN:HA	1:H:164:TYR:CD1	0.43	2.49	1	3
1:H:238:VAL:HG11	1:I:232:ALA:O	0.43	2.13	1	1
1:I:195:ASN:O	1:I:196:PRO:C	0.43	2.56	5	3
1:I:153:ILE:HD11	1:I:171:THR:OG1	0.43	2.13	2	2
1:K:191:VAL:HG13	1:K:192:GLN:N	0.43	2.29	2	2
1:K:215:MET:O	1:K:219:GLN:CB	0.43	2.67	2	2
1:G:153:ILE:O	1:G:193:ASN:ND2	0.43	2.52	3	2
1:I:160:PRO:O	1:I:164:TYR:N	0.43	2.52	3	2
3:I:301:2I4:C26	1:L:231:LEU:HD22	0.43	2.43	3	1
1:G:211:LEU:O	1:G:215:MET:HB2	0.43	2.13	4	1
1:H:153:ILE:HG12	1:H:171:THR:HG21	0.43	1.91	5	1
1:G:169:TYR:CE2	1:G:186:THR:OG1	0.42	2.67	2	1
1:G:194:ALA:O	1:G:195:ASN:O	0.42	2.36	2	1
1:H:201:ILE:O	1:H:205:LEU:N	0.42	2.52	2	1
1:H:168:PHE:CD2	1:H:168:PHE:C	0.42	2.93	3	1
1:K:153:ILE:HG21	1:K:168:PHE:HA	0.42	1.90	3	2
1:I:226:HIS:ND1	1:I:230:VAL:HG21	0.42	2.29	4	1
1:J:175:GLU:O	1:J:182:LYS:NZ	0.42	2.52	4	1
1:J:184:TRP:CZ3	1:J:188:THR:HG21	0.42	2.49	2	1
1:K:155:GLN:HB2	1:K:164:TYR:CG	0.42	2.49	2	1
1:L:226:HIS:CD2	1:L:230:VAL:HG21	0.42	2.49	2	1
1:J:190:LEU:O	1:J:194:ALA:CB	0.42	2.65	4	2
1:J:214:MET:O	1:J:218:CYS:HB2	0.42	2.14	5	2
1:J:219:GLN:C	1:J:221:VAL:H	0.42	2.18	4	1
1:G:231:LEU:O	1:G:235:MET:CB	0.42	2.67	5	1
1:K:172:LEU:HG	1:K:182:LYS:HD3	0.42	1.91	5	1
1:L:177:ALA:HB3	1:L:182:LYS:CG	0.42	2.44	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:202:LEU:CD2	1:G:214:MET:SD	0.42	3.07	1	1
1:L:165:VAL:O	1:L:169:TYR:HD1	0.42	1.97	1	1
1:L:231:LEU:O	1:L:235:MET:CB	0.42	2.68	1	1
1:I:155:GLN:HG3	1:I:164:TYR:CB	0.42	2.44	3	1
1:I:155:GLN:CG	1:I:164:TYR:HB2	0.42	2.44	3	1
1:G:169:TYR:N	1:G:169:TYR:CD1	0.42	2.86	2	3
1:G:226:HIS:CD2	1:G:230:VAL:HG21	0.42	2.49	5	2
1:K:168:PHE:CD2	1:K:168:PHE:C	0.42	2.93	1	1
1:K:178:SER:O	1:K:179:GLN:C	0.42	2.58	1	1
1:L:165:VAL:O	1:L:169:TYR:CD1	0.42	2.72	1	2
1:J:238:VAL:HG13	1:K:236:SER:CB	0.42	2.43	1	2
1:H:150:ILE:HG22	1:H:151:LEU:HD12	0.42	1.91	2	1
1:I:223:GLY:O	1:I:224:PRO:C	0.42	2.58	2	1
1:J:195:ASN:O	1:J:197:ASP:N	0.42	2.53	5	3
1:I:156:GLY:O	1:I:159:GLU:N	0.42	2.53	3	1
1:L:156:GLY:N	1:L:159:GLU:HB3	0.42	2.30	3	1
1:K:221:VAL:HG22	1:K:226:HIS:CD2	0.42	2.49	3	1
1:H:163:ASP:O	1:H:166:ASP:N	0.42	2.52	5	1
1:I:155:GLN:HA	1:I:164:TYR:CD1	0.42	2.50	1	3
1:G:153:ILE:O	1:G:193:ASN:HB3	0.42	2.15	2	1
1:I:210:THR:HG23	1:I:213:GLU:H	0.42	1.74	2	1
1:J:150:ILE:HD13	1:J:168:PHE:O	0.42	2.15	4	1
1:K:191:VAL:HG22	1:K:202:LEU:CD2	0.42	2.39	5	1
1:G:210:THR:HG23	1:G:213:GLU:H	0.42	1.74	2	1
1:H:191:VAL:HG22	1:H:202:LEU:CD2	0.42	2.45	5	1
1:K:150:ILE:HD11	1:K:168:PHE:CE2	0.42	2.50	1	1
1:L:155:GLN:HG3	1:L:164:TYR:HB2	0.42	1.90	2	1
1:J:180:GLU:O	1:J:184:TRP:HB3	0.42	2.14	4	1
1:J:169:TYR:CZ	1:J:186:THR:HG23	0.41	2.50	2	1
1:K:177:ALA:HB1	1:K:181:VAL:CG1	0.41	2.45	3	1
1:L:161:PHE:CG	1:L:218:CYS:SG	0.41	3.11	1	1
1:I:150:ILE:HD13	1:I:153:ILE:HG13	0.41	1.92	2	1
1:K:180:GLU:HG3	1:K:181:VAL:HG23	0.41	1.92	5	1
1:L:150:ILE:HG12	1:L:172:LEU:N	0.41	2.30	5	1
1:G:150:ILE:CD1	1:G:168:PHE:O	0.41	2.68	1	1
1:I:172:LEU:HD21	1:I:182:LYS:CB	0.41	2.44	1	1
1:J:169:TYR:CD1	1:J:169:TYR:N	0.41	2.88	1	1
1:H:161:PHE:HB2	1:H:218:CYS:HB2	0.41	1.92	2	1
1:I:164:TYR:CE2	1:I:190:LEU:CD1	0.41	3.03	4	1
1:J:150:ILE:HD11	1:J:168:PHE:CD1	0.41	2.48	4	1
1:K:153:ILE:HD12	1:K:167:ARG:CG	0.41	2.45	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:I:181:VAL:O	1:I:182:LYS:C	0.41	2.59	5	1
1:J:210:THR:O	1:J:211:LEU:C	0.41	2.57	5	1
1:G:150:ILE:HD11	1:G:168:PHE:CG	0.41	2.50	1	1
1:H:180:GLU:HG2	1:H:181:VAL:N	0.41	2.31	1	1
1:I:191:VAL:HG13	1:I:192:GLN:N	0.41	2.31	1	2
1:I:184:TRP:CD1	1:I:185:MET:N	0.41	2.89	3	1
1:H:181:VAL:O	1:H:184:TRP:CD1	0.41	2.73	4	1
1:G:224:PRO:CB	1:L:227:LYS:HG2	0.41	2.46	5	1
1:K:164:TYR:HE2	1:K:190:LEU:HD12	0.41	1.71	5	1
1:L:161:PHE:O	1:L:165:VAL:HG13	0.41	2.15	5	1
1:K:165:VAL:O	1:K:168:PHE:HB3	0.41	2.16	2	1
1:G:154:ARG:CG	1:G:193:ASN:HB2	0.41	2.46	3	1
1:L:153:ILE:HD11	1:L:171:THR:HG21	0.41	1.93	3	1
1:L:172:LEU:HD11	1:L:182:LYS:HG3	0.41	1.93	3	1
1:H:161:PHE:HB2	1:H:218:CYS:HB3	0.41	1.92	1	1
1:J:211:LEU:HD13	1:J:211:LEU:O	0.41	2.15	1	3
1:H:181:VAL:O	1:H:185:MET:HB2	0.41	2.15	2	1
1:I:221:VAL:HG13	1:I:226:HIS:CD2	0.41	2.50	2	1
1:K:184:TRP:CE3	1:K:188:THR:HG21	0.41	2.49	2	1
1:L:155:GLN:NE2	1:L:194:ALA:HB1	0.41	2.31	2	1
1:K:234:ALA:HB1	1:L:232:ALA:HA	0.41	1.93	3	1
1:J:198:CYS:O	1:J:202:LEU:HD12	0.41	2.15	4	1
1:H:177:ALA:HB1	1:H:181:VAL:HG12	0.41	1.89	5	1
1:J:186:THR:O	1:J:190:LEU:HB3	0.41	2.15	5	1
1:K:158:LYS:HB3	1:L:223:GLY:HA3	0.41	1.93	5	1
1:L:156:GLY:N	1:L:159:GLU:CB	0.41	2.84	2	1
1:K:186:THR:O	1:K:190:LEU:HB3	0.41	2.16	5	1
1:I:231:LEU:O	1:I:235:MET:HB2	0.41	2.16	1	1
1:L:215:MET:O	1:L:219:GLN:CB	0.41	2.69	1	1
1:H:157:PRO:HG3	1:I:219:GLN:O	0.41	2.15	3	1
1:J:179:GLN:O	1:J:183:ASN:N	0.41	2.53	3	1
1:I:153:ILE:HD12	1:I:167:ARG:O	0.41	2.16	4	1
1:K:221:VAL:HG13	1:K:226:HIS:CE1	0.41	2.51	5	1
1:L:164:TYR:HE2	1:L:190:LEU:HD12	0.41	1.73	5	1
1:H:169:TYR:CD1	1:H:169:TYR:N	0.41	2.88	1	2
1:I:211:LEU:O	1:I:211:LEU:HD13	0.41	2.16	1	1
1:J:155:GLN:N	1:J:164:TYR:CE1	0.41	2.88	1	1
1:L:161:PHE:HB2	1:L:218:CYS:HB2	0.41	1.93	1	1
1:L:214:MET:C	1:L:218:CYS:SG	0.41	2.99	1	1
1:G:161:PHE:HB2	1:G:218:CYS:HB3	0.41	1.92	3	1
1:G:197:ASP:O	1:G:200:THR:HG22	0.41	2.15	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:161:PHE:HB2	1:H:218:CYS:CB	0.41	2.46	3	1
1:I:201:ILE:O	1:I:204:ALA:HB3	0.41	2.15	5	2
1:J:155:GLN:OE1	1:J:159:GLU:O	0.41	2.39	4	1
1:L:198:CYS:C	1:L:202:LEU:HD12	0.41	2.36	4	1
1:I:177:ALA:HB3	1:I:182:LYS:HD3	0.41	1.91	5	1
1:J:218:CYS:O	1:J:221:VAL:HG23	0.41	2.14	1	1
1:L:194:ALA:O	1:L:195:ASN:HB3	0.41	2.16	3	1
1:J:185:MET:O	1:J:189:LEU:N	0.41	2.52	5	1
1:I:153:ILE:O	1:I:153:ILE:HG22	0.40	2.16	1	2
1:I:196:PRO:O	1:I:200:THR:HB	0.40	2.16	2	1
1:H:150:ILE:HG23	1:H:151:LEU:HD12	0.40	1.94	5	1
1:G:232:ALA:HB2	1:L:234:ALA:CB	0.40	2.39	2	1
1:I:172:LEU:O	1:I:175:GLU:O	0.40	2.38	2	1
1:I:168:PHE:CD2	1:I:168:PHE:O	0.40	2.74	3	1
1:K:238:VAL:HG22	1:L:236:SER:HB3	0.40	1.92	3	1
1:L:222:GLY:O	1:L:223:GLY:O	0.40	2.39	3	1
1:G:191:VAL:CG2	1:G:192:GLN:N	0.40	2.83	4	1
1:L:171:THR:HA	1:L:174:ALA:HB3	0.40	1.92	4	1
1:K:233:GLU:O	1:K:237:GLN:N	0.40	2.54	5	1
1:I:150:ILE:HD12	1:I:153:ILE:HG13	0.40	1.92	1	1
1:I:161:PHE:O	1:I:165:VAL:CG1	0.40	2.69	2	1
1:K:181:VAL:HA	1:K:184:TRP:CD1	0.40	2.51	2	1
1:L:155:GLN:HB2	1:L:164:TYR:CD2	0.40	2.51	2	1
1:L:177:ALA:HB3	1:L:182:LYS:HD2	0.40	1.92	2	1
1:G:195:ASN:OD1	1:G:195:ASN:C	0.40	2.59	3	1
1:I:237:GLN:O	1:I:241:THR:N	0.40	2.53	4	1
1:H:198:CYS:O	1:H:201:ILE:N	0.40	2.54	5	1
1:H:198:CYS:SG	1:H:221:VAL:HG11	0.40	2.56	5	1
1:K:155:GLN:N	1:K:164:TYR:CD1	0.40	2.90	5	1
1:J:192:GLN:HA	1:J:199:LYS:CD	0.40	2.47	1	1
1:H:191:VAL:HG23	1:H:202:LEU:HB2	0.40	1.93	2	1
1:H:209:ALA:O	1:H:214:MET:HE3	0.40	2.16	4	1
1:K:216:THR:O	1:K:219:GLN:HB3	0.40	2.15	5	1
1:J:155:GLN:CG	1:J:159:GLU:O	0.40	2.69	2	1
1:K:150:ILE:HG23	1:K:151:LEU:HD12	0.40	1.93	2	1
1:L:233:GLU:O	1:L:237:GLN:HB2	0.40	2.16	5	1

6.3 Torsion angles (i)

6.3.1 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 NMR 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	G	100/102 (98%)	92±2 (92±2%)	6±2 (6±2%)	2±0 (2±0%)	11 52
1	H	100/102 (98%)	91±3 (91±3%)	7±2 (7±2%)	3±1 (3±1%)	8 42
1	I	100/102 (98%)	86±3 (86±3%)	11±3 (11±3%)	3±1 (3±1%)	7 40
1	J	100/102 (98%)	88±1 (88±1%)	8±1 (8±1%)	4±0 (4±0%)	6 34
1	K	100/102 (98%)	87±2 (87±2%)	9±2 (9±2%)	3±1 (3±1%)	7 38
1	L	100/102 (98%)	86±2 (86±2%)	11±2 (11±2%)	3±1 (3±1%)	7 40
All	All	3000/3060 (98%)	2653 (88%)	259 (9%)	88 (3%)	7 41

All 34 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	G	195	ASN	5
1	G	196	PRO	5
1	H	195	ASN	5
1	H	196	PRO	5
1	I	195	ASN	5
1	I	196	PRO	5
1	J	195	ASN	5
1	J	196	PRO	5
1	K	195	ASN	5
1	L	195	ASN	5
1	K	196	PRO	4
1	L	196	PRO	4
1	J	223	GLY	3
1	J	224	PRO	3
1	K	153	ILE	2
1	L	145	GLY	2
1	L	153	ILE	2
1	K	148	THR	2
1	I	206	GLY	1
1	I	207	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	L	207	PRO	1
1	H	145	GLY	1
1	H	207	PRO	1
1	I	224	PRO	1
1	K	145	GLY	1
1	I	220	GLY	1
1	J	207	PRO	1
1	K	176	GLN	1
1	L	223	GLY	1
1	H	153	ILE	1
1	H	190	LEU	1
1	I	223	GLY	1
1	J	221	VAL	1
1	K	206	GLY	1

6.3.2 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 NMR 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	G	83/83 (100%)	74±3 (90±3%)	9±3 (10±3%)	10 55
1	H	83/83 (100%)	75±4 (90±4%)	8±4 (10±4%)	11 57
1	I	83/83 (100%)	72±2 (86±3%)	11±2 (14±3%)	7 47
1	J	83/83 (100%)	73±1 (88±1%)	10±1 (12±1%)	8 51
1	K	83/83 (100%)	75±1 (90±1%)	8±1 (10±1%)	11 56
1	L	83/83 (100%)	74±2 (89±3%)	9±2 (11±3%)	9 53
All	All	2490/2490 (100%)	2211 (89%)	279 (11%)	9 53

All 137 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	G	184	TRP	5
1	G	211	LEU	5
1	G	241	THR	5
1	H	241	THR	5

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Mol	Chain	Res	Type	Models (Total)
1	I	153	ILE	5
1	I	211	LEU	5
1	I	226	HIS	5
1	I	241	THR	5
1	J	202	LEU	5
1	J	211	LEU	5
1	J	241	THR	5
1	K	241	THR	5
1	L	184	TRP	5
1	L	241	THR	5
1	G	202	LEU	4
1	H	211	LEU	4
1	H	231	LEU	4
1	I	184	TRP	4
1	I	200	THR	4
1	J	186	THR	4
1	K	205	LEU	4
1	L	153	ILE	4
1	L	211	LEU	4
1	K	211	LEU	4
1	G	152	ASP	3
1	G	162	ARG	3
1	G	186	THR	3
1	H	186	THR	3
1	I	148	THR	3
1	I	186	THR	3
1	J	162	ARG	3
1	K	200	THR	3
1	K	202	LEU	3
1	K	226	HIS	3
1	L	186	THR	3
1	L	214	MET	3
1	J	153	ILE	3
1	L	233	GLU	3
1	L	202	LEU	3
1	G	197	ASP	2
1	G	219	GLN	2
1	I	152	ASP	2
1	J	158	LYS	2
1	J	195	ASN	2
1	J	231	LEU	2
1	J	235	MET	2

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Mol	Chain	Res	Type	Models (Total)
1	K	197	ASP	2
1	L	171	THR	2
1	H	152	ASP	2
1	H	214	MET	2
1	H	219	GLN	2
1	I	162	ARG	2
1	I	195	ASN	2
1	I	236	SER	2
1	J	152	ASP	2
1	J	180	GLU	2
1	K	154	ARG	2
1	K	186	THR	2
1	K	195	ASN	2
1	L	219	GLN	2
1	G	226	HIS	2
1	I	202	LEU	2
1	J	184	TRP	2
1	K	149	SER	2
1	J	226	HIS	2
1	G	163	ASP	1
1	H	195	ASN	1
1	H	238	VAL	1
1	I	227	LYS	1
1	I	235	MET	1
1	J	219	GLN	1
1	K	146	SER	1
1	K	227	LYS	1
1	L	197	ASP	1
1	G	153	ILE	1
1	G	178	SER	1
1	G	180	GLU	1
1	G	231	LEU	1
1	H	153	ILE	1
1	H	180	GLU	1
1	H	202	LEU	1
1	H	205	LEU	1
1	H	218	CYS	1
1	H	227	LYS	1
1	I	150	ILE	1
1	I	151	LEU	1
1	I	185	MET	1
1	I	197	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	I	219	GLN	1
1	J	210	THR	1
1	K	162	ARG	1
1	K	182	LYS	1
1	K	214	MET	1
1	K	219	GLN	1
1	L	161	PHE	1
1	L	162	ARG	1
1	L	180	GLU	1
1	L	203	LYS	1
1	L	231	LEU	1
1	G	235	MET	1
1	H	158	LYS	1
1	I	154	ARG	1
1	J	185	MET	1
1	J	214	MET	1
1	L	199	LYS	1
1	L	235	MET	1
1	H	148	THR	1
1	H	161	PHE	1
1	H	162	ARG	1
1	H	167	ARG	1
1	H	175	GLU	1
1	H	182	LYS	1
1	H	189	LEU	1
1	H	197	ASP	1
1	I	146	SER	1
1	I	176	GLN	1
1	I	214	MET	1
1	J	227	LYS	1
1	K	161	PHE	1
1	L	148	THR	1
1	L	185	MET	1
1	L	195	ASN	1
1	L	213	GLU	1
1	G	167	ARG	1
1	G	193	ASN	1
1	G	214	MET	1
1	H	184	TRP	1
1	H	199	LYS	1
1	I	182	LYS	1
1	I	233	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	J	175	GLU	1
1	J	199	LYS	1
1	J	200	THR	1
1	K	185	MET	1
1	K	193	ASN	1
1	K	245	MET	1
1	L	150	ILE	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	IHP	G	301	-	36,36,36	1.61±0.00	7±0 (19±0%)
3	2I4	I	301	-	46,46,46	2.89±0.01	16±0 (34±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	IHP	G	301	-	54,60,60	1.17±0.00	5±0 (10±0%)
3	2I4	I	301	-	77,78,78	2.37±0.00	28±0 (36±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
3	2I4	I	301	-	-	0±0,25,114,114	0±0,5,5,5
2	IHP	G	301	-	-	0±0,30,54,54	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	I	301	2I4	C33-C34	11.11	1.62	1.52	2	5
3	I	301	2I4	C17-C28	6.79	1.63	1.52	5	5
3	I	301	2I4	C6-C5	6.38	1.64	1.53	5	5
3	I	301	2I4	C8-C14	6.29	1.69	1.59	5	5
2	G	301	IHP	P2-O12	5.24	1.69	1.59	5	5
3	I	301	2I4	C19-C20	4.41	1.44	1.51	4	5
3	I	301	2I4	C11-C9	3.80	1.59	1.53	2	5
3	I	301	2I4	C18-C13	3.71	1.59	1.54	4	5
3	I	301	2I4	C14-C13	3.69	1.61	1.56	5	5
2	G	301	IHP	C4-C3	2.98	1.58	1.52	1	5
3	I	301	2I4	C4-C5	2.89	1.61	1.56	2	5
3	I	301	2I4	C22-C17	2.86	1.50	1.54	2	5
2	G	301	IHP	P4-O14	2.82	1.54	1.59	5	5
3	I	301	2I4	C32-C33	2.64	1.45	1.53	4	5
2	G	301	IHP	P5-O15	2.62	1.64	1.59	5	5
3	I	301	2I4	C35-C33	2.57	1.58	1.53	3	5
3	I	301	2I4	C7-C8	2.37	1.58	1.54	4	5
2	G	301	IHP	P6-O46	2.28	1.46	1.54	3	5
3	I	301	2I4	C21-C19	2.26	1.58	1.54	1	5
2	G	301	IHP	P4-O44	2.21	1.46	1.54	2	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	G	301	IHP	C5-C4	2.14	1.56	1.52	3	5
3	I	301	2I4	C12-C13	2.12	1.50	1.53	3	5
3	I	301	2I4	O6-C34	2.13	1.29	1.22	3	5

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	I	301	2I4	C22-C17-C18	6.89	93.57	101.11	5	5
3	I	301	2I4	C12-C13-C14	6.42	117.83	110.99	2	5
3	I	301	2I4	C18-C19-C20	5.67	126.72	117.03	4	5
3	I	301	2I4	C8-C14-C13	5.35	103.11	108.59	1	5
3	I	301	2I4	C21-C19-C18	4.95	98.02	103.33	4	5
3	I	301	2I4	C12-C13-C18	4.84	105.11	113.43	1	5
3	I	301	2I4	C17-C18-C13	4.79	106.47	112.32	1	5
3	I	301	2I4	C26-C8-C9	4.76	118.96	111.91	5	5
3	I	301	2I4	O1-C31-C32	4.16	103.68	111.21	3	5
3	I	301	2I4	C6-C5-C10	3.78	114.90	110.95	3	5
3	I	301	2I4	C26-C8-C7	3.75	101.43	107.84	3	5
3	I	301	2I4	C1-C2-C3	3.25	116.89	110.63	2	5
3	I	301	2I4	O1-C3-C2	3.25	114.05	108.48	3	5
2	G	301	IHP	C6-C1-C2	3.12	103.59	110.41	3	5
2	G	301	IHP	C5-C6-C1	2.86	104.14	110.41	4	5
3	I	301	2I4	C15-C16-C17	2.56	107.18	112.08	4	5
3	I	301	2I4	C11-C9-C8	2.54	114.00	110.87	3	5
3	I	301	2I4	C3-O1-C31	2.47	113.27	117.92	1	5
3	I	301	2I4	C7-C6-C5	2.44	106.33	111.07	4	5
2	G	301	IHP	O42-P2-O22	2.42	120.16	110.68	5	5
3	I	301	2I4	O6-C34-C33	2.38	119.48	122.87	4	5
3	I	301	2I4	O1-C31-O4	2.36	129.41	123.70	3	5
3	I	301	2I4	C35-C33-C34	2.33	104.12	109.05	5	5
2	G	301	IHP	C5-C4-C3	2.30	115.44	110.41	1	5
2	G	301	IHP	O32-P2-O12	2.29	116.25	105.99	4	5
3	I	301	2I4	C2-C3-C4	2.20	111.15	114.39	2	5
3	I	301	2I4	C15-C14-C8	2.19	112.75	110.77	2	5
3	I	301	2I4	C29-C20-C19	2.16	112.75	117.47	3	5
3	I	301	2I4	C24-C4-C3	2.16	114.20	109.38	4	5
3	I	301	2I4	C24-C4-C23	2.15	104.65	107.72	3	5
3	I	301	2I4	C18-C17-C28	2.15	116.94	114.29	1	5
3	I	301	2I4	C5-C4-C3	2.08	110.52	106.84	2	5
3	I	301	2I4	C36-C33-C34	2.08	113.44	109.05	3	5

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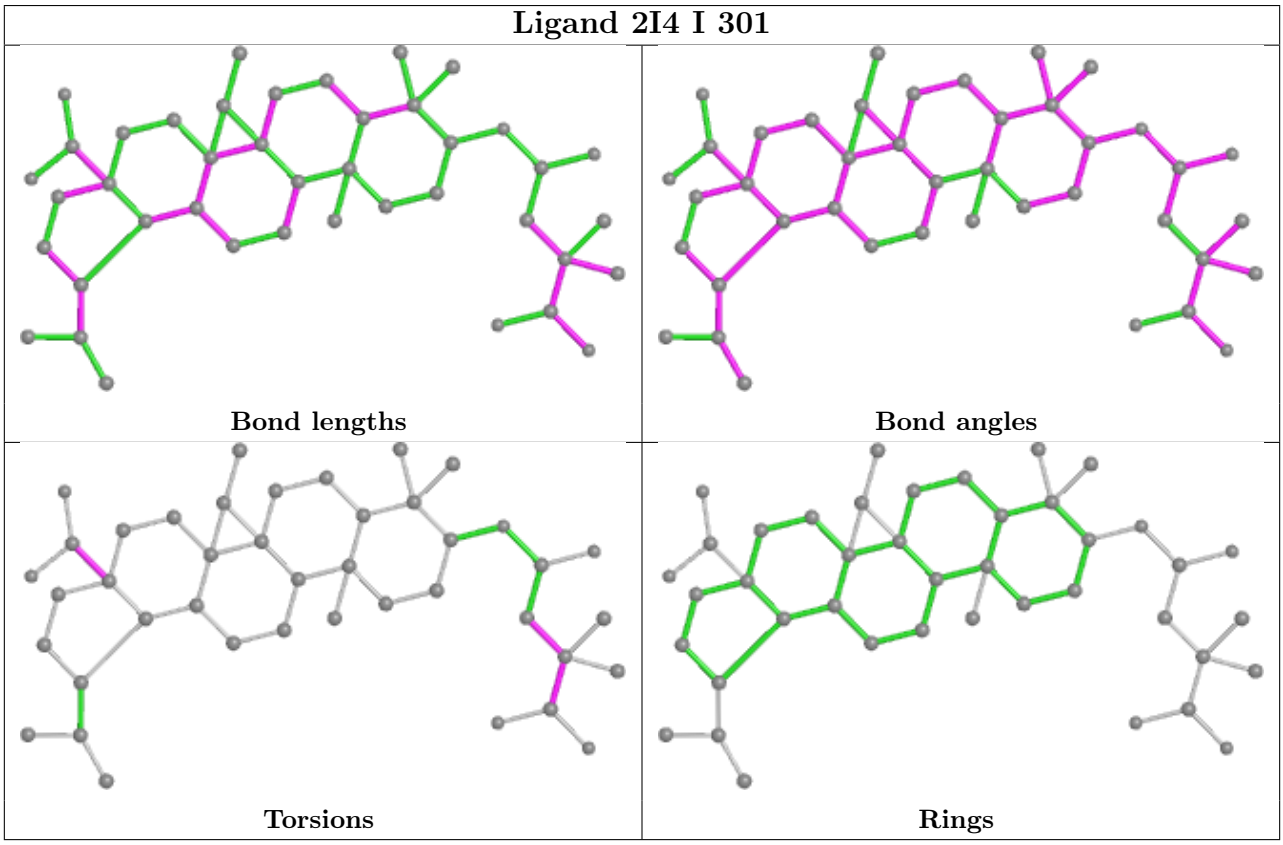
Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	G	301	IHP	C3-C2-C1	2.00	114.80	110.41	3	2

There are no chirality outliers.

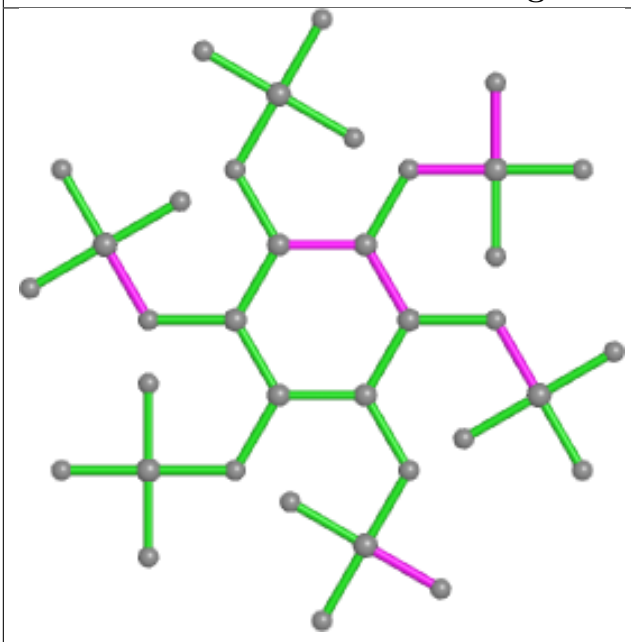
There are no torsion outliers.

There are no ring outliers.

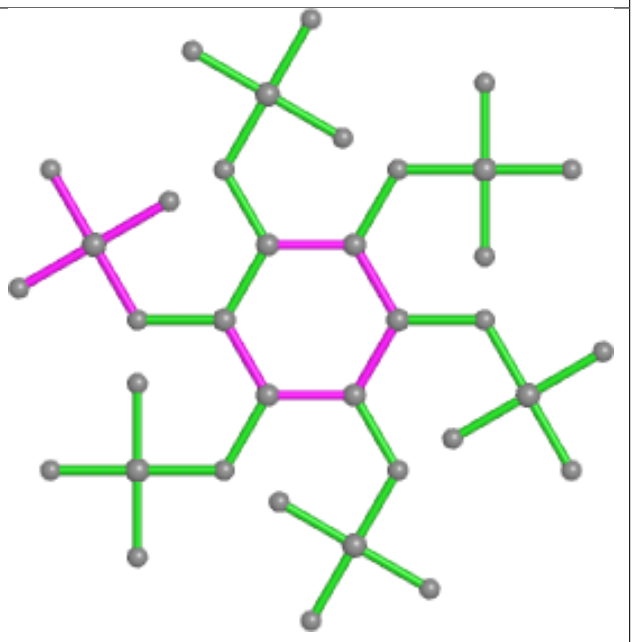
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



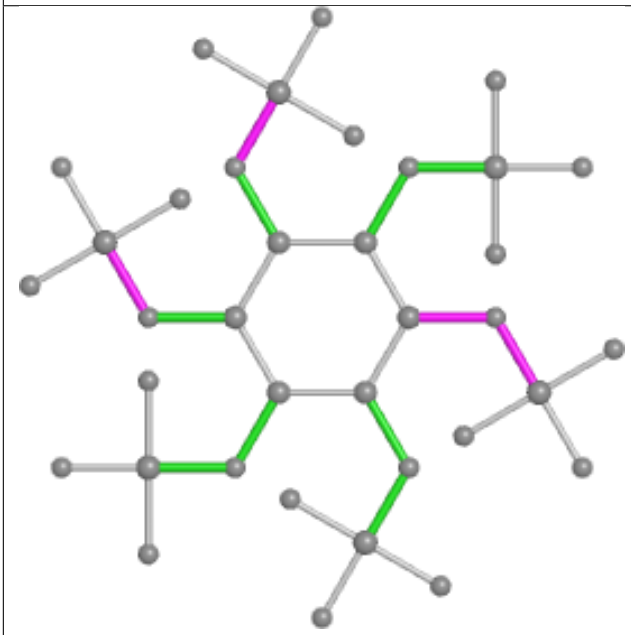
Ligand IHP G 301



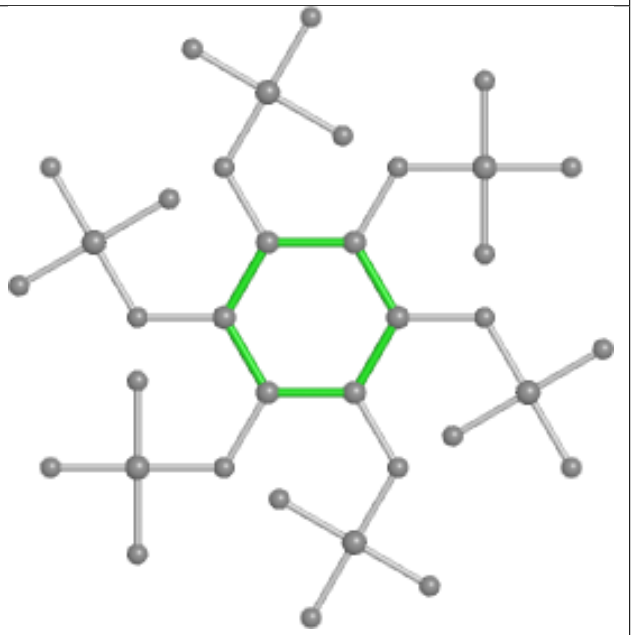
Bond lengths



Bond angles



Torsions



Rings

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 9% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *BVMIP6_chemicalshift_040721.str*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	770
Number of shifts mapped to atoms	770
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	98	-1.43 ± 0.74	None needed (imprecise)
$^{13}C_{\beta}$	88	0.27 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	93	-1.35 ± 0.46	Should be applied
^{15}N	95	-0.04 ± 0.78	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 9%, i.e. 744 atoms were assigned a chemical shift out of a possible 8047. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	398/3042 (13%)	117/1242 (9%)	191/1224 (16%)	90/576 (16%)
Sidechain	316/4662 (7%)	112/3036 (4%)	200/1440 (14%)	4/186 (2%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	30/343 (9%)	9/168 (5%)	18/162 (11%)	3/13 (23%)
Overall	744/8047 (9%)	238/4446 (5%)	409/2826 (14%)	97/775 (13%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 744 atoms were assigned a chemical shift out of a possible 8047. 0 out of 84 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	398/3042 (13%)	117/1242 (9%)	191/1224 (16%)	90/576 (16%)
Sidechain	316/4662 (7%)	112/3036 (4%)	200/1440 (14%)	4/186 (2%)
Aromatic	30/343 (9%)	9/168 (5%)	18/162 (11%)	3/13 (23%)
Overall	744/8047 (9%)	238/4446 (5%)	409/2826 (14%)	97/775 (13%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

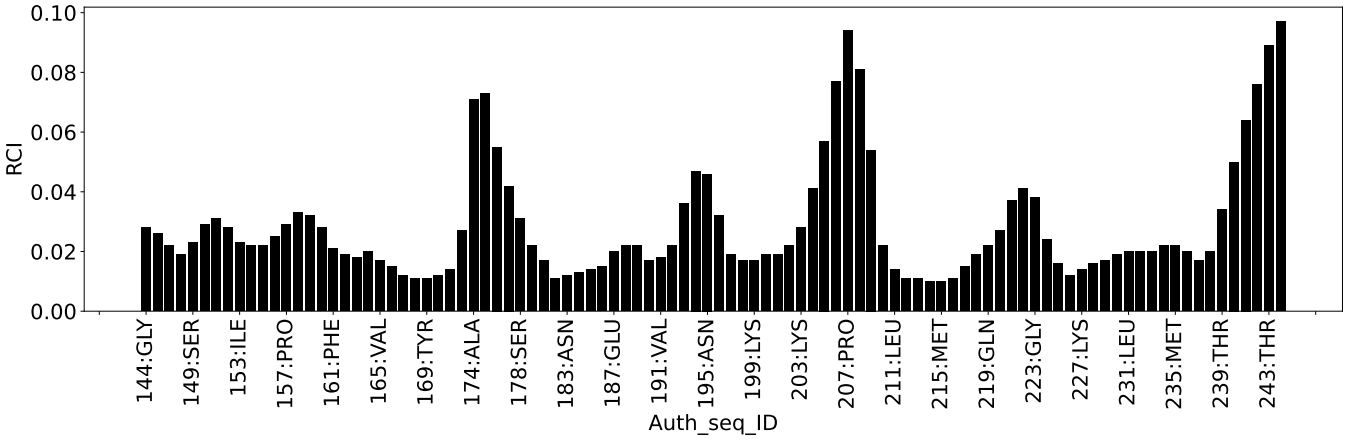
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain G:


RCI
0.10
0.08
0.06
0.04
0.02
0.00
144:GLY
149:SER
153:ILE
157:PRO
161:PHE
165:VAL
169:TYR
174:ALA
178:SER
183:ASN
187:GLU
191:VAL
195:ASN
199:LYS
203:LYS
207:PRO
211:LEU
215:MET
219:GLN
223:GLY
227:LYS
231:LEU
235:MET
239:THR
243:THR
Auth_seq_ID