



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 4LK1 / pdb_00004lk1
Title : Crystal Structure Analysis of the E.coli holoenzyme
Authors : Bae, B.; Darst, S.A.
Deposited on : 2013-07-05
Resolution : 3.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

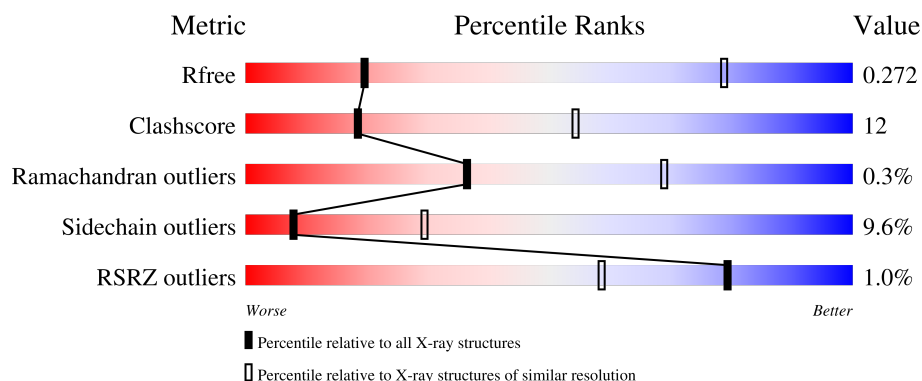
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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}	180053	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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

Mol	Chain	Length	Quality of chain
1	A	239	% 62% 28% • 6%
1	B	239	% 59% 29% • 8%
1	G	239	3% 62% 28% 5% 5%
1	H	239	% 56% 30% • 9%
2	C	1342	% 67% 29% •

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Mol	Chain	Length	Quality of chain
2	I	1342	% 68% 28%
3	D	1407	% 53% 26% 17%
3	J	1407	% 60% 31% 5%
4	E	91	67% 26%
4	K	91	57% 27% 13%
5	F	613	% 59% 26% 12%
5	L	613	% 59% 26% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 57170 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	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1334	Total	C	N	O	S	0	0	0
			10369	6513	1850	1957	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	542	Total	C	N	O	S	0	0	0
			4204	2625	752	801	26			
5	L	539	Total	C	N	O	S	0	0	0
			4196	2619	749	802	26			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

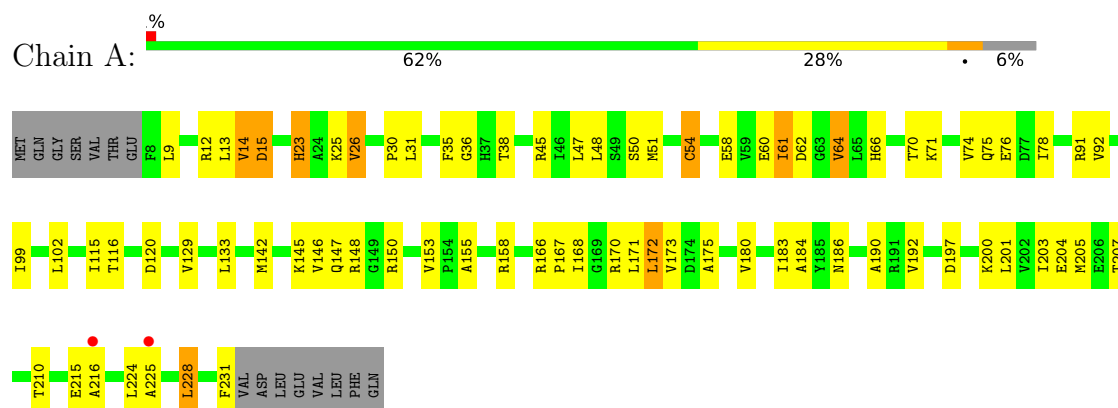
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

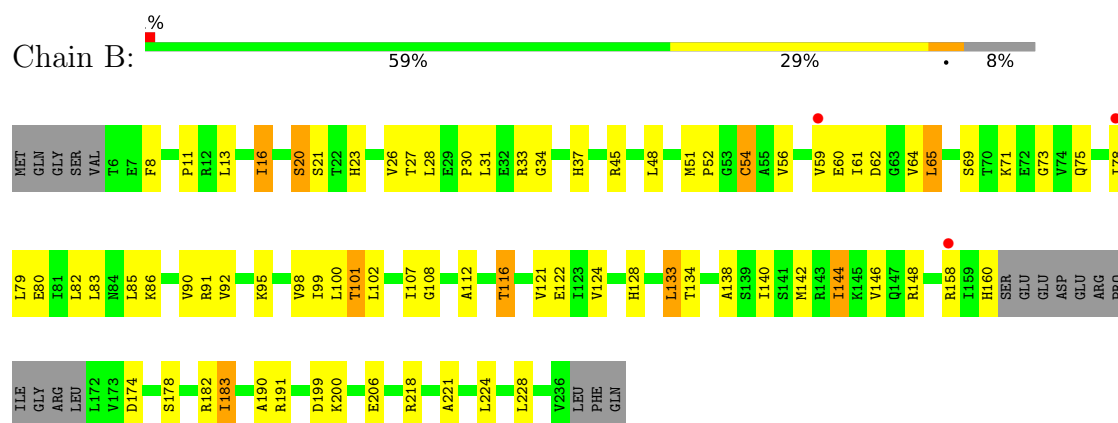
3 Residue-property plots [i](#)

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

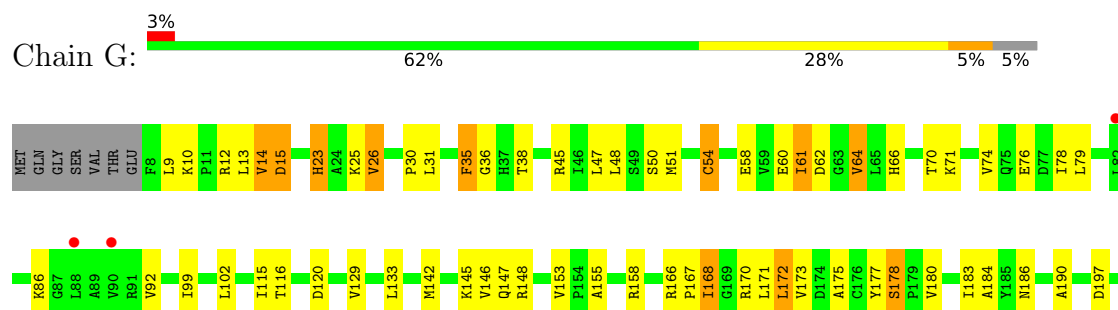
- Molecule 1: DNA-directed RNA polymerase subunit alpha



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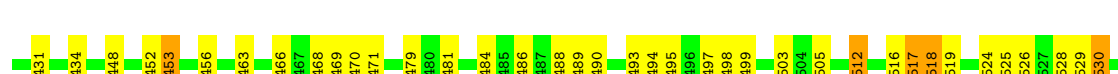
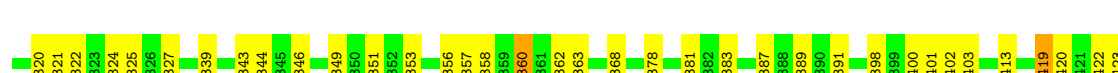


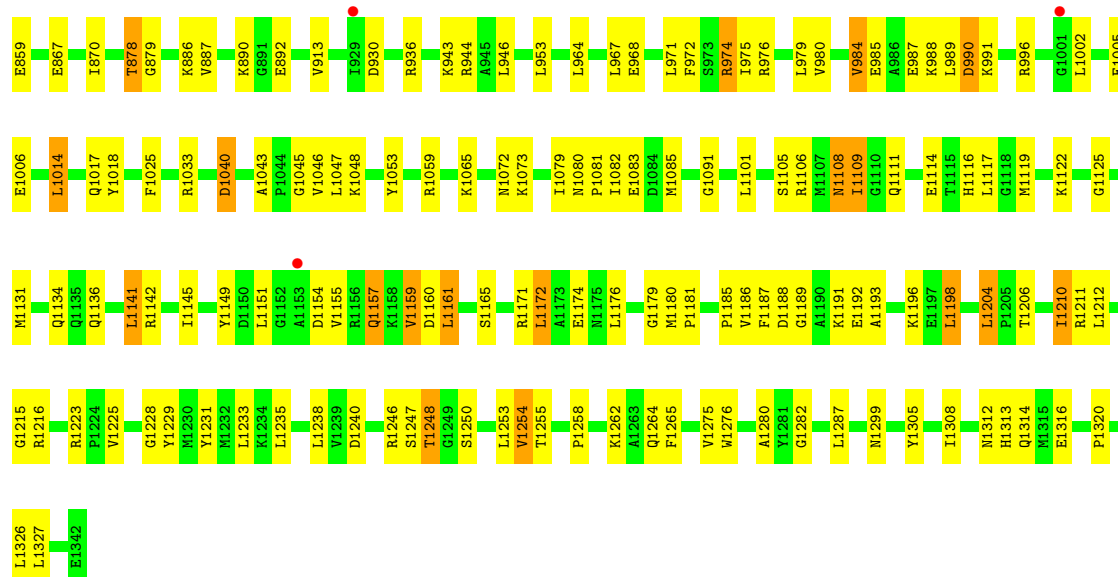


• Molecule 1: DNA-directed RNA polymerase subunit alpha

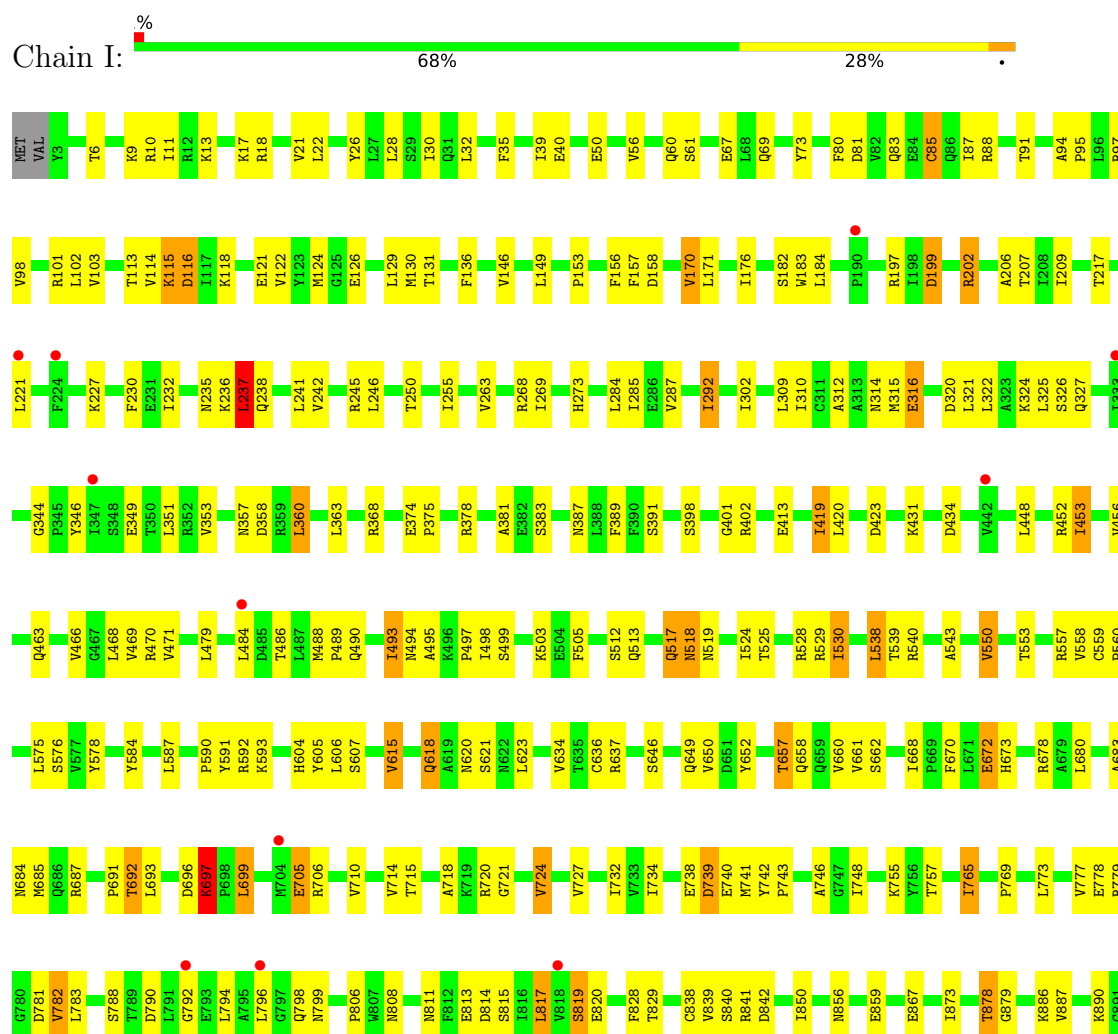


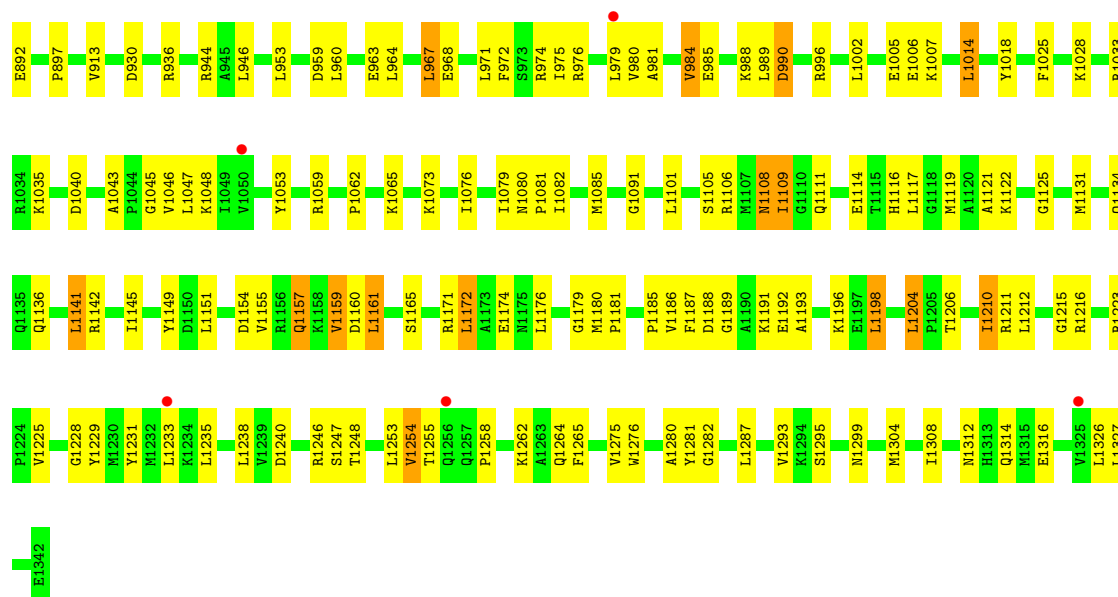
• Molecule 2: DNA-directed RNA polymerase subunit beta



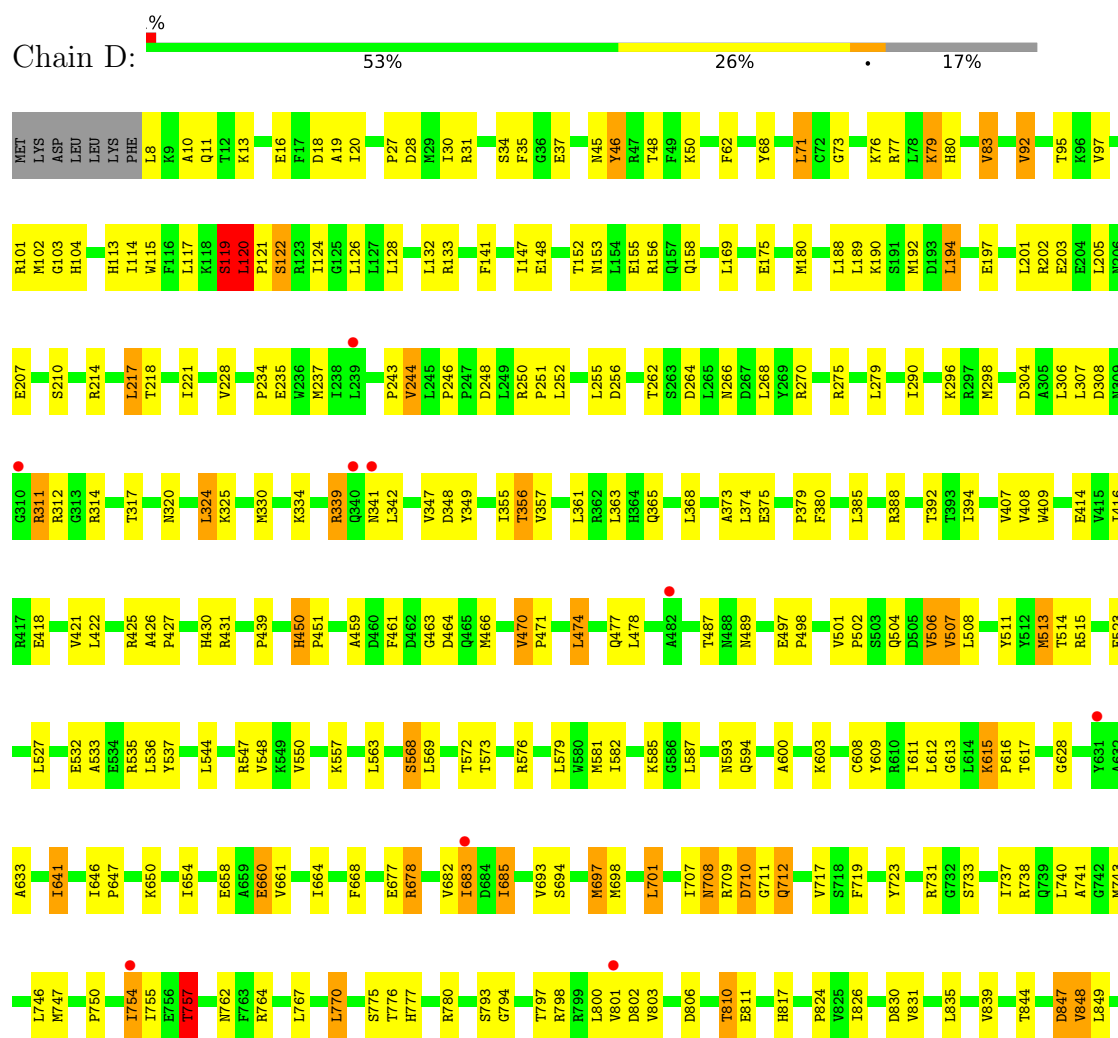


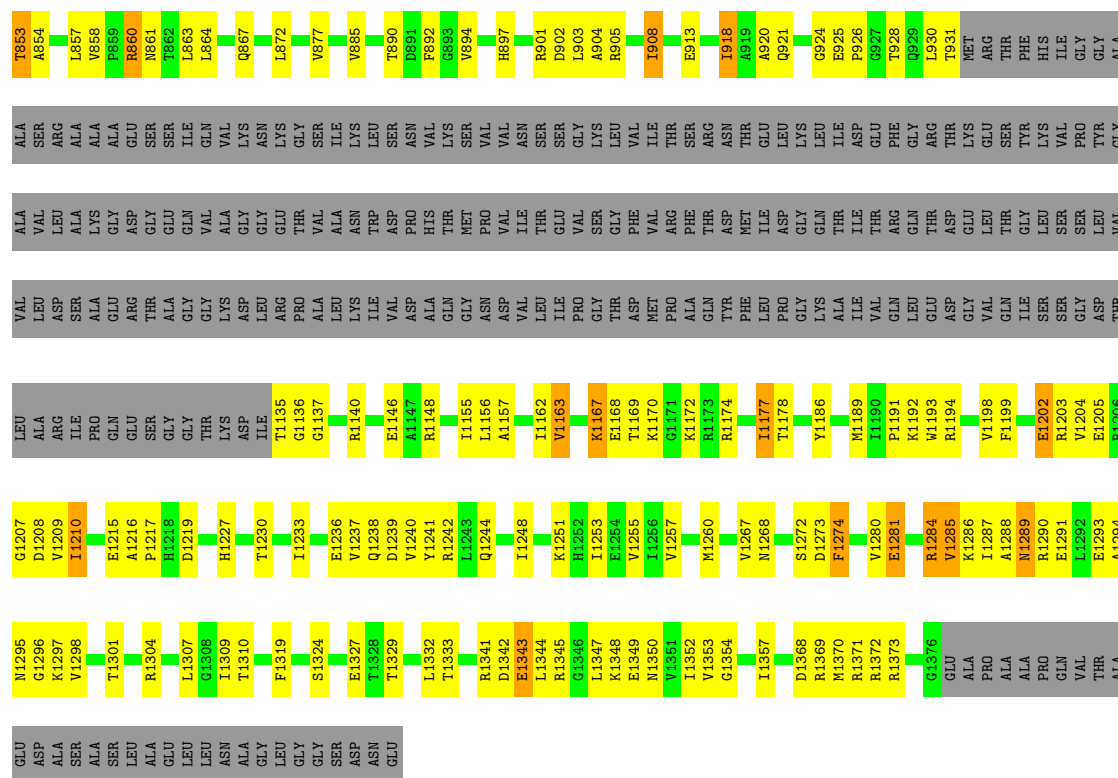
• Molecule 2: DNA-directed RNA polymerase subunit beta



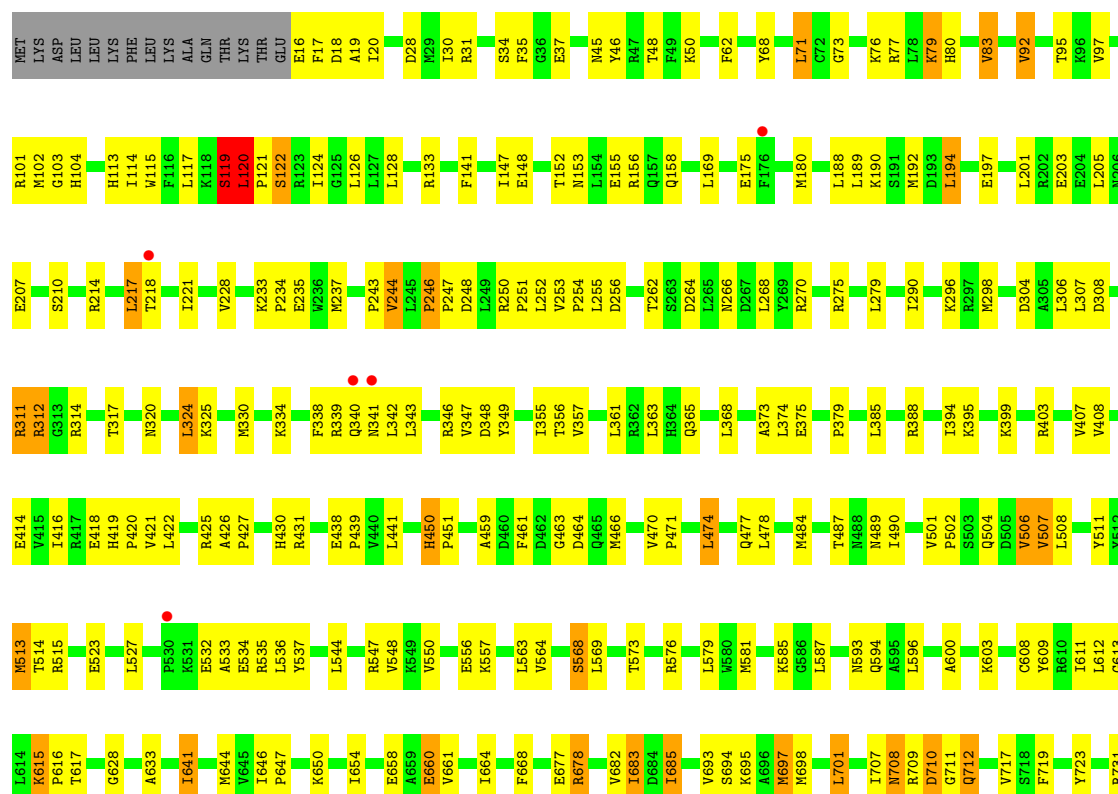


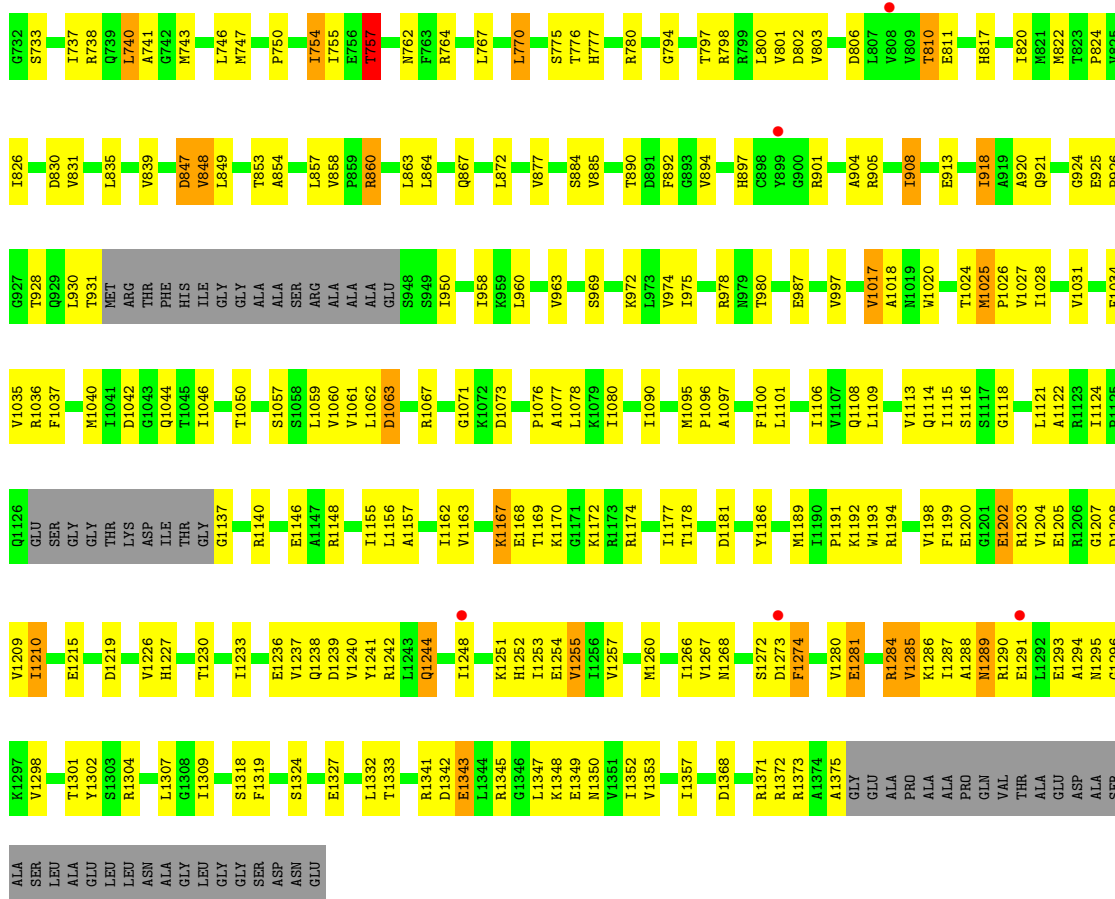
• Molecule 3: DNA-directed RNA polymerase subunit beta'



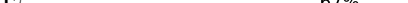


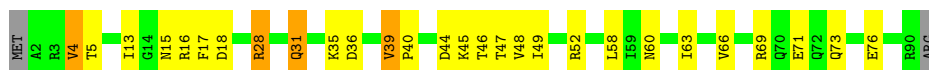
• Molecule 3: DNA-directed RNA polymerase subunit beta'



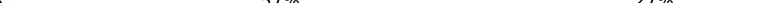


- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  67% 26% . . .

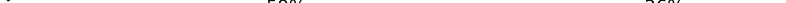


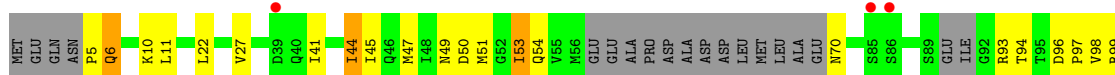
- Molecule 4: DNA-directed RNA polymerase subunit omega

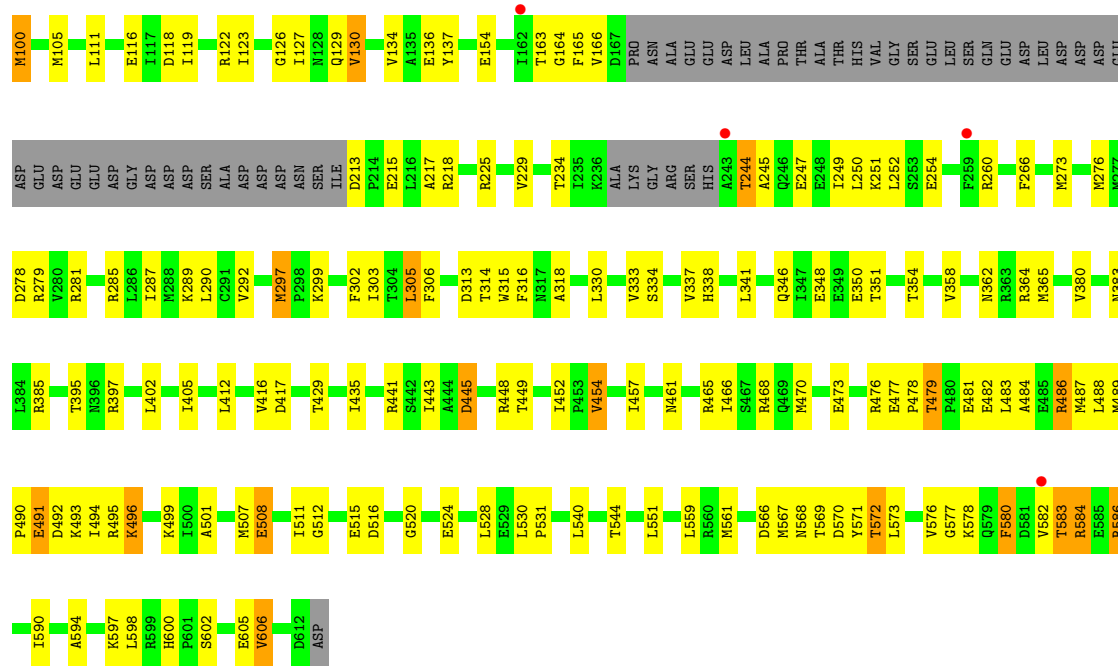
Chain K:  57% 27% • 13%



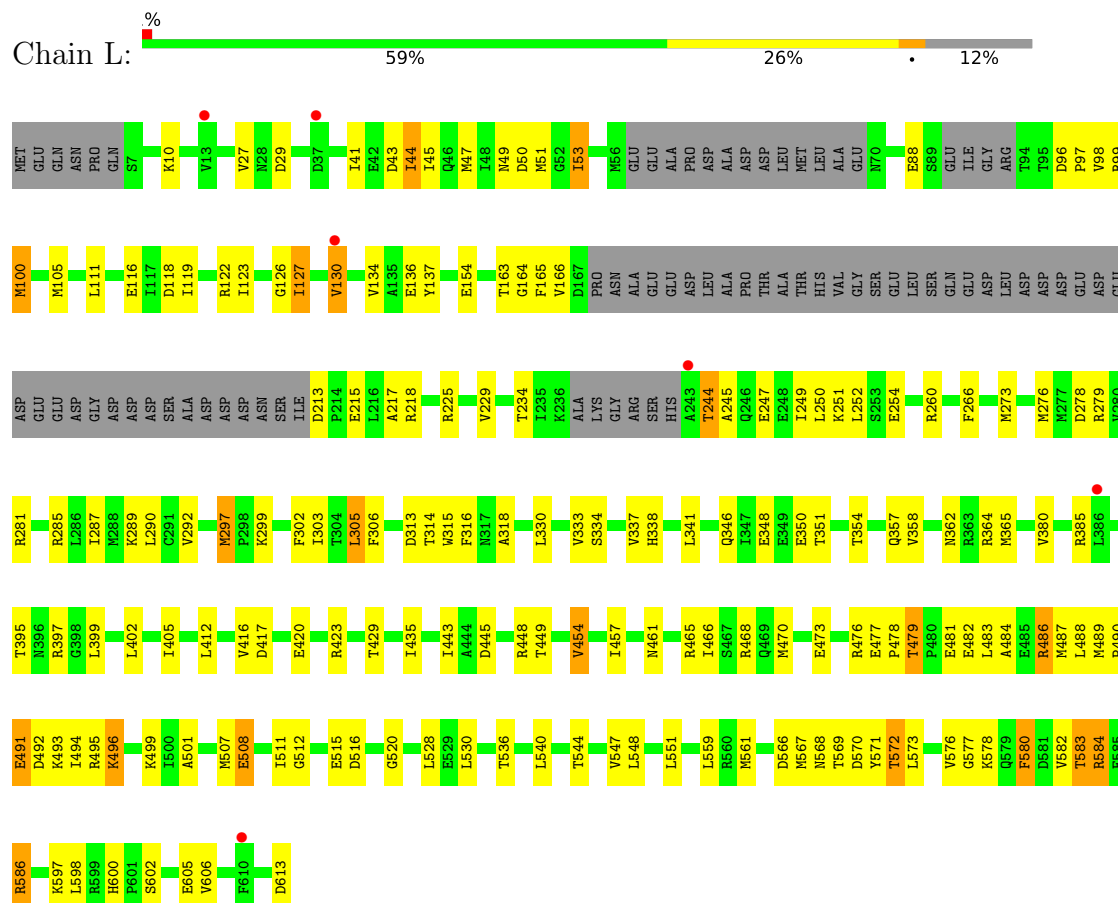
- Molecule 5: RNA polymerase sigma factor RpoD

Chain F:  59% 26% 12%





• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.68Å 206.39Å 308.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.78 – 3.84 44.78 – 3.84	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.78-3.84) 98.2 (44.78-3.84)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.224 , 0.272 0.224 , 0.272	Depositor DCC
R_{free} test set	5708 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	142.8	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	57170	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/1751	0.85	2/2373 (0.1%)
1	B	0.35	0/1707	0.84	3/2314 (0.1%)
1	G	0.34	0/1771	0.87	2/2401 (0.1%)
1	H	0.34	0/1686	0.83	3/2285 (0.1%)
2	C	0.36	0/10739	0.81	10/14489 (0.1%)
2	I	0.34	0/10735	0.80	9/14484 (0.1%)
3	D	0.37	0/9246	0.84	17/12478 (0.1%)
3	J	0.36	0/10525	0.83	17/14212 (0.1%)
4	E	0.37	0/693	0.82	0/935
4	K	0.35	0/629	0.83	0/847
5	F	0.37	0/4254	0.87	11/5731 (0.2%)
5	L	0.38	0/4246	0.85	7/5720 (0.1%)
All	All	0.36	0/57982	0.83	81/78269 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	4
3	J	0	2
5	F	0	2
5	L	0	1
All	All	0	10

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	11	LEU	N-CA-C	-11.49	86.33	110.80
3	D	120	LEU	CA-C-N	-10.09	107.23	119.84
3	D	120	LEU	C-N-CA	-10.09	107.23	119.84
5	L	53	ILE	N-CA-C	8.60	120.57	109.30
5	F	53	ILE	N-CA-C	8.58	120.53	109.30
5	F	51	MET	N-CA-C	8.26	122.14	112.72
3	D	339	ARG	N-CA-C	8.04	121.66	112.57
5	L	51	MET	N-CA-C	8.04	121.89	112.72
3	D	120	LEU	N-CA-C	6.97	125.21	109.81
3	J	120	LEU	N-CA-C	6.96	125.18	109.81
2	I	237	LEU	N-CA-C	6.91	125.53	110.80
3	J	757	THR	CA-C-N	6.83	127.76	120.11
3	J	757	THR	C-N-CA	6.83	127.76	120.11
3	D	757	THR	CA-C-N	6.83	127.75	120.11
3	D	757	THR	C-N-CA	6.83	127.75	120.11
5	F	6	GLN	N-CA-C	6.77	121.43	111.34
1	B	108	GLY	CA-C-N	6.65	126.67	119.89
1	B	108	GLY	C-N-CA	6.65	126.67	119.89
2	C	1157	GLN	N-CA-C	6.52	118.97	111.02
1	H	108	GLY	CA-C-N	6.51	126.53	119.89
1	H	108	GLY	C-N-CA	6.51	126.53	119.89
2	I	1157	GLN	N-CA-C	6.36	118.78	111.02
3	J	119	SER	N-CA-C	6.33	120.79	111.87
2	C	512	SER	CA-C-N	-6.32	112.07	122.11
2	C	512	SER	C-N-CA	-6.32	112.07	122.11
3	D	122	SER	N-CA-C	-5.94	101.11	109.96
3	D	1210	ILE	N-CA-C	-5.91	106.98	112.83
5	L	163	THR	N-CA-C	-5.84	106.02	113.02
3	J	1210	ILE	N-CA-C	-5.81	107.08	112.83
1	G	232	VAL	N-CA-C	5.76	121.33	109.34
5	F	163	THR	N-CA-C	-5.75	106.12	113.02
2	C	237	LEU	N-CA-C	5.68	122.89	110.80
2	I	236	LYS	N-CA-C	5.67	117.54	110.91
5	F	584	ARG	N-CA-C	5.62	116.31	108.00
5	F	5	PRO	N-CA-CB	5.61	109.18	103.00
2	C	1316	GLU	CA-C-N	5.61	124.80	118.97
2	C	1316	GLU	C-N-CA	5.61	124.80	118.97
2	I	1316	GLU	CA-C-N	5.60	124.79	118.97
2	I	1316	GLU	C-N-CA	5.60	124.79	118.97
1	A	23	HIS	N-CA-C	5.60	116.75	108.86
3	J	122	SER	N-CA-C	-5.57	101.66	109.96
5	L	584	ARG	N-CA-C	5.56	116.23	108.00
2	I	398	SER	CB-CA-C	-5.55	109.18	115.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	250	ARG	CA-C-N	5.54	125.47	119.76
3	D	250	ARG	C-N-CA	5.54	125.47	119.76
2	C	398	SER	CB-CA-C	-5.54	109.20	115.79
3	D	19	ALA	CB-CA-C	-5.51	109.23	115.79
5	F	213	ASP	CA-C-N	5.47	125.12	119.05
5	F	213	ASP	C-N-CA	5.47	125.12	119.05
2	I	1159	VAL	N-CA-C	5.46	120.69	109.34
5	L	213	ASP	CA-C-N	5.44	125.09	119.05
5	L	213	ASP	C-N-CA	5.44	125.09	119.05
1	H	20	SER	CB-CA-C	-5.40	109.89	117.23
2	I	513	GLN	N-CA-C	5.39	116.47	108.86
1	B	20	SER	CB-CA-C	-5.37	109.92	117.23
2	C	1159	VAL	N-CA-C	5.37	120.51	109.34
5	L	166	VAL	N-CA-C	-5.37	101.75	108.84
1	G	23	HIS	N-CA-C	5.34	116.39	108.86
3	J	19	ALA	CB-CA-C	-5.33	109.44	115.79
3	J	250	ARG	CA-C-N	5.32	125.24	119.76
3	J	250	ARG	C-N-CA	5.32	125.24	119.76
3	D	830	ASP	N-CA-C	5.29	117.89	109.96
3	J	450	HIS	CA-C-N	5.27	124.90	119.05
3	J	450	HIS	C-N-CA	5.27	124.90	119.05
5	F	166	VAL	N-CA-C	-5.25	101.91	108.84
3	D	450	HIS	CA-C-N	5.24	124.86	119.05
3	D	450	HIS	C-N-CA	5.24	124.86	119.05
3	J	830	ASP	N-CA-C	5.24	117.81	109.96
3	D	470	VAL	CA-C-N	5.19	126.32	119.84
3	D	470	VAL	C-N-CA	5.19	126.32	119.84
3	J	470	VAL	CA-C-N	5.18	126.31	119.84
3	J	470	VAL	C-N-CA	5.18	126.31	119.84
3	D	1344	LEU	CB-CA-C	-5.16	110.21	117.23
1	A	192	VAL	N-CA-C	-5.12	104.47	110.05
2	I	199	ASP	CB-CA-C	-5.10	109.20	116.34
2	C	199	ASP	CB-CA-C	-5.10	109.20	116.34
5	F	383	ASN	N-CA-C	5.07	119.56	113.17
2	C	573	ASN	CB-CA-C	-5.06	109.25	116.34
3	J	246	PRO	CA-C-N	5.03	124.64	119.05
3	J	246	PRO	C-N-CA	5.03	124.64	119.05
3	J	312	ARG	CB-CA-C	-5.01	109.32	116.34

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1161	LEU	Peptide
3	D	119	SER	Mainchain,Peptide
3	D	120	LEU	Peptide
3	D	1296	GLY	Peptide
5	F	10	LYS	Peptide
5	F	6	GLN	Peptide
3	J	120	LEU	Peptide
3	J	1296	GLY	Peptide
5	L	10	LYS	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	48	0
1	B	1687	0	1700	53	0
1	G	1750	0	1764	54	0
1	H	1667	0	1689	53	0
2	C	10570	0	10582	259	0
2	I	10566	0	10576	250	0
3	D	9107	0	9308	261	0
3	J	10369	0	10589	299	0
4	E	691	0	695	18	0
4	K	627	0	634	14	0
5	F	4204	0	4106	98	0
5	L	4196	0	4103	105	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	57170	0	57502	1381	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 (1381) 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:J:660:GLU:HB3	3:J:685:ILE:HD12	1.47	0.96
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.47	0.92
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.84
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.42	0.84
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.43	0.84
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.27	0.83
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.62	0.82
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.26	0.82
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.62	0.82
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.62	0.81
3:J:418:GLU:HG3	4:K:45:LYS:H	1.45	0.81
3:D:418:GLU:HG3	4:E:45:LYS:H	1.46	0.81
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.64	0.80
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.46	0.79
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.48	0.79
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.64	0.78
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.67	0.77
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.77
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.66	0.77
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.48	0.77
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.64	0.77
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.66	0.76
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.67	0.76
1:A:231:PHE:HZ	1:B:221:ALA:HB3	1.51	0.76
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.67	0.75
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.68	0.75
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.69	0.75
3:J:133:ARG:HB2	5:L:88:GLU:HA	1.68	0.74
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.69	0.74
5:F:470:MET:HA	5:F:473:GLU:HB3	1.68	0.74
3:D:514:THR:HG23	3:D:576:ARG:HG2	1.70	0.74
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.69	0.74
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.68	0.73
3:D:251:PRO:HD2	5:F:507:MET:HE1	1.69	0.73
5:L:470:MET:HA	5:L:473:GLU:HB3	1.69	0.73
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.69	0.73
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.69	0.73
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.22	0.73
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.71	0.73
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.22	0.73
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.71	0.72
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.70	0.72
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.71	0.72
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.71	0.72
1:H:59:VAL:O	1:H:171:LEU:N	2.23	0.72
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.72	0.71
5:L:561:MET:HA	5:L:567:MET:HE1	1.71	0.71
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.72	0.71
2:I:452:ARG:NH1	2:I:584:TYR:O	2.23	0.71
3:J:342:LEU:HD11	3:J:1324:SER:HB3	1.72	0.71
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.73	0.71
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.70	0.71
1:H:101:THR:HG22	1:H:116:THR:HB	1.73	0.70
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.73	0.70
2:C:452:ARG:NH1	2:C:584:TYR:O	2.25	0.70
5:F:561:MET:HA	5:F:567:MET:HE1	1.72	0.70
1:B:101:THR:HG22	1:B:116:THR:HB	1.73	0.70
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.73	0.70
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.71	0.70
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.73	0.69
2:C:528:ARG:NH2	2:C:576:SER:O	2.26	0.69
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.74	0.69
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.73	0.69
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.74	0.68
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.58	0.68
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.59	0.68
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.73	0.68
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.59	0.68
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.74	0.68
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.75	0.68
2:I:829:THR:HA	2:I:1059:ARG:HA	1.76	0.68
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.75	0.68
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.76	0.67
2:I:528:ARG:NH2	2:I:576:SER:O	2.26	0.67
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.75	0.67
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.76	0.67
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.75	0.67
2:C:18:ARG:NH2	2:C:620:ASN:OD1	2.27	0.67
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.76	0.67
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.77	0.67
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.59	0.67
2:I:18:ARG:NH2	2:I:620:ASN:OD1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.61	0.66
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.61	0.66
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.77	0.66
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.78	0.66
2:I:197:ARG:NH2	5:L:29:ASP:OD2	2.28	0.66
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.76	0.66
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.78	0.66
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.78	0.66
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.29	0.66
2:C:136:PHE:O	2:C:143:ARG:N	2.24	0.66
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.77	0.66
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.78	0.66
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.77	0.65
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.77	0.65
2:I:18:ARG:NH1	2:I:621:SER:O	2.29	0.65
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.77	0.65
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.78	0.65
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.76	0.65
2:C:829:THR:HA	2:C:1059:ARG:HA	1.77	0.65
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.78	0.65
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.78	0.65
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.77	0.65
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.78	0.65
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.79	0.65
3:J:120:LEU:HD22	3:J:121:PRO:HD3	1.79	0.65
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.79	0.65
1:A:166:ARG:O	1:A:168:ILE:N	2.29	0.65
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.77	0.65
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.77	0.65
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.60	0.65
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.65
2:C:18:ARG:NH1	2:C:621:SER:O	2.30	0.65
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.79	0.65
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.62	0.65
3:J:478:LEU:HG	4:K:47:THR:HG23	1.79	0.65
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.77	0.64
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.78	0.64
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.78	0.64
1:A:231:PHE:CZ	1:B:221:ALA:HB3	2.33	0.64
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.79	0.64
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.80	0.64
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.78	0.64
3:D:478:LEU:HG	4:E:47:THR:HG23	1.79	0.64
3:D:755:ILE:HG22	3:D:757:THR:H	1.62	0.64
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.80	0.64
1:G:230:ALA:HA	1:H:12:ARG:HG2	1.78	0.64
3:D:120:LEU:HD22	3:D:121:PRO:HD3	1.78	0.64
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.63	0.63
3:J:755:ILE:HG22	3:J:757:THR:H	1.62	0.63
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.32	0.63
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.79	0.63
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.81	0.63
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.81	0.63
2:I:88:ARG:NH2	2:I:1035:LYS:O	2.31	0.63
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.81	0.63
2:C:339:ASN:HB3	2:C:343:HIS:H	1.64	0.62
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.62	0.62
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.81	0.62
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.63	0.62
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.64	0.62
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.32	0.62
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.81	0.62
2:C:1119:MET:HE3	2:C:1204:LEU:HD13	1.82	0.62
2:I:1119:MET:HE3	2:I:1204:LEU:HD13	1.82	0.62
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.32	0.62
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	1.80	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.82	0.62
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.32	0.62
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.82	0.62
2:I:518:ASN:OD1	2:I:518:ASN:N	2.33	0.61
2:I:30:ILE:HD12	2:I:30:ILE:H	1.65	0.61
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.65	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.63	0.61
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.82	0.61
2:C:518:ASN:OD1	2:C:518:ASN:N	2.33	0.61
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.82	0.61
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.83	0.61
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.83	0.61
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.83	0.61
1:H:182:ARG:NH1	3:J:581:MET:SD	2.74	0.61
2:I:560:PRO:O	3:J:780:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:551:LEU:HD22	5:L:597:LYS:HD2	1.83	0.61
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.83	0.60
3:D:847:ASP:OD1	3:D:847:ASP:N	2.34	0.60
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.81	0.60
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.83	0.60
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.82	0.60
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.81	0.60
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.33	0.60
3:J:148:GLU:H	3:J:156:ARG:HG3	1.65	0.60
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.83	0.60
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.84	0.60
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.83	0.60
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.83	0.60
3:J:251:PRO:HD2	5:L:507:MET:HE1	1.82	0.60
2:I:738:GLU:HA	2:I:741:MET:HE2	1.84	0.60
2:C:494:ASN:OD1	2:C:495:ALA:N	2.32	0.60
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.84	0.60
2:I:494:ASN:OD1	2:I:495:ALA:N	2.33	0.60
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.34	0.60
2:C:738:GLU:HA	2:C:741:MET:HE2	1.83	0.60
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.84	0.60
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.84	0.60
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.84	0.59
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.83	0.59
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.84	0.59
5:L:476:ARG:HG2	5:L:477:GLU:HG2	1.84	0.59
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.84	0.59
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.84	0.59
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.84	0.59
3:D:148:GLU:H	3:D:156:ARG:HG3	1.67	0.59
5:F:476:ARG:HG2	5:F:477:GLU:HG2	1.84	0.59
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.84	0.59
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.85	0.59
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.85	0.59
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.84	0.59
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.84	0.59
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.85	0.59
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.85	0.59
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.33	0.59
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.68	0.59
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.85	0.59
2:C:560:PRO:O	3:D:780:ARG:NH2	2.35	0.58
3:D:308:ASP:OD2	3:D:311:ARG:NH2	2.35	0.58
3:D:356:THR:OG1	3:D:357:VAL:N	2.36	0.58
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.36	0.58
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.84	0.58
3:D:388:ARG:NH1	3:D:414:GLU:OE1	2.36	0.58
3:J:308:ASP:OD2	3:J:311:ARG:NH2	2.35	0.58
2:C:808:ASN:H	3:D:633:ALA:HB2	1.69	0.58
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.36	0.58
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.85	0.58
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.37	0.58
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.84	0.58
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.84	0.58
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.86	0.58
2:I:808:ASN:H	3:J:633:ALA:HB2	1.68	0.58
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.85	0.58
3:J:741:ALA:O	3:J:762:ASN:ND2	2.37	0.58
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.86	0.58
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.85	0.58
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.85	0.58
3:J:847:ASP:OD1	3:J:847:ASP:N	2.34	0.58
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.85	0.57
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.86	0.57
3:D:152:THR:OG1	3:D:153:ASN:N	2.37	0.57
3:D:741:ALA:O	3:D:762:ASN:ND2	2.37	0.57
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.85	0.57
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.86	0.57
5:F:276:MET:SD	5:F:279:ARG:NH1	2.77	0.57
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.85	0.57
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.86	0.57
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.37	0.57
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.87	0.57
3:J:77:ARG:HE	5:L:569:THR:HA	1.69	0.57
2:C:30:ILE:HD12	2:C:30:ILE:H	1.69	0.57
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.87	0.57
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.85	0.57
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.85	0.57
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.87	0.57
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.69	0.57
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.87	0.57
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.37	0.57
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.85	0.57
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.87	0.57
2:I:40:GLU:O	2:I:73:TYR:OH	2.22	0.57
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.87	0.57
5:L:482:GLU:O	5:L:486:ARG:NH2	2.38	0.57
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.70	0.57
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.87	0.57
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.86	0.57
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.87	0.57
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.87	0.57
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.87	0.56
2:C:40:GLU:O	2:C:73:TYR:OH	2.22	0.56
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.86	0.56
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.70	0.56
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.87	0.56
3:J:613:GLY:O	3:J:617:THR:OG1	2.23	0.56
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.70	0.56
3:D:682:VAL:O	3:D:685:ILE:HG12	2.05	0.56
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.86	0.56
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.68	0.56
3:J:152:THR:OG1	3:J:153:ASN:N	2.37	0.56
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.86	0.56
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.86	0.56
5:L:276:MET:SD	5:L:279:ARG:NH1	2.77	0.56
2:C:1250:SER:OG	5:F:524:GLU:OE1	2.24	0.56
3:D:794:GLY:O	3:D:797:THR:OG1	2.21	0.56
1:A:14:VAL:HG22	1:A:15:ASP:H	1.71	0.56
5:F:482:GLU:O	5:F:486:ARG:NH2	2.38	0.56
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.87	0.56
1:B:64:VAL:HG12	1:B:65:LEU:H	1.71	0.56
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.38	0.56
5:F:515:GLU:HG2	5:F:516:ASP:H	1.70	0.56
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.38	0.56
1:A:23:HIS:HB2	1:A:205:MET:O	2.06	0.56
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.70	0.56
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.88	0.56
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.88	0.56
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.88	0.56
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.88	0.56
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.70	0.56
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.88	0.56
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.88	0.56
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.38	0.56
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.88	0.56
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.88	0.55
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.36	0.55
3:J:682:VAL:O	3:J:685:ILE:HG12	2.05	0.55
5:L:134:VAL:HA	5:L:273:MET:HE1	1.87	0.55
2:C:207:THR:HG21	2:C:351:LEU:HG	1.88	0.55
2:C:227:LYS:O	2:C:245:ARG:NH2	2.39	0.55
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.88	0.55
3:J:356:THR:OG1	3:J:357:VAL:N	2.36	0.55
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.89	0.55
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.88	0.55
2:C:488:MET:O	2:C:490:GLN:N	2.34	0.55
3:J:794:GLY:O	3:J:797:THR:OG1	2.21	0.55
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	1.88	0.55
5:F:134:VAL:HA	5:F:273:MET:HE1	1.87	0.55
1:G:14:VAL:HG22	1:G:15:ASP:H	1.72	0.55
1:B:16:ILE:HG13	1:B:26:VAL:HG22	1.88	0.55
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.87	0.55
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.89	0.55
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.88	0.55
3:D:613:GLY:O	3:D:617:THR:OG1	2.24	0.55
3:J:120:LEU:HD12	5:L:43:ASP:HB3	1.88	0.55
2:I:227:LYS:O	2:I:245:ARG:NH2	2.40	0.55
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.89	0.55
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.37	0.54
2:I:207:THR:HG21	2:I:351:LEU:HG	1.88	0.54
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.90	0.54
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.41	0.54
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.89	0.54
1:G:23:HIS:HB2	1:G:205:MET:O	2.05	0.54
5:L:602:SER:H	5:L:605:GLU:HG3	1.72	0.54
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.90	0.54
1:H:64:VAL:HG12	1:H:65:LEU:H	1.72	0.54
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.90	0.54
5:L:515:GLU:HG2	5:L:516:ASP:H	1.71	0.54
3:J:115:TRP:O	3:J:119:SER:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.41	0.54
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.90	0.54
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.89	0.54
2:I:488:MET:O	2:I:490:GLN:N	2.35	0.54
3:J:425:ARG:HG2	3:J:426:ALA:H	1.72	0.54
3:D:770:LEU:H	3:D:770:LEU:HD22	1.72	0.54
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.71	0.54
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.89	0.54
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.90	0.54
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.89	0.54
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.89	0.54
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.42	0.54
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.21	0.54
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.90	0.54
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.89	0.54
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.90	0.54
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.88	0.54
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.90	0.54
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.89	0.54
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.88	0.54
3:D:210:SER:O	3:D:214:ARG:HG2	2.08	0.54
5:F:111:LEU:HD13	5:F:116:GLU:HG2	1.90	0.54
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.90	0.54
5:F:573:LEU:H	5:F:573:LEU:HD23	1.72	0.54
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.90	0.54
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.89	0.54
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.90	0.54
3:D:425:ARG:HG2	3:D:426:ALA:H	1.73	0.54
5:F:479:THR:HG23	5:F:481:GLU:H	1.72	0.54
3:J:34:SER:OG	3:J:104:HIS:ND1	2.28	0.54
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.90	0.54
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.90	0.54
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.90	0.53
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.90	0.53
3:J:210:SER:O	3:J:214:ARG:HG2	2.08	0.53
3:J:770:LEU:HD22	3:J:770:LEU:H	1.73	0.53
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.44	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.73	0.53
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.90	0.53
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.73	0.53
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1310:THR:HG21	5:F:70:ASN:HA	1.91	0.53
5:F:602:SER:H	5:F:605:GLU:HG3	1.72	0.53
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.73	0.53
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.90	0.53
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.73	0.53
5:L:111:LEU:HD13	5:L:116:GLU:HG2	1.90	0.53
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.44	0.53
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.91	0.53
4:K:73:GLN:HA	4:K:76:GLU:HB3	1.90	0.53
5:L:49:ASN:HA	5:L:53:ILE:HA	1.90	0.53
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.89	0.53
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.41	0.53
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.91	0.53
5:L:479:THR:HG23	5:L:481:GLU:H	1.74	0.53
1:A:74:VAL:HG22	1:A:76:GLU:H	1.73	0.53
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.53
5:F:511:ILE:HG13	5:F:512:GLY:H	1.74	0.53
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.41	0.53
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.89	0.53
3:D:34:SER:OG	3:D:104:HIS:ND1	2.29	0.53
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.90	0.53
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.89	0.53
1:B:11:PRO:HB3	1:B:30:PRO:O	2.08	0.53
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.91	0.53
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.89	0.53
5:L:511:ILE:HG13	5:L:512:GLY:H	1.74	0.53
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.91	0.53
2:C:9:LYS:HA	2:C:1171:ARG:HD2	1.91	0.53
2:C:324:LYS:O	2:C:327:GLN:NE2	2.42	0.53
3:D:202:ARG:HD3	3:J:1181:ASP:HA	1.90	0.53
5:L:548:LEU:HD21	5:L:559:LEU:HD23	1.91	0.53
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.09	0.52
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.42	0.52
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.90	0.52
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.10	0.52
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.08	0.52
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.91	0.52
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	1.90	0.52
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.90	0.52
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.43	0.52
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:ASP:H	1.74	0.52
1:A:172:LEU:HD12	1:A:172:LEU:H	1.74	0.52
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.43	0.52
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.92	0.52
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.90	0.52
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.44	0.52
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.91	0.52
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.27	0.52
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.21	0.52
1:G:74:VAL:HG22	1:G:76:GLU:H	1.74	0.52
2:I:324:LYS:O	2:I:327:GLN:NE2	2.43	0.52
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.73	0.52
3:J:338:PHE:CB	3:J:343:LEU:HB2	2.39	0.52
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.91	0.52
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.90	0.52
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.91	0.52
3:D:77:ARG:HE	5:F:569:THR:HA	1.74	0.52
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.90	0.52
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.90	0.52
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.44	0.52
3:J:119:SER:O	3:J:121:PRO:HD2	2.10	0.52
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.90	0.52
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.52
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.92	0.52
5:F:126:GLY:O	5:F:129:GLN:HB2	2.10	0.52
1:G:61:ILE:HG22	1:G:62:ASP:H	1.74	0.52
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.36	0.52
3:J:709:ARG:C	3:J:711:GLY:H	2.18	0.52
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.42	0.52
3:D:1297:LYS:HG2	3:J:1302:TYR:H	1.73	0.52
5:F:49:ASN:HA	5:F:53:ILE:HA	1.91	0.52
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.92	0.52
5:L:547:VAL:HG12	5:L:598:LEU:HD22	1.92	0.52
3:D:709:ARG:C	3:D:711:GLY:H	2.18	0.52
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.92	0.52
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.92	0.52
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.92	0.52
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.43	0.52
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.91	0.52
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.92	0.52
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.91	0.51
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.45	0.51
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.91	0.51
5:L:483:LEU:HD12	5:L:483:LEU:H	1.74	0.51
1:G:231:PHE:HZ	1:H:221:ALA:HB3	1.76	0.51
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.74	0.51
2:I:103:VAL:HB	2:I:113:THR:HG21	1.91	0.51
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.92	0.51
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.92	0.51
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.46	0.51
2:C:349:GLU:O	2:C:353:VAL:HG23	2.10	0.51
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.91	0.51
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.92	0.51
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.75	0.51
3:J:1170:LYS:C	3:J:1172:LYS:H	2.18	0.51
2:C:103:VAL:HB	2:C:113:THR:HG21	1.91	0.51
5:F:41:ILE:HA	5:F:44:ILE:HG23	1.93	0.51
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.92	0.51
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.43	0.51
3:J:1078:LEU:HB3	3:J:1121:LEU:HD13	1.92	0.51
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.75	0.51
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.76	0.51
1:H:11:PRO:HB3	1:H:30:PRO:O	2.10	0.51
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.93	0.51
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.93	0.51
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.93	0.51
1:G:172:LEU:HD12	1:G:172:LEU:H	1.76	0.51
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.93	0.51
3:J:568:SER:OG	3:J:569:LEU:N	2.43	0.51
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.27	0.51
5:L:448:ARG:NH1	5:L:501:ALA:O	2.35	0.51
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.26	0.51
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.93	0.51
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.46	0.51
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.92	0.51
2:C:1151:LEU:HD21	2:C:1198:LEU:HD23	1.92	0.51
3:D:1268:ASN:HD22	3:J:1268:ASN:HD22	1.59	0.51
5:F:316:PHE:HZ	5:F:334:SER:HA	1.76	0.51
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.92	0.51
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.46	0.51
5:L:126:GLY:O	5:L:130:VAL:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.46	0.51
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.46	0.51
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.92	0.51
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.44	0.51
5:F:483:LEU:HD12	5:F:483:LEU:H	1.75	0.51
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.92	0.51
2:I:349:GLU:O	2:I:353:VAL:HG23	2.11	0.51
5:L:487:MET:HA	5:L:487:MET:HE2	1.94	0.51
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.44	0.50
3:D:1170:LYS:C	3:D:1172:LYS:H	2.18	0.50
5:F:487:MET:HE2	5:F:487:MET:HA	1.93	0.50
5:F:551:LEU:HD11	5:F:598:LEU:HD21	1.92	0.50
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.93	0.50
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.93	0.50
1:A:91:ARG:HD3	1:A:210:THR:O	2.12	0.50
5:F:164:GLY:O	5:F:260:ARG:HB2	2.10	0.50
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.94	0.50
3:J:73:GLY:O	3:J:76:LYS:NZ	2.34	0.50
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.45	0.50
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.92	0.50
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.46	0.50
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.93	0.50
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.93	0.50
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.93	0.50
2:C:867:GLU:OE1	2:C:943:LYS:NZ	2.42	0.50
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.26	0.50
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.76	0.50
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.45	0.50
5:L:316:PHE:HZ	5:L:334:SER:HA	1.76	0.50
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.94	0.50
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.94	0.50
5:L:164:GLY:O	5:L:260:ARG:HB2	2.10	0.50
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.93	0.50
3:D:422:LEU:HD13	3:D:471:PRO:HG3	1.94	0.50
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.27	0.50
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.93	0.50
5:L:573:LEU:HD23	5:L:573:LEU:H	1.76	0.50
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.93	0.50
5:F:461:ASN:O	5:F:465:ARG:HG2	2.11	0.50
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.93	0.50
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:250:THR:HA	2:C:268:ARG:HA	1.93	0.50
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.94	0.50
2:C:842:ASP:N	2:C:1045:GLY:O	2.45	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49
3:J:697:MET:HE1	3:J:737:ILE:HG22	1.94	0.49
5:L:461:ASN:O	5:L:465:ARG:HG2	2.12	0.49
2:I:1151:LEU:HD21	2:I:1198:LEU:HD23	1.93	0.49
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.94	0.49
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.94	0.49
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.47	0.49
5:L:41:ILE:HA	5:L:44:ILE:HG23	1.93	0.49
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.95	0.49
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.93	0.49
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.94	0.49
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.95	0.49
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.95	0.49
2:I:739:ASP:OD1	2:I:739:ASP:N	2.38	0.49
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.94	0.49
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.19	0.49
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.94	0.49
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.93	0.49
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.20	0.49
5:F:281:ARG:O	5:F:285:ARG:HG3	2.13	0.49
2:I:402:ARG:NH2	2:I:419:ILE:O	2.46	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.13	0.49
2:I:842:ASP:N	2:I:1045:GLY:O	2.45	0.49
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.94	0.49
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.94	0.49
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.95	0.49
2:I:897:PRO:HG3	3:J:77:ARG:HH22	1.77	0.49
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.95	0.49
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.94	0.49
1:A:13:LEU:HD23	1:A:13:LEU:H	1.78	0.49
1:A:228:LEU:HD21	1:B:224:LEU:HD23	1.95	0.49
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.95	0.49
1:G:231:PHE:HB3	1:H:218:ARG:NH1	2.27	0.49
2:I:250:THR:HA	2:I:268:ARG:HA	1.94	0.49
2:I:746:ALA:HB3	2:I:971:LEU:HA	1.95	0.49
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.77	0.49
3:J:122:SER:O	3:J:126:LEU:HG	2.13	0.49
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:281:ARG:O	5:L:285:ARG:HG3	2.13	0.49
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.95	0.49
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.95	0.49
3:D:266:ASN:O	3:D:270:ARG:HB2	2.13	0.49
5:F:244:THR:O	5:F:247:GLU:HG2	2.13	0.49
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.93	0.49
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.13	0.49
5:L:297:MET:HE3	5:L:330:LEU:HD11	1.95	0.49
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.61	0.49
3:D:189:LEU:HD22	3:D:234:PRO:HB3	1.94	0.49
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.94	0.49
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.78	0.48
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.78	0.48
3:D:568:SER:OG	3:D:569:LEU:N	2.44	0.48
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.95	0.48
2:I:936:ARG:NH2	2:I:1043:ALA:O	2.46	0.48
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.95	0.48
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.94	0.48
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.94	0.48
2:C:255:ILE:HB	2:C:263:VAL:HB	1.96	0.48
2:C:878:THR:OG1	2:C:879:GLY:N	2.45	0.48
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.95	0.48
3:D:392:THR:HG21	5:F:606:VAL:HA	1.95	0.48
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.48	0.48
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.94	0.48
2:I:197:ARG:HH12	5:L:29:ASP:HB3	1.78	0.48
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.96	0.48
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.95	0.48
2:C:1313:HIS:N	4:E:31:GLN:OE1	2.39	0.48
5:F:297:MET:HE3	5:F:330:LEU:HD11	1.95	0.48
5:F:583:THR:HG22	5:F:584:ARG:H	1.79	0.48
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.94	0.48
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.94	0.48
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.96	0.48
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.78	0.48
3:J:1349:GLU:OE2	3:J:1349:GLU:N	2.33	0.48
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.95	0.48
2:C:692:THR:OG1	2:C:693:LEU:N	2.46	0.48
2:C:778:GLU:O	2:C:781:ASP:HB2	2.14	0.48
3:D:1268:ASN:HD22	3:J:1268:ASN:ND2	2.11	0.48
1:G:13:LEU:H	1:G:13:LEU:HD23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.95	0.48
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.93	0.48
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.78	0.48
3:J:266:ASN:O	3:J:270:ARG:HB2	2.13	0.48
3:J:341:ASN:HB2	3:J:1352:ILE:HD13	1.95	0.48
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.96	0.48
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.94	0.48
3:D:77:ARG:HG3	3:D:79:LYS:H	1.78	0.48
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.77	0.48
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.48	0.48
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.94	0.48
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.95	0.48
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.48
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.48	0.48
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.53	0.48
3:D:218:THR:HA	3:D:221:ILE:HG22	1.96	0.48
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.49	0.48
5:F:448:ARG:NH1	5:F:501:ALA:O	2.35	0.48
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.47	0.48
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.14	0.48
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.94	0.48
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	1.94	0.48
2:I:878:THR:OG1	2:I:879:GLY:N	2.46	0.48
3:J:77:ARG:HG3	3:J:79:LYS:H	1.78	0.48
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.77	0.48
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.95	0.48
5:L:244:THR:O	5:L:247:GLU:HG2	2.13	0.48
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.95	0.48
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.96	0.48
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.48	0.48
2:I:778:GLU:O	2:I:781:ASP:HB2	2.14	0.48
3:J:708:ASN:HB3	3:J:712:GLN:O	2.14	0.48
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.96	0.48
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.14	0.48
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.95	0.48
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.95	0.47
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.29	0.47
2:C:402:ARG:NH2	2:C:419:ILE:O	2.47	0.47
3:D:115:TRP:O	3:D:119:SER:HB2	2.14	0.47
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.96	0.47
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.96	0.47
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.62	0.47
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.96	0.47
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.95	0.47
5:F:580:PHE:C	5:F:582:VAL:H	2.21	0.47
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.95	0.47
1:H:95:LYS:NZ	1:H:98:VAL:HG23	2.29	0.47
3:D:733:SER:O	3:D:737:ILE:HG12	2.14	0.47
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.97	0.47
2:I:115:LYS:HE3	2:I:116:ASP:H	1.79	0.47
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.62	0.47
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.96	0.47
3:J:733:SER:O	3:J:737:ILE:HG12	2.15	0.47
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.95	0.47
3:D:13:LYS:HA	3:D:13:LYS:HD3	1.70	0.47
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.96	0.47
5:L:137:TYR:HE1	5:L:351:THR:HB	1.80	0.47
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.29	0.47
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.96	0.47
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.96	0.47
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.49	0.47
2:I:202:ARG:HH22	2:I:368:ARG:HH12	1.61	0.47
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.95	0.47
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.96	0.47
3:D:122:SER:O	3:D:126:LEU:HG	2.13	0.47
5:F:137:TYR:HE1	5:F:351:THR:HB	1.80	0.47
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.96	0.47
2:I:517:GLN:O	2:I:517:GLN:HG2	2.15	0.47
3:J:395:LYS:HE2	5:L:536:THR:HG21	1.96	0.47
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.49	0.47
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.97	0.47
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.95	0.47
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.96	0.47
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.97	0.47
2:C:115:LYS:HE3	2:C:116:ASP:H	1.78	0.47
2:C:232:ILE:HG12	2:C:237:LEU:HD13	1.96	0.47
2:C:560:PRO:HB3	3:D:776:THR:HG21	1.97	0.47
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.74	0.47
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.47	0.47
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.97	0.47
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.97	0.47
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.47	0.47
3:D:708:ASN:HB3	3:D:712:GLN:O	2.14	0.47
3:D:1287:ILE:HG13	3:D:1288:ALA:N	2.30	0.47
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.97	0.47
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.97	0.47
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.95	0.47
2:I:170:VAL:HG23	2:I:171:LEU:H	1.80	0.47
2:I:448:LEU:HB2	2:I:553:THR:HB	1.96	0.47
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.96	0.47
5:L:127:ILE:O	5:L:130:VAL:HG22	2.14	0.47
5:L:580:PHE:C	5:L:582:VAL:H	2.22	0.47
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.97	0.47
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.50	0.47
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.96	0.47
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.96	0.47
5:L:225:ARG:O	5:L:229:VAL:HG13	2.15	0.47
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.80	0.47
2:C:387:ASN:HA	2:C:391:SER:HB2	1.97	0.47
5:F:225:ARG:O	5:F:229:VAL:HG13	2.15	0.47
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.96	0.47
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.96	0.47
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.96	0.47
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.97	0.47
5:L:583:THR:HG22	5:L:584:ARG:H	1.79	0.47
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.46
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.79	0.46
2:I:170:VAL:HG23	2:I:171:LEU:N	2.30	0.46
3:J:1287:ILE:HG13	3:J:1288:ALA:N	2.30	0.46
5:L:507:MET:HG2	5:L:520:GLY:HA3	1.97	0.46
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.97	0.46
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.81	0.46
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.97	0.46
3:J:1167:LYS:HE3	3:J:1168:GLU:H	1.80	0.46
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.98	0.46
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.95	0.46
3:D:133:ARG:NH2	5:F:93:ARG:O	2.47	0.46
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.96	0.46
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.55	0.46
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.97	0.46
3:D:708:ASN:OD1	3:D:708:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.95	0.46
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.50	0.46
2:I:560:PRO:HB3	3:J:776:THR:HG21	1.97	0.46
3:J:79:LYS:HB2	5:L:569:THR:N	2.31	0.46
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.98	0.46
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.97	0.46
2:C:170:VAL:HG23	2:C:171:LEU:N	2.31	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.97	0.46
3:D:73:GLY:O	3:D:76:LYS:NZ	2.33	0.46
5:F:470:MET:HE3	5:F:478:PRO:HB3	1.98	0.46
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.96	0.46
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.28	0.46
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.55	0.46
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.96	0.46
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.97	0.46
2:I:98:VAL:HG21	2:I:124:MET:HE3	1.98	0.46
2:I:255:ILE:HB	2:I:263:VAL:HB	1.96	0.46
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.97	0.46
3:J:385:LEU:HD11	3:J:408:VAL:HG12	1.98	0.46
5:L:380:VAL:HG22	5:L:416:VAL:HG21	1.98	0.46
2:C:448:LEU:HB2	2:C:553:THR:HB	1.96	0.46
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.96	0.46
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.31	0.46
2:I:322:LEU:O	2:I:326:SER:OG	2.29	0.46
2:I:538:LEU:HD22	2:I:543:ALA:HB2	1.97	0.46
2:I:721:GLY:N	2:I:740:GLU:OE1	2.45	0.46
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.98	0.46
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.97	0.46
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.81	0.46
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.50	0.46
2:I:557:ARG:HH21	2:I:607:SER:C	2.24	0.46
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.97	0.46
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.96	0.46
3:J:695:LYS:HD3	3:J:695:LYS:HA	1.72	0.46
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.97	0.46
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.98	0.46
3:D:1341:ARG:HH22	3:D:1373:ARG:HH21	1.64	0.46
1:G:12:ARG:H	1:G:30:PRO:HD2	1.81	0.46
2:I:387:ASN:HA	2:I:391:SER:HB2	1.97	0.46
2:C:517:GLN:HG2	2:C:517:GLN:O	2.15	0.46
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.78	0.46
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.16	0.46
2:C:89:GLY:HA2	2:C:140:GLY:HA3	1.97	0.45
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.81	0.45
3:D:385:LEU:HD11	3:D:408:VAL:HG12	1.98	0.45
3:J:963:VAL:HB	3:J:980:THR:HG23	1.98	0.45
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.32	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.16	0.45
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.97	0.45
5:F:380:VAL:HG22	5:F:416:VAL:HG21	1.98	0.45
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.51	0.45
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.97	0.45
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.81	0.45
1:B:51:MET:HA	1:B:52:PRO:HD3	1.85	0.45
2:C:721:GLY:N	2:C:740:GLU:OE1	2.45	0.45
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	1.98	0.45
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.82	0.45
3:D:1349:GLU:OE2	3:D:1349:GLU:N	2.33	0.45
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.81	0.45
2:I:705:GLU:HB2	2:I:794:LEU:HB3	1.98	0.45
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.97	0.45
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.81	0.45
3:J:747:MET:HE2	3:J:775:SER:HA	1.98	0.45
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.97	0.45
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.31	0.45
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.48	0.45
5:F:507:MET:HG2	5:F:520:GLY:HA3	1.98	0.45
2:I:206:ALA:O	2:I:209:ILE:HG22	2.16	0.45
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.51	0.45
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.83	0.45
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.16	0.45
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.97	0.45
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.99	0.45
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.97	0.45
2:C:820:GLU:N	2:C:1080:ASN:O	2.50	0.45
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.98	0.45
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.16	0.45
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.32	0.45
4:K:60:ASN:HD21	4:K:63:ILE:HD13	1.81	0.45
2:C:113:THR:OG1	2:C:116:ASP:OD2	2.24	0.45
2:C:557:ARG:HH21	2:C:607:SER:C	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:680:LEU:O	2:C:684:ASN:HB2	2.17	0.45
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.99	0.45
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.98	0.45
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.99	0.45
2:I:820:GLU:N	2:I:1080:ASN:O	2.49	0.45
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.99	0.45
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.31	0.45
5:L:287:ILE:HG12	5:L:337:VAL:HG13	1.99	0.45
2:C:1085:MET:HE2	2:C:1085:MET:HA	1.98	0.45
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.98	0.45
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.99	0.45
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.98	0.45
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.81	0.45
5:F:44:ILE:HA	5:F:47:MET:HB2	1.98	0.45
5:F:137:TYR:HD2	5:F:273:MET:HE2	1.81	0.45
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.80	0.45
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.59	0.45
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.98	0.45
3:J:1244:GLN:HE21	3:J:1244:GLN:HB3	1.59	0.45
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.99	0.45
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.31	0.45
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.51	0.45
2:C:658:GLN:O	2:C:661:VAL:HG22	2.17	0.45
2:C:739:ASP:OD1	2:C:739:ASP:N	2.36	0.45
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.51	0.45
3:D:264:ASP:OD2	3:D:264:ASP:N	2.50	0.45
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.99	0.45
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.99	0.45
1:G:47:LEU:HD13	1:G:183:ILE:HG12	1.99	0.45
2:I:217:THR:HG23	2:I:351:LEU:HD13	1.97	0.45
2:I:1085:MET:HA	2:I:1085:MET:HE2	1.97	0.45
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.99	0.45
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.82	0.45
3:J:701:LEU:HD13	3:J:723:TYR:HB2	1.99	0.45
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.99	0.45
5:L:137:TYR:HD2	5:L:273:MET:HE2	1.81	0.45
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.98	0.45
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.52	0.45
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.32	0.45
3:D:50:LYS:HB3	3:D:71:LEU:HD21	1.98	0.45
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:654:ILE:O	3:J:658:GLU:HB2	2.17	0.45
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	1.99	0.45
5:L:249:ILE:O	5:L:252:LEU:HB3	2.16	0.45
5:L:470:MET:HE3	5:L:478:PRO:HB3	1.98	0.45
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.99	0.45
2:I:680:LEU:O	2:I:684:ASN:HB2	2.17	0.45
3:J:264:ASP:OD2	3:J:264:ASP:N	2.50	0.45
3:J:708:ASN:OD1	3:J:708:ASN:N	2.48	0.45
3:J:901:ARG:HA	3:J:908:ILE:HA	1.99	0.45
3:J:1061:VAL:HG21	3:J:1101:LEU:HB2	1.99	0.45
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.32	0.45
5:L:130:VAL:HB	5:L:365:MET:HG3	1.99	0.45
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.99	0.45
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.98	0.44
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.99	0.44
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.52	0.44
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.83	0.44
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.77	0.44
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.99	0.44
5:F:354:THR:O	5:F:358:VAL:HG23	2.17	0.44
2:I:113:THR:OG1	2:I:116:ASP:OD2	2.23	0.44
3:J:62:PHE:O	3:J:101:ARG:HD2	2.17	0.44
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.98	0.44
5:L:572:THR:O	5:L:576:VAL:HG23	2.17	0.44
1:B:79:LEU:HD23	1:B:79:LEU:H	1.82	0.44
3:D:747:MET:HE2	3:D:775:SER:HA	1.98	0.44
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.31	0.44
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.99	0.44
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.76	0.44
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.82	0.44
1:H:91:ARG:HG2	1:H:122:GLU:O	2.17	0.44
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.82	0.44
3:J:800:LEU:O	3:J:803:VAL:HG12	2.17	0.44
2:C:171:LEU:HD23	2:C:171:LEU:HA	1.91	0.44
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.53	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.44
5:F:346:GLN:O	5:F:350:GLU:HG3	2.17	0.44
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.99	0.44
1:G:197:ASP:OD1	1:G:197:ASP:N	2.51	0.44
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.99	0.44
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.53	0.44
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.99	0.44
3:D:800:LEU:O	3:D:803:VAL:HG12	2.17	0.44
3:D:1167:LYS:HE3	3:D:1168:GLU:H	1.80	0.44
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.82	0.44
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.99	0.44
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.99	0.44
3:J:709:ARG:O	3:J:711:GLY:N	2.50	0.44
3:J:1233:ILE:HG12	3:J:1260:MET:HE1	1.99	0.44
5:L:215:GLU:HG2	5:L:218:ARG:HH21	1.82	0.44
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.00	0.44
2:C:466:VAL:O	2:C:469:VAL:HG22	2.18	0.44
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.99	0.44
3:D:661:VAL:HG12	3:D:685:ILE:HD11	2.00	0.44
3:D:872:LEU:O	3:D:877:VAL:HG12	2.18	0.44
3:D:1233:ILE:HG12	3:D:1260:MET:HE1	2.00	0.44
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.00	0.44
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.82	0.44
2:I:1247:SER:HB3	3:J:375:GLU:O	2.17	0.44
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.52	0.44
3:J:203:GLU:O	3:J:207:GLU:HG2	2.17	0.44
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.82	0.44
5:L:314:THR:O	5:L:318:ALA:HB3	2.18	0.44
2:C:453:ILE:HD12	2:C:587:LEU:HD21	2.00	0.44
3:D:62:PHE:O	3:D:101:ARG:HD2	2.18	0.44
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.81	0.44
3:J:502:PRO:HB2	3:J:507:VAL:HG12	2.00	0.44
3:J:1198:VAL:HB	3:J:1210:ILE:HA	1.99	0.44
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.51	0.44
5:L:346:GLN:O	5:L:350:GLU:HG3	2.18	0.44
5:L:547:VAL:CG1	5:L:598:LEU:HD22	2.47	0.44
1:B:91:ARG:HG2	1:B:122:GLU:O	2.18	0.44
2:C:840:SER:O	2:C:1047:LEU:N	2.51	0.44
2:C:976:ARG:NH2	2:C:990:ASP:OD2	2.51	0.44
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.50	0.44
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.98	0.44
3:D:694:SER:OG	3:D:738:ARG:NE	2.42	0.44
3:D:860:ARG:HB3	3:D:861:ASN:H	1.57	0.44
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.33	0.44
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.99	0.44
1:G:25:LYS:HG2	1:G:204:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.99	0.44
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.82	0.44
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.83	0.44
5:L:97:PRO:HA	5:L:100:MET:HG3	2.00	0.44
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.83	0.44
1:A:12:ARG:H	1:A:30:PRO:HD2	1.82	0.44
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.82	0.44
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.18	0.44
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.99	0.44
5:F:249:ILE:O	5:F:252:LEU:HB3	2.17	0.44
2:I:453:ILE:HD12	2:I:587:LEU:HD21	2.00	0.44
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.98	0.44
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.99	0.44
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.23	0.44
5:L:44:ILE:HA	5:L:47:MET:HB2	2.00	0.44
5:L:234:THR:O	5:L:245:ALA:HB2	2.18	0.44
5:L:493:LYS:HA	5:L:496:LYS:HE2	2.00	0.44
2:C:316:GLU:CD	2:C:316:GLU:H	2.26	0.43
2:C:383:SER:O	2:C:387:ASN:HB2	2.18	0.43
2:C:453:ILE:HD11	2:C:530:ILE:HD12	2.00	0.43
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.83	0.43
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.99	0.43
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.83	0.43
5:F:136:GLU:OE1	5:F:364:ARG:NH2	2.51	0.43
5:F:572:THR:O	5:F:576:VAL:HG23	2.18	0.43
2:I:658:GLN:O	2:I:661:VAL:HG22	2.18	0.43
2:I:720:ARG:HA	2:I:779:ARG:HG3	2.00	0.43
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.65	0.43
3:J:325:LYS:HD3	5:L:508:GLU:HG2	2.00	0.43
2:C:1151:LEU:HD23	2:C:1151:LEU:HA	1.81	0.43
3:D:298:MET:SD	5:F:402:LEU:HB3	2.58	0.43
3:D:470:VAL:HA	3:D:471:PRO:HD3	1.79	0.43
3:D:527:LEU:HD22	3:D:533:ALA:HA	2.00	0.43
5:F:234:THR:O	5:F:245:ALA:HB2	2.18	0.43
3:J:1017:VAL:HG23	3:J:1018:ALA:H	1.82	0.43
3:J:1034:PHE:HA	3:J:1114:GLN:HA	2.00	0.43
1:B:98:VAL:HG22	1:B:99:ILE:H	1.84	0.43
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.16	0.43
3:D:45:ASN:HB3	3:D:48:THR:O	2.18	0.43
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.18	0.43
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:316:GLU:H	2:I:316:GLU:CD	2.26	0.43
2:I:466:VAL:O	2:I:469:VAL:HG22	2.18	0.43
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.58	0.43
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.53	0.43
3:J:314:ARG:HG2	3:J:314:ARG:HH11	1.83	0.43
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.78	0.43
3:D:654:ILE:O	3:D:658:GLU:HB2	2.17	0.43
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.99	0.43
5:F:493:LYS:HA	5:F:496:LYS:HE2	2.00	0.43
1:H:101:THR:HA	1:H:142:MET:O	2.18	0.43
2:I:183:TRP:HB2	2:I:199:ASP:HA	2.00	0.43
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.16	0.43
3:J:557:LYS:HA	3:J:563:LEU:HA	2.00	0.43
3:J:740:LEU:HA	3:J:740:LEU:HD12	1.85	0.43
3:J:810:THR:HG23	3:J:811:GLU:H	1.83	0.43
2:C:170:VAL:HG23	2:C:171:LEU:H	1.81	0.43
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.54	0.43
3:D:557:LYS:HA	3:D:563:LEU:HA	2.01	0.43
5:F:119:ILE:O	5:F:123:ILE:HG13	2.18	0.43
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.82	0.43
5:F:590:ILE:O	5:F:594:ALA:N	2.51	0.43
1:H:98:VAL:HG22	1:H:99:ILE:H	1.84	0.43
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.53	0.43
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.83	0.43
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.00	0.43
5:L:354:THR:O	5:L:358:VAL:HG23	2.18	0.43
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.34	0.43
1:A:224:LEU:HD22	1:B:228:LEU:HD11	2.00	0.43
1:A:231:PHE:HB3	1:B:218:ARG:HH11	1.82	0.43
1:B:20:SER:OG	1:B:21:SER:N	2.51	0.43
2:C:593:LYS:HD3	2:C:652:TYR:CZ	2.54	0.43
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.00	0.43
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.49	0.43
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.83	0.43
1:G:58:GLU:HB2	1:G:145:LYS:HB3	2.01	0.43
1:H:20:SER:OG	1:H:21:SER:N	2.51	0.43
1:H:79:LEU:HD23	1:H:79:LEU:H	1.83	0.43
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.59	0.43
2:I:840:SER:O	2:I:1047:LEU:N	2.51	0.43
2:I:976:ARG:NH2	2:I:990:ASP:OD2	2.52	0.43
3:J:45:ASN:HB3	3:J:48:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:527:LEU:HD22	3:J:533:ALA:HA	2.00	0.43
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.53	0.43
2:C:1247:SER:HB3	3:D:375:GLU:O	2.18	0.43
3:D:203:GLU:O	3:D:207:GLU:HG2	2.18	0.43
3:D:701:LEU:HD13	3:D:723:TYR:HB2	2.00	0.43
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.53	0.43
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.18	0.43
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.83	0.43
5:F:314:THR:O	5:F:318:ALA:HB3	2.19	0.43
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.34	0.43
2:I:453:ILE:HD11	2:I:530:ILE:HD12	2.01	0.43
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.52	0.43
1:A:47:LEU:HD13	1:A:183:ILE:HG12	1.99	0.43
1:B:101:THR:HA	1:B:142:MET:O	2.19	0.43
2:C:720:ARG:HA	2:C:779:ARG:HG3	2.00	0.43
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.01	0.43
3:D:848:VAL:HG22	3:D:858:VAL:CG2	2.48	0.43
3:D:1162:ILE:HA	3:D:1203:ARG:HA	2.01	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.01	0.43
3:J:661:VAL:HG12	3:J:685:ILE:HD11	2.00	0.43
5:L:511:ILE:HD12	5:L:511:ILE:HA	1.85	0.43
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.00	0.43
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.65	0.43
3:D:314:ARG:HG2	3:D:314:ARG:HH11	1.84	0.43
3:D:709:ARG:O	3:D:711:GLY:N	2.50	0.43
3:D:1236:GLU:O	3:D:1240:VAL:HG23	2.19	0.43
3:J:872:LEU:O	3:J:877:VAL:HG12	2.18	0.43
5:L:348:GLU:HG2	5:L:354:THR:HA	2.01	0.43
1:A:197:ASP:OD1	1:A:197:ASP:N	2.51	0.43
1:B:28:LEU:HG	1:B:31:LEU:HD21	2.01	0.43
2:C:980:VAL:HG13	2:C:984:VAL:HB	2.01	0.43
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.83	0.43
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.86	0.43
3:D:537:TYR:CE1	3:D:544:LEU:HB2	2.54	0.43
3:D:901:ARG:HA	3:D:908:ILE:HA	1.99	0.43
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.84	0.43
2:I:383:SER:O	2:I:387:ASN:HB2	2.18	0.43
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.54	0.43
1:B:34:GLY:HA3	2:C:1083:GLU:OE1	2.18	0.42
1:B:78:ILE:O	1:B:82:LEU:HG	2.19	0.42
3:D:317:THR:HB	3:D:324:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.18	0.42
3:D:925:GLU:HB3	3:D:926:PRO:HD3	2.01	0.42
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.01	0.42
1:H:28:LEU:HG	1:H:31:LEU:HD21	2.01	0.42
3:J:298:MET:SD	5:L:402:LEU:HB3	2.58	0.42
3:J:317:THR:HB	3:J:324:LEU:HB3	2.00	0.42
3:J:848:VAL:HG22	3:J:858:VAL:CG2	2.48	0.42
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.19	0.42
1:A:115:ILE:HG22	1:A:116:THR:H	1.84	0.42
2:C:360:LEU:HB2	2:C:378:ARG:HH21	1.84	0.42
2:C:964:LEU:HD22	2:C:1025:PHE:CG	2.54	0.42
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.54	0.42
3:D:347:VAL:HG12	3:D:348:ASP:O	2.19	0.42
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.42	0.42
1:G:115:ILE:HG22	1:G:116:THR:H	1.84	0.42
1:G:219:ARG:HE	1:G:219:ARG:HB2	1.56	0.42
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.54	0.42
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.01	0.42
3:J:1237:VAL:HG13	3:J:1253:ILE:HD13	2.00	0.42
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.84	0.42
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.88	0.42
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.59	0.42
2:C:692:THR:OG1	2:C:827:ARG:O	2.32	0.42
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.86	0.42
1:G:145:LYS:HB3	1:G:145:LYS:HE3	1.84	0.42
3:J:537:TYR:CE1	3:J:544:LEU:HB2	2.54	0.42
3:J:644:MET:HE3	3:J:644:MET:HB2	1.97	0.42
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.20	0.42
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.18	0.42
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.51	0.42
1:B:86:LYS:HD3	1:B:174:ASP:HB2	2.02	0.42
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.54	0.42
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.49	0.42
5:F:130:VAL:HB	5:F:365:MET:HG3	2.00	0.42
3:J:1162:ILE:HA	3:J:1203:ARG:HA	2.01	0.42
4:K:49:ILE:HA	4:K:52:ARG:HD3	2.01	0.42
1:A:25:LYS:HG2	1:A:204:GLU:HG3	2.01	0.42
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.99	0.42
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	2.02	0.42
5:F:97:PRO:HA	5:F:100:MET:HG3	2.01	0.42
1:G:51:MET:HE1	1:G:216:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.54	0.42
1:H:101:THR:H	1:H:116:THR:HG22	1.84	0.42
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.19	0.42
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.42
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.01	0.42
3:J:1090:ILE:HG13	3:J:1097:ALA:HB2	2.01	0.42
5:L:454:VAL:HA	5:L:457:ILE:HD12	2.02	0.42
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.01	0.42
1:A:75:GLN:HA	2:C:729:ALA:N	2.35	0.42
2:C:69:GLN:HE21	2:C:69:GLN:HB3	1.67	0.42
2:C:357:ASN:ND2	2:C:358:ASP:OD2	2.53	0.42
2:C:758:ARG:HD3	2:C:835:GLU:HB2	2.01	0.42
3:D:683:ILE:HD11	3:D:754:ILE:HG12	2.01	0.42
5:F:348:GLU:HG2	5:F:354:THR:HA	2.01	0.42
1:G:10:LYS:HE2	1:H:229:GLU:HB3	2.00	0.42
1:H:91:ARG:HG2	1:H:91:ARG:H	1.76	0.42
1:H:112:ALA:HB2	1:H:128:HIS:HB3	2.02	0.42
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.85	0.42
3:J:925:GLU:HB3	3:J:926:PRO:HD3	2.01	0.42
3:J:1146:GLU:HB3	3:J:1148:ARG:HG3	2.00	0.42
5:L:484:ALA:HB1	5:L:491:GLU:HB2	2.00	0.42
1:A:54:CYS:HA	1:A:148:ARG:HG3	2.02	0.42
1:B:90:VAL:HG11	1:B:146:VAL:HG11	2.01	0.42
3:D:1293:GLU:HB3	3:D:1294:ALA:H	1.69	0.42
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.55	0.42
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.83	0.42
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.54	0.42
3:J:128:LEU:HD23	3:J:192:MET:HE3	2.02	0.42
3:J:969:SER:HB3	3:J:1116:SER:HB2	2.00	0.42
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	2.01	0.42
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.34	0.42
2:I:710:VAL:HA	2:I:715:THR:HG21	2.01	0.42
2:I:967:LEU:HD12	2:I:967:LEU:HA	1.89	0.42
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.34	0.42
3:J:334:LYS:HD2	3:J:334:LYS:HA	1.50	0.42
3:J:694:SER:OG	3:J:738:ARG:NE	2.42	0.42
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.35	0.42
3:J:1341:ARG:HH22	3:J:1373:ARG:HH21	1.66	0.42
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.84	0.42
2:C:1080:ASN:HA	2:C:1081:PRO:HD3	1.96	0.42
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.35	0.42
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.53	0.42
5:F:454:VAL:HA	5:F:457:ILE:HD12	2.02	0.42
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.49	0.42
1:G:61:ILE:HG23	1:G:142:MET:HB3	2.01	0.42
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.50	0.42
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.91	0.42
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.87	0.42
1:A:61:ILE:HG23	1:A:142:MET:HB3	2.01	0.42
2:C:56:VAL:HG11	2:C:468:LEU:HB3	2.01	0.42
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.55	0.42
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.48	0.42
3:D:668:PHE:HB2	3:D:678:ARG:HG3	2.02	0.42
3:D:1293:GLU:HA	3:J:1226:VAL:H	1.85	0.42
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.86	0.42
2:I:10:ARG:HA	2:I:1172:LEU:HD23	2.02	0.42
2:I:980:VAL:HG13	2:I:984:VAL:HB	2.02	0.42
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.84	0.42
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.55	0.42
5:L:119:ILE:O	5:L:123:ILE:HG13	2.19	0.42
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.02	0.41
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.77	0.41
2:C:153:PRO:O	2:C:401:GLY:HA2	2.20	0.41
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.55	0.41
3:D:902:ASP:OD1	3:D:903:LEU:N	2.53	0.41
1:H:78:ILE:O	1:H:82:LEU:HG	2.19	0.41
1:H:178:SER:HA	1:H:179:PRO:HD3	1.94	0.41
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.02	0.41
2:I:782:VAL:HG11	2:I:792:GLY:HA2	2.02	0.41
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.54	0.41
3:J:347:VAL:HG12	3:J:348:ASP:O	2.20	0.41
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.91	0.41
5:L:569:THR:OG1	5:L:570:ASP:N	2.53	0.41
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.88	0.41
2:C:499:SER:O	2:C:503:LYS:HB2	2.20	0.41
3:D:355:ILE:HD13	3:D:466:MET:HG3	2.02	0.41
4:E:35:LYS:HZ1	4:E:71:GLU:CD	2.27	0.41
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.88	0.41
1:G:54:CYS:HA	1:G:148:ARG:HG3	2.01	0.41
2:I:518:ASN:O	2:I:691:PRO:HD3	2.20	0.41
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1285:VAL:O	3:J:1289:ASN:HB3	2.20	0.41
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.53	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.85	0.41
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.50	0.41
5:F:511:ILE:HD12	5:F:511:ILE:HA	1.86	0.41
1:H:86:LYS:HD3	1:H:174:ASP:HB2	2.02	0.41
1:H:151:GLY:O	1:H:177:TYR:HD2	2.04	0.41
1:H:158:ARG:HD2	1:H:158:ARG:HA	1.91	0.41
2:I:360:LEU:HB2	2:I:378:ARG:HH21	1.84	0.41
2:I:1295:SER:OG	3:J:346:ARG:O	2.31	0.41
3:J:124:ILE:H	3:J:124:ILE:HG13	1.63	0.41
3:J:1025:MET:SD	3:J:1124:ILE:HD12	2.60	0.41
3:J:1156:LEU:HD23	3:J:1219:ASP:HB3	2.02	0.41
3:J:1293:GLU:HB3	3:J:1294:ALA:H	1.69	0.41
5:L:299:LYS:O	5:L:303:ILE:HG12	2.20	0.41
5:L:357:GLN:H	5:L:357:GLN:HG3	1.62	0.41
5:L:465:ARG:HA	5:L:468:ARG:HH12	1.86	0.41
1:A:54:CYS:O	1:A:146:VAL:HG13	2.20	0.41
1:B:91:ARG:HG2	1:B:91:ARG:H	1.76	0.41
1:B:101:THR:H	1:B:116:THR:HG22	1.85	0.41
1:B:158:ARG:HD2	1:B:158:ARG:HA	1.90	0.41
1:B:182:ARG:NH1	3:D:581:MET:SD	2.94	0.41
3:D:190:LYS:HB2	3:D:190:LYS:HE2	1.87	0.41
3:D:361:LEU:HD22	3:D:365:GLN:HG3	2.01	0.41
3:D:810:THR:HG23	3:D:811:GLU:H	1.85	0.41
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.49	0.41
3:D:1285:VAL:O	3:D:1289:ASN:HB3	2.20	0.41
1:G:35:PHE:HD1	1:G:35:PHE:HA	1.70	0.41
2:I:470:ARG:NE	2:I:497:PRO:HB3	2.35	0.41
2:I:550:VAL:HG11	3:J:776:THR:HG22	2.02	0.41
1:A:51:MET:HE1	1:A:216:ALA:HA	2.02	0.41
1:B:182:ARG:HD2	3:D:581:MET:HE1	2.02	0.41
2:C:88:ARG:NE	2:C:1040:ASP:OD1	2.45	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.21	0.41
2:C:887:VAL:HB	2:C:913:VAL:HG21	2.01	0.41
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.55	0.41
3:D:27:PRO:O	3:D:31:ARG:HG3	2.21	0.41
3:D:128:LEU:HD23	3:D:192:MET:HE3	2.01	0.41
3:D:806:ASP:OD2	3:D:1347:LEU:N	2.48	0.41
3:D:1156:LEU:HD23	3:D:1219:ASP:HB3	2.02	0.41
5:F:582:VAL:HG22	5:F:586:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.55	0.41
2:I:499:SER:O	2:I:503:LYS:HB2	2.20	0.41
2:I:593:LYS:HD3	2:I:652:TYR:CZ	2.54	0.41
2:I:699:LEU:HD22	2:I:699:LEU:HA	1.95	0.41
2:I:959:ASP:O	2:I:963:GLU:HG2	2.21	0.41
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	2.02	0.41
3:J:79:LYS:HG3	3:J:80:HIS:N	2.35	0.41
3:J:441:LEU:HD13	3:J:441:LEU:HA	1.90	0.41
3:J:1236:GLU:O	3:J:1240:VAL:HG23	2.20	0.41
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.80	0.41
5:L:561:MET:HG3	5:L:571:TYR:HD2	1.84	0.41
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.70	0.41
5:L:582:VAL:HG22	5:L:586:ARG:HG2	2.02	0.41
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	2.02	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.92	0.41
3:D:793:SER:O	3:D:797:THR:HG23	2.20	0.41
2:I:122:VAL:HG21	2:I:493:ILE:HG23	2.03	0.41
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.88	0.41
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.56	0.41
3:J:556:GLU:O	3:J:564:VAL:N	2.33	0.41
3:J:668:PHE:HB2	3:J:678:ARG:HG3	2.02	0.41
3:J:1040:MET:HE3	3:J:1076:PRO:HB2	2.02	0.41
1:B:34:GLY:N	1:B:199:ASP:OD2	2.53	0.41
2:C:83:GLN:O	2:C:87:ILE:HG13	2.21	0.41
2:C:550:VAL:HG11	3:D:776:THR:HG22	2.03	0.41
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.21	0.41
3:D:1345:ARG:HD2	3:D:1370:MET:HE1	2.03	0.41
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.46	0.41
1:G:10:LYS:HE3	1:H:226:GLU:O	2.21	0.41
1:G:79:LEU:HD11	2:I:693:LEU:HD21	2.02	0.41
2:I:697:LYS:HB3	2:I:697:LYS:HE2	1.76	0.41
3:J:361:LEU:HD22	3:J:365:GLN:HG3	2.01	0.41
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.91	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.21	0.41
1:B:51:MET:HB3	1:B:178:SER:HA	2.01	0.41
2:C:312:ALA:HB3	2:C:315:MET:HE3	2.02	0.41
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.91	0.41
2:C:987:GLU:O	2:C:991:LYS:HG3	2.21	0.41
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.56	0.41
3:D:461:PHE:HD2	3:D:461:PHE:HA	1.77	0.41
3:D:746:LEU:HD22	3:D:754:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:44:ASP:HB3	4:E:48:VAL:HB	2.02	0.41
5:F:96:ASP:OD2	5:F:99:ARG:HB2	2.20	0.41
5:F:490:PRO:HG2	5:F:493:LYS:HE3	2.03	0.41
1:G:92:VAL:HA	1:G:120:ASP:O	2.21	0.41
1:H:34:GLY:N	1:H:199:ASP:OD2	2.53	0.41
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	2.03	0.41
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.02	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.86	0.41
1:B:112:ALA:HB2	1:B:128:HIS:HB3	2.01	0.41
2:C:403:MET:HE2	2:C:584:TYR:CG	2.56	0.41
2:C:470:ARG:NE	2:C:497:PRO:HB3	2.36	0.41
2:C:498:ILE:HD12	2:C:498:ILE:H	1.86	0.41
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.60	0.41
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.53	0.41
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.51	0.41
3:D:290:ILE:H	3:D:290:ILE:HD12	1.86	0.41
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	2.03	0.41
4:E:49:ILE:HA	4:E:52:ARG:HD3	2.02	0.41
5:F:22:LEU:H	5:F:54:GLN:CB	2.34	0.41
5:F:299:LYS:O	5:F:303:ILE:HG12	2.20	0.41
1:G:177:TYR:O	1:G:178:SER:HB2	2.20	0.41
1:H:61:ILE:HB	1:H:64:VAL:O	2.21	0.41
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.01	0.41
3:J:77:ARG:HG3	3:J:79:LYS:HB3	2.03	0.41
3:J:79:LYS:HB2	5:L:569:THR:H	1.84	0.41
3:J:233:LYS:HA	3:J:234:PRO:HD3	1.93	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.74	0.41
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.92	0.41
3:J:466:MET:HE2	3:J:466:MET:HB3	1.99	0.41
3:J:484:MET:HE2	3:J:484:MET:HB3	1.88	0.41
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.21	0.41
3:J:1348:LYS:HD2	3:J:1348:LYS:HA	1.87	0.41
4:K:35:LYS:HZ1	4:K:71:GLU:CD	2.27	0.41
5:L:96:ASP:OD2	5:L:99:ARG:HB2	2.20	0.41
2:C:468:LEU:HA	2:C:471:VAL:HG12	2.03	0.41
2:C:930:ASP:HB3	2:C:1053:TYR:HB2	2.01	0.41
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.53	0.41
2:I:468:LEU:HA	2:I:471:VAL:HG12	2.03	0.41
2:I:498:ILE:H	2:I:498:ILE:HD12	1.86	0.41
2:I:867:GLU:H	2:I:867:GLU:HG3	1.61	0.41
2:I:1121:ALA:HB1	2:I:1180:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:654:ILE:HG12	3:J:743:MET:HE1	2.03	0.41
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.21	0.41
5:L:250:LEU:O	5:L:254:GLU:HG2	2.21	0.41
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.90	0.40
2:C:60:GLN:HB3	2:C:67:GLU:HG3	2.02	0.40
2:C:516:ASP:H	2:C:526:HIS:HD1	1.69	0.40
2:C:972:PHE:CD2	2:C:975:ILE:HD12	2.56	0.40
3:D:77:ARG:HG3	3:D:79:LYS:HB3	2.03	0.40
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.21	0.40
1:H:90:VAL:HG11	1:H:146:VAL:HG11	2.02	0.40
2:I:32:LEU:HD23	2:I:32:LEU:HA	1.94	0.40
2:I:153:PRO:O	2:I:401:GLY:HA2	2.21	0.40
2:I:232:ILE:HG12	2:I:237:LEU:HD13	2.03	0.40
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.54	0.40
3:J:290:ILE:H	3:J:290:ILE:HD12	1.86	0.40
3:J:399:LYS:HG2	3:J:403:ARG:NH2	2.36	0.40
3:J:490:ILE:HD11	3:J:609:TYR:CD2	2.56	0.40
3:J:557:LYS:HB2	3:J:557:LYS:HE3	1.78	0.40
3:J:600:ALA:O	3:J:603:LYS:HG2	2.21	0.40
3:J:683:ILE:HD11	3:J:754:ILE:HG12	2.02	0.40
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.02	0.40
3:J:820:ILE:HD11	3:J:822:MET:HE2	2.02	0.40
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	2.03	0.40
4:K:44:ASP:HB3	4:K:48:VAL:HB	2.03	0.40
1:A:145:LYS:HB3	1:A:145:LYS:HE3	1.85	0.40
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.86	0.40
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.57	0.40
2:C:101:ARG:HH21	2:C:118:LYS:HE3	1.86	0.40
3:D:79:LYS:HG3	3:D:80:HIS:N	2.36	0.40
3:D:572:THR:OG1	3:D:573:THR:N	2.54	0.40
5:F:569:THR:OG1	5:F:570:ASP:N	2.53	0.40
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.56	0.40
2:I:1161:LEU:HD12	2:I:1161:LEU:HA	1.81	0.40
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.52	0.40
2:C:213:LEU:HD13	2:C:422:LYS:HG2	2.03	0.40
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.88	0.40
3:D:34:SER:HG	3:D:104:HIS:CG	2.30	0.40
3:D:197:GLU:O	3:D:201:LEU:HG	2.21	0.40
5:F:250:LEU:O	5:F:254:GLU:HG2	2.21	0.40
5:F:465:ARG:HA	5:F:468:ARG:HH12	1.87	0.40
1:G:54:CYS:O	1:G:146:VAL:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.77	0.40
1:H:213:PRO:O	1:H:217:ILE:HG13	2.22	0.40
3:J:660:GLU:O	3:J:664:ILE:HG12	2.21	0.40
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.51	0.40
1:B:61:ILE:HB	1:B:64:VAL:O	2.22	0.40
2:C:196:VAL:HG12	2:C:206:ALA:HA	2.04	0.40
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.85	0.40
3:D:579:LEU:HD12	3:D:582:ILE:HD12	2.03	0.40
3:D:844:THR:OG1	3:D:860:ARG:O	2.34	0.40
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.62	0.40
3:J:1100:PHE:HB2	3:J:1200:GLU:CD	2.46	0.40
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.52	0.40
2:C:202:ARG:NH2	2:C:368:ARG:HH12	2.20	0.40
2:C:356:THR:HG21	2:C:362:ALA:HA	2.03	0.40
3:D:581:MET:HE2	3:D:581:MET:HB3	2.01	0.40
3:D:600:ALA:O	3:D:603:LYS:HG2	2.21	0.40
4:E:4:VAL:HG22	4:E:5:THR:HG23	2.04	0.40
2:I:69:GLN:HE21	2:I:69:GLN:HB3	1.68	0.40
2:I:83:GLN:O	2:I:87:ILE:HG13	2.21	0.40
2:I:101:ARG:HH21	2:I:118:LYS:HE3	1.86	0.40
2:I:312:ALA:HB3	2:I:315:MET:HE3	2.03	0.40
2:I:742:TYR:CD2	2:I:743:PRO:HD2	2.57	0.40
2:I:930:ASP:HB3	2:I:1053:TYR:HB2	2.02	0.40
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	2.04	0.40
2:I:1109:ILE:HD12	2:I:1109:ILE:HA	1.81	0.40
3:J:197:GLU:O	3:J:201:LEU:HG	2.21	0.40
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	193 (87%)	27 (12%)	2 (1%)	14	47
1	B	216/239 (90%)	190 (88%)	26 (12%)	0	100	100
1	G	226/239 (95%)	196 (87%)	27 (12%)	3 (1%)	9	40
1	H	213/239 (89%)	190 (89%)	23 (11%)	0	100	100
2	C	1338/1342 (100%)	1233 (92%)	101 (8%)	4 (0%)	36	69
2	I	1338/1342 (100%)	1234 (92%)	99 (7%)	5 (0%)	30	64
3	D	1162/1407 (83%)	1061 (91%)	97 (8%)	4 (0%)	36	69
3	J	1328/1407 (94%)	1213 (91%)	111 (8%)	4 (0%)	36	69
4	E	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	480 (90%)	52 (10%)	0	100	100
5	L	529/613 (86%)	480 (91%)	49 (9%)	0	100	100
All	All	7268/7862 (92%)	6624 (91%)	622 (9%)	22 (0%)	36	69

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	120	LEU
3	J	120	LEU
2	C	170	VAL
2	I	170	VAL
2	I	237	LEU
3	J	340	GLN
2	C	697	LYS
2	C	1136	GLN
3	D	10	ALA
3	D	710	ASP
1	G	14	VAL
2	I	697	LYS
2	I	1136	GLN
3	J	710	ASP
1	A	14	VAL
2	C	1186	VAL
1	A	167	PRO
3	D	831	VAL
1	G	167	PRO
2	I	1186	VAL
3	J	831	VAL
1	G	178	SER

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%)	175 (92%)	16 (8%)	10	34
1	B	184/206 (89%)	166 (90%)	18 (10%)	7	28
1	G	191/206 (93%)	174 (91%)	17 (9%)	9	32
1	H	183/206 (89%)	166 (91%)	17 (9%)	8	30
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	9	33
2	I	1154/1157 (100%)	1053 (91%)	101 (9%)	9	33
3	D	975/1168 (84%)	871 (89%)	104 (11%)	6	25
3	J	1117/1168 (96%)	1005 (90%)	112 (10%)	7	28
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	24
4	K	67/75 (89%)	59 (88%)	8 (12%)	5	21
5	F	426/540 (79%)	382 (90%)	44 (10%)	7	27
5	L	428/540 (79%)	385 (90%)	43 (10%)	7	28
All	All	6143/6704 (92%)	5553 (90%)	590 (10%)	8	29

All (590) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	15	ASP
1	A	26	VAL
1	A	35	PHE
1	A	54	CYS
1	A	61	ILE
1	A	64	VAL
1	A	71	LYS
1	A	129	VAL
1	A	133	LEU
1	A	172	LEU
1	A	173	VAL
1	A	186	ASN
1	A	207	THR

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Mol	Chain	Res	Type
1	A	215	GLU
1	A	228	LEU
1	B	8	PHE
1	B	13	LEU
1	B	16	ILE
1	B	27	THR
1	B	54	CYS
1	B	60	GLU
1	B	65	LEU
1	B	75	GLN
1	B	80	GLU
1	B	92	VAL
1	B	101	THR
1	B	107	ILE
1	B	116	THR
1	B	124	VAL
1	B	133	LEU
1	B	144	ILE
1	B	160	HIS
1	B	183	ILE
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE
2	C	81	ASP
2	C	85	CYS
2	C	91	THR
2	C	114	VAL
2	C	115	LYS
2	C	116	ASP
2	C	131	THR
2	C	182	SER
2	C	202	ARG
2	C	235	ASN
2	C	285	ILE
2	C	292	ILE
2	C	316	GLU
2	C	320	ASP
2	C	321	LEU
2	C	360	LEU
2	C	413	GLU
2	C	419	ILE
2	C	423	ASP

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Mol	Chain	Res	Type
2	C	434	ASP
2	C	453	ILE
2	C	481	LEU
2	C	484	LEU
2	C	486	THR
2	C	493	ILE
2	C	512	SER
2	C	517	GLN
2	C	518	ASN
2	C	530	ILE
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	550	VAL
2	C	558	VAL
2	C	575	LEU
2	C	604	HIS
2	C	615	VAL
2	C	618	GLN
2	C	623	LEU
2	C	657	THR
2	C	660	VAL
2	C	672	GLU
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	706	ARG
2	C	714	VAL
2	C	724	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	782	VAL
2	C	788	SER
2	C	815	SER
2	C	817	LEU
2	C	819	SER
2	C	828	PHE
2	C	839	VAL
2	C	859	GLU

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Mol	Chain	Res	Type
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	946	LEU
2	C	967	LEU
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	990	ASP
2	C	1002	LEU
2	C	1005	GLU
2	C	1006	GLU
2	C	1014	LEU
2	C	1040	ASP
2	C	1082	ILE
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1141	LEU
2	C	1145	ILE
2	C	1155	VAL
2	C	1161	LEU
2	C	1172	LEU
2	C	1174	GLU
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1233	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1253	LEU
2	C	1254	VAL
2	C	1264	GLN
2	C	1265	PHE
2	C	1299	ASN
2	C	1326	LEU
2	C	1327	LEU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE

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Mol	Chain	Res	Type
3	D	46	TYR
3	D	71	LEU
3	D	79	LYS
3	D	83	VAL
3	D	92	VAL
3	D	95	THR
3	D	97	VAL
3	D	117	LEU
3	D	119	SER
3	D	120	LEU
3	D	132	LEU
3	D	169	LEU
3	D	175	GLU
3	D	194	LEU
3	D	217	LEU
3	D	237	MET
3	D	244	VAL
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	256	ASP
3	D	311	ARG
3	D	324	LEU
3	D	330	MET
3	D	339	ARG
3	D	356	THR
3	D	374	LEU
3	D	394	ILE
3	D	407	VAL
3	D	416	ILE
3	D	474	LEU
3	D	501	VAL
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	523	GLU
3	D	536	LEU
3	D	547	ARG
3	D	568	SER
3	D	593	ASN
3	D	594	GLN
3	D	615	LYS

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Mol	Chain	Res	Type
3	D	641	ILE
3	D	660	GLU
3	D	677	GLU
3	D	678	ARG
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	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	740	LEU
3	D	754	ILE
3	D	757	THR
3	D	767	LEU
3	D	770	LEU
3	D	810	THR
3	D	826	ILE
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	860	ARG
3	D	867	GLN
3	D	890	THR
3	D	897	HIS
3	D	908	ILE
3	D	913	GLU
3	D	918	ILE
3	D	928	THR
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1167	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1202	GLU
3	D	1209	VAL

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Mol	Chain	Res	Type
3	D	1215	GLU
3	D	1244	GLN
3	D	1251	LYS
3	D	1255	VAL
3	D	1272	SER
3	D	1274	PHE
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1307	LEU
3	D	1309	ILE
3	D	1327	GLU
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
4	E	4	VAL
4	E	13	ILE
4	E	28	ARG
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	27	VAL
5	F	44	ILE
5	F	45	ILE
5	F	50	ASP
5	F	94	THR
5	F	98	VAL
5	F	100	MET
5	F	118	ASP
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	244	THR
5	F	251	LYS
5	F	297	MET
5	F	305	LEU
5	F	306	PHE
5	F	341	LEU
5	F	395	THR

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Mol	Chain	Res	Type
5	F	417	ASP
5	F	429	THR
5	F	445	ASP
5	F	449	THR
5	F	454	VAL
5	F	479	THR
5	F	486	ARG
5	F	488	LEU
5	F	491	GLU
5	F	494	ILE
5	F	496	LYS
5	F	499	LYS
5	F	508	GLU
5	F	528	LEU
5	F	530	LEU
5	F	540	LEU
5	F	544	THR
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	578	LYS
5	F	580	PHE
5	F	583	THR
5	F	586	ARG
5	F	600	HIS
5	F	606	VAL
1	G	9	LEU
1	G	15	ASP
1	G	26	VAL
1	G	35	PHE
1	G	54	CYS
1	G	61	ILE
1	G	64	VAL
1	G	71	LYS
1	G	129	VAL
1	G	133	LEU
1	G	168	ILE
1	G	172	LEU
1	G	173	VAL
1	G	186	ASN
1	G	207	THR
1	G	215	GLU

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Mol	Chain	Res	Type
1	G	228	LEU
1	H	13	LEU
1	H	16	ILE
1	H	27	THR
1	H	54	CYS
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	80	GLU
1	H	92	VAL
1	H	101	THR
1	H	107	ILE
1	H	116	THR
1	H	124	VAL
1	H	133	LEU
1	H	144	ILE
1	H	183	ILE
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	81	ASP
2	I	85	CYS
2	I	91	THR
2	I	114	VAL
2	I	115	LYS
2	I	116	ASP
2	I	131	THR
2	I	182	SER
2	I	202	ARG
2	I	235	ASN
2	I	285	ILE
2	I	292	ILE
2	I	316	GLU
2	I	320	ASP
2	I	321	LEU
2	I	360	LEU
2	I	413	GLU
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	453	ILE

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Mol	Chain	Res	Type
2	I	484	LEU
2	I	486	THR
2	I	493	ILE
2	I	512	SER
2	I	517	GLN
2	I	518	ASN
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	550	VAL
2	I	558	VAL
2	I	575	LEU
2	I	604	HIS
2	I	615	VAL
2	I	618	GLN
2	I	623	LEU
2	I	657	THR
2	I	660	VAL
2	I	672	GLU
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	705	GLU
2	I	706	ARG
2	I	714	VAL
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	782	VAL
2	I	788	SER
2	I	815	SER
2	I	817	LEU
2	I	819	SER
2	I	828	PHE
2	I	839	VAL
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU

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Mol	Chain	Res	Type
2	I	946	LEU
2	I	967	LEU
2	I	974	ARG
2	I	979	LEU
2	I	984	VAL
2	I	990	ASP
2	I	1002	LEU
2	I	1005	GLU
2	I	1006	GLU
2	I	1014	LEU
2	I	1040	ASP
2	I	1082	ILE
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1141	LEU
2	I	1145	ILE
2	I	1155	VAL
2	I	1161	LEU
2	I	1172	LEU
2	I	1174	GLU
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1253	LEU
2	I	1254	VAL
2	I	1264	GLN
2	I	1265	PHE
2	I	1299	ASN
2	I	1326	LEU
2	I	1327	LEU
3	J	18	ASP
3	J	20	ILE
3	J	46	TYR
3	J	71	LEU
3	J	79	LYS
3	J	83	VAL
3	J	92	VAL

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Mol	Chain	Res	Type
3	J	95	THR
3	J	97	VAL
3	J	117	LEU
3	J	119	SER
3	J	120	LEU
3	J	169	LEU
3	J	175	GLU
3	J	194	LEU
3	J	217	LEU
3	J	237	MET
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	311	ARG
3	J	324	LEU
3	J	330	MET
3	J	339	ARG
3	J	374	LEU
3	J	394	ILE
3	J	407	VAL
3	J	416	ILE
3	J	474	LEU
3	J	501	VAL
3	J	506	VAL
3	J	507	VAL
3	J	513	MET
3	J	523	GLU
3	J	536	LEU
3	J	547	ARG
3	J	568	SER
3	J	593	ASN
3	J	594	GLN
3	J	596	LEU
3	J	615	LYS
3	J	641	ILE
3	J	660	GLU
3	J	677	GLU
3	J	678	ARG
3	J	683	ILE
3	J	685	ILE

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Mol	Chain	Res	Type
3	J	697	MET
3	J	698	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	740	LEU
3	J	754	ILE
3	J	757	THR
3	J	767	LEU
3	J	770	LEU
3	J	810	THR
3	J	826	ILE
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	860	ARG
3	J	867	GLN
3	J	890	THR
3	J	897	HIS
3	J	908	ILE
3	J	913	GLU
3	J	918	ILE
3	J	928	THR
3	J	931	THR
3	J	972	LYS
3	J	987	GLU
3	J	997	VAL
3	J	1017	VAL
3	J	1025	MET
3	J	1042	ASP
3	J	1062	LEU
3	J	1063	ASP
3	J	1073	ASP
3	J	1113	VAL
3	J	1115	ILE
3	J	1155	ILE
3	J	1163	VAL

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Mol	Chain	Res	Type
3	J	1167	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1202	GLU
3	J	1209	VAL
3	J	1215	GLU
3	J	1244	GLN
3	J	1251	LYS
3	J	1255	VAL
3	J	1272	SER
3	J	1274	PHE
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1307	LEU
3	J	1309	ILE
3	J	1327	GLU
3	J	1332	LEU
3	J	1333	THR
3	J	1343	GLU
4	K	4	VAL
4	K	13	ILE
4	K	28	ARG
4	K	31	GLN
4	K	36	ASP
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	27	VAL
5	L	44	ILE
5	L	45	ILE
5	L	50	ASP
5	L	98	VAL
5	L	100	MET
5	L	118	ASP
5	L	127	ILE
5	L	130	VAL
5	L	154	GLU
5	L	244	THR
5	L	251	LYS
5	L	297	MET

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Mol	Chain	Res	Type
5	L	305	LEU
5	L	306	PHE
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	429	THR
5	L	445	ASP
5	L	449	THR
5	L	454	VAL
5	L	479	THR
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU
5	L	494	ILE
5	L	496	LYS
5	L	499	LYS
5	L	508	GLU
5	L	528	LEU
5	L	530	LEU
5	L	540	LEU
5	L	544	THR
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	578	LYS
5	L	580	PHE
5	L	583	THR
5	L	586	ARG
5	L	600	HIS
5	L	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	84	ASN
1	B	194	GLN
2	C	510	GLN
2	C	513	GLN
2	C	618	GLN
2	C	684	ASN
2	C	1017	GLN
2	C	1108	ASN

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Mol	Chain	Res	Type
2	C	1111	GLN
2	C	1116	HIS
2	C	1264	GLN
2	C	1288	GLN
2	C	1312	ASN
2	C	1324	ASN
3	D	158	GLN
3	D	196	GLN
3	D	340	GLN
3	D	364	HIS
3	D	419	HIS
3	D	435	GLN
3	D	560	ASN
3	D	593	ASN
3	D	665	GLN
3	D	667	GLN
3	D	792	ASN
3	D	897	HIS
3	D	1295	ASN
3	D	1367	GLN
4	E	61	ASN
4	E	62	GLN
5	F	128	ASN
5	F	345	GLN
5	F	406	GLN
5	F	461	ASN
5	F	472	GLN
5	F	545	HIS
2	I	20	GLN
2	I	343	HIS
2	I	513	GLN
2	I	618	GLN
2	I	684	ASN
2	I	1017	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1288	GLN
2	I	1314	GLN
2	I	1324	ASN
3	J	158	GLN
3	J	196	GLN

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Mol	Chain	Res	Type
3	J	340	GLN
3	J	364	HIS
3	J	419	HIS
3	J	435	GLN
3	J	560	ASN
3	J	593	ASN
3	J	665	GLN
3	J	667	GLN
3	J	792	ASN
3	J	897	HIS
3	J	954	ASN
3	J	1126	GLN
3	J	1268	ASN
3	J	1295	ASN
3	J	1367	GLN
4	K	60	ASN
4	K	61	ASN
4	K	62	GLN
5	L	128	ASN
5	L	345	GLN
5	L	406	GLN
5	L	461	ASN
5	L	472	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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/239 (93%)	-0.31	2 (0%) 81 61	57, 89, 134, 170	0
1	B	220/239 (92%)	-0.24	3 (1%) 73 52	57, 121, 154, 165	0
1	G	228/239 (95%)	-0.22	7 (3%) 51 35	84, 122, 155, 170	0
1	H	217/239 (90%)	-0.26	2 (0%) 81 61	90, 134, 157, 166	0
2	C	1340/1342 (99%)	-0.25	10 (0%) 84 66	31, 86, 140, 175	0
2	I	1340/1342 (99%)	-0.29	16 (1%) 76 55	41, 105, 151, 183	0
3	D	1166/1407 (82%)	-0.33	9 (0%) 82 63	28, 78, 140, 170	0
3	J	1334/1407 (94%)	-0.29	10 (0%) 84 66	33, 99, 159, 185	0
4	E	89/91 (97%)	-0.54	0 100 100	38, 82, 122, 129	0
4	K	79/91 (86%)	-0.45	0 100 100	60, 96, 144, 154	0
5	F	542/613 (88%)	-0.21	7 (1%) 75 53	49, 127, 166, 196	0
5	L	539/613 (87%)	-0.24	6 (1%) 78 57	62, 125, 165, 179	0
All	All	7318/7862 (93%)	-0.28	72 (0%) 79 58	28, 102, 155, 196	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	341	ASN	4.2
3	J	1248	ILE	3.7
2	I	484	LEU	3.7
3	J	340	GLN	3.6
3	D	754	ILE	3.6
2	C	251	ALA	3.2
5	L	130	VAL	3.2
2	I	333	ILE	3.1
2	C	1001	GLY	3.1
2	I	190	PRO	3.0
1	H	233	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
3	D	310	GLY	3.0
1	G	88	LEU	2.9
1	G	235	GLU	2.9
2	C	929	ILE	2.9
5	F	85	SER	2.8
2	I	704	MET	2.8
3	D	631	TYR	2.8
2	I	792	GLY	2.8
5	L	386	LEU	2.7
1	A	216	ALA	2.7
2	I	347	ILE	2.7
5	L	13	VAL	2.7
2	C	206	ALA	2.6
3	D	482	ALA	2.6
1	H	234	LEU	2.6
3	D	683	ILE	2.6
2	I	796	LEU	2.6
5	L	610	PHE	2.6
3	J	218	THR	2.5
3	D	340	GLN	2.5
1	B	78	ILE	2.5
2	I	1256	GLN	2.5
2	I	818	VAL	2.4
5	F	162	ILE	2.4
3	D	341	ASN	2.4
1	B	158	ARG	2.4
2	I	221	LEU	2.4
2	C	184	LEU	2.3
1	B	59	VAL	2.3
5	L	243	ALA	2.3
2	I	442	VAL	2.3
1	G	234	LEU	2.3
1	A	225	ALA	2.3
3	J	176	PHE	2.3
3	J	1291	GLU	2.3
1	G	82	LEU	2.2
3	J	899	TYR	2.2
5	F	86	SER	2.2
1	G	90	VAL	2.2
3	J	1273	ASP	2.2
2	I	1050	VAL	2.2
2	C	575	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	217	ILE	2.2
3	J	808	VAL	2.1
2	I	224	PHE	2.1
5	F	243	ALA	2.1
3	J	530	PRO	2.1
2	I	979	LEU	2.1
2	C	1153	ALA	2.1
5	F	259	PHE	2.1
5	L	37	ASP	2.1
2	C	209	ILE	2.1
2	I	1233	LEU	2.0
3	D	239	LEU	2.0
3	D	801	VAL	2.0
1	G	233	ASP	2.0
2	I	1325	VAL	2.0
2	C	573	ASN	2.0
2	C	701	GLY	2.0
5	F	39	ASP	2.0
5	F	582	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	1501	1/1	0.60	0.20	72,72,72,72	0
6	MG	J	1501	1/1	0.74	0.20	74,74,74,74	0
7	ZN	D	1503	1/1	0.98	0.18	138,138,138,138	0
7	ZN	J	1502	1/1	0.99	0.06	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ZN	D	1502	1/1	1.00	0.04	103,103,103,103	0
7	ZN	J	1503	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.