



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 08:07 PM EDT

PDB ID : 4IQJ
Title : Structure of PolIIIalpha-Tauc-DNA complex suggests an atomic model of the replisome
Authors : Liu, B.; Lin, J.; Steitz, T.
Deposited on : 2013-01-11
Resolution : 3.20 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	:	2.27
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)	:	2.27

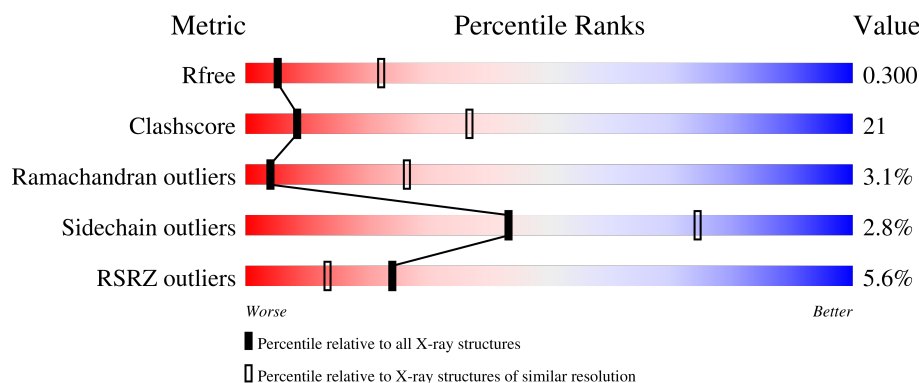
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	E	20	<div> <div>5%</div> <div>90%</div> <div>10%</div> </div>
1	G	20	<div> <div>15%</div> <div>75%</div> <div>20%</div> <div>5%</div> </div>
1	K	20	<div> <div>15%</div> <div>90%</div> <div>10%</div> </div>
2	F	28	<div> <div>18%</div> <div>50%</div> <div>14%</div> <div>7%</div> <div>29%</div> </div>
2	H	28	<div> <div>25%</div> <div>82%</div> <div>11%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	28	
2	L	28	
3	I	21	
4	A	1220	
4	B	1220	
4	C	1220	
4	D	1220	
5	M	177	
5	N	177	
5	O	177	
5	P	177	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DOC	I	21	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 45265 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 DNA chain called DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	20	Total	C	N	O	P	0	0	0
			411	193	83	115	20			
1	G	20	Total	C	N	O	P	0	0	0
			411	193	83	115	20			
1	K	20	Total	C	N	O	P	0	0	0
			411	193	83	115	20			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	20	Total	C	N	O	P	0	0	0
			409	194	70	125	20			
2	H	27	Total	C	N	O	P	0	0	0
			551	264	87	173	27			
2	J	23	Total	C	N	O	P	0	0	0
			471	224	79	145	23			
2	L	24	Total	C	N	O	P	0	0	0
			491	234	81	152	24			

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*AP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	21	Total	C	N	O	P	0	0	0
			429	202	86	120	21			

- Molecule 4 is a protein called DNA polymerase III subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1164	Total	C	N	O	S	0	0	0
			9280	5918	1620	1714	28			
4	B	1167	Total	C	N	O	S	0	0	0
			9295	5926	1623	1716	30			
4	C	1166	Total	C	N	O	S	0	0	0
			9293	5930	1621	1714	28			
4	D	1185	Total	C	N	O	S	0	0	0
			9445	6026	1651	1738	30			

- Molecule 5 is a protein called DNA polymerase III subunit gamma/tau.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	138	Total	C	N	O	S	0	0	0
			1103	702	203	197	1			
5	N	135	Total	C	N	O	S	0	0	0
			1078	687	200	190	1			
5	O	135	Total	C	N	O	S	0	0	0
			1078	687	200	190	1			
5	P	138	Total	C	N	O	S	0	0	0
			1093	695	203	194	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	367	HIS	-	expression tag	UNP A0A0M9ACL9
M	368	HIS	-	expression tag	UNP A0A0M9ACL9
M	369	HIS	-	expression tag	UNP A0A0M9ACL9
M	370	HIS	-	expression tag	UNP A0A0M9ACL9
M	371	HIS	-	expression tag	UNP A0A0M9ACL9
M	372	HIS	-	expression tag	UNP A0A0M9ACL9
M	373	LYS	GLU	conflict	UNP A0A0M9ACL9
M	541	MET	-	expression tag	UNP A0A0M9ACL9
M	542	PRO	-	expression tag	UNP A0A0M9ACL9
M	543	PRO	-	expression tag	UNP A0A0M9ACL9
N	367	HIS	-	expression tag	UNP A0A0M9ACL9
N	368	HIS	-	expression tag	UNP A0A0M9ACL9
N	369	HIS	-	expression tag	UNP A0A0M9ACL9
N	370	HIS	-	expression tag	UNP A0A0M9ACL9
N	371	HIS	-	expression tag	UNP A0A0M9ACL9
N	372	HIS	-	expression tag	UNP A0A0M9ACL9
N	373	LYS	GLU	conflict	UNP A0A0M9ACL9
N	541	MET	-	expression tag	UNP A0A0M9ACL9
N	542	PRO	-	expression tag	UNP A0A0M9ACL9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	543	PRO	-	expression tag	UNP A0A0M9ACL9
O	367	HIS	-	expression tag	UNP A0A0M9ACL9
O	368	HIS	-	expression tag	UNP A0A0M9ACL9
O	369	HIS	-	expression tag	UNP A0A0M9ACL9
O	370	HIS	-	expression tag	UNP A0A0M9ACL9
O	371	HIS	-	expression tag	UNP A0A0M9ACL9
O	372	HIS	-	expression tag	UNP A0A0M9ACL9
O	373	LYS	GLU	conflict	UNP A0A0M9ACL9
O	541	MET	-	expression tag	UNP A0A0M9ACL9
O	542	PRO	-	expression tag	UNP A0A0M9ACL9
O	543	PRO	-	expression tag	UNP A0A0M9ACL9
P	367	HIS	-	expression tag	UNP A0A0M9ACL9
P	368	HIS	-	expression tag	UNP A0A0M9ACL9
P	369	HIS	-	expression tag	UNP A0A0M9ACL9
P	370	HIS	-	expression tag	UNP A0A0M9ACL9
P	371	HIS	-	expression tag	UNP A0A0M9ACL9
P	372	HIS	-	expression tag	UNP A0A0M9ACL9
P	373	LYS	GLU	conflict	UNP A0A0M9ACL9
P	541	MET	-	expression tag	UNP A0A0M9ACL9
P	542	PRO	-	expression tag	UNP A0A0M9ACL9
P	543	PRO	-	expression tag	UNP A0A0M9ACL9

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Zn 3 3	0	0
6	B	3	Total Zn 3 3	0	0
6	C	3	Total Zn 3 3	0	0
6	D	3	Total Zn 3 3	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	Mg 1	0	0
7	D	1	Total 1	Mg 1	0	0

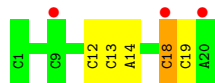
3 Residue-property plots [i](#)

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

- Molecule 1: DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*T P*GP*CP*CP*A)-3')



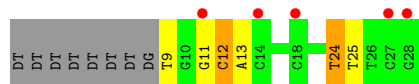
- Molecule 1: DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*T P*GP*CP*CP*A)-3')



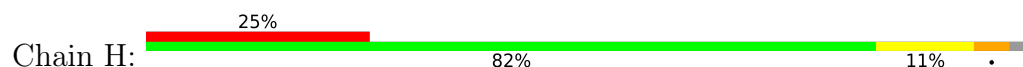
- Molecule 1: DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*T P*GP*CP*CP*A)-3')

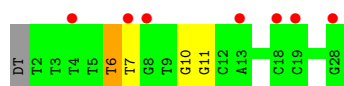


- Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP *GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3')

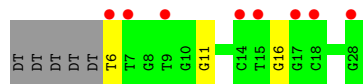


- Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP *GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3')

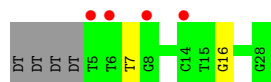
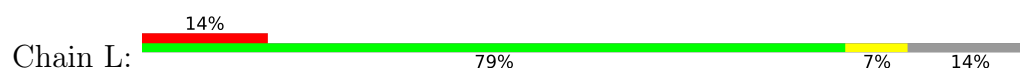




- Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3')



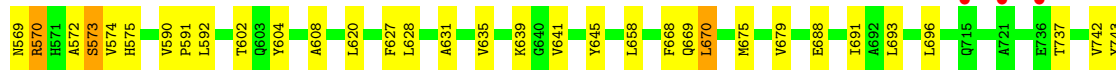
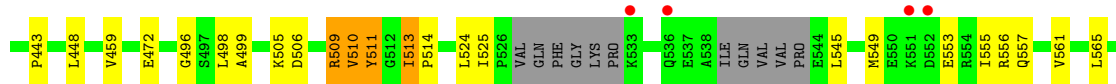
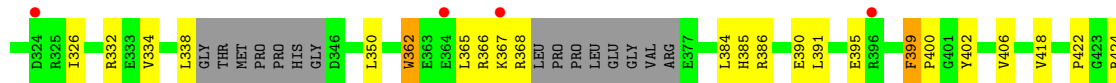
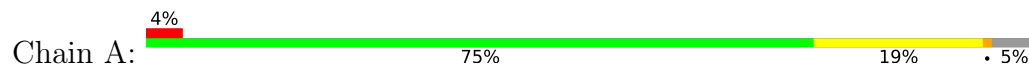
- Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*GP*TP*GP*GP*CP*AP*CP*TP*GP*GP*CP*CP*GP*TP*CP*GP*TP*TP*TP*CP*G)-3')

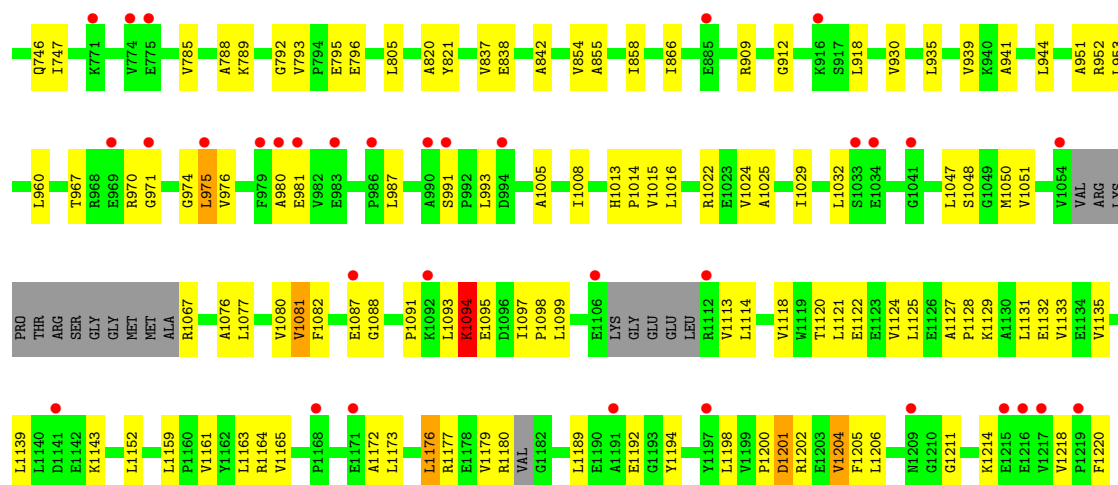


- Molecule 3: DNA (5'-D(P*CP*GP*AP*AP*AP*CP*GP*AP*CP*GP*GP*CP*CP*AP*GP*TP*P*GP*CP*CP*AP*(DOC))-3')

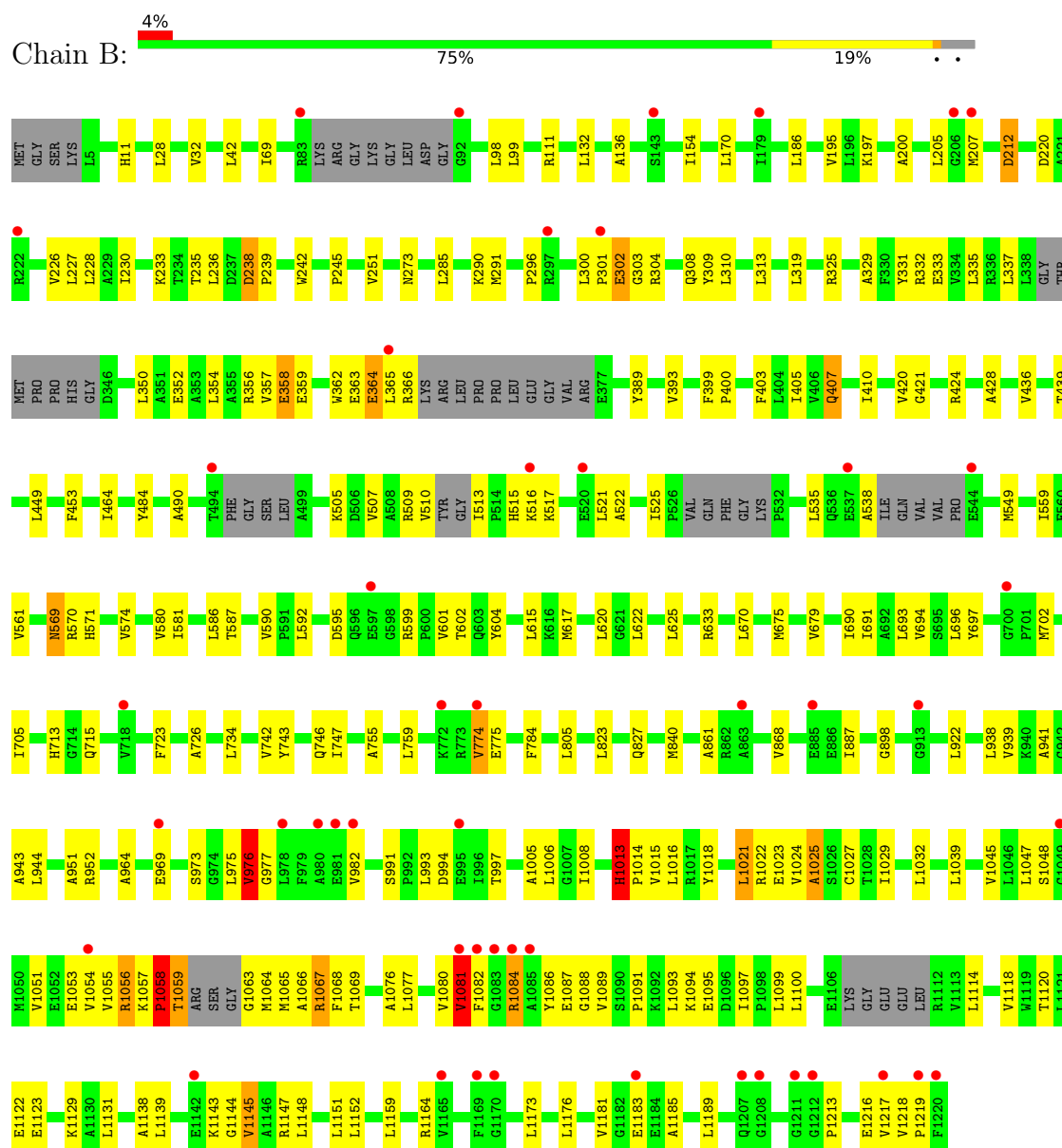


- Molecule 4: DNA polymerase III subunit alpha

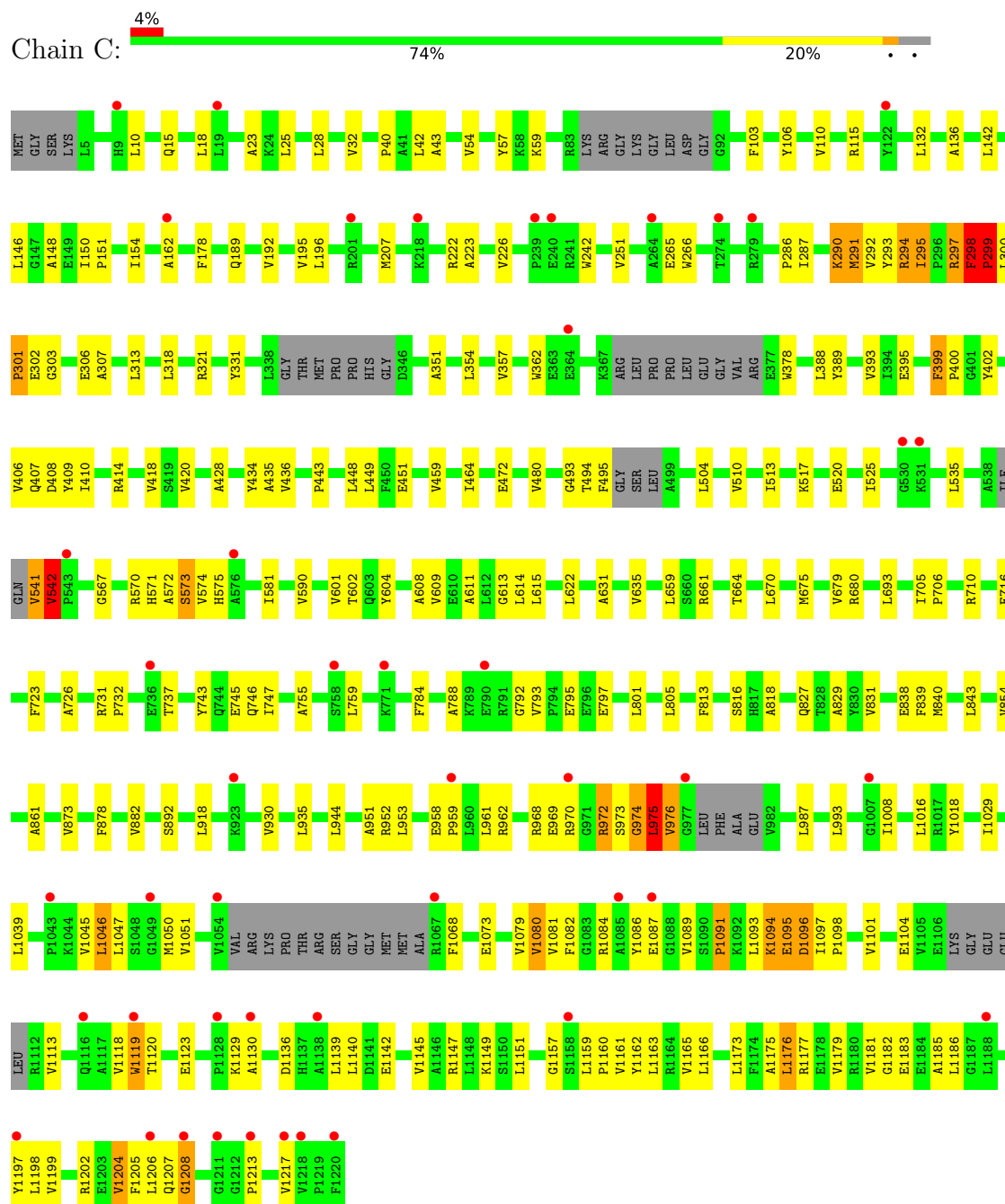




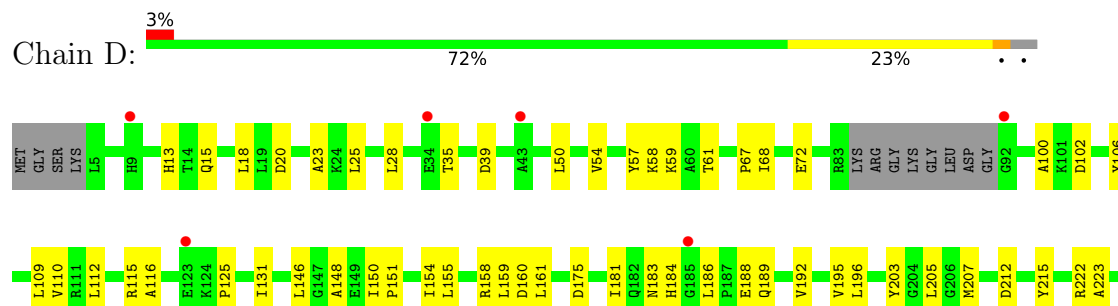
• Molecule 4: DNA polymerase III subunit alpha

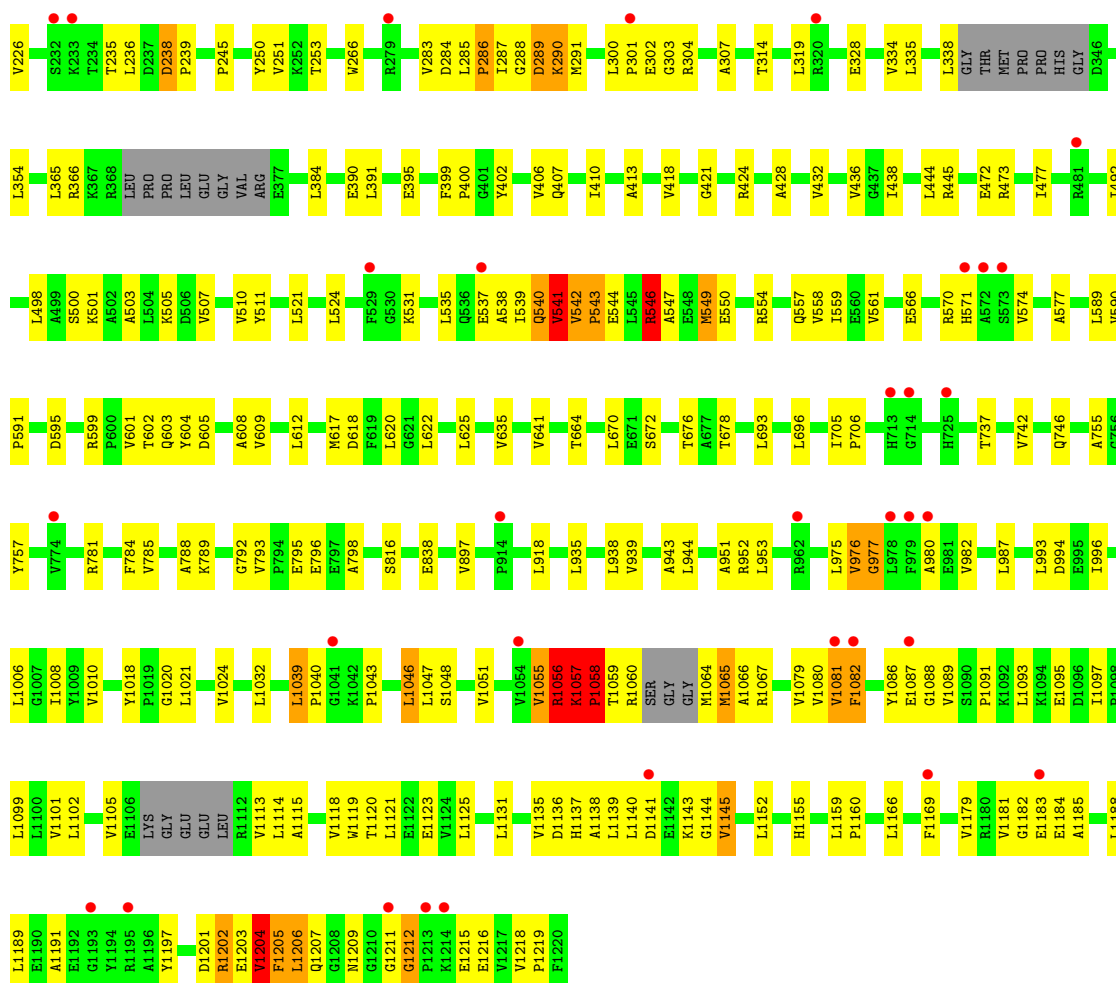


• Molecule 4: DNA polymerase III subunit alpha

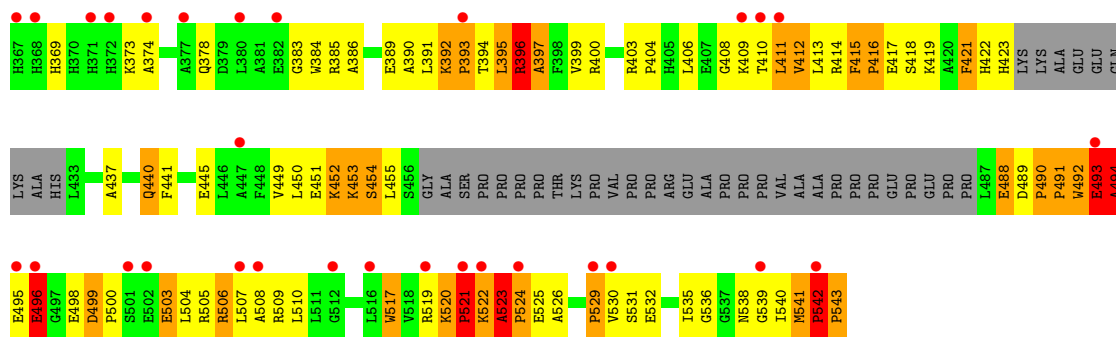
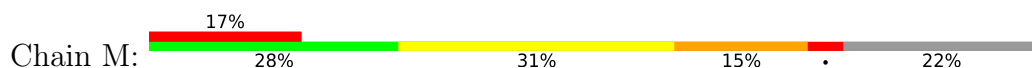


• Molecule 4: DNA polymerase III subunit alpha

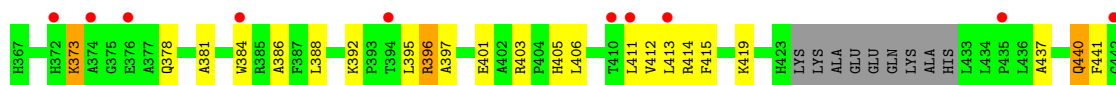


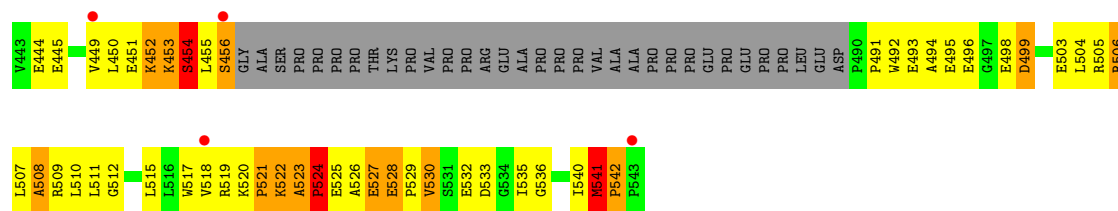


• Molecule 5: DNA polymerase III subunit gamma/tau

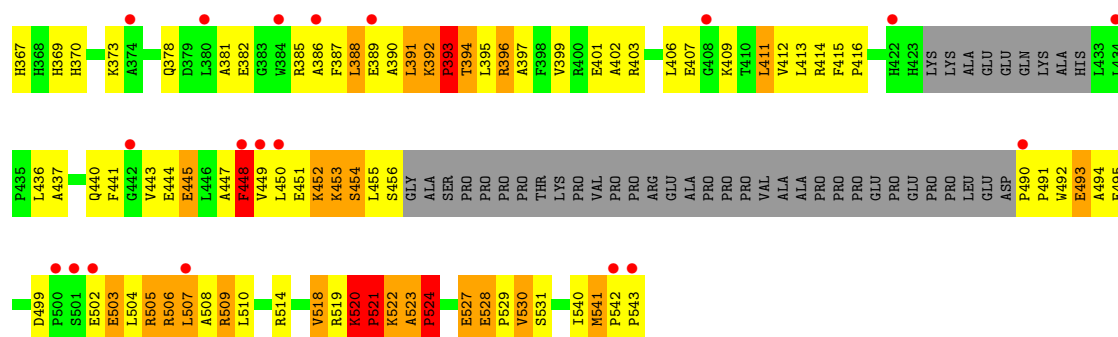
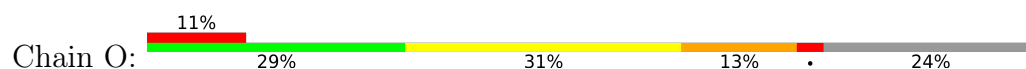


• Molecule 5: DNA polymerase III subunit gamma/tau

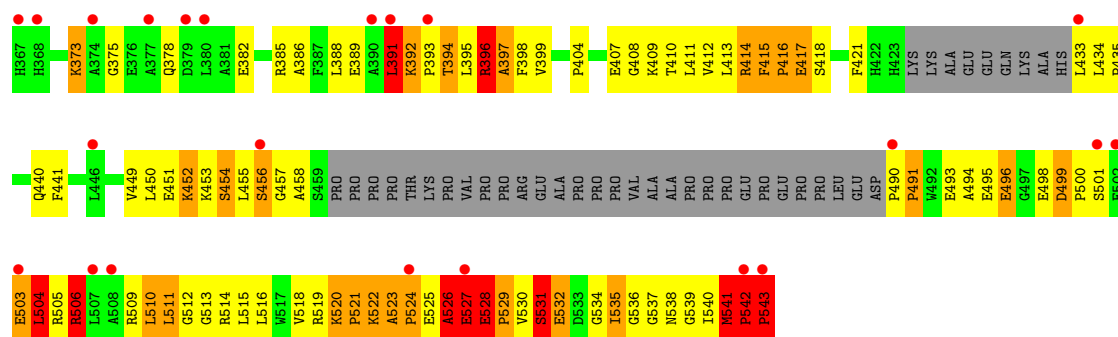
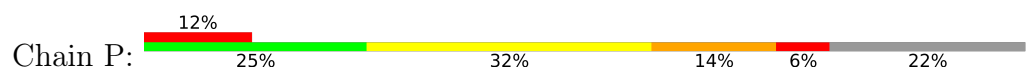




● Molecule 5: DNA polymerase III subunit gamma/tau



● Molecule 5: DNA polymerase III subunit gamma/tau



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	188.53Å 94.97Å 204.08Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-3.20) 96.0 (20.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.90 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.264 , 0.305 0.258 , 0.300	Depositor DCC
R_{free} test set	5710 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	99.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	45265	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: DOC, MG, ZN

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	E	0.31	0/462	0.78	0/710
1	G	0.34	0/462	0.81	1/710 (0.1%)
1	K	0.30	0/462	0.80	1/710 (0.1%)
2	F	0.31	0/456	0.88	2/702 (0.3%)
2	H	0.41	0/613	0.84	1/945 (0.1%)
2	J	0.34	0/525	0.85	1/809 (0.1%)
2	L	0.38	0/547	0.80	0/843
3	I	0.33	0/462	0.80	1/710 (0.1%)
4	A	0.50	2/9466 (0.0%)	0.60	5/12781 (0.0%)
4	B	0.50	1/9480 (0.0%)	0.61	2/12800 (0.0%)
4	C	0.51	3/9481 (0.0%)	0.61	3/12805 (0.0%)
4	D	0.52	1/9638 (0.0%)	0.62	10/13019 (0.1%)
5	M	0.85	7/1133 (0.6%)	1.06	11/1528 (0.7%)
5	N	0.63	0/1108	0.80	3/1493 (0.2%)
5	O	0.69	0/1108	0.87	5/1493 (0.3%)
5	P	0.82	2/1123 (0.2%)	1.05	7/1513 (0.5%)
All	All	0.53	16/46526 (0.0%)	0.67	53/63571 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1
4	B	0	1
4	C	0	3
4	D	0	4
5	M	0	7
5	N	0	1
5	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	P	0	7
All	All	0	26

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	543	PRO	N-CD	5.93	1.56	1.47
5	M	524	PRO	N-CD	5.75	1.55	1.47
5	M	416	PRO	N-CD	5.70	1.55	1.47
4	A	31	TRP	CD2-CE2	5.58	1.48	1.41
4	D	1058	PRO	N-CD	5.57	1.55	1.47
5	M	491	PRO	N-CD	5.44	1.55	1.47
5	M	517	TRP	CD2-CE2	5.43	1.47	1.41
5	M	543	PRO	N-CD	5.33	1.55	1.47
4	B	1058	PRO	N-CD	5.22	1.55	1.47
4	C	1119	TRP	CD2-CE2	5.21	1.47	1.41
5	P	524	PRO	N-CD	5.20	1.55	1.47
4	C	242	TRP	CD2-CE2	5.16	1.47	1.41
5	M	523	ALA	C-N	5.14	1.44	1.34
4	A	362	TRP	CD2-CE2	5.09	1.47	1.41
5	M	384	TRP	CD2-CE2	5.07	1.47	1.41
4	C	378	TRP	CD2-CE2	5.03	1.47	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	212	ASP	CB-CG-OD1	9.95	127.25	118.30
2	F	24	DT	P-O3'-C3'	9.83	131.50	119.70
5	P	541	MET	C-N-CD	8.76	146.79	128.40
5	P	415	PHE	C-N-CD	8.45	146.15	128.40
5	M	541	MET	C-N-CD	8.39	146.02	128.40
4	A	796	GLU	N-CA-C	-7.96	89.50	111.00
1	G	18	DC	P-O3'-C3'	7.73	128.97	119.70
2	F	12	DC	P-O3'-C3'	7.63	128.85	119.70
5	M	493	GLU	N-CA-C	7.27	130.64	111.00
2	H	6	DT	P-O3'-C3'	7.11	128.23	119.70
5	P	542	PRO	CA-N-CD	-7.08	101.58	111.50
4	D	542	VAL	N-CA-C	7.03	129.97	111.00
5	N	541	MET	C-N-CD	-6.90	105.43	120.60
5	O	523	ALA	C-N-CD	-6.59	106.11	120.60
5	M	542	PRO	CA-N-CD	-6.54	102.34	111.50
5	P	524	PRO	CA-N-CD	-6.53	102.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	494	ALA	N-CA-C	-6.45	93.59	111.00
5	O	520	LYS	C-N-CD	6.27	141.57	128.40
5	P	416	PRO	CA-N-CD	-6.22	102.80	111.50
5	O	524	PRO	CA-N-CD	-6.15	102.89	111.50
4	C	298	PHE	C-N-CD	6.12	141.25	128.40
4	D	1212	GLY	C-N-CD	6.03	141.07	128.40
4	D	1058	PRO	CA-N-CD	-6.00	103.11	111.50
4	C	295	ILE	C-N-CD	5.90	140.78	128.40
2	J	6	DT	P-O3'-C3'	5.89	126.77	119.70
5	M	520	LYS	C-N-CD	5.85	140.68	128.40
4	A	670	LEU	N-CA-CB	5.79	121.98	110.40
5	M	521	PRO	CA-N-CD	-5.75	103.45	111.50
4	A	796	GLU	N-CA-CB	5.69	120.85	110.60
1	K	17	DG	P-O3'-C3'	5.69	126.53	119.70
5	P	526	ALA	N-CA-C	5.62	126.17	111.00
5	N	524	PRO	CA-N-CD	-5.55	103.73	111.50
5	N	384	TRP	N-CA-C	5.53	125.93	111.00
5	M	392	LYS	C-N-CD	-5.52	108.45	120.60
5	M	542	PRO	C-N-CD	5.52	140.00	128.40
4	D	1056	ARG	O-C-N	-5.48	113.92	122.70
5	O	508	ALA	N-CA-C	5.37	125.51	111.00
5	M	490	PRO	C-N-CD	5.32	139.57	128.40
4	D	1056	ARG	C-N-CA	-5.32	108.41	121.70
4	D	20	ASP	CB-CG-OD1	-5.30	113.53	118.30
4	A	20	ASP	CB-CG-OD2	5.28	123.05	118.30
4	D	542	VAL	N-CA-CB	-5.27	99.90	111.50
4	D	796	GLU	N-CA-C	-5.25	96.81	111.00
4	C	975	LEU	C-N-CA	-5.21	108.68	121.70
5	O	521	PRO	CA-N-CD	-5.20	104.21	111.50
4	D	1184	GLU	N-CA-C	-5.11	97.19	111.00
5	P	542	PRO	C-N-CD	5.09	139.09	128.40
5	M	415	PHE	C-N-CD	5.09	139.09	128.40
4	B	1058	PRO	CA-N-CD	-5.08	104.38	111.50
3	I	18	DC	P-O3'-C3'	5.08	125.79	119.70
4	A	212	ASP	CB-CG-OD1	5.07	122.86	118.30
4	D	212	ASP	CB-CG-OD1	5.05	122.85	118.30
5	M	541	MET	N-CA-C	5.02	124.56	111.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	570	ARG	Peptide
4	B	1084	ARG	Sidechain
4	C	1080	VAL	Peptide
4	C	972	ARG	Mainchain
4	C	974	GLY	Peptide
4	D	1057	LYS	Peptide
4	D	1206	LEU	Peptide
4	D	541	VAL	Peptide
4	D	546	ARG	Sidechain
5	M	396	ARG	Peptide
5	M	397	ALA	Peptide
5	M	412	VAL	Peptide
5	M	493	GLU	Mainchain,Peptide
5	M	494	ALA	Mainchain
5	M	521	PRO	Peptide
5	N	508	ALA	Peptide
5	O	507	LEU	Peptide
5	O	509	ARG	Sidechain
5	P	391	LEU	Peptide
5	P	394	THR	Peptide
5	P	411	LEU	Mainchain,Peptide
5	P	504	LEU	Peptide
5	P	506	ARG	Peptide
5	P	531	SER	Peptide

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	E	411	0	222	2	0
1	G	411	0	222	5	0
1	K	411	0	222	1	0
2	F	409	0	227	5	0
2	H	551	0	310	4	0
2	J	471	0	262	2	0
2	L	491	0	274	2	0
3	I	429	0	233	5	0
4	A	9280	0	9298	227	2
4	B	9295	0	9323	298	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	9293	0	9318	274	0
4	D	9445	0	9488	387	2
5	M	1103	0	1085	176	0
5	N	1078	0	1065	134	1
5	O	1078	0	1065	143	0
5	P	1093	0	1078	208	2
6	A	3	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	45265	0	43692	1851	7

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 21.

All (1851) 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)
5:P:528:GLU:CG	5:P:529:PRO:HD3	1.29	1.53
5:O:387:PHE:CE2	5:O:441:PHE:CE2	2.03	1.47
4:D:1080:VAL:HG11	4:D:1082:PHE:CE2	1.50	1.45
5:P:523:ALA:CB	5:P:524:PRO:HA	1.38	1.43
4:D:1080:VAL:HA	4:D:1081:VAL:CG2	1.47	1.41
4:D:549:MET:CE	4:D:559:ILE:HD12	1.49	1.40
4:D:1082:PHE:CE1	4:D:1114:LEU:HG	1.58	1.39
5:O:519:ARG:HD3	5:O:520:LYS:NZ	1.35	1.35
4:D:1066:ALA:O	4:D:1081:VAL:HG13	1.27	1.30
5:N:523:ALA:CB	5:N:524:PRO:HA	1.63	1.29
4:D:1080:VAL:HA	4:D:1081:VAL:CB	1.59	1.27
5:P:524:PRO:HD2	5:P:525:GLU:O	1.30	1.25
4:D:1082:PHE:HE1	4:D:1114:LEU:CD1	1.51	1.24
4:D:1057:LYS:HG2	4:D:1064:MET:CA	1.67	1.23
4:B:1066:ALA:O	4:B:1081:VAL:HB	1.32	1.22
4:D:1057:LYS:CG	4:D:1064:MET:HA	1.69	1.22
4:D:1082:PHE:HE1	4:D:1114:LEU:CG	1.52	1.21
4:D:549:MET:CE	4:D:559:ILE:CD1	2.19	1.21
4:D:1082:PHE:CE1	4:D:1114:LEU:CG	2.23	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:492:TRP:O	5:M:493:GLU:HG2	1.37	1.20
4:B:357:VAL:HG12	4:B:358:GLU:HG3	1.21	1.19
4:D:1080:VAL:CA	4:D:1081:VAL:HG23	1.72	1.19
5:N:505:ARG:HD3	5:N:510:LEU:HD23	1.19	1.18
4:A:971:GLY:HA2	4:A:975:LEU:CB	1.74	1.17
4:B:1057:LYS:HE2	4:B:1064:MET:HE2	1.25	1.17
5:O:519:ARG:CD	5:O:520:LYS:HZ3	1.56	1.17
5:P:524:PRO:HD2	5:P:525:GLU:C	1.63	1.17
4:B:1056:ARG:HG3	4:B:1057:LYS:CG	1.75	1.16
5:O:387:PHE:CZ	5:O:441:PHE:CE2	2.32	1.16
5:O:519:ARG:CD	5:O:520:LYS:NZ	2.06	1.16
5:P:528:GLU:CG	5:P:529:PRO:CD	2.24	1.15
5:P:523:ALA:HB3	5:P:524:PRO:HA	1.27	1.15
4:D:549:MET:HE3	4:D:559:ILE:CD1	1.73	1.15
4:B:1066:ALA:O	4:B:1081:VAL:CB	1.94	1.13
4:C:1080:VAL:HG12	4:C:1082:PHE:CD2	1.81	1.13
4:B:357:VAL:HB	4:B:358:GLU:HB2	1.20	1.13
5:P:505:ARG:HB3	5:P:510:LEU:HD12	1.31	1.13
5:P:523:ALA:CB	5:P:524:PRO:CA	2.25	1.13
4:D:1080:VAL:HA	4:D:1081:VAL:HG23	1.23	1.12
5:O:450:LEU:HB3	5:O:451:GLU:C	1.69	1.12
4:B:1159:LEU:HD11	4:B:1183:GLU:HG3	1.13	1.12
4:A:1080:VAL:CG2	4:A:1114:LEU:HA	1.78	1.11
5:O:388:LEU:HD21	5:O:399:VAL:HG23	1.33	1.11
5:P:505:ARG:HD2	5:P:514:ARG:CZ	1.81	1.10
4:C:1080:VAL:HG12	4:C:1082:PHE:HD2	1.02	1.10
5:P:494:ALA:CB	5:P:495:GLU:HA	1.79	1.10
5:P:528:GLU:HG3	5:P:529:PRO:HD3	1.14	1.10
4:D:537:GLU:O	4:D:540:GLN:HG3	1.53	1.09
5:M:421:PHE:CD2	5:M:422:HIS:ND1	2.20	1.09
5:N:523:ALA:HB1	5:N:524:PRO:CA	1.83	1.09
5:O:387:PHE:CZ	5:O:441:PHE:CD2	2.41	1.08
4:B:1080:VAL:HA	4:B:1081:VAL:HG22	1.11	1.08
4:D:1065:MET:SD	4:D:1082:PHE:HA	1.92	1.08
5:N:506:ARG:HB2	5:N:510:LEU:HB2	1.16	1.08
4:C:1093:LEU:HD11	4:C:1097:ILE:CG2	1.83	1.08
4:D:1080:VAL:CG1	4:D:1082:PHE:CE2	2.35	1.08
4:D:1082:PHE:CE1	4:D:1114:LEU:CD1	2.36	1.08
5:N:494:ALA:CB	5:N:495:GLU:HA	1.82	1.08
4:D:537:GLU:HA	4:D:540:GLN:CG	1.84	1.07
5:P:505:ARG:HD2	5:P:514:ARG:NH2	1.69	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:532:GLU:HA	5:P:535:ILE:HD13	1.36	1.07
5:M:421:PHE:CE2	5:M:422:HIS:ND1	2.20	1.07
5:N:523:ALA:HB1	5:N:524:PRO:HA	1.32	1.07
5:P:505:ARG:CB	5:P:510:LEU:HD12	1.83	1.07
4:A:1080:VAL:HA	4:A:1081:VAL:HB	1.33	1.07
4:D:1080:VAL:CA	4:D:1081:VAL:CG2	2.32	1.06
5:N:505:ARG:CD	5:N:510:LEU:HD23	1.83	1.06
5:P:491:PRO:HB3	5:P:540:ILE:HG21	1.36	1.06
5:O:450:LEU:HB3	5:O:451:GLU:O	1.54	1.06
4:A:572:ALA:HB1	4:A:573:SER:HB2	1.36	1.06
4:B:1056:ARG:CG	4:B:1057:LYS:HG3	1.85	1.06
5:P:524:PRO:CD	5:P:525:GLU:O	2.03	1.06
4:A:572:ALA:HB1	4:A:573:SER:CB	1.84	1.06
4:B:1057:LYS:HB3	4:B:1058:PRO:HA	1.37	1.05
5:M:507:LEU:H	5:M:510:LEU:HD22	1.14	1.05
5:N:523:ALA:HB3	5:N:524:PRO:HA	1.37	1.05
4:C:292:VAL:O	4:C:294:ARG:NH2	1.88	1.05
5:M:519:ARG:HB3	5:M:520:LYS:HB2	1.08	1.05
5:N:524:PRO:HD2	5:N:525:GLU:HA	1.30	1.05
4:C:972:ARG:O	4:C:974:GLY:N	1.89	1.05
5:N:508:ALA:HA	5:N:510:LEU:H	1.19	1.05
4:A:1080:VAL:HG22	4:A:1114:LEU:HA	1.35	1.04
4:D:498:LEU:HD21	4:D:503:ALA:HB2	1.38	1.04
4:B:1057:LYS:HG2	4:B:1064:MET:CA	1.88	1.04
5:P:412:VAL:HB	5:P:415:PHE:CD2	1.92	1.04
4:B:1066:ALA:O	4:B:1081:VAL:CG1	2.06	1.03
5:O:523:ALA:HB1	5:O:524:PRO:HB3	1.35	1.03
5:P:528:GLU:HG2	5:P:529:PRO:CD	1.84	1.03
4:B:1057:LYS:CG	4:B:1064:MET:HA	1.89	1.03
4:D:1080:VAL:HA	4:D:1081:VAL:HB	1.34	1.03
4:B:1056:ARG:HD2	4:B:1057:LYS:HE3	1.42	1.02
5:P:523:ALA:HB1	5:P:524:PRO:HA	1.05	1.02
4:D:1080:VAL:CA	4:D:1081:VAL:CB	2.37	1.02
5:O:388:LEU:HD21	5:O:399:VAL:CG2	1.89	1.02
4:A:1080:VAL:HG21	4:A:1114:LEU:CD2	1.90	1.02
5:N:505:ARG:HB3	5:N:506:ARG:HB3	1.40	1.01
4:D:549:MET:HE3	4:D:559:ILE:HD12	1.06	1.01
5:O:494:ALA:CB	5:O:495:GLU:HA	1.90	1.01
5:P:501:SER:HB3	5:P:514:ARG:HD2	1.42	1.01
5:O:502:GLU:O	5:O:503:GLU:HB2	1.60	1.01
4:A:971:GLY:HA2	4:A:975:LEU:HB3	1.03	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1057:LYS:HB3	4:D:1058:PRO:HA	1.43	1.01
4:B:1093:LEU:HD11	4:B:1097:ILE:HG21	1.39	1.00
4:D:500:SER:HB3	4:D:535:LEU:CD1	1.91	1.00
5:N:505:ARG:HD2	5:N:510:LEU:HB3	1.42	1.00
5:P:501:SER:HB2	5:P:504:LEU:O	1.61	1.00
4:B:1080:VAL:HA	4:B:1081:VAL:CG2	1.92	1.00
4:B:1080:VAL:CA	4:B:1081:VAL:HG22	1.91	1.00
4:C:287:ILE:HA	4:C:291:MET:HB3	1.41	1.00
4:A:572:ALA:CB	4:A:573:SER:HB2	1.90	0.99
4:D:501:LYS:HE3	4:D:505:LYS:NZ	1.77	0.99
4:A:1080:VAL:HG21	4:A:1114:LEU:HD22	1.43	0.99
5:P:505:ARG:CZ	5:P:532:GLU:OE1	2.11	0.99
4:C:1093:LEU:HD11	4:C:1097:ILE:CB	1.93	0.99
4:D:549:MET:HE2	4:D:559:ILE:HD12	1.44	0.99
4:A:1029:ILE:HG23	4:A:1077:LEU:HD13	1.44	0.99
4:D:1080:VAL:HG11	4:D:1082:PHE:CD2	1.98	0.99
5:N:520:LYS:N	5:N:521:PRO:HD3	1.77	0.98
5:P:528:GLU:HG2	5:P:529:PRO:HD3	1.02	0.98
5:O:387:PHE:CE2	5:O:441:PHE:CZ	2.50	0.98
4:C:1129:LYS:HE2	4:C:1183:GLU:OE2	1.63	0.98
5:P:506:ARG:HB2	5:P:506:ARG:HH11	1.28	0.97
5:N:506:ARG:HB2	5:N:510:LEU:CB	1.94	0.97
4:D:1202:ARG:HG2	4:D:1202:ARG:HH11	1.25	0.97
5:M:519:ARG:CB	5:M:520:LYS:HB2	1.94	0.97
5:M:396:ARG:HA	5:M:397:ALA:HB3	1.44	0.97
5:M:519:ARG:HD3	5:M:520:LYS:HE2	1.45	0.97
4:D:1059:THR:HG22	4:D:1065:MET:HE3	1.47	0.96
5:N:494:ALA:HB3	5:N:495:GLU:HA	1.45	0.96
4:B:357:VAL:CG1	4:B:358:GLU:HG3	1.94	0.96
5:M:396:ARG:HB2	5:M:397:ALA:O	1.65	0.96
5:M:421:PHE:HE2	5:M:422:HIS:HD1	0.98	0.96
4:C:1080:VAL:HB	4:C:1082:PHE:N	1.79	0.96
5:N:523:ALA:CB	5:N:524:PRO:CA	2.34	0.96
5:N:524:PRO:HB2	5:N:525:GLU:C	1.84	0.96
5:P:494:ALA:HB3	5:P:495:GLU:HA	1.43	0.95
4:D:284:ASP:HB3	4:D:290:LYS:CE	1.96	0.95
4:B:1057:LYS:HE2	4:B:1064:MET:CE	1.96	0.95
4:D:1080:VAL:CA	4:D:1081:VAL:HB	1.96	0.95
4:B:1057:LYS:CE	4:B:1064:MET:HE2	1.96	0.95
4:D:1080:VAL:CG1	4:D:1082:PHE:HE2	1.76	0.95
4:A:971:GLY:CA	4:A:975:LEU:HB3	1.94	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1093:LEU:HD11	4:C:1097:ILE:HG21	1.43	0.95
4:D:1082:PHE:CE1	4:D:1114:LEU:HD12	1.99	0.95
5:M:505:ARG:HB3	5:M:506:ARG:HB3	1.48	0.95
4:A:1067:ARG:CA	4:A:1081:VAL:HG21	1.97	0.94
4:B:357:VAL:HB	4:B:358:GLU:CB	1.96	0.94
5:M:494:ALA:HB1	5:M:495:GLU:HA	1.47	0.94
4:D:1060:ARG:HG2	4:D:1060:ARG:HH11	1.33	0.94
5:P:528:GLU:HG3	5:P:529:PRO:CD	1.94	0.94
5:N:505:ARG:HB3	5:N:506:ARG:CB	1.96	0.94
4:D:501:LYS:HE3	4:D:505:LYS:HZ1	1.33	0.94
5:M:525:GLU:HG2	5:M:530:VAL:HG23	1.47	0.94
4:D:1080:VAL:HG21	4:D:1082:PHE:CE2	2.03	0.93
5:N:453:LYS:O	5:N:454:SER:HB2	1.64	0.93
5:P:412:VAL:HB	5:P:415:PHE:HD2	1.28	0.93
5:M:419:LYS:HA	5:M:422:HIS:CD2	2.04	0.93
5:P:532:GLU:HA	5:P:535:ILE:CD1	1.98	0.93
5:M:507:LEU:N	5:M:510:LEU:HD22	1.82	0.93
4:D:549:MET:HE1	4:D:559:ILE:HG21	1.50	0.93
5:M:418:SER:O	5:M:422:HIS:NE2	2.02	0.93
5:P:499:ASP:HB2	5:P:515:LEU:HD22	1.48	0.92
4:D:284:ASP:HB3	4:D:290:LYS:HE3	1.48	0.92
5:P:523:ALA:HB3	5:P:524:PRO:CA	1.95	0.92
4:D:994:ASP:HB2	5:P:528:GLU:OE1	1.69	0.92
4:D:1205:PHE:CD1	4:D:1206:LEU:HD12	2.04	0.92
5:N:505:ARG:NH2	5:N:532:GLU:OE1	2.02	0.92
4:A:1067:ARG:HA	4:A:1081:VAL:HG21	1.50	0.92
5:N:541:MET:N	5:N:542:PRO:HD2	1.85	0.92
5:M:413:LEU:C	5:M:416:PRO:HD2	1.89	0.92
5:O:390:ALA:HB3	5:O:393:PRO:CG	2.00	0.92
4:D:1056:ARG:HA	4:D:1066:ALA:HB2	1.52	0.92
5:N:524:PRO:CD	5:N:525:GLU:HA	1.98	0.91
5:P:540:ILE:HD12	5:P:541:MET:N	1.85	0.91
4:A:513:ILE:HG22	4:A:514:PRO:HD3	1.48	0.91
5:M:505:ARG:HB3	5:M:506:ARG:CB	1.99	0.91
5:P:505:ARG:CZ	5:P:510:LEU:HD13	2.00	0.91
5:P:522:LYS:HG3	5:P:523:ALA:H	1.34	0.91
5:N:395:LEU:HA	5:N:396:ARG:HB2	1.51	0.91
5:P:523:ALA:HB1	5:P:524:PRO:CA	1.93	0.91
4:D:1102:LEU:HD12	4:D:1206:LEU:HG	1.52	0.91
5:O:388:LEU:CD2	5:O:399:VAL:CG2	2.48	0.91
5:N:508:ALA:HA	5:N:510:LEU:N	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1093:LEU:HD11	4:B:1097:ILE:CG2	2.01	0.91
4:A:747:ILE:HG23	4:A:805:LEU:HD22	1.51	0.90
4:D:549:MET:HE1	4:D:559:ILE:CG2	2.01	0.90
4:B:1056:ARG:CD	4:B:1057:LYS:HE3	2.02	0.90
4:B:1159:LEU:CD1	4:B:1183:GLU:HG3	2.02	0.90
4:D:1102:LEU:CD1	4:D:1206:LEU:HG	2.02	0.90
4:A:1067:ARG:N	4:A:1081:VAL:HG21	1.88	0.89
4:B:1067:ARG:HA	4:B:1081:VAL:HG21	1.54	0.89
4:D:1082:PHE:CZ	4:D:1114:LEU:HA	2.07	0.89
4:D:1057:LYS:HB3	4:D:1058:PRO:CA	2.02	0.89
4:C:154:ILE:HD11	4:C:195:VAL:HB	1.54	0.88
4:C:494:THR:N	4:C:573:SER:O	2.06	0.88
5:O:494:ALA:HB1	5:O:495:GLU:HA	1.52	0.88
4:A:1133:VAL:CG2	4:A:1189:LEU:HD11	2.03	0.88
4:D:1006:LEU:HD13	4:D:1010:VAL:HG21	1.53	0.88
5:P:506:ARG:HB2	5:P:506:ARG:NH1	1.89	0.88
4:B:1013:HIS:NE2	4:B:1016:LEU:HD11	1.89	0.88
5:M:506:ARG:C	5:M:507:LEU:HD22	1.94	0.88
4:A:855:ALA:HB2	4:A:1008:ILE:HD11	1.56	0.88
5:M:519:ARG:HD3	5:M:520:LYS:CE	2.03	0.88
5:M:539:GLY:HA2	5:M:542:PRO:HD2	1.56	0.88
5:M:492:TRP:O	5:M:493:GLU:CG	2.22	0.87
4:D:1066:ALA:O	4:D:1081:VAL:CG1	2.19	0.87
5:M:523:ALA:HB1	5:M:524:PRO:O	1.75	0.87
4:A:1080:VAL:HA	4:A:1081:VAL:CB	2.05	0.87
4:B:357:VAL:HG12	4:B:358:GLU:CG	2.05	0.87
4:B:1057:LYS:HE2	4:B:1064:MET:CG	2.05	0.87
5:M:525:GLU:OE1	5:M:525:GLU:N	2.08	0.87
4:C:1080:VAL:CG1	4:C:1082:PHE:HD2	1.88	0.86
5:N:523:ALA:HB1	5:N:524:PRO:C	1.95	0.86
4:C:1080:VAL:CG1	4:C:1113:VAL:O	2.23	0.86
5:O:387:PHE:HE2	5:O:441:PHE:CZ	1.92	0.86
4:B:1057:LYS:CE	4:B:1064:MET:HG3	2.05	0.86
4:B:1056:ARG:HG3	4:B:1057:LYS:HG3	0.89	0.86
4:C:1129:LYS:CE	4:C:1183:GLU:OE2	2.23	0.86
5:N:541:MET:N	5:N:542:PRO:CD	2.37	0.86
4:D:537:GLU:HA	4:D:540:GLN:HG2	1.57	0.86
5:P:505:ARG:HG3	5:P:514:ARG:HE	1.39	0.86
4:C:968:ARG:O	4:C:972:ARG:HG3	1.75	0.85
4:C:1093:LEU:HD11	4:C:1097:ILE:HB	1.57	0.85
4:A:1032:LEU:HD11	4:A:1047:LEU:HD11	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1080:VAL:HG11	4:D:1082:PHE:HE2	0.90	0.85
5:O:389:GLU:HB2	5:O:445:GLU:HB2	1.57	0.85
5:O:390:ALA:HB3	5:O:393:PRO:HG2	1.57	0.85
5:M:421:PHE:HD2	5:M:422:HIS:ND1	1.72	0.85
5:P:529:PRO:HB2	5:P:530:VAL:HA	1.59	0.84
4:C:298:PHE:CD2	4:C:299:PRO:HD2	2.12	0.84
5:M:519:ARG:CD	5:M:520:LYS:HE2	2.08	0.84
5:O:450:LEU:CB	5:O:451:GLU:C	2.45	0.84
5:M:418:SER:O	5:M:422:HIS:CD2	2.31	0.84
4:A:572:ALA:CA	4:A:573:SER:HB2	2.07	0.84
4:A:1127:ALA:HB1	4:A:1128:PRO:HD2	1.57	0.84
4:C:970:ARG:HH21	4:C:975:LEU:CD2	1.90	0.84
4:B:1013:HIS:HB3	4:B:1014:PRO:HA	1.60	0.83
5:M:396:ARG:HB2	5:M:397:ALA:C	1.97	0.83
5:O:387:PHE:HE2	5:O:441:PHE:CE2	1.91	0.83
5:P:505:ARG:CG	5:P:514:ARG:HH21	1.91	0.83
5:N:506:ARG:HG2	5:N:507:LEU:N	1.92	0.83
4:A:1133:VAL:HG23	4:A:1189:LEU:HD11	1.60	0.83
4:D:1079:VAL:HG23	4:D:1113:VAL:HG11	1.60	0.83
5:M:392:LYS:HB3	5:M:395:LEU:O	1.78	0.83
5:O:389:GLU:HB2	5:O:445:GLU:CB	2.09	0.83
5:O:502:GLU:O	5:O:503:GLU:CB	2.26	0.83
4:A:513:ILE:HG22	4:A:514:PRO:CD	2.07	0.83
5:P:494:ALA:HB1	5:P:495:GLU:HA	1.61	0.83
5:P:532:GLU:CD	5:P:535:ILE:HD11	1.98	0.83
4:B:570:ARG:HG2	4:B:571:HIS:H	1.44	0.82
5:P:505:ARG:NE	5:P:510:LEU:CD1	2.43	0.82
4:D:1119:TRP:CH2	4:D:1206:LEU:HA	2.14	0.82
4:B:1057:LYS:CE	4:B:1064:MET:CE	2.56	0.82
4:B:1089:VAL:HG22	4:B:1118:VAL:HG12	1.62	0.82
5:M:396:ARG:CA	5:M:397:ALA:HB3	2.10	0.82
5:P:532:GLU:OE2	5:P:535:ILE:HD11	1.79	0.82
5:M:523:ALA:HB1	5:M:524:PRO:C	2.00	0.82
4:C:541:VAL:HG23	4:C:542:VAL:HA	1.61	0.82
5:O:450:LEU:HB3	5:O:451:GLU:HB2	1.61	0.82
5:P:396:ARG:O	5:P:397:ALA:O	1.96	0.82
4:B:1143:LYS:N	4:B:1144:GLY:HA2	1.94	0.81
4:D:549:MET:HE1	4:D:559:ILE:CB	2.09	0.81
4:D:539:ILE:O	4:D:541:VAL:HG23	1.78	0.81
5:P:501:SER:CB	5:P:504:LEU:O	2.28	0.81
4:B:1054:VAL:HG21	4:B:1094:LYS:NZ	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:539:GLY:CA	5:M:542:PRO:HD2	2.10	0.81
5:N:527:GLU:N	5:N:528:GLU:HA	1.95	0.81
5:P:539:GLY:O	5:P:542:PRO:HD2	1.80	0.81
4:B:1057:LYS:HG2	4:B:1064:MET:HA	0.93	0.81
4:D:1057:LYS:HE3	4:D:1064:MET:N	1.96	0.81
5:O:387:PHE:HZ	5:O:441:PHE:CD2	1.98	0.81
5:M:418:SER:O	5:M:422:HIS:CE1	2.34	0.81
4:D:549:MET:CE	4:D:559:ILE:HB	2.11	0.81
4:D:1080:VAL:CG1	4:D:1082:PHE:CD2	2.59	0.81
4:D:537:GLU:CA	4:D:540:GLN:CG	2.58	0.81
5:M:390:ALA:O	5:M:391:LEU:HD12	1.81	0.81
5:O:450:LEU:CB	5:O:451:GLU:HB2	2.11	0.81
5:O:387:PHE:CE2	5:O:441:PHE:HE2	1.94	0.81
5:N:453:LYS:O	5:N:454:SER:CB	2.21	0.80
4:C:1080:VAL:CG1	4:C:1082:PHE:CD2	2.62	0.80
5:O:505:ARG:HH11	5:O:505:ARG:HG2	1.47	0.80
5:M:389:GLU:O	5:M:390:ALA:HB3	1.79	0.80
5:M:408:GLY:HA3	5:M:415:PHE:HD1	1.46	0.80
4:D:1056:ARG:CA	4:D:1066:ALA:HB2	2.12	0.80
4:D:1079:VAL:O	4:D:1081:VAL:HG23	1.82	0.80
5:P:505:ARG:CD	5:P:514:ARG:CZ	2.58	0.80
5:N:520:LYS:N	5:N:521:PRO:CD	2.44	0.80
5:N:525:GLU:CG	5:N:528:GLU:O	2.30	0.80
4:D:284:ASP:HB3	4:D:290:LYS:NZ	1.95	0.80
5:M:505:ARG:HB3	5:M:506:ARG:CA	2.11	0.80
5:M:524:PRO:HB2	5:M:525:GLU:C	2.02	0.80
5:N:523:ALA:HB1	5:N:524:PRO:O	1.81	0.80
4:A:569:ASN:HA	4:A:570:ARG:HB3	1.60	0.80
5:P:505:ARG:CD	5:P:514:ARG:NH2	2.42	0.80
4:C:301:PRO:HB2	4:C:302:GLU:HB2	1.64	0.80
4:D:1059:THR:HG22	4:D:1065:MET:CE	2.11	0.80
5:N:506:ARG:HA	5:N:510:LEU:HD22	1.63	0.80
4:C:1080:VAL:HG13	4:C:1113:VAL:O	1.82	0.79
4:C:737:THR:HG21	4:C:746:GLN:HE22	1.47	0.79
5:O:388:LEU:HD23	5:O:394:THR:HG21	1.65	0.79
5:P:413:LEU:CA	5:P:416:PRO:HD2	2.13	0.79
4:A:967:THR:HG23	4:A:981:GLU:HG2	1.64	0.79
5:M:490:PRO:O	5:M:492:TRP:NE1	2.16	0.79
4:A:975:LEU:HD12	4:A:975:LEU:O	1.82	0.78
4:C:1093:LEU:CD1	4:C:1097:ILE:HG21	2.13	0.78
5:P:409:LYS:HG3	5:P:410:THR:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1054:VAL:CG2	4:B:1094:LYS:NZ	2.46	0.78
4:D:500:SER:HB3	4:D:535:LEU:HD13	1.64	0.78
4:C:407:GLN:OE1	4:C:436:VAL:HG11	1.84	0.78
5:P:505:ARG:NE	5:P:510:LEU:HD13	1.98	0.78
5:M:506:ARG:HA	5:M:510:LEU:HD23	1.64	0.78
5:P:490:PRO:HD2	5:P:522:LYS:HE3	1.63	0.78
4:D:1080:VAL:C	4:D:1081:VAL:HG23	2.01	0.78
4:D:1082:PHE:CZ	4:D:1114:LEU:CB	2.65	0.78
4:D:696:LEU:HD21	4:D:742:VAL:HG22	1.66	0.78
5:M:539:GLY:O	5:M:542:PRO:HD2	1.83	0.77
4:B:1057:LYS:CB	4:B:1058:PRO:HA	2.08	0.77
5:M:419:LYS:HA	5:M:422:HIS:HD2	1.49	0.77
5:M:539:GLY:C	5:M:542:PRO:HD2	2.04	0.77
5:N:494:ALA:CB	5:N:495:GLU:CA	2.62	0.77
5:M:494:ALA:CB	5:M:495:GLU:HA	2.15	0.77
3:I:19:DC:O2	2:J:11:DG:N2	2.18	0.77
4:C:1051:VAL:HG21	4:C:1094:LYS:O	1.85	0.77
4:D:302:GLU:HB3	4:D:303:GLY:CA	2.14	0.77
4:B:1057:LYS:NZ	4:B:1064:MET:CE	2.47	0.77
4:D:549:MET:CE	4:D:559:ILE:CB	2.63	0.77
5:M:413:LEU:O	5:M:417:GLU:HG3	1.85	0.77
5:M:505:ARG:HD2	5:M:510:LEU:HD23	1.66	0.77
5:N:505:ARG:HB3	5:N:506:ARG:CA	2.14	0.77
5:N:494:ALA:HB1	5:N:495:GLU:HA	1.64	0.76
4:D:1082:PHE:HZ	4:D:1114:LEU:CB	1.98	0.76
5:M:392:LYS:CG	5:M:397:ALA:HB2	2.16	0.76
5:M:521:PRO:HG2	5:M:522:LYS:O	1.85	0.76
5:M:394:THR:O	5:M:395:LEU:HB2	1.84	0.76
5:P:511:LEU:O	5:P:515:LEU:HD23	1.85	0.76
5:P:494:ALA:CB	5:P:495:GLU:CA	2.60	0.76
5:O:507:LEU:HD23	5:O:507:LEU:H	1.50	0.76
5:O:519:ARG:CD	5:O:520:LYS:HZ2	1.96	0.76
4:C:970:ARG:O	4:C:973:SER:N	2.18	0.76
5:P:412:VAL:O	5:P:415:PHE:N	2.17	0.76
5:O:390:ALA:CB	5:O:393:PRO:HG2	2.14	0.75
5:P:491:PRO:HB3	5:P:540:ILE:CG2	2.15	0.75
4:B:1013:HIS:CD2	4:B:1016:LEU:HD11	2.21	0.75
4:B:1056:ARG:HG2	4:B:1056:ARG:HH11	1.50	0.75
4:B:1057:LYS:HE3	4:B:1064:MET:HG3	1.66	0.75
5:P:524:PRO:CD	5:P:525:GLU:C	2.52	0.75
4:A:971:GLY:CA	4:A:975:LEU:CB	2.61	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1084:ARG:HD2	4:B:1089:VAL:CG1	2.17	0.75
4:B:1056:ARG:HA	4:B:1066:ALA:HB2	1.67	0.75
4:B:1057:LYS:HD3	4:B:1063:GLY:O	1.86	0.75
5:M:540:ILE:O	5:M:543:PRO:HD3	1.85	0.75
4:C:1129:LYS:NZ	4:C:1183:GLU:OE2	2.18	0.75
4:B:1054:VAL:HG23	4:B:1094:LYS:CE	2.16	0.75
5:O:396:ARG:HA	5:O:397:ALA:C	2.06	0.75
5:O:519:ARG:NE	5:O:520:LYS:NZ	2.35	0.75
4:C:590:VAL:HG13	4:C:604:TYR:CD1	2.22	0.74
5:O:541:MET:N	5:O:542:PRO:CD	2.50	0.74
4:D:542:VAL:HG13	4:D:543:PRO:HD3	1.67	0.74
4:D:939:VAL:HG22	4:D:944:LEU:HD12	1.67	0.74
5:N:411:LEU:CB	5:N:412:VAL:HA	2.17	0.74
5:P:409:LYS:HG3	5:P:410:THR:H	1.52	0.74
4:B:154:ILE:HD13	4:B:195:VAL:HB	1.69	0.74
4:D:537:GLU:HA	4:D:540:GLN:CD	2.06	0.74
4:D:1039:LEU:HD12	4:D:1040:PRO:CD	2.16	0.74
5:M:524:PRO:HD2	5:M:525:GLU:HA	1.69	0.74
5:O:390:ALA:HB3	5:O:393:PRO:HG3	1.67	0.74
4:B:679:VAL:HG22	4:B:693:LEU:HD21	1.69	0.74
4:B:1057:LYS:NZ	4:B:1064:MET:HE1	2.01	0.74
5:P:505:ARG:NH2	5:P:532:GLU:OE1	2.20	0.74
4:A:1051:VAL:HG21	4:A:1099:LEU:HD12	1.69	0.74
4:D:1080:VAL:CB	4:D:1081:VAL:HB	2.17	0.74
5:N:403:ARG:NE	5:N:437:ALA:HB1	2.02	0.74
5:P:522:LYS:HG3	5:P:523:ALA:N	2.02	0.74
5:M:506:ARG:HB2	5:M:510:LEU:HB3	1.67	0.74
5:P:499:ASP:CB	5:P:515:LEU:HD22	2.17	0.73
4:D:498:LEU:CD2	4:D:503:ALA:HB2	2.17	0.73
4:D:546:ARG:O	4:D:546:ARG:HD2	1.87	0.73
5:O:411:LEU:CB	5:O:412:VAL:HA	2.19	0.73
4:B:1056:ARG:HD2	4:B:1057:LYS:CE	2.17	0.73
5:N:411:LEU:HB2	5:N:412:VAL:HA	1.71	0.73
4:C:1080:VAL:HB	4:C:1082:PHE:H	1.52	0.73
4:D:542:VAL:HG13	4:D:543:PRO:CD	2.19	0.73
4:D:1080:VAL:CB	4:D:1082:PHE:CD2	2.71	0.73
5:M:539:GLY:HA2	5:M:542:PRO:CD	2.17	0.73
4:B:505:LYS:HE3	4:B:522:ALA:HB3	1.70	0.73
4:B:1159:LEU:HD11	4:B:1183:GLU:CG	2.07	0.73
4:D:541:VAL:HG13	4:D:544:GLU:HB2	1.69	0.73
5:O:450:LEU:CA	5:O:451:GLU:HB2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:291:MET:HE2	4:C:291:MET:O	1.88	0.73
4:A:980:ALA:C	4:A:981:GLU:HG3	2.09	0.73
4:B:1023:GLU:O	4:B:1164:ARG:NH2	2.22	0.73
5:O:494:ALA:CB	5:O:495:GLU:CA	2.67	0.73
5:M:505:ARG:CB	5:M:506:ARG:HB3	2.17	0.73
5:O:507:LEU:HD23	5:O:507:LEU:N	2.04	0.73
5:P:504:LEU:N	5:P:504:LEU:HD12	2.04	0.73
4:A:319:LEU:HD23	4:A:326:ILE:HG22	1.71	0.72
4:D:289:ASP:N	4:D:289:ASP:OD1	2.22	0.72
4:B:1013:HIS:CE1	4:B:1016:LEU:HD11	2.24	0.72
4:B:1054:VAL:HG21	4:B:1094:LYS:HZ2	1.53	0.72
4:D:546:ARG:HD2	4:D:546:ARG:C	2.09	0.72
4:D:1082:PHE:CZ	4:D:1114:LEU:CG	2.73	0.72
5:P:505:ARG:HB2	5:P:510:LEU:HD12	1.72	0.72
4:B:1066:ALA:O	4:B:1081:VAL:HG11	1.87	0.72
5:O:388:LEU:CD2	5:O:399:VAL:HG21	2.18	0.72
4:D:1135:VAL:HG11	4:D:1139:LEU:HD11	1.71	0.72
4:B:615:LEU:HD21	4:B:617:MET:CE	2.19	0.72
4:D:1080:VAL:HB	4:D:1082:PHE:CD2	2.24	0.72
4:D:1080:VAL:CG2	4:D:1082:PHE:CE2	2.72	0.72
5:M:421:PHE:CD2	5:M:422:HIS:CE1	2.78	0.72
5:N:505:ARG:CB	5:N:506:ARG:HB3	2.18	0.72
5:O:450:LEU:HA	5:O:451:GLU:HB2	1.71	0.72
5:O:505:ARG:HG2	5:O:505:ARG:NH1	2.01	0.72
4:C:1161:VAL:HG13	4:C:1176:LEU:HD23	1.71	0.72
4:A:572:ALA:HB1	4:A:573:SER:HB3	1.70	0.71
4:B:352:GLU:OE1	4:B:356:ARG:NH2	2.23	0.71
4:C:1161:VAL:CG1	4:C:1176:LEU:HD23	2.19	0.71
4:D:1080:VAL:HG21	4:D:1114:LEU:HA	1.72	0.71
5:O:519:ARG:HB3	5:O:520:LYS:HB2	1.71	0.71
4:B:1066:ALA:HB3	4:B:1084:ARG:CZ	2.19	0.71
4:C:1176:LEU:HD22	4:C:1179:VAL:HG23	1.72	0.71
5:O:411:LEU:HB2	5:O:412:VAL:HA	1.72	0.71
5:P:504:LEU:HB2	5:P:505:ARG:HG2	1.72	0.71
5:P:504:LEU:HB3	5:P:505:ARG:HA	1.72	0.71
4:B:363:GLU:O	4:B:366:ARG:HB2	1.90	0.71
4:C:407:GLN:CD	4:C:436:VAL:HG11	2.10	0.71
5:O:450:LEU:HB3	5:O:451:GLU:CB	2.20	0.71
4:B:1054:VAL:HG23	4:B:1094:LYS:HD3	1.71	0.71
4:D:498:LEU:HD21	4:D:503:ALA:CB	2.17	0.71
5:P:538:ASN:O	5:P:541:MET:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:506:ARG:CB	5:N:510:LEU:HB2	2.09	0.71
4:D:507:VAL:HG12	4:D:558:VAL:HG13	1.72	0.71
4:A:1029:ILE:HG23	4:A:1077:LEU:CD1	2.20	0.71
5:M:419:LYS:O	5:M:423:HIS:CE1	2.44	0.71
4:A:1159:LEU:O	4:A:1159:LEU:HD12	1.89	0.70
4:B:525:ILE:HD11	4:B:538:ALA:CB	2.20	0.70
4:D:537:GLU:O	4:D:540:GLN:CG	2.36	0.70
4:D:1119:TRP:HH2	4:D:1206:LEU:HA	1.55	0.70
5:O:495:GLU:HG3	5:O:503:GLU:HG3	1.73	0.70
5:M:507:LEU:O	5:M:510:LEU:HD13	1.90	0.70
4:C:1084:ARG:HG3	4:C:1089:VAL:HG22	1.73	0.70
4:C:1159:LEU:CD1	4:C:1183:GLU:HG3	2.22	0.70
5:M:532:GLU:O	5:M:535:ILE:HG22	1.91	0.70
5:N:524:PRO:HB2	5:N:525:GLU:CA	2.20	0.70
5:P:505:ARG:HB3	5:P:510:LEU:CD1	2.17	0.70
4:C:918:LEU:HD22	4:C:953:LEU:CD2	2.21	0.70
4:A:788:ALA:HB1	4:A:793:VAL:CG2	2.22	0.70
4:A:1161:VAL:HG21	4:A:1179:VAL:CG2	2.22	0.70
4:B:332:ARG:HG3	4:B:350:LEU:HD21	1.73	0.70
5:O:450:LEU:HB3	5:O:451:GLU:CA	2.21	0.70
4:C:1207:GLN:HB3	4:C:1208:GLY:HA2	1.73	0.70
5:M:415:PHE:HB2	5:M:416:PRO:HD3	1.74	0.70
5:P:538:ASN:O	5:P:542:PRO:HD3	1.91	0.70
5:M:506:ARG:HB2	5:M:510:LEU:CB	2.21	0.70
5:P:532:GLU:CA	5:P:535:ILE:HD13	2.18	0.70
4:B:310:LEU:HD13	4:B:403:PHE:CD2	2.27	0.69
4:C:854:VAL:HG23	4:C:1008:ILE:HD13	1.72	0.69
5:N:519:ARG:HB3	5:N:520:LYS:HB2	1.73	0.69
4:C:1176:LEU:HD22	4:C:1179:VAL:CG2	2.22	0.69
4:D:537:GLU:C	4:D:540:GLN:HG3	2.12	0.69
4:C:951:ALA:HB2	4:C:993:LEU:HG	1.72	0.69
4:D:1082:PHE:CZ	4:D:1114:LEU:HG	2.23	0.69
4:D:1082:PHE:CZ	4:D:1114:LEU:CA	2.75	0.69
5:M:519:ARG:HB3	5:M:520:LYS:CB	2.04	0.69
4:A:574:VAL:HG12	4:A:575:HIS:N	2.06	0.69
4:A:1080:VAL:HG21	4:A:1114:LEU:HD23	1.73	0.69
4:D:50:LEU:HD11	4:D:591:PRO:HG3	1.75	0.69
4:D:1080:VAL:CB	4:D:1082:PHE:CE2	2.75	0.69
4:B:1055:VAL:O	4:B:1066:ALA:CB	2.40	0.69
5:M:506:ARG:O	5:M:507:LEU:HD22	1.93	0.69
5:P:505:ARG:CG	5:P:514:ARG:NH2	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:520:LYS:H	5:N:521:PRO:HD3	1.53	0.69
4:B:357:VAL:CB	4:B:358:GLU:HB2	2.13	0.69
4:C:970:ARG:HH21	4:C:975:LEU:HD21	1.58	0.69
4:B:357:VAL:CB	4:B:358:GLU:HG3	2.22	0.69
4:D:590:VAL:HG13	4:D:604:TYR:CD1	2.27	0.69
4:A:1165:VAL:HG13	4:A:1172:ALA:HB3	1.75	0.68
4:B:515:HIS:HB2	4:B:516:LYS:HA	1.76	0.68
4:D:492:ILE:HA	4:D:602:THR:HG22	1.75	0.68
5:M:505:ARG:HB3	5:M:506:ARG:HA	1.73	0.68
5:P:494:ALA:HB1	5:P:495:GLU:CA	2.23	0.68
5:P:504:LEU:HB2	5:P:505:ARG:CG	2.23	0.68
4:D:635:VAL:HG12	4:D:641:VAL:HG13	1.75	0.68
4:D:1039:LEU:HD12	4:D:1040:PRO:HD2	1.74	0.68
5:M:524:PRO:CD	5:M:525:GLU:HA	2.24	0.68
4:C:154:ILE:CG2	4:C:192:VAL:HG22	2.23	0.68
4:D:116:ALA:HB1	4:D:125:PRO:HB2	1.76	0.68
4:B:186:LEU:HD21	4:B:245:PRO:HB2	1.75	0.68
4:D:1202:ARG:HG2	4:D:1202:ARG:NH1	1.98	0.68
4:D:994:ASP:CB	5:P:528:GLU:OE1	2.42	0.68
4:D:996:ILE:HD12	5:P:528:GLU:OE2	1.94	0.68
4:A:572:ALA:HA	4:A:573:SER:HB2	1.75	0.68
4:B:1066:ALA:C	4:B:1081:VAL:HB	2.14	0.68
4:D:538:ALA:O	4:D:541:VAL:HG22	1.93	0.68
4:D:1059:THR:CG2	4:D:1065:MET:CE	2.71	0.68
5:P:412:VAL:O	5:P:416:PRO:HD2	1.94	0.68
4:B:570:ARG:CG	4:B:571:HIS:H	2.03	0.68
4:B:1055:VAL:O	4:B:1066:ALA:HB1	1.93	0.67
5:M:411:LEU:N	5:M:412:VAL:HG22	2.09	0.67
5:O:541:MET:N	5:O:542:PRO:HD2	2.08	0.67
5:P:412:VAL:HB	5:P:415:PHE:CE2	2.29	0.67
4:B:357:VAL:O	4:B:362:TRP:CZ2	2.47	0.67
4:D:1060:ARG:HG2	4:D:1060:ARG:NH1	2.06	0.67
5:N:412:VAL:O	5:N:414:ARG:N	2.27	0.67
5:P:395:LEU:O	5:P:397:ALA:N	2.26	0.67
5:M:506:ARG:O	5:M:507:LEU:HD13	1.93	0.67
5:O:494:ALA:HB3	5:O:495:GLU:HA	1.71	0.67
5:P:392:LYS:N	5:P:393:PRO:CD	2.58	0.67
5:O:388:LEU:HD23	5:O:399:VAL:HG21	1.77	0.67
5:P:540:ILE:HD12	5:P:540:ILE:C	2.15	0.67
4:C:151:PRO:O	4:C:154:ILE:HG22	1.94	0.67
5:O:518:VAL:HG23	5:O:519:ARG:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:396:ARG:C	5:P:397:ALA:O	2.33	0.67
5:P:512:GLY:O	5:P:516:LEU:HG	1.93	0.67
4:A:498:LEU:HB3	4:A:499:ALA:HB2	1.77	0.67
4:B:352:GLU:CG	4:B:356:ARG:NH2	2.58	0.67
4:D:549:MET:HE2	4:D:559:ILE:HB	1.75	0.67
4:D:1080:VAL:HG21	4:D:1082:PHE:CZ	2.29	0.67
5:M:396:ARG:HA	5:M:397:ALA:CB	2.22	0.67
4:A:1080:VAL:CG2	4:A:1114:LEU:CD2	2.72	0.66
4:C:788:ALA:HB1	4:C:793:VAL:CG2	2.25	0.66
4:C:878:PHE:O	4:C:892:SER:OG	2.08	0.66
4:B:670:LEU:HD11	4:B:679:VAL:HG21	1.75	0.66
4:B:1095:GLU:O	4:B:1097:ILE:HD12	1.95	0.66
4:C:154:ILE:HD13	4:C:192:VAL:HA	1.76	0.66
5:M:505:ARG:CD	5:M:510:LEU:HD23	2.25	0.66
4:A:301:PRO:HA	4:A:302:GLU:HG2	1.77	0.66
4:A:1080:VAL:CG2	4:A:1114:LEU:HD23	2.25	0.66
4:A:1131:LEU:HD23	4:A:1132:GLU:N	2.11	0.66
4:B:359:GLU:HA	4:B:362:TRP:HD1	1.59	0.66
4:B:1054:VAL:HG23	4:B:1094:LYS:CD	2.24	0.66
4:C:659:LEU:HD11	4:C:829:ALA:HB1	1.78	0.66
5:M:507:LEU:O	5:M:510:LEU:HB2	1.95	0.66
5:N:494:ALA:HB1	5:N:495:GLU:CA	2.25	0.66
5:O:455:LEU:HA	5:O:456:SER:C	2.16	0.66
5:P:389:GLU:O	5:P:393:PRO:CD	2.44	0.66
4:B:352:GLU:HG2	4:B:356:ARG:NH2	2.11	0.66
4:D:1079:VAL:O	4:D:1081:VAL:CG2	2.43	0.66
4:D:1082:PHE:HZ	4:D:1114:LEU:HB2	1.58	0.66
5:P:408:GLY:O	5:P:409:LYS:C	2.33	0.66
5:P:456:SER:H	5:P:457:GLY:HA2	1.61	0.66
5:P:499:ASP:CB	5:P:515:LEU:CD2	2.74	0.66
4:C:975:LEU:HD23	4:C:975:LEU:C	2.15	0.66
4:A:975:LEU:HD12	4:A:975:LEU:C	2.16	0.66
4:B:357:VAL:CB	4:B:358:GLU:CB	2.73	0.66
4:D:737:THR:HG21	4:D:746:GLN:HE22	1.60	0.66
5:P:541:MET:O	5:P:541:MET:HE3	1.95	0.66
4:C:1095:GLU:HG2	4:C:1096:ASP:N	2.09	0.66
4:D:1093:LEU:HD22	4:D:1099:LEU:CD1	2.25	0.66
5:N:518:VAL:HG13	5:N:519:ARG:HB2	1.78	0.66
5:P:413:LEU:C	5:P:416:PRO:HD2	2.16	0.66
4:A:631:ALA:O	4:A:635:VAL:HG23	1.96	0.66
4:B:226:VAL:HG21	4:B:561:VAL:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1057:LYS:CE	4:B:1064:MET:CG	2.68	0.66
4:D:1159:LEU:HD21	4:D:1183:GLU:CG	2.26	0.66
5:N:525:GLU:CD	5:N:525:GLU:H	1.99	0.66
4:C:106:TYR:O	4:C:110:VAL:HG23	1.96	0.65
4:C:291:MET:HE1	4:C:613:GLY:CA	2.26	0.65
4:C:747:ILE:HG23	4:C:805:LEU:HD22	1.78	0.65
4:C:918:LEU:HD22	4:C:953:LEU:HD23	1.77	0.65
5:M:493:GLU:OE1	5:M:517:TRP:CD1	2.50	0.65
5:M:523:ALA:CB	5:M:524:PRO:HA	2.26	0.65
5:P:531:SER:O	5:P:534:GLY:N	2.29	0.65
4:A:980:ALA:O	4:A:981:GLU:HG3	1.96	0.65
4:B:226:VAL:HG21	4:B:561:VAL:CG1	2.26	0.65
4:B:941:ALA:HB1	4:B:1006:LEU:HD11	1.78	0.65
4:B:1057:LYS:HE2	4:B:1064:MET:CB	2.26	0.65
4:C:1051:VAL:CG2	4:C:1094:LYS:O	2.43	0.65
4:C:1093:LEU:O	4:C:1094:LYS:CB	2.44	0.65
5:M:392:LYS:HG3	5:M:397:ALA:HB2	1.77	0.65
4:A:668:PHE:O	4:A:669:GLN:CB	2.41	0.65
5:O:540:ILE:C	5:O:542:PRO:HD2	2.16	0.65
4:C:1161:VAL:HG12	4:C:1176:LEU:CD2	2.26	0.65
5:M:507:LEU:H	5:M:510:LEU:CD2	2.00	0.65
5:N:530:VAL:HG22	5:N:530:VAL:O	1.96	0.65
4:A:785:VAL:CG1	4:A:795:GLU:HG3	2.26	0.65
4:B:1057:LYS:HZ1	4:B:1064:MET:HE1	1.60	0.65
4:C:1029:ILE:HD13	4:C:1047:LEU:HD13	1.76	0.65
4:B:300:LEU:HD22	4:B:309:TYR:CD2	2.32	0.65
4:B:549:MET:HG2	4:B:559:ILE:HD12	1.79	0.65
4:D:549:MET:HE1	4:D:559:ILE:HB	1.73	0.65
4:A:951:ALA:HB2	4:A:993:LEU:CD2	2.27	0.65
4:A:980:ALA:O	4:A:981:GLU:CG	2.45	0.65
4:A:1133:VAL:HG21	4:A:1189:LEU:HD11	1.76	0.65
4:B:1008:ILE:O	4:B:1008:ILE:HD12	1.97	0.65
4:D:537:GLU:CA	4:D:540:GLN:HG2	2.25	0.65
5:M:538:ASN:O	5:M:542:PRO:HD3	1.96	0.65
5:N:499:ASP:OD2	5:N:515:LEU:HD11	1.96	0.65
4:D:1057:LYS:HG2	4:D:1064:MET:HA	0.79	0.65
5:M:421:PHE:HE2	5:M:422:HIS:ND1	1.73	0.65
5:O:505:ARG:HE	5:O:507:LEU:HD21	1.61	0.64
4:B:535:LEU:HD23	4:B:559:ILE:HG23	1.78	0.64
4:B:570:ARG:HG2	4:B:571:HIS:N	2.12	0.64
4:B:1054:VAL:CG2	4:B:1094:LYS:HD3	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:410:ILE:HG23	4:C:420:VAL:HG11	1.79	0.64
5:M:505:ARG:HD2	5:M:510:LEU:CD2	2.26	0.64
4:C:154:ILE:HG21	4:C:192:VAL:HG22	1.79	0.64
4:D:338:LEU:HD11	4:D:365:LEU:HD11	1.78	0.64
5:O:519:ARG:HD3	5:O:520:LYS:HZ3	0.65	0.64
4:A:785:VAL:HG11	4:A:795:GLU:HG3	1.79	0.64
4:D:1064:MET:O	4:D:1065:MET:HB2	1.96	0.64
5:P:521:PRO:O	5:P:522:LYS:HB3	1.96	0.64
5:P:535:ILE:HG12	5:P:536:GLY:N	2.13	0.64
4:B:1021:LEU:HD21	4:B:1100:LEU:HD13	1.79	0.64
4:B:1080:VAL:HG22	4:B:1114:LEU:HA	1.79	0.64
4:C:291:MET:HE1	4:C:613:GLY:HA3	1.80	0.64
4:C:590:VAL:HG11	4:C:602:THR:HG23	1.80	0.64
4:D:1101:VAL:HG22	4:D:1118:VAL:HG22	1.79	0.64
5:P:391:LEU:C	5:P:393:PRO:HD3	2.17	0.64
5:P:524:PRO:N	5:P:525:GLU:HA	2.13	0.64
4:B:1054:VAL:CG2	4:B:1094:LYS:HZ3	2.11	0.64
5:N:540:ILE:C	5:N:542:PRO:HD2	2.17	0.64
5:P:506:ARG:O	5:P:510:LEU:HG	1.98	0.64
4:D:222:ARG:O	4:D:226:VAL:HG13	1.98	0.63
4:D:542:VAL:HG22	4:D:543:PRO:HD3	1.80	0.63
5:M:495:GLU:HB2	5:M:496:GLU:HG2	1.79	0.63
4:B:509:ARG:HA	4:B:513:ILE:HG21	1.79	0.63
5:M:413:LEU:O	5:M:416:PRO:HD2	1.97	0.63
5:M:415:PHE:O	5:M:418:SER:HB3	1.98	0.63
5:N:525:GLU:HG3	5:N:529:PRO:HA	1.79	0.63
4:D:302:GLU:HB3	4:D:303:GLY:C	2.19	0.63
5:P:413:LEU:HA	5:P:416:PRO:HD2	1.79	0.63
4:A:1025:ALA:HB2	4:A:1048:SER:OG	1.98	0.63
4:B:1057:LYS:HE2	4:B:1064:MET:HB2	1.81	0.63
4:C:299:PRO:HG2	4:C:300:LEU:H	1.64	0.63
4:D:897:VAL:HG21	4:D:938:LEU:HD13	1.80	0.63
4:D:1136:ASP:OD2	4:D:1166:LEU:HD11	1.99	0.63
4:D:1205:PHE:HD1	4:D:1206:LEU:HD12	1.61	0.63
4:A:1135:VAL:HG13	4:A:1194:TYR:CE1	2.34	0.63
4:D:406:VAL:HG22	4:D:617:MET:HE1	1.81	0.63
5:O:504:LEU:HD13	5:O:514:ARG:HH22	1.63	0.63
5:O:505:ARG:HH11	5:O:505:ARG:CG	2.11	0.63
5:O:523:ALA:HB1	5:O:524:PRO:CB	2.20	0.63
5:P:505:ARG:HG3	5:P:514:ARG:NE	2.13	0.63
4:B:449:LEU:HD22	4:B:759:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:670:LEU:HD12	4:B:675:MET:HG3	1.79	0.62
4:B:1151:LEU:HD13	4:B:1189:LEU:HD13	1.80	0.62
4:D:547:ALA:O	4:D:550:GLU:N	2.29	0.62
5:N:411:LEU:N	5:N:412:VAL:HG22	2.14	0.62
5:P:532:GLU:O	5:P:535:ILE:HG12	1.98	0.62
4:A:918:LEU:HD22	4:A:953:LEU:HD23	1.80	0.62
4:A:1076:ALA:O	4:A:1077:LEU:HD12	1.99	0.62
4:D:226:VAL:CG1	4:D:510:VAL:HG11	2.29	0.62
4:D:50:LEU:HD12	4:D:50:LEU:O	1.99	0.62
5:P:416:PRO:HG2	5:P:417:GLU:N	2.14	0.62
4:D:635:VAL:CG1	4:D:641:VAL:HG13	2.30	0.62
4:D:1039:LEU:HD12	4:D:1040:PRO:HD3	1.80	0.62
5:P:513:GLY:HA2	5:P:516:LEU:HD12	1.79	0.62
4:A:1161:VAL:HG21	4:A:1179:VAL:HG21	1.80	0.62
4:D:181:ILE:HD12	4:D:207:MET:CE	2.30	0.62
5:M:523:ALA:HB1	5:M:524:PRO:CA	2.28	0.62
5:P:505:ARG:CD	5:P:514:ARG:NE	2.62	0.62
5:P:522:LYS:CG	5:P:523:ALA:N	2.62	0.62
4:B:1018:TYR:OH	5:N:530:VAL:HG12	2.00	0.62
4:B:1056:ARG:CG	4:B:1056:ARG:HH11	2.13	0.62
4:C:968:ARG:O	4:C:972:ARG:CG	2.48	0.62
5:N:499:ASP:OD1	5:N:515:LEU:HD21	1.99	0.62
5:O:388:LEU:HD23	5:O:399:VAL:CG2	2.30	0.62
5:P:537:GLY:O	5:P:540:ILE:HG13	1.99	0.62
4:B:354:LEU:O	4:B:362:TRP:CZ2	2.52	0.62
5:O:506:ARG:O	5:O:510:LEU:HD22	2.00	0.62
4:B:1064:MET:HE3	4:B:1087:GLU:OE1	2.00	0.62
4:B:1066:ALA:HB3	4:B:1084:ARG:NH1	2.15	0.62
4:B:976:VAL:HG11	4:C:115:ARG:HD3	1.82	0.62
4:C:1094:LYS:N	4:C:1094:LYS:HD2	2.14	0.62
4:D:284:ASP:CB	4:D:290:LYS:HE3	2.25	0.62
4:D:302:GLU:HB3	4:D:303:GLY:HA3	1.80	0.62
4:D:1135:VAL:CG1	4:D:1139:LEU:HD11	2.29	0.62
4:A:974:GLY:O	4:A:975:LEU:HB3	1.98	0.61
4:C:854:VAL:CG2	4:C:1008:ILE:HD13	2.30	0.61
5:N:526:ALA:C	5:N:528:GLU:HA	2.20	0.61
5:P:525:GLU:H	5:P:525:GLU:CD	2.03	0.61
4:B:615:LEU:HD21	4:B:617:MET:HE2	1.80	0.61
4:D:664:THR:OG1	4:D:676:THR:HG22	1.98	0.61
4:D:1006:LEU:CD1	4:D:1010:VAL:HG21	2.27	0.61
4:D:498:LEU:HD23	4:D:566:GLU:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:539:ILE:C	4:D:541:VAL:HG23	2.19	0.61
5:M:535:ILE:HG23	5:M:536:GLY:N	2.15	0.61
4:D:501:LYS:HE3	4:D:505:LYS:HZ2	1.63	0.61
5:P:413:LEU:HA	5:P:416:PRO:CD	2.31	0.61
4:A:668:PHE:O	4:A:669:GLN:HB2	2.01	0.61
4:A:1139:LEU:HD12	4:A:1143:LYS:HE3	1.81	0.61
4:B:1080:VAL:CB	4:B:1081:VAL:HG22	2.29	0.61
4:C:675:MET:O	4:C:679:VAL:HG23	2.00	0.61
4:C:1093:LEU:O	4:C:1094:LYS:HG2	2.00	0.61
4:C:1081:VAL:HG13	4:C:1081:VAL:O	2.01	0.61
5:M:408:GLY:CA	5:M:415:PHE:HD1	2.13	0.61
4:A:181:ILE:CD1	4:A:207:MET:HE3	2.31	0.61
4:B:670:LEU:HD11	4:B:679:VAL:CG2	2.30	0.61
4:D:181:ILE:HD12	4:D:207:MET:HE2	1.83	0.61
5:O:494:ALA:HB3	5:O:495:GLU:CA	2.29	0.61
4:B:1089:VAL:HG22	4:B:1118:VAL:CG1	2.28	0.61
5:O:450:LEU:CA	5:O:451:GLU:CB	2.77	0.61
4:B:1084:ARG:HD2	4:B:1089:VAL:HG12	1.82	0.61
4:D:795:GLU:O	4:D:795:GLU:HG2	2.00	0.61
4:C:1093:LEU:C	4:C:1094:LYS:HG2	2.21	0.61
5:N:411:LEU:H	5:N:412:VAL:HG22	1.66	0.61
4:A:1161:VAL:CG2	4:A:1179:VAL:HG22	2.31	0.60
4:D:549:MET:HE3	4:D:559:ILE:HD13	1.77	0.60
4:D:1181:VAL:HG11	4:D:1185:ALA:HB3	1.84	0.60
5:O:519:ARG:CB	5:O:520:LYS:HB2	2.31	0.60
4:B:1032:LEU:HD22	4:B:1077:LEU:HD11	1.84	0.60
4:B:1064:MET:HG2	4:B:1084:ARG:HH21	1.66	0.60
4:B:1066:ALA:HB3	4:B:1084:ARG:NH2	2.15	0.60
4:C:291:MET:CE	4:C:613:GLY:HA3	2.30	0.60
4:D:1204:VAL:HG22	4:D:1205:PHE:N	2.16	0.60
4:C:299:PRO:HG2	4:C:300:LEU:N	2.16	0.60
5:O:450:LEU:CB	5:O:451:GLU:O	2.41	0.60
5:O:450:LEU:HA	5:O:451:GLU:CB	2.30	0.60
4:A:1080:VAL:HB	4:A:1082:PHE:N	2.15	0.60
5:M:409:LYS:HB3	5:M:412:VAL:HG21	1.83	0.60
5:P:409:LYS:CG	5:P:410:THR:H	2.10	0.60
5:P:539:GLY:C	5:P:542:PRO:HD2	2.22	0.60
4:B:1054:VAL:CG2	4:B:1094:LYS:CD	2.79	0.60
5:M:390:ALA:C	5:M:391:LEU:HD12	2.21	0.60
4:A:1032:LEU:HD11	4:A:1047:LEU:CD1	2.30	0.60
4:D:507:VAL:CG1	4:D:558:VAL:HG13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:421:PHE:HD2	5:M:422:HIS:CE1	2.18	0.60
4:A:443:PRO:HA	4:A:448:LEU:HD12	1.83	0.60
4:D:549:MET:CE	4:D:559:ILE:CG1	2.79	0.60
5:M:499:ASP:HB3	5:M:500:PRO:HA	1.83	0.60
4:A:1161:VAL:CG2	4:A:1179:VAL:CG2	2.80	0.60
4:B:1054:VAL:CG2	4:B:1094:LYS:CE	2.80	0.60
4:B:1056:ARG:CG	4:B:1057:LYS:CG	2.63	0.60
4:D:300:LEU:HD22	4:D:304:ARG:HB2	1.84	0.59
4:D:1046:LEU:HD22	4:D:1205:PHE:CE2	2.36	0.59
5:O:388:LEU:HD23	5:O:394:THR:CG2	2.32	0.59
4:B:1057:LYS:NZ	4:B:1064:MET:HE2	2.16	0.59
4:D:1209:ASN:O	4:D:1211:GLY:N	2.31	0.59
4:B:774:VAL:HG12	4:B:775:GLU:HG3	1.83	0.59
4:C:298:PHE:CG	4:C:299:PRO:CD	2.85	0.59
4:D:537:GLU:CA	4:D:540:GLN:HG3	2.31	0.59
4:C:970:ARG:HH21	4:C:975:LEU:CD1	2.15	0.59
4:D:1081:VAL:O	4:D:1081:VAL:HG12	2.02	0.59
5:P:397:ALA:HA	5:P:398:PHE:O	2.03	0.59
4:A:1152:LEU:HD13	4:A:1179:VAL:HG21	1.83	0.59
4:D:1067:ARG:HA	4:D:1081:VAL:HG22	1.84	0.59
4:D:1204:VAL:O	4:D:1205:PHE:HD1	1.85	0.59
5:N:525:GLU:HG3	5:N:528:GLU:O	2.01	0.59
4:A:1165:VAL:CG1	4:A:1172:ALA:HB3	2.32	0.59
4:B:747:ILE:HG23	4:B:805:LEU:HD22	1.84	0.59
4:C:292:VAL:HG12	4:C:293:TYR:N	2.17	0.59
5:P:412:VAL:C	5:P:416:PRO:HD2	2.22	0.59
5:P:413:LEU:HA	5:P:416:PRO:CG	2.32	0.59
5:P:505:ARG:HG2	5:P:514:ARG:HH21	1.65	0.59
2:F:9:DT:O4	4:A:511:TYR:HA	2.02	0.59
4:C:839:PHE:CE2	4:C:843:LEU:HD11	2.38	0.59
4:D:334:VAL:HG21	4:D:384:LEU:HD11	1.84	0.59
4:A:226:VAL:HG21	4:A:561:VAL:HG11	1.85	0.59
4:B:389:TYR:O	4:B:393:VAL:HG23	2.02	0.59
4:B:1013:HIS:CE1	4:B:1016:LEU:HD21	2.36	0.59
4:C:57:TYR:CE2	4:C:287:ILE:HD11	2.38	0.59
5:N:525:GLU:HG2	5:N:528:GLU:O	2.02	0.59
5:N:529:PRO:CA	5:N:530:VAL:HB	2.33	0.59
4:B:333:GLU:O	4:B:337:LEU:HD12	2.03	0.59
4:D:300:LEU:HD22	4:D:304:ARG:CB	2.32	0.59
5:O:519:ARG:CG	5:O:520:LYS:HB2	2.32	0.59
4:A:1087:GLU:HG3	4:A:1088:GLY:HA3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:ALA:HB2	4:D:109:LEU:HD12	1.84	0.59
5:O:389:GLU:HB2	5:O:445:GLU:HB3	1.85	0.59
5:O:494:ALA:HB3	5:O:495:GLU:CD	2.22	0.59
4:B:1084:ARG:HD2	4:B:1089:VAL:HG11	1.84	0.58
4:C:975:LEU:HD23	4:C:976:VAL:N	2.18	0.58
4:B:319:LEU:HD23	4:B:319:LEU:C	2.22	0.58
4:C:1207:GLN:HB3	4:C:1208:GLY:CA	2.32	0.58
4:A:1161:VAL:HG22	4:A:1179:VAL:HG22	1.84	0.58
4:B:976:VAL:HG21	4:C:115:ARG:CZ	2.34	0.58
4:C:298:PHE:CG	4:C:299:PRO:HD2	2.37	0.58
4:D:1166:LEU:HD12	4:D:1166:LEU:O	2.02	0.58
4:B:233:LYS:HG2	4:B:510:VAL:HG11	1.85	0.58
4:C:428:ALA:HB3	4:C:816:SER:HB2	1.85	0.58
5:M:389:GLU:O	5:M:390:ALA:CB	2.49	0.58
5:M:525:GLU:H	5:M:525:GLU:CD	2.03	0.58
5:N:450:LEU:HB3	5:N:451:GLU:HB2	1.85	0.58
5:O:395:LEU:CB	5:O:396:ARG:HB2	2.34	0.58
5:M:524:PRO:N	5:M:525:GLU:HA	2.18	0.58
5:P:456:SER:N	5:P:457:GLY:HA2	2.18	0.58
4:A:639:LYS:O	4:A:641:VAL:HG23	2.03	0.58
4:A:1093:LEU:HD13	4:A:1099:LEU:HG	1.85	0.58
4:A:669:GLN:HE22	4:A:821:TYR:HB3	1.69	0.58
4:C:1165:VAL:O	4:C:1165:VAL:HG13	2.04	0.58
4:D:1119:TRP:CZ2	4:D:1206:LEU:HA	2.38	0.58
5:M:412:VAL:O	5:M:414:ARG:N	2.37	0.58
5:P:413:LEU:O	5:P:417:GLU:HB2	2.03	0.58
4:C:290:LYS:O	4:C:291:MET:HG3	2.03	0.58
4:D:1082:PHE:HZ	4:D:1114:LEU:CA	2.16	0.58
5:M:421:PHE:CE2	5:M:422:HIS:CE1	2.91	0.58
5:N:395:LEU:HA	5:N:396:ARG:CB	2.29	0.58
5:N:406:LEU:HD22	5:N:419:LYS:HG2	1.86	0.58
5:P:493:GLU:O	5:P:504:LEU:HD13	2.04	0.58
4:C:659:LEU:HD11	4:C:829:ALA:CB	2.33	0.58
5:P:524:PRO:HG2	5:P:526:ALA:HB2	1.86	0.58
5:P:529:PRO:CB	5:P:530:VAL:HA	2.30	0.58
4:C:1051:VAL:HG12	4:C:1068:PHE:CD1	2.39	0.57
4:D:1059:THR:CG2	4:D:1065:MET:HE3	2.25	0.57
5:M:421:PHE:CD2	5:M:422:HIS:N	2.72	0.57
5:P:456:SER:H	5:P:457:GLY:CA	2.17	0.57
4:A:1093:LEU:HD23	4:A:1094:LYS:O	2.04	0.57
4:A:1204:VAL:HG12	4:A:1205:PHE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:418:VAL:HG13	4:C:472:GLU:HB2	1.85	0.57
4:C:1129:LYS:HE2	4:C:1198:LEU:HD21	1.86	0.57
4:D:285:LEU:O	4:D:287:ILE:N	2.37	0.57
5:M:408:GLY:HA3	5:M:415:PHE:CD1	2.35	0.57
5:O:529:PRO:HA	5:O:530:VAL:HB	1.86	0.57
4:A:32:VAL:HG21	4:A:42:LEU:HD22	1.86	0.57
4:A:1080:VAL:CG2	4:A:1114:LEU:CA	2.70	0.57
4:B:1067:ARG:CA	4:B:1081:VAL:HG21	2.32	0.57
5:N:518:VAL:HG22	5:N:519:ARG:HG3	1.86	0.57
4:D:1201:ASP:O	4:D:1204:VAL:HG12	2.03	0.57
5:M:419:LYS:CA	5:M:422:HIS:CD2	2.84	0.57
5:O:453:LYS:O	5:O:454:SER:HB3	2.04	0.57
4:A:307:ALA:HB1	4:A:395:GLU:HG2	1.86	0.57
4:B:1056:ARG:HG3	4:B:1057:LYS:CD	2.34	0.57
4:C:541:VAL:N	4:C:542:VAL:HG13	2.19	0.57
4:D:951:ALA:HB2	4:D:993:LEU:HG	1.86	0.57
5:M:523:ALA:HB1	5:M:524:PRO:HA	1.87	0.57
5:O:490:PRO:HD2	5:O:522:LYS:HD2	1.86	0.57
4:A:1204:VAL:HG12	4:A:1205:PHE:N	2.20	0.57
4:C:1161:VAL:CG1	4:C:1176:LEU:CD2	2.83	0.57
4:B:354:LEU:O	4:B:362:TRP:CH2	2.58	0.57
4:D:418:VAL:HG13	4:D:472:GLU:HB2	1.85	0.57
4:D:1212:GLY:O	4:D:1216:GLU:HG2	2.04	0.57
5:M:524:PRO:HG2	5:M:526:ALA:CB	2.35	0.57
5:O:403:ARG:HE	5:O:437:ALA:HB3	1.70	0.57
4:B:525:ILE:HD11	4:B:538:ALA:HB2	1.86	0.57
4:D:159:LEU:HD22	4:D:195:VAL:HG11	1.86	0.57
4:D:1119:TRP:CZ2	4:D:1206:LEU:CA	2.88	0.57
4:D:1144:GLY:HA2	4:D:1145:VAL:HG13	1.85	0.57
5:M:403:ARG:HE	5:M:437:ALA:HB3	1.70	0.57
1:E:20:DA:N6	4:A:510:VAL:O	2.38	0.57
4:B:28:LEU:HD11	4:B:251:VAL:HG21	1.86	0.57
4:B:357:VAL:CG1	4:B:358:GLU:CG	2.75	0.57
4:C:1093:LEU:C	4:C:1094:LYS:CG	2.67	0.57
4:D:935:LEU:O	4:D:939:VAL:HG23	2.05	0.57
5:M:406:LEU:HA	5:M:419:LYS:HG2	1.86	0.57
5:M:523:ALA:CB	5:M:524:PRO:CA	2.83	0.57
5:O:392:LYS:HA	5:O:393:PRO:C	2.25	0.57
5:M:392:LYS:HG2	5:M:397:ALA:HB2	1.87	0.57
4:D:226:VAL:HG12	4:D:510:VAL:HG11	1.86	0.56
5:P:493:GLU:HB2	5:P:494:ALA:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:539:GLY:HA2	5:P:542:PRO:HD2	1.86	0.56
4:A:386:ARG:NH1	4:A:390:GLU:OE1	2.38	0.56
4:A:590:VAL:HG11	4:A:602:THR:HG23	1.87	0.56
4:B:490:ALA:O	4:B:580:VAL:HG12	2.05	0.56
4:D:444:LEU:HD12	4:D:445:ARG:N	2.21	0.56
5:M:413:LEU:CA	5:M:416:PRO:HD2	2.35	0.56
5:O:395:LEU:N	5:O:396:ARG:O	2.37	0.56
5:O:518:VAL:HA	5:O:519:ARG:HG3	1.88	0.56
4:C:331:TYR:CD2	4:C:354:LEU:HD11	2.40	0.56
4:C:1159:LEU:HD11	4:C:1183:GLU:HG3	1.88	0.56
4:C:1162:TYR:C	4:C:1163:LEU:HD12	2.26	0.56
4:D:67:PRO:O	4:D:68:ILE:HD13	2.04	0.56
4:D:106:TYR:O	4:D:110:VAL:HG23	2.04	0.56
4:D:975:LEU:CB	4:D:980:ALA:HB2	2.35	0.56
4:D:1032:LEU:HD12	4:D:1047:LEU:HD11	1.87	0.56
4:D:1055:VAL:HB	4:D:1066:ALA:HB1	1.88	0.56
5:O:530:VAL:HG13	5:O:530:VAL:O	2.05	0.56
5:P:392:LYS:N	5:P:393:PRO:HD3	2.20	0.56
4:B:132:LEU:O	4:B:136:ALA:HB2	2.05	0.56
4:B:235:THR:HG22	4:B:236:LEU:H	1.70	0.56
5:N:505:ARG:HH22	5:N:532:GLU:CD	2.09	0.56
5:O:402:ALA:O	5:O:406:LEU:HD13	2.05	0.56
5:P:389:GLU:HG2	5:P:393:PRO:HG2	1.87	0.56
5:M:418:SER:C	5:M:422:HIS:NE2	2.58	0.56
5:N:505:ARG:HD2	5:N:510:LEU:CB	2.26	0.56
5:P:540:ILE:O	5:P:543:PRO:HD3	2.04	0.56
4:B:357:VAL:CB	4:B:358:GLU:CG	2.84	0.56
5:M:506:ARG:HA	5:M:510:LEU:CD2	2.33	0.56
4:D:54:VAL:HG11	4:D:608:ALA:HB1	1.87	0.56
4:D:535:LEU:O	4:D:539:ILE:HG12	2.06	0.56
5:P:399:VAL:HG11	5:P:441:PHE:CZ	2.40	0.56
4:A:737:THR:HG21	4:A:746:GLN:HE22	1.69	0.56
4:D:192:VAL:HG12	4:D:196:LEU:CD1	2.35	0.56
4:D:287:ILE:O	4:D:290:LYS:HG3	2.05	0.56
4:A:1080:VAL:HG22	4:A:1113:VAL:O	2.05	0.56
4:D:188:GLU:O	4:D:192:VAL:HG23	2.06	0.56
4:D:1080:VAL:HG12	4:D:1081:VAL:HB	1.87	0.56
4:D:1205:PHE:CE1	4:D:1206:LEU:CD1	2.89	0.56
5:P:525:GLU:O	5:P:526:ALA:HB3	2.06	0.56
5:O:392:LYS:HD2	5:O:397:ALA:HB3	1.88	0.56
4:C:295:ILE:HG23	4:C:295:ILE:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1204:VAL:HG22	4:D:1205:PHE:H	1.71	0.55
5:N:504:LEU:HD13	5:N:535:ILE:HD12	1.88	0.55
5:O:506:ARG:O	5:O:510:LEU:HB2	2.06	0.55
5:P:518:VAL:HA	5:P:519:ARG:HG3	1.87	0.55
4:A:300:LEU:N	4:A:301:PRO:CD	2.70	0.55
5:N:505:ARG:HD2	5:N:510:LEU:HD23	1.78	0.55
5:N:529:PRO:HA	5:N:530:VAL:HB	1.88	0.55
4:C:351:ALA:HA	4:C:354:LEU:HD12	1.87	0.55
5:N:395:LEU:HD23	5:N:396:ARG:CB	2.36	0.55
5:N:529:PRO:CB	5:N:530:VAL:HB	2.36	0.55
4:A:399:PHE:N	4:A:400:PRO:CD	2.70	0.55
4:A:1133:VAL:HG13	4:A:1163:LEU:HD12	1.88	0.55
5:P:451:GLU:O	5:P:452:LYS:HB2	2.07	0.55
5:P:504:LEU:CB	5:P:505:ARG:HG2	2.36	0.55
4:C:590:VAL:HG11	4:C:602:THR:CG2	2.37	0.55
4:D:975:LEU:HB3	4:D:980:ALA:HB2	1.88	0.55
4:D:1102:LEU:CD1	4:D:1206:LEU:CG	2.82	0.55
4:B:1123:GLU:HG2	4:B:1216:GLU:HB3	1.88	0.55
4:D:286:PRO:HA	4:D:290:LYS:HB2	1.89	0.55
4:D:500:SER:HB3	4:D:535:LEU:HD12	1.86	0.55
4:D:1051:VAL:HG21	4:D:1093:LEU:CD2	2.37	0.55
5:P:499:ASP:HB3	5:P:515:LEU:CD2	2.37	0.55
4:D:1079:VAL:C	4:D:1081:VAL:HG23	2.26	0.55
4:B:569:ASN:O	4:B:570:ARG:HB3	2.07	0.55
4:B:1093:LEU:HD22	4:B:1099:LEU:HG	1.89	0.55
4:C:1079:VAL:HG12	4:C:1080:VAL:N	2.22	0.55
4:C:1093:LEU:CD1	4:C:1097:ILE:HB	2.34	0.55
5:M:535:ILE:O	5:M:538:ASN:HB3	2.07	0.55
4:B:1056:ARG:CG	4:B:1057:LYS:CD	2.84	0.55
4:D:664:THR:HG21	4:D:670:LEU:HD13	1.89	0.55
5:O:505:ARG:HH12	5:O:506:ARG:NH1	2.05	0.55
5:P:529:PRO:HB2	5:P:530:VAL:CA	2.32	0.55
1:G:19:DC:N4	2:H:10:DG:C6	2.75	0.54
4:C:788:ALA:HB1	4:C:793:VAL:HG21	1.89	0.54
5:P:396:ARG:O	5:P:397:ALA:C	2.45	0.54
5:P:498:GLU:HB2	5:P:499:ASP:HA	1.90	0.54
4:A:170:LEU:HD21	4:A:205:LEU:HD22	1.89	0.54
4:D:982:VAL:HG13	4:D:982:VAL:O	2.07	0.54
5:M:394:THR:O	5:M:394:THR:HG22	2.06	0.54
5:P:493:GLU:O	5:P:504:LEU:CD1	2.55	0.54
4:A:970:ARG:O	4:A:974:GLY:O	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1177:ARG:O	4:A:1179:VAL:HG13	2.07	0.54
4:B:670:LEU:HD12	4:B:675:MET:CG	2.37	0.54
4:B:696:LEU:HD21	4:B:742:VAL:HG22	1.89	0.54
4:B:1099:LEU:HD22	4:B:1118:VAL:HG22	1.90	0.54
4:D:537:GLU:C	4:D:540:GLN:CG	2.74	0.54
4:B:1053:GLU:HB3	4:B:1068:PHE:HA	1.89	0.54
4:C:154:ILE:CD1	4:C:195:VAL:HB	2.33	0.54
5:M:419:LYS:O	5:M:423:HIS:CD2	2.60	0.54
5:M:450:LEU:HB3	5:M:451:GLU:C	2.28	0.54
4:A:1013:HIS:CD2	4:A:1015:VAL:HG12	2.42	0.54
4:B:951:ALA:HB2	4:B:993:LEU:HG	1.90	0.54
5:M:541:MET:O	5:M:543:PRO:HD2	2.08	0.54
4:A:918:LEU:HD22	4:A:953:LEU:CD2	2.38	0.54
4:A:1080:VAL:HG23	4:A:1114:LEU:HA	1.81	0.54
4:C:723:PHE:HB3	4:C:726:ALA:HB3	1.88	0.54
4:D:287:ILE:HG22	4:D:288:GLY:N	2.22	0.54
4:D:1218:VAL:HB	4:D:1219:PRO:HD3	1.88	0.54
4:A:555:ILE:C	4:A:555:ILE:HD12	2.28	0.54
4:B:410:ILE:HG23	4:B:420:VAL:HG11	1.88	0.54
4:C:146:LEU:HD11	4:C:189:GLN:HG2	1.90	0.54
4:D:1087:GLU:HB3	4:D:1088:GLY:HA3	1.88	0.54
5:P:395:LEU:C	5:P:397:ALA:N	2.61	0.54
4:C:1093:LEU:O	4:C:1094:LYS:HB2	2.08	0.54
4:D:1057:LYS:CB	4:D:1058:PRO:CA	2.83	0.54
4:B:1058:PRO:HG2	4:B:1059:THR:N	2.22	0.54
4:C:854:VAL:HG23	4:C:1008:ILE:HG21	1.89	0.54
5:M:519:ARG:HD3	5:M:520:LYS:HE3	1.90	0.54
4:C:287:ILE:CA	4:C:291:MET:HB3	2.27	0.54
4:C:854:VAL:CG2	4:C:1008:ILE:HG21	2.38	0.54
4:C:1205:PHE:O	4:C:1206:LEU:HG	2.08	0.54
4:D:1080:VAL:CG2	4:D:1115:ALA:H	2.21	0.54
3:I:20:DA:C2	3:I:21:DOC:C2	2.91	0.53
4:A:1099:LEU:HD13	4:A:1118:VAL:HG11	1.90	0.53
4:D:589:LEU:HG	4:D:612:LEU:HD21	1.90	0.53
4:D:672:SER:O	4:D:676:THR:HG23	2.08	0.53
4:D:1095:GLU:O	4:D:1097:ILE:HD12	2.08	0.53
4:A:951:ALA:HB2	4:A:993:LEU:HD21	1.90	0.53
4:B:1080:VAL:HA	4:B:1081:VAL:CB	2.37	0.53
4:D:546:ARG:NH1	4:D:550:GLU:OE2	2.41	0.53
4:D:1159:LEU:HD21	4:D:1183:GLU:HG2	1.90	0.53
4:B:590:VAL:HG13	4:B:604:TYR:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1057:LYS:CB	4:B:1058:PRO:CA	2.84	0.53
4:C:28:LEU:HD11	4:C:251:VAL:HG21	1.90	0.53
4:C:631:ALA:O	4:C:635:VAL:HG23	2.08	0.53
5:N:395:LEU:HD23	5:N:396:ARG:CD	2.38	0.53
4:B:308:GLN:HE21	4:B:356:ARG:HA	1.74	0.53
4:D:28:LEU:CD1	4:D:251:VAL:HG21	2.39	0.53
4:D:535:LEU:O	4:D:538:ALA:HB3	2.08	0.53
4:D:788:ALA:HB1	4:D:793:VAL:CG2	2.38	0.53
4:A:170:LEU:HD21	4:A:205:LEU:CD2	2.38	0.53
4:C:1051:VAL:HG22	4:C:1097:ILE:O	2.07	0.53
4:D:1089:VAL:HG12	4:D:1091:PRO:HD3	1.89	0.53
4:D:1144:GLY:HA2	4:D:1145:VAL:CG1	2.38	0.53
4:D:1205:PHE:CD1	4:D:1206:LEU:CD1	2.85	0.53
4:A:691:ILE:HG22	4:A:743:TYR:OH	2.09	0.53
4:A:1067:ARG:N	4:A:1081:VAL:CG2	2.67	0.53
4:D:115:ARG:NH1	4:D:131:ILE:HD12	2.23	0.53
4:A:319:LEU:HD23	4:A:326:ILE:O	2.08	0.53
4:A:459:VAL:HG13	4:A:459:VAL:O	2.09	0.53
4:C:513:ILE:HG23	4:C:517:LYS:NZ	2.24	0.53
4:C:541:VAL:N	4:C:542:VAL:HG22	2.23	0.53
4:B:319:LEU:HD23	4:B:319:LEU:O	2.08	0.53
5:O:409:LYS:HD3	5:O:412:VAL:HG21	1.91	0.53
4:C:318:LEU:HD12	4:C:435:ALA:HB1	1.91	0.53
5:M:396:ARG:CB	5:M:397:ALA:HB3	2.39	0.53
5:N:378:GLN:HA	5:N:381:ALA:HB3	1.91	0.53
5:O:416:PRO:HB3	5:O:436:LEU:HD21	1.91	0.53
5:O:453:LYS:O	5:O:454:SER:CB	2.56	0.53
4:B:230:ILE:HG12	4:B:507:VAL:HG13	1.91	0.52
4:B:1181:VAL:CG1	4:B:1185:ALA:HB3	2.38	0.52
4:C:1129:LYS:O	4:C:1159:LEU:HD22	2.10	0.52
4:D:952:ARG:HD3	4:D:987:LEU:HD23	1.91	0.52
4:D:1205:PHE:O	4:D:1206:LEU:HD12	2.09	0.52
4:A:1121:LEU:HD11	4:A:1125:LEU:HD11	1.90	0.52
4:C:54:VAL:HG23	4:C:604:TYR:CE2	2.45	0.52
4:C:1081:VAL:HG23	4:C:1084:ARG:HB3	1.91	0.52
4:D:148:ALA:HB3	4:D:151:PRO:CG	2.38	0.52
4:D:158:ARG:HG2	4:D:161:LEU:HD22	1.91	0.52
5:N:505:ARG:CD	5:N:510:LEU:CD2	2.75	0.52
4:A:952:ARG:HD3	4:A:987:LEU:HD23	1.90	0.52
4:A:1080:VAL:CA	4:A:1081:VAL:HB	2.21	0.52
4:C:970:ARG:HE	4:C:975:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1213:PRO:O	4:C:1217:VAL:HG23	2.09	0.52
4:D:498:LEU:HD22	4:D:570:ARG:HH21	1.74	0.52
4:D:1065:MET:HG3	4:D:1081:VAL:O	2.09	0.52
5:N:512:GLY:HA2	5:N:515:LEU:HD13	1.91	0.52
2:F:24:DT:H1'	2:F:25:DT:H5''	1.90	0.52
4:A:1135:VAL:HG21	4:A:1163:LEU:HD11	1.91	0.52
4:B:1013:HIS:HB3	4:B:1014:PRO:CA	2.37	0.52
5:M:403:ARG:HG2	5:M:437:ALA:HB1	1.92	0.52
4:A:332:ARG:HG3	4:A:350:LEU:HD21	1.90	0.52
4:A:951:ALA:HB2	4:A:993:LEU:HG	1.92	0.52
4:C:970:ARG:NH2	4:C:975:LEU:CD1	2.73	0.52
4:C:1129:LYS:CE	4:C:1198:LEU:HD21	2.40	0.52
4:D:788:ALA:HB1	4:D:793:VAL:HG21	1.91	0.52
5:N:455:LEU:N	5:N:456:SER:CB	2.72	0.52
5:O:521:PRO:HD2	5:O:522:LYS:H	1.73	0.52
4:A:154:ILE:HD13	4:A:195:VAL:HB	1.92	0.52
4:A:569:ASN:HA	4:A:570:ARG:CB	2.34	0.52
4:A:574:VAL:CG1	4:A:575:HIS:N	2.73	0.52
4:D:1051:VAL:HB	4:D:1093:LEU:HD23	1.92	0.52
4:D:1055:VAL:HG21	4:D:1067:ARG:C	2.29	0.52
4:A:1016:LEU:HD23	4:A:1022:ARG:HD2	1.92	0.52
4:B:1122:GLU:OE2	5:N:530:VAL:HG11	2.09	0.52
4:C:1093:LEU:CD1	4:C:1097:ILE:CG2	2.71	0.52
4:C:1166:LEU:O	4:C:1166:LEU:HD12	2.10	0.52
4:D:112:LEU:CD2	4:D:131:ILE:HG22	2.38	0.52
5:M:385:ARG:HB2	5:M:386:ALA:HA	1.91	0.52
5:P:499:ASP:HB3	5:P:515:LEU:HD21	1.92	0.52
5:P:524:PRO:N	5:P:525:GLU:CA	2.73	0.52
4:A:424:ARG:CZ	4:A:620:LEU:HD22	2.39	0.52
4:B:1055:VAL:O	4:B:1066:ALA:HB2	2.08	0.52
5:O:395:LEU:HB2	5:O:396:ARG:O	2.09	0.52
4:A:1081:VAL:O	4:A:1081:VAL:HG12	2.09	0.52
4:C:574:VAL:HG12	4:C:575:HIS:O	2.09	0.52
4:C:1182:GLY:O	4:C:1183:GLU:HB2	2.10	0.52
5:M:505:ARG:CB	5:M:506:ARG:CA	2.82	0.52
5:M:524:PRO:HG2	5:M:526:ALA:HB3	1.92	0.52
5:N:524:PRO:CB	5:N:525:GLU:CA	2.86	0.52
4:A:561:VAL:O	4:A:565:LEU:HD13	2.10	0.52
4:A:1051:VAL:HB	4:A:1093:LEU:HD22	1.92	0.52
4:A:1080:VAL:CA	4:A:1081:VAL:CB	2.85	0.52
4:A:1159:LEU:HD11	4:A:1180:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1102:LEU:HD11	4:D:1206:LEU:HG	1.87	0.52
5:N:395:LEU:CA	5:N:396:ARG:HB2	2.31	0.52
5:P:504:LEU:CB	5:P:505:ARG:HA	2.36	0.52
1:E:15:DG:O6	2:F:13:DA:N6	2.43	0.51
4:B:615:LEU:HD21	4:B:617:MET:HE3	1.92	0.51
4:C:1080:VAL:HB	4:C:1081:VAL:C	2.29	0.51
4:D:537:GLU:HB3	4:D:540:GLN:NE2	2.26	0.51
4:D:1152:LEU:HD22	4:D:1181:VAL:HG21	1.92	0.51
5:O:519:ARG:HB3	5:O:520:LYS:CB	2.40	0.51
5:P:450:LEU:HB3	5:P:451:GLU:C	2.30	0.51
4:B:1056:ARG:C	4:B:1057:LYS:HG3	2.26	0.51
4:B:1147:ARG:HG3	4:B:1148:LEU:HD12	1.92	0.51
4:C:292:VAL:CG1	4:C:293:TYR:N	2.73	0.51
5:M:415:PHE:HB2	5:M:416:PRO:CD	2.41	0.51
4:A:291:MET:HG2	4:A:291:MET:O	2.10	0.51
4:A:971:GLY:HA2	4:A:975:LEU:HB2	1.85	0.51
4:A:1214:LYS:O	4:A:1218:VAL:HG23	2.09	0.51
4:C:293:TYR:N	4:C:293:TYR:CD1	2.78	0.51
5:M:535:ILE:CG2	5:M:536:GLY:N	2.72	0.51
5:N:455:LEU:HA	5:N:456:SER:C	2.30	0.51
5:O:407:GLU:OE1	5:O:436:LEU:HD22	2.10	0.51
4:B:1056:ARG:CZ	4:B:1056:ARG:HB2	2.38	0.51
4:C:293:TYR:N	4:C:293:TYR:HD1	2.07	0.51
4:C:399:PHE:N	4:C:400:PRO:CD	2.74	0.51
4:C:813:PHE:CE2	4:C:818:ALA:HB2	2.45	0.51
4:D:1120:THR:HG22	4:D:1121:LEU:H	1.76	0.51
5:P:416:PRO:HG2	5:P:417:GLU:H	1.75	0.51
4:A:795:GLU:O	4:A:795:GLU:HG2	2.10	0.51
4:B:357:VAL:HB	4:B:358:GLU:CG	2.41	0.51
4:C:301:PRO:HB2	4:C:302:GLU:CB	2.38	0.51
4:D:549:MET:CE	4:D:559:ILE:HD13	2.32	0.51
4:D:1057:LYS:CE	4:D:1064:MET:N	2.71	0.51
4:D:1159:LEU:CD2	4:D:1183:GLU:CG	2.88	0.51
4:B:690:ILE:O	4:B:694:VAL:HG23	2.10	0.51
4:B:982:VAL:O	4:B:982:VAL:HG13	2.11	0.51
4:D:1152:LEU:HB3	4:D:1179:VAL:HG11	1.93	0.51
5:N:494:ALA:HB1	5:N:495:GLU:C	2.30	0.51
5:N:505:ARG:HB3	5:N:506:ARG:HA	1.89	0.51
5:N:508:ALA:CA	5:N:510:LEU:N	2.67	0.51
5:P:539:GLY:HA2	5:P:542:PRO:CD	2.41	0.51
4:A:980:ALA:C	4:A:981:GLU:CG	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:407:GLN:HG3	4:B:436:VAL:HG12	1.92	0.51
4:B:1027:CYS:O	4:B:1047:LEU:HD13	2.11	0.51
4:B:1151:LEU:HD12	4:B:1152:LEU:CD1	2.41	0.51
4:C:54:VAL:HG23	4:C:604:TYR:CZ	2.45	0.51
4:C:504:LEU:HD12	4:C:525:ILE:HD11	1.92	0.51
4:C:1181:VAL:CG1	4:C:1185:ALA:HB3	2.41	0.51
4:D:146:LEU:HD11	4:D:189:GLN:HG3	1.92	0.51
5:N:395:LEU:HD23	5:N:396:ARG:HD2	1.92	0.51
4:D:1125:LEU:HD13	5:P:530:VAL:CG1	2.40	0.51
5:N:495:GLU:HB2	5:N:496:GLU:HB2	1.91	0.51
5:P:539:GLY:CA	5:P:542:PRO:HD2	2.41	0.51
4:A:106:TYR:O	4:A:110:VAL:HG23	2.10	0.51
4:B:1055:VAL:CG1	4:B:1066:ALA:HA	2.41	0.51
4:C:951:ALA:HB2	4:C:993:LEU:CG	2.41	0.51
4:C:952:ARG:HD3	4:C:987:LEU:HD23	1.93	0.51
4:C:976:VAL:O	4:C:976:VAL:HG13	2.10	0.51
4:C:1161:VAL:HG12	4:C:1176:LEU:HD21	1.93	0.51
4:D:1080:VAL:CG1	4:D:1081:VAL:HB	2.39	0.51
5:M:406:LEU:HD22	5:M:419:LYS:HG2	1.92	0.51
5:N:524:PRO:HD2	5:N:525:GLU:CA	2.21	0.51
5:O:447:ALA:O	5:O:448:PHE:CD1	2.64	0.51
5:P:528:GLU:H	5:P:529:PRO:CD	2.23	0.51
4:A:25:LEU:HD21	4:A:56:PHE:HA	1.93	0.51
4:C:226:VAL:HG12	4:C:510:VAL:HG11	1.92	0.51
5:M:543:PRO:HG2	5:M:543:PRO:O	2.11	0.51
4:C:975:LEU:HD23	4:C:976:VAL:HA	1.93	0.50
5:P:499:ASP:HB2	5:P:515:LEU:CD2	2.27	0.50
4:B:1024:VAL:O	4:B:1025:ALA:C	2.49	0.50
4:B:1027:CYS:SG	4:B:1045:VAL:HG11	2.51	0.50
4:B:1058:PRO:HG2	4:B:1059:THR:H	1.76	0.50
4:B:1058:PRO:CG	4:B:1059:THR:N	2.73	0.50
4:C:223:ALA:O	4:C:226:VAL:HG22	2.12	0.50
4:C:918:LEU:HD22	4:C:953:LEU:HD22	1.92	0.50
4:D:1080:VAL:C	4:D:1081:VAL:CG2	2.74	0.50
4:D:1080:VAL:N	4:D:1081:VAL:HG23	2.23	0.50
5:N:510:LEU:O	5:N:511:LEU:C	2.49	0.50
5:O:505:ARG:NE	5:O:507:LEU:HD21	2.24	0.50
3:I:14:DA:C2	2:J:16:DG:N2	2.80	0.50
4:A:1093:LEU:HD11	4:A:1097:ILE:HG22	1.93	0.50
4:C:154:ILE:HD11	4:C:195:VAL:CB	2.36	0.50
4:D:1159:LEU:CD1	4:D:1183:GLU:HG3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:362:TRP:CE3	4:A:365:LEU:HD12	2.47	0.50
4:B:227:LEU:HA	4:B:230:ILE:HD12	1.92	0.50
4:B:405:ILE:HG23	4:B:484:TYR:OH	2.11	0.50
4:B:515:HIS:HB2	4:B:516:LYS:CA	2.40	0.50
4:B:1151:LEU:HD12	4:B:1152:LEU:HD12	1.92	0.50
4:C:1089:VAL:HG23	4:C:1091:PRO:HD3	1.94	0.50
4:C:1093:LEU:O	4:C:1094:LYS:CG	2.59	0.50
4:D:537:GLU:HB3	4:D:540:GLN:HE21	1.76	0.50
5:N:440:GLN:CB	5:N:441:PHE:HA	2.41	0.50
4:A:186:LEU:HD21	4:A:245:PRO:HB2	1.93	0.50
4:D:1082:PHE:CZ	4:D:1114:LEU:HB2	2.39	0.50
5:M:369:HIS:O	5:M:378:GLN:NE2	2.44	0.50
5:O:494:ALA:HB3	5:O:495:GLU:CG	2.42	0.50
4:A:1093:LEU:HD13	4:A:1099:LEU:CG	2.41	0.50
4:C:604:TYR:HB3	4:C:608:ALA:HB3	1.93	0.50
4:C:1093:LEU:HD12	4:C:1097:ILE:HD12	1.92	0.50
4:C:1136:ASP:O	4:C:1139:LEU:HD23	2.11	0.50
5:M:406:LEU:HD22	5:M:419:LYS:CG	2.42	0.50
5:M:419:LYS:O	5:M:423:HIS:NE2	2.45	0.50
5:N:440:GLN:HB2	5:N:441:PHE:HB2	1.92	0.50
4:C:406:VAL:HG11	4:C:464:ILE:HG21	1.94	0.50
4:C:970:ARG:NE	4:C:975:LEU:HD13	2.26	0.50
4:D:1159:LEU:CD2	4:D:1183:GLU:HG3	2.42	0.50
5:O:385:ARG:HB2	5:O:386:ALA:HA	1.94	0.50
5:P:505:ARG:CG	5:P:514:ARG:HE	2.17	0.50
4:B:922:LEU:CD1	4:B:964:ALA:HB2	2.42	0.50
4:D:542:VAL:CG1	4:D:543:PRO:HD3	2.40	0.50
5:O:390:ALA:O	5:O:391:LEU:O	2.29	0.50
4:B:1218:VAL:N	4:B:1219:PRO:HD2	2.27	0.50
5:N:395:LEU:CA	5:N:396:ARG:CB	2.89	0.50
5:P:501:SER:OG	5:P:504:LEU:O	2.29	0.50
4:A:116:ALA:HB1	4:A:125:PRO:HB2	1.94	0.49
4:A:366:ARG:HD3	4:A:385:HIS:NE2	2.27	0.49
4:B:352:GLU:HG2	4:B:356:ARG:CZ	2.41	0.49
5:M:538:ASN:O	5:M:541:MET:HB3	2.12	0.49
5:P:542:PRO:C	5:P:543:PRO:OXT	2.51	0.49
2:L:7:DT:OP2	4:D:1067:ARG:NH1	2.45	0.49
4:A:513:ILE:CG2	4:A:514:PRO:CD	2.85	0.49
4:A:789:LYS:HE3	4:A:795:GLU:OE1	2.12	0.49
4:A:1152:LEU:HD13	4:A:1179:VAL:CG2	2.41	0.49
4:B:32:VAL:HG21	4:B:42:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1027:CYS:SG	4:B:1045:VAL:CG1	3.00	0.49
4:C:1173:LEU:HD13	4:C:1202:ARG:HH22	1.78	0.49
4:D:635:VAL:HG22	4:D:838:GLU:HG3	1.94	0.49
4:A:590:VAL:CG1	4:A:602:THR:HG23	2.42	0.49
4:A:628:LEU:HD22	4:A:645:TYR:CE2	2.47	0.49
4:D:154:ILE:C	4:D:154:ILE:HD12	2.33	0.49
4:B:590:VAL:CG1	4:B:602:THR:HG23	2.42	0.49
4:B:1099:LEU:HD23	4:B:1120:THR:HA	1.93	0.49
4:C:961:LEU:HD12	4:C:962:ARG:N	2.27	0.49
4:D:23:ALA:HB2	4:D:215:TYR:HA	1.94	0.49
4:D:1067:ARG:HA	4:D:1081:VAL:CG2	2.42	0.49
5:M:499:ASP:HB3	5:M:500:PRO:CA	2.42	0.49
5:N:395:LEU:HD23	5:N:396:ARG:HB3	1.93	0.49
5:O:452:LYS:HZ2	5:O:509:ARG:CZ	2.25	0.49
5:O:527:GLU:N	5:O:528:GLU:HA	2.26	0.49
4:B:1068:PHE:H	4:B:1081:VAL:HG11	1.75	0.49
4:C:28:LEU:CD1	4:C:251:VAL:HG21	2.42	0.49
4:C:32:VAL:HG21	4:C:42:LEU:HD22	1.94	0.49
4:C:132:LEU:O	4:C:136:ALA:HB2	2.12	0.49
4:C:661:ARG:O	4:C:680:ARG:NH1	2.46	0.49
5:P:389:GLU:O	5:P:393:PRO:HD2	2.13	0.49
4:B:1055:VAL:HG12	4:B:1056:ARG:N	2.26	0.49
4:B:1057:LYS:HE2	4:B:1064:MET:SD	2.51	0.49
4:C:148:ALA:HB3	4:C:151:PRO:CG	2.42	0.49
5:P:453:LYS:O	5:P:454:SER:HB3	2.13	0.49
4:A:1098:PRO:CG	4:A:1121:LEU:HD22	2.42	0.49
4:B:675:MET:HE1	4:B:697:TYR:HB3	1.94	0.49
4:D:319:LEU:HD11	4:D:328:GLU:OE2	2.13	0.49
5:O:412:VAL:O	5:O:414:ARG:N	2.45	0.49
5:N:526:ALA:O	5:N:527:GLU:HB2	2.13	0.49
5:O:403:ARG:HG2	5:O:437:ALA:HB1	1.95	0.49
5:O:505:ARG:NH1	5:O:506:ARG:NH1	2.60	0.49
5:P:417:GLU:O	5:P:418:SER:C	2.51	0.49
5:P:541:MET:C	5:P:543:PRO:HD3	2.33	0.49
4:A:54:VAL:HG13	4:A:287:ILE:HD11	1.94	0.49
4:A:181:ILE:HD13	4:A:266:TRP:CZ3	2.48	0.49
4:A:854:VAL:O	4:A:858:ILE:HG23	2.13	0.49
4:A:1098:PRO:HG2	4:A:1121:LEU:HD22	1.95	0.49
4:C:307:ALA:HB1	4:C:395:GLU:CD	2.32	0.49
4:D:1202:ARG:NH1	4:D:1202:ARG:CG	2.73	0.49
5:O:390:ALA:C	5:O:393:PRO:HG2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:504:LEU:N	5:P:504:LEU:CD1	2.73	0.49
4:A:1122:GLU:HB3	4:A:1220:PHE:CD1	2.48	0.49
5:N:498:GLU:HB2	5:N:499:ASP:HA	1.95	0.49
5:O:395:LEU:HB3	5:O:396:ARG:HB2	1.95	0.49
5:P:522:LYS:CG	5:P:523:ALA:H	2.13	0.49
4:C:362:TRP:CD1	4:C:388:LEU:HD13	2.48	0.48
4:D:996:ILE:CD1	5:P:528:GLU:OE2	2.59	0.48
4:D:1020:GLY:O	4:D:1024:VAL:HG23	2.13	0.48
4:D:1065:MET:SD	4:D:1082:PHE:CA	2.83	0.48
4:A:1014:PRO:HB2	4:A:1050:MET:HE3	1.95	0.48
4:B:358:GLU:C	4:B:362:TRP:CD1	2.86	0.48
4:C:975:LEU:HD23	4:C:976:VAL:CA	2.42	0.48
5:P:382:GLU:HG3	5:P:388:LEU:HD21	1.94	0.48
5:P:518:VAL:HG13	5:P:519:ARG:HB2	1.93	0.48
4:A:1189:LEU:O	4:A:1189:LEU:HD23	2.12	0.48
4:A:970:ARG:HG3	4:A:980:ALA:HA	1.95	0.48
4:A:1014:PRO:HB2	4:A:1050:MET:CE	2.44	0.48
4:A:1164:ARG:HG2	4:A:1173:LEU:HD21	1.94	0.48
4:B:1181:VAL:HG13	4:B:1185:ALA:HB3	1.95	0.48
4:D:335:LEU:HD21	4:D:354:LEU:HG	1.94	0.48
4:D:549:MET:HE2	4:D:559:ILE:CB	2.39	0.48
4:D:1046:LEU:HD13	4:D:1205:PHE:HD2	1.78	0.48
5:M:505:ARG:HD2	5:M:510:LEU:CG	2.43	0.48
5:P:494:ALA:HB1	5:P:495:GLU:C	2.34	0.48
4:D:1205:PHE:CE1	4:D:1206:LEU:HD12	2.45	0.48
5:N:493:GLU:HB2	5:N:494:ALA:HA	1.95	0.48
4:A:1124:VAL:HG13	4:A:1200:PRO:CG	2.42	0.48
4:C:679:VAL:HG22	4:C:693:LEU:HD21	1.96	0.48
4:C:1080:VAL:CB	4:C:1082:PHE:H	2.23	0.48
4:D:755:ALA:HB2	4:D:784:PHE:CD1	2.49	0.48
4:D:1119:TRP:CH2	4:D:1206:LEU:CA	2.93	0.48
4:A:574:VAL:HG12	4:A:575:HIS:H	1.76	0.48
4:B:356:ARG:O	4:B:357:VAL:CG1	2.62	0.48
4:B:1064:MET:CE	4:B:1087:GLU:OE1	2.62	0.48
4:D:589:LEU:HD21	4:D:612:LEU:HG	1.96	0.48
4:A:28:LEU:HD11	4:A:251:VAL:HG21	1.96	0.48
4:C:300:LEU:HB3	4:C:302:GLU:O	2.14	0.48
4:C:570:ARG:C	4:C:571:HIS:CG	2.87	0.48
4:C:1051:VAL:HG12	4:C:1068:PHE:CE1	2.48	0.48
5:M:411:LEU:CB	5:M:412:VAL:HA	2.43	0.48
5:N:527:GLU:N	5:N:528:GLU:CA	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:535:ILE:HG12	5:P:536:GLY:H	1.79	0.48
4:C:1101:VAL:HG22	4:C:1118:VAL:HG12	1.94	0.48
5:M:524:PRO:HB2	5:M:525:GLU:O	2.14	0.48
5:N:523:ALA:HB3	5:N:524:PRO:CA	2.24	0.48
5:N:525:GLU:HG3	5:N:530:VAL:HA	1.95	0.48
4:A:311:ARG:HG2	4:A:391:LEU:HD13	1.94	0.48
4:A:620:LEU:N	4:A:620:LEU:HD12	2.29	0.48
4:B:424:ARG:NE	4:B:620:LEU:HD22	2.28	0.48
4:B:1056:ARG:CG	4:B:1056:ARG:NH1	2.73	0.48
4:C:970:ARG:NH2	4:C:975:LEU:HD21	2.28	0.48
4:C:1086:TYR:HB2	4:C:1087:GLU:C	2.35	0.48
4:D:13:HIS:NE2	4:D:72:GLU:OE1	2.47	0.48
4:D:1099:LEU:HD23	4:D:1120:THR:HA	1.95	0.48
5:N:522:LYS:HG2	5:N:523:ALA:H	1.78	0.48
4:C:207:MET:HE3	4:C:266:TRP:CZ3	2.49	0.47
4:C:1096:ASP:O	4:C:1097:ILE:HG13	2.14	0.47
5:M:419:LYS:O	5:M:423:HIS:CG	2.66	0.47
4:B:356:ARG:O	4:B:357:VAL:HG13	2.13	0.47
4:B:517:LYS:O	4:B:521:LEU:HD13	2.13	0.47
4:B:941:ALA:CB	4:B:1006:LEU:HD11	2.45	0.47
4:D:154:ILE:HD11	4:D:192:VAL:HG22	1.96	0.47
4:D:307:ALA:HB1	4:D:395:GLU:CD	2.34	0.47
5:M:492:TRP:CZ3	5:M:495:GLU:O	2.68	0.47
2:F:11:DG:H2"	2:F:12:DC:C6	2.49	0.47
4:A:498:LEU:HB3	4:A:499:ALA:CB	2.43	0.47
4:A:525:ILE:H	4:A:525:ILE:HD12	1.79	0.47
4:C:389:TYR:O	4:C:393:VAL:HG23	2.14	0.47
4:C:1157:GLY:HA3	4:C:1182:GLY:HA2	1.95	0.47
4:D:15:GLN:N	4:D:23:ALA:O	2.47	0.47
4:D:314:THR:HG21	4:D:391:LEU:HD11	1.96	0.47
5:O:523:ALA:CB	5:O:524:PRO:HB3	2.25	0.47
4:A:1051:VAL:CG2	4:A:1099:LEU:HD12	2.43	0.47
4:B:951:ALA:HB2	4:B:993:LEU:CD2	2.45	0.47
4:C:287:ILE:HG22	4:C:611:ALA:O	2.14	0.47
4:D:574:VAL:HG22	4:D:601:VAL:HG21	1.95	0.47
4:D:918:LEU:HD22	4:D:953:LEU:CD2	2.44	0.47
4:D:1140:LEU:HG	4:D:1144:GLY:HA3	1.97	0.47
5:P:525:GLU:HB2	5:P:528:GLU:O	2.14	0.47
4:B:354:LEU:O	4:B:362:TRP:HZ2	1.98	0.47
4:B:590:VAL:HG11	4:B:602:THR:HG23	1.97	0.47
4:C:969:GLU:O	4:C:973:SER:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1140:LEU:HD12	4:C:1142:GLU:H	1.80	0.47
4:D:203:TYR:HB2	4:D:205:LEU:HD13	1.96	0.47
4:D:622:LEU:HD23	4:D:625:LEU:HD13	1.97	0.47
5:M:505:ARG:CB	5:M:506:ARG:HA	2.39	0.47
5:N:508:ALA:HB1	5:N:509:ARG:C	2.35	0.47
5:P:505:ARG:CG	5:P:514:ARG:NE	2.76	0.47
4:A:553:GLU:O	4:A:556:ARG:HG2	2.13	0.47
4:B:1029:ILE:HD13	4:B:1047:LEU:HD21	1.96	0.47
4:C:480:VAL:HG11	4:C:581:ILE:HD11	1.95	0.47
4:D:302:GLU:OE2	4:D:304:ARG:NH1	2.47	0.47
4:D:557:GLN:O	4:D:561:VAL:HG23	2.14	0.47
5:M:506:ARG:HB2	5:M:510:LEU:HB2	1.95	0.47
5:P:417:GLU:HG2	5:P:421:PHE:CE2	2.50	0.47
1:K:12:DC:N4	2:L:16:DG:O6	2.48	0.47
4:A:939:VAL:HG22	4:A:944:LEU:HD12	1.97	0.47
4:A:1173:LEU:HD12	4:A:1202:ARG:HD2	1.95	0.47
4:B:1080:VAL:HG21	4:B:1114:LEU:HD22	1.96	0.47
4:C:1094:LYS:N	4:C:1094:LYS:CD	2.72	0.47
4:D:181:ILE:CD1	4:D:207:MET:HE3	2.45	0.47
4:D:235:THR:HG22	4:D:236:LEU:H	1.80	0.47
4:D:399:PHE:N	4:D:400:PRO:CD	2.77	0.47
4:D:1099:LEU:HD22	4:D:1118:VAL:CG1	2.44	0.47
5:M:418:SER:O	5:M:422:HIS:CG	2.68	0.47
5:P:528:GLU:HG3	5:P:529:PRO:CG	2.43	0.47
2:F:12:DC:C4	2:F:13:DA:C6	3.02	0.47
4:B:238:ASP:HB3	4:B:239:PRO:CA	2.44	0.47
4:C:1176:LEU:HD12	4:C:1177:ARG:N	2.30	0.47
4:D:1093:LEU:HD11	4:D:1097:ILE:HG22	1.97	0.47
4:C:495:PHE:CD1	4:C:572:ALA:HB2	2.50	0.47
4:C:1197:TYR:CD2	4:C:1199:VAL:HG12	2.50	0.47
4:D:511:TYR:O	4:D:554:ARG:NH2	2.47	0.47
4:D:1211:GLY:N	4:D:1212:GLY:HA2	2.30	0.47
5:M:453:LYS:O	5:M:454:SER:CB	2.63	0.47
5:N:403:ARG:HE	5:N:437:ALA:HB1	1.80	0.47
5:N:505:ARG:CB	5:N:506:ARG:CA	2.85	0.47
5:O:390:ALA:CB	5:O:393:PRO:CG	2.78	0.47
5:P:505:ARG:NE	5:P:510:LEU:HD12	2.29	0.47
5:P:506:ARG:NH1	5:P:506:ARG:CB	2.72	0.47
2:H:6:DT:H2"	2:H:7:DT:OP2	2.15	0.47
4:B:331:TYR:O	4:B:335:LEU:HD13	2.15	0.47
4:C:970:ARG:NH2	4:C:975:LEU:HD11	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1080:VAL:HG11	4:C:1113:VAL:O	2.10	0.47
4:D:793:VAL:HG21	4:D:798:ALA:HB2	1.97	0.47
4:D:1043:PRO:HD2	4:D:1105:VAL:HG23	1.96	0.47
5:M:411:LEU:H	5:M:412:VAL:HG22	1.76	0.47
5:P:395:LEU:HG	5:P:396:ARG:N	2.29	0.47
4:B:675:MET:O	4:B:679:VAL:HG23	2.14	0.46
4:B:734:LEU:HD23	4:B:746:GLN:NE2	2.29	0.46
4:B:922:LEU:HD13	4:B:964:ALA:HB2	1.96	0.46
4:C:710:ARG:NH1	4:C:716:GLU:OE1	2.48	0.46
4:C:590:VAL:CG1	4:C:602:THR:HG23	2.45	0.46
4:D:1079:VAL:HG23	4:D:1113:VAL:CG1	2.40	0.46
5:M:373:LYS:O	5:M:374:ALA:HB3	2.15	0.46
5:O:378:GLN:HA	5:O:381:ALA:HB2	1.97	0.46
4:B:840:MET:HG2	4:B:861:ALA:HB2	1.96	0.46
4:D:595:ASP:OD1	4:D:599:ARG:N	2.44	0.46
4:D:1060:ARG:O	4:D:1060:ARG:HG3	2.16	0.46
4:D:1064:MET:O	4:D:1065:MET:HE2	2.16	0.46
4:D:1082:PHE:CE2	4:D:1113:VAL:O	2.69	0.46
5:M:525:GLU:HB3	5:M:529:PRO:CD	2.44	0.46
5:O:395:LEU:HB2	5:O:396:ARG:HB2	1.97	0.46
5:O:529:PRO:HB2	5:O:530:VAL:HG12	1.96	0.46
5:P:455:LEU:HA	5:P:456:SER:HB2	1.96	0.46
4:A:1099:LEU:HD23	4:A:1120:THR:HA	1.97	0.46
4:A:1161:VAL:HG11	4:A:1179:VAL:HG23	1.98	0.46
4:C:504:LEU:CD1	4:C:525:ILE:HD11	2.45	0.46
4:B:197:LYS:HG3	4:B:207:MET:HE1	1.98	0.46
4:B:399:PHE:N	4:B:400:PRO:CD	2.78	0.46
4:B:994:ASP:OD1	4:B:997:THR:HG22	2.16	0.46
4:D:215:TYR:CE1	4:D:250:TYR:HB3	2.50	0.46
4:D:549:MET:HE2	4:D:559:ILE:CG1	2.44	0.46
5:M:419:LYS:HA	5:M:419:LYS:HD2	1.61	0.46
5:M:519:ARG:NE	5:M:520:LYS:HE2	2.30	0.46
4:A:549:MET:HA	4:A:555:ILE:CD1	2.45	0.46
4:A:837:VAL:HA	4:A:866:ILE:HD13	1.97	0.46
4:B:622:LEU:HD23	4:B:625:LEU:HD13	1.97	0.46
4:B:1054:VAL:HG23	4:B:1094:LYS:HE2	1.95	0.46
4:C:291:MET:CE	4:C:613:GLY:CA	2.92	0.46
4:D:406:VAL:HG12	4:D:410:ILE:HD12	1.97	0.46
5:O:520:LYS:O	5:O:520:LYS:HG2	2.16	0.46
4:A:258:ARG:HG2	4:A:271:PHE:CZ	2.51	0.46
4:B:28:LEU:CD1	4:B:251:VAL:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1147:ARG:O	4:C:1151:LEU:HD13	2.15	0.46
4:C:1162:TYR:CD2	4:C:1175:ALA:HB2	2.50	0.46
4:D:57:TYR:CD2	4:D:287:ILE:HD12	2.50	0.46
4:D:1057:LYS:HB3	4:D:1058:PRO:CB	2.45	0.46
4:D:1160:PRO:CG	4:D:1201:ASP:OD2	2.63	0.46
4:B:98:LEU:O	4:B:99:LEU:HD23	2.16	0.46
4:B:331:TYR:HB3	4:B:350:LEU:HD23	1.97	0.46
4:B:702:MET:HG3	4:B:705:ILE:HD12	1.97	0.46
4:D:938:LEU:HG	4:D:943:ALA:HB3	1.97	0.46
4:D:1155:HIS:NE2	4:D:1188:LEU:HD21	2.31	0.46
5:O:411:LEU:H	5:O:412:VAL:HG22	1.81	0.46
5:P:412:VAL:O	5:P:415:PHE:HB2	2.16	0.46
5:P:495:GLU:H	5:P:496:GLU:HG2	1.81	0.46
2:H:10:DG:H2"	2:H:11:DG:C8	2.51	0.46
4:B:233:LYS:CG	4:B:510:VAL:HG11	2.45	0.46
4:C:28:LEU:O	4:C:32:VAL:HG23	2.16	0.46
4:C:602:THR:HG22	4:C:604:TYR:H	1.79	0.46
4:D:223:ALA:O	4:D:226:VAL:HG22	2.15	0.46
4:D:789:LYS:HG3	4:D:795:GLU:HB2	1.98	0.46
5:O:451:GLU:O	5:O:452:LYS:HB3	2.16	0.46
1:G:14:DA:OP1	4:B:898:GLY:HA2	2.16	0.46
4:A:402:TYR:O	4:A:406:VAL:HG23	2.16	0.46
4:A:1164:ARG:NH1	4:A:1173:LEU:HD11	2.31	0.46
4:B:357:VAL:HA	4:B:358:GLU:HG3	1.98	0.46
4:C:443:PRO:HA	4:C:448:LEU:HD12	1.97	0.46
4:C:525:ILE:HD11	4:C:535:LEU:HD21	1.98	0.46
4:D:207:MET:HE3	4:D:266:TRP:CZ3	2.51	0.46
5:M:524:PRO:HD2	5:M:526:ALA:N	2.30	0.46
5:N:536:GLY:O	5:N:540:ILE:HG12	2.16	0.46
5:P:541:MET:C	5:P:543:PRO:CD	2.85	0.46
4:A:226:VAL:HG21	4:A:561:VAL:CG1	2.47	0.45
4:A:604:TYR:HB3	4:A:608:ALA:HB3	1.98	0.45
4:A:1189:LEU:HD23	4:A:1194:TYR:O	2.16	0.45
4:B:308:GLN:NE2	4:B:356:ARG:HA	2.30	0.45
4:B:595:ASP:OD1	4:B:599:ARG:N	2.49	0.45
4:B:1016:LEU:C	4:B:1016:LEU:HD12	2.36	0.45
4:C:298:PHE:CZ	4:C:408:ASP:HB2	2.51	0.45
4:D:678:THR:HG22	4:D:693:LEU:HD11	1.98	0.45
4:D:785:VAL:HG13	4:D:795:GLU:HG3	1.97	0.45
5:O:521:PRO:O	5:O:522:LYS:CB	2.63	0.45
4:A:524:LEU:HD22	4:A:545:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:586:LEU:HD13	4:B:592:LEU:HD21	1.98	0.45
4:B:723:PHE:HB3	4:B:726:ALA:HB3	1.99	0.45
4:C:951:ALA:HB2	4:C:993:LEU:CD2	2.46	0.45
4:D:1080:VAL:CG2	4:D:1114:LEU:HA	2.44	0.45
5:M:450:LEU:HB3	5:M:451:GLU:HB2	1.97	0.45
4:A:557:GLN:O	4:A:561:VAL:HG23	2.17	0.45
4:A:658:LEU:HD23	4:A:658:LEU:C	2.37	0.45
4:B:939:VAL:HG22	4:B:944:LEU:HD12	1.99	0.45
4:B:1051:VAL:HG21	4:B:1093:LEU:HD23	1.97	0.45
4:B:1055:VAL:HG12	4:B:1066:ALA:HA	1.98	0.45
4:C:297:ARG:HD3	4:C:306:GLU:OE2	2.16	0.45
4:C:743:TYR:H	4:C:746:GLN:HE21	1.64	0.45
4:A:511:TYR:HB3	4:A:513:ILE:HD11	1.99	0.45
4:B:1015:VAL:HG13	4:B:1016:LEU:N	2.30	0.45
4:D:1043:PRO:O	4:D:1105:VAL:HG22	2.16	0.45
5:M:525:GLU:HB3	5:M:529:PRO:HD2	1.98	0.45
5:M:541:MET:C	5:M:543:PRO:CD	2.85	0.45
5:O:389:GLU:CB	5:O:445:GLU:HB3	2.46	0.45
5:O:529:PRO:CA	5:O:530:VAL:HB	2.46	0.45
4:A:302:GLU:O	4:A:304:ARG:N	2.49	0.45
4:B:238:ASP:HB3	4:B:239:PRO:HA	1.99	0.45
4:B:1057:LYS:HZ3	4:B:1064:MET:CE	2.28	0.45
4:B:1086:TYR:N	4:B:1087:GLU:HA	2.31	0.45
4:C:25:LEU:HD23	4:C:59:LYS:HD2	1.99	0.45
4:C:797:GLU:O	4:C:801:LEU:N	2.45	0.45
4:D:1137:HIS:O	4:D:1139:LEU:N	2.48	0.45
5:N:498:GLU:CB	5:N:499:ASP:CA	2.94	0.45
5:N:528:GLU:H	5:N:529:PRO:CD	2.29	0.45
5:P:494:ALA:HB1	5:P:495:GLU:O	2.15	0.45
4:C:590:VAL:HG13	4:C:604:TYR:CE1	2.52	0.45
5:M:488:GLU:HA	5:M:489:ASP:HA	1.71	0.45
5:N:386:ALA:HB1	5:N:388:LEU:HG	1.98	0.45
5:N:506:ARG:HD3	5:N:506:ARG:N	2.31	0.45
5:O:450:LEU:CB	5:O:451:GLU:CA	2.90	0.45
4:A:418:VAL:HG22	4:A:472:GLU:HB3	1.99	0.45
4:A:1127:ALA:HB1	4:A:1128:PRO:CD	2.37	0.45
4:B:421:GLY:N	4:B:625:LEU:HD21	2.31	0.45
4:B:755:ALA:HB2	4:B:784:PHE:CD1	2.51	0.45
4:B:1131:LEU:CD2	4:B:1181:VAL:HG21	2.47	0.45
4:C:1029:ILE:CD1	4:C:1047:LEU:HD13	2.44	0.45
4:C:1145:VAL:HG13	4:C:1149:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:451:GLU:O	5:M:452:LYS:HG2	2.16	0.45
5:M:507:LEU:N	5:M:507:LEU:HD22	2.31	0.45
5:N:506:ARG:CA	5:N:510:LEU:HD22	2.42	0.45
4:A:1205:PHE:O	4:A:1206:LEU:HD12	2.16	0.45
4:B:69:ILE:HD11	4:B:285:LEU:HD11	1.97	0.45
4:B:358:GLU:O	4:B:362:TRP:CD1	2.70	0.45
4:B:1143:LYS:N	4:B:1144:GLY:CA	2.74	0.45
4:C:755:ALA:HB2	4:C:784:PHE:CD1	2.52	0.45
4:C:840:MET:HG2	4:C:861:ALA:HB2	1.99	0.45
5:O:394:THR:HG21	5:O:399:VAL:CG2	2.47	0.45
5:P:434:LEU:N	5:P:435:PRO:CD	2.80	0.45
4:A:23:ALA:HB2	4:A:215:TYR:HA	1.99	0.45
4:A:549:MET:HA	4:A:555:ILE:HD13	1.98	0.45
4:C:570:ARG:O	4:C:571:HIS:CG	2.70	0.45
4:C:1095:GLU:HG2	4:C:1096:ASP:HB2	1.99	0.45
4:D:58:LYS:HA	4:D:61:THR:HG22	1.99	0.45
4:D:591:PRO:HG2	4:D:603:GLN:HB2	1.98	0.45
4:D:1080:VAL:CG1	4:D:1082:PHE:HD2	2.25	0.45
5:O:387:PHE:CD2	5:O:387:PHE:O	2.70	0.45
4:C:1207:GLN:CB	4:C:1208:GLY:CA	2.94	0.44
4:D:1140:LEU:CG	4:D:1144:GLY:HA3	2.46	0.44
4:D:1160:PRO:HG3	4:D:1201:ASP:OD2	2.16	0.44
5:M:490:PRO:O	5:M:492:TRP:CD1	2.70	0.44
5:O:369:HIS:CE1	5:O:370:HIS:NE2	2.84	0.44
5:P:412:VAL:O	5:P:415:PHE:HD2	1.99	0.44
5:P:499:ASP:HB3	5:P:500:PRO:HA	1.99	0.44
4:B:333:GLU:O	4:B:337:LEU:CD1	2.65	0.44
5:M:390:ALA:C	5:M:391:LEU:CD1	2.85	0.44
4:B:1029:ILE:HG21	4:B:1076:ALA:N	2.33	0.44
4:C:300:LEU:HD13	4:C:303:GLY:HA2	1.99	0.44
4:D:696:LEU:HD21	4:D:742:VAL:CG2	2.40	0.44
4:D:785:VAL:CG1	4:D:795:GLU:HG3	2.46	0.44
4:D:1051:VAL:CB	4:D:1093:LEU:HD23	2.47	0.44
5:N:454:SER:HA	5:N:456:SER:HB2	1.99	0.44
5:N:494:ALA:HB1	5:N:495:GLU:O	2.17	0.44
5:N:524:PRO:N	5:N:525:GLU:HA	2.28	0.44
5:P:412:VAL:O	5:P:415:PHE:CD2	2.70	0.44
4:A:191:LYS:O	4:A:195:VAL:HG23	2.17	0.44
4:A:941:ALA:HB2	4:A:1005:ALA:HB1	2.00	0.44
4:B:170:LEU:HD21	4:B:205:LEU:CD2	2.47	0.44
4:B:230:ILE:CG1	4:B:507:VAL:HG13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:235:THR:HG22	4:B:236:LEU:N	2.30	0.44
4:C:449:LEU:HD13	4:C:745:GLU:HB3	2.00	0.44
4:C:838:GLU:HB3	4:C:882:VAL:HG21	2.00	0.44
4:D:238:ASP:HB3	4:D:239:PRO:CA	2.47	0.44
5:N:508:ALA:HB2	5:N:511:LEU:HG	1.99	0.44
5:O:370:HIS:CE1	5:O:401:GLU:HG3	2.52	0.44
4:C:1104:GLU:O	4:C:1113:VAL:HG13	2.17	0.44
4:D:1205:PHE:CD1	4:D:1205:PHE:O	2.70	0.44
5:M:490:PRO:O	5:M:492:TRP:CE2	2.70	0.44
5:N:517:TRP:HH2	5:N:524:PRO:HD3	1.82	0.44
4:A:688:GLU:OE1	4:A:688:GLU:N	2.50	0.44
4:A:1024:VAL:HG11	4:A:1205:PHE:CE2	2.53	0.44
4:B:679:VAL:HG22	4:B:693:LEU:CD2	2.43	0.44
4:B:1087:GLU:HB3	4:B:1088:GLY:HA3	2.00	0.44
4:D:150:ILE:N	4:D:151:PRO:HD2	2.32	0.44
4:D:284:ASP:HB3	4:D:290:LYS:HZ2	1.81	0.44
4:D:421:GLY:N	4:D:625:LEU:HD21	2.33	0.44
4:D:781:ARG:O	4:D:785:VAL:HG23	2.18	0.44
5:M:505:ARG:HD2	5:M:510:LEU:HG	2.00	0.44
5:N:455:LEU:CA	5:N:456:SER:C	2.86	0.44
5:N:508:ALA:HB2	5:N:511:LEU:H	1.82	0.44
5:P:512:GLY:O	5:P:516:LEU:CD1	2.65	0.44
4:A:301:PRO:HA	4:A:302:GLU:O	2.18	0.44
4:A:951:ALA:HB2	4:A:993:LEU:CG	2.48	0.44
4:A:1095:GLU:O	4:A:1097:ILE:HD12	2.18	0.44
4:B:111:ARG:HG2	4:B:587:THR:HG22	2.00	0.44
4:B:302:GLU:CD	4:B:304:ARG:NH1	2.71	0.44
4:C:54:VAL:HG11	4:C:608:ALA:HB1	1.98	0.44
4:C:1130:ALA:HB1	4:C:1160:PRO:O	2.18	0.44
4:D:181:ILE:CD1	4:D:207:MET:CE	2.95	0.44
4:D:1188:LEU:HD12	4:D:1189:LEU:N	2.33	0.44
5:M:423:HIS:N	5:M:423:HIS:ND1	2.63	0.44
5:O:394:THR:HG21	5:O:399:VAL:HG21	2.00	0.44
5:O:493:GLU:HB2	5:O:494:ALA:HA	2.00	0.44
4:A:365:LEU:O	4:A:368:ARG:HB2	2.18	0.44
4:A:635:VAL:HG22	4:A:838:GLU:HG3	1.99	0.44
4:B:823:LEU:CD2	4:B:827:GLN:NE2	2.80	0.44
4:C:1081:VAL:O	4:C:1082:PHE:CD1	2.70	0.44
4:C:1205:PHE:O	4:C:1206:LEU:HD23	2.18	0.44
4:D:1203:GLU:O	4:D:1205:PHE:CE1	2.70	0.44
4:D:1204:VAL:O	4:D:1205:PHE:CD1	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:392:LYS:CD	5:O:397:ALA:HB3	2.48	0.44
5:P:382:GLU:CG	5:P:388:LEU:HD21	2.48	0.44
5:P:541:MET:C	5:P:541:MET:CE	2.85	0.44
4:C:15:GLN:NE2	4:C:567:GLY:O	2.50	0.44
4:C:705:ILE:N	4:C:706:PRO:CD	2.81	0.44
4:C:1204:VAL:HG12	4:C:1205:PHE:H	1.83	0.44
4:D:501:LYS:O	4:D:505:LYS:HG3	2.18	0.44
5:N:511:LEU:O	5:N:515:LEU:HD12	2.18	0.44
4:A:45:THR:HG22	4:A:70:GLY:HA3	2.00	0.43
4:B:525:ILE:HD11	4:B:538:ALA:HB3	1.98	0.43
4:B:1080:VAL:HG11	4:B:1082:PHE:CE2	2.53	0.43
4:C:737:THR:HG21	4:C:746:GLN:NE2	2.26	0.43
4:C:970:ARG:HH21	4:C:975:LEU:HD22	1.76	0.43
4:C:1093:LEU:CD1	4:C:1097:ILE:HD12	2.47	0.43
4:C:1182:GLY:O	4:C:1183:GLU:CB	2.66	0.43
5:M:491:PRO:O	5:M:492:TRP:CD2	2.70	0.43
5:P:450:LEU:HB3	5:P:451:GLU:HB2	1.99	0.43
4:B:11:HIS:CD2	4:B:212:ASP:OD1	2.70	0.43
4:C:146:LEU:HD11	4:C:189:GLN:CG	2.47	0.43
4:C:418:VAL:HG22	4:C:472:GLU:HB3	2.00	0.43
4:C:731:ARG:HB3	4:C:732:PRO:HD3	2.00	0.43
4:D:18:LEU:HD13	4:D:571:HIS:HA	2.00	0.43
4:D:302:GLU:HB3	4:D:304:ARG:N	2.32	0.43
4:D:1131:LEU:HD12	4:D:1197:TYR:O	2.17	0.43
5:M:406:LEU:HD11	5:M:440:GLN:NE2	2.33	0.43
5:M:419:LYS:HD2	5:M:422:HIS:CD2	2.52	0.43
5:P:505:ARG:HG3	5:P:514:ARG:HH21	1.79	0.43
5:P:505:ARG:NH1	5:P:532:GLU:OE1	2.48	0.43
4:D:307:ALA:HB1	4:D:395:GLU:HG2	1.99	0.43
4:D:542:VAL:CG2	4:D:543:PRO:HD3	2.48	0.43
4:D:1205:PHE:CD1	4:D:1205:PHE:C	2.90	0.43
5:M:491:PRO:C	5:M:492:TRP:CG	2.91	0.43
5:M:529:PRO:CB	5:M:530:VAL:HA	2.48	0.43
5:N:498:GLU:HB3	5:N:499:ASP:C	2.39	0.43
5:N:506:ARG:HG2	5:N:507:LEU:H	1.76	0.43
4:A:696:LEU:HD21	4:A:742:VAL:HG22	2.01	0.43
4:B:226:VAL:HG21	4:B:561:VAL:HG11	1.97	0.43
4:B:1145:VAL:O	4:B:1145:VAL:HG22	2.17	0.43
4:C:930:VAL:HG12	4:C:935:LEU:HG	2.00	0.43
4:D:577:ALA:HB1	4:D:618:ASP:HB3	2.00	0.43
4:D:1093:LEU:HD11	4:D:1097:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:401:GLU:O	5:N:405:HIS:CD2	2.71	0.43
4:A:555:ILE:HD12	4:A:556:ARG:N	2.34	0.43
4:B:424:ARG:CD	4:B:620:LEU:HD22	2.48	0.43
4:D:1093:LEU:HD22	4:D:1099:LEU:HD11	2.00	0.43
5:N:440:GLN:HB2	5:N:441:PHE:CB	2.47	0.43
5:O:542:PRO:N	5:O:543:PRO:CD	2.82	0.43
5:P:504:LEU:HB2	5:P:505:ARG:HG3	1.96	0.43
4:B:570:ARG:CG	4:B:571:HIS:N	2.73	0.43
4:B:938:LEU:HG	4:B:943:ALA:HB3	2.01	0.43
4:C:635:VAL:HG22	4:C:838:GLU:HG3	1.99	0.43
4:D:35:THR:HG23	4:D:253:THR:HG22	2.00	0.43
4:A:151:PRO:HB3	4:A:192:VAL:HG11	2.01	0.43
4:A:192:VAL:HG12	4:A:196:LEU:HD12	2.00	0.43
4:B:868:VAL:HG22	4:B:887:ILE:HB	2.01	0.43
4:C:290:LYS:O	4:C:291:MET:CG	2.67	0.43
4:C:297:ARG:CZ	4:C:306:GLU:HB2	2.49	0.43
4:C:574:VAL:HG22	4:C:601:VAL:HG21	2.00	0.43
4:D:155:LEU:HD13	4:D:192:VAL:HG22	2.01	0.43
4:D:390:GLU:OE2	4:D:432:VAL:HG23	2.19	0.43
5:N:518:VAL:HA	5:N:519:ARG:HG3	1.99	0.43
5:O:502:GLU:O	5:O:503:GLU:CG	2.66	0.43
4:A:788:ALA:HB1	4:A:793:VAL:HG22	2.00	0.43
4:C:150:ILE:HG23	4:C:162:ALA:HB1	2.00	0.43
4:C:357:VAL:HB	4:C:362:TRP:CH2	2.53	0.43
4:C:1080:VAL:CB	4:C:1082:PHE:CD2	3.01	0.43
5:M:489:ASP:O	5:M:490:PRO:C	2.57	0.43
5:M:524:PRO:HG2	5:M:526:ALA:HB2	2.01	0.43
4:A:366:ARG:O	4:A:368:ARG:N	2.43	0.43
4:A:930:VAL:HG12	4:A:935:LEU:HG	2.01	0.43
4:B:300:LEU:O	4:B:302:GLU:N	2.52	0.43
4:D:473:ARG:NH1	4:D:477:ILE:HD11	2.34	0.43
5:M:504:LEU:HD13	5:M:536:GLY:HA2	2.00	0.43
4:A:1099:LEU:HD22	4:A:1118:VAL:HG12	2.01	0.43
4:A:1099:LEU:CD2	4:A:1120:THR:HG22	2.48	0.43
4:C:1176:LEU:CD1	4:C:1177:ARG:N	2.81	0.43
4:D:1181:VAL:HG12	4:D:1182:GLY:N	2.34	0.43
5:M:391:LEU:O	5:M:392:LYS:C	2.57	0.43
4:A:334:VAL:HG21	4:A:384:LEU:HD11	2.00	0.42
4:A:338:LEU:HD11	4:A:365:LEU:HD11	2.02	0.42
4:A:572:ALA:CB	4:A:573:SER:CB	2.63	0.42
4:C:493:GLY:HA2	4:C:573:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1079:VAL:CG1	4:C:1080:VAL:N	2.82	0.42
4:D:100:ALA:HB2	4:D:109:LEU:CD1	2.49	0.42
5:P:504:LEU:CB	5:P:505:ARG:CG	2.94	0.42
4:A:150:ILE:HD11	4:A:166:LEU:HA	2.02	0.42
4:A:971:GLY:HA3	4:A:975:LEU:HD22	1.69	0.42
4:B:352:GLU:CD	4:B:356:ARG:NH2	2.72	0.42
4:B:1129:LYS:O	4:B:1159:LEU:HD22	2.18	0.42
4:D:1057:LYS:CD	4:D:1064:MET:N	2.82	0.42
5:M:403:ARG:HE	5:M:437:ALA:CB	2.32	0.42
4:B:574:VAL:HG22	4:B:601:VAL:HG21	2.00	0.42
4:C:459:VAL:HG23	4:C:459:VAL:O	2.19	0.42
5:O:493:GLU:O	5:O:504:LEU:HD12	2.19	0.42
5:O:519:ARG:HG2	5:O:520:LYS:HB2	1.98	0.42
5:P:385:ARG:HB3	5:P:386:ALA:HA	2.02	0.42
5:P:503:GLU:HB3	5:P:504:LEU:HD12	2.00	0.42
4:B:230:ILE:CD1	4:B:507:VAL:HG22	2.49	0.42
4:C:1119:TRP:CD1	4:C:1123:GLU:HB2	2.54	0.42
4:D:428:ALA:HB3	4:D:816:SER:HB2	2.01	0.42
5:N:440:GLN:CB	5:N:441:PHE:CA	2.97	0.42
4:A:28:LEU:CD1	4:A:251:VAL:HG21	2.50	0.42
4:B:1213:PRO:O	4:B:1217:VAL:HG23	2.19	0.42
4:C:103:PHE:CE1	4:C:286:PRO:HD3	2.54	0.42
4:C:827:GLN:O	4:C:831:VAL:HG23	2.19	0.42
4:C:1096:ASP:O	4:C:1097:ILE:CG1	2.67	0.42
4:D:1080:VAL:HG23	4:D:1115:ALA:H	1.83	0.42
4:D:1086:TYR:HB2	4:D:1087:GLU:C	2.40	0.42
5:M:440:GLN:CB	5:M:441:PHE:HA	2.50	0.42
5:M:490:PRO:HB2	5:M:492:TRP:CD1	2.55	0.42
5:M:494:ALA:CB	5:M:503:GLU:OE2	2.68	0.42
5:O:392:LYS:HA	5:O:394:THR:N	2.34	0.42
5:O:450:LEU:HA	5:O:451:GLU:HG3	2.01	0.42
5:P:455:LEU:N	5:P:456:SER:HA	2.33	0.42
5:P:498:GLU:HB2	5:P:499:ASP:CA	2.49	0.42
4:A:675:MET:O	4:A:679:VAL:HG23	2.20	0.42
4:B:357:VAL:CA	4:B:358:GLU:HG3	2.49	0.42
4:B:952:ARG:NH1	5:N:373:LYS:HB3	2.34	0.42
4:B:976:VAL:HG21	4:C:115:ARG:NH1	2.34	0.42
4:B:1093:LEU:HG	4:B:1097:ILE:HB	2.01	0.42
4:C:321:ARG:HD3	4:C:434:TYR:CE2	2.54	0.42
4:C:609:VAL:HG13	4:C:614:LEU:HD12	2.01	0.42
4:C:1050:MET:HE3	4:C:1098:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:LEU:HD21	4:D:245:PRO:HB2	2.01	0.42
4:D:1119:TRP:HZ2	4:D:1206:LEU:C	2.22	0.42
5:O:452:LYS:HZ2	5:O:509:ARG:NH2	2.18	0.42
5:P:505:ARG:CZ	5:P:510:LEU:CD1	2.80	0.42
5:P:532:GLU:HA	5:P:535:ILE:HD11	1.93	0.42
4:A:975:LEU:C	4:A:975:LEU:CD1	2.87	0.42
4:C:570:ARG:C	4:C:571:HIS:ND1	2.72	0.42
4:D:1102:LEU:HD11	4:D:1206:LEU:CG	2.46	0.42
4:B:313:LEU:HB3	4:B:436:VAL:HG13	2.02	0.42
4:C:321:ARG:HD3	4:C:434:TYR:CZ	2.55	0.42
4:C:541:VAL:CG2	4:C:542:VAL:HA	2.40	0.42
4:D:102:ASP:C	4:D:283:VAL:HG22	2.40	0.42
4:D:226:VAL:HB	4:D:510:VAL:HG21	2.01	0.42
4:D:424:ARG:NH1	4:D:620:LEU:HD22	2.35	0.42
4:D:554:ARG:O	4:D:558:VAL:HG23	2.20	0.42
4:D:1082:PHE:CZ	4:D:1113:VAL:O	2.73	0.42
5:M:495:GLU:N	5:M:496:GLU:C	2.73	0.42
4:A:237:ASP:OD1	4:A:237:ASP:N	2.53	0.42
4:B:364:GLU:C	4:B:366:ARG:H	2.23	0.42
4:C:406:VAL:HA	4:C:409:TYR:CE2	2.55	0.42
4:D:897:VAL:CG2	4:D:938:LEU:HD13	2.49	0.42
5:N:504:LEU:CD1	5:N:535:ILE:HD12	2.50	0.42
5:O:395:LEU:H	5:O:396:ARG:C	2.23	0.42
5:O:455:LEU:N	5:O:456:SER:HB3	2.35	0.42
3:I:18:DC:H2"	3:I:19:DC:C6	2.55	0.42
4:A:1161:VAL:HG23	4:A:1176:LEU:HD11	2.02	0.42
4:B:602:THR:HG22	4:B:604:TYR:H	1.84	0.42
4:B:1069:THR:HG23	4:B:1077:LEU:O	2.19	0.42
4:C:1082:PHE:C	4:C:1084:ARG:N	2.73	0.42
4:D:1093:LEU:HD22	4:D:1099:LEU:HD12	2.01	0.42
5:M:383:GLY:O	5:M:386:ALA:HB2	2.20	0.42
5:M:498:GLU:HB2	5:M:499:ASP:HA	2.02	0.42
5:N:524:PRO:CB	5:N:525:GLU:HA	2.49	0.42
5:O:443:VAL:HG13	5:O:444:GLU:N	2.35	0.42
5:O:505:ARG:HH12	5:O:506:ARG:HH12	1.67	0.42
5:P:524:PRO:HD2	5:P:526:ALA:CB	2.50	0.42
5:P:527:GLU:N	5:P:528:GLU:HA	2.35	0.42
4:B:200:ALA:HB3	4:B:207:MET:CE	2.50	0.41
4:B:335:LEU:HD12	4:B:354:LEU:HD21	2.02	0.41
4:C:958:GLU:HB3	4:C:959:PRO:HD3	2.02	0.41
4:C:1016:LEU:HD21	4:C:1073:GLU:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1186:LEU:HD23	4:C:1186:LEU:C	2.40	0.41
4:D:498:LEU:HD13	4:D:570:ARG:HE	1.85	0.41
4:D:952:ARG:HD2	5:P:375:GLY:H	1.85	0.41
4:D:1024:VAL:HG12	4:D:1046:LEU:CD1	2.50	0.41
5:M:524:PRO:HD2	5:M:525:GLU:CA	2.46	0.41
5:N:440:GLN:HB3	5:N:441:PHE:HA	2.02	0.41
5:P:540:ILE:C	5:P:540:ILE:CD1	2.85	0.41
4:B:691:ILE:HG22	4:B:743:TYR:OH	2.20	0.41
4:B:1021:LEU:HD22	4:B:1048:SER:CB	2.50	0.41
4:C:18:LEU:HD13	4:C:571:HIS:HB3	2.01	0.41
4:C:192:VAL:HG12	4:C:196:LEU:CD1	2.49	0.41
4:D:25:LEU:HD23	4:D:59:LYS:HD2	2.02	0.41
4:D:402:TYR:O	4:D:406:VAL:HG23	2.20	0.41
4:D:705:ILE:HB	4:D:706:PRO:HD3	2.01	0.41
4:D:939:VAL:CG2	4:D:944:LEU:HD12	2.44	0.41
5:M:400:ARG:O	5:M:404:PRO:CD	2.68	0.41
5:N:452:LYS:O	5:N:453:LYS:C	2.58	0.41
5:P:416:PRO:CG	5:P:417:GLU:N	2.80	0.41
5:P:522:LYS:O	5:P:523:ALA:C	2.57	0.41
4:A:909:ARG:O	4:A:912:GLY:O	2.37	0.41
4:C:142:LEU:HD23	4:C:178:PHE:HB2	2.02	0.41
4:C:297:ARG:HD3	4:C:297:ARG:HA	1.97	0.41
4:C:410:ILE:HG22	4:C:414:ARG:NH1	2.35	0.41
4:D:413:ALA:HB1	4:D:418:VAL:HB	2.01	0.41
4:D:1123:GLU:HG2	4:D:1216:GLU:HB3	2.02	0.41
5:M:393:PRO:O	5:M:394:THR:CB	2.68	0.41
5:O:521:PRO:HG2	5:O:523:ALA:H	1.83	0.41
5:P:528:GLU:HG2	5:P:528:GLU:H	1.58	0.41
4:A:216:VAL:HG12	4:A:217:ARG:HG3	2.02	0.41
4:B:941:ALA:HB2	4:B:1005:ALA:HB1	2.02	0.41
4:B:1008:ILE:HD12	4:B:1008:ILE:C	2.40	0.41
4:B:1021:LEU:HD22	4:B:1048:SER:OG	2.20	0.41
4:C:313:LEU:CD1	4:C:407:GLN:NE2	2.83	0.41
4:C:574:VAL:HG22	4:C:601:VAL:CG2	2.50	0.41
4:C:1045:VAL:HG12	4:C:1046:LEU:N	2.36	0.41
4:D:605:ASP:O	4:D:609:VAL:HG23	2.20	0.41
1:G:18:DC:H1'	1:G:19:DC:C5	2.56	0.41
1:G:19:DC:C4	2:H:10:DG:C6	3.08	0.41
4:A:1129:LYS:HB3	4:A:1198:LEU:HG	2.01	0.41
4:B:453:PHE:CZ	4:B:464:ILE:HD11	2.54	0.41
4:B:1089:VAL:CG2	4:B:1118:VAL:HG12	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:VAL:HG13	4:D:591:PRO:N	2.35	0.41
4:D:300:LEU:HD22	4:D:304:ARG:HB3	2.01	0.41
4:D:407:GLN:HG3	4:D:436:VAL:CG1	2.51	0.41
4:D:1008:ILE:O	4:D:1010:VAL:N	2.54	0.41
5:N:505:ARG:HD2	5:N:510:LEU:CD2	2.46	0.41
5:O:367:HIS:CE1	5:O:401:GLU:HG2	2.55	0.41
5:P:404:PRO:HA	5:P:433:LEU:HD13	2.02	0.41
5:P:412:VAL:CB	5:P:415:PHE:HD2	2.14	0.41
4:B:1032:LEU:CD2	4:B:1077:LEU:HD11	2.50	0.41
5:M:419:LYS:O	5:M:423:HIS:ND1	2.53	0.41
5:M:538:ASN:O	5:M:542:PRO:CD	2.66	0.41
5:N:506:ARG:CG	5:N:507:LEU:N	2.73	0.41
5:O:396:ARG:CA	5:O:397:ALA:C	2.84	0.41
5:P:519:ARG:HB3	5:P:520:LYS:CB	2.50	0.41
1:G:12:DC:H2"	1:G:13:DC:C6	2.55	0.41
4:A:1099:LEU:HD22	4:A:1118:VAL:CG1	2.51	0.41
4:B:1047:LEU:HD12	4:B:1048:SER:H	1.85	0.41
4:D:1099:LEU:HD22	4:D:1118:VAL:HG13	2.02	0.41
5:N:504:LEU:HD11	5:N:536:GLY:HA2	2.02	0.41
5:N:507:LEU:N	5:N:507:LEU:HD23	2.35	0.41
5:P:407:GLU:O	5:P:415:PHE:HB3	2.20	0.41
4:A:81:PHE:O	4:A:83:ARG:HG3	2.21	0.41
4:A:223:ALA:O	4:A:226:VAL:HG22	2.21	0.41
4:A:679:VAL:HG22	4:A:693:LEU:CD2	2.51	0.41
4:B:296:PRO:HG2	4:B:581:ILE:HG22	2.03	0.41
4:B:329:ALA:O	4:B:333:GLU:HG3	2.21	0.41
4:B:357:VAL:CA	4:B:358:GLU:CB	2.99	0.41
4:D:1008:ILE:O	4:D:1010:VAL:HG23	2.20	0.41
4:D:1057:LYS:HG2	4:D:1064:MET:N	2.28	0.41
4:D:1059:THR:HG23	4:D:1064:MET:O	2.21	0.41
5:P:395:LEU:HG	5:P:396:ARG:H	1.85	0.41
4:A:555:ILE:C	4:A:555:ILE:CD1	2.89	0.41
4:A:627:PHE:CE1	4:A:842:ALA:HB3	2.55	0.41
4:B:362:TRP:O	4:B:363:GLU:C	2.59	0.41
4:B:1054:VAL:HG13	4:B:1054:VAL:O	2.20	0.41
4:B:1080:VAL:HG11	4:B:1082:PHE:CD2	2.55	0.41
4:C:10:LEU:HA	4:C:43:ALA:HB3	2.03	0.41
4:C:664:THR:HG21	4:C:670:LEU:HD13	2.02	0.41
4:C:873:VAL:HG11	4:C:944:LEU:HD21	2.02	0.41
4:D:410:ILE:CD1	4:D:438:ILE:HG23	2.50	0.41
4:D:1021:LEU:HB3	4:D:1048:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1093:LEU:HD21	4:D:1097:ILE:O	2.21	0.41
4:D:1204:VAL:HG13	4:D:1205:PHE:H	1.86	0.41
5:N:530:VAL:O	5:N:530:VAL:CG2	2.66	0.41
5:P:373:LYS:HG2	5:P:378:GLN:HB2	2.03	0.41
5:P:520:LYS:N	5:P:521:PRO:HD3	2.36	0.41
5:P:526:ALA:O	5:P:527:GLU:CB	2.69	0.41
5:P:526:ALA:O	5:P:527:GLU:HG3	2.21	0.41
4:A:100:ALA:HB2	4:A:109:LEU:HD12	2.02	0.41
4:B:228:LEU:HD22	4:B:242:TRP:CE3	2.55	0.41
4:C:222:ARG:O	4:C:226:VAL:HG13	2.21	0.41
4:C:451:GLU:CD	4:C:759:LEU:HD23	2.41	0.41
4:C:451:GLU:OE1	4:C:451:GLU:N	2.53	0.41
4:D:521:LEU:HA	4:D:524:LEU:HD23	2.03	0.41
4:D:1065:MET:HE3	4:D:1065:MET:HB2	1.83	0.41
5:M:392:LYS:NZ	5:M:399:VAL:HG21	2.36	0.41
5:M:408:GLY:C	5:M:415:PHE:HD1	2.25	0.41
5:O:490:PRO:CD	5:O:522:LYS:HD2	2.51	0.41
5:P:540:ILE:O	5:P:543:PRO:CD	2.69	0.41
4:A:422:PRO:HG2	4:A:820:ALA:HB1	2.03	0.40
4:A:918:LEU:HD23	4:A:960:LEU:CD1	2.50	0.40
4:B:302:GLU:OE2	4:B:304:ARG:NH1	2.54	0.40
4:B:428:ALA:HA	4:B:439:THR:HG21	2.03	0.40
4:B:1081:VAL:O	4:B:1081:VAL:HG23	2.20	0.40
4:D:1065:MET:HB3	4:D:1066:ALA:H	1.18	0.40
5:O:519:ARG:CZ	5:O:520:LYS:HZ1	2.33	0.40
5:O:542:PRO:N	5:O:543:PRO:HD3	2.36	0.40
5:P:528:GLU:N	5:P:529:PRO:CD	2.82	0.40
4:A:591:PRO:C	4:A:592:LEU:HD12	2.41	0.40
4:B:509:ARG:CA	4:B:513:ILE:HG21	2.49	0.40
4:B:1056:ARG:CA	4:B:1066:ALA:HB2	2.46	0.40
4:D:1140:LEU:HD11	4:D:1144:GLY:HA3	2.02	0.40
4:D:1207:GLN:HG3	4:D:1207:GLN:O	2.20	0.40
4:D:1207:GLN:O	4:D:1207:GLN:CG	2.70	0.40
5:N:450:LEU:HB3	5:N:451:GLU:C	2.42	0.40
5:N:450:LEU:CB	5:N:451:GLU:HB2	2.50	0.40
5:N:495:GLU:HB2	5:N:496:GLU:CG	2.51	0.40
5:O:415:PHE:HB2	5:O:416:PRO:HD3	2.02	0.40
5:O:519:ARG:NE	5:O:520:LYS:HZ1	2.18	0.40
5:P:504:LEU:CB	5:P:505:ARG:CA	2.99	0.40
4:A:498:LEU:HB3	4:A:499:ALA:CA	2.51	0.40
4:A:505:LYS:HB3	4:A:509:ARG:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1094:LYS:CE	4:C:1094:LYS:CA	2.98	0.40
4:D:678:THR:CG2	4:D:693:LEU:HD11	2.52	0.40
4:D:1205:PHE:O	4:D:1206:LEU:CG	2.70	0.40
5:M:453:LYS:O	5:M:454:SER:HB3	2.22	0.40
5:O:373:LYS:HG2	5:O:378:GLN:HB2	2.02	0.40
5:P:498:GLU:CB	5:P:499:ASP:CA	3.00	0.40
5:P:504:LEU:HD12	5:P:504:LEU:H	1.82	0.40
5:P:512:GLY:O	5:P:516:LEU:CG	2.66	0.40
3:I:13:DC:H1'	3:I:14:DA:C8	2.57	0.40
4:A:1124:VAL:HG13	4:A:1200:PRO:HG2	2.04	0.40
4:B:620:LEU:HD12	4:B:620:LEU:N	2.36	0.40
4:B:1093:LEU:HD22	4:B:1099:LEU:CG	2.52	0.40
4:C:15:GLN:N	4:C:23:ALA:O	2.54	0.40
4:D:918:LEU:HD22	4:D:953:LEU:HD23	2.04	0.40
4:D:1058:PRO:O	4:D:1058:PRO:CD	2.70	0.40
4:D:1120:THR:HG22	4:D:1121:LEU:N	2.36	0.40
4:D:1188:LEU:O	4:D:1191:ALA:HB3	2.20	0.40
5:M:409:LYS:HB2	5:M:415:PHE:HE1	1.87	0.40
5:M:508:ALA:O	5:M:509:ARG:HB2	2.21	0.40
5:P:525:GLU:CD	5:P:525:GLU:N	2.72	0.40
4:B:574:VAL:HG22	4:B:601:VAL:CG2	2.52	0.40
4:C:402:TYR:HE1	4:C:615:LEU:HD11	1.87	0.40
4:C:788:ALA:HB1	4:C:793:VAL:HG22	1.99	0.40
4:D:183:ASN:OD1	4:D:184:HIS:O	2.39	0.40
4:D:976:VAL:HG23	4:D:977:GLY:H	1.87	0.40
4:D:1057:LYS:CB	4:D:1058:PRO:HA	2.29	0.40
5:M:414:ARG:HA	5:M:417:GLU:CD	2.41	0.40
5:O:518:VAL:CG2	5:O:519:ARG:HB2	2.46	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:ASP:OD1	5:P:414:ARG:NH1[2_655]	1.84	0.36
4:A:115:ARG:NE	4:A:976:VAL:CG1[2_555]	1.90	0.30
4:A:115:ARG:NH2	4:A:976:VAL:CG2[2_555]	1.95	0.25
4:B:363:GLU:OE2	4:B:969:GLU:OE2[1_545]	2.01	0.19
4:D:160:ASP:N	5:N:454:SER:OG[1_545]	2.01	0.19
4:B:715:GLN:OE1	5:P:413:LEU:CD2[2_655]	2.05	0.15
4:B:273:ASN:OD1	4:B:1057:LYS:O[2_646]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	A	1146/1220 (94%)	1036 (90%)	87 (8%)	23 (2%)	7	38
4	B	1147/1220 (94%)	1051 (92%)	76 (7%)	20 (2%)	9	42
4	C	1148/1220 (94%)	1056 (92%)	79 (7%)	13 (1%)	14	51
4	D	1173/1220 (96%)	1062 (90%)	94 (8%)	17 (1%)	11	46
5	M	132/177 (75%)	84 (64%)	31 (24%)	17 (13%)	0	1
5	N	129/177 (73%)	76 (59%)	28 (22%)	25 (19%)	0	0
5	O	129/177 (73%)	77 (60%)	28 (22%)	24 (19%)	0	0
5	P	132/177 (75%)	80 (61%)	33 (25%)	19 (14%)	0	1
All	All	5136/5588 (92%)	4522 (88%)	456 (9%)	158 (3%)	4	26

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	506	ASP
4	A	1081	VAL
4	A	1201	ASP
4	A	1204	VAL
4	B	301	PRO
4	B	1058	PRO
4	C	299	PRO
4	C	1204	VAL
4	D	301	PRO
4	D	543	PRO
4	D	1057	LYS
4	D	1065	MET
4	D	1081	VAL
5	M	393	PRO
5	M	452	LYS
5	M	454	SER
5	M	455	LEU

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Mol	Chain	Res	Type
5	M	493	GLU
5	M	521	PRO
5	M	523	ALA
5	N	396	ARG
5	N	413	LEU
5	N	444	GLU
5	N	445	GLU
5	N	452	LYS
5	N	453	LYS
5	N	454	SER
5	N	492	TRP
5	N	523	ALA
5	N	530	VAL
5	N	542	PRO
5	O	391	LEU
5	O	393	PRO
5	O	413	LEU
5	O	454	SER
5	O	492	TRP
5	O	524	PRO
5	O	530	VAL
5	P	392	LYS
5	P	397	ALA
5	P	452	LYS
5	P	521	PRO
5	P	523	ALA
5	P	527	GLU
4	A	303	GLY
4	A	511	TYR
4	A	1192	GLU
4	B	302	GLU
4	B	1013	HIS
4	B	1025	ALA
4	B	1081	VAL
4	B	1091	PRO
4	B	1176	LEU
4	C	976	VAL
4	D	286	PRO
4	D	977	GLY
4	D	1082	PHE
4	D	1138	ALA
4	D	1204	VAL

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Mol	Chain	Res	Type
5	M	449	VAL
5	M	453	LYS
5	M	488	GLU
5	N	373	LYS
5	N	397	ALA
5	N	440	GLN
5	N	491	PRO
5	N	527	GLU
5	O	394	THR
5	O	491	PRO
5	O	518	VAL
5	O	521	PRO
5	P	440	GLN
5	P	449	VAL
5	P	454	SER
4	A	290	LYS
4	A	302	GLU
4	A	367	LYS
4	A	573	SER
4	A	975	LEU
4	B	290	LYS
4	B	291	MET
4	B	365	LEU
4	B	977	GLY
4	C	265	GLU
4	C	298	PHE
4	C	542	VAL
4	D	238	ASP
4	D	1058	PRO
5	M	440	GLN
5	M	445	GLU
5	M	503	GLU
5	M	531	SER
5	N	415	PHE
5	N	503	GLU
5	O	396	ARG
5	O	411	LEU
5	O	440	GLN
5	O	445	GLU
5	O	448	PHE
5	O	493	GLU
5	O	503	GLU

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Mol	Chain	Res	Type
5	O	527	GLU
5	P	491	PRO
5	P	526	ALA
4	A	513	ILE
4	A	1094	LYS
4	B	238	ASP
4	B	1138	ALA
4	C	290	LYS
4	C	792	GLY
4	C	1176	LEU
4	D	541	VAL
4	D	1141	ASP
5	M	496	GLU
5	M	529	PRO
5	N	392	LYS
5	N	521	PRO
5	N	528	GLU
5	N	541	MET
5	O	452	LYS
5	O	528	GLU
5	O	531	SER
5	P	373	LYS
5	P	391	LEU
5	P	503	GLU
4	A	509	ARG
4	A	510	VAL
4	B	973	SER
4	D	792	GLY
4	D	1056	ARG
5	M	410	THR
5	N	522	LYS
5	O	541	MET
5	P	396	ARG
5	P	529	PRO
4	A	299	PRO
4	A	300	LEU
4	A	1091	PRO
4	B	975	LEU
4	C	1091	PRO
4	C	1208	GLY
5	P	456	SER
5	P	458	ALA

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Mol	Chain	Res	Type
4	B	774	VAL
4	B	976	VAL
5	N	449	VAL
4	A	792	GLY
4	A	1211	GLY
4	C	301	PRO
4	D	39	ASP
4	A	399	PHE
4	B	303	GLY
4	B	1145	VAL
4	C	399	PHE
4	A	496	GLY
5	O	449	VAL
5	P	528	GLU
5	N	524	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
4	A	965/1009 (96%)	958 (99%)	7 (1%)	84	94
4	B	968/1009 (96%)	946 (98%)	22 (2%)	50	78
4	C	968/1009 (96%)	949 (98%)	19 (2%)	55	80
4	D	984/1009 (98%)	961 (98%)	23 (2%)	50	78
5	M	112/144 (78%)	102 (91%)	10 (9%)	9	35
5	N	109/144 (76%)	104 (95%)	5 (5%)	27	63
5	O	109/144 (76%)	97 (89%)	12 (11%)	6	26
5	P	110/144 (76%)	89 (81%)	21 (19%)	1	8
All	All	4325/4612 (94%)	4206 (97%)	119 (3%)	43	74

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	235	THR
4	A	302	GLU
4	A	670	LEU
4	A	991	SER
4	A	1094	LYS
4	A	1176	LEU
4	A	1201	ASP
4	B	220	ASP
4	B	325	ARG
4	B	358	GLU
4	B	364	GLU
4	B	407	GLN
4	B	569	ASN
4	B	633	ARG
4	B	713	HIS
4	B	976	VAL
4	B	991	SER
4	B	1013	HIS
4	B	1021	LEU
4	B	1022	ARG
4	B	1039	LEU
4	B	1056	ARG
4	B	1058	PRO
4	B	1059	THR
4	B	1065	MET
4	B	1067	ARG
4	B	1081	VAL
4	B	1139	LEU
4	B	1173	LEU
4	C	40	PRO
4	C	291	MET
4	C	294	ARG
4	C	297	ARG
4	C	299	PRO
4	C	520	GLU
4	C	541	VAL
4	C	542	VAL
4	C	573	SER
4	C	622	LEU
4	C	795	GLU
4	C	975	LEU
4	C	1018	TYR
4	C	1039	LEU

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Mol	Chain	Res	Type
4	C	1046	LEU
4	C	1094	LYS
4	C	1095	GLU
4	C	1096	ASP
4	C	1120	THR
4	D	289	ASP
4	D	290	LYS
4	D	291	MET
4	D	366	ARG
4	D	531	LYS
4	D	540	GLN
4	D	546	ARG
4	D	549	MET
4	D	757	TYR
4	D	976	VAL
4	D	1018	TYR
4	D	1039	LEU
4	D	1046	LEU
4	D	1055	VAL
4	D	1056	ARG
4	D	1058	PRO
4	D	1143	LYS
4	D	1145	VAL
4	D	1169	PHE
4	D	1202	ARG
4	D	1204	VAL
4	D	1205	PHE
4	D	1215	GLU
5	M	395	LEU
5	M	396	ARG
5	M	411	LEU
5	M	421	PHE
5	M	492	TRP
5	M	496	GLU
5	M	499	ASP
5	M	506	ARG
5	M	522	LYS
5	M	542	PRO
5	N	454	SER
5	N	456	SER
5	N	499	ASP
5	N	506	ARG

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Mol	Chain	Res	Type
5	N	533	ASP
5	O	382	GLU
5	O	388	LEU
5	O	392	LYS
5	O	393	PRO
5	O	448	PHE
5	O	453	LYS
5	O	499	ASP
5	O	505	ARG
5	O	506	ARG
5	O	520	LYS
5	O	521	PRO
5	O	522	LYS
5	P	394	THR
5	P	396	ARG
5	P	414	ARG
5	P	417	GLU
5	P	496	GLU
5	P	499	ASP
5	P	504	LEU
5	P	506	ARG
5	P	509	ARG
5	P	510	LEU
5	P	511	LEU
5	P	520	LYS
5	P	522	LYS
5	P	527	GLU
5	P	528	GLU
5	P	531	SER
5	P	532	GLU
5	P	535	ILE
5	P	541	MET
5	P	542	PRO
5	P	543	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	273	ASN
4	A	411	ASN
4	A	669	GLN
4	A	746	GLN

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Mol	Chain	Res	Type
4	A	896	ASN
4	A	1013	HIS
4	B	308	GLN
4	B	827	GLN
4	B	874	ASN
4	B	896	ASN
4	C	26	GLN
4	C	407	GLN
4	C	746	GLN
4	C	778	GLN
4	D	411	ASN
4	D	440	ASN
4	D	540	GLN
4	D	799	ASN
4	D	896	ASN
5	M	378	GLN
5	M	440	GLN
5	N	367	HIS
5	N	405	HIS
5	N	423	HIS
5	O	369	HIS
5	O	371	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DOC	I	21	2,3	14,19,20	0.64	0	13,26,29	1.89	3 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DOC	I	21	2,3	-	1/4/18/19	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	21	DOC	C4-N3-C2	4.58	120.99	116.34
3	I	21	DOC	C3'-C2'-C1'	2.96	106.20	102.78
3	I	21	DOC	O4'-C4'-C3'	2.35	108.71	104.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	21	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	21	DOC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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

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	E	20/20 (100%)	0.86	1 (5%) 28 16	159, 177, 203, 209	0
1	G	20/20 (100%)	0.82	3 (15%) 2 1	160, 175, 204, 216	0
1	K	20/20 (100%)	0.94	3 (15%) 2 1	157, 168, 206, 213	0
2	F	20/28 (71%)	1.38	5 (25%) 0 0	165, 187, 208, 217	0
2	H	27/28 (96%)	1.25	7 (25%) 0 0	145, 168, 184, 186	0
2	J	23/28 (82%)	1.60	8 (34%) 0 0	148, 171, 192, 201	0
2	L	24/28 (85%)	1.41	4 (16%) 1 1	150, 176, 197, 204	0
3	I	20/21 (95%)	1.42	5 (25%) 0 0	198, 224, 252, 255	0
4	A	1164/1220 (95%)	0.19	50 (4%) 35 22	109, 140, 177, 212	0
4	B	1167/1220 (95%)	0.21	48 (4%) 37 24	107, 140, 174, 218	0
4	C	1166/1220 (95%)	0.22	46 (3%) 39 25	108, 148, 176, 203	0
4	D	1185/1220 (97%)	0.16	39 (3%) 46 30	111, 145, 175, 230	0
5	M	138/177 (77%)	1.09	30 (21%) 0 0	159, 176, 196, 209	0
5	N	135/177 (76%)	0.87	14 (10%) 6 4	143, 169, 187, 203	0
5	O	135/177 (76%)	1.03	19 (14%) 2 2	155, 181, 206, 227	0
5	P	138/177 (77%)	0.95	22 (15%) 1 1	139, 177, 202, 226	0
All	All	5402/5781 (93%)	0.31	304 (5%) 24 13	107, 147, 186, 255	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	446	LEU	9.6
4	D	714	GLY	6.0
4	D	1087	GLU	5.8
4	D	978	LEU	5.4
4	B	1085	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
4	B	978	LEU	5.2
4	A	92	GLY	5.2
5	O	442	GLY	5.2
4	A	980	ALA	5.0
5	N	456	SER	5.0
4	A	1041	GLY	4.9
5	O	374	ALA	4.9
5	N	449	VAL	4.8
4	A	367	LYS	4.8
5	N	410	THR	4.8
4	B	1208	GLY	4.7
2	H	19	DC	4.7
2	H	8	DG	4.6
5	N	543	PRO	4.6
2	F	27	DC	4.4
5	M	367	HIS	4.3
5	P	502	GLU	4.3
4	B	982	VAL	4.3
3	I	19	DC	4.2
5	M	542	PRO	4.2
4	A	774	VAL	4.2
5	P	542	PRO	4.2
4	D	1082	PHE	4.2
5	O	500	PRO	4.2
4	C	530	GLY	4.1
4	D	232	SER	4.0
4	B	1142	GLU	4.0
5	P	507	LEU	4.0
4	A	551	LYS	4.0
4	A	1215	GLU	3.9
4	C	1087	GLU	3.9
4	B	969	GLU	3.9
4	C	1138	ALA	3.8
5	P	527	GLU	3.8
4	A	533	LYS	3.8
3	I	18	DC	3.8
4	A	1219	PRO	3.7
5	N	411	LEU	3.7
2	J	28	DG	3.7
4	C	240	GLU	3.7
5	P	490	PRO	3.7
4	D	713	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
4	D	1141	ASP	3.7
4	A	1216	GLU	3.6
4	D	725	HIS	3.6
4	C	279	ARG	3.6
5	O	384	TRP	3.6
5	M	524	PRO	3.6
4	B	981	GLU	3.6
5	O	408	GLY	3.6
1	K	20	DA	3.5
5	M	530	VAL	3.5
4	C	239	PRO	3.5
4	A	979	PHE	3.5
4	B	1081	VAL	3.5
4	B	1207	GLN	3.5
4	A	1087	GLU	3.5
5	O	543	PRO	3.5
4	B	1083	GLY	3.4
5	M	411	LEU	3.4
4	C	19	LEU	3.4
4	C	531	LYS	3.4
4	B	1183	GLU	3.4
1	K	16	DT	3.4
2	L	8	DG	3.4
4	D	1214	LYS	3.4
4	C	977	GLY	3.3
4	D	980	ALA	3.3
5	N	372	HIS	3.3
4	B	1212	GLY	3.3
5	M	410	THR	3.3
5	N	518	VAL	3.3
5	M	409	LYS	3.3
5	M	539	GLY	3.3
5	O	380	LEU	3.3
4	B	1054	VAL	3.3
4	D	529	PHE	3.2
2	F	14	DC	3.2
4	B	1169	PHE	3.2
5	M	371	HIS	3.2
2	J	7	DT	3.2
4	C	264	ALA	3.2
5	P	377	ALA	3.2
5	N	413	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
5	M	372	HIS	3.2
4	C	1119	TRP	3.1
5	M	495	GLU	3.1
5	O	502	GLU	3.1
4	A	775	GLU	3.1
4	A	990	ALA	3.1
4	B	1082	PHE	3.1
4	B	92	GLY	3.1
4	A	981	GLU	3.1
4	D	1081	VAL	3.1
4	A	986	PRO	3.0
4	C	1218	VAL	3.0
4	B	1220	PHE	3.0
4	C	1067	ARG	3.0
5	M	521	PRO	3.0
5	P	391	LEU	3.0
5	O	389	GLU	3.0
4	A	715	GLN	3.0
5	M	502	GLU	3.0
5	P	508	ALA	2.9
4	C	1054	VAL	2.9
4	A	1171	GLU	2.9
4	B	1084	ARG	2.9
5	M	377	ALA	2.9
5	O	450	LEU	2.9
4	C	736	GLU	2.9
4	D	962	ARG	2.9
2	J	14	DC	2.9
4	D	774	VAL	2.9
4	C	1208	GLY	2.9
4	A	916	LYS	2.8
2	F	11	DG	2.8
4	C	122	TYR	2.8
4	A	971	GLY	2.8
4	A	1197	TYR	2.8
4	B	537	GLU	2.8
5	M	382	GLU	2.8
4	B	863	ALA	2.8
2	J	18	DC	2.8
4	B	544	GLU	2.8
5	P	503	GLU	2.8
5	O	490	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
4	A	736	GLU	2.8
4	A	969	GLU	2.8
4	C	543	PRO	2.8
4	A	991	SER	2.7
4	D	320	ARG	2.7
5	N	374	ALA	2.7
5	M	393	PRO	2.7
5	P	393	PRO	2.7
4	D	1195	ARG	2.7
5	M	501	SER	2.7
5	M	516	LEU	2.7
4	A	994	ASP	2.7
4	C	771	LYS	2.7
4	D	1054	VAL	2.7
4	C	364	GLU	2.7
4	A	1217	VAL	2.7
4	A	771	LYS	2.7
5	M	493	GLU	2.7
4	A	1209	ASN	2.7
4	A	1034	GLU	2.7
4	A	1112	ARG	2.7
4	B	494	THR	2.7
2	J	6	DT	2.7
4	C	9	HIS	2.6
4	B	143	SER	2.6
5	M	368	HIS	2.6
1	G	9	DC	2.6
4	B	1170	GLY	2.6
5	P	433	LEU	2.6
4	A	1054	VAL	2.6
4	C	1206	LEU	2.6
5	P	543	PRO	2.6
4	A	320	ARG	2.6
4	B	222	ARG	2.6
4	B	1211	GLY	2.6
4	D	233	LYS	2.6
4	C	162	ALA	2.6
4	B	885	GLU	2.6
5	O	542	PRO	2.6
1	G	18	DC	2.5
4	C	970	ARG	2.5
4	D	34	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
5	P	390	ALA	2.5
2	L	5	DT	2.5
4	B	772	LYS	2.5
4	A	1092	LYS	2.5
5	P	367	HIS	2.5
5	N	384	TRP	2.5
4	D	1211	GLY	2.5
2	H	28	DG	2.5
4	B	700	GLY	2.5
4	C	1007	GLY	2.5
4	A	6	LYS	2.5
5	M	374	ALA	2.5
4	D	571	HIS	2.5
4	D	573	SER	2.5
5	O	422	HIS	2.5
4	A	324	ASP	2.4
4	B	520	GLU	2.4
4	D	537	GLU	2.4
5	P	501	SER	2.4
4	C	1211	GLY	2.4
2	F	28	DG	2.4
5	M	447	ALA	2.4
4	D	301	PRO	2.4
4	D	1183	GLU	2.4
4	B	995	GLU	2.4
5	O	501	SER	2.4
4	B	718	VAL	2.4
5	M	529	PRO	2.4
5	N	435	PRO	2.4
2	J	15	DT	2.4
5	M	522	LYS	2.4
4	A	5	LEU	2.4
4	C	218	LYS	2.4
4	C	1128	PRO	2.4
4	D	9	HIS	2.4
4	D	43	ALA	2.3
2	H	18	DC	2.3
2	L	14	DC	2.3
4	C	1049	GLY	2.3
1	G	20	DA	2.3
4	C	758	SER	2.3
4	D	914	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
4	C	576	ALA	2.3
4	C	1197	TYR	2.3
4	A	1168	PRO	2.3
4	D	572	ALA	2.3
4	C	1217	VAL	2.3
4	B	83	ARG	2.3
4	C	790	GLU	2.3
5	P	374	ALA	2.3
4	B	206	GLY	2.3
5	N	442	GLY	2.3
4	B	365	LEU	2.3
5	M	380	LEU	2.3
4	A	1033	SER	2.3
5	M	496	GLU	2.3
3	I	20	DA	2.3
4	C	1116	GLN	2.3
4	A	364	GLU	2.2
5	O	434	LEU	2.2
4	B	516	LYS	2.2
4	C	1220	PHE	2.2
4	C	959	PRO	2.2
4	C	1130	ALA	2.2
4	D	1041	GLY	2.2
4	D	1193	GLY	2.2
4	D	123	GLU	2.2
5	P	368	HIS	2.2
4	B	1217	VAL	2.2
5	M	519	ARG	2.2
5	P	379	ASP	2.2
4	B	774	VAL	2.2
4	A	113	ALA	2.2
4	B	1049	GLY	2.2
5	P	524	PRO	2.2
4	D	481	ARG	2.2
4	A	536	GLN	2.2
4	A	1141	ASP	2.2
4	C	1213	PRO	2.2
2	H	4	DT	2.2
4	C	274	THR	2.2
2	F	18	DC	2.2
4	A	983	GLU	2.2
4	B	597	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
5	O	449	VAL	2.2
4	A	396	ARG	2.2
5	O	507	LEU	2.2
4	B	1219	PRO	2.2
4	D	979	PHE	2.2
4	A	1106	GLU	2.1
4	D	279	ARG	2.1
5	N	394	THR	2.1
4	C	1085	ALA	2.1
2	H	7	DT	2.1
1	E	11	DG	2.1
2	J	17	DG	2.1
4	B	179	ILE	2.1
5	N	376	GLU	2.1
5	M	512	GLY	2.1
4	B	301	PRO	2.1
4	C	1043	PRO	2.1
4	A	721	ALA	2.1
5	M	508	ALA	2.1
4	C	1188	LEU	2.1
4	A	885	GLU	2.1
1	K	17	DG	2.1
4	A	552	ASP	2.1
4	D	92	GLY	2.1
4	C	923	LYS	2.1
5	O	386	ALA	2.1
5	P	380	LEU	2.1
5	O	448	PHE	2.1
4	A	1191	ALA	2.1
3	I	17	DG	2.1
4	B	297	ARG	2.1
4	C	201	ARG	2.1
2	H	13	DA	2.0
4	C	1158	SER	2.0
2	L	6	DT	2.0
4	D	1213	PRO	2.0
4	B	980	ALA	2.0
5	M	507	LEU	2.0
2	J	9	DT	2.0
3	I	8	DA	2.0
4	D	1169	PHE	2.0
4	B	207	MET	2.0

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Mol	Chain	Res	Type	RSRZ
4	A	975	LEU	2.0
4	B	913	GLY	2.0
4	B	1165	VAL	2.0
5	P	456	SER	2.0
4	D	185	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	DOC	I	21	18/19	0.77	0.44	173,185,229,232	0

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
6	ZN	C	1301	1/1	0.76	0.14	197,197,197,197	0
7	MG	C	1304	1/1	0.79	0.07	177,177,177,177	0
6	ZN	D	1302	1/1	0.83	0.16	159,159,159,159	0
6	ZN	C	1303	1/1	0.83	0.20	179,179,179,179	0
7	MG	B	1304	1/1	0.84	0.27	132,132,132,132	0
6	ZN	A	1302	1/1	0.85	0.20	168,168,168,168	0
7	MG	A	1304	1/1	0.85	0.17	156,156,156,156	0
6	ZN	B	1302	1/1	0.88	0.15	141,141,141,141	0
6	ZN	C	1302	1/1	0.89	0.11	158,158,158,158	0
6	ZN	B	1303	1/1	0.90	0.21	166,166,166,166	0
6	ZN	D	1303	1/1	0.91	0.14	176,176,176,176	0
6	ZN	A	1301	1/1	0.91	0.17	187,187,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ZN	D	1301	1/1	0.93	0.11	233,233,233,233	0
6	ZN	A	1303	1/1	0.94	0.10	141,141,141,141	0
6	ZN	B	1301	1/1	0.95	0.14	163,163,163,163	0
7	MG	D	1304	1/1	0.95	0.28	139,139,139,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.