



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:15 PM BST

PDB ID : 4KN7  
Title : X-ray crystal structure of the Escherichia coli RNA polymerase in complex with Benzoxazinorifamycin-2c  
Authors : Murakami, K.S.  
Deposited on : 2013-05-08  
Resolution : 3.69 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](mailto: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.

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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 : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

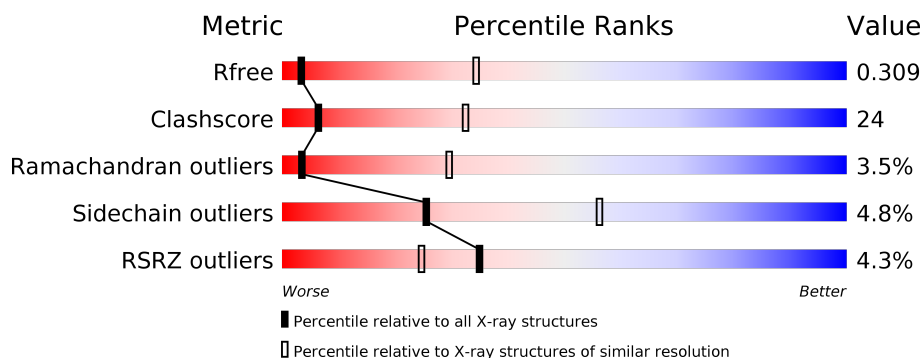
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.69 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	1013 (3.84-3.52)
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RSRZ outliers	127900	1471 (3.86-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	329	<div> <div>2%</div> <div> <div>62%</div> <div>33%</div> <div>• •</div> </div> </div>
1	B	329	<div> <div>3%</div> <div> <div>40%</div> <div>24%</div> <div>•</div> <div>33%</div> </div> </div>
1	F	329	<div> <div>4%</div> <div> <div>48%</div> <div>20%</div> <div>•</div> <div>30%</div> </div> </div>
1	G	329	<div> <div>5%</div> <div> <div>41%</div> <div>23%</div> <div>•</div> <div>34%</div> </div> </div>
2	C	1342	<div> <div>3%</div> <div> <div>53%</div> <div>41%</div> <div>5%</div> <div>•</div> </div> </div>
2	H	1342	<div> <div>5%</div> <div> <div>55%</div> <div>39%</div> <div>5%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div><div></div><div></div><div></div><div></div></div><div>2%40%38%5%18%</div></div>
3	I	1407	<div><div><div></div><div></div><div></div><div></div></div><div>4%41%37%•18%</div></div>
4	E	91	<div><div><div></div><div></div><div></div><div></div></div><div>%68%27%...</div></div>
4	J	91	<div><div><div></div><div></div><div></div><div></div></div><div>3%52%29%••16%</div></div>
5	X	613	<div><div><div></div><div></div><div></div><div></div></div><div>6%49%32%•16%</div></div>
5	Y	613	<div><div><div></div><div></div><div></div><div></div></div><div>5%44%29%•25%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56331 atoms, of which 117 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

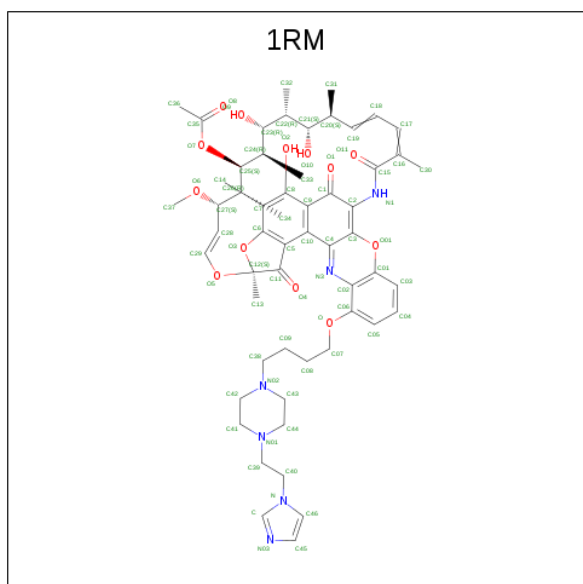
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is Benzoxazinorifamycin-2c (three-letter code: 1RM) (formula: C<sub>56</sub>H<sub>70</sub>N<sub>6</sub>O<sub>13</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			145	56	70	6	13		
6	H	1	Total	C	H	N	O	0	0
			105	43	47	2	13		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

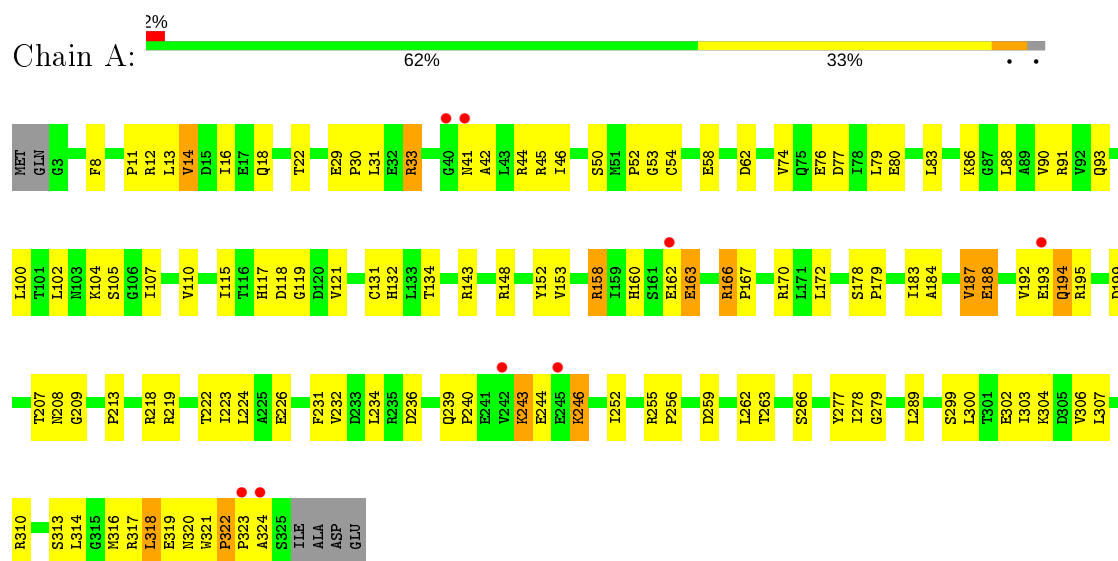
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	1	Total 1	Mg 1	0	0
8	D	1	Total 1	Mg 1	0	0

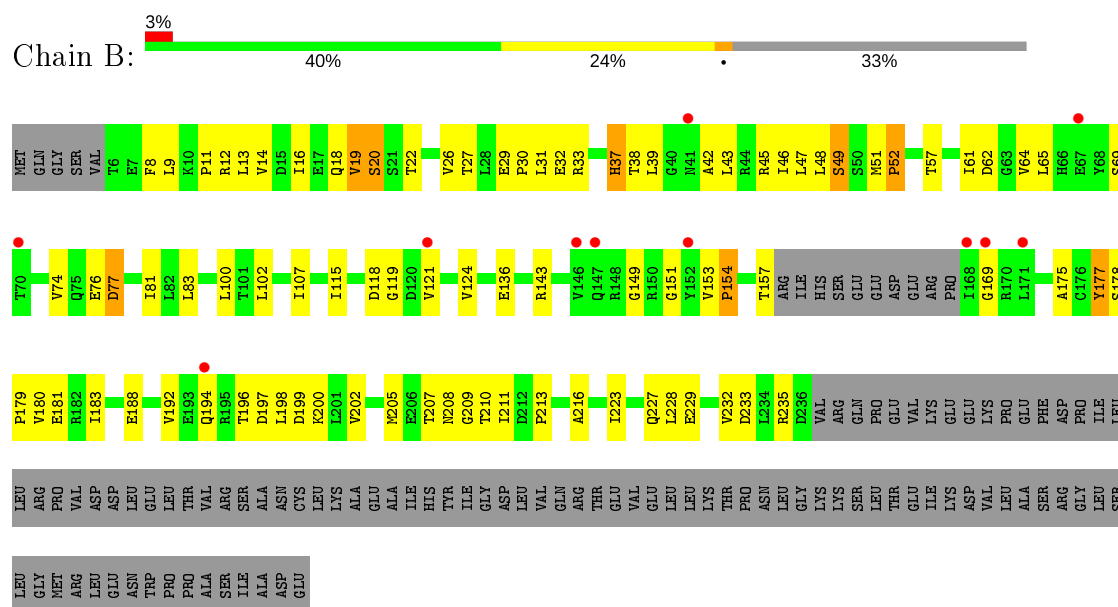
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

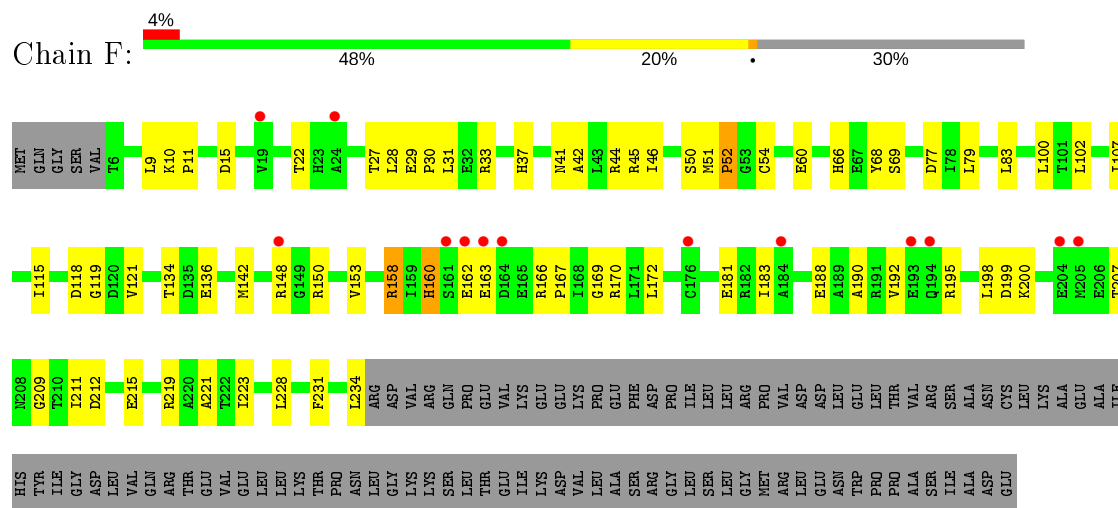
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



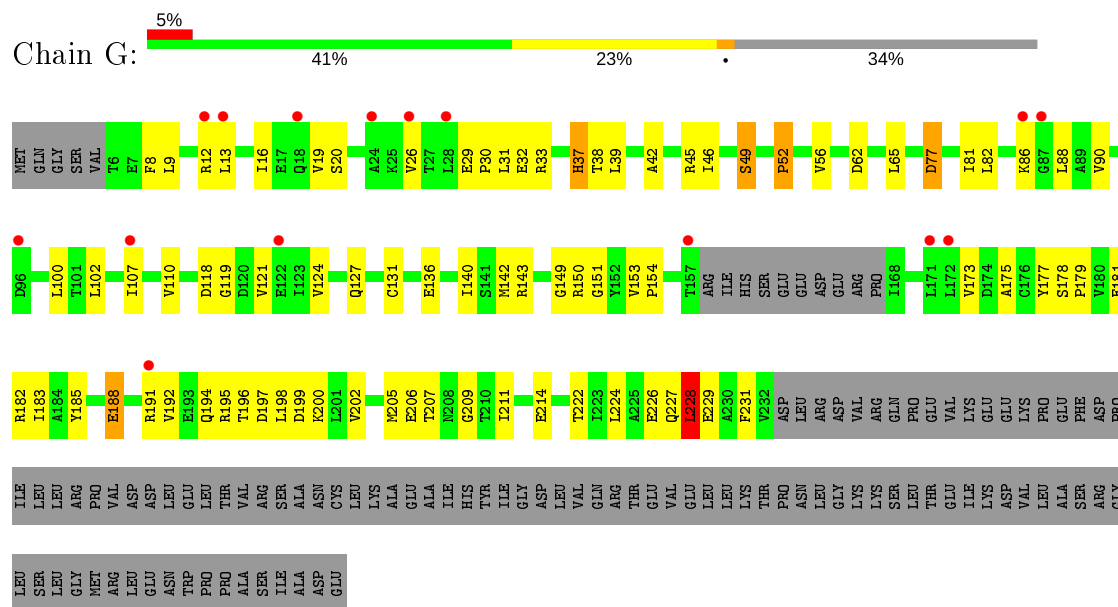
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



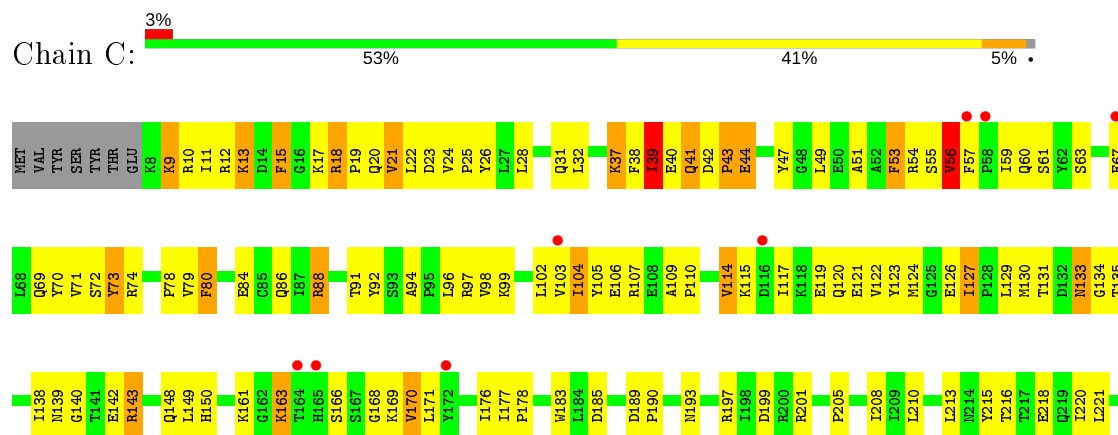
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



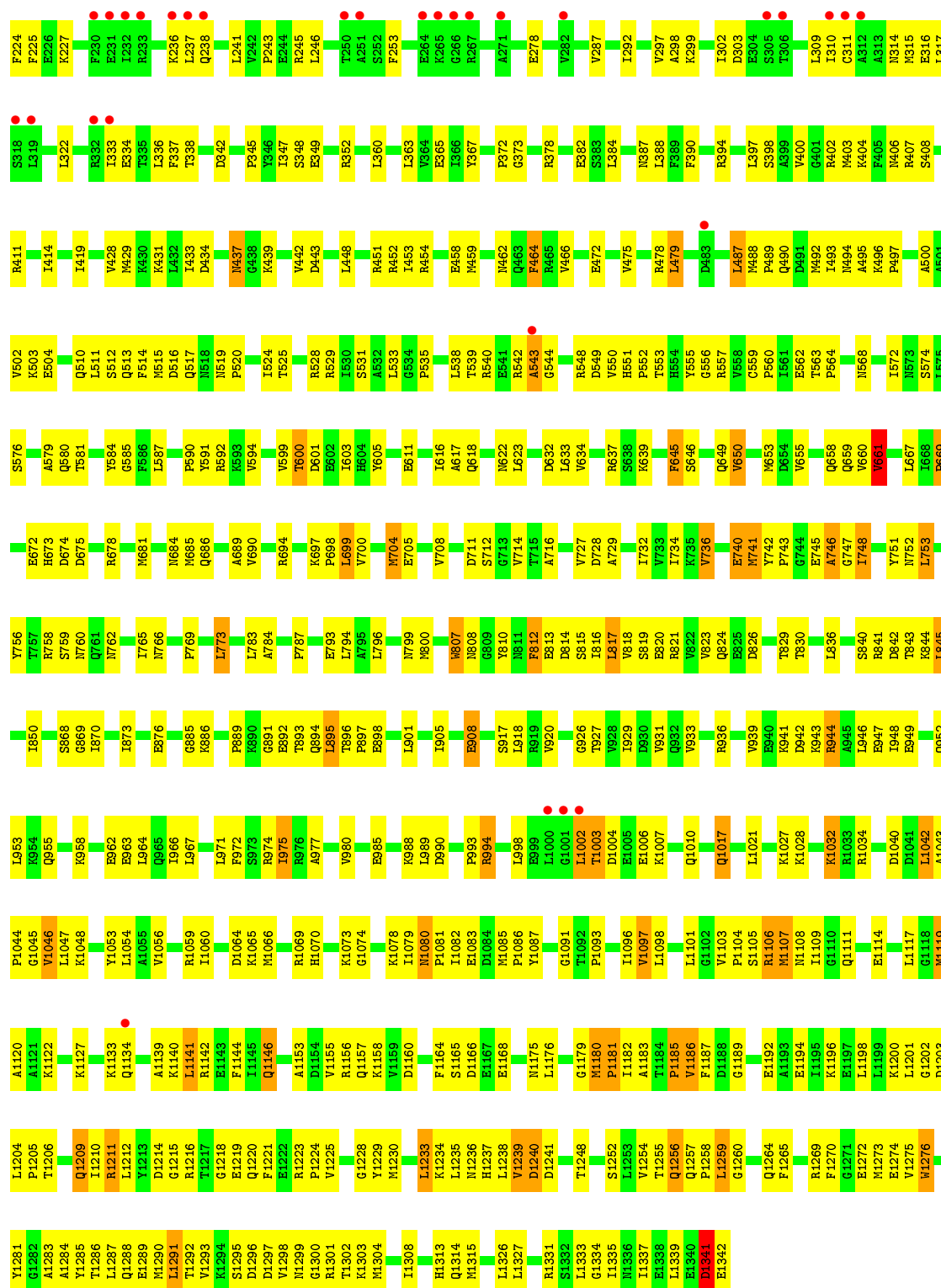
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta



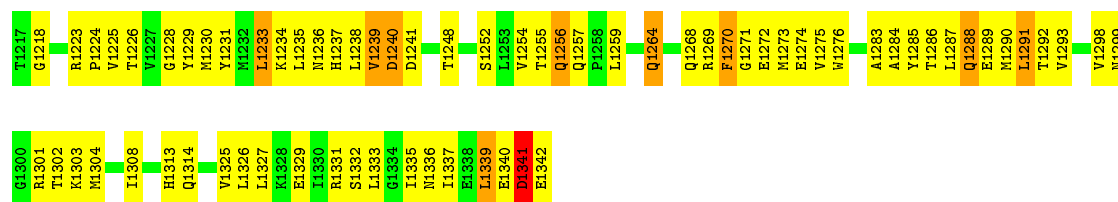




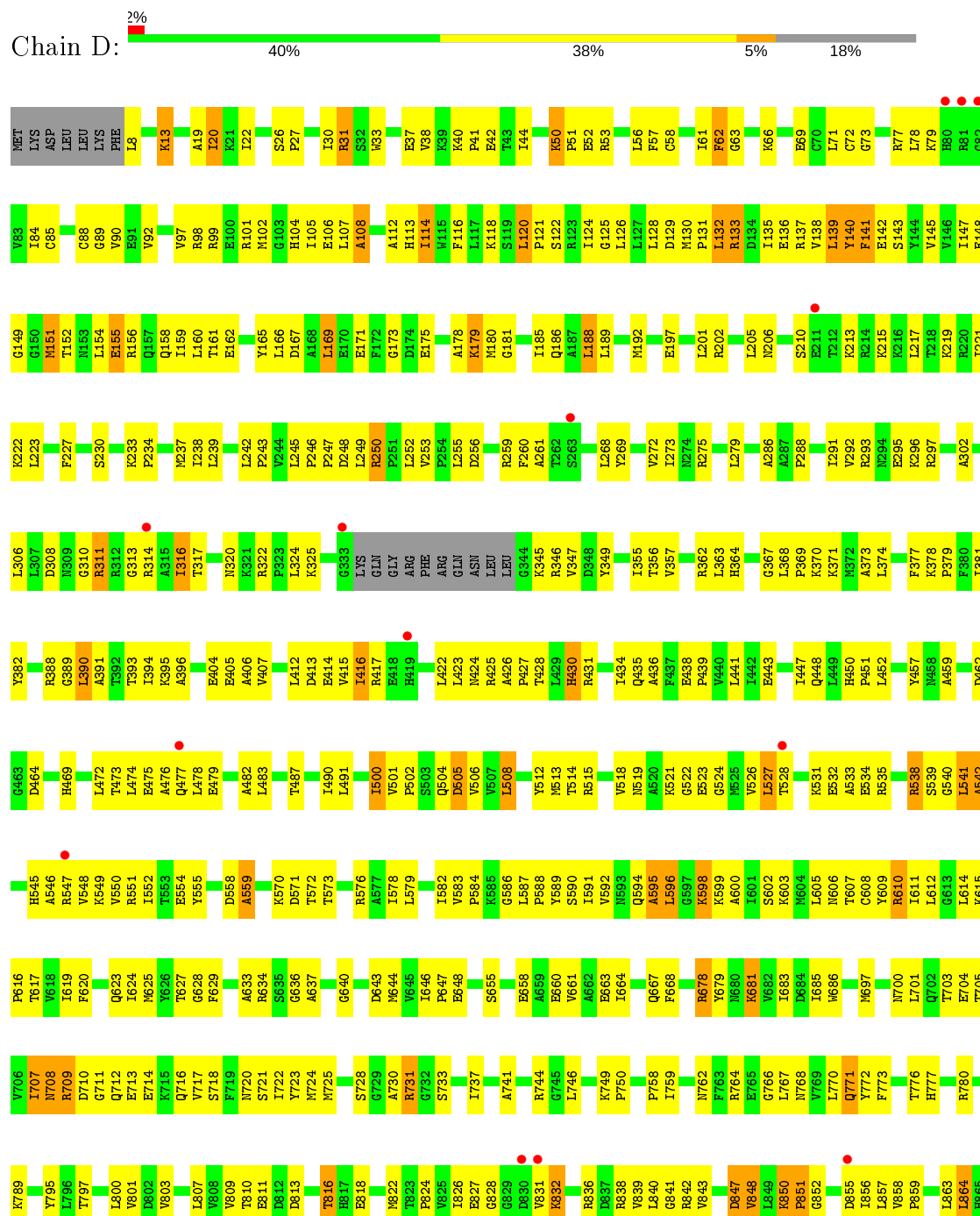
• Molecule 2: DNA-directed RNA polymerase subunit beta



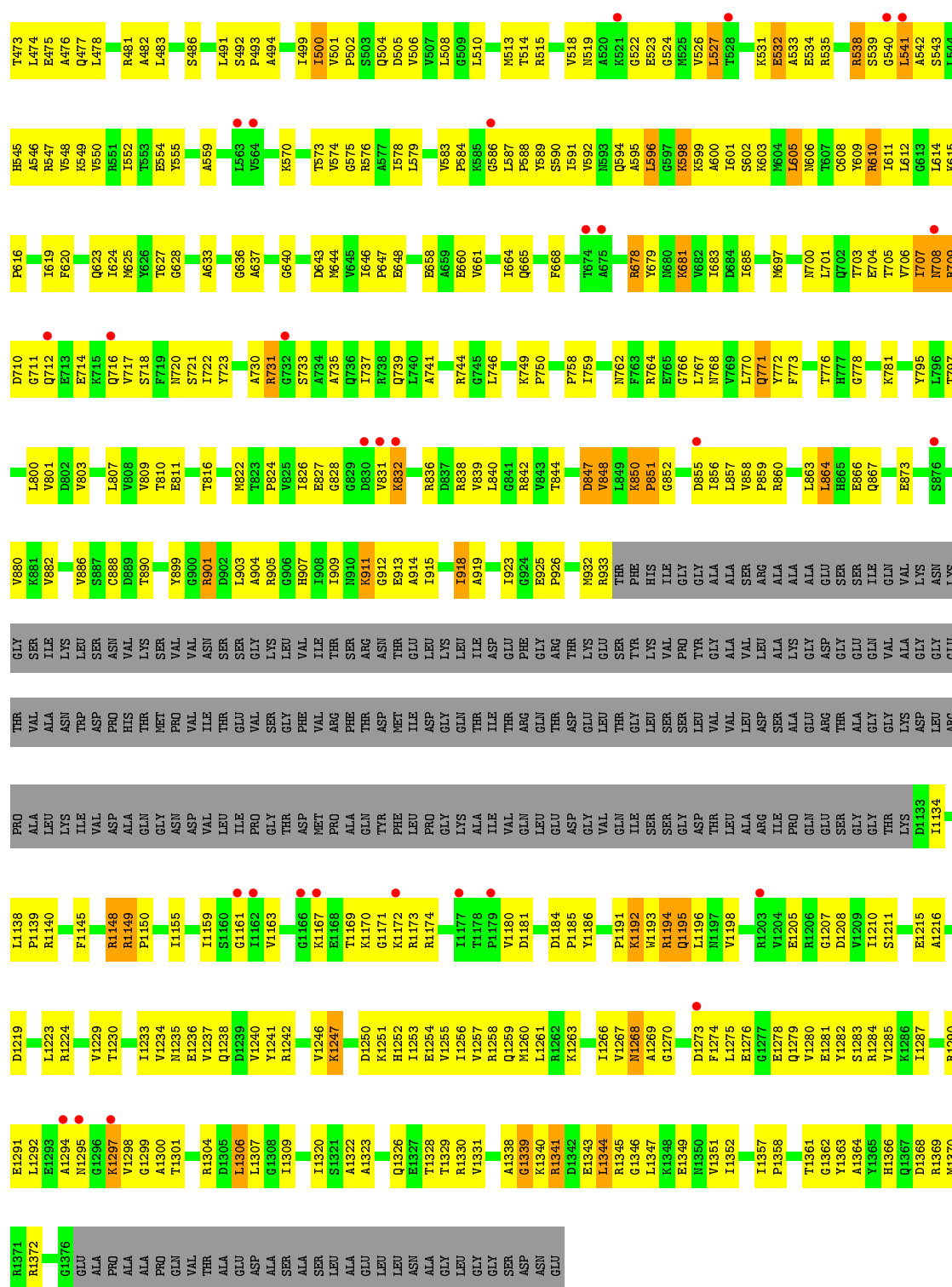




• Molecule 3: DNA-directed RNA polymerase subunit beta'





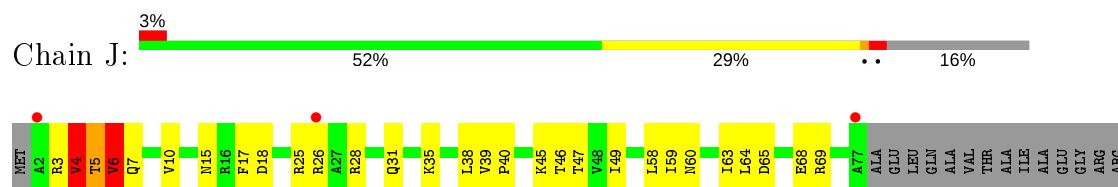


● Molecule 4: DNA-directed RNA polymerase subunit omega

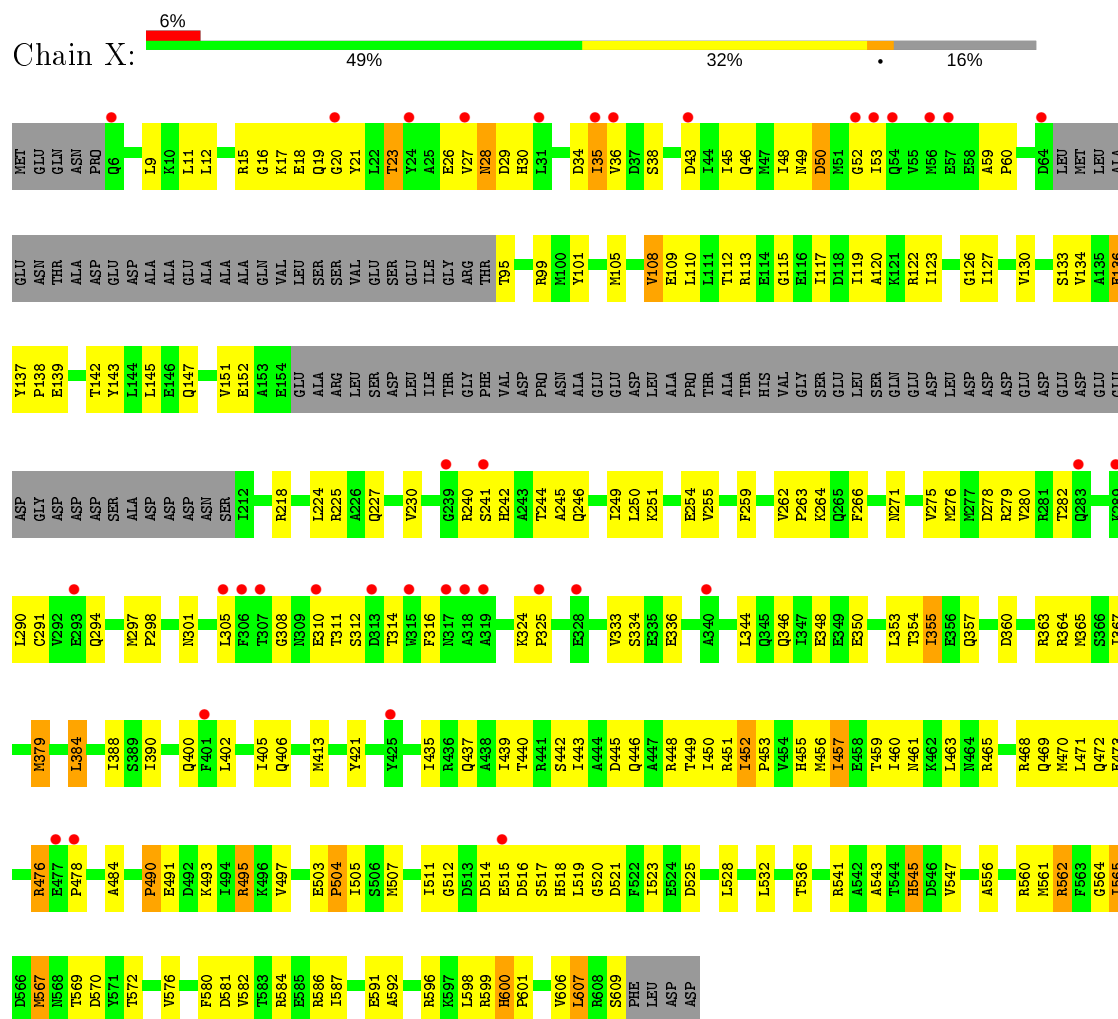
Chain E: 68% 27%



- Molecule 4: DNA-directed RNA polymerase subunit omega

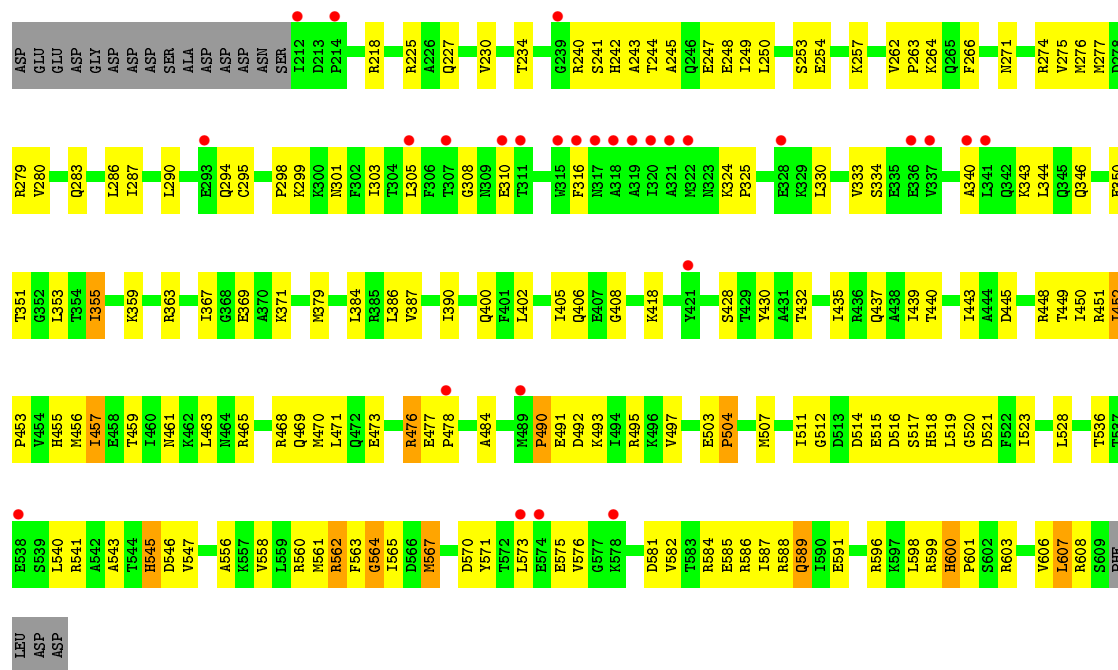


- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.83Å 204.58Å 308.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.69 29.88 – 3.69	Depositor EDS
% Data completeness (in resolution range)	93.1 (29.88-3.69) 87.0 (29.88-3.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 3.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.252 , 0.309 0.252 , 0.309	Depositor DCC
$R_{free}$ test set	5907 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 28.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	56331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, ZN, 1RM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.19	0/2548	0.37	0/3454
1	B	0.19	0/1725	0.41	0/2337
1	F	0.19	0/1797	0.40	0/2436
1	G	0.20	0/1690	0.40	0/2290
2	C	0.20	0/10690	0.39	0/14423
2	H	0.20	0/10690	0.39	0/14423
3	D	0.20	0/9198	0.40	0/12413
3	I	0.20	0/9198	0.40	0/12413
4	E	0.19	0/710	0.36	0/956
4	J	0.19	0/607	0.37	0/817
5	X	0.20	0/4253	0.37	0/5719
5	Y	0.20	0/3783	0.37	0/5083
All	All	0.20	0/56889	0.39	0/76764

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2514	0	2566	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1706	0	1738	86	0
1	F	1775	0	1800	65	0
1	G	1671	0	1706	80	0
2	C	10523	0	10546	566	0
2	H	10523	0	10546	538	0
3	D	9060	0	9257	589	0
3	I	9060	0	9256	532	0
4	E	708	0	719	31	0
4	J	605	0	612	28	0
5	X	4198	0	4250	180	0
5	Y	3732	0	3809	139	0
6	C	75	70	70	9	0
6	H	58	47	46	8	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56214	117	56921	2717	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2717) 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)
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.26	1.17
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.28	1.14
3:D:310:GLY:HA3	3:D:311:ARG:HB2	1.22	1.13
2:C:1119:MET:HG2	2:C:1228:GLY:HA2	1.31	1.10
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.29	1.09
3:I:186:GLN:HB2	3:I:238:ILE:HD11	1.35	1.08
2:H:488:MET:HB2	2:H:490:GLN:H	1.11	1.08
2:H:54:ARG:H	2:H:55:SER:HB2	1.20	1.06
2:C:42:ASP:HB3	2:C:43:PRO:HD2	1.36	1.04
3:I:858:VAL:HB	3:I:859:PRO:HD3	1.40	1.03
3:D:858:VAL:HB	3:D:859:PRO:HD3	1.40	1.03
3:I:850:LYS:HD2	3:I:851:PRO:HD2	1.40	1.00
2:H:1185:PRO:HD2	2:H:1189:GLY:HA2	1.43	0.99
2:H:1073:LYS:HD3	3:I:462:ASP:HB3	1.44	0.99
2:H:660:VAL:HG13	2:H:661:VAL:HG13	1.45	0.98
2:C:54:ARG:H	2:C:55:SER:HB2	1.23	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:487:LEU:HB3	2:H:488:MET:HA	1.46	0.97
3:D:186:GLN:HB2	3:D:238:ILE:HD11	1.43	0.97
3:D:610:ARG:HG3	3:D:864:LEU:HD13	1.46	0.96
2:H:1101:LEU:HD13	3:I:504:GLN:HB2	1.45	0.96
3:D:1261:LEU:HD21	3:D:1306:LEU:HD22	1.47	0.94
1:B:12:ARG:H	1:B:30:PRO:HG2	1.33	0.93
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.49	0.92
2:C:933:VAL:HG12	2:C:948:ILE:HD11	1.51	0.92
3:I:1263:LYS:HA	3:I:1279:GLN:HA	1.51	0.92
3:I:20:ILE:HD11	3:I:1320:ILE:HD11	1.53	0.91
2:H:488:MET:HB2	2:H:490:GLN:N	1.84	0.90
3:D:850:LYS:HD2	3:D:851:PRO:HD2	1.52	0.90
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.35	0.90
3:D:546:ALA:H	3:D:547:ARG:HA	1.37	0.89
1:A:45:ARG:HG3	2:C:1083:GLU:HB2	1.53	0.89
3:D:746:LEU:HD13	3:D:758:PRO:HG3	1.54	0.89
5:X:16:GLY:HA2	5:X:19:GLN:HG3	1.55	0.88
2:H:908:GLU:HG2	2:H:909:LYS:H	1.36	0.88
3:D:310:GLY:CA	3:D:311:ARG:HB2	2.03	0.88
3:D:128:LEU:HD21	3:D:188:LEU:HD13	1.55	0.88
2:H:13:LYS:HE3	2:H:1183:ALA:HB2	1.54	0.88
1:B:192:VAL:HG21	1:B:198:LEU:HD12	1.52	0.88
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.55	0.88
2:H:55:SER:HB3	2:H:56:VAL:HG13	1.55	0.88
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.54	0.88
3:D:1155:ILE:HG13	3:D:1210:ILE:HG23	1.56	0.88
3:D:310:GLY:HA3	3:D:311:ARG:CB	2.03	0.87
2:C:13:LYS:HE3	2:C:1183:ALA:HB2	1.57	0.87
3:D:1347:LEU:HD23	3:D:1358:PRO:HG2	1.55	0.87
1:F:231:PHE:HZ	1:G:39:LEU:HD13	1.40	0.87
2:C:816:ILE:HG13	2:C:1098:LEU:HD22	1.55	0.86
3:I:546:ALA:H	3:I:547:ARG:HA	1.40	0.86
3:I:749:LYS:HG3	3:I:750:PRO:HD2	1.57	0.86
6:H:1401:1RM:H23	6:H:1401:1RM:H26	1.55	0.86
2:H:487:LEU:CB	2:H:488:MET:HA	2.04	0.86
2:H:1269:ARG:HG3	3:I:346:ARG:HG2	1.56	0.85
2:C:55:SER:HB3	2:C:56:VAL:HG13	1.57	0.85
4:E:5:THR:HA	4:E:6:VAL:CB	2.04	0.85
2:C:131:THR:HG21	2:C:135:THR:HG22	1.58	0.85
2:H:488:MET:CB	2:H:490:GLN:H	1.89	0.85
4:J:5:THR:HA	4:J:6:VAL:CB	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49:LEU:HD11	2:C:464:PHE:HB3	1.59	0.84
3:D:905:ARG:HH22	4:E:10:VAL:HG11	1.43	0.84
1:F:100:LEU:HD21	1:F:121:VAL:HG21	1.59	0.84
2:H:489:PRO:HB2	2:H:492:MET:HB3	1.59	0.83
3:I:1173:ARG:HA	3:I:1174:ARG:CB	2.07	0.83
5:X:35:ILE:HG13	5:X:36:VAL:H	1.40	0.83
2:C:55:SER:HB3	2:C:56:VAL:HG22	1.60	0.83
2:H:55:SER:HB3	2:H:56:VAL:HG22	1.60	0.83
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.60	0.83
2:C:742:TYR:HB3	2:C:743:PRO:HD3	1.59	0.83
3:D:205:LEU:HD22	3:D:217:LEU:HD22	1.58	0.83
3:I:1149:ARG:HD3	3:I:1149:ARG:H	1.43	0.83
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.60	0.83
3:I:1280:VAL:HG11	3:I:1304:ARG:HE	1.44	0.83
3:I:746:LEU:HD13	3:I:758:PRO:HG3	1.60	0.82
2:H:700:VAL:HG11	2:H:1114:GLU:HG3	1.61	0.82
3:I:1347:LEU:HD23	3:I:1358:PRO:HG2	1.62	0.82
4:J:5:THR:HA	4:J:6:VAL:HB	1.62	0.82
1:F:228:LEU:HD21	1:G:224:LEU:HD23	1.62	0.81
2:H:816:ILE:HG13	2:H:1098:LEU:HD22	1.61	0.81
2:C:1117:LEU:HD11	2:C:1182:ILE:HD13	1.61	0.81
3:D:643:ASP:O	3:D:720:ASN:ND2	2.12	0.81
2:C:170:VAL:HG23	2:C:171:LEU:H	1.45	0.81
2:H:732:ILE:HD11	2:H:769:PRO:HB3	1.61	0.81
2:C:303:ASP:HB2	2:C:310:ILE:HD11	1.62	0.81
3:D:1173:ARG:HA	3:D:1174:ARG:CB	2.06	0.81
3:D:828:GLY:HA2	3:D:832:LYS:H	1.45	0.80
2:H:742:TYR:HB3	2:H:743:PRO:HD3	1.64	0.80
3:D:128:LEU:HD12	3:D:192:MET:HE3	1.62	0.80
1:G:182:ARG:HG2	1:G:206:GLU:HB3	1.62	0.80
2:H:303:ASP:HB2	2:H:310:ILE:HD11	1.64	0.80
2:H:487:LEU:HB3	2:H:488:MET:CA	2.11	0.80
3:I:1261:LEU:HD21	3:I:1306:LEU:HD22	1.62	0.80
3:D:749:LYS:HG3	3:D:750:PRO:HD2	1.63	0.80
4:E:5:THR:HA	4:E:6:VAL:HB	1.64	0.80
5:Y:511:ILE:HG23	5:Y:512:GLY:H	1.47	0.80
2:H:54:ARG:N	2:H:55:SER:HB2	1.96	0.79
2:C:131:THR:CG2	2:C:135:THR:HG22	2.13	0.79
2:C:38:PHE:HE2	2:C:49:LEU:HD12	1.45	0.79
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.63	0.79
2:H:660:VAL:HG22	2:H:661:VAL:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:660:VAL:HG22	2:C:661:VAL:H	1.47	0.79
3:D:572:THR:HG22	3:D:594:GLN:HE22	1.45	0.79
2:C:372:PRO:HB2	5:X:34:ASP:HB3	1.63	0.79
5:X:59:ALA:HB3	5:X:60:PRO:HD3	1.63	0.79
3:D:316:ILE:HG23	3:D:317:THR:H	1.47	0.79
5:X:240:ARG:HD3	5:X:244:THR:HB	1.65	0.79
3:D:230:SER:HB2	3:D:1339:GLY:H	1.47	0.78
3:I:1247:LYS:H	3:I:1247:LYS:HD3	1.47	0.78
2:C:105:TYR:CG	2:C:114:VAL:HG13	2.18	0.78
1:G:192:VAL:HG21	1:G:198:LEU:HD12	1.64	0.78
4:E:5:THR:HA	4:E:6:VAL:CG1	2.14	0.78
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.65	0.78
1:F:11:PRO:HG2	1:G:228:LEU:H	1.49	0.78
2:H:163:LYS:HD3	2:H:163:LYS:H	1.48	0.78
3:I:423:LEU:HD21	3:I:447:ILE:HD11	1.66	0.78
3:I:850:LYS:O	3:I:852:GLY:N	2.17	0.78
1:F:10:LYS:HE3	1:G:226:GLU:HB3	1.66	0.78
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.64	0.78
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.66	0.78
3:D:1247:LYS:HD3	3:D:1247:LYS:H	1.48	0.78
5:X:471:LEU:HB3	5:X:478:PRO:HD3	1.64	0.78
3:D:140:TYR:HA	3:D:181:GLY:HA2	1.66	0.77
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.67	0.77
3:I:205:LEU:HD22	3:I:217:LEU:HD22	1.64	0.77
2:C:400:VAL:HG12	2:C:404:LYS:HE2	1.66	0.77
2:C:54:ARG:N	2:C:55:SER:HB2	1.99	0.77
4:E:5:THR:HA	4:E:6:VAL:HG12	1.66	0.77
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.49	0.77
6:C:1401:1RM:H26	6:C:1401:1RM:H23	1.65	0.77
2:H:131:THR:HG21	2:H:135:THR:HG22	1.66	0.77
3:I:925:GLU:HB3	3:I:926:PRO:HD3	1.66	0.77
2:H:817:LEU:HB3	2:H:1097:VAL:HG13	1.66	0.77
3:D:120:LEU:HG	5:X:46:GLN:HB2	1.66	0.77
5:X:511:ILE:HG23	5:X:512:GLY:H	1.49	0.77
2:C:1073:LYS:HD3	3:D:462:ASP:HB3	1.67	0.76
2:H:142:GLU:HG2	2:H:515:MET:SD	2.25	0.76
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.66	0.76
3:I:905:ARG:HH22	4:J:10:VAL:HG11	1.50	0.76
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.66	0.76
3:I:1155:ILE:HG13	3:I:1210:ILE:HG23	1.67	0.76
1:A:80:GLU:HB2	2:C:694:ARG:HH22	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:598:LYS:HG3	3:I:599:LYS:HG3	1.68	0.76
3:D:546:ALA:H	3:D:547:ARG:CA	1.99	0.76
3:I:392:THR:HB	5:Y:606:VAL:HG21	1.65	0.76
3:D:1268:ASN:HB3	3:D:1300:ALA:HB1	1.68	0.75
2:H:131:THR:CG2	2:H:135:THR:HG22	2.16	0.75
3:I:643:ASP:O	3:I:720:ASN:ND2	2.14	0.75
3:D:545:HIS:HB2	3:D:546:ALA:HB2	1.67	0.75
2:H:360:LEU:HD13	2:H:378:ARG:HH11	1.51	0.75
1:F:163:GLU:HG3	1:F:170:ARG:HH12	1.50	0.75
3:I:230:SER:HB2	3:I:1339:GLY:H	1.49	0.75
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.67	0.75
4:J:15:ASN:HD22	4:J:18:ASP:H	1.34	0.75
1:F:11:PRO:HB3	1:F:31:LEU:HD21	1.69	0.75
1:B:11:PRO:HA	1:B:30:PRO:HB2	1.67	0.75
2:C:1140:LYS:HE2	2:C:1166:ASP:HB3	1.69	0.75
2:H:971:LEU:HD21	2:H:1017:GLN:NE2	2.02	0.75
3:I:600:ALA:HA	3:I:603:LYS:HB3	1.68	0.75
3:D:1301:THR:HG23	3:I:1301:THR:HG23	1.67	0.75
2:H:1042:LEU:H	2:H:1042:LEU:HD13	1.50	0.75
1:G:124:VAL:HG11	1:G:209:GLY:HA3	1.68	0.74
3:I:828:GLY:HA2	3:I:832:LYS:H	1.51	0.74
2:H:1101:LEU:HD21	3:I:508:LEU:HD12	1.69	0.74
2:C:454:ARG:HD3	2:C:459:MET:HG2	1.70	0.74
2:C:487:LEU:HB2	2:C:489:PRO:HD3	1.70	0.74
3:D:600:ALA:HA	3:D:603:LYS:HB3	1.69	0.74
4:E:38:LEU:HD13	4:E:58:LEU:HD23	1.68	0.74
2:C:43:PRO:HD3	2:C:47:TYR:CD2	2.23	0.74
2:C:1211:ARG:O	2:C:1211:ARG:NE	2.20	0.74
3:D:1149:ARG:H	3:D:1149:ARG:HD3	1.52	0.73
5:Y:262:VAL:HG13	5:Y:263:PRO:HD2	1.70	0.73
2:C:562:GLU:HG2	2:C:574:SER:CB	2.19	0.73
3:D:1343:GLU:HA	3:D:1344:LEU:HB2	1.70	0.73
3:D:822:MET:SD	3:D:838:ARG:NH1	2.61	0.73
2:C:727:VAL:HG22	2:C:773:LEU:HB3	1.70	0.73
2:H:21:VAL:HG13	2:H:22:LEU:H	1.54	0.73
2:H:845:LEU:HD23	2:H:889:PRO:HG2	1.71	0.73
3:D:598:LYS:HG3	3:D:599:LYS:HG3	1.71	0.73
2:H:38:PHE:HE2	2:H:49:LEU:HD12	1.53	0.73
2:H:403:MET:HG2	2:H:407:ARG:HH12	1.53	0.73
4:J:5:THR:HA	4:J:6:VAL:CG1	2.19	0.73
5:X:139:GLU:HA	5:X:142:THR:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:564:GLY:HA3	5:X:570:ASP:HB3	1.71	0.73
3:D:850:LYS:O	3:D:852:GLY:N	2.21	0.73
2:C:1269:ARG:HG2	3:D:346:ARG:HG2	1.70	0.73
1:G:45:ARG:O	3:I:538:ARG:NH2	2.22	0.73
2:H:876:GLU:HG3	2:H:927:THR:HG22	1.70	0.73
5:X:457:ILE:O	5:X:461:ASN:ND2	2.22	0.73
3:I:474:LEU:HA	3:I:477:GLN:HE21	1.54	0.73
2:C:736:VAL:HG11	2:C:740:GLU:HA	1.71	0.72
2:H:699:LEU:HD11	2:H:1179:GLY:HA3	1.69	0.72
3:I:120:LEU:HB2	3:I:121:PRO:HD3	1.71	0.72
3:D:546:ALA:N	3:D:547:ARG:HA	2.03	0.72
2:C:309:LEU:HD23	2:C:309:LEU:H	1.54	0.72
3:D:120:LEU:CB	3:D:121:PRO:HD3	2.19	0.72
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.71	0.72
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.71	0.72
2:H:127:ILE:HD13	2:H:127:ILE:H	1.54	0.72
1:F:29:GLU:HB3	1:F:30:PRO:HD3	1.72	0.72
2:C:54:ARG:HG2	2:C:55:SER:HB2	1.70	0.72
3:I:1173:ARG:HB3	3:I:1174:ARG:O	1.88	0.72
3:I:1268:ASN:HB3	3:I:1300:ALA:HB1	1.69	0.72
3:I:426:ALA:HB3	3:I:427:PRO:HD3	1.71	0.72
3:I:546:ALA:H	3:I:547:ARG:CA	2.02	0.72
1:B:37:HIS:CD2	2:C:1216:ARG:HB3	2.24	0.72
2:H:1335:ILE:HD11	3:I:22:ILE:HD11	1.72	0.71
3:I:378:LYS:HB3	3:I:379:PRO:HD3	1.70	0.71
3:I:828:GLY:HA2	3:I:832:LYS:N	2.05	0.71
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.70	0.71
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.71	0.71
2:H:55:SER:HB3	2:H:56:VAL:CG1	2.20	0.71
5:Y:453:PRO:HD2	5:Y:456:MET:HB2	1.73	0.71
1:A:11:PRO:HB3	1:A:31:LEU:HD21	1.73	0.71
2:H:131:THR:HG23	2:H:133:ASN:H	1.54	0.71
2:C:745:GLU:HB2	2:C:1017:GLN:HG3	1.71	0.71
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.71	0.71
2:H:434:ASP:HB3	2:H:439:LYS:HB2	1.73	0.71
3:I:822:MET:SD	3:I:838:ARG:NH1	2.64	0.71
3:I:803:VAL:HG13	3:I:1259:GLN:HE22	1.56	0.71
1:B:29:GLU:HA	1:B:200:LYS:CB	2.20	0.71
3:D:1280:VAL:HA	3:D:1283:SER:HB2	1.72	0.71
5:Y:108:VAL:HG23	5:Y:109:GLU:H	1.56	0.70
3:D:1311:LYS:NZ	5:X:50:ASP:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:368:LEU:HD12	3:D:369:PRO:HD2	1.73	0.70
1:F:231:PHE:CZ	1:G:39:LEU:HD13	2.26	0.70
4:J:5:THR:HA	4:J:6:VAL:HG12	1.72	0.70
5:X:298:PRO:HB2	5:X:301:ASN:HD22	1.55	0.70
3:I:546:ALA:N	3:I:547:ARG:HA	2.04	0.70
5:Y:290:LEU:HB3	5:Y:333:VAL:HG21	1.73	0.70
2:H:49:LEU:HD11	2:H:464:PHE:HB3	1.72	0.70
2:H:59:ILE:HG21	2:H:479:LEU:HB3	1.72	0.70
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.74	0.70
2:C:714:VAL:HG23	2:C:787:PRO:HD2	1.73	0.70
3:D:828:GLY:HA2	3:D:832:LYS:N	2.07	0.70
2:H:151:ARG:HH22	2:H:175:ARG:HH11	1.39	0.70
3:D:1225:GLY:HA2	3:I:1294:ALA:HA	1.74	0.70
3:I:1280:VAL:HA	3:I:1283:SER:HB2	1.73	0.70
4:J:5:THR:CA	4:J:6:VAL:HB	2.21	0.70
2:C:131:THR:HG23	2:C:133:ASN:H	1.56	0.70
1:A:231:PHE:CZ	1:B:39:LEU:HD13	2.27	0.70
5:X:108:VAL:HG23	5:X:109:GLU:H	1.57	0.70
3:D:1292:LEU:HD21	3:I:1284:ARG:HH22	1.55	0.69
3:D:836:ARG:HH12	3:D:839:VAL:HB	1.57	0.69
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.06	0.69
3:D:450:HIS:CD2	3:D:451:PRO:HD2	2.27	0.69
3:I:120:LEU:CB	3:I:121:PRO:HD3	2.21	0.69
5:X:390:ILE:HD11	5:X:435:ILE:HG22	1.74	0.69
2:C:49:LEU:HD11	2:C:464:PHE:CB	2.21	0.69
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.75	0.69
2:H:727:VAL:HG22	2:H:773:LEU:HB3	1.74	0.69
2:H:1065:LYS:NZ	3:I:462:ASP:O	2.25	0.69
2:C:1042:LEU:H	2:C:1042:LEU:HD13	1.58	0.69
2:C:15:PHE:CE2	2:C:1182:ILE:HD11	2.27	0.69
3:D:932:MET:O	3:D:933:ARG:HG3	1.91	0.69
2:H:170:VAL:HG23	2:H:171:LEU:H	1.57	0.69
2:C:189:ASP:OD1	2:C:193:ASN:N	2.21	0.69
2:H:664:GLY:O	2:H:686:GLN:NE2	2.25	0.69
3:I:848:VAL:HG11	3:I:880:VAL:HA	1.75	0.69
5:Y:137:TYR:CE2	5:Y:139:GLU:HB2	2.27	0.69
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.74	0.69
2:C:568:ASN:HB3	2:C:572:ILE:HD12	1.75	0.69
1:G:65:LEU:H	1:G:65:LEU:HD23	1.56	0.69
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.75	0.69
2:C:517:GLN:HE21	2:C:760:ASN:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:309:LEU:H	2:H:309:LEU:HD23	1.55	0.69
2:H:42:ASP:HB2	2:H:47:TYR:CD2	2.28	0.69
2:H:55:SER:CB	2:H:56:VAL:HG22	2.23	0.69
2:C:634:VAL:HG22	2:C:645:PHE:CE2	2.29	0.69
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.75	0.68
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.75	0.68
3:D:1173:ARG:HB3	3:D:1174:ARG:O	1.93	0.68
3:I:864:LEU:HD11	3:I:901:ARG:HH12	1.58	0.68
2:C:55:SER:HB3	2:C:56:VAL:CG1	2.23	0.68
3:D:1167:LYS:HE3	3:D:1173:ARG:HH12	1.57	0.68
1:F:107:ILE:HD11	1:F:136:GLU:HG3	1.75	0.68
3:I:545:HIS:HB2	3:I:546:ALA:HB2	1.76	0.68
2:H:55:SER:HB3	2:H:56:VAL:CG2	2.24	0.68
1:A:18:GLN:HE22	1:A:213:PRO:HG2	1.59	0.68
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.57	0.68
2:H:704:MET:HA	2:H:704:MET:HE3	1.74	0.68
3:I:450:HIS:CD2	3:I:451:PRO:HD2	2.28	0.68
2:H:902:LEU:HD21	5:Y:608:ARG:HG3	1.76	0.68
2:C:817:LEU:HB3	2:C:1097:VAL:HG13	1.76	0.68
2:H:637:ARG:HE	3:I:770:LEU:HD23	1.59	0.68
3:I:145:VAL:HG13	3:I:180:MET:HB3	1.74	0.68
5:X:28:ASN:ND2	5:X:29:ASP:OD2	2.26	0.68
2:C:13:LYS:HD3	2:C:1181:PRO:HG2	1.75	0.68
4:J:25:ARG:NH2	4:J:68:GLU:OE1	2.27	0.68
2:H:794:LEU:HD21	2:H:796:LEU:HG	1.74	0.68
1:G:49:SER:OG	3:I:538:ARG:NH2	2.27	0.68
1:B:62:ASP:OD1	1:B:143:ARG:NH1	2.27	0.68
1:G:37:HIS:CD2	2:H:1216:ARG:HB3	2.29	0.68
2:H:510:GLN:O	2:H:513:GLN:NE2	2.27	0.68
5:X:476:ARG:H	5:X:476:ARG:HD2	1.59	0.68
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.76	0.68
3:D:711:GLY:O	3:D:712:GLN:HG2	1.93	0.68
3:D:803:VAL:HG13	3:D:1259:GLN:HE22	1.58	0.68
2:H:1252:SER:OG	2:H:1255:THR:O	2.12	0.67
3:D:259:ARG:HH21	5:X:504:PRO:HB2	1.58	0.67
5:Y:457:ILE:O	5:Y:461:ASN:ND2	2.27	0.67
2:C:926:GLY:HA3	2:C:1056:VAL:HG12	1.77	0.67
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.76	0.67
2:C:37:LYS:HE3	2:C:37:LYS:HA	1.76	0.67
3:D:151:MET:N	3:D:151:MET:SD	2.68	0.67
2:H:13:LYS:HD3	2:H:1181:PRO:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:133:ARG:O	3:I:133:ARG:NH2	2.26	0.67
2:H:829:THR:HG22	2:H:1059:ARG:HG2	1.76	0.67
2:H:674:ASP:OD2	2:H:1070:HIS:ND1	2.28	0.67
5:Y:470:MET:HB2	5:Y:478:PRO:HB3	1.75	0.67
1:F:52:PRO:HG2	1:F:219:ARG:HH21	1.59	0.67
3:I:1343:GLU:HA	3:I:1344:LEU:HB2	1.77	0.67
2:C:55:SER:CB	2:C:56:VAL:HG22	2.25	0.67
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.77	0.67
3:D:573:THR:HG22	3:D:576:ARG:HG3	1.77	0.67
1:F:11:PRO:CG	1:G:228:LEU:H	2.07	0.67
2:C:127:ILE:HD13	2:C:127:ILE:H	1.60	0.67
1:G:192:VAL:HG12	1:G:194:GLN:HG2	1.76	0.67
3:I:1297:LYS:NZ	3:I:1297:LYS:HA	2.09	0.67
2:C:1180:MET:HB3	2:C:1181:PRO:CA	2.25	0.67
2:H:564:PRO:HA	2:H:684:ASN:HD21	1.60	0.67
3:I:140:TYR:HA	3:I:181:GLY:HA2	1.77	0.67
2:H:185:ASP:HB2	2:H:197:ARG:HB2	1.76	0.66
3:I:139:LEU:HD21	3:I:185:ILE:HD13	1.77	0.66
2:C:1254:VAL:HG23	2:C:1255:THR:H	1.60	0.66
3:D:1341:ARG:NH2	3:D:1343:GLU:OE1	2.28	0.66
3:D:56:LEU:HB3	3:D:250:ARG:HH21	1.59	0.66
2:H:971:LEU:HD21	2:H:1017:GLN:HE21	1.59	0.66
3:I:518:VAL:HG12	3:I:519:ASN:HD22	1.60	0.66
5:X:152:GLU:OE2	5:X:218:ARG:NH1	2.29	0.66
3:D:1261:LEU:CD2	3:D:1306:LEU:HD22	2.23	0.66
3:I:145:VAL:HG22	3:I:180:MET:SD	2.35	0.66
5:X:442:SER:OG	5:X:446:GLN:NE2	2.28	0.66
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.76	0.66
3:D:405:GLU:O	3:D:407:VAL:N	2.29	0.66
3:D:848:VAL:HG11	3:D:880:VAL:HA	1.77	0.66
2:H:488:MET:HE3	2:H:489:PRO:HA	1.77	0.66
3:I:744:ARG:HB2	3:I:759:ILE:HB	1.77	0.66
5:Y:138:PRO:HG3	5:Y:353:LEU:HD21	1.78	0.66
5:Y:469:GLN:HE21	5:Y:473:GLU:HG3	1.60	0.66
3:I:259:ARG:HH21	5:Y:504:PRO:HB2	1.60	0.66
3:D:1362:GLY:O	3:D:1364:ALA:N	2.29	0.66
2:C:1335:ILE:HD11	3:D:22:ILE:HD11	1.77	0.66
3:D:245:LEU:O	3:D:250:ARG:NH1	2.29	0.66
3:D:572:THR:HG22	3:D:594:GLN:NE2	2.10	0.66
2:H:54:ARG:H	2:H:55:SER:CB	2.04	0.66
2:H:54:ARG:HG2	2:H:55:SER:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:876:GLU:HG3	2:C:927:THR:HG22	1.78	0.66
1:A:163:GLU:HB3	1:A:166:ARG:HB3	1.78	0.66
2:C:20:GLN:O	2:C:22:LEU:N	2.29	0.66
3:I:903:LEU:HD11	3:I:909:ILE:HG22	1.77	0.66
1:B:29:GLU:HA	1:B:200:LYS:HB2	1.77	0.66
2:C:1295:SER:HB2	3:D:347:VAL:HG12	1.78	0.66
3:I:1159:ILE:HD12	3:I:1186:TYR:HE2	1.61	0.66
5:X:290:LEU:HB3	5:X:333:VAL:HG21	1.77	0.66
1:F:211:ILE:HD11	1:F:215:GLU:HG3	1.77	0.65
2:C:1117:LEU:HD11	2:C:1182:ILE:CD1	2.26	0.65
2:C:794:LEU:HD21	2:C:796:LEU:HG	1.76	0.65
3:D:423:LEU:HD21	3:D:447:ILE:HD11	1.79	0.65
2:H:143:ARG:NH1	2:H:512:SER:O	2.29	0.65
5:X:262:VAL:HG13	5:X:263:PRO:HD2	1.77	0.65
2:C:488:MET:N	2:C:489:PRO:HD3	2.11	0.65
3:D:1177:ILE:HD11	3:D:1196:LEU:HD11	1.77	0.65
2:H:400:VAL:HG12	2:H:404:LYS:HE2	1.78	0.65
5:Y:145:LEU:HD21	5:Y:225:ARG:HH21	1.60	0.65
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.76	0.65
3:D:720:ASN:O	3:D:722:ILE:N	2.29	0.65
1:F:11:PRO:HD3	1:G:227:GLN:HG3	1.78	0.65
2:H:660:VAL:O	2:H:661:VAL:HG22	1.95	0.65
1:B:192:VAL:HG12	1:B:194:GLN:HG2	1.78	0.65
2:C:972:PHE:HA	2:C:975:ILE:HG22	1.79	0.65
3:D:128:LEU:HD11	3:D:188:LEU:HD22	1.79	0.65
2:H:487:LEU:HB3	2:H:488:MET:HG3	1.79	0.65
2:H:616:ILE:HB	2:H:637:ARG:HB2	1.79	0.65
3:I:320:ASN:HB3	3:I:322:ARG:HG2	1.79	0.65
2:C:55:SER:HB3	2:C:56:VAL:CG2	2.25	0.65
2:C:845:LEU:H	2:C:845:LEU:HD13	1.62	0.65
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.79	0.65
3:D:589:TYR:O	3:D:591:ILE:N	2.28	0.65
2:C:634:VAL:H	2:C:645:PHE:HE2	1.45	0.65
1:F:11:PRO:HB3	1:F:31:LEU:CD2	2.26	0.65
2:H:628:HIS:HB3	2:H:647:ARG:NH2	2.12	0.65
4:J:38:LEU:HD13	4:J:58:LEU:HD23	1.77	0.65
5:X:145:LEU:HD11	5:X:225:ARG:NH2	2.12	0.65
5:Y:298:PRO:HB2	5:Y:301:ASN:HD22	1.60	0.65
2:C:618:GLN:OE1	2:C:637:ARG:NH1	2.30	0.65
2:H:1180:MET:HB3	2:H:1181:PRO:CA	2.26	0.65
2:H:908:GLU:HG2	2:H:909:LYS:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1171:GLY:HA3	3:D:1172:LYS:HB2	1.79	0.65
2:H:11:ILE:HG21	2:H:697:LYS:NZ	2.12	0.65
2:H:99:LYS:N	2:H:99:LYS:HD3	2.12	0.65
3:I:827:GLU:O	3:I:831:VAL:HG12	1.96	0.65
5:Y:98:VAL:HB	5:Y:402:LEU:HD21	1.77	0.65
2:C:660:VAL:O	2:C:661:VAL:HG22	1.97	0.65
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.79	0.65
2:H:1254:VAL:HG23	2:H:1255:THR:H	1.60	0.65
2:H:21:VAL:HG21	2:H:592:ARG:HD3	1.78	0.65
3:I:242:LEU:HD12	3:I:243:PRO:HD2	1.78	0.65
3:I:720:ASN:O	3:I:722:ILE:N	2.30	0.65
3:I:858:VAL:HB	3:I:859:PRO:CD	2.24	0.65
3:D:1254:GLU:O	3:D:1257:VAL:HG12	1.97	0.64
5:X:517:SER:O	5:X:518:HIS:ND1	2.30	0.64
3:D:759:ILE:HG23	3:D:771:GLN:HG3	1.79	0.64
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.08	0.64
2:C:59:ILE:HG21	2:C:479:LEU:HB3	1.80	0.64
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.62	0.64
3:D:154:LEU:HD21	3:D:160:LEU:HD21	1.80	0.64
2:H:557:ARG:HB3	2:H:587:LEU:HD23	1.80	0.64
3:I:151:MET:N	3:I:151:MET:SD	2.70	0.64
3:I:584:PRO:HG2	3:I:587:LEU:HD13	1.79	0.64
3:I:711:GLY:O	3:I:712:GLN:HG2	1.97	0.64
3:I:759:ILE:HG23	3:I:771:GLN:HG3	1.78	0.64
2:C:1239:VAL:O	2:C:1241:ASP:N	2.29	0.64
2:H:255:ILE:HD12	2:H:263:VAL:HB	1.79	0.64
1:A:62:ASP:OD1	1:A:143:ARG:NH1	2.31	0.64
1:F:102:LEU:HG	1:F:115:ILE:HG12	1.80	0.64
1:F:150:ARG:HH12	1:G:8:PHE:HA	1.63	0.64
2:H:816:ILE:HD13	2:H:1074:GLY:HA3	1.80	0.64
2:H:800:MET:HE2	2:H:800:MET:HA	1.79	0.64
2:C:678:ARG:HE	2:C:1106:ARG:HG2	1.62	0.64
2:C:1200:LYS:O	2:C:1202:GLY:N	2.31	0.64
4:E:5:THR:HB	4:E:7:GLN:HB2	1.80	0.64
3:I:541:LEU:H	3:I:541:LEU:HD23	1.61	0.64
5:X:112:THR:HG22	5:X:113:ARG:H	1.62	0.64
1:B:227:GLN:O	1:B:228:LEU:HG	1.97	0.64
3:D:1320:ILE:HG22	3:D:1352:ILE:HD11	1.80	0.64
2:C:142:GLU:HG2	2:C:515:MET:SD	2.38	0.64
3:I:1297:LYS:HZ3	3:I:1297:LYS:HA	1.61	0.64
5:Y:152:GLU:OE2	5:Y:218:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:138:PRO:HD2	5:Y:353:LEU:HD11	1.80	0.64
2:C:1237:HIS:O	2:C:1238:LEU:HG	1.99	0.63
2:C:568:ASN:HB3	2:C:572:ILE:CD1	2.28	0.63
3:D:50:LYS:HG2	3:D:51:PRO:HD2	1.79	0.63
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.31	0.63
3:D:316:ILE:HG23	3:D:317:THR:N	2.13	0.63
1:A:318:LEU:O	1:A:320:ASN:N	2.31	0.63
2:C:94:ALA:N	2:C:126:GLU:OE2	2.24	0.63
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.79	0.63
4:E:5:THR:CA	4:E:6:VAL:HB	2.28	0.63
2:H:933:VAL:HG12	2:H:948:ILE:HD11	1.80	0.63
3:I:325:LYS:HZ3	3:I:330:MET:HG2	1.63	0.63
3:I:368:LEU:HD12	3:I:369:PRO:HD2	1.80	0.63
5:X:12:LEU:CD2	5:X:27:VAL:HG21	2.28	0.63
5:Y:517:SER:O	5:Y:518:HIS:ND1	2.32	0.63
2:C:452:ARG:NH2	2:C:458:GLU:OE1	2.31	0.63
2:C:54:ARG:HG2	2:C:55:SER:CB	2.29	0.63
2:C:660:VAL:HG13	2:C:661:VAL:CG1	2.26	0.63
2:H:1176:LEU:HD22	2:H:1180:MET:O	1.99	0.63
2:H:1210:ILE:HG23	2:H:1211:ARG:NH1	2.14	0.63
2:H:568:ASN:HB3	2:H:572:ILE:CD1	2.29	0.63
3:I:139:LEU:HD13	3:I:140:TYR:N	2.14	0.63
3:I:533:ALA:HB2	3:I:578:ILE:HD13	1.81	0.63
1:A:224:LEU:HD23	1:B:228:LEU:HD22	1.81	0.63
2:H:1272:GLU:HA	2:H:1275:VAL:HG22	1.80	0.62
5:X:264:LYS:HD2	5:X:264:LYS:H	1.64	0.62
2:C:13:LYS:CD	2:C:1181:PRO:HG2	2.29	0.62
3:D:664:ILE:HD12	3:D:681:LYS:HE3	1.81	0.62
2:C:529:ARG:HB2	2:C:529:ARG:HH11	1.64	0.62
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.81	0.62
2:H:1239:VAL:HG12	2:H:1240:ASP:H	1.64	0.62
2:H:68:LEU:HG	2:H:100:LEU:HD23	1.81	0.62
3:I:42:GLU:HG3	5:Y:451:ARG:NH2	2.14	0.62
2:C:592:ARG:HB2	2:C:653:MET:HB3	1.81	0.62
2:H:1237:HIS:O	2:H:1238:LEU:HG	1.99	0.62
3:I:128:LEU:HD12	3:I:192:MET:HE3	1.80	0.62
2:H:618:GLN:OE1	3:I:770:LEU:HB2	1.99	0.62
2:H:660:VAL:HG13	2:H:661:VAL:CG1	2.26	0.62
2:C:841:ARG:NH1	3:D:256:ASP:HB3	2.15	0.62
2:C:1313:HIS:CG	4:E:31:GLN:HE22	2.17	0.62
3:D:522:GLY:HA2	3:D:545:HIS:CG	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1338:ALA:O	3:I:1340:LYS:N	2.33	0.62
5:X:137:TYR:CE2	5:X:139:GLU:HB2	2.34	0.62
3:D:56:LEU:HB3	3:D:250:ARG:NH2	2.14	0.62
2:H:1288:GLN:HE21	2:H:1288:GLN:HA	1.65	0.62
2:H:716:ALA:HB3	2:H:784:ALA:HB3	1.82	0.62
2:H:705:GLU:HB2	2:H:794:LEU:HB3	1.82	0.62
2:C:816:ILE:HD13	2:C:1074:GLY:HA3	1.82	0.62
3:D:606:ASN:OD1	3:D:610:ARG:NH1	2.32	0.62
3:I:1148:ARG:NH2	3:I:1149:ARG:O	2.33	0.62
3:I:1171:GLY:HA3	3:I:1172:LYS:HB2	1.81	0.62
4:J:31:GLN:HB2	4:J:46:THR:HG21	1.80	0.62
2:C:1255:THR:O	2:C:1257:GLN:N	2.33	0.61
3:D:1338:ALA:O	3:D:1340:LYS:N	2.33	0.61
3:D:320:ASN:HB3	3:D:322:ARG:HG2	1.82	0.61
3:D:38:VAL:HG11	3:D:56:LEU:HD13	1.81	0.61
2:H:94:ALA:N	2:H:126:GLU:OE2	2.25	0.61
2:H:55:SER:HB3	2:H:56:VAL:CB	2.30	0.61
2:C:519:ASN:HB2	2:C:520:PRO:HD2	1.82	0.61
2:H:1335:ILE:HD11	3:I:22:ILE:CD1	2.30	0.61
2:H:845:LEU:H	2:H:845:LEU:HD13	1.64	0.61
3:I:423:LEU:CD2	3:I:447:ILE:HD11	2.30	0.61
5:X:240:ARG:O	5:X:242:HIS:N	2.33	0.61
2:C:302:ILE:HA	2:C:309:LEU:HA	1.81	0.61
3:D:139:LEU:HD13	3:D:140:TYR:N	2.16	0.61
3:D:77:ARG:HG3	3:D:78:LEU:H	1.63	0.61
2:H:62:TYR:HD2	2:H:480:SER:HB3	1.65	0.61
3:I:1155:ILE:HG12	3:I:1211:SER:HB2	1.81	0.61
2:C:1252:SER:OG	2:C:1255:THR:O	2.18	0.61
2:C:91:THR:HG21	2:C:503:LYS:HE3	1.82	0.61
2:C:681:MET:O	2:C:685:MET:HG2	2.00	0.61
2:C:1127:LYS:HG2	2:C:1144:PHE:CZ	2.35	0.61
2:C:714:VAL:CG2	2:C:787:PRO:HD2	2.30	0.61
1:B:196:THR:OG1	3:D:443:GLU:HG3	2.01	0.61
3:D:524:GLY:HA2	3:D:548:VAL:HG23	1.81	0.61
3:D:863:LEU:HB2	3:D:866:GLU:HB2	1.83	0.61
2:H:13:LYS:CD	2:H:1181:PRO:HG2	2.31	0.61
3:I:1191:PRO:O	3:I:1193:TRP:N	2.33	0.61
3:I:50:LYS:NZ	3:I:50:LYS:HB3	2.15	0.61
3:I:836:ARG:HH12	3:I:839:VAL:HB	1.65	0.61
3:I:863:LEU:HB2	3:I:866:GLU:HB2	1.83	0.61
2:C:1078:LYS:HG2	2:C:1079:ILE:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1191:PRO:O	3:D:1193:TRP:N	2.31	0.61
2:H:1078:LYS:HG2	2:H:1079:ILE:H	1.66	0.61
2:H:590:PRO:O	2:H:659:GLN:NE2	2.34	0.61
2:H:892:GLU:O	2:H:893:THR:OG1	2.18	0.61
2:C:403:MET:HG3	2:C:414:ILE:HB	1.83	0.61
2:C:562:GLU:HG2	2:C:574:SER:HB3	1.83	0.61
2:C:898:GLU:N	2:C:898:GLU:OE1	2.31	0.61
2:H:510:GLN:NE2	2:H:534:GLY:HA2	2.15	0.61
3:I:1362:GLY:O	3:I:1364:ALA:N	2.33	0.61
3:I:422:LEU:HA	3:I:436:ALA:HA	1.83	0.61
3:I:422:LEU:HD11	3:I:469:HIS:HB2	1.83	0.61
3:I:541:LEU:HB2	3:I:545:HIS:CE1	2.36	0.61
2:C:39:ILE:HG22	2:C:40:GLU:HG2	1.81	0.61
2:C:901:LEU:O	2:C:905:ILE:HG13	2.01	0.61
3:D:500:ILE:H	3:D:500:ILE:HD13	1.66	0.61
2:H:1186:VAL:HG13	2:H:1187:PHE:H	1.66	0.61
2:H:1200:LYS:O	2:H:1202:GLY:N	2.33	0.61
2:H:459:MET:SD	2:H:511:LEU:HD22	2.40	0.61
3:I:222:LYS:NZ	3:I:1276:GLU:HB2	2.16	0.61
3:I:514:THR:HG23	3:I:576:ARG:HE	1.66	0.61
5:Y:139:GLU:HA	5:Y:142:THR:HG22	1.81	0.61
2:C:645:PHE:CE1	2:C:650:VAL:HB	2.36	0.61
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.82	0.61
3:D:50:LYS:NZ	3:D:50:LYS:HB3	2.16	0.61
1:F:221:ALA:HB1	1:G:228:LEU:HD12	1.83	0.61
2:H:18:ARG:HG3	2:H:19:PRO:HD2	1.82	0.61
3:I:425:ARG:HD2	3:I:459:ALA:HB2	1.83	0.61
3:I:88:CYS:O	3:I:90:VAL:N	2.34	0.61
5:X:445:ASP:N	5:X:445:ASP:OD1	2.34	0.61
5:X:448:ARG:HD3	5:X:450:ILE:HG13	1.83	0.61
3:I:838:ARG:NH2	3:I:1250:ASP:OD2	2.34	0.60
3:I:120:LEU:HD22	3:I:1330:ARG:HD3	1.82	0.60
5:X:35:ILE:HG23	5:X:36:VAL:HG13	1.82	0.60
1:B:49:SER:HA	1:B:151:GLY:HA2	1.83	0.60
2:C:166:SER:O	2:C:168:GLY:N	2.33	0.60
2:H:146:VAL:HG13	2:H:513:GLN:HG3	1.83	0.60
2:H:528:ARG:NH2	2:H:576:SER:O	2.34	0.60
5:Y:112:THR:HG22	5:Y:113:ARG:H	1.65	0.60
5:Y:556:ALA:O	5:Y:560:ARG:HB2	2.00	0.60
2:C:163:LYS:HD3	2:C:163:LYS:H	1.64	0.60
2:H:714:VAL:HG23	2:H:787:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1268:ASN:HB3	3:I:1300:ALA:CB	2.31	0.60
3:I:20:ILE:CD1	3:I:1320:ILE:HD11	2.30	0.60
3:I:186:GLN:CB	3:I:238:ILE:HD11	2.22	0.60
3:I:828:GLY:HA2	3:I:832:LYS:CA	2.31	0.60
5:X:12:LEU:HD23	5:X:27:VAL:HG21	1.83	0.60
2:C:106:GLU:N	2:C:107:ARG:HA	2.14	0.60
2:C:1081:PRO:HB2	2:C:1083:GLU:HG2	1.82	0.60
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.33	0.60
1:F:190:ALA:HB2	1:F:200:LYS:HB3	1.83	0.60
3:I:526:VAL:HG12	3:I:549:LYS:HB2	1.83	0.60
3:D:1269:ALA:H	3:D:1300:ALA:HB2	1.66	0.60
3:D:389:GLY:O	3:D:391:ALA:N	2.35	0.60
3:D:474:LEU:HA	3:D:477:GLN:HE21	1.66	0.60
3:D:858:VAL:HB	3:D:859:PRO:CD	2.24	0.60
5:X:138:PRO:HD2	5:X:353:LEU:HD11	1.83	0.60
2:C:201:ARG:NH1	5:X:36:VAL:HG11	2.16	0.60
1:B:227:GLN:O	1:B:229:GLU:N	2.29	0.60
2:C:21:VAL:HG13	2:C:22:LEU:H	1.66	0.60
1:F:158:ARG:HH11	1:F:172:LEU:HD11	1.64	0.60
3:I:128:LEU:HD21	3:I:188:LEU:HD13	1.84	0.60
3:I:245:LEU:O	3:I:250:ARG:NH1	2.34	0.60
3:I:842:ARG:HD2	3:I:882:VAL:HG21	1.83	0.60
3:D:120:LEU:HB2	3:D:121:PRO:CD	2.31	0.60
3:D:1155:ILE:HG12	3:D:1211:SER:HB2	1.83	0.60
2:H:817:LEU:HB3	2:H:1097:VAL:CG1	2.32	0.60
2:H:1298:VAL:HG23	2:H:1299:ASN:H	1.66	0.60
2:H:208:ILE:HD11	2:H:365:GLU:HB3	1.83	0.60
2:H:20:GLN:O	2:H:22:LEU:N	2.34	0.60
2:H:403:MET:HG2	2:H:407:ARG:NH1	2.16	0.60
3:I:213:LYS:O	3:I:217:LEU:HG	2.01	0.60
3:I:422:LEU:CD1	3:I:469:HIS:HB2	2.31	0.60
3:I:708:ASN:OD1	3:I:712:GLN:HB2	2.02	0.60
2:C:1180:MET:HB3	2:C:1181:PRO:O	2.01	0.60
2:C:808:ASN:H	3:D:633:ALA:HB2	1.67	0.60
2:H:55:SER:CB	2:H:56:VAL:HG13	2.28	0.60
3:I:473:THR:HG22	3:I:475:GLU:HG2	1.84	0.60
5:Y:445:ASP:OD1	5:Y:445:ASP:N	2.35	0.60
2:C:402:ARG:NH2	2:C:419:ILE:O	2.35	0.60
2:H:1252:SER:HB3	2:H:1259:LEU:HD21	1.84	0.60
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.33	0.60
2:C:572:ILE:HD13	6:C:1401:1RM:O1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:ARG:HD2	3:D:714:GLU:HB2	1.84	0.60
2:H:106:GLU:N	2:H:107:ARG:HA	2.16	0.60
2:H:1255:THR:O	2:H:1257:GLN:N	2.35	0.60
2:H:452:ARG:NH2	2:H:458:GLU:OE1	2.34	0.60
2:H:898:GLU:OE1	2:H:898:GLU:N	2.33	0.60
2:H:936:ARG:HD2	2:H:1047:LEU:H	1.67	0.60
3:I:768:ASN:O	3:I:771:GLN:NE2	2.35	0.60
2:C:487:LEU:CD1	2:C:488:MET:H	2.15	0.59
2:C:11:ILE:HD13	2:C:697:LYS:NZ	2.17	0.59
2:C:746:ALA:HB2	2:C:971:LEU:HD23	1.84	0.59
3:D:1237:VAL:O	3:D:1240:VAL:HG22	2.02	0.59
2:C:408:SER:O	2:C:431:LYS:NZ	2.28	0.59
3:D:1287:ILE:HG22	3:D:1290:ARG:HE	1.67	0.59
3:I:886:VAL:CG1	3:I:1230:THR:HG21	2.33	0.59
3:I:615:LYS:HB3	3:I:616:PRO:HD3	1.83	0.59
3:I:824:PRO:O	3:I:826:ILE:HG13	2.03	0.59
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.31	0.59
2:C:1255:THR:HG22	2:C:1257:GLN:HG3	1.84	0.59
2:H:1142:ARG:NH2	2:H:1165:SER:O	2.35	0.59
3:D:546:ALA:HB3	3:D:547:ARG:O	2.02	0.59
3:D:703:THR:HA	3:D:717:VAL:HA	1.82	0.59
3:D:903:LEU:HD11	3:D:909:ILE:HG22	1.83	0.59
2:H:1127:LYS:HG2	2:H:1144:PHE:CZ	2.38	0.59
3:I:681:LYS:NZ	3:I:681:LYS:HB2	2.17	0.59
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.84	0.59
2:C:936:ARG:HD2	2:C:1047:LEU:H	1.66	0.59
2:H:1239:VAL:O	2:H:1241:ASP:N	2.35	0.59
2:H:557:ARG:NH1	2:H:611:GLU:OE1	2.35	0.59
3:I:31:ARG:NH2	3:I:106:GLU:OE2	2.34	0.59
5:X:28:ASN:HD22	5:X:29:ASP:N	2.00	0.59
2:C:1293:VAL:HG23	2:C:1301:ARG:HA	1.83	0.59
3:D:245:LEU:HD12	3:D:246:PRO:HD2	1.84	0.59
2:H:568:ASN:HB3	2:H:572:ILE:HD12	1.83	0.59
2:H:592:ARG:HB2	2:H:653:MET:HB3	1.84	0.59
2:C:387:ASN:HB3	2:C:394:ARG:HG3	1.85	0.59
3:D:124:ILE:HG13	3:D:189:LEU:HD11	1.85	0.59
2:H:1087:TYR:HE2	2:H:1215:GLY:HA2	1.67	0.59
2:H:645:PHE:CE1	2:H:650:VAL:HB	2.37	0.59
5:Y:507:MET:HB3	5:Y:520:GLY:HA3	1.85	0.59
2:C:448:LEU:HB2	2:C:553:THR:CG2	2.32	0.59
2:C:55:SER:CB	2:C:56:VAL:HG13	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:708:ASN:OD1	3:D:712:GLN:HB2	2.02	0.59
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.85	0.59
3:D:608:CYS:O	3:D:612:LEU:HB2	2.03	0.59
3:I:1261:LEU:CD2	3:I:1306:LEU:HD22	2.33	0.59
1:B:179:PRO:O	1:B:207:THR:OG1	2.16	0.59
2:C:700:VAL:HG11	2:C:1114:GLU:CG	2.32	0.59
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.68	0.59
2:C:542:ARG:O	2:C:544:GLY:N	2.32	0.59
2:C:550:VAL:HG11	3:D:776:THR:HG23	1.84	0.59
2:H:1148:ALA:HA	2:H:1201:LEU:HD21	1.85	0.59
3:I:1284:ARG:HA	3:I:1287:ILE:HG12	1.85	0.59
5:X:120:ALA:HB3	5:X:421:TYR:HB3	1.84	0.59
1:B:65:LEU:HA	1:B:169:GLY:HA2	1.84	0.58
2:C:1273:MET:HB3	3:D:428:THR:HB	1.85	0.58
5:X:108:VAL:HB	5:X:110:LEU:HG	1.84	0.58
5:X:453:PRO:HD2	5:X:456:MET:HB2	1.85	0.58
1:B:65:LEU:HD23	1:B:65:LEU:H	1.67	0.58
1:B:83:LEU:HD11	3:D:527:LEU:HA	1.84	0.58
2:C:54:ARG:H	2:C:55:SER:CB	2.07	0.58
3:D:19:ALA:CB	3:D:1343:GLU:HB3	2.33	0.58
3:D:658:GLU:HA	3:D:661:VAL:HG12	1.85	0.58
5:X:561:MET:HA	5:X:567:MET:SD	2.43	0.58
2:C:55:SER:HB3	2:C:56:VAL:CB	2.34	0.58
3:D:768:ASN:O	3:D:771:GLN:NE2	2.36	0.58
2:H:454:ARG:HD3	2:H:459:MET:HG2	1.84	0.58
3:I:40:LYS:HB3	3:I:42:GLU:HG2	1.86	0.58
5:X:514:ASP:C	5:X:516:ASP:HA	2.24	0.58
3:I:120:LEU:HB2	3:I:121:PRO:CD	2.33	0.58
3:I:125:GLY:O	3:I:129:ASP:N	2.36	0.58
5:X:562:ARG:NH1	5:X:591:GLU:OE2	2.36	0.58
5:Y:264:LYS:H	5:Y:264:LYS:HD2	1.69	0.58
4:E:3:ARG:NH2	4:E:44:ASP:OD2	2.31	0.58
2:H:1141:LEU:HD13	2:H:1141:LEU:H	1.68	0.58
3:I:1257:VAL:HA	3:I:1260:MET:HB3	1.86	0.58
3:I:77:ARG:HG3	3:I:78:LEU:H	1.68	0.58
2:C:616:ILE:HB	2:C:637:ARG:HB2	1.85	0.58
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.84	0.58
3:D:142:GLU:HG2	3:D:293:ARG:HB2	1.84	0.58
4:E:4:VAL:O	4:E:5:THR:OG1	2.22	0.58
2:H:1283:ALA:HB1	2:H:1286:THR:HB	1.84	0.58
3:I:405:GLU:O	3:I:407:VAL:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:274:ARG:NH1	5:Y:369:GLU:OE2	2.37	0.58
2:C:10:ARG:HD3	2:C:1175:ASN:HD21	1.69	0.58
2:C:752:ASN:O	2:C:753:LEU:HG	2.03	0.58
3:D:518:VAL:HG12	3:D:519:ASN:HD22	1.67	0.58
2:H:1180:MET:HB3	2:H:1181:PRO:O	2.03	0.58
2:H:26:TYR:CE2	2:H:28:LEU:HB2	2.39	0.58
3:I:768:ASN:ND2	3:I:771:GLN:OE1	2.36	0.58
2:C:163:LYS:H	2:C:163:LYS:CD	2.16	0.58
3:D:125:GLY:O	3:D:129:ASP:N	2.37	0.58
2:H:600:THR:HG22	2:H:601:ASP:H	1.68	0.58
2:H:634:VAL:H	2:H:645:PHE:HE2	1.52	0.58
2:H:747:GLY:O	2:H:748:ILE:HG13	2.03	0.58
3:I:1291:GLU:HB2	3:I:1292:LEU:HD12	1.86	0.58
3:D:120:LEU:CB	3:D:121:PRO:CD	2.80	0.58
3:D:681:LYS:HB2	3:D:681:LYS:NZ	2.18	0.58
2:H:753:LEU:HD12	2:H:753:LEU:O	2.04	0.58
1:B:181:GLU:HG2	3:D:531:LYS:HD3	1.85	0.57
1:A:41:ASN:OD1	2:C:1218:GLY:HA3	2.02	0.57
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.86	0.57
2:H:1141:LEU:CD1	2:H:1141:LEU:H	2.17	0.57
2:H:684:ASN:HA	2:H:687:ARG:HD3	1.86	0.57
3:D:527:LEU:HD13	3:D:531:LYS:HB3	1.85	0.57
1:F:234:LEU:HD22	1:G:214:GLU:OE2	2.03	0.57
2:H:54:ARG:HG2	2:H:55:SER:CB	2.34	0.57
2:H:985:GLU:HG2	2:H:989:LEU:HD13	1.86	0.57
3:I:1320:ILE:HG22	3:I:1352:ILE:HD11	1.84	0.57
3:I:606:ASN:OD1	3:I:610:ARG:NH1	2.38	0.57
3:D:1268:ASN:HB3	3:D:1300:ALA:CB	2.34	0.57
3:D:768:ASN:ND2	3:D:771:GLN:OE1	2.37	0.57
3:I:1344:LEU:H	3:I:1345:ARG:HG3	1.68	0.57
1:B:64:VAL:HG13	1:B:69:SER:OG	2.04	0.57
1:F:66:HIS:CE1	1:F:69:SER:HB2	2.40	0.57
2:H:245:ARG:HB3	2:H:337:PHE:CZ	2.39	0.57
5:Y:465:ARG:O	5:Y:468:ARG:HG2	2.04	0.57
2:C:528:ARG:NH2	2:C:576:SER:O	2.38	0.57
2:C:699:LEU:HD23	2:C:799:ASN:CG	2.24	0.57
3:D:19:ALA:HB2	3:D:1343:GLU:HB3	1.87	0.57
3:D:1369:ARG:NH1	3:D:1369:ARG:HB3	2.18	0.57
3:D:579:LEU:HD23	3:D:627:THR:HG21	1.86	0.57
3:D:905:ARG:NH2	4:E:10:VAL:HG11	2.17	0.57
3:I:1254:GLU:O	3:I:1257:VAL:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:400:VAL:HG12	2:C:404:LYS:CE	2.34	0.57
2:H:1339:LEU:H	2:H:1339:LEU:HD12	1.69	0.57
1:A:53:GLY:HA3	1:A:179:PRO:HG3	1.86	0.57
2:C:1111:GLN:HE21	2:C:1230:MET:HE1	1.69	0.57
3:D:528:THR:HG22	3:D:551:ARG:HB2	1.86	0.57
1:G:29:GLU:HA	1:G:200:LYS:CB	2.35	0.57
2:C:1176:LEU:HD22	2:C:1180:MET:O	2.05	0.57
2:C:38:PHE:CE2	2:C:49:LEU:HD12	2.34	0.57
3:D:213:LYS:O	3:D:217:LEU:HG	2.04	0.57
3:D:858:VAL:CB	3:D:859:PRO:HD3	2.25	0.57
2:H:801:ARG:NH1	2:H:1093:PRO:O	2.37	0.57
3:I:367:GLY:HA3	3:I:448:GLN:HB2	1.87	0.57
5:Y:355:ILE:O	5:Y:355:ILE:HD13	2.03	0.57
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.39	0.57
2:C:765:ILE:HG13	2:C:787:PRO:HG2	1.86	0.57
3:D:40:LYS:HB3	3:D:42:GLU:HG2	1.87	0.57
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.37	0.57
5:X:363:ARG:O	5:X:367:ILE:HG12	2.05	0.57
1:A:8:PHE:CE1	1:B:223:ILE:HG12	2.40	0.57
2:C:829:THR:HG22	2:C:1059:ARG:HG2	1.87	0.57
2:C:1335:ILE:HD11	3:D:22:ILE:CD1	2.34	0.57
2:C:478:ARG:HD3	2:C:492:MET:HG3	1.87	0.57
3:D:136:GLU:HA	3:D:139:LEU:HD12	1.87	0.57
3:I:128:LEU:HD13	3:I:189:LEU:HD23	1.87	0.57
3:I:389:GLY:O	3:I:391:ALA:N	2.38	0.57
3:D:395:LYS:HG3	5:X:536:THR:HG21	1.86	0.57
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.87	0.56
2:C:92:TYR:CD1	2:C:129:LEU:HB2	2.40	0.56
2:C:360:LEU:HD13	2:C:378:ARG:HH11	1.68	0.56
2:C:933:VAL:CG1	2:C:948:ILE:HD11	2.31	0.56
2:H:504:GLU:O	2:H:508:SER:HB3	2.05	0.56
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.87	0.56
3:D:423:LEU:CD2	3:D:447:ILE:HD11	2.35	0.56
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.40	0.56
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.88	0.56
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.87	0.56
3:D:85:CYS:HB3	3:D:88:CYS:O	2.05	0.56
4:E:45:LYS:O	4:E:49:ILE:HG12	2.06	0.56
2:H:106:GLU:HB3	2:H:107:ARG:HA	1.86	0.56
2:H:516:ASP:HB2	6:H:1401:1RM:H10	1.86	0.56
2:H:531:SER:OG	6:H:1401:1RM:O2	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:901:LEU:O	2:H:905:ILE:HG13	2.05	0.56
3:I:205:LEU:HD13	3:I:217:LEU:HD22	1.87	0.56
3:I:382:TYR:HE1	3:I:401:VAL:HG21	1.70	0.56
3:I:85:CYS:HB3	3:I:88:CYS:O	2.04	0.56
5:Y:402:LEU:HD13	5:Y:405:ILE:HD11	1.87	0.56
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.69	0.56
2:H:478:ARG:HD3	2:H:492:MET:HG3	1.86	0.56
3:I:128:LEU:HD12	3:I:192:MET:CE	2.35	0.56
5:X:448:ARG:HD2	5:X:452:ILE:HD12	1.87	0.56
3:D:767:LEU:HB3	3:D:771:GLN:NE2	2.20	0.56
1:F:45:ARG:NH2	2:H:1216:ARG:O	2.38	0.56
2:H:406:ASN:HB3	2:H:411:ARG:HB2	1.86	0.56
3:I:245:LEU:HD12	3:I:246:PRO:HD2	1.88	0.56
3:I:704:GLU:HB2	3:I:718:SER:OG	2.06	0.56
3:D:173:GLY:O	3:D:175:GLU:HG3	2.06	0.56
3:D:422:LEU:CD1	3:D:469:HIS:HB2	2.35	0.56
2:H:1340:GLU:OE2	3:I:1341:ARG:NH1	2.34	0.56
2:H:73:TYR:HD2	2:H:74:ARG:H	1.53	0.56
5:X:515:GLU:N	5:X:516:ASP:HA	2.20	0.56
5:Y:503:GLU:HB3	5:Y:504:PRO:O	2.06	0.56
2:C:753:LEU:O	2:C:753:LEU:HD12	2.06	0.56
2:H:122:VAL:HG23	2:H:490:GLN:HG3	1.86	0.56
3:I:122:SER:HB2	3:I:132:LEU:HD22	1.87	0.56
3:I:778:GLY:HA2	3:I:781:LYS:HE3	1.87	0.56
2:C:143:ARG:NH1	2:C:512:SER:O	2.39	0.56
2:C:316:GLU:HG3	2:C:352:ARG:HH12	1.69	0.56
3:D:554:GLU:HA	3:D:589:TYR:CD2	2.40	0.56
3:D:51:PRO:HB3	3:D:57:PHE:O	2.06	0.56
3:D:591:ILE:HD12	3:D:592:VAL:N	2.21	0.56
3:I:644:MET:O	3:I:764:ARG:NH1	2.39	0.56
3:I:824:PRO:HB3	3:I:836:ARG:HD3	1.86	0.56
5:X:503:GLU:HB3	5:X:504:PRO:O	2.05	0.56
2:C:302:ILE:HG22	2:C:309:LEU:HB3	1.88	0.56
2:C:812:PHE:CD2	2:C:813:GLU:HG3	2.41	0.56
2:H:9:LYS:HD3	2:H:9:LYS:N	2.19	0.56
3:I:1274:PHE:HD2	3:I:1275:LEU:HG	1.70	0.56
5:Y:283:GLN:NE2	5:Y:343:LYS:HD2	2.21	0.56
1:B:29:GLU:HA	1:B:200:LYS:HB3	1.87	0.56
3:D:120:LEU:CG	5:X:46:GLN:HB2	2.36	0.56
5:Y:240:ARG:HD3	5:Y:244:THR:HB	1.88	0.56
5:Y:571:TYR:HB3	5:Y:575:GLU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:ASP:O	2:C:44:GLU:HG2	2.06	0.56
2:C:897:PRO:HB3	5:X:564:GLY:O	2.06	0.56
3:D:107:LEU:HD12	3:D:107:LEU:H	1.70	0.56
3:D:589:TYR:O	3:D:591:ILE:HG13	2.06	0.56
1:G:33:ARG:HE	1:G:197:ASP:HB2	1.71	0.56
1:G:42:ALA:O	1:G:46:ILE:HG12	2.06	0.56
2:H:218:GLU:HG2	2:H:299:LYS:HA	1.88	0.56
3:I:57:PHE:CZ	3:I:252:LEU:HD22	2.41	0.56
3:I:919:ALA:O	3:I:923:ILE:HG12	2.06	0.56
5:X:503:GLU:N	5:X:504:PRO:HA	2.21	0.56
5:Y:564:GLY:HA3	5:Y:570:ASP:HB3	1.88	0.56
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.88	0.56
2:C:1180:MET:HB3	2:C:1181:PRO:C	2.26	0.56
2:C:572:ILE:HD13	6:C:1401:1RM:C1	2.35	0.56
1:B:49:SER:OG	3:D:538:ARG:NH2	2.39	0.56
3:I:107:LEU:HD12	3:I:107:LEU:H	1.70	0.56
5:X:136:GLU:OE2	5:X:364:ARG:NH2	2.39	0.56
1:A:219:ARG:O	1:A:223:ILE:HG13	2.07	0.55
2:C:149:LEU:HD12	2:C:452:ARG:O	2.06	0.55
2:C:892:GLU:O	2:C:893:THR:OG1	2.21	0.55
1:F:44:ARG:HG3	1:F:183:ILE:HG22	1.88	0.55
2:H:1043:ALA:HB1	2:H:1044:PRO:HD2	1.88	0.55
2:H:1268:GLN:O	3:I:346:ARG:HA	2.06	0.55
3:I:388:ARG:NH2	3:I:414:GLU:OE2	2.39	0.55
3:I:412:LEU:O	3:I:416:ILE:HG23	2.05	0.55
3:I:502:PRO:HB3	3:I:506:VAL:HG11	1.88	0.55
3:I:589:TYR:O	3:I:591:ILE:N	2.35	0.55
5:Y:476:ARG:HD2	5:Y:476:ARG:H	1.71	0.55
5:Y:503:GLU:N	5:Y:504:PRO:HA	2.21	0.55
2:C:747:GLY:O	2:C:748:ILE:HG13	2.05	0.55
2:C:618:GLN:OE1	3:D:770:LEU:HB2	2.05	0.55
3:D:809:VAL:HG13	3:D:912:GLY:H	1.71	0.55
4:E:5:THR:CA	4:E:6:VAL:CB	2.83	0.55
1:G:49:SER:HA	1:G:151:GLY:HA2	1.88	0.55
2:H:1211:ARG:O	2:H:1211:ARG:NE	2.34	0.55
1:F:41:ASN:OD1	2:H:1218:GLY:HA3	2.06	0.55
2:H:487:LEU:HB3	2:H:488:MET:CG	2.36	0.55
4:J:15:ASN:HD21	4:J:17:PHE:HB2	1.71	0.55
3:D:393:THR:HG21	5:X:607:LEU:HD22	1.87	0.55
5:Y:363:ARG:O	5:Y:367:ILE:HG12	2.05	0.55
1:A:11:PRO:HD3	1:B:227:GLN:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:ILE:HD11	2:C:115:LYS:HB2	1.88	0.55
2:C:127:ILE:HG22	2:C:502:VAL:HG11	1.88	0.55
2:C:11:ILE:HD13	2:C:697:LYS:HZ1	1.70	0.55
2:C:9:LYS:N	2:C:9:LYS:HD3	2.20	0.55
3:D:1291:GLU:HB2	3:D:1292:LEU:HD12	1.89	0.55
2:H:342:ASP:HA	2:H:437:ASN:HB3	1.88	0.55
2:H:448:LEU:HB2	2:H:553:THR:CG2	2.36	0.55
2:H:800:MET:HA	2:H:800:MET:CE	2.36	0.55
3:I:640:GLY:N	3:I:643:ASP:OD2	2.39	0.55
2:C:106:GLU:HG2	2:C:109:ALA:H	1.72	0.55
2:C:131:THR:HG22	2:C:135:THR:N	2.22	0.55
3:D:179:LYS:H	3:D:179:LYS:HD3	1.69	0.55
2:H:18:ARG:N	2:H:1188:ASP:OD2	2.30	0.55
3:I:828:GLY:HA2	3:I:832:LYS:HA	1.88	0.55
3:I:886:VAL:HG11	3:I:1230:THR:HG21	1.89	0.55
2:C:105:TYR:CD1	2:C:114:VAL:HG13	2.41	0.55
2:C:842:ASP:N	2:C:1046:VAL:HG11	2.22	0.55
2:H:484:LEU:H	2:H:484:LEU:HD22	1.70	0.55
3:I:1274:PHE:CD2	3:I:1275:LEU:HG	2.41	0.55
3:I:325:LYS:NZ	3:I:330:MET:HG2	2.20	0.55
3:D:396:ALA:HB2	5:X:606:VAL:HG11	1.89	0.55
5:Y:279:ARG:NH2	5:Y:350:GLU:OE1	2.39	0.55
3:D:120:LEU:HG	5:X:46:GLN:CB	2.36	0.55
3:D:388:ARG:NH2	3:D:414:GLU:OE2	2.40	0.55
5:X:584:ARG:O	5:X:587:ILE:HG22	2.07	0.55
3:D:932:MET:SD	3:D:932:MET:N	2.70	0.55
1:A:104:LYS:HD3	1:A:105:SER:N	2.22	0.55
2:C:600:THR:HG22	2:C:601:ASP:H	1.70	0.55
2:H:926:GLY:HA3	2:H:1056:VAL:HG12	1.89	0.55
2:H:519:ASN:HB2	2:H:520:PRO:HD2	1.88	0.55
2:H:62:TYR:CD2	2:H:480:SER:HB3	2.42	0.55
2:H:660:VAL:HG22	2:H:661:VAL:N	2.20	0.55
2:H:700:VAL:HG11	2:H:1114:GLU:CG	2.36	0.55
2:C:841:ARG:HH12	3:D:256:ASP:HB3	1.72	0.55
3:D:1257:VAL:HA	3:D:1260:MET:HB3	1.88	0.55
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.87	0.55
3:D:108:ALA:HB3	3:D:279:LEU:HD12	1.89	0.55
3:D:864:LEU:HD11	3:D:901:ARG:HH12	1.70	0.55
2:H:69:GLN:HE22	2:H:101:ARG:HH21	1.54	0.55
2:H:1256:GLN:HB3	2:H:1301:ARG:HH22	1.72	0.55
5:Y:598:LEU:O	5:Y:599:ARG:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1347:LEU:HD22	3:D:1357:ILE:CG2	2.37	0.55
3:D:186:GLN:CB	3:D:238:ILE:HD11	2.27	0.55
2:H:496:LYS:N	2:H:497:PRO:HD2	2.22	0.55
3:I:426:ALA:HB3	3:I:427:PRO:CD	2.37	0.55
1:A:158:ARG:HB2	1:A:158:ARG:NH2	2.22	0.54
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.88	0.54
3:D:422:LEU:HA	3:D:436:ALA:HA	1.89	0.54
2:H:582:ASN:HB2	2:H:588:GLU:HG3	1.88	0.54
2:H:59:ILE:HD11	2:H:63:SER:HB3	1.88	0.54
3:I:554:GLU:HA	3:I:589:TYR:HD2	1.72	0.54
2:C:105:TYR:CD1	2:C:106:GLU:HB2	2.43	0.54
3:D:56:LEU:O	3:D:250:ARG:NH2	2.34	0.54
3:D:422:LEU:HD11	3:D:469:HIS:HB2	1.89	0.54
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.41	0.54
3:D:474:LEU:HD13	3:D:478:LEU:HD13	1.90	0.54
2:H:1313:HIS:CG	4:J:31:GLN:HE22	2.25	0.54
2:H:1336:ASN:HB2	3:I:33:TRP:HH2	1.71	0.54
2:H:505:PHE:O	2:H:512:SER:OG	2.24	0.54
3:I:19:ALA:CB	3:I:1343:GLU:HB3	2.36	0.54
2:C:1141:LEU:H	2:C:1141:LEU:CD1	2.19	0.54
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.90	0.54
3:D:824:PRO:HB3	3:D:836:ARG:HD3	1.88	0.54
1:G:118:ASP:OD1	1:G:119:GLY:N	2.41	0.54
3:I:252:LEU:HD23	3:I:252:LEU:H	1.71	0.54
3:I:591:ILE:HD12	3:I:592:VAL:N	2.21	0.54
2:H:808:ASN:H	3:I:633:ALA:HB2	1.70	0.54
1:A:158:ARG:HH11	1:A:172:LEU:HD11	1.73	0.54
2:C:645:PHE:HE1	2:C:650:VAL:HB	1.72	0.54
2:H:21:VAL:HG13	2:H:22:LEU:N	2.21	0.54
3:I:131:PRO:HG2	3:I:135:ILE:HD13	1.88	0.54
3:I:253:VAL:HG11	5:Y:523:ILE:HG21	1.88	0.54
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.90	0.54
2:C:1186:VAL:HG13	2:C:1187:PHE:H	1.72	0.54
2:C:41:GLN:CD	2:C:42:ASP:H	2.10	0.54
2:C:660:VAL:HG22	2:C:661:VAL:N	2.20	0.54
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.08	0.54
3:D:27:PRO:O	3:D:31:ARG:HD3	2.07	0.54
3:D:573:THR:HG22	3:D:576:ARG:CG	2.37	0.54
3:D:827:GLU:O	3:D:831:VAL:HG12	2.08	0.54
5:X:17:LYS:N	5:X:18:GLU:HA	2.22	0.54
5:Y:108:VAL:HB	5:Y:110:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ALA:O	1:B:46:ILE:HG12	2.07	0.54
3:D:105:ILE:HD13	3:D:273:ILE:HD11	1.89	0.54
2:H:1014:LEU:O	2:H:1017:GLN:NE2	2.41	0.54
3:I:120:LEU:CB	3:I:121:PRO:CD	2.86	0.54
3:I:491:LEU:HB2	3:I:904:ALA:HA	1.90	0.54
5:Y:448:ARG:HD3	5:Y:450:ILE:HG13	1.90	0.54
2:C:311:CYS:SG	2:C:315:MET:HB2	2.48	0.54
2:C:843:THR:HG22	2:C:844:LYS:H	1.72	0.54
2:C:894:GLN:O	2:C:895:LEU:HB2	2.07	0.54
2:H:105:TYR:CG	2:H:114:VAL:HG13	2.43	0.54
2:H:152:SER:HG	2:H:404:LYS:HZ2	1.53	0.54
2:H:740:GLU:HB2	2:H:741:MET:SD	2.47	0.54
3:I:246:PRO:HB2	3:I:249:LEU:HD13	1.90	0.54
3:I:292:VAL:HG22	3:I:296:LYS:HE3	1.90	0.54
3:I:573:THR:HG22	3:I:576:ARG:HG3	1.89	0.54
5:X:518:HIS:HB2	5:X:521:ASP:OD2	2.08	0.54
5:Y:518:HIS:HB2	5:Y:521:ASP:OD2	2.08	0.54
2:C:843:THR:HB	2:C:845:LEU:HD22	1.89	0.54
2:C:873:ILE:HD11	2:C:931:VAL:HG22	1.90	0.54
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.07	0.54
3:D:1261:LEU:HD21	3:D:1306:LEU:CD2	2.30	0.54
3:D:522:GLY:HA2	3:D:545:HIS:CD2	2.43	0.54
4:E:38:LEU:HD13	4:E:58:LEU:CD2	2.36	0.54
2:H:1140:LYS:HE2	2:H:1166:ASP:HB3	1.90	0.54
2:C:533:LEU:HG	6:C:1401:1RM:H05	1.89	0.54
3:D:746:LEU:CD1	3:D:758:PRO:HG3	2.33	0.54
3:D:88:CYS:O	3:D:90:VAL:N	2.41	0.54
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.42	0.54
2:H:765:ILE:HG13	2:H:787:PRO:HG2	1.89	0.54
3:I:1138:LEU:HB3	3:I:1139:PRO:HD3	1.90	0.54
2:C:1296:ASP:OD1	3:D:345:LYS:NZ	2.38	0.54
3:D:426:ALA:HB3	3:D:427:PRO:CD	2.38	0.54
1:G:31:LEU:HB2	1:G:199:ASP:O	2.08	0.54
3:I:450:HIS:HD2	3:I:451:PRO:HD2	1.73	0.54
1:A:263:THR:HG23	1:A:266:SER:H	1.74	0.53
3:D:316:ILE:HG13	3:D:317:THR:N	2.24	0.53
3:D:767:LEU:HB3	3:D:771:GLN:HE22	1.73	0.53
1:G:62:ASP:OD1	1:G:143:ARG:NH1	2.40	0.53
2:H:811:ASN:O	2:H:1099:ASN:ND2	2.38	0.53
3:I:1322:ALA:HB3	3:I:1331:VAL:HG21	1.89	0.53
3:I:381:ILE:HD11	3:I:412:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:546:ALA:HB3	3:I:547:ARG:O	2.07	0.53
2:H:1223:ARG:HD2	3:I:637:ALA:HA	1.90	0.53
3:I:733:SER:O	3:I:737:ILE:HG12	2.08	0.53
1:B:33:ARG:HE	1:B:197:ASP:HB2	1.73	0.53
2:C:487:LEU:HD13	2:C:488:MET:H	1.72	0.53
1:F:118:ASP:OD1	1:F:119:GLY:N	2.41	0.53
2:H:960:LEU:HD12	2:H:1032:LYS:HD3	1.88	0.53
4:J:5:THR:HB	4:J:7:GLN:HB2	1.91	0.53
1:B:77:ASP:O	1:B:81:ILE:HG13	2.08	0.53
2:C:245:ARG:HB3	2:C:337:PHE:CZ	2.43	0.53
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.42	0.53
3:D:412:LEU:O	3:D:416:ILE:HG23	2.07	0.53
2:H:189:ASP:HB2	2:H:190:PRO:HD2	1.91	0.53
3:I:508:LEU:HD23	3:I:508:LEU:O	2.08	0.53
5:Y:573:LEU:HD21	5:Y:588:ARG:HD3	1.91	0.53
2:C:11:ILE:HG21	2:C:697:LYS:HZ2	1.73	0.53
3:D:828:GLY:HA2	3:D:832:LYS:CA	2.38	0.53
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.89	0.53
2:H:49:LEU:HD11	2:H:464:PHE:CB	2.38	0.53
3:I:809:VAL:HG13	3:I:912:GLY:H	1.74	0.53
4:J:39:VAL:HG13	4:J:40:PRO:HD2	1.90	0.53
4:J:45:LYS:O	4:J:49:ILE:HG12	2.08	0.53
3:D:545:HIS:HB2	3:D:546:ALA:CB	2.38	0.53
1:G:56:VAL:HG12	1:G:173:VAL:HG11	1.89	0.53
2:H:1014:LEU:HA	2:H:1017:GLN:OE1	2.09	0.53
2:H:1314:GLN:HG3	4:J:28:ARG:NH1	2.24	0.53
2:H:230:PHE:HB2	2:H:333:ILE:HB	1.90	0.53
3:I:1266:ILE:HG13	3:I:1274:PHE:O	2.09	0.53
3:I:527:LEU:HD13	3:I:531:LYS:CB	2.39	0.53
3:I:57:PHE:CE1	3:I:252:LEU:HD22	2.43	0.53
2:C:12:ARG:O	2:C:13:LYS:HG2	2.09	0.53
2:C:557:ARG:HB3	2:C:587:LEU:HD23	1.89	0.53
2:C:590:PRO:O	2:C:659:GLN:NE2	2.41	0.53
3:D:541:LEU:H	3:D:541:LEU:HD23	1.74	0.53
3:D:640:GLY:N	3:D:643:ASP:OD2	2.42	0.53
5:X:402:LEU:HD13	5:X:405:ILE:HD11	1.90	0.53
1:A:243:LYS:NZ	1:A:243:LYS:HB2	2.24	0.53
2:H:562:GLU:HG2	2:H:574:SER:CB	2.39	0.53
2:H:844:LYS:NZ	2:H:844:LYS:HB2	2.24	0.53
3:I:189:LEU:HB3	3:I:234:PRO:HB2	1.90	0.53
4:J:4:VAL:O	4:J:5:THR:OG1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:355:ILE:HD13	5:X:355:ILE:O	2.07	0.53
1:A:192:VAL:O	1:A:194:GLN:N	2.40	0.53
2:C:1341:ASP:HB2	2:C:1342:GLU:OE1	2.08	0.53
2:C:496:LYS:N	2:C:497:PRO:HD2	2.23	0.53
3:D:1256:ILE:HG13	3:D:1257:VAL:N	2.23	0.53
2:H:901:LEU:HD13	5:Y:563:PHE:CE2	2.43	0.53
3:I:450:HIS:HE1	3:I:452:LEU:HD12	1.74	0.53
5:X:143:TYR:O	5:X:147:GLN:HG2	2.09	0.53
3:D:252:LEU:HD23	3:D:252:LEU:H	1.73	0.53
2:H:1180:MET:HB3	2:H:1181:PRO:C	2.28	0.53
3:I:1287:ILE:HG22	3:I:1290:ARG:HE	1.73	0.53
3:I:527:LEU:HD13	3:I:531:LYS:HB3	1.90	0.53
3:I:546:ALA:N	3:I:547:ARG:CA	2.68	0.53
3:I:66:LYS:HB2	3:I:69:GLU:HG2	1.91	0.53
5:X:301:ASN:O	5:X:305:LEU:HD13	2.09	0.53
5:X:598:LEU:O	5:X:599:ARG:HD2	2.07	0.53
1:B:118:ASP:OD1	1:B:119:GLY:N	2.42	0.53
2:C:728:ASP:OD2	2:C:729:ALA:N	2.42	0.53
3:D:1198:VAL:HB	3:D:1210:ILE:HD13	1.91	0.53
3:D:202:ARG:O	3:D:206:ASN:ND2	2.42	0.53
3:D:546:ALA:N	3:D:547:ARG:CA	2.67	0.53
2:H:302:ILE:HG22	2:H:309:LEU:HB3	1.91	0.53
3:I:120:LEU:HD22	3:I:1330:ARG:CD	2.38	0.53
3:I:918:ILE:HD13	3:I:919:ALA:N	2.23	0.53
1:A:88:LEU:HD22	1:A:90:VAL:HG23	1.91	0.52
2:C:1119:MET:HG2	2:C:1228:GLY:CA	2.22	0.52
2:C:946:LEU:O	2:C:949:GLU:HG3	2.09	0.52
3:D:1193:TRP:O	3:D:1194:ARG:HB2	2.09	0.52
1:G:16:ILE:HG12	1:G:26:VAL:HG22	1.90	0.52
2:H:384:LEU:O	2:H:388:LEU:HG	2.10	0.52
2:H:179:TYR:HE2	2:H:462:ASN:HD21	1.55	0.52
2:H:488:MET:HE2	2:H:488:MET:N	2.24	0.52
2:H:843:THR:HG22	2:H:844:LYS:H	1.74	0.52
3:I:222:LYS:HZ3	3:I:1276:GLU:HB2	1.74	0.52
5:X:115:GLY:O	5:X:119:ILE:HG12	2.09	0.52
5:Y:387:VAL:HG13	5:Y:408:GLY:HA3	1.91	0.52
2:C:131:THR:HG22	2:C:135:THR:H	1.73	0.52
1:A:80:GLU:HA	2:C:694:ARG:HH12	1.74	0.52
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.44	0.52
1:F:15:ASP:HB3	1:F:27:THR:OG1	2.09	0.52
2:H:1210:ILE:HG23	2:H:1211:ARG:HH11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:222:LYS:HE2	3:I:1273:ASP:CG	2.29	0.52
3:I:709:ARG:O	3:I:711:GLY:N	2.42	0.52
2:C:1239:VAL:HG12	2:C:1240:ASP:H	1.75	0.52
3:D:554:GLU:HA	3:D:589:TYR:HD2	1.74	0.52
2:H:496:LYS:HE2	5:Y:471:LEU:HD22	1.91	0.52
5:X:138:PRO:HG3	5:X:353:LEU:HD21	1.91	0.52
1:A:256:PRO:HA	1:A:277:TYR:HA	1.90	0.52
1:B:102:LEU:HG	1:B:115:ILE:HG12	1.91	0.52
2:C:1002:LEU:CD1	2:C:1003:THR:H	2.22	0.52
2:C:516:ASP:HB2	6:C:1401:1RM:H10	1.90	0.52
3:I:305:ALA:O	3:I:309:ASN:ND2	2.43	0.52
5:Y:514:ASP:C	5:Y:516:ASP:HA	2.30	0.52
2:C:91:THR:HG22	2:C:139:ASN:H	1.74	0.52
2:C:59:ILE:CG2	2:C:479:LEU:HB3	2.39	0.52
3:D:709:ARG:O	3:D:711:GLY:N	2.42	0.52
1:F:212:ASP:OD2	1:F:215:GLU:HG2	2.09	0.52
2:H:1064:ASP:OD1	2:H:1239:VAL:HG23	2.09	0.52
2:H:728:ASP:OD2	2:H:729:ALA:N	2.42	0.52
2:H:838:CYS:HB2	2:H:918:LEU:HB2	1.92	0.52
5:X:600:HIS:HB2	5:X:601:PRO:HD3	1.90	0.52
5:Y:511:ILE:HG23	5:Y:512:GLY:N	2.23	0.52
1:B:27:THR:HG22	1:B:202:VAL:HG13	1.91	0.52
1:A:45:ARG:CG	2:C:1083:GLU:HB2	2.35	0.52
2:C:314:ASN:HD21	2:C:348:SER:HA	1.74	0.52
3:D:1145:PHE:CE2	3:D:1256:ILE:HD11	2.44	0.52
3:D:149:GLY:HA2	3:D:156:ARG:HG2	1.91	0.52
3:D:450:HIS:HD2	3:D:451:PRO:HD2	1.75	0.52
3:D:828:GLY:HA2	3:D:832:LYS:HA	1.90	0.52
1:F:41:ASN:HD21	2:H:1218:GLY:HA3	1.75	0.52
2:H:1336:ASN:HB2	3:I:33:TRP:CH2	2.44	0.52
3:I:1256:ILE:HG13	3:I:1257:VAL:N	2.25	0.52
1:A:42:ALA:O	1:A:46:ILE:HG12	2.09	0.52
2:C:1142:ARG:HH22	2:C:1165:SER:N	2.08	0.52
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.92	0.52
3:D:1169:THR:HA	3:D:1173:ARG:HB3	1.92	0.52
3:D:185:ILE:HG22	3:D:238:ILE:HD13	1.91	0.52
3:D:527:LEU:HD13	3:D:531:LYS:CB	2.40	0.52
1:F:9:LEU:O	1:G:227:GLN:NE2	2.43	0.52
2:H:119:GLU:HG2	2:H:120:GLN:N	2.25	0.52
2:H:241:LEU:HD11	2:H:246:LEU:HD11	1.91	0.52
2:H:453:ILE:HG22	2:H:585:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:634:VAL:HG22	2:H:645:PHE:CE2	2.45	0.52
2:H:752:ASN:O	2:H:753:LEU:HG	2.10	0.52
2:H:843:THR:HB	2:H:845:LEU:HD22	1.91	0.52
3:I:1280:VAL:HG21	3:I:1304:ARG:NH2	2.25	0.52
3:I:316:ILE:HD13	3:I:316:ILE:H	1.74	0.52
3:I:646:ILE:HG22	3:I:741:ALA:O	2.10	0.52
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.38	0.52
2:C:936:ARG:NH1	5:X:495:ARG:HD3	2.25	0.52
3:D:137:ARG:NH1	5:X:95:THR:HG23	2.24	0.52
1:F:42:ALA:O	1:F:46:ILE:HG12	2.10	0.52
2:H:105:TYR:HA	2:H:106:GLU:HB2	1.92	0.52
2:H:12:ARG:O	2:H:13:LYS:HG2	2.10	0.52
3:I:142:GLU:HG2	3:I:293:ARG:HB2	1.91	0.52
3:I:701:LEU:HD21	3:I:723:TYR:HB2	1.92	0.52
2:C:669:PRO:HG2	2:C:1070:HIS:CE1	2.45	0.52
2:C:818:VAL:HG22	2:C:819:SER:H	1.75	0.52
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.91	0.52
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.44	0.52
3:D:535:ARG:HB3	3:D:541:LEU:HD21	1.92	0.52
2:H:678:ARG:HE	2:H:1106:ARG:HG2	1.74	0.52
2:H:204:LEU:HD11	2:H:369:MET:HG3	1.92	0.52
2:H:36:GLN:O	2:H:39:ILE:HG22	2.10	0.52
3:I:534:GLU:O	3:I:538:ARG:HB2	2.10	0.52
3:I:701:LEU:CD2	3:I:723:TYR:HB2	2.40	0.52
1:A:152:TYR:CD2	2:C:824:GLN:HG2	2.45	0.52
3:D:120:LEU:HD22	3:D:1330:ARG:HD2	1.90	0.52
4:E:10:VAL:HG21	4:E:16:ARG:HG2	1.92	0.52
2:H:106:GLU:HG2	2:H:109:ALA:H	1.75	0.52
3:I:803:VAL:HG22	3:I:1259:GLN:OE1	2.09	0.52
3:I:50:LYS:HG2	3:I:51:PRO:HD2	1.92	0.52
2:C:1304:MET:O	2:C:1308:ILE:HG13	2.09	0.51
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.92	0.51
2:C:740:GLU:OE2	2:C:974:ARG:NH2	2.43	0.51
2:H:658:GLN:HB3	2:H:1186:VAL:HG11	1.93	0.51
2:H:59:ILE:HB	2:H:480:SER:OG	2.10	0.51
3:I:552:ILE:HD13	3:I:570:LYS:HB2	1.92	0.51
3:I:800:LEU:O	3:I:803:VAL:HG12	2.10	0.51
5:Y:301:ASN:O	5:Y:305:LEU:HD13	2.10	0.51
1:B:83:LEU:HD13	3:D:526:VAL:HG23	1.92	0.51
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.45	0.51
3:D:316:ILE:O	3:D:317:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:LEU:HD12	3:D:535:ARG:NE	2.25	0.51
1:B:45:ARG:O	3:D:538:ARG:NH2	2.42	0.51
3:D:552:ILE:HD13	3:D:570:LYS:HB2	1.91	0.51
1:F:158:ARG:NH2	1:F:162:GLU:HB3	2.26	0.51
2:H:807:TRP:HH2	2:H:1216:ARG:HE	1.57	0.51
2:H:360:LEU:HD13	2:H:378:ARG:NH1	2.22	0.51
2:H:557:ARG:HH12	2:H:611:GLU:CD	2.14	0.51
5:X:27:VAL:HA	5:X:30:HIS:HD2	1.75	0.51
5:Y:471:LEU:HB3	5:Y:478:PRO:HD3	1.91	0.51
1:A:58:GLU:HG2	1:A:172:LEU:HD23	1.92	0.51
2:C:1120:ALA:HB1	2:C:1198:LEU:HB3	1.92	0.51
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.93	0.51
3:D:1357:ILE:H	3:D:1357:ILE:HD12	1.76	0.51
3:D:646:ILE:HG22	3:D:741:ALA:O	2.10	0.51
3:D:744:ARG:HB2	3:D:759:ILE:HB	1.92	0.51
3:D:842:ARG:HB3	3:D:882:VAL:HG21	1.91	0.51
2:H:91:THR:HG22	2:H:139:ASN:H	1.76	0.51
3:I:1167:LYS:HB3	3:I:1170:LYS:HD2	1.91	0.51
3:I:310:GLY:HA2	3:I:314:ARG:HE	1.75	0.51
3:I:807:LEU:O	3:I:807:LEU:HD12	2.11	0.51
5:Y:515:GLU:N	5:Y:516:ASP:HA	2.26	0.51
5:Y:585:GLU:HB3	5:Y:589:GLN:HE22	1.76	0.51
1:A:80:GLU:HB2	2:C:694:ARG:NH2	2.22	0.51
2:C:634:VAL:HG22	2:C:645:PHE:CZ	2.45	0.51
2:C:742:TYR:CB	2:C:743:PRO:HD3	2.35	0.51
3:D:1270:GLY:HA3	3:D:1299:GLY:HA2	1.92	0.51
3:D:233:LYS:HD2	3:D:234:PRO:HD2	1.91	0.51
3:D:363:LEU:HA	3:D:450:HIS:ND1	2.25	0.51
2:H:1101:LEU:HD21	3:I:508:LEU:CD1	2.40	0.51
2:H:166:SER:O	2:H:168:GLY:N	2.41	0.51
2:H:628:HIS:HB3	2:H:647:ARG:HH22	1.74	0.51
2:H:741:MET:N	2:H:741:MET:SD	2.82	0.51
5:X:379:MET:CE	5:X:379:MET:HA	2.40	0.51
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.92	0.51
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.93	0.51
2:C:21:VAL:HG13	2:C:22:LEU:N	2.25	0.51
2:C:678:ARG:HD3	2:C:681:MET:HG3	1.92	0.51
3:D:1323:ALA:O	3:D:1328:THR:HG22	2.11	0.51
3:D:152:THR:O	3:D:154:LEU:N	2.41	0.51
2:H:543:ALA:HB1	2:H:548:ARG:HD2	1.92	0.51
2:H:814:ASP:O	2:H:1074:GLY:HA2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:818:VAL:HG22	2:H:819:SER:H	1.76	0.51
3:I:1323:ALA:O	3:I:1328:THR:HG22	2.10	0.51
3:I:155:GLU:CG	3:I:158:GLN:HB2	2.40	0.51
3:I:394:ILE:HG23	5:Y:536:THR:HG22	1.91	0.51
3:I:500:ILE:HD13	3:I:500:ILE:H	1.75	0.51
3:D:260:PHE:O	5:X:504:PRO:HG2	2.11	0.51
1:B:19:VAL:O	1:B:20:SER:HB3	2.10	0.51
2:C:448:LEU:HB2	2:C:553:THR:HG21	1.92	0.51
2:C:99:LYS:NZ	2:C:99:LYS:HB3	2.26	0.51
3:D:141:PHE:O	3:D:297:ARG:HD3	2.10	0.51
3:D:647:PRO:HG3	3:D:697:MET:HA	1.92	0.51
1:G:179:PRO:O	1:G:207:THR:OG1	2.20	0.51
1:G:52:PRO:HG3	1:G:150:ARG:HH12	1.75	0.51
2:H:145:ILE:CG2	2:H:456:VAL:HG22	2.40	0.51
3:I:1145:PHE:HB3	3:I:1309:ILE:HD13	1.92	0.51
3:I:197:GLU:O	3:I:201:LEU:HD23	2.10	0.51
3:I:227:PHE:O	3:I:230:SER:OG	2.23	0.51
3:I:513:MET:O	3:I:575:GLY:HA3	2.11	0.51
2:H:637:ARG:NE	3:I:770:LEU:HD23	2.24	0.51
4:J:60:ASN:H	4:J:63:ILE:HB	1.76	0.51
1:A:163:GLU:HG3	1:A:170:ARG:NH1	2.26	0.51
2:C:1046:VAL:HG22	2:C:1047:LEU:HD13	1.92	0.51
1:A:134:THR:HG21	2:C:727:VAL:O	2.10	0.51
3:D:131:PRO:HG2	3:D:135:ILE:HD13	1.92	0.51
1:B:83:LEU:CD2	3:D:551:ARG:HG3	2.40	0.51
3:D:810:THR:OG1	3:D:811:GLU:N	2.42	0.51
1:F:68:TYR:HB3	2:H:756:TYR:CD1	2.46	0.51
2:H:672:GLU:HG3	2:H:673:HIS:CD2	2.45	0.51
2:H:11:ILE:HG21	2:H:697:LYS:HZ2	1.74	0.51
3:I:1346:GLY:HA3	3:I:1349:GLU:OE2	2.10	0.51
2:C:106:GLU:H	2:C:107:ARG:HA	1.76	0.51
3:D:1155:ILE:HG13	3:D:1210:ILE:CG2	2.36	0.51
3:D:120:LEU:CD2	5:X:46:GLN:HB2	2.41	0.51
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.93	0.51
3:D:609:TYR:HD1	3:D:610:ARG:HD2	1.76	0.51
3:I:1358:PRO:HB3	3:I:1366:HIS:CD2	2.46	0.51
3:I:38:VAL:HG11	3:I:56:LEU:HD13	1.93	0.51
1:A:44:ARG:HG3	1:A:183:ILE:CG2	2.41	0.51
1:A:79:LEU:O	1:A:83:LEU:HD13	2.11	0.51
2:C:297:VAL:HB	2:C:317:LEU:HD21	1.93	0.51
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1322:ALA:HB1	3:D:1326:GLN:NE2	2.25	0.51
1:F:52:PRO:HG2	1:F:219:ARG:NH2	2.25	0.51
1:G:37:HIS:CE1	2:H:1216:ARG:HD3	2.46	0.51
2:H:189:ASP:OD1	2:H:193:ASN:N	2.35	0.51
2:H:494:ASN:OD1	2:H:495:ALA:N	2.43	0.51
3:I:543:SER:O	3:I:574:VAL:HB	2.11	0.51
3:I:56:LEU:HB3	3:I:250:ARG:NH2	2.26	0.51
3:I:707:ILE:HG22	3:I:708:ASN:H	1.75	0.51
5:X:457:ILE:HG23	5:X:461:ASN:HD21	1.76	0.51
2:C:106:GLU:HB3	2:C:107:ARG:HA	1.92	0.51
2:C:685:MET:HE3	2:C:1235:LEU:HD11	1.92	0.51
2:C:699:LEU:H	2:C:799:ASN:HD21	1.58	0.51
3:D:518:VAL:HG23	3:D:716:GLN:OE1	2.11	0.51
1:F:192:VAL:HG21	1:F:198:LEU:HD12	1.92	0.51
3:I:554:GLU:HA	3:I:589:TYR:CD2	2.45	0.51
5:Y:541:ARG:O	5:Y:545:HIS:HB2	2.10	0.51
2:C:67:GLU:HG2	2:C:103:VAL:HG12	1.93	0.50
2:C:517:GLN:HG3	2:C:759:SER:OG	2.10	0.50
2:C:975:ILE:HD13	2:C:975:ILE:O	2.11	0.50
1:F:223:ILE:HD13	1:G:8:PHE:CE1	2.47	0.50
2:H:237:LEU:HD13	2:H:292:ILE:HD12	1.92	0.50
3:I:316:ILE:N	3:I:316:ILE:HD13	2.26	0.50
5:X:493:LYS:O	5:X:497:VAL:HG23	2.11	0.50
1:A:300:LEU:CD1	1:A:304:LYS:HE2	2.41	0.50
2:C:539:THR:O	2:C:540:ARG:HG3	2.11	0.50
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.47	0.50
3:D:1284:ARG:HH22	3:I:1292:LEU:HD21	1.75	0.50
3:D:648:GLU:N	3:D:648:GLU:OE2	2.43	0.50
2:H:18:ARG:HD3	2:H:619:ALA:O	2.11	0.50
5:X:35:ILE:HG13	5:X:36:VAL:N	2.20	0.50
5:Y:243:ALA:O	5:Y:247:GLU:HG3	2.12	0.50
2:C:685:MET:CE	2:C:1235:LEU:HD11	2.41	0.50
2:C:836:LEU:HB3	2:C:918:LEU:HD21	1.94	0.50
2:C:72:SER:O	2:C:98:VAL:HG23	2.11	0.50
3:D:1295:ASN:O	3:D:1298:VAL:HG12	2.11	0.50
3:D:704:GLU:HB2	3:D:718:SER:OG	2.12	0.50
2:H:105:TYR:CD1	2:H:114:VAL:HG13	2.47	0.50
2:H:1180:MET:HB3	2:H:1181:PRO:HA	1.93	0.50
2:H:572:ILE:HD13	6:H:1401:IRM:O1	2.11	0.50
3:I:112:ALA:HA	3:I:238:ILE:HG22	1.92	0.50
3:I:1261:LEU:HD21	3:I:1306:LEU:CD2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:288:PRO:HB2	3:I:291:ILE:HG12	1.93	0.50
5:X:600:HIS:H	5:X:601:PRO:HD2	1.76	0.50
5:Y:600:HIS:HB2	5:Y:601:PRO:HD3	1.93	0.50
3:I:1237:VAL:O	3:I:1240:VAL:HG22	2.11	0.50
3:I:450:HIS:CE1	3:I:452:LEU:HD12	2.46	0.50
4:J:3:ARG:O	4:J:4:VAL:HG13	2.10	0.50
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.12	0.50
3:D:746:LEU:H	3:D:746:LEU:HD22	1.76	0.50
2:H:10:ARG:HD3	2:H:1175:ASN:HD21	1.75	0.50
3:I:1195:GLN:N	3:I:1195:GLN:OE1	2.45	0.50
3:I:658:GLU:HA	3:I:661:VAL:HG12	1.93	0.50
3:I:746:LEU:H	3:I:746:LEU:HD22	1.76	0.50
5:X:35:ILE:HG23	5:X:36:VAL:N	2.26	0.50
3:D:205:LEU:HD22	3:D:217:LEU:CD2	2.36	0.50
2:H:1274:GLU:N	2:H:1274:GLU:OE1	2.44	0.50
2:H:403:MET:HG3	2:H:414:ILE:HB	1.93	0.50
2:H:448:LEU:HB2	2:H:553:THR:HG21	1.92	0.50
3:I:1366:HIS:O	3:I:1370:MET:HB2	2.12	0.50
3:I:152:THR:O	3:I:154:LEU:N	2.40	0.50
3:I:221:ILE:HG13	3:I:222:LYS:N	2.27	0.50
3:I:478:LEU:HD12	4:J:47:THR:HG23	1.94	0.50
1:B:183:ILE:HD11	1:B:205:MET:HE2	1.91	0.50
3:D:1320:ILE:HG22	3:D:1352:ILE:CD1	2.42	0.50
3:D:66:LYS:HG3	3:D:69:GLU:OE2	2.11	0.50
3:D:899:TYR:CZ	3:D:915:ILE:HD12	2.47	0.50
2:H:127:ILE:O	2:H:127:ILE:HG12	2.11	0.50
2:H:842:ASP:CB	2:H:1046:VAL:HG11	2.40	0.50
3:I:271:ARG:HH12	3:I:317:THR:HG21	1.76	0.50
3:I:905:ARG:HE	3:I:907:HIS:HB2	1.75	0.50
2:C:1192:GLU:O	2:C:1196:LYS:HD3	2.11	0.50
2:C:88:ARG:NH2	2:C:1040:ASP:OD1	2.44	0.50
1:F:79:LEU:O	1:F:83:LEU:HD13	2.12	0.50
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.93	0.50
3:I:1295:ASN:O	3:I:1298:VAL:HG12	2.11	0.50
3:I:450:HIS:NE2	3:I:625:MET:SD	2.84	0.50
5:X:101:TYR:OH	5:X:384:LEU:HD11	2.12	0.50
5:X:379:MET:HE2	5:X:379:MET:HA	1.94	0.50
2:H:898:GLU:HB2	5:Y:540:LEU:HD21	1.94	0.50
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.92	0.50
2:C:1274:GLU:N	2:C:1274:GLU:OE1	2.44	0.50
2:C:127:ILE:HD13	2:C:127:ILE:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:221:LEU:HD21	2:C:314:ASN:HD22	1.76	0.50
2:C:11:ILE:HG21	2:C:697:LYS:NZ	2.26	0.50
2:C:699:LEU:HD11	2:C:1179:GLY:HA3	1.94	0.50
2:H:747:GLY:C	2:H:748:ILE:HG13	2.32	0.50
3:I:1357:ILE:H	3:I:1357:ILE:HD12	1.75	0.50
3:I:279:LEU:HD23	3:I:295:GLU:HB3	1.94	0.50
3:D:394:ILE:HG21	5:X:536:THR:HA	1.93	0.50
1:B:33:ARG:NH1	2:C:820:GLU:OE2	2.44	0.49
2:C:105:TYR:CG	2:C:106:GLU:HB2	2.47	0.49
2:C:807:TRP:HE1	2:C:1086:PRO:HD3	1.77	0.49
2:C:1156:ARG:HH11	2:C:1157:GLN:H	1.60	0.49
2:C:98:VAL:HG11	2:C:124:MET:SD	2.52	0.49
1:F:158:ARG:HB2	1:F:158:ARG:NH2	2.27	0.49
1:F:50:SER:HB3	1:G:8:PHE:CZ	2.47	0.49
2:H:105:TYR:CD1	2:H:106:GLU:HB2	2.46	0.49
2:H:511:LEU:HA	2:H:513:GLN:HE21	1.76	0.49
3:I:1193:TRP:O	3:I:1194:ARG:HB2	2.11	0.49
3:I:1251:LYS:O	3:I:1255:VAL:HG23	2.12	0.49
3:I:510:LEU:HD12	3:I:601:ILE:HD11	1.94	0.49
2:C:1042:LEU:HD13	2:C:1042:LEU:N	2.26	0.49
2:C:756:TYR:H	2:C:766:ASN:HB3	1.78	0.49
3:D:803:VAL:HG22	3:D:1259:GLN:OE1	2.12	0.49
3:D:205:LEU:CD2	3:D:217:LEU:HD22	2.36	0.49
3:D:515:ARG:HH22	3:D:717:VAL:C	2.15	0.49
1:F:195:ARG:HH21	1:F:198:LEU:HD21	1.77	0.49
2:H:1046:VAL:HG22	2:H:1047:LEU:HD13	1.93	0.49
2:H:1122:LYS:HG2	2:H:1229:TYR:CE2	2.47	0.49
5:X:264:LYS:N	5:X:264:LYS:HD2	2.28	0.49
3:D:1255:VAL:O	3:D:1258:ARG:HB3	2.11	0.49
3:D:1346:GLY:HA3	3:D:1349:GLU:OE2	2.12	0.49
3:D:733:SER:O	3:D:737:ILE:HG12	2.13	0.49
3:D:899:TYR:CD2	3:D:909:ILE:HG12	2.47	0.49
1:F:41:ASN:ND2	2:H:1218:GLY:HA3	2.28	0.49
3:I:1282:TYR:HA	3:I:1285:VAL:HG22	1.94	0.49
5:Y:600:HIS:H	5:Y:601:PRO:HD2	1.76	0.49
1:A:207:THR:OG1	1:A:208:ASN:N	2.42	0.49
2:C:520:PRO:HB3	2:C:714:VAL:HG11	1.93	0.49
2:C:756:TYR:H	2:C:766:ASN:CB	2.25	0.49
2:C:842:ASP:HB2	2:C:1046:VAL:HG21	1.94	0.49
2:C:942:ASP:HB2	2:C:1048:LYS:NZ	2.28	0.49
3:D:50:LYS:HB3	3:D:50:LYS:HZ2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:807:LEU:O	3:D:807:LEU:HD12	2.12	0.49
3:D:822:MET:HG2	3:D:839:VAL:CG2	2.43	0.49
2:H:127:ILE:HD13	2:H:127:ILE:N	2.26	0.49
2:H:263:VAL:HA	2:H:267:ARG:HH21	1.78	0.49
2:H:510:GLN:HE22	2:H:534:GLY:HA2	1.75	0.49
3:D:1225:GLY:CA	3:I:1294:ALA:HA	2.42	0.49
3:I:474:LEU:HD13	3:I:478:LEU:HD13	1.95	0.49
3:I:550:VAL:HG23	3:I:552:ILE:HD11	1.94	0.49
3:I:648:GLU:OE2	3:I:648:GLU:N	2.43	0.49
1:A:239:GLN:HG3	1:A:240:PRO:HD2	1.93	0.49
2:C:1153:ALA:HB2	2:C:1194:GLU:HG2	1.94	0.49
2:C:1284:ALA:HB3	3:D:1361:THR:HB	1.94	0.49
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.94	0.49
3:D:221:ILE:HG13	3:D:222:LYS:N	2.27	0.49
2:H:817:LEU:CB	2:H:1097:VAL:HG13	2.40	0.49
2:H:1284:ALA:HB3	3:I:1361:THR:HB	1.94	0.49
5:X:511:ILE:HG23	5:X:512:GLY:N	2.25	0.49
5:Y:119:ILE:HD12	5:Y:122:ARG:HH21	1.77	0.49
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.33	0.49
1:B:83:LEU:HD21	3:D:551:ARG:HG3	1.93	0.49
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.95	0.49
2:C:556:GLY:O	2:C:579:ALA:HB2	2.13	0.49
2:C:893:THR:O	2:C:895:LEU:N	2.40	0.49
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.94	0.49
3:D:57:PHE:HB3	3:D:98:ARG:NH1	2.27	0.49
3:D:515:ARG:NH2	3:D:717:VAL:HG12	2.28	0.49
2:H:1325:VAL:O	2:H:1329:GLU:HG3	2.13	0.49
3:I:1255:VAL:O	3:I:1258:ARG:HB3	2.12	0.49
3:I:160:LEU:HA	3:I:164:GLN:NE2	2.27	0.49
3:I:515:ARG:NH2	3:I:717:VAL:HG12	2.26	0.49
3:I:515:ARG:NH2	3:I:718:SER:O	2.46	0.49
5:X:126:GLY:O	5:X:130:VAL:HG23	2.12	0.49
5:X:580:PHE:O	5:X:582:VAL:N	2.46	0.49
1:A:118:ASP:OD1	1:A:119:GLY:N	2.45	0.49
1:B:37:HIS:CE1	2:C:1216:ARG:HD3	2.47	0.49
2:C:747:GLY:C	2:C:748:ILE:HG13	2.33	0.49
3:D:1283:SER:O	3:D:1287:ILE:HG23	2.12	0.49
3:D:539:SER:OG	3:D:540:GLY:N	2.46	0.49
1:G:149:GLY:HA3	1:G:177:TYR:CD2	2.48	0.49
2:H:1225:VAL:HG12	3:I:636:GLY:O	2.13	0.49
2:H:1293:VAL:HG23	2:H:1301:ARG:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1341:ASP:HB2	2:H:1342:GLU:OE1	2.13	0.49
2:H:453:ILE:HG23	2:H:453:ILE:O	2.13	0.49
3:I:1283:SER:O	3:I:1287:ILE:HG23	2.12	0.49
3:I:518:VAL:HG23	3:I:716:GLN:OE1	2.13	0.49
3:I:504:GLN:HA	3:I:730:ALA:HA	1.92	0.49
2:C:936:ARG:HH11	5:X:495:ARG:HD3	1.78	0.49
2:C:1066:MET:HG3	2:C:1234:LYS:HA	1.95	0.49
2:C:119:GLU:HG2	2:C:120:GLN:N	2.28	0.49
2:C:403:MET:HG2	2:C:407:ARG:NH1	2.28	0.49
2:C:845:LEU:N	2:C:845:LEU:HD13	2.28	0.49
3:D:584:PRO:O	3:D:589:TYR:OH	2.28	0.49
4:E:6:VAL:HG23	4:E:51:LEU:HD13	1.95	0.49
3:I:111:THR:HG23	3:I:300:GLN:NE2	2.27	0.49
3:I:42:GLU:HG3	5:Y:451:ARG:HH21	1.77	0.49
3:I:588:PRO:HG2	3:I:591:ILE:HD11	1.95	0.49
5:X:279:ARG:NH2	5:X:350:GLU:OE1	2.46	0.49
5:Y:115:GLY:O	5:Y:119:ILE:HG12	2.12	0.49
5:Y:600:HIS:H	5:Y:601:PRO:CD	2.25	0.49
2:C:337:PHE:O	2:C:338:THR:OG1	2.27	0.49
2:C:453:ILE:HG23	2:C:453:ILE:O	2.13	0.49
2:C:891:GLY:O	2:C:893:THR:HG23	2.13	0.49
2:C:91:THR:HG22	2:C:138:ILE:HA	1.95	0.49
3:D:1171:GLY:N	3:D:1172:LYS:O	2.44	0.49
3:D:128:LEU:HA	3:D:192:MET:HE3	1.95	0.49
3:D:57:PHE:CZ	3:D:252:LEU:HD22	2.48	0.49
2:H:1156:ARG:HH11	2:H:1157:GLN:H	1.59	0.49
2:H:1331:ARG:NH2	2:H:1337:ILE:O	2.46	0.49
2:H:38:PHE:O	2:H:39:ILE:HB	2.12	0.49
2:H:176:ILE:HD11	2:H:428:VAL:HG21	1.94	0.49
2:H:488:MET:HB2	2:H:489:PRO:CA	2.43	0.49
2:H:119:GLU:OE1	2:H:490:GLN:HB2	2.12	0.49
2:H:562:GLU:HG2	2:H:574:SER:HB2	1.95	0.49
2:H:645:PHE:CD1	2:H:650:VAL:HB	2.48	0.49
2:H:678:ARG:HD3	2:H:681:MET:HG3	1.94	0.49
2:H:756:TYR:H	2:H:766:ASN:HB3	1.78	0.49
3:I:428:THR:HG23	3:I:433:GLY:HA3	1.93	0.49
3:I:535:ARG:HB3	3:I:541:LEU:HD11	1.95	0.49
3:I:810:THR:OG1	3:I:811:GLU:N	2.42	0.49
5:X:105:MET:HG3	5:X:384:LEU:HD12	1.93	0.49
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.46	0.49
2:C:513:GLN:HG2	6:C:1401:1RM:C34	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:355:ILE:HG12	3:D:464:ASP:O	2.13	0.49
3:D:44:ILE:HG22	5:X:450:ILE:HG22	1.94	0.49
3:D:762:ASN:OD1	3:D:764:ARG:HB3	2.13	0.49
3:D:919:ALA:O	3:D:923:ILE:HG12	2.12	0.49
2:H:1289:GLU:HG3	2:H:1290:MET:N	2.28	0.49
2:H:735:LYS:HA	2:H:748:ILE:HA	1.95	0.49
2:H:699:LEU:HD23	2:H:799:ASN:CG	2.33	0.49
3:I:349:TYR:HE2	3:I:379:PRO:HG2	1.77	0.49
5:Y:290:LEU:O	5:Y:294:GLN:HB3	2.13	0.49
1:A:243:LYS:HD3	1:A:243:LYS:N	2.28	0.48
2:C:611:GLU:CG	2:C:616:ILE:HD11	2.43	0.48
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.24	0.48
3:D:1145:PHE:HB3	3:D:1309:ILE:HD13	1.95	0.48
1:F:207:THR:HG23	1:F:209:GLY:H	1.77	0.48
3:I:140:TYR:OH	3:I:312:ARG:NH1	2.41	0.48
3:I:161:THR:HG22	3:I:162:GLU:H	1.78	0.48
3:I:425:ARG:HG2	3:I:427:PRO:HD2	1.95	0.48
3:D:118:LYS:NZ	5:X:43:ASP:OD2	2.41	0.48
2:C:493:ILE:O	5:X:472:GLN:NE2	2.45	0.48
5:Y:543:ALA:O	5:Y:547:VAL:HG23	2.13	0.48
1:A:243:LYS:HZ2	1:A:243:LYS:HB2	1.78	0.48
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.48	0.48
2:C:812:PHE:H	2:C:815:SER:HB2	1.77	0.48
3:D:1205:GLU:HB2	3:D:1208:ASP:OD1	2.12	0.48
3:D:138:VAL:O	3:D:143:SER:HB3	2.12	0.48
3:D:227:PHE:O	3:D:230:SER:OG	2.24	0.48
3:D:609:TYR:HA	3:D:617:THR:OG1	2.13	0.48
3:D:50:LYS:HD3	3:D:71:LEU:HD11	1.93	0.48
2:H:1146:GLN:NE2	2:H:1160:ASP:HB2	2.28	0.48
2:H:646:SER:HB2	2:H:649:GLN:HG3	1.95	0.48
2:H:1335:ILE:CD1	3:I:22:ILE:HD11	2.43	0.48
3:I:238:ILE:HG13	3:I:238:ILE:O	2.14	0.48
5:Y:459:THR:O	5:Y:463:LEU:HD13	2.13	0.48
2:C:1146:GLN:CD	2:C:1160:ASP:HB2	2.33	0.48
2:C:510:GLN:O	2:C:511:LEU:HB2	2.13	0.48
3:D:1195:GLN:OE1	3:D:1195:GLN:N	2.46	0.48
3:D:197:GLU:O	3:D:201:LEU:HD23	2.12	0.48
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.96	0.48
4:E:39:VAL:HG13	4:E:40:PRO:HD2	1.93	0.48
1:G:183:ILE:HD11	1:G:205:MET:HE2	1.95	0.48
2:H:812:PHE:H	2:H:815:SER:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:888:THR:O	2:H:914:LYS:N	2.40	0.48
3:I:202:ARG:O	3:I:206:ASN:ND2	2.41	0.48
3:I:614:LEU:HG	4:J:7:GLN:HG3	1.95	0.48
2:C:1106:ARG:O	2:C:1108:ASN:N	2.43	0.48
2:C:514:PHE:HB2	6:C:1401:IRM:O8	2.12	0.48
5:X:384:LEU:O	5:X:384:LEU:HD13	2.13	0.48
1:A:244:GLU:HB2	1:A:246:LYS:NZ	2.28	0.48
2:C:667:LEU:O	2:C:1069:ARG:NH2	2.46	0.48
2:C:51:ALA:C	2:C:53:PHE:H	2.17	0.48
2:C:13:LYS:NZ	2:C:793:GLU:OE1	2.35	0.48
3:D:1284:ARG:NH2	3:I:1292:LEU:HD11	2.27	0.48
3:D:646:ILE:HD12	3:D:646:ILE:O	2.14	0.48
2:C:1104:PRO:HG3	3:D:725:MET:SD	2.53	0.48
4:E:44:ASP:HB2	4:E:49:ILE:HD11	1.96	0.48
1:G:86:LYS:NZ	3:I:526:VAL:O	2.47	0.48
2:H:13:LYS:CE	2:H:1183:ALA:HB2	2.37	0.48
2:H:297:VAL:HB	2:H:317:LEU:HD21	1.95	0.48
2:H:387:ASN:HB3	2:H:394:ARG:HG3	1.94	0.48
2:H:59:ILE:HD13	2:H:479:LEU:HD12	1.95	0.48
3:I:589:TYR:O	3:I:591:ILE:HG13	2.14	0.48
3:I:608:CYS:O	3:I:612:LEU:HB2	2.13	0.48
3:I:856:ILE:HG13	3:I:857:LEU:O	2.13	0.48
5:X:582:VAL:HG11	5:X:586:ARG:HG2	1.94	0.48
5:X:600:HIS:H	5:X:601:PRO:CD	2.26	0.48
1:A:44:ARG:HA	1:A:183:ILE:HG21	1.95	0.48
2:C:1272:GLU:HA	2:C:1275:VAL:HG22	1.95	0.48
2:C:224:PHE:CG	2:C:347:ILE:HG13	2.49	0.48
2:C:453:ILE:HG22	2:C:585:GLY:O	2.13	0.48
2:C:933:VAL:HG12	2:C:948:ILE:CD1	2.33	0.48
3:D:800:LEU:O	3:D:803:VAL:HG12	2.12	0.48
3:D:850:LYS:HD2	3:D:851:PRO:CD	2.35	0.48
2:H:1186:VAL:HG13	2:H:1187:PHE:N	2.28	0.48
3:I:1205:GLU:HB2	3:I:1208:ASP:OD1	2.14	0.48
3:I:482:ALA:C	3:I:483:LEU:HD12	2.34	0.48
3:I:762:ASN:OD1	3:I:764:ARG:HB3	2.13	0.48
5:X:354:THR:HG23	5:X:357:GLN:HB3	1.94	0.48
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.49	0.48
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.96	0.48
3:D:1251:LYS:O	3:D:1255:VAL:HG23	2.13	0.48
3:D:205:LEU:HD13	3:D:217:LEU:HA	1.96	0.48
3:D:253:VAL:HG11	5:X:523:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:541:LEU:HB2	3:D:545:HIS:CE1	2.48	0.48
2:H:1028:LYS:O	2:H:1032:LYS:HG2	2.14	0.48
2:H:106:GLU:CB	2:H:107:ARG:HA	2.43	0.48
2:H:223:LEU:HD13	2:H:426:ILE:HD13	1.95	0.48
2:H:484:LEU:HB3	2:H:486:THR:HG22	1.95	0.48
5:Y:250:LEU:O	5:Y:254:GLU:HG2	2.13	0.48
5:Y:283:GLN:CD	5:Y:343:LYS:HD2	2.34	0.48
5:Y:324:LYS:HB3	5:Y:325:PRO:HD2	1.95	0.48
5:Y:493:LYS:O	5:Y:497:VAL:HG23	2.14	0.48
5:Y:558:VAL:O	5:Y:562:ARG:HB2	2.14	0.48
1:B:18:GLN:C	1:B:20:SER:H	2.16	0.48
2:C:91:THR:HG22	2:C:139:ASN:N	2.29	0.48
2:C:963:GLU:O	2:C:967:LEU:HD13	2.13	0.48
3:D:1297:LYS:HA	3:D:1297:LYS:NZ	2.28	0.48
3:D:515:ARG:NH2	3:D:718:SER:O	2.47	0.48
6:H:1401:1RM:H26	6:H:1401:1RM:C31	2.35	0.48
2:H:839:VAL:O	2:H:886:LYS:NZ	2.32	0.48
2:H:843:THR:HB	2:H:845:LEU:CD2	2.44	0.48
3:I:136:GLU:HA	3:I:139:LEU:HD12	1.95	0.48
3:I:50:LYS:HB3	3:I:50:LYS:HZ2	1.78	0.48
5:X:133:SER:OG	5:X:365:MET:HB2	2.13	0.48
1:B:107:ILE:HD11	1:B:136:GLU:HG2	1.96	0.48
2:C:842:ASP:CB	2:C:1046:VAL:HG21	2.44	0.48
2:C:348:SER:O	2:C:352:ARG:HG3	2.13	0.48
2:C:434:ASP:HB3	2:C:439:LYS:HB2	1.96	0.48
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.95	0.48
3:D:856:ILE:HG13	3:D:857:LEU:O	2.13	0.48
3:D:918:ILE:HD11	3:D:1252:HIS:HE2	1.77	0.48
3:D:614:LEU:HG	4:E:7:GLN:HG3	1.94	0.48
2:H:963:GLU:O	2:H:967:LEU:HD13	2.13	0.48
3:I:619:ILE:O	3:I:623:GLN:HG2	2.14	0.48
3:I:700:ASN:O	3:I:704:GLU:HG2	2.14	0.48
5:X:145:LEU:HD21	5:X:225:ARG:HE	1.79	0.48
5:Y:316:PHE:HZ	5:Y:334:SER:HA	1.79	0.48
2:C:1238:LEU:HD12	2:C:1239:VAL:O	2.13	0.48
2:C:1064:ASP:OD1	2:C:1239:VAL:HG23	2.14	0.48
2:C:494:ASN:OD1	2:C:495:ALA:N	2.46	0.48
2:C:639:LYS:HA	2:C:639:LYS:HE2	1.96	0.48
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.96	0.48
2:H:989:LEU:HG	2:H:990:ASP:H	1.79	0.48
3:I:394:ILE:CG2	5:Y:536:THR:HG22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:413:ASP:HA	3:I:416:ILE:HD12	1.95	0.48
3:I:609:TYR:HD1	3:I:610:ARG:HD2	1.78	0.48
1:B:151:GLY:O	1:B:177:TYR:HB2	2.14	0.47
2:C:105:TYR:HA	2:C:106:GLU:HB2	1.95	0.47
2:C:1186:VAL:HG13	2:C:1187:PHE:N	2.29	0.47
2:C:18:ARG:HG3	2:C:19:PRO:HD2	1.96	0.47
2:C:403:MET:HE1	2:C:584:TYR:CD1	2.48	0.47
3:D:120:LEU:HG	5:X:46:GLN:NE2	2.29	0.47
3:D:1297:LYS:HA	3:D:1297:LYS:HZ2	1.79	0.47
3:D:412:LEU:O	3:D:416:ILE:HD12	2.13	0.47
4:E:82:ALA:O	4:E:86:ILE:HG13	2.13	0.47
1:G:12:ARG:H	1:G:30:PRO:HG2	1.79	0.47
1:G:149:GLY:HA3	1:G:177:TYR:CE2	2.49	0.47
2:H:442:VAL:HG12	2:H:443:ASP:H	1.79	0.47
3:I:205:LEU:CD2	3:I:217:LEU:HD22	2.39	0.47
5:X:507:MET:HB3	5:X:520:GLY:HA3	1.96	0.47
5:Y:139:GLU:HG3	5:Y:351:THR:HA	1.95	0.47
2:C:1209:GLN:O	2:C:1210:ILE:HG13	2.14	0.47
2:C:943:LYS:O	2:C:947:GLU:HG2	2.13	0.47
3:D:105:ILE:HD13	3:D:273:ILE:CD1	2.43	0.47
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.48	0.47
3:D:840:LEU:O	3:D:840:LEU:HD12	2.14	0.47
2:H:1252:SER:HB3	2:H:1259:LEU:CD2	2.44	0.47
1:F:134:THR:HG21	2:H:727:VAL:O	2.14	0.47
3:I:660:GLU:O	3:I:664:ILE:HG12	2.13	0.47
5:Y:262:VAL:HG13	5:Y:263:PRO:CD	2.43	0.47
5:Y:390:ILE:HD11	5:Y:435:ILE:HG22	1.96	0.47
5:Y:546:ASP:HB3	5:Y:603:ARG:NH2	2.28	0.47
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.29	0.47
3:D:238:ILE:HG13	3:D:238:ILE:O	2.13	0.47
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.96	0.47
2:H:639:LYS:HE2	2:H:639:LYS:HA	1.95	0.47
2:H:71:VAL:O	2:H:72:SER:OG	2.25	0.47
3:I:840:LEU:HD12	3:I:840:LEU:O	2.15	0.47
2:C:227:LYS:NZ	2:C:334:GLU:OE2	2.42	0.47
2:C:342:ASP:HA	2:C:437:ASN:HB3	1.95	0.47
2:C:442:VAL:HG12	2:C:443:ASP:H	1.79	0.47
2:C:529:ARG:HB2	2:C:529:ARG:NH1	2.27	0.47
3:D:573:THR:CG2	3:D:576:ARG:HG3	2.44	0.47
1:G:29:GLU:HA	1:G:200:LYS:HB2	1.96	0.47
2:H:163:LYS:CD	2:H:163:LYS:H	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:365:GLU:OE2	2:H:368:ARG:NH2	2.48	0.47
2:H:698:PRO:HB3	2:H:1231:TYR:CZ	2.50	0.47
2:H:812:PHE:CD2	2:H:813:GLU:HG3	2.48	0.47
2:H:975:ILE:HD13	2:H:975:ILE:O	2.13	0.47
1:A:318:LEU:HD13	1:A:318:LEU:N	2.29	0.47
2:C:1180:MET:HB3	2:C:1181:PRO:HA	1.95	0.47
2:C:989:LEU:HG	2:C:990:ASP:H	1.79	0.47
3:D:1174:ARG:HA	3:D:1192:LYS:HG3	1.96	0.47
3:D:114:ILE:HG21	3:D:308:ASP:HB3	1.96	0.47
2:H:924:VAL:HG12	2:H:1058:ARG:HH22	1.80	0.47
2:H:868:SER:OG	2:H:942:ASP:OD1	2.28	0.47
3:I:811:GLU:OE2	3:I:890:THR:OG1	2.28	0.47
1:A:54:CYS:SG	1:A:148:ARG:HD3	2.54	0.47
1:B:118:ASP:HB3	1:B:121:VAL:HB	1.96	0.47
1:B:19:VAL:O	1:B:20:SER:CB	2.63	0.47
2:C:131:THR:HG23	2:C:133:ASN:N	2.28	0.47
2:C:510:GLN:HG3	2:C:535:PRO:HD3	1.96	0.47
2:C:845:LEU:HD23	2:C:889:PRO:HG2	1.97	0.47
3:D:395:LYS:NZ	5:X:607:LEU:O	2.45	0.47
2:H:130:MET:HG3	2:H:134:GLY:HA2	1.97	0.47
2:H:263:VAL:HG22	2:H:273:HIS:CD2	2.48	0.47
3:I:1347:LEU:O	3:I:1351:VAL:HG23	2.14	0.47
3:I:425:ARG:NH2	3:I:464:ASP:OD2	2.47	0.47
3:I:545:HIS:HB2	3:I:546:ALA:CB	2.43	0.47
3:I:773:PHE:O	3:I:776:THR:HG22	2.13	0.47
2:C:689:ALA:HB2	2:C:1233:LEU:HD22	1.96	0.47
2:C:127:ILE:HG12	2:C:127:ILE:O	2.14	0.47
2:C:843:THR:HB	2:C:845:LEU:CD2	2.45	0.47
3:D:451:PRO:HG2	3:D:625:MET:SD	2.54	0.47
3:D:63:GLY:O	3:D:98:ARG:NH2	2.47	0.47
1:F:60:GLU:HG3	1:F:169:GLY:O	2.14	0.47
2:H:1303:LYS:HE2	2:H:1303:LYS:HA	1.97	0.47
2:H:1327:LEU:HA	2:H:1337:ILE:HD11	1.95	0.47
2:H:714:VAL:CG2	2:H:787:PRO:HD2	2.45	0.47
3:I:145:VAL:HG21	3:I:165:TYR:CD2	2.49	0.47
3:I:393:THR:HG23	3:I:396:ALA:H	1.79	0.47
3:I:370:LYS:HA	3:I:441:LEU:HD12	1.97	0.47
3:I:473:THR:HB	3:I:476:ALA:HB2	1.97	0.47
3:I:822:MET:HG2	3:I:839:VAL:CG2	2.44	0.47
3:D:137:ARG:CZ	5:X:95:THR:HG23	2.44	0.47
2:C:1285:TYR:CG	3:D:475:GLU:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1401:IRM:H	5:X:515:GLU:HB2	1.95	0.47
2:C:59:ILE:HD13	2:C:479:LEU:HD22	1.96	0.47
2:C:91:THR:HB	2:C:138:ILE:HD13	1.96	0.47
2:H:578:TYR:CD2	2:H:659:GLN:HA	2.49	0.47
2:H:699:LEU:H	2:H:799:ASN:HD21	1.62	0.47
2:H:979:LEU:HD12	2:H:1002:LEU:HD23	1.97	0.47
3:I:194:LEU:O	3:I:198:CYS:HB2	2.15	0.47
3:I:797:THR:O	3:I:801:VAL:HG23	2.14	0.47
3:I:832:LYS:HZ2	3:I:832:LYS:HB2	1.79	0.47
5:X:333:VAL:HG22	5:X:336:GLU:HB2	1.95	0.47
2:C:122:VAL:HG22	2:C:123:TYR:N	2.29	0.47
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.80	0.47
2:C:1219:GLU:OE2	3:D:634:ARG:NH1	2.47	0.47
3:D:914:ALA:O	3:D:918:ILE:HG22	2.15	0.47
3:I:292:VAL:O	3:I:296:LYS:HG3	2.15	0.47
3:I:66:LYS:HG3	3:I:69:GLU:OE2	2.14	0.47
3:I:707:ILE:HD11	3:I:716:GLN:HG3	1.97	0.47
5:Y:245:ALA:O	5:Y:249:ILE:HG13	2.15	0.47
2:C:17:LYS:HG2	2:C:1155:VAL:HG11	1.97	0.47
2:C:1276:TRP:CE3	2:C:1276:TRP:HA	2.50	0.47
3:D:275:ARG:HD2	3:D:302:ALA:HB2	1.97	0.47
3:D:533:ALA:HB2	3:D:578:ILE:HD13	1.96	0.47
3:D:700:ASN:O	3:D:704:GLU:HG2	2.15	0.47
3:D:824:PRO:O	3:D:826:ILE:HG13	2.14	0.47
2:H:488:MET:H	2:H:489:PRO:HA	1.79	0.47
3:I:646:ILE:HD12	3:I:646:ILE:O	2.14	0.47
5:X:119:ILE:HD12	5:X:122:ARG:HH21	1.80	0.47
1:A:158:ARG:HE	1:A:172:LEU:HD13	1.79	0.47
2:C:102:LEU:HB3	2:C:117:ILE:HD11	1.97	0.47
3:D:1173:ARG:CZ	3:D:1176:VAL:HG21	2.45	0.47
3:D:918:ILE:HD11	3:D:1252:HIS:NE2	2.30	0.47
3:D:1287:ILE:HA	3:D:1290:ARG:HG2	1.96	0.47
3:D:139:LEU:HD22	3:D:139:LEU:O	2.15	0.47
3:D:620:PHE:O	3:D:624:ILE:HG23	2.14	0.47
3:D:655:SER:O	3:D:658:GLU:HG2	2.14	0.47
2:H:1223:ARG:HG3	2:H:1224:PRO:HD2	1.97	0.47
2:H:500:ALA:O	2:H:504:GLU:HB2	2.15	0.47
3:I:1215:GLU:OE1	3:I:1224:ARG:NH2	2.47	0.47
3:I:166:LEU:HD12	3:I:167:ASP:N	2.29	0.47
3:I:205:LEU:HB3	3:I:217:LEU:HB3	1.97	0.47
3:I:481:ARG:HG2	4:J:6:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:253:SER:O	5:Y:257:LYS:HG3	2.14	0.47
5:Y:428:SER:O	5:Y:432:THR:OG1	2.27	0.47
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.97	0.46
2:C:634:VAL:HG22	2:C:645:PHE:HE2	1.80	0.46
2:C:71:VAL:O	2:C:72:SER:OG	2.28	0.46
3:D:1346:GLY:O	3:D:1350:ASN:HB2	2.15	0.46
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.97	0.46
3:I:19:ALA:HB1	3:I:1343:GLU:HB3	1.97	0.46
3:I:217:LEU:O	3:I:221:ILE:HG12	2.14	0.46
5:X:17:LYS:NZ	5:X:17:LYS:HB3	2.30	0.46
5:Y:316:PHE:CZ	5:Y:334:SER:HA	2.49	0.46
3:D:166:LEU:HD12	3:D:167:ASP:N	2.31	0.46
3:D:377:PHE:O	3:D:381:ILE:HG13	2.15	0.46
3:D:704:GLU:HB2	3:D:718:SER:HG	1.79	0.46
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.98	0.46
2:H:106:GLU:HB3	2:H:107:ARG:CA	2.45	0.46
2:H:524:ILE:HD12	2:H:708:VAL:HG13	1.97	0.46
3:I:262:THR:OG1	3:I:266:ASN:ND2	2.30	0.46
3:I:390:LEU:HD21	3:I:407:VAL:HG11	1.97	0.46
1:A:107:ILE:HG12	1:A:134:THR:O	2.16	0.46
2:C:236:LYS:HE3	2:C:238:GLN:HE21	1.80	0.46
2:C:97:ARG:HA	2:C:122:VAL:O	2.15	0.46
2:H:514:PHE:HB2	6:H:1401:1RM:O8	2.14	0.46
2:H:632:ASP:O	2:H:633:LEU:HD23	2.16	0.46
2:H:634:VAL:HG22	2:H:645:PHE:CZ	2.50	0.46
3:I:233:LYS:HD2	3:I:234:PRO:HD2	1.98	0.46
5:X:448:ARG:NH1	5:X:452:ILE:HD12	2.31	0.46
5:X:459:THR:O	5:X:463:LEU:HD13	2.15	0.46
1:B:31:LEU:HB2	1:B:199:ASP:O	2.15	0.46
2:C:1165:SER:O	2:C:1168:GLU:HB3	2.16	0.46
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.50	0.46
3:D:362:ARG:HD2	3:D:364:HIS:HE1	1.81	0.46
2:H:106:GLU:H	2:H:107:ARG:HA	1.81	0.46
2:H:1105:SER:HB2	3:I:731:ARG:HD3	1.96	0.46
2:H:1301:ARG:HG3	2:H:1302:THR:N	2.30	0.46
3:I:141:PHE:O	3:I:297:ARG:HD3	2.15	0.46
3:I:596:LEU:HD23	3:I:596:LEU:N	2.30	0.46
5:Y:448:ARG:HD2	5:Y:452:ILE:HD12	1.98	0.46
5:Y:449:THR:OG1	5:Y:503:GLU:O	2.34	0.46
5:Y:576:VAL:HG12	5:Y:587:ILE:HG12	1.97	0.46
1:A:321:TRP:HA	1:A:322:PRO:HA	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:VAL:HG12	1:B:76:GLU:H	1.81	0.46
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.98	0.46
2:C:43:PRO:HD3	2:C:47:TYR:CE2	2.50	0.46
3:D:1369:ARG:HH11	3:D:1369:ARG:HB3	1.80	0.46
3:D:514:THR:HG21	3:D:595:ALA:O	2.15	0.46
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.97	0.46
3:D:583:VAL:CG1	3:D:584:PRO:HD2	2.46	0.46
1:G:227:GLN:C	1:G:228:LEU:HD23	2.36	0.46
1:F:150:ARG:HD2	1:G:8:PHE:CZ	2.51	0.46
2:H:1133:LYS:HG3	2:H:1134:GLN:HG3	1.97	0.46
2:H:1255:THR:HG22	2:H:1257:GLN:HG3	1.98	0.46
3:I:1322:ALA:HB1	3:I:1326:GLN:NE2	2.30	0.46
5:Y:582:VAL:HB	5:Y:586:ARG:HG2	1.97	0.46
1:B:149:GLY:HA3	1:B:177:TYR:CE2	2.49	0.46
3:D:1297:LYS:HE3	3:I:1267:VAL:HB	1.97	0.46
3:D:161:THR:HG22	3:D:162:GLU:H	1.79	0.46
3:D:797:THR:O	3:D:801:VAL:HG23	2.15	0.46
3:D:909:ILE:O	3:D:909:ILE:HD12	2.16	0.46
1:G:110:VAL:HB	1:G:131:CYS:HB2	1.96	0.46
2:H:91:THR:HG22	2:H:139:ASN:N	2.30	0.46
2:H:551:HIS:CG	2:H:552:PRO:HD2	2.50	0.46
2:H:756:TYR:H	2:H:766:ASN:CB	2.27	0.46
2:H:998:LEU:O	2:H:998:LEU:HD13	2.16	0.46
3:I:265:LEU:HD11	3:I:330:MET:SD	2.56	0.46
3:I:494:ALA:HA	3:I:1252:HIS:HE1	1.80	0.46
3:I:8:LEU:N	3:I:8:LEU:HD23	2.31	0.46
5:X:316:PHE:CZ	5:X:334:SER:HA	2.51	0.46
5:Y:126:GLY:O	5:Y:130:VAL:HG23	2.15	0.46
1:A:11:PRO:HA	1:A:30:PRO:O	2.16	0.46
1:A:218:ARG:NH1	1:B:233:ASP:OD2	2.48	0.46
2:C:1233:LEU:O	2:C:1233:LEU:HD12	2.15	0.46
2:C:1276:TRP:HE3	2:C:1276:TRP:HA	1.80	0.46
2:C:15:PHE:CD2	2:C:1182:ILE:HD11	2.51	0.46
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.98	0.46
2:C:740:GLU:HB2	2:C:741:MET:SD	2.56	0.46
3:D:122:SER:HB2	3:D:132:LEU:HD13	1.97	0.46
3:D:292:VAL:HG22	3:D:296:LYS:HE3	1.97	0.46
3:D:396:ALA:CB	5:X:606:VAL:HG11	2.46	0.46
3:D:8:LEU:HD23	3:D:8:LEU:N	2.30	0.46
3:I:139:LEU:HD22	3:I:139:LEU:O	2.15	0.46
3:I:205:LEU:HD22	3:I:217:LEU:CD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:119:ILE:O	5:X:123:ILE:HG13	2.15	0.46
3:D:286:ALA:HB3	5:X:413:MET:SD	2.55	0.46
5:X:465:ARG:O	5:X:468:ARG:HG2	2.15	0.46
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.16	0.46
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.51	0.46
2:C:1254:VAL:O	3:D:99:ARG:NH1	2.46	0.46
1:F:190:ALA:HB2	1:F:200:LYS:CB	2.46	0.46
2:H:1006:GLU:H	2:H:1006:GLU:CD	2.19	0.46
2:H:337:PHE:O	2:H:338:THR:OG1	2.26	0.46
3:I:1145:PHE:CE2	3:I:1256:ILE:HD11	2.51	0.46
3:I:492:SER:HB2	3:I:499:ILE:HB	1.97	0.46
3:I:766:GLY:C	3:I:767:LEU:HD22	2.36	0.46
5:X:346:GLN:O	5:X:350:GLU:HG3	2.15	0.46
5:Y:286:LEU:HD23	5:Y:340:ALA:HB2	1.96	0.46
5:Y:484:ALA:HB1	5:Y:490:PRO:O	2.16	0.46
5:Y:546:ASP:HB3	5:Y:603:ARG:HH22	1.79	0.46
1:B:180:VAL:HG11	1:B:183:ILE:HG12	1.98	0.46
2:C:11:ILE:HD11	2:C:1181:PRO:HD3	1.98	0.46
2:C:11:ILE:HD13	2:C:697:LYS:CE	2.46	0.46
2:C:1223:ARG:HD2	3:D:637:ALA:HA	1.97	0.46
2:C:1254:VAL:HG23	2:C:1255:THR:N	2.29	0.46
1:G:191:ARG:NH2	3:I:442:ILE:HA	2.31	0.46
1:G:9:LEU:H	1:G:9:LEU:HD23	1.81	0.46
2:H:999:GLU:HG2	2:H:1000:LEU:H	1.81	0.46
2:H:1209:GLN:O	2:H:1210:ILE:HG13	2.16	0.46
3:I:1169:THR:HA	3:I:1173:ARG:HB3	1.98	0.46
3:I:1171:GLY:N	3:I:1172:LYS:O	2.48	0.46
3:I:522:GLY:HA2	3:I:545:HIS:CD2	2.51	0.46
5:X:250:LEU:O	5:X:254:GLU:HG2	2.15	0.46
2:C:1214:ASP:HA	2:C:1221:PHE:CZ	2.51	0.46
3:D:482:ALA:C	3:D:483:LEU:HD12	2.35	0.46
3:D:508:LEU:HD22	3:D:508:LEU:O	2.16	0.46
2:H:1081:PRO:HB2	2:H:1083:GLU:HG2	1.98	0.46
2:H:122:VAL:HG13	2:H:124:MET:HG3	1.98	0.46
2:H:91:THR:HB	2:H:138:ILE:HD13	1.98	0.46
2:H:589:THR:HG23	2:H:591:TYR:CE2	2.51	0.46
3:I:149:GLY:HA2	3:I:156:ARG:HG2	1.98	0.46
3:I:377:PHE:O	3:I:381:ILE:HG13	2.16	0.46
3:I:909:ILE:O	3:I:909:ILE:HD12	2.16	0.46
5:Y:119:ILE:O	5:Y:123:ILE:HG13	2.16	0.46
3:I:260:PHE:O	5:Y:504:PRO:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:HB2	1:A:30:PRO:HG2	1.98	0.45
1:A:300:LEU:O	1:A:300:LEU:HD13	2.16	0.45
1:B:16:ILE:HG12	1:B:26:VAL:HG22	1.98	0.45
1:B:61:ILE:HB	1:B:64:VAL:HB	1.98	0.45
2:C:170:VAL:O	2:C:171:LEU:HB2	2.15	0.45
3:D:145:VAL:HG22	3:D:180:MET:SD	2.57	0.45
3:D:619:ILE:O	3:D:623:GLN:HG2	2.15	0.45
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.51	0.45
2:C:560:PRO:HB2	3:D:776:THR:OG1	2.16	0.45
2:H:178:PRO:HA	2:H:397:LEU:HD23	1.98	0.45
2:H:902:LEU:HD11	5:Y:608:ARG:HA	1.97	0.45
3:I:1184:ASP:HA	3:I:1185:PRO:HD3	1.71	0.45
3:I:37:GLU:HB2	3:I:104:HIS:CE1	2.51	0.45
5:X:123:ILE:O	5:X:127:ILE:HG12	2.17	0.45
5:X:9:LEU:HD22	5:X:60:PRO:HB3	1.98	0.45
2:C:57:PHE:CE1	2:C:472:GLU:HA	2.50	0.45
3:D:526:VAL:HG12	3:D:549:LYS:O	2.15	0.45
2:H:607:SER:H	2:H:610:GLU:HB2	1.81	0.45
2:H:766:ASN:H	2:H:787:PRO:HG3	1.80	0.45
2:H:840:SER:HB3	2:H:850:ILE:HD11	1.98	0.45
3:I:264:ASP:OD2	3:I:324:LEU:HD12	2.17	0.45
3:I:767:LEU:HB3	3:I:771:GLN:HE22	1.80	0.45
1:B:22:THR:HG22	1:B:208:ASN:O	2.16	0.45
2:C:216:THR:O	2:C:220:ILE:HG13	2.16	0.45
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.51	0.45
3:D:169:LEU:HD13	3:D:173:GLY:HA3	1.98	0.45
3:D:549:LYS:HG2	3:D:571:ASP:OD1	2.16	0.45
3:D:77:ARG:HD2	3:D:77:ARG:HA	1.73	0.45
2:H:1238:LEU:HD12	2:H:1239:VAL:O	2.15	0.45
2:H:994:ARG:N	2:H:994:ARG:HD3	2.30	0.45
3:I:886:VAL:HG13	3:I:1230:THR:HG21	1.98	0.45
3:I:275:ARG:HD3	3:I:298:MET:HB3	1.97	0.45
4:J:65:ASP:O	4:J:69:ARG:HG3	2.16	0.45
5:X:310:GLU:O	5:X:344:LEU:HD23	2.16	0.45
5:Y:271:ASN:O	5:Y:275:VAL:HG23	2.16	0.45
5:Y:561:MET:HA	5:Y:567:MET:SD	2.57	0.45
2:C:130:MET:CG	2:C:134:GLY:HA2	2.47	0.45
2:C:590:PRO:HB3	2:C:605:TYR:CE1	2.51	0.45
3:D:915:ILE:O	3:D:918:ILE:HG23	2.15	0.45
1:G:227:GLN:O	1:G:229:GLU:N	2.50	0.45
2:H:706:ARG:HA	2:H:793:GLU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:242:HIS:HA	5:X:245:ALA:HB3	1.98	0.45
1:A:158:ARG:NH2	1:A:162:GLU:HB3	2.31	0.45
1:A:222:THR:O	1:A:226:GLU:HG3	2.17	0.45
2:C:92:TYR:HD1	2:C:129:LEU:HB2	1.80	0.45
3:D:217:LEU:O	3:D:221:ILE:HG12	2.15	0.45
3:D:818:GLU:HA	3:D:881:LYS:HE2	1.99	0.45
2:H:1087:TYR:CE2	2:H:1215:GLY:HA2	2.48	0.45
2:H:1304:MET:O	2:H:1308:ILE:HG13	2.16	0.45
2:H:908:GLU:H	2:H:908:GLU:CD	2.20	0.45
2:H:946:LEU:O	2:H:949:GLU:HG3	2.15	0.45
3:I:1280:VAL:HG11	3:I:1304:ARG:NE	2.23	0.45
2:H:1287:LEU:HD23	3:I:1357:ILE:HG12	1.98	0.45
3:I:313:GLY:O	3:I:314:ARG:HB2	2.16	0.45
3:I:858:VAL:CB	3:I:859:PRO:HD3	2.25	0.45
4:J:15:ASN:ND2	4:J:18:ASP:H	2.09	0.45
5:X:271:ASN:O	5:X:275:VAL:HG23	2.16	0.45
1:A:45:ARG:HH22	2:C:1216:ARG:CA	2.24	0.45
1:B:232:VAL:O	1:B:233:ASP:HB2	2.16	0.45
2:C:11:ILE:HD13	2:C:697:LYS:HE3	1.99	0.45
2:C:1292:THR:OG1	2:C:1293:VAL:N	2.47	0.45
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.98	0.45
3:D:112:ALA:HA	3:D:238:ILE:HG22	1.98	0.45
3:D:1148:ARG:HB2	3:D:1148:ARG:NH2	2.32	0.45
3:D:133:ARG:NH2	3:D:133:ARG:HB2	2.32	0.45
3:D:527:LEU:HB2	3:D:535:ARG:CZ	2.47	0.45
2:H:131:THR:HG23	2:H:133:ASN:N	2.27	0.45
2:H:572:ILE:HD13	6:H:1401:1RM:C1	2.47	0.45
2:H:549:ASP:OD1	2:H:550:VAL:N	2.49	0.45
3:I:502:PRO:HB3	3:I:506:VAL:CG1	2.47	0.45
3:I:767:LEU:HB3	3:I:771:GLN:NE2	2.32	0.45
5:X:311:THR:HG21	5:X:348:GLU:CD	2.37	0.45
3:D:291:ILE:HD11	5:X:384:LEU:HD21	1.98	0.45
5:Y:295:CYS:SG	5:Y:330:LEU:HD23	2.56	0.45
5:Y:596:ARG:HE	5:Y:596:ARG:HA	1.81	0.45
1:A:289:LEU:HD11	1:A:314:LEU:HD11	1.98	0.45
2:C:1314:GLN:HG3	4:E:28:ARG:NH1	2.31	0.45
2:C:197:ARG:NH1	2:C:201:ARG:O	2.49	0.45
2:C:929:ILE:HG12	2:C:1053:TYR:O	2.17	0.45
3:D:120:LEU:CD2	3:D:1330:ARG:HD2	2.46	0.45
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.52	0.45
3:D:697:MET:SD	3:D:741:ALA:HB3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1111:GLN:HE21	2:H:1230:MET:HE1	1.81	0.45
2:H:489:PRO:HB2	2:H:492:MET:CB	2.40	0.45
2:H:842:ASP:HB2	2:H:1046:VAL:HG11	1.99	0.45
3:I:1194:ARG:HD2	3:I:1194:ARG:N	2.32	0.45
3:I:1238:GLN:O	3:I:1242:ARG:HG2	2.17	0.45
3:I:1287:ILE:HA	3:I:1290:ARG:HG2	1.99	0.45
3:I:147:ILE:HD12	3:I:178:ALA:CB	2.46	0.45
3:I:56:LEU:HB3	3:I:250:ARG:HH21	1.80	0.45
3:I:412:LEU:O	3:I:415:VAL:HG22	2.17	0.45
3:I:697:MET:SD	3:I:741:ALA:HB3	2.57	0.45
5:X:543:ALA:O	5:X:547:VAL:HG23	2.16	0.45
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.98	0.45
3:D:269:TYR:HA	3:D:272:VAL:HG12	1.98	0.45
3:D:573:THR:HG23	3:D:576:ARG:H	1.81	0.45
3:D:905:ARG:HH12	4:E:10:VAL:HG12	1.81	0.45
2:H:170:VAL:O	2:H:171:LEU:HB2	2.17	0.45
3:I:147:ILE:HD12	3:I:178:ALA:HB2	1.98	0.45
3:I:194:LEU:HD21	3:I:234:PRO:HG3	1.98	0.45
3:I:370:LYS:HG3	3:I:371:LYS:H	1.82	0.45
3:I:679:TYR:CZ	3:I:683:ILE:HD11	2.52	0.45
5:X:357:GLN:NE2	5:X:360:ASP:OD2	2.50	0.45
1:A:158:ARG:HB2	1:A:158:ARG:HH21	1.82	0.45
1:A:184:ALA:HB2	2:C:1091:GLY:N	2.32	0.45
2:C:751:TYR:CE1	2:C:783:LEU:HD12	2.51	0.45
3:D:269:TYR:CG	3:D:306:LEU:HD11	2.52	0.45
3:D:512:TYR:HD2	3:D:724:MET:HE3	1.82	0.45
2:H:1254:VAL:O	3:I:99:ARG:NH1	2.48	0.45
3:I:1269:ALA:H	3:I:1300:ALA:HB2	1.81	0.45
3:I:513:MET:HE2	3:I:579:LEU:HB2	1.99	0.45
3:I:850:LYS:HD2	3:I:851:PRO:CD	2.29	0.45
5:Y:113:ARG:O	5:Y:117:ILE:HD13	2.16	0.45
2:C:452:ARG:HH22	2:C:458:GLU:CD	2.20	0.45
3:D:313:GLY:O	3:D:314:ARG:HB2	2.17	0.45
3:D:368:LEU:HG	3:D:373:ALA:HB2	1.99	0.45
3:D:424:ASN:HB2	3:D:434:ILE:HG13	1.99	0.45
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.99	0.45
2:H:207:THR:O	2:H:211:ARG:HG3	2.17	0.45
2:H:42:ASP:HB2	2:H:47:TYR:CG	2.51	0.45
2:H:53:PHE:HA	2:H:56:VAL:HG23	1.99	0.45
2:H:51:ALA:C	2:H:53:PHE:H	2.19	0.45
3:I:147:ILE:HG23	3:I:156:ARG:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:539:SER:OG	3:I:540:GLY:N	2.47	0.45
1:A:90:VAL:HG13	1:A:121:VAL:HG13	2.00	0.44
2:C:1284:ALA:HA	3:D:1357:ILE:HD13	1.99	0.44
2:C:1303:LYS:HE2	2:C:1303:LYS:HA	1.98	0.44
2:C:170:VAL:HG23	2:C:171:LEU:N	2.24	0.44
3:D:1274:PHE:HD2	3:D:1275:LEU:HG	1.81	0.44
3:D:596:LEU:N	3:D:596:LEU:HD23	2.32	0.44
3:D:703:THR:O	3:D:718:SER:N	2.50	0.44
1:G:179:PRO:HB2	1:G:211:ILE:HG22	1.99	0.44
2:H:67:GLU:HG2	2:H:103:VAL:HG12	1.99	0.44
2:H:1233:LEU:O	2:H:1233:LEU:HD12	2.17	0.44
2:H:1254:VAL:HG23	2:H:1255:THR:N	2.29	0.44
2:H:1276:TRP:HA	2:H:1276:TRP:CE3	2.52	0.44
2:H:469:VAL:O	2:H:472:GLU:HB3	2.17	0.44
2:H:97:ARG:HA	2:H:122:VAL:O	2.17	0.44
3:I:26:SER:O	3:I:30:ILE:HG12	2.17	0.44
3:I:579:LEU:HD23	3:I:627:THR:HG21	1.98	0.44
5:Y:585:GLU:O	5:Y:589:GLN:N	2.45	0.44
1:B:37:HIS:NE2	2:C:1216:ARG:HD3	2.32	0.44
2:C:841:ARG:HA	2:C:1046:VAL:CG1	2.47	0.44
2:C:1272:GLU:HG3	2:C:1276:TRP:CE2	2.53	0.44
2:C:24:VAL:HA	2:C:25:PRO:HD3	1.82	0.44
2:C:896:THR:HG22	2:C:898:GLU:OE1	2.17	0.44
3:D:316:ILE:HD11	3:D:320:ASN:O	2.17	0.44
3:D:701:LEU:CD2	3:D:723:TYR:HB2	2.47	0.44
2:H:1276:TRP:HE3	2:H:1276:TRP:HA	1.82	0.44
2:H:1333:LEU:HB2	2:H:1335:ILE:HG22	1.99	0.44
2:H:546:GLU:O	2:H:548:ARG:N	2.45	0.44
2:H:943:LYS:O	2:H:947:GLU:HG2	2.16	0.44
3:I:681:LYS:O	3:I:685:ILE:HG13	2.18	0.44
3:I:857:LEU:HB2	3:I:860:ARG:HB2	1.99	0.44
5:X:242:HIS:O	5:X:246:GLN:HB2	2.18	0.44
5:X:470:MET:HB2	5:X:478:PRO:HB3	1.99	0.44
5:Y:408:GLY:HA2	5:Y:435:ILE:HG23	1.99	0.44
1:A:102:LEU:HD12	1:A:115:ILE:HG12	1.99	0.44
2:C:819:SER:HB2	2:C:1085:MET:SD	2.57	0.44
2:C:475:VAL:O	2:C:479:LEU:HB2	2.17	0.44
2:C:533:LEU:HD23	2:C:533:LEU:H	1.82	0.44
2:C:741:MET:SD	2:C:741:MET:N	2.90	0.44
2:C:816:ILE:HG13	2:C:1098:LEU:CD2	2.38	0.44
2:C:826:ASP:HA	2:C:829:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:SER:CB	3:D:132:LEU:HD13	2.48	0.44
3:D:355:ILE:HA	3:D:447:ILE:HG23	1.98	0.44
4:E:16:ARG:O	4:E:20:VAL:HG23	2.17	0.44
1:F:45:ARG:HG2	2:H:1083:GLU:HB2	1.99	0.44
2:H:1065:LYS:HG2	2:H:1235:LEU:HD12	1.99	0.44
2:H:105:TYR:CG	2:H:106:GLU:HB2	2.52	0.44
2:H:517:GLN:HE21	2:H:760:ASN:H	1.65	0.44
3:I:12:THR:O	3:I:13:LYS:HD2	2.17	0.44
3:I:138:VAL:O	3:I:143:SER:HB3	2.17	0.44
2:C:201:ARG:HH12	5:X:36:VAL:HG11	1.82	0.44
5:X:449:THR:HG23	5:X:503:GLU:OE1	2.18	0.44
5:Y:264:LYS:N	5:Y:264:LYS:HD2	2.30	0.44
1:A:178:SER:HA	1:A:179:PRO:HD3	1.79	0.44
2:C:429:MET:O	2:C:433:ILE:HG13	2.18	0.44
2:C:817:LEU:HB3	2:C:1097:VAL:CG1	2.46	0.44
2:H:1066:MET:HG3	2:H:1234:LYS:HA	1.99	0.44
2:H:169:LYS:HA	2:H:169:LYS:HD3	1.73	0.44
3:I:124:ILE:HG13	3:I:189:LEU:HD11	1.98	0.44
3:I:1290:ARG:HD2	3:I:1299:GLY:HA3	2.00	0.44
3:I:384:LYS:HD2	3:I:384:LYS:HA	1.84	0.44
5:X:278:ASP:O	5:X:282:THR:OG1	2.22	0.44
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.16	0.44
2:C:213:LEU:HD21	2:C:390:PHE:CZ	2.51	0.44
2:C:818:VAL:HG22	2:C:819:SER:N	2.33	0.44
3:D:105:ILE:CD1	3:D:273:ILE:HD11	2.47	0.44
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.98	0.44
3:D:746:LEU:N	3:D:746:LEU:HD22	2.33	0.44
4:E:15:ASN:OD1	4:E:17:PHE:HB2	2.17	0.44
2:H:1287:LEU:O	2:H:1291:LEU:HB2	2.17	0.44
2:H:130:MET:SD	2:H:134:GLY:HA2	2.57	0.44
1:A:14:VAL:HG21	1:A:29:GLU:HB2	1.98	0.44
1:B:192:VAL:HG21	1:B:198:LEU:CD1	2.34	0.44
1:B:9:LEU:H	1:B:9:LEU:HD23	1.83	0.44
2:C:31:GLN:HG3	2:C:130:MET:HE1	1.99	0.44
3:D:116:PHE:HB3	3:D:237:MET:CE	2.48	0.44
3:D:1184:ASP:HA	3:D:1185:PRO:HD3	1.79	0.44
3:D:1264:ALA:HB1	3:D:1303:SER:O	2.18	0.44
3:D:145:VAL:HG13	3:D:180:MET:HB3	1.99	0.44
1:G:110:VAL:HG11	1:G:140:ILE:HD11	1.99	0.44
2:H:236:LYS:HE3	2:H:238:GLN:HE21	1.83	0.44
2:H:478:ARG:CD	2:H:492:MET:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:818:VAL:HG22	2:H:819:SER:N	2.33	0.44
3:I:1180:VAL:HG22	3:I:1185:PRO:HA	1.99	0.44
3:I:413:ASP:HA	3:I:416:ILE:CD1	2.46	0.44
3:I:588:PRO:CG	3:I:591:ILE:HD11	2.48	0.44
5:X:519:LEU:HD13	5:X:519:LEU:O	2.18	0.44
5:X:52:GLY:O	5:X:53:ILE:HB	2.18	0.44
5:Y:386:LEU:O	5:Y:390:ILE:HG23	2.18	0.44
1:A:310:ARG:HA	1:A:310:ARG:NE	2.33	0.44
1:B:47:LEU:HD13	1:B:205:MET:HE2	2.00	0.44
2:C:367:TYR:CD1	2:C:384:LEU:HD13	2.52	0.44
3:D:531:LYS:NZ	3:D:531:LYS:HB3	2.33	0.44
2:H:1204:LEU:CD2	2:H:1205:PRO:HD2	2.48	0.44
2:H:1214:ASP:HB3	2:H:1218:GLY:H	1.83	0.44
2:H:578:TYR:HE2	2:H:658:GLN:HG3	1.82	0.44
3:I:1357:ILE:N	3:I:1357:ILE:HD12	2.33	0.44
3:I:510:LEU:HD12	3:I:601:ILE:CD1	2.47	0.44
3:I:77:ARG:HD2	3:I:77:ARG:HA	1.75	0.44
5:Y:234:THR:HG21	5:Y:248:GLU:OE2	2.17	0.44
5:Y:439:ILE:O	5:Y:443:ILE:HG13	2.16	0.44
2:C:1006:GLU:H	2:C:1006:GLU:CD	2.20	0.44
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.17	0.44
2:C:1204:LEU:CD2	2:C:1205:PRO:HD2	2.48	0.44
2:C:563:THR:HG21	3:D:780:ARG:CZ	2.48	0.44
2:C:591:TYR:CE1	2:C:616:ILE:HG23	2.53	0.44
3:D:1269:ALA:N	3:D:1300:ALA:HB2	2.32	0.44
3:D:165:TYR:O	3:D:169:LEU:HB2	2.17	0.44
3:D:217:LEU:O	3:D:221:ILE:HG23	2.17	0.44
3:D:704:GLU:O	3:D:705:THR:OG1	2.28	0.44
3:D:72:CYS:SG	3:D:73:GLY:N	2.91	0.44
2:H:122:VAL:HG22	2:H:123:TYR:N	2.32	0.44
2:H:170:VAL:HG23	2:H:171:LEU:N	2.29	0.44
2:H:26:TYR:HE2	2:H:28:LEU:HB2	1.81	0.44
2:H:54:ARG:N	2:H:55:SER:CB	2.75	0.44
2:H:555:TYR:HE2	2:H:616:ILE:HD13	1.83	0.44
3:I:363:LEU:HA	3:I:450:HIS:ND1	2.32	0.44
3:I:515:ARG:HH22	3:I:717:VAL:C	2.18	0.44
3:I:583:VAL:CG1	3:I:584:PRO:HD2	2.48	0.44
3:I:555:TYR:HD1	3:I:589:TYR:HE2	1.66	0.44
3:I:720:ASN:ND2	3:I:720:ASN:O	2.51	0.44
5:X:324:LYS:HB3	5:X:325:PRO:HD2	1.99	0.44
5:Y:227:GLN:HA	5:Y:230:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:HD21	2:C:1218:GLY:CA	2.31	0.44
1:B:153:VAL:O	1:B:175:ALA:N	2.50	0.44
2:C:1042:LEU:HB2	2:C:1043:ALA:H	1.68	0.44
2:C:998:LEU:HD13	2:C:998:LEU:O	2.18	0.44
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.44	0.44
3:D:50:LYS:HG2	3:D:51:PRO:CD	2.47	0.44
3:D:664:ILE:HG21	3:D:681:LYS:HD2	2.00	0.44
1:F:11:PRO:CD	1:G:227:GLN:HG3	2.48	0.44
2:H:1129:ASN:OD1	2:H:1177:ARG:NH1	2.49	0.44
2:H:342:ASP:N	2:H:342:ASP:OD1	2.46	0.44
2:H:57:PHE:CE2	2:H:472:GLU:HG3	2.53	0.44
2:H:511:LEU:HA	2:H:513:GLN:NE2	2.33	0.44
2:H:697:LYS:HG3	2:H:698:PRO:HD2	2.00	0.44
3:I:478:LEU:CD1	4:J:47:THR:HG23	2.47	0.44
5:X:130:VAL:O	5:X:134:VAL:HG23	2.18	0.44
5:X:245:ALA:O	5:X:249:ILE:HG13	2.18	0.44
1:A:299:SER:O	1:A:303:ILE:HG12	2.18	0.43
1:B:192:VAL:CG1	1:B:194:GLN:HG2	2.45	0.43
2:C:130:MET:HG3	2:C:134:GLY:HA2	2.00	0.43
2:C:310:ILE:O	2:C:311:CYS:HB3	2.18	0.43
2:C:646:SER:HB2	2:C:649:GLN:HG3	2.00	0.43
2:C:559:CYS:SG	2:C:661:VAL:HA	2.57	0.43
2:C:985:GLU:HG3	2:C:988:LYS:HB2	2.00	0.43
3:D:1247:LYS:H	3:D:1247:LYS:CD	2.24	0.43
3:D:395:LYS:HG3	5:X:536:THR:CG2	2.48	0.43
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.53	0.43
3:D:588:PRO:HG2	3:D:591:ILE:HD11	2.00	0.43
3:D:504:GLN:HA	3:D:730:ALA:HA	2.00	0.43
2:H:1103:VAL:N	2:H:1104:PRO:HD2	2.33	0.43
2:H:1269:ARG:N	2:H:1269:ARG:HD3	2.33	0.43
2:H:1332:SER:O	3:I:243:PRO:HG2	2.18	0.43
2:H:157:PHE:CZ	2:H:431:LYS:HD3	2.53	0.43
2:H:59:ILE:HG22	2:H:476:LYS:HA	2.00	0.43
3:I:390:LEU:HD12	3:I:390:LEU:N	2.32	0.43
5:X:291:CYS:O	5:X:297:MET:HB3	2.18	0.43
5:X:138:PRO:CD	5:X:353:LEU:HD11	2.47	0.43
3:I:44:ILE:HG22	5:Y:450:ILE:HG22	2.00	0.43
5:Y:596:ARG:HH21	5:Y:599:ARG:CZ	2.31	0.43
2:C:1141:LEU:HD13	2:C:1141:LEU:H	1.83	0.43
2:C:149:LEU:HD23	2:C:451:ARG:HH21	1.83	0.43
2:C:452:ARG:HH11	2:C:585:GLY:HA3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:ARG:HG2	2:C:55:SER:OG	2.18	0.43
1:A:152:TYR:CE2	2:C:824:GLN:HG2	2.53	0.43
2:C:1287:LEU:HD23	3:D:1357:ILE:HG12	2.00	0.43
3:D:452:LEU:HG	3:D:625:MET:SD	2.58	0.43
1:F:200:LYS:O	1:F:200:LYS:HG3	2.19	0.43
1:G:178:SER:HA	1:G:179:PRO:HD3	1.88	0.43
5:Y:240:ARG:O	5:Y:242:HIS:N	2.52	0.43
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.33	0.43
2:C:237:LEU:HD13	2:C:292:ILE:HD12	1.99	0.43
2:C:49:LEU:HD11	2:C:464:PHE:CG	2.53	0.43
2:C:617:ALA:HB2	2:C:650:VAL:CG2	2.46	0.43
2:C:843:THR:HG22	2:C:844:LYS:N	2.32	0.43
2:C:985:GLU:HG2	2:C:989:LEU:HD13	2.00	0.43
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.82	0.43
3:D:546:ALA:H	3:D:547:ARG:C	2.21	0.43
1:G:29:GLU:HA	1:G:200:LYS:HB3	1.98	0.43
2:H:106:GLU:HG3	2:H:108:GLU:N	2.34	0.43
2:H:1084:ASP:HB2	2:H:1216:ARG:HG2	2.00	0.43
2:H:505:PHE:O	2:H:509:SER:HB3	2.18	0.43
2:H:73:TYR:O	2:H:74:ARG:HB2	2.17	0.43
3:I:33:TRP:O	3:I:102:MET:HB2	2.18	0.43
3:I:31:ARG:HD2	3:I:104:HIS:CD2	2.54	0.43
3:I:392:THR:CG2	5:Y:606:VAL:HG11	2.48	0.43
3:I:703:THR:O	3:I:718:SER:N	2.52	0.43
5:X:592:ALA:O	5:X:596:ARG:HG2	2.18	0.43
2:C:1002:LEU:HG	2:C:1007:LYS:HG2	2.00	0.43
2:C:243:PRO:HB2	2:C:278:GLU:HG3	2.00	0.43
2:C:511:LEU:HD13	2:C:535:PRO:HD3	2.00	0.43
2:C:580:GLN:HG2	2:C:581:THR:N	2.34	0.43
2:C:24:VAL:HG11	2:C:704:MET:HE1	2.01	0.43
2:C:936:ARG:HB3	2:C:939:VAL:CG2	2.48	0.43
3:D:1216:ALA:O	3:D:1220:ILE:HG13	2.18	0.43
3:D:413:ASP:HA	3:D:416:ILE:CD1	2.48	0.43
3:D:686:TRP:HB3	3:D:758:PRO:HG2	1.99	0.43
2:H:24:VAL:HA	2:H:25:PRO:HD3	1.87	0.43
2:H:468:LEU:O	2:H:471:VAL:HG22	2.18	0.43
2:H:667:LEU:O	2:H:1069:ARG:NH2	2.51	0.43
2:H:69:GLN:HE22	2:H:101:ARG:NH2	2.16	0.43
3:I:1307:LEU:HD23	3:I:1307:LEU:N	2.33	0.43
3:I:165:TYR:O	3:I:169:LEU:HB2	2.18	0.43
3:I:531:LYS:NZ	3:I:531:LYS:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:611:ILE:HG13	3:I:612:LEU:HD23	2.00	0.43
3:I:647:PRO:HG3	3:I:697:MET:HA	1.99	0.43
3:I:72:CYS:SG	3:I:73:GLY:N	2.90	0.43
3:I:749:LYS:CG	3:I:750:PRO:HD2	2.37	0.43
5:X:514:ASP:HB2	5:X:517:SER:OG	2.18	0.43
5:Y:130:VAL:O	5:Y:134:VAL:HG23	2.18	0.43
1:B:22:THR:HB	1:B:207:THR:O	2.19	0.43
2:C:1223:ARG:HG3	2:C:1224:PRO:HD2	2.01	0.43
2:C:130:MET:SD	2:C:134:GLY:HA2	2.59	0.43
2:C:1314:GLN:O	3:D:473:THR:HG23	2.18	0.43
2:C:205:PRO:O	2:C:208:ILE:HG22	2.19	0.43
2:C:363:LEU:HD13	2:C:382:GLU:HG2	2.00	0.43
2:C:519:ASN:ND2	2:C:689:ALA:O	2.52	0.43
2:C:734:ILE:O	2:C:748:ILE:HA	2.18	0.43
3:D:720:ASN:ND2	3:D:720:ASN:O	2.51	0.43
1:F:41:ASN:HD21	2:H:1218:GLY:CA	2.32	0.43
1:G:191:ARG:HH22	3:I:442:ILE:HA	1.84	0.43
2:H:92:TYR:CE1	2:H:129:LEU:HB2	2.54	0.43
2:H:131:THR:HG22	2:H:135:THR:N	2.34	0.43
2:H:966:ILE:HG23	2:H:967:LEU:HD12	2.01	0.43
3:I:108:ALA:HB3	3:I:279:LEU:HD12	1.99	0.43
3:I:161:THR:HG22	3:I:162:GLU:N	2.34	0.43
3:I:165:TYR:CE1	3:I:169:LEU:HD23	2.54	0.43
3:I:522:GLY:HA2	3:I:545:HIS:CG	2.53	0.43
5:X:437:GLN:HA	5:X:440:THR:HG22	1.99	0.43
3:D:395:LYS:HD3	5:X:607:LEU:HD13	2.01	0.43
1:A:131:CYS:O	1:A:132:HIS:ND1	2.52	0.43
1:A:320:ASN:O	1:A:323:PRO:HD3	2.19	0.43
3:D:390:LEU:HD12	3:D:390:LEU:N	2.33	0.43
1:G:195:ARG:HH21	1:G:198:LEU:HD21	1.84	0.43
2:H:1116:HIS:HE1	2:H:1226:THR:HG23	1.84	0.43
2:H:519:ASN:ND2	2:H:689:ALA:O	2.51	0.43
2:H:555:TYR:OH	2:H:637:ARG:NH2	2.51	0.43
2:H:972:PHE:HA	2:H:975:ILE:HG22	1.99	0.43
3:I:1155:ILE:HG13	3:I:1210:ILE:CG2	2.43	0.43
3:I:1229:VAL:O	3:I:1233:ILE:HG13	2.18	0.43
3:I:185:ILE:HD12	3:I:185:ILE:HA	1.92	0.43
3:I:205:LEU:HB3	3:I:217:LEU:HD13	2.00	0.43
3:I:412:LEU:HA	3:I:415:VAL:HG22	1.99	0.43
3:I:678:ARG:O	3:I:681:LYS:HG3	2.18	0.43
5:Y:452:ILE:HG21	5:Y:457:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HG22	1:A:278:ILE:HD11	2.00	0.43
1:A:317:ARG:C	1:A:318:LEU:HD13	2.39	0.43
1:B:179:PRO:HB3	1:B:210:THR:HB	2.00	0.43
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.53	0.43
2:C:169:LYS:HA	2:C:169:LYS:HD3	1.73	0.43
2:C:618:GLN:HG2	2:C:637:ARG:NH2	2.33	0.43
2:C:886:LYS:H	2:C:917:SER:HB3	1.82	0.43
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.43
3:D:126:LEU:HD21	3:D:223:LEU:HD13	2.00	0.43
3:D:205:LEU:HD13	3:D:217:LEU:HD22	2.00	0.43
3:D:393:THR:HG23	3:D:396:ALA:H	1.83	0.43
3:D:395:LYS:HZ1	5:X:609:SER:HB3	1.83	0.43
3:D:58:CYS:SG	3:D:61:ILE:HG13	2.58	0.43
3:D:505:ASP:HB3	3:D:629:PHE:HE2	1.83	0.43
1:G:19:VAL:O	1:G:20:SER:OG	2.19	0.43
2:H:1042:LEU:N	2:H:1042:LEU:HD13	2.25	0.43
2:H:1106:ARG:O	2:H:1108:ASN:N	2.45	0.43
1:G:191:ARG:NH2	3:I:441:LEU:O	2.51	0.43
5:X:290:LEU:HD13	5:X:336:GLU:HB3	2.01	0.43
3:D:313:GLY:H	5:X:38:SER:HB3	1.81	0.43
5:X:525:ASP:OD1	5:X:528:LEU:HG	2.19	0.43
1:B:179:PRO:HA	1:B:208:ASN:HD21	1.84	0.43
2:C:1327:LEU:HA	2:C:1337:ILE:HD11	1.99	0.43
3:D:1357:ILE:N	3:D:1357:ILE:HD12	2.33	0.43
3:D:268:LEU:HD22	3:D:324:LEU:HD23	2.01	0.43
1:G:185:TYR:HA	1:G:202:VAL:O	2.19	0.43
1:G:77:ASP:O	1:G:81:ILE:HG13	2.19	0.43
2:H:1292:THR:OG1	2:H:1293:VAL:N	2.47	0.43
2:H:170:VAL:CG2	2:H:171:LEU:H	2.23	0.43
2:H:591:TYR:HD2	2:H:606:LEU:HD23	1.84	0.43
2:H:681:MET:O	2:H:685:MET:HG2	2.19	0.43
2:H:923:GLY:HA2	3:I:371:LYS:HE3	2.01	0.43
3:I:1270:GLY:HA3	3:I:1299:GLY:HA2	2.01	0.43
3:I:19:ALA:HB2	3:I:1343:GLU:HB3	1.99	0.43
3:I:435:GLN:HB2	3:I:457:TYR:OH	2.18	0.43
3:I:546:ALA:H	3:I:547:ARG:C	2.21	0.43
5:X:224:LEU:HB2	5:X:259:PHE:CE1	2.53	0.43
5:X:556:ALA:O	5:X:560:ARG:HB2	2.18	0.43
5:Y:299:LYS:O	5:Y:303:ILE:HG12	2.18	0.43
2:C:73:TYR:CD2	2:C:73:TYR:N	2.87	0.43
3:D:1148:ARG:HB2	3:D:1148:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1234:VAL:HG13	3:D:1235:ASN:N	2.34	0.43
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.85	0.43
3:D:413:ASP:HA	3:D:416:ILE:HD12	2.00	0.43
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.18	0.43
3:D:773:PHE:O	3:D:776:THR:HG22	2.19	0.43
3:D:97:VAL:O	3:D:101:ARG:HG2	2.18	0.43
1:F:51:MET:HA	1:F:52:PRO:HD3	1.83	0.43
2:H:1045:GLY:O	2:H:1046:VAL:HB	2.18	0.43
2:H:807:TRP:HE1	2:H:1086:PRO:CD	2.30	0.43
2:H:73:TYR:CD2	2:H:73:TYR:N	2.87	0.43
2:H:866:ASP:HA	2:H:872:TYR:OH	2.19	0.43
3:I:1196:LEU:HG	3:I:1210:ILE:HD11	2.01	0.43
3:I:1281:GLU:O	3:I:1285:VAL:HG13	2.19	0.43
3:I:1287:ILE:O	3:I:1291:GLU:HG2	2.19	0.43
1:A:246:LYS:N	1:A:246:LYS:HD3	2.34	0.43
1:A:236:ASP:HA	1:B:14:VAL:HB	2.00	0.43
1:A:45:ARG:NE	1:B:38:THR:OG1	2.45	0.43
2:C:1141:LEU:HD22	2:C:1141:LEU:O	2.18	0.43
2:C:56:VAL:HB	2:C:57:PHE:H	1.52	0.43
3:D:1322:ALA:HB3	3:D:1331:VAL:HG21	2.00	0.43
3:D:905:ARG:HG2	3:D:907:HIS:H	1.84	0.43
1:G:227:GLN:C	1:G:229:GLU:H	2.22	0.43
2:H:578:TYR:HD2	2:H:659:GLN:HA	1.84	0.43
2:H:734:ILE:HG23	2:H:749:ASP:HB2	2.01	0.43
2:H:759:SER:HB3	2:H:763:THR:H	1.83	0.43
3:I:1170:LYS:C	3:I:1173:ARG:HD2	2.39	0.43
3:I:235:GLU:N	3:I:235:GLU:OE1	2.52	0.43
3:I:363:LEU:O	3:I:486:SER:OG	2.25	0.43
2:H:1314:GLN:O	3:I:473:THR:HG23	2.18	0.43
3:I:746:LEU:N	3:I:746:LEU:HD22	2.34	0.43
5:X:439:ILE:O	5:X:443:ILE:HG13	2.19	0.43
5:Y:120:ALA:HA	5:Y:123:ILE:HD12	1.99	0.43
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.54	0.42
2:C:177:ILE:HD12	2:C:177:ILE:N	2.35	0.42
2:C:185:ASP:HB2	2:C:197:ARG:HB2	2.00	0.42
2:C:73:TYR:O	2:C:74:ARG:HB2	2.18	0.42
3:D:1170:LYS:C	3:D:1173:ARG:HD2	2.39	0.42
3:D:155:GLU:CG	3:D:158:GLN:HB2	2.48	0.42
3:D:246:PRO:HB2	3:D:249:LEU:HD13	2.01	0.42
3:D:26:SER:O	3:D:30:ILE:HG12	2.19	0.42
3:D:325:LYS:HB3	3:D:325:LYS:HE2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:42:GLU:HG3	5:X:451:ARG:HH21	1.84	0.42
3:D:771:GLN:HE21	3:D:772:TYR:N	2.17	0.42
3:D:832:LYS:HB2	3:D:832:LYS:HZ2	1.84	0.42
3:D:843:VAL:HG12	3:D:883:ARG:HD3	2.00	0.42
1:F:45:ARG:NE	1:G:38:THR:OG1	2.49	0.42
2:H:106:GLU:CB	2:H:107:ARG:CA	2.96	0.42
2:H:820:GLU:O	2:H:824:GLN:HG3	2.19	0.42
2:H:999:GLU:HG2	2:H:1000:LEU:N	2.34	0.42
3:I:1278:GLU:HG3	3:I:1279:GLN:N	2.34	0.42
3:I:524:GLY:HA2	3:I:548:VAL:HG23	2.01	0.42
3:I:51:PRO:HB3	3:I:57:PHE:O	2.19	0.42
3:I:586:GLY:O	3:I:587:LEU:HB2	2.19	0.42
3:I:661:VAL:O	3:I:665:GLN:HG3	2.19	0.42
5:X:117:ILE:HG13	5:X:421:TYR:HB2	2.01	0.42
5:X:101:TYR:HE2	5:X:388:ILE:HD11	1.83	0.42
5:X:484:ALA:HB1	5:X:490:PRO:O	2.17	0.42
5:X:532:LEU:O	5:X:536:THR:HG23	2.19	0.42
1:A:91:ARG:NH2	1:A:209:GLY:O	2.52	0.42
1:B:57:THR:HG21	1:B:177:TYR:OH	2.19	0.42
2:C:745:GLU:HA	2:C:1017:GLN:OE1	2.19	0.42
2:C:345:PRO:O	2:C:349:GLU:HG2	2.19	0.42
2:C:524:ILE:HD11	2:C:712:SER:HB2	2.00	0.42
2:C:727:VAL:CG2	2:C:773:LEU:HB3	2.44	0.42
2:C:844:LYS:HB2	2:C:844:LYS:NZ	2.33	0.42
2:C:1335:ILE:CD1	3:D:22:ILE:HD11	2.47	0.42
3:D:595:ALA:HB1	3:D:596:LEU:HD23	2.01	0.42
1:F:54:CYS:SG	1:F:148:ARG:HD3	2.58	0.42
1:G:196:THR:OG1	3:I:443:GLU:HG3	2.18	0.42
1:G:192:VAL:CG2	1:G:198:LEU:HD12	2.43	0.42
1:G:82:LEU:O	1:G:86:LYS:HG3	2.19	0.42
2:H:1212:LEU:HD12	2:H:1225:VAL:HG21	2.01	0.42
2:H:429:MET:O	2:H:433:ILE:HG13	2.19	0.42
5:X:48:ILE:HG13	5:X:49:ASN:H	1.84	0.42
1:A:22:THR:HB	1:A:207:THR:O	2.19	0.42
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.53	0.42
2:C:42:ASP:HB3	2:C:43:PRO:CD	2.28	0.42
2:C:462:ASN:O	2:C:466:VAL:HG23	2.20	0.42
2:C:850:ILE:HG23	2:C:885:GLY:O	2.20	0.42
2:C:948:ILE:O	2:C:952:GLN:HG3	2.19	0.42
3:D:22:ILE:HG12	3:D:1336:ALA:HA	2.02	0.42
3:D:355:ILE:HA	3:D:447:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:66:LYS:HB2	3:D:69:GLU:HG2	2.00	0.42
3:D:701:LEU:HD21	3:D:723:TYR:HB2	2.02	0.42
1:G:153:VAL:HA	1:G:154:PRO:HD3	1.85	0.42
2:H:1270:PHE:HB3	2:H:1271:GLY:H	1.58	0.42
2:H:1339:LEU:N	2:H:1339:LEU:HD12	2.33	0.42
2:H:977:ALA:O	2:H:980:VAL:HG12	2.19	0.42
2:H:99:LYS:H	2:H:99:LYS:HD3	1.80	0.42
3:I:1140:ARG:HH21	3:I:1236:GLU:CG	2.32	0.42
3:I:252:LEU:HG	3:I:252:LEU:O	2.20	0.42
3:I:326:SER:O	3:I:330:MET:HG3	2.18	0.42
4:J:15:ASN:ND2	4:J:17:PHE:HB2	2.32	0.42
5:X:120:ALA:CB	5:X:421:TYR:HB3	2.47	0.42
5:X:276:MET:O	5:X:280:VAL:HG23	2.20	0.42
5:X:45:ILE:HD12	5:X:45:ILE:C	2.40	0.42
1:B:179:PRO:HB2	1:B:211:ILE:HG22	2.00	0.42
2:C:748:ILE:HD12	2:C:748:ILE:C	2.40	0.42
3:D:886:VAL:CG1	3:D:1230:THR:HG21	2.48	0.42
3:D:161:THR:HG22	3:D:162:GLU:N	2.34	0.42
3:D:245:LEU:CD1	3:D:246:PRO:HD2	2.48	0.42
3:D:295:GLU:OE1	5:X:406:GLN:HG2	2.19	0.42
3:D:678:ARG:O	3:D:681:LYS:HG3	2.20	0.42
1:F:44:ARG:HG3	1:F:183:ILE:CG2	2.49	0.42
1:G:181:GLU:HB2	1:G:206:GLU:O	2.19	0.42
2:H:576:SER:HB3	2:H:579:ALA:HB2	2.02	0.42
3:I:1247:LYS:CD	3:I:1247:LYS:H	2.20	0.42
3:I:412:LEU:O	3:I:416:ILE:HD12	2.19	0.42
3:I:704:GLU:HB2	3:I:718:SER:HG	1.82	0.42
3:I:771:GLN:HE21	3:I:772:TYR:N	2.17	0.42
3:I:856:ILE:HD12	3:I:857:LEU:N	2.35	0.42
5:Y:453:PRO:HD2	5:Y:456:MET:CB	2.44	0.42
2:C:1087:TYR:HE2	2:C:1215:GLY:HA2	1.83	0.42
2:C:1108:ASN:O	2:C:1108:ASN:ND2	2.50	0.42
2:C:1297:ASP:OD1	2:C:1300:GLY:HA3	2.19	0.42
2:C:53:PHE:HD1	2:C:57:PHE:CD2	2.36	0.42
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	2.02	0.42
3:D:707:ILE:HD11	3:D:716:GLN:CD	2.40	0.42
3:D:813:ASP:OD1	3:D:896:ALA:HB3	2.18	0.42
1:F:102:LEU:HB3	1:F:142:MET:HG2	2.02	0.42
2:H:1259:LEU:O	2:H:1259:LEU:HD12	2.19	0.42
2:H:1298:VAL:HG23	2:H:1299:ASN:N	2.33	0.42
2:H:310:ILE:HG21	2:H:324:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:948:ILE:O	2:H:952:GLN:HG3	2.19	0.42
2:C:1027:LYS:HB2	2:C:1027:LYS:NZ	2.35	0.42
2:C:333:ILE:N	2:C:333:ILE:HD12	2.34	0.42
2:C:603:ILE:HD12	2:C:603:ILE:O	2.19	0.42
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.99	0.42
3:D:521:LYS:HB2	3:D:542:ALA:HB2	2.00	0.42
3:D:588:PRO:CG	3:D:591:ILE:HD11	2.50	0.42
3:D:607:THR:O	3:D:611:ILE:HG12	2.19	0.42
3:D:79:LYS:HE3	5:X:569:THR:N	2.35	0.42
4:E:5:THR:HB	4:E:7:GLN:H	1.84	0.42
1:F:28:LEU:HD13	1:G:231:PHE:CE2	2.55	0.42
2:H:105:TYR:HA	2:H:106:GLU:HA	1.89	0.42
2:H:1192:GLU:O	2:H:1196:LYS:HD3	2.20	0.42
2:H:153:PRO:HD2	2:H:452:ARG:HD3	2.01	0.42
2:H:748:ILE:HD12	2:H:748:ILE:C	2.40	0.42
3:I:1216:ALA:HB3	3:I:1219:ASP:OD1	2.20	0.42
3:I:1234:VAL:HA	3:I:1253:ILE:HG21	2.02	0.42
3:I:385:LEU:CD2	3:I:411:ILE:HG13	2.49	0.42
2:H:1273:MET:HB3	3:I:428:THR:HB	2.00	0.42
5:Y:147:GLN:O	5:Y:151:VAL:HG23	2.20	0.42
1:B:213:PRO:HA	1:B:216:ALA:HB3	2.01	0.42
2:C:384:LEU:O	2:C:388:LEU:HG	2.20	0.42
2:C:490:GLN:O	5:X:472:GLN:HG3	2.20	0.42
2:C:57:PHE:HE1	2:C:472:GLU:HA	1.84	0.42
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.19	0.42
3:D:1141:VAL:HG22	3:D:1240:VAL:HG21	2.01	0.42
3:D:1307:LEU:HD23	3:D:1307:LEU:N	2.34	0.42
3:D:130:MET:HA	3:D:131:PRO:HD3	1.95	0.42
3:D:147:ILE:HG13	3:D:148:GLU:N	2.34	0.42
3:D:252:LEU:HA	3:D:261:ALA:O	2.19	0.42
3:D:899:TYR:CE1	3:D:915:ILE:HD12	2.55	0.42
4:E:5:THR:HB	4:E:7:GLN:N	2.35	0.42
6:H:1401:1RM:O2	6:H:1401:1RM:O1	2.37	0.42
2:H:148:GLN:HB2	2:H:511:LEU:HD21	2.02	0.42
2:H:177:ILE:N	2:H:177:ILE:HD12	2.34	0.42
2:H:475:VAL:O	2:H:479:LEU:HB2	2.19	0.42
2:H:47:TYR:CD1	2:H:70:TYR:HE2	2.37	0.42
2:H:768:MET:O	2:H:785:ASP:N	2.46	0.42
2:H:850:ILE:HG23	2:H:885:GLY:O	2.19	0.42
3:I:1140:ARG:HH21	3:I:1236:GLU:HG2	1.85	0.42
3:I:120:LEU:N	3:I:120:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1297:LYS:HB3	3:I:1297:LYS:HZ2	1.84	0.42
2:H:1285:TYR:HD2	3:I:1361:THR:HG21	1.85	0.42
3:I:269:TYR:HA	3:I:272:VAL:HG12	2.02	0.42
3:I:844:THR:CG2	3:I:848:VAL:HG23	2.50	0.42
5:X:560:ARG:HG2	5:X:565:ILE:HG23	2.01	0.42
5:Y:148:TYR:OH	5:Y:218:ARG:HG2	2.20	0.42
5:Y:540:LEU:HD13	5:Y:607:LEU:HD22	2.01	0.42
1:A:74:VAL:HG12	1:A:76:GLU:O	2.20	0.42
1:B:33:ARG:NE	1:B:197:ASP:HB2	2.34	0.42
1:B:19:VAL:HG12	1:B:19:VAL:O	2.20	0.42
2:C:106:GLU:CB	2:C:107:ARG:HA	2.49	0.42
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.33	0.42
2:C:531:SER:OG	6:C:1401:1RM:O2	2.19	0.42
2:C:225:PHE:HB2	2:C:336:LEU:HD22	2.01	0.42
3:D:1241:TYR:HB3	3:D:1246:VAL:HG23	2.01	0.42
2:C:812:PHE:HB2	3:D:357:VAL:HG21	2.02	0.42
3:D:513:MET:HE2	3:D:513:MET:HB3	1.91	0.42
2:H:1108:ASN:ND2	2:H:1108:ASN:O	2.50	0.42
1:F:45:ARG:HH12	2:H:1216:ARG:HA	1.85	0.42
2:H:812:PHE:N	2:H:815:SER:HB2	2.34	0.42
2:H:993:PRO:HB2	2:H:994:ARG:H	1.60	0.42
3:I:1230:THR:O	3:I:1234:VAL:HG12	2.20	0.42
5:X:227:GLN:O	5:X:230:VAL:HG12	2.20	0.42
1:A:80:GLU:HG3	2:C:694:ARG:NH1	2.34	0.42
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.26	0.42
2:C:342:ASP:O	2:C:437:ASN:ND2	2.53	0.42
2:C:538:LEU:HD12	2:C:538:LEU:N	2.35	0.42
2:C:92:TYR:CE1	2:C:129:LEU:HB2	2.55	0.42
2:C:958:LYS:O	2:C:962:GLU:HG2	2.20	0.42
3:D:33:TRP:O	3:D:102:MET:HB2	2.19	0.42
3:D:167:ASP:O	3:D:171:GLU:HG2	2.20	0.42
3:D:185:ILE:HA	3:D:185:ILE:HD12	1.92	0.42
3:D:681:LYS:O	3:D:685:ILE:HG13	2.19	0.42
3:D:841:GLY:HA3	3:D:901:ARG:HD3	2.02	0.42
1:G:33:ARG:NE	1:G:197:ASP:HB2	2.33	0.42
3:I:911:LYS:O	3:I:911:LYS:HD2	2.20	0.42
5:Y:562:ARG:NH1	5:Y:591:GLU:OE2	2.53	0.42
1:A:88:LEU:HD22	1:A:90:VAL:CG2	2.50	0.42
2:C:971:LEU:HD21	2:C:1017:GLN:HE22	1.85	0.42
2:C:59:ILE:HD11	2:C:63:SER:OG	2.20	0.42
3:D:122:SER:OG	3:D:132:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:678:ARG:HD2	3:D:678:ARG:C	2.41	0.42
2:H:1054:LEU:O	2:H:1054:LEU:HD12	2.20	0.42
2:H:1120:ALA:HB2	2:H:1199:LEU:HD23	2.02	0.42
2:H:133:ASN:O	2:H:527:LYS:NZ	2.43	0.42
2:H:241:LEU:HD22	2:H:285:ILE:HD13	2.02	0.42
2:H:333:ILE:N	2:H:333:ILE:HD12	2.35	0.42
2:H:344:GLY:HA2	2:H:345:PRO:HD3	1.83	0.42
2:H:37:LYS:HE3	2:H:37:LYS:HA	2.01	0.42
3:I:1234:VAL:HG13	3:I:1235:ASN:N	2.35	0.42
1:A:110:VAL:HB	1:A:131:CYS:HB2	2.01	0.41
1:A:303:ILE:O	1:A:307:LEU:HD13	2.20	0.41
2:C:1002:LEU:HD13	2:C:1003:THR:H	1.85	0.41
2:C:106:GLU:HB3	2:C:107:ARG:CA	2.49	0.41
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	2.02	0.41
2:C:210:LEU:O	2:C:215:TYR:HB2	2.19	0.41
2:C:510:GLN:C	2:C:512:SER:H	2.24	0.41
2:C:60:GLN:O	2:C:61:SER:OG	2.33	0.41
3:D:1229:VAL:O	3:D:1233:ILE:HG13	2.20	0.41
3:D:20:ILE:HD13	3:D:1320:ILE:HD11	2.02	0.41
3:D:288:PRO:O	3:D:292:VAL:HG12	2.20	0.41
3:D:356:THR:O	3:D:448:GLN:HA	2.19	0.41
2:H:1027:LYS:NZ	2:H:1027:LYS:HB2	2.35	0.41
2:H:1117:LEU:HD11	2:H:1182:ILE:HD13	2.01	0.41
2:H:618:GLN:OE1	2:H:637:ARG:NH1	2.52	0.41
2:H:771:VAL:HG23	2:H:775:GLU:CD	2.40	0.41
3:I:41:PRO:HB3	3:I:270:ARG:HG3	2.01	0.41
3:I:709:ARG:HD2	3:I:714:GLU:HB2	2.02	0.41
3:I:909:ILE:H	3:I:909:ILE:HG13	1.55	0.41
5:Y:99:ARG:HD3	5:Y:99:ARG:O	2.20	0.41
1:A:104:LYS:HD2	1:A:110:VAL:HG22	2.01	0.41
1:A:302:GLU:O	1:A:306:VAL:HG22	2.19	0.41
1:B:227:GLN:C	1:B:229:GLU:H	2.18	0.41
1:B:51:MET:HA	1:B:52:PRO:HD3	1.86	0.41
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.35	0.41
2:C:812:PHE:N	2:C:815:SER:HB2	2.35	0.41
3:D:159:ILE:HD12	3:D:159:ILE:N	2.35	0.41
3:D:189:LEU:HB3	3:D:234:PRO:HB2	2.02	0.41
1:F:167:PRO:HD2	1:F:170:ARG:NE	2.36	0.41
1:F:22:THR:HB	1:F:207:THR:O	2.21	0.41
3:I:1149:ARG:HA	3:I:1150:PRO:HD3	1.92	0.41
3:I:1207:GLY:HA2	3:I:1223:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:506:VAL:HG23	3:I:628:GLY:HA3	2.01	0.41
5:X:147:GLN:O	5:X:151:VAL:HG23	2.20	0.41
1:A:234:LEU:HD12	1:A:234:LEU:N	2.35	0.41
1:B:154:PRO:O	1:B:157:THR:HG22	2.20	0.41
2:C:1287:LEU:O	2:C:1291:LEU:HB2	2.20	0.41
2:C:17:LYS:N	2:C:17:LYS:HD2	2.35	0.41
2:C:622:ASN:OD1	2:C:623:LEU:N	2.53	0.41
2:C:816:ILE:HD13	2:C:1074:GLY:CA	2.50	0.41
2:C:823:VAL:HG22	2:C:1060:ILE:HG13	2.01	0.41
2:C:868:SER:OG	2:C:942:ASP:OD1	2.25	0.41
3:D:1368:ASP:O	3:D:1372:ARG:HB2	2.19	0.41
2:C:1281:TYR:O	3:D:483:LEU:HD23	2.20	0.41
3:D:522:GLY:O	3:D:523:GLU:HG2	2.21	0.41
3:D:644:MET:O	3:D:764:ARG:NH1	2.52	0.41
3:D:766:GLY:C	3:D:767:LEU:HD22	2.41	0.41
2:H:253:PHE:CZ	2:H:287:VAL:HG12	2.55	0.41
2:H:338:THR:OG1	2:H:345:PRO:HG3	2.21	0.41
3:I:1161:GLY:HA2	3:I:1181:ASP:HB2	2.02	0.41
3:I:311:ARG:HH21	3:I:1329:THR:HG21	1.85	0.41
3:I:425:ARG:CD	3:I:459:ALA:HB2	2.50	0.41
5:Y:310:GLU:O	5:Y:344:LEU:HD23	2.20	0.41
5:Y:437:GLN:HA	5:Y:440:THR:HG22	2.01	0.41
5:Y:528:LEU:HD12	5:Y:528:LEU:O	2.21	0.41
2:C:1166:ASP:C	2:C:1168:GLU:H	2.23	0.41
2:C:96:LEU:HD22	2:C:127:ILE:HD12	2.03	0.41
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.20	0.41
3:D:1290:ARG:HD2	3:D:1299:GLY:HA3	2.02	0.41
3:D:502:PRO:HB3	3:D:506:VAL:HG11	2.03	0.41
3:D:646:ILE:H	3:D:646:ILE:HG13	1.64	0.41
3:D:660:GLU:O	3:D:664:ILE:HG12	2.20	0.41
4:E:18:ASP:O	4:E:22:VAL:HG12	2.20	0.41
2:H:130:MET:CG	2:H:134:GLY:HA2	2.50	0.41
2:H:58:PRO:O	2:H:476:LYS:HE3	2.21	0.41
2:H:734:ILE:O	2:H:749:ASP:N	2.53	0.41
2:H:866:ASP:HA	2:H:872:TYR:CZ	2.56	0.41
2:H:92:TYR:HE1	2:H:129:LEU:HD12	1.85	0.41
3:I:147:ILE:HG13	3:I:148:GLU:N	2.34	0.41
3:I:355:ILE:HG12	3:I:464:ASP:O	2.21	0.41
3:I:605:LEU:HD13	3:I:605:LEU:O	2.20	0.41
3:I:735:ALA:O	3:I:739:GLN:HG3	2.20	0.41
4:J:26:ARG:HD3	4:J:64:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:492:ASP:HA	5:Y:495:ARG:HG3	2.01	0.41
2:C:1004:ASP:N	2:C:1004:ASP:OD1	2.54	0.41
2:C:1196:LYS:HG3	2:C:1206:THR:OG1	2.20	0.41
2:C:397:LEU:O	2:C:398:SER:OG	2.31	0.41
2:C:406:ASN:HB3	2:C:411:ARG:HB2	2.01	0.41
3:D:252:LEU:O	3:D:252:LEU:HG	2.20	0.41
3:D:40:LYS:HA	3:D:41:PRO:HD3	1.80	0.41
2:H:1086:PRO:HG2	2:H:1094:VAL:HG21	2.02	0.41
2:H:705:GLU:HG2	2:H:793:GLU:HG3	2.02	0.41
2:H:896:THR:HG22	2:H:898:GLU:OE1	2.20	0.41
2:H:944:ARG:HD3	2:H:944:ARG:O	2.21	0.41
3:I:824:PRO:CB	3:I:836:ARG:HD3	2.50	0.41
5:X:528:LEU:HD12	5:X:528:LEU:O	2.18	0.41
5:Y:343:LYS:O	5:Y:346:GLN:HB3	2.21	0.41
5:Y:277:MET:HE1	5:Y:359:LYS:HE2	2.02	0.41
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.85	0.41
2:C:1272:GLU:HG3	2:C:1276:TRP:CZ2	2.56	0.41
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.68	0.41
2:C:80:PHE:O	2:C:84:GLU:HB3	2.19	0.41
3:D:205:LEU:HB3	3:D:217:LEU:HB3	2.02	0.41
2:C:1258:PRO:HG2	3:D:346:ARG:CB	2.50	0.41
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.91	0.41
3:D:501:VAL:HA	3:D:502:PRO:HD3	1.97	0.41
3:D:591:ILE:HD12	3:D:592:VAL:HG13	2.03	0.41
3:D:77:ARG:CG	3:D:78:LEU:H	2.33	0.41
3:D:918:ILE:HD13	3:D:919:ALA:N	2.36	0.41
2:H:669:PRO:HG2	2:H:1070:HIS:CE1	2.55	0.41
2:H:120:GLN:HG3	2:H:121:GLU:N	2.36	0.41
2:H:157:PHE:HD2	2:H:174:ALA:HB2	1.85	0.41
3:I:1297:LYS:CE	3:I:1297:LYS:HA	2.50	0.41
3:I:294:ASN:ND2	5:Y:406:GLN:OE1	2.54	0.41
3:I:271:ARG:NH1	3:I:317:THR:HG21	2.35	0.41
3:I:368:LEU:HG	3:I:373:ALA:HB2	2.02	0.41
3:I:591:ILE:HD12	3:I:592:VAL:HG13	2.02	0.41
5:X:262:VAL:HG12	5:X:264:LYS:H	1.85	0.41
5:X:456:MET:O	5:X:460:ILE:HG13	2.20	0.41
5:X:514:ASP:HB3	5:X:515:GLU:H	1.65	0.41
5:Y:562:ARG:HG3	5:Y:591:GLU:OE1	2.19	0.41
2:C:892:GLU:C	2:C:894:GLN:H	2.24	0.41
2:C:977:ALA:O	2:C:980:VAL:HG12	2.20	0.41
3:D:13:LYS:HA	3:D:13:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:ALA:HB2	3:D:1343:GLU:CB	2.48	0.41
3:D:126:LEU:HD21	3:D:223:LEU:CD1	2.50	0.41
3:D:412:LEU:O	3:D:415:VAL:HG22	2.21	0.41
3:D:473:THR:HB	3:D:476:ALA:HB2	2.01	0.41
3:D:586:GLY:O	3:D:587:LEU:HB2	2.20	0.41
3:D:66:LYS:HB3	3:D:66:LYS:NZ	2.36	0.41
2:H:161:LYS:HB3	2:H:161:LYS:NZ	2.36	0.41
2:H:488:MET:HB2	2:H:489:PRO:HA	2.02	0.41
2:H:773:LEU:CD1	2:H:773:LEU:H	2.32	0.41
2:H:886:LYS:HD3	2:H:916:SER:O	2.20	0.41
3:I:179:LYS:N	3:I:179:LYS:HD3	2.36	0.41
3:I:210:SER:O	3:I:214:ARG:HG3	2.21	0.41
3:I:382:TYR:HE1	3:I:401:VAL:CG2	2.31	0.41
3:I:492:SER:HA	3:I:493:PRO:HD3	1.95	0.41
3:I:579:LEU:HD13	3:I:579:LEU:O	2.19	0.41
3:I:905:ARG:HG2	3:I:907:HIS:H	1.85	0.41
4:J:26:ARG:HB2	4:J:64:LEU:HD11	2.01	0.41
5:X:23:THR:HG22	5:X:26:GLU:HG2	2.03	0.41
5:Y:262:VAL:HG12	5:Y:264:LYS:H	1.85	0.41
5:Y:276:MET:O	5:Y:280:VAL:HG23	2.21	0.41
5:Y:587:ILE:HD12	5:Y:587:ILE:HA	1.95	0.41
1:A:207:THR:HG23	1:A:209:GLY:H	1.85	0.41
1:A:316:MET:HB2	1:A:316:MET:HE2	1.90	0.41
2:C:317:LEU:HD13	2:C:322:LEU:HD21	2.02	0.41
2:C:658:GLN:HB3	2:C:1186:VAL:HG11	2.02	0.41
2:C:758:ARG:NH1	2:C:762:ASN:OD1	2.54	0.41
3:D:62:PHE:O	3:D:101:ARG:HG3	2.20	0.41
3:D:490:ILE:HG23	3:D:500:ILE:HD11	2.03	0.41
3:D:527:LEU:H	3:D:550:VAL:HG12	1.85	0.41
3:D:84:ILE:HG13	3:D:84:ILE:H	1.78	0.41
3:D:905:ARG:HH12	4:E:10:VAL:CG1	2.32	0.41
1:F:31:LEU:HB2	1:F:199:ASP:O	2.21	0.41
1:F:11:PRO:HD2	1:G:227:GLN:HA	2.02	0.41
2:H:187:GLU:OE2	2:H:203:LYS:HD3	2.20	0.41
2:H:699:LEU:HB2	2:H:799:ASN:ND2	2.36	0.41
2:H:843:THR:HG22	2:H:844:LYS:N	2.36	0.41
3:I:1368:ASP:O	3:I:1372:ARG:HB2	2.20	0.41
3:I:526:VAL:CG1	3:I:549:LYS:HB2	2.47	0.41
3:I:532:GLU:OE2	3:I:574:VAL:HG13	2.19	0.41
5:X:290:LEU:O	5:X:294:GLN:HB3	2.21	0.41
5:X:453:PRO:HB2	5:X:455:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1045:GLY:O	2:C:1046:VAL:HB	2.21	0.41
2:C:548:ARG:O	3:D:780:ARG:NH1	2.54	0.41
2:C:814:ASP:O	2:C:1074:GLY:HA2	2.21	0.41
2:C:966:ILE:HG23	2:C:967:LEU:HD12	2.03	0.41
3:D:789:LYS:HD2	3:D:932:MET:SD	2.61	0.41
3:D:886:VAL:HG13	3:D:1230:THR:HG21	2.02	0.41
1:G:222:THR:O	1:G:226:GLU:HG2	2.21	0.41
2:H:10:ARG:CZ	2:H:1171:ARG:HH21	2.33	0.41
2:H:1101:LEU:O	2:H:1104:PRO:HD2	2.21	0.41
2:H:1264:GLN:HB3	2:H:1264:GLN:HE21	1.72	0.41
2:H:157:PHE:CD2	2:H:174:ALA:HB2	2.56	0.41
2:H:848:GLU:CD	2:H:888:THR:HG22	2.41	0.41
3:I:270:ARG:HE	5:Y:449:THR:HG22	1.85	0.41
3:I:611:ILE:HG13	3:I:612:LEU:CD2	2.51	0.41
3:I:620:PHE:O	3:I:624:ILE:HG23	2.20	0.41
5:X:469:GLN:HE21	5:X:473:GLU:HG3	1.85	0.41
5:X:572:THR:O	5:X:576:VAL:HG23	2.21	0.41
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.81	0.41
2:C:1211:ARG:HB2	2:C:1220:GLN:HE21	1.85	0.41
2:C:1225:VAL:HG12	3:D:636:GLY:O	2.21	0.41
2:C:1333:LEU:HB2	2:C:1335:ILE:HG22	2.03	0.41
2:C:22:LEU:HD13	2:C:23:ASP:O	2.21	0.41
2:C:817:LEU:HD21	2:C:1080:ASN:HB2	2.03	0.41
3:D:19:ALA:HB1	3:D:1343:GLU:HB3	2.03	0.41
3:D:215:LYS:O	3:D:219:LYS:HG3	2.21	0.41
2:H:138:ILE:HB	2:H:143:ARG:HD2	2.03	0.41
2:H:603:ILE:HD12	2:H:603:ILE:O	2.21	0.41
2:H:707:ALA:O	2:H:710:VAL:HG12	2.21	0.41
2:H:869:GLY:C	2:H:870:ILE:HD12	2.41	0.41
3:I:1241:TYR:HB3	3:I:1246:VAL:HG23	2.02	0.41
3:I:1247:LYS:N	3:I:1247:LYS:HD3	2.25	0.41
3:I:222:LYS:HZ2	3:I:1276:GLU:HB2	1.85	0.41
3:I:230:SER:CB	3:I:1339:GLY:H	2.28	0.41
3:I:19:ALA:HB2	3:I:1343:GLU:CB	2.51	0.41
3:I:40:LYS:HE3	3:I:42:GLU:HG3	2.02	0.41
3:I:421:VAL:HB	3:I:439:PRO:HG3	2.03	0.41
3:I:501:VAL:HG21	3:I:602:SER:HB2	2.03	0.41
3:I:587:LEU:HD12	3:I:611:ILE:HD11	2.03	0.41
3:I:899:TYR:CE1	3:I:915:ILE:HD12	2.56	0.41
5:X:145:LEU:HD11	5:X:225:ARG:HH21	1.84	0.41
5:Y:455:HIS:O	5:Y:459:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:GLN:HB2	2:C:511:LEU:HD21	2.03	0.41
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.21	0.41
2:C:555:TYR:OH	2:C:637:ARG:NH2	2.54	0.41
2:C:697:LYS:HG3	2:C:698:PRO:HD2	2.03	0.41
2:C:821:ARG:HB2	2:C:1082:ILE:CD1	2.51	0.41
3:D:1266:ILE:HG13	3:D:1274:PHE:O	2.20	0.41
3:D:1347:LEU:CD2	3:D:1358:PRO:HG2	2.38	0.41
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.51	0.41
1:G:200:LYS:O	1:G:200:LYS:HG3	2.21	0.41
2:H:1010:GLN:HE21	2:H:1010:GLN:HB2	1.66	0.41
3:I:41:PRO:HG3	3:I:273:ILE:HG22	2.03	0.41
5:X:119:ILE:CD1	5:X:122:ARG:HH21	2.34	0.41
5:X:312:SER:OG	5:X:314:THR:HG23	2.21	0.41
2:C:1105:SER:HB2	3:D:731:ARG:HB2	2.03	0.40
2:C:1133:LYS:O	2:C:1134:GLN:HB2	2.22	0.40
2:C:96:LEU:HB2	2:C:127:ILE:CD1	2.52	0.40
2:C:54:ARG:N	2:C:55:SER:C	2.75	0.40
2:C:632:ASP:O	2:C:633:LEU:HD23	2.22	0.40
2:C:732:ILE:HD11	2:C:769:PRO:CB	2.50	0.40
3:D:147:ILE:HD12	3:D:178:ALA:HB2	2.03	0.40
3:D:378:LYS:HD2	3:D:382:TYR:OH	2.20	0.40
3:D:555:TYR:HD1	3:D:589:TYR:HE2	1.70	0.40
3:D:558:ASP:OD1	3:D:559:ALA:N	2.53	0.40
1:G:102:LEU:HB3	1:G:142:MET:HG2	2.03	0.40
1:F:45:ARG:NH2	1:G:37:HIS:HB3	2.37	0.40
2:H:347:ILE:HD11	2:H:433:ILE:HD11	2.02	0.40
2:H:54:ARG:HG2	2:H:55:SER:OG	2.21	0.40
3:I:1346:GLY:HA3	3:I:1349:GLU:CD	2.42	0.40
3:I:1347:LEU:CD2	3:I:1358:PRO:HG2	2.42	0.40
3:I:438:GLU:HA	3:I:439:PRO:HD3	1.88	0.40
3:I:522:GLY:O	3:I:523:GLU:HG2	2.21	0.40
3:I:545:HIS:HA	3:I:546:ALA:HA	1.78	0.40
5:X:541:ARG:O	5:X:545:HIS:HB2	2.22	0.40
5:Y:138:PRO:CG	5:Y:353:LEU:HD21	2.49	0.40
5:Y:418:LYS:O	5:Y:430:TYR:OH	2.33	0.40
2:C:542:ARG:HG2	2:C:543:ALA:N	2.35	0.40
2:C:994:ARG:HD3	2:C:994:ARG:N	2.36	0.40
3:D:1347:LEU:HD22	3:D:1357:ILE:HG23	2.03	0.40
3:D:155:GLU:CD	3:D:155:GLU:H	2.24	0.40
3:D:292:VAL:O	3:D:296:LYS:HG3	2.22	0.40
3:D:374:LEU:HD22	3:D:381:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1103:VAL:H	2:H:1104:PRO:HD2	1.84	0.40
2:H:936:ARG:HH11	5:Y:495:ARG:HH11	1.68	0.40
3:I:109:SER:HA	3:I:110:PRO:HD3	1.98	0.40
3:I:205:LEU:HD13	3:I:217:LEU:CD2	2.50	0.40
3:I:382:TYR:CE1	3:I:401:VAL:HG21	2.52	0.40
3:I:704:GLU:HB3	3:I:705:THR:H	1.71	0.40
5:X:112:THR:HG22	5:X:113:ARG:N	2.31	0.40
5:X:251:LYS:O	5:X:255:VAL:HG23	2.21	0.40
5:X:504:PRO:HB2	5:X:505:ILE:H	1.63	0.40
5:Y:240:ARG:HD3	5:Y:244:THR:CB	2.50	0.40
5:Y:519:LEU:O	5:Y:519:LEU:HD13	2.21	0.40
1:A:187:VAL:O	1:A:188:GLU:HB2	2.21	0.40
2:C:818:VAL:HA	2:C:1096:ILE:HG22	2.03	0.40
2:C:119:GLU:OE2	2:C:489:PRO:HB2	2.21	0.40
2:C:1203:ASP:O	2:C:1204:LEU:HG	2.21	0.40
2:C:400:VAL:O	2:C:404:LYS:HE2	2.20	0.40
2:C:690:VAL:HG11	2:C:830:THR:HG21	2.04	0.40
3:D:1226:VAL:HA	3:D:1229:VAL:HG12	2.03	0.40
3:D:1324:SER:CB	3:D:1348:LYS:HD3	2.52	0.40
3:D:610:ARG:HG3	3:D:864:LEU:CD1	2.34	0.40
3:D:582:ILE:HG22	3:D:620:PHE:CE1	2.56	0.40
1:G:188:GLU:O	1:G:200:LYS:HG2	2.22	0.40
1:F:28:LEU:HD13	1:G:231:PHE:HE2	1.86	0.40
2:H:1304:MET:HE1	3:I:472:LEU:HD13	2.04	0.40
2:H:1276:TRP:CE3	3:I:801:VAL:HG11	2.57	0.40
3:I:842:ARG:HB3	3:I:882:VAL:HG21	2.02	0.40
5:X:240:ARG:HD3	5:X:244:THR:CB	2.45	0.40
1:A:313:SER:OG	1:A:314:LEU:N	2.54	0.40
1:B:48:LEU:HD22	3:D:534:GLU:HG3	2.04	0.40
2:C:820:GLU:HB2	2:C:1081:PRO:HA	2.04	0.40
2:C:1185:PRO:HB2	2:C:1186:VAL:H	1.67	0.40
2:C:500:ALA:O	2:C:504:GLU:HB2	2.20	0.40
2:C:525:THR:O	2:C:529:ARG:NH1	2.54	0.40
2:C:54:ARG:N	2:C:55:SER:CB	2.77	0.40
2:C:869:GLY:C	2:C:870:ILE:HD12	2.41	0.40
3:D:97:VAL:HG13	3:D:101:ARG:CZ	2.51	0.40
3:D:1190:ILE:HD12	3:D:1190:ILE:N	2.37	0.40
3:D:370:LYS:HG3	3:D:371:LYS:H	1.85	0.40
2:C:1315:MET:HE2	3:D:473:THR:OG1	2.21	0.40
3:D:479:GLU:O	3:D:483:LEU:HB2	2.22	0.40
3:D:545:HIS:HA	3:D:546:ALA:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:816:THR:OG1	3:D:818:GLU:OE1	2.29	0.40
3:D:901:ARG:CB	3:D:908:ILE:HA	2.52	0.40
1:G:90:VAL:HG13	1:G:121:VAL:HG13	2.02	0.40
1:G:33:ARG:NH1	2:H:820:GLU:OE2	2.55	0.40
2:H:131:THR:HG22	2:H:135:THR:H	1.86	0.40
3:I:1159:ILE:HD12	3:I:1186:TYR:CE2	2.48	0.40
3:I:1297:LYS:NZ	3:I:1297:LYS:CA	2.81	0.40
3:I:139:LEU:HD22	3:I:139:LEU:C	2.42	0.40
3:I:27:PRO:HD3	3:I:236:TRP:CE3	2.57	0.40
5:X:11:LEU:HB3	5:X:15:ARG:NH1	2.36	0.40
5:Y:283:GLN:O	5:Y:287:ILE:HG13	2.22	0.40
1:B:178:SER:HA	1:B:179:PRO:HD3	1.91	0.40
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.56	0.40
2:C:1054:LEU:HD12	2:C:1054:LEU:O	2.21	0.40
2:C:1085:MET:HB3	2:C:1085:MET:HE2	1.96	0.40
2:C:1164:PHE:HB3	2:C:1168:GLU:HG2	2.04	0.40
2:C:161:LYS:HB3	2:C:161:LYS:NZ	2.36	0.40
2:C:539:THR:HB	2:C:540:ARG:H	1.65	0.40
2:C:931:VAL:HG21	2:C:944:ARG:CZ	2.52	0.40
3:D:1167:LYS:HB3	3:D:1170:LYS:HB2	2.03	0.40
3:D:1170:LYS:O	3:D:1173:ARG:HD2	2.21	0.40
3:D:292:VAL:HG13	3:D:293:ARG:N	2.36	0.40
3:D:52:GLU:OE1	5:X:451:ARG:HD2	2.21	0.40
3:D:514:THR:HG23	3:D:576:ARG:HE	1.87	0.40
3:D:663:GLU:O	3:D:667:GLN:HG3	2.22	0.40
3:D:749:LYS:CG	3:D:750:PRO:HD2	2.43	0.40
1:F:181:GLU:OE1	1:F:181:GLU:N	2.54	0.40
1:F:44:ARG:HA	1:F:183:ILE:HG21	2.03	0.40
2:H:468:LEU:HA	2:H:468:LEU:HD12	1.96	0.40
2:H:892:GLU:C	2:H:894:GLN:H	2.25	0.40
2:H:988:LYS:HB3	2:H:988:LYS:NZ	2.36	0.40
3:I:1174:ARG:HA	3:I:1192:LYS:HG3	2.03	0.40
3:I:1163:VAL:HG21	3:I:1198:VAL:HG11	2.03	0.40
3:I:1278:GLU:HG3	3:I:1279:GLN:H	1.86	0.40
3:I:1307:LEU:HD23	3:I:1307:LEU:H	1.86	0.40
5:Y:584:ARG:O	5:Y:587:ILE:HG22	2.20	0.40

There are no symmetry-related clashes.

## 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	
1	A	321/329 (98%)	266 (83%)	40 (12%)	15 (5%)	2	22
1	B	217/329 (66%)	187 (86%)	22 (10%)	8 (4%)	3	28
1	F	227/329 (69%)	196 (86%)	25 (11%)	6 (3%)	5	33
1	G	213/329 (65%)	187 (88%)	22 (10%)	4 (2%)	8	40
2	C	1333/1342 (99%)	1069 (80%)	216 (16%)	48 (4%)	3	29
2	H	1333/1342 (99%)	1069 (80%)	215 (16%)	49 (4%)	3	28
3	D	1154/1407 (82%)	918 (80%)	194 (17%)	42 (4%)	3	29
3	I	1154/1407 (82%)	920 (80%)	192 (17%)	42 (4%)	3	29
4	E	88/91 (97%)	78 (89%)	5 (6%)	5 (6%)	1	19
4	J	74/91 (81%)	65 (88%)	4 (5%)	5 (7%)	1	16
5	X	511/613 (83%)	449 (88%)	49 (10%)	13 (2%)	5	34
5	Y	454/613 (74%)	410 (90%)	34 (8%)	10 (2%)	6	37
All	All	7079/8222 (86%)	5814 (82%)	1018 (14%)	247 (4%)	3	29

All (247) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	319	GLU
1	B	20	SER
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE
2	C	43	PRO
2	C	110	PRO
2	C	114	VAL
2	C	170	VAL
2	C	661	VAL
2	C	669	PRO

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Mol	Chain	Res	Type
2	C	686	GLN
2	C	748	ILE
2	C	753	LEU
2	C	993	PRO
2	C	1185	PRO
2	C	1186	VAL
3	D	120	LEU
3	D	311	ARG
3	D	390	LEU
3	D	406	ALA
3	D	595	ALA
3	D	708	ASN
3	D	847	ASP
3	D	1268	ASN
3	D	1339	GLY
4	E	6	VAL
4	E	35	LYS
5	X	241	SER
5	X	490	PRO
1	F	52	PRO
1	G	52	PRO
2	H	21	VAL
2	H	39	ILE
2	H	79	VAL
2	H	110	PRO
2	H	114	VAL
2	H	661	VAL
2	H	748	ILE
2	H	993	PRO
2	H	1185	PRO
2	H	1341	ASP
3	I	120	LEU
3	I	390	LEU
3	I	404	GLU
3	I	406	ALA
3	I	595	ALA
3	I	710	ASP
3	I	851	PRO
3	I	1339	GLY
4	J	6	VAL
4	J	35	LYS
5	Y	241	SER

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Mol	Chain	Res	Type
1	A	193	GLU
1	B	19	VAL
1	B	188	GLU
2	C	53	PHE
2	C	79	VAL
2	C	437	ASN
2	C	699	LEU
2	C	1236	ASN
2	C	1239	VAL
2	C	1256	GLN
2	C	1341	ASP
3	D	89	GLY
3	D	155	GLU
3	D	255	LEU
3	D	316	ILE
3	D	404	GLU
3	D	417	ARG
3	D	542	ALA
3	D	590	SER
3	D	710	ASP
3	D	721	SER
3	D	851	PRO
3	D	901	ARG
3	D	913	GLU
3	D	914	ALA
5	X	23	THR
5	X	581	ASP
1	F	188	GLU
1	G	188	GLU
2	H	53	PHE
2	H	78	PRO
2	H	170	VAL
2	H	535	PRO
2	H	669	PRO
2	H	753	LEU
2	H	1186	VAL
2	H	1236	ASN
2	H	1239	VAL
2	H	1256	GLN
3	I	53	ARG
3	I	89	GLY
3	I	155	GLU

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Mol	Chain	Res	Type
3	I	345	LYS
3	I	417	ARG
3	I	542	ALA
3	I	707	ILE
3	I	708	ASN
3	I	721	SER
3	I	847	ASP
3	I	914	ALA
3	I	1268	ASN
4	J	4	VAL
5	Y	490	PRO
1	A	14	VAL
1	A	160	HIS
1	A	166	ARG
2	C	44	GLU
2	C	56	VAL
2	C	78	PRO
2	C	143	ARG
2	C	298	ALA
2	C	740	GLU
2	C	1107	MET
2	C	1240	ASP
2	C	1270	PHE
3	D	53	ARG
3	D	108	ALA
3	D	132	LEU
3	D	559	ALA
3	D	707	ILE
3	D	731	ARG
3	D	1344	LEU
3	D	1363	TYR
4	E	4	VAL
5	X	20	GLY
5	X	308	GLY
5	X	491	GLU
2	H	44	GLU
2	H	56	VAL
2	H	298	ALA
2	H	437	ASN
2	H	740	GLU
2	H	1270	PHE
3	I	108	ALA

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Mol	Chain	Res	Type
3	I	132	LEU
3	I	210	SER
3	I	255	LEU
3	I	559	ALA
3	I	731	ARG
3	I	901	ARG
3	I	913	GLU
3	I	1195	GLN
3	I	1363	TYR
5	Y	108	VAL
5	Y	308	GLY
5	Y	491	GLU
1	A	93	GLN
1	A	194	GLN
1	B	235	ARG
2	C	543	ALA
2	C	1003	THR
2	C	1080	ASN
2	C	1139	ALA
3	D	62	PHE
3	D	210	SER
3	D	596	LEU
3	D	1195	GLN
4	E	5	THR
5	X	50	ASP
5	X	504	PRO
5	X	567	MET
1	F	153	VAL
1	F	160	HIS
1	F	166	ARG
1	G	228	LEU
2	H	13	LYS
2	H	143	ARG
2	H	487	LEU
2	H	488	MET
2	H	699	LEU
2	H	895	LEU
2	H	1003	THR
2	H	1080	ASN
2	H	1093	PRO
2	H	1107	MET
2	H	1240	ASP

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Mol	Chain	Res	Type
3	I	62	PHE
3	I	598	LYS
3	I	888	CYS
3	I	1344	LEU
5	Y	504	PRO
5	Y	567	MET
5	Y	581	ASP
1	A	187	VAL
1	A	188	GLU
1	A	195	ARG
1	A	322	PRO
1	B	177	TYR
2	C	13	LYS
2	C	69	GLN
2	C	746	ALA
2	C	812	PHE
2	C	895	LEU
3	D	598	LYS
3	D	848	VAL
3	D	888	CYS
5	X	600	HIS
1	F	33	ARG
2	H	736	VAL
2	H	746	ALA
2	H	1046	VAL
2	H	1139	ALA
3	I	590	SER
3	I	596	LEU
4	J	5	THR
5	Y	600	HIS
1	A	163	GLU
1	B	49	SER
2	C	908	GLU
2	C	1093	PRO
2	C	1201	LEU
3	D	728	SER
3	D	855	ASP
3	D	1174	ARG
4	E	59	ILE
5	X	108	VAL
1	G	49	SER
2	H	516	ASP

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Mol	Chain	Res	Type
2	H	812	PHE
2	H	908	GLU
3	I	848	VAL
3	I	850	LYS
3	I	855	ASP
3	I	1192	LYS
3	I	1194	ARG
2	H	43	PRO
4	J	59	ILE
1	A	232	VAL
2	C	104	ILE
2	C	373	GLY
2	C	736	VAL
2	C	1046	VAL
5	X	35	ILE
2	H	104	ILE
1	A	153	VAL
2	H	373	GLY
3	D	850	LYS
5	Y	564	GLY
1	B	154	PRO
3	I	706	VAL
2	H	489	PRO
2	H	1181	PRO
2	C	1181	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	
1	A	281/286 (98%)	273 (97%)	8 (3%)	43	67
1	B	189/286 (66%)	186 (98%)	3 (2%)	62	79
1	F	197/286 (69%)	193 (98%)	4 (2%)	55	74
1	G	185/286 (65%)	179 (97%)	6 (3%)	39	64
2	C	1150/1157 (99%)	1083 (94%)	67 (6%)	20	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	1150/1157 (99%)	1085 (94%)	65 (6%)	20	52
3	D	971/1168 (83%)	920 (95%)	51 (5%)	22	54
3	I	971/1168 (83%)	920 (95%)	51 (5%)	22	54
4	E	74/75 (99%)	72 (97%)	2 (3%)	44	68
4	J	65/75 (87%)	63 (97%)	2 (3%)	40	65
5	X	460/540 (85%)	443 (96%)	17 (4%)	34	61
5	Y	407/540 (75%)	391 (96%)	16 (4%)	32	60
All	All	6100/7024 (87%)	5808 (95%)	292 (5%)	25	56

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	77	ASP
1	A	117	HIS
1	A	158	ARG
1	A	243	LYS
1	A	246	LYS
1	A	262	LEU
1	A	318	LEU
1	B	13	LEU
1	B	37	HIS
1	B	77	ASP
2	C	9	LYS
2	C	15	PHE
2	C	18	ARG
2	C	32	LEU
2	C	37	LYS
2	C	39	ILE
2	C	41	GLN
2	C	56	VAL
2	C	70	TYR
2	C	73	TYR
2	C	80	PHE
2	C	88	ARG
2	C	121	GLU
2	C	127	ILE
2	C	133	ASN
2	C	150	HIS
2	C	163	LYS

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Mol	Chain	Res	Type
2	C	464	PHE
2	C	479	LEU
2	C	487	LEU
2	C	600	THR
2	C	645	PHE
2	C	650	VAL
2	C	661	VAL
2	C	704	MET
2	C	711	ASP
2	C	741	MET
2	C	773	LEU
2	C	800	MET
2	C	807	TRP
2	C	817	LEU
2	C	845	LEU
2	C	908	GLU
2	C	920	VAL
2	C	941	LYS
2	C	944	ARG
2	C	953	LEU
2	C	955	GLN
2	C	964	LEU
2	C	975	ILE
2	C	994	ARG
2	C	1002	LEU
2	C	1010	GLN
2	C	1017	GLN
2	C	1032	LYS
2	C	1034	ARG
2	C	1042	LEU
2	C	1097	VAL
2	C	1106	ARG
2	C	1119	MET
2	C	1141	LEU
2	C	1146	GLN
2	C	1158	LYS
2	C	1180	MET
2	C	1209	GLN
2	C	1211	ARG
2	C	1233	LEU
2	C	1248	THR
2	C	1259	LEU

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Mol	Chain	Res	Type
2	C	1264	GLN
2	C	1265	PHE
2	C	1276	TRP
2	C	1288	GLN
2	C	1291	LEU
2	C	1326	LEU
2	C	1339	LEU
2	C	1341	ASP
3	D	13	LYS
3	D	20	ILE
3	D	31	ARG
3	D	50	LYS
3	D	92	VAL
3	D	114	ILE
3	D	133	ARG
3	D	139	LEU
3	D	140	TYR
3	D	141	PHE
3	D	151	MET
3	D	169	LEU
3	D	179	LYS
3	D	188	LEU
3	D	239	LEU
3	D	250	ARG
3	D	416	ILE
3	D	430	HIS
3	D	500	ILE
3	D	505	ASP
3	D	508	LEU
3	D	527	LEU
3	D	532	GLU
3	D	538	ARG
3	D	541	LEU
3	D	605	LEU
3	D	610	ARG
3	D	668	PHE
3	D	678	ARG
3	D	681	LYS
3	D	709	ARG
3	D	713	GLU
3	D	771	GLN
3	D	795	TYR

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Mol	Chain	Res	Type
3	D	816	THR
3	D	832	LYS
3	D	847	ASP
3	D	864	LEU
3	D	867	GLN
3	D	873	GLU
3	D	911	LYS
3	D	918	ILE
3	D	932	MET
3	D	933	ARG
3	D	1134	ILE
3	D	1148	ARG
3	D	1149	ARG
3	D	1188	GLU
3	D	1247	LYS
3	D	1306	LEU
3	D	1341	ARG
4	E	4	VAL
4	E	6	VAL
5	X	21	TYR
5	X	28	ASN
5	X	99	ARG
5	X	136	GLU
5	X	266	PHE
5	X	355	ILE
5	X	379	MET
5	X	384	LEU
5	X	400	GLN
5	X	452	ILE
5	X	457	ILE
5	X	476	ARG
5	X	495	ARG
5	X	545	HIS
5	X	562	ARG
5	X	565	ILE
5	X	607	LEU
1	F	37	HIS
1	F	77	ASP
1	F	158	ARG
1	F	160	HIS
1	G	13	LEU
1	G	37	HIS

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Mol	Chain	Res	Type
1	G	77	ASP
1	G	88	LEU
1	G	127	GLN
1	G	228	LEU
2	H	9	LYS
2	H	15	PHE
2	H	18	ARG
2	H	32	LEU
2	H	37	LYS
2	H	41	GLN
2	H	42	ASP
2	H	46	GLN
2	H	56	VAL
2	H	70	TYR
2	H	73	TYR
2	H	80	PHE
2	H	88	ARG
2	H	99	LYS
2	H	127	ILE
2	H	150	HIS
2	H	163	LYS
2	H	311	CYS
2	H	464	PHE
2	H	479	LEU
2	H	488	MET
2	H	514	PHE
2	H	600	THR
2	H	645	PHE
2	H	661	VAL
2	H	704	MET
2	H	711	ASP
2	H	773	LEU
2	H	800	MET
2	H	807	TRP
2	H	817	LEU
2	H	844	LYS
2	H	845	LEU
2	H	920	VAL
2	H	941	LYS
2	H	944	ARG
2	H	953	LEU
2	H	955	GLN

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Mol	Chain	Res	Type
2	H	964	LEU
2	H	971	LEU
2	H	975	ILE
2	H	994	ARG
2	H	1002	LEU
2	H	1005	GLU
2	H	1007	LYS
2	H	1010	GLN
2	H	1017	GLN
2	H	1032	LYS
2	H	1034	ARG
2	H	1042	LEU
2	H	1106	ARG
2	H	1119	MET
2	H	1141	LEU
2	H	1158	LYS
2	H	1180	MET
2	H	1209	GLN
2	H	1211	ARG
2	H	1233	LEU
2	H	1248	THR
2	H	1264	GLN
2	H	1288	GLN
2	H	1291	LEU
2	H	1326	LEU
2	H	1339	LEU
2	H	1341	ASP
3	I	31	ARG
3	I	50	LYS
3	I	92	VAL
3	I	114	ILE
3	I	133	ARG
3	I	139	LEU
3	I	140	TYR
3	I	141	PHE
3	I	151	MET
3	I	169	LEU
3	I	179	LYS
3	I	188	LEU
3	I	239	LEU
3	I	250	ARG
3	I	316	ILE

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Mol	Chain	Res	Type
3	I	325	LYS
3	I	416	ILE
3	I	430	HIS
3	I	500	ILE
3	I	505	ASP
3	I	527	LEU
3	I	532	GLU
3	I	538	ARG
3	I	541	LEU
3	I	594	GLN
3	I	605	LEU
3	I	610	ARG
3	I	668	PHE
3	I	678	ARG
3	I	681	LYS
3	I	709	ARG
3	I	771	GLN
3	I	795	TYR
3	I	816	THR
3	I	832	LYS
3	I	847	ASP
3	I	864	LEU
3	I	867	GLN
3	I	873	GLU
3	I	911	LYS
3	I	918	ILE
3	I	932	MET
3	I	933	ARG
3	I	1134	ILE
3	I	1148	ARG
3	I	1149	ARG
3	I	1247	LYS
3	I	1297	LYS
3	I	1306	LEU
3	I	1341	ARG
3	I	1369	ARG
4	J	4	VAL
4	J	6	VAL
5	Y	136	GLU
5	Y	266	PHE
5	Y	355	ILE
5	Y	371	LYS

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Mol	Chain	Res	Type
5	Y	379	MET
5	Y	384	LEU
5	Y	400	GLN
5	Y	452	ILE
5	Y	457	ILE
5	Y	476	ARG
5	Y	477	GLU
5	Y	545	HIS
5	Y	562	ARG
5	Y	565	ILE
5	Y	589	GLN
5	Y	607	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	75	GLN
1	A	227	GLN
1	A	239	GLN
1	B	66	HIS
1	B	84	ASN
2	C	69	GLN
2	C	238	GLN
2	C	273	HIS
2	C	314	ASN
2	C	510	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	673	HIS
2	C	684	ASN
2	C	799	ASN
2	C	955	GLN
2	C	1010	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1134	GLN
2	C	1146	GLN
2	C	1175	ASN
2	C	1220	GLN
2	C	1264	GLN

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Mol	Chain	Res	Type
3	D	94	GLN
3	D	164	GLN
3	D	364	HIS
3	D	419	HIS
3	D	477	GLN
3	D	504	GLN
3	D	519	ASN
3	D	875	ASN
3	D	921	GLN
3	D	1197	ASN
3	D	1268	ASN
3	D	1326	GLN
3	D	1350	ASN
4	E	31	GLN
5	X	8	GLN
5	X	28	ASN
5	X	30	HIS
5	X	40	GLN
5	X	46	GLN
5	X	54	GLN
5	X	301	ASN
5	X	406	GLN
5	X	437	GLN
5	X	446	GLN
5	X	461	ASN
5	X	469	GLN
2	H	46	GLN
2	H	69	GLN
2	H	238	GLN
2	H	510	GLN
2	H	513	GLN
2	H	517	GLN
2	H	526	HIS
2	H	684	ASN
2	H	686	GLN
2	H	725	GLN
2	H	799	ASN
2	H	894	GLN
2	H	922	ASN
2	H	952	GLN
2	H	1010	GLN
2	H	1134	GLN

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Mol	Chain	Res	Type
2	H	1175	ASN
2	H	1220	GLN
2	H	1264	GLN
2	H	1288	GLN
2	H	1313	HIS
3	I	274	ASN
3	I	300	GLN
3	I	309	ASN
3	I	419	HIS
3	I	477	GLN
3	I	504	GLN
3	I	519	ASN
3	I	1268	ASN
4	J	15	ASN
4	J	31	GLN
5	Y	242	HIS
5	Y	301	ASN
5	Y	342	GLN
5	Y	437	GLN
5	Y	461	ASN
5	Y	469	GLN
5	Y	589	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	1RM	H	1401	-	58,63,82	2.04	18 (31%)	82,96,120	1.72	18 (21%)
6	1RM	C	1401	-	76,82,82	1.81	14 (18%)	104,120,120	1.82	26 (25%)

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
6	1RM	H	1401	-	-	31/55/74/97	0/5/6/8
6	1RM	C	1401	-	-	40/68/97/97	0/7/8/8

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1401	1RM	O3-C6	7.86	1.52	1.37
6	C	1401	1RM	O3-C6	7.84	1.52	1.37
6	C	1401	1RM	C4-C10	5.03	1.51	1.43
6	H	1401	1RM	C4-C10	4.66	1.50	1.43
6	C	1401	1RM	C15-N1	4.64	1.45	1.35
6	C	1401	1RM	O7-C25	-4.55	1.37	1.44
6	H	1401	1RM	C15-N1	4.54	1.45	1.35
6	H	1401	1RM	O7-C25	-4.45	1.38	1.44
6	H	1401	1RM	C12-C11	-3.98	1.38	1.54
6	C	1401	1RM	C12-C11	-3.90	1.39	1.54
6	C	1401	1RM	C02-N3	3.43	1.43	1.37
6	H	1401	1RM	C02-N3	3.20	1.43	1.37
6	C	1401	1RM	C32-C22	-2.55	1.48	1.53
6	H	1401	1RM	C32-C22	-2.53	1.48	1.53
6	H	1401	1RM	C18-C17	2.39	1.50	1.43
6	H	1401	1RM	O-C06	2.32	1.42	1.36
6	C	1401	1RM	O9-C23	-2.28	1.37	1.43
6	C	1401	1RM	C18-C17	2.27	1.50	1.43
6	C	1401	1RM	O10-C21	-2.22	1.37	1.43
6	H	1401	1RM	O9-C23	-2.22	1.37	1.43
6	H	1401	1RM	O10-C21	-2.21	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	1RM	C3-C4	2.19	1.52	1.47
6	C	1401	1RM	O6-C27	-2.17	1.38	1.43
6	C	1401	1RM	C2-N1	2.16	1.45	1.38
6	H	1401	1RM	O6-C27	-2.15	1.38	1.43
6	H	1401	1RM	C14-C7	2.13	1.56	1.51
6	H	1401	1RM	C6-C7	2.10	1.43	1.39
6	H	1401	1RM	C2-N1	2.09	1.45	1.38
6	H	1401	1RM	C4-N3	-2.07	1.29	1.32
6	H	1401	1RM	C18-C19	2.04	1.41	1.33
6	C	1401	1RM	C14-C7	2.03	1.55	1.51
6	H	1401	1RM	C3-C4	2.03	1.51	1.47

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	1RM	C38-N02-C42	5.35	124.91	111.23
6	C	1401	1RM	C12-O3-C6	-4.90	99.42	107.68
6	H	1401	1RM	C12-O3-C6	-4.56	99.99	107.68
6	H	1401	1RM	O7-C35-C36	4.47	119.31	111.09
6	C	1401	1RM	O7-C35-C36	4.28	118.96	111.09
6	H	1401	1RM	C37-O6-C27	4.15	122.97	113.01
6	C	1401	1RM	C39-N01-C44	4.00	121.47	111.23
6	H	1401	1RM	O4-C11-C5	-3.75	124.65	131.81
6	C	1401	1RM	O4-C11-C5	-3.74	124.68	131.81
6	H	1401	1RM	C06-C02-N3	3.73	121.08	117.33
6	H	1401	1RM	C12-C11-C5	3.64	114.43	107.30
6	C	1401	1RM	C37-O6-C27	3.63	121.71	113.01
6	C	1401	1RM	C5-C10-C9	-3.61	113.08	119.66
6	C	1401	1RM	O-C06-C02	3.51	119.47	115.16
6	C	1401	1RM	C44-N01-C41	3.41	116.51	108.83
6	H	1401	1RM	C5-C10-C9	-3.35	113.56	119.66
6	C	1401	1RM	C12-C11-C5	3.32	113.80	107.30
6	C	1401	1RM	C06-C02-N3	3.21	121.78	118.97
6	H	1401	1RM	C31-C20-C21	3.18	117.97	111.31
6	C	1401	1RM	C18-C17-C16	-3.13	117.39	126.61
6	C	1401	1RM	C17-C18-C19	-3.08	117.07	124.53
6	C	1401	1RM	C25-O7-C35	3.03	122.41	117.72
6	C	1401	1RM	C31-C20-C21	2.99	117.58	111.31
6	H	1401	1RM	C18-C17-C16	-2.92	118.03	126.61
6	C	1401	1RM	C1-C9-C8	-2.88	115.72	119.17
6	H	1401	1RM	C25-O7-C35	2.84	122.12	117.72
6	H	1401	1RM	C17-C18-C19	-2.80	117.73	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	1RM	C43-C44-N01	2.78	116.34	110.64
6	C	1401	1RM	O01-C3-C2	2.58	119.36	116.12
6	C	1401	1RM	C6-C5-C11	-2.57	100.59	106.79
6	H	1401	1RM	O01-C3-C2	2.53	119.30	116.12
6	H	1401	1RM	C6-C5-C11	-2.34	101.15	106.79
6	H	1401	1RM	C1-C9-C8	-2.32	116.39	119.17
6	C	1401	1RM	C42-C41-N01	2.30	115.37	110.64
6	C	1401	1RM	C38-N02-C43	2.25	116.98	111.23
6	H	1401	1RM	C20-C19-C18	-2.24	121.46	126.16
6	C	1401	1RM	C39-N01-C41	2.19	116.85	111.23
6	C	1401	1RM	C12-O5-C29	2.17	123.21	117.84
6	C	1401	1RM	C20-C19-C18	-2.14	121.66	126.16
6	H	1401	1RM	C12-O5-C29	2.14	123.12	117.84
6	H	1401	1RM	C13-C12-C11	-2.14	108.60	113.90
6	C	1401	1RM	C8-C9-C10	2.13	123.77	119.41
6	H	1401	1RM	C30-C16-C17	-2.04	118.49	123.42
6	C	1401	1RM	O11-C15-N1	-2.01	119.64	123.92

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	1401	1RM	C11-C12-O5-C29
6	H	1401	1RM	C13-C12-O5-C29
6	H	1401	1RM	O3-C12-O5-C29
6	H	1401	1RM	C15-C16-C17-C18
6	H	1401	1RM	C30-C16-C17-C18
6	H	1401	1RM	C19-C20-C21-C22
6	H	1401	1RM	C19-C20-C21-O10
6	H	1401	1RM	C31-C20-C21-C22
6	H	1401	1RM	C21-C22-C23-C24
6	H	1401	1RM	C21-C22-C23-O9
6	H	1401	1RM	C32-C22-C23-C24
6	H	1401	1RM	C32-C22-C23-O9
6	H	1401	1RM	C23-C24-C25-C26
6	H	1401	1RM	C33-C24-C25-C26
6	H	1401	1RM	C33-C24-C25-O7
6	H	1401	1RM	O7-C25-C26-C34
6	H	1401	1RM	C26-C27-C28-C29
6	C	1401	1RM	C11-C12-O5-C29
6	C	1401	1RM	C13-C12-O5-C29
6	C	1401	1RM	O3-C12-O5-C29

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Mol	Chain	Res	Type	Atoms
6	C	1401	1RM	C30-C16-C17-C18
6	C	1401	1RM	C31-C20-C21-C22
6	C	1401	1RM	C21-C22-C23-C24
6	C	1401	1RM	C21-C22-C23-O9
6	C	1401	1RM	C32-C22-C23-C24
6	C	1401	1RM	C32-C22-C23-O9
6	C	1401	1RM	C23-C24-C25-C26
6	C	1401	1RM	C33-C24-C25-C26
6	C	1401	1RM	C33-C24-C25-O7
6	C	1401	1RM	O7-C25-C26-C34
6	C	1401	1RM	C26-C27-C28-C29
6	H	1401	1RM	C23-C24-C25-O7
6	C	1401	1RM	C23-C24-C25-O7
6	C	1401	1RM	C36-C35-O7-C25
6	H	1401	1RM	C17-C18-C19-C20
6	C	1401	1RM	C17-C18-C19-C20
6	C	1401	1RM	N01-C39-C40-N
6	H	1401	1RM	O7-C25-C26-C27
6	C	1401	1RM	O7-C25-C26-C27
6	C	1401	1RM	O8-C35-O7-C25
6	C	1401	1RM	C09-C38-N02-C42
6	H	1401	1RM	C31-C20-C21-O10
6	C	1401	1RM	C19-C20-C21-O10
6	C	1401	1RM	C19-C20-C21-C22
6	H	1401	1RM	O8-C35-O7-C25
6	H	1401	1RM	C36-C35-O7-C25
6	C	1401	1RM	C15-C16-C17-C18
6	H	1401	1RM	C28-C29-O5-C12
6	H	1401	1RM	C16-C17-C18-C19
6	C	1401	1RM	C31-C20-C21-O10
6	C	1401	1RM	C02-C06-O-C07
6	C	1401	1RM	C05-C06-O-C07
6	C	1401	1RM	C16-C17-C18-C19
6	C	1401	1RM	C28-C29-O5-C12
6	C	1401	1RM	N1-C15-C16-C17
6	C	1401	1RM	O11-C15-C16-C17
6	C	1401	1RM	O-C07-C08-C09
6	C	1401	1RM	O6-C27-C28-C29
6	H	1401	1RM	C24-C25-C26-C34
6	C	1401	1RM	C24-C25-C26-C34
6	C	1401	1RM	C39-C40-N-C
6	C	1401	1RM	C40-C39-N01-C44

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Mol	Chain	Res	Type	Atoms
6	C	1401	1RM	C39-C40-N-C46
6	H	1401	1RM	N1-C15-C16-C17
6	H	1401	1RM	O11-C15-C16-C17
6	H	1401	1RM	C28-C27-O6-C37
6	H	1401	1RM	O6-C27-C28-C29
6	C	1401	1RM	C24-C25-C26-C27
6	H	1401	1RM	C24-C25-C26-C27
6	C	1401	1RM	N1-C15-C16-C30
6	C	1401	1RM	O11-C15-C16-C30

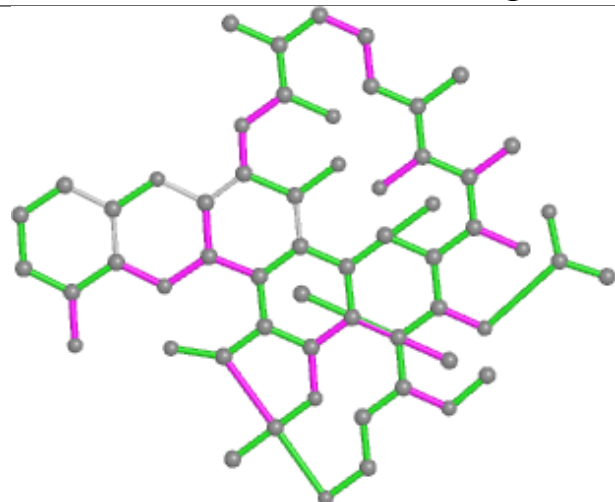
There are no ring outliers.

2 monomers are involved in 17 short contacts:

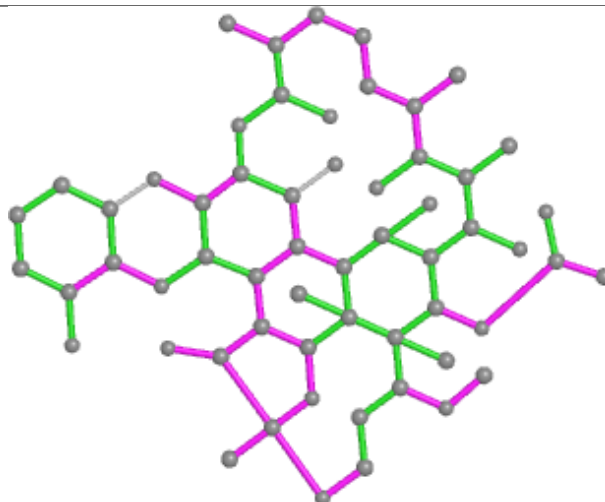
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1401	1RM	8	0
6	C	1401	1RM	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

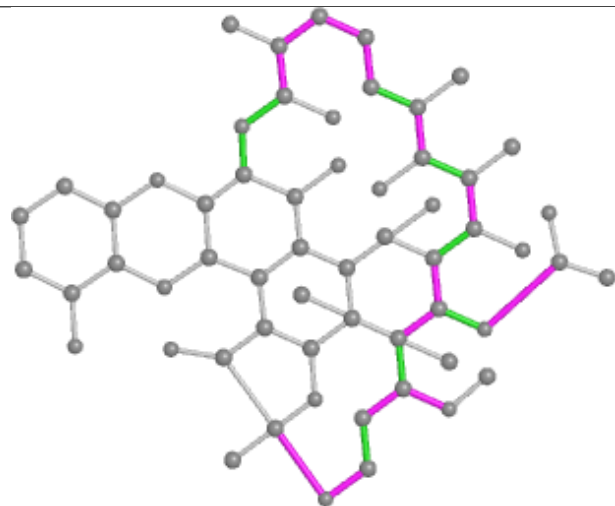
## Ligand 1RM H 1401



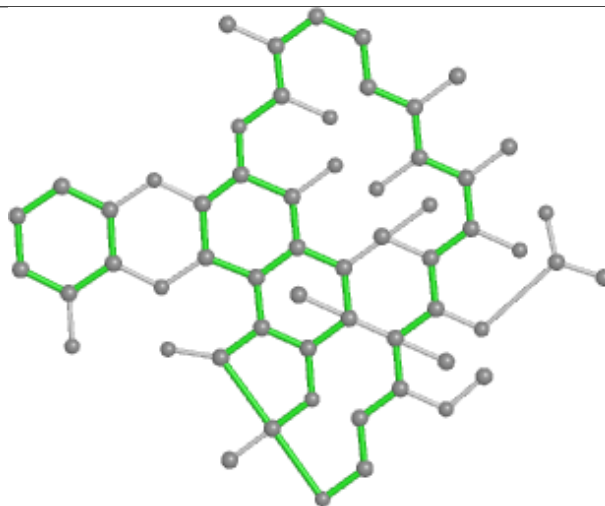
Bond lengths



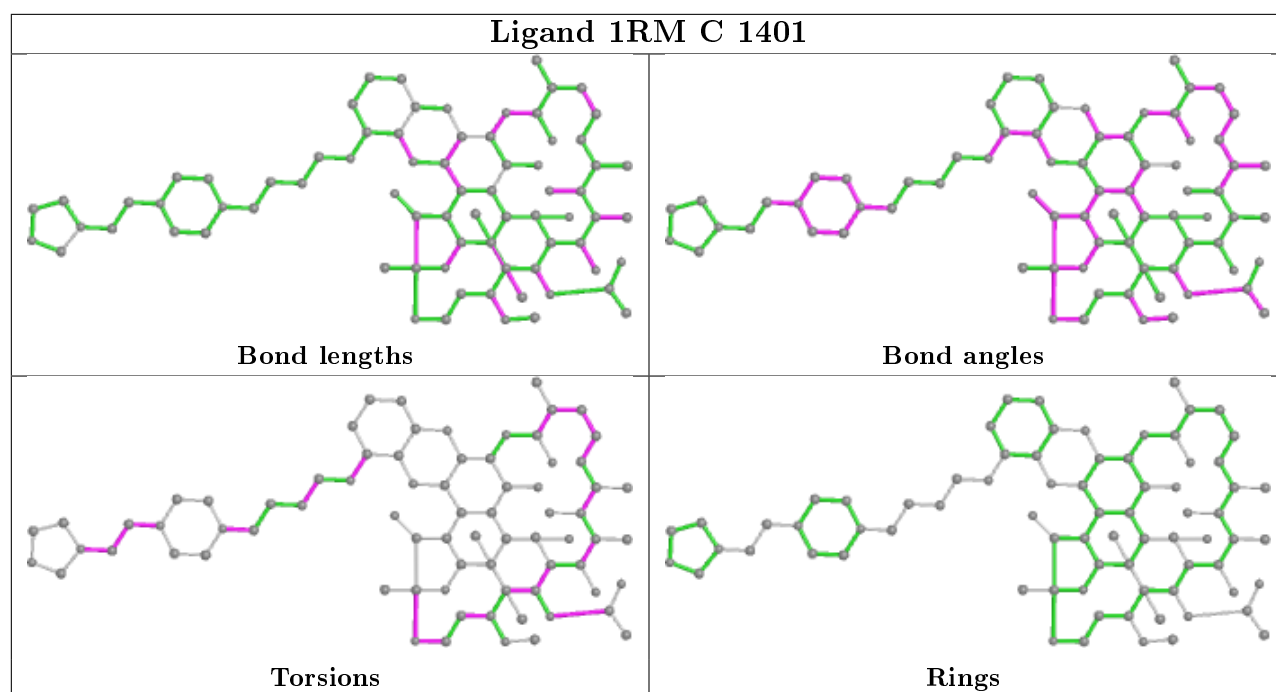
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	323/329 (98%)	-0.12	8 (2%) 57 43	0, 59, 154, 247	0
1	B	221/329 (67%)	0.14	11 (4%) 28 20	5, 86, 172, 210	0
1	F	229/329 (69%)	0.19	13 (5%) 23 16	20, 107, 186, 257	0
1	G	217/329 (65%)	0.26	15 (6%) 16 11	23, 106, 166, 211	0
2	C	1335/1342 (99%)	-0.22	38 (2%) 53 39	0, 35, 155, 279	0
2	H	1335/1342 (99%)	0.03	73 (5%) 25 17	1, 78, 192, 314	0
3	D	1160/1407 (82%)	-0.16	27 (2%) 60 47	0, 30, 149, 264	0
3	I	1160/1407 (82%)	-0.01	52 (4%) 33 23	1, 49, 170, 288	0
4	E	90/91 (98%)	-0.40	1 (1%) 80 70	0, 32, 101, 141	0
4	J	76/91 (83%)	-0.06	3 (3%) 39 27	7, 72, 156, 198	0
5	X	517/613 (84%)	0.11	36 (6%) 16 10	1, 95, 219, 329	0
5	Y	458/613 (74%)	0.11	28 (6%) 21 14	2, 98, 217, 320	0
All	All	7121/8222 (86%)	-0.04	305 (4%) 35 25	0, 62, 183, 329	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	10	ALA	11.8
2	H	1002	LEU	9.5
2	H	1003	THR	7.8
5	Y	239	GLY	7.6
5	X	24	TYR	7.2
3	I	11	GLN	7.2
3	I	212	THR	7.0
2	C	311	CYS	6.9
2	H	998	LEU	6.9
5	Y	212	ILE	6.9
5	Y	337	VAL	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	238	GLN	6.1
1	F	162	GLU	6.0
2	H	982	GLY	5.9
2	H	986	ALA	5.9
5	Y	315	TRP	5.8
5	Y	319	ALA	5.8
5	X	319	ALA	5.7
5	Y	318	ALA	5.6
2	C	231	GLU	5.6
3	D	1203	ARG	5.6
2	H	1004	ASP	5.5
3	I	12	THR	5.4
2	C	282	VAL	5.4
5	Y	310	GLU	5.4
5	X	306	PHE	5.3
3	D	1171	GLY	5.3
2	C	251	ALA	5.1
2	H	981	ALA	5.1
2	H	332	ARG	5.0
2	H	258	ASN	5.0
5	Y	320	ILE	5.0
3	I	1203	ARG	4.9
3	I	9	LYS	4.8
3	I	1167	LYS	4.7
5	Y	293	GLU	4.7
5	X	289	LYS	4.7
5	X	52	GLY	4.7
5	X	305	LEU	4.6
3	I	540	GLY	4.6
2	H	999	GLU	4.6
5	X	56	MET	4.6
5	X	307	THR	4.5
2	C	165	HIS	4.5
5	Y	311	THR	4.5
3	I	13	LYS	4.4
3	I	830	ASP	4.4
2	C	267	ARG	4.4
2	C	483	ASP	4.4
2	C	116	ASP	4.4
2	H	1000	LEU	4.3
5	Y	317	ASN	4.3
5	X	313	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	232	ILE	4.2
2	H	1001	GLY	4.2
3	I	1161	GLY	4.2
5	Y	305	LEU	4.2
5	X	293	GLU	4.2
5	Y	340	ALA	4.2
3	I	563	LEU	4.1
1	G	12	ARG	4.1
2	H	334	GLU	4.1
2	H	60	GLN	4.1
2	C	237	LEU	4.0
1	G	157	THR	4.0
5	X	53	ILE	4.0
1	G	171	LEU	4.0
1	B	147	GLN	4.0
2	C	332	ARG	3.9
2	H	990	ASP	3.9
5	X	27	VAL	3.9
1	F	148	ARG	3.9
2	H	375	PRO	3.9
5	Y	322	MET	3.9
2	H	969	ALA	3.9
3	D	1170	LYS	3.9
2	H	1020	GLU	3.8
3	I	521	LYS	3.8
2	C	266	GLY	3.8
1	B	169	GLY	3.8
2	H	1006	GLU	3.8
5	X	325	PRO	3.7
1	F	194	GLN	3.7
3	I	208	THR	3.7
5	X	310	GLU	3.7
5	X	43	ASP	3.7
1	G	172	LEU	3.7
2	H	970	GLY	3.6
5	Y	489	MET	3.6
3	D	878	ASP	3.6
3	D	830	ASP	3.6
2	C	1002	LEU	3.5
2	H	165	HIS	3.5
2	H	974	ARG	3.5
2	C	250	THR	3.5

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Mol	Chain	Res	Type	RSRZ
3	I	205	LEU	3.4
4	J	2	ALA	3.4
2	C	230	PHE	3.4
2	C	67	GLU	3.4
3	I	708	ASN	3.4
2	C	265	LYS	3.3
5	X	340	ALA	3.3
1	G	107	ILE	3.3
5	X	54	GLN	3.3
5	Y	307	THR	3.3
5	X	35	ILE	3.3
5	X	315	TRP	3.3
3	I	213	LYS	3.3
3	I	216	LYS	3.3
2	H	975	ILE	3.3
3	I	876	SER	3.2
2	H	987	GLU	3.2
4	E	91	ARG	3.2
2	H	984	VAL	3.2
3	I	675	ALA	3.2
2	H	972	PHE	3.1
5	X	328	GLU	3.1
2	C	233	ARG	3.1
2	C	172	TYR	3.1
3	I	8	LEU	3.1
2	C	264	GLU	3.1
3	I	732	GLY	3.1
2	H	107	ARG	3.1
1	A	41	ASN	3.1
3	I	177	ASP	3.1
5	X	36	VAL	3.1
5	Y	336	GLU	3.1
2	H	983	GLY	3.0
3	I	564	VAL	3.0
2	H	742	TYR	3.0
3	I	541	LEU	3.0
2	H	333	ILE	3.0
5	X	425	TYR	3.0
5	Y	316	PHE	3.0
2	H	1005	GLU	2.9
3	D	333	GLY	2.9
3	I	204	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	163	LYS	2.9
3	D	1199	PHE	2.9
3	I	1295	ASN	2.9
3	I	1162	ILE	2.9
3	I	1179	PRO	2.9
2	H	232	ILE	2.9
3	D	932	MET	2.9
3	I	1273	ASP	2.9
3	D	1196	LEU	2.9
5	X	6	GLN	2.9
1	F	161	SER	2.9
1	B	171	LEU	2.9
2	C	310	ILE	2.8
3	D	1185	PRO	2.8
3	I	1172	LYS	2.8
1	F	193	GLU	2.8
2	C	236	LYS	2.8
1	G	191	ARG	2.8
3	I	1166	GLY	2.8
1	G	18	GLN	2.8
2	H	104	ILE	2.8
2	H	662	SER	2.8
1	B	168	ILE	2.8
3	I	80	HIS	2.7
2	H	473	ARG	2.7
2	C	305	SER	2.7
5	X	57	GLU	2.7
5	Y	341	LEU	2.7
5	X	241	SER	2.7
5	Y	214	PRO	2.7
2	H	1019	ASP	2.7
2	H	264	GLU	2.7
1	F	184	ALA	2.7
2	H	1010	GLN	2.7
3	D	80	HIS	2.7
5	Y	421	TYR	2.7
3	I	174	ASP	2.7
1	B	70	THR	2.7
5	Y	321	ALA	2.7
1	A	245	GLU	2.6
2	H	230	PHE	2.6
3	D	855	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	61	SER	2.6
3	I	1294	ALA	2.6
3	D	477	GLN	2.6
1	F	205	MET	2.6
5	Y	478	PRO	2.6
2	H	169	LYS	2.5
5	Y	538	GLU	2.5
2	H	988	LYS	2.5
3	I	674	THR	2.5
1	B	41	ASN	2.5
1	G	13	LEU	2.5
1	F	19	VAL	2.5
1	F	164	ASP	2.5
5	X	31	LEU	2.5
2	H	103	VAL	2.5
2	H	269	ILE	2.5
1	A	40	GLY	2.5
5	Y	578	LYS	2.5
1	B	146	VAL	2.4
1	G	87	GLY	2.4
2	C	164	THR	2.4
3	D	314	ARG	2.4
5	X	477	GLU	2.4
3	D	1133	ASP	2.4
2	C	312	ALA	2.4
2	C	103	VAL	2.4
5	Y	574	GLU	2.4
5	X	478	PRO	2.4
2	H	996	ARG	2.4
2	C	1000	LEU	2.4
2	H	483	ASP	2.4
3	D	1198	VAL	2.4
4	J	26	ARG	2.4
1	F	204	GLU	2.4
2	C	543	ALA	2.4
2	C	319	LEU	2.4
5	X	20	GLY	2.4
2	H	1032	LYS	2.4
2	H	725	GLN	2.3
2	H	718	ALA	2.3
5	X	318	ALA	2.3
5	Y	573	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	414	ILE	2.3
3	D	1186	TYR	2.3
2	H	231	GLU	2.3
3	I	133	ARG	2.3
5	X	283	GLN	2.3
5	X	317	ASN	2.3
1	F	24	ALA	2.3
1	A	193	GLU	2.3
3	D	547	ARG	2.3
3	D	831	VAL	2.3
2	C	57	PHE	2.3
2	H	973	SER	2.3
1	G	122	GLU	2.3
2	H	997	TRP	2.3
2	C	271	ALA	2.3
1	G	24	ALA	2.3
1	A	324	ALA	2.2
5	X	64	ASP	2.2
2	H	167	SER	2.2
2	H	1008	GLN	2.2
3	D	1179	PRO	2.2
5	X	239	GLY	2.2
1	A	242	VAL	2.2
1	B	194	GLN	2.2
3	D	419	HIS	2.2
1	G	28	LEU	2.2
2	C	333	ILE	2.2
2	H	254	ASP	2.2
3	I	333	GLY	2.2
3	I	154	LEU	2.2
3	I	586	GLY	2.2
5	X	401	PHE	2.2
3	I	218	THR	2.2
2	C	1134	GLN	2.2
2	H	252	SER	2.2
2	H	978	VAL	2.2
2	H	908	GLU	2.2
2	C	306	THR	2.1
2	H	979	LEU	2.1
2	H	1025	PHE	2.1
2	C	1001	GLY	2.1
3	D	82	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	233	ARG	2.1
1	B	152	TYR	2.1
1	G	96	ASP	2.1
1	B	67	GLU	2.1
1	A	323	PRO	2.1
1	F	176	CYS	2.1
2	H	111	GLU	2.1
2	H	374	GLU	2.1
2	H	62	TYR	2.1
3	D	1172	LYS	2.1
3	I	712	GLN	2.1
2	C	58	PRO	2.1
1	G	86	LYS	2.1
2	H	492	MET	2.1
3	I	832	LYS	2.1
1	G	26	VAL	2.1
2	H	1029	LEU	2.1
3	D	263	SER	2.1
5	Y	328	GLU	2.1
2	H	906	PHE	2.1
3	I	1297	LYS	2.1
3	I	392	THR	2.1
1	A	162	GLU	2.1
2	H	985	GLU	2.1
3	D	211	GLU	2.1
5	X	515	GLU	2.1
3	I	222	LYS	2.0
3	I	528	THR	2.0
3	I	831	VAL	2.0
4	J	77	ALA	2.0
3	I	855	ASP	2.0
2	H	265	LYS	2.0
3	D	528	THR	2.0
1	F	163	GLU	2.0
3	D	81	ARG	2.0
3	I	1177	ILE	2.0
1	B	121	VAL	2.0
2	H	168	GLY	2.0
2	H	251	ALA	2.0
2	C	318	SER	2.0
3	I	716	GLN	2.0
3	I	210	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

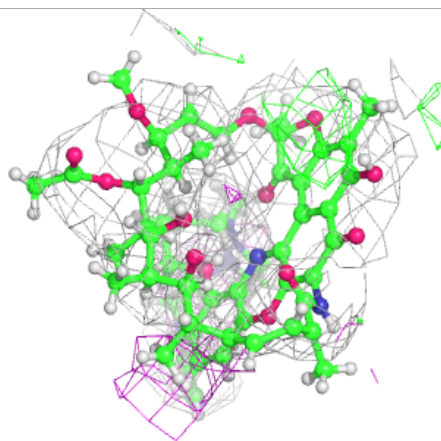
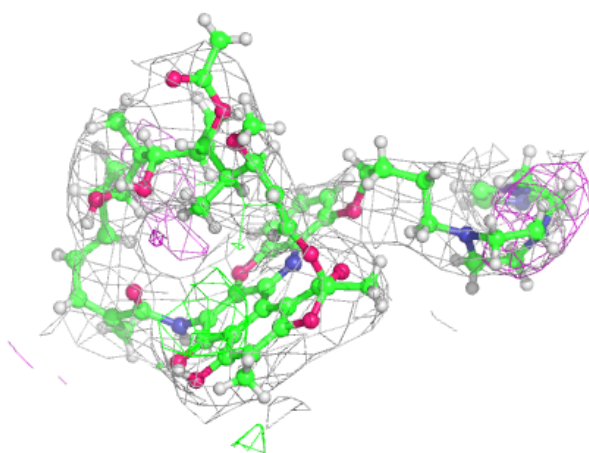
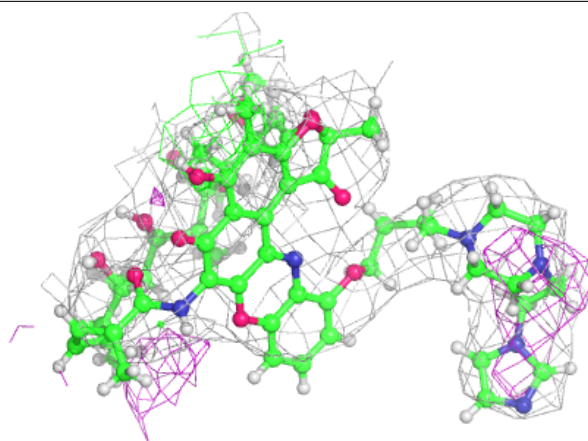
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	1RM	C	1401	75/75	0.76	0.37	20,20,20,20	0
6	1RM	H	1401	58/75	0.83	0.32	20,20,20,20	0
8	MG	D	1503	1/1	0.86	0.49	24,24,24,24	0
8	MG	I	1503	1/1	0.93	0.74	20,20,20,20	0
7	ZN	I	1501	1/1	0.96	0.10	60,60,60,60	0
7	ZN	I	1502	1/1	0.97	0.15	49,49,49,49	0
7	ZN	D	1502	1/1	0.97	0.20	8,8,8,8	0
7	ZN	D	1501	1/1	0.98	0.10	54,54,54,54	0

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

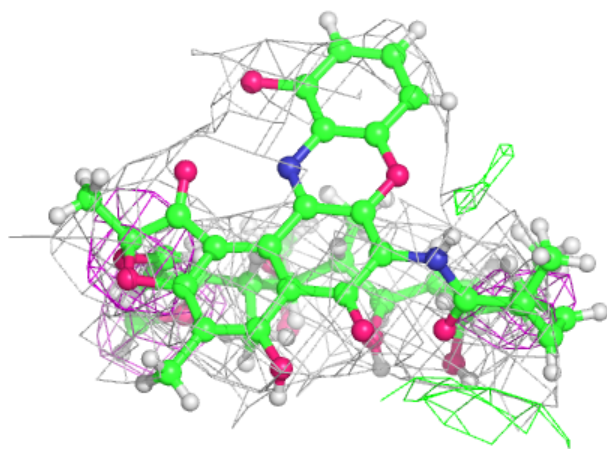
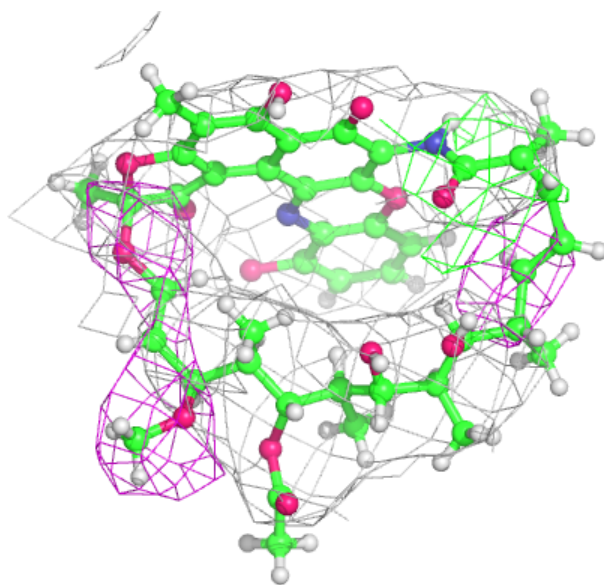
**Electron density around 1RM C 1401:**

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



**Electron density around 1RM H 1401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.