



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:43 am GMT

PDB ID : 1DE4  
Title : HEMOCHROMATOSIS PROTEIN HFE COMPLEXED WITH TRANSFERRIN RECEPTOR  
Authors : Bennett, M.J.; Lebron, J.A.; Bjorkman, P.J.  
Deposited on : 1999-11-12  
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

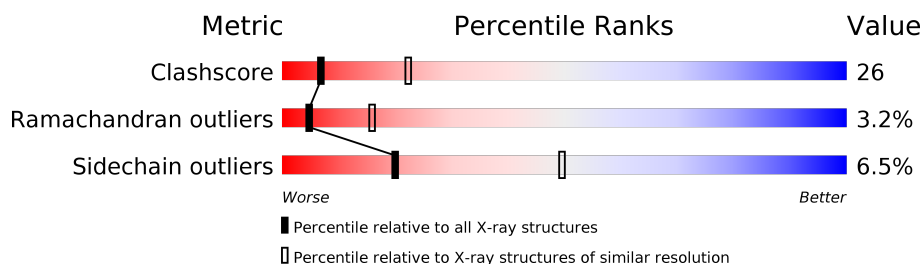
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	
1	D	275	
1	G	275	
2	B	99	
2	E	99	
2	H	99	
3	C	640	

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Mol	Chain	Length	Quality of chain
3	F	640	<div><div></div><div>56%39%5% •</div></div>
3	I	640	<div><div></div><div>58%36%5% •</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24315 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HEMOCHROMATOSIS PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			
1	D	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			
1	G	272	Total	C	N	O	S	0	0	0
			2242	1424	390	416	12			

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			
2	E	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			
2	H	99	Total	C	N	O	S	0	0	0
			821	522	138	158	3			

- Molecule 3 is a protein called TRANSFERRIN RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			
3	F	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			
3	I	635	Total	C	N	O	S	0	0	0
			5022	3223	845	940	14			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

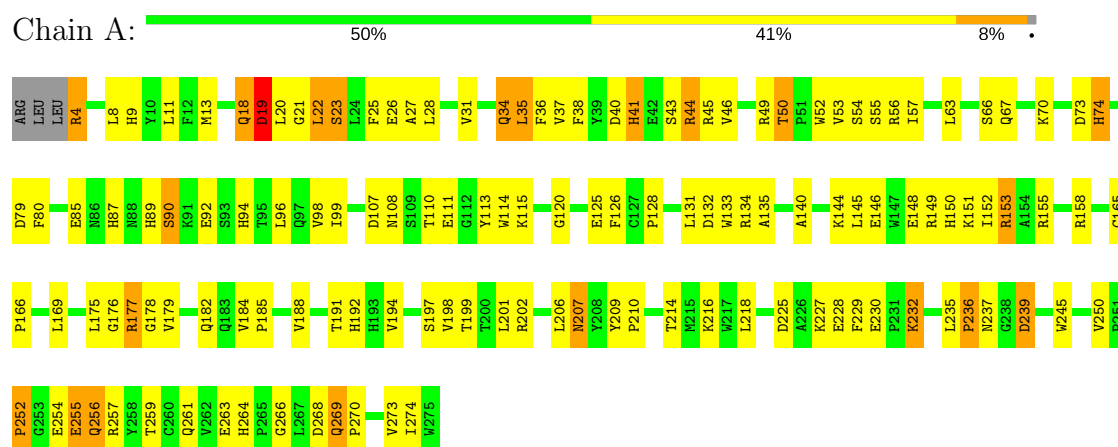
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	4	Total	O	0	0
			4	4		
7	F	2	Total	O	0	0
			2	2		
7	I	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

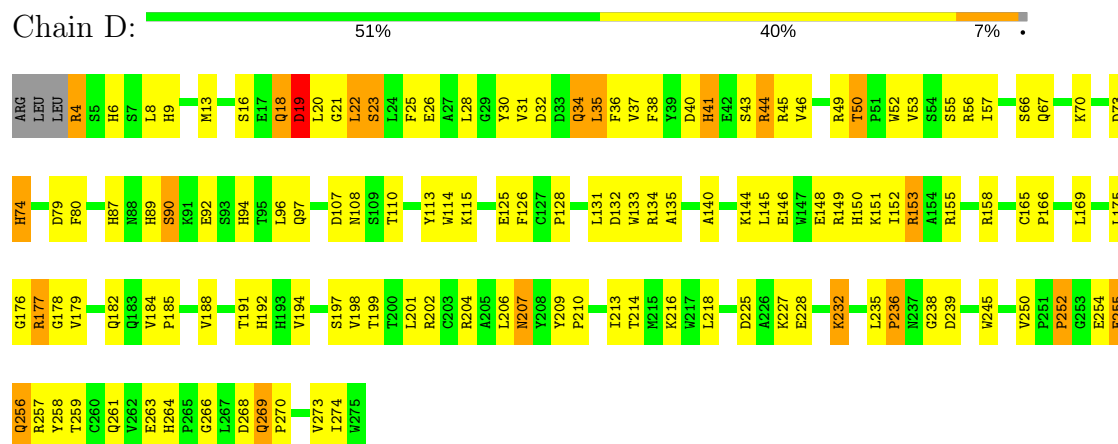
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

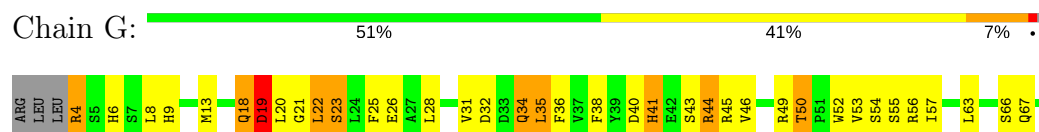
#### • Molecule 1: HEMOCHROMATOSIS PROTEIN

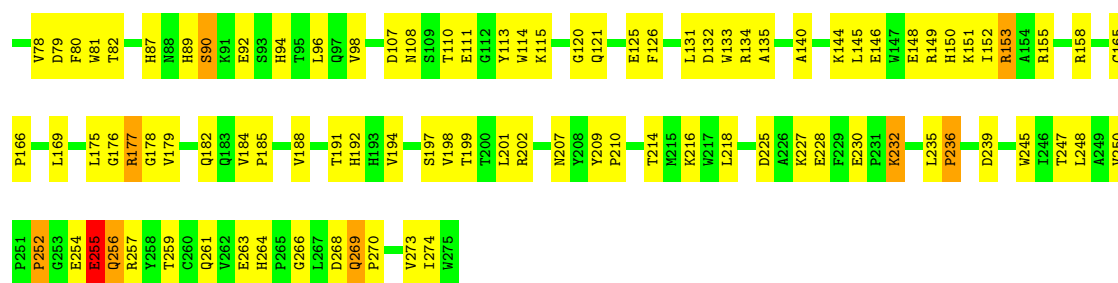


#### • Molecule 1: HEMOCHROMATOSIS PROTEIN



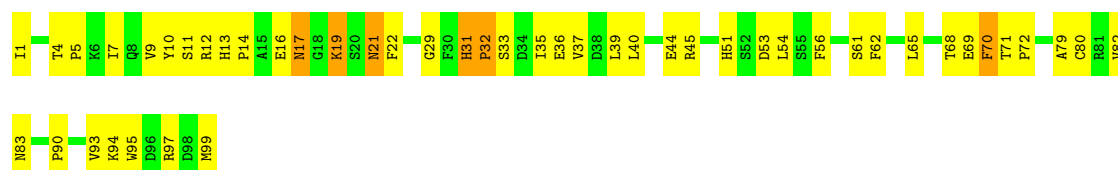
#### • Molecule 1: HEMOCHROMATOSIS PROTEIN





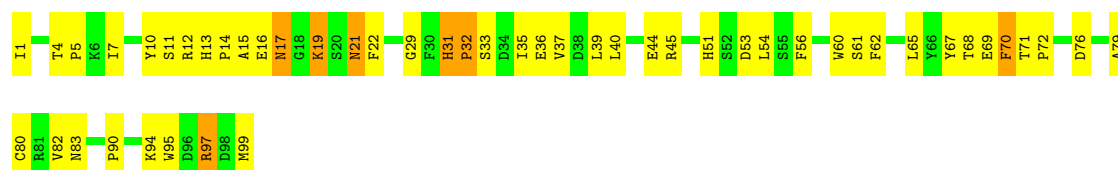
• Molecule 2: BETA-2-MICROGLOBULIN

Chain B: 52% 42% 6%



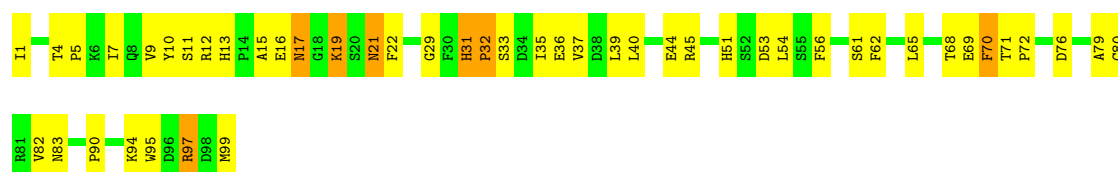
• Molecule 2: BETA-2-MICROGLOBULIN

Chain E: 49% 43% 7%



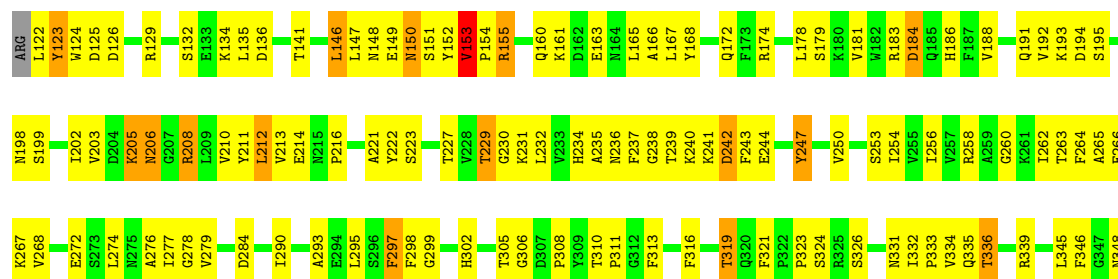
• Molecule 2: BETA-2-MICROGLOBULIN

Chain H: 52% 41% 7%



• Molecule 3: TRANSFERRIN RECEPTOR

Chain C: 55% 39% 5%







K371	L501	V586	H699
N372	L502	A587	V700
K374	L506	R588	F701
L375	E507	A589	W702
T376	K508	A590	G703
N377	T509	E591	S704
S378	M510	E592	G705
	Q511	V593	S706
I386	N512	A594	H707
	V513	Q595	T708
F390	K514	F597	L709
	H515	V598	P710
Y402	P516	I599	A711
	V517	K600	L712
R409	T518	H603	L713
G413	Q519	N608	L716
P414	Q520		K717
		Y611	L718
S419	W528	E612	Q721
K428	A529	L618	N722
		L619	N723
N432	E533		G724
	K534	V622	A725
D435	L535	R623	F726
K439	N539	L624	N727
D440	A540	G626	E728
G441	A541	Q627	R732
	F542	Y628	
S447	P543	R629	N747
I448	F544		D752
	S548	I632	V753
V453	P551	H635	I756
S454	A552		ASP
A455	V553	L639	ASN
F458	S554	Q640	GLU
	F555	Y643	PHE
V461	C556		
	F557	R646	
L467	C558		
	E559	R655	
Y470	M570	L656	
L474	D571	T657	
	T572		
F479	Y573	E664	
	K574	R665	
N483	E575	T666	
		D667	
N493	R579	V670	
F494	I580		
K495		E682	
V496	L583		
S497	N584		
A498	K585	V690	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.40Å 144.40Å 327.10Å 90.00° 93.60° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	94.3 (30.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.231 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.34	0/2310	0.60	0/3143
1	D	0.34	0/2310	0.60	0/3143
1	G	0.35	0/2310	0.60	0/3143
2	B	0.33	0/844	0.56	0/1144
2	E	0.34	0/844	0.56	0/1144
2	H	0.33	0/844	0.56	0/1144
3	C	0.40	0/5142	0.65	2/6973 (0.0%)
3	F	0.40	0/5142	0.65	1/6973 (0.0%)
3	I	0.43	0/5142	0.66	2/6973 (0.0%)
All	All	0.38	0/24888	0.63	5/33780 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	557	PHE	N-CA-C	-6.66	93.01	111.00
3	F	557	PHE	N-CA-C	-6.58	93.23	111.00
3	I	557	PHE	N-CA-C	-6.44	93.61	111.00
3	C	363	CYS	CA-CB-SG	5.07	123.13	114.00
3	I	363	CYS	CA-CB-SG	5.03	123.05	114.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2242	0	2126	136	0
1	D	2242	0	2126	139	0
1	G	2242	0	2126	133	0
2	B	821	0	772	51	0
2	E	821	0	772	55	0
2	H	821	0	772	50	0
3	C	5022	0	4965	253	0
3	F	5022	0	4965	250	0
3	I	5022	0	4965	238	0
4	C	14	0	13	0	0
4	F	14	0	13	0	0
4	I	14	0	13	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
6	G	6	0	8	3	0
7	C	4	0	0	0	0
7	F	2	0	0	0	0
7	I	3	0	0	0	0
All	All	24315	0	23636	1231	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 26.

All (1231) 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)
3:C:708:THR:HG22	3:C:711:ALA:H	1.18	1.09
3:C:708:THR:HG23	3:C:710:PRO:HD2	1.29	1.08
3:I:708:THR:HG23	3:I:710:PRO:HD2	1.29	1.07
3:F:708:THR:HG23	3:F:710:PRO:HD2	1.31	1.04
3:I:708:THR:HG22	3:I:711:ALA:H	1.18	1.03
3:F:708:THR:HG22	3:F:711:ALA:H	1.19	1.02
3:I:493:ASN:HD22	3:I:495:LYS:HZ1	1.03	1.00
3:I:539:ASN:HD22	3:I:541:ALA:H	1.11	0.99
3:C:493:ASN:HD22	3:C:495:LYS:HZ1	1.05	0.97
3:C:539:ASN:HD22	3:C:541:ALA:H	1.10	0.96
1:A:146:GLU:HG2	3:C:640:GLN:HE21	1.31	0.96
3:F:239:THR:HG22	3:F:241:LYS:H	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:515:HIS:HD2	3:F:517:VAL:H	1.14	0.95
3:F:539:ASN:HD22	3:F:541:ALA:H	1.14	0.95
3:C:515:HIS:HD2	3:C:517:VAL:H	1.12	0.94
1:D:22:LEU:HD12	3:F:619:LEU:HD23	1.48	0.94
3:F:493:ASN:HD22	3:F:495:LYS:HZ1	1.04	0.93
3:I:202:ILE:HB	3:I:211:TYR:HB2	1.50	0.93
1:D:202:ARG:HE	2:E:99:MET:HG2	1.33	0.92
3:I:239:THR:HG22	3:I:241:LYS:H	1.35	0.91
3:I:515:HIS:HD2	3:I:517:VAL:H	1.14	0.91
3:C:239:THR:HG22	3:C:241:LYS:H	1.35	0.91
3:I:204:ASP:O	3:I:206:ASN:N	2.05	0.90
1:G:146:GLU:HG2	3:I:640:GLN:HE21	1.37	0.88
3:C:664:GLU:CD	3:C:664:GLU:H	1.80	0.85
2:E:31:HIS:HB3	2:E:32:PRO:HD3	1.58	0.85
2:B:31:HIS:HB3	2:B:32:PRO:HD3	1.57	0.84
2:H:31:HIS:HB3	2:H:32:PRO:HD3	1.59	0.84
3:F:664:GLU:H	3:F:664:GLU:CD	1.80	0.83
3:I:708:THR:HG23	3:I:710:PRO:CD	2.09	0.83
3:C:386:ILE:HG23	3:C:454:SER:HB3	1.61	0.83
1:A:146:GLU:HG2	3:C:640:GLN:NE2	1.95	0.82
3:I:664:GLU:H	3:I:664:GLU:CD	1.83	0.81
3:F:386:ILE:HG23	3:F:454:SER:HB3	1.60	0.81
3:C:239:THR:HB	3:C:242:ASP:OD1	1.81	0.80
3:C:655:ARG:HH11	3:C:655:ARG:HB2	1.45	0.80
3:C:153:VAL:HG23	3:C:154:PRO:HD2	1.64	0.80
3:F:655:ARG:HB2	3:F:655:ARG:HH11	1.44	0.80
3:C:515:HIS:CD2	3:C:517:VAL:H	1.99	0.80
3:C:708:THR:HG23	3:C:710:PRO:CD	2.10	0.80
2:E:79:ALA:HB2	2:E:94:LYS:HA	1.63	0.80
1:G:57:ILE:HA	1:G:175:LEU:HD21	1.64	0.80
1:D:206:LEU:HD11	2:E:14:PRO:HD3	1.62	0.79
2:B:79:ALA:HB2	2:B:94:LYS:HA	1.63	0.79
2:H:79:ALA:HB2	2:H:94:LYS:HA	1.64	0.79
3:I:386:ILE:HG23	3:I:454:SER:HB3	1.62	0.79
3:I:153:VAL:HG23	3:I:154:PRO:HD2	1.64	0.79
3:I:539:ASN:ND2	3:I:541:ALA:H	1.81	0.79
3:F:708:THR:HG23	3:F:710:PRO:CD	2.11	0.79
1:G:26:GLU:HG3	1:G:41:HIS:ND1	1.98	0.79
1:G:36:PHE:HB2	1:G:53:VAL:HG11	1.65	0.78
3:I:239:THR:HB	3:I:242:ASP:OD1	1.83	0.78
1:D:26:GLU:HG3	1:D:41:HIS:ND1	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:153:VAL:HG23	3:F:154:PRO:HD2	1.64	0.78
1:A:57:ILE:HA	1:A:175:LEU:HD21	1.65	0.77
3:C:539:ASN:ND2	3:C:541:ALA:H	1.82	0.77
3:F:239:THR:HB	3:F:242:ASP:OD1	1.84	0.77
1:D:22:LEU:HD12	3:F:619:LEU:CD2	2.14	0.77
1:A:36:PHE:HB2	1:A:53:VAL:HG11	1.66	0.77
1:D:36:PHE:HB2	1:D:53:VAL:HG11	1.65	0.77
1:A:26:GLU:HG3	1:A:41:HIS:ND1	2.00	0.77
3:I:655:ARG:HH11	3:I:655:ARG:HB2	1.47	0.76
1:D:202:ARG:NE	2:E:99:MET:HG2	2.01	0.76
3:I:209:LEU:HD12	3:I:210:VAL:H	1.49	0.76
1:G:146:GLU:HG2	3:I:640:GLN:NE2	2.01	0.76
1:D:198:VAL:HA	1:D:252:PRO:HG3	1.67	0.76
3:F:515:HIS:CD2	3:F:517:VAL:H	2.02	0.76
1:G:56:ARG:O	1:G:175:LEU:HD11	1.85	0.76
1:D:145:LEU:HD22	1:D:149:ARG:NH2	2.01	0.76
6:G:309:GOL:H32	3:I:646:ARG:HH21	1.51	0.76
1:D:259:THR:HG22	1:D:274:ILE:HG22	1.67	0.75
1:D:268:ASP:HB2	1:D:269:GLN:HE21	1.51	0.75
1:D:57:ILE:HA	1:D:175:LEU:HD21	1.66	0.75
1:A:268:ASP:HB2	1:A:269:GLN:HE21	1.52	0.75
3:F:495:LYS:HD3	3:F:558:CYS:SG	2.27	0.75
1:G:259:THR:HG22	1:G:274:ILE:HG22	1.68	0.75
3:F:539:ASN:ND2	3:F:541:ALA:H	1.84	0.75
1:A:259:THR:HG22	1:A:274:ILE:HG22	1.69	0.75
1:G:268:ASP:HB2	1:G:269:GLN:HE21	1.51	0.75
1:A:202:ARG:HE	2:B:99:MET:HG2	1.50	0.74
3:F:655:ARG:CB	3:F:655:ARG:HH11	1.99	0.74
1:G:165:CYS:HB3	1:G:166:PRO:HD3	1.69	0.74
1:D:56:ARG:O	1:D:175:LEU:HD11	1.86	0.74
1:D:146:GLU:HG2	3:F:640:GLN:HE21	1.52	0.74
1:D:207:ASN:HD21	2:E:13:HIS:CD2	2.04	0.74
3:C:202:ILE:HB	3:C:211:TYR:HB2	1.68	0.74
1:D:21:GLY:C	1:D:22:LEU:HD23	2.08	0.74
2:E:19:LYS:HD2	2:E:19:LYS:N	2.03	0.74
3:I:515:HIS:CD2	3:I:517:VAL:H	2.02	0.74
2:B:19:LYS:N	2:B:19:LYS:HD2	2.03	0.73
1:G:21:GLY:C	1:G:22:LEU:HD23	2.08	0.73
3:I:210:VAL:HG12	3:I:211:TYR:HD1	1.54	0.73
1:A:20:LEU:HD13	1:A:20:LEU:O	1.89	0.73
1:D:165:CYS:HB3	1:D:166:PRO:HD3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:655:ARG:HH11	3:I:655:ARG:CB	2.01	0.73
1:A:198:VAL:HA	1:A:252:PRO:HG3	1.70	0.73
3:C:655:ARG:HH11	3:C:655:ARG:CB	2.01	0.73
1:G:145:LEU:HD22	1:G:149:ARG:NH2	2.03	0.73
3:F:263:THR:HG22	3:F:265:ALA:N	2.04	0.72
3:C:495:LYS:HD3	3:C:558:CYS:SG	2.29	0.72
1:G:18:GLN:O	1:G:19:ASP:HB2	1.89	0.72
2:H:19:LYS:N	2:H:19:LYS:HD2	2.05	0.72
3:I:428:LYS:HA	3:I:428:LYS:HE2	1.71	0.72
1:D:206:LEU:CD1	2:E:14:PRO:HD3	2.19	0.72
1:D:25:PHE:O	1:D:44:ARG:NH1	2.23	0.72
3:F:428:LYS:HA	3:F:428:LYS:HE2	1.71	0.72
3:I:263:THR:HG22	3:I:265:ALA:N	2.05	0.72
3:C:153:VAL:HG23	3:C:161:LYS:HE3	1.72	0.72
1:A:21:GLY:C	1:A:22:LEU:HD23	2.08	0.72
1:D:18:GLN:O	1:D:19:ASP:HB2	1.90	0.72
3:C:122:LEU:O	3:C:123:TYR:HB2	1.90	0.71
3:F:635:MET:CE	3:F:728:GLU:HG3	2.20	0.71
3:I:495:LYS:HD3	3:I:558:CYS:SG	2.29	0.71
1:A:56:ARG:O	1:A:175:LEU:HD11	1.90	0.71
3:C:497:SER:HB3	3:C:535:LEU:HD13	1.71	0.71
1:D:194:VAL:HG22	1:D:199:THR:HG23	1.73	0.71
3:I:705:GLY:O	3:I:708:THR:HB	1.90	0.71
1:G:198:VAL:HA	1:G:252:PRO:HG3	1.73	0.71
1:G:20:LEU:O	1:G:20:LEU:HD13	1.91	0.71
3:C:263:THR:HG22	3:C:265:ALA:N	2.05	0.71
1:G:202:ARG:HE	2:H:99:MET:HG2	1.54	0.71
3:C:211:TYR:O	3:C:212:LEU:HB3	1.91	0.71
1:A:18:GLN:O	1:A:19:ASP:HB2	1.89	0.71
3:C:428:LYS:HE2	3:C:428:LYS:HA	1.73	0.71
3:F:153:VAL:HG23	3:F:161:LYS:HE3	1.72	0.71
1:A:202:ARG:NE	2:B:99:MET:HG2	2.05	0.70
1:D:20:LEU:O	1:D:20:LEU:HD13	1.91	0.70
3:C:705:GLY:O	3:C:708:THR:HB	1.90	0.70
3:F:239:THR:HG22	3:F:241:LYS:N	2.04	0.70
1:G:150:HIS:HD2	1:G:153:ARG:H	1.40	0.70
1:A:165:CYS:HB3	1:A:166:PRO:HD3	1.71	0.70
1:G:150:HIS:CD2	1:G:152:ILE:HB	2.26	0.70
1:A:194:VAL:HG22	1:A:199:THR:HG23	1.73	0.70
3:I:497:SER:HB3	3:I:535:LEU:HD13	1.72	0.70
3:I:122:LEU:O	3:I:123:TYR:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:635:MET:CE	3:C:728:GLU:HG3	2.22	0.70
1:D:150:HIS:HD2	1:D:153:ARG:H	1.38	0.70
1:D:28:LEU:HD23	1:D:38:PHE:HD1	1.56	0.70
3:F:122:LEU:O	3:F:123:TYR:HB2	1.92	0.70
1:G:50:THR:O	1:G:53:VAL:HG22	1.91	0.69
3:F:306:GLY:HA2	3:F:461:VAL:HA	1.75	0.69
3:C:239:THR:HG22	3:C:241:LYS:N	2.08	0.69
3:I:306:GLY:HA2	3:I:461:VAL:HA	1.73	0.69
2:E:39:LEU:HD23	2:E:80:CYS:HB3	1.75	0.69
1:D:50:THR:O	1:D:53:VAL:HG22	1.92	0.69
1:A:145:LEU:HD22	1:A:149:ARG:NH2	2.08	0.69
3:C:626:ASN:HA	3:C:629:ARG:HG3	1.75	0.69
3:C:206:ASN:C	3:C:206:ASN:HD22	1.94	0.69
1:A:50:THR:O	1:A:53:VAL:HG22	1.93	0.68
1:D:185:PRO:HB3	1:D:266:GLY:O	1.93	0.68
3:I:153:VAL:HG23	3:I:161:LYS:HE3	1.74	0.68
3:F:497:SER:HB3	3:F:535:LEU:HD13	1.76	0.68
1:D:52:TRP:O	1:D:56:ARG:HB2	1.93	0.68
3:F:626:ASN:HA	3:F:629:ARG:HG3	1.74	0.68
1:G:194:VAL:HG22	1:G:199:THR:HG23	1.74	0.68
2:H:31:HIS:O	2:H:33:SER:N	2.26	0.68
3:I:239:THR:HG22	3:I:241:LYS:N	2.06	0.68
1:A:22:LEU:HD12	3:C:619:LEU:HD23	1.75	0.68
3:C:153:VAL:HB	3:C:154:PRO:HD3	1.76	0.68
3:C:753:VAL:HG13	3:F:473:SER:HB3	1.74	0.68
1:A:198:VAL:HG22	1:A:199:THR:N	2.09	0.68
2:H:39:LEU:HD23	2:H:80:CYS:HB3	1.75	0.68
2:B:39:LEU:HD23	2:B:80:CYS:HB3	1.75	0.68
3:C:306:GLY:HA2	3:C:461:VAL:HA	1.74	0.68
3:C:600:LYS:HD2	3:C:608:ASN:ND2	2.09	0.68
1:D:198:VAL:HG22	1:D:199:THR:N	2.09	0.68
2:E:31:HIS:O	2:E:33:SER:N	2.26	0.68
1:G:185:PRO:HB3	1:G:266:GLY:O	1.93	0.68
1:G:202:ARG:NE	2:H:99:MET:HG2	2.09	0.68
3:I:626:ASN:HA	3:I:629:ARG:HG3	1.76	0.68
3:C:708:THR:CG2	3:C:711:ALA:H	2.02	0.67
3:F:153:VAL:HB	3:F:154:PRO:HD3	1.75	0.67
3:F:213:VAL:HG11	3:F:345:LEU:HD22	1.74	0.67
3:F:600:LYS:HD2	3:F:608:ASN:ND2	2.09	0.67
3:C:718:LEU:HD13	3:C:725:ALA:HB1	1.75	0.67
3:F:705:GLY:O	3:F:708:THR:HB	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:402:TYR:HB3	3:I:447:SER:HB2	1.76	0.67
3:F:236:ASN:HB3	3:F:242:ASP:OD2	1.93	0.67
3:F:718:LEU:HD13	3:F:725:ALA:HB1	1.77	0.67
1:G:52:TRP:O	1:G:56:ARG:HB2	1.93	0.67
3:C:539:ASN:HD22	3:C:541:ALA:N	1.91	0.67
1:D:150:HIS:CD2	1:D:152:ILE:HB	2.29	0.67
3:F:188:VAL:HG21	3:F:386:ILE:HD11	1.76	0.67
3:I:470:TYR:O	3:I:474:LEU:HD13	1.94	0.67
1:A:133:TRP:O	1:A:144:LYS:HE2	1.95	0.67
3:F:198:ASN:HD21	3:F:378:SER:H	1.42	0.67
3:I:497:SER:HB3	3:I:535:LEU:CD1	2.23	0.67
3:F:498:ALA:HB2	3:F:553:VAL:HG23	1.76	0.67
3:F:708:THR:CG2	3:F:711:ALA:H	2.02	0.67
3:I:213:VAL:HG11	3:I:345:LEU:HD22	1.75	0.67
1:A:28:LEU:HD23	1:A:38:PHE:HD1	1.59	0.67
1:D:133:TRP:O	1:D:144:LYS:HE2	1.95	0.67
1:A:150:HIS:CD2	1:A:152:ILE:HB	2.29	0.67
3:C:263:THR:HG22	3:C:265:ALA:H	1.59	0.67
2:B:31:HIS:O	2:B:33:SER:N	2.28	0.67
3:C:188:VAL:HG21	3:C:386:ILE:HD11	1.77	0.67
3:I:236:ASN:HB3	3:I:242:ASP:OD2	1.95	0.67
1:A:4:ARG:N	1:A:4:ARG:HD3	2.10	0.67
3:C:402:TYR:HB3	3:C:447:SER:HB2	1.77	0.67
3:C:198:ASN:ND2	3:C:378:SER:H	1.93	0.66
1:D:4:ARG:HD3	1:D:4:ARG:N	2.10	0.66
1:G:25:PHE:O	1:G:44:ARG:NH1	2.27	0.66
2:H:31:HIS:O	2:H:32:PRO:C	2.34	0.66
3:C:236:ASN:HB3	3:C:242:ASP:OD2	1.95	0.66
3:C:470:TYR:O	3:C:474:LEU:HD13	1.96	0.66
3:F:402:TYR:HB3	3:F:447:SER:HB2	1.76	0.66
3:I:153:VAL:HB	3:I:154:PRO:HD3	1.76	0.66
3:C:635:MET:HE2	3:C:728:GLU:HG3	1.76	0.66
3:F:198:ASN:ND2	3:F:378:SER:H	1.92	0.66
3:F:263:THR:HG22	3:F:265:ALA:H	1.60	0.66
3:I:718:LEU:HD13	3:I:725:ALA:HB1	1.78	0.66
3:F:540:ALA:O	3:F:543:PRO:HD2	1.94	0.66
1:G:198:VAL:HG22	1:G:199:THR:N	2.10	0.66
1:A:150:HIS:HD2	1:A:153:ARG:H	1.41	0.66
1:A:52:TRP:O	1:A:56:ARG:HB2	1.96	0.66
3:C:236:ASN:C	3:C:238:GLY:H	1.99	0.66
1:G:4:ARG:HD3	1:G:4:ARG:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:699:HIS:HD2	3:I:702:TRP:H	1.43	0.66
3:C:297:PHE:O	3:C:336:THR:HG21	1.96	0.66
3:F:236:ASN:C	3:F:238:GLY:H	1.99	0.66
1:A:214:THR:HB	1:A:263:GLU:HB2	1.78	0.66
1:D:214:THR:HB	1:D:263:GLU:HB2	1.77	0.66
3:I:345:LEU:HB3	3:I:349:MET:HE2	1.78	0.66
3:I:493:ASN:ND2	3:I:495:LYS:HZ1	1.87	0.66
3:F:297:PHE:O	3:F:336:THR:HG21	1.96	0.66
1:G:225:ASP:OD2	1:G:227:LYS:HB3	1.96	0.66
1:D:28:LEU:CD2	1:D:38:PHE:HD1	2.09	0.65
3:C:323:PRO:HG3	3:F:729:THR:HG22	1.76	0.65
3:I:708:THR:CG2	3:I:711:ALA:H	2.02	0.65
1:A:185:PRO:HB3	1:A:266:GLY:O	1.96	0.65
1:D:225:ASP:OD2	1:D:227:LYS:HB3	1.95	0.65
3:F:635:MET:HE2	3:F:728:GLU:HG3	1.76	0.65
3:C:198:ASN:HD21	3:C:378:SER:H	1.42	0.65
3:C:497:SER:HB3	3:C:535:LEU:CD1	2.27	0.65
3:F:699:HIS:HD2	3:F:702:TRP:H	1.45	0.65
3:I:198:ASN:ND2	3:I:378:SER:H	1.93	0.65
3:I:635:MET:CE	3:I:728:GLU:HG3	2.26	0.65
1:A:28:LEU:CD2	1:A:38:PHE:HD1	2.10	0.65
1:A:67:GLN:HE22	3:C:657:THR:HB	1.62	0.65
3:I:498:ALA:HB2	3:I:553:VAL:HG23	1.79	0.65
3:C:699:HIS:HD2	3:C:702:TRP:H	1.45	0.65
3:I:297:PHE:O	3:I:336:THR:HG21	1.96	0.65
3:I:600:LYS:HD2	3:I:608:ASN:ND2	2.11	0.65
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.79	0.65
3:I:205:LYS:HE3	3:I:370:SER:HA	1.79	0.65
3:C:278:GLY:HA2	3:C:333:PRO:O	1.97	0.65
1:A:225:ASP:OD2	1:A:227:LYS:HB3	1.97	0.64
2:H:33:SER:HB2	2:H:54:LEU:HD21	1.78	0.64
2:B:31:HIS:HB3	2:B:32:PRO:CD	2.28	0.64
2:B:31:HIS:O	2:B:32:PRO:C	2.35	0.64
3:F:470:TYR:O	3:F:474:LEU:HD13	1.98	0.64
1:G:214:THR:HB	1:G:263:GLU:HB2	1.78	0.64
3:I:278:GLY:HA2	3:I:333:PRO:O	1.97	0.64
3:F:497:SER:HB3	3:F:535:LEU:CD1	2.27	0.64
3:I:236:ASN:C	3:I:238:GLY:H	1.99	0.64
1:G:28:LEU:HD23	1:G:38:PHE:HD1	1.62	0.64
6:G:309:GOL:H32	3:I:646:ARG:NH2	2.12	0.64
3:C:213:VAL:HG11	3:C:345:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:575:GLU:O	3:F:579:ARG:HG3	1.98	0.64
3:I:635:MET:HE2	3:I:728:GLU:HG3	1.80	0.64
3:C:345:LEU:HB3	3:C:349:MET:HE2	1.79	0.63
3:C:498:ALA:HB2	3:C:553:VAL:HG23	1.78	0.63
3:F:278:GLY:HA2	3:F:333:PRO:O	1.97	0.63
3:F:345:LEU:HB3	3:F:349:MET:HE2	1.79	0.63
2:E:31:HIS:O	2:E:32:PRO:C	2.35	0.63
3:I:198:ASN:HD21	3:I:378:SER:H	1.45	0.63
1:D:145:LEU:HD22	1:D:149:ARG:HH22	1.64	0.63
1:G:28:LEU:CD2	1:G:38:PHE:HD1	2.10	0.63
3:I:155:ARG:HD2	3:I:409:ARG:O	1.98	0.62
1:A:132:ASP:HB2	1:A:148:GLU:OE2	1.98	0.62
3:F:204:ASP:O	3:F:206:ASN:N	2.32	0.62
1:G:133:TRP:O	1:G:144:LYS:HE2	1.98	0.62
2:E:31:HIS:HB3	2:E:32:PRO:CD	2.28	0.62
2:E:7:ILE:HD12	2:E:7:ILE:H	1.64	0.62
1:A:25:PHE:O	1:A:44:ARG:NH1	2.29	0.62
3:F:319:THR:HG22	3:F:321:PHE:H	1.64	0.62
3:I:188:VAL:HG21	3:I:386:ILE:HD11	1.81	0.62
3:I:667:ASP:HB3	3:I:670:VAL:HG12	1.81	0.62
1:G:218:LEU:HB2	1:G:259:THR:OG1	2.00	0.62
3:I:192:VAL:HG12	3:I:193:LYS:N	2.15	0.62
3:F:192:VAL:HG12	3:F:193:LYS:N	2.15	0.62
3:I:153:VAL:HB	3:I:154:PRO:CD	2.30	0.62
3:I:263:THR:HG22	3:I:265:ALA:H	1.63	0.62
1:D:236:PRO:HG2	2:E:65:LEU:HD22	1.82	0.61
1:D:74:HIS:HB3	3:F:646:ARG:NH1	2.14	0.61
3:F:258:ARG:HD2	3:F:284:ASP:OD1	2.00	0.61
3:F:302:HIS:HE1	3:F:326:SER:OG	1.83	0.61
1:G:132:ASP:HB2	1:G:148:GLU:OE2	2.00	0.61
3:I:618:LEU:HD13	3:I:701:PHE:HZ	1.65	0.61
2:H:31:HIS:HB3	2:H:32:PRO:CD	2.30	0.61
3:C:263:THR:HB	3:C:266:GLU:HG3	1.82	0.61
1:D:132:ASP:HB2	1:D:148:GLU:OE2	2.00	0.61
2:B:7:ILE:H	2:B:7:ILE:HD12	1.66	0.61
2:H:16:GLU:HG2	2:H:19:LYS:HD3	1.82	0.61
3:C:575:GLU:O	3:C:579:ARG:HG3	1.99	0.61
3:C:590:ALA:O	3:C:593:VAL:HG22	2.01	0.61
3:F:618:LEU:HD13	3:F:701:PHE:HZ	1.66	0.61
3:C:153:VAL:HB	3:C:154:PRO:CD	2.30	0.61
3:C:192:VAL:HG12	3:C:193:LYS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:ARG:HD2	3:C:409:ARG:O	2.00	0.61
2:E:33:SER:HB2	2:E:54:LEU:HD21	1.81	0.60
3:F:539:ASN:HD22	3:F:541:ALA:N	1.93	0.60
3:I:203:VAL:HG11	3:I:207:GLY:HA2	1.81	0.60
3:F:209:LEU:HD12	3:F:210:VAL:H	1.65	0.60
2:E:79:ALA:CB	2:E:94:LYS:HA	2.31	0.60
2:H:79:ALA:CB	2:H:94:LYS:HA	2.31	0.60
3:C:319:THR:HG22	3:C:321:PHE:H	1.66	0.60
3:F:153:VAL:HB	3:F:154:PRO:CD	2.30	0.60
3:F:618:LEU:CD1	3:F:701:PHE:HZ	2.14	0.60
3:I:319:THR:HG22	3:I:321:PHE:H	1.66	0.60
3:C:155:ARG:HH12	3:C:419:SER:HB3	1.66	0.60
3:C:611:TYR:CZ	3:C:656:LEU:HD23	2.37	0.60
1:D:218:LEU:HB2	1:D:259:THR:OG1	2.02	0.60
1:G:43:SER:O	1:G:45:ARG:N	2.35	0.60
3:I:501:LEU:HD23	3:I:611:TYR:HA	1.83	0.60
2:E:7:ILE:HD12	2:E:7:ILE:N	2.16	0.60
1:A:43:SER:O	1:A:45:ARG:N	2.35	0.60
3:F:611:TYR:CZ	3:F:656:LEU:HD23	2.36	0.60
3:I:590:ALA:O	3:I:593:VAL:HG22	2.02	0.60
3:F:667:ASP:HB3	3:F:670:VAL:HG12	1.83	0.60
3:I:540:ALA:O	3:I:543:PRO:HD2	2.02	0.60
3:C:174:ARG:HG2	3:C:174:ARG:HH11	1.67	0.59
3:C:386:ILE:CG2	3:C:454:SER:HB3	2.32	0.59
3:C:540:ALA:O	3:C:543:PRO:HD2	2.02	0.59
3:I:258:ARG:HD2	3:I:284:ASP:OD1	2.02	0.59
2:B:16:GLU:HG2	2:B:19:LYS:HD3	1.83	0.59
3:F:580:ILE:HD11	3:F:586:VAL:HG21	1.84	0.59
3:I:580:ILE:HD11	3:I:586:VAL:HG21	1.83	0.59
3:F:155:ARG:HD2	3:F:409:ARG:O	2.02	0.59
2:H:7:ILE:H	2:H:7:ILE:HD12	1.67	0.59
2:B:12:ARG:NH2	2:B:22:PHE:CE2	2.70	0.59
1:D:146:GLU:HG2	3:F:640:GLN:NE2	2.18	0.59
3:F:263:THR:HB	3:F:266:GLU:HG3	1.84	0.59
1:D:74:HIS:HB3	3:F:646:ARG:HH12	1.68	0.59
3:I:263:THR:HB	3:I:266:GLU:HG3	1.84	0.59
3:C:600:LYS:HB3	3:C:608:ASN:HD22	1.67	0.59
3:I:174:ARG:HH11	3:I:174:ARG:HG2	1.66	0.59
2:B:79:ALA:CB	2:B:94:LYS:HA	2.30	0.59
1:D:21:GLY:O	1:D:22:LEU:O	2.20	0.59
1:A:184:VAL:HG12	1:A:209:TYR:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:ARG:HD2	3:C:284:ASP:OD1	2.03	0.59
2:E:31:HIS:O	2:E:62:PHE:HD2	1.85	0.59
1:G:145:LEU:HD22	1:G:149:ARG:HH22	1.66	0.59
3:I:539:ASN:HD22	3:I:541:ALA:N	1.91	0.59
1:A:63:LEU:HD21	3:C:657:THR:HG22	1.85	0.58
3:C:618:LEU:HD13	3:C:701:PHE:HZ	1.68	0.58
1:D:43:SER:O	1:D:45:ARG:N	2.35	0.58
2:B:7:ILE:N	2:B:7:ILE:HD12	2.19	0.58
3:F:141:THR:OG1	3:F:584:ASN:HB2	2.03	0.58
3:F:590:ALA:O	3:F:593:VAL:HG22	2.03	0.58
3:I:575:GLU:O	3:I:579:ARG:HG3	2.03	0.58
3:I:600:LYS:HB3	3:I:608:ASN:HD22	1.68	0.58
3:C:146:LEU:HD22	3:C:146:LEU:O	2.03	0.58
1:A:87:HIS:HB3	1:A:89:HIS:CE1	2.38	0.58
3:F:155:ARG:HH12	3:F:419:SER:HB3	1.67	0.58
3:I:203:VAL:CG1	3:I:204:ASP:N	2.67	0.58
1:D:150:HIS:HE1	3:F:641:TRP:HA	1.69	0.58
3:C:580:ILE:HD11	3:C:586:VAL:HG21	1.86	0.58
3:C:667:ASP:HB3	3:C:670:VAL:HG12	1.85	0.58
3:I:721:GLN:O	3:I:723:ASN:N	2.36	0.58
2:B:31:HIS:O	2:B:62:PHE:HD2	1.86	0.58
3:C:501:LEU:HD23	3:C:611:TYR:HA	1.86	0.58
3:F:600:LYS:HB3	3:F:608:ASN:HD22	1.69	0.58
1:D:53:VAL:HB	1:D:57:ILE:CD1	2.33	0.58
2:E:12:ARG:NH2	2:E:22:PHE:CE2	2.72	0.58
3:I:295:LEU:HD22	3:I:570:MET:HE2	1.84	0.58
3:I:699:HIS:CD2	3:I:702:TRP:CD1	2.91	0.58
3:F:174:ARG:HH11	3:F:174:ARG:HG2	1.68	0.58
3:I:501:LEU:CD2	3:I:611:TYR:HA	2.33	0.58
3:C:699:HIS:CD2	3:C:702:TRP:CD1	2.92	0.58
3:C:618:LEU:CD1	3:C:701:PHE:HZ	2.17	0.57
1:D:268:ASP:HB2	1:D:269:GLN:NE2	2.18	0.57
3:F:721:GLN:O	3:F:723:ASN:N	2.37	0.57
3:F:496:VAL:HG11	3:F:506:ILE:HD13	1.87	0.57
3:C:473:SER:HB3	3:F:753:VAL:HG13	1.86	0.57
1:G:184:VAL:HG12	1:G:209:TYR:HB3	1.85	0.57
2:H:12:ARG:NH2	2:H:22:PHE:CE2	2.71	0.57
2:H:31:HIS:O	2:H:62:PHE:HD2	1.87	0.57
3:I:611:TYR:CZ	3:I:656:LEU:HD23	2.39	0.57
3:I:155:ARG:HH12	3:I:419:SER:HB3	1.68	0.57
3:C:493:ASN:HB2	3:C:495:LYS:NZ	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:VAL:HG12	1:D:209:TYR:HB3	1.86	0.57
1:D:87:HIS:HB3	1:D:89:HIS:CE1	2.39	0.57
1:A:43:SER:O	1:A:45:ARG:HG2	2.04	0.57
1:D:43:SER:O	1:D:45:ARG:HG2	2.04	0.57
3:C:721:GLN:O	3:C:723:ASN:N	2.37	0.57
3:F:153:VAL:HG23	3:F:154:PRO:CD	2.34	0.57
3:I:496:VAL:HG11	3:I:506:ILE:HD13	1.87	0.57
3:C:141:THR:HG23	3:C:573:TYR:OH	2.05	0.57
3:F:467:LEU:HD21	3:F:544:PHE:CE2	2.40	0.57
1:A:218:LEU:HB2	1:A:259:THR:OG1	2.03	0.56
3:C:141:THR:OG1	3:C:584:ASN:HB2	2.05	0.56
3:C:230:GLY:O	3:C:372:ASN:HB2	2.05	0.56
2:H:7:ILE:N	2:H:7:ILE:HD12	2.20	0.56
3:C:728:GLU:O	3:C:732:ARG:HG3	2.06	0.56
1:D:80:PHE:HA	1:D:96:LEU:HD22	1.86	0.56
2:E:16:GLU:HG2	2:E:19:LYS:HD3	1.86	0.56
1:A:149:ARG:O	1:A:151:LYS:HG2	2.04	0.56
1:G:43:SER:O	1:G:45:ARG:HG2	2.06	0.56
3:I:551:PRO:HD3	3:I:682:GLU:HG2	1.87	0.56
3:C:150:ASN:O	3:C:153:VAL:HG22	2.05	0.56
3:F:493:ASN:ND2	3:F:495:LYS:HZ1	1.88	0.56
3:F:728:GLU:O	3:F:732:ARG:HG3	2.05	0.56
2:H:19:LYS:O	2:H:72:PRO:HD2	2.06	0.56
3:I:141:THR:OG1	3:I:584:ASN:HB2	2.05	0.56
1:A:21:GLY:O	1:A:22:LEU:O	2.23	0.56
3:F:386:ILE:CG2	3:F:454:SER:HB3	2.32	0.56
3:I:150:ASN:O	3:I:153:VAL:HG22	2.04	0.56
3:F:501:LEU:CD2	3:F:611:TYR:HA	2.35	0.56
1:D:79:ASP:OD1	1:D:153:ARG:NH2	2.39	0.56
3:F:146:LEU:HD22	3:F:146:LEU:O	2.04	0.56
1:G:225:ASP:OD1	1:G:228:GLU:HG2	2.06	0.56
3:C:295:LEU:HD22	3:C:570:MET:HE2	1.88	0.56
1:D:192:HIS:HB2	1:D:201:LEU:HD23	1.88	0.56
3:I:153:VAL:HG23	3:I:154:PRO:CD	2.34	0.56
1:A:216:LYS:HE3	1:A:261:GLN:NE2	2.20	0.56
1:D:225:ASP:OD1	1:D:228:GLU:HG2	2.06	0.56
1:G:268:ASP:HB2	1:G:269:GLN:NE2	2.17	0.56
3:I:295:LEU:HD22	3:I:570:MET:CE	2.36	0.56
1:A:80:PHE:HA	1:A:96:LEU:HD22	1.87	0.56
3:F:501:LEU:HD23	3:F:611:TYR:HA	1.86	0.56
1:G:192:HIS:HB2	1:G:201:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:HB2	1:A:269:GLN:NE2	2.18	0.56
3:C:346:PHE:HA	3:C:349:MET:HE3	1.88	0.56
2:E:19:LYS:O	2:E:72:PRO:HD2	2.06	0.56
3:I:302:HIS:HE1	3:I:326:SER:OG	1.89	0.56
3:C:153:VAL:HG23	3:C:154:PRO:CD	2.35	0.55
3:F:346:PHE:HA	3:F:349:MET:HE3	1.88	0.55
2:B:19:LYS:O	2:B:72:PRO:HD2	2.06	0.55
1:D:191:THR:HG23	1:D:202:ARG:HB3	1.88	0.55
1:A:151:LYS:O	1:A:155:ARG:HG3	2.06	0.55
3:F:213:VAL:HG11	3:F:345:LEU:CD2	2.36	0.55
3:C:699:HIS:CD2	3:C:702:TRP:H	2.24	0.55
1:D:235:LEU:HD13	2:E:10:TYR:CE1	2.41	0.55
3:C:134:LYS:NZ	3:C:435:ASP:HB3	2.22	0.55
1:G:21:GLY:O	1:G:22:LEU:O	2.23	0.55
1:G:87:HIS:HB3	1:G:89:HIS:CE1	2.42	0.55
3:I:134:LYS:NZ	3:I:435:ASP:HB3	2.22	0.55
3:F:428:LYS:CA	3:F:428:LYS:HE2	2.37	0.55
3:F:493:ASN:HB2	3:F:495:LYS:NZ	2.21	0.55
3:F:699:HIS:CD2	3:F:702:TRP:H	2.24	0.55
3:I:493:ASN:HB2	3:I:495:LYS:NZ	2.22	0.55
3:C:632:ILE:HG21	3:C:639:LEU:HD13	1.88	0.55
3:F:231:LYS:O	3:F:253:SER:HB2	2.07	0.55
1:A:35:LEU:HD22	1:A:49:ARG:HG3	1.88	0.55
3:F:514:LYS:HD2	3:F:519:GLY:O	2.06	0.55
3:F:632:ILE:HG21	3:F:639:LEU:HD13	1.89	0.55
3:I:618:LEU:CD1	3:I:701:PHE:HZ	2.19	0.55
1:A:192:HIS:HB2	1:A:201:LEU:HD23	1.88	0.55
1:A:225:ASP:OD1	1:A:228:GLU:HG2	2.07	0.55
3:F:134:LYS:NZ	3:F:435:ASP:HB3	2.21	0.55
1:G:149:ARG:O	1:G:151:LYS:HG2	2.07	0.55
1:G:151:LYS:O	1:G:155:ARG:HG3	2.07	0.55
1:G:50:THR:HG22	1:G:52:TRP:HD1	1.71	0.55
1:A:53:VAL:HB	1:A:57:ILE:CD1	2.36	0.54
1:G:191:THR:HG23	1:G:202:ARG:HB3	1.88	0.54
3:I:632:ILE:HG21	3:I:639:LEU:HD13	1.89	0.54
1:D:97:GLN:HB2	2:E:60:TRP:CE3	2.42	0.54
3:F:295:LEU:HD22	3:F:570:MET:CE	2.37	0.54
3:F:297:PHE:N	3:F:297:PHE:CD2	2.75	0.54
3:I:297:PHE:N	3:I:297:PHE:CD2	2.75	0.54
3:F:150:ASN:O	3:F:153:VAL:HG22	2.07	0.54
3:I:141:THR:HG23	3:I:573:TYR:OH	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:501:LEU:CD2	3:C:611:TYR:HA	2.37	0.54
3:C:514:LYS:HD2	3:C:519:GLY:O	2.07	0.54
3:F:231:LYS:HG3	3:F:253:SER:HB3	1.89	0.54
1:D:206:LEU:HD22	2:E:12:ARG:O	2.08	0.54
3:I:213:VAL:HG11	3:I:345:LEU:CD2	2.37	0.54
1:A:145:LEU:HD22	1:A:149:ARG:HH22	1.71	0.54
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.42	0.54
3:C:153:VAL:CB	3:C:154:PRO:CD	2.86	0.54
1:D:216:LYS:HE3	1:D:261:GLN:NE2	2.23	0.54
3:F:153:VAL:CB	3:F:154:PRO:CD	2.85	0.54
3:F:664:GLU:N	3:F:664:GLU:CD	2.57	0.54
3:I:231:LYS:O	3:I:253:SER:HB2	2.07	0.54
1:A:198:VAL:HG22	1:A:199:THR:H	1.72	0.54
3:C:254:ILE:HA	3:C:277:ILE:O	2.08	0.54
3:F:655:ARG:CG	3:F:655:ARG:HH11	2.21	0.54
3:C:231:LYS:HG3	3:C:253:SER:HB3	1.89	0.54
1:D:151:LYS:O	1:D:155:ARG:HG3	2.08	0.54
1:G:79:ASP:OD1	1:G:153:ARG:NH2	2.41	0.54
3:C:213:VAL:HG11	3:C:345:LEU:CD2	2.38	0.54
1:D:50:THR:HG22	1:D:52:TRP:HD1	1.72	0.53
3:I:153:VAL:CB	3:I:154:PRO:CD	2.86	0.53
1:D:232:LYS:HD2	1:D:232:LYS:O	2.08	0.53
1:G:198:VAL:HG22	1:G:199:THR:H	1.73	0.53
3:I:728:GLU:O	3:I:732:ARG:HG3	2.08	0.53
3:C:231:LYS:O	3:C:253:SER:HB2	2.08	0.53
1:D:198:VAL:HG22	1:D:199:THR:H	1.71	0.53
3:F:214:GLU:O	3:F:216:PRO:HD3	2.09	0.53
1:A:79:ASP:OD1	1:A:153:ARG:NH2	2.42	0.53
3:C:295:LEU:HD22	3:C:570:MET:CE	2.37	0.53
3:C:278:GLY:H	3:C:332:ILE:HB	1.74	0.53
3:C:496:VAL:HG11	3:C:506:ILE:HD13	1.90	0.53
3:C:214:GLU:O	3:C:216:PRO:HD3	2.09	0.53
3:C:234:HIS:ND1	3:C:235:ALA:O	2.41	0.53
3:C:250:VAL:CG1	3:C:276:ALA:HB2	2.38	0.53
3:F:154:PRO:HD2	3:F:161:LYS:HE3	1.91	0.53
3:I:346:PHE:HA	3:I:349:MET:HE3	1.91	0.53
3:I:655:ARG:CG	3:I:655:ARG:HH11	2.21	0.53
3:C:297:PHE:N	3:C:297:PHE:CD2	2.76	0.53
3:I:278:GLY:H	3:I:332:ILE:HB	1.74	0.53
1:A:125:GLU:HB3	1:A:134:ARG:HG2	1.90	0.53
3:C:134:LYS:HZ1	3:C:435:ASP:HB3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:635:MET:HE1	3:C:726:PHE:HZ	1.74	0.53
1:D:235:LEU:HD13	2:E:10:TYR:CZ	2.44	0.53
3:F:699:HIS:CD2	3:F:702:TRP:CD1	2.96	0.53
1:A:50:THR:HG22	1:A:52:TRP:HD1	1.73	0.53
3:C:154:PRO:HD2	3:C:161:LYS:HE3	1.90	0.53
1:D:125:GLU:HB3	1:D:134:ARG:HG2	1.89	0.53
1:G:216:LYS:HE3	1:G:261:GLN:NE2	2.23	0.53
1:A:191:THR:HG23	1:A:202:ARG:HB3	1.91	0.53
3:C:493:ASN:ND2	3:C:495:LYS:HZ1	1.89	0.53
3:F:310:THR:HG22	3:F:313:PHE:CE1	2.44	0.53
1:G:80:PHE:HA	1:G:96:LEU:HD22	1.91	0.53
3:C:302:HIS:HE1	3:C:326:SER:OG	1.91	0.52
3:C:199:SER:OG	3:C:376:THR:HG23	2.08	0.52
3:C:664:GLU:N	3:C:664:GLU:CD	2.57	0.52
2:E:71:THR:HG23	2:E:71:THR:O	2.09	0.52
2:H:71:THR:HG23	2:H:71:THR:O	2.10	0.52
3:I:230:GLY:O	3:I:372:ASN:HB2	2.09	0.52
3:I:467:LEU:HD21	3:I:544:PHE:CE2	2.43	0.52
1:D:35:LEU:HD22	1:D:49:ARG:HG3	1.91	0.52
3:F:135:LEU:HD23	3:F:432:MET:SD	2.50	0.52
3:F:295:LEU:HD22	3:F:570:MET:HE2	1.91	0.52
3:I:146:LEU:HD22	3:I:146:LEU:O	2.09	0.52
3:I:250:VAL:CG1	3:I:276:ALA:HB2	2.40	0.52
3:C:231:LYS:HG3	3:C:253:SER:CB	2.38	0.52
3:C:551:PRO:HD3	3:C:682:GLU:HG2	1.91	0.52
3:F:134:LYS:HZ1	3:F:435:ASP:HB3	1.74	0.52
1:G:150:HIS:NE2	1:G:152:ILE:HB	2.24	0.52
3:I:386:ILE:CG2	3:I:454:SER:HB3	2.36	0.52
3:I:514:LYS:HD2	3:I:519:GLY:O	2.08	0.52
3:C:206:ASN:C	3:C:206:ASN:ND2	2.63	0.52
3:F:230:GLY:O	3:F:372:ASN:HB2	2.09	0.52
1:D:206:LEU:HD11	2:E:14:PRO:CD	2.36	0.52
3:F:254:ILE:HA	3:F:277:ILE:O	2.10	0.52
3:F:278:GLY:H	3:F:332:ILE:HB	1.75	0.52
3:C:729:THR:HG22	3:F:323:PRO:HG3	1.92	0.52
1:G:50:THR:CG2	1:G:52:TRP:HD1	2.22	0.52
3:F:141:THR:HG23	3:F:573:TYR:OH	2.08	0.52
3:F:203:VAL:CG1	3:F:204:ASP:N	2.71	0.52
1:G:125:GLU:HB3	1:G:134:ARG:HG2	1.91	0.52
1:G:188:VAL:HB	1:G:273:VAL:HG21	1.91	0.52
3:C:354:PRO:HD3	3:C:365:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ASP:O	1:D:108:ASN:HB2	2.10	0.52
2:H:33:SER:HB3	2:H:62:PHE:CE2	2.45	0.52
3:C:150:ASN:HA	3:C:153:VAL:HG22	1.92	0.51
3:F:184:ASP:HB2	3:F:390:PHE:HE1	1.75	0.51
3:F:237:PHE:O	3:F:267:LYS:HG2	2.10	0.51
1:G:35:LEU:HD22	1:G:49:ARG:HG3	1.91	0.51
1:G:49:ARG:O	1:G:50:THR:HB	2.10	0.51
1:G:81:TRP:CH2	3:I:623:ARG:HB2	2.44	0.51
3:I:231:LYS:HG3	3:I:253:SER:HB3	1.92	0.51
3:I:699:HIS:CD2	3:I:702:TRP:H	2.24	0.51
1:D:50:THR:CG2	1:D:52:TRP:HD1	2.23	0.51
1:D:53:VAL:HB	1:D:57:ILE:HD12	1.92	0.51
3:F:250:VAL:CG1	3:F:276:ALA:HB2	2.41	0.51
3:F:297:PHE:HD2	3:F:297:PHE:N	2.07	0.51
3:I:297:PHE:HD2	3:I:297:PHE:N	2.08	0.51
3:I:310:THR:HG22	3:I:313:PHE:CE1	2.45	0.51
3:I:354:PRO:HD3	3:I:365:MET:SD	2.51	0.51
3:C:414:PRO:HB2	3:C:571:ASP:O	2.10	0.51
1:A:107:ASP:O	1:A:108:ASN:HB2	2.09	0.51
3:C:122:LEU:O	3:C:123:TYR:CB	2.59	0.51
3:C:237:PHE:O	3:C:267:LYS:HG2	2.10	0.51
1:D:150:HIS:NE2	1:D:152:ILE:HB	2.25	0.51
3:F:205:LYS:HE3	3:F:370:SER:HA	1.93	0.51
3:F:231:LYS:HG3	3:F:253:SER:CB	2.40	0.51
1:G:8:LEU:HB2	1:G:169:LEU:HD13	1.92	0.51
1:A:50:THR:CG2	1:A:52:TRP:HD1	2.23	0.51
1:G:53:VAL:HB	1:G:57:ILE:CD1	2.40	0.51
3:I:254:ILE:HA	3:I:277:ILE:O	2.11	0.51
3:I:625:LEU:HD13	3:I:713:LEU:HD21	1.91	0.51
1:A:49:ARG:O	1:A:50:THR:HB	2.11	0.51
1:D:67:GLN:HE22	3:F:657:THR:HB	1.75	0.51
3:F:551:PRO:HD3	3:F:682:GLU:HG2	1.92	0.51
3:I:305:THR:HG21	3:I:543:PRO:HG3	1.93	0.51
3:I:414:PRO:HB2	3:I:571:ASP:O	2.10	0.51
3:F:229:THR:HG22	3:F:374:LYS:HG3	1.93	0.51
3:I:154:PRO:HD2	3:I:161:LYS:HE3	1.92	0.51
3:I:231:LYS:HG3	3:I:253:SER:CB	2.41	0.51
3:I:150:ASN:HA	3:I:153:VAL:HG22	1.92	0.51
3:I:199:SER:OG	3:I:376:THR:HG23	2.10	0.51
1:D:49:ARG:O	1:D:50:THR:HB	2.11	0.51
3:F:414:PRO:HB2	3:F:571:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:625:LEU:HD13	3:C:713:LEU:HD21	1.92	0.51
1:D:264:HIS:ND1	1:D:266:GLY:N	2.48	0.51
3:F:708:THR:HG22	3:F:711:ALA:N	2.04	0.51
1:G:232:LYS:HD2	1:G:232:LYS:O	2.11	0.51
1:A:188:VAL:HB	1:A:273:VAL:HG21	1.93	0.50
2:B:71:THR:O	2:B:71:THR:HG23	2.10	0.50
3:C:236:ASN:O	3:C:238:GLY:N	2.44	0.50
3:C:135:LEU:HD23	3:C:432:MET:SD	2.51	0.50
1:D:22:LEU:CD1	3:F:619:LEU:HD23	2.31	0.50
1:A:53:VAL:HB	1:A:57:ILE:HD12	1.92	0.50
1:D:149:ARG:O	1:D:151:LYS:HG2	2.12	0.50
3:F:518:THR:C	3:F:520:GLN:H	2.15	0.50
3:F:625:LEU:HD13	3:F:713:LEU:HD21	1.93	0.50
2:H:29:GLY:HA2	2:H:61:SER:HB2	1.93	0.50
3:I:229:THR:HG22	3:I:374:LYS:HG3	1.92	0.50
3:C:428:LYS:HE2	3:C:428:LYS:CA	2.39	0.50
3:C:747:ASN:HB3	3:C:756:ILE:HD13	1.93	0.50
3:I:428:LYS:HE2	3:I:428:LYS:CA	2.39	0.50
3:C:297:PHE:HD2	3:C:297:PHE:N	2.09	0.50
1:D:92:GLU:HB2	1:D:94:HIS:NE2	2.27	0.50
3:F:354:PRO:HD3	3:F:365:MET:SD	2.51	0.50
1:G:263:GLU:HG2	1:G:270:PRO:HB3	1.94	0.50
3:I:203:VAL:HG13	3:I:204:ASP:N	2.27	0.50
3:F:199:SER:OG	3:F:376:THR:HG23	2.11	0.50
3:I:236:ASN:O	3:I:238:GLY:N	2.43	0.50
3:I:635:MET:HE1	3:I:726:PHE:HZ	1.77	0.50
3:C:229:THR:HG22	3:C:374:LYS:HG3	1.94	0.50
3:C:184:ASP:HB2	3:C:390:PHE:HE1	1.76	0.50
3:C:467:LEU:HD22	3:C:548:SER:OG	2.12	0.50
1:D:198:VAL:HA	1:D:252:PRO:CG	2.38	0.50
1:D:46:VAL:HG21	1:D:66:SER:HA	1.93	0.50
1:A:232:LYS:O	1:A:232:LYS:HD2	2.12	0.50
1:D:207:ASN:HD21	2:E:13:HIS:HD2	1.57	0.50
3:F:498:ALA:HB2	3:F:553:VAL:HA	1.93	0.50
3:I:147:LEU:C	3:I:148:ASN:HD22	2.14	0.50
3:C:305:THR:HG21	3:C:543:PRO:HG3	1.94	0.50
1:G:107:ASP:O	1:G:108:ASN:HB2	2.10	0.50
3:I:690:VAL:HG11	3:I:707:HIS:HB3	1.94	0.50
3:F:622:VAL:HG13	3:F:643:TYR:CE2	2.47	0.50
3:I:279:VAL:HB	3:I:334:VAL:HG13	1.94	0.50
1:A:92:GLU:HB2	1:A:94:HIS:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLU:HG2	1:D:270:PRO:HB3	1.94	0.49
3:F:150:ASN:HA	3:F:153:VAL:HG22	1.92	0.49
3:I:345:LEU:HB3	3:I:349:MET:CE	2.41	0.49
3:C:236:ASN:C	3:C:238:GLY:N	2.65	0.49
3:C:467:LEU:HD21	3:C:544:PHE:CE2	2.47	0.49
3:F:234:HIS:ND1	3:F:235:ALA:O	2.45	0.49
3:F:236:ASN:O	3:F:238:GLY:N	2.44	0.49
1:G:18:GLN:O	1:G:19:ASP:CB	2.59	0.49
3:I:236:ASN:C	3:I:238:GLY:N	2.65	0.49
3:I:135:LEU:HD23	3:I:432:MET:SD	2.52	0.49
2:E:33:SER:HB3	2:E:62:PHE:CE2	2.47	0.49
3:F:502:LEU:O	3:F:506:ILE:HG13	2.12	0.49
3:C:147:LEU:C	3:C:148:ASN:HD22	2.15	0.49
1:D:131:LEU:HD21	1:D:158:ARG:CZ	2.43	0.49
1:D:188:VAL:HB	1:D:273:VAL:HG21	1.93	0.49
1:D:238:GLY:HA3	2:E:67:TYR:CZ	2.48	0.49
3:I:192:VAL:HG12	3:I:193:LYS:H	1.76	0.49
3:I:209:LEU:HD12	3:I:210:VAL:N	2.22	0.49
3:I:234:HIS:ND1	3:I:235:ALA:O	2.46	0.49
1:A:198:VAL:HA	1:A:252:PRO:CG	2.42	0.49
3:C:518:THR:C	3:C:520:GLN:H	2.15	0.49
3:F:166:ALA:HB1	3:F:389:ILE:CD1	2.43	0.49
1:G:150:HIS:O	1:G:151:LYS:HB2	2.12	0.49
3:I:237:PHE:O	3:I:267:LYS:HG2	2.13	0.49
1:A:228:GLU:OE2	1:G:134:ARG:NH2	2.46	0.49
3:C:655:ARG:HH11	3:C:655:ARG:CG	2.24	0.49
3:C:753:VAL:HG13	3:F:473:SER:CB	2.41	0.49
1:D:8:LEU:HB2	1:D:169:LEU:HD13	1.94	0.49
3:F:209:LEU:HD12	3:F:210:VAL:N	2.27	0.49
1:G:18:GLN:H	1:G:18:GLN:NE2	2.10	0.49
3:I:184:ASP:HB2	3:I:390:PHE:HE1	1.77	0.49
1:A:135:ALA:HB1	1:A:140:ALA:HB3	1.95	0.48
3:C:494:PHE:HA	3:C:556:CYS:O	2.13	0.48
1:D:23:SER:OG	1:D:73:ASP:OD2	2.30	0.48
3:F:203:VAL:HG11	3:F:207:GLY:HA2	1.94	0.48
3:F:345:LEU:HB3	3:F:349:MET:CE	2.43	0.48
1:G:31:VAL:O	1:G:34:GLN:HB2	2.12	0.48
3:I:664:GLU:N	3:I:664:GLU:CD	2.60	0.48
1:A:18:GLN:O	1:A:19:ASP:CB	2.59	0.48
1:A:35:LEU:CD2	1:A:49:ARG:HG3	2.42	0.48
3:F:305:THR:HG21	3:F:543:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:GLU:HB2	1:G:94:HIS:NE2	2.28	0.48
1:G:22:LEU:HD12	3:I:619:LEU:HD23	1.95	0.48
1:A:150:HIS:NE2	1:A:152:ILE:HB	2.27	0.48
1:A:57:ILE:HG12	1:A:175:LEU:CD2	2.43	0.48
1:A:198:VAL:CG2	1:A:199:THR:N	2.75	0.48
1:A:31:VAL:O	1:A:34:GLN:HB2	2.13	0.48
3:C:310:THR:HG22	3:C:313:PHE:CE1	2.48	0.48
3:C:595:GLY:O	3:C:599:ILE:HG12	2.13	0.48
3:F:236:ASN:C	3:F:238:GLY:N	2.65	0.48
3:F:279:VAL:HB	3:F:334:VAL:HG13	1.96	0.48
1:G:57:ILE:HG12	1:G:175:LEU:CD2	2.43	0.48
2:H:1:ILE:O	2:H:1:ILE:HG23	2.13	0.48
3:F:192:VAL:HG12	3:F:193:LYS:H	1.77	0.48
3:F:247:TYR:CD1	3:F:247:TYR:N	2.81	0.48
1:G:135:ALA:HB1	1:G:140:ALA:HB3	1.96	0.48
1:G:46:VAL:HG21	1:G:66:SER:HA	1.96	0.48
3:I:595:GLY:O	3:I:599:ILE:HG12	2.12	0.48
1:A:22:LEU:O	1:A:23:SER:O	2.32	0.48
1:A:263:GLU:HG2	1:A:270:PRO:HB3	1.96	0.48
1:D:31:VAL:O	1:D:34:GLN:HB2	2.12	0.48
3:F:690:VAL:HG11	3:F:707:HIS:HB3	1.94	0.48
1:G:131:LEU:HD21	1:G:158:ARG:CZ	2.44	0.48
3:C:414:PRO:HG2	3:C:572:THR:HG22	1.96	0.48
1:G:198:VAL:CG2	1:G:199:THR:N	2.77	0.48
1:A:236:PRO:HG2	2:B:65:LEU:HD22	1.96	0.48
3:C:191:GLN:NE2	3:C:222:TYR:H	2.12	0.48
3:C:625:LEU:HD13	3:C:713:LEU:CD2	2.43	0.48
1:D:191:THR:O	1:D:192:HIS:HB3	2.14	0.48
3:I:214:GLU:O	3:I:216:PRO:HD3	2.14	0.48
3:C:664:GLU:C	3:C:666:THR:H	2.16	0.48
1:D:191:THR:CG2	1:D:202:ARG:HB3	2.44	0.48
1:G:53:VAL:HB	1:G:57:ILE:HD12	1.95	0.48
3:I:467:LEU:HD22	3:I:548:SER:OG	2.13	0.48
1:A:18:GLN:NE2	1:A:18:GLN:H	2.11	0.48
1:D:18:GLN:NE2	1:D:18:GLN:H	2.12	0.48
1:D:198:VAL:CG2	1:D:199:THR:N	2.76	0.48
3:F:155:ARG:NH1	3:F:419:SER:HB3	2.29	0.48
3:I:166:ALA:HB1	3:I:389:ILE:CD1	2.44	0.48
3:I:134:LYS:HZ1	3:I:435:ASP:HB3	1.78	0.48
3:C:622:VAL:HG13	3:C:643:TYR:CE2	2.49	0.48
1:D:57:ILE:HG12	1:D:175:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:GLN:HE22	1:D:257:ARG:HG3	1.79	0.48
2:E:56:PHE:HB3	2:E:62:PHE:CD1	2.49	0.48
3:F:122:LEU:O	3:F:123:TYR:CB	2.61	0.48
3:F:147:LEU:C	3:F:148:ASN:HD22	2.16	0.48
3:C:247:TYR:N	3:C:247:TYR:CD1	2.81	0.47
3:C:155:ARG:NH1	3:C:419:SER:HB3	2.28	0.47
1:A:49:ARG:O	1:A:50:THR:CB	2.61	0.47
2:H:21:ASN:CG	2:H:22:PHE:H	2.17	0.47
3:I:247:TYR:N	3:I:247:TYR:CD1	2.81	0.47
3:I:518:THR:C	3:I:520:GLN:H	2.17	0.47
1:G:35:LEU:CD2	1:G:49:ARG:HG3	2.44	0.47
1:G:23:SER:OG	1:G:73:ASP:OD2	2.32	0.47
3:C:502:LEU:O	3:C:506:ILE:HG13	2.14	0.47
3:C:724:GLY:O	3:C:726:PHE:N	2.48	0.47
1:G:264:HIS:ND1	1:G:266:GLY:N	2.47	0.47
1:A:25:PHE:CD1	1:A:25:PHE:N	2.82	0.47
1:A:264:HIS:ND1	1:A:266:GLY:N	2.49	0.47
3:C:122:LEU:O	3:C:126:ASP:OD2	2.33	0.47
1:D:49:ARG:O	1:D:50:THR:CB	2.62	0.47
3:F:203:VAL:HG13	3:F:204:ASP:N	2.29	0.47
3:F:494:PHE:HA	3:F:556:CYS:O	2.14	0.47
1:G:191:THR:CG2	1:G:202:ARG:HB3	2.45	0.47
1:A:8:LEU:HB2	1:A:169:LEU:HD13	1.95	0.47
1:A:46:VAL:HG21	1:A:66:SER:HA	1.97	0.47
6:G:309:GOL:C3	3:I:646:ARG:HH21	2.24	0.47
3:I:664:GLU:C	3:I:666:THR:H	2.18	0.47
1:A:191:THR:O	1:A:192:HIS:HB3	2.14	0.47
3:C:205:LYS:HB2	3:C:370:SER:O	2.14	0.47
3:C:690:VAL:HG11	3:C:707:HIS:HB3	1.96	0.47
1:D:22:LEU:O	1:D:23:SER:O	2.33	0.47
3:I:708:THR:HG22	3:I:711:ALA:N	2.03	0.47
3:C:192:VAL:HG12	3:C:193:LYS:H	1.77	0.47
1:D:28:LEU:CD2	1:D:38:PHE:CD1	2.95	0.47
3:F:479:PHE:O	3:F:551:PRO:HG2	2.15	0.47
1:G:120:GLY:CA	2:H:31:HIS:CE1	2.98	0.47
3:C:345:LEU:HB3	3:C:349:MET:CE	2.45	0.47
1:D:150:HIS:CD2	1:D:153:ARG:H	2.27	0.47
1:D:35:LEU:CD2	1:D:49:ARG:HG3	2.45	0.47
1:A:92:GLU:CB	1:A:94:HIS:NE2	2.78	0.47
3:C:236:ASN:O	3:C:237:PHE:HB2	2.15	0.47
1:G:236:PRO:HG2	2:H:65:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:163:GLU:O	3:I:167:LEU:HD13	2.14	0.47
3:I:622:VAL:HG13	3:I:643:TYR:CE2	2.50	0.47
3:I:724:GLY:O	3:I:725:ALA:C	2.53	0.47
3:C:747:ASN:HD22	3:C:747:ASN:N	2.13	0.46
3:F:149:GLU:O	3:F:151:SER:N	2.48	0.46
3:F:635:MET:HE1	3:F:726:PHE:HZ	1.79	0.46
1:A:191:THR:CG2	1:A:202:ARG:HB3	2.46	0.46
3:C:628:TYR:O	3:C:632:ILE:HG12	2.15	0.46
3:C:699:HIS:CD2	3:C:701:PHE:HB2	2.50	0.46
1:D:179:VAL:O	1:D:179:VAL:HG12	2.16	0.46
3:I:747:ASN:HB3	3:I:756:ILE:HD13	1.97	0.46
3:C:483:ASN:ND2	3:C:540:ALA:HB3	2.31	0.46
1:D:209:TYR:HA	1:D:210:PRO:O	2.15	0.46
3:F:153:VAL:CG2	3:F:154:PRO:CD	2.94	0.46
3:F:747:ASN:HB3	3:F:756:ILE:HD13	1.97	0.46
1:G:256:GLN:HE22	1:G:257:ARG:HG3	1.79	0.46
3:C:166:ALA:HB1	3:C:389:ILE:CD1	2.46	0.46
1:D:92:GLU:CB	1:D:94:HIS:NE2	2.79	0.46
3:C:231:LYS:CG	3:C:253:SER:HB3	2.46	0.46
1:D:194:VAL:HG22	1:D:199:THR:CG2	2.44	0.46
1:A:207:ASN:HD21	2:B:13:HIS:CD2	2.33	0.46
3:C:153:VAL:CG2	3:C:154:PRO:CD	2.94	0.46
2:E:29:GLY:HA2	2:E:61:SER:HB2	1.97	0.46
2:H:36:GLU:HG2	2:H:83:ASN:HB3	1.98	0.46
3:I:155:ARG:NH1	3:I:419:SER:HB3	2.29	0.46
2:B:56:PHE:HB3	2:B:62:PHE:CD1	2.51	0.46
2:E:17:ASN:HA	2:E:72:PRO:O	2.16	0.46
2:H:45:ARG:HG3	2:H:45:ARG:O	2.16	0.46
3:I:724:GLY:O	3:I:726:PHE:N	2.47	0.46
3:C:639:LEU:HA	3:C:639:LEU:HD12	1.73	0.46
1:D:135:ALA:HB1	1:D:140:ALA:HB3	1.97	0.46
1:G:22:LEU:O	1:G:23:SER:O	2.33	0.46
2:H:56:PHE:HB3	2:H:62:PHE:CD1	2.51	0.46
1:A:150:HIS:O	1:A:151:LYS:HB2	2.15	0.46
3:F:625:LEU:HD13	3:F:713:LEU:CD2	2.45	0.46
1:G:50:THR:CG2	1:G:52:TRP:CD1	2.99	0.46
3:I:625:LEU:HD13	3:I:713:LEU:CD2	2.45	0.46
1:A:144:LYS:O	1:A:148:GLU:HG3	2.16	0.46
3:I:153:VAL:CG2	3:I:154:PRO:CD	2.94	0.46
1:A:4:ARG:N	1:A:4:ARG:CD	2.79	0.45
1:D:4:ARG:O	1:D:4:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:231:LYS:CG	3:F:253:SER:HB3	2.46	0.45
1:G:49:ARG:O	1:G:50:THR:CB	2.63	0.45
1:G:4:ARG:HG2	1:G:4:ARG:O	2.16	0.45
3:I:414:PRO:HG2	3:I:572:THR:HG22	1.97	0.45
1:A:178:GLY:O	1:A:182:GLN:HB2	2.16	0.45
1:A:66:SER:O	1:A:70:LYS:HG3	2.17	0.45
1:D:25:PHE:N	1:D:25:PHE:CD1	2.83	0.45
2:E:54:LEU:HD11	2:E:62:PHE:HB3	1.99	0.45
3:F:747:ASN:N	3:F:747:ASN:HD22	2.14	0.45
1:G:198:VAL:HA	1:G:252:PRO:CG	2.44	0.45
1:G:25:PHE:CD1	1:G:25:PHE:N	2.84	0.45
3:C:149:GLU:O	3:C:151:SER:N	2.50	0.45
3:C:279:VAL:HB	3:C:334:VAL:HG13	1.98	0.45
1:D:150:HIS:O	1:D:151:LYS:HB2	2.17	0.45
3:F:699:HIS:CD2	3:F:701:PHE:H	2.34	0.45
3:C:316:PHE:CD1	3:F:740:TRP:CH2	3.04	0.45
2:H:35:ILE:HD11	2:H:82:VAL:CG1	2.46	0.45
3:I:236:ASN:O	3:I:237:PHE:HB2	2.17	0.45
3:I:316:PHE:O	3:I:319:THR:HB	2.16	0.45
3:I:544:PHE:O	3:I:548:SER:HB2	2.16	0.45
2:B:21:ASN:CG	2:B:22:PHE:H	2.18	0.45
1:D:110:THR:HG21	1:D:166:PRO:HG3	1.98	0.45
1:D:4:ARG:N	1:D:4:ARG:CD	2.79	0.45
1:G:146:GLU:CD	3:I:629:ARG:HH22	2.19	0.45
1:G:22:LEU:O	1:G:23:SER:HB3	2.16	0.45
3:I:600:LYS:HB3	3:I:608:ASN:ND2	2.32	0.45
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.97	0.45
2:E:35:ILE:HD11	2:E:82:VAL:CG1	2.46	0.45
3:F:507:GLU:O	3:F:511:GLN:HG3	2.17	0.45
3:F:664:GLU:C	3:F:666:THR:H	2.18	0.45
1:G:178:GLY:O	1:G:182:GLN:HB2	2.16	0.45
1:G:209:TYR:HA	1:G:210:PRO:O	2.16	0.45
1:A:209:TYR:HA	1:A:210:PRO:O	2.16	0.45
1:A:23:SER:OG	1:A:73:ASP:OD2	2.34	0.45
1:A:74:HIS:HB3	3:C:646:ARG:NH1	2.32	0.45
2:E:21:ASN:CG	2:E:22:PHE:H	2.19	0.45
3:F:316:PHE:O	3:F:319:THR:HB	2.16	0.45
1:G:92:GLU:CB	1:G:94:HIS:NE2	2.80	0.45
3:I:494:PHE:HA	3:I:556:CYS:O	2.16	0.45
3:I:496:VAL:HG22	3:I:555:PHE:HB3	1.99	0.45
3:C:448:ILE:HD13	3:C:598:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:232:LEU:HD11	3:F:256:ILE:HB	1.99	0.45
1:A:49:ARG:HD2	2:B:53:ASP:OD2	2.16	0.45
1:D:176:GLY:O	1:D:177:ARG:C	2.54	0.45
3:F:414:PRO:HG2	3:F:572:THR:HG22	1.98	0.45
2:H:17:ASN:HA	2:H:72:PRO:O	2.17	0.45
3:I:618:LEU:HA	3:I:618:LEU:HD12	1.81	0.45
3:C:232:LEU:HB3	3:C:367:THR:HG23	1.98	0.45
3:C:310:THR:N	3:C:311:PRO:CD	2.79	0.45
3:C:316:PHE:O	3:C:319:THR:HB	2.16	0.45
1:D:144:LYS:O	1:D:148:GLU:HG3	2.16	0.45
2:E:36:GLU:HG2	2:E:83:ASN:HB3	1.99	0.45
1:G:144:LYS:O	1:G:148:GLU:HG3	2.17	0.45
2:H:54:LEU:HD11	2:H:62:PHE:HB3	1.98	0.45
2:B:1:ILE:HG23	2:B:1:ILE:O	2.16	0.45
3:C:186:HIS:CE1	3:C:316:PHE:CE2	3.05	0.45
1:D:53:VAL:HA	1:D:57:ILE:HG13	1.99	0.45
3:F:518:THR:HG22	3:F:520:GLN:HB2	1.99	0.45
1:G:179:VAL:O	1:G:179:VAL:HG12	2.17	0.45
1:A:50:THR:CG2	1:A:52:TRP:CD1	3.00	0.44
2:B:17:ASN:HA	2:B:72:PRO:O	2.17	0.44
2:B:68:THR:HG22	2:B:69:GLU:O	2.17	0.44
2:B:35:ILE:HD11	2:B:82:VAL:CG1	2.47	0.44
3:C:724:GLY:O	3:C:725:ALA:C	2.55	0.44
1:D:114:TRP:HB3	1:D:126:PHE:HB3	1.99	0.44
1:D:178:GLY:O	1:D:182:GLN:HB2	2.17	0.44
2:E:35:ILE:HD11	2:E:82:VAL:HG13	2.00	0.44
3:F:122:LEU:O	3:F:126:ASP:OD2	2.35	0.44
3:F:724:GLY:O	3:F:725:ALA:C	2.55	0.44
3:I:507:GLU:O	3:I:511:GLN:HG3	2.17	0.44
1:A:114:TRP:HB3	1:A:126:PHE:HB3	1.99	0.44
3:C:240:LYS:HE3	3:C:240:LYS:HB2	1.87	0.44
3:F:724:GLY:O	3:F:726:PHE:N	2.50	0.44
2:H:35:ILE:HD11	2:H:82:VAL:HG13	1.99	0.44
3:I:231:LYS:CG	3:I:253:SER:HB3	2.46	0.44
3:I:186:HIS:CE1	3:I:316:PHE:CE2	3.05	0.44
1:A:85:GLU:HG3	3:C:629:ARG:HD3	2.00	0.44
3:F:163:GLU:O	3:F:167:LEU:HD13	2.17	0.44
3:F:595:GLY:O	3:F:599:ILE:HG12	2.16	0.44
1:G:53:VAL:C	1:G:55:SER:H	2.21	0.44
1:D:18:GLN:O	1:D:19:ASP:CB	2.60	0.44
2:E:45:ARG:HG3	2:E:45:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:HIS:HB3	1:D:113:TYR:OH	2.18	0.44
3:F:515:HIS:CD2	3:F:518:THR:H	2.35	0.44
3:F:640:GLN:OE1	3:F:643:TYR:HD1	2.01	0.44
1:G:114:TRP:HB3	1:G:126:PHE:HB3	1.99	0.44
3:I:149:GLU:O	3:I:151:SER:N	2.50	0.44
3:I:479:PHE:O	3:I:551:PRO:HG2	2.18	0.44
3:I:588:ARG:HH11	3:I:588:ARG:HG3	1.83	0.44
1:A:256:GLN:HE22	1:A:257:ARG:HG3	1.82	0.44
2:B:31:HIS:CB	2:B:32:PRO:CD	2.96	0.44
2:B:39:LEU:CD2	2:B:80:CYS:HB3	2.47	0.44
3:C:147:LEU:CD2	3:C:165:LEU:HD11	2.48	0.44
3:C:635:MET:HE1	3:C:726:PHE:CZ	2.51	0.44
3:F:483:ASN:ND2	3:F:540:ALA:HB3	2.32	0.44
3:I:122:LEU:O	3:I:126:ASP:OD2	2.35	0.44
3:I:528:TRP:CG	3:I:529:ALA:N	2.85	0.44
1:A:110:THR:HG21	1:A:166:PRO:HG3	1.99	0.44
1:A:176:GLY:O	1:A:177:ARG:C	2.55	0.44
2:B:54:LEU:HD11	2:B:62:PHE:HB3	2.00	0.44
1:D:22:LEU:O	1:D:23:SER:HB3	2.18	0.44
1:D:50:THR:CG2	1:D:52:TRP:CD1	3.01	0.44
2:E:1:ILE:HG23	2:E:1:ILE:O	2.18	0.44
3:F:191:GLN:NE2	3:F:222:TYR:H	2.16	0.44
3:C:476:LEU:HB2	3:F:680:ARG:HH22	1.83	0.44
1:G:28:LEU:CD2	1:G:38:PHE:CD1	2.97	0.44
1:G:4:ARG:CD	1:G:4:ARG:N	2.79	0.44
3:I:240:LYS:HE3	3:I:240:LYS:HB2	1.90	0.44
2:B:45:ARG:HG3	2:B:45:ARG:O	2.17	0.44
3:C:163:GLU:O	3:C:167:LEU:HD13	2.17	0.44
3:C:221:ALA:O	3:C:222:TYR:HB2	2.17	0.44
1:D:115:LYS:HE3	1:D:125:GLU:OE2	2.18	0.44
1:D:90:SER:C	1:D:92:GLU:H	2.20	0.44
1:D:204:ARG:NH2	2:E:11:SER:O	2.51	0.44
3:F:211:TYR:O	3:F:212:LEU:HB3	2.18	0.44
3:I:448:ILE:HD13	3:I:598:VAL:HG11	2.00	0.44
3:I:747:ASN:N	3:I:747:ASN:HD22	2.15	0.44
1:A:28:LEU:CD2	1:A:38:PHE:CD1	2.96	0.44
3:C:272:GLU:OE1	3:C:331:ASN:HB2	2.17	0.44
3:C:498:ALA:HB2	3:C:553:VAL:HA	1.98	0.44
3:F:348:ASN:HD22	3:F:348:ASN:N	2.15	0.44
2:H:31:HIS:O	2:H:62:PHE:CD2	2.71	0.44
3:I:628:TYR:O	3:I:632:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:SER:HA	2:H:22:PHE:O	2.18	0.43
2:B:36:GLU:HG2	2:B:83:ASN:HB3	1.98	0.43
3:C:588:ARG:HH11	3:C:588:ARG:HG3	1.84	0.43
2:E:39:LEU:CD2	2:E:80:CYS:HB3	2.47	0.43
2:B:4:THR:OG1	2:B:5:PRO:HD2	2.18	0.43
3:C:232:LEU:HD11	3:C:256:ILE:HB	1.99	0.43
3:C:712:LEU:HD23	3:C:712:LEU:C	2.38	0.43
1:G:121:GLN:NE2	2:H:1:ILE:CG2	2.81	0.43
1:G:191:THR:O	1:G:192:HIS:HB3	2.16	0.43
1:G:90:SER:C	1:G:92:GLU:H	2.21	0.43
3:I:348:ASN:HD22	3:I:348:ASN:N	2.16	0.43
3:I:699:HIS:CD2	3:I:701:PHE:HB2	2.53	0.43
2:B:35:ILE:HD11	2:B:82:VAL:HG13	2.01	0.43
3:C:493:ASN:HB2	3:C:495:LYS:HZ2	1.83	0.43
3:C:528:TRP:CG	3:C:529:ALA:N	2.87	0.43
2:E:31:HIS:CB	2:E:32:PRO:CD	2.96	0.43
3:F:236:ASN:O	3:F:237:PHE:HB2	2.18	0.43
3:F:293:ALA:HB2	3:F:339:ARG:NH1	2.33	0.43
1:A:115:LYS:HE3	1:A:125:GLU:OE2	2.18	0.43
1:A:126:PHE:CE2	1:A:128:PRO:HG3	2.54	0.43
1:A:90:SER:C	1:A:92:GLU:H	2.20	0.43
1:A:98:VAL:HA	1:A:115:LYS:O	2.19	0.43
3:C:664:GLU:C	3:C:666:THR:N	2.72	0.43
3:F:190:ILE:HB	3:F:458:PHE:CE2	2.54	0.43
3:F:628:TYR:O	3:F:632:ILE:HG12	2.18	0.43
2:H:9:VAL:HG21	2:H:95:TRP:HA	1.99	0.43
3:I:125:ASP:O	3:I:129:ARG:HG3	2.19	0.43
3:I:310:THR:N	3:I:311:PRO:CD	2.81	0.43
3:I:515:HIS:CD2	3:I:518:THR:H	2.36	0.43
1:A:57:ILE:CA	1:A:175:LEU:HD21	2.43	0.43
3:C:122:LEU:HD12	3:C:122:LEU:N	2.34	0.43
2:E:68:THR:HG22	2:E:69:GLU:O	2.18	0.43
3:F:699:HIS:CD2	3:F:701:PHE:HB2	2.53	0.43
3:F:717:LYS:O	3:F:720:LYS:HG2	2.19	0.43
1:G:78:VAL:HG22	3:I:622:VAL:HG11	2.01	0.43
3:I:448:ILE:HD13	3:I:598:VAL:CG1	2.48	0.43
1:A:194:VAL:HG22	1:A:199:THR:CG2	2.45	0.43
3:C:178:LEU:O	3:C:179:SER:C	2.55	0.43
3:C:243:PHE:HB3	3:C:274:LEU:HD11	2.00	0.43
3:C:268:VAL:HG21	3:C:334:VAL:HG21	2.01	0.43
3:C:290:ILE:O	3:C:339:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:SER:HB3	3:C:394:LYS:HG3	2.01	0.43
2:H:31:HIS:CB	2:H:32:PRO:CD	2.97	0.43
3:I:483:ASN:ND2	3:I:540:ALA:HB3	2.33	0.43
1:A:131:LEU:HD21	1:A:158:ARG:CZ	2.48	0.43
1:A:53:VAL:C	1:A:55:SER:H	2.21	0.43
3:C:135:LEU:HD13	3:C:592:GLU:HB2	2.01	0.43
3:C:194:ASP:CG	3:C:195:SER:N	2.73	0.43
3:C:515:HIS:CD2	3:C:518:THR:H	2.37	0.43
2:E:21:ASN:N	2:E:70:PHE:O	2.46	0.43
3:F:122:LEU:N	3:F:122:LEU:HD12	2.34	0.43
3:F:125:ASP:O	3:F:129:ARG:HG3	2.19	0.43
3:F:496:VAL:HG22	3:F:555:PHE:HB3	1.99	0.43
3:F:504:THR:HG22	3:F:508:LYS:HE2	2.01	0.43
3:F:528:TRP:CG	3:F:529:ALA:N	2.86	0.43
3:C:699:HIS:CD2	3:C:701:PHE:H	2.36	0.43
2:E:37:VAL:HG22	2:E:82:VAL:HG22	2.00	0.43
3:F:178:LEU:O	3:F:179:SER:C	2.55	0.43
3:F:531:LYS:C	3:F:531:LYS:HD3	2.39	0.43
3:F:467:LEU:HD22	3:F:548:SER:OG	2.19	0.43
1:G:115:LYS:HE3	1:G:125:GLU:OE2	2.18	0.43
1:A:22:LEU:HD12	3:C:619:LEU:CD2	2.46	0.43
2:B:21:ASN:N	2:B:70:PHE:O	2.46	0.43
3:C:129:ARG:HB3	3:C:129:ARG:HH11	1.84	0.43
3:C:348:ASN:HD22	3:C:348:ASN:N	2.17	0.43
3:C:544:PHE:O	3:C:548:SER:HB2	2.19	0.43
1:D:198:VAL:CG2	1:D:199:THR:H	2.32	0.43
1:G:53:VAL:HG23	1:G:54:SER:N	2.34	0.43
3:I:229:THR:CG2	3:I:374:LYS:HG3	2.49	0.43
3:I:243:PHE:HB3	3:I:274:LEU:HD11	2.01	0.43
3:I:600:LYS:O	3:I:608:ASN:ND2	2.52	0.43
1:A:40:ASP:OD2	1:A:40:ASP:C	2.57	0.42
1:A:4:ARG:HG2	1:A:4:ARG:O	2.18	0.42
2:B:9:VAL:HG21	2:B:95:TRP:HA	2.01	0.42
3:C:600:LYS:HB3	3:C:608:ASN:ND2	2.32	0.42
3:C:618:LEU:HA	3:C:618:LEU:HD12	1.81	0.42
1:D:49:ARG:NH1	2:E:53:ASP:OD2	2.38	0.42
3:F:588:ARG:HG3	3:F:588:ARG:HH11	1.84	0.42
1:G:28:LEU:HD21	1:G:38:PHE:CD1	2.54	0.42
3:I:502:LEU:O	3:I:506:ILE:HG13	2.19	0.42
3:I:603:HIS:C	3:I:603:HIS:CD2	2.92	0.42
1:A:254:GLU:OE2	1:A:257:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:147:LEU:CD2	3:F:165:LEU:HD11	2.48	0.42
1:G:176:GLY:O	1:G:177:ARG:C	2.57	0.42
2:H:40:LEU:HA	2:H:44:GLU:O	2.19	0.42
3:I:129:ARG:HH11	3:I:129:ARG:HB3	1.84	0.42
3:I:518:THR:HG22	3:I:520:GLN:HB2	2.00	0.42
3:C:205:LYS:O	3:C:208:ARG:NH1	2.52	0.42
1:D:126:PHE:CE2	1:D:128:PRO:HG3	2.54	0.42
2:E:40:LEU:HA	2:E:44:GLU:O	2.18	0.42
3:F:290:ILE:O	3:F:339:ARG:NH2	2.52	0.42
3:F:229:THR:HA	3:F:373:VAL:O	2.19	0.42
1:G:202:ARG:CZ	2:H:99:MET:HG2	2.48	0.42
3:I:122:LEU:N	3:I:122:LEU:HD12	2.34	0.42
3:I:268:VAL:HG21	3:I:334:VAL:HG21	2.01	0.42
3:I:349:MET:HG2	3:I:367:THR:HA	2.01	0.42
3:C:580:ILE:HA	3:C:581:PRO:HD2	1.88	0.42
3:F:335:GLN:NE2	3:F:336:THR:H	2.17	0.42
1:G:235:LEU:HD13	2:H:10:TYR:CZ	2.54	0.42
3:I:135:LEU:HD13	3:I:592:GLU:HB2	2.01	0.42
3:I:178:LEU:O	3:I:179:SER:C	2.57	0.42
3:I:232:LEU:HB3	3:I:367:THR:HG23	2.00	0.42
3:C:229:THR:CG2	3:C:374:LYS:HG3	2.49	0.42
1:G:192:HIS:CB	1:G:201:LEU:HD23	2.49	0.42
1:G:66:SER:O	1:G:70:LYS:HG3	2.18	0.42
2:H:68:THR:HG22	2:H:69:GLU:O	2.19	0.42
3:I:664:GLU:C	3:I:666:THR:N	2.73	0.42
1:A:110:THR:HG22	1:A:111:GLU:N	2.35	0.42
3:C:222:TYR:CE2	3:C:308:PRO:HG3	2.54	0.42
3:C:479:PHE:O	3:C:551:PRO:HG2	2.19	0.42
2:E:31:HIS:O	2:E:62:PHE:CD2	2.69	0.42
3:F:243:PHE:HB3	3:F:274:LEU:HD11	2.01	0.42
3:I:293:ALA:HB2	3:I:339:ARG:NH1	2.35	0.42
3:I:635:MET:HE1	3:I:726:PHE:CZ	2.54	0.42
1:A:206:LEU:CD1	2:B:14:PRO:HD3	2.50	0.42
3:F:129:ARG:HH11	3:F:129:ARG:HB3	1.84	0.42
3:F:211:TYR:CE2	3:F:344:LYS:HD2	2.55	0.42
3:F:349:MET:HG2	3:F:367:THR:HA	2.00	0.42
3:F:509:THR:O	3:F:513:VAL:HG23	2.18	0.42
3:I:509:THR:O	3:I:513:VAL:HG23	2.20	0.42
1:G:63:LEU:HD21	3:I:657:THR:HG22	2.02	0.42
3:C:263:THR:HG22	3:C:264:PHE:N	2.35	0.42
3:C:349:MET:HG2	3:C:367:THR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:SER:O	1:D:70:LYS:HG3	2.19	0.42
3:F:455:ALA:CB	3:F:461:VAL:HB	2.50	0.42
2:B:37:VAL:HG22	2:B:82:VAL:HG22	2.02	0.42
3:C:640:GLN:OE1	3:C:643:TYR:HD1	2.02	0.42
3:F:310:THR:N	3:F:311:PRO:CD	2.82	0.42
3:F:580:ILE:HA	3:F:581:PRO:HD2	1.88	0.42
3:F:639:LEU:HA	3:F:639:LEU:HD12	1.73	0.42
1:G:198:VAL:HG23	1:G:250:VAL:O	2.20	0.42
2:H:37:VAL:HG22	2:H:82:VAL:HG22	2.01	0.42
3:I:186:HIS:CE1	3:I:316:PHE:CZ	3.08	0.42
1:A:192:HIS:CB	1:A:201:LEU:HD23	2.50	0.42
1:A:237:ASN:O	1:A:239:ASP:N	2.50	0.42
2:B:40:LEU:HA	2:B:44:GLU:O	2.19	0.42
3:C:124:TRP:HH2	3:C:596:GLN:HG2	1.83	0.42
1:D:22:LEU:HD12	3:F:619:LEU:CG	2.49	0.42
1:D:37:VAL:HG22	1:D:38:PHE:N	2.35	0.42
3:F:723:ASN:O	3:F:725:ALA:N	2.53	0.42
1:G:255:GLU:OE1	1:G:255:GLU:N	2.52	0.42
2:H:16:GLU:O	2:H:17:ASN:C	2.58	0.42
2:H:4:THR:OG1	2:H:5:PRO:HD2	2.20	0.42
1:G:82:THR:HG23	3:I:629:ARG:NH2	2.35	0.42
3:I:699:HIS:CD2	3:I:701:PHE:H	2.37	0.42
3:C:168:TYR:O	3:C:172:GLN:HG2	2.20	0.41
3:C:507:GLU:O	3:C:511:GLN:HG3	2.20	0.41
3:C:518:THR:HG22	3:C:520:GLN:HB2	2.01	0.41
3:C:539:ASN:ND2	3:C:541:ALA:HB3	2.35	0.41
3:C:664:GLU:O	3:C:666:THR:N	2.53	0.41
1:D:150:HIS:ND1	3:F:640:GLN:HB3	2.35	0.41
1:D:254:GLU:OE2	1:D:257:ARG:NH1	2.53	0.41
2:E:15:ALA:HB2	2:E:95:TRP:CZ2	2.55	0.41
3:F:539:ASN:ND2	3:F:541:ALA:HB3	2.35	0.41
1:G:110:THR:HG22	1:G:111:GLU:N	2.34	0.41
3:I:192:VAL:CG1	3:I:193:LYS:N	2.83	0.41
3:I:290:ILE:O	3:I:339:ARG:NH2	2.53	0.41
3:I:154:PRO:HA	3:I:413:GLY:O	2.19	0.41
1:A:99:ILE:HG23	1:A:99:ILE:O	2.20	0.41
3:C:715:ASN:ND2	3:C:731:PHE:HB2	2.34	0.41
3:F:149:GLU:C	3:F:151:SER:N	2.72	0.41
3:F:229:THR:CG2	3:F:374:LYS:HG3	2.50	0.41
3:F:655:ARG:NH1	3:F:655:ARG:CG	2.81	0.41
3:F:664:GLU:C	3:F:666:THR:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:498:ALA:HB2	3:I:553:VAL:HA	2.01	0.41
1:A:22:LEU:O	1:A:23:SER:HB3	2.20	0.41
1:D:235:LEU:HB3	2:E:10:TYR:OH	2.20	0.41
1:D:40:ASP:C	1:D:40:ASP:OD2	2.59	0.41
1:D:53:VAL:C	1:D:55:SER:H	2.24	0.41
2:E:12:ARG:NH2	2:E:22:PHE:CD2	2.78	0.41
3:F:298:PHE:CG	3:F:299:GLY:N	2.88	0.41
3:F:446:ARG:HH11	3:F:602:THR:HA	1.85	0.41
3:F:709:LEU:HA	3:F:709:LEU:HD12	1.84	0.41
1:G:254:GLU:OE2	1:G:257:ARG:NH1	2.53	0.41
1:G:98:VAL:HA	1:G:115:LYS:O	2.21	0.41
3:I:593:VAL:HG23	3:I:594:ALA:N	2.35	0.41
3:I:551:PRO:HD3	3:I:682:GLU:CB	2.50	0.41
1:A:9:HIS:HB3	1:A:113:TYR:OH	2.20	0.41
1:A:179:VAL:O	1:A:179:VAL:HG12	2.18	0.41
1:A:53:VAL:HG23	1:A:54:SER:N	2.34	0.41
2:B:12:ARG:NH2	2:B:22:PHE:CD2	2.77	0.41
1:A:49:ARG:NH1	2:B:53:ASP:OD2	2.37	0.41
3:C:293:ALA:HB2	3:C:339:ARG:NH1	2.36	0.41
3:F:154:PRO:HA	3:F:413:GLY:O	2.20	0.41
3:F:192:VAL:CG1	3:F:193:LYS:N	2.82	0.41
3:F:518:THR:HG22	3:F:520:GLN:CG	2.50	0.41
3:F:712:LEU:HD23	3:F:712:LEU:C	2.40	0.41
1:G:235:LEU:HD13	2:H:10:TYR:CE1	2.55	0.41
1:G:40:ASP:OD2	1:G:40:ASP:C	2.59	0.41
2:H:12:ARG:HG2	2:H:13:HIS:CE1	2.54	0.41
3:I:168:TYR:O	3:I:172:GLN:HG2	2.20	0.41
3:I:210:VAL:HG12	3:I:211:TYR:CD1	2.44	0.41
3:I:705:GLY:HA3	3:I:707:HIS:CE1	2.55	0.41
1:A:229:PHE:HD1	1:A:230:GLU:O	2.03	0.41
1:A:35:LEU:HD23	1:A:36:PHE:N	2.36	0.41
3:C:150:ASN:C	3:C:153:VAL:HG22	2.41	0.41
3:C:518:THR:HG22	3:C:520:GLN:CG	2.50	0.41
3:C:603:HIS:C	3:C:603:HIS:CD2	2.93	0.41
1:D:192:HIS:CB	1:D:201:LEU:HD23	2.50	0.41
1:G:150:HIS:CD2	1:G:153:ARG:H	2.29	0.41
1:G:35:LEU:CD2	1:G:35:LEU:C	2.89	0.41
1:G:121:GLN:CG	2:H:1:ILE:HG22	2.50	0.41
3:I:149:GLU:C	3:I:151:SER:N	2.73	0.41
3:I:191:GLN:NE2	3:I:222:TYR:H	2.18	0.41
1:A:198:VAL:HG23	1:A:250:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD11	2:B:14:PRO:HD3	2.02	0.41
2:B:16:GLU:O	2:B:17:ASN:C	2.58	0.41
2:B:79:ALA:HB1	2:B:93:VAL:O	2.20	0.41
3:C:205:LYS:HB3	3:C:205:LYS:NZ	2.35	0.41
3:C:263:THR:CG2	3:C:264:PHE:N	2.84	0.41
3:C:353:CYS:HB2	3:C:363:CYS:O	2.21	0.41
3:F:232:LEU:HB3	3:F:367:THR:HG23	2.01	0.41
3:F:493:ASN:HB2	3:F:495:LYS:HZ2	1.86	0.41
1:G:110:THR:CG2	1:G:111:GLU:N	2.83	0.41
1:G:49:ARG:HD2	2:H:53:ASP:OD2	2.21	0.41
2:H:21:ASN:N	2:H:70:PHE:O	2.45	0.41
3:I:124:TRP:HH2	3:I:596:GLN:HG2	1.85	0.41
3:I:704:SER:O	3:I:707:HIS:CE1	2.74	0.41
3:I:712:LEU:HD23	3:I:712:LEU:C	2.40	0.41
3:I:723:ASN:O	3:I:725:ALA:N	2.53	0.41
1:A:110:THR:CG2	1:A:111:GLU:N	2.83	0.41
2:E:4:THR:OG1	2:E:5:PRO:HD2	2.21	0.41
3:F:603:HIS:CD2	3:F:603:HIS:C	2.94	0.41
1:D:146:GLU:CD	3:F:629:ARG:HH22	2.24	0.41
1:G:9:HIS:HB3	1:G:113:TYR:OH	2.20	0.41
1:G:35:LEU:HD23	1:G:36:PHE:N	2.35	0.41
3:I:147:LEU:CD2	3:I:165:LEU:HD11	2.50	0.41
3:I:298:PHE:CG	3:I:299:GLY:N	2.88	0.41
1:A:120:GLY:CA	2:B:31:HIS:CE1	3.04	0.41
3:F:166:ALA:HB1	3:F:389:ILE:HD13	2.02	0.41
3:F:241:LYS:O	3:F:244:GLU:HB3	2.21	0.41
3:F:236:ASN:HD21	3:F:258:ARG:HE	1.68	0.41
1:G:194:VAL:HG22	1:G:199:THR:CG2	2.44	0.41
3:I:655:ARG:CG	3:I:655:ARG:NH1	2.81	0.41
3:I:667:ASP:HB3	3:I:670:VAL:CG1	2.48	0.41
3:C:125:ASP:O	3:C:129:ARG:HG3	2.20	0.41
3:C:241:LYS:O	3:C:244:GLU:HB3	2.21	0.41
3:C:260:GLY:C	3:C:262:ILE:H	2.22	0.41
1:D:57:ILE:HG12	1:D:175:LEU:HD21	2.03	0.41
1:D:213:ILE:HG12	1:D:214:THR:N	2.36	0.41
3:F:194:ASP:CG	3:F:195:SER:N	2.74	0.41
1:A:198:VAL:CG2	1:A:199:THR:H	2.32	0.41
1:A:11:LEU:O	1:A:27:ALA:HA	2.21	0.41
1:A:37:VAL:HG22	1:A:38:PHE:N	2.35	0.41
2:B:12:ARG:HG2	2:B:13:HIS:CE1	2.56	0.41
3:C:298:PHE:CG	3:C:299:GLY:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:268:VAL:HG21	3:F:334:VAL:HG21	2.02	0.41
3:C:229:THR:HA	3:C:373:VAL:O	2.21	0.41
3:C:531:LYS:HD3	3:C:531:LYS:C	2.41	0.41
3:C:723:ASN:O	3:C:725:ALA:N	2.54	0.41
1:D:28:LEU:HD21	1:D:38:PHE:CD1	2.55	0.41
2:E:76:ASP:O	2:E:97:ARG:NH2	2.54	0.41
3:F:429:LEU:O	3:F:433:PHE:HD1	2.04	0.41
3:F:551:PRO:HD3	3:F:682:GLU:CB	2.51	0.41
1:G:230:GLU:H	1:G:230:GLU:CD	2.25	0.41
2:H:15:ALA:HB2	2:H:95:TRP:CZ2	2.56	0.41
2:H:76:ASP:O	2:H:97:ARG:NH2	2.54	0.41
1:A:235:LEU:HD13	2:B:10:TYR:CE1	2.56	0.40
2:B:11:SER:HA	2:B:22:PHE:O	2.20	0.40
2:B:13:HIS:O	2:B:21:ASN:OD1	2.39	0.40
3:C:149:GLU:C	3:C:151:SER:N	2.74	0.40
3:C:392:VAL:HG22	3:C:393:ILE:N	2.36	0.40
3:C:455:ALA:CB	3:C:461:VAL:HB	2.51	0.40
3:C:705:GLY:HA3	3:C:707:HIS:CE1	2.56	0.40
1:D:6:HIS:HA	1:D:32:ASP:OD1	2.21	0.40
3:F:448:ILE:HD13	3:F:598:VAL:CG1	2.51	0.40
3:F:704:SER:O	3:F:707:HIS:CE1	2.75	0.40
1:G:6:HIS:HA	1:G:32:ASP:OD1	2.21	0.40
1:G:74:HIS:HB3	3:I:646:ARG:NH1	2.36	0.40
3:I:150:ASN:C	3:I:153:VAL:HG22	2.41	0.40
3:I:350:GLU:O	3:I:365:MET:O	2.39	0.40
3:I:505:LEU:HD12	3:I:505:LEU:O	2.21	0.40
3:I:518:THR:HG22	3:I:520:GLN:CG	2.50	0.40
1:G:67:GLN:HE22	3:I:657:THR:HB	1.85	0.40
1:A:28:LEU:HD21	1:A:38:PHE:CD1	2.56	0.40
1:A:53:VAL:HA	1:A:57:ILE:HG13	2.02	0.40
3:C:186:HIS:CE1	3:C:316:PHE:CZ	3.10	0.40
3:C:319:THR:CG2	3:C:321:PHE:H	2.32	0.40
3:C:691:SER:HA	3:C:692:PRO:HD3	1.94	0.40
1:D:145:LEU:HB3	1:D:149:ARG:NH2	2.36	0.40
3:F:593:VAL:HG23	3:F:594:ALA:N	2.36	0.40
3:I:190:ILE:HB	3:I:458:PHE:CE2	2.55	0.40
3:I:263:THR:HB	3:I:266:GLU:CG	2.50	0.40
3:I:353:CYS:HB2	3:I:363:CYS:O	2.22	0.40
3:C:154:PRO:HA	3:C:413:GLY:O	2.21	0.40
3:C:335:GLN:NE2	3:C:336:THR:H	2.19	0.40
1:D:9:HIS:CE1	1:D:30:TYR:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:168:TYR:O	3:F:172:GLN:HG2	2.21	0.40
3:F:272:GLU:OE1	3:F:331:ASN:HB2	2.22	0.40
3:F:518:THR:HG22	3:F:520:GLN:CB	2.51	0.40
3:F:664:GLU:O	3:F:666:THR:N	2.54	0.40
1:G:247:THR:CG2	1:G:248:LEU:N	2.85	0.40
3:I:455:ALA:HB3	3:I:461:VAL:HB	2.04	0.40
1:A:50:THR:HG22	1:A:52:TRP:CD1	2.56	0.40
3:C:132:SER:O	3:C:136:ASP:OD1	2.39	0.40
3:C:435:ASP:O	3:C:436:MET:C	2.60	0.40
3:C:448:ILE:HD13	3:C:598:VAL:CG1	2.51	0.40
2:E:68:THR:HG22	2:E:69:GLU:N	2.36	0.40
3:F:618:LEU:HA	3:F:618:LEU:HD12	1.84	0.40
1:G:110:THR:HG21	1:G:166:PRO:HG3	2.02	0.40
3:I:194:ASP:CG	3:I:195:SER:N	2.75	0.40
1:A:35:LEU:CD2	1:A:35:LEU:C	2.90	0.40
3:C:153:VAL:HG23	3:C:161:LYS:CE	2.47	0.40
3:C:203:VAL:HG22	3:C:210:VAL:HG12	2.04	0.40
3:C:350:GLU:O	3:C:365:MET:O	2.39	0.40
3:C:163:GLU:HG3	3:C:387:LEU:HD12	2.03	0.40
3:C:551:PRO:HD3	3:C:682:GLU:CB	2.52	0.40
3:C:496:VAL:HG22	3:C:555:PHE:HB3	2.03	0.40
3:C:708:THR:HG22	3:C:711:ALA:N	2.03	0.40
1:D:250:VAL:HG11	1:D:258:TYR:CE1	2.57	0.40
3:F:150:ASN:HA	3:F:153:VAL:HG13	2.03	0.40
3:F:386:ILE:HG22	3:F:387:LEU:N	2.37	0.40
3:F:435:ASP:O	3:F:436:MET:C	2.59	0.40
3:F:506:ILE:O	3:F:510:MET:HG3	2.22	0.40
3:F:600:LYS:HB3	3:F:608:ASN:ND2	2.33	0.40
3:I:122:LEU:O	3:I:123:TYR:CB	2.59	0.40
3:I:439:LYS:C	3:I:441:GLY:H	2.25	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	270/275 (98%)	233 (86%)	24 (9%)	13 (5%)	2	8
1	D	270/275 (98%)	230 (85%)	26 (10%)	14 (5%)	2	7
1	G	270/275 (98%)	230 (85%)	27 (10%)	13 (5%)	2	8
2	B	97/99 (98%)	83 (86%)	9 (9%)	5 (5%)	2	7
2	E	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	2	7
2	H	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	2	7
3	C	633/640 (99%)	575 (91%)	45 (7%)	13 (2%)	8	27
3	F	633/640 (99%)	572 (90%)	47 (7%)	14 (2%)	8	26
3	I	633/640 (99%)	573 (90%)	47 (7%)	13 (2%)	8	27
All	All	3000/3042 (99%)	2664 (89%)	241 (8%)	95 (3%)	5	16

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	22	LEU
1	A	44	ARG
2	B	31	HIS
3	C	153	VAL
3	C	722	ASN
3	C	724	GLY
3	C	725	ALA
3	C	752	ASP
1	D	19	ASP
1	D	22	LEU
1	D	44	ARG
2	E	31	HIS
3	F	153	VAL
3	F	205	LYS
3	F	722	ASN
3	F	724	GLY
3	F	725	ALA
3	F	752	ASP
1	G	19	ASP
1	G	22	LEU
1	G	44	ARG
2	H	31	HIS

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Mol	Chain	Res	Type
3	I	153	VAL
3	I	205	LYS
3	I	722	ASN
3	I	724	GLY
3	I	725	ALA
3	I	752	ASP
1	A	177	ARG
2	B	17	ASN
3	C	212	LEU
3	C	366	VAL
3	C	440	ASP
1	D	177	ARG
1	D	255	GLU
1	D	256	GLN
2	E	17	ASN
3	F	366	VAL
3	F	440	ASP
1	G	177	ARG
2	H	17	ASN
3	I	210	VAL
3	I	366	VAL
3	I	440	ASP
1	A	23	SER
1	A	90	SER
1	A	255	GLU
1	A	256	GLN
2	B	32	PRO
3	C	150	ASN
3	C	208	ARG
1	D	23	SER
1	D	90	SER
2	E	32	PRO
3	F	150	ASN
1	G	23	SER
1	G	90	SER
1	G	255	GLU
1	G	256	GLN
2	H	32	PRO
3	I	150	ASN
1	A	50	THR
1	A	239	ASP
2	B	97	ARG

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Mol	Chain	Res	Type
3	C	123	TYR
3	C	360	ASP
3	C	665	LYS
1	D	50	THR
1	D	207	ASN
2	E	97	ARG
3	F	360	ASP
1	G	50	THR
1	G	207	ASN
2	H	97	ARG
1	A	207	ASN
1	D	239	ASP
3	F	123	TYR
3	F	665	LYS
1	G	239	ASP
3	I	123	TYR
3	I	360	ASP
1	A	236	PRO
1	D	16	SER
1	D	236	PRO
2	E	90	PRO
3	F	237	PHE
1	G	236	PRO
2	H	90	PRO
3	I	237	PHE
2	B	90	PRO
1	D	252	PRO
1	G	252	PRO
1	A	252	PRO
3	F	210	VAL

### 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	244/249 (98%)	230 (94%)	14 (6%)	24 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	244/249 (98%)	230 (94%)	14 (6%)	24	56
1	G	244/249 (98%)	230 (94%)	14 (6%)	24	56
2	B	92/94 (98%)	88 (96%)	4 (4%)	33	67
2	E	92/94 (98%)	88 (96%)	4 (4%)	33	67
2	H	92/94 (98%)	88 (96%)	4 (4%)	33	67
3	C	544/549 (99%)	504 (93%)	40 (7%)	16	42
3	F	544/549 (99%)	506 (93%)	38 (7%)	18	45
3	I	544/549 (99%)	505 (93%)	39 (7%)	17	43
All	All	2640/2676 (99%)	2469 (94%)	171 (6%)	20	49

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	13	MET
1	A	18	GLN
1	A	19	ASP
1	A	34	GLN
1	A	35	LEU
1	A	41	HIS
1	A	74	HIS
1	A	153	ARG
1	A	197	SER
1	A	232	LYS
1	A	245	TRP
1	A	255	GLU
1	A	269	GLN
2	B	19	LYS
2	B	21	ASN
2	B	51	HIS
2	B	70	PHE
3	C	146	LEU
3	C	152	TYR
3	C	153	VAL
3	C	155	ARG
3	C	160	GLN
3	C	181	VAL
3	C	183	ARG
3	C	184	ASP

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Mol	Chain	Res	Type
3	C	205	LYS
3	C	206	ASN
3	C	223	SER
3	C	227	THR
3	C	229	THR
3	C	242	ASP
3	C	247	TYR
3	C	297	PHE
3	C	319	THR
3	C	324	SER
3	C	336	THR
3	C	353	CYS
3	C	365	MET
3	C	376	THR
3	C	453	TRP
3	C	533	GLU
3	C	535	LEU
3	C	539	ASN
3	C	558	CYS
3	C	559	GLU
3	C	583	LEU
3	C	588	ARG
3	C	612	GLU
3	C	618	LEU
3	C	639	LEU
3	C	646	ARG
3	C	655	ARG
3	C	664	GLU
3	C	708	THR
3	C	709	LEU
3	C	716	LEU
3	C	753	VAL
1	D	4	ARG
1	D	13	MET
1	D	18	GLN
1	D	19	ASP
1	D	34	GLN
1	D	35	LEU
1	D	41	HIS
1	D	74	HIS
1	D	153	ARG
1	D	197	SER

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Mol	Chain	Res	Type
1	D	232	LYS
1	D	245	TRP
1	D	255	GLU
1	D	269	GLN
2	E	19	LYS
2	E	21	ASN
2	E	51	HIS
2	E	70	PHE
3	F	146	LEU
3	F	152	TYR
3	F	153	VAL
3	F	155	ARG
3	F	160	GLN
3	F	181	VAL
3	F	183	ARG
3	F	184	ASP
3	F	223	SER
3	F	227	THR
3	F	229	THR
3	F	242	ASP
3	F	247	TYR
3	F	297	PHE
3	F	319	THR
3	F	324	SER
3	F	336	THR
3	F	353	CYS
3	F	365	MET
3	F	376	THR
3	F	453	TRP
3	F	533	GLU
3	F	535	LEU
3	F	539	ASN
3	F	558	CYS
3	F	559	GLU
3	F	583	LEU
3	F	588	ARG
3	F	612	GLU
3	F	618	LEU
3	F	639	LEU
3	F	646	ARG
3	F	655	ARG
3	F	664	GLU

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Mol	Chain	Res	Type
3	F	708	THR
3	F	709	LEU
3	F	716	LEU
3	F	753	VAL
1	G	4	ARG
1	G	13	MET
1	G	18	GLN
1	G	19	ASP
1	G	34	GLN
1	G	35	LEU
1	G	41	HIS
1	G	74	HIS
1	G	153	ARG
1	G	197	SER
1	G	232	LYS
1	G	245	TRP
1	G	255	GLU
1	G	269	GLN
2	H	19	LYS
2	H	21	ASN
2	H	51	HIS
2	H	70	PHE
3	I	146	LEU
3	I	152	TYR
3	I	153	VAL
3	I	155	ARG
3	I	160	GLN
3	I	181	VAL
3	I	183	ARG
3	I	184	ASP
3	I	204	ASP
3	I	223	SER
3	I	227	THR
3	I	229	THR
3	I	242	ASP
3	I	247	TYR
3	I	297	PHE
3	I	319	THR
3	I	324	SER
3	I	336	THR
3	I	353	CYS
3	I	365	MET

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Mol	Chain	Res	Type
3	I	376	THR
3	I	453	TRP
3	I	533	GLU
3	I	535	LEU
3	I	539	ASN
3	I	558	CYS
3	I	559	GLU
3	I	583	LEU
3	I	588	ARG
3	I	612	GLU
3	I	618	LEU
3	I	639	LEU
3	I	646	ARG
3	I	655	ARG
3	I	664	GLU
3	I	708	THR
3	I	709	LEU
3	I	716	LEU
3	I	753	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	18	GLN
1	A	67	GLN
1	A	74	HIS
1	A	87	HIS
1	A	97	GLN
1	A	121	GLN
1	A	123	HIS
1	A	150	HIS
1	A	156	GLN
1	A	157	ASN
1	A	168	GLN
1	A	256	GLN
1	A	261	GLN
1	A	269	GLN
2	B	13	HIS
2	B	21	ASN
2	B	31	HIS
2	B	51	HIS

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Mol	Chain	Res	Type
2	B	83	ASN
3	C	160	GLN
3	C	191	GLN
3	C	198	ASN
3	C	206	ASN
3	C	215	ASN
3	C	236	ASN
3	C	302	HIS
3	C	379	ASN
3	C	483	ASN
3	C	493	ASN
3	C	515	HIS
3	C	539	ASN
3	C	603	HIS
3	C	608	ASN
3	C	640	GLN
3	C	684	HIS
3	C	699	HIS
3	C	747	ASN
1	D	9	HIS
1	D	18	GLN
1	D	64	GLN
1	D	67	GLN
1	D	74	HIS
1	D	87	HIS
1	D	97	GLN
1	D	121	GLN
1	D	123	HIS
1	D	150	HIS
1	D	157	ASN
1	D	168	GLN
1	D	207	ASN
1	D	222	GLN
1	D	256	GLN
1	D	261	GLN
1	D	269	GLN
2	E	21	ASN
2	E	51	HIS
2	E	83	ASN
3	F	160	GLN
3	F	191	GLN
3	F	198	ASN

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Mol	Chain	Res	Type
3	F	215	ASN
3	F	236	ASN
3	F	302	HIS
3	F	318	HIS
3	F	379	ASN
3	F	401	HIS
3	F	483	ASN
3	F	493	ASN
3	F	515	HIS
3	F	539	ASN
3	F	603	HIS
3	F	608	ASN
3	F	684	HIS
3	F	699	HIS
3	F	743	GLN
3	F	747	ASN
1	G	9	HIS
1	G	18	GLN
1	G	67	GLN
1	G	87	HIS
1	G	97	GLN
1	G	121	GLN
1	G	150	HIS
1	G	156	GLN
1	G	157	ASN
1	G	168	GLN
1	G	222	GLN
1	G	256	GLN
1	G	261	GLN
1	G	269	GLN
2	H	21	ASN
2	H	31	HIS
2	H	51	HIS
2	H	83	ASN
3	I	160	GLN
3	I	191	GLN
3	I	198	ASN
3	I	215	ASN
3	I	236	ASN
3	I	302	HIS
3	I	318	HIS
3	I	379	ASN

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Mol	Chain	Res	Type
3	I	483	ASN
3	I	493	ASN
3	I	515	HIS
3	I	539	ASN
3	I	603	HIS
3	I	608	ASN
3	I	640	GLN
3	I	699	HIS
3	I	743	GLN
3	I	747	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	C	900	3	14,14,15	0.63	0	15,19,21	0.83	1 (6%)
4	NAG	F	901	3	14,14,15	0.56	0	15,19,21	0.90	1 (6%)
6	GOL	G	309	-	5,5,5	1.77	2 (40%)	5,5,5	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	I	902	3	14,14,15	0.44	0	15,19,21	1.08	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	900	3	-	0/6/23/26	0/1/1/1
4	NAG	F	901	3	-	0/6/23/26	0/1/1/1
6	GOL	G	309	-	-	0/4/4/4	0/0/0/0
4	NAG	I	902	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	309	GOL	C3-C2	2.13	1.60	1.52
6	G	309	GOL	O2-C2	2.90	1.52	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	901	NAG	C2-N2-C7	-2.59	119.16	122.94
4	I	902	NAG	C2-N2-C7	-2.46	119.36	122.94
4	C	900	NAG	C2-N2-C7	-2.32	119.56	122.94
4	I	902	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	309	GOL	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.