



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:31 am BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

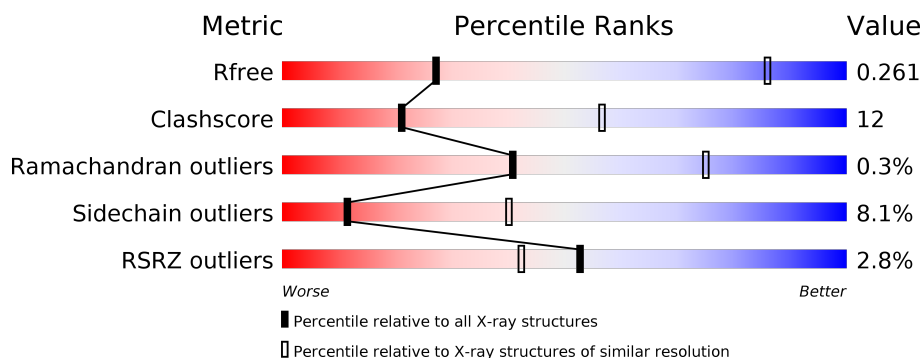
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	239	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>32%</div> <div>6%</div> </div> </div>
1	B	239	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>8%</div> </div> </div>
1	G	239	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>5%</div> </div> </div>
1	H	239	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>27%</div> <div>9%</div> </div> </div>
2	C	1342	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div></div> </div> </div>
2	I	1342	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div></div> </div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	D	1501	-	-	-	X

## 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 1	Mg 1	0	0
7	D	1	Total 1	Mg 1	0	0

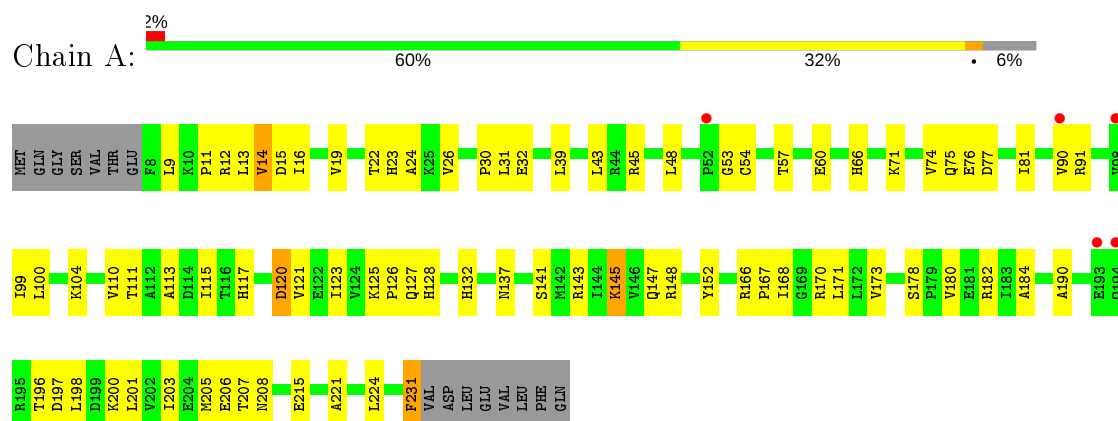
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

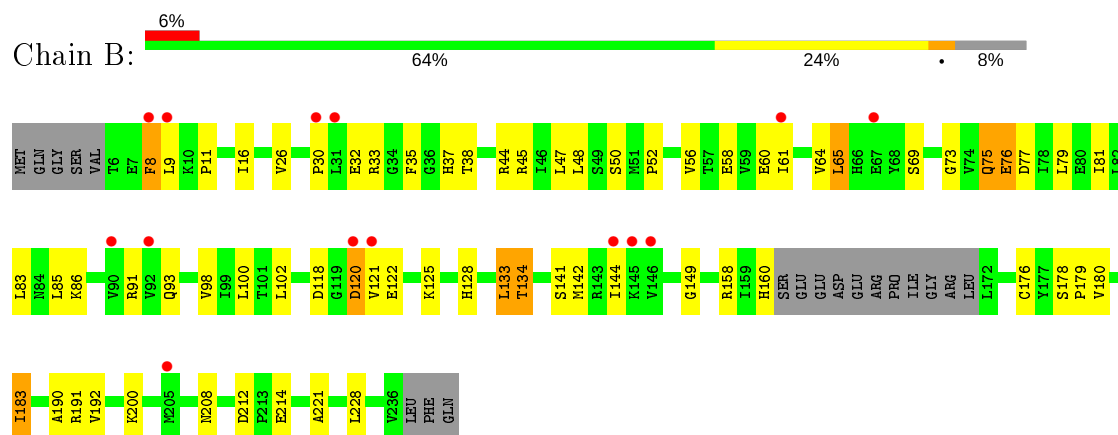
### 3 Residue-property plots [i](#)

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

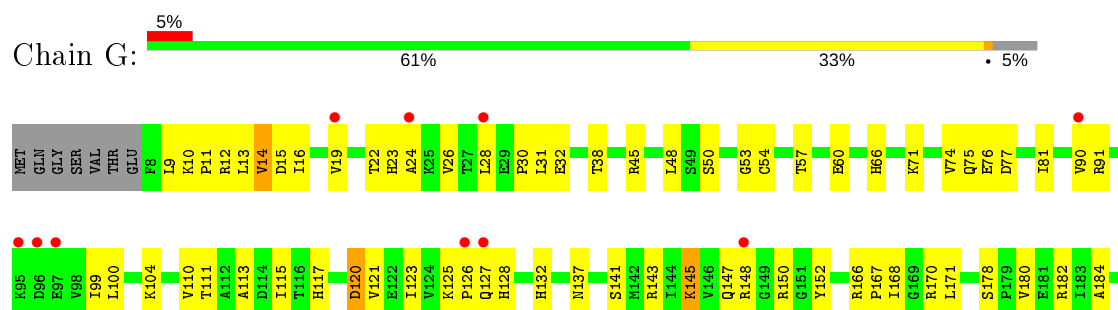
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



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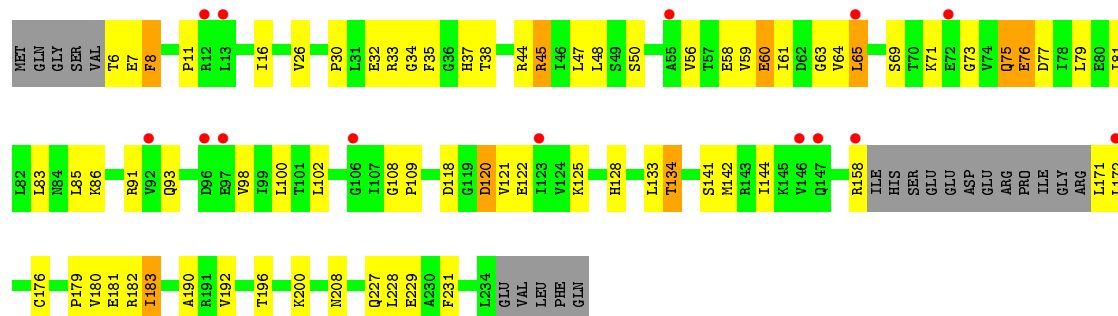


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

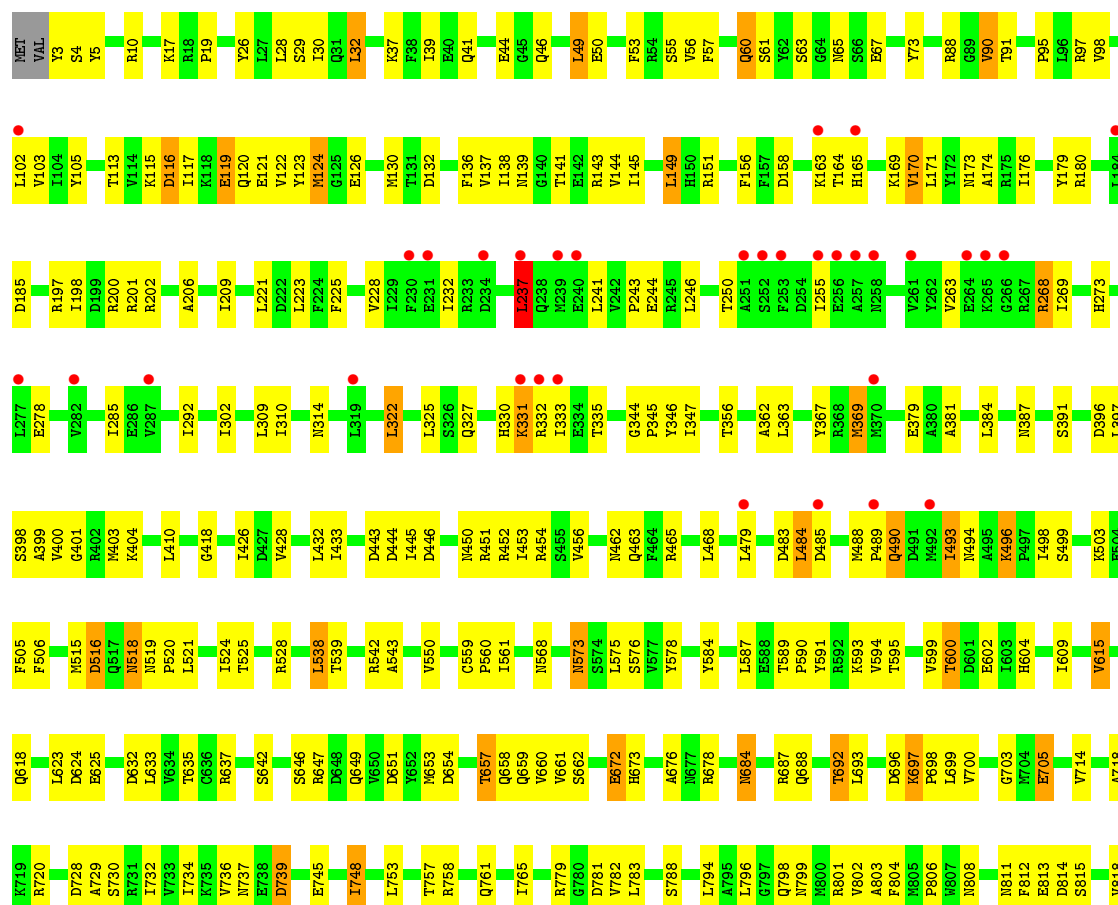


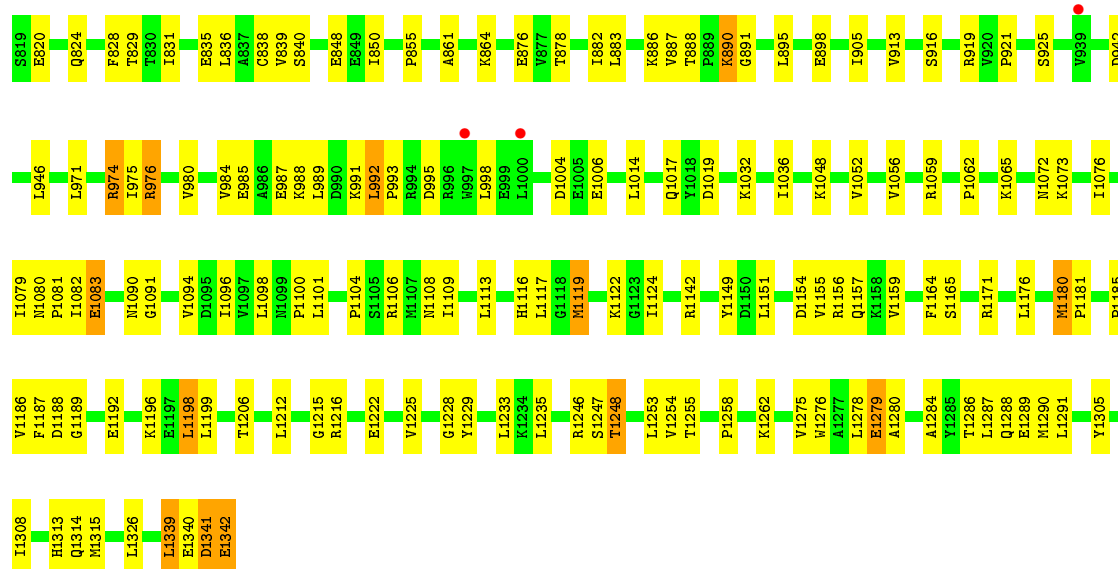


• Molecule 1: DNA-directed RNA polymerase subunit alpha

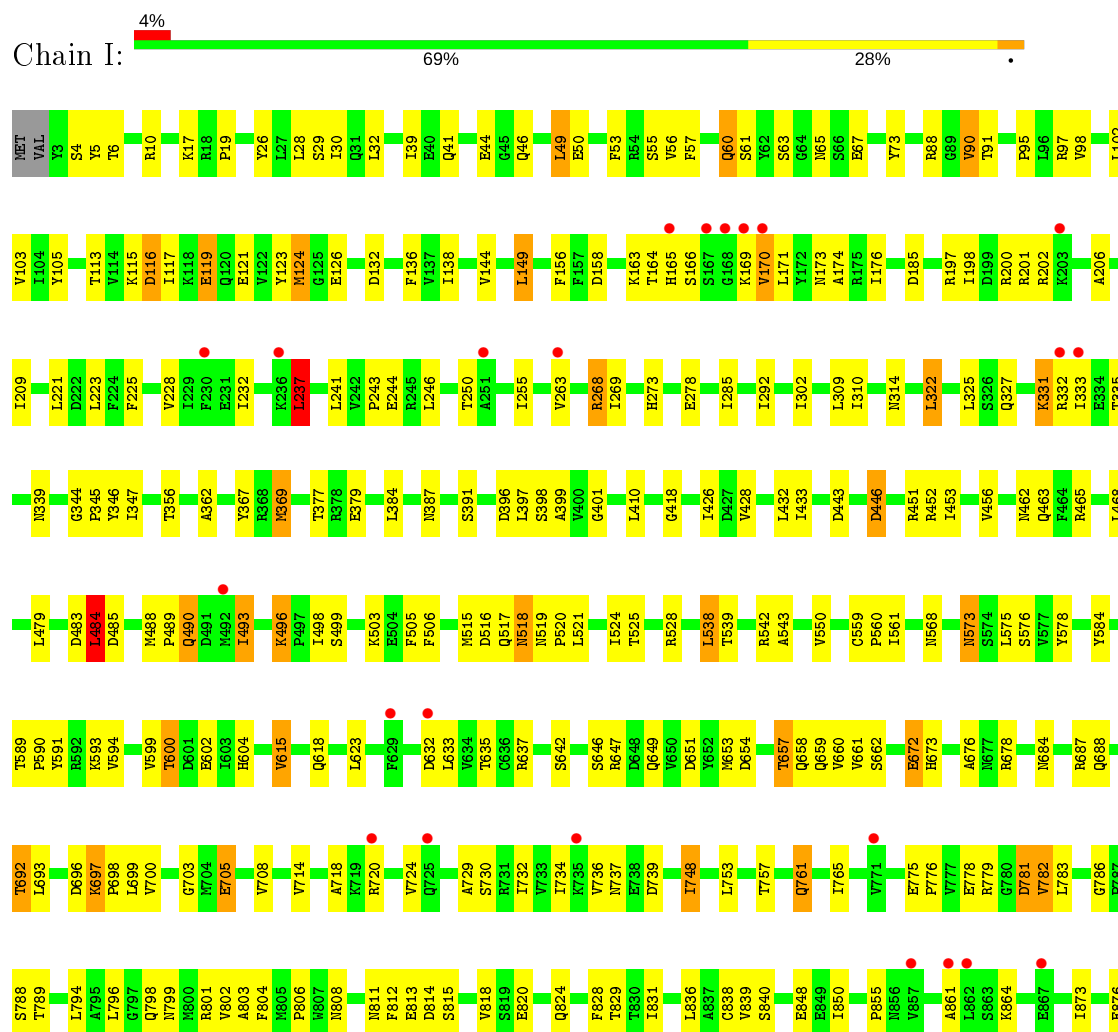


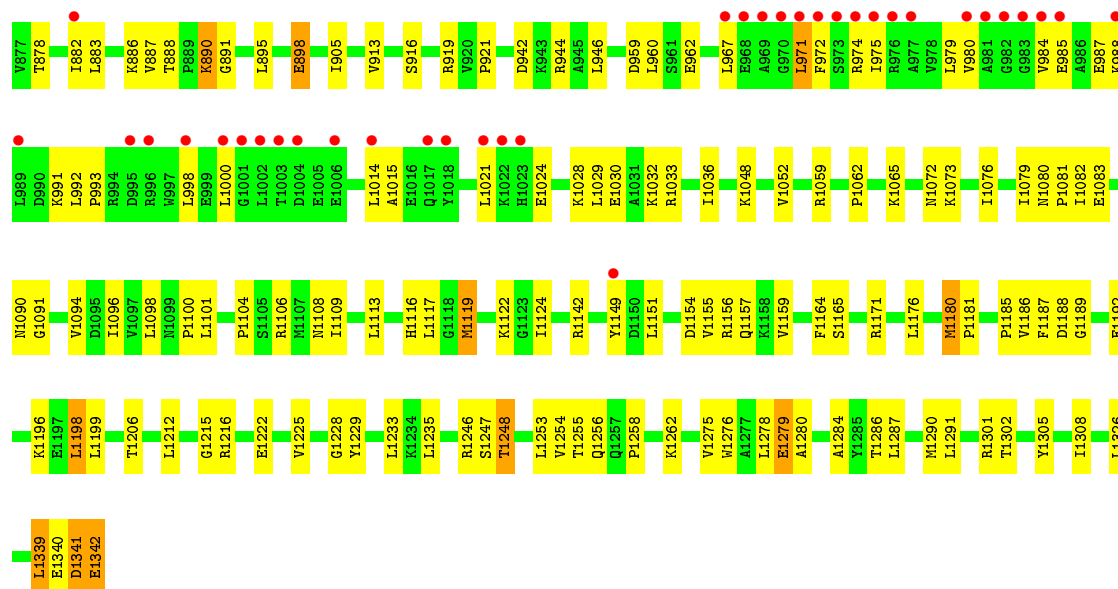
• Molecule 2: DNA-directed RNA polymerase subunit beta



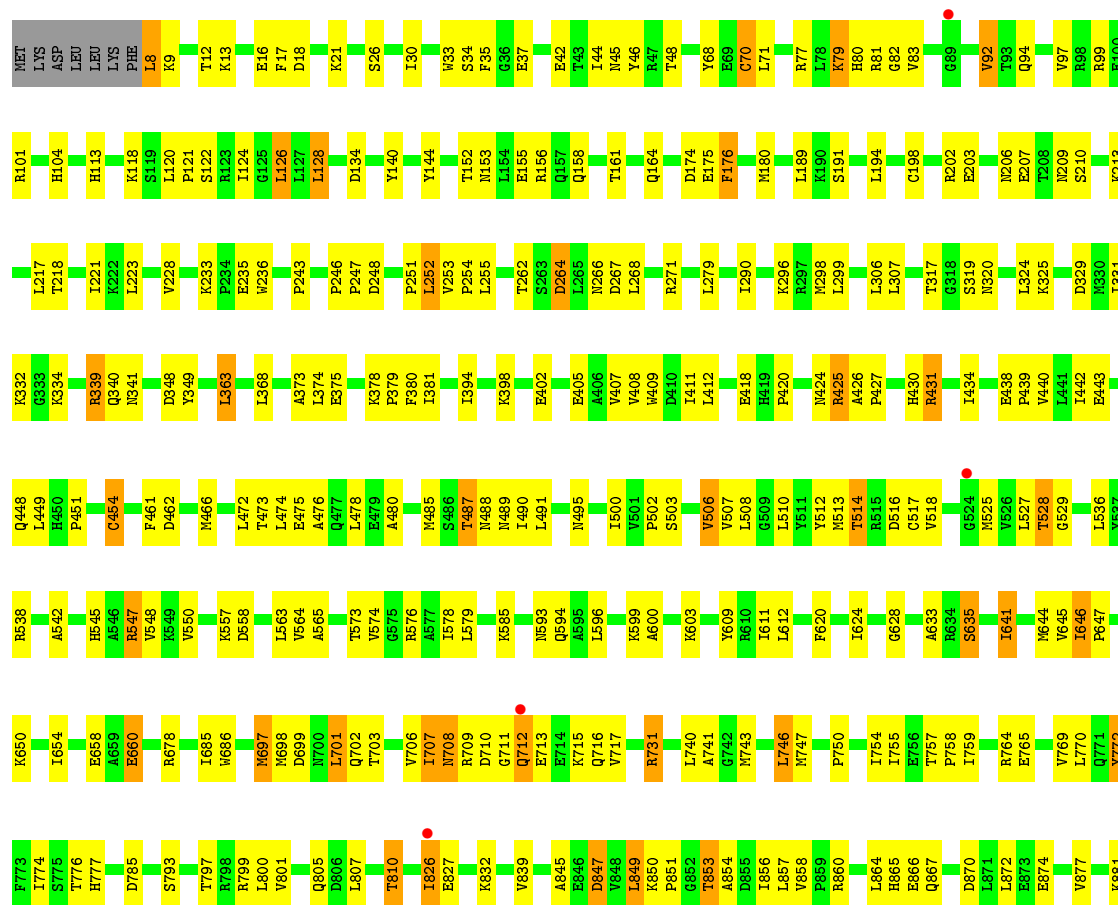


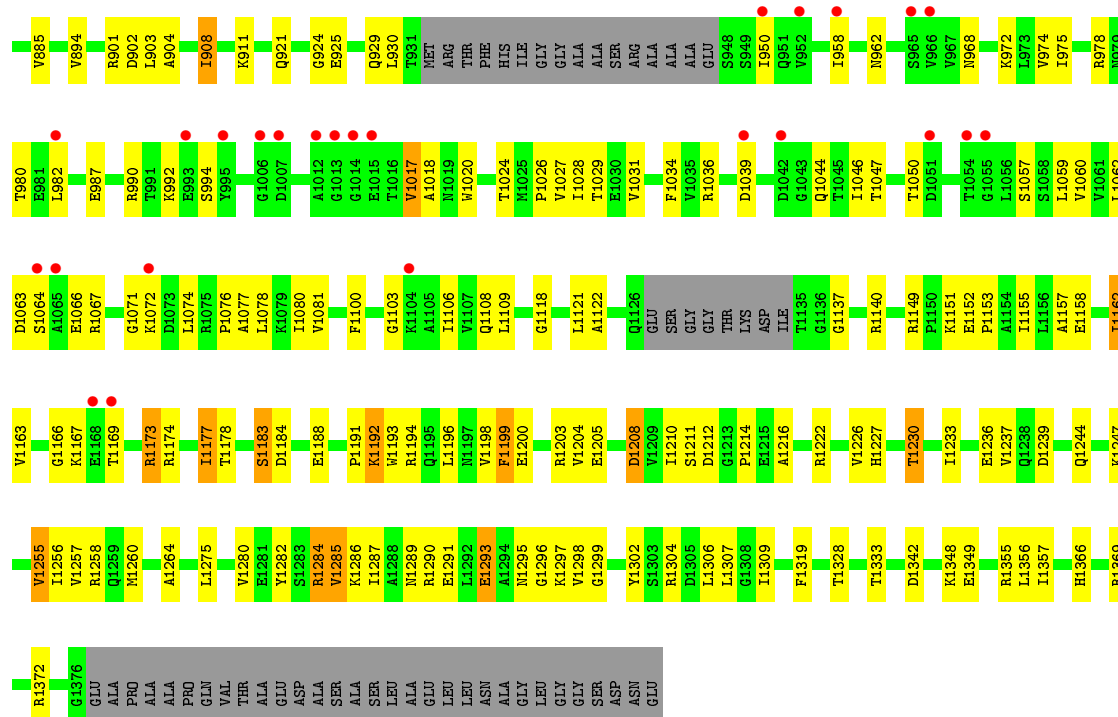
• Molecule 2: DNA-directed RNA polymerase subunit beta



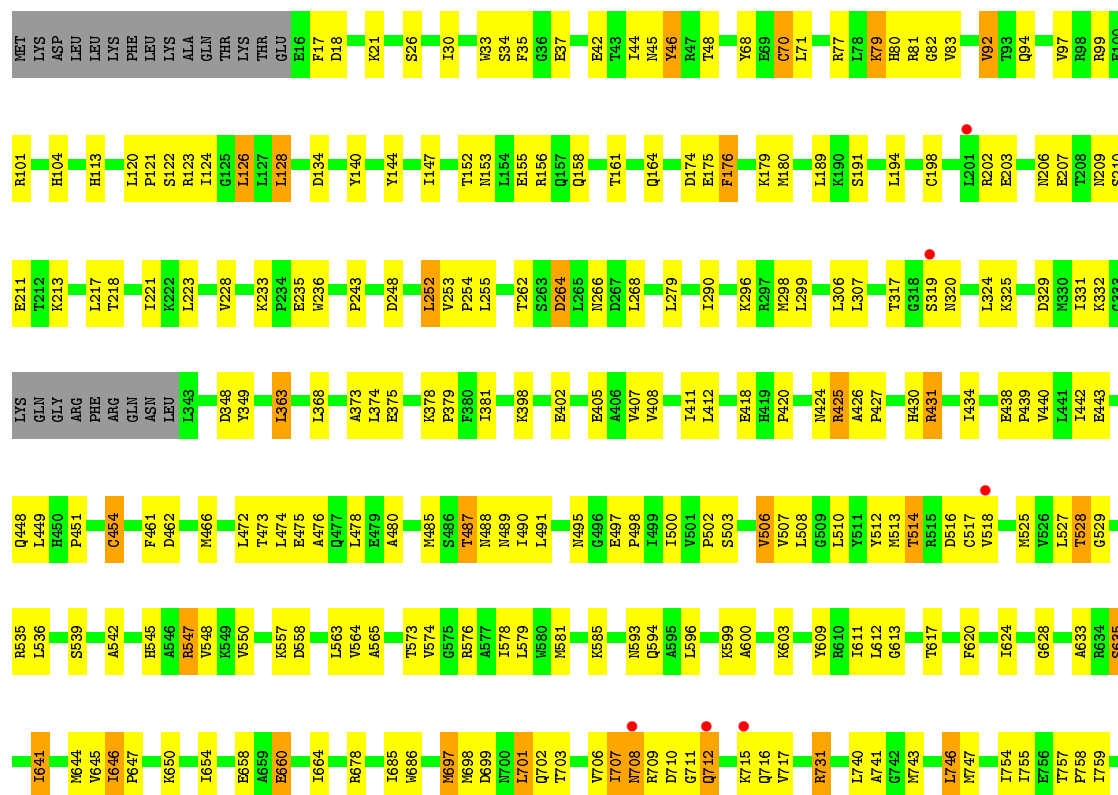


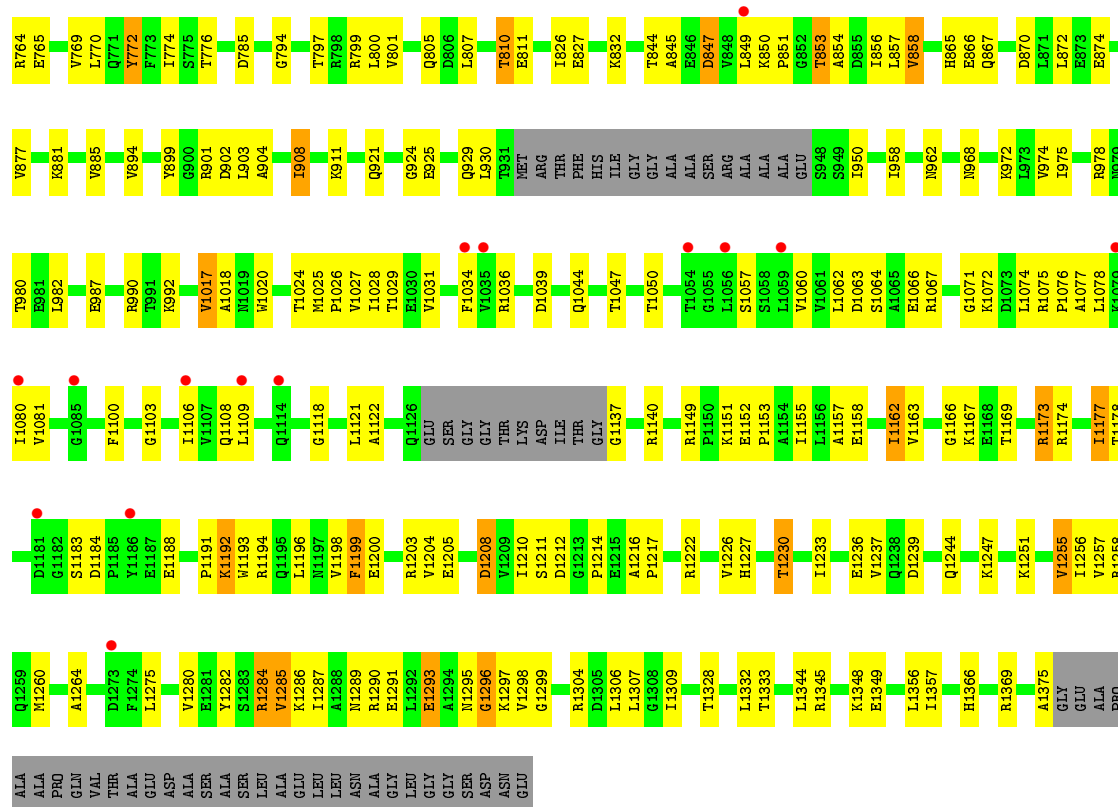
• Molecule 3: DNA-directed RNA polymerase subunit beta'



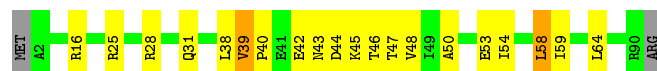
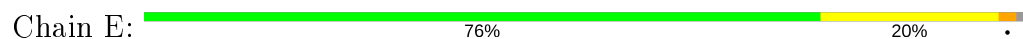


• Molecule 3: DNA-directed RNA polymerase subunit beta'

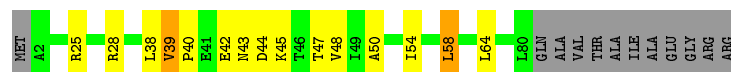




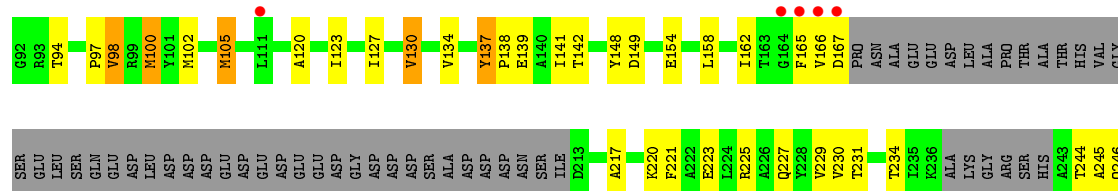
- Molecule 4: DNA-directed RNA polymerase subunit omega

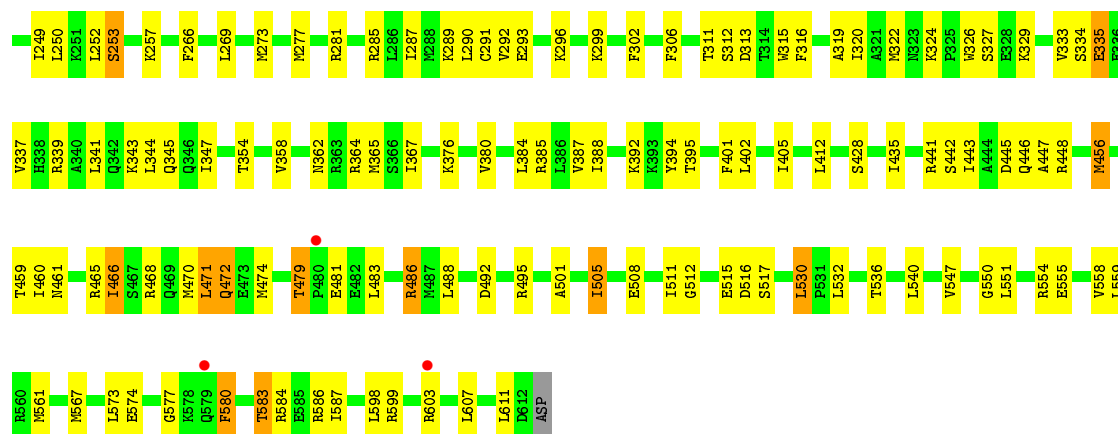


- Molecule 4: DNA-directed RNA polymerase subunit omega

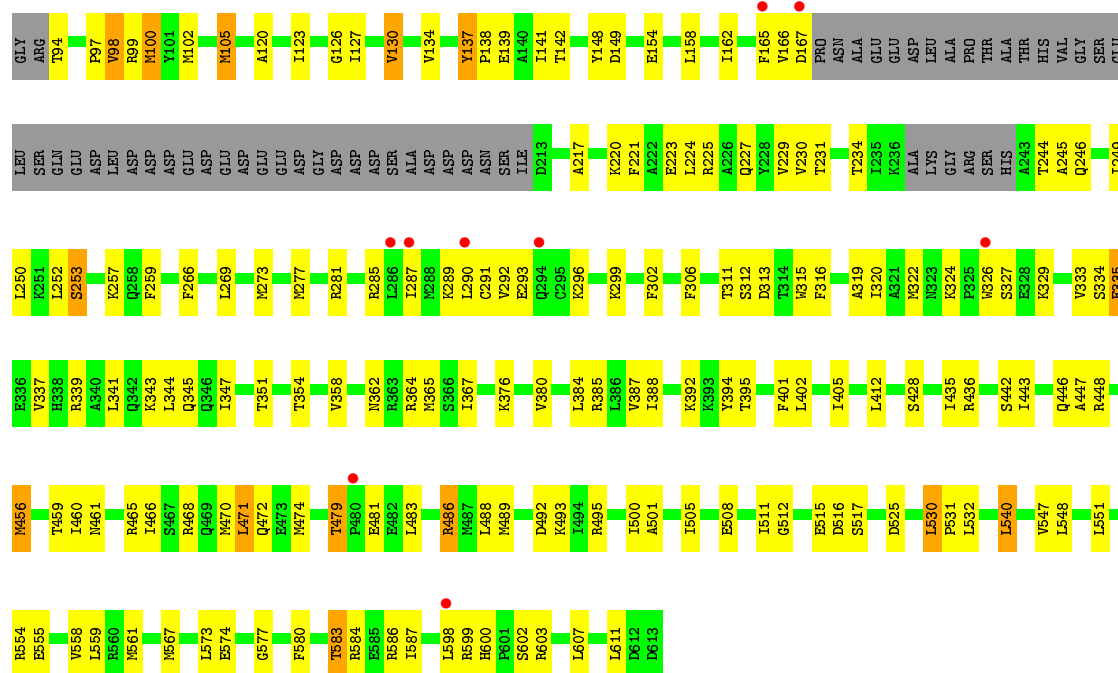


- Molecule 5: RNA polymerase sigma factor RpoD

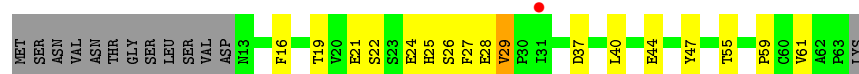




• Molecule 5: RNA polymerase sigma factor RpoD



• 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, $\alpha$ , $\beta$ , $\gamma$	186.36 Å   206.28 Å   308.00 Å 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 3.87 Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.219   ,   0.260 0.220   ,   0.261	Depositor DCC
$R_{free}$ test set	5023 reflections (5.03%)	wwPDB-VP
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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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( $^{\circ}$ )	Ideal( $^{\circ}$ )
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
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.66	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
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
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.68	0.74
5:F:515:GLU:HG2	5:F:516:ASP:H	1.52	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
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.73	0.69
3:D:152:THR:OG1	3:D:153:ASN:N	2.24	0.69
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.74	0.69
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.74	0.69
2:I:166:SER:HA	6:N:23:SER:HB3	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
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.76	0.67
3:J:489:ASN:HA	3:J:904:ALA:HB1	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
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.60	0.66
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.60	0.66
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.28	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
5:F:561:MET:HA	5:F:567:MET:HE1	1.78	0.66
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.79	0.65
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.77	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
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.60	0.65
2:I:292:ILE:HD12	2:I:322:LEU:HD11	1.78	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
3:D:885:VAL:HG21	3:D:1255:VAL:HG12	1.80	0.64
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.79	0.64
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.78	0.64
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.31	0.64
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.80	0.64
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.80	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
5:L:126:GLY:O	5:L:130:VAL:HG13	1.97	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:485:MET:HG3	3:D:487:THR:HG23	1.80	0.63
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.80	0.63
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.79	0.63
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.31	0.63
3:D:510:LEU:O	3:D:514:THR:OG1	2.16	0.63
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.80	0.63
3:J:1264:ALA:HB2	3:J:1280:VAL:CG2	2.29	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:485:MET:HG3	3:J:487:THR:HG23	1.81	0.62
3:J:557:LYS:HA	3:J:563:LEU:HA	1.78	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
1:A:12:ARG:H	1:A:30:PRO:HD2	1.64	0.62
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.80	0.62
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.65	0.62
1:G:166:ARG:O	1:G:168:ILE:N	2.33	0.62
2:C:237:LEU:H	2:C:237:LEU:HD22	1.64	0.62
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.82	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
3:D:1297:LYS:HG3	3:D:1299:GLY:H	1.65	0.61
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.83	0.61
5:F:583:THR:HG22	5:F:584:ARG:H	1.64	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
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
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.82	0.61
1:G:45:ARG:HG2	1:H:38:THR:HB	1.82	0.61
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.82	0.61
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.81	0.61
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.83	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
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.65	0.60
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.82	0.60
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.36	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:1050:THR:HG23	3:D:1057:SER:HB3	1.83	0.60
3:D:1108:GLN:HG3	3:D:1109:LEU:HD13	1.83	0.60
1:G:74:VAL:HG22	1:G:76:GLU:H	1.66	0.60
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.84	0.60
1:G:182:ARG:H	1:G:206:GLU:HB3	1.67	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
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.84	0.60
3:D:218:THR:HA	3:D:221:ILE:HG22	1.83	0.60
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.83	0.59
3:J:218:THR:HA	3:J:221:ILE:HG22	1.83	0.59
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.83	0.59
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.35	0.59
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.83	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
1:A:182:ARG:H	1:A:206:GLU:HB3	1.67	0.59
3:D:424:ASN:HD22	3:D:434:ILE:HG12	1.67	0.59
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.84	0.59
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.83	0.59
3:J:1191:PRO:HB2	3:J:1193:TRP:CD1	2.38	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
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.85	0.58
5:F:479:THR:HG23	5:F:481:GLU:H	1.68	0.58
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.17	0.58
2:C:255:ILE:HB	2:C:263:VAL:HB	1.85	0.58
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.84	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
2:C:250:THR:HA	2:C:268:ARG:HA	1.86	0.58
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.86	0.58
2:I:1278:LEU:HD12	2:I:1287:LEU:HD12	1.86	0.58
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.18	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
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.85	0.57
5:F:547:VAL:HG11	5:F:607:LEU:HD11	1.86	0.57
2:I:518:ASN:N	2:I:518:ASN:OD1	2.35	0.57
2:I:1073:LYS:HD3	3:J:462:ASP:HB2	1.85	0.57
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.86	0.57
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.86	0.57
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.85	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
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.68	0.57
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.87	0.57
2:I:166:SER:HB2	6:N:23:SER:N	2.19	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:D:495:ASN:ND2	3:D:1247:LYS:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:232:ILE:HG13	2:I:331:LYS:O	2.05	0.57
3:J:1297:LYS:HG3	3:J:1299:GLY:H	1.68	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:518:ASN:OD1	2:C:518:ASN:N	2.36	0.57
2:C:1073:LYS:HD3	3:D:462:ASP:HB2	1.86	0.57
1:G:26:VAL:HG23	1:G:203:ILE:HB	1.87	0.57
2:C:1305:TYR:HE1	3:D:379:PRO:HG3	1.70	0.57
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.87	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
2:C:1278:LEU:HD12	2:C:1287:LEU:HD12	1.87	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
3:J:34:SER:OG	3:J:104:HIS:ND1	2.24	0.56
3:J:1063:ASP:HB3	3:J:1103:GLY:HA3	1.87	0.56
2:C:615:VAL:HG13	2:C:651:ASP:H	1.70	0.56
3:D:1077:ALA:HA	3:D:1100:PHE:HA	1.87	0.56
3:D:325:LYS:HG2	3:D:329:ASP:HB2	1.88	0.56
3:D:77:ARG:HG3	3:D:79:LYS:H	1.69	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
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.87	0.56
2:I:615:VAL:HG13	2:I:651:ASP:H	1.70	0.56
2:I:992:LEU:HD11	2:I:1000:LEU:HD11	1.86	0.56
3:D:1063:ASP:HB3	3:D:1103:GLY:HA3	1.87	0.56
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.86	0.56
3:J:1077:ALA:HA	3:J:1100:PHE:HA	1.87	0.56
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.87	0.56
1:A:11:PRO:HA	1:A:30:PRO:HB2	1.87	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:77:ARG:HG3	3:J:79:LYS:H	1.70	0.56
3:D:381:ILE:HD11	3:D:412:LEU:HD12	1.87	0.56
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.88	0.56
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.87	0.56
3:J:853:THR:HG22	3:J:854:ALA:H	1.70	0.56
2:I:488:MET:O	2:I:490:GLN:N	2.35	0.56
3:J:1192:LYS:HG2	3:J:1196:LEU:HD11	1.88	0.56
3:J:325:LYS:HG2	3:J:329:ASP:HB2	1.88	0.56
3:J:827:GLU:HG2	3:J:832:LYS:HD2	1.86	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
3:D:847:ASP:HB3	3:D:856:ILE:HG23	1.87	0.56
2:I:967:LEU:HD21	2:I:1021:LEU:HD13	1.87	0.56
5:L:166:VAL:O	5:L:167:ASP:HB2	2.05	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
3:J:490:ILE:HG22	3:J:500:ILE:HG13	1.88	0.56
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.88	0.56
2:I:808:ASN:H	3:J:633:ALA:HB2	1.69	0.56
5:L:316:PHE:HZ	5:L:334:SER:HA	1.71	0.56
1:A:26:VAL:HG23	1:A:203:ILE:HB	1.87	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.69	0.56
2:I:520:PRO:HG3	2:I:714:VAL:HG11	1.88	0.56
3:J:1211:SER:OG	3:J:1212:ASP:N	2.39	0.56
3:J:381:ILE:HD11	3:J:412:LEU:HD12	1.86	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
3:J:495:ASN:ND2	3:J:1247:LYS:O	2.39	0.56
5:L:281:ARG:O	5:L:285:ARG:HG3	2.06	0.56
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.87	0.55
2:C:19:PRO:HA	2:C:1156:ARG:HD3	1.87	0.55
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.87	0.55
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.88	0.55
1:A:48:LEU:HA	1:A:180:VAL:HG21	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
5:L:530:LEU:HD23	5:L:530:LEU:H	1.71	0.55
2:C:560:PRO:HB3	3:D:776:THR:HG21	1.87	0.55
3:D:1192:LYS:HG2	3:D:1196:LEU:HD11	1.89	0.55
5:F:511:ILE:HG13	5:F:512:GLY:H	1.72	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
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.22	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
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
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.89	0.55
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.86	0.55
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.89	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
5:F:281:ARG:O	5:F:285:ARG:HG3	2.07	0.55
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.88	0.55
5:L:511:ILE:HG13	5:L:512:GLY:H	1.72	0.55
2:C:488:MET:O	2:C:490:GLN:N	2.35	0.55
5:F:554:ARG:HB2	5:F:580:PHE:HE2	1.72	0.55
3:J:847:ASP:HB3	3:J:856:ILE:HG23	1.87	0.55
5:L:551:LEU:HD11	5:L:598:LEU:HD11	1.89	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
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.88	0.55
5:L:97:PRO:HA	5:L:100:MET:HG3	1.89	0.55
2:C:149:LEU:HD21	2:C:451:ARG:NH1	2.22	0.55
4:E:38:LEU:HD23	4:E:58:LEU:HD13	1.87	0.55
5:F:316:PHE:HZ	5:F:334:SER:HA	1.71	0.55
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.89	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
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.90	0.54
5:F:316:PHE:O	5:F:320:ILE:HG13	2.07	0.54
3:J:1191:PRO:HB2	3:J:1193:TRP:HD1	1.72	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: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:672:GLU:HG2	2:C:1187:PHE:HA	1.89	0.54
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.89	0.54
2:I:41:GLN:NE2	2:I:73:TYR:O	2.40	0.54
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.89	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
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.90	0.54
2:I:149:LEU:HD21	2:I:451:ARG:NH1	2.23	0.54
2:I:39:ILE:HA	2:I:49:LEU:HD12	1.89	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)
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.73	0.54
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:102:LEU:HB2	2:C:489:PRO:HG3	1.90	0.54
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.88	0.54
1:G:19:VAL:HG12	1:G:24:ALA:HA	1.90	0.54
2:I:102:LEU:HB2	2:I:489:PRO:HG3	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
1:A:60:GLU:OE1	1:A:143:ARG:NH2	2.41	0.54
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.89	0.54
3:D:516:ASP:HB3	3:D:573:THR:HG21	1.90	0.54
5:L:554:ARG:HB2	5:L:580:PHE:HE2	1.72	0.54
3:D:1191:PRO:HB2	3:D:1193:TRP:HD1	1.72	0.54
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.72	0.54
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.23	0.54
5:L:316:PHE:O	5:L:320:ILE:HG13	2.08	0.54
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.43	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
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.41	0.53
2:C:815:SER:HB3	3:D:461:PHE:HB3	1.90	0.53
3:D:1167:LYS:HG3	3:D:1174:ARG:HD2	1.91	0.53
4:E:42:GLU:O	4:E:43:ASN:HB2	2.09	0.53
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.91	0.53
3:D:978:ARG:HB2	3:D:1199:PHE:CZ	2.43	0.53
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.90	0.53
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.90	0.53
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.89	0.53
5:L:130:VAL:HB	5:L:365:MET:HG3	1.90	0.53
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.90	0.53
1:B:8:PHE:HD1	1:B:9:LEU:H	1.55	0.53
5:F:97:PRO:HA	5:F:100:MET:HG3	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
6:N:21:GLU:HG3	6:N:26:SER:HB3	1.90	0.53
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.90	0.53
2:C:120:GLN:HG2	2:C:121:GLU:H	1.73	0.53
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:818:VAL:HG13	2:C:1096:ILE:HG12	1.90	0.53
5:F:470:MET:O	5:F:474:MET:HB2	2.07	0.53
2:I:593:LYS:HB3	2:I:602:GLU:HG3	1.89	0.53
2:I:60:GLN:HB3	2:I:67:GLU:HG3	1.91	0.53
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.89	0.53
2:I:815:SER:HB3	3:J:461:PHE:HB3	1.90	0.53
3:J:1167:LYS:HG3	3:J:1174:ARG:HD2	1.90	0.53
3:J:709:ARG:C	3:J:711:GLY:H	2.12	0.53
2:C:804:PHE:HB3	2:C:1100:PRO:HG3	1.91	0.53
2:C:1247:SER:HB3	3:D:375:GLU:O	2.09	0.53
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.91	0.53
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.91	0.53
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.90	0.53
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.90	0.53
1:G:60:GLU:OE1	1:G:143:ARG:NH2	2.42	0.53
2:I:176:ILE:HD11	2:I:428:VAL:HG21	1.90	0.53
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.43	0.53
4:K:42:GLU:O	4:K:43:ASN:HB2	2.08	0.53
5:L:234:THR:O	5:L:245:ALA:HB2	2.09	0.53
1:B:75:GLN:OE1	1:B:76:GLU:HG3	2.09	0.53
2:C:387:ASN:HA	2:C:391:SER:HB2	1.91	0.53
3:D:1039:ASP:OD1	3:D:1074:LEU:HB3	2.09	0.53
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.39	0.53
2:I:387:ASN:HA	2:I:391:SER:HB2	1.90	0.53
1:B:64:VAL:HG21	1:B:69:SER: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
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.90	0.53
5:L:577:GLY:HA3	5:L:583:THR:HA	1.91	0.53
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.89	0.53
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.91	0.53
3:D:1191:PRO:HD3	6:M:55:THR:O	2.08	0.53
5:F:166:VAL:O	5:F:167:ASP:HB2	2.07	0.53
1:A:14:VAL:HG22	1:A:15:ASP:H	1.74	0.52
1:H:75:GLN:OE1	1:H:76:GLU:HG3	2.09	0.52
2:I:356:THR:HG21	2:I:362:ALA:HA	1.90	0.52
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	1.91	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
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.92	0.52
3:J:475:GLU:OE2	4:K:28:ARG:NH2	2.39	0.52
1:B:64:VAL:HG12	1:B:65:LEU:H	1.74	0.52
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.92	0.52
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.91	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
3:D:1078:LEU:HD13	3:D:1121:LEU:HD22	1.91	0.52
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.92	0.52
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.91	0.52
2:C:861:ALA:HB1	2:C:882:ILE:HD13	1.91	0.52
2:I:5:TYR:CE1	2:I:776:PRO:HB2	2.44	0.52
3:J:1162:ILE:HA	3:J:1203:ARG:HA	1.92	0.52
3:J:332:LYS:HG2	3:J:1328:THR:HB	1.92	0.52
1:B:125:LYS:HE2	1:B:128:HIS:HB2	1.91	0.52
2:C:703:GLY:N	2:C:705:GLU:OE2	2.42	0.52
3:D:974:VAL:HG21	3:D:1118:GLY:HA2	1.92	0.52
3:D:198:CYS:O	3:D:202:ARG:HG3	2.10	0.52
2:C:356:THR:HG21	2:C:362:ALA:HA	1.91	0.52
3:D:709:ARG:C	3:D:711:GLY:H	2.12	0.52
1:G:50:SER:HB3	1:H:8:PHE:CZ	2.45	0.52
2:I:367:TYR:HD1	2:I:384:LEU:HD22	1.74	0.52
2:I:980:VAL:O	2:I:984:VAL:HB	2.10	0.52
3:J:1029:THR:HG21	3:J:1080:ILE:HD11	1.91	0.52
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.91	0.52
3:J:516:ASP:HB3	3:J:573:THR:HG21	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: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
2:I:600:THR:HB	2:I:602:GLU:HG2	1.92	0.52
3:J:502:PRO:HB2	3:J:507:VAL:HG12	1.92	0.52
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.90	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
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.92	0.51
2:I:119:GLU:HG3	2:I:488:MET:HB3	1.90	0.51
2:I:861:ALA:HB1	2:I:882:ILE:HD13	1.91	0.51

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.92	0.50
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.76	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
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	1.93	0.50
5:L:343:LYS:H	5:L:343:LYS:HD2	1.76	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
1:A:120:ASP:OD2	1:A:120:ASP:N	2.44	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
2:C:225:PHE:HE1	2:C:345:PRO:HA	1.77	0.50
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.93	0.50
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.93	0.50
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.93	0.50
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.47	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:699:ASP:HA	3:J:702:GLN:HG2	1.92	0.50
3:J:847:ASP:N	3:J:847:ASP:OD1	2.43	0.50
2:C:206:ALA:O	2:C:209:ILE:HG22	2.11	0.50
2:C:55:SER:OG	2:C:56:VAL:N	2.45	0.50
2:C:632:ASP:HA	2:C:647:ARG:HB2	1.93	0.50
3:D:697:MET:HG3	3:D:698:MET:N	2.26	0.50
3:D:902:ASP:OD1	3:D:903:LEU:N	2.45	0.50
2:I:331:LYS:HB2	2:I:332:ARG:NH2	2.26	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:C:170:VAL:HG23	2:C:171:LEU:N	2.27	0.49
3:D:576:ARG:NH1	3:D:593:ASN:O	2.44	0.49
3:D:870:ASP:O	3:D:874:GLU:HG2	2.12	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
2:I:688:GLN:HB2	2:I:1235:LEU:HD22	1.93	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.12	0.49
3:D:564:VAL:HG12	3:D:565:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:708:ASN:HB3	3:D:712:GLN:O	2.11	0.49
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.93	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.76	0.49
3:D:298:MET:SD	5:F:402:LEU:HB3	2.52	0.49
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.76	0.49
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.93	0.49
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.95	0.49
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.47	0.49
5:F:141:ILE:HG21	5:F:252:LEU:HD11	1.93	0.49
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.93	0.49
3:D:1227:HIS:ND1	3:J:1293:GLU:HG2	2.27	0.49
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.48	0.49
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.94	0.49
2:I:225:PHE:HE1	2:I:345:PRO:HA	1.77	0.49
3:J:451:PRO:O	3:J:454:CYS:HB2	2.13	0.49
3:J:902:ASP:OD1	3:J:903:LEU:N	2.46	0.49
2:C:829:THR:HG23	2:C:1059:ARG:HA	1.95	0.49
2:C:688:GLN:HB2	2:C:1235:LEU:HD22	1.93	0.49
3:D:332:LYS:HG2	3:D:1328:THR:HB	1.92	0.49
3:D:826:ILE:HD12	3:D:994:SER:HB2	1.94	0.49
5:F:461:ASN:O	5:F:465:ARG:HG2	2.12	0.49
2:I:632:ASP:HA	2:I:647:ARG:HB2	1.94	0.49
3:J:564:VAL:HG12	3:J:565:ALA:H	1.78	0.49
5:L:134:VAL:HG22	5:L:273:MET:HE1	1.95	0.49
1:A:197:ASP:N	1:A:197:ASP:OD1	2.45	0.49
2:C:1247:SER:OG	2:C:1248:THR:N	2.44	0.49
2:C:1106:ARG:NE	3:D:731:ARG:HH21	2.10	0.49
2:C:30:ILE:H	2:C:30:ILE:HD12	1.76	0.49
2:C:180:ARG:CZ	2:C:465:ARG:HH12	2.26	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
1:B:44:ARG:HG3	1:B:183:ILE:HB	1.94	0.49
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.12	0.49
3:D:755:ILE:HG22	3:D:757:THR:H	1.78	0.49
5:F:250:LEU:O	5:F:253:SER:OG	2.27	0.49
1:G:197:ASP:N	1:G:197:ASP:OD1	2.45	0.49
3:J:708:ASN:HB3	3:J:712:GLN:O	2.12	0.49
3:D:398:LYS:O	3:D:402:GLU:HB2	2.13	0.49
3:D:451:PRO:O	3:D:454:CYS:HB2	2.13	0.49
3:D:845:ALA:HB3	3:D:881:LYS:HB3	1.95	0.49
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.77	0.49
5:L:245:ALA:O	5:L:249:ILE:HG13	2.12	0.49
5:L:343:LYS:O	5:L:347:ILE:HG13	2.13	0.49
5:F:343:LYS:O	5:F:347:ILE:HG13	2.13	0.49
1:H:44:ARG:HG3	1:H:183:ILE:HB	1.94	0.49
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.48	0.49
3:J:576:ARG:NH1	3:J:593:ASN:O	2.45	0.49
6:N:16:PHE:HD1	6:N:59:PRO:HA	1.78	0.49
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.48	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: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
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.95	0.48
3:D:978:ARG:HB2	3:D:1199:PHE:HZ	1.77	0.48
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.95	0.48
2:I:528:ARG:NH2	2:I:576:SER:O	2.46	0.48
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.10	0.48
5:L:250:LEU:O	5:L:253:SER:OG	2.28	0.48
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.96	0.48
3:D:478:LEU:HG	4:E:47:THR:HG23	1.94	0.48
2:I:1149:TYR:OH	2:I:1176:LEU:HD11	2.14	0.48
2:I:55:SER:OG	2:I:56:VAL:N	2.46	0.48
3:J:398:LYS:O	3:J:402:GLU:HB2	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: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:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.94	0.48
3:J:1062:LEU:CD2	3:J:1066:GLU:HB3	2.44	0.48
2:C:1149:TYR:OH	2:C:1176:LEU:HD11	2.14	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.95	0.48
2:C:232:ILE:HD11	2:C:333:ILE:HD11	1.95	0.48
3:D:1264:ALA:CB	3:D:1280:VAL:HG22	2.44	0.48
2:C:1246:ARG:NH2	3:D:348:ASP:OD1	2.46	0.48
3:D:807:LEU:HD11	3:D:894:VAL:HG23	1.95	0.48
3:J:298:MET:SD	5:L:402:LEU:HB3	2.53	0.48
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.95	0.48

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

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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:G:10:LYS:HE2	1:H:229:GLU:HB3	1.95	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
5:L:130:VAL:O	5:L:134:VAL:HG23	2.14	0.47
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.96	0.47
5:F:138:PRO:O	5:F:142:THR:HG23	2.14	0.47
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.13	0.47
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.96	0.47
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.97	0.47
3:D:144:TYR:CD1	3:D:180:MET:HB3	2.50	0.47
3:D:405:GLU:O	3:D:408:VAL:HG22	2.14	0.47
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.96	0.47
3:J:850:LYS:HG2	3:J:851:PRO:HD2	1.95	0.47
5:L:489:MET:HE2	5:L:493:LYS:HG3	1.97	0.47
2:C:151:ARG:HG2	2:C:445:ILE:HG23	1.97	0.47
2:C:225:PHE:CE1	2:C:345:PRO:HA	2.50	0.47
3:D:1062:LEU:HD21	3:D:1066:GLU:HB3	1.95	0.47
3:D:525:MET:O	3:D:548:VAL:HG13	2.13	0.47
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.96	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
2:I:890:LYS:NZ	2:I:891:GLY:O	2.47	0.47
3:J:1064:SER:HB2	3:J:1173:ARG:NH1	2.25	0.47
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.96	0.47
3:J:122:SER:O	3:J:126:LEU:HG	2.15	0.47
6:M:16:PHE:HD1	6:M:59:PRO:HA	1.78	0.47
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.97	0.47
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.79	0.47
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.97	0.47
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.46	0.47
5:L:220:LYS:O	5:L:223:GLU:HB3	2.15	0.47
3:D:442:ILE:HG22	3:D:443:GLU:O	2.15	0.47
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.48	0.47
5:F:598:LEU:HA	5:F:603:ARG:HB2	1.96	0.47
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.96	0.47
2:C:4:SER:OG	2:C:5:TYR:N	2.47	0.47
3:D:1062:LEU:CD2	3:D:1066:GLU:HB3	2.44	0.47
3:D:1282:TYR:O	3:D:1285:VAL:HG12	2.15	0.47
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.96	0.47
3:D:853:THR:HG21	3:J:1375:ALA:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:61:ILE:HB	1:H:64:VAL:O	2.14	0.47
3:J:1260:MET:HG2	3:J:1307:LEU:O	2.14	0.47
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.97	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.97	0.47
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.97	0.47
1:G:75:GLN:HA	2:I:729:ALA:N	2.30	0.47
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.45	0.47
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.97	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
2:C:499:SER:O	2:C:503:LYS:HB2	2.15	0.47
3:D:1153:PRO:HA	3:D:1214:PRO:O	2.15	0.47
5:F:470:MET:HG3	5:F:486:ARG:HH22	1.78	0.47
5:L:598:LEU:HA	5:L:603:ARG:HB2	1.97	0.47
1:A:45:ARG:NE	2:C:1083:GLU:HB3	2.29	0.47
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.15	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
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.49	0.47
2:C:883:LEU:HD22	2:C:1052:VAL:HG11	1.97	0.47
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.14	0.47
1:H:73:GLY:CA	1:H:134:THR:HG22	2.44	0.47
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.96	0.47
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.50	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
1:A:207:THR:HG22	1:A:208:ASN:H	1.80	0.46
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.45	0.46
3:D:1260:MET:HG2	3:D:1307:LEU:O	2.15	0.46
2:C:1253:LEU:HD11	3:D:251:PRO:HG2	1.96	0.46
3:D:574:VAL:O	3:D:578:ILE:HG13	2.16	0.46
2:I:1116:HIS:O	2:I:1119:MET:HB3	2.15	0.46
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.97	0.46
5:L:362:ASN:HB2	5:L:365:MET:HE1	1.97	0.46
5:L:547:VAL:HG21	5:L:607:LEU:HD11	1.98	0.46
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.98	0.46
2:C:1113:LEU:HD11	3:D:641:ILE:HG13	1.97	0.46
3:D:122:SER:O	3:D:126:LEU:HG	2.15	0.46
3:D:290:ILE:HD12	3:D:290:ILE:H	1.81	0.46
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.97	0.46
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.96	0.46
3:J:156:ARG:NH2	3:J:191:SER:OG	2.48	0.46
6:N:40:LEU:O	6:N:44:GLU:HG2	2.16	0.46
2:C:1279:GLU:HG3	3:D:1357:ILE:HD13	1.97	0.46
3:D:654:ILE:O	3:D:658:GLU:HB2	2.16	0.46
1:G:201:LEU:HG	1:G:203:ILE:HG13	1.96	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
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
2:I:5:TYR:HD2	2:I:778:GLU:HB2	1.80	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
3:D:1100:PHE:HB2	3:D:1200:GLU:CD	2.36	0.46
3:D:156:ARG:NH2	3:D:191:SER:OG	2.47	0.46
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.97	0.46
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.97	0.46
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.49	0.46
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.98	0.46
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.96	0.46
2:I:225:PHE:CE1	2:I:345:PRO:HA	2.50	0.46
1:G:75:GLN:HA	2:I:729:ALA:H	1.80	0.46
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.97	0.46
3:J:574:VAL:O	3:J:578:ILE:HG13	2.16	0.46
1:B:47:LEU:HB3	1:B:180:VAL:HG11	1.98	0.46
1:B:75:GLN:HG3	1:B:75:GLN:H	1.60	0.46
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.97	0.46
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.97	0.46
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.49	0.46
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.80	0.46
2:I:1113:LEU:HD11	3:J:641:ILE:HG13	1.97	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)
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.81	0.46
3:J:144:TYR:CD1	3:J:180:MET:HB3	2.50	0.46
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
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:D:334:LYS:HD2	3:D:334:LYS:HA	1.70	0.46
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.98	0.46
3:D:650:LYS:O	3:D:654:ILE:HG13	2.16	0.46
3:J:1158:GLU:OE2	3:J:1222:ARG:NH1	2.48	0.46
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.45	0.45
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.81	0.45
2:I:883:LEU:HD22	2:I:1052:VAL:HG11	1.97	0.45
2:I:705:GLU:O	2:I:794:LEU:N	2.49	0.45
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.98	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
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.97	0.45
4:E:50:ALA:O	4:E:54:ILE:HG12	2.16	0.45
5:F:311:THR:HB	5:F:345:GLN:HG2	1.99	0.45
5:F:446:GLN:O	5:F:448:ARG:N	2.49	0.45
2:I:960:LEU:HA	2:I:960:LEU:HD13	1.87	0.45
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.97	0.45
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.64	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
2:C:123:TYR:OH	2:C:126:GLU:HG3	2.17	0.45
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.96	0.45
3:D:1078:LEU:HB2	3:D:1121:LEU:HD13	1.98	0.45
3:D:1167:LYS:O	3:D:1169:THR:N	2.50	0.45
3:D:1158:GLU:OE2	3:D:1222:ARG:NH1	2.50	0.45
5:F:362:ASN:HB2	5:F:365:MET:HE1	1.98	0.45
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.31	0.45
3:J:1062:LEU:O	3:J:1067:ARG:NE	2.45	0.45
2:I:1279:GLU:HG3	3:J:1357:ILE:HD13	1.98	0.45
6:N:19:THR:OG1	6:N:55:THR:HB	2.17	0.45
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.52	0.45
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.52	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
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:J:1027:VAL:HG21	3:J:1122:ALA:HB3	1.98	0.45
3:J:1167:LYS:O	3:J:1169:THR:N	2.49	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
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
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	1.99	0.45
3:J:363:LEU:HD21	3:J:487:THR:HA	1.97	0.45
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.51	0.45
2:C:705:GLU:O	2:C:794:LEU:N	2.49	0.45
3:D:1027:VAL:HG21	3:D:1122:ALA:HB3	1.97	0.45
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.49	0.45
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.17	0.45
3:J:378:LYS:HB3	3:J:379:PRO:HD3	1.99	0.45
3:J:424:ASN:ND2	3:J:434:ILE:HG12	2.31	0.45
5:L:446:GLN:O	5:L:448:ARG:N	2.50	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
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.47	0.45
2:I:673:HIS:HB3	2:I:1109:ILE:CG2	2.47	0.45
3:J:1166:GLY:O	3:J:1174:ARG:HB2	2.17	0.45
3:J:950:ILE:HG13	3:J:1020:TRP:CZ3	2.52	0.45
6:N:29:VAL:HG21	6:N:47:TYR:OH	2.17	0.45
1:B:73:GLY:CA	1:B:134:THR:HG22	2.44	0.45
2:C:976:ARG:O	2:C:980:VAL:HG23	2.16	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
2:C:1326:LEU:HD11	3:D:331:ILE:HG23	1.98	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.17	0.45
2:C:519:ASN:OD1	2:C:521:LEU:N	2.50	0.45
3:D:473:THR:HG23	3:D:476:ALA:H	1.81	0.45
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.81	0.45
3:J:1064:SER:O	3:J:1072:LYS:HE2	2.17	0.45
3:J:1078:LEU:HB2	3:J:1121:LEU:HD13	1.98	0.45
3:J:770:LEU:HD22	3:J:770:LEU:H	1.81	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
1:H:32:GLU:HB2	1:H:35:PHE:CD1	2.52	0.45
2:I:971:LEU:HD22	2:I:1021:LEU:HD12	1.98	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

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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
3:D:1349:GLU:CD	3:D:1349:GLU:H	2.20	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
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.65	0.44
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.53	0.44
1:A:104:LYS:HG2	1:A:110:VAL:HG22	2.00	0.44
2:C:971:LEU:HD23	2:C:975:ILE:HD11	1.99	0.44
3:D:418:GLU:H	4:E:45:LYS:NZ	2.15	0.44
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.99	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
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.72	0.44
3:D:958:ILE:HD11	3:D:1017:VAL:HG11	2.00	0.44
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.98	0.44
5:F:220:LYS:O	5:F:223:GLU:HB3	2.17	0.44
5:F:335:GLU:O	5:F:339:ARG:HG2	2.18	0.44
5:F:354:THR:O	5:F:358:VAL:HG23	2.16	0.44
1:H:172:LEU:H	1:H:172:LEU:HD12	1.82	0.44
1:H:47:LEU:HB3	1:H:180:VAL:HG11	1.99	0.44
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	2.00	0.44
2:I:174:ALA:HB2	2:I:432:LEU:HD13	2.00	0.44
3:J:1282:TYR:O	3:J:1285:VAL:HG12	2.17	0.44
3:J:233:LYS:HB3	3:J:235:GLU:OE2	2.17	0.44
1:H:196:THR:HG23	3:J:443:GLU:HG3	2.00	0.44
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.17	0.44
3:D:334:LYS:HB3	5:F:516:ASP:OD2	2.16	0.44
1:H:93:GLN:HB2	1:H:120:ASP:HB3	2.00	0.44
1:H:81:ILE:O	1:H:85:LEU:HG	2.18	0.44
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.97	0.44
2:I:396:ASP:OD1	2:I:418:GLY:HA3	2.18	0.44
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.32	0.44
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.98	0.44
3:J:743:MET:HB2	3:J:759:ILE:O	2.17	0.44
1:B:93:GLN:HB2	1:B:120:ASP:HB3	1.99	0.44
1:B:178:SER:HA	1:B:179:PRO:HD3	1.71	0.44
1:B:32:GLU:HB2	1:B:35:PHE:CD1	2.53	0.44
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.32	0.44
5:F:253:SER:O	5:F:257:LYS:HG3	2.17	0.44
2:I:992:LEU:HB2	2:I:993:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:794:GLY:O	3:J:797:THR:OG1	2.31	0.44
1:A:231:PHE:CE1	1:B:221:ALA:HB3	2.53	0.44
2:C:657:THR:HG23	2:C:658:GLN:HG3	2.00	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:D:706:VAL:HG12	3:D:715:LYS:HB3	2.00	0.44
4:E:44:ASP:HB3	4:E:48:VAL:HB	2.00	0.44
1:H:79:LEU:HD23	1:H:79:LEU:H	1.82	0.44
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.17	0.44
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.99	0.44
3:J:26:SER:HB2	3:J:236:TRP:CE2	2.53	0.44
3:J:613:GLY:O	3:J:617:THR:OG1	2.33	0.44
3:J:418:GLU:H	4:K:45:LYS:NZ	2.15	0.44
4:K:44:ASP:HB3	4:K:48:VAL:HB	2.00	0.44
1:B:30:PRO:HB3	1:B:192:VAL:HG21	1.99	0.44
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.32	0.44
3:D:800:LEU:HD12	3:D:1309:ILE:HD13	2.00	0.44
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.16	0.44
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.87	0.44
3:D:440:VAL:O	3:D:442:ILE:HG12	2.18	0.44
3:D:363:LEU:HD21	3:D:487:THR:HA	1.98	0.44
3:D:490:ILE:HD11	3:D:609:TYR:CE2	2.53	0.44
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.47	0.44
2:I:1326:LEU:HD11	3:J:331:ILE:HG23	1.99	0.44
3:J:490:ILE:HD11	3:J:609:TYR:CE2	2.53	0.44
3:J:958:ILE:HG23	3:J:982:LEU:HD11	2.00	0.44
5:L:312:SER:OG	5:L:313:ASP:N	2.51	0.44
1:B:102:LEU:O	1:B:141:SER:OG	2.29	0.44
1:B:52:PRO:HA	1:B:149:GLY:O	2.18	0.44
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.00	0.44
2:C:137:VAL:HA	2:C:141:THR:O	2.18	0.44
2:C:980:VAL:HG13	2:C:984:VAL:HG23	1.99	0.44
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.18	0.44
3:D:18:ASP:OD1	3:D:18:ASP:N	2.50	0.44
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.79	0.44
5:F:324:LYS:HB2	5:F:327:SER:HB2	2.00	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
2:I:657:THR:HG23	2:I:658:GLN:HG3	2.00	0.44
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.53	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)
1:B:79:LEU:HD23	1:B:79:LEU:H	1.84	0.43
2:C:396:ASP:OD1	2:C:418:GLY:HA3	2.18	0.43
2:C:403:MET:HG3	2:C:584:TYR:CZ	2.53	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
3:D:743:MET:HB2	3:D:759:ILE:O	2.17	0.43
5:F:468:ARG:O	5:F:471:LEU:HB2	2.18	0.43
1:G:11:PRO:HB3	1:G:31:LEU:HD23	2.00	0.43
2:I:1142:ARG:HH22	2:I:1165:SER:HA	1.82	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.00	0.43
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.16	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
3:J:702:GLN:HG3	3:J:703:THR:N	2.33	0.43
3:J:697:MET:SD	3:J:741:ALA:HB3	2.58	0.43
3:J:747:MET:HB2	3:J:774:ILE:HG22	2.00	0.43
3:J:990:ARG:NH1	3:J:992:LYS:HD3	2.33	0.43
5:L:354:THR:O	5:L:358:VAL:HG23	2.18	0.43
2:I:905:ILE:O	5:L:599:ARG:NH1	2.51	0.43
2:C:174:ALA:HB2	2:C:432:LEU:HD13	2.01	0.43
3:D:1062:LEU:O	3:D:1067:ARG:NE	2.45	0.43
3:D:518:VAL:O	3:D:547:ARG:NH1	2.51	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
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.98	0.43
1:G:16:ILE:HG23	1:G:26:VAL:HG12	2.00	0.43
5:L:287:ILE:HG23	5:L:337:VAL:HG13	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
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.99	0.43
1:B:81:ILE:O	1:B:85:LEU:HG	2.18	0.43
2:C:905:ILE:O	5:F:599:ARG:NH1	2.51	0.43
3:D:1067:ARG:HB2	3:D:1072:LYS:HG3	2.00	0.43
3:D:747:MET:HB2	3:D:774:ILE:HG22	2.00	0.43
5:F:312:SER:OG	5:F:313:ASP:N	2.51	0.43
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.33	0.43
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.18	0.43
3:J:1067:ARG:HB2	3:J:1072:LYS:HG3	2.01	0.43
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.48	0.43
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.53	0.43
5:F:137:TYR:CE1	5:F:139:GLU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:302:PHE:O	5:F:306:PHE:HB2	2.18	0.43
3:J:440:VAL:O	3:J:442:ILE:HG12	2.18	0.43
3:J:46:TYR:O	5:L:500:ILE:HG21	2.18	0.43
5:L:253:SER:O	5:L:257:LYS:HG3	2.18	0.43
6:M:29:VAL:HG21	6:M:47:TYR:OH	2.17	0.43
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.18	0.43
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	2.01	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
3:D:958:ILE:HG23	3:D:982:LEU:HD11	2.01	0.43
1:G:137:ASN:N	1:G:137:ASN:OD1	2.51	0.43
2:I:1100:PRO:O	2:I:1104:PRO:HD3	2.18	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
3:J:1349:GLU:H	3:J:1349:GLU:CD	2.19	0.43
3:J:518:VAL:O	3:J:547:ARG:NH1	2.51	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:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.51	0.43
5:F:394:TYR:HB3	5:F:443:ILE:HD11	2.01	0.43
1:G:53:GLY:O	1:G:148:ARG:HG3	2.19	0.43
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	2.00	0.43
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.83	0.43
1:A:77:ASP:O	1:A:81:ILE:HG13	2.19	0.43
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	2.00	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.59	0.43
3:D:26:SER:HB2	3:D:236:TRP:CE2	2.54	0.43
3:D:339:ARG:O	3:D:341:ASN:N	2.44	0.43
3:D:512:TYR:CD2	3:D:635:SER:HB2	2.53	0.43
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.01	0.43
3:D:564:VAL:HG12	3:D:565:ALA:N	2.34	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.54	0.43
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.58	0.43
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.00	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:527:LEU:HD21	3:J:536:LEU:HG	2.01	0.43
3:J:746:LEU:HD13	3:J:754:ILE:HD11	2.00	0.43
5:L:127:ILE:O	5:L:130:VAL:HG22	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:555:GLU:HA	5:L:558:VAL:HG12	2.01	0.43
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	1.99	0.43
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.54	0.43
2:C:3:TYR:HB3	2:C:4:SER:H	1.64	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:I:1280:ALA:HB3	3:J:431:ARG:HB3	2.01	0.43
2:I:1286:THR:O	2:I:1290:MET:HB2	2.19	0.43
2:I:339:ASN:O	2:I:344:GLY:HA2	2.18	0.43
2:I:697:LYS:HG2	2:I:698:PRO:O	2.19	0.43
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.87	0.43
3:J:800:LEU:HD12	3:J:1309:ILE:HD13	2.00	0.43
1:A:53:GLY:O	1:A:148:ARG:HG3	2.19	0.43
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.87	0.43
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.43
3:D:990:ARG:NH1	3:D:992:LYS:HD3	2.34	0.43
2:I:708:VAL:HG11	2:I:794:LEU:HD22	2.01	0.43
3:J:161:THR:HG22	3:J:164:GLN:CD	2.39	0.43
2:I:1339:LEU:HB3	3:J:17:PHE:CD1	2.54	0.43
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	2.01	0.43
1:A:90:VAL:HG22	1:A:91:ARG:H	1.84	0.43
2:C:985:GLU:O	2:C:989:LEU:HB2	2.18	0.43
3:D:702:GLN:HG3	3:D:703:THR:N	2.34	0.43
3:D:475:GLU:CD	4:E:28:ARG:HH22	2.23	0.43
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.84	0.43
2:I:519:ASN:OD1	2:I:521:LEU:N	2.51	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
3:J:174:ASP:C	3:J:176:PHE:H	2.22	0.43
3:J:124:ILE:HG23	3:J:189:LEU:HD11	2.00	0.43
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.43
3:J:702:GLN:HG3	3:J:703:THR:H	1.83	0.43
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.00	0.43
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.81	0.43
5:L:266:PHE:HA	5:L:269:LEU:HD12	2.00	0.43
5:L:324:LYS:HB2	5:L:327:SER:HB2	2.01	0.43
5:L:515:GLU:C	5:L:517:SER:H	2.23	0.43
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.84	0.42
2:C:1339:LEU:HB3	3:D:17:PHE:CD1	2.54	0.42
5:F:141:ILE:H	5:F:141:ILE:HG12	1.68	0.42
5:F:266:PHE:HA	5:F:269:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:573:LEU:H	5:F:573:LEU:HD23	1.83	0.42
5:F:584:ARG:HA	5:F:584:ARG:NH1	2.34	0.42
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.87	0.42
1:A:117:HIS:NE2	1:A:121:VAL:O	2.53	0.42
2:C:53:PHE:O	2:C:57:PHE:HB2	2.19	0.42
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.92	0.42
2:C:980:VAL:O	2:C:984:VAL:HB	2.19	0.42
3:D:746:LEU:HD13	3:D:754:ILE:HD11	2.00	0.42
2:I:228:VAL:HB	2:I:335:THR:OG1	2.19	0.42
2:I:637:ARG:HA	2:I:642:SER:HA	2.01	0.42
2:I:946:LEU:HD23	2:I:946:LEU:HA	1.85	0.42
5:L:296:LYS:HD3	5:L:296:LYS:HA	1.79	0.42
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	2.01	0.42
2:C:637:ARG:HA	2:C:642:SER:HA	2.00	0.42
2:C:992:LEU:HD23	2:C:992:LEU:H	1.84	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
3:J:1155:ILE:HD12	3:J:1210:ILE:HB	2.02	0.42
3:J:512:TYR:CD2	3:J:635:SER:HB2	2.54	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
5:L:387:VAL:HG22	5:L:435:ILE:HD13	2.02	0.42
1:A:208:ASN:N	1:A:208:ASN:OD1	2.49	0.42
2:C:1253:LEU:CD1	3:D:251:PRO:HG2	2.50	0.42
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.88	0.42
2:C:179:TYR:HE1	2:C:454:ARG:HH21	1.67	0.42
3:D:1046:ILE:HD12	3:D:1059:LEU:HD13	2.02	0.42
3:D:264:ASP:N	3:D:264:ASP:OD2	2.52	0.42
3:D:8:LEU:HD23	3:D:9:LYS:N	2.34	0.42
5:F:227:GLN:HA	5:F:230:VAL:HG12	2.01	0.42
5:F:515:GLU:C	5:F:517:SER:H	2.23	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:1341:ASP:HB3	2:I:1342:GLU:H	1.49	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
3:J:81:ARG:HG3	3:J:82:GLY:H	1.83	0.42
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.29	0.42
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.86	0.42
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	2.01	0.42
3:D:203:GLU:O	3:D:207:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:653:MET:HG2	2:I:654:ASP:N	2.35	0.42
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.84	0.42
2:I:88:ARG:NH1	2:I:88:ARG:HB2	2.34	0.42
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	2.02	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
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.51	0.42
3:D:424:ASN:ND2	3:D:434:ILE:HG12	2.33	0.42
5:F:134:VAL:HG22	5:F:273:MET:HE1	2.01	0.42
5:F:105:MET:HE3	5:F:384:LEU:HB2	2.02	0.42
3:J:264:ASP:OD2	3:J:264:ASP:N	2.53	0.42
3:J:480:ALA:O	3:J:485:MET:N	2.52	0.42
5:L:302:PHE:O	5:L:306:PHE:HB2	2.19	0.42
1:A:75:GLN:HA	2:C:729:ALA:N	2.34	0.42
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	2.01	0.42
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.84	0.42
2:C:520:PRO:HG3	2:C:714:VAL:HG11	2.01	0.42
2:C:676:ALA:HB2	3:D:772:TYR:HE1	1.85	0.42
3:D:1063:ASP:O	3:D:1067:ARG:HG3	2.20	0.42
5:F:505:ILE:HD12	5:F:505:ILE:HA	1.84	0.42
1:G:77:ASP:O	1:G:81:ILE:HG13	2.19	0.42
2:I:347:ILE:HD11	2:I:433:ILE:HD11	2.02	0.42
5:L:137:TYR:CE1	5:L:139:GLU:HB2	2.54	0.42
5:L:364:ARG:HA	5:L:367:ILE:HD12	2.02	0.42
5:L:394:TYR:HB3	5:L:443:ILE:HD11	2.00	0.42
6:M:19:THR:HG1	6:M:55:THR:HB	1.84	0.42
1:A:11:PRO:HB3	1:A:31:LEU:HD23	2.01	0.42
2:C:138:ILE:HG22	2:C:139:ASN:N	2.34	0.42
2:C:452:ARG:HG2	2:C:453:ILE:N	2.35	0.42
2:C:484:LEU:CD1	2:C:485:ASP:H	2.32	0.42
3:D:118:LYS:HA	3:D:118:LYS:HD2	1.81	0.42
3:D:1256:ILE:HG22	3:D:1260:MET:HE2	2.02	0.42
3:D:702:GLN:HG3	3:D:703:THR:H	1.83	0.42
5:F:120:ALA:HA	5:F:123:ILE:HD12	2.02	0.42
1:G:125:LYS:HE2	1:G:128:HIS:HB2	2.01	0.42
2:I:672:GLU:HG3	2:I:672:GLU:H	1.57	0.42
3:J:203:GLU:O	3:J:207:GLU:HG2	2.20	0.42
5:L:577:GLY:HA3	5:L:583:THR:HG23	2.01	0.42
3:D:12:THR:HG22	3:D:13:LYS:HG2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:291:CYS:O	5:F:296:LYS:N	2.53	0.42
2:I:53:PHE:O	2:I:57:PHE:HB2	2.20	0.42
2:I:975:ILE:O	2:I:979:LEU:HB2	2.19	0.42
3:J:611:ILE:HG22	3:J:612:LEU:HD12	2.02	0.42
2:I:676:ALA:HB2	3:J:772:TYR:HE1	1.85	0.42
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.35	0.42
5:L:291:CYS:O	5:L:296:LYS:N	2.53	0.42
5:L:584:ARG:NH1	5:L:584:ARG:HA	2.34	0.42
1:A:75:GLN:HA	2:C:729:ALA:H	1.85	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
2:C:848:GLU:HG2	2:C:888:THR:HG22	2.02	0.42
2:C:925:SER:O	2:C:1056:VAL:HG13	2.20	0.42
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.35	0.42
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.95	0.42
3:D:70:CYS:SG	3:D:71:LEU:N	2.92	0.42
5:F:387:VAL:HG22	5:F:435:ILE:HD13	2.02	0.42
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.01	0.42
2:I:898:GLU:HB3	5:L:540:LEU:HD22	2.02	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
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	2.02	0.41
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.02	0.41
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	0.41
3:D:161:THR:HG22	3:D:164:GLN:CD	2.40	0.41
3:D:44:ILE:HD13	3:D:252:LEU:HD13	2.02	0.41
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
3:D:645:VAL:HB	3:D:701:LEU:HD23	2.02	0.41
3:D:697:MET:SD	3:D:741:ALA:HB3	2.60	0.41
3:D:9:LYS:HE2	3:D:9:LYS:HB3	1.93	0.41
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.34	0.41
5:F:287:ILE:HG23	5:F:337:VAL:HG13	2.01	0.41
5:F:376:LYS:O	5:F:380:VAL:HG23	2.20	0.41
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.88	0.41
2:I:446:ASP:N	2:I:446:ASP:OD1	2.53	0.41
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.50	0.41
5:L:584:ARG:O	5:L:587:ILE:HG22	2.20	0.41
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:NH1	2:C:88:ARG:HB2	2.35	0.41
3:D:425:ARG:HG2	3:D:426:ALA:N	2.35	0.41
3:D:620:PHE:O	3:D:624:ILE:HG13	2.20	0.41
3:D:644:MET:SD	3:D:740:LEU:HD23	2.60	0.41
5:F:441:ARG:O	5:F:445:ASP:HB2	2.20	0.41
5:F:550:GLY:HA3	5:F:603:ARG:NH1	2.36	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
2:I:1028:LYS:HE2	2:I:1028:LYS:HB2	1.71	0.41
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.20	0.41
2:I:452:ARG:HG2	2:I:453:ILE:N	2.35	0.41
2:I:730:SER:O	2:I:753:LEU:HB2	2.20	0.41
3:J:564:VAL:HG12	3:J:565:ALA:N	2.35	0.41
5:L:573:LEU:HD23	5:L:573:LEU:H	1.84	0.41
2:C:379:GLU:CD	2:C:379:GLU:H	2.23	0.41
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.50	0.41
3:D:528:THR:HG23	3:D:529:GLY:H	1.85	0.41
3:D:712:GLN:HG2	3:D:713:GLU:H	1.85	0.41
5:F:225:ARG:O	5:F:229:VAL:HG13	2.20	0.41
1:G:111:THR:HB	1:G:126:PRO:O	2.21	0.41
1:H:11:PRO:HB3	1:H:30:PRO:O	2.20	0.41
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	2.02	0.41
3:J:1183:SER:OG	3:J:1184:ASP:N	2.51	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:J:449:LEU:HD22	3:J:466:MET:SD	2.60	0.41
3:J:620:PHE:O	3:J:624:ILE:HG13	2.20	0.41
5:L:551:LEU:HD21	5:L:598:LEU:HD21	2.01	0.41
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	2.02	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.19	0.41
2:C:228:VAL:HB	2:C:335:THR:OG1	2.20	0.41
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	2.02	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.88	0.41
5:F:344:LEU:HA	5:F:344:LEU:HD12	1.86	0.41
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.47	0.41
2:I:198:ILE:O	2:I:201:ARG:HB2	2.20	0.41
2:I:959:ASP:O	2:I:962:GLU:HB2	2.21	0.41
5:L:470:MET:HB3	5:L:474:MET:HG3	2.01	0.41
2:C:1124:ILE:HB	2:C:1180:MET:HB2	2.02	0.41
2:C:246:LEU:HD12	2:C:246:LEU:H	1.85	0.41
2:C:697:LYS:HG2	2:C:698:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1024:THR:HG22	3:D:1026:PRO:HD3	2.02	0.41
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	2.02	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
5:F:470:MET:HB3	5:F:474:MET:HG3	2.01	0.41
1:G:208:ASN:N	1:G:208:ASN:OD1	2.50	0.41
1:G:28:LEU:HD23	1:H:231:PHE:CZ	2.56	0.41
3:J:1348:LYS:HD2	3:J:1348:LYS:HA	1.89	0.41
3:J:407:VAL:O	3:J:411:ILE:HG12	2.20	0.41
3:J:528:THR:HG23	3:J:529:GLY:H	1.85	0.41
5:L:120:ALA:HA	5:L:123:ILE:HD12	2.02	0.41
5:L:388:ILE:HG22	5:L:392:LYS:HE3	2.02	0.41
1:A:137:ASN:OD1	1:A:137:ASN:N	2.51	0.41
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.88	0.41
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.51	0.41
3:D:155:GLU:HB2	3:D:158:GLN:HB2	2.02	0.41
3:D:449:LEU:HD22	3:D:466:MET:SD	2.61	0.41
2:I:169:LYS:O	2:I:170:VAL:HG22	2.18	0.41
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.55	0.41
2:I:484:LEU:CD1	2:I:485:ASP:H	2.34	0.41
2:I:573:ASN:N	2:I:573:ASN:OD1	2.54	0.41
2:I:848:GLU:HG2	2:I:888:THR:HG22	2.01	0.41
3:J:490:ILE:HA	3:J:500:ILE:HG12	2.03	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
1:A:111:THR:HB	1:A:126:PRO:O	2.21	0.41
1:A:45:ARG:HG2	1:B:38:THR:CB	2.50	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
1:G:117:HIS:NE2	1:G:121:VAL:O	2.53	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
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.21	0.41
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.34	0.41
3:J:18:ASP:N	3:J:18:ASP:OD1	2.54	0.41
5:L:554:ARG:HB2	5:L:580:PHE:CE2	2.55	0.41
3:D:1183:SER:OG	3:D:1184:ASP:N	2.51	0.41
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.02	0.41
4:E:53:GLU:HB3	4:E:59:ILE:HG13	2.03	0.41
5:F:554:ARG:HB2	5:F:580:PHE:CE2	2.55	0.41
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:ILE:H	1:G:115:ILE:HG13	1.70	0.41
1:H:102:LEU:O	1:H:141:SER:OG	2.28	0.41
1:H:63:GLY:HA3	1:H:71:LYS:HD3	2.03	0.41
2:I:1124:ILE:HB	2:I:1180:MET:HB2	2.02	0.41
2:I:1340:GLU:OE2	3:J:21:LYS:HE3	2.20	0.41
2:I:985:GLU:HB3	2:I:988:LYS:HB2	2.03	0.41
3:J:844:THR:HG21	3:J:858:VAL:HG21	2.02	0.41
1:A:57:THR:O	1:A:173:VAL:HG22	2.21	0.41
2:C:462:ASN:O	2:C:465:ARG:HB3	2.21	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
4:E:31:GLN:HB2	4:E:46:THR:HG21	2.03	0.41
2:I:980:VAL:HG13	2:I:984:VAL:HG23	2.03	0.41
3:J:646:ILE:HG22	3:J:647:PRO:HD2	2.03	0.41
5:L:224:LEU:HB2	5:L:259:PHE:CZ	2.56	0.41
2:C:1340:GLU:OE2	3:D:21:LYS:HE3	2.21	0.41
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.03	0.41
2:C:624:ASP:OD1	2:C:625:GLU:HG3	2.21	0.41
3:D:860:ARG:HD2	3:D:860:ARG:HA	1.89	0.41
5:F:466:ILE:HG13	5:F:466:ILE:H	1.41	0.41
1:H:108:GLY:HA2	1:H:109:PRO:HD3	1.92	0.41
1:G:221:ALA:HB1	1:H:228:LEU:HD22	2.02	0.41
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	2.02	0.41
2:I:496:LYS:HA	2:I:499:SER:HB3	2.03	0.41
2:C:673:HIS:O	2:C:1109:ILE:HG22	2.21	0.41
2:C:730:SER:O	2:C:753:LEU:HB2	2.20	0.41
2:C:91:THR:HG21	2:C:503:LYS:CE	2.50	0.41
3:D:646:ILE:HG22	3:D:647:PRO:HD2	2.02	0.41
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.03	0.41
1:H:59:VAL:O	1:H:171:LEU:HA	2.21	0.41
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.20	0.41
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.51	0.41
2:I:786:GLY:N	2:I:789:THR:OG1	2.42	0.41
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	2.03	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.87	0.41
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.56	0.41
3:J:645:VAL:HB	3:J:701:LEU:HD23	2.02	0.41
3:J:70:CYS:SG	3:J:71:LEU:N	2.94	0.41
3:J:475:GLU:CD	4:K:28:ARG:HH22	2.23	0.41
5:L:269:LEU:O	5:L:273:MET:HG3	2.20	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)
1:A:39:LEU:O	1:A:43:LEU:HG	2.22	0.40
2:C:573:ASN:N	2:C:573:ASN:OD1	2.54	0.40
3:D:1162:ILE:O	3:D:1178:THR:OG1	2.19	0.40
3:D:849:LEU:HD22	3:D:849:LEU:H	1.86	0.40
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.78	0.40
2:I:246:LEU:HD12	2:I:246:LEU:H	1.85	0.40
2:I:724:VAL:HG23	2:I:775:GLU:O	2.21	0.40
3:J:1177:ILE:HG13	3:J:1177:ILE:H	1.69	0.40
3:J:123:ARG:HA	3:J:123:ARG:HD3	1.87	0.40
3:J:1256:ILE:HG22	3:J:1260:MET:HE2	2.03	0.40
3:J:1332:LEU:HA	3:J:1332:LEU:HD13	1.93	0.40
3:J:418:GLU:O	3:J:420:PRO:HD3	2.21	0.40
3:J:425:ARG:HG2	3:J:426:ALA:N	2.35	0.40
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.87	0.40
3:J:488:ASN:HA	3:J:488:ASN:HD22	1.68	0.40
3:J:810:THR:HG23	3:J:811:GLU:H	1.87	0.40
5:L:376:LYS:O	5:L:380:VAL:HG23	2.22	0.40
1:A:125:LYS:HE2	1:A:128:HIS:HB2	2.02	0.40
2:C:519:ASN:HA	2:C:520:PRO:HD3	1.95	0.40
2:C:758:ARG:HD2	2:C:835:GLU:HB2	2.04	0.40
2:C:992:LEU:HB2	2:C:993:PRO:HD2	2.03	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:D:793:SER:O	3:D:797:THR:HG23	2.21	0.40
5:F:364:ARG:HA	5:F:367:ILE:HD12	2.02	0.40
5:F:584:ARG:O	5:F:587:ILE:HG22	2.21	0.40
1:G:38:THR:OG1	1:H:45:ARG:HD3	2.21	0.40
1:H:182:ARG:NH1	3:J:581:MET:SD	2.94	0.40
2:I:521:LEU:HA	2:I:524:ILE:HG22	2.02	0.40
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.21	0.40
3:J:899:TYR:O	3:J:1251:LYS:HD3	2.21	0.40
3:J:709:ARG:O	3:J:711:GLY:N	2.53	0.40
5:L:105:MET:HE3	5:L:384:LEU:HB2	2.02	0.40
5:L:225:ARG:O	5:L:229:VAL:HG13	2.21	0.40
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.57	0.40
3:D:140:TYR:HB3	5:F:100:MET:SD	2.61	0.40
5:F:339:ARG:HA	5:F:339:ARG:HD2	1.97	0.40
5:F:551:LEU:HD21	5:F:598:LEU:HD21	2.03	0.40
1:G:152:TYR:CZ	2:I:824:GLN:HA	2.57	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)
3:J:140:TYR:HB3	5:L:100:MET:SD	2.61	0.40
6:N:13:ASN:N	6:N:34:GLU:HG2	2.36	0.40
1:A:60:GLU:HB2	1:A:170:ARG:HG2	2.03	0.40
2:C:1289:GLU:HB3	2:C:1315:MET:SD	2.61	0.40
2:C:232:ILE:HD12	2:C:330:HIS:O	2.21	0.40
2:C:496:LYS:HA	2:C:499:SER:HB3	2.03	0.40
5:F:388:ILE:HG22	5:F:392:LYS:HE3	2.02	0.40
1:G:11:PRO:HD2	1:H:227:GLN:HA	2.02	0.40
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.86	0.40
2:I:462:ASN:O	2:I:465:ARG:HB3	2.21	0.40
3:J:124:ILE:O	3:J:128:LEU:HG	2.22	0.40
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.21	0.40
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.94	0.40
5:L:139:GLU:HG3	5:L:351:THR:HA	2.03	0.40
1:B:212:ASP:OD1	1:B:214:GLU:HB3	2.22	0.40
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.47	0.40
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.22	0.40
2:C:32:LEU:HA	2:C:130:MET:SD	2.62	0.40
2:C:363:LEU:HB3	2:C:381:ALA:HB1	2.04	0.40
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.21	0.40
3:D:124:ILE:O	3:D:128:LEU:HG	2.21	0.40
3:D:407:VAL:O	3:D:411:ILE:HG12	2.21	0.40
3:D:488:ASN:HD22	3:D:488:ASN:HA	1.67	0.40
3:D:746:LEU:HB2	3:D:754:ILE:HD11	2.04	0.40
5:F:555:GLU:HA	5:F:558:VAL:HG12	2.02	0.40
1:G:60:GLU:HB2	1:G:170:ARG:HG2	2.03	0.40
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	2.02	0.40
2:I:379:GLU:H	2:I:379:GLU:CD	2.24	0.40
3:J:1075:ARG:HH21	3:J:1166:GLY:HA2	1.87	0.40
5:L:394:TYR:OH	5:L:436:ARG:HG2	2.21	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%)	8	41
1	B	216/239 (90%)	189 (88%)	27 (12%)	0	100	100
1	G	226/239 (95%)	202 (89%)	20 (9%)	4 (2%)	8	41
1	H	213/239 (89%)	187 (88%)	26 (12%)	0	100	100
2	C	1338/1342 (100%)	1213 (91%)	121 (9%)	4 (0%)	41	75
2	I	1338/1342 (100%)	1216 (91%)	117 (9%)	5 (0%)	34	71
3	D	1339/1407 (95%)	1217 (91%)	120 (9%)	2 (0%)	51	83
3	J	1317/1407 (94%)	1201 (91%)	115 (9%)	1 (0%)	51	83
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%)	47	79
5	L	463/522 (89%)	415 (90%)	47 (10%)	1 (0%)	47	79
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%)	41	75

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%)	20	49
1	B	184/206 (89%)	167 (91%)	17 (9%)	9	34
1	G	191/206 (93%)	180 (94%)	11 (6%)	20	49
1	H	183/206 (89%)	166 (91%)	17 (9%)	9	33
2	C	1155/1157 (100%)	1052 (91%)	103 (9%)	9	36
2	I	1154/1157 (100%)	1056 (92%)	98 (8%)	10	39
3	D	1125/1168 (96%)	1036 (92%)	89 (8%)	12	41
3	J	1110/1168 (95%)	1023 (92%)	87 (8%)	12	41
4	E	72/75 (96%)	69 (96%)	3 (4%)	30	57
4	K	67/75 (89%)	65 (97%)	2 (3%)	41	64
5	F	417/462 (90%)	383 (92%)	34 (8%)	11	39
5	L	418/462 (90%)	386 (92%)	32 (8%)	13	41
6	M	44/56 (79%)	38 (86%)	6 (14%)	3	21
6	N	44/56 (79%)	38 (86%)	6 (14%)	3	21
All	All	6355/6660 (95%)	5839 (92%)	516 (8%)	11	40

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	224/239 (93%)	0.06	5 (2%) 62 52	48, 85, 138, 169	0
1	B	220/239 (92%)	0.37	14 (6%) 19 15	46, 110, 148, 166	0
1	G	228/239 (95%)	0.08	13 (5%) 23 20	48, 94, 141, 167	0
1	H	217/239 (90%)	0.33	14 (6%) 18 15	48, 111, 150, 167	0
2	C	1340/1342 (99%)	-0.08	36 (2%) 54 44	12, 74, 129, 163	0
2	I	1340/1342 (99%)	0.04	59 (4%) 34 29	12, 78, 143, 189	0
3	D	1345/1407 (95%)	-0.08	29 (2%) 62 52	13, 61, 142, 194	0
3	J	1325/1407 (94%)	-0.14	21 (1%) 72 62	10, 63, 139, 195	0
4	E	89/91 (97%)	-0.22	0 100 100	30, 77, 122, 138	0
4	K	79/91 (86%)	-0.28	0 100 100	32, 76, 121, 164	0
5	F	470/522 (90%)	-0.16	8 (1%) 70 61	25, 98, 147, 179	0
5	L	469/522 (89%)	-0.16	9 (1%) 66 58	28, 96, 150, 181	0
6	M	51/64 (79%)	0.53	1 (1%) 65 56	66, 115, 146, 158	0
6	N	51/64 (79%)	0.31	3 (5%) 22 18	64, 112, 143, 149	0
All	All	7448/7808 (95%)	-0.04	212 (2%) 53 42	10, 79, 142, 195	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.6
2	I	981	ALA	8.1
3	J	1059	LEU	6.5
2	I	995	ASP	5.6
1	B	146	VAL	5.5
2	I	985	GLU	5.1
2	C	258	ASN	5.0
5	F	167	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
2	I	967	LEU	4.9
1	G	95	LYS	4.8
2	C	165	HIS	4.5
2	I	1018	TYR	4.4
1	B	8	PHE	4.4
1	H	146	VAL	4.4
2	I	1022	LYS	4.3
2	I	972	PHE	4.2
5	L	167	ASP	4.2
2	I	1002	LEU	4.2
5	L	165	PHE	4.2
2	I	971	LEU	4.2
2	I	977	ALA	4.1
5	L	287	ILE	4.1
1	B	121	VAL	4.1
1	B	120	ASP	4.0
5	F	603	ARG	4.0
2	I	968	GLU	4.0
2	I	998	LEU	3.9
2	C	251	ALA	3.9
1	A	193	GLU	3.8
2	C	489	PRO	3.8
5	F	165	PHE	3.8
2	I	970	GLY	3.8
1	H	96	ASP	3.8
3	J	1080	ILE	3.8
3	D	1054	THR	3.7
2	I	973	SER	3.7
2	I	1021	LEU	3.7
5	L	294	GLN	3.6
5	L	480	PRO	3.6
2	I	975	ILE	3.6
3	D	952	VAL	3.6
2	C	332	ARG	3.6
1	B	92	VAL	3.5
2	I	996	ARG	3.5
3	D	1065	ALA	3.5
3	J	1054	THR	3.5
1	G	97	GLU	3.5
1	H	97	GLU	3.5
2	I	867	GLU	3.4
2	C	231	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	282	VAL	3.3
2	I	168	GLY	3.3
1	H	72	GLU	3.3
2	C	333	ILE	3.3
5	F	579	GLN	3.2
1	G	96	ASP	3.2
5	L	290	LEU	3.2
1	H	172	LEU	3.2
2	C	252	SER	3.1
5	L	326	TRP	3.1
3	J	1273	ASP	3.0
1	H	12	ARG	3.0
1	B	90	VAL	3.0
2	C	237	LEU	3.0
2	I	1017	GLN	3.0
3	J	201	LEU	3.0
3	J	1035	VAL	3.0
2	C	184	LEU	2.9
2	I	988	LYS	2.9
2	I	974	ARG	2.9
5	L	286	LEU	2.9
1	B	145	LYS	2.9
3	D	1064	SER	2.9
3	D	1168	GLU	2.9
1	A	90	VAL	2.9
3	D	958	ILE	2.8
3	J	1114	GLN	2.8
2	I	882	ILE	2.8
2	C	277	LEU	2.8
2	C	261	VAL	2.8
2	I	492	MET	2.8
2	I	969	ALA	2.8
2	I	169	LYS	2.8
1	H	92	VAL	2.8
2	I	984	VAL	2.7
3	J	1181	ASP	2.7
2	C	266	GLY	2.7
1	H	123	ILE	2.7
1	B	30	PRO	2.7
1	H	158	ARG	2.7
3	D	965	SER	2.7
3	D	712	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	I	989	LEU	2.7
1	H	55	ALA	2.7
1	A	194	GLN	2.7
3	J	1034	PHE	2.7
2	C	331	LYS	2.7
6	N	63	PRO	2.7
2	C	253	PHE	2.7
2	I	725	GLN	2.7
2	I	857	VAL	2.7
3	D	1039	ASP	2.7
3	D	993	GLU	2.6
2	C	479	LEU	2.6
2	C	240	GLU	2.6
2	I	980	VAL	2.6
3	D	1055	GLY	2.6
2	I	629	PHE	2.6
2	C	102	LEU	2.6
3	J	1079	LYS	2.6
2	I	1023	HIS	2.6
2	I	236	LYS	2.6
3	J	319	SER	2.6
2	I	165	HIS	2.6
2	I	1003	THR	2.6
2	I	251	ALA	2.6
1	B	9	LEU	2.5
2	I	1004	ASP	2.5
1	G	28	LEU	2.5
2	I	1014	LEU	2.5
2	C	997	TRP	2.5
2	I	332	ARG	2.5
3	D	826	ILE	2.5
2	I	1001	GLY	2.5
2	I	167	SER	2.5
1	H	106	GLY	2.5
2	C	265	LYS	2.5
2	C	255	ILE	2.4
3	D	89	GLY	2.4
6	M	31	ILE	2.4
1	B	144	ILE	2.4
3	D	1013	GLY	2.4
3	D	1015	GLU	2.4
2	C	230	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	1012	ALA	2.4
3	D	1006	GLY	2.4
2	C	485	ASP	2.4
2	I	735	LYS	2.4
2	C	319	LEU	2.4
1	B	67	GLU	2.3
1	G	127	GLN	2.3
1	G	193	GLU	2.3
1	G	194	GLN	2.3
5	F	111	LEU	2.3
3	D	1007	ASP	2.3
2	I	720	ARG	2.3
2	I	861	ALA	2.3
2	I	1006	GLU	2.3
6	N	31	ILE	2.3
3	J	1109	LEU	2.3
2	I	203	LYS	2.2
2	I	1000	LEU	2.2
3	J	518	VAL	2.2
3	D	524	GLY	2.2
3	D	1014	GLY	2.2
2	I	983	GLY	2.2
3	D	950	ILE	2.2
3	J	712	GLN	2.2
1	H	13	LEU	2.2
3	J	708	ASN	2.2
6	N	52	PHE	2.2
2	C	370	MET	2.2
1	B	31	LEU	2.2
1	H	65	LEU	2.2
1	H	147	GLN	2.2
1	A	52	PRO	2.2
2	I	263	VAL	2.2
2	I	230	PHE	2.2
5	F	164	GLY	2.2
2	I	1149	TYR	2.2
1	A	98	VAL	2.2
2	C	1000	LEU	2.2
5	F	480	PRO	2.1
2	C	239	MET	2.1
2	C	163	LYS	2.1
2	I	632	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	1104	LYS	2.1
1	B	205	MET	2.1
3	J	849	LEU	2.1
3	D	995	TYR	2.1
5	F	166	VAL	2.1
1	G	19	VAL	2.1
2	C	939	VAL	2.1
2	C	256	GLU	2.1
2	I	862	LEU	2.1
3	D	982	LEU	2.1
3	J	1056	LEU	2.1
2	C	257	ALA	2.1
1	G	148	ARG	2.1
1	G	24	ALA	2.1
3	D	966	VAL	2.1
3	D	1169	THR	2.1
3	J	1186	TYR	2.1
1	G	126	PRO	2.1
2	C	234	ASP	2.0
2	I	333	ILE	2.0
3	D	1042	ASP	2.0
5	L	598	LEU	2.0
1	B	61	ILE	2.0
2	C	492	MET	2.0
2	C	264	GLU	2.0
2	I	976	ARG	2.0
1	G	214	GLU	2.0
3	D	1051	ASP	2.0
2	I	170	VAL	2.0
2	I	771	VAL	2.0
1	G	90	VAL	2.0
2	C	287	VAL	2.0
3	J	715	LYS	2.0
3	J	1085	GLY	2.0
3	J	1106	ILE	2.0
3	D	1072	LYS	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	D	1501	1/1	0.70	0.44	41,41,41,41	0
7	MG	J	1501	1/1	0.81	0.35	40,40,40,40	0
8	ZN	D	1502	1/1	0.90	0.18	193,193,193,193	0
8	ZN	J	1502	1/1	0.98	0.06	71,71,71,71	0
8	ZN	D	1503	1/1	0.99	0.21	36,36,36,36	0
8	ZN	J	1503	1/1	1.00	0.15	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.