



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2022 – 06:36 PM EST

PDB ID : 7K6V
Title : Crystal Structure of Virus-like Particles of GII.4 Norovirus Houston virus (HOV)
Authors : Hu, L.; Prasad, B.V.V.
Deposited on : 2020-09-21
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

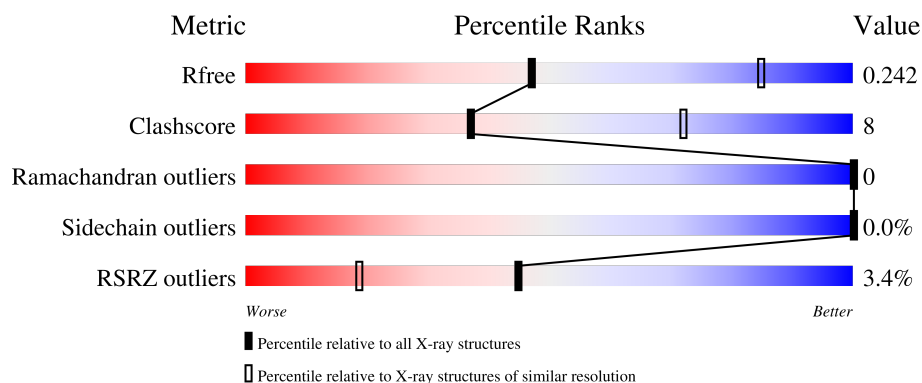
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	540	<div> <div>0%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	AB	540	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>•</div> </div>
1	AC	540	<div> <div>2%</div> <div>77%</div> <div>17%</div> <div>6%</div> </div>
1	BA	540	<div> <div>3%</div> <div>77%</div> <div>16%</div> <div>8%</div> </div>
1	BB	540	<div> <div>2%</div> <div>78%</div> <div>19%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	BC	540	
1	CA	540	
1	CB	540	
1	CC	540	
1	DA	540	
1	DB	540	
1	DC	540	
1	EA	540	
1	EB	540	
1	EC	540	
1	FA	540	
1	FB	540	
1	FC	540	
1	GA	540	
1	GB	540	
1	GC	540	
1	HA	540	
1	HB	540	
1	HC	540	
1	IA	540	
1	IB	540	
1	IC	540	
1	JA	540	
1	JB	540	
1	JC	540	

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Mol	Chain	Length	Quality of chain
1	KA	540	
1	KB	540	
1	KC	540	
1	LA	540	
1	LB	540	
1	LC	540	
1	MA	540	
1	MB	540	
1	MC	540	
1	NA	540	
1	NB	540	
1	NC	540	
1	OA	540	
1	OB	540	
1	OC	540	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 176522 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	500	Total	C	N	O	S	0	0	0
			3860	2474	656	715	15			
1	AB	523	Total	C	N	O	S	0	0	0
			4013	2560	681	757	15			
1	AC	508	Total	C	N	O	S	0	0	0
			3921	2506	668	732	15			
1	BA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	BB	523	Total	C	N	O	S	0	0	0
			4019	2563	684	757	15			
1	BC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	CA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	CB	523	Total	C	N	O	S	0	0	0
			4013	2560	681	757	15			
1	CC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	DA	498	Total	C	N	O	S	0	0	0
			3845	2464	654	713	14			
1	DB	523	Total	C	N	O	S	0	0	0
			4013	2560	681	757	15			
1	DC	506	Total	C	N	O	S	0	0	0
			3906	2497	665	730	14			
1	EA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	EB	523	Total	C	N	O	S	0	0	0
			4013	2560	681	757	15			
1	EC	493	Total	C	N	O	S	0	0	0
			3814	2442	651	709	12			
1	FA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	FB	523	Total	C	N	O	S	0	0	0
			4019	2563	684	757	15			
1	FC	509	Total	C	N	O	S	0	0	0
			3928	2511	669	733	15			
1	GA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	GB	523	Total	C	N	O	S	0	0	0
			4016	2562	684	755	15			
1	GC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	HA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	HB	523	Total	C	N	O	S	0	0	0
			4015	2561	684	755	15			
1	HC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	IA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	IB	523	Total	C	N	O	S	0	0	0
			4019	2564	685	755	15			
1	IC	503	Total	C	N	O	S	0	0	0
			3885	2487	660	723	15			
1	JA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	JB	523	Total	C	N	O	S	0	0	0
			4007	2558	681	753	15			
1	JC	506	Total	C	N	O	S	0	0	0
			3906	2497	665	730	14			
1	KA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	KB	523	Total	C	N	O	S	0	0	0
			4009	2558	681	755	15			
1	KC	507	Total	C	N	O	S	0	0	0
			3913	2502	666	730	15			
1	LA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	LB	523	Total	C	N	O	S	0	0	0
			4003	2556	681	751	15			
1	LC	502	Total	C	N	O	S	0	0	0
			3865	2474	657	719	15			
1	MA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	MB	523	Total	C	N	O	S	0	0	0
			4010	2559	681	755	15			
1	MC	506	Total	C	N	O	S	0	0	0
			3906	2497	665	730	14			
1	NA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	NB	523	Total	C	N	O	S	0	0	0
			4017	2564	685	753	15			
1	NC	506	Total	C	N	O	S	0	0	0
			3899	2494	665	726	14			
1	OA	499	Total	C	N	O	S	0	0	0
			3853	2469	655	714	15			
1	OB	523	Total	C	N	O	S	0	0	0
			4017	2564	685	753	15			
1	OC	498	Total	C	N	O	S	0	0	0
			3851	2464	656	719	12			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AA	3	Total	Cl	0	0
			3	3		
2	AB	1	Total	Cl	0	0
			1	1		
2	AC	1	Total	Cl	0	0
			1	1		
2	BA	2	Total	Cl	0	0
			2	2		
2	BC	1	Total	Cl	0	0
			1	1		
2	CA	2	Total	Cl	0	0
			2	2		
2	CC	3	Total	Cl	0	0
			3	3		
2	DA	1	Total	Cl	0	0
			1	1		
2	DB	1	Total	Cl	0	0
			1	1		
2	DC	2	Total	Cl	0	0
			2	2		
2	EA	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	FA	2	Total 2	Cl 2	0	0
2	GA	1	Total 1	Cl 1	0	0
2	GC	2	Total 2	Cl 2	0	0
2	HA	1	Total 1	Cl 1	0	0
2	HC	1	Total 1	Cl 1	0	0
2	IA	3	Total 3	Cl 3	0	0
2	JA	3	Total 3	Cl 3	0	0
2	KA	2	Total 2	Cl 2	0	0
2	KC	2	Total 2	Cl 2	0	0
2	LA	1	Total 1	Cl 1	0	0
2	LC	2	Total 2	Cl 2	0	0
2	MA	3	Total 3	Cl 3	0	0
2	MC	2	Total 2	Cl 2	0	0
2	NA	2	Total 2	Cl 2	0	0
2	NC	1	Total 1	Cl 1	0	0
2	OA	2	Total 2	Cl 2	0	0

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AC	1	Total 1	Cd 1	0	0
3	BA	1	Total 1	Cd 1	0	0
3	BC	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	CA	1	Total	Cd	0	0
			1	1		
3	DA	1	Total	Cd	0	0
			1	1		
3	EA	1	Total	Cd	0	0
			1	1		
3	EB	1	Total	Cd	0	0
			1	1		
3	EC	1	Total	Cd	0	0
			1	1		
3	FA	1	Total	Cd	0	0
			1	1		
3	FC	1	Total	Cd	0	0
			1	1		
3	GA	1	Total	Cd	0	0
			1	1		
3	GB	1	Total	Cd	0	0
			1	1		
3	HC	1	Total	Cd	0	0
			1	1		
3	IA	1	Total	Cd	0	0
			1	1		
3	JA	1	Total	Cd	0	0
			1	1		
3	JC	1	Total	Cd	0	0
			1	1		
3	KA	1	Total	Cd	0	0
			1	1		
3	KB	1	Total	Cd	0	0
			1	1		
3	MA	1	Total	Cd	0	0
			1	1		
3	MB	1	Total	Cd	0	0
			1	1		
3	NC	1	Total	Cd	0	0
			1	1		
3	OA	1	Total	Cd	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	JA	1	Total	C	O	0	0
			4	2	2		

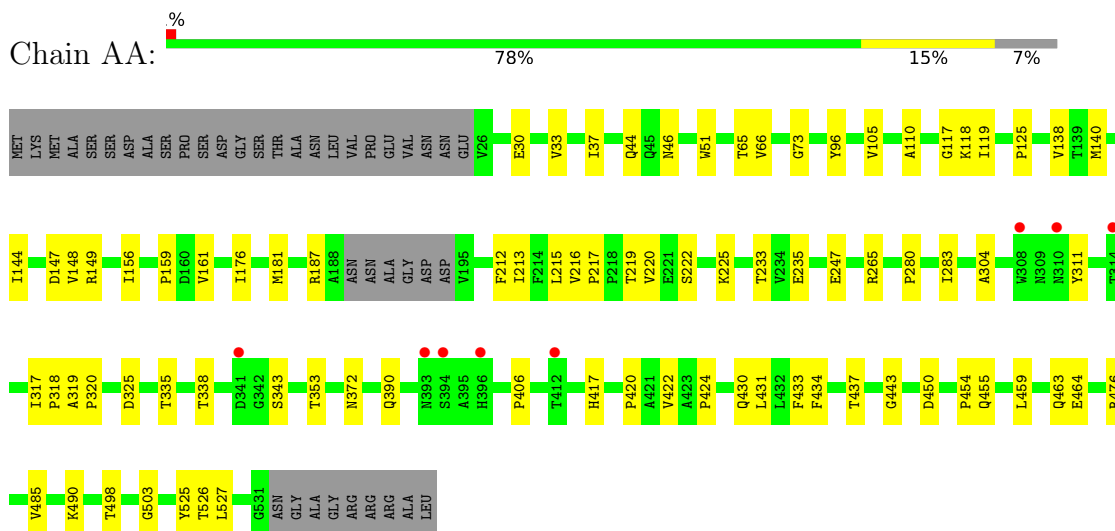
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	HC	1	Total	O	0	0
			1	1		
5	OA	1	Total	O	0	0
			1	1		
5	OB	1	Total	O	0	0
			1	1		

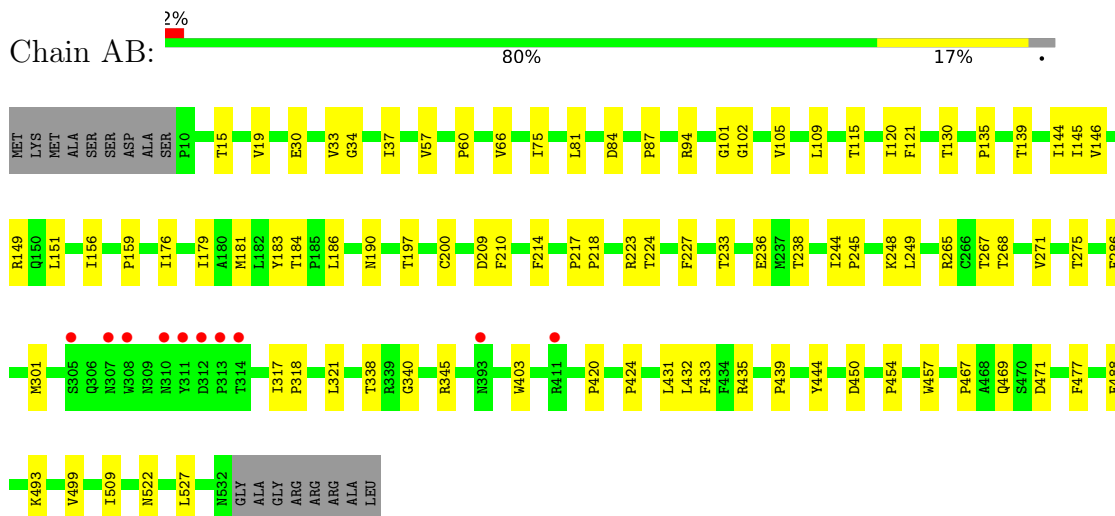
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

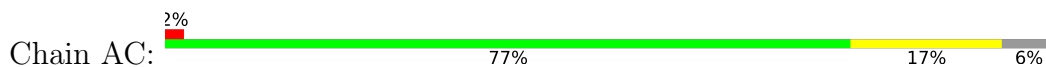
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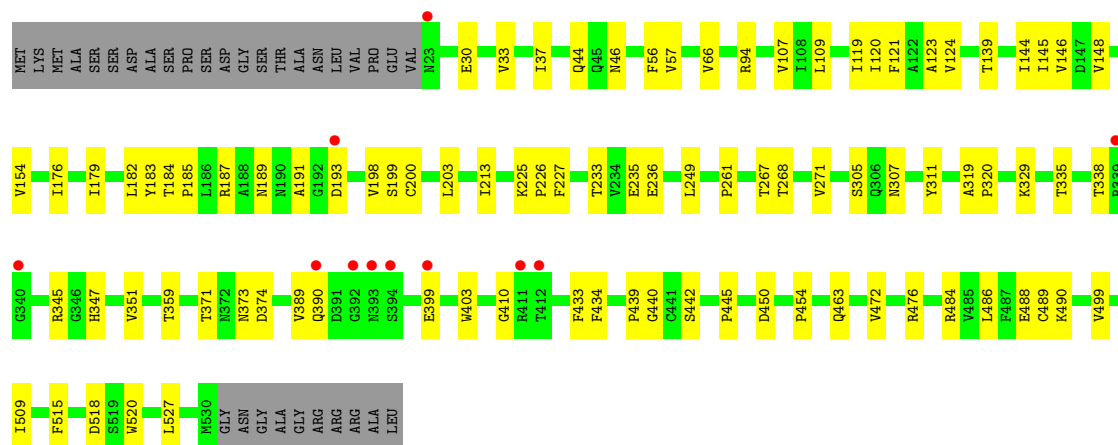


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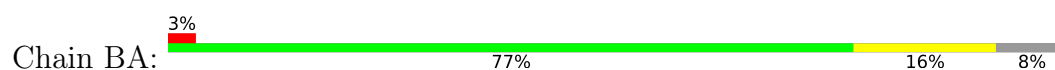


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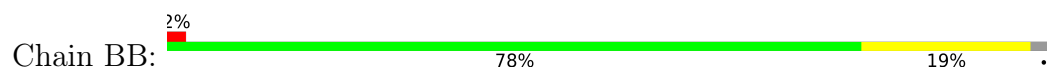


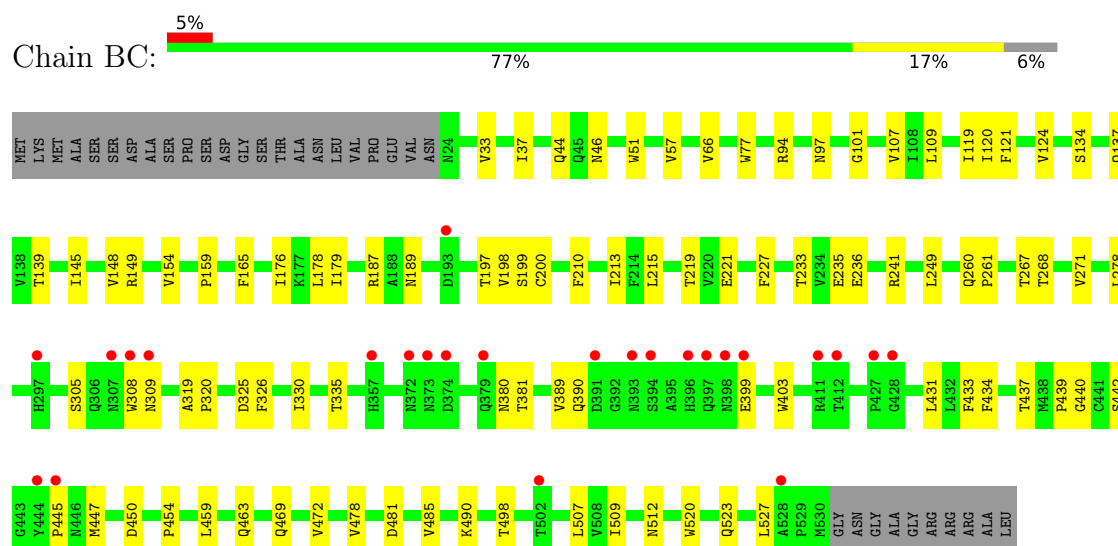


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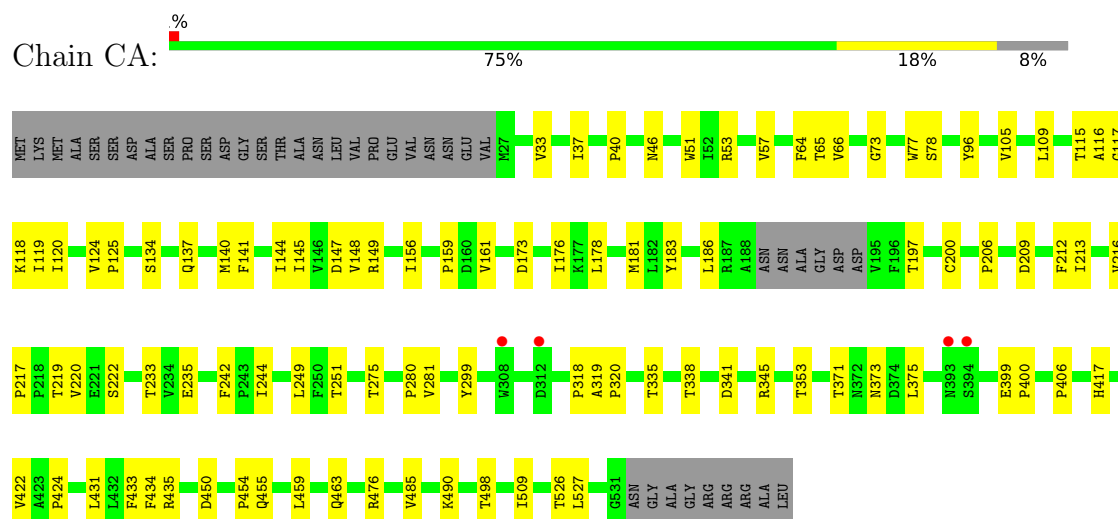


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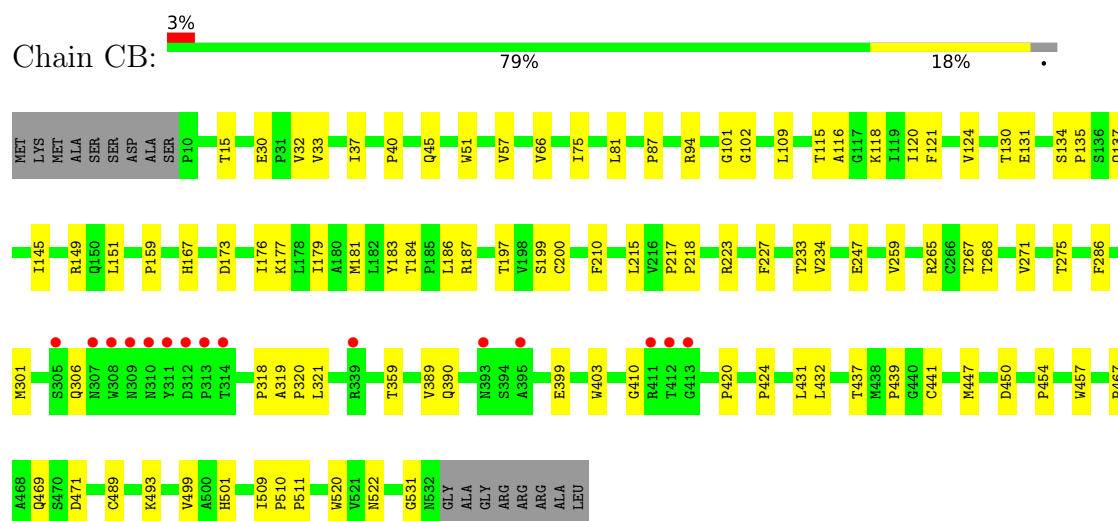




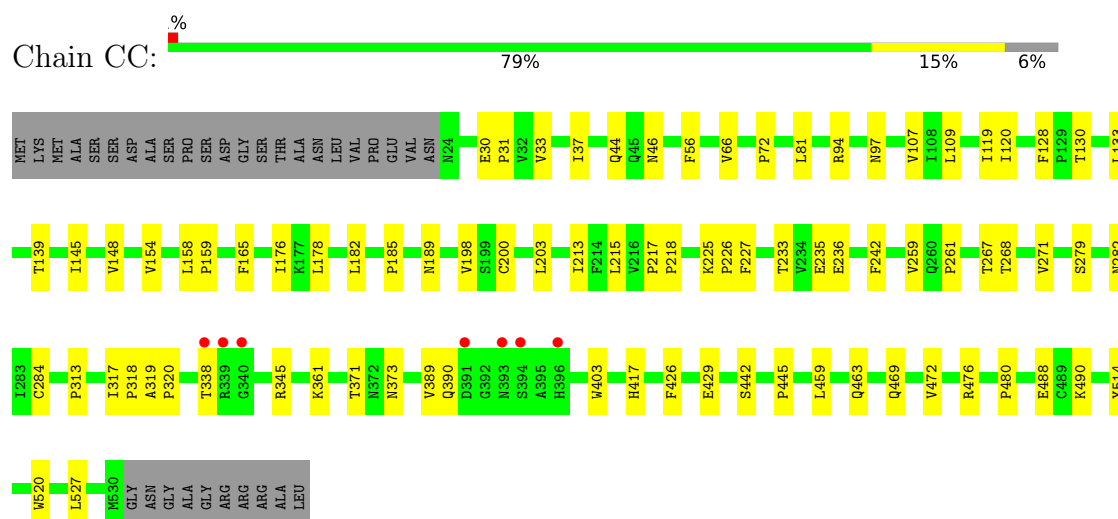
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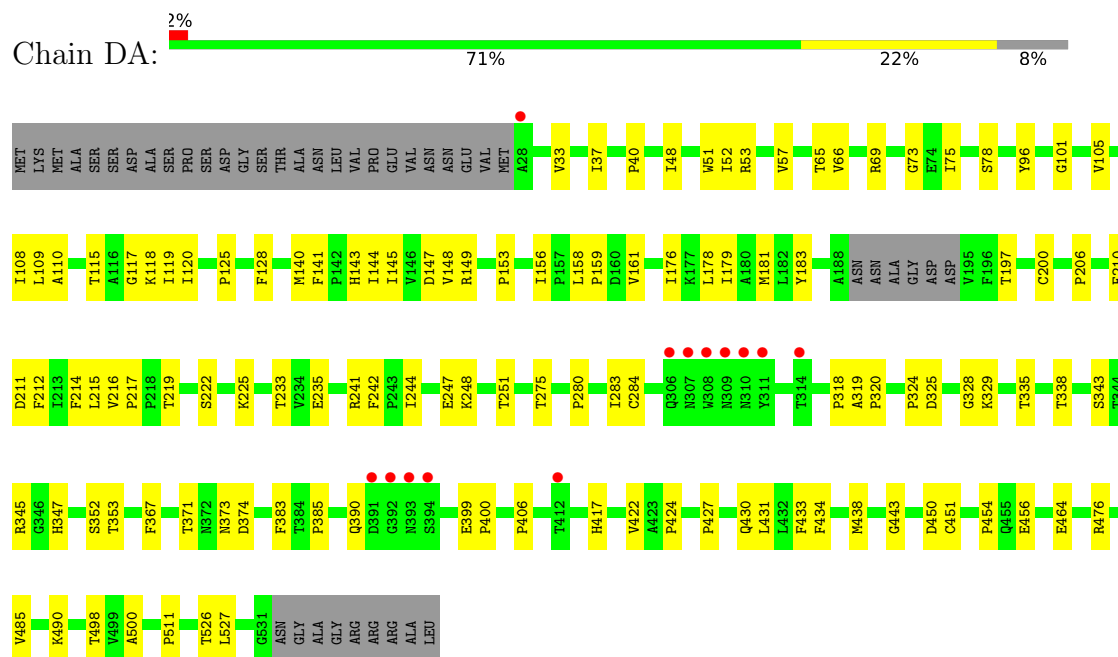
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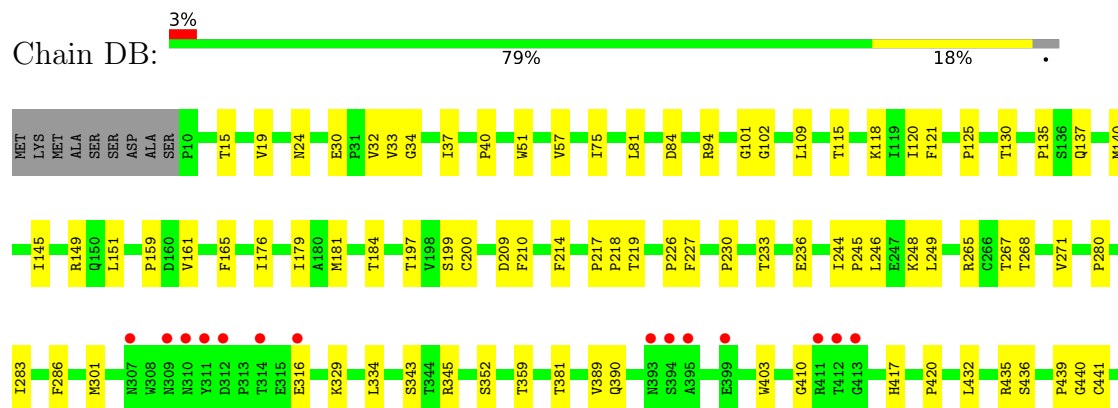
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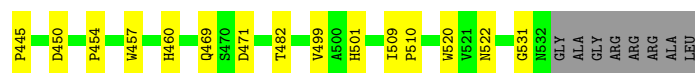


- Molecule 1: Capsid protein VP1

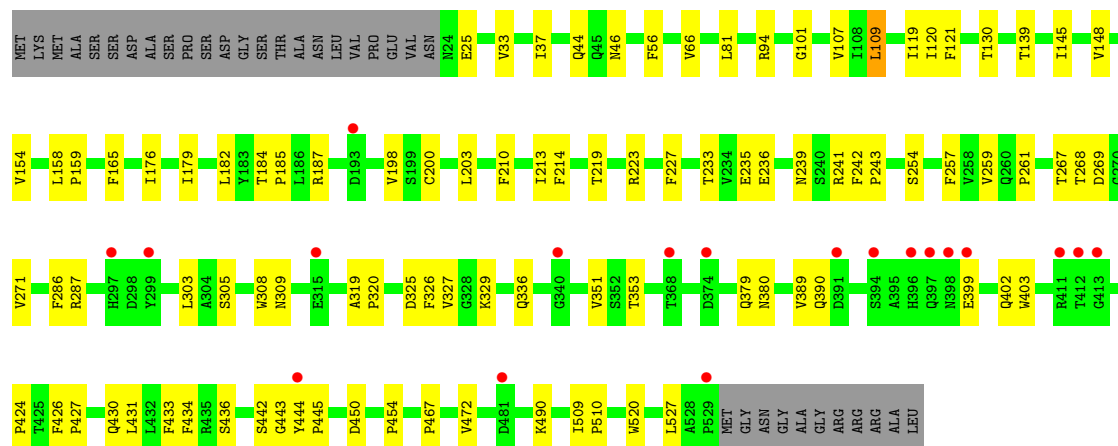
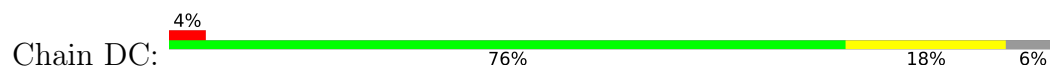


- Molecule 1: Capsid protein VP1

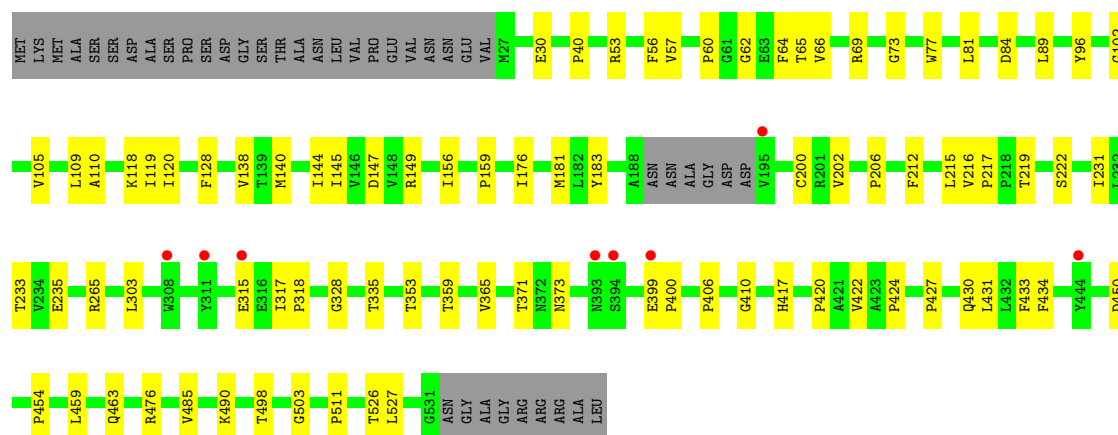
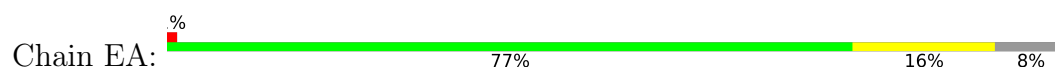




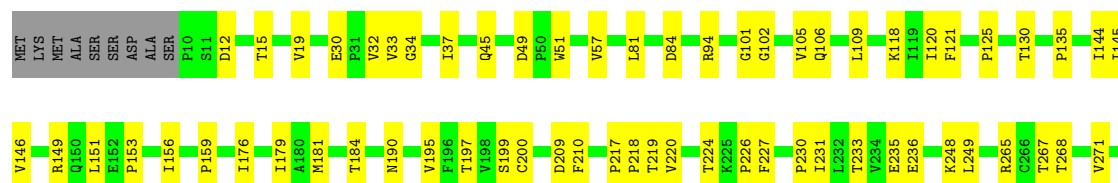
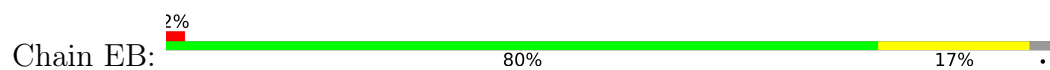
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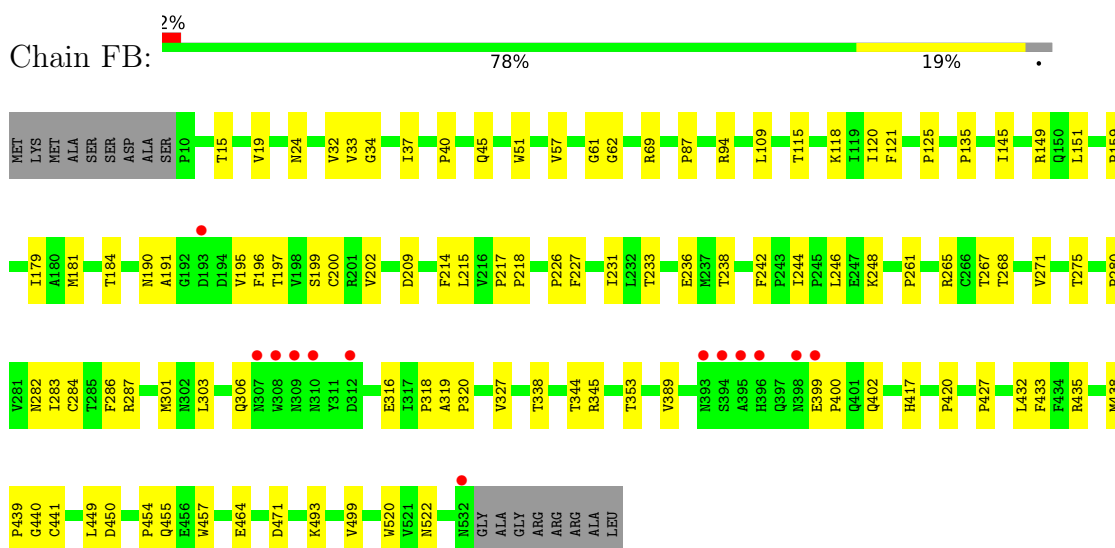
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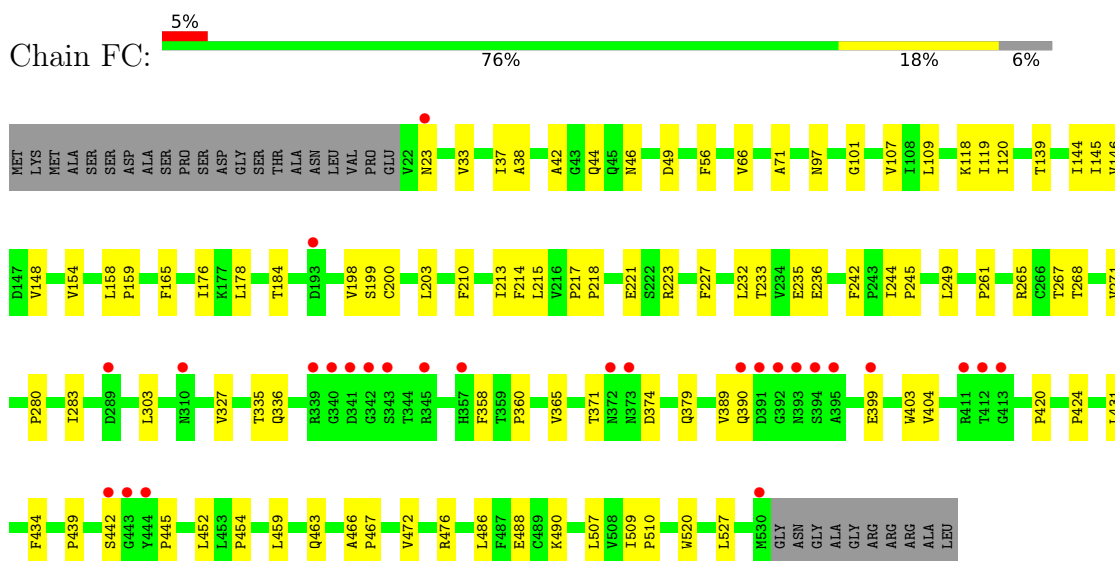
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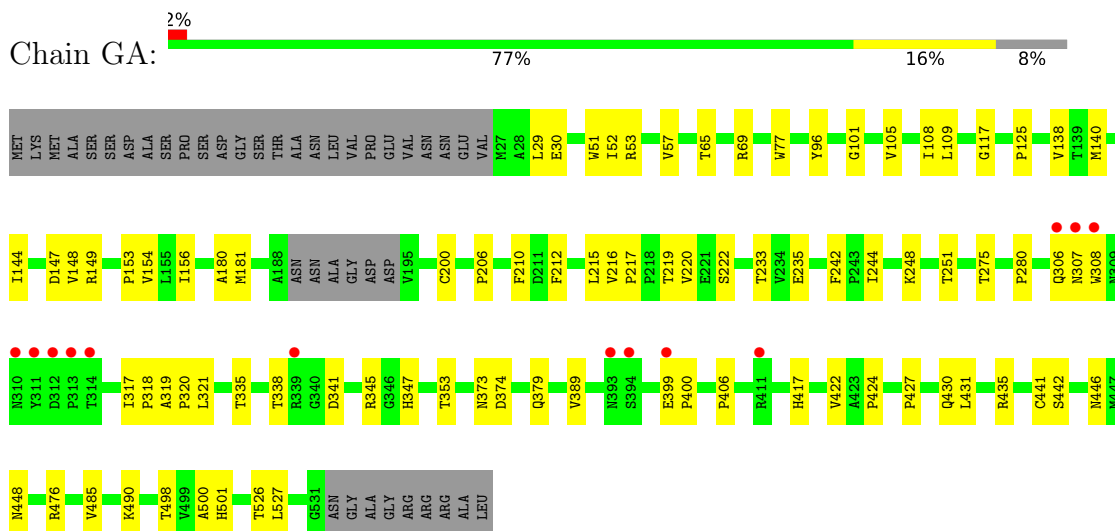




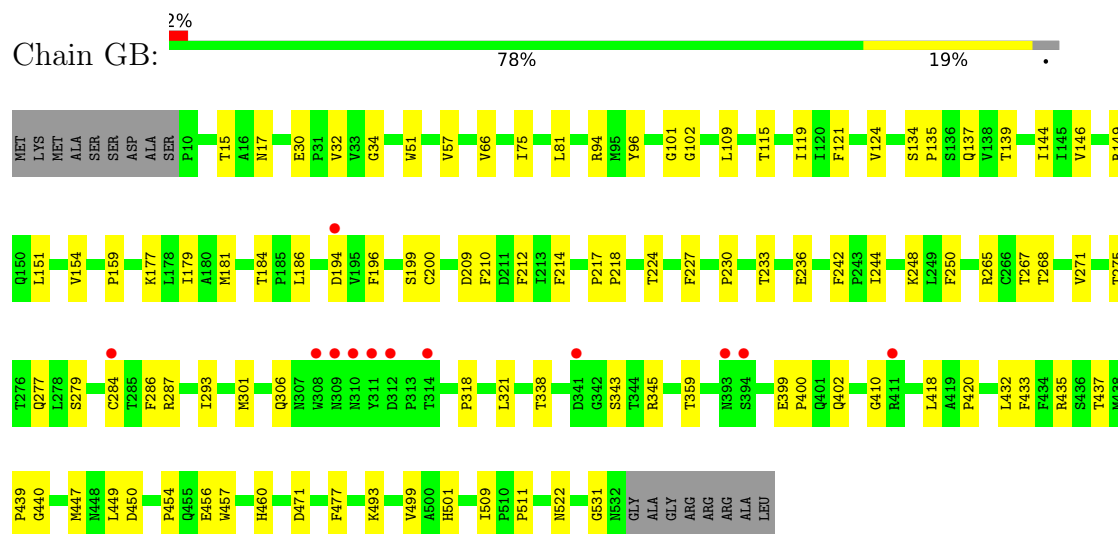
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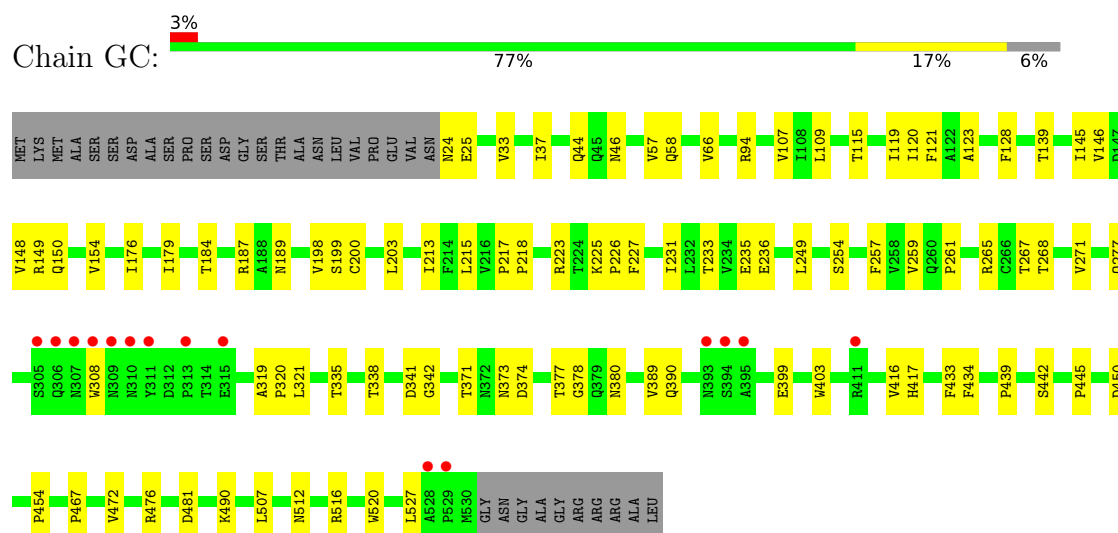
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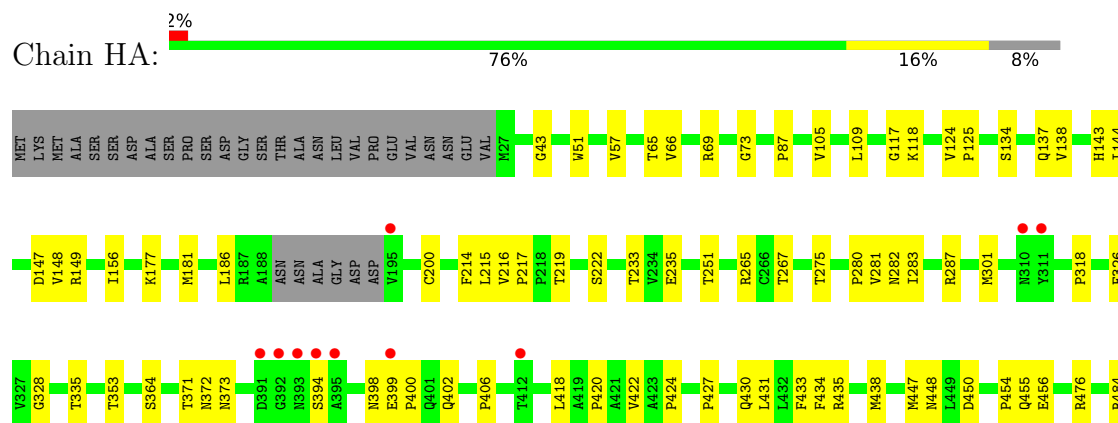
- Molecule 1: Capsid protein VP1



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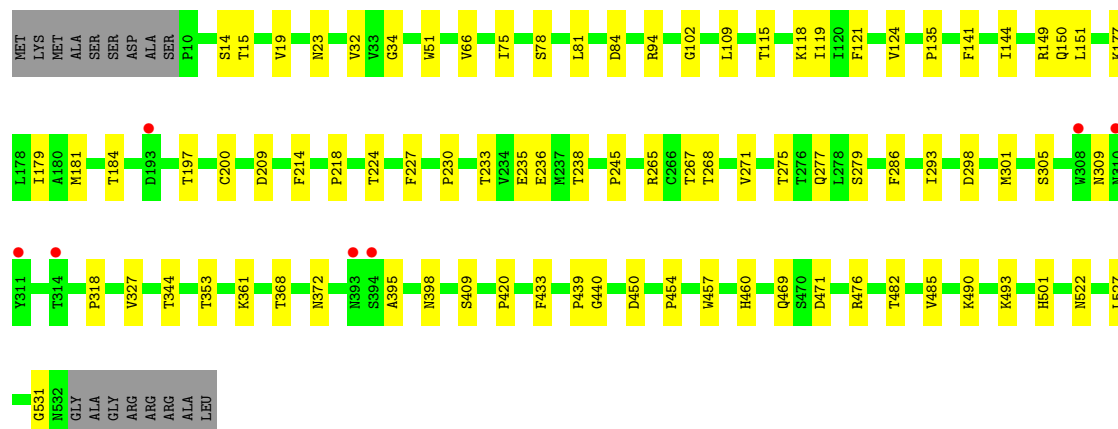
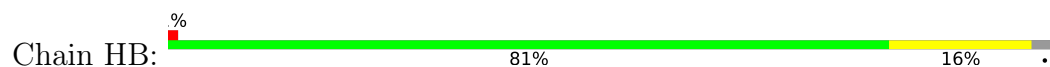


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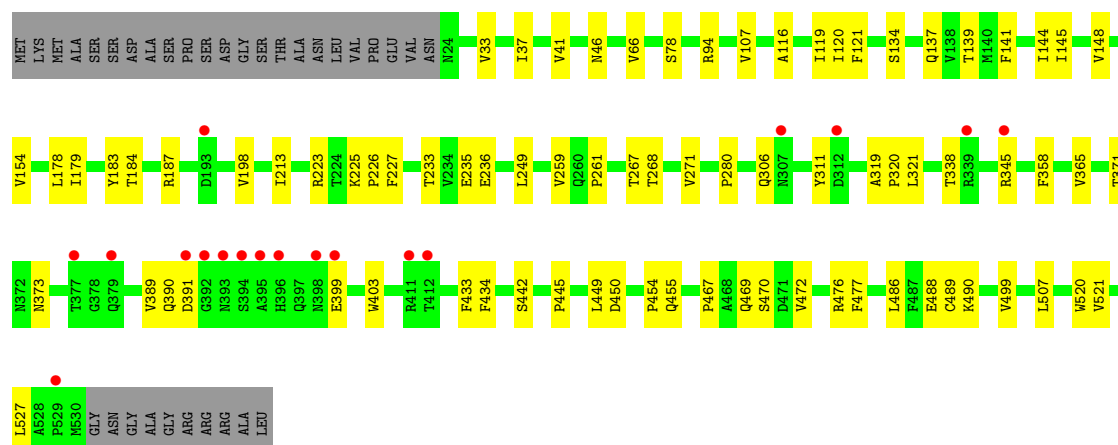
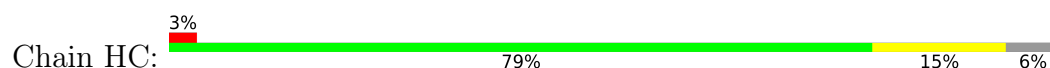




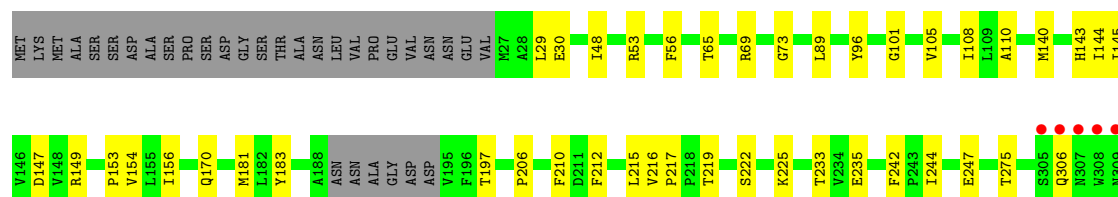
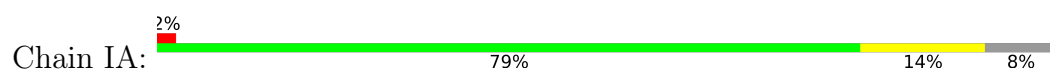
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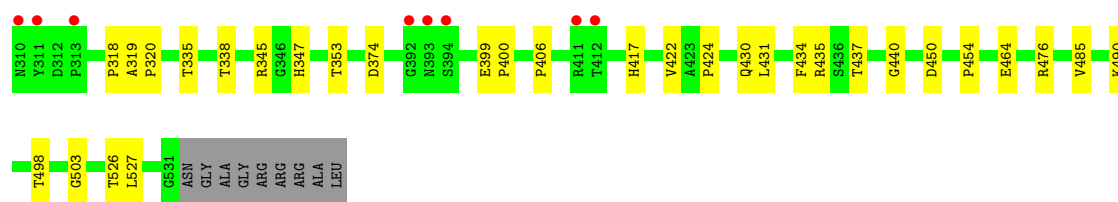


• Molecule 1: Capsid protein VP1

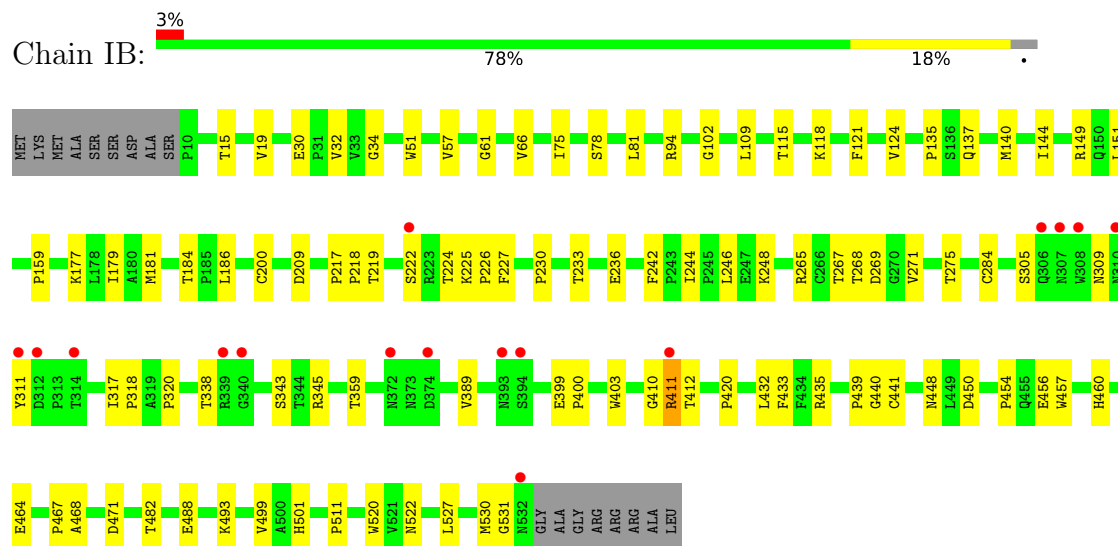


• Molecule 1: Capsid protein VP1

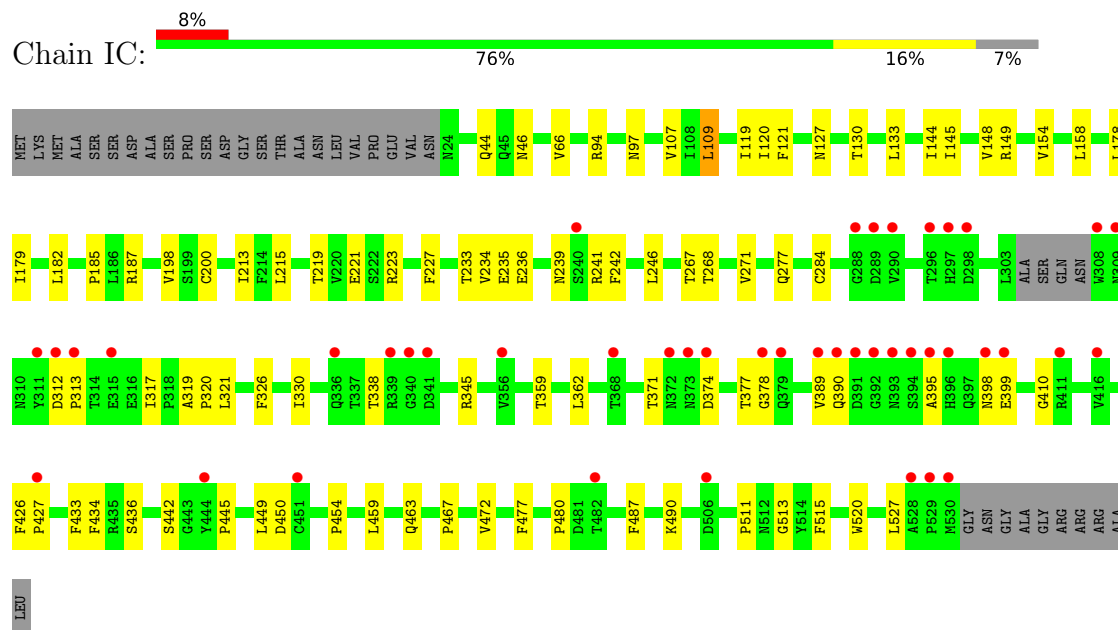




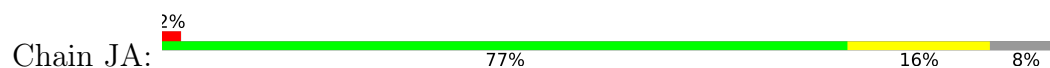
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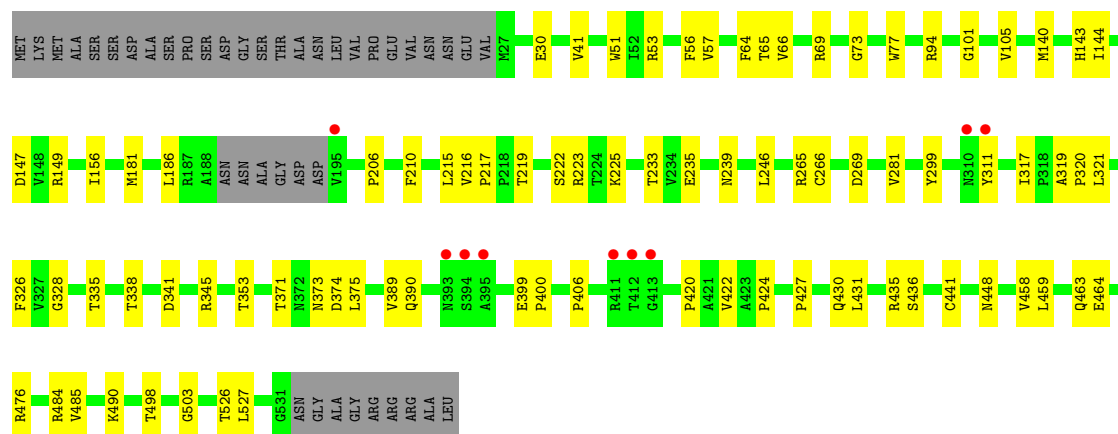


• Molecule 1: Capsid protein VP1

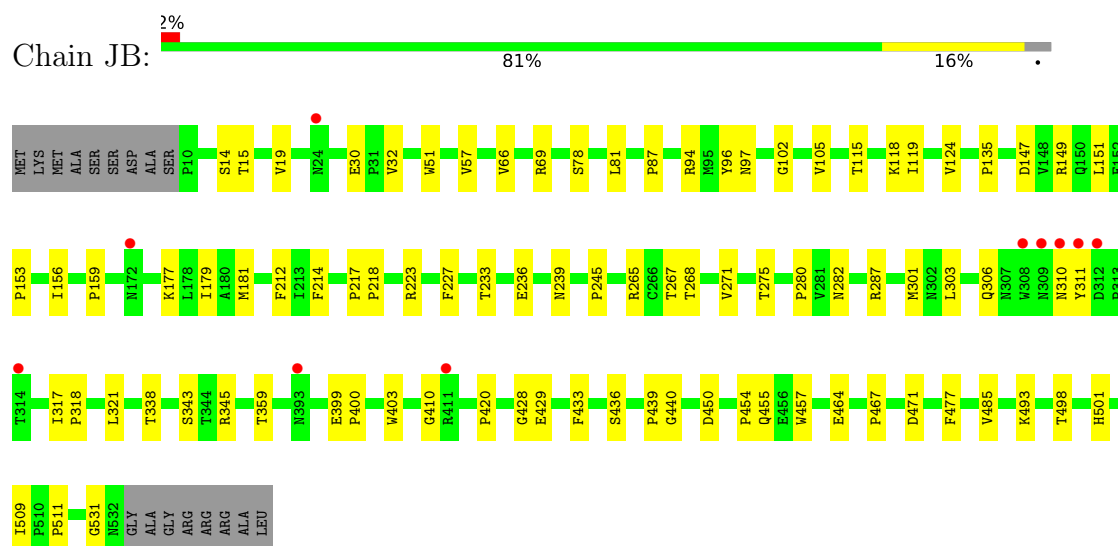


• Molecule 1: Capsid protein VP1

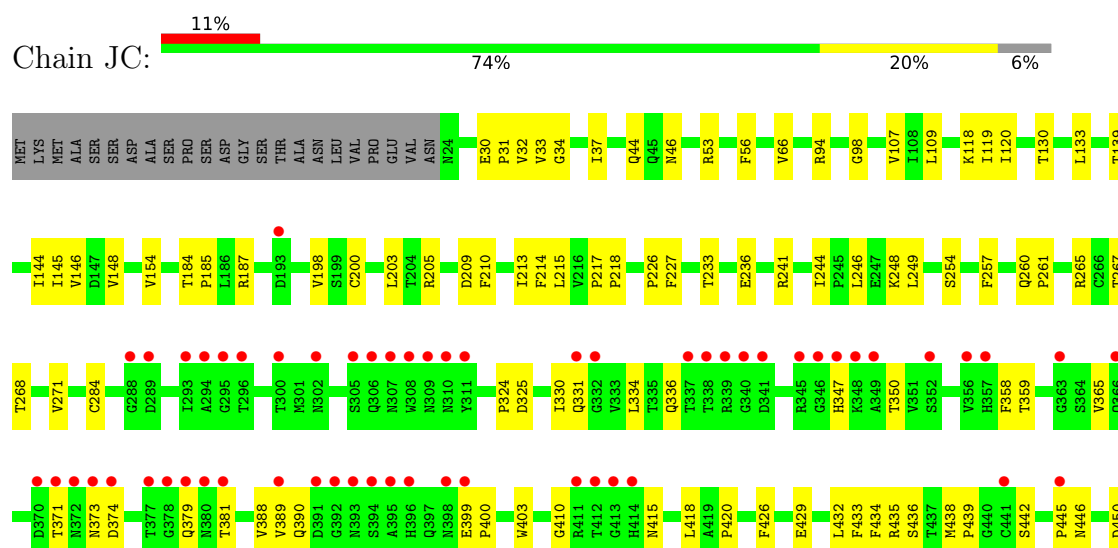


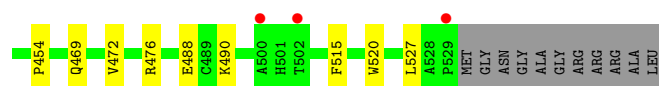


● Molecule 1: Capsid protein VP1

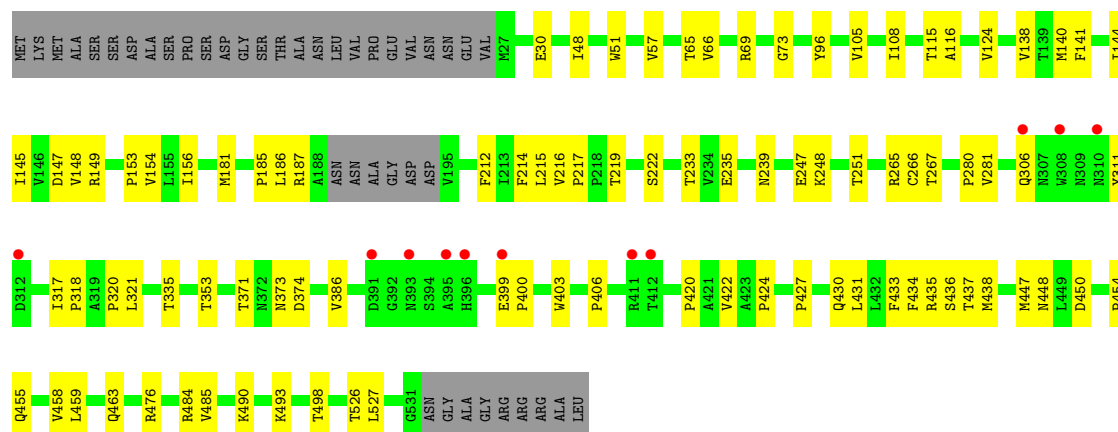
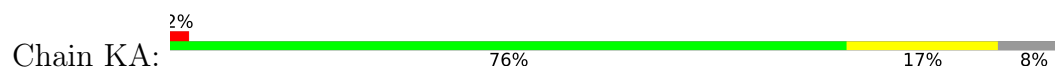


● Molecule 1: Capsid protein VP1

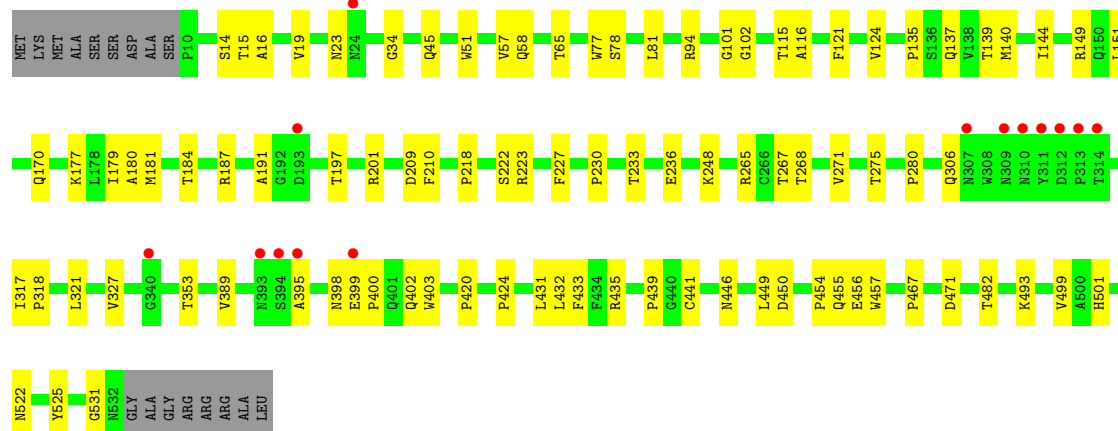
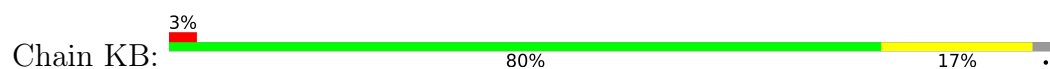




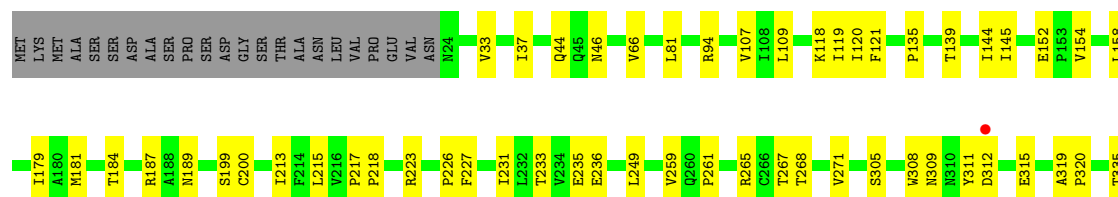
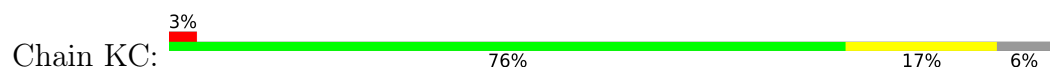
• Molecule 1: Capsid protein VP1

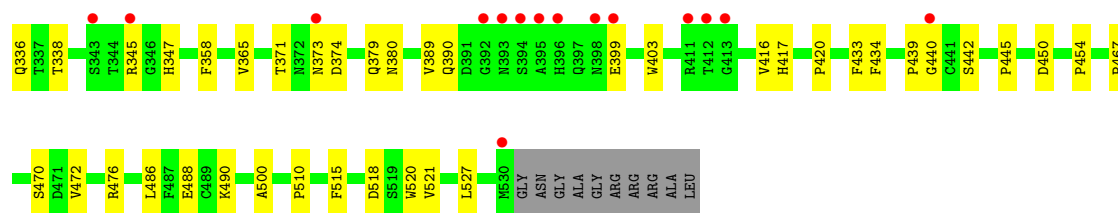


• Molecule 1: Capsid protein VP1

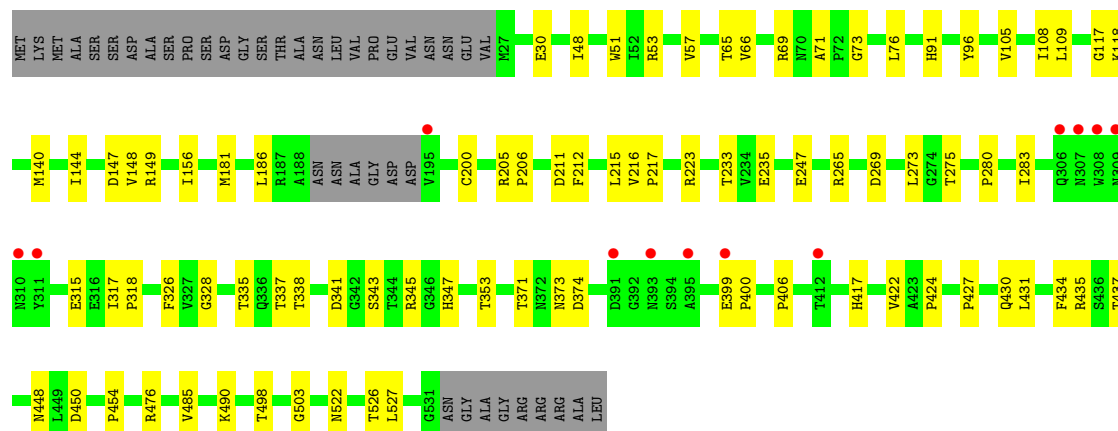
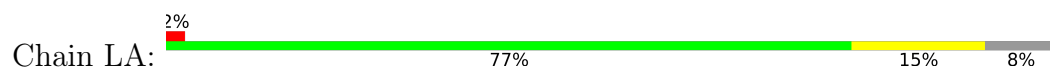


• Molecule 1: Capsid protein VP1

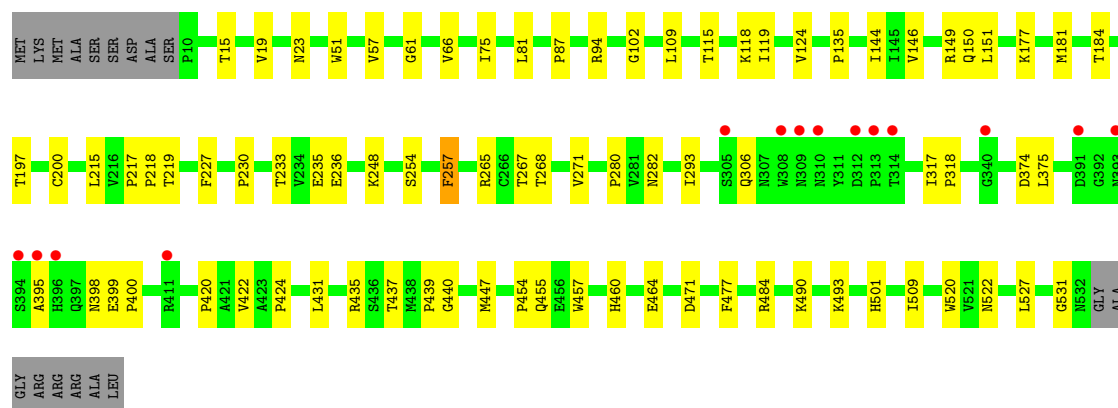
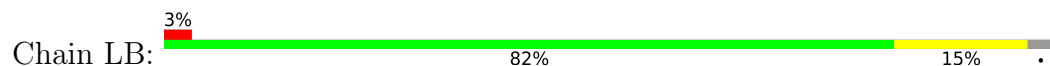




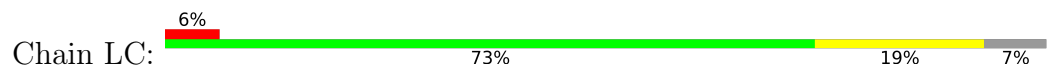
● Molecule 1: Capsid protein VP1

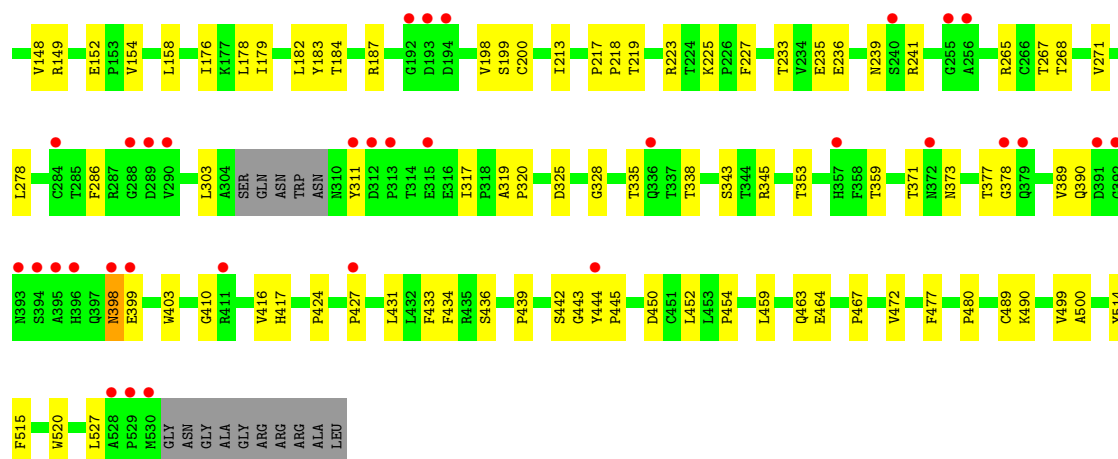


● Molecule 1: Capsid protein VP1

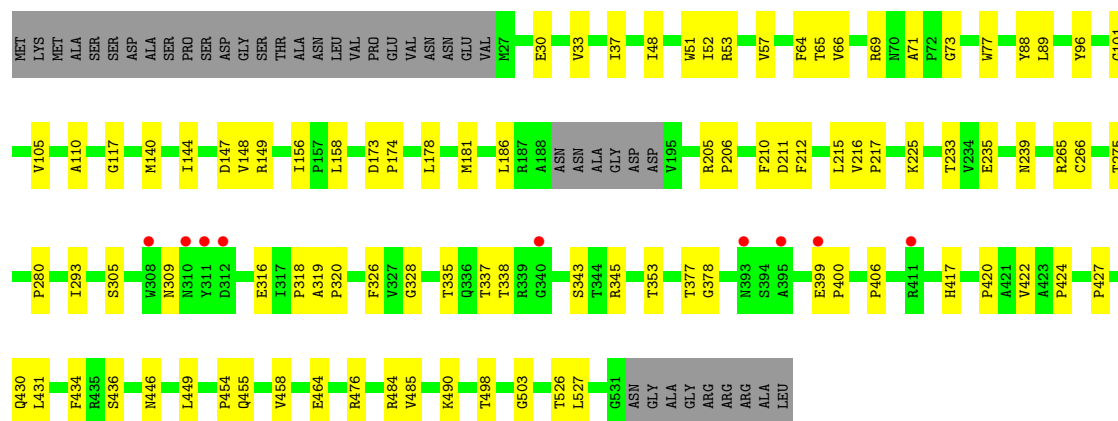
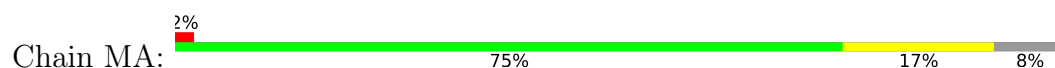


● Molecule 1: Capsid protein VP1

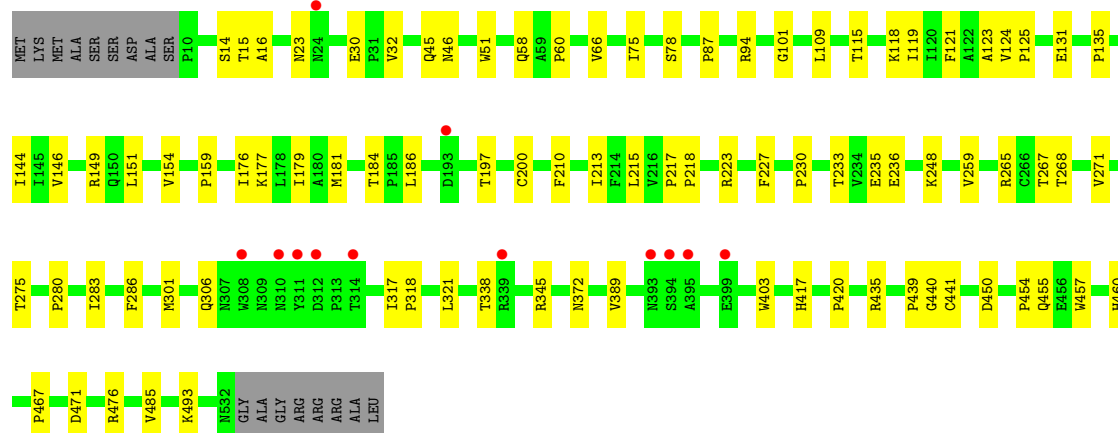
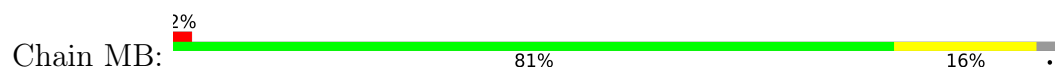




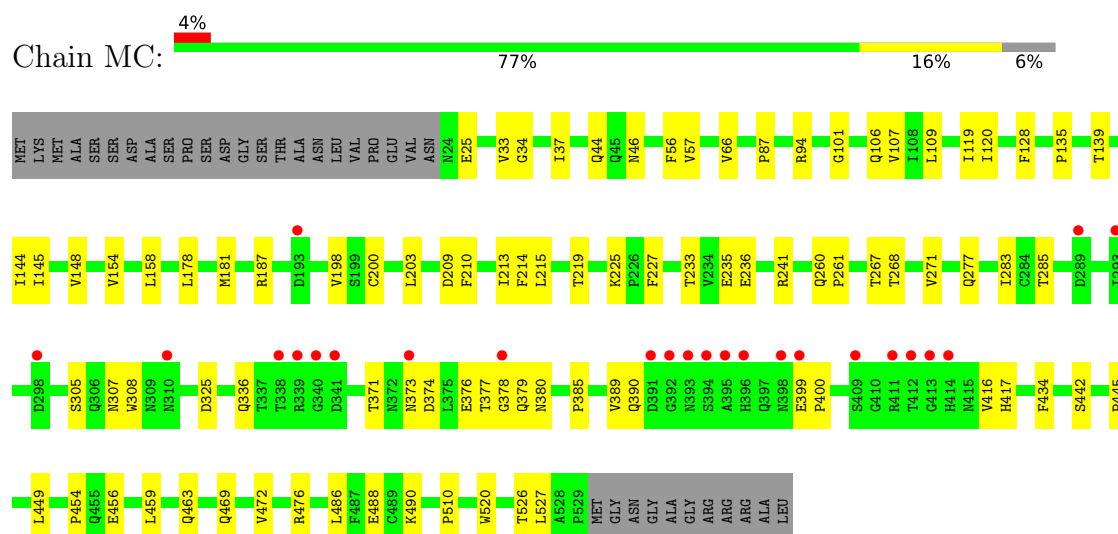
• Molecule 1: Capsid protein VP1



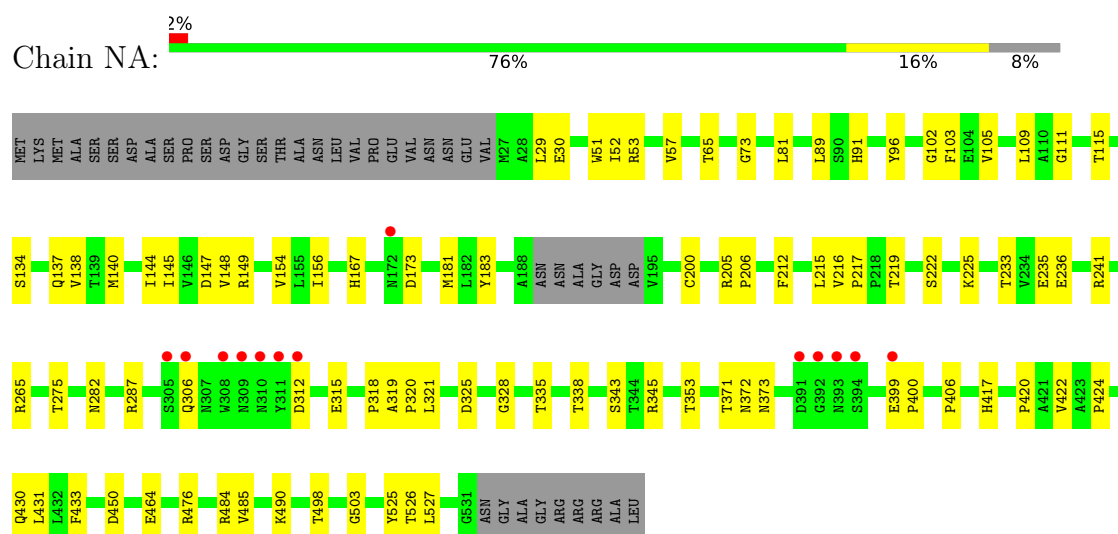
• Molecule 1: Capsid protein VP1



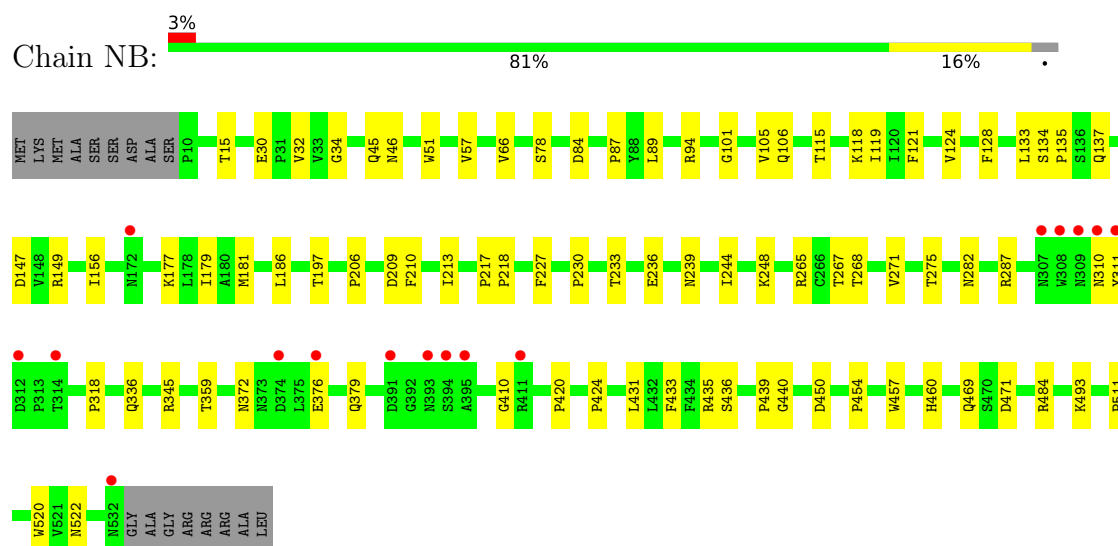
• Molecule 1: Capsid protein VP1



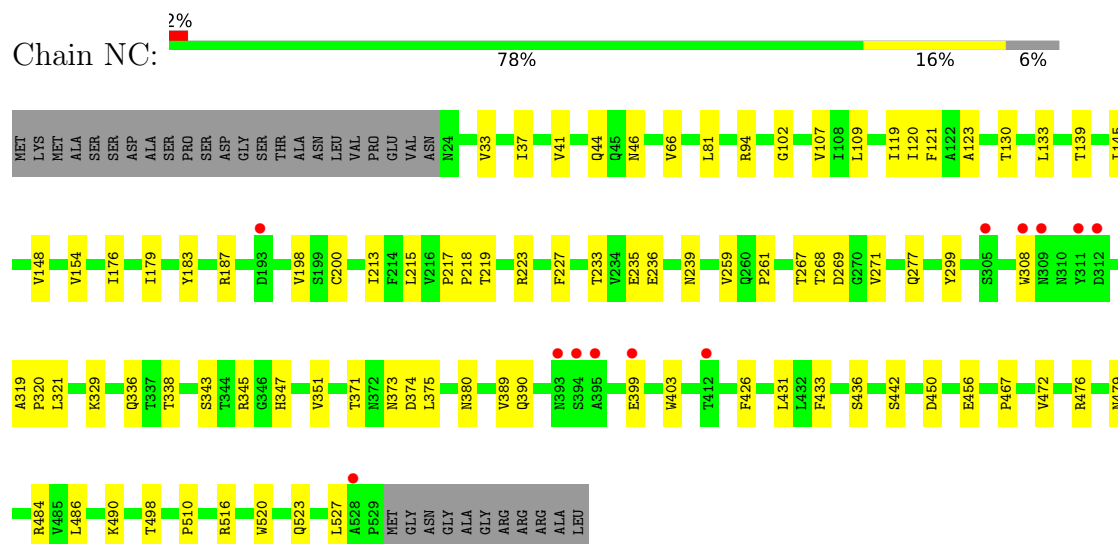
• Molecule 1: Capsid protein VP1



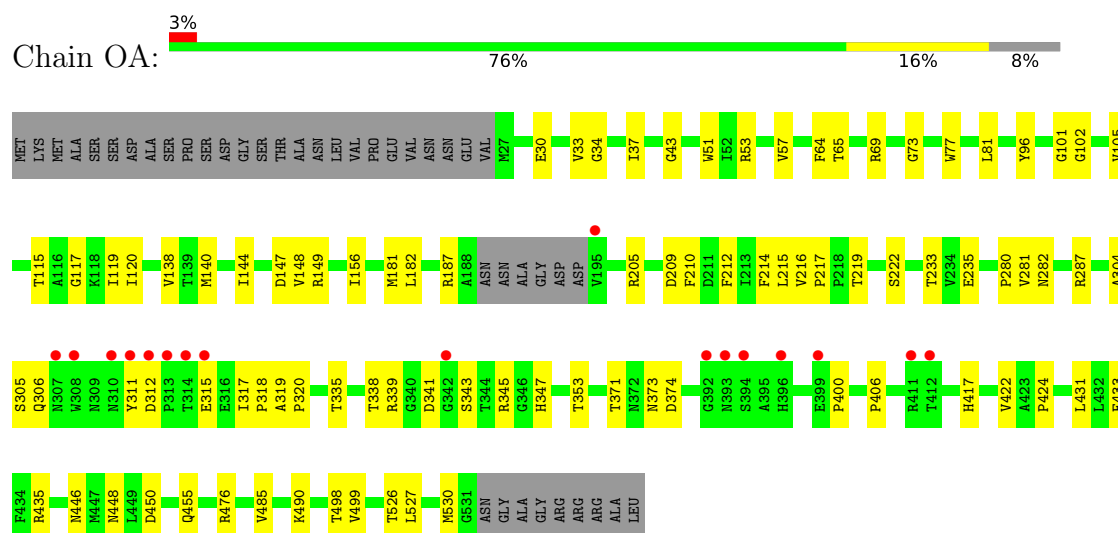
• Molecule 1: Capsid protein VP1



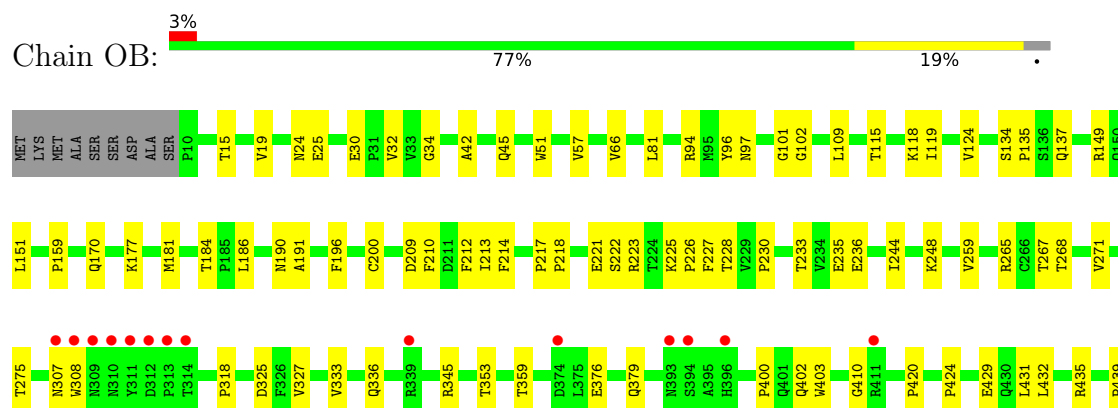
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

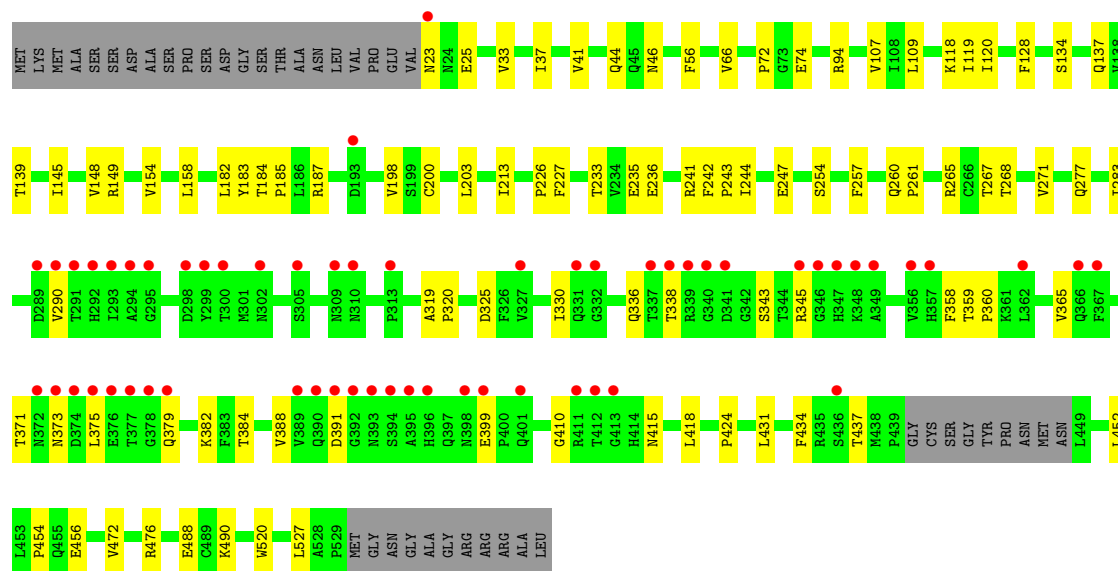
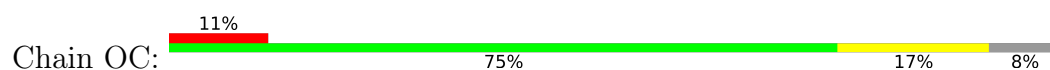


- Molecule 1: Capsid protein VP1





● Molecule 1: Capsid protein VP1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	420.17Å 446.60Å 463.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-3.00) 95.7 (30.00-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.207 , 0.242 0.207 , 0.242	Depositor DCC
R_{free} test set	40708 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	176522	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CD, CL, EDO

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	AA	0.27	0/3978	0.50	0/5458
1	AB	0.27	0/4134	0.50	0/5677
1	AC	0.27	0/4040	0.51	0/5545
1	BA	0.27	0/3971	0.49	0/5448
1	BB	0.27	0/4140	0.52	0/5684
1	BC	0.27	0/4032	0.51	0/5534
1	CA	0.27	0/3971	0.50	1/5448 (0.0%)
1	CB	0.28	0/4134	0.52	0/5677
1	CC	0.27	0/4032	0.51	0/5534
1	DA	0.27	0/3963	0.50	0/5438
1	DB	0.28	0/4134	0.52	0/5677
1	DC	0.27	0/4025	0.52	1/5525 (0.0%)
1	EA	0.27	0/3971	0.51	0/5448
1	EB	0.28	0/4134	0.51	0/5677
1	EC	0.27	0/3929	0.51	0/5392
1	FA	0.27	0/3971	0.49	0/5448
1	FB	0.27	0/4140	0.52	0/5684
1	FC	0.27	0/4047	0.52	0/5555
1	GA	0.27	0/3971	0.49	0/5448
1	GB	0.27	0/4137	0.52	0/5680
1	GC	0.27	0/4032	0.51	0/5534
1	HA	0.27	0/3971	0.50	0/5448
1	HB	0.27	0/4136	0.52	0/5679
1	HC	0.27	0/4032	0.51	0/5534
1	IA	0.27	0/3971	0.49	0/5448
1	IB	0.28	0/4140	0.52	0/5683
1	IC	0.27	0/4003	0.51	1/5493 (0.0%)
1	JA	0.27	0/3971	0.49	0/5448
1	JB	0.27	0/4128	0.51	0/5669
1	JC	0.26	0/4025	0.50	0/5525
1	KA	0.27	0/3971	0.49	0/5448
1	KB	0.27	0/4130	0.50	0/5672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	KC	0.26	0/4032	0.51	0/5534
1	LA	0.27	0/3971	0.50	0/5448
1	LB	0.27	0/4124	0.51	0/5664
1	LC	0.27	0/3981	0.51	1/5462 (0.0%)
1	MA	0.27	0/3971	0.49	0/5448
1	MB	0.36	1/4131 (0.0%)	0.52	0/5673
1	MC	0.27	0/4025	0.51	0/5525
1	NA	0.27	0/3971	0.49	0/5448
1	NB	0.27	0/4138	0.51	0/5680
1	NC	0.27	0/4018	0.51	0/5516
1	OA	0.27	0/3971	0.50	0/5448
1	OB	0.28	0/4138	0.52	0/5680
1	OC	0.27	0/3967	0.50	0/5445
All	All	0.27	1/181802 (0.0%)	0.51	4/249529 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	MB	217	PRO	N-CD	-15.17	1.26	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DC	109	LEU	CA-CB-CG	5.13	127.10	115.30
1	IC	109	LEU	CA-CB-CG	5.09	127.02	115.30
1	CA	173	ASP	CB-CG-OD1	5.06	122.86	118.30
1	LC	109	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3860	0	3758	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	4013	0	3874	62	0
1	AC	3921	0	3802	63	0
1	BA	3853	0	3749	60	0
1	BB	4019	0	3885	66	0
1	BC	3913	0	3796	68	0
1	CA	3853	0	3749	76	0
1	CB	4013	0	3874	63	0
1	CC	3913	0	3796	55	0
1	DA	3845	0	3740	82	0
1	DB	4013	0	3874	74	0
1	DC	3906	0	3787	67	0
1	EA	3853	0	3749	62	0
1	EB	4013	0	3874	63	0
1	EC	3814	0	3705	76	0
1	FA	3853	0	3749	81	0
1	FB	4019	0	3885	74	0
1	FC	3928	0	3811	67	0
1	GA	3853	0	3749	70	0
1	GB	4016	0	3883	72	0
1	GC	3913	0	3796	66	0
1	HA	3853	0	3749	64	0
1	HB	4015	0	3881	63	0
1	HC	3913	0	3796	57	0
1	IA	3853	0	3749	55	0
1	IB	4019	0	3892	71	0
1	IC	3885	0	3771	63	0
1	JA	3853	0	3749	68	0
1	JB	4007	0	3870	60	0
1	JC	3906	0	3787	72	0
1	KA	3853	0	3749	69	0
1	KB	4009	0	3870	69	0
1	KC	3913	0	3796	61	0
1	LA	3853	0	3749	64	0
1	LB	4003	0	3866	56	0
1	LC	3865	0	3758	79	0
1	MA	3853	0	3749	72	0
1	MB	4010	0	3872	68	0
1	MC	3906	0	3787	61	0
1	NA	3853	0	3749	67	0
1	NB	4017	0	3892	57	0
1	NC	3899	0	3781	62	0
1	OA	3853	0	3749	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	OB	4017	0	3892	71	0
1	OC	3851	0	3739	62	0
2	AA	3	0	0	0	0
2	AB	1	0	0	0	0
2	AC	1	0	0	0	0
2	BA	2	0	0	0	0
2	BC	1	0	0	0	0
2	CA	2	0	0	0	0
2	CC	3	0	0	1	0
2	DA	1	0	0	0	0
2	DB	1	0	0	0	0
2	DC	2	0	0	0	0
2	EA	3	0	0	0	0
2	FA	2	0	0	0	0
2	GA	1	0	0	0	0
2	GC	2	0	0	0	0
2	HA	1	0	0	0	0
2	HC	1	0	0	0	0
2	IA	3	0	0	0	0
2	JA	3	0	0	0	0
2	KA	2	0	0	0	0
2	KC	2	0	0	0	0
2	LA	1	0	0	0	0
2	LC	2	0	0	0	0
2	MA	3	0	0	0	0
2	MC	2	0	0	1	0
2	NA	2	0	0	0	0
2	NC	1	0	0	0	0
2	OA	2	0	0	0	0
3	AC	1	0	0	0	0
3	BA	1	0	0	0	0
3	BC	1	0	0	0	0
3	CA	1	0	0	0	0
3	DA	1	0	0	0	0
3	EA	1	0	0	0	0
3	EB	1	0	0	0	0
3	EC	1	0	0	0	0
3	FA	1	0	0	0	0
3	FC	1	0	0	0	0
3	GA	1	0	0	0	0
3	GB	1	0	0	0	0
3	HC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	IA	1	0	0	0	0
3	JA	1	0	0	0	0
3	JC	1	0	0	0	0
3	KA	1	0	0	0	0
3	KB	1	0	0	0	0
3	MA	1	0	0	0	0
3	MB	1	0	0	0	0
3	NC	1	0	0	0	0
3	OA	1	0	0	0	0
4	JA	4	0	6	0	0
5	HC	1	0	0	0	0
5	OA	1	0	0	0	0
5	OB	1	0	0	0	0
All	All	176522	0	171133	2696	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 8.

All (2696) 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:NA:65:THR:HG21	1:NA:526:THR:H	1.25	1.01
1:GA:65:THR:HG21	1:GA:526:THR:H	1.25	1.01
1:AA:65:THR:HG21	1:AA:526:THR:H	1.23	1.00
1:MA:65:THR:HG21	1:MA:526:THR:H	1.28	0.98
1:CA:65:THR:HG21	1:CA:526:THR:H	1.30	0.96
1:OA:65:THR:HG21	1:OA:526:THR:H	1.30	0.96
1:FA:65:THR:HG21	1:FA:526:THR:H	1.27	0.96
1:BA:65:THR:HG21	1:BA:526:THR:H	1.32	0.95
1:HA:65:THR:HG21	1:HA:526:THR:H	1.29	0.95
1:KA:65:THR:HG21	1:KA:526:THR:H	1.32	0.95
1:LA:65:THR:HG21	1:LA:526:THR:H	1.32	0.93
1:DA:65:THR:HG21	1:DA:526:THR:H	1.32	0.93
1:JA:65:THR:HG21	1:JA:526:THR:H	1.30	0.93
1:EA:65:THR:HG21	1:EA:526:THR:H	1.37	0.88
1:FA:120:ILE:HG12	1:FA:145:ILE:HG12	1.56	0.88
1:KC:267:THR:HG22	1:KC:271:VAL:H	1.39	0.87
1:CA:46:ASN:ND2	1:CA:213:ILE:O	2.07	0.87
1:EC:94:ARG:HD2	1:EC:219:THR:HG22	1.57	0.86
1:AA:46:ASN:ND2	1:AA:213:ILE:O	2.10	0.84
1:DC:94:ARG:HD2	1:DC:219:THR:HG22	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:120:ILE:HG12	1:DA:145:ILE:HG12	1.58	0.82
1:CB:223:ARG:HA	1:CB:467:PRO:HG3	1.62	0.82
1:HC:371:THR:HG22	1:HC:373:ASN:H	1.42	0.82
1:FB:120:ILE:HG12	1:FB:145:ILE:HG12	1.62	0.80
1:JB:267:THR:HG22	1:JB:271:VAL:H	1.47	0.80
1:GC:371:THR:HG22	1:GC:373:ASN:H	1.47	0.80
1:LC:371:THR:HG22	1:LC:373:ASN:H	1.47	0.79
1:EB:12:ASP:OD1	1:GB:17:ASN:ND2	2.13	0.79
1:IC:94:ARG:HD2	1:IC:219:THR:HG22	1.63	0.79
1:MC:486:LEU:HD11	1:MC:510:PRO:HD2	1.63	0.79
1:NA:306:GLN:NE2	1:NA:321:LEU:O	2.16	0.79
1:FB:439:PRO:HB3	1:GA:335:THR:HG21	1.65	0.78
1:IB:265:ARG:NH2	1:IB:420:PRO:O	2.17	0.78
1:OC:382:LYS:NZ	1:OC:384:THR:OG1	2.17	0.78
1:GB:277:GLN:HE22	1:GB:279:SER:HB3	1.49	0.78
1:DB:15:THR:HG21	1:DB:151:LEU:HD11	1.66	0.78
1:MB:267:THR:HG22	1:MB:271:VAL:H	1.48	0.78
1:GC:46:ASN:ND2	1:GC:213:ILE:O	2.17	0.78
1:BC:268:THR:HG21	1:BC:520:TRP:HH2	1.49	0.77
1:GC:233:THR:HB	1:GC:236:GLU:HG3	1.65	0.77
1:EA:120:ILE:HG12	1:EA:145:ILE:HG12	1.66	0.77
1:NC:267:THR:HG22	1:NC:271:VAL:H	1.50	0.77
1:CC:371:THR:HG22	1:CC:373:ASN:H	1.48	0.77
1:AA:144:ILE:HD12	1:AA:156:ILE:HG12	1.64	0.77
1:DB:120:ILE:HG12	1:DB:145:ILE:HG12	1.66	0.77
1:NB:15:THR:HG22	1:OC:149:ARG:HE	1.47	0.77
1:EB:135:PRO:HA	1:EB:181:MET:HE1	1.67	0.77
1:IB:121:PHE:HB2	1:IB:144:ILE:HG22	1.64	0.77
1:HB:15:THR:HG21	1:HB:151:LEU:HD11	1.66	0.76
1:JA:265:ARG:NH2	1:JA:420:PRO:O	2.17	0.76
1:LC:94:ARG:HD2	1:LC:219:THR:HG22	1.67	0.76
1:GB:248:LYS:HE3	1:GB:435:ARG:HD2	1.66	0.76
1:IA:65:THR:HG21	1:IA:526:THR:HB	1.68	0.76
1:EC:359:THR:HG22	1:EC:410:GLY:HA3	1.68	0.76
1:IC:267:THR:HG22	1:IC:271:VAL:H	1.50	0.76
1:GC:268:THR:HG21	1:GC:520:TRP:HH2	1.51	0.76
1:EA:265:ARG:NH2	1:EA:420:PRO:O	2.19	0.75
1:DC:268:THR:HG21	1:DC:520:TRP:HH2	1.49	0.75
1:JC:233:THR:HB	1:JC:236:GLU:HG3	1.68	0.75
1:DB:439:PRO:HB3	1:EA:335:THR:HG21	1.68	0.75
1:DA:120:ILE:HG13	1:DA:183:TYR:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:484:ARG:NH2	1:OA:69:ARG:O	2.20	0.75
1:BC:94:ARG:HD2	1:BC:219:THR:HG22	1.68	0.74
1:MC:371:THR:HG22	1:MC:373:ASN:H	1.52	0.74
1:NC:94:ARG:HD2	1:NC:219:THR:HG22	1.66	0.74
1:KB:223:ARG:HA	1:KB:467:PRO:HG3	1.69	0.74
1:DC:267:THR:HG22	1:DC:271:VAL:H	1.51	0.74
1:AC:476:ARG:HD3	1:AC:488:GLU:HB3	1.67	0.74
1:DB:267:THR:HG22	1:DB:271:VAL:H	1.51	0.74
1:IB:248:LYS:HE3	1:IB:435:ARG:HD2	1.68	0.74
1:MA:149:ARG:NH1	1:NA:111:GLY:O	2.20	0.74
1:AC:268:THR:HG21	1:AC:520:TRP:HH2	1.52	0.74
1:EA:120:ILE:HG13	1:EA:183:TYR:HB2	1.70	0.74
1:NA:265:ARG:NH2	1:NA:420:PRO:O	2.19	0.74
1:KC:46:ASN:ND2	1:KC:213:ILE:O	2.19	0.74
1:OB:135:PRO:HA	1:OB:181:MET:HE1	1.68	0.74
1:HB:267:THR:HG22	1:HB:271:VAL:H	1.53	0.73
1:EB:120:ILE:HG12	1:EB:145:ILE:HG12	1.70	0.73
1:KB:265:ARG:NH2	1:KB:420:PRO:O	2.21	0.73
1:AC:359:THR:HG22	1:AC:410:GLY:H	1.54	0.73
1:CB:267:THR:HG22	1:CB:271:VAL:H	1.52	0.73
1:JC:371:THR:HG22	1:JC:373:ASN:H	1.53	0.73
1:LB:248:LYS:HE3	1:LB:435:ARG:HD2	1.71	0.73
1:OB:15:THR:HG21	1:OB:151:LEU:HD11	1.69	0.73
1:AC:267:THR:HG22	1:AC:271:VAL:H	1.54	0.73
1:EA:303:LEU:HD11	1:EA:365:VAL:HG22	1.71	0.73
1:FA:120:ILE:HG13	1:FA:183:TYR:HB2	1.70	0.73
1:GB:15:THR:HG21	1:GB:151:LEU:HD11	1.69	0.73
1:AC:371:THR:HG22	1:AC:373:ASN:H	1.52	0.73
1:EA:144:ILE:HD12	1:EA:156:ILE:HG12	1.70	0.73
1:FC:33:VAL:HG11	1:FC:37:ILE:HG13	1.70	0.73
1:IC:46:ASN:ND2	1:IC:213:ILE:O	2.20	0.73
1:HA:282:ASN:OD1	1:HA:287:ARG:NH2	2.22	0.73
1:LC:268:THR:HG21	1:LC:520:TRP:HH2	1.52	0.73
1:AB:267:THR:HG22	1:AB:271:VAL:H	1.52	0.72
1:NC:233:THR:HB	1:NC:236:GLU:HG3	1.71	0.72
1:BB:267:THR:HG22	1:BB:271:VAL:H	1.54	0.72
1:EC:233:THR:HB	1:EC:236:GLU:HG3	1.71	0.72
1:EC:334:LEU:HD22	1:EC:381:THR:HG22	1.71	0.72
1:BB:345:ARG:NH2	1:BB:376:GLU:OE1	2.23	0.72
1:HA:233:THR:HG22	1:HA:235:GLU:H	1.54	0.72
1:HC:268:THR:HG21	1:HC:520:TRP:HH2	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:135:PRO:HA	1:AB:181:MET:HE1	1.69	0.72
1:HA:251:THR:HG22	1:HA:430:GLN:HE21	1.54	0.72
1:IC:268:THR:HG21	1:IC:520:TRP:HH2	1.53	0.72
1:JA:338:THR:OG1	1:JA:345:ARG:NH2	2.17	0.72
1:HC:233:THR:HB	1:HC:236:GLU:HG3	1.70	0.72
1:FC:267:THR:HG22	1:FC:271:VAL:H	1.55	0.72
1:JB:317:ILE:HG13	1:JB:318:PRO:HD2	1.71	0.72
1:JC:268:THR:HG21	1:JC:520:TRP:HH2	1.55	0.72
1:AB:120:ILE:HG12	1:AB:145:ILE:HG12	1.71	0.72
1:EC:316:GLU:OE1	1:EC:417:HIS:NE2	2.22	0.72
1:KC:268:THR:HG21	1:KC:520:TRP:HH2	1.55	0.72
1:LC:390:GLN:HG2	1:LC:399:GLU:HG2	1.72	0.72
1:BA:144:ILE:HD12	1:BA:156:ILE:HG12	1.72	0.71
1:EC:46:ASN:ND2	1:EC:213:ILE:O	2.21	0.71
1:LB:135:PRO:HA	1:LB:181:MET:HE1	1.71	0.71
1:CB:439:PRO:HB3	1:DA:335:THR:HG21	1.70	0.71
1:KB:170:GLN:NE2	1:KB:222:SER:O	2.22	0.71
1:DB:135:PRO:HA	1:DB:181:MET:HE1	1.71	0.71
1:FA:312:ASP:HB3	1:FA:315:GLU:HG3	1.72	0.71
1:IA:69:ARG:O	1:JA:484:ARG:NH2	2.24	0.71
1:MA:265:ARG:NH2	1:MA:420:PRO:O	2.24	0.71
1:FA:338:THR:OG1	1:FA:345:ARG:NH2	2.22	0.71
1:LC:267:THR:HG22	1:LC:271:VAL:H	1.55	0.71
1:FA:335:THR:HG21	1:JB:439:PRO:HB3	1.72	0.71
1:IB:94:ARG:HG2	1:IB:224:THR:HG23	1.73	0.71
1:LA:233:THR:HG22	1:LA:235:GLU:H	1.54	0.71
1:AC:233:THR:HB	1:AC:236:GLU:HG3	1.72	0.71
1:IB:411:ARG:NH1	1:IB:412:THR:OG1	2.24	0.71
1:BB:135:PRO:HA	1:BB:181:MET:HE1	1.72	0.71
1:FB:15:THR:HG21	1:FB:151:LEU:HD11	1.73	0.71
1:OC:268:THR:HG21	1:OC:520:TRP:HH2	1.55	0.71
1:IC:44:GLN:NE2	1:IC:215:LEU:H	1.89	0.70
1:MC:336:GLN:HE21	1:MC:379:GLN:HB2	1.55	0.70
1:EA:476:ARG:HD3	1:EA:485:VAL:HG11	1.73	0.70
1:OB:265:ARG:NH2	1:OB:420:PRO:O	2.24	0.70
1:IB:225:LYS:HE3	1:IB:464:GLU:HG3	1.72	0.70
1:KC:338:THR:OG1	1:KC:345:ARG:NH2	2.24	0.70
1:HB:439:PRO:HB3	1:IA:335:THR:HG21	1.72	0.70
1:FA:216:VAL:HG22	1:FA:217:PRO:HD2	1.74	0.70
1:FC:97:ASN:ND2	1:FC:221:GLU:OE2	2.25	0.70
1:MB:223:ARG:HA	1:MB:467:PRO:HG3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OB:248:LYS:HE3	1:OB:435:ARG:HD2	1.74	0.70
1:AA:265:ARG:NH2	1:AA:420:PRO:O	2.25	0.69
1:GA:476:ARG:HD3	1:GA:485:VAL:HG11	1.74	0.69
1:CC:233:THR:HB	1:CC:236:GLU:HG3	1.73	0.69
1:FC:66:VAL:HG21	1:FC:119:ILE:HD11	1.74	0.69
1:KB:267:THR:HG22	1:KB:271:VAL:H	1.57	0.69
1:MA:338:THR:OG1	1:MA:345:ARG:NH2	2.25	0.69
1:MB:439:PRO:HB3	1:NA:335:THR:HG21	1.75	0.69
1:IB:439:PRO:HB3	1:JA:335:THR:HG21	1.73	0.69
1:KC:66:VAL:HG21	1:KC:119:ILE:HD11	1.73	0.69
1:FC:439:PRO:HB3	1:LC:335:THR:HG21	1.73	0.69
1:HA:147:ASP:OD1	1:HA:149:ARG:HG2	1.92	0.69
1:OB:275:THR:HG23	1:OB:318:PRO:HG2	1.72	0.69
1:BC:33:VAL:HG11	1:BC:37:ILE:HG13	1.75	0.69
1:DB:244:ILE:HD11	1:DB:439:PRO:HD3	1.74	0.69
1:KA:149:ARG:NH2	1:LA:149:ARG:O	2.26	0.69
1:KB:23:ASN:HD22	1:KB:144:ILE:HD11	1.55	0.69
1:OA:140:MET:HB2	1:OB:217:PRO:HG3	1.75	0.69
1:CB:197:THR:O	1:DC:187:ARG:NH1	2.25	0.69
1:GB:275:THR:HG23	1:GB:318:PRO:HG2	1.74	0.69
1:DC:33:VAL:HG11	1:DC:37:ILE:HG13	1.73	0.69
1:JB:135:PRO:HA	1:JB:181:MET:HE1	1.74	0.69
1:JB:265:ARG:NH2	1:JB:420:PRO:O	2.26	0.68
1:AA:216:VAL:HG22	1:AA:217:PRO:HD2	1.76	0.68
1:DA:73:GLY:H	1:DA:181:MET:HE3	1.58	0.68
1:BC:233:THR:HB	1:BC:236:GLU:HG3	1.74	0.68
1:KA:335:THR:HG21	1:OB:439:PRO:HB3	1.74	0.68
1:MA:69:ARG:HH21	1:MA:427:PRO:HB2	1.58	0.68
1:BB:439:PRO:HB3	1:CA:335:THR:HG21	1.76	0.68
1:AA:140:MET:HB2	1:AB:217:PRO:HG3	1.76	0.68
1:MC:66:VAL:HG21	1:MC:119:ILE:HD11	1.75	0.68
1:BC:66:VAL:HG21	1:BC:119:ILE:HD11	1.74	0.68
1:OC:391:ASP:H	1:OC:399:GLU:HG3	1.58	0.68
1:AA:335:THR:HG21	1:EB:439:PRO:HB3	1.75	0.68
1:FB:33:VAL:HG21	1:FB:37:ILE:HG13	1.76	0.68
1:IC:233:THR:HB	1:IC:236:GLU:HG3	1.74	0.68
1:KB:197:THR:HB	1:LC:187:ARG:HH11	1.59	0.68
1:NC:44:GLN:NE2	1:NC:215:LEU:H	1.92	0.68
1:CC:267:THR:HG22	1:CC:271:VAL:H	1.57	0.68
1:FA:149:ARG:O	1:JA:149:ARG:NH2	2.27	0.68
1:HC:267:THR:HG22	1:HC:271:VAL:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LC:66:VAL:HG21	1:LC:119:ILE:HD11	1.74	0.68
1:MC:233:THR:HB	1:MC:236:GLU:HG3	1.76	0.68
1:GB:121:PHE:HB2	1:GB:144:ILE:HG22	1.76	0.68
1:HC:66:VAL:HG21	1:HC:119:ILE:HD11	1.74	0.68
1:JC:66:VAL:HG21	1:JC:119:ILE:HD11	1.75	0.68
1:CA:216:VAL:HG22	1:CA:217:PRO:HD2	1.75	0.67
1:FB:62:GLY:HA2	1:FB:202:VAL:HB	1.76	0.67
1:IC:66:VAL:HG21	1:IC:119:ILE:HD11	1.75	0.67
1:KB:275:THR:HG23	1:KB:318:PRO:HG2	1.76	0.67
1:HB:23:ASN:ND2	1:HB:144:ILE:HD11	2.09	0.67
1:AC:439:PRO:HB3	1:GC:335:THR:HG21	1.76	0.67
1:BA:424:PRO:HD3	1:BA:431:LEU:HD13	1.76	0.67
1:IB:94:ARG:HD3	1:IB:226:PRO:HD3	1.75	0.67
1:DC:390:GLN:HB2	1:DC:445:PRO:HB3	1.76	0.67
1:GB:135:PRO:HA	1:GB:181:MET:HE1	1.77	0.67
1:AB:439:PRO:HB3	1:BA:335:THR:HG21	1.77	0.67
1:EA:105:VAL:HG13	1:EA:156:ILE:HB	1.74	0.67
1:HB:265:ARG:NH2	1:HB:420:PRO:O	2.26	0.67
1:FB:231:ILE:HD11	1:GA:220:VAL:HG11	1.75	0.67
1:FC:371:THR:HG21	1:FC:374:ASP:HB2	1.77	0.67
1:MB:15:THR:HG21	1:MB:151:LEU:HD11	1.77	0.67
1:MC:267:THR:HG22	1:MC:271:VAL:H	1.59	0.67
1:BC:335:THR:HG21	1:KC:439:PRO:HB3	1.76	0.67
1:CC:46:ASN:ND2	1:CC:213:ILE:O	2.27	0.67
1:DC:66:VAL:HG21	1:DC:119:ILE:HD11	1.76	0.67
1:NB:439:PRO:HB3	1:OA:335:THR:HG21	1.77	0.67
1:NC:223:ARG:HA	1:NC:467:PRO:HG2	1.76	0.67
1:DA:476:ARG:HD3	1:DA:485:VAL:HG11	1.77	0.67
1:IA:353:THR:HG22	1:IA:406:PRO:HB3	1.76	0.66
1:EA:73:GLY:H	1:EA:181:MET:HE3	1.60	0.66
1:LA:371:THR:HG22	1:LA:373:ASN:H	1.61	0.66
1:LB:265:ARG:NH2	1:LB:420:PRO:O	2.28	0.66
1:CC:66:VAL:HG21	1:CC:119:ILE:HD11	1.77	0.66
1:CC:268:THR:HG21	1:CC:520:TRP:HH2	1.60	0.66
1:FA:144:ILE:HD12	1:FA:156:ILE:HG12	1.76	0.66
1:GB:439:PRO:HB3	1:HA:335:THR:HG21	1.76	0.66
1:GC:44:GLN:NE2	1:GC:215:LEU:H	1.94	0.66
1:NC:268:THR:HG21	1:NC:520:TRP:HH2	1.60	0.66
1:OA:490:LYS:HB2	1:OA:498:THR:HG22	1.78	0.66
1:GB:233:THR:HB	1:GB:236:GLU:HG3	1.78	0.66
1:GC:66:VAL:HG21	1:GC:119:ILE:HD11	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LC:433:PHE:HB3	1:LC:450:ASP:HB3	1.78	0.66
1:DA:251:THR:HG22	1:DA:430:GLN:HE21	1.60	0.66
1:IB:15:THR:HG21	1:IB:151:LEU:HD11	1.77	0.66
1:JB:15:THR:HG21	1:JB:151:LEU:HD11	1.78	0.66
1:KA:317:ILE:HG13	1:KA:318:PRO:HD2	1.77	0.66
1:KB:135:PRO:HA	1:KB:181:MET:HE1	1.78	0.66
1:EC:120:ILE:HG12	1:EC:145:ILE:HG12	1.78	0.66
1:GB:338:THR:OG1	1:GB:345:ARG:NH2	2.28	0.66
1:IC:120:ILE:HG12	1:IC:145:ILE:HG12	1.78	0.66
1:KC:233:THR:HB	1:KC:236:GLU:HG3	1.77	0.66
1:LB:215:LEU:HD21	1:MA:52:ILE:HD13	1.78	0.66
1:AA:490:LYS:HB2	1:AA:498:THR:HG22	1.78	0.66
1:HB:471:ASP:HA	1:HB:493:LYS:HD2	1.78	0.66
1:LB:267:THR:HG22	1:LB:271:VAL:H	1.61	0.66
1:CA:33:VAL:HG11	1:CA:37:ILE:HG13	1.78	0.66
1:AB:33:VAL:HG21	1:AB:37:ILE:HG13	1.79	0.65
1:BB:15:THR:HG21	1:BB:151:LEU:HD11	1.77	0.65
1:GC:120:ILE:HG12	1:GC:145:ILE:HG12	1.78	0.65
1:GC:390:GLN:HG2	1:GC:399:GLU:HG3	1.78	0.65
1:IA:233:THR:HG22	1:IA:235:GLU:H	1.61	0.65
1:BB:24:ASN:ND2	1:KC:152:GLU:OE2	2.28	0.65
1:JA:69:ARG:HH21	1:JA:427:PRO:HB2	1.60	0.65
1:KB:15:THR:HG21	1:KB:151:LEU:HD11	1.77	0.65
1:KC:390:GLN:HB2	1:KC:445:PRO:HB3	1.77	0.65
1:LC:120:ILE:HG12	1:LC:145:ILE:HG12	1.79	0.65
1:CA:73:GLY:H	1:CA:181:MET:HE3	1.62	0.65
1:CA:120:ILE:HD11	1:CA:183:TYR:CD1	2.31	0.65
1:NA:490:LYS:HB2	1:NA:498:THR:HG22	1.79	0.65
1:IB:135:PRO:HA	1:IB:181:MET:HE1	1.78	0.65
1:LA:140:MET:HB2	1:LB:217:PRO:HG3	1.78	0.65
1:BB:306:GLN:NE2	1:BB:321:LEU:O	2.30	0.65
1:BB:307:ASN:ND2	1:BB:309:ASN:OD1	2.30	0.65
1:DC:233:THR:HB	1:DC:236:GLU:HG3	1.77	0.65
1:HA:69:ARG:HH21	1:HA:427:PRO:HB2	1.60	0.65
1:JC:44:GLN:NE2	1:JC:215:LEU:H	1.94	0.65
1:LA:149:ARG:NH2	1:MA:149:ARG:O	2.30	0.65
1:KA:306:GLN:NE2	1:KA:321:LEU:O	2.30	0.65
1:LA:216:VAL:HG22	1:LA:217:PRO:HD2	1.78	0.65
1:AA:65:THR:HG21	1:AA:526:THR:N	2.05	0.65
1:BA:66:VAL:HG12	1:BA:186:LEU:HD22	1.79	0.65
1:IB:222:SER:HB3	1:IB:467:PRO:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OB:233:THR:HB	1:OB:236:GLU:HG3	1.79	0.65
1:BA:490:LYS:HB2	1:BA:498:THR:HG22	1.77	0.65
1:FB:267:THR:HG22	1:FB:271:VAL:H	1.62	0.65
1:AC:66:VAL:HG21	1:AC:119:ILE:HD11	1.77	0.64
1:GA:216:VAL:HG22	1:GA:217:PRO:HD2	1.78	0.64
1:HB:135:PRO:HA	1:HB:181:MET:HE1	1.78	0.64
1:LB:439:PRO:HB3	1:MA:335:THR:HG21	1.79	0.64
1:CB:306:GLN:NE2	1:CB:321:LEU:O	2.30	0.64
1:DB:248:LYS:HE3	1:DB:435:ARG:HD2	1.78	0.64
1:EB:33:VAL:HG21	1:EB:37:ILE:HG13	1.79	0.64
1:EB:265:ARG:NH2	1:EB:420:PRO:O	2.30	0.64
1:LC:121:PHE:HB2	1:LC:144:ILE:HG22	1.80	0.64
1:BA:149:ARG:NH2	1:CA:149:ARG:O	2.31	0.64
1:FC:476:ARG:HD3	1:FC:488:GLU:HB3	1.79	0.64
1:CB:15:THR:HG21	1:CB:151:LEU:HD11	1.80	0.64
1:CC:33:VAL:HG11	1:CC:37:ILE:HG13	1.79	0.64
1:CC:476:ARG:HD3	1:CC:488:GLU:HB3	1.80	0.64
1:FA:389:VAL:HG12	1:FA:441:CYS:HB2	1.79	0.64
1:IB:217:PRO:HB2	1:IB:219:THR:HG22	1.80	0.64
1:NC:46:ASN:ND2	1:NC:213:ILE:O	2.28	0.64
1:BB:94:ARG:HG3	1:BB:224:THR:HG23	1.78	0.64
1:BC:97:ASN:ND2	1:BC:221:GLU:OE2	2.30	0.64
1:EA:353:THR:HG22	1:EA:406:PRO:HB3	1.80	0.64
1:HB:197:THR:O	1:IC:187:ARG:NH1	2.31	0.64
1:OA:490:LYS:HG3	1:OA:527:LEU:HD11	1.78	0.64
1:AA:147:ASP:OD1	1:AA:149:ARG:HG2	1.97	0.64
1:BC:267:THR:HG22	1:BC:271:VAL:H	1.62	0.64
1:CB:265:ARG:NH2	1:CB:420:PRO:O	2.30	0.64
1:FA:476:ARG:HD3	1:FA:485:VAL:HG11	1.78	0.64
1:IA:476:ARG:HD3	1:IA:485:VAL:HG11	1.78	0.64
1:JA:73:GLY:H	1:JA:181:MET:HE3	1.62	0.64
1:AB:248:LYS:HE3	1:AB:435:ARG:HD2	1.80	0.64
1:AC:187:ARG:HH22	1:EB:197:THR:HB	1.63	0.64
1:FA:66:VAL:HG21	1:FA:119:ILE:HD11	1.78	0.64
1:JA:66:VAL:HG12	1:JA:186:LEU:HD22	1.78	0.64
1:KA:233:THR:HG22	1:KA:235:GLU:H	1.62	0.64
1:KB:439:PRO:HB3	1:LA:335:THR:HG21	1.79	0.64
1:KC:120:ILE:HG12	1:KC:145:ILE:HG12	1.79	0.64
1:OC:66:VAL:HG21	1:OC:119:ILE:HD11	1.80	0.64
1:CA:140:MET:HB2	1:CB:217:PRO:HG3	1.80	0.64
1:AC:184:THR:HG23	1:EB:199:SER:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:424:PRO:HD3	1:FA:431:LEU:HD13	1.79	0.64
1:NA:476:ARG:HD3	1:NA:485:VAL:HG11	1.80	0.64
1:AB:265:ARG:NH2	1:AB:420:PRO:O	2.32	0.63
1:DA:140:MET:HB2	1:DB:217:PRO:HG3	1.80	0.63
1:IC:359:THR:HG22	1:IC:410:GLY:HA3	1.80	0.63
1:NA:65:THR:HG21	1:NA:526:THR:N	2.07	0.63
1:EA:66:VAL:HG21	1:EA:119:ILE:HD11	1.80	0.63
1:GC:373:ASN:OD1	1:GC:374:ASP:N	2.31	0.63
1:HB:395:ALA:HB3	1:HB:398:ASN:ND2	2.14	0.63
1:MA:233:THR:HG22	1:MA:235:GLU:H	1.62	0.63
1:BA:144:ILE:HG21	1:BA:154:VAL:HG11	1.78	0.63
1:CA:120:ILE:HG13	1:CA:183:TYR:HB2	1.79	0.63
1:CB:130:THR:HG23	1:CB:179:ILE:HD11	1.80	0.63
1:EB:130:THR:HG23	1:EB:179:ILE:HD11	1.79	0.63
1:AA:304:ALA:O	1:AA:311:TYR:HB2	1.98	0.63
1:BA:490:LYS:HG3	1:BA:527:LEU:HD11	1.80	0.63
1:CA:233:THR:HG22	1:CA:235:GLU:H	1.64	0.63
1:CB:33:VAL:HG21	1:CB:37:ILE:HG13	1.78	0.63
1:CB:75:ILE:O	1:CB:522:ASN:ND2	2.32	0.63
1:JA:233:THR:HG22	1:JA:235:GLU:H	1.64	0.63
1:MC:476:ARG:HD3	1:MC:488:GLU:HB3	1.80	0.63
1:BB:46:ASN:ND2	1:BB:213:ILE:O	2.30	0.63
1:GB:471:ASP:HA	1:GB:493:LYS:HD2	1.79	0.63
1:JC:472:VAL:HG11	1:JC:490:LYS:HD2	1.79	0.63
1:KC:371:THR:HG22	1:KC:373:ASN:H	1.63	0.63
1:OA:233:THR:HG22	1:OA:235:GLU:H	1.61	0.63
1:EB:471:ASP:HA	1:EB:493:LYS:HD2	1.81	0.63
1:FB:184:THR:HG23	1:LC:199:SER:HB2	1.81	0.63
1:GA:353:THR:HG22	1:GA:406:PRO:HB3	1.79	0.63
1:LC:233:THR:HB	1:LC:236:GLU:HG3	1.79	0.63
1:MB:275:THR:HG23	1:MB:318:PRO:HG2	1.81	0.63
1:NA:424:PRO:HD3	1:NA:431:LEU:HD13	1.80	0.63
1:CA:144:ILE:HD12	1:CA:156:ILE:HG13	1.80	0.63
1:CC:120:ILE:HG12	1:CC:145:ILE:HG12	1.80	0.63
1:DA:37:ILE:HD11	1:DB:40:PRO:HB2	1.79	0.63
1:LA:147:ASP:OD1	1:LA:149:ARG:HG2	1.99	0.62
1:NB:275:THR:HG23	1:NB:318:PRO:HG2	1.81	0.62
1:KA:69:ARG:HH21	1:KA:427:PRO:HB2	1.65	0.62
1:AC:120:ILE:HG12	1:AC:145:ILE:HG12	1.81	0.62
1:BC:390:GLN:HB2	1:BC:445:PRO:HB3	1.81	0.62
1:FA:73:GLY:H	1:FA:181:MET:HE3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:24:ASN:CG	1:GC:25:GLU:H	2.03	0.62
1:DC:223:ARG:HA	1:DC:467:PRO:HG2	1.81	0.62
1:DC:286:PHE:HB3	1:DC:303:LEU:HD21	1.82	0.62
1:GA:233:THR:HG22	1:GA:235:GLU:H	1.63	0.62
1:KA:490:LYS:HB2	1:KA:498:THR:HG22	1.81	0.62
1:OC:371:THR:HG22	1:OC:373:ASN:H	1.64	0.62
1:DA:66:VAL:HG21	1:DA:119:ILE:HD11	1.80	0.62
1:EA:490:LYS:HG3	1:EA:527:LEU:HD11	1.80	0.62
1:GC:267:THR:HG22	1:GC:271:VAL:H	1.65	0.62
1:MA:66:VAL:HG12	1:MA:186:LEU:HD22	1.82	0.62
1:AC:335:THR:HG21	1:GC:439:PRO:HB3	1.82	0.62
1:BC:390:GLN:HG2	1:BC:399:GLU:HG3	1.81	0.62
1:EA:490:LYS:HB2	1:EA:498:THR:HG22	1.81	0.62
1:FC:233:THR:HB	1:FC:236:GLU:HG3	1.81	0.62
1:CC:44:GLN:NE2	1:CC:215:LEU:H	1.97	0.62
1:EA:233:THR:HG22	1:EA:235:GLU:H	1.65	0.62
1:JB:306:GLN:NE2	1:JB:321:LEU:O	2.33	0.62
1:KC:486:LEU:HD11	1:KC:510:PRO:HD2	1.82	0.62
1:BB:464:GLU:O	1:BB:464:GLU:HG3	2.00	0.62
1:CA:147:ASP:OD1	1:CA:149:ARG:HG2	2.00	0.62
1:FA:147:ASP:OD1	1:FA:149:ARG:HG2	1.99	0.62
1:HC:261:PRO:HG3	1:HC:403:TRP:HZ3	1.65	0.62
1:DA:69:ARG:HH21	1:DA:427:PRO:HB2	1.65	0.62
1:KA:65:THR:HG21	1:KA:526:THR:N	2.12	0.62
1:NC:261:PRO:HG3	1:NC:403:TRP:HZ3	1.64	0.62
1:OA:424:PRO:HD3	1:OA:431:LEU:HD13	1.81	0.62
1:OC:233:THR:HB	1:OC:236:GLU:HG3	1.82	0.62
1:DC:120:ILE:HG12	1:DC:145:ILE:HG12	1.82	0.61
1:JA:490:LYS:HB2	1:JA:498:THR:HG22	1.81	0.61
1:LC:223:ARG:HA	1:LC:467:PRO:HG2	1.80	0.61
1:LC:500:ALA:HB2	1:LC:527:LEU:HG	1.82	0.61
1:AA:66:VAL:HG21	1:AA:119:ILE:HD11	1.81	0.61
1:BC:433:PHE:HB3	1:BC:450:ASP:HB3	1.81	0.61
1:FA:248:LYS:HE2	1:FA:435:ARG:HD2	1.81	0.61
1:OA:476:ARG:HD3	1:OA:485:VAL:HG11	1.82	0.61
1:FA:147:ASP:OD2	1:FA:149:ARG:NH1	2.33	0.61
1:HC:120:ILE:HG12	1:HC:145:ILE:HG12	1.83	0.61
1:JC:400:PRO:HG2	1:JC:446:ASN:HB3	1.82	0.61
1:BC:46:ASN:ND2	1:BC:213:ILE:O	2.32	0.61
1:JA:490:LYS:HG3	1:JA:527:LEU:HD11	1.83	0.61
1:NA:282:ASN:OD1	1:NA:287:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:439:PRO:HB3	1:KC:335:THR:HG21	1.82	0.61
1:FC:268:THR:HG21	1:FC:520:TRP:HH2	1.66	0.61
1:FC:390:GLN:HG2	1:FC:399:GLU:HG3	1.82	0.61
1:JA:105:VAL:HG13	1:JA:156:ILE:HB	1.81	0.61
1:LA:490:LYS:HG3	1:LA:527:LEU:HD11	1.83	0.61
1:BA:147:ASP:OD1	1:BA:149:ARG:HG2	2.01	0.61
1:FA:140:MET:HB2	1:FB:217:PRO:HG3	1.83	0.61
1:JA:371:THR:HG22	1:JA:373:ASN:H	1.66	0.61
1:MC:44:GLN:NE2	1:MC:215:LEU:H	1.99	0.61
1:BB:33:VAL:HG21	1:BB:37:ILE:HG13	1.82	0.61
1:KA:239:ASN:ND2	1:KA:436:SER:OG	2.34	0.61
1:BC:120:ILE:HG12	1:BC:145:ILE:HG12	1.81	0.61
1:JB:94:ARG:HB3	1:JB:218:PRO:O	2.01	0.61
1:JB:275:THR:HG23	1:JB:318:PRO:HG2	1.83	0.61
1:MB:23:ASN:ND2	1:MB:144:ILE:HD11	2.15	0.61
1:NA:140:MET:HB2	1:NB:217:PRO:HG3	1.82	0.61
1:OC:415:ASN:HB3	1:OC:418:LEU:HD11	1.82	0.61
1:DC:81:LEU:HD12	1:DC:158:LEU:HG	1.84	0.60
1:LA:338:THR:OG1	1:LA:345:ARG:NH2	2.26	0.60
1:MA:147:ASP:OD1	1:MA:149:ARG:HG2	2.01	0.60
1:MA:316:GLU:OE1	1:MA:417:HIS:NE2	2.33	0.60
1:OC:33:VAL:HG11	1:OC:37:ILE:HB	1.82	0.60
1:LC:328:GLY:H	1:LC:353:THR:HG1	1.47	0.60
1:MC:158:LEU:HD13	1:MC:178:LEU:HG	1.82	0.60
1:NC:66:VAL:HG21	1:NC:119:ILE:HD11	1.83	0.60
1:BB:389:VAL:HG12	1:BB:441:CYS:HB2	1.84	0.60
1:EA:422:VAL:HG12	1:EA:431:LEU:HD21	1.84	0.60
1:FA:161:VAL:HB	1:FA:176:ILE:HD11	1.84	0.60
1:AB:197:THR:O	1:BC:187:ARG:NH1	2.34	0.60
1:CB:469:GLN:OE1	1:CB:520:TRP:NE1	2.34	0.60
1:DA:233:THR:HG22	1:DA:235:GLU:H	1.65	0.60
1:DC:254:SER:HA	1:DC:257:PHE:CE1	2.36	0.60
1:GC:261:PRO:HG3	1:GC:403:TRP:HZ3	1.67	0.60
1:HC:472:VAL:HG11	1:HC:490:LYS:HD2	1.84	0.60
1:IB:233:THR:HB	1:IB:236:GLU:HG3	1.83	0.60
1:KC:476:ARG:HD3	1:KC:488:GLU:HB3	1.82	0.60
1:BA:69:ARG:HH21	1:BA:427:PRO:HB2	1.66	0.60
1:FC:46:ASN:ND2	1:FC:213:ILE:O	2.31	0.60
1:GB:267:THR:HG22	1:GB:271:VAL:H	1.66	0.60
1:IC:97:ASN:ND2	1:IC:221:GLU:OE2	2.34	0.60
1:KA:490:LYS:HG3	1:KA:527:LEU:HD11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JB:471:ASP:HA	1:JB:493:LYS:HD2	1.83	0.60
1:HC:121:PHE:HB2	1:HC:144:ILE:HG22	1.84	0.60
1:KB:15:THR:HG22	1:LC:149:ARG:HE	1.66	0.60
1:OA:280:PRO:HB3	1:OA:455:GLN:HG2	1.82	0.60
1:DA:159:PRO:O	1:DA:176:ILE:HD12	2.02	0.60
1:BB:433:PHE:HB3	1:BB:450:ASP:HB3	1.84	0.60
1:FB:275:THR:HG23	1:FB:318:PRO:HG2	1.83	0.60
1:IA:490:LYS:HG3	1:IA:527:LEU:HD11	1.83	0.60
1:NA:144:ILE:HD12	1:NA:154:VAL:HG11	1.84	0.60
1:DC:109:LEU:HD13	1:DC:200:CYS:SG	2.42	0.59
1:JC:46:ASN:ND2	1:JC:213:ILE:O	2.35	0.59
1:JC:120:ILE:HG12	1:JC:145:ILE:HG12	1.83	0.59
1:AA:233:THR:HG22	1:AA:235:GLU:H	1.66	0.59
1:DA:490:LYS:HB2	1:DA:498:THR:HG22	1.82	0.59
1:HC:33:VAL:HG11	1:HC:37:ILE:HB	1.84	0.59
1:KC:223:ARG:HA	1:KC:467:PRO:HG2	1.83	0.59
1:NA:73:GLY:H	1:NA:181:MET:HE3	1.67	0.59
1:CB:135:PRO:HA	1:CB:181:MET:HE1	1.84	0.59
1:GA:65:THR:HG21	1:GA:526:THR:N	2.06	0.59
1:NB:135:PRO:HA	1:NB:181:MET:HE1	1.82	0.59
1:DA:216:VAL:HG22	1:DA:217:PRO:HD2	1.84	0.59
1:EB:267:THR:HG22	1:EB:271:VAL:H	1.66	0.59
1:FA:159:PRO:O	1:FA:176:ILE:HD12	2.02	0.59
1:FA:233:THR:HG22	1:FA:235:GLU:H	1.66	0.59
1:KA:147:ASP:OD2	1:KA:149:ARG:NH1	2.36	0.59
1:LB:94:ARG:O	1:LB:218:PRO:HA	2.03	0.59
1:NA:225:LYS:HD3	1:NA:464:GLU:HG3	1.84	0.59
1:BA:66:VAL:HG21	1:BA:119:ILE:HD11	1.85	0.59
1:HA:73:GLY:H	1:HA:181:MET:HE3	1.68	0.59
1:AA:159:PRO:O	1:AA:176:ILE:HD12	2.03	0.59
1:DA:275:THR:HG23	1:DA:318:PRO:HG2	1.83	0.59
1:IC:472:VAL:HG11	1:IC:490:LYS:HD2	1.85	0.59
1:NA:105:VAL:HG13	1:NA:156:ILE:HB	1.85	0.59
1:NC:338:THR:OG1	1:NC:345:ARG:NH2	2.35	0.59
1:AA:220:VAL:HG11	1:EB:231:ILE:HD11	1.85	0.59
1:DB:197:THR:O	1:EC:187:ARG:NH1	2.36	0.59
1:EC:343:SER:OG	1:EC:345:ARG:NH1	2.36	0.59
1:HA:147:ASP:OD2	1:HA:149:ARG:NH1	2.36	0.59
1:IC:246:LEU:HA	1:IC:436:SER:HB3	1.85	0.59
1:NC:120:ILE:HG12	1:NC:145:ILE:HG12	1.84	0.59
1:NA:147:ASP:OD1	1:NA:149:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:275:THR:HG23	1:NA:318:PRO:HG2	1.85	0.59
1:GA:317:ILE:HG22	1:GA:318:PRO:HD2	1.83	0.59
1:MB:121:PHE:HB2	1:MB:144:ILE:HG22	1.84	0.59
1:FA:490:LYS:HB2	1:FA:498:THR:HG22	1.85	0.59
1:NA:353:THR:HG22	1:NA:406:PRO:HB3	1.85	0.59
1:AA:149:ARG:NH2	1:BA:149:ARG:O	2.36	0.58
1:AC:189:ASN:HD21	1:EB:190:ASN:HB2	1.68	0.58
1:EC:476:ARG:HD3	1:EC:488:GLU:HB3	1.83	0.58
1:HA:371:THR:HG22	1:HA:373:ASN:H	1.67	0.58
1:IB:94:ARG:HH22	1:JA:94:ARG:HH12	1.49	0.58
1:NC:371:THR:HG22	1:NC:373:ASN:H	1.68	0.58
1:CB:471:ASP:HA	1:CB:493:LYS:HD2	1.85	0.58
1:DB:101:GLY:HA3	1:DB:210:PHE:HA	1.85	0.58
1:HA:490:LYS:HG3	1:HA:527:LEU:HD11	1.85	0.58
1:KB:14:SER:O	1:KB:16:ALA:N	2.36	0.58
1:OC:120:ILE:HG12	1:OC:145:ILE:HG12	1.85	0.58
1:AA:105:VAL:HG13	1:AA:156:ILE:HB	1.84	0.58
1:BA:476:ARG:HD3	1:BA:485:VAL:HG11	1.85	0.58
1:OA:147:ASP:OD1	1:OA:149:ARG:HG2	2.03	0.58
1:CA:37:ILE:HD11	1:CB:40:PRO:HB2	1.84	0.58
1:EA:216:VAL:HG22	1:EA:217:PRO:HD2	1.85	0.58
1:GB:242:PHE:HD1	1:GB:284:CYS:HG	1.51	0.58
1:LC:338:THR:HB	1:LC:343:SER:HB3	1.85	0.58
1:LC:472:VAL:HG11	1:LC:490:LYS:HD2	1.84	0.58
1:AA:73:GLY:H	1:AA:181:MET:HE3	1.67	0.58
1:AC:261:PRO:HG3	1:AC:403:TRP:HZ3	1.68	0.58
1:AC:338:THR:OG1	1:AC:345:ARG:NH2	2.35	0.58
1:FB:433:PHE:HB3	1:FB:450:ASP:HB3	1.86	0.58
1:MA:216:VAL:HG22	1:MA:217:PRO:HD2	1.85	0.58
1:MB:135:PRO:HA	1:MB:181:MET:HE1	1.86	0.58
1:MC:472:VAL:HG11	1:MC:490:LYS:HD2	1.85	0.58
1:BB:277:GLN:OE1	1:BB:279:SER:N	2.34	0.58
1:FA:37:ILE:HD11	1:FB:40:PRO:HB2	1.85	0.58
1:KB:471:ASP:HA	1:KB:493:LYS:HD2	1.85	0.58
1:KC:261:PRO:HG3	1:KC:403:TRP:HZ3	1.67	0.58
1:CA:338:THR:OG1	1:CA:345:ARG:NH2	2.30	0.58
1:CB:389:VAL:HG12	1:CB:441:CYS:HB2	1.86	0.58
1:DC:390:GLN:HG2	1:DC:399:GLU:HG3	1.86	0.58
1:HC:249:LEU:HB3	1:HC:507:LEU:HD12	1.86	0.58
1:IB:488:GLU:HG3	1:IB:527:LEU:HD22	1.85	0.58
1:EC:44:GLN:NE2	1:EC:215:LEU:H	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:470:SER:OG	1:HC:521:VAL:O	2.13	0.58
1:LB:233:THR:HB	1:LB:236:GLU:HG3	1.85	0.58
1:OC:434:PHE:CE2	1:OC:454:PRO:HD3	2.39	0.58
1:DA:225:LYS:HD3	1:DA:464:GLU:HG3	1.85	0.58
1:FC:227:PHE:CE1	1:FC:268:THR:HG23	2.39	0.58
1:HB:482:THR:HG21	1:IC:427:PRO:HD3	1.86	0.58
1:JB:69:ARG:NH1	1:JB:428:GLY:HA3	2.18	0.58
1:JC:284:CYS:HB2	1:JC:324:PRO:HG3	1.85	0.58
1:MB:109:LEU:HD23	1:MB:200:CYS:SG	2.44	0.58
1:OC:476:ARG:HD3	1:OC:488:GLU:HB3	1.86	0.58
1:AC:199:SER:HB2	1:GB:184:THR:HG23	1.86	0.58
1:KA:105:VAL:HG13	1:KA:156:ILE:HB	1.86	0.58
1:AA:490:LYS:HG3	1:AA:527:LEU:HD11	1.85	0.57
1:BB:275:THR:HG23	1:BB:318:PRO:HG2	1.84	0.57
1:NA:216:VAL:HG22	1:NA:217:PRO:HD2	1.85	0.57
1:AC:227:PHE:CE1	1:AC:268:THR:HG23	2.38	0.57
1:CA:490:LYS:HB2	1:CA:498:THR:HG22	1.85	0.57
1:EC:66:VAL:HG21	1:EC:119:ILE:HD11	1.86	0.57
1:GA:306:GLN:NE2	1:GA:321:LEU:O	2.37	0.57
1:HA:275:THR:HG23	1:HA:318:PRO:HG2	1.86	0.57
1:KB:395:ALA:HB3	1:KB:398:ASN:ND2	2.17	0.57
1:OA:353:THR:HG22	1:OA:406:PRO:HB3	1.86	0.57
1:CB:94:ARG:O	1:CB:218:PRO:HA	2.05	0.57
1:IA:149:ARG:NH2	1:JA:149:ARG:O	2.37	0.57
1:LC:239:ASN:ND2	1:LC:436:SER:OG	2.35	0.57
1:MC:371:THR:HG21	1:MC:374:ASP:HB2	1.86	0.57
1:DC:261:PRO:HG3	1:DC:403:TRP:HZ3	1.69	0.57
1:IC:121:PHE:HB2	1:IC:144:ILE:HG22	1.86	0.57
1:LC:398:ASN:ND2	1:LC:398:ASN:O	2.38	0.57
1:MA:319:ALA:HB1	1:MA:320:PRO:HD2	1.85	0.57
1:NA:144:ILE:HD13	1:NA:156:ILE:HG12	1.87	0.57
1:AC:390:GLN:HG2	1:AC:399:GLU:HG3	1.86	0.57
1:CB:120:ILE:HG12	1:CB:145:ILE:HG12	1.86	0.57
1:DA:105:VAL:HG13	1:DA:156:ILE:HB	1.86	0.57
1:EA:424:PRO:HD3	1:EA:431:LEU:HD13	1.85	0.57
1:FA:490:LYS:HG3	1:FA:527:LEU:HD11	1.86	0.57
1:FB:233:THR:HB	1:FB:236:GLU:HG3	1.85	0.57
1:IA:216:VAL:HG22	1:IA:217:PRO:HD2	1.87	0.57
1:LC:227:PHE:CE1	1:LC:268:THR:HG23	2.39	0.57
1:EB:30:GLU:HG3	1:EC:44:GLN:HA	1.84	0.57
1:LA:476:ARG:HD3	1:LA:485:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:437:THR:HG23	1:CB:447:MET:HB3	1.86	0.57
1:JA:216:VAL:HG22	1:JA:217:PRO:HD2	1.87	0.57
1:BB:109:LEU:HD23	1:BB:200:CYS:SG	2.45	0.57
1:FC:120:ILE:HG12	1:FC:145:ILE:HG12	1.86	0.57
1:GB:306:GLN:NE2	1:GB:321:LEU:O	2.38	0.57
1:HC:46:ASN:ND2	1:HC:213:ILE:O	2.37	0.57
1:IA:105:VAL:HG13	1:IA:156:ILE:HB	1.86	0.57
1:LB:464:GLU:HG3	1:LB:464:GLU:O	2.05	0.57
1:NC:371:THR:HG21	1:NC:374:ASP:HB2	1.86	0.57
1:OC:46:ASN:ND2	1:OC:213:ILE:O	2.34	0.57
1:CA:490:LYS:HG3	1:CA:527:LEU:HD11	1.87	0.57
1:IA:53:ARG:HB3	1:IA:206:PRO:HG2	1.87	0.57
1:LA:147:ASP:OD2	1:LA:149:ARG:NH1	2.38	0.57
1:MA:328:GLY:H	1:MA:353:THR:HB	1.68	0.57
1:MB:23:ASN:HD22	1:MB:144:ILE:HD11	1.70	0.57
1:MC:109:LEU:HD13	1:MC:200:CYS:SG	2.44	0.57
1:MC:434:PHE:CE2	1:MC:454:PRO:HD3	2.40	0.57
1:OB:471:ASP:HA	1:OB:493:LYS:HD2	1.87	0.57
1:GC:254:SER:HA	1:GC:257:PHE:CE1	2.40	0.57
1:IB:246:LEU:HD11	1:IB:454:PRO:HB3	1.87	0.57
1:MC:268:THR:HG21	1:MC:520:TRP:HH2	1.68	0.57
1:EB:118:LYS:H	1:EB:184:THR:HB	1.70	0.56
1:EC:159:PRO:O	1:EC:176:ILE:HD12	2.05	0.56
1:HC:227:PHE:CE1	1:HC:268:THR:HG23	2.40	0.56
1:LA:69:ARG:HH21	1:LA:427:PRO:HB2	1.70	0.56
1:LB:197:THR:O	1:MC:187:ARG:NH1	2.38	0.56
1:OC:267:THR:HG22	1:OC:271:VAL:H	1.69	0.56
1:MC:94:ARG:HD2	1:MC:219:THR:HG22	1.86	0.56
1:AC:33:VAL:HG11	1:AC:37:ILE:HB	1.87	0.56
1:BC:268:THR:HG21	1:BC:520:TRP:CH2	2.36	0.56
1:FB:227:PHE:CE1	1:FB:268:THR:HG23	2.40	0.56
1:FC:335:THR:HG21	1:LC:439:PRO:HB3	1.86	0.56
1:JB:227:PHE:CE1	1:JB:268:THR:HG23	2.40	0.56
1:KC:390:GLN:HG2	1:KC:399:GLU:HG3	1.86	0.56
1:MA:490:LYS:HB2	1:MA:498:THR:HG22	1.87	0.56
1:MB:123:ALA:HB1	1:MB:176:ILE:HD11	1.86	0.56
1:MC:120:ILE:HG12	1:MC:145:ILE:HG12	1.87	0.56
1:AB:94:ARG:O	1:AB:218:PRO:HA	2.05	0.56
1:BC:199:SER:HB2	1:KB:184:THR:HG23	1.86	0.56
1:DA:144:ILE:HD12	1:DA:156:ILE:HG12	1.88	0.56
1:FB:471:ASP:HA	1:FB:493:LYS:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HC:476:ARG:HD3	1:HC:488:GLU:HB3	1.86	0.56
1:OB:248:LYS:NZ	1:OB:506:ASP:OD2	2.32	0.56
1:CC:242:PHE:HD1	1:CC:284:CYS:HG	1.53	0.56
1:DA:149:ARG:NH2	1:EA:149:ARG:O	2.38	0.56
1:FC:199:SER:HB2	1:LB:184:THR:HG23	1.88	0.56
1:IC:227:PHE:CE1	1:IC:268:THR:HG23	2.41	0.56
1:BB:30:GLU:HG3	1:BC:44:GLN:HA	1.87	0.56
1:JB:477:PHE:CE2	1:JB:509:ILE:HD12	2.41	0.56
1:KB:248:LYS:HE3	1:KB:435:ARG:HD2	1.86	0.56
1:LB:75:ILE:O	1:LB:522:ASN:ND2	2.39	0.56
1:DB:359:THR:HG22	1:DB:410:GLY:HA3	1.87	0.56
1:DC:46:ASN:ND2	1:DC:213:ILE:O	2.39	0.56
1:EB:19:VAL:HG23	1:EB:149:ARG:HB3	1.88	0.56
1:GA:144:ILE:HD13	1:GA:156:ILE:HG12	1.88	0.56
1:GB:287:ARG:HD2	1:GB:306:GLN:HA	1.88	0.56
1:GC:233:THR:HG22	1:GC:235:GLU:H	1.71	0.56
1:HA:149:ARG:NH2	1:IA:149:ARG:O	2.38	0.56
1:IB:267:THR:HG22	1:IB:271:VAL:H	1.71	0.56
1:DC:148:VAL:HG13	1:DC:198:VAL:HG21	1.88	0.56
1:IA:73:GLY:H	1:IA:181:MET:HE3	1.70	0.56
1:IA:490:LYS:HB2	1:IA:498:THR:HG22	1.87	0.56
1:JC:415:ASN:HB3	1:JC:418:LEU:HD21	1.86	0.56
1:KA:149:ARG:O	1:OA:149:ARG:NH2	2.39	0.56
1:AB:338:THR:OG1	1:AB:345:ARG:NH2	2.38	0.56
1:MB:58:GLN:H	1:NC:139:THR:HG21	1.71	0.56
1:NB:30:GLU:HG3	1:NC:44:GLN:HA	1.87	0.56
1:NB:227:PHE:CE1	1:NB:268:THR:HG23	2.41	0.56
1:AC:46:ASN:ND2	1:AC:213:ILE:O	2.38	0.56
1:CA:476:ARG:HD3	1:CA:485:VAL:HG11	1.88	0.56
1:CB:30:GLU:HG3	1:CC:44:GLN:HA	1.88	0.56
1:DB:244:ILE:CD1	1:DB:439:PRO:HD3	2.36	0.56
1:KC:135:PRO:HA	1:KC:181:MET:HE1	1.87	0.56
1:KC:476:ARG:HG3	1:KC:518:ASP:OD2	2.05	0.56
1:OB:267:THR:HG22	1:OB:271:VAL:H	1.71	0.56
1:JB:267:THR:CG2	1:JB:271:VAL:H	2.19	0.55
1:OA:319:ALA:HB1	1:OA:320:PRO:HD2	1.87	0.55
1:OC:472:VAL:HG11	1:OC:490:LYS:HD2	1.87	0.55
1:CB:120:ILE:HG13	1:CB:183:TYR:HB2	1.89	0.55
1:IB:242:PHE:HD1	1:IB:284:CYS:HG	1.53	0.55
1:MB:454:PRO:HG2	1:MB:457:TRP:CG	2.41	0.55
1:AA:147:ASP:OD2	1:AA:149:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:19:VAL:HG23	1:LB:149:ARG:HB3	1.88	0.55
1:FB:464:GLU:HG3	1:FB:464:GLU:O	2.07	0.55
1:HA:490:LYS:HB2	1:HA:498:THR:HG22	1.88	0.55
1:HB:454:PRO:HG2	1:HB:457:TRP:CG	2.41	0.55
1:HC:306:GLN:NE2	1:HC:321:LEU:O	2.40	0.55
1:IA:147:ASP:OD2	1:IA:149:ARG:NH1	2.40	0.55
1:JC:527:LEU:HD23	1:JC:527:LEU:H	1.72	0.55
1:NA:422:VAL:HG12	1:NA:431:LEU:HD21	1.89	0.55
1:AA:476:ARG:HD3	1:AA:485:VAL:HG11	1.88	0.55
1:DB:265:ARG:NH2	1:DB:420:PRO:O	2.38	0.55
1:GB:109:LEU:HD23	1:GB:200:CYS:SG	2.47	0.55
1:HC:390:GLN:HB2	1:HC:445:PRO:HB3	1.89	0.55
1:IC:395:ALA:HB3	1:IC:398:ASN:HD22	1.72	0.55
1:EB:248:LYS:HD2	1:EB:435:ARG:HD2	1.89	0.55
1:HB:286:PHE:HB3	1:HB:301:MET:HE2	1.88	0.55
1:KA:216:VAL:HG22	1:KA:217:PRO:HD2	1.88	0.55
1:OA:73:GLY:H	1:OA:181:MET:HE3	1.70	0.55
1:EA:40:PRO:HB2	1:EC:37:ILE:HD11	1.88	0.55
1:EA:128:PHE:CZ	1:EB:220:VAL:HG11	2.42	0.55
1:EA:371:THR:HG22	1:EA:373:ASN:H	1.72	0.55
1:IB:482:THR:HG22	1:JC:426:PHE:HD1	1.70	0.55
1:KA:251:THR:HG22	1:KA:430:GLN:HE21	1.71	0.55
1:LC:109:LEU:HD13	1:LC:200:CYS:SG	2.46	0.55
1:MC:527:LEU:HD23	1:MC:527:LEU:H	1.72	0.55
1:NA:338:THR:OG1	1:NA:345:ARG:NH2	2.39	0.55
1:BB:118:LYS:H	1:BB:184:THR:HB	1.72	0.55
1:BC:159:PRO:O	1:BC:176:ILE:HD12	2.06	0.55
1:DA:147:ASP:OD1	1:DA:149:ARG:HG2	2.07	0.55
1:EB:275:THR:HG23	1:EB:318:PRO:HG2	1.88	0.55
1:HA:476:ARG:HD3	1:HA:485:VAL:HG11	1.89	0.55
1:KA:147:ASP:OD1	1:KA:149:ARG:HG2	2.07	0.55
1:LA:422:VAL:HG12	1:LA:431:LEU:HD21	1.89	0.55
1:NC:390:GLN:HG2	1:NC:399:GLU:HG3	1.88	0.55
1:OA:312:ASP:HB3	1:OA:315:GLU:HG3	1.89	0.55
1:DA:329:LYS:HE2	1:DA:352:SER:HB2	1.89	0.55
1:HC:389:VAL:HG23	1:HC:442:SER:HB3	1.88	0.55
1:IB:109:LEU:HD23	1:IB:200:CYS:SG	2.47	0.55
1:JB:78:SER:HB2	1:JB:179:ILE:HD13	1.89	0.55
1:KC:527:LEU:HD23	1:KC:527:LEU:H	1.72	0.55
1:LC:46:ASN:ND2	1:LC:213:ILE:O	2.37	0.55
1:EB:144:ILE:HG22	1:EB:146:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:233:THR:HB	1:EB:236:GLU:HG3	1.89	0.55
1:MC:233:THR:HG22	1:MC:235:GLU:H	1.70	0.55
1:MC:305:SER:HB2	1:MC:307:ASN:OD1	2.06	0.55
1:NA:233:THR:HG22	1:NA:235:GLU:H	1.72	0.55
1:OC:94:ARG:NH1	1:OC:226:PRO:HD3	2.22	0.55
1:DB:130:THR:HG23	1:DB:179:ILE:HD11	1.89	0.54
1:EB:15:THR:HG21	1:EB:151:LEU:HD11	1.89	0.54
1:FA:149:ARG:NH2	1:GA:149:ARG:O	2.40	0.54
1:HB:121:PHE:HB2	1:HB:144:ILE:HG22	1.89	0.54
1:AB:267:THR:CG2	1:AB:271:VAL:H	2.18	0.54
1:AC:148:VAL:HG13	1:AC:198:VAL:HG21	1.88	0.54
1:DB:159:PRO:O	1:DB:176:ILE:HD12	2.06	0.54
1:HA:66:VAL:HG12	1:HA:186:LEU:HD22	1.90	0.54
1:IB:275:THR:HG23	1:IB:318:PRO:HG2	1.89	0.54
1:AA:149:ARG:O	1:EA:149:ARG:NH2	2.39	0.54
1:AB:159:PRO:O	1:AB:176:ILE:HD12	2.07	0.54
1:CC:390:GLN:HB2	1:CC:445:PRO:HB3	1.88	0.54
1:FB:389:VAL:HG12	1:FB:441:CYS:HB2	1.89	0.54
1:JA:430:GLN:HE22	1:JA:503:GLY:H	1.54	0.54
1:MB:471:ASP:HA	1:MB:493:LYS:HD2	1.89	0.54
1:MC:148:VAL:HG13	1:MC:198:VAL:HG21	1.90	0.54
1:BC:389:VAL:HG23	1:BC:442:SER:HB3	1.89	0.54
1:FC:244:ILE:HG22	1:FC:245:PRO:HD2	1.89	0.54
1:HB:277:GLN:OE1	1:HB:279:SER:N	2.37	0.54
1:HC:477:PHE:HD1	1:HC:486:LEU:HD12	1.72	0.54
1:KB:399:GLU:HB3	1:KB:400:PRO:HD3	1.88	0.54
1:NC:338:THR:HB	1:NC:343:SER:HB3	1.89	0.54
1:OB:170:GLN:NE2	1:OB:222:SER:O	2.40	0.54
1:FA:33:VAL:HG11	1:FA:37:ILE:HG13	1.89	0.54
1:FC:23:ASN:HD22	1:JB:153:PRO:HG3	1.72	0.54
1:GB:196:PHE:HA	1:HC:187:ARG:HD2	1.90	0.54
1:IC:158:LEU:HD13	1:IC:178:LEU:HG	1.90	0.54
1:NB:94:ARG:O	1:NB:218:PRO:HA	2.08	0.54
1:NC:233:THR:HG22	1:NC:235:GLU:H	1.71	0.54
1:DC:527:LEU:HD23	1:DC:527:LEU:H	1.73	0.54
1:GA:490:LYS:HG3	1:GA:527:LEU:HD11	1.88	0.54
1:AA:161:VAL:HB	1:AA:176:ILE:HD11	1.89	0.54
1:DC:472:VAL:HG11	1:DC:490:LYS:HD2	1.90	0.54
1:IC:433:PHE:HB3	1:IC:450:ASP:HB3	1.89	0.54
1:LC:403:TRP:CZ2	1:LC:450:ASP:HB2	2.42	0.54
1:BB:190:ASN:HB2	1:CC:189:ASN:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:53:ARG:HB3	1:EA:206:PRO:HG2	1.90	0.54
1:EC:472:VAL:HG11	1:EC:490:LYS:HD2	1.90	0.54
1:IC:223:ARG:HA	1:IC:467:PRO:HG2	1.90	0.54
1:JC:227:PHE:CE1	1:JC:268:THR:HG23	2.42	0.54
1:LB:227:PHE:CE1	1:LB:268:THR:HG23	2.43	0.54
1:CC:56:PHE:HB3	1:CC:203:LEU:HB3	1.90	0.54
1:GA:424:PRO:HD3	1:GA:431:LEU:HD13	1.89	0.54
1:LA:275:THR:HG23	1:LA:318:PRO:HG2	1.89	0.54
1:OC:254:SER:HA	1:OC:257:PHE:CE1	2.43	0.54
1:AA:33:VAL:HG11	1:AA:37:ILE:HB	1.90	0.54
1:AB:184:THR:HG23	1:GC:199:SER:HB2	1.88	0.54
1:BB:227:PHE:CE1	1:BB:268:THR:HG23	2.43	0.54
1:EC:243:PRO:HG3	1:EC:283:ILE:HB	1.89	0.54
1:IB:454:PRO:HG2	1:IB:457:TRP:CG	2.43	0.54
1:LA:430:GLN:HE22	1:LA:503:GLY:H	1.56	0.54
1:OC:227:PHE:CE1	1:OC:268:THR:HG23	2.43	0.54
1:OC:343:SER:OG	1:OC:345:ARG:NH1	2.41	0.54
1:AC:191:ALA:HB1	1:GB:194:ASP:HB3	1.90	0.53
1:BC:109:LEU:HD13	1:BC:200:CYS:SG	2.48	0.53
1:BC:472:VAL:HG11	1:BC:490:LYS:HD2	1.89	0.53
1:FB:34:GLY:HA3	1:FB:209:ASP:HB2	1.91	0.53
1:JA:435:ARG:NH1	1:JA:448:ASN:HB3	2.23	0.53
1:KB:121:PHE:HB2	1:KB:144:ILE:HG22	1.90	0.53
1:LA:73:GLY:H	1:LA:181:MET:HE3	1.71	0.53
1:MA:140:MET:HG2	1:NA:57:VAL:HG21	1.90	0.53
1:MA:399:GLU:HB3	1:MA:400:PRO:HD3	1.90	0.53
1:NB:233:THR:HG21	1:NB:511:PRO:O	2.08	0.53
1:OA:338:THR:OG1	1:OA:345:ARG:NH2	2.33	0.53
1:DC:227:PHE:CE1	1:DC:268:THR:HG23	2.44	0.53
1:HB:84:ASP:HB3	1:HB:469:GLN:OE1	2.09	0.53
1:NA:430:GLN:HE22	1:NA:503:GLY:H	1.54	0.53
1:AA:430:GLN:HE22	1:AA:503:GLY:H	1.56	0.53
1:AC:305:SER:HB2	1:AC:307:ASN:OD1	2.07	0.53
1:BB:184:THR:HG23	1:KC:199:SER:HB2	1.90	0.53
1:FC:233:THR:HG22	1:FC:235:GLU:H	1.74	0.53
1:FC:249:LEU:HB2	1:FC:509:ILE:HD11	1.90	0.53
1:IC:390:GLN:HA	1:IC:399:GLU:OE1	2.07	0.53
1:KA:215:LEU:HD12	1:OB:51:TRP:HB3	1.89	0.53
1:BC:77:TRP:HZ3	1:BC:178:LEU:HD22	1.73	0.53
1:CB:45:GLN:O	1:DA:51:TRP:NE1	2.42	0.53
1:CC:261:PRO:HG3	1:CC:403:TRP:HZ3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:65:THR:HG21	1:FA:526:THR:N	2.10	0.53
1:GC:109:LEU:HD13	1:GC:200:CYS:SG	2.48	0.53
1:IC:312:ASP:HB3	1:IC:313:PRO:HD2	1.90	0.53
1:LB:471:ASP:HA	1:LB:493:LYS:HG3	1.89	0.53
1:NC:268:THR:HG21	1:NC:520:TRP:CH2	2.43	0.53
1:AA:353:THR:HG22	1:AA:406:PRO:HB3	1.90	0.53
1:GA:490:LYS:HB2	1:GA:498:THR:HG22	1.91	0.53
1:MB:227:PHE:CE1	1:MB:268:THR:HG23	2.44	0.53
1:MC:25:GLU:OE1	1:MC:25:GLU:N	2.41	0.53
1:MC:227:PHE:CE1	1:MC:268:THR:HG23	2.44	0.53
1:NB:248:LYS:HD2	1:NB:435:ARG:HD2	1.90	0.53
1:BC:308:TRP:CZ3	1:BC:380:ASN:HB3	2.44	0.53
1:DB:32:VAL:HB	1:DB:159:PRO:HB2	1.90	0.53
1:EA:147:ASP:OD2	1:EA:149:ARG:NH1	2.42	0.53
1:EC:268:THR:HG21	1:EC:520:TRP:HH2	1.74	0.53
1:FC:527:LEU:HD23	1:FC:527:LEU:H	1.73	0.53
1:HC:433:PHE:HB3	1:HC:450:ASP:HB3	1.89	0.53
1:IB:57:VAL:HA	1:JC:139:THR:HG22	1.89	0.53
1:CB:199:SER:HB2	1:DC:184:THR:HG23	1.91	0.53
1:IC:239:ASN:ND2	1:IC:436:SER:OG	2.35	0.53
1:LB:66:VAL:HG21	1:LB:119:ILE:HD11	1.91	0.53
1:LB:267:THR:CG2	1:LB:271:VAL:H	2.22	0.53
1:AB:94:ARG:HG2	1:AB:224:THR:HB	1.90	0.53
1:CC:109:LEU:HD13	1:CC:200:CYS:SG	2.49	0.53
1:CC:472:VAL:HG11	1:CC:490:LYS:HD2	1.90	0.53
1:HC:338:THR:OG1	1:HC:345:ARG:NH2	2.20	0.53
1:IA:147:ASP:OD1	1:IA:149:ARG:HG2	2.09	0.53
1:KC:472:VAL:HG11	1:KC:490:LYS:HD2	1.90	0.53
1:MC:390:GLN:HB2	1:MC:445:PRO:HB3	1.91	0.53
1:CB:109:LEU:HD23	1:CB:200:CYS:SG	2.49	0.53
1:GA:101:GLY:HA3	1:GA:210:PHE:HA	1.91	0.53
1:KC:433:PHE:HB3	1:KC:450:ASP:HB3	1.91	0.53
1:NC:239:ASN:ND2	1:NC:436:SER:OG	2.39	0.53
1:BB:57:VAL:HA	1:CC:139:THR:HG22	1.91	0.53
1:BB:249:LEU:HB2	1:BB:509:ILE:HD11	1.91	0.53
1:GA:105:VAL:HG13	1:GA:156:ILE:HB	1.90	0.53
1:GA:319:ALA:HB1	1:GA:320:PRO:HD2	1.90	0.53
1:GC:338:THR:HB	1:GC:341:ASP:OD1	2.09	0.53
1:HB:501:HIS:ND1	1:HB:531:GLY:HA3	2.23	0.53
1:HC:223:ARG:HA	1:HC:467:PRO:HG2	1.91	0.53
1:KA:311:TYR:CE1	1:KA:320:PRO:HG3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:308:TRP:CZ3	1:KC:380:ASN:HB3	2.44	0.53
1:BC:267:THR:CG2	1:BC:271:VAL:H	2.22	0.52
1:DC:268:THR:HG21	1:DC:520:TRP:CH2	2.38	0.52
1:EA:433:PHE:HB3	1:EA:450:ASP:HB3	1.91	0.52
1:JA:223:ARG:NH2	1:JA:269:ASP:HB2	2.24	0.52
1:JC:359:THR:HG22	1:JC:410:GLY:H	1.74	0.52
1:BB:245:PRO:O	1:BB:436:SER:OG	2.19	0.52
1:EA:159:PRO:O	1:EA:176:ILE:HD12	2.09	0.52
1:EB:359:THR:HG22	1:EB:410:GLY:HA3	1.90	0.52
1:FC:37:ILE:HG22	1:FC:165:PHE:HD1	1.74	0.52
1:FC:159:PRO:O	1:FC:176:ILE:HD12	2.07	0.52
1:FC:486:LEU:HD11	1:FC:510:PRO:CD	2.40	0.52
1:GA:144:ILE:HD12	1:GA:154:VAL:HG11	1.92	0.52
1:AB:15:THR:HG21	1:AB:151:LEU:HD11	1.90	0.52
1:EB:94:ARG:HD3	1:EB:226:PRO:HD3	1.91	0.52
1:EB:159:PRO:O	1:EB:176:ILE:HD12	2.09	0.52
1:GB:30:GLU:HG3	1:GC:44:GLN:HA	1.91	0.52
1:HB:14:SER:HA	1:IC:149:ARG:O	2.08	0.52
1:IC:338:THR:OG1	1:IC:345:ARG:NH2	2.38	0.52
1:JA:328:GLY:H	1:JA:353:THR:HB	1.74	0.52
1:JB:338:THR:OG1	1:JB:345:ARG:NH2	2.41	0.52
1:JC:434:PHE:CE2	1:JC:454:PRO:HD3	2.44	0.52
1:LC:338:THR:OG1	1:LC:345:ARG:NH2	2.40	0.52
1:MB:338:THR:OG1	1:MB:345:ARG:NH2	2.31	0.52
1:OA:105:VAL:HG13	1:OA:156:ILE:HB	1.90	0.52
1:OB:94:ARG:O	1:OB:218:PRO:HA	2.09	0.52
1:OB:124:VAL:HG22	1:OB:177:LYS:HB2	1.91	0.52
1:AA:422:VAL:HG12	1:AA:431:LEU:HD21	1.92	0.52
1:CA:147:ASP:OD2	1:CA:149:ARG:NH1	2.41	0.52
1:CB:159:PRO:O	1:CB:176:ILE:HD12	2.09	0.52
1:DB:482:THR:HG22	1:EC:426:PHE:HD1	1.72	0.52
1:EB:94:ARG:O	1:EB:218:PRO:HA	2.10	0.52
1:EB:233:THR:HG22	1:EB:235:GLU:H	1.75	0.52
1:EB:464:GLU:HG3	1:EB:464:GLU:O	2.09	0.52
1:FA:105:VAL:HG13	1:FA:156:ILE:HB	1.90	0.52
1:FA:306:GLN:H	1:FA:306:GLN:CD	2.13	0.52
1:FB:338:THR:OG1	1:FB:345:ARG:NH2	2.35	0.52
1:IA:275:THR:HG23	1:IA:318:PRO:HG2	1.90	0.52
1:AC:472:VAL:HG11	1:AC:490:LYS:HD2	1.92	0.52
1:BA:216:VAL:HG22	1:BA:217:PRO:HD2	1.92	0.52
1:CC:527:LEU:HD23	1:CC:527:LEU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:57:VAL:HA	1:HC:139:THR:HG22	1.91	0.52
1:GC:227:PHE:CE1	1:GC:268:THR:HG23	2.44	0.52
1:JA:147:ASP:OD2	1:JA:149:ARG:NH1	2.41	0.52
1:LC:33:VAL:HG11	1:LC:37:ILE:HB	1.91	0.52
1:OC:527:LEU:HD23	1:OC:527:LEU:H	1.73	0.52
1:AA:433:PHE:HB3	1:AA:450:ASP:HB3	1.90	0.52
1:AB:120:ILE:HG13	1:AB:183:TYR:HB2	1.91	0.52
1:AB:433:PHE:HB3	1:AB:450:ASP:HB3	1.89	0.52
1:FC:249:LEU:HB3	1:FC:507:LEU:HD12	1.92	0.52
1:GC:472:VAL:HG11	1:GC:490:LYS:HD2	1.92	0.52
1:HB:94:ARG:HG2	1:HB:224:THR:HB	1.92	0.52
1:KC:434:PHE:CE2	1:KC:454:PRO:HD3	2.45	0.52
1:MB:197:THR:HB	1:NC:187:ARG:HH12	1.75	0.52
1:NB:45:GLN:O	1:OA:51:TRP:NE1	2.42	0.52
1:NC:33:VAL:HG11	1:NC:37:ILE:HB	1.91	0.52
1:NC:227:PHE:CE1	1:NC:268:THR:HG23	2.44	0.52
1:BA:328:GLY:H	1:BA:353:THR:HB	1.74	0.52
1:EB:227:PHE:CE1	1:EB:268:THR:HG23	2.44	0.52
1:GA:53:ARG:HB3	1:GA:206:PRO:HG2	1.92	0.52
1:HC:319:ALA:HB1	1:HC:320:PRO:HD2	1.91	0.52
1:KB:454:PRO:HG2	1:KB:457:TRP:CG	2.44	0.52
1:LC:389:VAL:HG23	1:LC:442:SER:HB3	1.91	0.52
1:NB:101:GLY:HA3	1:NB:210:PHE:HA	1.92	0.52
1:NB:197:THR:HB	1:OC:187:ARG:HH11	1.74	0.52
1:NB:424:PRO:HD3	1:NB:431:LEU:HG	1.91	0.52
1:OB:225:LYS:HD2	1:OB:226:PRO:HD2	1.91	0.52
1:AB:233:THR:HB	1:AB:236:GLU:HG3	1.91	0.52
1:AC:267:THR:CG2	1:AC:271:VAL:H	2.21	0.52
1:IB:81:LEU:HD11	1:IB:102:GLY:HA2	1.90	0.52
1:MA:73:GLY:H	1:MA:181:MET:HE3	1.74	0.52
1:MA:225:LYS:HD2	1:MA:464:GLU:HG3	1.92	0.52
1:NC:347:HIS:CE1	1:NC:374:ASP:HB3	2.45	0.52
1:CA:424:PRO:HD3	1:CA:431:LEU:HD13	1.91	0.52
1:EB:81:LEU:HD11	1:EB:102:GLY:HA2	1.91	0.52
1:EC:33:VAL:HG11	1:EC:37:ILE:HG13	1.91	0.52
1:HA:318:PRO:HB3	1:HA:418:LEU:HD23	1.92	0.52
1:HA:326:PHE:O	1:HA:353:THR:HG21	2.10	0.52
1:JB:464:GLU:O	1:JB:464:GLU:HG3	2.10	0.52
1:KC:305:SER:HB2	1:KC:309:ASN:H	1.74	0.52
1:LA:53:ARG:HB3	1:LA:206:PRO:HG2	1.92	0.52
1:LA:233:THR:HG22	1:LA:235:GLU:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MA:140:MET:HG2	1:NA:57:VAL:CG2	2.40	0.52
1:MB:267:THR:CG2	1:MB:271:VAL:H	2.22	0.52
1:MC:46:ASN:ND2	1:MC:213:ILE:O	2.42	0.52
1:MC:456:GLU:OE1	1:MC:456:GLU:N	2.43	0.52
1:CA:65:THR:HG21	1:CA:526:THR:N	2.12	0.52
1:CC:267:THR:CG2	1:CC:271:VAL:H	2.23	0.52
1:GB:286:PHE:HB3	1:GB:301:MET:HE2	1.92	0.52
1:HB:267:THR:CG2	1:HB:271:VAL:H	2.22	0.52
1:IA:144:ILE:HD12	1:IA:154:VAL:HG11	1.91	0.52
1:LC:233:THR:HG22	1:LC:235:GLU:H	1.74	0.52
1:AB:244:ILE:HA	1:BA:281:VAL:HG11	1.91	0.51
1:BC:478:VAL:HG22	1:BC:485:VAL:HG22	1.92	0.51
1:CA:109:LEU:HD22	1:CA:200:CYS:SG	2.50	0.51
1:EC:391:ASP:H	1:EC:399:GLU:HG3	1.74	0.51
1:FA:328:GLY:H	1:FA:353:THR:HB	1.74	0.51
1:FC:44:GLN:NE2	1:FC:215:LEU:HD23	2.25	0.51
1:JA:476:ARG:HD3	1:JA:485:VAL:HG11	1.92	0.51
1:JB:282:ASN:OD1	1:JB:287:ARG:NH2	2.42	0.51
1:MB:115:THR:O	1:MB:149:ARG:HD3	2.11	0.51
1:NA:53:ARG:O	1:NA:205:ARG:HD2	2.10	0.51
1:AB:471:ASP:HA	1:AB:493:LYS:CD	2.40	0.51
1:BB:359:THR:HG22	1:BB:410:GLY:HA3	1.93	0.51
1:FA:101:GLY:HA3	1:FA:210:PHE:HA	1.92	0.51
1:FA:117:GLY:O	1:FA:148:VAL:HG22	2.10	0.51
1:GC:416:VAL:HG12	1:GC:417:HIS:CD2	2.45	0.51
1:KA:424:PRO:HD3	1:KA:431:LEU:HD13	1.93	0.51
1:NA:490:LYS:HG3	1:NA:527:LEU:HD11	1.91	0.51
1:BA:248:LYS:HE2	1:BA:435:ARG:HD2	1.91	0.51
1:BC:335:THR:HG23	1:KC:440:GLY:O	2.10	0.51
1:CB:101:GLY:HA3	1:CB:210:PHE:HA	1.92	0.51
1:FB:94:ARG:O	1:FB:218:PRO:HA	2.10	0.51
1:FB:94:ARG:HD3	1:FB:226:PRO:HD3	1.92	0.51
1:GA:77:TRP:HB3	1:GA:180:ALA:HB3	1.93	0.51
1:HC:233:THR:HG22	1:HC:235:GLU:H	1.75	0.51
1:JB:454:PRO:HG2	1:JB:457:TRP:CG	2.45	0.51
1:LB:81:LEU:HD11	1:LB:102:GLY:HA2	1.91	0.51
1:OB:501:HIS:CE1	1:OB:531:GLY:HA3	2.46	0.51
1:AB:249:LEU:HB2	1:AB:509:ILE:HD11	1.91	0.51
1:CC:37:ILE:HG22	1:CC:165:PHE:HD1	1.76	0.51
1:DC:433:PHE:HB3	1:DC:450:ASP:HB3	1.91	0.51
1:IA:30:GLU:HG3	1:JA:51:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:244:ILE:HA	1:JA:281:VAL:HG11	1.92	0.51
1:JB:343:SER:OG	1:JB:345:ARG:NH2	2.42	0.51
1:LB:15:THR:HG21	1:LB:151:LEU:HD11	1.93	0.51
1:MB:197:THR:HB	1:NC:187:ARG:NH1	2.25	0.51
1:FA:422:VAL:HG12	1:FA:431:LEU:HD21	1.92	0.51
1:FA:484:ARG:NH2	1:JA:69:ARG:O	2.40	0.51
1:FB:57:VAL:HA	1:GC:139:THR:HG22	1.91	0.51
1:FB:69:ARG:HD3	1:FB:427:PRO:HB2	1.91	0.51
1:GA:389:VAL:HG12	1:GA:441:CYS:HB2	1.93	0.51
1:GC:94:ARG:NH1	1:GC:226:PRO:HD3	2.25	0.51
1:HA:105:VAL:HG13	1:HA:156:ILE:HB	1.91	0.51
1:IA:306:GLN:OE1	1:IA:306:GLN:N	2.41	0.51
1:KA:233:THR:HG22	1:KA:235:GLU:N	2.26	0.51
1:KB:389:VAL:HG12	1:KB:441:CYS:HB2	1.93	0.51
1:MC:56:PHE:HB3	1:MC:203:LEU:HB3	1.91	0.51
1:OA:216:VAL:HG22	1:OA:217:PRO:HD2	1.92	0.51
1:AC:56:PHE:HB3	1:AC:203:LEU:HB3	1.92	0.51
1:BA:138:VAL:HG21	1:BA:181:MET:SD	2.50	0.51
1:FB:32:VAL:HB	1:FB:159:PRO:HB2	1.93	0.51
1:FC:434:PHE:CE2	1:FC:454:PRO:HD3	2.46	0.51
1:HA:353:THR:CG2	1:HA:406:PRO:HB3	2.40	0.51
1:HB:19:VAL:HG23	1:HB:149:ARG:HB3	1.92	0.51
1:IC:233:THR:HG22	1:IC:235:GLU:H	1.74	0.51
1:KB:115:THR:O	1:KB:149:ARG:HD3	2.11	0.51
1:MB:30:GLU:HG3	1:MC:44:GLN:HA	1.93	0.51
1:MB:233:THR:HG22	1:MB:235:GLU:HG2	1.91	0.51
1:NA:241:ARG:NE	1:NA:325:ASP:OD2	2.44	0.51
1:NC:148:VAL:HG13	1:NC:198:VAL:HG21	1.92	0.51
1:NC:389:VAL:HG23	1:NC:442:SER:HB3	1.92	0.51
1:AA:51:TRP:CH2	1:EA:30:GLU:HG3	2.45	0.51
1:AA:117:GLY:O	1:AA:148:VAL:HG22	2.10	0.51
1:AB:227:PHE:CE1	1:AB:268:THR:HG23	2.46	0.51
1:FC:56:PHE:HB3	1:FC:203:LEU:HB3	1.93	0.51
1:GC:267:THR:CG2	1:GC:271:VAL:H	2.24	0.51
1:HC:107:VAL:CG1	1:HC:154:VAL:HB	2.41	0.51
1:HC:434:PHE:CE2	1:HC:454:PRO:HD3	2.46	0.51
1:AC:390:GLN:HB2	1:AC:445:PRO:HB3	1.92	0.51
1:LA:490:LYS:HB2	1:LA:498:THR:HG22	1.93	0.51
1:LC:527:LEU:HD23	1:LC:527:LEU:H	1.75	0.51
1:MA:117:GLY:O	1:MA:148:VAL:HG22	2.11	0.51
1:MA:430:GLN:HE22	1:MA:503:GLY:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:227:PHE:CE1	1:EC:268:THR:HG23	2.46	0.51
1:GB:267:THR:CG2	1:GB:271:VAL:H	2.24	0.51
1:HB:230:PRO:HG2	1:HB:457:TRP:CD1	2.46	0.51
1:HB:275:THR:HG23	1:HB:318:PRO:HG2	1.93	0.51
1:IB:30:GLU:HG3	1:IC:44:GLN:HA	1.93	0.51
1:JC:56:PHE:HB3	1:JC:203:LEU:HB3	1.93	0.51
1:KC:189:ASN:HD21	1:OB:190:ASN:HB2	1.75	0.51
1:LB:57:VAL:HA	1:MC:139:THR:HG22	1.92	0.51
1:NB:66:VAL:HG12	1:NB:186:LEU:HB2	1.93	0.51
1:NB:471:ASP:HA	1:NB:493:LYS:CD	2.41	0.51
1:NC:267:THR:CG2	1:NC:271:VAL:H	2.22	0.51
1:BA:147:ASP:OD2	1:BA:149:ARG:NH1	2.44	0.51
1:BC:51:TRP:CG	1:KC:44:GLN:NE2	2.79	0.51
1:DB:94:ARG:O	1:DB:218:PRO:HA	2.10	0.51
1:IA:65:THR:HG23	1:IA:197:THR:HG23	1.93	0.51
1:JA:225:LYS:HE3	1:JA:464:GLU:HG3	1.92	0.51
1:MC:336:GLN:NE2	1:MC:379:GLN:HB2	2.24	0.51
1:CA:105:VAL:HG13	1:CA:156:ILE:HB	1.93	0.50
1:FB:267:THR:CG2	1:FB:271:VAL:H	2.24	0.50
1:GC:481:ASP:OD1	1:GC:512:ASN:ND2	2.39	0.50
1:IC:109:LEU:HD13	1:IC:200:CYS:SG	2.51	0.50
1:JB:359:THR:HG22	1:JB:410:GLY:HA3	1.92	0.50
1:MA:101:GLY:HA3	1:MA:210:PHE:HA	1.93	0.50
1:NA:53:ARG:HB3	1:NA:206:PRO:HG2	1.93	0.50
1:NB:134:SER:OG	1:NB:137:GLN:HG3	2.11	0.50
1:AC:57:VAL:HA	1:GB:139:THR:HG22	1.93	0.50
1:BA:125:PRO:HG3	1:BB:214:PHE:CD1	2.46	0.50
1:BA:140:MET:CE	1:BB:218:PRO:HD3	2.41	0.50
1:EA:62:GLY:HA2	1:EA:202:VAL:HB	1.92	0.50
1:EB:267:THR:CG2	1:EB:271:VAL:H	2.24	0.50
1:HC:338:THR:HG1	1:HC:345:ARG:HH22	1.54	0.50
1:IB:338:THR:OG1	1:IB:345:ARG:NH2	2.45	0.50
1:JB:501:HIS:ND1	1:JB:531:GLY:HA3	2.26	0.50
1:MB:101:GLY:HA3	1:MB:210:PHE:HA	1.92	0.50
1:NB:84:ASP:HB3	1:NB:469:GLN:OE1	2.11	0.50
1:NB:267:THR:HG22	1:NB:271:VAL:H	1.76	0.50
1:OB:228:THR:OG1	1:OB:464:GLU:OE2	2.27	0.50
1:FB:118:LYS:H	1:FB:184:THR:HB	1.76	0.50
1:GA:233:THR:HG22	1:GA:235:GLU:N	2.26	0.50
1:GC:434:PHE:CE2	1:GC:454:PRO:HD3	2.47	0.50
1:HC:267:THR:CG2	1:HC:271:VAL:H	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JB:399:GLU:HB3	1:JB:400:PRO:HD3	1.93	0.50
1:KC:233:THR:HG22	1:KC:235:GLU:H	1.76	0.50
1:LC:286:PHE:HB3	1:LC:303:LEU:HD21	1.93	0.50
1:MA:490:LYS:HG3	1:MA:527:LEU:HD11	1.92	0.50
1:MC:399:GLU:HB3	1:MC:400:PRO:HD3	1.93	0.50
1:NC:472:VAL:HG11	1:NC:490:LYS:HD2	1.93	0.50
1:AA:138:VAL:HG21	1:AA:181:MET:SD	2.50	0.50
1:BA:438:MET:O	1:BA:447:MET:HG2	2.11	0.50
1:DC:389:VAL:HG23	1:DC:442:SER:HB3	1.94	0.50
1:EC:37:ILE:HG22	1:EC:165:PHE:HD1	1.76	0.50
1:EC:527:LEU:HD23	1:EC:527:LEU:H	1.76	0.50
1:FC:101:GLY:HA3	1:FC:210:PHE:HA	1.93	0.50
1:IB:94:ARG:O	1:IB:218:PRO:HA	2.11	0.50
1:JA:390:GLN:HG2	1:JA:399:GLU:HB2	1.93	0.50
1:JC:109:LEU:HD13	1:JC:200:CYS:SG	2.51	0.50
1:MA:140:MET:CE	1:MB:218:PRO:HD3	2.41	0.50
1:MA:490:LYS:HE3	1:MA:527:LEU:HG	1.93	0.50
1:NB:115:THR:O	1:NB:149:ARG:HD3	2.11	0.50
1:AB:275:THR:HG23	1:AB:318:PRO:HG2	1.94	0.50
1:BB:265:ARG:HE	1:BB:419:ALA:HB1	1.76	0.50
1:BC:227:PHE:CE1	1:BC:268:THR:HG23	2.46	0.50
1:CB:57:VAL:HA	1:DC:139:THR:HG22	1.93	0.50
1:CC:227:PHE:CE1	1:CC:268:THR:HG23	2.47	0.50
1:DB:233:THR:HB	1:DB:236:GLU:HG3	1.92	0.50
1:EC:434:PHE:CE2	1:EC:454:PRO:HD3	2.47	0.50
1:FA:53:ARG:HB3	1:FA:206:PRO:HG2	1.94	0.50
1:HB:115:THR:O	1:HB:149:ARG:HD3	2.12	0.50
1:JA:53:ARG:HB3	1:JA:206:PRO:HG2	1.92	0.50
1:JC:244:ILE:HD13	1:JC:438:MET:HA	1.93	0.50
1:KB:227:PHE:CE1	1:KB:268:THR:HG23	2.46	0.50
1:KC:109:LEU:HD13	1:KC:200:CYS:SG	2.52	0.50
1:LA:353:THR:CG2	1:LA:406:PRO:HB3	2.42	0.50
1:MB:233:THR:HB	1:MB:236:GLU:HG3	1.93	0.50
1:NB:15:THR:HG22	1:OC:149:ARG:NE	2.23	0.50
1:AB:190:ASN:HB2	1:BC:189:ASN:HD21	1.76	0.50
1:BB:277:GLN:HB3	1:BB:321:LEU:HB3	1.92	0.50
1:DB:118:LYS:H	1:DB:184:THR:HB	1.77	0.50
1:JB:233:THR:HB	1:JB:236:GLU:HG3	1.93	0.50
1:KC:81:LEU:HD12	1:KC:158:LEU:HG	1.94	0.50
1:LC:416:VAL:HG12	1:LC:417:HIS:ND1	2.26	0.50
1:MA:353:THR:HG22	1:MA:406:PRO:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:463:GLN:HA	1:GC:231:ILE:HD11	1.94	0.50
1:BB:233:THR:HB	1:BB:236:GLU:HG3	1.94	0.50
1:CA:159:PRO:O	1:CA:176:ILE:HD12	2.11	0.50
1:CA:280:PRO:HB3	1:CA:455:GLN:HG2	1.94	0.50
1:EB:249:LEU:HB2	1:EB:509:ILE:HD11	1.93	0.50
1:GA:30:GLU:HG3	1:HA:51:TRP:CH2	2.47	0.50
1:GC:33:VAL:HG11	1:GC:37:ILE:HB	1.92	0.50
1:HC:527:LEU:HD23	1:HC:527:LEU:H	1.77	0.50
1:LC:265:ARG:HD3	1:LC:452:LEU:HD12	1.94	0.50
1:MB:197:THR:O	1:NC:187:ARG:NH1	2.44	0.50
1:NB:128:PHE:HE1	1:NB:133:LEU:HD21	1.77	0.50
1:HA:280:PRO:HB3	1:HA:455:GLN:HG2	1.94	0.50
1:IA:422:VAL:HG12	1:IA:431:LEU:HD21	1.93	0.50
1:IB:94:ARG:HG2	1:IB:224:THR:CG2	2.42	0.50
1:IB:124:VAL:HG22	1:IB:177:LYS:HB2	1.94	0.50
1:JA:105:VAL:CG1	1:JA:156:ILE:HB	2.42	0.50
1:JB:245:PRO:O	1:JB:436:SER:OG	2.19	0.50
1:JC:185:PRO:HG2	1:JC:187:ARG:HE	1.77	0.50
1:MB:440:GLY:O	1:NA:335:THR:HG23	2.12	0.50
1:NB:310:ASN:OD1	1:NB:311:TYR:N	2.45	0.50
1:OA:317:ILE:HG22	1:OA:318:PRO:HD2	1.94	0.50
1:OB:400:PRO:HG2	1:OB:446:ASN:HB3	1.94	0.50
1:AC:123:ALA:HB1	1:AC:176:ILE:HD11	1.93	0.50
1:AC:527:LEU:H	1:AC:527:LEU:HD23	1.77	0.50
1:BA:371:THR:HG22	1:BA:373:ASN:H	1.77	0.50
1:CA:40:PRO:HB2	1:CC:37:ILE:HD11	1.94	0.50
1:CA:319:ALA:HB1	1:CA:320:PRO:HD2	1.93	0.50
1:FA:353:THR:CG2	1:FA:406:PRO:HB3	2.42	0.50
1:FA:435:ARG:NH1	1:FA:448:ASN:HB3	2.26	0.50
1:FC:265:ARG:HD3	1:FC:452:LEU:HD12	1.93	0.50
1:GA:69:ARG:HH21	1:GA:427:PRO:HB2	1.76	0.50
1:GA:248:LYS:HE2	1:GA:435:ARG:HD2	1.94	0.50
1:HC:469:GLN:HB2	1:HC:520:TRP:CG	2.46	0.50
1:IA:101:GLY:HA3	1:IA:210:PHE:HA	1.94	0.50
1:IA:144:ILE:HD13	1:IA:156:ILE:HG12	1.94	0.50
1:IA:225:LYS:HD3	1:IA:464:GLU:HG3	1.94	0.50
1:OC:243:PRO:HG3	1:OC:283:ILE:HB	1.93	0.50
1:AC:109:LEU:HD13	1:AC:200:CYS:SG	2.51	0.49
1:BA:96:TYR:CG	1:BA:212:PHE:HB3	2.47	0.49
1:BA:433:PHE:HB3	1:BA:450:ASP:HB3	1.94	0.49
1:BC:37:ILE:HG22	1:BC:165:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:124:VAL:HG21	1:BC:179:ILE:HD12	1.94	0.49
1:CC:148:VAL:HG13	1:CC:198:VAL:HG21	1.94	0.49
1:EC:249:LEU:HB3	1:EC:507:LEU:HD12	1.93	0.49
1:FB:24:ASN:ND2	1:LC:152:GLU:OE2	2.44	0.49
1:FB:399:GLU:HB3	1:FB:400:PRO:HD3	1.94	0.49
1:IA:424:PRO:HD3	1:IA:431:LEU:HD13	1.94	0.49
1:MA:158:LEU:HD13	1:MA:178:LEU:HD13	1.93	0.49
1:NB:34:GLY:HA3	1:NB:209:ASP:HB2	1.94	0.49
1:OA:96:TYR:CG	1:OA:212:PHE:HB3	2.46	0.49
1:CC:94:ARG:NH1	1:CC:226:PRO:HD3	2.26	0.49
1:DB:33:VAL:HG21	1:DB:37:ILE:CD1	2.41	0.49
1:EA:65:THR:CG2	1:EA:526:THR:H	2.19	0.49
1:EA:69:ARG:HH21	1:EA:427:PRO:HB2	1.77	0.49
1:FA:75:ILE:HG23	1:FA:179:ILE:HG23	1.94	0.49
1:FC:336:GLN:NE2	1:FC:379:GLN:HB2	2.27	0.49
1:HA:399:GLU:HB3	1:HA:400:PRO:HD3	1.94	0.49
1:KA:265:ARG:NH2	1:KA:420:PRO:O	2.40	0.49
1:LA:353:THR:HG22	1:LA:406:PRO:HB3	1.94	0.49
1:LC:123:ALA:HB1	1:LC:176:ILE:HD11	1.94	0.49
1:OC:148:VAL:HG13	1:OC:198:VAL:HG21	1.94	0.49
1:BA:233:THR:HG21	1:BA:511:PRO:O	2.12	0.49
1:BB:32:VAL:HB	1:BB:159:PRO:HB2	1.94	0.49
1:FC:486:LEU:HD11	1:FC:510:PRO:HD2	1.93	0.49
1:IB:501:HIS:CE1	1:IB:531:GLY:HA3	2.47	0.49
1:JA:399:GLU:HB3	1:JA:400:PRO:HD3	1.95	0.49
1:JA:424:PRO:HD3	1:JA:431:LEU:HD13	1.93	0.49
1:KB:233:THR:HB	1:KB:236:GLU:HG3	1.94	0.49
1:NB:106:GLN:HE22	1:OC:23:ASN:N	2.10	0.49
1:NB:433:PHE:HB3	1:NB:450:ASP:HB3	1.95	0.49
1:DA:109:LEU:HD22	1:DA:200:CYS:SG	2.51	0.49
1:DA:353:THR:CG2	1:DA:406:PRO:HB3	2.42	0.49
1:DB:199:SER:HB2	1:EC:184:THR:HG23	1.95	0.49
1:FA:215:LEU:HD12	1:JB:51:TRP:HB3	1.93	0.49
1:GA:109:LEU:HD22	1:GA:200:CYS:SG	2.52	0.49
1:IC:389:VAL:HG23	1:IC:442:SER:HB3	1.94	0.49
1:KA:422:VAL:HG12	1:KA:431:LEU:HD21	1.93	0.49
1:MA:233:THR:HG22	1:MA:235:GLU:N	2.27	0.49
1:MB:389:VAL:HG12	1:MB:441:CYS:HB2	1.95	0.49
1:AB:30:GLU:HG3	1:AC:44:GLN:HA	1.93	0.49
1:AC:94:ARG:NH1	1:AC:226:PRO:HD3	2.27	0.49
1:BC:527:LEU:HD23	1:BC:527:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:267:THR:CG2	1:DB:271:VAL:H	2.24	0.49
1:HA:435:ARG:NH1	1:HA:448:ASN:HB3	2.28	0.49
1:JA:144:ILE:HD11	1:JA:156:ILE:HD11	1.95	0.49
1:JB:267:THR:HG22	1:JB:271:VAL:N	2.22	0.49
1:LC:148:VAL:HG13	1:LC:198:VAL:HG21	1.95	0.49
1:AA:125:PRO:HG3	1:AB:214:PHE:CD1	2.48	0.49
1:AB:81:LEU:HD11	1:AB:102:GLY:HA2	1.95	0.49
1:BC:434:PHE:CE2	1:BC:454:PRO:HD3	2.48	0.49
1:DA:319:ALA:HB1	1:DA:320:PRO:HD2	1.94	0.49
1:EB:101:GLY:HA3	1:EB:210:PHE:HA	1.94	0.49
1:FC:44:GLN:NE2	1:LC:51:TRP:CG	2.81	0.49
1:GC:377:THR:HG22	1:GC:378:GLY:H	1.77	0.49
1:GC:433:PHE:HB3	1:GC:450:ASP:HB3	1.93	0.49
1:JC:30:GLU:HG3	1:JC:31:PRO:HD2	1.94	0.49
1:KA:247:GLU:OE1	1:KA:437:THR:HG22	2.11	0.49
1:LB:233:THR:HG22	1:LB:235:GLU:H	1.77	0.49
1:BB:115:THR:O	1:BB:149:ARG:HD3	2.12	0.49
1:DB:57:VAL:HA	1:EC:139:THR:HG22	1.94	0.49
1:GB:75:ILE:HD13	1:GB:179:ILE:HD12	1.95	0.49
1:GB:359:THR:HG22	1:GB:410:GLY:HA3	1.95	0.49
1:GB:471:ASP:HA	1:GB:493:LYS:CD	2.40	0.49
1:KC:33:VAL:HG11	1:KC:37:ILE:HB	1.95	0.49
1:NB:239:ASN:HD22	1:NB:436:SER:HB3	1.77	0.49
1:OC:118:LYS:H	1:OC:184:THR:HB	1.78	0.49
1:BB:159:PRO:O	1:BB:176:ILE:HD12	2.13	0.49
1:BC:261:PRO:HG3	1:BC:403:TRP:HZ3	1.78	0.49
1:DB:227:PHE:CE1	1:DB:268:THR:HG23	2.47	0.49
1:DB:501:HIS:CE1	1:DB:531:GLY:HA3	2.48	0.49
1:FB:265:ARG:NH2	1:FB:420:PRO:O	2.46	0.49
1:FC:33:VAL:CG1	1:FC:37:ILE:HG13	2.42	0.49
1:GC:107:VAL:CG1	1:GC:154:VAL:HB	2.43	0.49
1:GC:476:ARG:HG3	1:GC:516:ARG:HH21	1.78	0.49
1:IB:115:THR:O	1:IB:149:ARG:HD3	2.13	0.49
1:JA:65:THR:HG21	1:JA:526:THR:N	2.12	0.49
1:JA:147:ASP:OD1	1:JA:149:ARG:HG2	2.13	0.49
1:JA:233:THR:HG22	1:JA:235:GLU:N	2.28	0.49
1:MA:48:ILE:HD12	1:MA:211:ASP:HA	1.95	0.49
1:BB:14:SER:O	1:BB:15:THR:OG1	2.24	0.49
1:EB:403:TRP:CZ2	1:EB:450:ASP:HB2	2.48	0.49
1:HC:390:GLN:HG2	1:HC:399:GLU:HG3	1.94	0.49
1:IB:389:VAL:HG12	1:IB:441:CYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:389:VAL:HG23	1:KC:442:SER:HB3	1.94	0.49
1:MA:71:ALA:HB3	1:NA:484:ARG:HG3	1.95	0.49
1:MC:336:GLN:NE2	1:MC:376:GLU:O	2.40	0.49
1:AC:434:PHE:CE2	1:AC:454:PRO:HD3	2.47	0.49
1:AC:476:ARG:HG3	1:AC:518:ASP:OD2	2.12	0.49
1:FB:195:VAL:HG13	1:FB:196:PHE:N	2.27	0.49
1:GA:422:VAL:HG12	1:GA:431:LEU:HD21	1.95	0.49
1:JB:310:ASN:OD1	1:JB:311:TYR:N	2.46	0.49
1:MB:131:GLU:N	1:MB:131:GLU:OE1	2.46	0.49
1:MB:286:PHE:HB3	1:MB:301:MET:CE	2.43	0.49
1:CC:317:ILE:HG13	1:CC:318:PRO:HD2	1.95	0.48
1:EC:358:PHE:HD1	1:EC:365:VAL:HG13	1.78	0.48
1:FC:424:PRO:HD3	1:FC:431:LEU:HG	1.93	0.48
1:HB:32:VAL:HG13	1:HC:41:VAL:HA	1.95	0.48
1:IB:118:LYS:H	1:IB:184:THR:HB	1.78	0.48
1:JA:223:ARG:HH22	1:JA:269:ASP:HB2	1.76	0.48
1:MA:343:SER:HB3	1:MA:345:ARG:HH12	1.78	0.48
1:CB:424:PRO:HD3	1:CB:431:LEU:HG	1.95	0.48
1:EC:434:PHE:CD2	1:EC:454:PRO:HD3	2.48	0.48
1:FB:125:PRO:HG3	1:FC:214:PHE:CD1	2.49	0.48
1:IA:105:VAL:CG1	1:IA:156:ILE:HB	2.42	0.48
1:IA:140:MET:HB2	1:IB:217:PRO:HG3	1.96	0.48
1:IA:145:ILE:HD13	1:IA:183:TYR:CE2	2.48	0.48
1:IA:430:GLN:HE22	1:IA:503:GLY:H	1.60	0.48
1:IB:456:GLU:OE1	1:IB:456:GLU:N	2.45	0.48
1:IC:277:GLN:HB3	1:IC:321:LEU:HB3	1.94	0.48
1:KA:140:MET:CE	1:KB:218:PRO:HD3	2.42	0.48
1:KA:399:GLU:HB3	1:KA:400:PRO:HD3	1.95	0.48
1:KC:187:ARG:HD2	1:OB:196:PHE:HA	1.95	0.48
1:LA:105:VAL:HG13	1:LA:156:ILE:HB	1.95	0.48
1:LC:158:LEU:HD13	1:LC:178:LEU:HG	1.95	0.48
1:OA:305:SER:OG	1:OA:306:GLN:N	2.45	0.48
1:BA:422:VAL:HG12	1:BA:431:LEU:HD21	1.94	0.48
1:CA:433:PHE:HB3	1:CA:450:ASP:HB3	1.95	0.48
1:DB:439:PRO:CB	1:EA:335:THR:HG21	2.40	0.48
1:DB:454:PRO:HG2	1:DB:457:TRP:CG	2.48	0.48
1:EC:182:LEU:HD21	1:EC:185:PRO:HA	1.94	0.48
1:FB:115:THR:O	1:FB:149:ARG:HD3	2.13	0.48
1:HB:238:THR:HA	1:HB:245:PRO:HA	1.95	0.48
1:IC:426:PHE:CD1	1:IC:427:PRO:HD2	2.49	0.48
1:JB:239:ASN:HD22	1:JB:436:SER:HB3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:57:VAL:HG21	1:OA:140:MET:HG2	1.95	0.48
1:KB:267:THR:CG2	1:KB:271:VAL:H	2.23	0.48
1:LC:267:THR:CG2	1:LC:271:VAL:H	2.24	0.48
1:BA:101:GLY:HA3	1:BA:210:PHE:HA	1.95	0.48
1:BB:388:VAL:HG21	1:BB:400:PRO:HB3	1.95	0.48
1:BC:233:THR:HG22	1:BC:235:GLU:H	1.79	0.48
1:CA:53:ARG:HB3	1:CA:206:PRO:HG2	1.94	0.48
1:CA:371:THR:HG22	1:CA:373:ASN:H	1.77	0.48
1:EA:459:LEU:O	1:EA:463:GLN:HG3	2.14	0.48
1:EC:107:VAL:CG1	1:EC:154:VAL:HB	2.44	0.48
1:EC:336:GLN:NE2	1:EC:379:GLN:HB2	2.29	0.48
1:HB:109:LEU:HD23	1:HB:200:CYS:SG	2.52	0.48
1:IA:143:HIS:HE1	1:JA:56:PHE:O	1.96	0.48
1:IA:347:HIS:NE2	1:IA:374:ASP:HB3	2.27	0.48
1:KA:51:TRP:CH2	1:OA:30:GLU:HG3	2.49	0.48
1:KB:116:ALA:N	1:KB:187:ARG:O	2.38	0.48
1:LA:71:ALA:HB3	1:MA:484:ARG:HG3	1.94	0.48
1:MA:275:THR:HG23	1:MA:318:PRO:HG2	1.94	0.48
1:NC:527:LEU:HD23	1:NC:527:LEU:H	1.78	0.48
1:OB:19:VAL:HG13	1:OB:149:ARG:O	2.12	0.48
1:OB:359:THR:HG22	1:OB:410:GLY:HA3	1.94	0.48
1:BA:40:PRO:HB2	1:BC:37:ILE:HD11	1.95	0.48
1:BB:317:ILE:HD13	1:BB:321:LEU:HD21	1.94	0.48
1:DA:353:THR:HG22	1:DA:406:PRO:HB3	1.95	0.48
1:DC:319:ALA:HB1	1:DC:320:PRO:HD2	1.95	0.48
1:EA:434:PHE:CE1	1:EA:454:PRO:HD3	2.49	0.48
1:GA:338:THR:OG1	1:GA:345:ARG:NH2	2.40	0.48
1:JC:358:PHE:HD1	1:JC:365:VAL:HG13	1.78	0.48
1:MB:32:VAL:HB	1:MB:159:PRO:HB2	1.95	0.48
1:MC:34:GLY:HA3	1:MC:209:ASP:HB2	1.96	0.48
1:NA:81:LEU:HD11	1:NA:102:GLY:HA2	1.95	0.48
1:AB:34:GLY:HA3	1:AB:209:ASP:HB2	1.96	0.48
1:AC:139:THR:HG22	1:EB:57:VAL:HA	1.94	0.48
1:DA:140:MET:HG2	1:EA:57:VAL:HG21	1.94	0.48
1:DA:490:LYS:HG3	1:DA:527:LEU:HD11	1.95	0.48
1:DB:115:THR:O	1:DB:149:ARG:HD3	2.13	0.48
1:EC:290:VAL:HG21	1:EC:375:LEU:HD13	1.94	0.48
1:GC:341:ASP:OD1	1:GC:342:GLY:N	2.47	0.48
1:IB:78:SER:HB2	1:IB:179:ILE:HD13	1.94	0.48
1:IB:432:LEU:HB2	1:IB:499:VAL:HG13	1.95	0.48
1:JB:115:THR:O	1:JB:149:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:94:ARG:NH1	1:KC:226:PRO:HD3	2.29	0.48
1:KC:139:THR:HG22	1:OB:57:VAL:HA	1.96	0.48
1:LC:434:PHE:CE2	1:LC:454:PRO:HD3	2.48	0.48
1:MA:422:VAL:HG12	1:MA:431:LEU:HD21	1.96	0.48
1:NA:96:TYR:CG	1:NA:212:PHE:HB3	2.49	0.48
1:NB:57:VAL:HA	1:OC:139:THR:HG22	1.96	0.48
1:NC:109:LEU:HD13	1:NC:200:CYS:SG	2.54	0.48
1:DB:94:ARG:HD3	1:DB:226:PRO:HD3	1.96	0.48
1:EB:84:ASP:HB3	1:EB:469:GLN:OE1	2.14	0.48
1:FA:43:GLY:HA3	1:FA:214:PHE:HE1	1.78	0.48
1:FC:109:LEU:HD13	1:FC:200:CYS:SG	2.53	0.48
1:FC:390:GLN:HB2	1:FC:445:PRO:HB3	1.96	0.48
1:GB:454:PRO:HG2	1:GB:457:TRP:CG	2.48	0.48
1:IA:233:THR:HG22	1:IA:235:GLU:N	2.26	0.48
1:IC:377:THR:HG22	1:IC:378:GLY:H	1.79	0.48
1:LB:280:PRO:HB3	1:LB:455:GLN:HG2	1.96	0.48
1:LC:359:THR:HG22	1:LC:410:GLY:HA3	1.96	0.48
1:MB:230:PRO:HD3	1:MB:460:HIS:CD2	2.48	0.48
1:OC:290:VAL:HG11	1:OC:375:LEU:HD13	1.96	0.48
1:AA:118:LYS:HE2	1:BA:110:ALA:HA	1.96	0.48
1:AA:424:PRO:HD3	1:AA:431:LEU:HD13	1.93	0.48
1:FC:336:GLN:HE21	1:FC:379:GLN:HB2	1.79	0.48
1:JC:469:GLN:HB2	1:JC:520:TRP:CD1	2.49	0.48
1:NB:244:ILE:HA	1:OA:281:VAL:HG11	1.95	0.48
1:AA:215:LEU:HD12	1:EB:51:TRP:HB3	1.95	0.48
1:AA:216:VAL:CG2	1:AA:217:PRO:HD2	2.44	0.48
1:AB:130:THR:HG23	1:AB:179:ILE:HD11	1.94	0.48
1:BB:128:PHE:HE1	1:BB:133:LEU:HD21	1.79	0.48
1:EA:147:ASP:OD1	1:EA:149:ARG:HG2	2.13	0.48
1:GA:138:VAL:HG21	1:GA:181:MET:SD	2.53	0.48
1:HB:230:PRO:HD3	1:HB:460:HIS:ND1	2.28	0.48
1:IB:530:MET:HG3	1:IB:531:GLY:N	2.28	0.48
1:LA:328:GLY:H	1:LA:353:THR:HB	1.78	0.48
1:MC:377:THR:HG22	1:MC:378:GLY:H	1.78	0.48
1:NA:233:THR:HB	1:NA:236:GLU:HG2	1.96	0.48
1:NB:484:ARG:HG3	1:OC:74:GLU:OE2	2.13	0.48
1:OC:247:GLU:CD	1:OC:437:THR:H	2.17	0.48
1:BA:353:THR:CG2	1:BA:406:PRO:HB3	2.44	0.48
1:CB:267:THR:HG22	1:CB:271:VAL:N	2.27	0.48
1:LA:315:GLU:HB3	1:LA:317:ILE:HG13	1.94	0.48
1:BA:430:GLN:HE22	1:BA:503:GLY:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:124:VAL:HG22	1:BB:177:LYS:HB2	1.95	0.47
1:BC:463:GLN:HA	1:KC:231:ILE:HD11	1.94	0.47
1:CB:454:PRO:HG2	1:CB:457:TRP:CG	2.49	0.47
1:EC:429:GLU:OE2	1:EC:490:LYS:HE2	2.13	0.47
1:FC:46:ASN:HD21	1:FC:213:ILE:C	2.15	0.47
1:FC:472:VAL:HG11	1:FC:490:LYS:HD2	1.96	0.47
1:GA:96:TYR:CG	1:GA:212:PHE:HB3	2.48	0.47
1:HA:43:GLY:HA3	1:HA:214:PHE:HE1	1.79	0.47
1:HA:433:PHE:HB3	1:HA:450:ASP:HB3	1.96	0.47
1:HB:471:ASP:HA	1:HB:493:LYS:CD	2.43	0.47
1:JB:69:ARG:HH12	1:JB:428:GLY:HA3	1.78	0.47
1:KB:471:ASP:HA	1:KB:493:LYS:CD	2.43	0.47
1:LC:443:GLY:O	1:LC:444:TYR:HD1	1.97	0.47
1:MC:285:THR:HG22	1:MC:385:PRO:HD2	1.96	0.47
1:NB:66:VAL:HG21	1:NB:119:ILE:HD11	1.95	0.47
1:NC:259:VAL:HG13	1:NC:403:TRP:CZ3	2.49	0.47
1:AA:319:ALA:HB1	1:AA:320:PRO:HD2	1.96	0.47
1:AC:107:VAL:CG1	1:AC:154:VAL:HB	2.44	0.47
1:BB:34:GLY:HA3	1:BB:209:ASP:HB2	1.95	0.47
1:DB:343:SER:OG	1:DB:345:ARG:NH2	2.48	0.47
1:DC:336:GLN:OE1	1:DC:379:GLN:HB2	2.13	0.47
1:FA:343:SER:HB3	1:FA:345:ARG:HH12	1.78	0.47
1:GA:147:ASP:OD1	1:GA:149:ARG:HG2	2.14	0.47
1:GB:81:LEU:HD11	1:GB:102:GLY:HA2	1.95	0.47
1:KC:121:PHE:HB2	1:KC:144:ILE:HG22	1.96	0.47
1:KC:227:PHE:CE1	1:KC:268:THR:HG23	2.49	0.47
1:LA:317:ILE:HG22	1:LA:318:PRO:HD2	1.96	0.47
1:LB:265:ARG:HH22	1:LB:422:VAL:HG23	1.79	0.47
1:NB:51:TRP:HB3	1:OA:215:LEU:HD12	1.96	0.47
1:OB:459:LEU:O	1:OB:463:GLN:HG3	2.15	0.47
1:DA:33:VAL:HG11	1:DA:37:ILE:HG13	1.96	0.47
1:DB:432:LEU:HB2	1:DB:499:VAL:HG13	1.96	0.47
1:GB:477:PHE:CE2	1:GB:509:ILE:HD12	2.50	0.47
1:GC:123:ALA:HB1	1:GC:176:ILE:HD11	1.97	0.47
1:KA:371:THR:HG22	1:KA:373:ASN:H	1.79	0.47
1:KB:14:SER:O	1:KB:15:THR:OG1	2.26	0.47
1:LB:501:HIS:ND1	1:LB:531:GLY:HA3	2.30	0.47
1:LC:107:VAL:HG13	1:LC:154:VAL:HB	1.96	0.47
1:MC:459:LEU:O	1:MC:463:GLN:HG3	2.14	0.47
1:OC:265:ARG:HD3	1:OC:452:LEU:HD12	1.96	0.47
1:AA:338:THR:HB	1:AA:343:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:115:THR:O	1:AB:149:ARG:HD3	2.14	0.47
1:CA:353:THR:HG22	1:CA:406:PRO:HB3	1.97	0.47
1:CC:159:PRO:O	1:CC:176:ILE:HD12	2.14	0.47
1:EA:105:VAL:CG1	1:EA:156:ILE:HB	2.42	0.47
1:EA:359:THR:HG22	1:EA:410:GLY:HA3	1.96	0.47
1:EB:109:LEU:HD23	1:EB:200:CYS:SG	2.55	0.47
1:FB:238:THR:HG21	1:GA:280:PRO:HD2	1.95	0.47
1:GA:149:ARG:NH2	1:HA:149:ARG:O	2.47	0.47
1:GC:148:VAL:HG13	1:GC:198:VAL:HG21	1.97	0.47
1:HB:75:ILE:O	1:HB:522:ASN:ND2	2.47	0.47
1:KA:66:VAL:HG12	1:KA:186:LEU:HD22	1.95	0.47
1:KA:433:PHE:HB3	1:KA:450:ASP:HB3	1.95	0.47
1:KA:438:MET:O	1:KA:447:MET:HG2	2.14	0.47
1:KB:81:LEU:HD11	1:KB:102:GLY:HA2	1.96	0.47
1:KB:482:THR:HG21	1:LC:427:PRO:HD3	1.97	0.47
1:KC:44:GLN:HE22	1:KC:215:LEU:HD23	1.78	0.47
1:KC:358:PHE:HD1	1:KC:365:VAL:HG13	1.78	0.47
1:LA:424:PRO:HD3	1:LA:431:LEU:HD13	1.96	0.47
1:LB:306:GLN:CD	1:LB:306:GLN:H	2.18	0.47
1:MA:52:ILE:HD12	1:MA:88:TYR:HB3	1.94	0.47
1:MA:89:LEU:HD11	1:MA:206:PRO:HB3	1.96	0.47
1:MA:476:ARG:HD3	1:MA:485:VAL:HG11	1.94	0.47
1:MB:75:ILE:HD13	1:MB:179:ILE:HD12	1.96	0.47
1:NC:308:TRP:CH2	1:NC:380:ASN:HB3	2.49	0.47
1:OB:267:THR:CG2	1:OB:271:VAL:H	2.26	0.47
1:AB:15:THR:HG22	1:BC:149:ARG:HE	1.80	0.47
1:BB:432:LEU:HB2	1:BB:499:VAL:HG13	1.96	0.47
1:DC:25:GLU:O	1:DC:25:GLU:HG3	2.14	0.47
1:DC:37:ILE:HG22	1:DC:165:PHE:HD1	1.78	0.47
1:EA:318:PRO:HD3	1:EA:417:HIS:O	2.14	0.47
1:EC:477:PHE:HD2	1:EC:515:PHE:CE1	2.33	0.47
1:HC:94:ARG:NH1	1:HC:225:LYS:HA	2.29	0.47
1:JC:254:SER:HA	1:JC:257:PHE:CE1	2.49	0.47
1:KC:311:TYR:CZ	1:KC:320:PRO:HD3	2.48	0.47
1:LA:140:MET:HG2	1:MA:57:VAL:HG21	1.96	0.47
1:MB:306:GLN:H	1:MB:306:GLN:CD	2.18	0.47
1:NA:319:ALA:HB1	1:NA:320:PRO:HD2	1.96	0.47
1:AA:140:MET:CE	1:AB:218:PRO:HD2	2.44	0.47
1:BB:440:GLY:O	1:CA:335:THR:HG23	2.15	0.47
1:DB:84:ASP:HB3	1:DB:469:GLN:OE1	2.14	0.47
1:FC:148:VAL:HG13	1:FC:198:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:527:LEU:HD23	1:GC:527:LEU:H	1.80	0.47
1:HA:265:ARG:NH2	1:HA:420:PRO:O	2.37	0.47
1:JC:148:VAL:HG13	1:JC:198:VAL:HG21	1.95	0.47
1:KA:138:VAL:HG21	1:KA:181:MET:SD	2.54	0.47
1:KC:107:VAL:HG13	1:KC:154:VAL:HB	1.97	0.47
1:MB:318:PRO:HD3	1:MB:417:HIS:O	2.14	0.47
1:NC:107:VAL:CG1	1:NC:154:VAL:HB	2.44	0.47
1:OC:424:PRO:HD3	1:OC:431:LEU:HG	1.96	0.47
1:AB:66:VAL:HG12	1:AB:186:LEU:HB2	1.97	0.47
1:AC:233:THR:HG22	1:AC:235:GLU:H	1.79	0.47
1:BB:454:PRO:HG2	1:BB:457:TRP:CG	2.50	0.47
1:BC:107:VAL:CG1	1:BC:154:VAL:HB	2.45	0.47
1:CA:73:GLY:H	1:CA:181:MET:CE	2.26	0.47
1:CA:422:VAL:HG12	1:CA:431:LEU:HD21	1.95	0.47
1:CC:318:PRO:HG3	1:CC:417:HIS:O	2.14	0.47
1:FC:389:VAL:HG23	1:FC:442:SER:HB3	1.96	0.47
1:GC:390:GLN:HB2	1:GC:445:PRO:HB3	1.97	0.47
1:HB:94:ARG:O	1:HB:218:PRO:HA	2.15	0.47
1:IA:338:THR:OG1	1:IA:345:ARG:NH2	2.37	0.47
1:IB:230:PRO:HD3	1:IB:460:HIS:CD2	2.50	0.47
1:IB:471:ASP:OD1	1:IB:522:ASN:HA	2.15	0.47
1:KA:115:THR:HG22	1:KA:148:VAL:HG21	1.97	0.47
1:KA:140:MET:HG2	1:LA:57:VAL:HG21	1.96	0.47
1:LA:347:HIS:NE2	1:LA:374:ASP:HB3	2.29	0.47
1:LC:107:VAL:CG1	1:LC:154:VAL:HB	2.44	0.47
1:MA:424:PRO:HD3	1:MA:431:LEU:HD13	1.95	0.47
1:MB:46:ASN:ND2	1:MB:213:ILE:O	2.39	0.47
1:MB:78:SER:HB2	1:MB:179:ILE:HD13	1.96	0.47
1:MB:265:ARG:NH2	1:MB:420:PRO:O	2.40	0.47
1:NA:105:VAL:CG1	1:NA:156:ILE:HB	2.44	0.47
1:OA:341:ASP:OD2	1:OA:343:SER:OG	2.28	0.47
1:BA:371:THR:CG2	1:BA:374:ASP:H	2.27	0.47
1:BB:144:ILE:HG22	1:BB:146:VAL:HG23	1.97	0.47
1:CB:115:THR:O	1:CB:149:ARG:HD3	2.14	0.47
1:CB:227:PHE:CE1	1:CB:268:THR:HG23	2.50	0.47
1:DB:75:ILE:O	1:DB:522:ASN:ND2	2.48	0.47
1:DB:230:PRO:HD3	1:DB:460:HIS:CD2	2.50	0.47
1:DB:389:VAL:HG12	1:DB:441:CYS:HB2	1.97	0.47
1:EC:109:LEU:HD22	1:EC:200:CYS:SG	2.54	0.47
1:FB:471:ASP:OD1	1:FB:522:ASN:HA	2.14	0.47
1:GB:433:PHE:HB3	1:GB:450:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:277:GLN:HB3	1:GC:321:LEU:HB3	1.97	0.47
1:IC:480:PRO:HD3	1:IC:513:GLY:HA2	1.97	0.47
1:KB:34:GLY:HA3	1:KB:209:ASP:HB2	1.96	0.47
1:LA:48:ILE:HD12	1:LA:211:ASP:HA	1.97	0.47
1:LA:318:PRO:HD3	1:LA:417:HIS:O	2.15	0.47
1:MC:277:GLN:HE21	1:MC:283:ILE:HD13	1.80	0.47
1:OB:81:LEU:HD11	1:OB:102:GLY:HA2	1.96	0.47
1:OC:120:ILE:HG13	1:OC:183:TYR:HB2	1.96	0.47
1:FA:275:THR:HG23	1:FA:318:PRO:HG2	1.96	0.47
1:FB:454:PRO:HG2	1:FB:457:TRP:CG	2.50	0.47
1:HA:353:THR:HG23	1:HA:406:PRO:HB3	1.97	0.47
1:HB:305:SER:HB3	1:HB:309:ASN:HB2	1.97	0.47
1:IB:471:ASP:HA	1:IB:493:LYS:CD	2.45	0.47
1:KB:94:ARG:HB3	1:KB:218:PRO:O	2.15	0.47
1:KB:471:ASP:OD1	1:KB:522:ASN:HA	2.14	0.47
1:MC:107:VAL:CG1	1:MC:154:VAL:HB	2.44	0.47
1:OB:32:VAL:HG13	1:OC:41:VAL:HA	1.95	0.47
1:OB:227:PHE:CE1	1:OB:268:THR:HG23	2.50	0.47
1:AA:30:GLU:HG3	1:BA:51:TRP:CZ2	2.50	0.47
1:AA:51:TRP:NE1	1:EB:45:GLN:O	2.47	0.47
1:AA:247:GLU:OE1	1:AA:437:THR:HG22	2.15	0.47
1:AC:249:LEU:HD21	1:AC:515:PHE:HZ	1.80	0.47
1:AC:389:VAL:HG23	1:AC:442:SER:HB3	1.97	0.47
1:CA:125:PRO:HA	1:CA:176:ILE:HG12	1.97	0.47
1:EB:230:PRO:HD3	1:EB:460:HIS:ND1	2.30	0.47
1:GC:249:LEU:HB3	1:GC:507:LEU:HD12	1.96	0.47
1:HA:422:VAL:HG12	1:HA:431:LEU:HD21	1.97	0.47
1:IB:75:ILE:HD13	1:IB:179:ILE:HD12	1.97	0.47
1:LA:399:GLU:HB3	1:LA:400:PRO:HD3	1.97	0.47
1:LB:424:PRO:HD3	1:LB:431:LEU:HG	1.96	0.47
1:OC:56:PHE:HB3	1:OC:203:LEU:HB3	1.97	0.47
1:AA:318:PRO:HD3	1:AA:417:HIS:O	2.16	0.46
1:EB:230:PRO:HG2	1:EB:457:TRP:CD1	2.50	0.46
1:EB:280:PRO:HB3	1:EB:455:GLN:HG2	1.97	0.46
1:FB:45:GLN:O	1:GA:51:TRP:NE1	2.48	0.46
1:GA:275:THR:HG23	1:GA:318:PRO:HG2	1.97	0.46
1:GB:51:TRP:HB3	1:HA:215:LEU:HD12	1.97	0.46
1:GC:223:ARG:HA	1:GC:467:PRO:HG2	1.96	0.46
1:HA:118:LYS:HE2	1:IA:110:ALA:HA	1.96	0.46
1:JC:476:ARG:HD3	1:JC:488:GLU:HB3	1.98	0.46
1:LA:223:ARG:NH2	1:LA:269:ASP:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LB:144:ILE:HG22	1:LB:146:VAL:HG23	1.97	0.46
1:MB:45:GLN:O	1:NA:51:TRP:NE1	2.47	0.46
1:NA:353:THR:CG2	1:NA:406:PRO:HB3	2.45	0.46
1:AA:46:ASN:HB3	1:EB:49:ASP:OD2	2.16	0.46
1:AA:434:PHE:CE1	1:AA:454:PRO:HD3	2.50	0.46
1:DA:117:GLY:O	1:DA:148:VAL:HG22	2.16	0.46
1:DA:338:THR:OG1	1:DA:345:ARG:NH2	2.46	0.46
1:DC:233:THR:HG22	1:DC:235:GLU:H	1.81	0.46
1:DC:305:SER:HB2	1:DC:309:ASN:H	1.81	0.46
1:FB:244:ILE:HD13	1:FB:438:MET:HA	1.98	0.46
1:GB:399:GLU:HB3	1:GB:400:PRO:HD3	1.96	0.46
1:HB:233:THR:CG2	1:HB:235:GLU:HG2	2.46	0.46
1:IB:32:VAL:HB	1:IB:159:PRO:HB2	1.96	0.46
1:LC:225:LYS:HE3	1:LC:464:GLU:HB3	1.97	0.46
1:NC:433:PHE:HB3	1:NC:450:ASP:HB3	1.97	0.46
1:OC:107:VAL:CG1	1:OC:154:VAL:HB	2.45	0.46
1:BA:30:GLU:HG3	1:CA:51:TRP:CZ2	2.49	0.46
1:CA:233:THR:HG22	1:CA:235:GLU:N	2.29	0.46
1:CC:469:GLN:HB2	1:CC:520:TRP:CG	2.50	0.46
1:DB:286:PHE:HB3	1:DB:301:MET:CE	2.45	0.46
1:EA:96:TYR:CG	1:EA:212:PHE:HB3	2.51	0.46
1:EA:109:LEU:HD22	1:EA:200:CYS:SG	2.56	0.46
1:FA:219:THR:HG22	1:FA:222:SER:OG	2.16	0.46
1:FC:139:THR:HG22	1:JB:57:VAL:HA	1.97	0.46
1:HA:326:PHE:HB2	1:HA:402:GLN:HA	1.98	0.46
1:LB:399:GLU:HB3	1:LB:400:PRO:HD3	1.97	0.46
1:MB:267:THR:HG22	1:MB:271:VAL:N	2.22	0.46
1:NB:78:SER:HB2	1:NB:179:ILE:HD13	1.96	0.46
1:OB:424:PRO:HD3	1:OB:431:LEU:HG	1.97	0.46
1:AC:267:THR:HG22	1:AC:271:VAL:N	2.28	0.46
1:CB:81:LEU:HD11	1:CB:102:GLY:HA2	1.98	0.46
1:DA:65:THR:CG2	1:DA:526:THR:H	2.16	0.46
1:DC:239:ASN:ND2	1:DC:436:SER:OG	2.47	0.46
1:EB:433:PHE:HB3	1:EB:450:ASP:HB3	1.97	0.46
1:EB:471:ASP:HA	1:EB:493:LYS:CD	2.43	0.46
1:EB:471:ASP:OD1	1:EB:522:ASN:HA	2.16	0.46
1:FA:282:ASN:OD1	1:FA:287:ARG:NH2	2.48	0.46
1:FA:371:THR:HG22	1:FA:373:ASN:H	1.80	0.46
1:FA:430:GLN:HE22	1:FA:503:GLY:H	1.62	0.46
1:GB:199:SER:HB2	1:HC:184:THR:HG23	1.98	0.46
1:HB:15:THR:HG22	1:IC:149:ARG:HE	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:51:TRP:NE1	1:OB:45:GLN:O	2.48	0.46
1:LA:434:PHE:CE1	1:LA:454:PRO:HD3	2.50	0.46
1:LC:268:THR:HG21	1:LC:520:TRP:CH2	2.42	0.46
1:BB:230:PRO:HD3	1:BB:460:HIS:ND1	2.31	0.46
1:BC:305:SER:HB2	1:BC:309:ASN:H	1.81	0.46
1:DC:424:PRO:HD3	1:DC:431:LEU:HG	1.98	0.46
1:EC:299:TYR:CE2	1:EC:375:LEU:HB2	2.50	0.46
1:FC:223:ARG:HA	1:FC:467:PRO:HG2	1.97	0.46
1:GC:115:THR:O	1:GC:149:ARG:HD3	2.15	0.46
1:HB:78:SER:HB2	1:HB:179:ILE:HD13	1.98	0.46
1:HC:78:SER:HB2	1:HC:179:ILE:HD13	1.97	0.46
1:JC:248:LYS:HE3	1:JC:435:ARG:HD3	1.98	0.46
1:KB:19:VAL:HG13	1:KB:149:ARG:O	2.16	0.46
1:KB:501:HIS:ND1	1:KB:531:GLY:HA3	2.30	0.46
1:KC:500:ALA:HB2	1:KC:527:LEU:HG	1.97	0.46
1:LB:501:HIS:CE1	1:LB:531:GLY:HA3	2.51	0.46
1:MB:286:PHE:HB3	1:MB:301:MET:HE1	1.98	0.46
1:MC:225:LYS:NZ	2:MC:602:CL:CL	2.85	0.46
1:NC:46:ASN:HD21	1:NC:213:ILE:C	2.18	0.46
1:NC:479:ASN:ND2	1:NC:510:PRO:HG3	2.31	0.46
1:OA:147:ASP:OD2	1:OA:149:ARG:NH1	2.49	0.46
1:OC:267:THR:CG2	1:OC:271:VAL:H	2.26	0.46
1:BA:187:ARG:NH2	1:CA:197:THR:O	2.49	0.46
1:BC:278:LEU:HD22	1:BC:459:LEU:HD23	1.96	0.46
1:CC:429:GLU:OE2	1:CC:490:LYS:HE2	2.16	0.46
1:DB:246:LEU:HD11	1:DB:454:PRO:HB3	1.96	0.46
1:FA:96:TYR:CG	1:FA:212:PHE:HB3	2.51	0.46
1:FC:267:THR:CG2	1:FC:271:VAL:H	2.26	0.46
1:GA:125:PRO:HG3	1:GB:214:PHE:CD1	2.51	0.46
1:IB:51:TRP:HB3	1:JA:215:LEU:HD12	1.96	0.46
1:JB:501:HIS:CE1	1:JB:531:GLY:HA3	2.51	0.46
1:KB:51:TRP:HB3	1:LA:215:LEU:HD12	1.98	0.46
1:KB:78:SER:HB2	1:KB:179:ILE:HD13	1.97	0.46
1:KB:94:ARG:NH2	1:LA:91:HIS:HE1	2.12	0.46
1:LB:115:THR:O	1:LB:149:ARG:HD3	2.15	0.46
1:LB:197:THR:HB	1:MC:187:ARG:NH1	2.31	0.46
1:NB:267:THR:CG2	1:NB:271:VAL:H	2.28	0.46
1:NB:372:ASN:OD1	1:NB:372:ASN:N	2.48	0.46
1:OC:359:THR:HG22	1:OC:410:GLY:H	1.80	0.46
1:AA:110:ALA:HA	1:EA:118:LYS:HE2	1.97	0.46
1:AB:101:GLY:HA3	1:AB:210:PHE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:267:THR:HG22	1:AB:271:VAL:N	2.26	0.46
1:BC:101:GLY:HA3	1:BC:210:PHE:HA	1.96	0.46
1:BC:249:LEU:HB2	1:BC:509:ILE:HD11	1.98	0.46
1:CA:318:PRO:HD3	1:CA:417:HIS:O	2.15	0.46
1:CB:233:THR:HG21	1:CB:511:PRO:O	2.16	0.46
1:FA:78:SER:HA	1:FA:178:LEU:O	2.16	0.46
1:FC:265:ARG:NH2	1:FC:420:PRO:O	2.39	0.46
1:GA:219:THR:HG22	1:GA:222:SER:OG	2.16	0.46
1:GB:471:ASP:OD1	1:GB:522:ASN:HA	2.16	0.46
1:HB:81:LEU:HD11	1:HB:102:GLY:HA2	1.97	0.46
1:MC:389:VAL:HG23	1:MC:442:SER:HB3	1.98	0.46
1:OC:330:ILE:HG12	1:OC:388:VAL:HG12	1.96	0.46
1:AC:182:LEU:HD21	1:AC:185:PRO:HA	1.98	0.46
1:CA:140:MET:HG2	1:DA:57:VAL:HG21	1.97	0.46
1:CA:434:PHE:CE1	1:CA:454:PRO:HD3	2.51	0.46
1:EB:454:PRO:HG2	1:EB:457:TRP:CG	2.50	0.46
1:FA:57:VAL:HG21	1:JA:140:MET:HG2	1.97	0.46
1:FB:319:ALA:HB1	1:FB:320:PRO:HD2	1.98	0.46
1:HA:138:VAL:HG21	1:HA:181:MET:SD	2.56	0.46
1:JA:459:LEU:O	1:JA:463:GLN:HG3	2.16	0.46
1:KA:73:GLY:HA2	1:KA:181:MET:HE3	1.97	0.46
1:LA:53:ARG:O	1:LA:205:ARG:HD2	2.16	0.46
1:MB:317:ILE:HD13	1:MB:321:LEU:HD21	1.98	0.46
1:MC:241:ARG:HB2	1:MC:449:LEU:HD21	1.97	0.46
1:OB:464:GLU:O	1:OB:464:GLU:HG3	2.15	0.46
1:AA:51:TRP:CZ2	1:EA:30:GLU:HG3	2.51	0.46
1:AC:144:ILE:HG22	1:AC:146:VAL:HG23	1.97	0.46
1:CA:96:TYR:CG	1:CA:212:PHE:HB3	2.51	0.46
1:CC:158:LEU:HD13	1:CC:178:LEU:HG	1.96	0.46
1:DA:216:VAL:CG2	1:DA:217:PRO:HD2	2.46	0.46
1:DA:233:THR:HG22	1:DA:235:GLU:N	2.31	0.46
1:DA:318:PRO:HD3	1:DA:417:HIS:O	2.15	0.46
1:DA:399:GLU:HB3	1:DA:400:PRO:HD3	1.97	0.46
1:DB:81:LEU:HD11	1:DB:102:GLY:HA2	1.98	0.46
1:DC:267:THR:CG2	1:DC:271:VAL:H	2.24	0.46
1:DC:434:PHE:CE2	1:DC:454:PRO:HD3	2.51	0.46
1:EC:409:SER:HB2	1:EC:412:THR:O	2.16	0.46
1:FA:56:PHE:O	1:JA:143:HIS:HE1	1.99	0.46
1:FB:215:LEU:HD21	1:GA:52:ILE:HG12	1.98	0.46
1:FB:402:GLN:OE1	1:FB:449:LEU:HA	2.16	0.46
1:GA:400:PRO:HG2	1:GA:446:ASN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:233:THR:HG21	1:GB:511:PRO:O	2.16	0.46
1:GB:432:LEU:HB2	1:GB:499:VAL:HG13	1.97	0.46
1:HB:471:ASP:OD1	1:HB:471:ASP:N	2.43	0.46
1:JB:217:PRO:HA	1:JB:218:PRO:HD3	1.62	0.46
1:JB:471:ASP:HA	1:JB:493:LYS:CD	2.46	0.46
1:JC:44:GLN:HE22	1:JC:215:LEU:HB2	1.81	0.46
1:JC:241:ARG:NE	1:JC:325:ASP:OD2	2.49	0.46
1:JC:244:ILE:HD11	1:JC:439:PRO:HD3	1.98	0.46
1:KC:44:GLN:NE2	1:KC:215:LEU:HD23	2.31	0.46
1:KC:336:GLN:OE1	1:KC:379:GLN:HB2	2.16	0.46
1:DA:96:TYR:CG	1:DA:212:PHE:HB3	2.51	0.46
1:FB:316:GLU:OE1	1:FB:417:HIS:NE2	2.49	0.46
1:HB:75:ILE:HD13	1:HB:179:ILE:HD12	1.97	0.46
1:IB:227:PHE:CE1	1:IB:268:THR:HG23	2.51	0.46
1:JB:19:VAL:HG13	1:JB:149:ARG:O	2.15	0.46
1:JB:280:PRO:HB3	1:JB:455:GLN:HG2	1.97	0.46
1:JC:390:GLN:HB2	1:JC:445:PRO:HB3	1.97	0.46
1:KC:470:SER:OG	1:KC:521:VAL:O	2.20	0.46
1:MB:94:ARG:NH2	1:NA:91:HIS:HE1	2.14	0.46
1:NA:149:ARG:NH2	1:OA:149:ARG:O	2.48	0.46
1:CB:275:THR:HG23	1:CB:318:PRO:HG2	1.98	0.45
1:EC:217:PRO:HA	1:EC:218:PRO:HD3	1.85	0.45
1:EC:426:PHE:HD2	1:EC:429:GLU:OE2	2.00	0.45
1:FA:318:PRO:HD3	1:FA:417:HIS:O	2.16	0.45
1:FB:432:LEU:HB2	1:FB:499:VAL:HG13	1.98	0.45
1:GA:338:THR:HG23	1:GA:379:GLN:NE2	2.31	0.45
1:HB:233:THR:HG22	1:HB:235:GLU:HG2	1.97	0.45
1:HB:327:VAL:HA	1:HB:353:THR:OG1	2.15	0.45
1:IA:140:MET:HG2	1:JA:57:VAL:HG21	1.97	0.45
1:IB:267:THR:CG2	1:IB:271:VAL:H	2.29	0.45
1:JA:353:THR:CG2	1:JA:406:PRO:HB3	2.46	0.45
1:KA:280:PRO:HB3	1:KA:455:GLN:HG2	1.97	0.45
1:MB:118:LYS:H	1:MB:184:THR:HB	1.80	0.45
1:MC:267:THR:CG2	1:MC:271:VAL:H	2.26	0.45
1:NA:219:THR:HG22	1:NA:222:SER:OG	2.15	0.45
1:NB:345:ARG:NE	1:NB:376:GLU:OE1	2.49	0.45
1:NB:469:GLN:HG3	1:NB:520:TRP:NE1	2.31	0.45
1:NC:121:PHE:HA	1:NC:179:ILE:O	2.16	0.45
1:NC:299:TYR:CE2	1:NC:375:LEU:HB2	2.51	0.45
1:NC:456:GLU:OE1	1:NC:456:GLU:N	2.48	0.45
1:NC:476:ARG:HG3	1:NC:516:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OC:242:PHE:O	1:OC:244:ILE:N	2.49	0.45
1:BA:73:GLY:H	1:BA:181:MET:HE3	1.81	0.45
1:DA:125:PRO:HG3	1:DB:214:PHE:CD1	2.52	0.45
1:FC:242:PHE:HD2	1:FC:244:ILE:HD11	1.81	0.45
1:GB:94:ARG:HB3	1:GB:218:PRO:O	2.16	0.45
1:GC:107:VAL:HG13	1:GC:154:VAL:HB	1.99	0.45
1:MA:266:CYS:HB2	1:MA:458:VAL:HG13	1.99	0.45
1:NB:46:ASN:ND2	1:NB:213:ILE:O	2.49	0.45
1:NC:431:LEU:HD23	1:NC:498:THR:HG22	1.98	0.45
1:AB:84:ASP:HB3	1:AB:469:GLN:OE1	2.16	0.45
1:AB:471:ASP:HA	1:AB:493:LYS:HD2	1.97	0.45
1:CA:118:LYS:HE2	1:DA:110:ALA:HA	1.99	0.45
1:CB:267:THR:CG2	1:CB:271:VAL:H	2.25	0.45
1:CC:30:GLU:HG3	1:CC:31:PRO:HD2	1.99	0.45
1:DB:471:ASP:OD1	1:DB:471:ASP:N	2.49	0.45
1:DC:107:VAL:CG1	1:DC:154:VAL:HB	2.46	0.45
1:EB:105:VAL:HG22	1:EB:156:ILE:HB	1.98	0.45
1:FB:280:PRO:HB3	1:FB:455:GLN:HG2	1.99	0.45
1:FB:301:MET:HE2	1:FB:303:LEU:HD23	1.98	0.45
1:GA:347:HIS:NE2	1:GA:374:ASP:HB3	2.31	0.45
1:IA:219:THR:HG22	1:IA:222:SER:OG	2.16	0.45
1:IC:377:THR:HG22	1:IC:378:GLY:N	2.31	0.45
1:KB:45:GLN:O	1:LA:51:TRP:NE1	2.47	0.45
1:MA:65:THR:HG21	1:MA:526:THR:N	2.12	0.45
1:NC:319:ALA:HB1	1:NC:320:PRO:HD2	1.99	0.45
1:AC:193:ASP:OD1	1:AC:193:ASP:N	2.42	0.45
1:AC:489:CYS:HB3	1:AC:499:VAL:HG12	1.97	0.45
1:BA:434:PHE:CE1	1:BA:454:PRO:HD3	2.51	0.45
1:CA:105:VAL:CG1	1:CA:156:ILE:HB	2.46	0.45
1:CC:225:LYS:NZ	2:CC:601:CL:CL	2.86	0.45
1:DB:109:LEU:HD23	1:DB:200:CYS:SG	2.57	0.45
1:DC:148:VAL:CG1	1:DC:198:VAL:HG21	2.47	0.45
1:DC:308:TRP:CZ3	1:DC:380:ASN:HB3	2.52	0.45
1:GA:490:LYS:HE3	1:GA:527:LEU:HG	1.99	0.45
1:GC:268:THR:HG21	1:GC:520:TRP:CH2	2.42	0.45
1:HB:227:PHE:CE1	1:HB:268:THR:HG23	2.51	0.45
1:IB:19:VAL:HG13	1:IB:149:ARG:O	2.16	0.45
1:JB:105:VAL:HG22	1:JB:156:ILE:HB	1.99	0.45
1:LA:280:PRO:HA	1:LA:283:ILE:HD11	1.99	0.45
1:LB:124:VAL:HG22	1:LB:177:LYS:HB2	1.98	0.45
1:LC:118:LYS:H	1:LC:184:THR:HB	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LC:459:LEU:O	1:LC:463:GLN:HG3	2.17	0.45
1:MA:216:VAL:CG2	1:MA:217:PRO:HD2	2.47	0.45
1:AA:44:GLN:HA	1:AC:30:GLU:HG2	1.98	0.45
1:AB:477:PHE:CE2	1:AB:509:ILE:HG23	2.52	0.45
1:BA:221:GLU:OE1	1:BA:221:GLU:N	2.49	0.45
1:BB:403:TRP:CZ2	1:BB:450:ASP:HB2	2.52	0.45
1:CA:219:THR:HG22	1:CA:222:SER:OG	2.17	0.45
1:DA:338:THR:HB	1:DA:343:SER:HB2	1.98	0.45
1:EC:372:ASN:OD1	1:EC:372:ASN:N	2.49	0.45
1:JB:301:MET:HE2	1:JB:303:LEU:HD23	1.99	0.45
1:JC:336:GLN:NE2	1:JC:379:GLN:HB2	2.32	0.45
1:JC:389:VAL:HG23	1:JC:442:SER:HB3	1.98	0.45
1:LB:471:ASP:HA	1:LB:493:LYS:HE2	1.97	0.45
1:LB:490:LYS:HG3	1:LB:527:LEU:HD21	1.96	0.45
1:NA:115:THR:HG22	1:NA:148:VAL:HG21	1.99	0.45
1:OA:105:VAL:CG1	1:OA:156:ILE:HB	2.45	0.45
1:OA:433:PHE:HB3	1:OA:450:ASP:HB3	1.97	0.45
1:OC:456:GLU:OE1	1:OC:456:GLU:N	2.49	0.45
1:BB:81:LEU:HD11	1:BB:102:GLY:HA2	1.98	0.45
1:BB:130:THR:HG23	1:BB:179:ILE:HD11	1.99	0.45
1:BB:242:PHE:HD1	1:BB:284:CYS:HG	1.62	0.45
1:CC:389:VAL:HG23	1:CC:442:SER:HB3	1.98	0.45
1:DA:424:PRO:HD3	1:DA:431:LEU:HD13	1.98	0.45
1:DC:267:THR:HG22	1:DC:271:VAL:N	2.26	0.45
1:EA:233:THR:HG22	1:EA:235:GLU:N	2.29	0.45
1:EB:218:PRO:O	1:EB:219:THR:HG22	2.17	0.45
1:FA:223:ARG:HH21	1:FA:269:ASP:HB2	1.82	0.45
1:HA:109:LEU:HD22	1:HA:200:CYS:SG	2.57	0.45
1:HC:477:PHE:CD1	1:HC:486:LEU:HD12	2.51	0.45
1:IA:434:PHE:CE1	1:IA:454:PRO:HD3	2.51	0.45
1:IC:267:THR:CG2	1:IC:271:VAL:H	2.26	0.45
1:JC:118:LYS:H	1:JC:184:THR:HB	1.81	0.45
1:JC:249:LEU:HD23	1:JC:432:LEU:HD21	1.97	0.45
1:KA:476:ARG:HD3	1:KA:485:VAL:HG11	1.97	0.45
1:LC:390:GLN:HB2	1:LC:445:PRO:HB3	1.98	0.45
1:MC:416:VAL:HG12	1:MC:417:HIS:N	2.32	0.45
1:OB:115:THR:O	1:OB:149:ARG:HD3	2.17	0.45
1:OB:230:PRO:HD3	1:OB:460:HIS:CD2	2.52	0.45
1:OC:358:PHE:HD1	1:OC:365:VAL:HG13	1.81	0.45
1:AB:57:VAL:HG23	1:AB:87:PRO:HD2	1.98	0.45
1:CB:121:PHE:HA	1:CB:179:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:75:ILE:HG23	1:DA:179:ILE:HG23	1.99	0.45
1:DA:161:VAL:HB	1:DA:176:ILE:HD11	1.98	0.45
1:DB:280:PRO:HA	1:DB:283:ILE:HD11	1.98	0.45
1:FC:217:PRO:HA	1:FC:218:PRO:HD3	1.85	0.45
1:GA:105:VAL:CG1	1:GA:156:ILE:HB	2.46	0.45
1:HB:34:GLY:HA3	1:HB:209:ASP:HB2	1.97	0.45
1:HB:440:GLY:O	1:IA:335:THR:HG23	2.16	0.45
1:IC:527:LEU:H	1:IC:527:LEU:HD23	1.82	0.45
1:JC:347:HIS:NE2	1:JC:374:ASP:HB3	2.31	0.45
1:KA:371:THR:HG21	1:KA:374:ASP:HB2	1.99	0.45
1:MA:173:ASP:OD1	1:MA:174:PRO:HD2	2.16	0.45
1:MB:60:PRO:HD3	1:MB:87:PRO:HD3	1.99	0.45
1:NB:230:PRO:HD3	1:NB:460:HIS:CD2	2.52	0.45
1:OB:34:GLY:HA3	1:OB:209:ASP:HB2	1.97	0.45
1:AB:454:PRO:HG2	1:AB:457:TRP:CG	2.52	0.45
1:CA:120:ILE:CG1	1:CA:183:TYR:HB2	2.47	0.45
1:CB:32:VAL:HB	1:CB:159:PRO:HB2	1.98	0.45
1:CC:107:VAL:CG1	1:CC:154:VAL:HB	2.47	0.45
1:FA:223:ARG:NH2	1:FA:269:ASP:HB2	2.32	0.45
1:GB:115:THR:O	1:GB:149:ARG:HD3	2.17	0.45
1:HB:233:THR:HB	1:HB:236:GLU:HG3	1.99	0.45
1:JA:101:GLY:HA3	1:JA:210:PHE:HA	1.98	0.45
1:KB:57:VAL:HA	1:LC:139:THR:HG22	1.98	0.45
1:KC:107:VAL:CG1	1:KC:154:VAL:HB	2.47	0.45
1:LC:241:ARG:NE	1:LC:325:ASP:OD2	2.45	0.45
1:NB:265:ARG:NH2	1:NB:420:PRO:O	2.44	0.45
1:OB:403:TRP:CZ2	1:OB:450:ASP:HB2	2.52	0.45
1:OC:148:VAL:CG1	1:OC:198:VAL:HG21	2.47	0.45
1:OC:233:THR:HG22	1:OC:235:GLU:H	1.81	0.45
1:AB:109:LEU:HD23	1:AB:200:CYS:SG	2.56	0.45
1:AB:424:PRO:HD3	1:AB:431:LEU:HG	1.98	0.45
1:AC:124:VAL:HG21	1:AC:179:ILE:HD12	1.99	0.45
1:BA:326:PHE:O	1:BA:353:THR:HG21	2.17	0.45
1:BB:24:ASN:OD1	1:BB:25:GLU:N	2.49	0.45
1:BB:482:THR:HG22	1:CC:426:PHE:HD1	1.81	0.45
1:DA:347:HIS:NE2	1:DA:374:ASP:HB3	2.32	0.45
1:DA:371:THR:HG22	1:DA:373:ASN:H	1.82	0.45
1:DC:130:THR:HG23	1:DC:179:ILE:HD11	1.98	0.45
1:FB:199:SER:HB2	1:GC:184:THR:HG23	1.99	0.45
1:FC:118:LYS:H	1:FC:184:THR:HB	1.80	0.45
1:IC:371:THR:CG2	1:IC:374:ASP:H	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:395:ALA:HB3	1:KB:398:ASN:HD22	1.81	0.45
1:LB:51:TRP:HB3	1:MA:215:LEU:HD12	1.98	0.45
1:LC:148:VAL:CG1	1:LC:198:VAL:HG21	2.47	0.45
1:NA:318:PRO:HD3	1:NA:417:HIS:O	2.17	0.45
1:OA:371:THR:HG22	1:OA:373:ASN:H	1.81	0.45
1:OB:233:THR:CG2	1:OB:235:GLU:HG2	2.46	0.45
1:BA:116:ALA:O	1:BA:186:LEU:HD12	2.17	0.45
1:CA:161:VAL:HB	1:CA:176:ILE:HD11	1.99	0.45
1:CA:399:GLU:HB3	1:CA:400:PRO:HD3	1.98	0.45
1:CC:267:THR:HG22	1:CC:271:VAL:N	2.30	0.45
1:DB:121:PHE:HA	1:DB:179:ILE:O	2.17	0.45
1:DB:197:THR:HB	1:EC:187:ARG:NH1	2.31	0.45
1:DB:316:GLU:OE1	1:DB:417:HIS:NE2	2.50	0.45
1:DC:426:PHE:CD1	1:DC:427:PRO:HD2	2.51	0.45
1:FC:107:VAL:CG1	1:FC:154:VAL:HB	2.47	0.45
1:GA:108:ILE:HG12	1:GA:153:PRO:HB3	1.98	0.45
1:HA:43:GLY:HA3	1:HA:214:PHE:CE1	2.52	0.45
1:HA:267:THR:HG23	1:HA:493:LYS:O	2.17	0.45
1:HB:51:TRP:HB3	1:IA:215:LEU:HD12	1.99	0.45
1:KC:312:ASP:HB3	1:KC:315:GLU:HG3	1.99	0.45
1:LA:435:ARG:HG3	1:LA:450:ASP:OD1	2.17	0.45
1:LB:118:LYS:H	1:LB:184:THR:HB	1.82	0.45
1:MB:215:LEU:HD21	1:NA:52:ILE:HG12	2.00	0.45
1:NB:454:PRO:HG2	1:NB:457:TRP:CD1	2.52	0.45
1:OB:30:GLU:HG3	1:OC:44:GLN:HA	1.97	0.45
1:AC:249:LEU:HB2	1:AC:509:ILE:HD11	1.99	0.44
1:CA:140:MET:HG2	1:DA:57:VAL:CG2	2.47	0.44
1:CC:130:THR:O	1:CC:133:LEU:HD23	2.17	0.44
1:CC:338:THR:OG1	1:CC:345:ARG:NH2	2.41	0.44
1:DB:482:THR:HG22	1:EC:426:PHE:CD1	2.52	0.44
1:EB:32:VAL:HB	1:EB:159:PRO:HB2	1.99	0.44
1:GA:216:VAL:CG2	1:GA:217:PRO:HD2	2.45	0.44
1:GA:399:GLU:HB3	1:GA:400:PRO:HD3	1.98	0.44
1:HA:219:THR:HG22	1:HA:222:SER:OG	2.17	0.44
1:JA:389:VAL:HG12	1:JA:441:CYS:HB2	1.98	0.44
1:JB:30:GLU:HG3	1:JC:44:GLN:HA	1.98	0.44
1:KA:248:LYS:HE2	1:KA:435:ARG:HD2	1.99	0.44
1:KC:118:LYS:H	1:KC:184:THR:HB	1.82	0.44
1:LA:118:LYS:HE2	1:MA:110:ALA:HA	2.00	0.44
1:LC:424:PRO:HD3	1:LC:431:LEU:HG	1.99	0.44
1:MB:14:SER:O	1:MB:15:THR:OG1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OB:222:SER:O	1:OB:223:ARG:HB2	2.18	0.44
1:OB:325:ASP:OD1	1:OB:325:ASP:N	2.50	0.44
1:CA:105:VAL:HG11	1:CA:178:LEU:HD22	2.00	0.44
1:EC:25:GLU:HG3	1:EC:25:GLU:O	2.17	0.44
1:FB:195:VAL:HG13	1:FB:197:THR:H	1.82	0.44
1:FB:471:ASP:HA	1:FB:493:LYS:CD	2.46	0.44
1:FC:303:LEU:HD11	1:FC:365:VAL:HG23	1.98	0.44
1:HA:125:PRO:HG3	1:HB:214:PHE:CD1	2.53	0.44
1:KA:30:GLU:HG3	1:LA:51:TRP:CH2	2.51	0.44
1:LC:477:PHE:HD2	1:LC:515:PHE:CE1	2.35	0.44
1:NA:30:GLU:HG3	1:OA:51:TRP:CH2	2.52	0.44
1:OC:182:LEU:HD21	1:OC:185:PRO:HA	1.99	0.44
1:AB:338:THR:HG22	1:AB:340:GLY:H	1.82	0.44
1:BC:44:GLN:HE21	1:BC:215:LEU:HD23	1.83	0.44
1:CA:115:THR:HG22	1:CA:148:VAL:CG2	2.48	0.44
1:CA:275:THR:HG23	1:CA:318:PRO:HG2	1.99	0.44
1:CB:134:SER:OG	1:CB:137:GLN:HG3	2.18	0.44
1:FA:317:ILE:HD13	1:FA:321:LEU:HD21	2.00	0.44
1:GB:124:VAL:HG22	1:GB:177:LYS:HB2	1.99	0.44
1:GB:343:SER:OG	1:GB:345:ARG:NH2	2.50	0.44
1:GB:456:GLU:OE1	1:GB:456:GLU:N	2.46	0.44
1:IA:247:GLU:OE1	1:IA:437:THR:HG22	2.16	0.44
1:KB:424:PRO:HD3	1:KB:431:LEU:HG	1.99	0.44
1:OA:499:VAL:HG21	1:OA:530:MET:HE3	1.99	0.44
1:AB:144:ILE:HG22	1:AB:146:VAL:HG23	2.00	0.44
1:CA:251:THR:HG23	1:CA:431:LEU:O	2.17	0.44
1:CB:489:CYS:HB3	1:CB:499:VAL:HG12	1.99	0.44
1:DB:219:THR:HG22	1:DB:219:THR:O	2.18	0.44
1:DB:249:LEU:HB2	1:DB:509:ILE:HD11	1.99	0.44
1:DC:434:PHE:CD2	1:DC:454:PRO:HD3	2.52	0.44
1:EC:130:THR:O	1:EC:133:LEU:HD23	2.17	0.44
1:FB:196:PHE:HA	1:GC:187:ARG:HD2	2.00	0.44
1:FC:158:LEU:HD13	1:FC:178:LEU:HG	1.98	0.44
1:GC:416:VAL:HG12	1:GC:417:HIS:CG	2.53	0.44
1:HA:216:VAL:HG22	1:HA:217:PRO:HD2	2.00	0.44
1:HA:233:THR:HG22	1:HA:235:GLU:N	2.29	0.44
1:IC:434:PHE:CE2	1:IC:454:PRO:HD3	2.52	0.44
1:JB:233:THR:HG21	1:JB:511:PRO:O	2.16	0.44
1:JB:429:GLU:HB3	1:JB:498:THR:CG2	2.47	0.44
1:KA:281:VAL:HG11	1:OB:244:ILE:HA	1.99	0.44
1:MA:53:ARG:HB3	1:MA:206:PRO:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OA:216:VAL:HG21	1:OC:128:PHE:CD1	2.52	0.44
1:OB:233:THR:HG22	1:OB:235:GLU:HG2	1.99	0.44
1:BC:319:ALA:HB1	1:BC:320:PRO:HD2	1.99	0.44
1:DB:37:ILE:HG22	1:DB:165:PHE:CD1	2.53	0.44
1:EA:430:GLN:HE22	1:EA:503:GLY:H	1.65	0.44
1:EB:345:ARG:NE	1:EB:376:GLU:OE1	2.51	0.44
1:EC:66:VAL:HB	1:EC:198:VAL:HB	2.00	0.44
1:GB:34:GLY:HA3	1:GB:209:ASP:HB2	2.00	0.44
1:GC:217:PRO:HA	1:GC:218:PRO:HD3	1.63	0.44
1:JC:426:PHE:HD2	1:JC:429:GLU:OE2	1.99	0.44
1:JC:429:GLU:OE2	1:JC:490:LYS:HE2	2.17	0.44
1:LA:66:VAL:HG12	1:LA:186:LEU:HD22	1.99	0.44
1:LA:341:ASP:OD1	1:LA:341:ASP:N	2.51	0.44
1:LB:219:THR:HG22	1:LB:219:THR:O	2.17	0.44
1:LC:278:LEU:HD22	1:LC:459:LEU:HD23	2.00	0.44
1:MC:46:ASN:HD21	1:MC:213:ILE:C	2.20	0.44
1:NA:372:ASN:OD1	1:NA:372:ASN:N	2.51	0.44
1:NC:269:ASP:OD1	1:NC:269:ASP:N	2.47	0.44
1:OC:241:ARG:NE	1:OC:325:ASP:OD2	2.47	0.44
1:BB:464:GLU:O	1:BB:466:ALA:N	2.49	0.44
1:BC:57:VAL:HA	1:KB:139:THR:HG22	2.00	0.44
1:CA:66:VAL:HG21	1:CA:119:ILE:HD11	2.00	0.44
1:DC:269:ASP:OD1	1:DC:269:ASP:N	2.51	0.44
1:EA:231:ILE:HD12	1:EA:231:ILE:H	1.83	0.44
1:FC:227:PHE:HD1	1:FC:466:ALA:HB1	1.82	0.44
1:GA:117:GLY:O	1:GA:148:VAL:HG22	2.17	0.44
1:IC:459:LEU:O	1:IC:463:GLN:HG3	2.18	0.44
1:KA:96:TYR:HA	1:KA:214:PHE:O	2.17	0.44
1:KA:108:ILE:HG12	1:KA:153:PRO:HB3	2.00	0.44
1:LC:241:ARG:NH1	1:LC:450:ASP:O	2.43	0.44
1:NA:312:ASP:O	1:NA:315:GLU:HG3	2.18	0.44
1:OB:477:PHE:CE2	1:OB:509:ILE:HD12	2.52	0.44
1:AA:96:TYR:CG	1:AA:212:PHE:HB3	2.53	0.44
1:BB:278:LEU:HD22	1:BB:459:LEU:HD23	1.98	0.44
1:CB:118:LYS:H	1:CB:184:THR:HB	1.82	0.44
1:CB:247:GLU:OE2	1:CB:437:THR:N	2.51	0.44
1:EA:399:GLU:HB3	1:EA:400:PRO:HD3	2.00	0.44
1:EB:121:PHE:HA	1:EB:179:ILE:O	2.17	0.44
1:EC:57:VAL:HG11	1:EC:87:PRO:HD2	2.00	0.44
1:FC:459:LEU:O	1:FC:463:GLN:HG3	2.18	0.44
1:IA:318:PRO:HD3	1:IA:417:HIS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IC:242:PHE:HD1	1:IC:284:CYS:HG	1.66	0.44
1:IC:319:ALA:HB1	1:IC:320:PRO:HD2	1.99	0.44
1:JB:32:VAL:HB	1:JB:159:PRO:HB2	1.98	0.44
1:JC:469:GLN:HB2	1:JC:520:TRP:CG	2.52	0.44
1:KA:386:VAL:HG11	1:OB:333:VAL:HB	1.99	0.44
1:LB:282:ASN:HD22	1:LB:306:GLN:HB3	1.81	0.44
1:MA:239:ASN:ND2	1:MA:436:SER:OG	2.49	0.44
1:DC:159:PRO:O	1:DC:176:ILE:HD12	2.18	0.44
1:FA:66:VAL:HG12	1:FA:186:LEU:HD22	2.00	0.44
1:FA:468:ALA:HA	1:FA:520:TRP:CH2	2.53	0.44
1:FC:327:VAL:HG23	1:FC:404:VAL:O	2.17	0.44
1:HC:489:CYS:HB3	1:HC:499:VAL:HG12	2.00	0.44
1:IB:34:GLY:HA3	1:IB:209:ASP:HB2	2.00	0.44
1:IB:230:PRO:HG2	1:IB:457:TRP:CD1	2.53	0.44
1:KA:73:GLY:CA	1:KA:181:MET:HE3	2.47	0.44
1:OB:230:PRO:HG2	1:OB:457:TRP:CD1	2.53	0.44
1:OC:319:ALA:HB1	1:OC:320:PRO:HD2	1.99	0.44
1:AB:317:ILE:HD13	1:AB:321:LEU:HD21	1.99	0.44
1:CA:341:ASP:OD1	1:CA:341:ASP:N	2.46	0.44
1:CC:81:LEU:HD12	1:CC:158:LEU:HG	1.99	0.44
1:DA:158:LEU:HD13	1:DA:178:LEU:HD13	2.00	0.44
1:DA:390:GLN:O	1:DA:443:GLY:HA3	2.18	0.44
1:DC:424:PRO:HG3	1:DC:430:GLN:HA	2.00	0.44
1:EA:219:THR:HG22	1:EA:222:SER:OG	2.17	0.44
1:FA:51:TRP:CH2	1:JA:30:GLU:HG3	2.52	0.44
1:FB:121:PHE:HA	1:FB:179:ILE:O	2.18	0.44
1:FC:148:VAL:CG1	1:FC:198:VAL:HG21	2.47	0.44
1:HA:105:VAL:CG1	1:HA:156:ILE:HB	2.48	0.44
1:HB:361:LYS:HD2	1:HB:409:SER:OG	2.18	0.44
1:HC:116:ALA:HB3	1:HC:187:ARG:HB2	2.00	0.44
1:IC:107:VAL:CG1	1:IC:154:VAL:HB	2.48	0.44
1:JC:53:ARG:NH2	1:JC:210:PHE:O	2.37	0.44
1:KC:347:HIS:NE2	1:KC:374:ASP:HB3	2.32	0.44
1:MB:51:TRP:HB3	1:NA:215:LEU:HD12	2.00	0.44
1:MB:233:THR:CG2	1:MB:235:GLU:HG2	2.48	0.44
1:NB:124:VAL:HG22	1:NB:177:LYS:HB2	1.99	0.44
1:OA:33:VAL:HG11	1:OA:37:ILE:HB	1.99	0.44
1:OA:304:ALA:O	1:OA:311:TYR:HB2	2.18	0.44
1:OB:345:ARG:NH2	1:OB:376:GLU:OE2	2.48	0.44
1:AB:19:VAL:HG13	1:AB:149:ARG:O	2.17	0.43
1:BA:64:PHE:CG	1:BA:77:TRP:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:107:VAL:HG13	1:BC:154:VAL:HB	1.98	0.43
1:CA:299:TYR:CE2	1:CA:375:LEU:HB2	2.53	0.43
1:CB:471:ASP:HA	1:CB:493:LYS:CD	2.47	0.43
1:DC:403:TRP:CZ2	1:DC:450:ASP:HB2	2.53	0.43
1:EC:25:GLU:OE1	1:EC:154:VAL:HG13	2.17	0.43
1:EC:106:GLN:HB3	1:EC:203:LEU:HB2	1.99	0.43
1:EC:469:GLN:HB2	1:EC:520:TRP:CG	2.53	0.43
1:EC:500:ALA:HB3	1:EC:529:PRO:HA	1.99	0.43
1:GC:58:GLN:HA	1:GC:203:LEU:HD13	2.00	0.43
1:HA:372:ASN:OD1	1:HA:372:ASN:N	2.49	0.43
1:HB:23:ASN:HD21	1:HB:144:ILE:HD11	1.83	0.43
1:HC:259:VAL:HG13	1:HC:403:TRP:CZ3	2.53	0.43
1:JC:334:LEU:HD22	1:JC:381:THR:HG22	1.99	0.43
1:KC:319:ALA:HB1	1:KC:320:PRO:HD2	1.99	0.43
1:LA:326:PHE:O	1:LA:353:THR:HG21	2.17	0.43
1:MB:248:LYS:HD2	1:MB:435:ARG:HD2	2.00	0.43
1:MC:25:GLU:HA	1:MC:144:ILE:HG23	2.00	0.43
1:NC:484:ARG:HH11	1:NC:486:LEU:HD23	1.83	0.43
1:OA:347:HIS:NE2	1:OA:374:ASP:HB3	2.32	0.43
1:AA:390:GLN:O	1:AA:443:GLY:HA3	2.17	0.43
1:BC:523:GLN:HG3	1:BC:523:GLN:O	2.17	0.43
1:DC:259:VAL:HG13	1:DC:403:TRP:CZ3	2.53	0.43
1:EC:124:VAL:HG21	1:EC:179:ILE:HD12	1.99	0.43
1:FA:140:MET:HG2	1:GA:57:VAL:CG2	2.47	0.43
1:FC:232:LEU:HD11	1:LC:459:LEU:HD22	2.00	0.43
1:IB:343:SER:OG	1:IB:345:ARG:NH2	2.51	0.43
1:JA:311:TYR:OH	1:JA:320:PRO:HD3	2.18	0.43
1:JA:317:ILE:HG21	1:JA:321:LEU:HD21	2.00	0.43
1:JC:330:ILE:HG12	1:JC:388:VAL:HG12	2.00	0.43
1:KA:105:VAL:CG1	1:KA:156:ILE:HB	2.48	0.43
1:KB:400:PRO:HD2	1:KB:446:ASN:H	1.81	0.43
1:KB:433:PHE:HB3	1:KB:450:ASP:HB3	2.00	0.43
1:MB:280:PRO:HB3	1:MB:455:GLN:HG2	2.00	0.43
1:NA:138:VAL:HG21	1:NA:181:MET:SD	2.58	0.43
1:OC:46:ASN:HD21	1:OC:213:ILE:C	2.18	0.43
1:BC:46:ASN:HD21	1:BC:213:ILE:C	2.20	0.43
1:DB:125:PRO:HG3	1:DC:214:PHE:CD1	2.52	0.43
1:DB:161:VAL:HB	1:DB:176:ILE:HD11	2.01	0.43
1:EC:260:GLN:N	1:EC:261:PRO:HD3	2.34	0.43
1:FA:216:VAL:CG2	1:FA:217:PRO:HD2	2.45	0.43
1:FB:440:GLY:O	1:GA:335:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:230:PRO:HG2	1:GB:457:TRP:CD1	2.53	0.43
1:IA:48:ILE:HD11	1:IA:89:LEU:CD2	2.48	0.43
1:IC:130:THR:O	1:IC:133:LEU:HD23	2.18	0.43
1:KC:121:PHE:HA	1:KC:179:ILE:O	2.18	0.43
1:MA:53:ARG:O	1:MA:205:ARG:HD2	2.17	0.43
1:MA:377:THR:OG1	1:MA:378:GLY:N	2.52	0.43
1:MB:14:SER:O	1:MB:16:ALA:N	2.43	0.43
1:MB:125:PRO:HG3	1:MC:214:PHE:CD1	2.53	0.43
1:NC:479:ASN:HD22	1:NC:510:PRO:HG3	1.82	0.43
1:OA:117:GLY:O	1:OA:148:VAL:HG22	2.17	0.43
1:CA:435:ARG:HG3	1:CA:450:ASP:OD1	2.18	0.43
1:CB:124:VAL:HG22	1:CB:177:LYS:HB2	2.00	0.43
1:DA:367:PHE:HE2	1:DA:383:PHE:CG	2.36	0.43
1:DB:230:PRO:HG2	1:DB:457:TRP:CD1	2.53	0.43
1:FB:306:GLN:CD	1:FB:306:GLN:H	2.22	0.43
1:GB:437:THR:HG23	1:GB:447:MET:HB3	2.00	0.43
1:GC:377:THR:HG22	1:GC:378:GLY:N	2.33	0.43
1:IB:359:THR:HG22	1:IB:410:GLY:HA3	1.99	0.43
1:JC:107:VAL:CG1	1:JC:154:VAL:HB	2.49	0.43
1:JC:359:THR:HG22	1:JC:410:GLY:N	2.33	0.43
1:LB:57:VAL:HG23	1:LB:87:PRO:HD2	2.00	0.43
1:OB:109:LEU:HD23	1:OB:200:CYS:SG	2.58	0.43
1:AB:488:GLU:HG3	1:AB:527:LEU:HD22	2.01	0.43
1:AC:120:ILE:HG13	1:AC:183:TYR:HB2	2.01	0.43
1:BC:241:ARG:NE	1:BC:325:ASP:OD2	2.50	0.43
1:BC:260:GLN:N	1:BC:261:PRO:HD3	2.33	0.43
1:CA:216:VAL:CG2	1:CA:217:PRO:HD2	2.47	0.43
1:CB:57:VAL:HG23	1:CB:87:PRO:HD2	2.01	0.43
1:CC:72:PRO:HA	1:CC:182:LEU:O	2.18	0.43
1:CC:148:VAL:CG1	1:CC:198:VAL:HG21	2.47	0.43
1:DA:500:ALA:HB2	1:DA:527:LEU:HB2	2.00	0.43
1:DB:286:PHE:HB3	1:DB:301:MET:HE1	2.01	0.43
1:DC:257:PHE:H	1:DC:257:PHE:HD1	1.65	0.43
1:EB:424:PRO:HD3	1:EB:431:LEU:HG	2.00	0.43
1:FA:30:GLU:HG3	1:GA:51:TRP:CZ2	2.53	0.43
1:FB:280:PRO:HA	1:FB:283:ILE:HD11	1.99	0.43
1:GB:124:VAL:CG2	1:GB:177:LYS:HB2	2.48	0.43
1:GC:24:ASN:CG	1:GC:25:GLU:N	2.70	0.43
1:HA:328:GLY:H	1:HA:353:THR:HB	1.83	0.43
1:HC:268:THR:HG21	1:HC:520:TRP:CH2	2.43	0.43
1:IB:454:PRO:HG2	1:IB:457:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IC:234:VAL:O	1:IC:246:LEU:HB2	2.18	0.43
1:JA:246:LEU:HA	1:JA:436:SER:HB3	2.00	0.43
1:JA:319:ALA:HB1	1:JA:320:PRO:HD2	2.00	0.43
1:JB:124:VAL:CG2	1:JB:177:LYS:HB2	2.47	0.43
1:JC:433:PHE:HB3	1:JC:450:ASP:HB3	2.01	0.43
1:KA:116:ALA:O	1:KA:186:LEU:HD12	2.18	0.43
1:KC:265:ARG:NH2	1:KC:420:PRO:O	2.26	0.43
1:LB:109:LEU:HD23	1:LB:200:CYS:SG	2.58	0.43
1:LB:484:ARG:HH21	1:MC:526:THR:HG21	1.83	0.43
1:MA:33:VAL:HG11	1:MA:37:ILE:HB	2.00	0.43
1:MB:66:VAL:HG12	1:MB:186:LEU:HB2	2.01	0.43
1:MC:308:TRP:CH2	1:MC:380:ASN:HB3	2.53	0.43
1:NC:148:VAL:CG1	1:NC:198:VAL:HG21	2.48	0.43
1:AA:372:ASN:OD1	1:AA:372:ASN:N	2.52	0.43
1:AC:433:PHE:HB3	1:AC:450:ASP:HB3	1.99	0.43
1:BA:140:MET:HG2	1:CA:57:VAL:CG2	2.49	0.43
1:DA:101:GLY:HA3	1:DA:210:PHE:HA	2.00	0.43
1:DA:433:PHE:HB3	1:DA:450:ASP:HB3	2.00	0.43
1:DB:249:LEU:HD12	1:DB:509:ILE:HD11	2.01	0.43
1:DC:101:GLY:HA3	1:DC:210:PHE:HA	2.01	0.43
1:DC:326:PHE:HB2	1:DC:402:GLN:HA	2.00	0.43
1:EA:60:PRO:HD2	1:EA:84:ASP:O	2.18	0.43
1:EC:390:GLN:HG2	1:EC:399:GLU:HG3	2.01	0.43
1:GA:29:LEU:HA	1:GA:29:LEU:HD23	1.79	0.43
1:GB:265:ARG:NH2	1:GB:420:PRO:O	2.49	0.43
1:IA:108:ILE:HG12	1:IA:153:PRO:HB3	1.99	0.43
1:IC:390:GLN:HB2	1:IC:445:PRO:HB3	2.00	0.43
1:JB:97:ASN:HB3	1:JB:214:PHE:HB3	2.00	0.43
1:KA:144:ILE:HD12	1:KA:154:VAL:HG11	2.01	0.43
1:KA:145:ILE:HG21	1:LA:108:ILE:HD13	2.00	0.43
1:LA:216:VAL:HG21	1:LC:128:PHE:CD1	2.54	0.43
1:MA:326:PHE:O	1:MA:353:THR:HG21	2.18	0.43
1:NC:120:ILE:HG13	1:NC:183:TYR:HB2	2.00	0.43
1:NC:336:GLN:HE22	1:NC:375:LEU:HA	1.83	0.43
1:OB:432:LEU:HB2	1:OB:499:VAL:HG13	2.00	0.43
1:FB:286:PHE:HB3	1:FB:301:MET:CE	2.48	0.43
1:HA:394:SER:OG	1:HA:398:ASN:ND2	2.42	0.43
1:IA:29:LEU:HD23	1:IA:29:LEU:HA	1.81	0.43
1:IA:216:VAL:CG2	1:IA:217:PRO:HD2	2.48	0.43
1:IC:182:LEU:HD21	1:IC:185:PRO:HA	2.00	0.43
1:IC:233:THR:HG21	1:IC:511:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JC:148:VAL:CG1	1:JC:198:VAL:HG21	2.48	0.43
1:KA:434:PHE:CE1	1:KA:454:PRO:HD3	2.53	0.43
1:MC:106:GLN:HB3	1:MC:203:LEU:HB2	1.99	0.43
1:MC:416:VAL:HG12	1:MC:417:HIS:H	1.83	0.43
1:OB:336:GLN:NE2	1:OB:379:GLN:HB2	2.34	0.43
1:AC:371:THR:HG21	1:AC:374:ASP:HB2	1.99	0.43
1:DB:24:ASN:OD1	1:DB:24:ASN:N	2.51	0.43
1:DB:267:THR:HG22	1:DB:271:VAL:N	2.27	0.43
1:FA:105:VAL:CG1	1:FA:156:ILE:HB	2.49	0.43
1:FB:327:VAL:HA	1:FB:353:THR:OG1	2.18	0.43
1:GB:96:TYR:CG	1:GB:212:PHE:HB3	2.54	0.43
1:IA:96:TYR:CG	1:IA:212:PHE:HB3	2.54	0.43
1:IA:242:PHE:O	1:IA:244:ILE:N	2.51	0.43
1:IC:449:LEU:HD12	1:IC:449:LEU:HA	1.91	0.43
1:JB:66:VAL:HG21	1:JB:119:ILE:HD11	2.01	0.43
1:JC:94:ARG:NH1	1:JC:226:PRO:HD3	2.32	0.43
1:KB:101:GLY:HA3	1:KB:210:PHE:HA	1.99	0.43
1:LC:57:VAL:HG11	1:LC:87:PRO:HD2	2.00	0.43
1:LC:317:ILE:HD12	1:LC:319:ALA:O	2.18	0.43
1:MB:280:PRO:HA	1:MB:283:ILE:HD11	2.01	0.43
1:NA:328:GLY:H	1:NA:353:THR:HB	1.84	0.43
1:NB:121:PHE:HA	1:NB:179:ILE:O	2.18	0.43
1:NB:454:PRO:HG2	1:NB:457:TRP:CG	2.54	0.43
1:NC:81:LEU:HD11	1:NC:102:GLY:HA2	2.01	0.43
1:AB:57:VAL:HA	1:BC:139:THR:HG22	2.00	0.43
1:BA:341:ASP:OD2	1:BA:341:ASP:N	2.51	0.43
1:CA:134:SER:OG	1:CA:137:GLN:HG3	2.18	0.43
1:CA:249:LEU:HD12	1:CA:509:ILE:HD11	2.01	0.43
1:CB:131:GLU:OE1	1:CB:131:GLU:N	2.52	0.43
1:CB:259:VAL:HG13	1:CB:403:TRP:CZ3	2.54	0.43
1:DA:219:THR:HG22	1:DA:222:SER:OG	2.19	0.43
1:EA:138:VAL:HG21	1:EA:181:MET:SD	2.59	0.43
1:EB:403:TRP:HZ2	1:EB:450:ASP:HB2	1.83	0.43
1:FA:43:GLY:HA3	1:FA:214:PHE:CE1	2.54	0.43
1:FC:280:PRO:HA	1:FC:283:ILE:HD11	2.01	0.43
1:GB:66:VAL:HG21	1:GB:119:ILE:HD11	2.01	0.43
1:GB:101:GLY:HA3	1:GB:210:PHE:HA	2.01	0.43
1:GB:471:ASP:OD1	1:GB:471:ASP:N	2.52	0.43
1:GC:233:THR:HG22	1:GC:235:GLU:N	2.34	0.43
1:GC:259:VAL:HG13	1:GC:403:TRP:CZ3	2.54	0.43
1:HB:23:ASN:HB3	1:HB:150:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:435:ARG:NH1	1:IB:448:ASN:HB3	2.34	0.43
1:MA:144:ILE:O	1:MA:144:ILE:HG13	2.19	0.43
1:MB:230:PRO:HG2	1:MB:457:TRP:CD1	2.54	0.43
1:NA:140:MET:HG2	1:OA:57:VAL:HG21	2.00	0.43
1:OA:53:ARG:O	1:OA:205:ARG:HD2	2.19	0.43
1:OA:81:LEU:HD11	1:OA:102:GLY:HA2	2.00	0.43
1:OA:422:VAL:HG12	1:OA:431:LEU:HD21	2.01	0.43
1:AA:280:PRO:HA	1:AA:283:ILE:HD11	2.00	0.43
1:DA:78:SER:HA	1:DA:178:LEU:O	2.18	0.43
1:EB:195:VAL:O	1:EB:195:VAL:HG12	2.19	0.43
1:EC:118:LYS:H	1:EC:184:THR:HB	1.82	0.43
1:FA:96:TYR:HA	1:FA:214:PHE:O	2.19	0.43
1:FA:307:ASN:O	1:FA:309:ASN:N	2.52	0.43
1:FA:319:ALA:HB1	1:FA:320:PRO:HD2	2.00	0.43
1:HC:134:SER:OG	1:HC:137:GLN:HG3	2.19	0.43
1:HC:311:TYR:CZ	1:HC:320:PRO:HD3	2.54	0.43
1:HC:469:GLN:HB2	1:HC:520:TRP:CD1	2.54	0.43
1:IB:317:ILE:CG2	1:IB:318:PRO:HD2	2.49	0.43
1:IC:317:ILE:HD12	1:IC:319:ALA:O	2.19	0.43
1:JA:216:VAL:CG2	1:JA:217:PRO:HD2	2.48	0.43
1:JC:399:GLU:HB2	1:JC:400:PRO:HD3	2.01	0.43
1:JC:434:PHE:CD2	1:JC:454:PRO:HD3	2.54	0.43
1:LA:265:ARG:HG3	1:LA:273:LEU:HD12	2.01	0.43
1:LB:374:ASP:O	1:LB:375:LEU:HD23	2.19	0.43
1:LC:403:TRP:HZ2	1:LC:450:ASP:HB2	1.83	0.43
1:MB:146:VAL:HG11	1:MB:154:VAL:HG21	2.01	0.43
1:NB:57:VAL:HG23	1:NB:87:PRO:HD2	2.01	0.43
1:NB:440:GLY:O	1:OA:335:THR:HG23	2.18	0.43
1:OB:471:ASP:OD1	1:OB:471:ASP:N	2.49	0.43
1:AC:57:VAL:HA	1:GB:139:THR:CG2	2.49	0.42
1:AC:94:ARG:NH1	1:AC:225:LYS:HA	2.34	0.42
1:CA:64:PHE:HB3	1:CA:77:TRP:CD1	2.53	0.42
1:DA:434:PHE:CE1	1:DA:454:PRO:HD3	2.53	0.42
1:DB:245:PRO:O	1:DB:436:SER:OG	2.30	0.42
1:FA:44:GLN:HE22	1:FA:215:LEU:HB2	1.83	0.42
1:FA:57:VAL:CG2	1:JA:140:MET:HG2	2.49	0.42
1:FA:233:THR:HG22	1:FA:235:GLU:N	2.32	0.42
1:FB:344:THR:O	1:GA:442:SER:HA	2.19	0.42
1:IB:61:GLY:HA2	1:IB:520:TRP:O	2.19	0.42
1:KA:219:THR:HG22	1:KA:222:SER:OG	2.19	0.42
1:KB:317:ILE:HD13	1:KB:321:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:327:VAL:HA	1:KB:353:THR:OG1	2.19	0.42
1:KC:217:PRO:HA	1:KC:218:PRO:HD3	1.64	0.42
1:MA:216:VAL:HG21	1:MC:128:PHE:CD2	2.54	0.42
1:MC:148:VAL:CG1	1:MC:198:VAL:HG21	2.49	0.42
1:NA:145:ILE:HD13	1:NA:183:TYR:CE2	2.54	0.42
1:OA:34:GLY:HA3	1:OA:209:ASP:O	2.19	0.42
1:OA:318:PRO:HD3	1:OA:417:HIS:O	2.18	0.42
1:OB:307:ASN:O	1:OB:308:TRP:HB2	2.19	0.42
1:BA:109:LEU:HD22	1:BA:200:CYS:SG	2.60	0.42
1:BC:44:GLN:NE2	1:BC:215:LEU:HD23	2.34	0.42
1:CC:182:LEU:HD21	1:CC:185:PRO:HA	2.01	0.42
1:DA:247:GLU:HG2	1:DA:248:LYS:HE3	2.01	0.42
1:DA:422:VAL:HG12	1:DA:431:LEU:HD21	2.01	0.42
1:EC:265:ARG:NH2	1:EC:420:PRO:O	2.48	0.42
1:EC:473:ALA:HB2	1:EC:520:TRP:CZ3	2.54	0.42
1:FA:125:PRO:HG3	1:FB:214:PHE:CD1	2.54	0.42
1:FB:61:GLY:HA2	1:FB:520:TRP:O	2.19	0.42
1:FB:109:LEU:HD23	1:FB:200:CYS:SG	2.58	0.42
1:FB:246:LEU:HD11	1:FB:454:PRO:HB3	2.01	0.42
1:GA:373:ASN:OD1	1:GA:373:ASN:N	2.51	0.42
1:HA:456:GLU:OE1	1:HA:456:GLU:N	2.51	0.42
1:HB:476:ARG:HD3	1:HB:485:VAL:HG11	2.02	0.42
1:HC:280:PRO:HB3	1:HC:455:GLN:HG2	2.00	0.42
1:IB:311:TYR:OH	1:IB:320:PRO:HD3	2.19	0.42
1:JA:374:ASP:O	1:JA:375:LEU:HD23	2.19	0.42
1:KA:267:THR:HG23	1:KA:493:LYS:O	2.19	0.42
1:KB:137:GLN:HA	1:KB:140:MET:HE3	2.01	0.42
1:MB:372:ASN:OD1	1:MB:372:ASN:N	2.52	0.42
1:MC:260:GLN:N	1:MC:261:PRO:HD3	2.34	0.42
1:NB:230:PRO:HG2	1:NB:457:TRP:CD1	2.54	0.42
1:NC:130:THR:O	1:NC:133:LEU:HD23	2.19	0.42
1:NC:217:PRO:HA	1:NC:218:PRO:HD3	1.87	0.42
1:AB:121:PHE:HA	1:AB:179:ILE:O	2.20	0.42
1:AC:329:LYS:HA	1:AC:351:VAL:O	2.18	0.42
1:AC:440:GLY:O	1:GC:335:THR:HG23	2.19	0.42
1:BC:434:PHE:CD2	1:BC:454:PRO:HD3	2.54	0.42
1:BC:481:ASP:OD1	1:BC:512:ASN:ND2	2.51	0.42
1:DA:328:GLY:H	1:DA:353:THR:HB	1.83	0.42
1:DB:34:GLY:HA3	1:DB:209:ASP:HB2	2.01	0.42
1:DB:509:ILE:HG22	1:DB:510:PRO:O	2.20	0.42
1:EA:81:LEU:HD11	1:EA:102:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:290:VAL:HG22	1:EB:299:TYR:HB3	2.01	0.42
1:EB:488:GLU:HG3	1:EB:527:LEU:HD22	2.02	0.42
1:EC:101:GLY:HA3	1:EC:210:PHE:HA	2.00	0.42
1:FA:65:THR:HG22	1:FA:525:TYR:HA	2.02	0.42
1:FA:87:PRO:HG2	1:JA:140:MET:HE3	2.00	0.42
1:GB:440:GLY:O	1:HA:335:THR:HG23	2.18	0.42
1:GC:225:LYS:HA	1:GC:226:PRO:HD3	1.93	0.42
1:HA:143:HIS:HE1	1:IA:56:PHE:O	2.02	0.42
1:HC:94:ARG:NH1	1:HC:226:PRO:HD3	2.34	0.42
1:JB:223:ARG:HA	1:JB:467:PRO:HG3	2.01	0.42
1:JC:265:ARG:NH2	1:JC:420:PRO:O	2.48	0.42
1:KA:144:ILE:HD13	1:KA:156:ILE:HG12	2.00	0.42
1:NC:123:ALA:HB1	1:NC:176:ILE:HD11	2.01	0.42
1:OB:97:ASN:HB3	1:OB:214:PHE:HB3	2.02	0.42
1:OB:223:ARG:HA	1:OB:467:PRO:HG3	2.00	0.42
1:BC:326:PHE:CZ	1:BC:330:ILE:HD11	2.54	0.42
1:CB:319:ALA:HB1	1:CB:320:PRO:HD2	2.01	0.42
1:CC:313:PRO:HB3	1:CC:361:LYS:O	2.19	0.42
1:DB:19:VAL:HG13	1:DB:149:ARG:O	2.20	0.42
1:DC:121:PHE:HA	1:DC:179:ILE:O	2.20	0.42
1:DC:257:PHE:CD2	1:DC:403:TRP:CD1	3.08	0.42
1:FA:120:ILE:HD11	1:FA:183:TYR:CD1	2.53	0.42
1:JC:33:VAL:HG11	1:JC:37:ILE:HB	2.01	0.42
1:JC:46:ASN:HD21	1:JC:213:ILE:C	2.21	0.42
1:KC:416:VAL:HG12	1:KC:417:HIS:N	2.34	0.42
1:MA:69:ARG:O	1:NA:484:ARG:NH2	2.45	0.42
1:MA:337:THR:HA	1:MA:343:SER:O	2.19	0.42
1:MA:353:THR:CG2	1:MA:406:PRO:HB3	2.49	0.42
1:MB:66:VAL:HG21	1:MB:119:ILE:HD11	2.00	0.42
1:MC:434:PHE:CD2	1:MC:454:PRO:HD3	2.53	0.42
1:NA:109:LEU:HD22	1:NA:200:CYS:SG	2.60	0.42
1:NA:371:THR:HG22	1:NA:373:ASN:H	1.84	0.42
1:OB:429:GLU:HB3	1:OB:498:THR:CG2	2.49	0.42
1:OC:338:THR:OG1	1:OC:345:ARG:NH2	2.41	0.42
1:AC:311:TYR:CZ	1:AC:320:PRO:HD3	2.54	0.42
1:BA:115:THR:HG22	1:BA:148:VAL:CG2	2.50	0.42
1:DA:325:ASP:OD1	1:DA:325:ASP:N	2.52	0.42
1:DC:329:LYS:HA	1:DC:351:VAL:O	2.20	0.42
1:FB:51:TRP:HB3	1:GA:215:LEU:HD12	2.02	0.42
1:FC:144:ILE:HG22	1:FC:146:VAL:HG23	2.00	0.42
1:GA:140:MET:HG2	1:HA:57:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:319:ALA:HB1	1:GC:320:PRO:HD2	2.01	0.42
1:HB:501:HIS:CE1	1:HB:531:GLY:HA3	2.54	0.42
1:HC:148:VAL:HG13	1:HC:198:VAL:HG21	2.00	0.42
1:JB:124:VAL:HG22	1:JB:177:LYS:HB2	2.00	0.42
1:JC:246:LEU:HA	1:JC:436:SER:HB3	2.00	0.42
1:KA:435:ARG:HH12	1:KA:448:ASN:HB3	1.85	0.42
1:KB:222:SER:OG	1:KB:223:ARG:N	2.52	0.42
1:LA:30:GLU:HG3	1:MA:51:TRP:CZ2	2.55	0.42
1:LA:216:VAL:CG2	1:LA:217:PRO:HD2	2.46	0.42
1:MB:476:ARG:HD3	1:MB:485:VAL:HG11	2.01	0.42
1:NB:282:ASN:OD1	1:NB:287:ARG:NH2	2.49	0.42
1:NB:336:GLN:NE2	1:NB:379:GLN:HB2	2.34	0.42
1:NC:267:THR:HG22	1:NC:271:VAL:N	2.26	0.42
1:OA:282:ASN:OD1	1:OA:287:ARG:NH2	2.50	0.42
1:OC:158:LEU:HD12	1:OC:158:LEU:HA	1.88	0.42
1:BB:471:ASP:N	1:BB:471:ASP:OD1	2.52	0.42
1:BC:267:THR:HG22	1:BC:271:VAL:N	2.33	0.42
1:CA:64:PHE:HB3	1:CA:77:TRP:HD1	1.85	0.42
1:CA:459:LEU:O	1:CA:463:GLN:HG3	2.19	0.42
1:CB:390:GLN:HA	1:CB:399:GLU:OE1	2.20	0.42
1:DA:241:ARG:HG3	1:DA:451:CYS:HB3	2.02	0.42
1:FC:261:PRO:HG3	1:FC:403:TRP:HZ3	1.85	0.42
1:GC:389:VAL:HG23	1:GC:442:SER:HB3	2.02	0.42
1:HA:233:THR:HG21	1:HA:511:PRO:O	2.19	0.42
1:IC:246:LEU:HD13	1:IC:434:PHE:HB3	2.00	0.42
1:JB:403:TRP:CZ2	1:JB:450:ASP:HB2	2.55	0.42
1:JC:260:GLN:N	1:JC:261:PRO:HD3	2.35	0.42
1:LA:223:ARG:HH22	1:LA:269:ASP:HB2	1.85	0.42
1:LB:61:GLY:HA2	1:LB:520:TRP:O	2.19	0.42
1:MA:30:GLU:HG3	1:NA:51:TRP:CZ2	2.54	0.42
1:AB:105:VAL:CG2	1:AB:156:ILE:HB	2.49	0.42
1:AB:403:TRP:CZ2	1:AB:450:ASP:HB2	2.55	0.42
1:BA:219:THR:HG22	1:BA:222:SER:OG	2.19	0.42
1:BC:197:THR:O	1:KB:187:ARG:HG2	2.20	0.42
1:EB:106:GLN:HG3	1:EB:153:PRO:HB3	2.01	0.42
1:FB:135:PRO:HA	1:FB:181:MET:HE3	1.99	0.42
1:FB:190:ASN:HB2	1:GC:189:ASN:HD21	1.85	0.42
1:GA:341:ASP:OD1	1:GA:341:ASP:N	2.44	0.42
1:HB:66:VAL:HG21	1:HB:119:ILE:HD11	2.02	0.42
1:LB:437:THR:HG23	1:LB:447:MET:HB3	2.01	0.42
1:LC:267:THR:HG22	1:LC:271:VAL:N	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LC:377:THR:HG22	1:LC:378:GLY:N	2.35	0.42
1:NB:105:VAL:CG2	1:NB:156:ILE:HB	2.50	0.42
1:OA:144:ILE:O	1:OA:144:ILE:HG13	2.19	0.42
1:OB:94:ARG:HD3	1:OB:226:PRO:HD3	2.01	0.42
1:OC:72:PRO:HA	1:OC:182:LEU:O	2.20	0.42
1:OC:109:LEU:HD13	1:OC:200:CYS:SG	2.59	0.42
1:CA:149:ARG:NH2	1:DA:149:ARG:O	2.46	0.42
1:CC:279:SER:HB3	1:CC:282:ASN:HB2	2.01	0.42
1:DA:143:HIS:HE1	1:EA:56:PHE:O	2.02	0.42
1:DC:308:TRP:CH2	1:DC:380:ASN:HB3	2.54	0.42
1:DC:443:GLY:C	1:DC:444:TYR:HD1	2.23	0.42
1:GB:267:THR:HG22	1:GB:271:VAL:N	2.34	0.42
1:IB:440:GLY:O	1:JA:335:THR:HG23	2.20	0.42
1:IB:482:THR:HG22	1:JC:426:PHE:CD1	2.53	0.42
1:IC:326:PHE:CZ	1:IC:330:ILE:HD11	2.55	0.42
1:IC:359:THR:HB	1:IC:362:LEU:HD12	2.02	0.42
1:JA:371:THR:HG21	1:JA:374:ASP:HB2	2.01	0.42
1:JC:34:GLY:HA3	1:JC:209:ASP:HB2	2.02	0.42
1:KB:403:TRP:CZ2	1:KB:450:ASP:HB2	2.55	0.42
1:MA:280:PRO:HB3	1:MA:455:GLN:HG2	2.01	0.42
1:MC:135:PRO:HA	1:MC:181:MET:HE3	2.01	0.42
1:NC:390:GLN:HG2	1:NC:399:GLU:CG	2.49	0.42
1:OA:339:ARG:H	1:OA:339:ARG:HG2	1.70	0.42
1:OB:118:LYS:H	1:OB:184:THR:HB	1.84	0.42
1:OC:260:GLN:N	1:OC:261:PRO:HD3	2.34	0.42
1:OC:268:THR:HG21	1:OC:520:TRP:CH2	2.44	0.42
1:BA:29:LEU:HD23	1:BA:29:LEU:HA	1.81	0.42
1:BC:148:VAL:CG1	1:BC:198:VAL:HG21	2.50	0.42
1:CB:66:VAL:HG12	1:CB:186:LEU:HB2	2.01	0.42
1:DB:244:ILE:HD13	1:DB:244:ILE:HG21	1.84	0.42
1:FC:242:PHE:CD2	1:FC:244:ILE:HD11	2.55	0.42
1:GA:430:GLN:HG3	1:GA:501:HIS:O	2.20	0.42
1:HA:134:SER:OG	1:HA:137:GLN:HG3	2.19	0.42
1:HB:124:VAL:HG12	1:HB:141:PHE:CD2	2.55	0.42
1:HB:298:ASP:OD1	1:HB:368:THR:HG22	2.20	0.42
1:HC:120:ILE:HG13	1:HC:183:TYR:HB2	2.01	0.42
1:HC:267:THR:HG22	1:HC:271:VAL:N	2.32	0.42
1:IC:241:ARG:NH1	1:IC:450:ASP:O	2.48	0.42
1:JC:347:HIS:CE1	1:JC:374:ASP:HB3	2.55	0.42
1:KB:230:PRO:HG2	1:KB:457:TRP:CD1	2.54	0.42
1:LA:337:THR:HA	1:LA:343:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:435:ARG:NH1	1:LA:448:ASN:HB3	2.35	0.42
1:LC:70:ASN:HB3	1:LC:182:LEU:HD22	2.02	0.42
1:MC:325:ASP:OD1	1:MC:325:ASP:N	2.53	0.42
1:MC:469:GLN:HB2	1:MC:520:TRP:CG	2.55	0.42
1:AC:121:PHE:HA	1:AC:179:ILE:O	2.20	0.42
1:AC:148:VAL:CG1	1:AC:198:VAL:HG21	2.50	0.42
1:CB:432:LEU:HB2	1:CB:499:VAL:HG13	2.01	0.42
1:CC:480:PRO:HG3	1:CC:514:TYR:CD1	2.54	0.42
1:EA:233:THR:HG21	1:EA:511:PRO:O	2.20	0.42
1:EC:24:ASN:O	1:EC:25:GLU:HB3	2.20	0.42
1:EC:150:GLN:NE2	1:EC:154:VAL:HG22	2.35	0.42
1:EC:486:LEU:HD11	1:EC:510:PRO:HG3	2.02	0.42
1:FC:71:ALA:HB3	1:JB:485:VAL:HB	2.02	0.42
1:GB:32:VAL:HB	1:GB:159:PRO:HB2	2.02	0.42
1:GB:217:PRO:HA	1:GB:218:PRO:HD3	1.73	0.42
1:HA:144:ILE:HG13	1:HA:144:ILE:O	2.20	0.42
1:IB:305:SER:HB3	1:IB:309:ASN:H	1.84	0.42
1:IB:433:PHE:HB3	1:IB:450:ASP:HB3	2.02	0.42
1:KB:58:GLN:H	1:LC:139:THR:HG21	1.85	0.42
1:KB:280:PRO:HB3	1:KB:455:GLN:HG2	2.02	0.42
1:MB:94:ARG:O	1:MB:218:PRO:HA	2.20	0.42
1:OB:42:ALA:HB1	1:OB:213:ILE:HG23	2.02	0.42
1:OB:233:THR:HG22	1:OB:235:GLU:H	1.85	0.42
1:OB:259:VAL:HG13	1:OB:403:TRP:CZ3	2.55	0.42
1:AA:233:THR:HG22	1:AA:235:GLU:N	2.34	0.41
1:AA:325:ASP:OD1	1:AA:325:ASP:N	2.54	0.41
1:BB:231:ILE:HD11	1:CA:220:VAL:HG11	2.02	0.41
1:CA:116:ALA:O	1:CA:186:LEU:HD12	2.20	0.41
1:CC:426:PHE:HD2	1:CC:429:GLU:OE2	2.02	0.41
1:FC:46:ASN:ND2	1:FC:213:ILE:C	2.73	0.41
1:GA:318:PRO:HD3	1:GA:417:HIS:O	2.20	0.41
1:GB:501:HIS:CE1	1:GB:531:GLY:HA3	2.55	0.41
1:HA:301:MET:O	1:HA:364:SER:HA	2.20	0.41
1:IB:399:GLU:HB3	1:IB:400:PRO:HD3	2.02	0.41
1:JA:219:THR:HG22	1:JA:222:SER:OG	2.20	0.41
1:JA:326:PHE:O	1:JA:353:THR:HG21	2.20	0.41
1:JB:57:VAL:HG23	1:JB:87:PRO:HD2	2.01	0.41
1:KB:454:PRO:HG2	1:KB:457:TRP:CD1	2.55	0.41
1:LC:120:ILE:HG13	1:LC:183:TYR:HB2	2.02	0.41
1:NB:359:THR:HG22	1:NB:410:GLY:HA3	2.01	0.41
1:AA:317:ILE:HG22	1:AA:318:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BC:134:SER:OG	1:BC:137:GLN:HG3	2.20	0.41
1:BC:469:GLN:HB2	1:BC:520:TRP:CG	2.55	0.41
1:CB:124:VAL:CG2	1:CB:177:LYS:HB2	2.50	0.41
1:DA:242:PHE:CZ	1:DA:385:PRO:HB2	2.55	0.41
1:DC:287:ARG:HB3	1:DC:308:TRP:CH2	2.55	0.41
1:EC:32:VAL:HB	1:EC:159:PRO:HB2	2.02	0.41
1:EC:241:ARG:HH12	1:EC:402:GLN:HG3	1.85	0.41
1:EC:318:PRO:HG3	1:EC:417:HIS:O	2.19	0.41
1:FB:57:VAL:HG23	1:FB:87:PRO:HD2	2.02	0.41
1:FB:261:PRO:HG2	1:FB:265:ARG:HD3	2.02	0.41
1:GB:318:PRO:HB3	1:GB:418:LEU:HD23	2.02	0.41
1:HA:434:PHE:CE1	1:HA:454:PRO:HD3	2.55	0.41
1:JC:213:ILE:HG23	1:JC:214:PHE:N	2.36	0.41
1:KB:306:GLN:CD	1:KB:306:GLN:H	2.23	0.41
1:LB:230:PRO:HD3	1:LB:460:HIS:CD2	2.55	0.41
1:MA:305:SER:HB3	1:MA:309:ASN:H	1.84	0.41
1:NC:329:LYS:HA	1:NC:351:VAL:O	2.19	0.41
1:OA:119:ILE:HD13	1:OA:182:LEU:HD23	2.01	0.41
1:OA:219:THR:HG22	1:OA:222:SER:OG	2.20	0.41
1:OB:24:ASN:OD1	1:OB:25:GLU:N	2.53	0.41
1:AB:223:ARG:HA	1:AB:467:PRO:HG3	2.02	0.41
1:AB:435:ARG:NH1	1:AB:450:ASP:OD1	2.54	0.41
1:AC:319:ALA:HB1	1:AC:320:PRO:HD2	2.01	0.41
1:BA:301:MET:O	1:BA:364:SER:HA	2.19	0.41
1:BB:191:ALA:HB3	1:OB:191:ALA:HB3	2.02	0.41
1:BC:121:PHE:HA	1:BC:179:ILE:O	2.21	0.41
1:DA:284:CYS:SG	1:DA:324:PRO:HG3	2.60	0.41
1:FB:231:ILE:CD1	1:GA:220:VAL:HG11	2.48	0.41
1:GA:435:ARG:HH12	1:GA:448:ASN:HB3	1.85	0.41
1:IC:148:VAL:CG1	1:IC:198:VAL:HG21	2.51	0.41
1:JC:144:ILE:HG22	1:JC:146:VAL:HG23	2.01	0.41
1:JC:249:LEU:HD21	1:JC:515:PHE:HZ	1.84	0.41
1:KA:96:TYR:CG	1:KA:212:PHE:HB3	2.55	0.41
1:KA:185:PRO:HB2	1:KA:187:ARG:NH1	2.35	0.41
1:KA:266:CYS:HB2	1:KA:458:VAL:HG13	2.01	0.41
1:KB:482:THR:HG21	1:LC:427:PRO:CD	2.51	0.41
1:LA:117:GLY:O	1:LA:148:VAL:HG22	2.20	0.41
1:LB:267:THR:HG22	1:LB:271:VAL:N	2.32	0.41
1:LC:179:ILE:HA	1:LC:179:ILE:HD13	1.81	0.41
1:LC:489:CYS:HB3	1:LC:499:VAL:HG12	2.02	0.41
1:MB:124:VAL:HG22	1:MB:177:LYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MC:33:VAL:HG11	1:MC:37:ILE:HB	2.01	0.41
1:OA:115:THR:HG22	1:OA:148:VAL:CG2	2.50	0.41
1:OA:435:ARG:NH1	1:OA:448:ASN:HB3	2.36	0.41
1:OB:327:VAL:HA	1:OB:353:THR:OG1	2.21	0.41
1:BA:242:PHE:O	1:BA:244:ILE:N	2.52	0.41
1:BA:275:THR:HG23	1:BA:318:PRO:HG2	2.03	0.41
1:BC:335:THR:O	1:BC:381:THR:HA	2.20	0.41
1:CC:217:PRO:HA	1:CC:218:PRO:HD3	1.86	0.41
1:DA:233:THR:HG21	1:DA:511:PRO:O	2.20	0.41
1:DB:390:GLN:HB2	1:DB:445:PRO:HB3	2.02	0.41
1:DC:327:VAL:HA	1:DC:353:THR:OG1	2.20	0.41
1:EA:328:GLY:H	1:EA:353:THR:HB	1.86	0.41
1:EB:105:VAL:CG2	1:EB:156:ILE:HB	2.51	0.41
1:GB:293:ILE:HD13	1:GB:293:ILE:HA	1.92	0.41
1:HA:216:VAL:HG23	1:HC:141:PHE:CE1	2.55	0.41
1:HA:438:MET:O	1:HA:447:MET:HG2	2.20	0.41
1:HB:267:THR:HG22	1:HB:271:VAL:N	2.27	0.41
1:IB:66:VAL:HG12	1:IB:186:LEU:HB2	2.02	0.41
1:IB:217:PRO:HA	1:IB:218:PRO:HD3	1.96	0.41
1:IC:434:PHE:HE1	1:IC:515:PHE:HE2	1.67	0.41
1:JA:239:ASN:ND2	1:JA:436:SER:OG	2.40	0.41
1:JC:267:THR:HG22	1:JC:271:VAL:H	1.84	0.41
1:LA:144:ILE:O	1:LA:144:ILE:HG13	2.20	0.41
1:LB:454:PRO:HG2	1:LB:457:TRP:CG	2.55	0.41
1:MA:149:ARG:NH2	1:NA:149:ARG:O	2.51	0.41
1:MA:318:PRO:HD3	1:MA:417:HIS:O	2.20	0.41
1:MB:58:GLN:N	1:NC:139:THR:HG21	2.35	0.41
1:MB:403:TRP:CZ2	1:MB:450:ASP:HB2	2.56	0.41
1:MB:471:ASP:HA	1:MB:493:LYS:CD	2.50	0.41
1:NA:167:HIS:ND1	1:NA:173:ASP:OD2	2.49	0.41
1:OA:43:GLY:HA3	1:OA:214:PHE:CE1	2.56	0.41
1:OA:64:PHE:CG	1:OA:77:TRP:HB2	2.55	0.41
1:OA:216:VAL:CG2	1:OA:217:PRO:HD2	2.51	0.41
1:OB:32:VAL:HB	1:OB:159:PRO:HB2	2.02	0.41
1:OB:402:GLN:OE1	1:OB:449:LEU:HA	2.21	0.41
1:BA:53:ARG:HB3	1:BA:206:PRO:HG2	2.01	0.41
1:BA:216:VAL:CG2	1:BA:217:PRO:HD2	2.50	0.41
1:BB:403:TRP:HZ2	1:BB:450:ASP:HB2	1.85	0.41
1:BC:431:LEU:HD23	1:BC:498:THR:HG22	2.03	0.41
1:CB:167:HIS:ND1	1:CB:173:ASP:OD2	2.48	0.41
1:CB:509:ILE:HG22	1:CB:510:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:96:TYR:HA	1:DA:214:PHE:O	2.20	0.41
1:DA:244:ILE:HD13	1:DA:438:MET:HA	2.03	0.41
1:EB:34:GLY:HA3	1:EB:209:ASP:HB2	2.03	0.41
1:EC:158:LEU:HD13	1:EC:178:LEU:HG	2.02	0.41
1:EC:305:SER:HB2	1:EC:307:ASN:OD1	2.21	0.41
1:FC:37:ILE:HG22	1:FC:165:PHE:CD1	2.54	0.41
1:GA:307:ASN:O	1:GA:308:TRP:HB2	2.20	0.41
1:GB:134:SER:OG	1:GB:137:GLN:HG3	2.21	0.41
1:GB:146:VAL:HG11	1:GB:154:VAL:HG21	2.03	0.41
1:GB:402:GLN:OE1	1:GB:449:LEU:HA	2.21	0.41
1:GC:257:PHE:CE2	1:GC:403:TRP:CD1	3.08	0.41
1:IB:403:TRP:CZ2	1:IB:450:ASP:HB2	2.55	0.41
1:JA:144:ILE:O	1:JA:144:ILE:HG13	2.21	0.41
1:JC:130:THR:O	1:JC:133:LEU:HD23	2.20	0.41
1:KB:65:THR:HG23	1:KB:525:TYR:CE1	2.56	0.41
1:LA:96:TYR:CG	1:LA:212:PHE:HB3	2.55	0.41
1:MA:64:PHE:CG	1:MA:77:TRP:HB2	2.55	0.41
1:MA:434:PHE:CE1	1:MA:454:PRO:HD3	2.55	0.41
1:NA:343:SER:HB3	1:NA:345:ARG:HH12	1.86	0.41
1:OB:170:GLN:HE21	1:OB:221:GLU:HB3	1.85	0.41
1:AB:60:PRO:HD3	1:AB:87:PRO:HD3	2.03	0.41
1:AB:139:THR:HG22	1:GC:57:VAL:HA	2.02	0.41
1:CA:145:ILE:HD13	1:CA:183:TYR:CE2	2.56	0.41
1:DA:40:PRO:HB2	1:DC:37:ILE:HD11	2.02	0.41
1:DA:53:ARG:HB3	1:DA:206:PRO:HG2	2.01	0.41
1:DC:443:GLY:O	1:DC:444:TYR:HD1	2.02	0.41
1:FA:390:GLN:HB3	1:FA:444:TYR:H	1.86	0.41
1:GC:308:TRP:CH2	1:GC:380:ASN:HB3	2.56	0.41
1:HB:124:VAL:HG22	1:HB:177:LYS:HB2	2.02	0.41
1:HC:391:ASP:H	1:HC:399:GLU:HG3	1.86	0.41
1:IC:395:ALA:HB3	1:IC:398:ASN:ND2	2.35	0.41
1:JB:403:TRP:HZ2	1:JB:450:ASP:HB2	1.85	0.41
1:KA:57:VAL:CG2	1:OA:140:MET:HG2	2.50	0.41
1:KB:471:ASP:OD1	1:KB:471:ASP:N	2.54	0.41
1:LA:76:LEU:C	1:LA:522:ASN:HD21	2.24	0.41
1:LB:254:SER:HA	1:LB:257:PHE:CE1	2.55	0.41
1:LB:477:PHE:CE2	1:LB:509:ILE:HD12	2.55	0.41
1:LC:325:ASP:N	1:LC:325:ASP:OD1	2.52	0.41
1:MA:105:VAL:CG1	1:MA:156:ILE:HB	2.51	0.41
1:NB:32:VAL:HG13	1:NC:41:VAL:HA	2.03	0.41
1:NC:277:GLN:HB3	1:NC:321:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NC:426:PHE:HZ	1:NC:523:GLN:O	2.03	0.41
1:OC:134:SER:OG	1:OC:137:GLN:HG3	2.20	0.41
1:AB:238:THR:HA	1:AB:245:PRO:HA	2.02	0.41
1:AB:286:PHE:HB3	1:AB:301:MET:HE2	2.02	0.41
1:BB:66:VAL:HG21	1:BB:119:ILE:HD11	2.01	0.41
1:BB:490:LYS:HG3	1:BB:527:LEU:HD21	2.02	0.41
1:BC:249:LEU:HB3	1:BC:507:LEU:HD12	2.03	0.41
1:CB:359:THR:HG22	1:CB:410:GLY:HA3	2.03	0.41
1:DA:108:ILE:HG12	1:DA:153:PRO:HB3	2.02	0.41
1:DA:456:GLU:OE1	1:DA:456:GLU:N	2.52	0.41
1:DB:403:TRP:CZ2	1:DB:450:ASP:HB2	2.56	0.41
1:EA:140:MET:HB2	1:EB:217:PRO:HG3	2.02	0.41
1:EB:94:ARG:HG2	1:EB:224:THR:HB	2.03	0.41
1:EC:371:THR:HG22	1:EC:373:ASN:H	1.85	0.41
1:FA:371:THR:CG2	1:FA:374:ASP:H	2.34	0.41
1:FB:449:LEU:HA	1:FB:449:LEU:HD12	1.89	0.41
1:GB:454:PRO:HG2	1:GB:457:TRP:CD1	2.55	0.41
1:JC:98:GLY:N	1:JC:213:ILE:HG22	2.36	0.41
1:JC:217:PRO:HA	1:JC:218:PRO:HD3	1.85	0.41
1:KB:317:ILE:HG22	1:KB:318:PRO:HD2	2.02	0.41
1:KC:259:VAL:HG13	1:KC:403:TRP:CZ3	2.56	0.41
1:LB:395:ALA:HB3	1:LB:398:ASN:HD22	1.85	0.41
1:LB:440:GLY:O	1:MA:335:THR:HG23	2.21	0.41
1:NA:433:PHE:HB3	1:NA:450:ASP:HB3	2.01	0.41
1:NB:233:THR:HB	1:NB:236:GLU:HG3	2.03	0.41
1:NC:403:TRP:CZ2	1:NC:450:ASP:HB2	2.56	0.41
1:OB:134:SER:OG	1:OB:137:GLN:HG3	2.21	0.41
1:OB:471:ASP:HA	1:OB:493:LYS:CD	2.49	0.41
1:AC:484:ARG:HH11	1:AC:486:LEU:HD23	1.86	0.41
1:CB:116:ALA:N	1:CB:187:ARG:O	2.49	0.41
1:DC:509:ILE:HG22	1:DC:510:PRO:O	2.20	0.41
1:EA:64:PHE:CG	1:EA:77:TRP:HB2	2.56	0.41
1:EA:315:GLU:HB3	1:EA:317:ILE:HG13	2.02	0.41
1:FB:242:PHE:HD1	1:FB:284:CYS:HG	1.64	0.41
1:GA:69:ARG:O	1:HA:484:ARG:NH2	2.50	0.41
1:GB:121:PHE:HA	1:GB:179:ILE:O	2.19	0.41
1:HB:118:LYS:H	1:HB:184:THR:HB	1.86	0.41
1:IA:399:GLU:HB3	1:IA:400:PRO:HD3	2.02	0.41
1:IC:371:THR:HG21	1:IC:374:ASP:HB3	2.03	0.41
1:JA:64:PHE:CG	1:JA:77:TRP:HB2	2.56	0.41
1:JA:266:CYS:HB2	1:JA:458:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:299:TYR:CE2	1:JA:375:LEU:HB2	2.55	0.41
1:JB:96:TYR:CG	1:JB:212:PHE:HB3	2.56	0.41
1:KB:267:THR:HG22	1:KB:271:VAL:N	2.29	0.41
1:LA:247:GLU:OE1	1:LA:437:THR:HG22	2.21	0.41
1:LC:46:ASN:HD21	1:LC:213:ILE:C	2.23	0.41
1:NA:216:VAL:CG2	1:NA:217:PRO:HD2	2.48	0.41
1:OA:43:GLY:HA3	1:OA:214:PHE:HE1	1.85	0.41
1:OC:25:GLU:CD	1:OC:25:GLU:H	2.23	0.41
1:AB:471:ASP:OD1	1:AB:522:ASN:HA	2.21	0.41
1:BA:399:GLU:HB3	1:BA:400:PRO:HD3	2.02	0.41
1:BB:105:VAL:CG2	1:BB:156:ILE:HB	2.51	0.41
1:BB:121:PHE:HA	1:BB:179:ILE:O	2.20	0.41
1:CB:51:TRP:HB3	1:DA:215:LEU:HD12	2.02	0.41
1:CB:501:HIS:CE1	1:CB:531:GLY:HA3	2.56	0.41
1:CC:178:LEU:HD23	1:CC:178:LEU:HA	1.87	0.41
1:DA:280:PRO:HA	1:DA:283:ILE:HD11	2.03	0.41
1:DB:137:GLN:HA	1:DB:140:MET:HE3	2.03	0.41
1:DB:329:LYS:HE2	1:DB:352:SER:HB2	2.03	0.41
1:DC:182:LEU:HD21	1:DC:185:PRO:HA	2.02	0.41
1:EB:125:PRO:HG3	1:EC:214:PHE:CD1	2.56	0.41
1:EC:78:SER:HA	1:EC:178:LEU:O	2.21	0.41
1:EC:406:PRO:HG2	1:EC:408:TYR:CE1	2.56	0.41
1:EC:414:HIS:O	1:EC:416:VAL:HG23	2.21	0.41
1:FA:115:THR:HG22	1:FA:148:VAL:CG2	2.51	0.41
1:FA:335:THR:HG23	1:JB:440:GLY:O	2.21	0.41
1:FB:19:VAL:HG13	1:FB:149:ARG:O	2.20	0.41
1:FB:267:THR:HG22	1:FB:271:VAL:N	2.34	0.41
1:GA:140:MET:HE3	1:HA:87:PRO:HG2	2.02	0.41
1:GA:242:PHE:O	1:GA:244:ILE:N	2.53	0.41
1:GB:94:ARG:HG2	1:GB:224:THR:HB	2.03	0.41
1:GB:250:PHE:CD2	1:GB:435:ARG:NH2	2.89	0.41
1:GC:121:PHE:HA	1:GC:179:ILE:O	2.20	0.41
1:HA:117:GLY:O	1:HA:148:VAL:HG22	2.21	0.41
1:HA:280:PRO:HA	1:HA:283:ILE:HD11	2.03	0.41
1:HB:344:THR:HG21	1:IA:440:GLY:HA3	2.02	0.41
1:IA:319:ALA:HB1	1:IA:320:PRO:HD2	2.03	0.41
1:IC:121:PHE:HA	1:IC:179:ILE:O	2.20	0.41
1:JA:422:VAL:HG12	1:JA:431:LEU:HD21	2.02	0.41
1:JB:81:LEU:HD11	1:JB:102:GLY:HA2	2.03	0.41
1:KA:459:LEU:O	1:KA:463:GLN:HG3	2.21	0.41
1:KB:77:TRP:HB3	1:KB:180:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:456:GLU:OE1	1:KB:456:GLU:N	2.51	0.41
1:LA:105:VAL:CG1	1:LA:156:ILE:HB	2.50	0.41
1:LB:293:ILE:HD13	1:LB:293:ILE:HA	1.94	0.41
1:LB:317:ILE:HG22	1:LB:318:PRO:HD2	2.03	0.41
1:MA:400:PRO:HG2	1:MA:446:ASN:O	2.21	0.41
1:MB:121:PHE:HB2	1:MB:144:ILE:CG2	2.50	0.41
1:NA:134:SER:OG	1:NA:137:GLN:HG3	2.20	0.41
1:NB:89:LEU:HD11	1:NB:206:PRO:HB3	2.03	0.41
1:OA:120:ILE:HD13	1:OA:138:VAL:HG12	2.02	0.41
1:OC:358:PHE:CZ	1:OC:360:PRO:HG3	2.56	0.41
1:AA:280:PRO:HB3	1:AA:455:GLN:HG2	2.03	0.41
1:AA:459:LEU:O	1:AA:463:GLN:HG3	2.21	0.41
1:AC:390:GLN:HG2	1:AC:399:GLU:CG	2.50	0.41
1:BA:318:PRO:HD3	1:BA:417:HIS:O	2.21	0.41
1:BB:435:ARG:NH1	1:BB:448:ASN:HB3	2.36	0.41
1:CA:242:PHE:O	1:CA:244:ILE:N	2.54	0.41
1:CC:233:THR:HG22	1:CC:235:GLU:H	1.86	0.41
1:DB:30:GLU:HG3	1:DC:44:GLN:HA	2.03	0.41
1:EC:148:VAL:CG1	1:EC:198:VAL:HG21	2.52	0.41
1:FB:248:LYS:HD2	1:FB:435:ARG:HD2	2.02	0.41
1:FB:439:PRO:CB	1:GA:335:THR:HG21	2.44	0.41
1:GB:244:ILE:HA	1:HA:281:VAL:HG11	2.03	0.41
1:HB:372:ASN:OD1	1:HB:372:ASN:N	2.53	0.41
1:HC:121:PHE:HA	1:HC:179:ILE:O	2.21	0.41
1:IC:434:PHE:CD2	1:IC:454:PRO:HD3	2.57	0.41
1:IC:477:PHE:HD2	1:IC:487:PHE:CE1	2.38	0.41
1:JA:341:ASP:OD1	1:JA:341:ASP:N	2.53	0.41
1:JC:331:GLN:HG2	1:JC:350:THR:OG1	2.21	0.41
1:KA:353:THR:CG2	1:KA:406:PRO:HB3	2.51	0.41
1:KA:353:THR:HG22	1:KA:406:PRO:HB3	2.03	0.41
1:KB:402:GLN:OE1	1:KB:449:LEU:HA	2.20	0.41
1:LA:109:LEU:HD22	1:LA:200:CYS:SG	2.61	0.41
1:LC:311:TYR:HE1	1:LC:320:PRO:HB3	1.86	0.41
1:LC:480:PRO:HG3	1:LC:514:TYR:CE1	2.55	0.41
1:MC:101:GLY:HA3	1:MC:210:PHE:HA	2.02	0.41
1:AA:187:ARG:NH2	1:BA:197:THR:O	2.54	0.40
1:AB:75:ILE:O	1:AB:522:ASN:ND2	2.54	0.40
1:AC:347:HIS:NE2	1:AC:374:ASP:HB3	2.36	0.40
1:BA:282:ASN:OD1	1:BA:287:ARG:NH2	2.53	0.40
1:CA:209:ASP:OD1	1:CA:209:ASP:N	2.53	0.40
1:CB:120:ILE:HD11	1:CB:183:TYR:CD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:403:TRP:CZ2	1:CB:450:ASP:HB2	2.55	0.40
1:CC:259:VAL:HG13	1:CC:403:TRP:CZ3	2.56	0.40
1:DA:48:ILE:HD12	1:DA:211:ASP:HA	2.03	0.40
1:FA:120:ILE:HD13	1:FA:120:ILE:HG21	1.79	0.40
1:FA:244:ILE:HD13	1:FA:438:MET:HA	2.03	0.40
1:FC:49:ASP:OD2	1:LC:46:ASN:HB3	2.20	0.40
1:GA:216:VAL:HG21	1:GC:128:PHE:CD1	2.56	0.40
1:GA:251:THR:HG22	1:GA:430:GLN:HE21	1.86	0.40
1:GB:227:PHE:CE1	1:GB:268:THR:HG23	2.56	0.40
1:HB:433:PHE:HB3	1:HB:450:ASP:HB3	2.02	0.40
1:IB:121:PHE:HA	1:IB:179:ILE:O	2.21	0.40
1:IB:233:THR:HG21	1:IB:511:PRO:O	2.21	0.40
1:JA:41:VAL:HA	1:JC:32:VAL:HG13	2.02	0.40
1:JB:454:PRO:HG2	1:JB:457:TRP:CD1	2.55	0.40
1:MB:124:VAL:CG2	1:MB:177:LYS:HB2	2.50	0.40
1:NA:89:LEU:HD12	1:NA:103:PHE:HE2	1.85	0.40
1:OA:341:ASP:N	1:OA:341:ASP:OD1	2.55	0.40
1:OA:400:PRO:HG2	1:OA:446:ASN:HB3	2.03	0.40
1:OB:66:VAL:HG21	1:OB:119:ILE:HD11	2.03	0.40
1:AA:225:LYS:HD3	1:AA:464:GLU:HG3	2.03	0.40
1:BB:286:PHE:HB3	1:BB:301:MET:HE2	2.03	0.40
1:BC:440:GLY:O	1:KC:335:THR:HG23	2.20	0.40
1:CA:117:GLY:O	1:CA:148:VAL:HG22	2.21	0.40
1:CA:124:VAL:HG23	1:CA:141:PHE:CE1	2.57	0.40
1:DB:51:TRP:HB3	1:EA:215:LEU:HD12	2.02	0.40
1:DB:440:GLY:O	1:EA:335:THR:HG23	2.21	0.40
1:DC:241:ARG:NE	1:DC:325:ASP:OD2	2.52	0.40
1:EA:216:VAL:CG2	1:EA:217:PRO:HD2	2.49	0.40
1:EC:242:PHE:O	1:EC:244:ILE:N	2.52	0.40
1:EC:395:ALA:HB3	1:EC:398:ASN:HD22	1.85	0.40
1:FA:433:PHE:HB3	1:FA:450:ASP:HB3	2.03	0.40
1:FB:282:ASN:OD1	1:FB:287:ARG:NH2	2.53	0.40
1:GA:144:ILE:CD1	1:GA:156:ILE:HG12	2.51	0.40
1:GC:146:VAL:HG13	1:GC:150:GLN:OE1	2.21	0.40
1:HB:233:THR:HG22	1:HB:235:GLU:H	1.85	0.40
1:HC:449:LEU:HD12	1:HC:449:LEU:HA	1.93	0.40
1:IA:435:ARG:HG3	1:IA:450:ASP:OD1	2.20	0.40
1:JA:353:THR:HG22	1:JA:406:PRO:HB3	2.03	0.40
1:KB:124:VAL:HG22	1:KB:177:LYS:HB2	2.03	0.40
1:LB:23:ASN:HB3	1:LB:150:GLN:NE2	2.36	0.40
1:MA:293:ILE:HD13	1:MA:293:ILE:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:399:GLU:HB3	1:NA:400:PRO:HD3	2.02	0.40
1:NB:471:ASP:N	1:NB:471:ASP:OD1	2.54	0.40
1:OB:96:TYR:CG	1:OB:212:PHE:HB3	2.56	0.40
1:AA:219:THR:HG22	1:AA:222:SER:OG	2.21	0.40
1:AB:432:LEU:HB2	1:AB:499:VAL:HG13	2.03	0.40
1:BB:244:ILE:HA	1:CA:281:VAL:HG11	2.04	0.40
1:CA:216:VAL:HG21	1:CC:128:PHE:CD1	2.56	0.40
1:CB:233:THR:HG22	1:CB:234:VAL:N	2.36	0.40
1:DA:65:THR:OG1	1:DA:197:THR:HG23	2.22	0.40
1:DA:371:THR:CG2	1:DA:374:ASP:H	2.35	0.40
1:DB:94:ARG:HH11	1:DB:94:ARG:HD2	1.78	0.40
1:DB:469:GLN:HG3	1:DB:520:TRP:NE1	2.36	0.40
1:DC:56:PHE:HB3	1:DC:203:LEU:HB3	2.03	0.40
1:DC:242:PHE:CD2	1:DC:243:PRO:HD2	2.57	0.40
1:EA:89:LEU:HD11	1:EA:206:PRO:HB3	2.03	0.40
1:FA:403:TRP:CZ2	1:FA:450:ASP:HB2	2.56	0.40
1:FB:191:ALA:CB	1:KB:191:ALA:HB3	2.51	0.40
1:FC:358:PHE:CZ	1:FC:360:PRO:HG3	2.56	0.40
1:GB:66:VAL:HG12	1:GB:186:LEU:HB2	2.04	0.40
1:GB:230:PRO:HD3	1:GB:460:HIS:CD2	2.57	0.40
1:GC:265:ARG:HA	1:GC:265:ARG:HD2	1.94	0.40
1:HA:124:VAL:HG13	1:HA:177:LYS:HB3	2.03	0.40
1:HA:216:VAL:CG2	1:HA:217:PRO:HD2	2.52	0.40
1:HC:178:LEU:HD23	1:HC:178:LEU:HA	1.88	0.40
1:IA:490:LYS:HE3	1:IA:527:LEU:HG	2.02	0.40
1:IB:179:ILE:HD13	1:IB:179:ILE:HA	1.97	0.40
1:JB:14:SER:O	1:JB:15:THR:OG1	2.31	0.40
1:JB:118:LYS:HD3	1:JB:147:ASP:HA	2.03	0.40
1:KB:201:ARG:HG3	1:LC:183:TYR:CE2	2.56	0.40
1:KC:179:ILE:HD13	1:KC:179:ILE:HA	1.83	0.40
1:KC:249:LEU:HD21	1:KC:515:PHE:HZ	1.87	0.40
1:LC:217:PRO:HA	1:LC:218:PRO:HD3	1.89	0.40
1:MC:57:VAL:HG11	1:MC:87:PRO:HD2	2.02	0.40
1:NA:65:THR:HG22	1:NA:525:TYR:HA	2.02	0.40
1:OC:336:GLN:NE2	1:OC:379:GLN:HB2	2.36	0.40
1:BA:403:TRP:CZ2	1:BA:450:ASP:HB2	2.56	0.40
1:BB:411:ARG:H	1:BB:411:ARG:HG2	1.72	0.40
1:BC:437:THR:HG23	1:BC:447:MET:HB3	2.03	0.40
1:CB:215:LEU:HD21	1:DA:52:ILE:HG12	2.02	0.40
1:CB:286:PHE:HB3	1:CB:301:MET:CE	2.51	0.40
1:CC:319:ALA:HB1	1:CC:320:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CC:459:LEU:O	1:CC:463:GLN:HG3	2.22	0.40
1:DA:118:LYS:HE2	1:EA:110:ALA:HA	2.03	0.40
1:DA:128:PHE:CE1	1:DA:141:PHE:HZ	2.39	0.40
1:DB:161:VAL:CG2	1:DB:176:ILE:HD11	2.51	0.40
1:EC:135:PRO:HA	1:EC:181:MET:HE1	2.04	0.40
1:FA:115:THR:HG23	1:FA:186:LEU:HD11	2.03	0.40
1:FB:94:ARG:HH11	1:FB:94:ARG:HD2	1.77	0.40
1:FC:38:ALA:O	1:FC:42:ALA:N	2.52	0.40
1:GB:306:GLN:H	1:GB:306:GLN:CD	2.24	0.40
1:HA:424:PRO:HD3	1:HA:431:LEU:CD1	2.51	0.40
1:HB:490:LYS:HG3	1:HB:527:LEU:HD11	2.04	0.40
1:IA:170:GLN:HG3	1:IC:127:ASN:O	2.22	0.40
1:IB:269:ASP:HB3	1:IB:467:PRO:HA	2.03	0.40
1:IC:148:VAL:HG13	1:IC:198:VAL:HG21	2.03	0.40
1:JB:433:PHE:HB3	1:JB:450:ASP:HB3	2.04	0.40
1:JC:53:ARG:O	1:JC:205:ARG:HD2	2.21	0.40
1:JC:390:GLN:HG2	1:JC:399:GLU:HG3	2.03	0.40
1:KA:48:ILE:HD11	1:KA:212:PHE:CD2	2.56	0.40
1:KA:51:TRP:CZ2	1:OA:30:GLU:HG3	2.57	0.40
1:KA:124:VAL:HG23	1:KA:141:PHE:CE1	2.56	0.40
1:KA:403:TRP:CZ2	1:KA:450:ASP:HB2	2.56	0.40
1:KB:432:LEU:HB2	1:KB:499:VAL:HG13	2.04	0.40
1:LB:395:ALA:HB3	1:LB:398:ASN:ND2	2.37	0.40
1:MA:96:TYR:CG	1:MA:212:PHE:HB3	2.56	0.40
1:MB:259:VAL:HG13	1:MB:403:TRP:CZ3	2.57	0.40
1:NA:29:LEU:HD23	1:NA:29:LEU:HA	1.78	0.40
1:NB:118:LYS:HD3	1:NB:147:ASP:HA	2.03	0.40
1:NB:471:ASP:OD1	1:NB:522:ASN:HA	2.22	0.40
1:OA:101:GLY:HA3	1:OA:210:PHE:HA	2.03	0.40
1:OB:101:GLY:HA3	1:OB:210:PHE:HA	2.02	0.40
1:AA:65:THR:HG22	1:AA:525:TYR:HA	2.02	0.40
1:AB:444:TYR:HE2	1:BA:341:ASP:HB2	1.87	0.40
1:BB:307:ASN:ND2	1:CA:235:GLU:OE2	2.55	0.40
1:CA:78:SER:HA	1:CA:178:LEU:O	2.21	0.40
1:DA:115:THR:HG22	1:DA:148:VAL:CG2	2.51	0.40
1:DB:334:LEU:HD22	1:DB:381:THR:HG22	2.03	0.40
1:GA:500:ALA:HB2	1:GA:527:LEU:HB2	2.02	0.40
1:HB:293:ILE:HD13	1:HB:293:ILE:HA	1.91	0.40
1:HB:454:PRO:HG2	1:HB:457:TRP:CD1	2.57	0.40
1:HC:358:PHE:HD1	1:HC:365:VAL:HG13	1.87	0.40
1:HC:390:GLN:HG2	1:HC:399:GLU:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:137:GLN:HA	1:IB:140:MET:CE	2.51	0.40
1:IB:468:ALA:HA	1:IB:520:TRP:CH2	2.57	0.40
1:JC:213:ILE:CG2	1:JC:214:PHE:N	2.85	0.40
1:JC:261:PRO:HG3	1:JC:403:TRP:HZ3	1.87	0.40
1:KA:216:VAL:CG2	1:KA:217:PRO:HD2	2.50	0.40
1:LA:144:ILE:HD13	1:LA:156:ILE:HG12	2.03	0.40
1:LC:434:PHE:CD2	1:LC:454:PRO:HD3	2.57	0.40
1:MA:449:LEU:HD12	1:MA:449:LEU:HA	1.87	0.40
1:OB:66:VAL:HG12	1:OB:186:LEU:HB2	2.03	0.40
1:OC:107:VAL:HG13	1:OC:154:VAL:HB	2.04	0.40
1:OC:277:GLN:NE2	1:OC:283:ILE:HD13	2.37	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 X-ray entries followed by that with respect to entries of similar resolution.

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	AA	496/540 (92%)	482 (97%)	14 (3%)	0	100	100
1	AB	521/540 (96%)	505 (97%)	16 (3%)	0	100	100
1	AC	506/540 (94%)	489 (97%)	17 (3%)	0	100	100
1	BA	495/540 (92%)	480 (97%)	15 (3%)	0	100	100
1	BB	521/540 (96%)	502 (96%)	19 (4%)	0	100	100
1	BC	505/540 (94%)	488 (97%)	17 (3%)	0	100	100
1	CA	495/540 (92%)	481 (97%)	14 (3%)	0	100	100
1	CB	521/540 (96%)	501 (96%)	20 (4%)	0	100	100
1	CC	505/540 (94%)	488 (97%)	17 (3%)	0	100	100
1	DA	494/540 (92%)	480 (97%)	14 (3%)	0	100	100
1	DB	521/540 (96%)	501 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DC	504/540 (93%)	489 (97%)	15 (3%)	0	100	100
1	EA	495/540 (92%)	484 (98%)	11 (2%)	0	100	100
1	EB	521/540 (96%)	505 (97%)	16 (3%)	0	100	100
1	EC	489/540 (91%)	475 (97%)	14 (3%)	0	100	100
1	FA	495/540 (92%)	473 (96%)	22 (4%)	0	100	100
1	FB	521/540 (96%)	502 (96%)	19 (4%)	0	100	100
1	FC	507/540 (94%)	491 (97%)	16 (3%)	0	100	100
1	GA	495/540 (92%)	478 (97%)	17 (3%)	0	100	100
1	GB	521/540 (96%)	500 (96%)	21 (4%)	0	100	100
1	GC	505/540 (94%)	488 (97%)	17 (3%)	0	100	100
1	HA	495/540 (92%)	481 (97%)	14 (3%)	0	100	100
1	HB	521/540 (96%)	499 (96%)	22 (4%)	0	100	100
1	HC	505/540 (94%)	491 (97%)	14 (3%)	0	100	100
1	IA	495/540 (92%)	481 (97%)	14 (3%)	0	100	100
1	IB	521/540 (96%)	497 (95%)	24 (5%)	0	100	100
1	IC	499/540 (92%)	485 (97%)	14 (3%)	0	100	100
1	JA	495/540 (92%)	479 (97%)	16 (3%)	0	100	100
1	JB	521/540 (96%)	501 (96%)	20 (4%)	0	100	100
1	JC	504/540 (93%)	487 (97%)	17 (3%)	0	100	100
1	KA	495/540 (92%)	479 (97%)	16 (3%)	0	100	100
1	KB	521/540 (96%)	505 (97%)	16 (3%)	0	100	100
1	KC	505/540 (94%)	491 (97%)	14 (3%)	0	100	100
1	LA	495/540 (92%)	477 (96%)	18 (4%)	0	100	100
1	LB	521/540 (96%)	503 (96%)	18 (4%)	0	100	100
1	LC	498/540 (92%)	480 (96%)	18 (4%)	0	100	100
1	MA	495/540 (92%)	483 (98%)	12 (2%)	0	100	100
1	MB	521/540 (96%)	506 (97%)	15 (3%)	0	100	100
1	MC	504/540 (93%)	490 (97%)	14 (3%)	0	100	100
1	NA	495/540 (92%)	480 (97%)	15 (3%)	0	100	100
1	NB	521/540 (96%)	505 (97%)	16 (3%)	0	100	100
1	NC	504/540 (93%)	486 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OA	495/540 (92%)	482 (97%)	13 (3%)	0	100	100
1	OB	521/540 (96%)	502 (96%)	19 (4%)	0	100	100
1	OC	494/540 (92%)	476 (96%)	18 (4%)	0	100	100
All	All	22774/24300 (94%)	22028 (97%)	746 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	AA	427/457 (93%)	427 (100%)	0	100	100
1	AB	444/457 (97%)	444 (100%)	0	100	100
1	AC	434/457 (95%)	434 (100%)	0	100	100
1	BA	426/457 (93%)	426 (100%)	0	100	100
1	BB	445/457 (97%)	445 (100%)	0	100	100
1	BC	433/457 (95%)	433 (100%)	0	100	100
1	CA	426/457 (93%)	426 (100%)	0	100	100
1	CB	444/457 (97%)	444 (100%)	0	100	100
1	CC	433/457 (95%)	432 (100%)	1 (0%)	93	98
1	DA	425/457 (93%)	425 (100%)	0	100	100
1	DB	444/457 (97%)	444 (100%)	0	100	100
1	DC	432/457 (94%)	432 (100%)	0	100	100
1	EA	426/457 (93%)	426 (100%)	0	100	100
1	EB	444/457 (97%)	444 (100%)	0	100	100
1	EC	421/457 (92%)	421 (100%)	0	100	100
1	FA	426/457 (93%)	426 (100%)	0	100	100
1	FB	445/457 (97%)	445 (100%)	0	100	100
1	FC	435/457 (95%)	435 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GA	426/457 (93%)	426 (100%)	0	100	100
1	GB	444/457 (97%)	444 (100%)	0	100	100
1	GC	433/457 (95%)	433 (100%)	0	100	100
1	HA	426/457 (93%)	426 (100%)	0	100	100
1	HB	444/457 (97%)	444 (100%)	0	100	100
1	HC	433/457 (95%)	433 (100%)	0	100	100
1	IA	426/457 (93%)	426 (100%)	0	100	100
1	IB	445/457 (97%)	444 (100%)	1 (0%)	93	98
1	IC	430/457 (94%)	430 (100%)	0	100	100
1	JA	426/457 (93%)	426 (100%)	0	100	100
1	JB	442/457 (97%)	442 (100%)	0	100	100
1	JC	432/457 (94%)	432 (100%)	0	100	100
1	KA	426/457 (93%)	426 (100%)	0	100	100
1	KB	443/457 (97%)	443 (100%)	0	100	100
1	KC	433/457 (95%)	433 (100%)	0	100	100
1	LA	426/457 (93%)	426 (100%)	0	100	100
1	LB	441/457 (96%)	440 (100%)	1 (0%)	93	98
1	LC	427/457 (93%)	426 (100%)	1 (0%)	93	98
1	MA	426/457 (93%)	426 (100%)	0	100	100
1	MB	443/457 (97%)	443 (100%)	0	100	100
1	MC	432/457 (94%)	432 (100%)	0	100	100
1	NA	426/457 (93%)	426 (100%)	0	100	100
1	NB	444/457 (97%)	444 (100%)	0	100	100
1	NC	430/457 (94%)	430 (100%)	0	100	100
1	OA	426/457 (93%)	425 (100%)	1 (0%)	93	98
1	OB	444/457 (97%)	444 (100%)	0	100	100
1	OC	426/457 (93%)	426 (100%)	0	100	100
All	All	19510/20565 (95%)	19505 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CC	97	ASN

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Mol	Chain	Res	Type
1	IB	411	ARG
1	LB	257	PHE
1	LC	398	ASN
1	OA	187	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	BC	44	GLN
1	CC	44	GLN
1	EC	44	GLN
1	FA	44	GLN
1	FA	306	GLN
1	FC	23	ASN
1	FC	297	HIS
1	GB	277	GLN
1	GC	44	GLN
1	GC	417	HIS
1	HA	430	GLN
1	HC	309	ASN
1	IC	44	GLN
1	IC	398	ASN
1	JC	44	GLN
1	LB	396	HIS
1	MB	309	ASN
1	MC	44	GLN
1	NC	44	GLN
1	OB	170	GLN
1	OC	336	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 72 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	JA	601	-	3,3,3	0.49	0	2,2,2	0.29	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	EDO	JA	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	500/540 (92%)	-0.44	8 (1%) 72 44	34, 56, 104, 132	0
1	AB	523/540 (96%)	-0.45	10 (1%) 66 37	34, 58, 105, 138	0
1	AC	508/540 (94%)	-0.43	11 (2%) 62 33	33, 58, 104, 143	0
1	BA	499/540 (92%)	-0.38	15 (3%) 50 22	35, 56, 110, 140	0
1	BB	523/540 (96%)	-0.38	12 (2%) 60 31	33, 57, 107, 140	0
1	BC	507/540 (93%)	-0.17	25 (4%) 29 11	32, 68, 131, 159	0
1	CA	499/540 (92%)	-0.43	4 (0%) 86 65	36, 57, 105, 131	0
1	CB	523/540 (96%)	-0.43	15 (2%) 51 23	33, 57, 106, 141	0
1	CC	507/540 (93%)	-0.43	7 (1%) 75 49	33, 59, 105, 152	0
1	DA	498/540 (92%)	-0.36	13 (2%) 56 27	36, 57, 107, 152	0
1	DB	523/540 (96%)	-0.38	14 (2%) 54 26	35, 58, 115, 148	0
1	DC	506/540 (93%)	-0.20	19 (3%) 40 16	35, 69, 130, 168	0
1	EA	499/540 (92%)	-0.35	8 (1%) 72 44	35, 58, 113, 139	0
1	EB	523/540 (96%)	-0.43	11 (2%) 63 34	34, 56, 109, 148	0
1	EC	493/540 (91%)	0.16	58 (11%) 4 1	34, 81, 168, 194	0
1	FA	499/540 (92%)	-0.39	10 (2%) 65 36	36, 59, 111, 137	0
1	FB	523/540 (96%)	-0.46	13 (2%) 57 29	32, 54, 101, 132	0
1	FC	509/540 (94%)	-0.17	27 (5%) 26 10	34, 74, 127, 175	0
1	GA	499/540 (92%)	-0.43	13 (2%) 56 27	36, 53, 103, 138	0
1	GB	523/540 (96%)	-0.37	12 (2%) 60 31	34, 55, 110, 139	0
1	GC	507/540 (93%)	-0.35	15 (2%) 50 22	34, 59, 109, 148	0
1	HA	499/540 (92%)	-0.39	10 (2%) 65 36	36, 57, 109, 138	0
1	HB	523/540 (96%)	-0.43	7 (1%) 77 51	35, 55, 101, 145	0
1	HC	507/540 (93%)	-0.24	18 (3%) 42 17	33, 67, 124, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	IA	499/540 (92%)	-0.38	13 (2%) 56 27	35, 55, 104, 144	0
1	IB	523/540 (96%)	-0.35	16 (3%) 49 21	34, 58, 119, 149	0
1	IC	503/540 (93%)	0.07	44 (8%) 10 3	34, 81, 142, 174	0
1	JA	499/540 (92%)	-0.38	9 (1%) 68 40	35, 59, 117, 156	0
1	JB	523/540 (96%)	-0.39	10 (1%) 66 37	36, 58, 113, 145	0
1	JC	506/540 (93%)	0.21	61 (12%) 4 1	34, 85, 178, 204	0
1	KA	499/540 (92%)	-0.32	11 (2%) 62 33	36, 59, 111, 137	0
1	KB	523/540 (96%)	-0.42	14 (2%) 54 26	35, 55, 106, 144	0
1	KC	507/540 (93%)	-0.24	16 (3%) 47 20	34, 67, 123, 145	0
1	LA	499/540 (92%)	-0.38	12 (2%) 59 30	36, 56, 102, 151	0
1	LB	523/540 (96%)	-0.36	14 (2%) 54 26	31, 58, 118, 142	0
1	LC	502/540 (92%)	-0.03	33 (6%) 18 5	35, 81, 137, 167	0
1	MA	499/540 (92%)	-0.38	9 (1%) 68 40	34, 59, 111, 143	0
1	MB	523/540 (96%)	-0.46	12 (2%) 60 31	35, 53, 98, 142	0
1	MC	506/540 (93%)	-0.16	24 (4%) 31 11	33, 73, 128, 153	0
1	NA	499/540 (92%)	-0.44	13 (2%) 56 27	35, 53, 103, 144	0
1	NB	523/540 (96%)	-0.35	16 (3%) 49 21	34, 58, 114, 145	0
1	NC	506/540 (93%)	-0.36	12 (2%) 59 30	33, 60, 111, 171	0
1	OA	499/540 (92%)	-0.36	17 (3%) 45 19	35, 59, 116, 141	0
1	OB	523/540 (96%)	-0.35	16 (3%) 49 21	35, 58, 115, 147	0
1	OC	498/540 (92%)	0.21	58 (11%) 4 1	37, 83, 171, 191	0
All	All	22902/24300 (94%)	-0.31	785 (3%) 45 19	31, 59, 123, 204	0

All (785) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	OC	346	GLY	8.9
1	JC	349	ALA	7.9
1	OC	412	THR	7.9
1	JC	412	THR	6.6
1	NC	393	ASN	6.2
1	JC	348	LYS	6.2
1	DA	307	ASN	6.2
1	DC	396	HIS	6.0
1	EC	346	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
1	JC	295	GLY	5.7
1	BC	391	ASP	5.7
1	OC	349	ALA	5.6
1	FC	393	ASN	5.6
1	EC	349	ALA	5.6
1	OC	413	GLY	5.5
1	EC	393	ASN	5.4
1	OC	300	THR	5.4
1	OC	373	ASN	5.4
1	EC	332	GLY	5.3
1	HC	393	ASN	5.3
1	EC	347	HIS	5.3
1	JC	393	ASN	5.2
1	JC	413	GLY	5.2
1	JC	373	ASN	5.1
1	IC	372	ASN	5.1
1	HB	393	ASN	5.1
1	LA	307	ASN	5.1
1	BC	399	GLU	5.0
1	MB	310	ASN	5.0
1	HA	393	ASN	5.0
1	EC	394	SER	4.9
1	OC	291	THR	4.9
1	IC	308	TRP	4.8
1	EC	414	HIS	4.8
1	LC	528	ALA	4.7
1	JC	372	ASN	4.7
1	EC	395	ALA	4.7
1	OC	294	ALA	4.6
1	JC	377	THR	4.6
1	KB	314	THR	4.6
1	OC	347	HIS	4.6
1	IA	307	ASN	4.6
1	CC	393	ASN	4.6
1	GB	310	ASN	4.6
1	LC	393	ASN	4.6
1	JC	395	ALA	4.6
1	OC	295	GLY	4.5
1	OC	377	THR	4.5
1	MC	413	GLY	4.5
1	NC	394	SER	4.5
1	FC	340	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	EA	393	ASN	4.5
1	AC	393	ASN	4.4
1	OC	390	GLN	4.4
1	IA	308	TRP	4.4
1	KC	393	ASN	4.4
1	KC	412	THR	4.3
1	FC	394	SER	4.3
1	OC	396	HIS	4.3
1	OC	332	GLY	4.2
1	OC	395	ALA	4.2
1	IC	528	ALA	4.2
1	IC	529	PRO	4.2
1	OA	393	ASN	4.2
1	IC	311	TYR	4.2
1	EC	396	HIS	4.2
1	AA	393	ASN	4.1
1	IC	398	ASN	4.1
1	KC	413	GLY	4.1
1	EC	391	ASP	4.1
1	DB	307	ASN	4.1
1	OC	393	ASN	4.1
1	JC	340	GLY	4.1
1	MC	340	GLY	4.1
1	DB	413	GLY	4.0
1	GC	309	ASN	4.0
1	JA	310	ASN	4.0
1	JC	394	SER	4.0
1	OC	374	ASP	4.0
1	BB	393	ASN	4.0
1	IC	411	ARG	4.0
1	OB	311	TYR	4.0
1	LB	310	ASN	4.0
1	DC	411	ARG	4.0
1	JC	339	ARG	4.0
1	IC	427	PRO	4.0
1	OB	314	THR	4.0
1	JC	399	GLU	4.0
1	MC	341	ASP	4.0
1	BB	312	ASP	4.0
1	IC	391	ASP	4.0
1	FC	395	ALA	3.9
1	MC	339	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	OC	292	HIS	3.9
1	LA	306	GLN	3.9
1	EC	338	THR	3.9
1	JB	393	ASN	3.9
1	JC	306	GLN	3.9
1	LC	289	ASP	3.9
1	JC	332	GLY	3.9
1	OB	313	PRO	3.8
1	OC	339	ARG	3.8
1	EC	289	ASP	3.8
1	EC	412	THR	3.8
1	MA	393	ASN	3.8
1	NB	310	ASN	3.8
1	OC	340	GLY	3.8
1	CC	394	SER	3.8
1	IB	222	SER	3.8
1	LC	312	ASP	3.7
1	FC	412	THR	3.7
1	DC	412	THR	3.7
1	GC	305	SER	3.7
1	NB	411	ARG	3.7
1	OB	308	TRP	3.7
1	JA	393	ASN	3.7
1	EC	339	ARG	3.7
1	JC	392	GLY	3.7
1	DB	310	ASN	3.7
1	EB	308	TRP	3.7
1	JC	357	HIS	3.7
1	GB	393	ASN	3.7
1	OC	310	ASN	3.7
1	FC	339	ARG	3.6
1	NA	393	ASN	3.6
1	LC	255	GLY	3.6
1	BA	394	SER	3.6
1	IC	393	ASN	3.6
1	EC	340	GLY	3.6
1	LA	310	ASN	3.6
1	MC	393	ASN	3.6
1	JC	411	ARG	3.6
1	BB	313	PRO	3.6
1	EC	295	GLY	3.6
1	FC	399	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	EC	302	ASN	3.6
1	NA	308	TRP	3.6
1	EB	314	THR	3.6
1	JC	381	THR	3.6
1	LC	193	ASP	3.6
1	NB	393	ASN	3.5
1	OC	389	VAL	3.5
1	MC	411	ARG	3.5
1	EA	311	TYR	3.5
1	BC	398	ASN	3.5
1	OA	311	TYR	3.5
1	DB	393	ASN	3.5
1	JC	391	ASP	3.5
1	JC	305	SER	3.5
1	IA	310	ASN	3.5
1	MC	373	ASN	3.5
1	DA	311	TYR	3.5
1	FB	394	SER	3.5
1	NC	399	GLU	3.5
1	OC	399	GLU	3.5
1	BA	393	ASN	3.5
1	LC	395	ALA	3.4
1	EB	307	ASN	3.4
1	EA	394	SER	3.4
1	DC	368	THR	3.4
1	BB	310	ASN	3.4
1	EC	373	ASN	3.4
1	KB	312	ASP	3.4
1	MC	395	ALA	3.4
1	OC	394	SER	3.4
1	LA	393	ASN	3.4
1	LC	530	MET	3.4
1	GB	314	THR	3.4
1	IB	314	THR	3.4
1	IC	368	THR	3.4
1	OC	293	ILE	3.4
1	GC	308	TRP	3.4
1	CB	310	ASN	3.4
1	AB	314	THR	3.4
1	JC	337	THR	3.4
1	JB	312	ASP	3.4
1	EC	337	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	CB	411	ARG	3.4
1	DA	393	ASN	3.4
1	IB	311	TYR	3.4
1	IA	305	SER	3.4
1	EC	341	ASP	3.3
1	GA	393	ASN	3.3
1	MC	412	THR	3.3
1	HC	411	ARG	3.3
1	CB	393	ASN	3.3
1	IA	393	ASN	3.3
1	HC	394	SER	3.3
1	OC	298	ASP	3.3
1	OC	398	ASN	3.3
1	BA	395	ALA	3.3
1	NC	308	TRP	3.3
1	CB	307	ASN	3.3
1	JC	338	THR	3.3
1	NA	391	ASP	3.3
1	IC	297	HIS	3.3
1	MA	310	ASN	3.3
1	NA	306	GLN	3.3
1	JC	289	ASP	3.3
1	IC	341	ASP	3.3
1	JC	345	ARG	3.3
1	NA	310	ASN	3.3
1	BA	307	ASN	3.2
1	FA	393	ASN	3.2
1	FC	442	SER	3.2
1	IB	394	SER	3.2
1	IC	309	ASN	3.2
1	KC	395	ALA	3.2
1	KC	411	ARG	3.2
1	AB	313	PRO	3.2
1	DA	314	THR	3.2
1	HC	399	GLU	3.2
1	JC	293	ILE	3.2
1	LB	393	ASN	3.2
1	LC	399	GLU	3.2
1	EC	392	GLY	3.2
1	IA	311	TYR	3.2
1	IB	393	ASN	3.2
1	HC	529	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	LC	256	ALA	3.2
1	EC	398	ASN	3.2
1	IC	399	GLU	3.2
1	GC	528	ALA	3.2
1	BC	411	ARG	3.2
1	IC	378	GLY	3.2
1	NB	394	SER	3.2
1	KC	399	GLU	3.2
1	IC	373	ASN	3.2
1	KA	411	ARG	3.2
1	DB	314	THR	3.2
1	EC	356	VAL	3.2
1	FC	411	ARG	3.1
1	EC	399	GLU	3.1
1	MC	398	ASN	3.1
1	BB	314	THR	3.1
1	FC	341	ASP	3.1
1	EC	354	GLY	3.1
1	LA	308	TRP	3.1
1	OC	392	GLY	3.1
1	BA	310	ASN	3.1
1	JB	310	ASN	3.1
1	MB	311	TYR	3.1
1	BC	396	HIS	3.1
1	KB	393	ASN	3.1
1	OC	302	ASN	3.1
1	NC	312	ASP	3.1
1	JC	378	GLY	3.1
1	OA	307	ASN	3.1
1	LB	313	PRO	3.1
1	JC	308	TRP	3.1
1	GA	312	ASP	3.1
1	OC	193	ASP	3.1
1	HC	395	ALA	3.1
1	IC	379	GLN	3.1
1	KA	393	ASN	3.1
1	KB	313	PRO	3.1
1	OC	372	ASN	3.1
1	DA	310	ASN	3.1
1	JA	412	THR	3.1
1	CB	309	ASN	3.0
1	FA	399	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	LA	412	THR	3.0
1	OB	531	GLY	3.0
1	LB	308	TRP	3.0
1	OC	290	VAL	3.0
1	NA	311	TYR	3.0
1	OC	378	GLY	3.0
1	EC	377	THR	3.0
1	OC	411	ARG	3.0
1	DB	312	ASP	3.0
1	AB	305	SER	3.0
1	IC	392	GLY	3.0
1	BB	411	ARG	3.0
1	IB	308	TRP	3.0
1	OC	341	ASP	3.0
1	MB	393	ASN	3.0
1	BC	444	TYR	3.0
1	IC	451	CYS	3.0
1	IC	296	THR	3.0
1	BA	308	TRP	3.0
1	JC	288	GLY	3.0
1	MB	308	TRP	3.0
1	KB	311	TYR	3.0
1	LB	312	ASP	3.0
1	LC	391	ASP	3.0
1	KC	343	SER	3.0
1	JC	347	HIS	3.0
1	JC	396	HIS	3.0
1	OC	338	THR	3.0
1	OC	379	GLN	3.0
1	DC	399	GLU	3.0
1	DA	308	TRP	2.9
1	MB	312	ASP	2.9
1	NB	312	ASP	2.9
1	EC	390	GLN	2.9
1	JA	395	ALA	2.9
1	EC	298	ASP	2.9
1	KC	396	HIS	2.9
1	MB	193	ASP	2.9
1	BC	428	GLY	2.9
1	HB	310	ASN	2.9
1	AA	308	TRP	2.9
1	IB	312	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	IB	340	GLY	2.9
1	BC	307	ASN	2.9
1	MB	399	GLU	2.9
1	OC	376	GLU	2.9
1	FC	391	ASP	2.9
1	EC	401	GLN	2.9
1	EC	300	THR	2.9
1	JB	308	TRP	2.9
1	DA	309	ASN	2.9
1	DA	394	SER	2.9
1	FA	394	SER	2.9
1	HA	310	ASN	2.9
1	AB	311	TYR	2.9
1	JC	346	GLY	2.9
1	IA	412	THR	2.9
1	BC	379	GLN	2.9
1	JC	366	GLN	2.9
1	MC	399	GLU	2.9
1	FC	443	GLY	2.9
1	HA	394	SER	2.9
1	KA	310	ASN	2.9
1	LC	290	VAL	2.9
1	IA	306	GLN	2.9
1	DA	391	ASP	2.9
1	FC	193	ASP	2.9
1	BA	311	TYR	2.8
1	GA	306	GLN	2.8
1	JC	294	ALA	2.8
1	AB	312	ASP	2.8
1	EB	393	ASN	2.8
1	GC	310	ASN	2.8
1	HA	311	TYR	2.8
1	IB	310	ASN	2.8
1	EB	339	ARG	2.8
1	IB	411	ARG	2.8
1	BC	445	PRO	2.8
1	CA	308	TRP	2.8
1	OB	394	SER	2.8
1	GC	393	ASN	2.8
1	EC	389	VAL	2.8
1	CC	391	ASP	2.8
1	AB	307	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	JA	195	VAL	2.8
1	OB	393	ASN	2.8
1	EC	369	THR	2.8
1	HC	377	THR	2.8
1	OC	289	ASP	2.8
1	DB	311	TYR	2.8
1	GB	308	TRP	2.8
1	JC	379	GLN	2.8
1	KA	306	GLN	2.8
1	KC	398	ASN	2.8
1	GA	313	PRO	2.8
1	OC	401	GLN	2.8
1	FC	373	ASN	2.8
1	LB	314	THR	2.8
1	HC	391	ASP	2.8
1	CA	393	ASN	2.7
1	GB	311	TYR	2.7
1	BA	399	GLU	2.7
1	EC	310	ASN	2.7
1	JB	314	THR	2.7
1	BB	394	SER	2.7
1	BC	297	HIS	2.7
1	JC	310	ASN	2.7
1	LC	398	ASN	2.7
1	EC	348	LYS	2.7
1	EC	294	ALA	2.7
1	LA	391	ASP	2.7
1	FC	342	GLY	2.7
1	NA	399	GLU	2.7
1	DC	394	SER	2.7
1	OA	394	SER	2.7
1	KA	308	TRP	2.7
1	LC	288	GLY	2.7
1	EC	357	HIS	2.7
1	FB	310	ASN	2.7
1	KB	340	GLY	2.7
1	CC	396	HIS	2.7
1	LC	411	ARG	2.7
1	MC	409	SER	2.7
1	FB	393	ASN	2.7
1	BC	412	THR	2.7
1	MA	311	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	OA	392	GLY	2.7
1	EB	399	GLU	2.7
1	EB	310	ASN	2.7
1	FA	308	TRP	2.7
1	LC	372	ASN	2.7
1	DA	306	GLN	2.7
1	GC	306	GLN	2.7
1	IC	390	GLN	2.7
1	AA	310	ASN	2.7
1	OC	391	ASP	2.7
1	MA	340	GLY	2.7
1	BC	394	SER	2.6
1	EC	400	PRO	2.6
1	JC	445	PRO	2.6
1	GC	394	SER	2.6
1	FB	532	ASN	2.6
1	NA	312	ASP	2.6
1	FC	392	GLY	2.6
1	BB	399	GLU	2.6
1	DC	391	ASP	2.6
1	EB	312	ASP	2.6
1	IC	530	MET	2.6
1	CB	339	ARG	2.6
1	BC	309	ASN	2.6
1	EC	374	ASP	2.6
1	IC	298	ASP	2.6
1	IC	312	ASP	2.6
1	JA	411	ARG	2.6
1	LC	313	PRO	2.6
1	OC	357	HIS	2.6
1	EB	411	ARG	2.6
1	EC	413	GLY	2.6
1	IA	309	ASN	2.6
1	IB	372	ASN	2.6
1	BB	412	THR	2.6
1	BA	392	GLY	2.6
1	OA	396	HIS	2.6
1	IC	416	VAL	2.6
1	JC	374	ASP	2.6
1	EC	309	ASN	2.6
1	JC	302	ASN	2.6
1	LC	529	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	IC	394	SER	2.6
1	JB	411	ARG	2.6
1	MA	411	ARG	2.6
1	FA	310	ASN	2.6
1	JC	307	ASN	2.6
1	JC	529	PRO	2.6
1	EC	292	HIS	2.6
1	FC	390	GLN	2.6
1	IB	306	GLN	2.6
1	FC	289	ASP	2.6
1	GA	394	SER	2.6
1	JA	311	TYR	2.6
1	KC	373	ASN	2.6
1	KA	412	THR	2.6
1	LA	311	TYR	2.6
1	IC	288	GLY	2.6
1	LB	411	ARG	2.6
1	MB	395	ALA	2.6
1	OC	331	GLN	2.6
1	BC	373	ASN	2.6
1	OC	375	LEU	2.6
1	IC	395	ALA	2.5
1	KA	312	ASP	2.5
1	JC	296	THR	2.5
1	BA	306	GLN	2.5
1	GA	307	ASN	2.5
1	OC	23	ASN	2.5
1	FB	399	GLU	2.5
1	HB	311	TYR	2.5
1	NC	412	THR	2.5
1	HC	392	GLY	2.5
1	GB	312	ASP	2.5
1	IC	289	ASP	2.5
1	BA	313	PRO	2.5
1	EC	293	ILE	2.5
1	IC	340	GLY	2.5
1	EC	530	MET	2.5
1	AC	193	ASP	2.5
1	FB	312	ASP	2.5
1	LB	395	ALA	2.5
1	MA	395	ALA	2.5
1	IC	396	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	DC	340	GLY	2.5
1	MC	394	SER	2.5
1	NB	374	ASP	2.5
1	DA	392	GLY	2.5
1	JA	394	SER	2.5
1	KC	394	SER	2.5
1	LC	394	SER	2.5
1	NC	305	SER	2.5
1	HB	308	TRP	2.5
1	BC	502	THR	2.5
1	LA	395	ALA	2.5
1	OC	356	VAL	2.5
1	CB	308	TRP	2.5
1	GA	411	ARG	2.5
1	AB	310	ASN	2.5
1	JC	398	ASN	2.5
1	JC	341	ASP	2.5
1	LB	305	SER	2.5
1	LB	396	HIS	2.5
1	OB	309	ASN	2.4
1	DC	529	PRO	2.4
1	BA	391	ASP	2.4
1	OA	312	ASP	2.4
1	HC	307	ASN	2.4
1	KB	307	ASN	2.4
1	OC	337	THR	2.4
1	FB	193	ASP	2.4
1	KA	391	ASP	2.4
1	LB	391	ASP	2.4
1	CB	395	ALA	2.4
1	EA	315	GLU	2.4
1	HA	412	THR	2.4
1	HC	379	GLN	2.4
1	DC	297	HIS	2.4
1	FB	396	HIS	2.4
1	IC	290	VAL	2.4
1	NB	391	ASP	2.4
1	OC	305	SER	2.4
1	AC	412	THR	2.4
1	NB	307	ASN	2.4
1	BB	311	TYR	2.4
1	OC	367	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	OB	532	ASN	2.4
1	IA	392	GLY	2.4
1	AA	341	ASP	2.4
1	DC	374	ASP	2.4
1	JC	441	CYS	2.4
1	NC	193	ASP	2.4
1	MB	394	SER	2.4
1	GC	529	PRO	2.4
1	DC	444	TYR	2.4
1	EC	193	ASP	2.4
1	IB	374	ASP	2.4
1	CB	413	GLY	2.4
1	CC	340	GLY	2.4
1	JC	502	THR	2.4
1	CB	313	PRO	2.4
1	DB	394	SER	2.4
1	FC	23	ASN	2.4
1	IB	307	ASN	2.4
1	LA	309	ASN	2.4
1	OA	313	PRO	2.4
1	MC	338	THR	2.4
1	HA	391	ASP	2.4
1	MC	298	ASP	2.4
1	CA	394	SER	2.4
1	IA	394	SER	2.4
1	JC	352	SER	2.3
1	NC	311	TYR	2.3
1	FC	345	ARG	2.3
1	IB	339	ARG	2.3
1	CA	312	ASP	2.3
1	EC	370	ASP	2.3
1	OB	312	ASP	2.3
1	EC	409	SER	2.3
1	LC	427	PRO	2.3
1	BB	307	ASN	2.3
1	EC	23	ASN	2.3
1	EC	368	THR	2.3
1	KC	440	GLY	2.3
1	OC	327	VAL	2.3
1	AC	23	ASN	2.3
1	BC	372	ASN	2.3
1	BC	193	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	EA	195	VAL	2.3
1	OC	348	LYS	2.3
1	AC	411	ARG	2.3
1	DC	397	GLN	2.3
1	FA	309	ASN	2.3
1	LC	315	GLU	2.3
1	OB	310	ASN	2.3
1	EC	451	CYS	2.3
1	JB	311	TYR	2.3
1	FC	343	SER	2.3
1	FC	310	ASN	2.3
1	BC	528	ALA	2.3
1	GA	399	GLU	2.3
1	GC	315	GLU	2.3
1	KB	394	SER	2.3
1	NB	308	TRP	2.3
1	OB	396	HIS	2.3
1	CC	338	THR	2.3
1	JC	311	TYR	2.3
1	LC	311	TYR	2.3
1	OA	310	ASN	2.3
1	BA	195	VAL	2.3
1	LC	392	GLY	2.3
1	GB	284	CYS	2.3
1	EC	379	GLN	2.3
1	DB	395	ALA	2.3
1	IC	444	TYR	2.3
1	FC	413	GLY	2.3
1	HC	193	ASP	2.3
1	MC	193	ASP	2.3
1	OA	342	GLY	2.3
1	OA	412	THR	2.3
1	AC	394	SER	2.3
1	EA	308	TRP	2.3
1	EC	327	VAL	2.3
1	NB	395	ALA	2.3
1	AC	340	GLY	2.3
1	JC	300	THR	2.3
1	BC	397	GLN	2.3
1	AB	308	TRP	2.3
1	FB	395	ALA	2.3
1	KB	399	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	FC	372	ASN	2.3
1	LB	309	ASN	2.3
1	MA	312	ASP	2.3
1	NC	309	ASN	2.3
1	CB	311	TYR	2.3
1	HC	396	HIS	2.3
1	GB	309	ASN	2.2
1	NB	532	ASN	2.2
1	OC	345	ARG	2.2
1	AC	390	GLN	2.2
1	DC	413	GLY	2.2
1	GA	308	TRP	2.2
1	OA	315	GLU	2.2
1	DB	411	ARG	2.2
1	GA	339	ARG	2.2
1	IC	506	ASP	2.2
1	MB	314	THR	2.2
1	LA	195	VAL	2.2
1	AC	399	GLU	2.2
1	AC	339	ARG	2.2
1	GB	411	ARG	2.2
1	IC	240	SER	2.2
1	BA	309	ASN	2.2
1	GB	194	ASP	2.2
1	HC	312	ASP	2.2
1	IC	482	THR	2.2
1	KB	310	ASN	2.2
1	DB	316	GLU	2.2
1	LA	399	GLU	2.2
1	NA	394	SER	2.2
1	DC	193	ASP	2.2
1	AC	392	GLY	2.2
1	DB	412	THR	2.2
1	EC	372	ASN	2.2
1	GB	341	ASP	2.2
1	IC	313	PRO	2.2
1	LC	378	GLY	2.2
1	LC	444	TYR	2.2
1	MA	399	GLU	2.2
1	OB	411	ARG	2.2
1	NA	305	SER	2.2
1	FB	398	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	GA	310	ASN	2.2
1	IA	313	PRO	2.2
1	JC	309	ASN	2.2
1	OA	308	TRP	2.2
1	HA	195	VAL	2.2
1	JC	356	VAL	2.2
1	MB	339	ARG	2.2
1	OC	436	SER	2.2
1	KB	193	ASP	2.2
1	DB	309	ASN	2.2
1	MC	310	ASN	2.2
1	AA	396	HIS	2.2
1	FC	357	HIS	2.2
1	IA	411	ARG	2.2
1	OB	374	ASP	2.2
1	AA	412	THR	2.2
1	FB	309	ASN	2.2
1	GC	307	ASN	2.2
1	BC	308	TRP	2.2
1	DC	315	GLU	2.2
1	GA	311	TYR	2.2
1	NC	395	ALA	2.2
1	HB	193	ASP	2.2
1	KC	530	MET	2.2
1	IB	532	ASN	2.2
1	KC	345	ARG	2.2
1	CB	305	SER	2.2
1	EC	352	SER	2.2
1	KB	395	ALA	2.2
1	IC	374	ASP	2.2
1	MC	293	ILE	2.2
1	JA	413	GLY	2.2
1	JB	172	ASN	2.2
1	JC	414	HIS	2.2
1	KA	396	HIS	2.2
1	KB	24	ASN	2.2
1	MC	414	HIS	2.2
1	NB	314	THR	2.2
1	LC	379	GLN	2.1
1	EA	399	GLU	2.1
1	KC	312	ASP	2.1
1	OB	339	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	AB	393	ASN	2.1
1	DA	28	ALA	2.1
1	DB	399	GLU	2.1
1	BC	374	ASP	2.1
1	LC	192	GLY	2.1
1	MC	378	GLY	2.1
1	FA	412	THR	2.1
1	JB	309	ASN	2.1
1	IC	339	ARG	2.1
1	IC	356	VAL	2.1
1	JC	389	VAL	2.1
1	LC	240	SER	2.1
1	AB	411	ARG	2.1
1	FB	307	ASN	2.1
1	GA	314	THR	2.1
1	HC	398	ASN	2.1
1	KB	309	ASN	2.1
1	LC	396	HIS	2.1
1	OA	314	THR	2.1
1	LC	336	GLN	2.1
1	LB	340	GLY	2.1
1	DC	299	TYR	2.1
1	EC	345	ARG	2.1
1	MC	289	ASP	2.1
1	GC	395	ALA	2.1
1	JC	500	ALA	2.1
1	LC	357	HIS	2.1
1	HA	399	GLU	2.1
1	JC	371	THR	2.1
1	KA	399	GLU	2.1
1	MB	24	ASN	2.1
1	NA	309	ASN	2.1
1	BA	305	SER	2.1
1	OC	313	PRO	2.1
1	DC	481	ASP	2.1
1	HA	395	ALA	2.1
1	CB	314	THR	2.1
1	EB	309	ASN	2.1
1	IC	389	VAL	2.1
1	EC	288	GLY	2.1
1	IC	336	GLN	2.1
1	GC	313	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	LC	194	ASP	2.1
1	MC	391	ASP	2.1
1	BC	357	HIS	2.1
1	MC	396	HIS	2.1
1	HB	314	THR	2.1
1	NA	172	ASN	2.1
1	OC	309	ASN	2.1
1	EA	444	TYR	2.1
1	GB	394	SER	2.1
1	FA	391	ASP	2.1
1	KC	392	GLY	2.1
1	OC	366	GLN	2.1
1	BC	393	ASN	2.1
1	DC	398	ASN	2.1
1	FA	314	THR	2.1
1	NB	309	ASN	2.1
1	BC	427	PRO	2.1
1	NB	311	TYR	2.1
1	OC	299	TYR	2.1
1	EC	378	GLY	2.1
1	HA	392	GLY	2.1
1	HC	412	THR	2.1
1	JC	363	GLY	2.1
1	MC	392	GLY	2.1
1	JC	331	GLN	2.1
1	FA	307	ASN	2.1
1	OA	399	GLU	2.1
1	AA	394	SER	2.1
1	EC	387	GLY	2.1
1	HB	394	SER	2.1
1	NA	392	GLY	2.1
1	MA	308	TRP	2.0
1	DA	412	THR	2.0
1	EB	412	THR	2.0
1	JB	24	ASN	2.0
1	CC	339	ARG	2.0
1	EC	331	GLN	2.0
1	FC	530	MET	2.0
1	FC	444	TYR	2.0
1	LC	284	CYS	2.0
1	NC	528	ALA	2.0
1	CB	412	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	NB	172	ASN	2.0
1	OB	307	ASN	2.0
1	GC	411	ARG	2.0
1	FB	308	TRP	2.0
1	IC	315	GLU	2.0
1	JC	193	ASP	2.0
1	LB	394	SER	2.0
1	NB	376	GLU	2.0
1	KA	395	ALA	2.0
1	OA	195	VAL	2.0
1	AA	314	THR	2.0
1	HC	345	ARG	2.0
1	CB	312	ASP	2.0
1	GC	311	TYR	2.0
1	OA	411	ARG	2.0
1	JC	370	ASP	2.0
1	BB	309	ASN	2.0
1	JC	380	ASN	2.0
1	HC	339	ARG	2.0
1	OC	362	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	JA	601	4/4	0.72	0.29	69,69,69,69	0
3	CD	MB	601	1/1	0.79	0.07	140,140,140,140	0
2	CL	AA	603	1/1	0.82	0.16	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CD	KA	601	1/1	0.82	0.07	142,142,142,142	0
2	CL	IA	603	1/1	0.85	0.18	78,78,78,78	0
2	CL	CC	603	1/1	0.85	0.09	79,79,79,79	0
2	CL	EA	603	1/1	0.86	0.27	80,80,80,80	0
3	CD	EA	601	1/1	0.88	0.07	144,144,144,144	0
2	CL	CC	602	1/1	0.89	0.15	95,95,95,95	0
3	CD	GB	601	1/1	0.90	0.08	149,149,149,149	0
3	CD	JC	601	1/1	0.90	0.09	176,176,176,176	0
2	CL	AB	601	1/1	0.90	0.21	67,67,67,67	0
2	CL	JA	604	1/1	0.90	0.28	82,82,82,82	0
2	CL	GC	601	1/1	0.90	0.32	63,63,63,63	0
3	CD	JA	602	1/1	0.91	0.06	136,136,136,136	0
2	CL	KC	602	1/1	0.91	0.15	74,74,74,74	0
2	CL	BC	602	1/1	0.91	0.25	55,55,55,55	0
3	CD	EC	601	1/1	0.91	0.17	195,195,195,195	0
2	CL	CC	601	1/1	0.91	0.22	56,56,56,56	0
3	CD	IA	601	1/1	0.92	0.05	135,135,135,135	0
3	CD	KB	601	1/1	0.92	0.07	138,138,138,138	0
3	CD	DA	601	1/1	0.92	0.08	136,136,136,136	0
2	CL	LC	601	1/1	0.92	0.21	59,59,59,59	0
3	CD	BA	601	1/1	0.93	0.07	142,142,142,142	0
3	CD	EB	601	1/1	0.93	0.06	133,133,133,133	0
3	CD	MA	601	1/1	0.93	0.05	138,138,138,138	0
2	CL	DB	601	1/1	0.93	0.11	65,65,65,65	0
3	CD	FA	601	1/1	0.93	0.05	134,134,134,134	0
2	CL	KA	603	1/1	0.94	0.18	76,76,76,76	0
2	CL	EA	604	1/1	0.94	0.31	46,46,46,46	0
3	CD	NC	601	1/1	0.94	0.08	128,128,128,128	0
2	CL	DC	601	1/1	0.94	0.31	56,56,56,56	0
2	CL	AC	602	1/1	0.95	0.18	76,76,76,76	0
3	CD	GA	601	1/1	0.95	0.06	127,127,127,127	0
3	CD	CA	601	1/1	0.95	0.04	136,136,136,136	0
2	CL	MC	602	1/1	0.95	0.22	58,58,58,58	0
3	CD	BC	601	1/1	0.96	0.07	127,127,127,127	0
3	CD	OA	601	1/1	0.96	0.05	139,139,139,139	0
2	CL	LA	601	1/1	0.96	0.17	49,49,49,49	0
2	CL	MA	604	1/1	0.97	0.26	76,76,76,76	0
2	CL	MC	601	1/1	0.97	0.21	54,54,54,54	0
3	CD	HC	601	1/1	0.97	0.05	127,127,127,127	0
2	CL	AA	602	1/1	0.97	0.29	43,43,43,43	0
2	CL	NC	602	1/1	0.97	0.06	68,68,68,68	0
2	CL	JA	603	1/1	0.97	0.21	51,51,51,51	0

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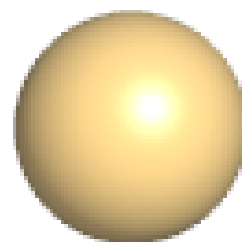
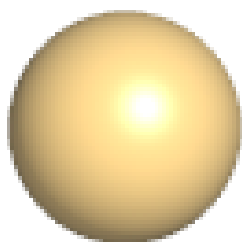
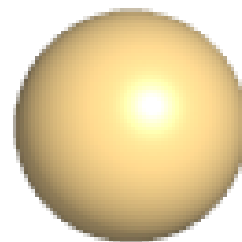
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CL	BA	602	1/1	0.97	0.21	45,45,45,45	0
2	CL	KA	602	1/1	0.97	0.24	48,48,48,48	0
2	CL	FA	603	1/1	0.97	0.22	47,47,47,47	0
2	CL	DC	602	1/1	0.97	0.30	44,44,44,44	0
2	CL	HA	601	1/1	0.97	0.25	48,48,48,48	0
2	CL	HC	602	1/1	0.97	0.41	45,45,45,45	0
2	CL	LC	602	1/1	0.97	0.25	40,40,40,40	0
2	CL	MA	603	1/1	0.98	0.25	50,50,50,50	0
3	CD	FC	601	1/1	0.98	0.04	127,127,127,127	0
2	CL	DA	602	1/1	0.98	0.26	48,48,48,48	0
2	CL	CA	603	1/1	0.98	0.19	44,44,44,44	0
2	CL	JA	605	1/1	0.98	0.30	44,44,44,44	0
2	CL	GA	602	1/1	0.98	0.27	41,41,41,41	0
2	CL	OA	602	1/1	0.98	0.24	50,50,50,50	0
3	CD	AC	601	1/1	0.98	0.07	121,121,121,121	0
2	CL	BA	603	1/1	0.98	0.34	48,48,48,48	0
2	CL	KC	601	1/1	0.98	0.30	42,42,42,42	0
2	CL	AA	601	1/1	0.98	0.24	49,49,49,49	0
2	CL	EA	602	1/1	0.98	0.19	50,50,50,50	0
2	CL	CA	602	1/1	0.98	0.28	42,42,42,42	0
2	CL	IA	604	1/1	0.98	0.33	41,41,41,41	0
2	CL	MA	602	1/1	0.98	0.32	41,41,41,41	0
2	CL	OA	603	1/1	0.99	0.30	47,47,47,47	0
2	CL	GC	602	1/1	0.99	0.41	46,46,46,46	0
2	CL	NA	601	1/1	0.99	0.31	37,37,37,37	0
2	CL	NA	602	1/1	0.99	0.25	42,42,42,42	0
2	CL	IA	602	1/1	0.99	0.25	47,47,47,47	0
2	CL	FA	602	1/1	0.99	0.30	42,42,42,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

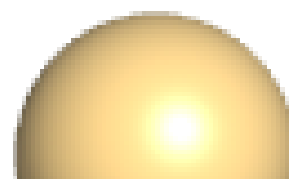
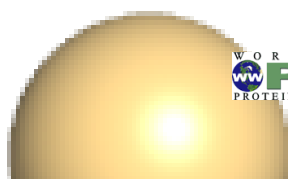
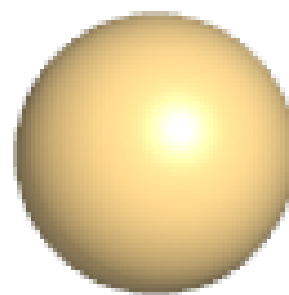
Electron density around CD MB 601:

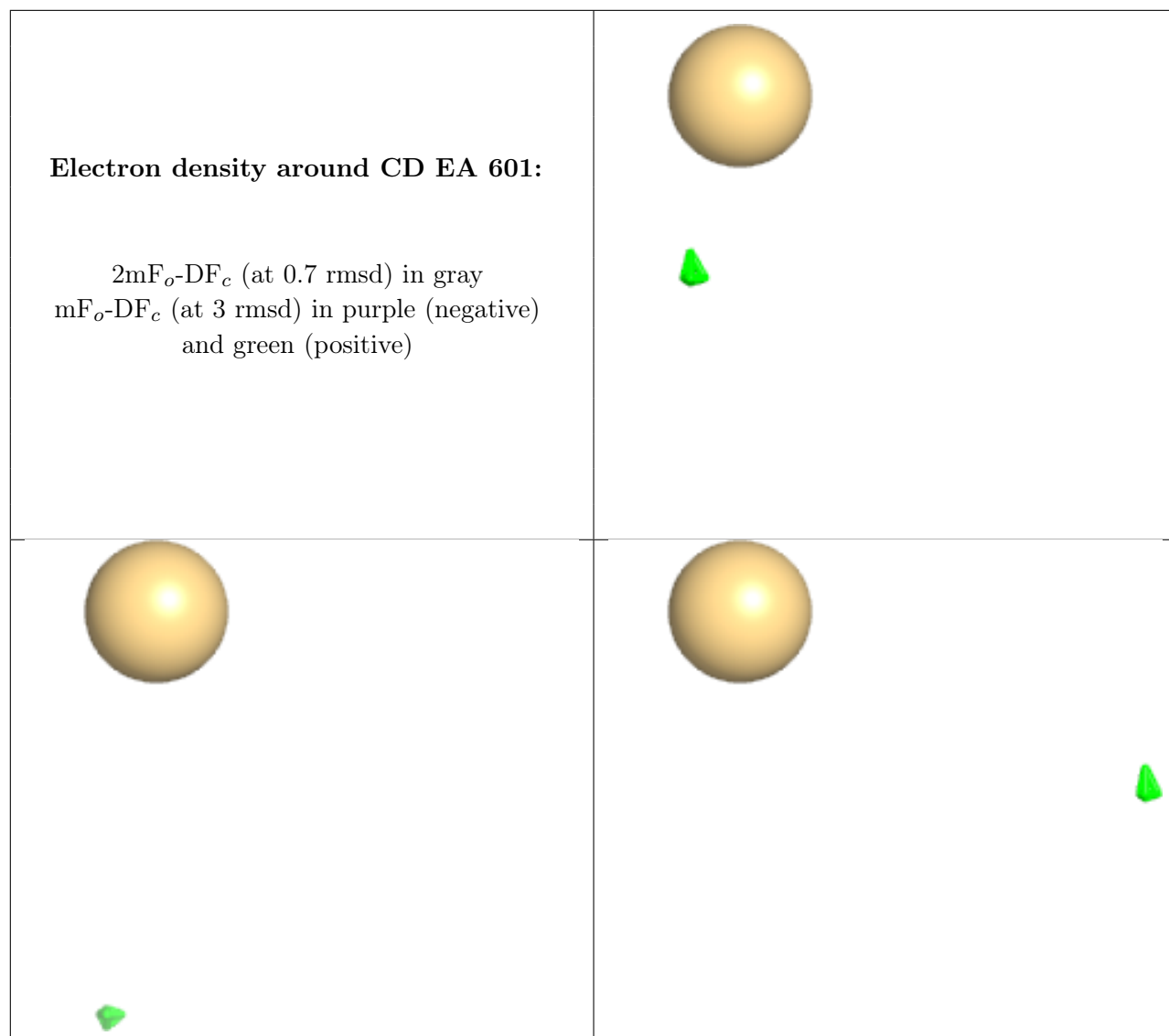
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CD KA 601:

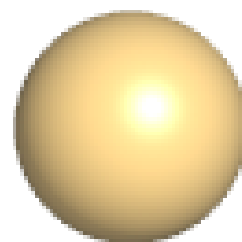
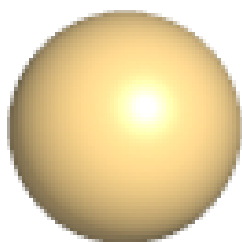
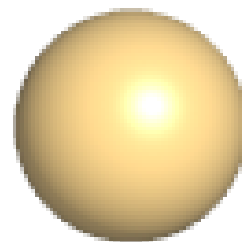
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





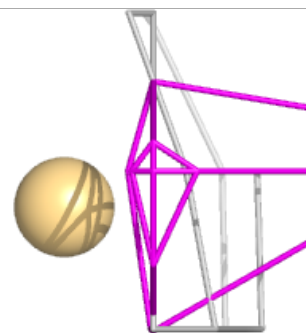
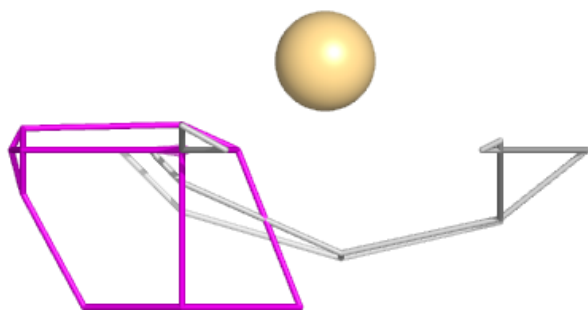
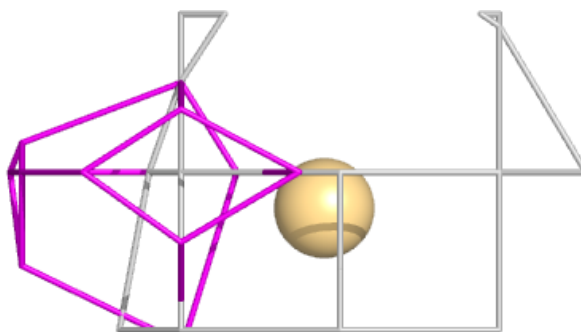
Electron density around CD GB 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



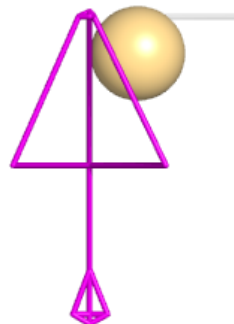
Electron density around CD JC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



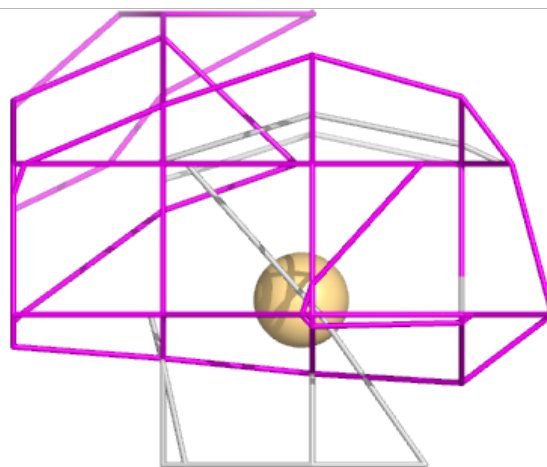
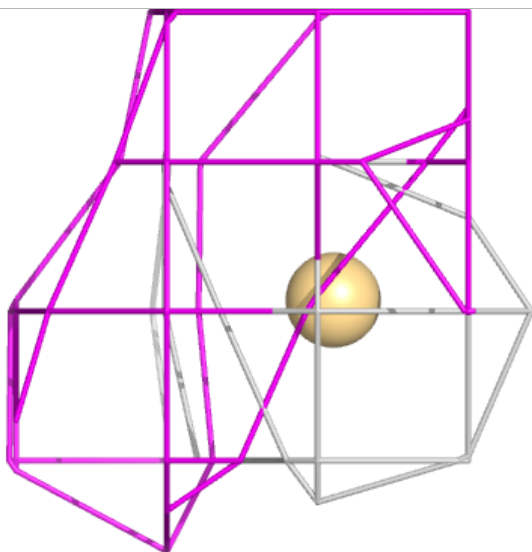
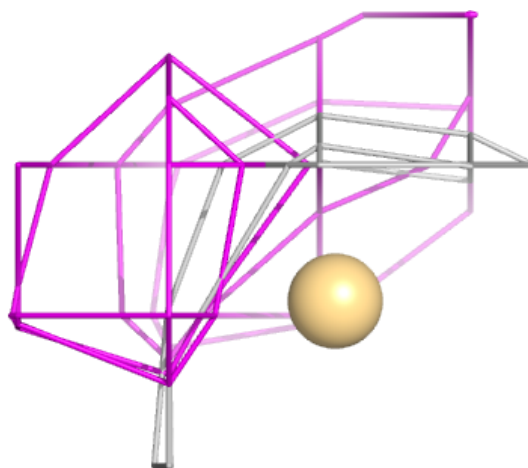
Electron density around CD JA 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



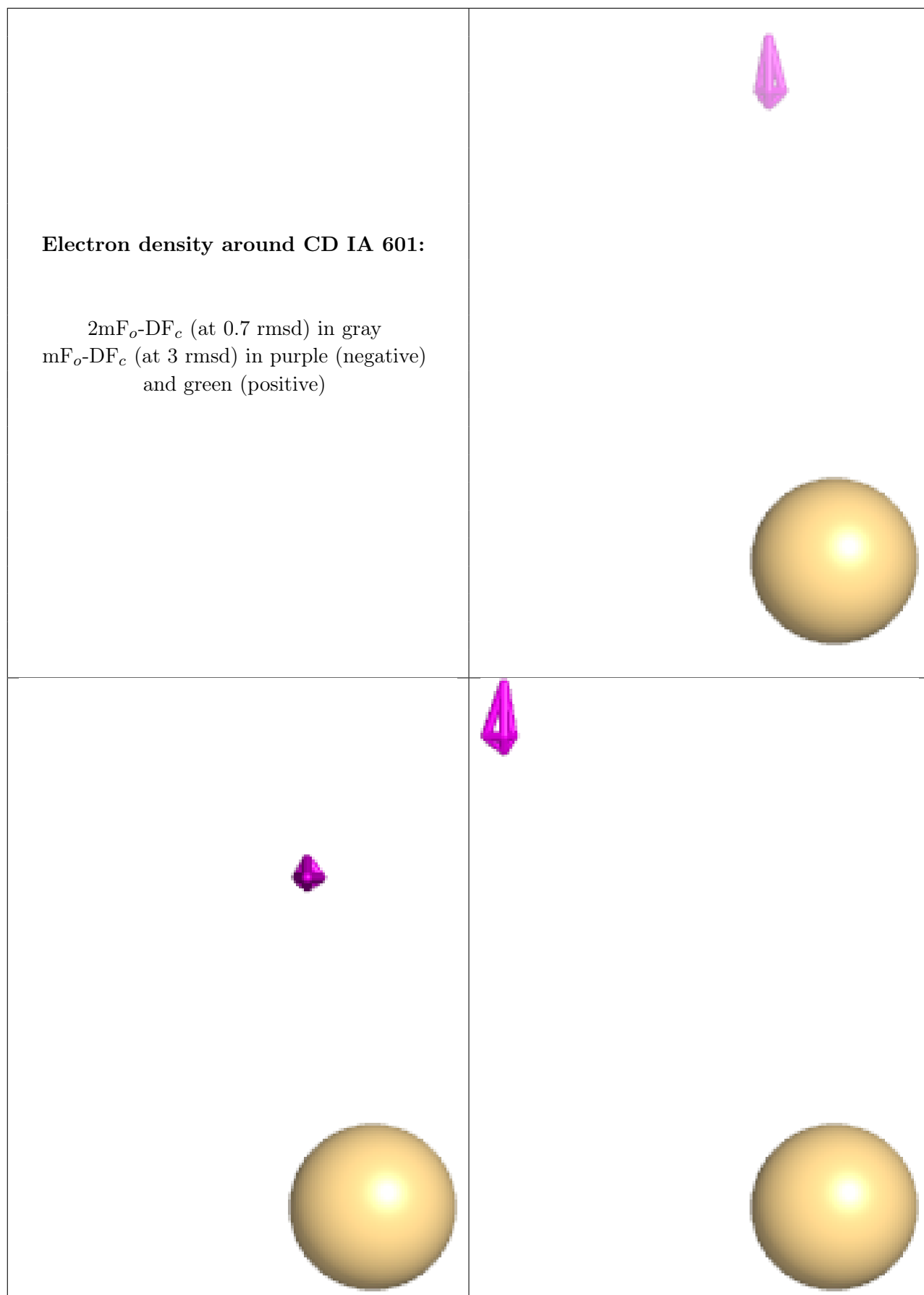
Electron density around CD EC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



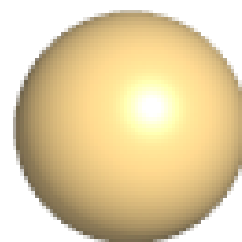
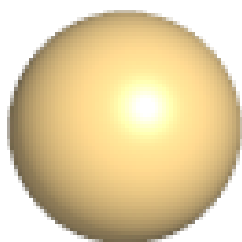
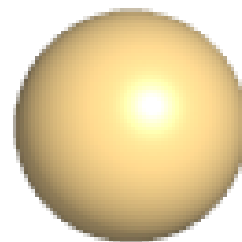
Electron density around CD IA 601:

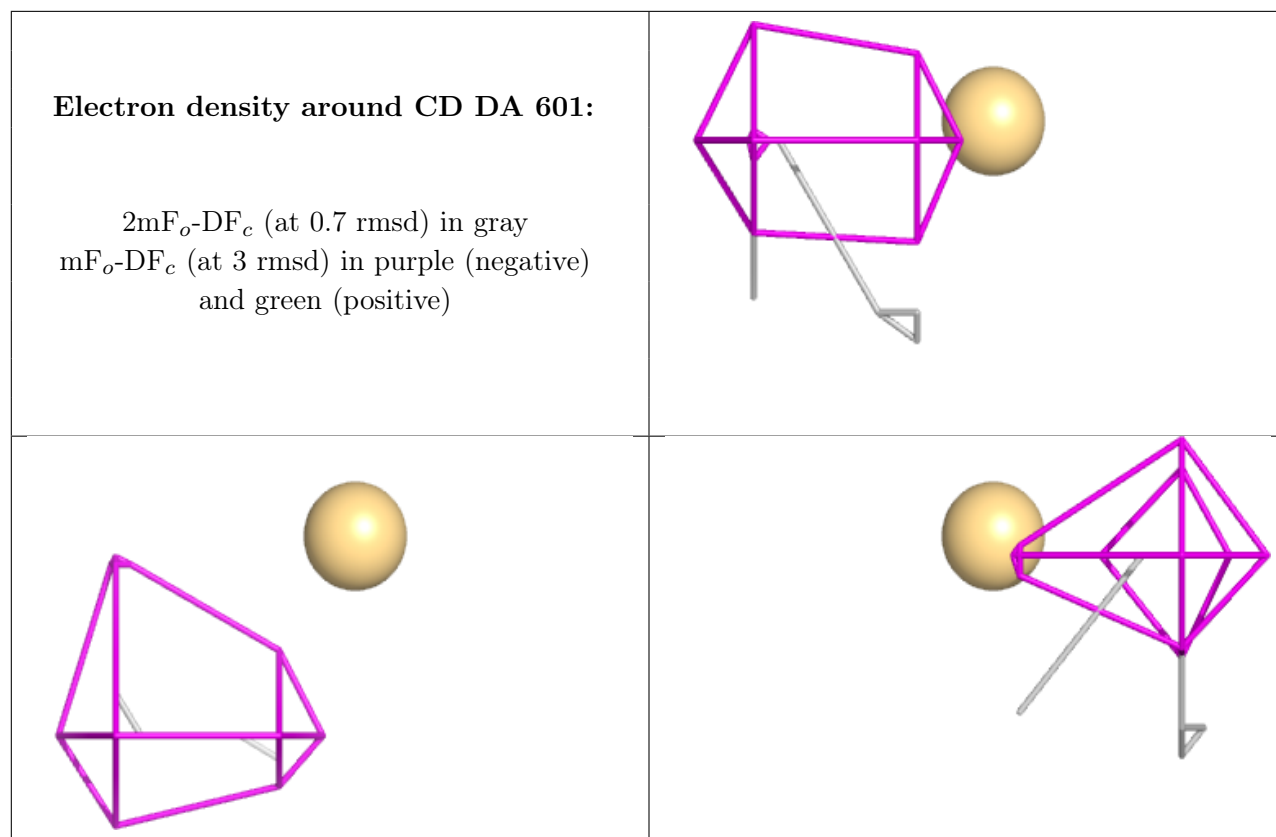
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CD KB 601:

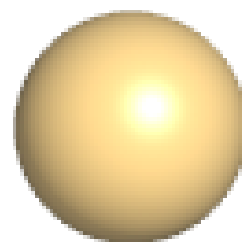
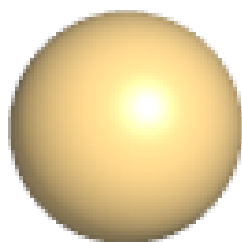
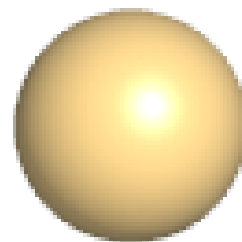
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





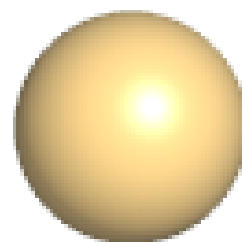
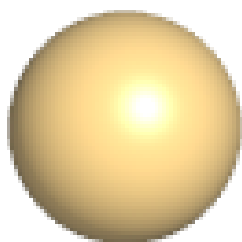
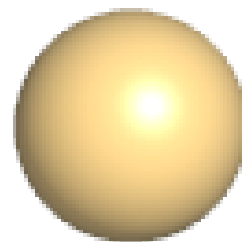
Electron density around CD BA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



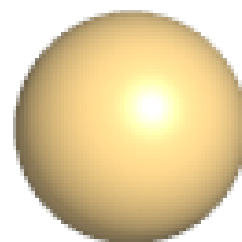
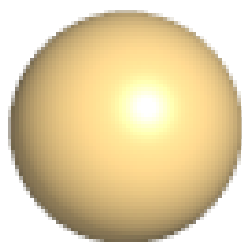
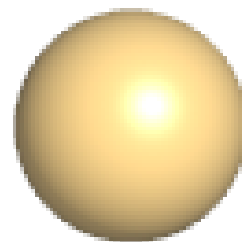
Electron density around CD EB 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



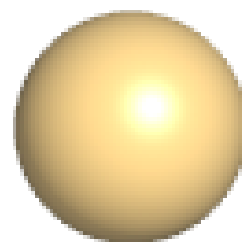
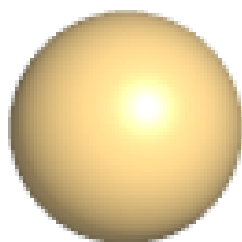
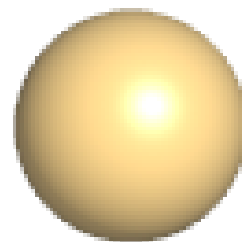
Electron density around CD MA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



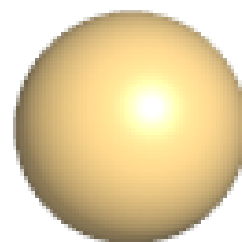
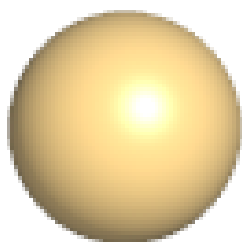
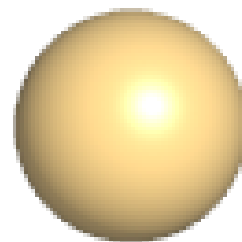
Electron density around CD FA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



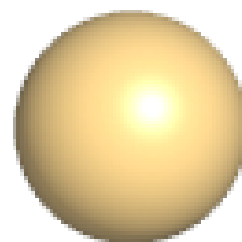
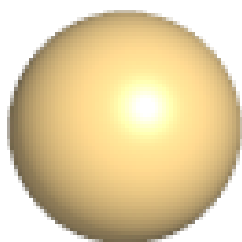
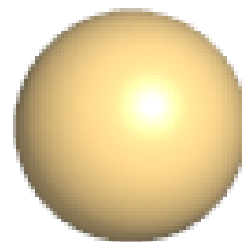
Electron density around CD NC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



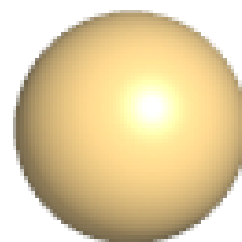
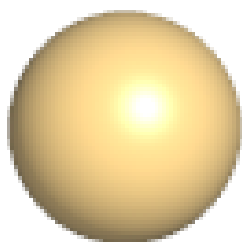
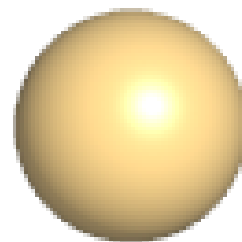
Electron density around CD GA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



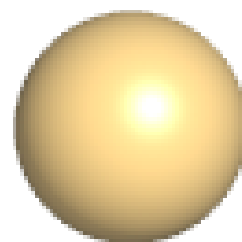
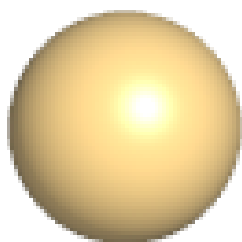
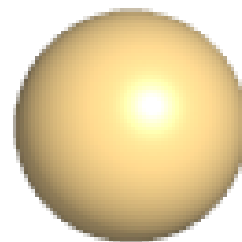
Electron density around CD CA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



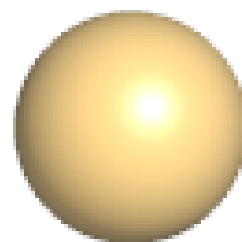
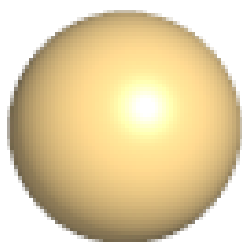
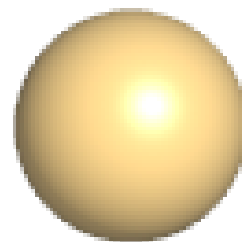
Electron density around CD BC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



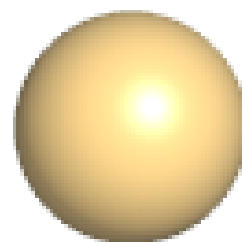
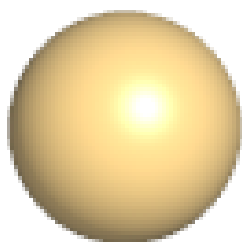
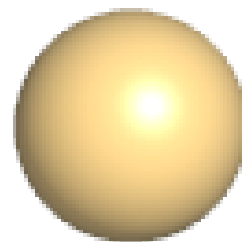
Electron density around CD OA 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



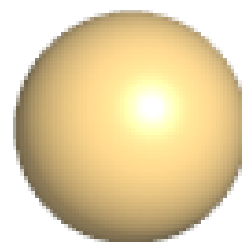
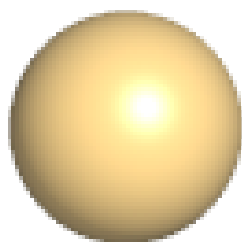
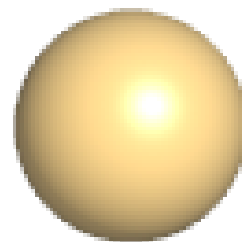
Electron density around CD HC 601:

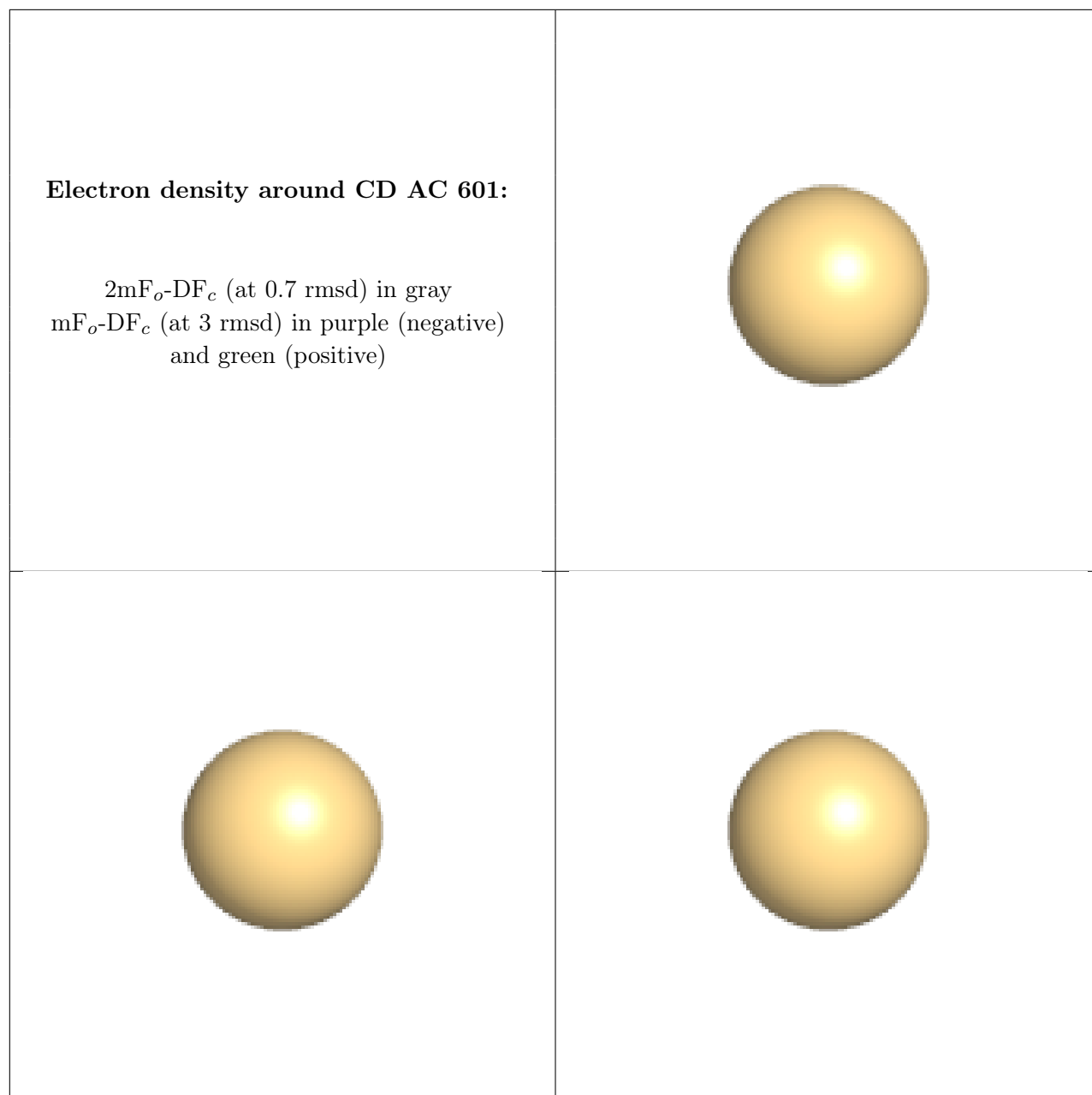
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CD FC 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.