



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 PM GMT

PDB ID : 4LK0  
Title : Crystal Structure Analysis of the E.coli holoenzyme/T7 Gp2 complex  
Authors : Bae, B.; Darst, S.A.  
Deposited on : 2013-07-05  
Resolution : 3.91 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

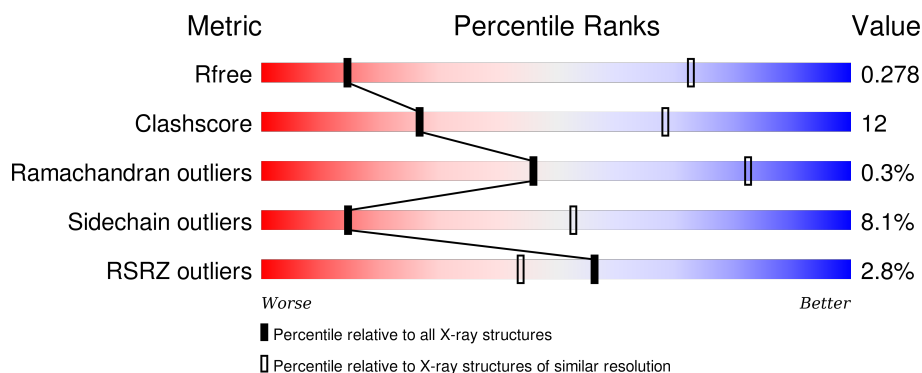
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.91 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))
$R_{free}$	91344	1047 (4.32-3.52)
Clashscore	102246	1008 (4.26-3.58)
Ramachandran outliers	100387	1044 (4.30-3.54)
Sidechain outliers	100360	1035 (4.30-3.54)
RSRZ outliers	91569	1002 (4.30-3.54)

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.

Mol	Chain	Length	Quality of chain
1	A	239	
1	B	239	
1	G	239	
1	H	239	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	522	
5	L	522	
6	M	64	
6	N	64	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58505 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	B	220	Total	C	N	O	S	0	0	0
			1687	1053	298	330	6			
1	G	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
A	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
A	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
A	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
A	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
B	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
B	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
B	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
B	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
B	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
G	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
G	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
G	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
G	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
G	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
H	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
H	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
H	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
H	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
H	239	GLN	-	EXPRESSION TAG	UNP C9QXI7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1345	Total	C	N	O	S	0	0	0
			10447	6560	1864	1974	49			
3	J	1325	Total	C	N	O	S	0	0	0
			10295	6470	1831	1945	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	470	Total	C	N	O	S	0	0	0
			3822	2394	680	725	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called Bacterial RNA polymerase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	51	Total	C	N	O	S	0	0	0
			413	268	65	79	1			
6	N	51	Total	C	N	O	S	0	0	0
			413	268	65	79	1			

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

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

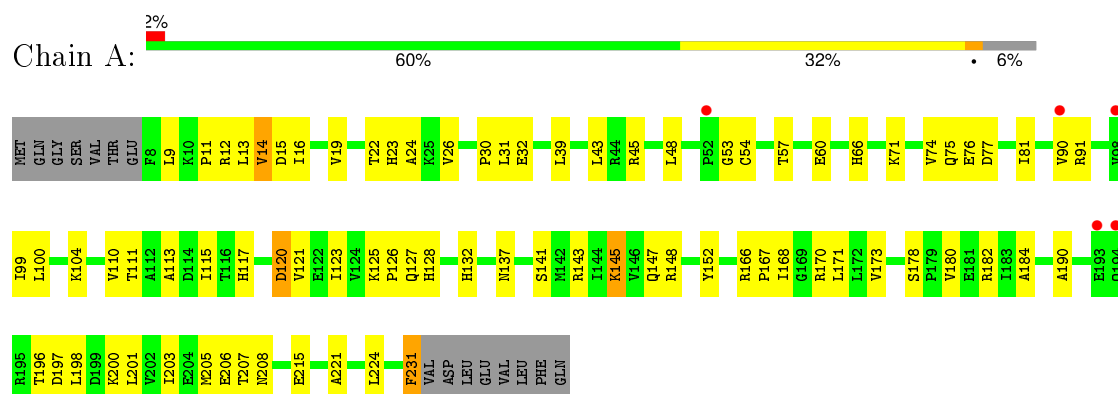
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		

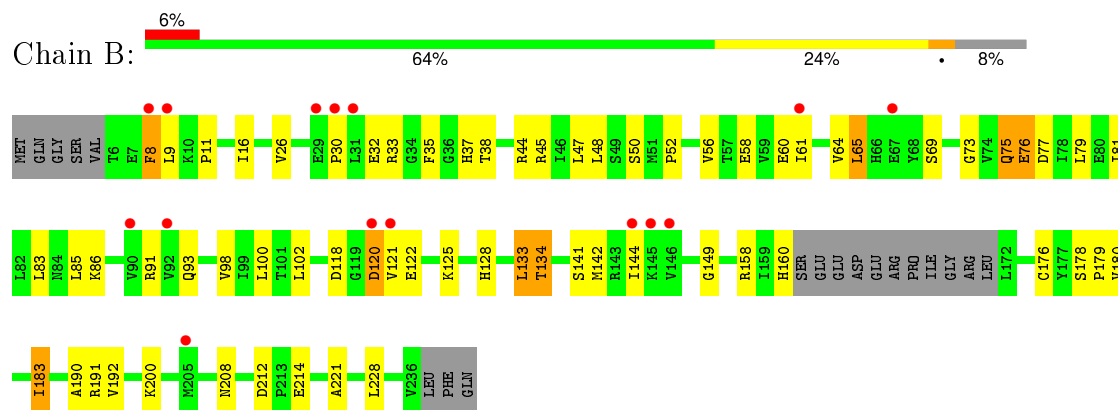
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

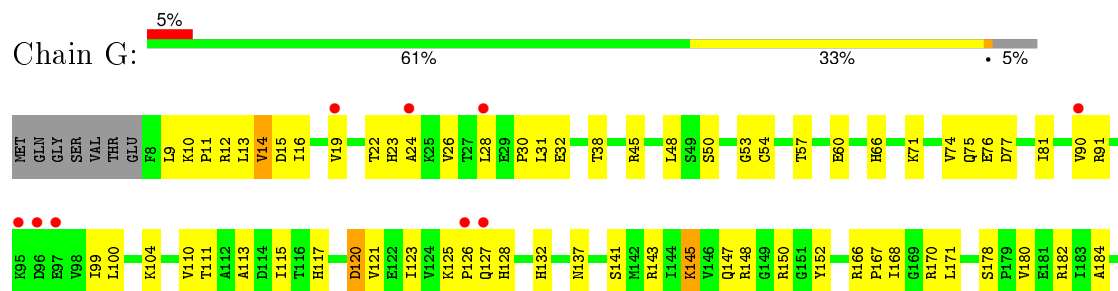
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

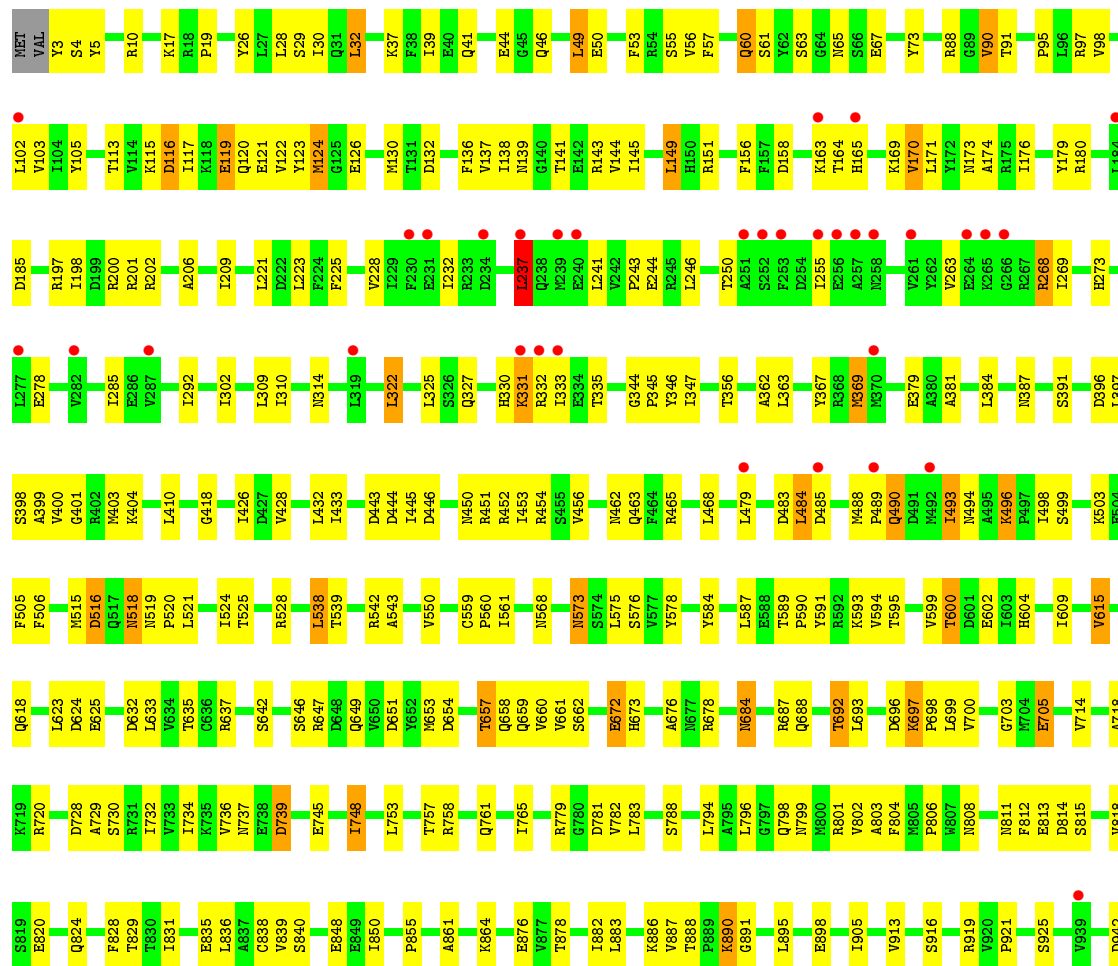


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

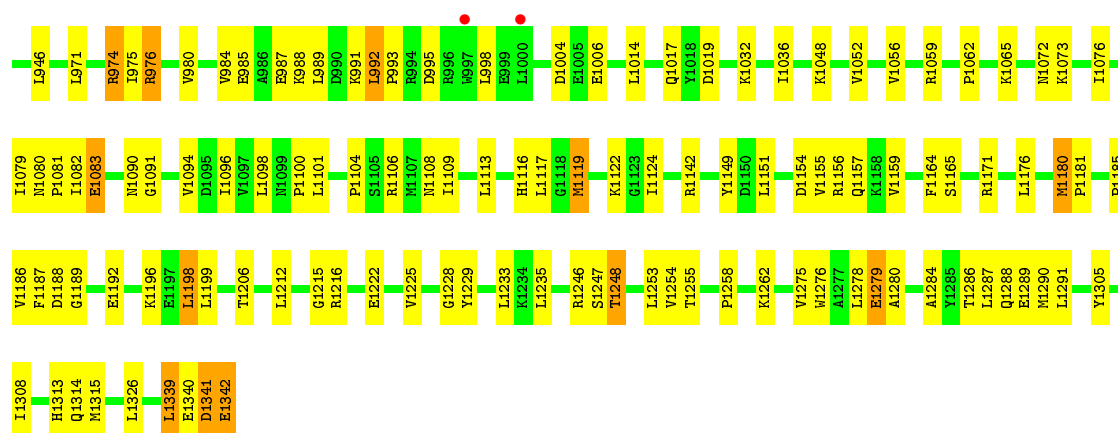


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

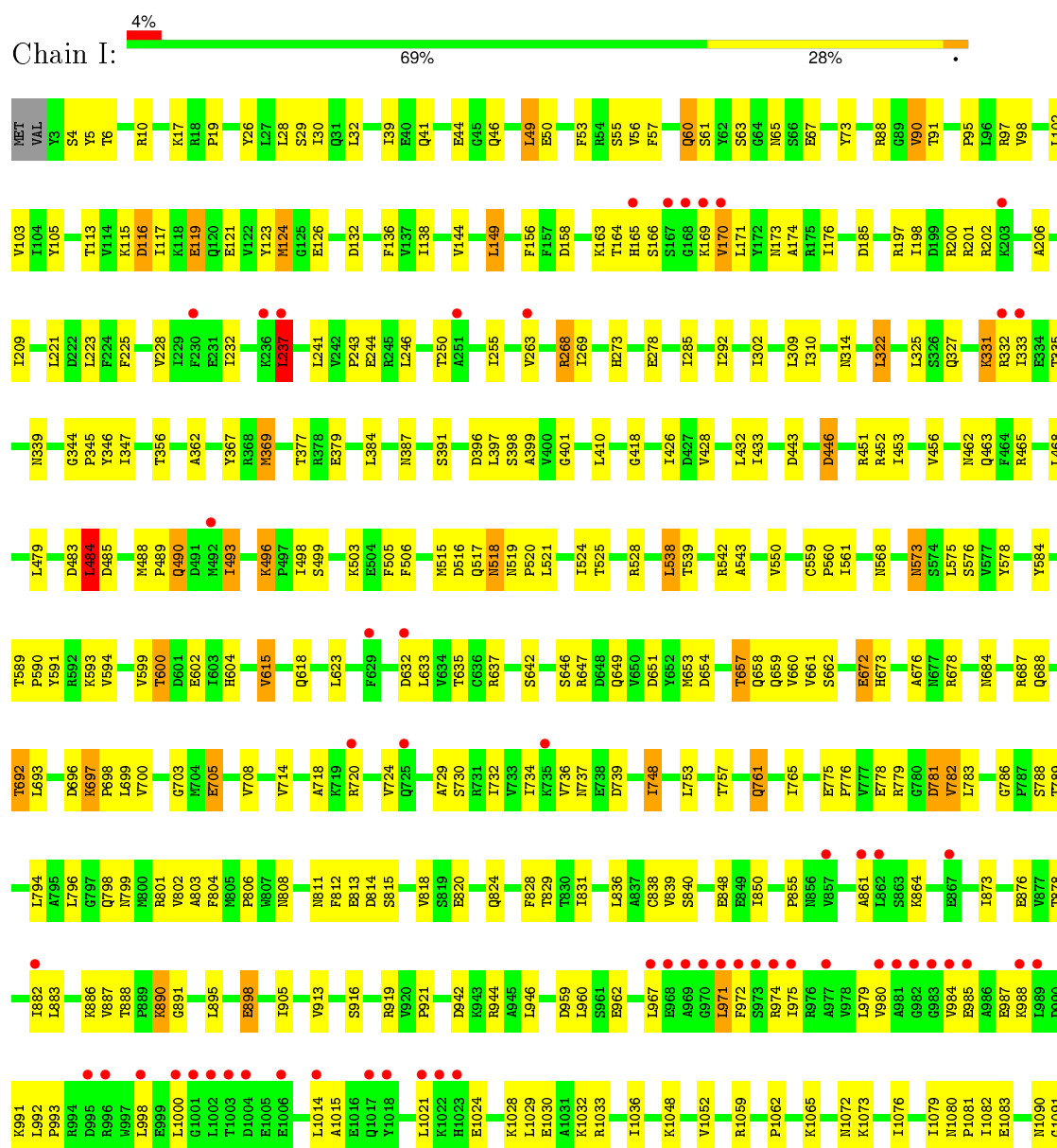


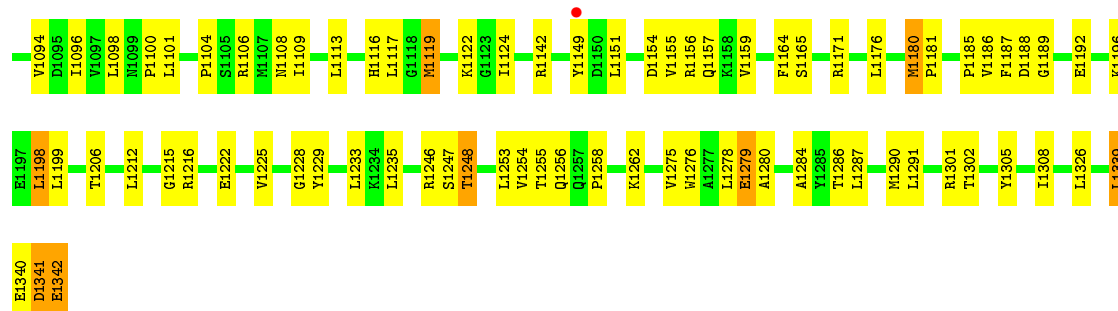




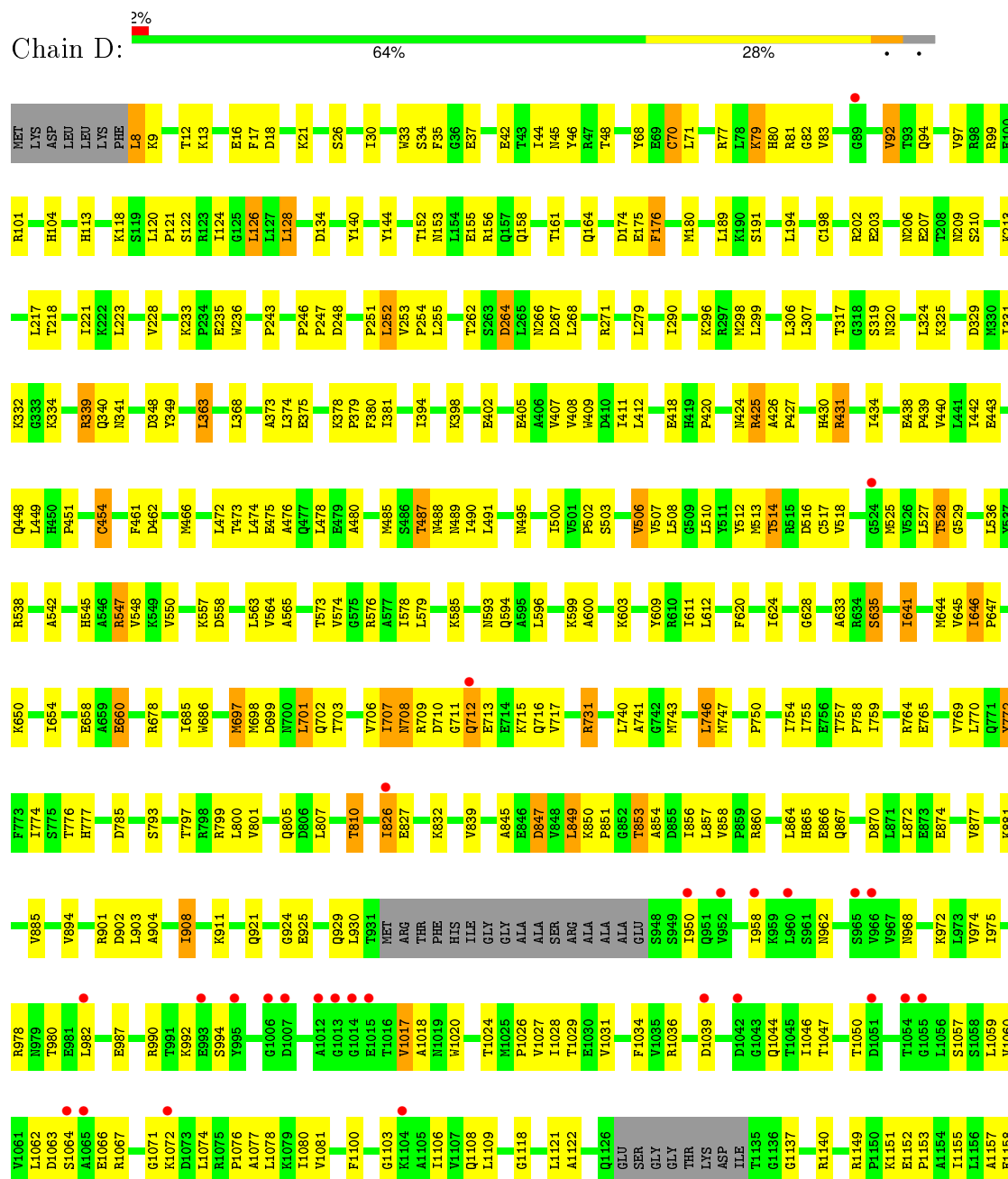


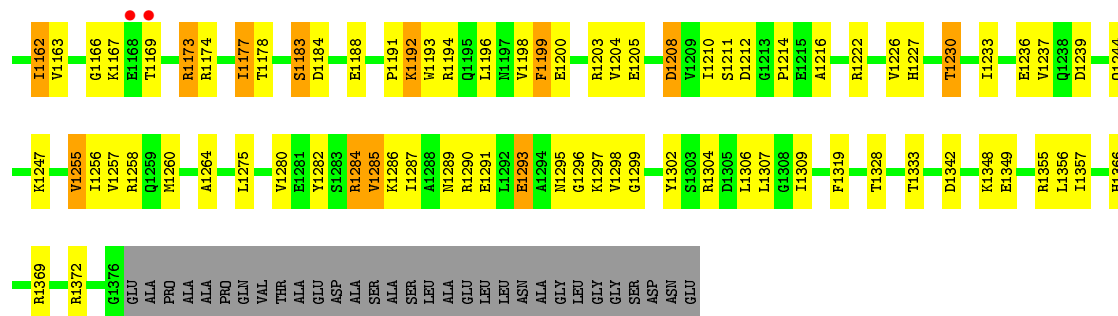
• Molecule 2: DNA-directed RNA polymerase subunit beta



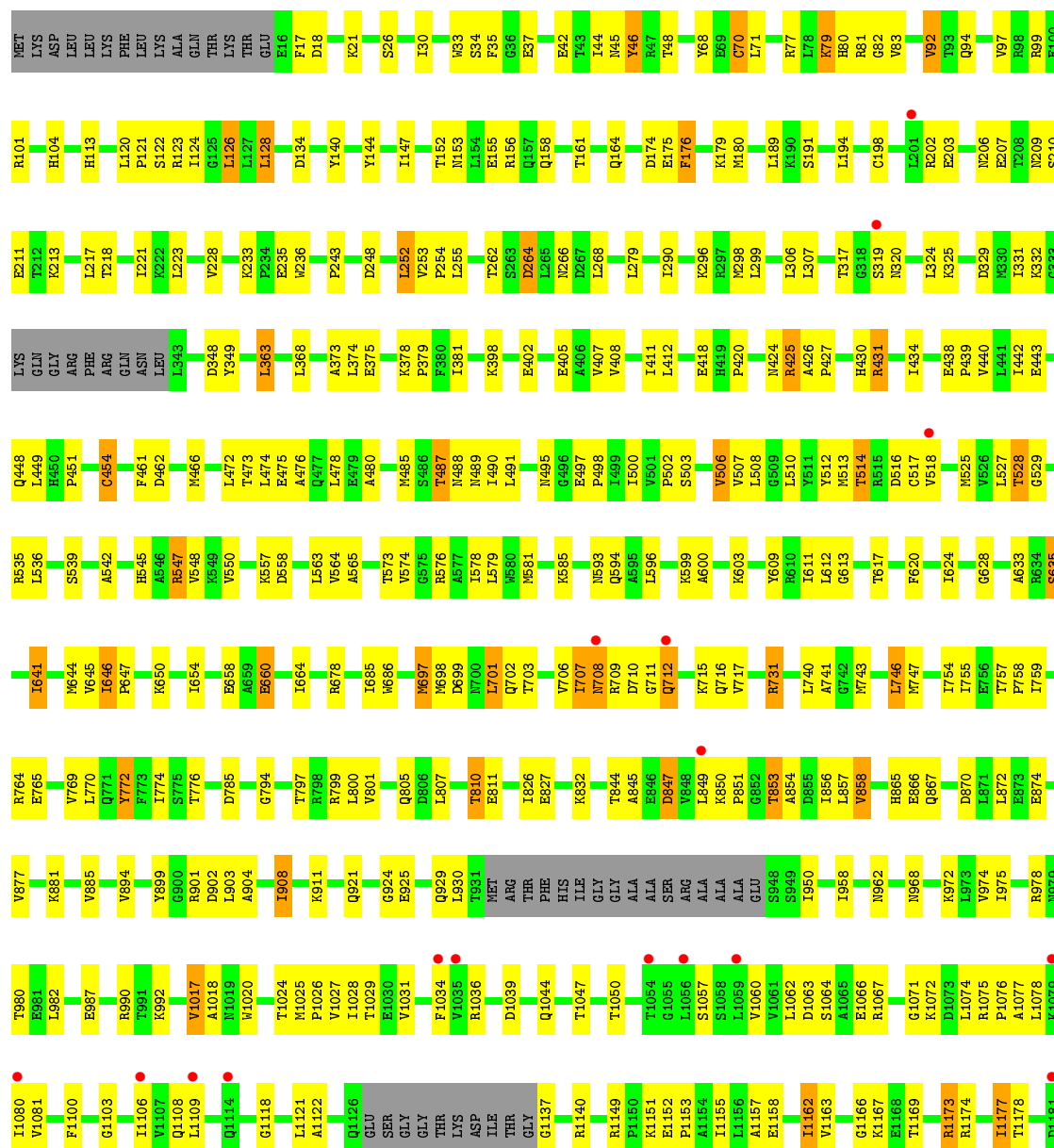


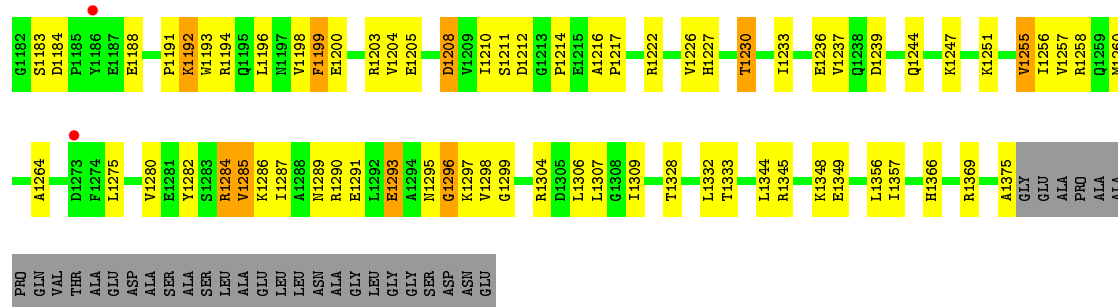
• Molecule 3: DNA-directed RNA polymerase subunit beta'





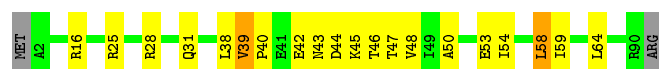
• Molecule 3: DNA-directed RNA polymerase subunit beta'





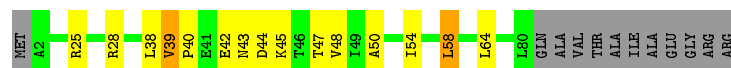
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



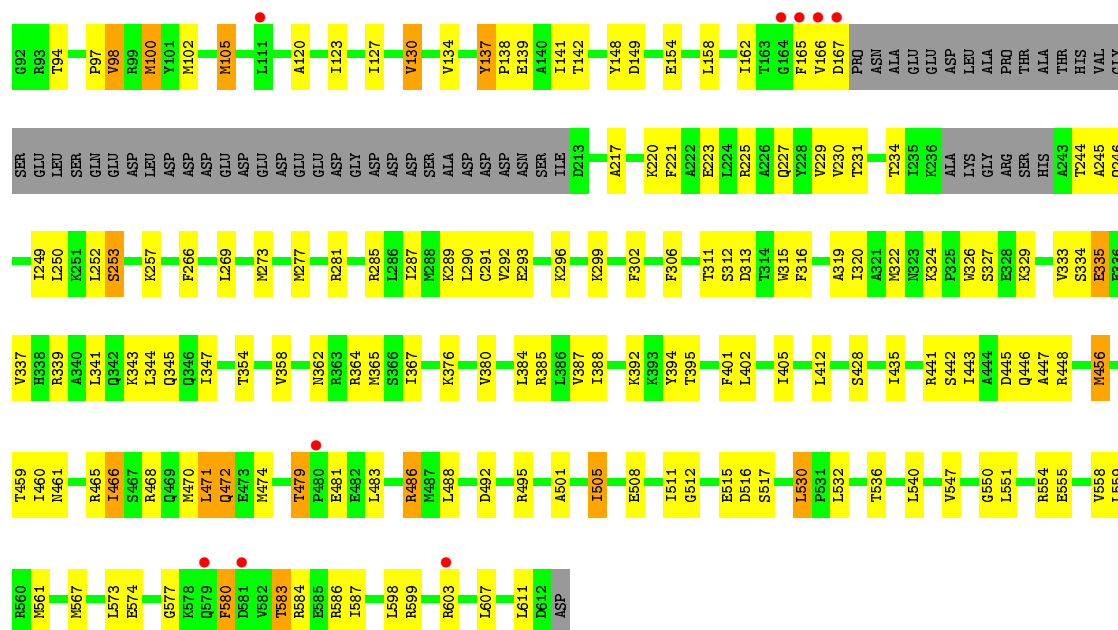
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:



- Molecule 5: RNA polymerase sigma factor RpoD

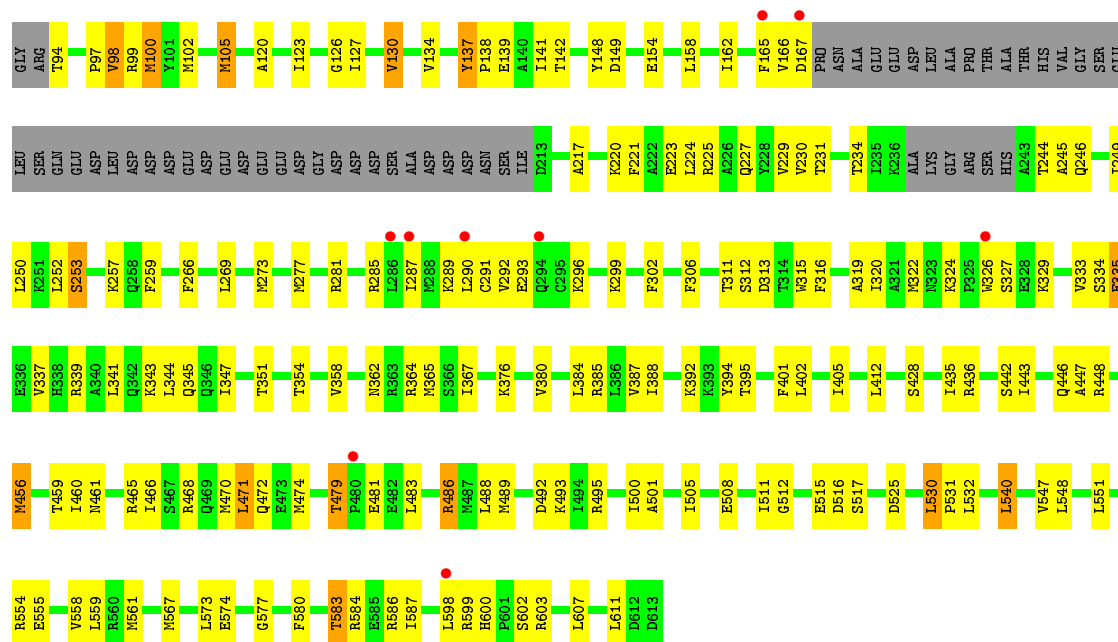
Chain F:



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L:

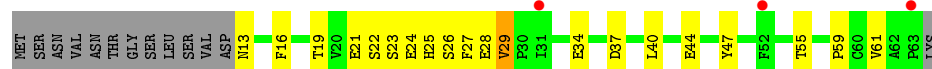




- Molecule 6: Bacterial RNA polymerase inhibitor



- Molecule 6: Bacterial RNA polymerase inhibitor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.36Å 206.28Å 308.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.94 – 3.91 39.94 – 3.91	Depositor EDS
% Data completeness (in resolution range)	92.8 (39.94-3.91) 92.9 (39.94-3.91)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 3.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.219 , 0.260 0.244 , 0.278	Depositor DCC
$R_{free}$ test set	5023 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	120.8	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 99934 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	58505	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: ZN, MG

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	0.25	0/1751	0.51	0/2373
1	B	0.27	0/1707	0.51	0/2314
1	G	0.25	0/1771	0.52	0/2401
1	H	0.27	0/1686	0.51	0/2285
2	C	0.26	0/10739	0.49	2/14489 (0.0%)
2	I	0.26	0/10735	0.49	2/14484 (0.0%)
3	D	0.25	0/10603	0.48	0/14316
3	J	0.25	0/10450	0.47	0/14112
4	E	0.24	0/693	0.47	0/935
4	K	0.23	0/629	0.47	0/847
5	F	0.26	0/3873	0.49	1/5206 (0.0%)
5	L	0.27	0/3872	0.49	1/5205 (0.0%)
6	M	0.25	0/426	0.41	0/583
6	N	0.24	0/426	0.41	0/583
All	All	0.25	0/59361	0.48	6/80133 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	237	LEU	CA-CB-CG	6.80	130.94	115.30
2	C	237	LEU	CA-CB-CG	6.68	130.67	115.30
2	I	516	ASP	CB-CG-OD2	5.27	123.04	118.30
2	C	516	ASP	CB-CG-OD2	5.18	122.96	118.30
5	F	149	ASP	CB-CG-OD2	5.17	122.95	118.30
5	L	149	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1296	GLY	Peptide
3	J	1296	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1730	0	1756	53	0
1	B	1687	0	1700	43	0
1	G	1750	0	1764	57	0
1	H	1667	0	1689	49	0
2	C	10570	0	10582	269	0
2	I	10566	0	10576	248	0
3	D	10447	0	10672	304	0
3	J	10295	0	10511	292	0
4	E	691	0	695	15	0
4	K	627	0	634	12	0
5	F	3822	0	3885	101	0
5	L	3821	0	3884	105	0
6	M	413	0	389	10	0
6	N	413	0	389	13	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	58505	0	59126	1420	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 12.

All (1420) 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:D:206:ASN:ND2	3:J:1183:SER:OG	2.04	0.90
3:D:1183:SER:OG	3:J:206:ASN:ND2	2.08	0.87
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.60	0.83
2:C:452:ARG:NH1	2:C:584:TYR:O	2.11	0.83
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.60	0.81
3:D:418:GLU:HG3	4:E:45:LYS:H	1.44	0.81
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.64	0.80
2:I:452:ARG:NH1	2:I:584:TYR:O	2.12	0.80
5:F:448:ARG:NH2	5:F:501:ALA:O	2.15	0.80
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.64	0.80
3:J:418:GLU:HG3	4:K:45:LYS:H	1.44	0.80
5:L:448:ARG:NH2	5:L:501:ALA:O	2.15	0.78
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.65	0.78
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.65	0.78
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.66	0.78
3:D:1044:GLN:HB3	3:D:1071:GLY:HA3	1.65	0.77
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.50	0.77
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.66	0.77
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.66	0.77
6:M:19:THR:HG22	6:M:28:GLU:HG2	1.67	0.76
2:I:398:SER:OG	2:I:399:ALA:N	2.17	0.76
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.50	0.76
6:N:19:THR:HG22	6:N:28:GLU:HG2	1.66	0.76
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.66	0.76
2:C:398:SER:OG	2:C:399:ALA:N	2.18	0.75
1:G:113:ALA:HB2	1:G:126:PRO:HB3	1.68	0.75
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.68	0.75
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.52	0.74
5:F:515:GLU:HG2	5:F:516:ASP:H	1.52	0.74
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.68	0.74
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.51	0.74
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.68	0.74
2:I:166:SER:HB2	6:N:23:SER:H	1.51	0.74
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.70	0.74
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.68	0.73
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.70	0.73
3:J:1064:SER:HB2	3:J:1173:ARG:HH12	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.70	0.73
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.70	0.73
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.71	0.73
5:L:515:GLU:HG2	5:L:516:ASP:H	1.53	0.73
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.53	0.72
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.72	0.72
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.72	0.71
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.72	0.71
2:C:684:ASN:OD1	2:C:687:ARG:NH2	2.23	0.71
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.72	0.71
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.73	0.71
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.54	0.71
3:D:1188:GLU:HG2	6:M:59:PRO:HD2	1.71	0.71
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.71	0.70
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.73	0.70
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.73	0.70
3:J:152:THR:OG1	3:J:153:ASN:N	2.24	0.70
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.73	0.70
3:J:1188:GLU:HG2	6:N:59:PRO:HD2	1.73	0.69
3:D:152:THR:OG1	3:D:153:ASN:N	2.24	0.69
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.73	0.69
2:I:166:SER:HA	6:N:23:SER:HB3	1.74	0.69
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.74	0.69
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.74	0.69
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.73	0.69
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.58	0.69
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.74	0.68
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.58	0.68
3:J:930:LEU:HD23	3:J:1244:GLN:HG3	1.74	0.68
2:C:516:ASP:O	2:C:516:ASP:OD1	2.11	0.68
5:F:492:ASP:HA	5:F:495:ARG:HH12	1.58	0.68
5:L:492:ASP:HA	5:L:495:ARG:HH12	1.57	0.68
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.60	0.67
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.77	0.67
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.74	0.67
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.76	0.67
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.76	0.67
1:A:224:LEU:HD22	1:B:228:LEU:HD11	1.77	0.67
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.77	0.67
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.77	0.67
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.60	0.66
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.60	0.66
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.60	0.66
3:D:1152:GLU:HG2	3:D:1194:ARG:HH21	1.60	0.66
1:H:60:GLU:HA	1:H:171:LEU:HD23	1.76	0.66
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.28	0.66
5:F:561:MET:HA	5:F:567:MET:HE1	1.78	0.66
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.77	0.65
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.79	0.65
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.60	0.65
5:L:561:MET:HA	5:L:567:MET:HE1	1.76	0.65
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.78	0.65
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.76	0.65
2:C:243:PRO:HG2	2:C:278:GLU:HG3	1.78	0.65
2:I:292:ILE:HD12	2:I:322:LEU:HD11	1.78	0.65
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.60	0.65
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.78	0.65
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.79	0.65
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.79	0.65
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	1.79	0.64
3:J:1152:GLU:HG2	3:J:1194:ARG:HH21	1.60	0.64
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.77	0.64
3:D:557:LYS:HA	3:D:563:LEU:HA	1.78	0.64
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.79	0.64
3:D:1264:ALA:HB2	3:D:1280:VAL:HG22	1.79	0.64
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.80	0.64
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.79	0.64
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.80	0.64
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.80	0.64
2:C:292:ILE:HD12	2:C:322:LEU:HD11	1.80	0.64
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.79	0.64
3:D:885:VAL:HG21	3:D:1255:VAL:HG12	1.80	0.64
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.80	0.64
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.78	0.64
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.79	0.64
2:I:243:PRO:HG2	2:I:278:GLU:HG3	1.78	0.64
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.31	0.64
5:L:126:GLY:O	5:L:130:VAL:HG13	1.97	0.64
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.80	0.64
3:J:510:LEU:O	3:J:514:THR:OG1	2.16	0.63
3:D:1060:VAL:HG22	3:D:1106:ILE:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.80	0.63
3:D:485:MET:HG3	3:D:487:THR:HG23	1.80	0.63
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.31	0.63
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.79	0.63
3:D:510:LEU:O	3:D:514:THR:OG1	2.16	0.63
3:J:1264:ALA:HB2	3:J:1280:VAL:CG2	2.29	0.63
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.80	0.63
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.80	0.63
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.79	0.63
5:L:583:THR:HG22	5:L:584:ARG:H	1.64	0.63
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.80	0.63
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.79	0.62
3:J:557:LYS:HA	3:J:563:LEU:HA	1.78	0.62
3:J:485:MET:HG3	3:J:487:THR:HG23	1.81	0.62
1:A:166:ARG:O	1:A:168:ILE:N	2.32	0.62
3:D:950:ILE:HB	3:D:1018:ALA:HB3	1.82	0.62
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.80	0.62
3:D:1264:ALA:HB2	3:D:1280:VAL:CG2	2.29	0.62
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.79	0.62
1:G:12:ARG:H	1:G:30:PRO:HD2	1.63	0.62
5:L:548:LEU:HD23	5:L:551:LEU:HD12	1.81	0.62
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.82	0.62
2:I:237:LEU:HD22	2:I:237:LEU:H	1.64	0.62
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.82	0.62
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.65	0.62
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.80	0.62
1:A:12:ARG:H	1:A:30:PRO:HD2	1.64	0.62
1:G:166:ARG:O	1:G:168:ILE:N	2.33	0.62
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.82	0.62
2:C:237:LEU:H	2:C:237:LEU:HD22	1.64	0.62
3:J:885:VAL:HG21	3:J:1255:VAL:HG12	1.81	0.62
1:A:74:VAL:HG22	1:A:76:GLU:H	1.65	0.61
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.81	0.61
1:A:45:ARG:HG2	1:B:38:THR:HB	1.83	0.61
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.82	0.61
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.83	0.61
3:D:1297:LYS:HG3	3:D:1299:GLY:H	1.65	0.61
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	1.83	0.61
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.66	0.61
5:F:583:THR:HG22	5:F:584:ARG:H	1.64	0.61
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.81	0.61
1:G:45:ARG:HG2	1:H:38:THR:HB	1.82	0.61
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.82	0.61
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.82	0.61
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.83	0.61
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.81	0.61
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.35	0.61
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.82	0.61
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.36	0.60
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.82	0.60
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.65	0.60
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	1.83	0.60
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.83	0.60
2:C:123:TYR:HB3	5:F:472:GLN:HB2	1.83	0.60
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.82	0.60
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.82	0.60
1:H:48:LEU:HD21	3:J:539:SER:HB3	1.83	0.60
3:D:1108:GLN:HG3	3:D:1109:LEU:HD13	1.83	0.60
3:D:1050:THR:HG23	3:D:1057:SER:HB3	1.83	0.60
1:G:74:VAL:HG22	1:G:76:GLU:H	1.66	0.60
1:G:182:ARG:H	1:G:206:GLU:HB3	1.67	0.60
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.84	0.60
3:J:45:ASN:HB3	3:J:48:THR:O	2.02	0.60
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.84	0.60
3:D:218:THR:HA	3:D:221:ILE:HG22	1.83	0.60
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.84	0.60
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.83	0.59
3:J:218:THR:HA	3:J:221:ILE:HG22	1.83	0.59
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.83	0.59
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.83	0.59
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.35	0.59
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.82	0.59
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.35	0.59
3:D:424:ASN:HD22	3:D:434:ILE:HG12	1.67	0.59
1:A:182:ARG:H	1:A:206:GLU:HB3	1.67	0.59
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.84	0.59
3:J:1191:PRO:HB2	3:J:1193:TRP:CD1	2.38	0.59
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.83	0.59
3:D:853:THR:HG22	3:D:854:ALA:H	1.68	0.59
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.85	0.59
3:D:978:ARG:HH21	3:D:1199:PHE:HE1	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.37	0.59
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.18	0.59
5:L:479:THR:HG23	5:L:481:GLU:H	1.68	0.59
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.84	0.59
2:I:103:VAL:HB	2:I:113:THR:HG21	1.84	0.58
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.83	0.58
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.38	0.58
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.17	0.58
5:F:479:THR:HG23	5:F:481:GLU:H	1.68	0.58
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.85	0.58
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.84	0.58
2:C:255:ILE:HB	2:C:263:VAL:HB	1.85	0.58
2:I:255:ILE:HB	2:I:263:VAL:HB	1.85	0.58
3:D:45:ASN:HB3	3:D:48:THR:O	2.02	0.58
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.86	0.58
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.18	0.58
2:I:1278:LEU:HD12	2:I:1287:LEU:HD12	1.86	0.58
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.86	0.58
2:C:250:THR:HA	2:C:268:ARG:HA	1.86	0.58
3:D:1191:PRO:HB2	3:D:1193:TRP:CD1	2.38	0.58
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.34	0.58
2:I:538:LEU:HD22	2:I:543:ALA:HB2	1.85	0.58
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.85	0.58
1:G:23:HIS:HB2	1:G:205:MET:O	2.04	0.58
1:A:23:HIS:HB2	1:A:205:MET:O	2.04	0.58
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.85	0.58
2:I:1073:LYS:HD3	3:J:462:ASP:HB2	1.85	0.57
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.85	0.57
2:I:518:ASN:N	2:I:518:ASN:OD1	2.35	0.57
5:F:547:VAL:HG11	5:F:607:LEU:HD11	1.86	0.57
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.86	0.57
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.85	0.57
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.86	0.57
2:I:166:SER:HB2	6:N:23:SER:N	2.19	0.57
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.87	0.57
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.68	0.57
2:C:232:ILE:HG13	2:C:331:LYS:O	2.05	0.57
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.86	0.57
3:D:827:GLU:HG2	3:D:832:LYS:HD2	1.86	0.57
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.86	0.57
3:J:1297:LYS:HG3	3:J:1299:GLY:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:495:ASN:ND2	3:D:1247:LYS:O	2.37	0.57
2:I:232:ILE:HG13	2:I:331:LYS:O	2.05	0.57
1:G:26:VAL:HG23	1:G:203:ILE:HB	1.87	0.57
2:C:103:VAL:HB	2:C:113:THR:HG21	1.84	0.57
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.87	0.57
2:C:1073:LYS:HD3	3:D:462:ASP:HB2	1.86	0.57
2:C:518:ASN:OD1	2:C:518:ASN:N	2.36	0.57
2:C:1305:TYR:HE1	3:D:379:PRO:HG3	1.70	0.57
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.87	0.57
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.70	0.57
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.87	0.57
2:C:1278:LEU:HD12	2:C:1287:LEU:HD12	1.87	0.56
3:J:1063:ASP:HB3	3:J:1103:GLY:HA3	1.87	0.56
3:J:34:SER:OG	3:J:104:HIS:ND1	2.24	0.56
3:D:1026:PRO:HB2	3:D:1028:ILE:HG23	1.86	0.56
2:I:560:PRO:HB3	3:J:776:THR:HG21	1.87	0.56
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.87	0.56
3:D:77:ARG:HG3	3:D:79:LYS:H	1.69	0.56
2:I:615:VAL:HG13	2:I:651:ASP:H	1.70	0.56
3:D:325:LYS:HG2	3:D:329:ASP:HB2	1.88	0.56
2:I:992:LEU:HD11	2:I:1000:LEU:HD11	1.86	0.56
2:C:615:VAL:HG13	2:C:651:ASP:H	1.70	0.56
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.70	0.56
1:G:50:SER:HB3	1:H:8:PHE:HZ	1.70	0.56
3:D:1077:ALA:HA	3:D:1100:PHE:HA	1.87	0.56
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.86	0.56
1:A:11:PRO:HA	1:A:30:PRO:HB2	1.87	0.56
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.87	0.56
3:J:1077:ALA:HA	3:J:1100:PHE:HA	1.87	0.56
3:D:1063:ASP:HB3	3:D:1103:GLY:HA3	1.87	0.56
3:J:77:ARG:HG3	3:J:79:LYS:H	1.70	0.56
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.86	0.56
3:D:17:PHE:O	3:D:1369:ARG:NH2	2.34	0.56
3:J:853:THR:HG22	3:J:854:ALA:H	1.70	0.56
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.87	0.56
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.88	0.56
3:D:381:ILE:HD11	3:D:412:LEU:HD12	1.87	0.56
3:J:827:GLU:HG2	3:J:832:LYS:HD2	1.86	0.56
3:J:1192:LYS:HG2	3:J:1196:LEU:HD11	1.88	0.56
2:I:488:MET:O	2:I:490:GLN:N	2.35	0.56
3:J:325:LYS:HG2	3:J:329:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1151:LYS:NZ	6:N:22:SER:O	2.39	0.56
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.88	0.56
5:L:166:VAL:O	5:L:167:ASP:HB2	2.05	0.56
2:I:967:LEU:HD21	2:I:1021:LEU:HD13	1.87	0.56
3:D:847:ASP:HB3	3:D:856:ILE:HG23	1.87	0.56
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.88	0.56
3:J:490:ILE:HG22	3:J:500:ILE:HG13	1.88	0.56
2:I:808:ASN:H	3:J:633:ALA:HB2	1.69	0.56
2:I:250:THR:HA	2:I:268:ARG:HA	1.86	0.56
3:J:424:ASN:HD22	3:J:434:ILE:HG12	1.69	0.56
5:L:316:PHE:HZ	5:L:334:SER:HA	1.71	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.69	0.56
1:A:26:VAL:HG23	1:A:203:ILE:HB	1.87	0.56
3:J:381:ILE:HD11	3:J:412:LEU:HD12	1.86	0.56
3:J:1211:SER:OG	3:J:1212:ASP:N	2.39	0.56
2:I:520:PRO:HG3	2:I:714:VAL:HG11	1.88	0.56
2:I:19:PRO:HA	2:I:1156:ARG:HD3	1.87	0.56
3:D:1198:VAL:HG22	3:D:1199:PHE:H	1.70	0.56
5:L:281:ARG:O	5:L:285:ARG:HG3	2.06	0.56
3:J:495:ASN:ND2	3:J:1247:LYS:O	2.39	0.56
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.87	0.55
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.88	0.55
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.87	0.55
2:C:19:PRO:HA	2:C:1156:ARG:HD3	1.87	0.55
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.88	0.55
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.71	0.55
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.87	0.55
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.87	0.55
5:L:530:LEU:HD23	5:L:530:LEU:H	1.71	0.55
3:D:1192:LYS:HG2	3:D:1196:LEU:HD11	1.89	0.55
2:C:560:PRO:HB3	3:D:776:THR:HG21	1.87	0.55
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.88	0.55
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.87	0.55
5:F:511:ILE:HG13	5:F:512:GLY:H	1.72	0.55
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.22	0.55
3:J:1198:VAL:HG22	3:J:1199:PHE:H	1.70	0.55
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.89	0.55
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.88	0.55
5:F:530:LEU:H	5:F:530:LEU:HD23	1.71	0.55
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.89	0.55
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.87	0.55
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.86	0.55
5:L:470:MET:O	5:L:474:MET:HB2	2.07	0.55
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.89	0.55
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.88	0.55
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.88	0.55
5:F:281:ARG:O	5:F:285:ARG:HG3	2.07	0.55
5:L:511:ILE:HG13	5:L:512:GLY:H	1.72	0.55
5:L:551:LEU:HD11	5:L:598:LEU:HD11	1.89	0.55
2:C:488:MET:O	2:C:490:GLN:N	2.35	0.55
3:J:847:ASP:HB3	3:J:856:ILE:HG23	1.87	0.55
5:F:554:ARG:HB2	5:F:580:PHE:HE2	1.72	0.55
2:C:39:ILE:HA	2:C:49:LEU:HD12	1.89	0.55
3:D:1029:THR:HG21	3:D:1080:ILE:HD11	1.89	0.55
3:D:1211:SER:OG	3:D:1212:ASP:N	2.39	0.55
5:L:97:PRO:HA	5:L:100:MET:HG3	1.89	0.55
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.88	0.55
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.89	0.55
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.88	0.55
4:E:38:LEU:HD23	4:E:58:LEU:HD13	1.87	0.55
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.89	0.55
2:C:149:LEU:HD21	2:C:451:ARG:NH1	2.22	0.55
5:F:316:PHE:HZ	5:F:334:SER:HA	1.71	0.55
3:J:1191:PRO:HB2	3:J:1193:TRP:HD1	1.72	0.54
5:F:316:PHE:O	5:F:320:ILE:HG13	2.07	0.54
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.90	0.54
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.90	0.54
2:I:998:LEU:HD23	2:I:1015:ALA:HA	1.89	0.54
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.73	0.54
2:C:593:LYS:HB3	2:C:602:GLU:HG3	1.90	0.54
3:D:490:ILE:HG22	3:D:500:ILE:HG13	1.89	0.54
2:I:41:GLN:NE2	2:I:73:TYR:O	2.40	0.54
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.89	0.54
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.89	0.54
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.89	0.54
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.90	0.54
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.72	0.54
5:F:551:LEU:HD11	5:F:598:LEU:HD11	1.89	0.54
2:I:39:ILE:HA	2:I:49:LEU:HD12	1.89	0.54
2:I:149:LEU:HD21	2:I:451:ARG:NH1	2.23	0.54
2:C:41:GLN:NE2	2:C:73:TYR:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:650:LYS:NZ	3:D:765:GLU:OE2	2.41	0.54
3:J:968:ASN:HB3	3:J:1118:GLY:HA3	1.88	0.54
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.73	0.54
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.90	0.54
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.88	0.54
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.90	0.54
1:G:19:VAL:HG12	1:G:24:ALA:HA	1.90	0.54
5:F:577:GLY:HA3	5:F:583:THR:HA	1.90	0.54
6:M:21:GLU:HG3	6:M:26:SER:HB3	1.90	0.54
2:C:736:VAL:HG23	2:C:748:ILE:HA	1.89	0.54
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.89	0.54
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.89	0.54
5:L:554:ARG:HB2	5:L:580:PHE:HE2	1.72	0.54
1:A:60:GLU:OE1	1:A:143:ARG:NH2	2.41	0.54
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.90	0.54
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.23	0.54
3:D:1191:PRO:HB2	3:D:1193:TRP:HD1	1.72	0.54
5:L:316:PHE:O	5:L:320:ILE:HG13	2.08	0.54
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.72	0.54
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.41	0.53
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.89	0.53
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.90	0.53
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.43	0.53
2:C:815:SER:HB3	3:D:461:PHE:HB3	1.90	0.53
4:E:42:GLU:O	4:E:43:ASN:HB2	2.09	0.53
3:D:1167:LYS:HG3	3:D:1174:ARG:HD2	1.91	0.53
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.90	0.53
5:L:130:VAL:HB	5:L:365:MET:HG3	1.90	0.53
3:D:978:ARG:HB2	3:D:1199:PHE:CZ	2.43	0.53
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.89	0.53
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.91	0.53
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.90	0.53
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.90	0.53
5:F:234:THR:O	5:F:245:ALA:HB2	2.09	0.53
2:I:91:THR:HG21	2:I:503:LYS:HE2	1.90	0.53
1:B:8:PHE:HD1	1:B:9:LEU:H	1.55	0.53
6:N:21:GLU:HG3	6:N:26:SER:HB3	1.90	0.53
5:F:97:PRO:HA	5:F:100:MET:HG3	1.90	0.53
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.90	0.53
2:I:815:SER:HB3	3:J:461:PHE:HB3	1.90	0.53
2:I:60:GLN:HB3	2:I:67:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:593:LYS:HB3	2:I:602:GLU:HG3	1.89	0.53
2:C:120:GLN:HG2	2:C:121:GLU:H	1.73	0.53
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.90	0.53
5:F:470:MET:O	5:F:474:MET:HB2	2.07	0.53
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.89	0.53
3:J:709:ARG:C	3:J:711:GLY:H	2.12	0.53
2:C:818:VAL:HG13	2:C:1096:ILE:HG12	1.90	0.53
3:J:1167:LYS:HG3	3:J:1174:ARG:HD2	1.90	0.53
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.91	0.53
2:C:1247:SER:HB3	3:D:375:GLU:O	2.09	0.53
2:C:804:PHE:HB3	2:C:1100:PRO:HG3	1.91	0.53
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.91	0.53
5:L:234:THR:O	5:L:245:ALA:HB2	2.09	0.53
1:G:60:GLU:OE1	1:G:143:ARG:NH2	2.42	0.53
4:K:42:GLU:O	4:K:43:ASN:HB2	2.08	0.53
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.90	0.53
2:I:176:ILE:HD11	2:I:428:VAL:HG21	1.90	0.53
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.90	0.53
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.43	0.53
2:C:387:ASN:HA	2:C:391:SER:HB2	1.91	0.53
1:B:75:GLN:OE1	1:B:76:GLU:HG3	2.09	0.53
2:I:387:ASN:HA	2:I:391:SER:HB2	1.90	0.53
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.39	0.53
3:D:1039:ASP:OD1	3:D:1074:LEU:HB3	2.09	0.53
5:L:577:GLY:HA3	5:L:583:THR:HA	1.91	0.53
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.90	0.53
3:D:968:ASN:HB3	3:D:1118:GLY:HA3	1.90	0.53
3:D:425:ARG:HG2	3:D:426:ALA:H	1.74	0.53
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.90	0.53
3:D:1191:PRO:HD3	6:M:55:THR:O	2.08	0.53
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.91	0.53
5:F:166:VAL:O	5:F:167:ASP:HB2	2.07	0.53
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.89	0.53
1:H:75:GLN:OE1	1:H:76:GLU:HG3	2.09	0.52
1:A:14:VAL:HG22	1:A:15:ASP:H	1.74	0.52
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	1.91	0.52
2:I:356:THR:HG21	2:I:362:ALA:HA	1.90	0.52
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.74	0.52
2:I:1247:SER:OG	2:I:1248:THR:N	2.42	0.52
3:D:1151:LYS:NZ	6:M:22:SER:O	2.42	0.52
1:H:125:LYS:HE2	1:H:128:HIS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:818:VAL:HG13	2:I:1096:ILE:HG12	1.91	0.52
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.91	0.52
3:J:475:GLU:OE2	4:K:28:ARG:NH2	2.39	0.52
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.92	0.52
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.91	0.52
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.92	0.52
1:B:64:VAL:HG12	1:B:65:LEU:H	1.74	0.52
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.90	0.52
1:G:14:VAL:HG22	1:G:15:ASP:H	1.74	0.52
3:J:425:ARG:HG2	3:J:426:ALA:H	1.74	0.52
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.91	0.52
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.92	0.52
3:D:1078:LEU:HD13	3:D:1121:LEU:HD22	1.91	0.52
2:I:5:TYR:CE1	2:I:776:PRO:HB2	2.44	0.52
2:C:861:ALA:HB1	2:C:882:ILE:HD13	1.91	0.52
3:J:332:LYS:HG2	3:J:1328:THR:HB	1.92	0.52
3:J:1162:ILE:HA	3:J:1203:ARG:HA	1.92	0.52
3:D:974:VAL:HG21	3:D:1118:GLY:HA2	1.92	0.52
1:B:125:LYS:HE2	1:B:128:HIS:HB2	1.91	0.52
3:D:198:CYS:O	3:D:202:ARG:HG3	2.10	0.52
2:C:703:GLY:N	2:C:705:GLU:OE2	2.42	0.52
1:G:50:SER:HB3	1:H:8:PHE:CZ	2.45	0.52
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.91	0.52
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.91	0.52
2:I:980:VAL:O	2:I:984:VAL:HB	2.10	0.52
3:D:709:ARG:C	3:D:711:GLY:H	2.12	0.52
2:I:367:TYR:HD1	2:I:384:LEU:HD22	1.74	0.52
2:C:356:THR:HG21	2:C:362:ALA:HA	1.91	0.52
3:J:1029:THR:HG21	3:J:1080:ILE:HD11	1.91	0.52
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.92	0.52
1:H:64:VAL:HG12	1:H:65:LEU:H	1.75	0.52
2:I:600:THR:HB	2:I:602:GLU:HG2	1.92	0.52
2:I:1247:SER:HB3	3:J:375:GLU:O	2.10	0.52
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.92	0.52
3:J:502:PRO:HB2	3:J:507:VAL:HG12	1.92	0.52
2:I:119:GLU:HG3	2:I:488:MET:HB3	1.90	0.51
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.90	0.51
3:J:474:LEU:O	3:J:478:LEU:HD12	2.10	0.51
2:I:861:ALA:HB1	2:I:882:ILE:HD13	1.91	0.51
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.91	0.51
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.92	0.51
3:D:474:LEU:O	3:D:478:LEU:HD12	2.10	0.51
1:G:74:VAL:HG23	1:G:132:HIS:O	2.10	0.51
3:J:198:CYS:O	3:J:202:ARG:HG3	2.11	0.51
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.92	0.51
3:J:1039:ASP:OD1	3:J:1074:LEU:HB3	2.09	0.51
3:J:697:MET:HG3	3:J:698:MET:N	2.26	0.51
5:F:130:VAL:HB	5:F:365:MET:HG3	1.93	0.51
3:J:1100:PHE:HB2	3:J:1200:GLU:CD	2.30	0.51
2:C:600:THR:HB	2:C:602:GLU:HG2	1.93	0.51
2:I:804:PHE:HB3	2:I:1100:PRO:HG3	1.91	0.51
3:D:699:ASP:HA	3:D:702:GLN:HG2	1.92	0.51
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.93	0.51
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.92	0.51
3:J:810:THR:O	3:J:911:LYS:HE3	2.10	0.51
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.93	0.51
2:I:119:GLU:HB2	2:I:489:PRO:HD2	1.92	0.51
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.91	0.51
2:I:864:LYS:NZ	2:I:876:GLU:O	2.43	0.51
3:J:901:ARG:HA	3:J:908:ILE:HA	1.92	0.51
5:L:289:LYS:HE3	5:L:293:GLU:HG2	1.93	0.51
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.92	0.51
3:D:901:ARG:HA	3:D:908:ILE:HA	1.92	0.51
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.91	0.51
5:F:289:LYS:HE3	5:F:293:GLU:HG2	1.92	0.51
3:D:810:THR:O	3:D:911:LYS:HE3	2.10	0.51
5:F:158:LEU:HD22	5:F:162:ILE:HD11	1.93	0.51
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.93	0.51
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.76	0.51
3:J:978:ARG:HB2	3:J:1199:PHE:CZ	2.46	0.51
2:I:206:ALA:O	2:I:209:ILE:HG22	2.11	0.51
1:G:120:ASP:OD2	1:G:120:ASP:N	2.44	0.51
3:J:644:MET:HE3	3:J:764:ARG:HG3	1.93	0.51
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.93	0.51
3:D:34:SER:OG	3:D:104:HIS:ND1	2.26	0.51
2:C:864:LYS:NZ	2:C:876:GLU:O	2.43	0.51
1:B:191:ARG:NH2	3:D:409:TRP:HB3	2.26	0.51
3:D:644:MET:HE3	3:D:764:ARG:HG3	1.94	0.50
1:A:74:VAL:HG23	1:A:132:HIS:O	2.10	0.50
5:L:158:LEU:HD22	5:L:162:ILE:HD11	1.93	0.50
3:D:847:ASP:N	3:D:847:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	1.93	0.50
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.76	0.50
5:L:343:LYS:H	5:L:343:LYS:HD2	1.76	0.50
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.92	0.50
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.93	0.50
2:I:802:VAL:HG23	2:I:1098:LEU:HD13	1.94	0.50
5:F:245:ALA:O	5:F:249:ILE:HG13	2.12	0.50
2:C:331:LYS:HB2	2:C:332:ARG:NH2	2.26	0.50
3:D:1064:SER:HB2	3:D:1173:ARG:HH12	1.77	0.50
2:C:1314:GLN:HG2	4:E:28:ARG:NH1	2.27	0.50
3:J:1162:ILE:O	3:J:1178:THR:OG1	2.18	0.50
3:J:478:LEU:HG	4:K:47:THR:HG23	1.94	0.50
3:D:1077:ALA:HB2	3:D:1100:PHE:CD1	2.47	0.50
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.93	0.50
1:A:120:ASP:OD2	1:A:120:ASP:N	2.44	0.50
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.47	0.50
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.93	0.50
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.93	0.50
2:C:225:PHE:HE1	2:C:345:PRO:HA	1.77	0.50
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.93	0.50
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.46	0.50
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.94	0.50
3:J:847:ASP:N	3:J:847:ASP:OD1	2.43	0.50
3:J:699:ASP:HA	3:J:702:GLN:HG2	1.92	0.50
2:I:331:LYS:HB2	2:I:332:ARG:NH2	2.26	0.50
2:C:55:SER:OG	2:C:56:VAL:N	2.45	0.50
3:D:697:MET:HG3	3:D:698:MET:N	2.26	0.50
2:C:206:ALA:O	2:C:209:ILE:HG22	2.11	0.50
3:D:902:ASP:OD1	3:D:903:LEU:N	2.45	0.50
2:C:632:ASP:HA	2:C:647:ARG:HB2	1.93	0.50
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.12	0.50
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.47	0.50
2:I:688:GLN:HB2	2:I:1235:LEU:HD22	1.93	0.49
3:D:576:ARG:NH1	3:D:593:ASN:O	2.44	0.49
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.12	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49
3:D:870:ASP:O	3:D:874:GLU:HG2	2.12	0.49
2:C:170:VAL:HG23	2:C:171:LEU:N	2.27	0.49
2:I:170:VAL:HG23	2:I:171:LEU:N	2.27	0.49
2:I:30:ILE:HD12	2:I:30:ILE:H	1.77	0.49
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:298:MET:SD	5:F:402:LEU:HB3	2.52	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.76	0.49
3:D:564:VAL:HG12	3:D:565:ALA:H	1.77	0.49
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.76	0.49
3:D:708:ASN:HB3	3:D:712:GLN:O	2.11	0.49
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.95	0.49
5:F:141:ILE:HG21	5:F:252:LEU:HD11	1.93	0.49
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.93	0.49
3:D:1227:HIS:ND1	3:J:1293:GLU:HG2	2.27	0.49
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.47	0.49
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.93	0.49
2:I:225:PHE:HE1	2:I:345:PRO:HA	1.77	0.49
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.94	0.49
3:J:902:ASP:OD1	3:J:903:LEU:N	2.46	0.49
3:J:451:PRO:O	3:J:454:CYS:HB2	2.13	0.49
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.48	0.49
2:C:688:GLN:HB2	2:C:1235:LEU:HD22	1.93	0.49
5:L:134:VAL:HG22	5:L:273:MET:HE1	1.95	0.49
2:I:632:ASP:HA	2:I:647:ARG:HB2	1.94	0.49
3:D:826:ILE:HD12	3:D:994:SER:HB2	1.94	0.49
3:J:564:VAL:HG12	3:J:565:ALA:H	1.78	0.49
5:F:461:ASN:O	5:F:465:ARG:HG2	2.12	0.49
2:C:829:THR:HG23	2:C:1059:ARG:HA	1.95	0.49
3:D:332:LYS:HG2	3:D:1328:THR:HB	1.92	0.49
2:C:1247:SER:OG	2:C:1248:THR:N	2.44	0.49
1:A:197:ASP:N	1:A:197:ASP:OD1	2.45	0.49
5:F:442:SER:O	5:F:446:GLN:HG2	2.12	0.49
4:K:25:ARG:HD3	4:K:64:LEU:HD13	1.93	0.49
2:C:1106:ARG:NE	3:D:731:ARG:HH21	2.10	0.49
2:C:180:ARG:CZ	2:C:465:ARG:HH12	2.26	0.49
2:C:30:ILE:H	2:C:30:ILE:HD12	1.76	0.49
1:B:44:ARG:HG3	1:B:183:ILE:HB	1.94	0.49
5:F:250:LEU:O	5:F:253:SER:OG	2.27	0.49
3:D:755:ILE:HG22	3:D:757:THR:H	1.78	0.49
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.12	0.49
3:J:708:ASN:HB3	3:J:712:GLN:O	2.12	0.49
1:G:197:ASP:N	1:G:197:ASP:OD1	2.45	0.49
5:L:245:ALA:O	5:L:249:ILE:HG13	2.12	0.49
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.77	0.49
5:L:343:LYS:O	5:L:347:ILE:HG13	2.13	0.49
3:D:398:LYS:O	3:D:402:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.94	0.49
3:D:845:ALA:HB3	3:D:881:LYS:HB3	1.95	0.49
3:D:451:PRO:O	3:D:454:CYS:HB2	2.13	0.49
6:N:16:PHE:HD1	6:N:59:PRO:HA	1.78	0.49
1:H:44:ARG:HG3	1:H:183:ILE:HB	1.94	0.49
3:J:576:ARG:NH1	3:J:593:ASN:O	2.45	0.49
5:F:343:LYS:O	5:F:347:ILE:HG13	2.13	0.49
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.48	0.49
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.13	0.48
5:L:470:MET:HG3	5:L:486:ARG:HH22	1.78	0.48
3:D:850:LYS:HG2	3:D:851:PRO:HD2	1.95	0.48
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.77	0.48
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.13	0.48
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.48	0.48
3:D:978:ARG:HB2	3:D:1199:PHE:HZ	1.77	0.48
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.10	0.48
2:I:528:ARG:NH2	2:I:576:SER:O	2.46	0.48
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.95	0.48
5:L:250:LEU:O	5:L:253:SER:OG	2.28	0.48
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.95	0.48
2:I:1149:TYR:OH	2:I:1176:LEU:HD11	2.14	0.48
3:D:478:LEU:HG	4:E:47:THR:HG23	1.94	0.48
2:I:55:SER:OG	2:I:56:VAL:N	2.46	0.48
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.96	0.48
3:J:398:LYS:O	3:J:402:GLU:HB2	2.13	0.48
3:D:418:GLU:H	4:E:45:LYS:HZ2	1.62	0.48
2:I:232:ILE:HD11	2:I:333:ILE:HD11	1.96	0.48
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.95	0.48
3:J:870:ASP:O	3:J:874:GLU:HG2	2.13	0.48
2:C:802:VAL:HG23	2:C:1098:LEU:HD13	1.94	0.48
2:C:444:ASP:O	2:C:450:ASN:ND2	2.39	0.48
3:J:1062:LEU:CD2	3:J:1066:GLU:HB3	2.44	0.48
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.94	0.48
3:D:1264:ALA:CB	3:D:1280:VAL:HG22	2.44	0.48
2:C:1149:TYR:OH	2:C:1176:LEU:HD11	2.14	0.48
3:D:807:LEU:HD11	3:D:894:VAL:HG23	1.95	0.48
2:C:232:ILE:HD11	2:C:333:ILE:HD11	1.95	0.48
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.95	0.48
3:J:298:MET:SD	5:L:402:LEU:HB3	2.53	0.48
2:C:1246:ARG:NH2	3:D:348:ASP:OD1	2.46	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.94	0.48
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.95	0.48
2:C:692:THR:OG1	2:C:693:LEU:N	2.46	0.48
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.96	0.48
3:D:1226:VAL:HG23	3:J:1296:GLY:HA2	1.96	0.48
3:J:99:ARG:HA	3:J:248:ASP:HB2	1.96	0.48
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.95	0.48
2:I:1246:ARG:NH2	3:J:348:ASP:OD1	2.46	0.48
3:J:17:PHE:O	3:J:1369:ARG:NH2	2.38	0.48
2:C:739:ASP:OD1	2:C:739:ASP:N	2.43	0.48
1:B:73:GLY:O	1:B:134:THR:N	2.35	0.48
3:D:1067:ARG:HH22	3:D:1076:PRO:HD3	1.79	0.48
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.96	0.48
5:L:141:ILE:HG21	5:L:252:LEU:HD11	1.94	0.48
3:J:755:ILE:HG22	3:J:757:THR:H	1.77	0.48
5:L:138:PRO:O	5:L:142:THR:HG23	2.14	0.48
2:C:528:ARG:NH2	2:C:576:SER:O	2.47	0.48
5:L:319:ALA:HA	5:L:322:MET:HG3	1.94	0.48
2:C:403:MET:HE2	2:C:584:TYR:CD1	2.49	0.48
3:J:1062:LEU:HD21	3:J:1066:GLU:HB3	1.95	0.48
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.96	0.48
1:G:207:THR:HG22	1:G:208:ASN:H	1.79	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.96	0.48
3:J:1264:ALA:CB	3:J:1280:VAL:HG22	2.44	0.48
3:J:1067:ARG:HH22	3:J:1076:PRO:HD3	1.79	0.48
1:A:57:THR:OG1	1:A:147:GLN:HG2	2.14	0.48
3:J:807:LEU:HD11	3:J:894:VAL:HG23	1.96	0.48
5:F:130:VAL:O	5:F:134:VAL:HG23	2.14	0.48
3:J:525:MET:O	3:J:548:VAL:HG13	2.14	0.48
1:B:61:ILE:HB	1:B:64:VAL:O	2.14	0.48
2:I:4:SER:OG	2:I:5:TYR:N	2.47	0.48
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.47	0.48
5:F:98:VAL:O	5:F:102:MET:HB2	2.14	0.48
2:I:703:GLY:N	2:I:705:GLU:OE2	2.43	0.48
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.95	0.48
5:F:319:ALA:HA	5:F:322:MET:HG3	1.95	0.47
3:D:99:ARG:HA	3:D:248:ASP:HB2	1.96	0.47
3:J:845:ALA:HB3	3:J:881:LYS:HB3	1.96	0.47
1:H:181:GLU:HA	3:J:535:ARG:NH2	2.29	0.47
5:L:130:VAL:O	5:L:134:VAL:HG23	2.14	0.47
1:G:10:LYS:HE2	1:H:229:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:890:LYS:NZ	2:C:891:GLY:O	2.47	0.47
1:B:16:ILE:HG13	1:B:26:VAL:HG22	1.96	0.47
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.79	0.47
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.96	0.47
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.79	0.47
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.13	0.47
5:F:138:PRO:O	5:F:142:THR:HG23	2.14	0.47
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.96	0.47
3:J:850:LYS:HG2	3:J:851:PRO:HD2	1.95	0.47
3:D:405:GLU:O	3:D:408:VAL:HG22	2.14	0.47
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.96	0.47
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.96	0.47
3:D:144:TYR:CD1	3:D:180:MET:HB3	2.50	0.47
5:L:489:MET:HE2	5:L:493:LYS:HG3	1.97	0.47
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.97	0.47
3:J:1064:SER:HB2	3:J:1173:ARG:NH1	2.25	0.47
6:M:16:PHE:HD1	6:M:59:PRO:HA	1.78	0.47
3:D:525:MET:O	3:D:548:VAL:HG13	2.13	0.47
3:D:1062:LEU:HD21	3:D:1066:GLU:HB3	1.95	0.47
2:I:499:SER:O	2:I:503:LYS:HB2	2.15	0.47
2:I:5:TYR:CD2	2:I:778:GLU:HB2	2.50	0.47
3:J:122:SER:O	3:J:126:LEU:HG	2.15	0.47
2:C:225:PHE:CE1	2:C:345:PRO:HA	2.50	0.47
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.96	0.47
2:I:890:LYS:NZ	2:I:891:GLY:O	2.47	0.47
2:C:151:ARG:HG2	2:C:445:ILE:HG23	1.97	0.47
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.96	0.47
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.46	0.47
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.97	0.47
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.79	0.47
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.97	0.47
5:L:220:LYS:O	5:L:223:GLU:HB3	2.15	0.47
3:D:853:THR:HG21	3:J:1375:ALA:CB	2.45	0.47
3:D:1062:LEU:CD2	3:D:1066:GLU:HB3	2.44	0.47
1:H:61:ILE:HB	1:H:64:VAL:O	2.14	0.47
5:F:598:LEU:HA	5:F:603:ARG:HB2	1.96	0.47
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.96	0.47
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.48	0.47
3:D:442:ILE:HG22	3:D:443:GLU:O	2.15	0.47
2:C:4:SER:OG	2:C:5:TYR:N	2.47	0.47
3:D:1282:TYR:O	3:D:1285:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.96	0.47
3:J:1260:MET:HG2	3:J:1307:LEU:O	2.14	0.47
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.97	0.47
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.45	0.47
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.15	0.47
5:L:98:VAL:O	5:L:102:MET:HB2	2.15	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.97	0.47
1:G:75:GLN:HA	2:I:729:ALA:N	2.30	0.47
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.97	0.47
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.97	0.47
5:L:598:LEU:HA	5:L:603:ARG:HB2	1.97	0.47
2:C:499:SER:O	2:C:503:LYS:HB2	2.15	0.47
5:F:470:MET:HG3	5:F:486:ARG:HH22	1.78	0.47
3:D:1153:PRO:HA	3:D:1214:PRO:O	2.15	0.47
1:A:45:ARG:NE	2:C:1083:GLU:HB3	2.29	0.47
1:H:73:GLY:CA	1:H:134:THR:HG22	2.44	0.47
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.15	0.47
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.96	0.47
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.49	0.47
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.50	0.47
2:C:883:LEU:HD22	2:C:1052:VAL:HG11	1.97	0.47
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.97	0.47
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.96	0.47
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.14	0.47
2:C:120:GLN:HG2	2:C:121:GLU:HG2	1.96	0.46
2:C:494:ASN:HD21	5:F:468:ARG:HG2	1.80	0.46
3:J:442:ILE:HG22	3:J:443:GLU:O	2.15	0.46
5:L:362:ASN:HB2	5:L:365:MET:HE1	1.97	0.46
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.45	0.46
2:I:1116:HIS:O	2:I:1119:MET:HB3	2.15	0.46
3:D:574:VAL:O	3:D:578:ILE:HG13	2.16	0.46
5:L:547:VAL:HG21	5:L:607:LEU:HD11	1.98	0.46
2:C:1253:LEU:HD11	3:D:251:PRO:HG2	1.96	0.46
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.97	0.46
1:A:207:THR:HG22	1:A:208:ASN:H	1.80	0.46
3:D:1260:MET:HG2	3:D:1307:LEU:O	2.15	0.46
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.96	0.46
3:D:122:SER:O	3:D:126:LEU:HG	2.15	0.46
2:C:1113:LEU:HD11	3:D:641:ILE:HG13	1.97	0.46
3:J:156:ARG:NH2	3:J:191:SER:OG	2.48	0.46
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.98	0.46
6:N:40:LEU:O	6:N:44:GLU:HG2	2.16	0.46
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.97	0.46
3:D:290:ILE:HD12	3:D:290:ILE:H	1.81	0.46
2:C:1279:GLU:HG3	3:D:1357:ILE:HD13	1.97	0.46
1:G:201:LEU:HG	1:G:203:ILE:HG13	1.96	0.46
3:D:654:ILE:O	3:D:658:GLU:HB2	2.16	0.46
2:I:90:VAL:HG12	2:I:91:THR:H	1.80	0.46
5:L:456:MET:O	5:L:460:ILE:HG13	2.15	0.46
6:M:40:LEU:O	6:M:44:GLU:HG2	2.15	0.46
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.97	0.46
2:C:855:PRO:HG3	2:C:913:VAL:HG13	1.97	0.46
2:I:5:TYR:HD2	2:I:778:GLU:HB2	1.80	0.46
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.98	0.46
2:I:223:LEU:HD22	2:I:426:ILE:HG21	1.97	0.46
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.49	0.46
3:D:1100:PHE:HB2	3:D:1200:GLU:CD	2.36	0.46
2:I:225:PHE:CE1	2:I:345:PRO:HA	2.50	0.46
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.97	0.46
1:G:75:GLN:HA	2:I:729:ALA:H	1.80	0.46
3:D:156:ARG:NH2	3:D:191:SER:OG	2.47	0.46
3:J:574:VAL:O	3:J:578:ILE:HG13	2.16	0.46
2:C:136:PHE:O	2:C:143:ARG:N	2.37	0.46
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.97	0.46
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.96	0.46
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.98	0.46
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.97	0.46
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.97	0.46
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.97	0.46
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.49	0.46
1:B:75:GLN:HG3	1:B:75:GLN:H	1.60	0.46
2:I:1113:LEU:HD11	3:J:641:ILE:HG13	1.97	0.46
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.80	0.46
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.97	0.46
1:B:47:LEU:HB3	1:B:180:VAL:HG11	1.98	0.46
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.46	0.46
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.59	0.46
5:F:456:MET:O	5:F:460:ILE:HG13	2.15	0.46
3:J:405:GLU:O	3:J:408:VAL:HG22	2.15	0.46
5:L:311:THR:HB	5:L:345:GLN:HG2	1.98	0.46
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:473:THR:HG23	3:J:476:ALA:H	1.81	0.46
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.46
3:J:144:TYR:CD1	3:J:180:MET:HB3	2.50	0.46
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.81	0.46
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.70	0.46
3:D:650:LYS:O	3:D:654:ILE:HG13	2.16	0.46
2:C:1109:ILE:HA	2:C:1109:ILE:HD12	1.80	0.46
2:C:223:LEU:HD22	2:C:426:ILE:HG21	1.98	0.46
3:J:1158:GLU:OE2	3:J:1222:ARG:NH1	2.48	0.46
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.98	0.46
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.45	0.45
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.98	0.45
2:I:705:GLU:O	2:I:794:LEU:N	2.49	0.45
2:I:883:LEU:HD22	2:I:1052:VAL:HG11	1.97	0.45
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.81	0.45
5:F:446:GLN:O	5:F:448:ARG:N	2.49	0.45
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.64	0.45
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.97	0.45
1:B:44:ARG:NH2	3:D:538:ARG:HH21	2.14	0.45
2:C:90:VAL:HG12	2:C:91:THR:H	1.79	0.45
4:E:50:ALA:O	4:E:54:ILE:HG12	2.16	0.45
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.97	0.45
5:F:311:THR:HB	5:F:345:GLN:HG2	1.99	0.45
2:I:960:LEU:HA	2:I:960:LEU:HD13	1.87	0.45
6:N:19:THR:OG1	6:N:55:THR:HB	2.17	0.45
2:I:1279:GLU:HG3	3:J:1357:ILE:HD13	1.98	0.45
3:J:1062:LEU:O	3:J:1067:ARG:NE	2.45	0.45
2:C:123:TYR:OH	2:C:126:GLU:HG3	2.17	0.45
5:F:362:ASN:HB2	5:F:365:MET:HE1	1.98	0.45
3:D:1167:LYS:O	3:D:1169:THR:N	2.50	0.45
3:D:1078:LEU:HB2	3:D:1121:LEU:HD13	1.98	0.45
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.96	0.45
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.31	0.45
2:C:1142:ARG:HH22	2:C:1165:SER:HA	1.81	0.45
3:D:1158:GLU:OE2	3:D:1222:ARG:NH1	2.50	0.45
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.31	0.45
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.52	0.45
3:J:650:LYS:O	3:J:654:ILE:HG13	2.16	0.45
3:J:654:ILE:O	3:J:658:GLU:HB2	2.16	0.45
3:J:1167:LYS:O	3:J:1169:THR:N	2.49	0.45
2:I:5:TYR:HB2	2:I:781:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.52	0.45
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	1.98	0.45
3:D:600:ALA:O	3:D:603:LYS:HG2	2.16	0.45
1:H:30:PRO:HB3	1:H:192:VAL:HG21	1.98	0.45
3:J:363:LEU:HD21	3:J:487:THR:HA	1.97	0.45
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	1.99	0.45
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.47	0.45
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.51	0.45
5:L:446:GLN:O	5:L:448:ARG:N	2.50	0.45
3:J:378:LYS:HB3	3:J:379:PRO:HD3	1.99	0.45
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.17	0.45
3:J:424:ASN:ND2	3:J:434:ILE:HG12	2.31	0.45
2:C:705:GLU:O	2:C:794:LEU:N	2.49	0.45
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.49	0.45
3:D:1027:VAL:HG21	3:D:1122:ALA:HB3	1.97	0.45
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.51	0.45
3:J:211:GLU:HG3	6:N:13:ASN:O	2.16	0.45
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.27	0.45
3:J:950:ILE:HG13	3:J:1020:TRP:CZ3	2.52	0.45
3:J:1166:GLY:O	3:J:1174:ARG:HB2	2.17	0.45
2:I:673:HIS:HB3	2:I:1109:ILE:CG2	2.47	0.45
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.47	0.45
6:N:29:VAL:HG21	6:N:47:TYR:OH	2.17	0.45
2:C:976:ARG:O	2:C:980:VAL:HG23	2.16	0.45
1:B:73:GLY:CA	1:B:134:THR:HG22	2.44	0.45
3:D:1166:GLY:O	3:D:1174:ARG:HB2	2.17	0.45
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.17	0.45
3:J:1064:SER:O	3:J:1072:LYS:HE2	2.17	0.45
3:J:770:LEU:HD22	3:J:770:LEU:H	1.81	0.45
2:C:519:ASN:OD1	2:C:521:LEU:N	2.50	0.45
3:J:1078:LEU:HB2	3:J:1121:LEU:HD13	1.98	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.17	0.45
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.81	0.45
2:C:1326:LEU:HD11	3:D:331:ILE:HG23	1.98	0.45
3:D:473:THR:HG23	3:D:476:ALA:H	1.81	0.45
2:I:971:LEU:HD22	2:I:1021:LEU:HD12	1.98	0.45
2:C:121:GLU:HG2	2:C:121:GLU:H	1.59	0.45
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.99	0.45
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.52	0.45
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.98	0.45
1:H:32:GLU:HB2	1:H:35:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.98	0.44
3:D:1302:TYR:CZ	3:J:1297:LYS:HD3	2.52	0.44
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.65	0.44
3:J:600:ALA:O	3:J:603:LYS:HG2	2.16	0.44
3:D:1349:GLU:CD	3:D:1349:GLU:H	2.20	0.44
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.53	0.44
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.65	0.44
3:D:418:GLU:H	4:E:45:LYS:NZ	2.15	0.44
5:L:442:SER:O	5:L:446:GLN:HG2	2.18	0.44
6:M:19:THR:OG1	6:M:55:THR:HB	2.16	0.44
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.99	0.44
2:C:971:LEU:HD23	2:C:975:ILE:HD11	1.99	0.44
1:A:104:LYS:HG2	1:A:110:VAL:HG22	2.00	0.44
1:H:196:THR:HG23	3:J:443:GLU:HG3	2.00	0.44
5:F:335:GLU:O	5:F:339:ARG:HG2	2.18	0.44
3:J:1282:TYR:O	3:J:1285:VAL:HG12	2.17	0.44
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.98	0.44
5:F:354:THR:O	5:F:358:VAL:HG23	2.16	0.44
3:D:958:ILE:HD11	3:D:1017:VAL:HG11	2.00	0.44
3:J:233:LYS:HB3	3:J:235:GLU:OE2	2.17	0.44
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	2.00	0.44
1:H:47:LEU:HB3	1:H:180:VAL:HG11	1.99	0.44
2:I:174:ALA:HB2	2:I:432:LEU:HD13	2.00	0.44
5:F:220:LYS:O	5:F:223:GLU:HB3	2.17	0.44
1:H:172:LEU:H	1:H:172:LEU:HD12	1.82	0.44
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.72	0.44
3:D:334:LYS:HB3	5:F:516:ASP:OD2	2.16	0.44
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.32	0.44
2:I:396:ASP:OD1	2:I:418:GLY:HA3	2.18	0.44
1:H:81:ILE:O	1:H:85:LEU:HG	2.18	0.44
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.17	0.44
1:H:93:GLN:HB2	1:H:120:ASP:HB3	2.00	0.44
3:J:743:MET:HB2	3:J:759:ILE:O	2.17	0.44
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.97	0.44
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.98	0.44
3:J:794:GLY:O	3:J:797:THR:OG1	2.31	0.44
2:I:992:LEU:HB2	2:I:993:PRO:HD2	1.99	0.44
5:F:253:SER:O	5:F:257:LYS:HG3	2.17	0.44
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.32	0.44
1:B:178:SER:HA	1:B:179:PRO:HD3	1.71	0.44
1:B:93:GLN:HB2	1:B:120:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:HB2	1:B:35:PHE:CD1	2.53	0.44
3:J:418:GLU:H	4:K:45:LYS:NZ	2.15	0.44
3:D:950:ILE:HG13	3:D:1020:TRP:CZ3	2.52	0.44
3:D:430:HIS:CE1	3:D:925:GLU:HG3	2.52	0.44
3:J:26:SER:HB2	3:J:236:TRP:CE2	2.53	0.44
1:A:231:PHE:CE1	1:B:221:ALA:HB3	2.53	0.44
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.17	0.44
4:K:44:ASP:HB3	4:K:48:VAL:HB	2.00	0.44
4:E:44:ASP:HB3	4:E:48:VAL:HB	2.00	0.44
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.99	0.44
3:J:613:GLY:O	3:J:617:THR:OG1	2.33	0.44
3:D:706:VAL:HG12	3:D:715:LYS:HB3	2.00	0.44
1:H:79:LEU:HD23	1:H:79:LEU:H	1.82	0.44
2:C:657:THR:HG23	2:C:658:GLN:HG3	2.00	0.44
3:D:363:LEU:HD21	3:D:487:THR:HA	1.98	0.44
3:J:490:ILE:HD11	3:J:609:TYR:CE2	2.53	0.44
3:D:490:ILE:HD11	3:D:609:TYR:CE2	2.53	0.44
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.16	0.44
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.32	0.44
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.47	0.44
3:D:440:VAL:O	3:D:442:ILE:HG12	2.18	0.44
3:J:958:ILE:HG23	3:J:982:LEU:HD11	2.00	0.44
3:D:800:LEU:HD12	3:D:1309:ILE:HD13	2.00	0.44
2:I:1326:LEU:HD11	3:J:331:ILE:HG23	1.99	0.44
1:B:30:PRO:HB3	1:B:192:VAL:HG21	1.99	0.44
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.87	0.44
5:L:312:SER:OG	5:L:313:ASP:N	2.51	0.44
2:C:980:VAL:HG13	2:C:984:VAL:HG23	1.99	0.44
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.53	0.44
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.00	0.44
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.18	0.44
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	2.00	0.44
2:I:594:VAL:HG22	2:I:599:VAL:HA	2.00	0.44
1:B:52:PRO:HA	1:B:149:GLY:O	2.18	0.44
1:B:102:LEU:O	1:B:141:SER:OG	2.29	0.44
2:C:137:VAL:HA	2:C:141:THR:O	2.18	0.44
5:F:324:LYS:HB2	5:F:327:SER:HB2	2.00	0.44
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.79	0.44
2:I:657:THR:HG23	2:I:658:GLN:HG3	2.00	0.44
3:D:18:ASP:OD1	3:D:18:ASP:N	2.50	0.44
5:L:335:GLU:O	5:L:339:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:403:MET:HG3	2:C:584:TYR:CZ	2.53	0.43
1:G:11:PRO:HB3	1:G:31:LEU:HD23	2.00	0.43
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.16	0.43
3:J:697:MET:SD	3:J:741:ALA:HB3	2.58	0.43
3:J:702:GLN:HG3	3:J:703:THR:N	2.33	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.00	0.43
5:F:468:ARG:O	5:F:471:LEU:HB2	2.18	0.43
3:J:747:MET:HB2	3:J:774:ILE:HG22	2.00	0.43
5:L:354:THR:O	5:L:358:VAL:HG23	2.18	0.43
3:D:743:MET:HB2	3:D:759:ILE:O	2.17	0.43
2:C:594:VAL:HG22	2:C:599:VAL:HA	2.00	0.43
3:D:124:ILE:HG23	3:D:189:LEU:HD11	2.00	0.43
2:C:396:ASP:OD1	2:C:418:GLY:HA3	2.18	0.43
2:I:1142:ARG:HH22	2:I:1165:SER:HA	1.82	0.43
2:I:905:ILE:O	5:L:599:ARG:NH1	2.51	0.43
3:J:990:ARG:NH1	3:J:992:LYS:HD3	2.33	0.43
1:B:79:LEU:HD23	1:B:79:LEU:H	1.84	0.43
3:J:290:ILE:HD12	3:J:290:ILE:H	1.81	0.43
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.89	0.43
1:G:16:ILE:HG23	1:G:26:VAL:HG12	2.00	0.43
3:D:1062:LEU:O	3:D:1067:ARG:NE	2.45	0.43
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	2.00	0.43
3:D:394:ILE:HG21	5:F:536:THR:HA	2.00	0.43
5:L:461:ASN:O	5:L:465:ARG:HG2	2.17	0.43
5:L:468:ARG:O	5:L:471:LEU:HB2	2.18	0.43
2:C:174:ALA:HB2	2:C:432:LEU:HD13	2.01	0.43
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.98	0.43
3:D:518:VAL:O	3:D:547:ARG:NH1	2.51	0.43
5:L:287:ILE:HG23	5:L:337:VAL:HG13	2.00	0.43
3:J:1067:ARG:HB2	3:J:1072:LYS:HG3	2.01	0.43
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.18	0.43
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.99	0.43
3:D:1067:ARG:HB2	3:D:1072:LYS:HG3	2.00	0.43
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.33	0.43
1:B:81:ILE:O	1:B:85:LEU:HG	2.18	0.43
3:D:747:MET:HB2	3:D:774:ILE:HG22	2.00	0.43
2:C:905:ILE:O	5:F:599:ARG:NH1	2.51	0.43
5:F:312:SER:OG	5:F:313:ASP:N	2.51	0.43
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.53	0.43
5:L:253:SER:O	5:L:257:LYS:HG3	2.18	0.43
3:J:440:VAL:O	3:J:442:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:46:TYR:O	5:L:500:ILE:HG21	2.18	0.43
6:M:29:VAL:HG21	6:M:47:TYR:OH	2.17	0.43
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.48	0.43
5:F:302:PHE:O	5:F:306:PHE:HB2	2.18	0.43
5:F:137:TYR:CE1	5:F:139:GLU:HB2	2.53	0.43
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.18	0.43
3:D:1064:SER:O	3:D:1072:LYS:HE2	2.18	0.43
3:D:1177:ILE:HG13	3:D:1177:ILE:H	1.69	0.43
2:I:1100:PRO:O	2:I:1104:PRO:HD3	2.18	0.43
3:D:958:ILE:HG23	3:D:982:LEU:HD11	2.01	0.43
2:I:517:GLN:O	2:I:761:GLN:HB2	2.19	0.43
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.99	0.43
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	2.01	0.43
3:J:518:VAL:O	3:J:547:ARG:NH1	2.51	0.43
1:G:137:ASN:N	1:G:137:ASN:OD1	2.51	0.43
3:J:1349:GLU:H	3:J:1349:GLU:CD	2.19	0.43
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.18	0.43
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	2.00	0.43
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	2.00	0.43
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.51	0.43
1:G:53:GLY:O	1:G:148:ARG:HG3	2.19	0.43
5:F:394:TYR:HB3	5:F:443:ILE:HD11	2.01	0.43
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.83	0.43
5:L:127:ILE:O	5:L:130:VAL:HG22	2.18	0.43
3:J:1227:HIS:O	3:J:1230:THR:HG22	2.19	0.43
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.19	0.43
3:J:746:LEU:HD13	3:J:754:ILE:HD11	2.00	0.43
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.00	0.43
3:D:564:VAL:HG12	3:D:565:ALA:N	2.34	0.43
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.58	0.43
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.01	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.59	0.43
3:J:527:LEU:HD21	3:J:536:LEU:HG	2.01	0.43
2:I:1302:THR:HG22	5:L:531:PRO:HB3	2.00	0.43
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.18	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.54	0.43
5:L:555:GLU:HA	5:L:558:VAL:HG12	2.01	0.43
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	2.00	0.43
3:D:26:SER:HB2	3:D:236:TRP:CE2	2.54	0.43
3:D:512:TYR:CD2	3:D:635:SER:HB2	2.53	0.43
3:D:339:ARG:O	3:D:341:ASN:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:O	1:A:81:ILE:HG13	2.19	0.43
2:I:697:LYS:HG2	2:I:698:PRO:O	2.19	0.43
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	1.99	0.43
2:I:339:ASN:O	2:I:344:GLY:HA2	2.18	0.43
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.99	0.43
3:D:1227:HIS:O	3:D:1230:THR:HG22	2.19	0.43
2:C:3:TYR:HB3	2:C:4:SER:H	1.64	0.43
2:I:1286:THR:O	2:I:1290:MET:HB2	2.19	0.43
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.87	0.43
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.54	0.43
3:J:800:LEU:HD12	3:J:1309:ILE:HD13	2.00	0.43
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	2.01	0.43
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.43
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	2.01	0.43
2:I:1339:LEU:HB3	3:J:17:PHE:CD1	2.54	0.43
2:I:708:VAL:HG11	2:I:794:LEU:HD22	2.01	0.43
1:A:53:GLY:O	1:A:148:ARG:HG3	2.19	0.43
3:J:161:THR:HG22	3:J:164:GLN:CD	2.39	0.43
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.87	0.43
3:D:990:ARG:NH1	3:D:992:LYS:HD3	2.34	0.43
2:C:985:GLU:O	2:C:989:LEU:HB2	2.18	0.43
5:L:515:GLU:C	5:L:517:SER:H	2.23	0.43
5:L:266:PHE:HA	5:L:269:LEU:HD12	2.00	0.43
2:I:519:ASN:OD1	2:I:521:LEU:N	2.51	0.43
3:D:475:GLU:CD	4:E:28:ARG:HH22	2.23	0.43
1:A:90:VAL:HG22	1:A:91:ARG:H	1.84	0.43
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.43
3:D:702:GLN:HG3	3:D:703:THR:N	2.34	0.43
3:J:702:GLN:HG3	3:J:703:THR:H	1.83	0.43
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.81	0.43
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.51	0.43
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	2.01	0.43
5:L:324:LYS:HB2	5:L:327:SER:HB2	2.01	0.43
3:J:124:ILE:HG23	3:J:189:LEU:HD11	2.00	0.43
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.00	0.43
3:J:174:ASP:C	3:J:176:PHE:H	2.22	0.43
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.84	0.43
5:F:584:ARG:HA	5:F:584:ARG:NH1	2.34	0.42
5:F:266:PHE:HA	5:F:269:LEU:HD12	2.00	0.42
2:C:1339:LEU:HB3	3:D:17:PHE:CD1	2.54	0.42
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:141:ILE:H	5:F:141:ILE:HG12	1.68	0.42
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.87	0.42
5:F:573:LEU:H	5:F:573:LEU:HD23	1.83	0.42
2:C:980:VAL:O	2:C:984:VAL:HB	2.19	0.42
2:I:637:ARG:HA	2:I:642:SER:HA	2.01	0.42
3:D:746:LEU:HD13	3:D:754:ILE:HD11	2.00	0.42
2:C:53:PHE:O	2:C:57:PHE:HB2	2.19	0.42
2:I:228:VAL:HB	2:I:335:THR:OG1	2.19	0.42
5:L:296:LYS:HD3	5:L:296:LYS:HA	1.79	0.42
1:A:117:HIS:NE2	1:A:121:VAL:O	2.53	0.42
2:I:946:LEU:HD23	2:I:946:LEU:HA	1.85	0.42
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.92	0.42
2:C:637:ARG:HA	2:C:642:SER:HA	2.00	0.42
3:J:1155:ILE:HD12	3:J:1210:ILE:HB	2.02	0.42
3:D:1031:VAL:HG23	3:D:1080:ILE:HG21	2.00	0.42
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.18	0.42
5:L:387:VAL:HG22	5:L:435:ILE:HD13	2.02	0.42
3:J:701:LEU:HD22	3:J:701:LEU:HA	1.91	0.42
3:J:94:GLN:O	3:J:97:VAL:HG23	2.19	0.42
2:C:992:LEU:HD23	2:C:992:LEU:H	1.84	0.42
3:J:512:TYR:CD2	3:J:635:SER:HB2	2.54	0.42
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	2.01	0.42
5:F:515:GLU:C	5:F:517:SER:H	2.23	0.42
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.29	0.42
5:F:577:GLY:HA3	5:F:583:THR:HG23	2.01	0.42
1:G:90:VAL:HG22	1:G:91:ARG:H	1.84	0.42
2:I:91:THR:HG21	2:I:503:LYS:CE	2.49	0.42
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.94	0.42
2:C:1253:LEU:CD1	3:D:251:PRO:HG2	2.50	0.42
1:A:208:ASN:N	1:A:208:ASN:OD1	2.49	0.42
3:D:8:LEU:HD23	3:D:9:LYS:N	2.34	0.42
3:J:81:ARG:HG3	3:J:82:GLY:H	1.83	0.42
5:F:227:GLN:HA	5:F:230:VAL:HG12	2.01	0.42
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.49	0.42
3:D:1046:ILE:HD12	3:D:1059:LEU:HD13	2.02	0.42
2:C:179:TYR:HE1	2:C:454:ARG:HH21	1.67	0.42
3:D:264:ASP:N	3:D:264:ASP:OD2	2.52	0.42
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.88	0.42
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	2.01	0.42
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.84	0.42
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:203:GLU:O	3:D:207:GLU:HG2	2.19	0.42
2:I:653:MET:HG2	2:I:654:ASP:N	2.35	0.42
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.86	0.42
2:I:88:ARG:NH1	2:I:88:ARG:HB2	2.34	0.42
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.51	0.42
5:F:105:MET:HE3	5:F:384:LEU:HB2	2.02	0.42
3:J:480:ALA:O	3:J:485:MET:N	2.52	0.42
5:F:134:VAL:HG22	5:F:273:MET:HE1	2.01	0.42
3:D:424:ASN:ND2	3:D:434:ILE:HG12	2.33	0.42
1:B:11:PRO:HB3	1:B:30:PRO:O	2.19	0.42
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.20	0.42
5:L:302:PHE:O	5:L:306:PHE:HB2	2.19	0.42
3:J:264:ASP:OD2	3:J:264:ASP:N	2.53	0.42
6:M:19:THR:HG1	6:M:55:THR:HB	1.84	0.42
3:D:1063:ASP:O	3:D:1067:ARG:HG3	2.20	0.42
2:C:520:PRO:HG3	2:C:714:VAL:HG11	2.01	0.42
5:L:394:TYR:HB3	5:L:443:ILE:HD11	2.00	0.42
2:C:676:ALA:HB2	3:D:772:TYR:HE1	1.85	0.42
5:L:364:ARG:HA	5:L:367:ILE:HD12	2.02	0.42
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	2.01	0.42
2:I:347:ILE:HD11	2:I:433:ILE:HD11	2.02	0.42
1:G:77:ASP:O	1:G:81:ILE:HG13	2.19	0.42
1:A:75:GLN:HA	2:C:729:ALA:N	2.34	0.42
5:L:137:TYR:CE1	5:L:139:GLU:HB2	2.54	0.42
5:F:505:ILE:HD12	5:F:505:ILE:HA	1.84	0.42
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.84	0.42
2:C:452:ARG:HG2	2:C:453:ILE:N	2.35	0.42
5:L:577:GLY:HA3	5:L:583:THR:HG23	2.01	0.42
1:A:11:PRO:HB3	1:A:31:LEU:HD23	2.01	0.42
2:I:672:GLU:HG3	2:I:672:GLU:H	1.57	0.42
2:C:138:ILE:HG22	2:C:139:ASN:N	2.34	0.42
3:D:702:GLN:HG3	3:D:703:THR:H	1.83	0.42
3:D:1256:ILE:HG22	3:D:1260:MET:HE2	2.02	0.42
2:C:484:LEU:CD1	2:C:485:ASP:H	2.32	0.42
3:J:203:GLU:O	3:J:207:GLU:HG2	2.20	0.42
1:G:125:LYS:HE2	1:G:128:HIS:HB2	2.01	0.42
5:F:120:ALA:HA	5:F:123:ILE:HD12	2.02	0.42
3:D:118:LYS:HA	3:D:118:LYS:HD2	1.81	0.42
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.35	0.42
5:L:584:ARG:NH1	5:L:584:ARG:HA	2.34	0.42
3:J:611:ILE:HG22	3:J:612:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:291:CYS:O	5:L:296:LYS:N	2.53	0.42
2:I:53:PHE:O	2:I:57:PHE:HB2	2.20	0.42
2:I:676:ALA:HB2	3:J:772:TYR:HE1	1.85	0.42
2:I:975:ILE:O	2:I:979:LEU:HB2	2.19	0.42
3:D:750:PRO:HA	3:D:777:HIS:NE2	2.35	0.42
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.42
5:F:291:CYS:O	5:F:296:LYS:N	2.53	0.42
3:D:12:THR:HG22	3:D:13:LYS:HG2	2.02	0.42
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.35	0.42
2:C:521:LEU:HA	2:C:524:ILE:HG22	2.02	0.42
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.95	0.42
5:F:387:VAL:HG22	5:F:435:ILE:HD13	2.02	0.42
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.35	0.42
1:A:75:GLN:HA	2:C:729:ALA:H	1.85	0.42
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.01	0.42
3:D:70:CYS:SG	3:D:71:LEU:N	2.92	0.42
2:C:848:GLU:HG2	2:C:888:THR:HG22	2.02	0.42
2:I:898:GLU:HB3	5:L:540:LEU:HD22	2.02	0.42
2:C:925:SER:O	2:C:1056:VAL:HG13	2.20	0.42
5:L:227:GLN:HA	5:L:230:VAL:HG12	2.01	0.42
5:L:344:LEU:HA	5:L:344:LEU:HD12	1.85	0.42
3:D:418:GLU:O	3:D:420:PRO:HD3	2.20	0.41
3:D:480:ALA:O	3:D:485:MET:N	2.52	0.41
5:L:584:ARG:O	5:L:587:ILE:HG22	2.20	0.41
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.34	0.41
3:D:697:MET:SD	3:D:741:ALA:HB3	2.60	0.41
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.50	0.41
3:D:9:LYS:HE2	3:D:9:LYS:HB3	1.93	0.41
5:F:287:ILE:HG23	5:F:337:VAL:HG13	2.01	0.41
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	2.02	0.41
3:D:645:VAL:HB	3:D:701:LEU:HD23	2.02	0.41
3:D:44:ILE:HD13	3:D:252:LEU:HD13	2.02	0.41
5:F:376:LYS:O	5:F:380:VAL:HG23	2.20	0.41
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.02	0.41
3:D:161:THR:HG22	3:D:164:GLN:CD	2.40	0.41
2:I:446:ASP:N	2:I:446:ASP:OD1	2.53	0.41
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.88	0.41
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	0.41
2:I:452:ARG:HG2	2:I:453:ILE:N	2.35	0.41
1:G:45:ARG:NH1	1:H:34:GLY:O	2.52	0.41
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:644:MET:SD	3:D:740:LEU:HD23	2.60	0.41
5:F:550:GLY:HA3	5:F:603:ARG:NH1	2.36	0.41
3:D:425:ARG:HG2	3:D:426:ALA:N	2.35	0.41
3:J:564:VAL:HG12	3:J:565:ALA:N	2.35	0.41
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.20	0.41
2:I:1028:LYS:HE2	2:I:1028:LYS:HB2	1.71	0.41
5:F:441:ARG:O	5:F:445:ASP:HB2	2.20	0.41
2:C:1286:THR:O	2:C:1290:MET:HB2	2.20	0.41
2:C:198:ILE:O	2:C:201:ARG:HB2	2.20	0.41
2:I:730:SER:O	2:I:753:LEU:HB2	2.20	0.41
3:D:620:PHE:O	3:D:624:ILE:HG13	2.20	0.41
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.87	0.41
2:C:88:ARG:NH1	2:C:88:ARG:HB2	2.35	0.41
5:L:573:LEU:HD23	5:L:573:LEU:H	1.84	0.41
3:J:1183:SER:OG	3:J:1184:ASP:N	2.51	0.41
1:G:111:THR:HB	1:G:126:PRO:O	2.21	0.41
5:L:551:LEU:HD21	5:L:598:LEU:HD21	2.01	0.41
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	2.02	0.41
3:D:712:GLN:HG2	3:D:713:GLU:H	1.85	0.41
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.50	0.41
1:H:11:PRO:HB3	1:H:30:PRO:O	2.20	0.41
3:J:147:ILE:HD11	3:J:179:LYS:HG2	2.03	0.41
3:J:155:GLU:HB2	3:J:158:GLN:HB2	2.02	0.41
3:D:528:THR:HG23	3:D:529:GLY:H	1.85	0.41
5:F:225:ARG:O	5:F:229:VAL:HG13	2.20	0.41
3:J:620:PHE:O	3:J:624:ILE:HG13	2.20	0.41
3:J:449:LEU:HD22	3:J:466:MET:SD	2.60	0.41
2:C:379:GLU:CD	2:C:379:GLU:H	2.23	0.41
5:L:470:MET:HB3	5:L:474:MET:HG3	2.01	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.19	0.41
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	2.02	0.41
2:I:959:ASP:O	2:I:962:GLU:HB2	2.21	0.41
2:I:198:ILE:O	2:I:201:ARG:HB2	2.20	0.41
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	2.02	0.41
2:C:228:VAL:HB	2:C:335:THR:OG1	2.20	0.41
5:F:344:LEU:HA	5:F:344:LEU:HD12	1.86	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.88	0.41
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.47	0.41
2:C:697:LYS:HG2	2:C:698:PRO:O	2.20	0.41
3:D:1024:THR:HG22	3:D:1026:PRO:HD3	2.02	0.41
5:F:470:MET:HB3	5:F:474:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1348:LYS:HA	3:J:1348:LYS:HD2	1.89	0.41
3:D:709:ARG:O	3:D:711:GLY:N	2.52	0.41
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.35	0.41
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	2.02	0.41
1:G:208:ASN:N	1:G:208:ASN:OD1	2.50	0.41
2:C:246:LEU:HD12	2:C:246:LEU:H	1.85	0.41
1:G:28:LEU:HD23	1:H:231:PHE:CZ	2.56	0.41
5:L:388:ILE:HG22	5:L:392:LYS:HE3	2.02	0.41
3:J:407:VAL:O	3:J:411:ILE:HG12	2.20	0.41
5:L:120:ALA:HA	5:L:123:ILE:HD12	2.02	0.41
3:J:528:THR:HG23	3:J:529:GLY:H	1.85	0.41
2:C:1124:ILE:HB	2:C:1180:MET:HB2	2.02	0.41
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.51	0.41
3:J:644:MET:SD	3:J:740:LEU:HD23	2.60	0.41
3:J:660:GLU:O	3:J:664:ILE:HG12	2.20	0.41
3:J:490:ILE:HA	3:J:500:ILE:HG12	2.03	0.41
2:I:169:LYS:O	2:I:170:VAL:HG22	2.18	0.41
2:I:484:LEU:CD1	2:I:485:ASP:H	2.34	0.41
3:D:449:LEU:HD22	3:D:466:MET:SD	2.61	0.41
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.55	0.41
2:I:848:GLU:HG2	2:I:888:THR:HG22	2.01	0.41
3:D:155:GLU:HB2	3:D:158:GLN:HB2	2.02	0.41
1:A:137:ASN:OD1	1:A:137:ASN:N	2.51	0.41
2:I:573:ASN:N	2:I:573:ASN:OD1	2.54	0.41
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.88	0.41
1:A:111:THR:HB	1:A:126:PRO:O	2.21	0.41
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.21	0.41
1:A:45:ARG:HG2	1:B:38:THR:CB	2.50	0.41
5:L:554:ARG:HB2	5:L:580:PHE:CE2	2.55	0.41
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.34	0.41
2:C:728:ASP:OD1	2:C:729:ALA:N	2.53	0.41
3:D:1036:ARG:HE	3:D:1081:VAL:HG11	1.86	0.41
3:J:1034:PHE:HB2	3:J:1081:VAL:HG23	2.03	0.41
3:J:1036:ARG:HE	3:J:1081:VAL:HG11	1.86	0.41
1:G:117:HIS:NE2	1:G:121:VAL:O	2.53	0.41
3:J:18:ASP:N	3:J:18:ASP:OD1	2.54	0.41
3:D:1183:SER:OG	3:D:1184:ASP:N	2.51	0.41
5:F:554:ARG:HB2	5:F:580:PHE:CE2	2.55	0.41
1:G:115:ILE:H	1:G:115:ILE:HG13	1.70	0.41
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.02	0.41
2:I:1124:ILE:HB	2:I:1180:MET:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:844:THR:HG21	3:J:858:VAL:HG21	2.02	0.41
4:E:53:GLU:HB3	4:E:59:ILE:HG13	2.03	0.41
2:I:985:GLU:HB3	2:I:988:LYS:HB2	2.03	0.41
1:H:63:GLY:HA3	1:H:71:LYS:HD3	2.03	0.41
2:I:1340:GLU:OE2	3:J:21:LYS:HE3	2.20	0.41
1:H:102:LEU:O	1:H:141:SER:OG	2.28	0.41
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.82	0.41
1:A:57:THR:O	1:A:173:VAL:HG22	2.21	0.41
3:J:646:ILE:HG22	3:J:647:PRO:HD2	2.03	0.41
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.03	0.41
2:I:496:LYS:HA	2:I:499:SER:HB3	2.03	0.41
2:I:980:VAL:HG13	2:I:984:VAL:HG23	2.03	0.41
2:C:462:ASN:O	2:C:465:ARG:HB3	2.21	0.41
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	2.02	0.41
1:G:221:ALA:HB1	1:H:228:LEU:HD22	2.02	0.41
4:E:31:GLN:HB2	4:E:46:THR:HG21	2.03	0.41
3:D:174:ASP:C	3:D:176:PHE:H	2.23	0.41
3:D:94:GLN:O	3:D:97:VAL:HG23	2.20	0.41
5:L:224:LEU:HB2	5:L:259:PHE:CZ	2.56	0.41
1:H:108:GLY:HA2	1:H:109:PRO:HD3	1.92	0.41
2:C:1340:GLU:OE2	3:D:21:LYS:HE3	2.21	0.41
2:C:624:ASP:OD1	2:C:625:GLU:HG3	2.21	0.41
5:F:466:ILE:H	5:F:466:ILE:HG13	1.41	0.41
3:D:860:ARG:HA	3:D:860:ARG:HD2	1.89	0.41
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.51	0.41
3:D:646:ILE:HG22	3:D:647:PRO:HD2	2.02	0.41
1:H:59:VAL:O	1:H:171:LEU:HA	2.21	0.41
5:L:269:LEU:O	5:L:273:MET:HG3	2.20	0.41
2:C:91:THR:HG21	2:C:503:LYS:CE	2.50	0.41
3:J:475:GLU:CD	4:K:28:ARG:HH22	2.23	0.41
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.21	0.41
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	2.03	0.41
3:J:645:VAL:HB	3:J:701:LEU:HD23	2.02	0.41
2:C:730:SER:O	2:C:753:LEU:HB2	2.20	0.41
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.03	0.41
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.20	0.41
2:I:786:GLY:N	2:I:789:THR:OG1	2.42	0.41
3:J:70:CYS:SG	3:J:71:LEU:N	2.94	0.41
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.56	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.87	0.41
5:L:600:HIS:O	5:L:602:SER:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:418:GLU:O	3:J:420:PRO:HD3	2.21	0.40
3:D:1162:ILE:O	3:D:1178:THR:OG1	2.19	0.40
3:J:1177:ILE:HG13	3:J:1177:ILE:H	1.69	0.40
3:J:425:ARG:HG2	3:J:426:ALA:N	2.35	0.40
3:J:810:THR:HG23	3:J:811:GLU:H	1.87	0.40
3:J:1256:ILE:HG22	3:J:1260:MET:HE2	2.03	0.40
2:I:246:LEU:HD12	2:I:246:LEU:H	1.85	0.40
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.78	0.40
2:I:724:VAL:HG23	2:I:775:GLU:O	2.21	0.40
5:L:376:LYS:O	5:L:380:VAL:HG23	2.22	0.40
1:A:39:LEU:O	1:A:43:LEU:HG	2.22	0.40
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.87	0.40
2:C:573:ASN:N	2:C:573:ASN:OD1	2.54	0.40
3:J:488:ASN:HA	3:J:488:ASN:HD22	1.68	0.40
3:D:849:LEU:HD22	3:D:849:LEU:H	1.86	0.40
3:J:123:ARG:HA	3:J:123:ARG:HD3	1.87	0.40
3:J:1332:LEU:HA	3:J:1332:LEU:HD13	1.93	0.40
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.21	0.40
5:L:105:MET:HE3	5:L:384:LEU:HB2	2.02	0.40
3:D:793:SER:O	3:D:797:THR:HG23	2.21	0.40
5:F:584:ARG:O	5:F:587:ILE:HG22	2.21	0.40
2:C:519:ASN:HA	2:C:520:PRO:HD3	1.95	0.40
2:I:521:LEU:HA	2:I:524:ILE:HG22	2.02	0.40
3:J:709:ARG:O	3:J:711:GLY:N	2.53	0.40
2:C:992:LEU:HB2	2:C:993:PRO:HD2	2.03	0.40
2:C:758:ARG:HD2	2:C:835:GLU:HB2	2.04	0.40
5:F:364:ARG:HA	5:F:367:ILE:HD12	2.02	0.40
1:G:38:THR:OG1	1:H:45:ARG:HD3	2.21	0.40
1:A:125:LYS:HE2	1:A:128:HIS:HB2	2.02	0.40
1:H:182:ARG:NH1	3:J:581:MET:SD	2.94	0.40
3:J:899:TYR:O	3:J:1251:LYS:HD3	2.21	0.40
5:L:225:ARG:O	5:L:229:VAL:HG13	2.21	0.40
3:D:16:GLU:OE2	3:D:1355:ARG:NH2	2.53	0.40
3:D:267:ASP:OD1	3:D:271:ARG:NH2	2.55	0.40
3:J:140:TYR:HB3	5:L:100:MET:SD	2.61	0.40
5:F:551:LEU:HD21	5:F:598:LEU:HD21	2.03	0.40
3:D:140:TYR:HB3	5:F:100:MET:SD	2.61	0.40
6:N:13:ASN:N	6:N:34:GLU:HG2	2.36	0.40
5:F:339:ARG:HA	5:F:339:ARG:HD2	1.97	0.40
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.56	0.40
3:J:44:ILE:HD13	3:J:252:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:TYR:CZ	2:I:824:GLN:HA	2.57	0.40
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.57	0.40
1:G:11:PRO:HD2	1:H:227:GLN:HA	2.02	0.40
2:C:232:ILE:HD12	2:C:330:HIS:O	2.21	0.40
1:A:60:GLU:HB2	1:A:170:ARG:HG2	2.03	0.40
2:C:496:LYS:HA	2:C:499:SER:HB3	2.03	0.40
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.94	0.40
2:C:1289:GLU:HB3	2:C:1315:MET:SD	2.61	0.40
3:J:124:ILE:O	3:J:128:LEU:HG	2.22	0.40
5:L:139:GLU:HG3	5:L:351:THR:HA	2.03	0.40
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.86	0.40
5:F:388:ILE:HG22	5:F:392:LYS:HE3	2.02	0.40
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.21	0.40
2:I:462:ASN:O	2:I:465:ARG:HB3	2.21	0.40
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.21	0.40
3:D:746:LEU:HB2	3:D:754:ILE:HD11	2.04	0.40
3:J:1075:ARG:HH21	3:J:1166:GLY:HA2	1.87	0.40
1:G:60:GLU:HB2	1:G:170:ARG:HG2	2.03	0.40
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.22	0.40
3:D:124:ILE:O	3:D:128:LEU:HG	2.21	0.40
5:L:394:TYR:OH	5:L:436:ARG:HG2	2.21	0.40
1:B:212:ASP:OD1	1:B:214:GLU:HB3	2.22	0.40
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	2.02	0.40
5:F:555:GLU:HA	5:F:558:VAL:HG12	2.02	0.40
3:D:407:VAL:O	3:D:411:ILE:HG12	2.21	0.40
2:C:363:LEU:HB3	2:C:381:ALA:HB1	2.04	0.40
2:C:32:LEU:HA	2:C:130:MET:SD	2.62	0.40
2:I:379:GLU:H	2:I:379:GLU:CD	2.24	0.40
3:D:488:ASN:HD22	3:D:488:ASN:HA	1.67	0.40
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.47	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	222/239 (93%)	197 (89%)	21 (10%)	4 (2%)	11	54
1	B	216/239 (90%)	189 (88%)	27 (12%)	0	100	100
1	G	226/239 (95%)	202 (89%)	20 (9%)	4 (2%)	11	54
1	H	213/239 (89%)	187 (88%)	26 (12%)	0	100	100
2	C	1338/1342 (100%)	1213 (91%)	121 (9%)	4 (0%)	46	82
2	I	1338/1342 (100%)	1216 (91%)	117 (9%)	5 (0%)	39	79
3	D	1339/1407 (95%)	1217 (91%)	120 (9%)	2 (0%)	56	90
3	J	1317/1407 (94%)	1201 (91%)	115 (9%)	1 (0%)	56	90
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	70 (91%)	7 (9%)	0	100	100
5	F	464/522 (89%)	415 (89%)	48 (10%)	1 (0%)	52	86
5	L	463/522 (89%)	415 (90%)	47 (10%)	1 (0%)	52	86
6	M	49/64 (77%)	42 (86%)	7 (14%)	0	100	100
6	N	49/64 (77%)	42 (86%)	7 (14%)	0	100	100
All	All	7398/7808 (95%)	6685 (90%)	691 (9%)	22 (0%)	46	82

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	170	VAL
2	I	170	VAL
3	D	340	GLN
1	G	167	PRO
2	I	484	LEU
1	A	14	VAL
1	A	167	PRO
1	A	196	THR
2	C	63	SER
2	C	697	LYS
1	G	14	VAL
1	G	196	THR
2	I	63	SER
2	I	697	LYS
5	F	447	ALA
5	L	447	ALA

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Mol	Chain	Res	Type
2	C	1186	VAL
2	I	1186	VAL
1	A	178	SER
3	D	826	ILE
1	G	178	SER
3	J	826	ILE

### 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	191/206 (93%)	180 (94%)	11 (6%)	25	64
1	B	184/206 (89%)	167 (91%)	17 (9%)	11	46
1	G	191/206 (93%)	180 (94%)	11 (6%)	25	64
1	H	183/206 (89%)	166 (91%)	17 (9%)	11	46
2	C	1155/1157 (100%)	1052 (91%)	103 (9%)	12	48
2	I	1154/1157 (100%)	1056 (92%)	98 (8%)	13	51
3	D	1125/1168 (96%)	1036 (92%)	89 (8%)	15	54
3	J	1110/1168 (95%)	1023 (92%)	87 (8%)	16	54
4	E	72/75 (96%)	69 (96%)	3 (4%)	36	72
4	K	67/75 (89%)	65 (97%)	2 (3%)	48	79
5	F	417/462 (90%)	383 (92%)	34 (8%)	14	52
5	L	418/462 (90%)	386 (92%)	32 (8%)	16	55
6	M	44/56 (79%)	38 (86%)	6 (14%)	5	29
6	N	44/56 (79%)	38 (86%)	6 (14%)	5	29
All	All	6355/6660 (95%)	5839 (92%)	516 (8%)	15	53

All (516) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU

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Mol	Chain	Res	Type
1	A	13	LEU
1	A	22	THR
1	A	54	CYS
1	A	71	LYS
1	A	120	ASP
1	A	127	GLN
1	A	141	SER
1	A	145	LYS
1	A	215	GLU
1	A	231	PHE
1	B	8	PHE
1	B	45	ARG
1	B	50	SER
1	B	58	GLU
1	B	60	GLU
1	B	65	LEU
1	B	75	GLN
1	B	76	GLU
1	B	77	ASP
1	B	120	ASP
1	B	133	LEU
1	B	134	THR
1	B	142	MET
1	B	158	ARG
1	B	160	HIS
1	B	176	CYS
1	B	183	ILE
2	C	29	SER
2	C	32	LEU
2	C	44	GLU
2	C	46	GLN
2	C	49	LEU
2	C	60	GLN
2	C	90	VAL
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	119	GLU
2	C	124	MET
2	C	132	ASP
2	C	149	LEU
2	C	164	THR

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Mol	Chain	Res	Type
2	C	165	HIS
2	C	185	ASP
2	C	197	ARG
2	C	200	ARG
2	C	237	LEU
2	C	244	GLU
2	C	268	ARG
2	C	285	ILE
2	C	322	LEU
2	C	327	GLN
2	C	331	LYS
2	C	369	MET
2	C	410	LEU
2	C	443	ASP
2	C	446	ASP
2	C	483	ASP
2	C	484	LEU
2	C	490	GLN
2	C	493	ILE
2	C	496	LYS
2	C	518	ASN
2	C	538	LEU
2	C	539	THR
2	C	542	ARG
2	C	561	ILE
2	C	568	ASN
2	C	573	ASN
2	C	589	THR
2	C	600	THR
2	C	604	HIS
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU
2	C	635	THR
2	C	657	THR
2	C	659	GLN
2	C	672	GLU
2	C	684	ASN
2	C	692	THR
2	C	699	LEU
2	C	705	GLU

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Mol	Chain	Res	Type
2	C	737	ASN
2	C	739	ASP
2	C	748	ILE
2	C	761	GLN
2	C	779	ARG
2	C	781	ASP
2	C	782	VAL
2	C	788	SER
2	C	799	ASN
2	C	814	ASP
2	C	828	PHE
2	C	831	ILE
2	C	839	VAL
2	C	878	THR
2	C	890	LYS
2	C	895	LEU
2	C	898	GLU
2	C	919	ARG
2	C	942	ASP
2	C	974	ARG
2	C	976	ARG
2	C	992	LEU
2	C	995	ASP
2	C	998	LEU
2	C	1004	ASP
2	C	1006	GLU
2	C	1019	ASP
2	C	1080	ASN
2	C	1082	ILE
2	C	1083	GLU
2	C	1090	ASN
2	C	1108	ASN
2	C	1119	MET
2	C	1155	VAL
2	C	1164	PHE
2	C	1171	ARG
2	C	1180	MET
2	C	1198	LEU
2	C	1222	GLU
2	C	1233	LEU
2	C	1248	THR
2	C	1279	GLU

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Mol	Chain	Res	Type
2	C	1291	LEU
2	C	1339	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	33	TRP
3	D	42	GLU
3	D	46	TYR
3	D	70	CYS
3	D	79	LYS
3	D	92	VAL
3	D	126	LEU
3	D	128	LEU
3	D	134	ASP
3	D	175	GLU
3	D	176	PHE
3	D	209	ASN
3	D	217	LEU
3	D	252	LEU
3	D	255	LEU
3	D	264	ASP
3	D	299	LEU
3	D	319	SER
3	D	324	LEU
3	D	339	ARG
3	D	363	LEU
3	D	374	LEU
3	D	425	ARG
3	D	431	ARG
3	D	448	GLN
3	D	454	CYS
3	D	472	LEU
3	D	487	THR
3	D	506	VAL
3	D	514	THR
3	D	517	CYS
3	D	528	THR
3	D	545	HIS
3	D	547	ARG
3	D	558	ASP
3	D	594	GLN
3	D	596	LEU

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Mol	Chain	Res	Type
3	D	635	SER
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	678	ARG
3	D	686	TRP
3	D	697	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	731	ARG
3	D	746	LEU
3	D	769	VAL
3	D	772	TYR
3	D	785	ASP
3	D	805	GLN
3	D	810	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	908	ILE
3	D	929	GLN
3	D	962	ASN
3	D	972	LYS
3	D	987	GLU
3	D	1017	VAL
3	D	1047	THR
3	D	1162	ILE
3	D	1173	ARG
3	D	1177	ILE
3	D	1183	SER
3	D	1192	LYS
3	D	1199	PHE
3	D	1204	VAL
3	D	1208	ASP
3	D	1230	THR
3	D	1239	ASP

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Mol	Chain	Res	Type
3	D	1255	VAL
3	D	1258	ARG
3	D	1275	LEU
3	D	1284	ARG
3	D	1285	VAL
3	D	1293	GLU
3	D	1306	LEU
3	D	1333	THR
3	D	1366	HIS
4	E	16	ARG
4	E	39	VAL
4	E	58	LEU
5	F	94	THR
5	F	98	VAL
5	F	100	MET
5	F	105	MET
5	F	127	ILE
5	F	130	VAL
5	F	137	TYR
5	F	154	GLU
5	F	221	PHE
5	F	244	THR
5	F	246	GLN
5	F	253	SER
5	F	335	GLU
5	F	395	THR
5	F	401	PHE
5	F	428	SER
5	F	456	MET
5	F	459	THR
5	F	466	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	483	LEU
5	F	486	ARG
5	F	488	LEU
5	F	505	ILE
5	F	508	GLU
5	F	530	LEU
5	F	540	LEU
5	F	574	GLU

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Mol	Chain	Res	Type
5	F	580	PHE
5	F	583	THR
5	F	586	ARG
5	F	611	LEU
1	G	9	LEU
1	G	13	LEU
1	G	22	THR
1	G	54	CYS
1	G	71	LYS
1	G	120	ASP
1	G	127	GLN
1	G	141	SER
1	G	145	LYS
1	G	215	GLU
1	G	231	PHE
1	H	7	GLU
1	H	8	PHE
1	H	45	ARG
1	H	50	SER
1	H	58	GLU
1	H	60	GLU
1	H	65	LEU
1	H	75	GLN
1	H	76	GLU
1	H	77	ASP
1	H	120	ASP
1	H	133	LEU
1	H	134	THR
1	H	142	MET
1	H	158	ARG
1	H	176	CYS
1	H	183	ILE
2	I	29	SER
2	I	32	LEU
2	I	44	GLU
2	I	46	GLN
2	I	49	LEU
2	I	60	GLN
2	I	90	VAL
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE

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Mol	Chain	Res	Type
2	I	119	GLU
2	I	124	MET
2	I	132	ASP
2	I	149	LEU
2	I	164	THR
2	I	165	HIS
2	I	185	ASP
2	I	197	ARG
2	I	200	ARG
2	I	237	LEU
2	I	244	GLU
2	I	268	ARG
2	I	285	ILE
2	I	322	LEU
2	I	327	GLN
2	I	331	LYS
2	I	369	MET
2	I	377	THR
2	I	410	LEU
2	I	443	ASP
2	I	446	ASP
2	I	483	ASP
2	I	484	LEU
2	I	490	GLN
2	I	493	ILE
2	I	496	LYS
2	I	518	ASN
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
2	I	561	ILE
2	I	568	ASN
2	I	573	ASN
2	I	589	THR
2	I	600	THR
2	I	604	HIS
2	I	615	VAL
2	I	623	LEU
2	I	633	LEU
2	I	635	THR
2	I	657	THR
2	I	659	GLN

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Mol	Chain	Res	Type
2	I	672	GLU
2	I	684	ASN
2	I	692	THR
2	I	699	LEU
2	I	705	GLU
2	I	737	ASN
2	I	739	ASP
2	I	748	ILE
2	I	761	GLN
2	I	779	ARG
2	I	781	ASP
2	I	782	VAL
2	I	788	SER
2	I	799	ASN
2	I	814	ASP
2	I	828	PHE
2	I	831	ILE
2	I	839	VAL
2	I	878	THR
2	I	890	LYS
2	I	895	LEU
2	I	898	GLU
2	I	919	ARG
2	I	942	ASP
2	I	971	LEU
2	I	972	PHE
2	I	1029	LEU
2	I	1080	ASN
2	I	1082	ILE
2	I	1083	GLU
2	I	1090	ASN
2	I	1108	ASN
2	I	1119	MET
2	I	1155	VAL
2	I	1164	PHE
2	I	1171	ARG
2	I	1180	MET
2	I	1198	LEU
2	I	1222	GLU
2	I	1233	LEU
2	I	1248	THR
2	I	1279	GLU

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Mol	Chain	Res	Type
2	I	1291	LEU
2	I	1339	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	33	TRP
3	J	42	GLU
3	J	46	TYR
3	J	70	CYS
3	J	79	LYS
3	J	92	VAL
3	J	126	LEU
3	J	128	LEU
3	J	134	ASP
3	J	175	GLU
3	J	176	PHE
3	J	209	ASN
3	J	217	LEU
3	J	252	LEU
3	J	255	LEU
3	J	264	ASP
3	J	299	LEU
3	J	319	SER
3	J	324	LEU
3	J	363	LEU
3	J	374	LEU
3	J	425	ARG
3	J	431	ARG
3	J	448	GLN
3	J	454	CYS
3	J	472	LEU
3	J	487	THR
3	J	506	VAL
3	J	514	THR
3	J	517	CYS
3	J	528	THR
3	J	545	HIS
3	J	547	ARG
3	J	558	ASP
3	J	594	GLN
3	J	596	LEU
3	J	635	SER
3	J	641	ILE

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Mol	Chain	Res	Type
3	J	646	ILE
3	J	660	GLU
3	J	678	ARG
3	J	686	TRP
3	J	697	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	731	ARG
3	J	746	LEU
3	J	769	VAL
3	J	772	TYR
3	J	785	ASP
3	J	805	GLN
3	J	810	THR
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	908	ILE
3	J	929	GLN
3	J	962	ASN
3	J	972	LYS
3	J	987	GLU
3	J	1017	VAL
3	J	1025	MET
3	J	1047	THR
3	J	1162	ILE
3	J	1173	ARG
3	J	1177	ILE
3	J	1192	LYS
3	J	1199	PHE
3	J	1204	VAL
3	J	1208	ASP
3	J	1230	THR
3	J	1239	ASP
3	J	1255	VAL
3	J	1258	ARG

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Mol	Chain	Res	Type
3	J	1275	LEU
3	J	1284	ARG
3	J	1285	VAL
3	J	1293	GLU
3	J	1306	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	39	VAL
4	K	58	LEU
5	L	94	THR
5	L	98	VAL
5	L	100	MET
5	L	105	MET
5	L	130	VAL
5	L	137	TYR
5	L	154	GLU
5	L	221	PHE
5	L	244	THR
5	L	246	GLN
5	L	253	SER
5	L	335	GLU
5	L	395	THR
5	L	401	PHE
5	L	428	SER
5	L	456	MET
5	L	459	THR
5	L	466	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	483	LEU
5	L	486	ARG
5	L	488	LEU
5	L	505	ILE
5	L	508	GLU
5	L	530	LEU
5	L	540	LEU
5	L	574	GLU
5	L	583	THR
5	L	586	ARG
5	L	611	LEU
6	M	24	GLU

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Mol	Chain	Res	Type
6	M	25	HIS
6	M	27	PHE
6	M	29	VAL
6	M	37	ASP
6	M	61	VAL
6	N	24	GLU
6	N	25	HIS
6	N	27	PHE
6	N	29	VAL
6	N	37	ASP
6	N	61	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	686	GLN
2	C	1257	GLN
3	D	206	ASN
5	F	446	GLN
2	I	686	GLN
3	J	206	ASN
5	L	446	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	224/239 (93%)	0.08	5 (2%) 65 54	48, 85, 138, 169	0
1	B	220/239 (92%)	0.39	15 (6%) 20 13	46, 110, 148, 166	0
1	G	228/239 (95%)	0.10	12 (5%) 30 22	48, 94, 141, 167	0
1	H	217/239 (90%)	0.36	14 (6%) 22 14	48, 111, 150, 167	0
2	C	1340/1342 (99%)	-0.05	36 (2%) 58 46	12, 74, 129, 163	0
2	I	1340/1342 (99%)	0.06	58 (4%) 39 28	12, 78, 143, 189	0
3	D	1345/1407 (95%)	-0.05	30 (2%) 65 54	13, 61, 142, 194	0
3	J	1325/1407 (94%)	-0.11	19 (1%) 78 68	10, 63, 139, 195	0
4	E	89/91 (97%)	-0.19	0 100 100	30, 77, 122, 138	0
4	K	79/91 (86%)	-0.26	0 100 100	32, 76, 121, 164	0
5	F	470/522 (90%)	-0.14	9 (1%) 70 59	25, 98, 147, 179	0
5	L	469/522 (89%)	-0.13	9 (1%) 70 59	28, 96, 150, 181	0
6	M	51/64 (79%)	0.56	2 (3%) 43 32	66, 115, 146, 158	0
6	N	51/64 (79%)	0.34	3 (5%) 26 17	64, 112, 143, 149	0
All	All	7448/7808 (95%)	-0.02	212 (2%) 56 44	10, 79, 142, 195	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.3
2	I	981	ALA	8.0
3	J	1059	LEU	6.4
2	I	995	ASP	5.7
1	B	146	VAL	5.6
2	I	985	GLU	5.3
5	F	167	ASP	5.1
2	C	258	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
2	I	967	LEU	4.8
1	G	95	LYS	4.7
2	I	1018	TYR	4.5
2	C	165	HIS	4.4
1	H	146	VAL	4.4
1	B	8	PHE	4.3
5	L	167	ASP	4.3
2	I	1002	LEU	4.2
2	I	972	PHE	4.2
2	I	971	LEU	4.2
2	I	977	ALA	4.2
2	I	1022	LYS	4.2
1	B	121	VAL	4.2
5	L	165	PHE	4.1
2	I	968	GLU	4.1
5	L	287	ILE	4.0
1	A	193	GLU	4.0
1	B	120	ASP	4.0
5	F	603	ARG	3.8
2	C	251	ALA	3.8
5	F	165	PHE	3.8
3	J	1080	ILE	3.8
2	I	998	LEU	3.8
2	I	970	GLY	3.8
2	I	973	SER	3.8
1	H	96	ASP	3.7
2	C	489	PRO	3.7
2	I	1021	LEU	3.7
5	L	294	GLN	3.6
3	D	1054	THR	3.6
1	B	92	VAL	3.6
1	G	97	GLU	3.6
3	D	952	VAL	3.6
5	L	480	PRO	3.6
2	I	975	ILE	3.5
2	C	332	ARG	3.5
2	C	231	GLU	3.5
2	I	867	GLU	3.4
3	D	1065	ALA	3.4
2	I	996	ARG	3.4
1	H	72	GLU	3.4
1	H	97	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
3	J	1054	THR	3.4
2	C	282	VAL	3.3
2	C	333	ILE	3.3
1	G	96	ASP	3.3
5	L	290	LEU	3.3
2	I	168	GLY	3.3
5	F	579	GLN	3.2
1	H	172	LEU	3.2
5	L	326	TRP	3.2
2	I	1017	GLN	3.1
3	J	1273	ASP	3.1
2	C	252	SER	3.1
3	J	201	LEU	3.0
1	H	12	ARG	3.0
3	J	1035	VAL	3.0
1	B	90	VAL	3.0
2	C	237	LEU	2.9
1	A	90	VAL	2.9
2	C	184	LEU	2.9
2	I	988	LYS	2.9
3	D	1064	SER	2.9
1	B	145	LYS	2.9
3	D	1168	GLU	2.9
3	D	1039	ASP	2.9
5	L	286	LEU	2.9
2	I	974	ARG	2.9
2	I	969	ALA	2.8
3	D	958	ILE	2.8
2	C	277	LEU	2.8
3	D	993	GLU	2.8
2	I	492	MET	2.8
2	C	261	VAL	2.8
3	J	1181	ASP	2.8
1	A	194	GLN	2.8
2	I	882	ILE	2.8
3	D	965	SER	2.8
1	B	30	PRO	2.8
1	H	55	ALA	2.8
3	J	1114	GLN	2.8
2	I	989	LEU	2.7
3	J	1034	PHE	2.7
6	N	63	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	I	725	GLN	2.7
1	H	123	ILE	2.7
2	I	984	VAL	2.7
3	J	319	SER	2.7
2	C	266	GLY	2.7
2	I	169	LYS	2.7
2	C	240	GLU	2.7
2	C	331	LYS	2.7
1	H	92	VAL	2.7
1	H	158	ARG	2.7
3	D	712	GLN	2.7
2	I	857	VAL	2.7
2	I	629	PHE	2.7
2	C	479	LEU	2.6
3	J	1079	LYS	2.6
2	I	1004	ASP	2.6
2	I	980	VAL	2.6
2	I	1014	LEU	2.6
2	C	997	TRP	2.6
2	C	102	LEU	2.6
2	C	253	PHE	2.6
2	I	165	HIS	2.6
2	I	251	ALA	2.6
1	B	9	LEU	2.5
2	I	1003	THR	2.5
3	D	1055	GLY	2.5
2	I	167	SER	2.5
2	I	1001	GLY	2.5
2	I	1023	HIS	2.5
3	D	1015	GLU	2.5
3	D	1007	ASP	2.5
2	I	332	ARG	2.5
2	I	236	LYS	2.5
3	D	826	ILE	2.5
2	C	230	PHE	2.5
1	G	28	LEU	2.4
1	H	106	GLY	2.4
2	C	255	ILE	2.4
3	D	1006	GLY	2.4
1	G	127	GLN	2.4
3	D	1012	ALA	2.4
1	B	144	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
6	M	31	ILE	2.4
1	G	193	GLU	2.4
3	D	1013	GLY	2.4
1	B	67	GLU	2.4
3	D	89	GLY	2.4
2	C	265	LYS	2.4
1	G	194	GLN	2.4
2	C	485	ASP	2.4
2	I	1006	GLU	2.4
2	I	861	ALA	2.3
1	H	147	GLN	2.3
2	I	735	LYS	2.3
3	J	712	GLN	2.3
2	C	319	LEU	2.3
5	F	111	LEU	2.3
2	I	230	PHE	2.3
3	J	708	ASN	2.3
2	I	720	ARG	2.3
1	H	13	LEU	2.2
3	D	524	GLY	2.2
2	I	1000	LEU	2.2
6	N	52	PHE	2.2
3	J	518	VAL	2.2
3	D	1014	GLY	2.2
6	N	31	ILE	2.2
3	J	1109	LEU	2.2
1	A	52	PRO	2.2
3	D	995	TYR	2.2
2	C	256	GLU	2.2
1	A	98	VAL	2.2
2	I	203	LYS	2.2
2	I	1149	TYR	2.2
2	C	370	MET	2.2
1	B	31	LEU	2.2
1	H	65	LEU	2.2
2	I	632	ASP	2.2
2	I	263	VAL	2.2
2	C	234	ASP	2.2
5	F	480	PRO	2.2
1	G	19	VAL	2.2
5	F	164	GLY	2.2
2	C	239	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	939	VAL	2.1
2	I	983	GLY	2.1
3	D	950	ILE	2.1
5	F	166	VAL	2.1
1	B	205	MET	2.1
2	C	1000	LEU	2.1
1	G	214	GLU	2.1
2	C	264	GLU	2.1
3	D	982	LEU	2.1
3	J	849	LEU	2.1
2	C	257	ALA	2.1
3	J	1186	TYR	2.1
2	I	862	LEU	2.1
3	J	1106	ILE	2.1
3	D	1042	ASP	2.1
1	G	24	ALA	2.1
2	I	333	ILE	2.1
2	C	163	LYS	2.1
5	L	598	LEU	2.1
3	D	966	VAL	2.1
3	D	1104	LYS	2.1
3	D	1169	THR	2.0
1	B	61	ILE	2.0
3	D	1072	LYS	2.0
1	G	126	PRO	2.0
2	C	492	MET	2.0
6	M	26	SER	2.0
3	D	1051	ASP	2.0
3	J	1056	LEU	2.0
1	G	90	VAL	2.0
2	I	170	VAL	2.0
1	B	29	GLU	2.0
2	C	287	VAL	2.0
5	F	581	ASP	2.0
2	I	237	LEU	2.0
3	D	960	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	D	1503	1/1	0.99	0.21	-0.40	36,36,36,36	0
8	ZN	J	1503	1/1	1.00	0.15	-0.40	23,23,23,23	0
8	ZN	D	1502	1/1	0.90	0.18	-0.82	193,193,193,193	0
8	ZN	J	1502	1/1	0.98	0.06	-1.51	71,71,71,71	0
7	MG	J	1501	1/1	0.81	0.36	-	40,40,40,40	0
7	MG	D	1501	1/1	0.70	0.44	-	41,41,41,41	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.