



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:33 PM UTC

PDB ID : 4LLG / pdb_00004llg
Title : Crystal Structure Analysis of the E.coli holoenzyme/Gp2 complex
Authors : Bae, B.; Darst, S.A.
Deposited on : 2013-07-09
Resolution : 3.79 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:

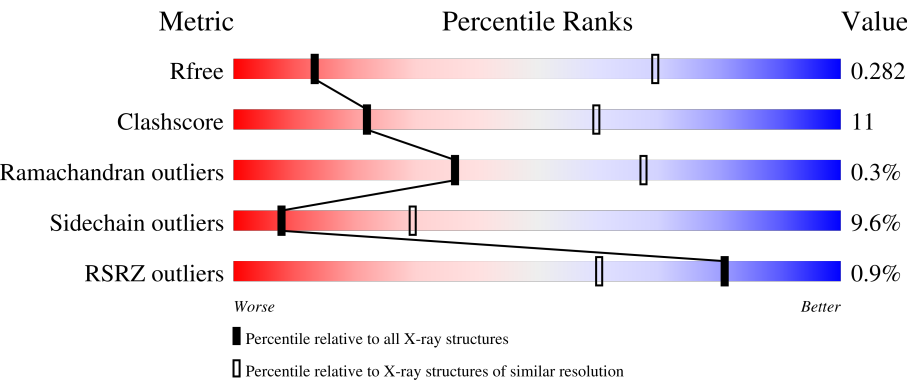
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	% 57%31%8%
1	G	239	% 63%29%5%
1	H	239	% 58%29%9%
2	C	1342	% 69%27%

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Mol	Chain	Length	Quality of chain
2	I	1342	70% 26% .
3	D	1407	65% 27% . .
3	J	1407	65% 26% . 6%
4	E	91	73% 22% . . .
4	K	91	58% 26% . . 13%
5	F	613	59% 22% . 15%
5	L	613	58% 23% . 15%
6	M	64	50% 23% 5% 22%
6	N	64	47% 22% 5% . 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 59147 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 20 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	521	Total	C	N	O	S	0	0	0
			4161	2609	735	791	26			
5	L	519	Total	C	N	O	S	0	0	0
			4155	2605	733	791	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	50	Total	C	N	O	S	0	0	0
			406	264	63	78	1			
6	N	48	Total	C	N	O	S	0	0	0
			389	253	60	75	1			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

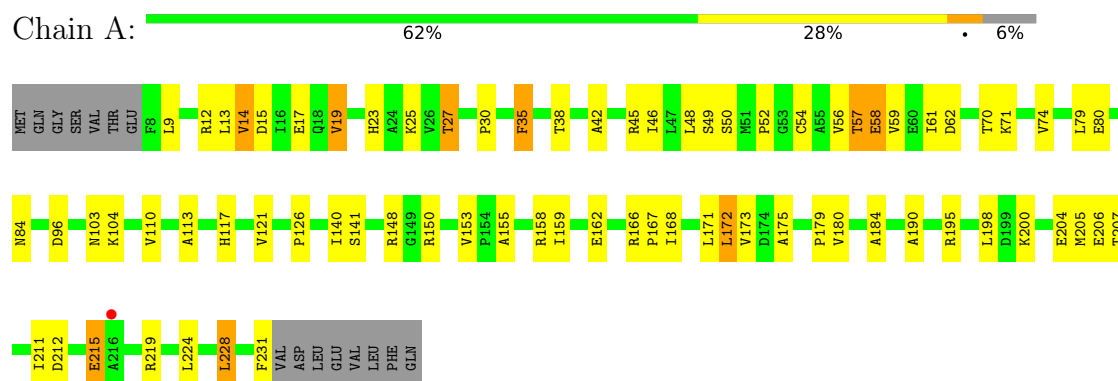
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

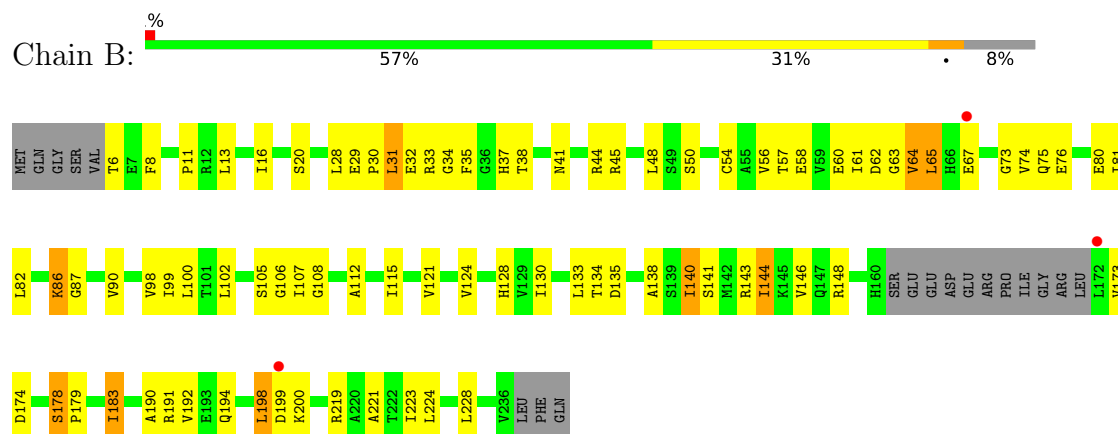
3 Residue-property plots [i](#)

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.

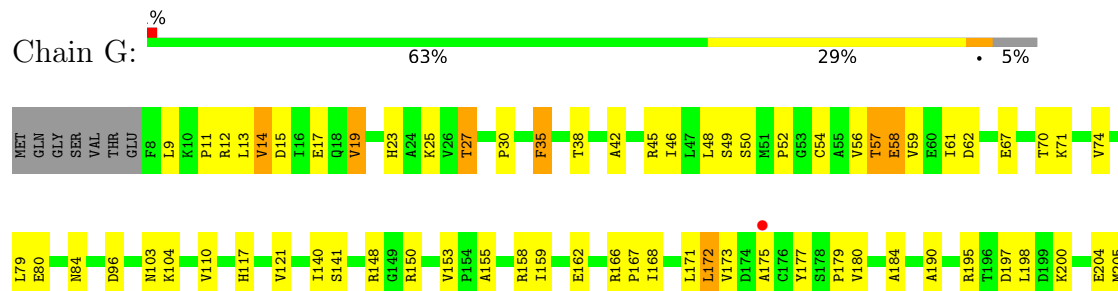
- Molecule 1: DNA-directed RNA polymerase subunit alpha

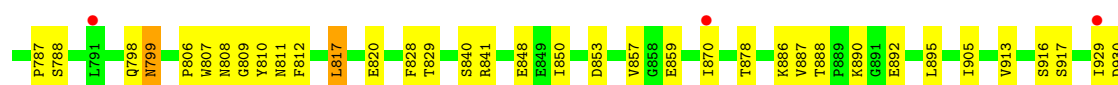


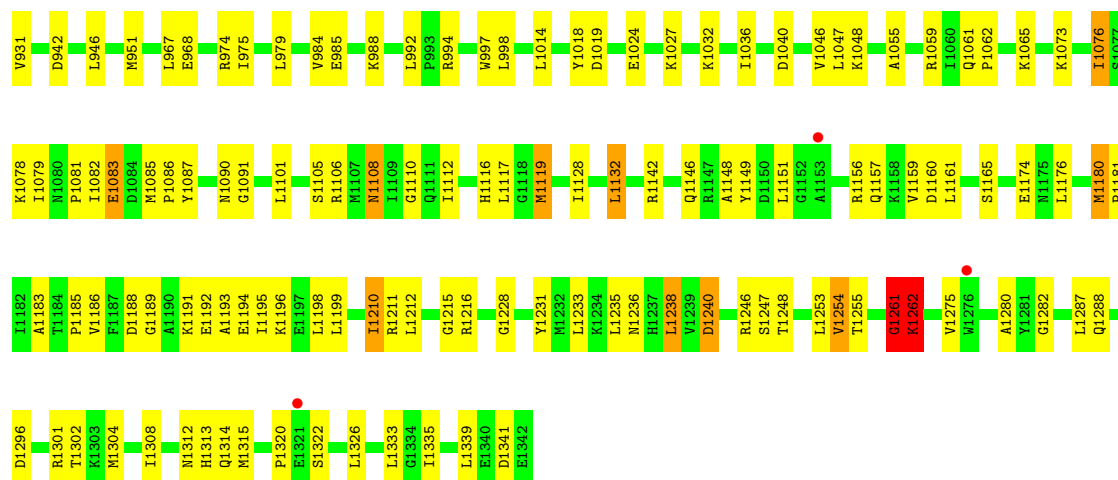
- Molecule 1: DNA-directed RNA polymerase subunit alpha



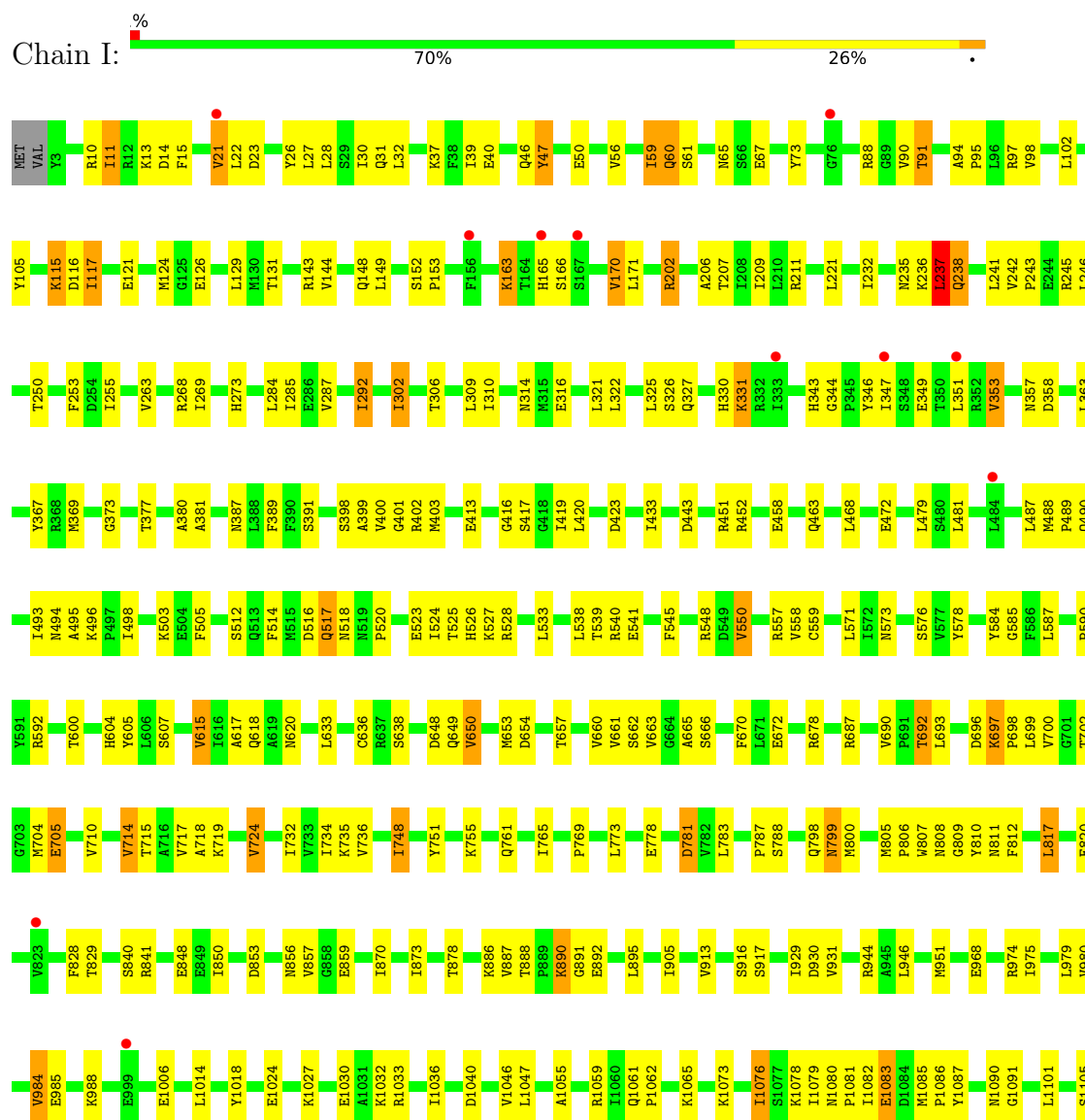
- Molecule 1: DNA-directed RNA polymerase subunit alpha



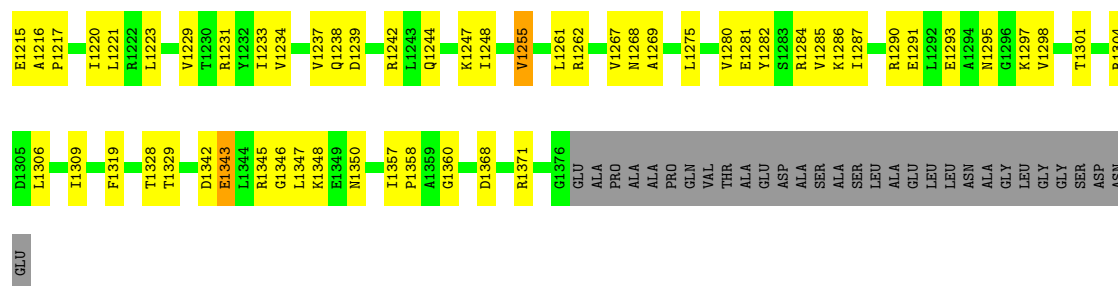




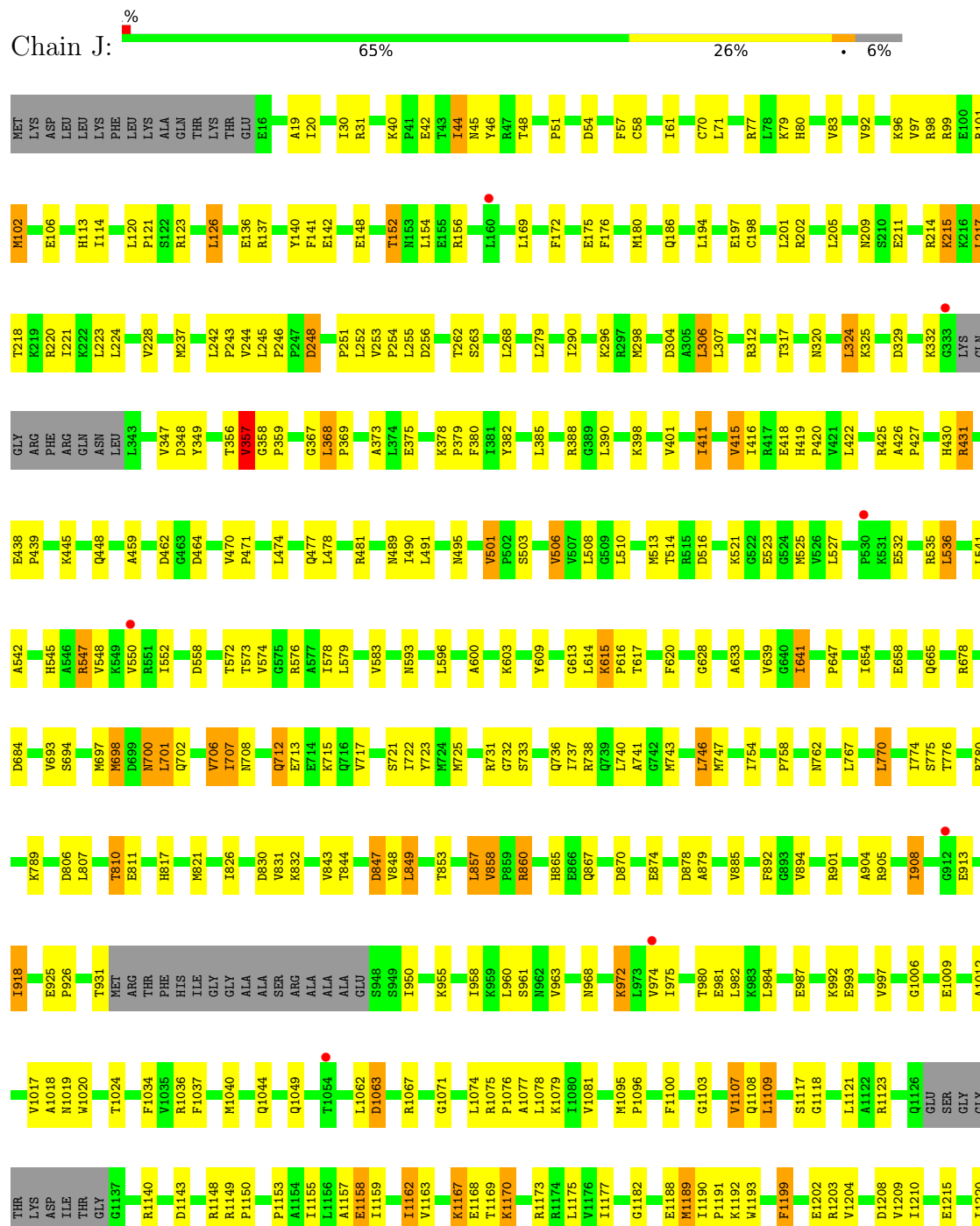
• Molecule 2: DNA-directed RNA polymerase subunit beta

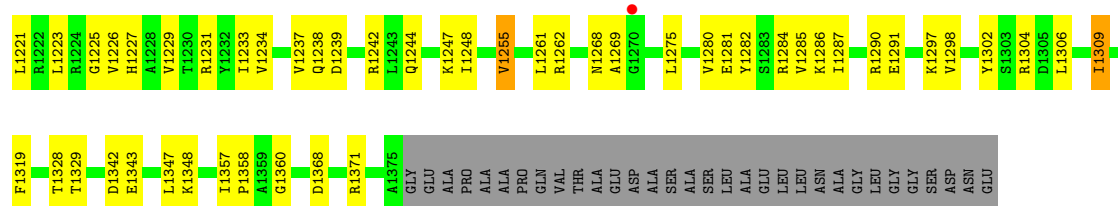




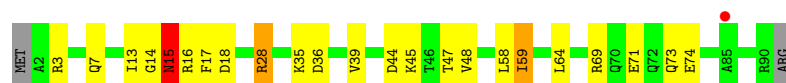


• Molecule 3: DNA-directed RNA polymerase subunit beta'





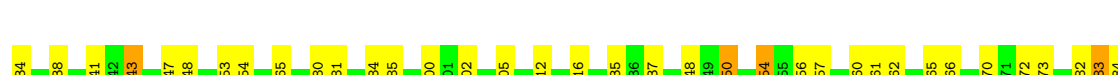
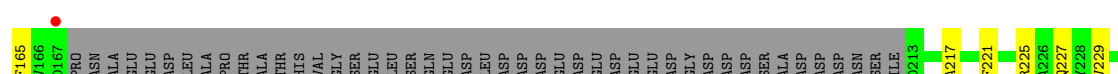
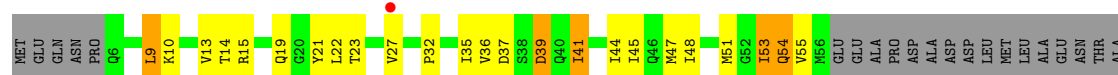
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 4: DNA-directed RNA polymerase subunit omega

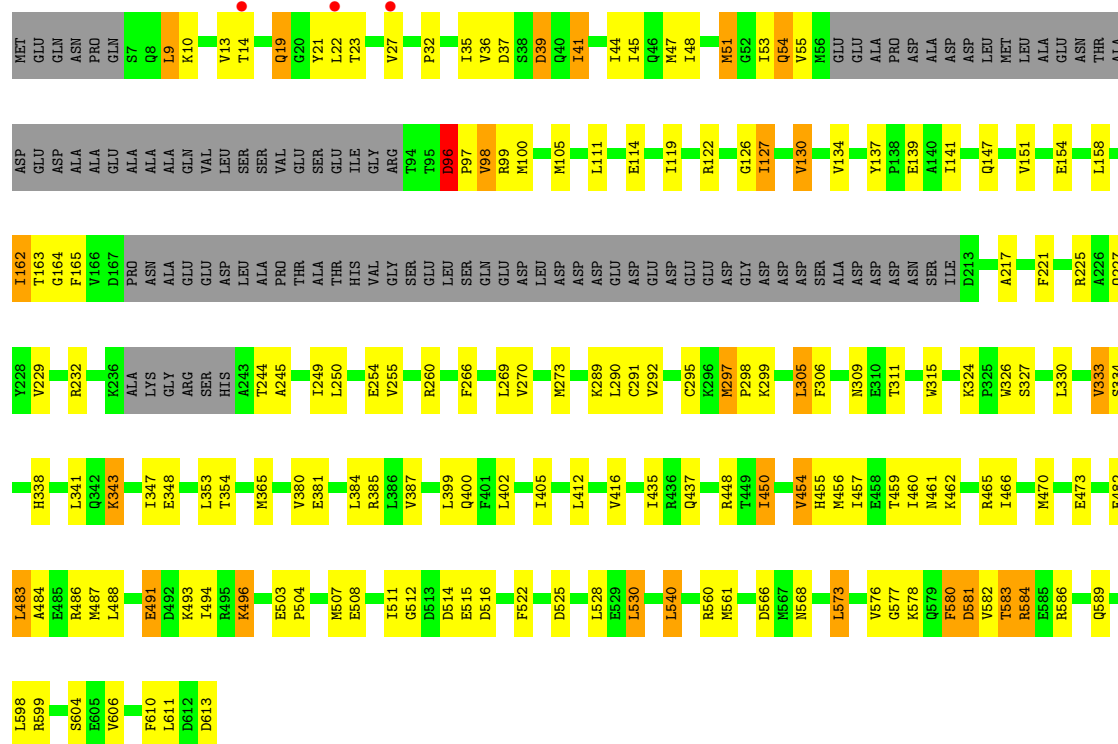


- Molecule 5: RNA polymerase sigma factor RpoD



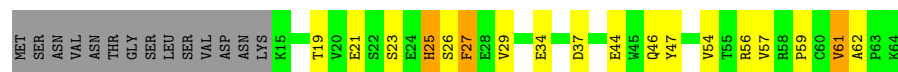
- Molecule 5: RNA polymerase sigma factor RpoD

Chain L:  58% 23% 15%



• Molecule 6: Bacterial RNA polymerase inhibitor

Chain M:  50% 23% 5% 22%



• Molecule 6: Bacterial RNA polymerase inhibitor

Chain N:  47% 22% 5% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.51Å 205.04Å 308.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.21 – 3.79 45.21 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.21-3.79) 98.1 (45.21-3.79)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.243 , 0.282 0.242 , 0.282	Depositor DCC
R_{free} test set	5844 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	126.7	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	59147	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: MG, ZN

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	0.31	0/1751	0.81	0/2373
1	B	0.32	0/1707	0.79	5/2314 (0.2%)
1	G	0.31	0/1771	0.82	0/2401
1	H	0.32	0/1686	0.80	5/2285 (0.2%)
2	C	0.33	2/10739 (0.0%)	0.78	7/14489 (0.0%)
2	I	0.33	2/10735 (0.0%)	0.78	5/14484 (0.0%)
3	D	0.32	2/10603 (0.0%)	0.78	11/14316 (0.1%)
3	J	0.32	2/10450 (0.0%)	0.77	9/14112 (0.1%)
4	E	0.32	0/693	0.81	0/935
4	K	0.31	0/629	0.80	0/847
5	F	0.34	0/4214	0.81	8/5673 (0.1%)
5	L	0.36	0/4208	0.82	5/5665 (0.1%)
6	M	0.43	0/419	0.86	2/572 (0.3%)
6	N	0.42	0/401	0.86	3/549 (0.5%)
All	All	0.33	8/60006 (0.0%)	0.79	60/81015 (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
2	I	0	1
4	E	0	1
4	K	0	1
5	L	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	31	GLN	CD-NE2	-10.54	1.11	1.33
2	I	31	GLN	CD-NE2	-10.20	1.11	1.33
2	I	31	GLN	CD-OE1	-9.01	1.06	1.23
2	C	31	GLN	CD-OE1	-8.81	1.06	1.23
3	D	477	GLN	CD-NE2	-7.64	1.17	1.33
3	J	477	GLN	CD-NE2	-7.43	1.17	1.33
3	D	477	GLN	CD-OE1	-5.18	1.13	1.23
3	J	477	GLN	CD-OE1	-5.17	1.13	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	19	GLN	CA-C-N	7.36	134.94	121.70
5	L	19	GLN	C-N-CA	7.36	134.94	121.70
2	I	237	LEU	CB-CA-C	-7.08	107.36	115.79
2	C	237	LEU	CB-CA-C	-7.07	107.38	115.79
5	F	19	GLN	CA-C-N	6.58	134.30	121.41
5	F	19	GLN	C-N-CA	6.58	134.30	121.41
5	F	96	ASP	CA-C-N	6.50	126.19	119.56
5	F	96	ASP	C-N-CA	6.50	126.19	119.56
3	J	1225	GLY	N-CA-C	6.36	118.51	112.08
2	I	1261	GLY	N-CA-C	6.20	127.87	113.18
2	C	1261	GLY	N-CA-C	6.19	127.84	113.18
6	M	23	SER	CB-CA-C	-6.06	109.57	116.54
3	J	1182	GLY	N-CA-C	6.00	127.39	113.18
6	N	25	HIS	N-CA-C	5.92	116.38	108.38
6	M	25	HIS	N-CA-C	5.90	116.34	108.38
3	D	1182	GLY	N-CA-C	5.89	127.14	113.18
1	H	178	SER	CA-C-N	5.88	125.50	119.56
1	H	178	SER	C-N-CA	5.88	125.50	119.56
1	B	178	SER	CA-C-N	5.62	125.71	119.87
1	B	178	SER	C-N-CA	5.62	125.71	119.87
3	D	1295	ASN	N-CA-C	-5.56	101.97	110.14
5	F	19	GLN	O-C-N	5.55	128.48	122.15
6	N	23	SER	CB-CA-C	-5.54	110.17	116.54
1	H	20	SER	CB-CA-C	-5.54	110.21	116.63
1	B	108	GLY	CA-C-N	5.52	125.47	119.78
1	B	108	GLY	C-N-CA	5.52	125.47	119.78
1	H	108	GLY	CA-C-N	5.51	125.45	119.78
1	H	108	GLY	C-N-CA	5.51	125.45	119.78
1	B	20	SER	CB-CA-C	-5.51	110.24	116.63
2	I	984	VAL	N-CA-C	5.50	116.36	108.93
3	J	40	LYS	CA-C-N	5.48	125.09	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	40	LYS	C-N-CA	5.48	125.09	119.56
3	D	40	LYS	CA-C-N	5.47	125.08	119.56
3	D	40	LYS	C-N-CA	5.47	125.08	119.56
3	D	253	VAL	CA-C-N	5.45	125.45	120.21
3	D	253	VAL	C-N-CA	5.45	125.45	120.21
3	J	470	VAL	CA-C-N	5.44	126.64	119.84
3	J	470	VAL	C-N-CA	5.44	126.64	119.84
3	D	470	VAL	CA-C-N	5.43	126.63	119.84
3	D	470	VAL	C-N-CA	5.43	126.63	119.84
2	I	650	VAL	N-CA-C	5.43	116.41	109.30
2	C	650	VAL	N-CA-C	5.39	116.36	109.30
3	D	19	ALA	CB-CA-C	-5.35	109.42	115.79
3	J	19	ALA	CB-CA-C	-5.29	109.50	115.79
2	C	512	SER	CA-C-N	-5.26	112.66	121.75
2	C	512	SER	C-N-CA	-5.26	112.66	121.75
5	F	53	ILE	N-CA-C	5.21	115.71	108.84
5	F	37	ASP	N-CA-C	5.14	117.09	109.69
2	C	984	VAL	N-CA-C	5.12	115.84	108.93
3	D	501	VAL	CA-C-N	5.07	125.06	119.89
3	D	501	VAL	C-N-CA	5.07	125.06	119.89
3	J	501	VAL	CA-C-N	5.05	125.05	119.89
3	J	501	VAL	C-N-CA	5.05	125.05	119.89
5	F	584	ARG	N-CA-C	5.04	115.45	108.00
5	L	37	ASP	N-CA-C	5.03	116.93	109.69
6	N	61	VAL	CB-CA-C	5.03	119.53	111.29
2	I	31	GLN	OE1-CD-NE2	-5.03	117.58	122.60
5	L	96	ASP	N-CA-C	5.02	120.90	109.81
2	C	398	SER	CB-CA-C	-5.02	109.82	115.79
5	L	584	ARG	N-CA-C	5.00	115.41	108.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1261	GLY	Peptide
4	E	14	GLY	Peptide
2	I	1261	GLY	Peptide
4	K	14	GLY	Peptide
5	L	19	GLN	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	47	0
1	B	1687	0	1700	49	0
1	G	1750	0	1764	48	0
1	H	1667	0	1689	42	0
2	C	10570	0	10582	243	0
2	I	10566	0	10576	229	0
3	D	10447	0	10671	262	0
3	J	10295	0	10510	241	0
4	E	691	0	695	16	0
4	K	627	0	634	18	0
5	F	4161	0	4171	89	0
5	L	4155	0	4168	94	0
6	M	406	0	383	10	0
6	N	389	0	363	13	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	59147	0	59662	1269	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 11.

All (1269) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1173:ARG:HE	3:D:1192:LYS:HG3	1.29	0.97
3:J:1173:ARG:HE	3:J:1192:LYS:HG3	1.28	0.97
3:D:418:GLU:HG3	4:E:45:LYS:H	1.42	0.85
3:J:1006:GLY:H	3:J:1009:GLU:HG3	1.41	0.85
3:J:418:GLU:HG3	4:K:45:LYS:H	1.41	0.83
3:D:1006:GLY:H	3:D:1009:GLU:HG3	1.42	0.83
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.44	0.83
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.44	0.82
2:C:517:GLN:HB2	2:C:523:GLU:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:517:GLN:HB2	2:I:523:GLU:HG2	1.63	0.79
5:F:32:PRO:HG2	5:F:35:ILE:HD12	1.63	0.79
5:L:32:PRO:HG2	5:L:35:ILE:HD12	1.64	0.79
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.65	0.78
2:C:1322:SER:HB2	3:D:340:GLN:HG2	1.65	0.77
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.67	0.77
5:L:130:VAL:HB	5:L:365:MET:HG3	1.66	0.77
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.66	0.76
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.00	0.76
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.66	0.76
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.67	0.75
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.00	0.75
5:F:130:VAL:HB	5:F:365:MET:HG3	1.68	0.75
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.68	0.74
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.70	0.73
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.22	0.73
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.71	0.72
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.72	0.72
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.71	0.72
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.72	0.72
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.72	0.71
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.72	0.71
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.72	0.71
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.72	0.71
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.72	0.71
1:A:159:ILE:HG13	1:A:162:GLU:HB2	1.73	0.70
1:G:104:LYS:HD3	1:G:110:VAL:HG22	1.73	0.69
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.74	0.69
3:J:1075:ARG:HH22	3:J:1173:ARG:NH1	1.90	0.69
5:L:324:LYS:HB2	5:L:327:SER:HB2	1.74	0.69
5:F:134:VAL:HG22	5:F:273:MET:HE1	1.74	0.69
5:F:324:LYS:HB2	5:F:327:SER:HB2	1.74	0.69
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.74	0.69
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.74	0.69
2:I:211:ARG:NH1	2:I:357:ASN:O	2.26	0.69
5:L:134:VAL:HG22	5:L:273:MET:HE1	1.74	0.69
1:A:104:LYS:HD3	1:A:110:VAL:HG22	1.73	0.68
2:C:490:GLN:HG2	5:F:472:GLN:HE21	1.56	0.68
1:G:159:ILE:HG13	1:G:162:GLU:HB2	1.73	0.68
1:G:58:GLU:HG2	1:G:158:ARG:HH22	1.59	0.68
2:C:211:ARG:NH1	2:C:357:ASN:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1108:GLN:HG3	3:D:1109:LEU:HD13	1.76	0.68
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.75	0.68
3:D:358:GLY:H	3:D:359:PRO:HD3	1.59	0.68
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.76	0.68
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.59	0.68
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.76	0.68
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	1.76	0.67
3:D:885:VAL:HG21	3:D:1255:VAL:HG12	1.75	0.67
3:J:358:GLY:H	3:J:359:PRO:HD3	1.59	0.67
3:J:885:VAL:HG21	3:J:1255:VAL:HG12	1.76	0.67
3:J:1075:ARG:HH22	3:J:1173:ARG:HH12	1.43	0.67
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.76	0.67
4:E:15:ASN:OD1	4:E:18:ASP:N	2.26	0.67
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.57	0.67
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.57	0.67
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.76	0.67
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.77	0.66
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.76	0.66
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.28	0.66
4:K:15:ASN:OD1	4:K:18:ASP:N	2.26	0.66
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.60	0.66
2:I:452:ARG:NH1	2:I:584:TYR:O	2.29	0.66
2:C:115:LYS:HE3	2:C:116:ASP:H	1.62	0.65
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.78	0.65
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.78	0.65
5:L:39:ASP:OD1	5:L:39:ASP:N	2.22	0.65
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.78	0.65
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.62	0.65
3:J:209:ASN:HA	3:J:214:ARG:HE	1.62	0.65
3:J:722:ILE:HD11	3:J:737:ILE:HD12	1.78	0.65
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.79	0.65
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.78	0.65
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.62	0.65
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.80	0.64
3:D:77:ARG:HG3	3:D:79:LYS:H	1.62	0.64
3:D:251:PRO:HD2	5:F:507:MET:HE1	1.79	0.64
2:C:452:ARG:NH1	2:C:584:TYR:O	2.31	0.64
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.78	0.64
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.78	0.64
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.78	0.64
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:ASP:OD1	1:G:141:SER:OG	2.16	0.64
3:J:77:ARG:HG3	3:J:79:LYS:H	1.62	0.64
3:J:152:THR:HG21	3:J:176:PHE:HB2	1.80	0.64
3:D:722:ILE:HD11	3:D:737:ILE:HD12	1.78	0.64
3:J:1155:ILE:HG13	3:J:1210:ILE:HB	1.80	0.64
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.78	0.64
3:D:1044:GLN:HB3	3:D:1071:GLY:HA3	1.79	0.64
3:D:209:ASN:HA	3:D:214:ARG:HE	1.62	0.64
3:D:1188:GLU:HG2	6:M:59:PRO:HD2	1.80	0.64
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.80	0.64
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.63	0.63
3:J:481:ARG:NH1	4:K:3:ARG:O	2.31	0.63
3:J:1162:ILE:HA	3:J:1203:ARG:HA	1.80	0.63
1:B:107:ILE:HG23	1:B:135:ASP:HA	1.80	0.63
6:N:44:GLU:HG2	6:N:54:VAL:HG21	1.81	0.63
3:D:152:THR:HG21	3:D:176:PHE:HB2	1.80	0.63
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.81	0.63
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.79	0.63
3:D:481:ARG:NH1	4:E:3:ARG:O	2.32	0.63
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.81	0.63
2:I:528:ARG:NH2	2:I:576:SER:O	2.31	0.63
2:C:528:ARG:NH2	2:C:576:SER:O	2.31	0.63
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.81	0.63
3:D:1155:ILE:HG13	3:D:1210:ILE:HB	1.80	0.63
6:M:61:VAL:HG13	6:M:62:ALA:H	1.63	0.63
5:F:493:LYS:HA	5:F:496:LYS:HE3	1.80	0.62
6:M:44:GLU:HG2	6:M:54:VAL:HG21	1.80	0.62
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.81	0.62
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.81	0.62
5:F:483:LEU:O	5:F:486:ARG:NH1	2.32	0.62
2:I:115:LYS:HE3	2:I:116:ASP:H	1.61	0.62
5:L:10:LYS:O	5:L:14:THR:OG1	2.10	0.62
2:I:702:THR:OG1	2:I:705:GLU:OE2	2.13	0.62
2:I:1119:MET:HE1	2:I:1210:ILE:HD11	1.81	0.62
1:A:62:ASP:OD1	1:A:141:SER:OG	2.17	0.62
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.64	0.62
5:L:493:LYS:HA	5:L:496:LYS:HE3	1.80	0.62
3:D:821:MET:HE2	3:D:879:ALA:HB1	1.82	0.62
2:C:1119:MET:HE1	2:C:1210:ILE:HD11	1.81	0.62
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.81	0.62
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:613:GLY:O	3:D:617:THR:OG1	2.17	0.61
5:L:483:LEU:O	5:L:486:ARG:NH1	2.32	0.61
2:C:59:ILE:HG21	2:C:472:GLU:HG3	1.82	0.61
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.81	0.61
2:I:886:LYS:HB3	2:I:917:SER:HA	1.81	0.61
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.81	0.61
3:J:821:MET:HE2	3:J:879:ALA:HB1	1.83	0.61
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.81	0.61
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.81	0.61
2:C:886:LYS:HB3	2:C:917:SER:HA	1.81	0.61
2:I:59:ILE:HG21	2:I:472:GLU:HG3	1.82	0.61
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.66	0.61
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.32	0.61
3:J:1188:GLU:HG2	6:N:59:PRO:HD2	1.81	0.60
2:C:702:THR:OG1	2:C:705:GLU:OE2	2.13	0.60
3:D:126:LEU:HD13	3:D:223:LEU:HD21	1.84	0.60
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.83	0.60
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.66	0.60
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.84	0.60
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.32	0.60
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.84	0.60
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.84	0.60
2:C:250:THR:HA	2:C:268:ARG:HA	1.84	0.59
1:G:166:ARG:O	1:G:168:ILE:N	2.35	0.59
3:J:356:THR:OG1	3:J:357:VAL:N	2.35	0.59
5:F:10:LYS:O	5:F:14:THR:OG1	2.09	0.59
3:J:613:GLY:O	3:J:617:THR:OG1	2.18	0.59
1:A:166:ARG:O	1:A:168:ILE:N	2.35	0.59
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.85	0.59
3:D:356:THR:OG1	3:D:357:VAL:N	2.35	0.59
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.83	0.59
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.84	0.59
3:D:737:ILE:HA	3:D:740:LEU:HD12	1.85	0.59
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.85	0.59
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.32	0.59
3:D:694:SER:OG	3:D:738:ARG:NE	2.35	0.59
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.84	0.59
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.83	0.59
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.83	0.59
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.85	0.59
3:D:1262:ARG:O	3:D:1280:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:14:ASP:HA	2:I:1183:ALA:HB3	1.84	0.59
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.84	0.58
2:I:250:THR:HA	2:I:268:ARG:HA	1.84	0.58
3:J:1347:LEU:HD12	3:J:1358:PRO:HG2	1.84	0.58
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.36	0.58
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.86	0.58
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.85	0.58
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.03	0.58
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.68	0.58
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.86	0.58
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.85	0.58
3:D:1347:LEU:HD12	3:D:1358:PRO:HG2	1.84	0.58
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.85	0.58
1:H:57:THR:HG22	1:H:58:GLU:HG2	1.85	0.58
3:D:1067:ARG:NH1	3:D:1074:LEU:O	2.36	0.58
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.84	0.58
3:J:694:SER:OG	3:J:738:ARG:NE	2.35	0.58
3:J:737:ILE:HA	3:J:740:LEU:HD12	1.85	0.58
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.85	0.58
1:A:12:ARG:H	1:A:30:PRO:HD2	1.69	0.58
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.68	0.58
1:G:158:ARG:HH21	1:G:172:LEU:HB3	1.69	0.58
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.69	0.58
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.85	0.58
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.86	0.58
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.86	0.58
1:B:57:THR:HG22	1:B:58:GLU:HG2	1.85	0.57
1:G:79:LEU:HD11	2:I:693:LEU:HD21	1.86	0.57
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.86	0.57
2:I:166:SER:HB3	6:N:23:SER:N	2.19	0.57
1:B:64:VAL:HG12	1:B:65:LEU:H	1.69	0.57
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.85	0.57
2:C:1261:GLY:O	2:C:1262:LYS:HB2	2.04	0.57
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.86	0.57
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.86	0.57
1:A:54:CYS:HB3	1:A:148:ARG:HG2	1.86	0.57
3:D:1173:ARG:HH21	3:D:1192:LYS:HE3	1.68	0.57
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.86	0.57
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.86	0.57
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.70	0.57
3:J:789:LYS:NZ	3:J:931:THR:O	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.87	0.57
1:G:54:CYS:HB3	1:G:148:ARG:HG2	1.86	0.57
2:I:398:SER:OG	2:I:399:ALA:N	2.32	0.57
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.86	0.57
3:D:746:LEU:HB2	3:D:754:ILE:HD11	1.86	0.57
3:J:958:ILE:HG23	3:J:982:LEU:HD11	1.87	0.57
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.86	0.57
3:J:251:PRO:HD2	5:L:507:MET:HE1	1.87	0.57
3:J:746:LEU:HB2	3:J:754:ILE:HD11	1.86	0.57
4:K:35:LYS:NZ	4:K:71:GLU:OE2	2.36	0.57
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.87	0.57
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.87	0.57
2:I:1261:GLY:O	2:I:1262:LYS:HB2	2.04	0.57
3:J:388:ARG:HB2	3:J:390:LEU:HD13	1.87	0.57
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.87	0.57
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.87	0.57
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.69	0.57
1:H:90:VAL:HG11	1:H:146:VAL:HG11	1.86	0.57
3:J:44:ILE:HG13	5:L:450:ILE:HG22	1.86	0.57
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.87	0.57
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.86	0.57
2:C:357:ASN:ND2	2:C:358:ASP:OD2	2.38	0.56
2:C:840:SER:O	2:C:1047:LEU:N	2.38	0.56
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.87	0.56
3:J:1067:ARG:NH1	3:J:1074:LEU:O	2.36	0.56
3:D:701:LEU:HD12	3:D:723:TYR:HB2	1.87	0.56
2:I:166:SER:HB3	6:N:23:SER:CA	2.35	0.56
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.38	0.56
2:I:1254:VAL:O	3:J:99:ARG:NH2	2.38	0.56
3:J:51:PRO:HB2	3:J:58:CYS:HA	1.86	0.56
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.87	0.56
3:J:1173:ARG:HH21	3:J:1192:LYS:HE3	1.70	0.56
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.86	0.56
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.87	0.56
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.87	0.56
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.87	0.56
3:J:701:LEU:HD12	3:J:723:TYR:HB2	1.87	0.56
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.87	0.56
2:C:975:ILE:HG12	2:C:1014:LEU:HD13	1.88	0.56
3:D:218:THR:HA	3:D:221:ILE:HG22	1.88	0.56
2:C:829:THR:HG23	2:C:1059:ARG:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.33	0.56
2:I:930:ASP:OD2	2:I:931:VAL:N	2.39	0.56
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.70	0.56
3:D:388:ARG:HB2	3:D:390:LEU:HD13	1.87	0.56
3:D:51:PRO:HB2	3:D:58:CYS:HA	1.86	0.56
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.87	0.56
3:J:218:THR:HA	3:J:221:ILE:HG22	1.88	0.56
3:J:1173:ARG:NE	3:J:1192:LYS:HG3	2.11	0.56
1:B:11:PRO:HG3	1:B:31:LEU:HD13	1.88	0.56
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.69	0.56
1:G:12:ARG:H	1:G:30:PRO:HD2	1.69	0.55
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.87	0.55
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.87	0.55
1:H:11:PRO:HG3	1:H:31:LEU:HD13	1.87	0.55
2:I:373:GLY:O	5:L:99:ARG:NH1	2.39	0.55
1:B:74:VAL:HG11	1:B:81:ILE:HD11	1.88	0.55
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.39	0.55
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.86	0.55
5:F:573:LEU:H	5:F:573:LEU:HD23	1.70	0.55
1:G:45:ARG:HE	1:H:38:THR:HB	1.71	0.55
2:I:840:SER:O	2:I:1047:LEU:N	2.39	0.55
5:F:560:ARG:NH1	5:F:566:ASP:OD1	2.40	0.55
5:L:560:ARG:NH1	5:L:566:ASP:OD1	2.39	0.55
5:F:39:ASP:OD1	5:F:39:ASP:N	2.22	0.55
1:G:96:ASP:HA	1:G:148:ARG:HD3	1.89	0.55
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.86	0.55
2:I:165:HIS:CD2	5:L:51:MET:HE2	2.42	0.55
5:F:583:THR:HG22	5:F:584:ARG:H	1.72	0.55
3:J:1143:ASP:OD1	3:J:1148:ARG:NH1	2.39	0.55
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.87	0.55
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.72	0.55
3:D:1297:LYS:HG2	3:J:1302:TYR:H	1.70	0.55
3:D:958:ILE:HG23	3:D:982:LEU:HD11	1.87	0.55
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.89	0.55
2:C:398:SER:OG	2:C:399:ALA:N	2.32	0.55
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.89	0.55
5:L:9:LEU:HD22	6:N:46:GLN:O	2.07	0.55
5:L:573:LEU:HD23	5:L:573:LEU:H	1.71	0.55
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.21	0.54
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.87	0.54
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:930:ASP:OD2	2:C:931:VAL:N	2.39	0.54
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.54
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.90	0.54
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.88	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.89	0.54
5:L:583:THR:HG22	5:L:584:ARG:H	1.72	0.54
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.22	0.54
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.42	0.54
5:F:330:LEU:O	5:F:334:SER:OG	2.21	0.54
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.89	0.54
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.72	0.54
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.89	0.54
3:D:1036:ARG:HG2	3:D:1037:PHE:H	1.73	0.54
5:F:270:VAL:HA	5:F:273:MET:HE3	1.90	0.54
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.90	0.54
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.43	0.54
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.42	0.54
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.89	0.54
5:F:21:TYR:HB3	5:F:54:GLN:HG3	1.90	0.54
5:L:21:TYR:HB3	5:L:54:GLN:HG3	1.88	0.54
1:H:64:VAL:HG12	1:H:65:LEU:H	1.73	0.54
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.90	0.54
1:H:61:ILE:HG22	1:H:63:GLY:H	1.73	0.54
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.73	0.54
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.90	0.53
3:D:394:ILE:HG21	5:F:536:THR:HA	1.90	0.53
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.89	0.53
1:A:96:ASP:HA	1:A:148:ARG:HD3	1.89	0.53
3:D:44:ILE:HG13	5:F:450:ILE:HG22	1.91	0.53
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.23	0.53
5:F:530:LEU:HD23	5:F:530:LEU:H	1.74	0.53
1:G:117:HIS:NE2	1:G:121:VAL:O	2.41	0.53
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.90	0.53
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.23	0.53
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.74	0.53
5:L:330:LEU:O	5:L:334:SER:OG	2.21	0.53
1:A:14:VAL:HG22	1:A:15:ASP:H	1.74	0.53
2:C:1160:ASP:O	2:C:1161:LEU:HB2	2.08	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.74	0.53
1:G:14:VAL:HG22	1:G:15:ASP:H	1.74	0.53
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:712:GLN:HG2	3:J:713:GLU:H	1.73	0.53
2:I:905:ILE:O	5:L:599:ARG:NH1	2.41	0.53
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.42	0.53
5:L:229:VAL:HG12	5:L:232:ARG:HH12	1.73	0.53
2:C:905:ILE:O	5:F:599:ARG:NH1	2.42	0.53
1:G:80:GLU:O	1:G:84:ASN:ND2	2.42	0.53
2:I:1296:ASP:HB3	2:I:1320:PRO:HB3	1.91	0.53
5:L:270:VAL:HA	5:L:273:MET:HE3	1.90	0.53
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.91	0.53
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.90	0.53
1:B:61:ILE:HG22	1:B:63:GLY:H	1.73	0.53
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.91	0.53
2:I:520:PRO:HG3	2:I:714:VAL:HG11	1.90	0.53
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.33	0.53
3:J:1199:PHE:CD2	3:J:1202:GLU:HB3	2.44	0.53
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.74	0.53
2:C:520:PRO:HG3	2:C:714:VAL:HG11	1.90	0.53
2:C:1296:ASP:HB3	2:C:1320:PRO:HB3	1.89	0.53
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.42	0.53
5:L:530:LEU:H	5:L:530:LEU:HD23	1.73	0.53
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.91	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.44	0.52
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.91	0.52
1:A:13:LEU:HD23	1:A:13:LEU:H	1.74	0.52
2:I:1160:ASP:O	2:I:1161:LEU:HB2	2.08	0.52
1:A:117:HIS:NE2	1:A:121:VAL:O	2.42	0.52
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.92	0.52
3:D:712:GLN:HG2	3:D:713:GLU:H	1.73	0.52
5:F:309:ASN:C	5:F:311:THR:H	2.18	0.52
2:I:719:LYS:H	2:I:751:TYR:HH	1.58	0.52
2:I:886:LYS:H	2:I:917:SER:HB3	1.74	0.52
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.74	0.52
1:G:13:LEU:H	1:G:13:LEU:HD23	1.74	0.52
1:A:80:GLU:O	1:A:84:ASN:ND2	2.42	0.52
3:D:1199:PHE:CD2	3:D:1202:GLU:HB3	2.44	0.52
5:F:229:VAL:HG12	5:F:232:ARG:HH12	1.73	0.52
5:F:511:ILE:HG12	5:F:512:GLY:H	1.73	0.52
1:G:23:HIS:HB2	1:G:206:GLU:HA	1.91	0.52
2:I:30:ILE:HD12	2:I:30:ILE:H	1.75	0.52
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.92	0.52
5:L:511:ILE:HG12	5:L:512:GLY:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:558:VAL:HG11	2:C:573:ASN:HB3	1.92	0.52
5:F:9:LEU:HD22	6:M:46:GLN:O	2.10	0.52
3:J:527:LEU:HB2	3:J:550:VAL:HG12	1.91	0.52
5:L:309:ASN:C	5:L:311:THR:H	2.18	0.52
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.92	0.51
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.92	0.51
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.92	0.51
3:J:136:GLU:OE2	3:J:312:ARG:NH1	2.42	0.51
2:C:886:LYS:H	2:C:917:SER:HB3	1.74	0.51
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.42	0.51
3:D:847:ASP:OD1	3:D:847:ASP:N	2.42	0.51
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.75	0.51
2:C:1086:PRO:HB2	2:C:1212:LEU:HD23	1.92	0.51
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.18	0.51
2:C:232:ILE:HG13	2:C:331:LYS:O	2.10	0.51
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.91	0.51
3:D:961:SER:HB2	3:D:981:GLU:HB3	1.93	0.51
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.46	0.51
3:J:961:SER:HB2	3:J:981:GLU:HB3	1.93	0.51
5:F:10:LYS:HA	5:F:13:VAL:HG12	1.93	0.51
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.93	0.51
1:H:13:LEU:HD23	1:H:13:LEU:H	1.76	0.51
2:I:558:VAL:HG11	2:I:573:ASN:HB3	1.92	0.51
1:A:23:HIS:HB2	1:A:206:GLU:HA	1.91	0.51
3:D:1173:ARG:NE	3:D:1192:LYS:HG3	2.12	0.51
2:I:1086:PRO:HB2	2:I:1212:LEU:HD23	1.92	0.51
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.45	0.51
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.93	0.51
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.91	0.51
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.92	0.51
5:L:491:GLU:HG3	5:L:491:GLU:O	2.11	0.51
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.93	0.51
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.92	0.51
3:D:1280:VAL:CG2	3:D:1304:ARG:HE	2.24	0.51
3:J:425:ARG:HG2	3:J:426:ALA:H	1.76	0.51
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.93	0.51
2:C:180:ARG:CZ	2:C:465:ARG:HH12	2.24	0.50
3:D:1167:LYS:HB2	3:D:1167:LYS:NZ	2.26	0.50
2:I:255:ILE:HB	2:I:263:VAL:HB	1.93	0.50
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.93	0.50
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.92	0.50
3:D:425:ARG:HG2	3:D:426:ALA:H	1.75	0.50
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.92	0.50
3:D:978:ARG:HB2	3:D:1199:PHE:CZ	2.46	0.50
5:F:491:GLU:O	5:F:491:GLU:HG3	2.11	0.50
3:J:1150:PRO:O	6:N:26:SER:OG	2.29	0.50
5:L:127:ILE:O	5:L:130:VAL:HG22	2.11	0.50
5:F:98:VAL:HG22	5:F:402:LEU:HD11	1.93	0.50
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.93	0.50
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.93	0.50
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.45	0.50
5:L:10:LYS:HA	5:L:13:VAL:HG12	1.92	0.50
5:L:98:VAL:HG22	5:L:402:LEU:HD11	1.93	0.50
2:C:255:ILE:HB	2:C:263:VAL:HB	1.93	0.50
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.45	0.50
1:H:59:VAL:O	1:H:171:LEU:N	2.45	0.50
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.93	0.50
3:J:290:ILE:H	3:J:290:ILE:HD12	1.77	0.50
3:J:1280:VAL:CG2	3:J:1304:ARG:HE	2.24	0.50
3:D:665:GLN:OE1	3:D:678:ARG:NH2	2.44	0.50
3:D:1077:ALA:HB2	3:D:1100:PHE:CD1	2.46	0.50
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.75	0.50
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.18	0.50
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.47	0.50
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.93	0.50
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.94	0.50
3:D:140:TYR:CD2	5:F:100:MET:HE1	2.47	0.50
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.76	0.50
5:F:53:ILE:O	5:F:54:GLN:NE2	2.36	0.50
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.42	0.50
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.94	0.50
2:I:1024:GLU:HA	2:I:1027:LYS:HG2	1.93	0.50
1:A:228:LEU:HD21	1:B:224:LEU:HD23	1.93	0.50
3:D:1293:GLU:HG3	3:J:1227:HIS:HB2	1.93	0.50
1:G:208:ASN:OD1	1:G:208:ASN:N	2.44	0.50
3:J:665:GLN:OE1	3:J:678:ARG:NH2	2.44	0.50
6:M:19:THR:HB	6:M:56:ARG:HB3	1.93	0.50
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.42	0.50
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.94	0.50
1:B:13:LEU:H	1:B:13:LEU:HD23	1.76	0.49
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.12	0.49
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	1.94	0.49
3:D:847:ASP:HB3	3:D:860:ARG:H	1.77	0.49
6:N:19:THR:HB	6:N:56:ARG:HB3	1.93	0.49
1:H:34:GLY:N	1:H:199:ASP:OD2	2.46	0.49
2:I:232:ILE:HG13	2:I:331:LYS:O	2.10	0.49
3:D:54:ASP:HA	3:D:61:ILE:HD11	1.95	0.49
1:G:211:ILE:HD12	1:G:215:GLU:HG2	1.94	0.49
2:I:808:ASN:H	3:J:633:ALA:HB2	1.76	0.49
3:J:733:SER:O	3:J:737:ILE:HG12	2.12	0.49
5:L:165:PHE:CZ	5:L:217:ALA:HA	2.47	0.49
3:D:963:VAL:HB	3:D:980:THR:HG23	1.94	0.49
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.45	0.49
1:G:23:HIS:HB2	1:G:205:MET:O	2.13	0.49
1:H:86:LYS:HE2	1:H:174:ASP:HB2	1.94	0.49
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.78	0.49
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.30	0.49
2:C:808:ASN:H	3:D:633:ALA:HB2	1.76	0.49
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.47	0.49
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.93	0.49
3:J:847:ASP:HB3	3:J:860:ARG:H	1.78	0.49
5:L:126:GLY:O	5:L:130:VAL:HG13	2.11	0.49
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.94	0.49
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.94	0.49
3:D:349:TYR:CE2	3:D:379:PRO:HG2	2.48	0.49
1:H:32:GLU:HA	1:H:198:LEU:HD12	1.95	0.49
3:D:290:ILE:HD12	3:D:290:ILE:H	1.77	0.49
3:D:576:ARG:NH1	3:D:593:ASN:O	2.46	0.49
5:F:515:GLU:HG2	5:F:516:ASP:H	1.78	0.49
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.94	0.49
2:I:1254:VAL:HG22	2:I:1255:THR:HG23	1.94	0.49
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.94	0.49
3:J:198:CYS:O	3:J:202:ARG:HG3	2.13	0.49
3:J:963:VAL:HB	3:J:980:THR:HG23	1.94	0.49
5:F:165:PHE:CZ	5:F:217:ALA:HA	2.47	0.49
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.94	0.49
2:C:516:ASP:OD1	2:C:516:ASP:O	2.31	0.49
2:C:1105:SER:HA	3:D:736:GLN:NE2	2.28	0.49
2:C:1301:ARG:HG3	2:C:1302:THR:H	1.78	0.49
3:D:198:CYS:O	3:D:202:ARG:HG3	2.13	0.49
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:297:MET:HB2	5:L:326:TRP:HB2	1.95	0.49
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.95	0.48
3:D:700:ASN:ND2	3:D:700:ASN:O	2.46	0.48
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	1.95	0.48
5:F:164:GLY:O	5:F:260:ARG:HB2	2.13	0.48
2:I:117:ILE:HG21	2:I:488:MET:HG2	1.95	0.48
2:I:232:ILE:HA	2:I:237:LEU:HA	1.94	0.48
3:J:700:ASN:O	3:J:700:ASN:ND2	2.46	0.48
1:A:23:HIS:HB2	1:A:205:MET:O	2.13	0.48
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.94	0.48
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.94	0.48
2:I:349:GLU:O	2:I:353:VAL:HG23	2.13	0.48
2:I:516:ASP:OD1	2:I:516:ASP:O	2.30	0.48
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.13	0.48
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.48	0.48
3:D:733:SER:O	3:D:737:ILE:HG12	2.12	0.48
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.48	0.48
5:F:266:PHE:HA	5:F:269:LEU:HD12	1.95	0.48
3:J:732:GLY:HA2	3:J:736:GLN:NE2	2.29	0.48
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.48	0.48
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.95	0.48
2:C:60:GLN:HA	2:C:67:GLU:HA	1.95	0.48
3:D:1297:LYS:HB3	3:J:1302:TYR:O	2.13	0.48
3:J:54:ASP:HA	3:J:61:ILE:HD11	1.94	0.48
1:A:211:ILE:HD12	1:A:215:GLU:HG2	1.94	0.48
2:C:117:ILE:HG21	2:C:488:MET:HG2	1.95	0.48
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.36	0.48
5:F:291:CYS:HA	5:F:295:CYS:HB2	1.95	0.48
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.94	0.48
3:D:490:ILE:HG13	3:D:491:LEU:HG	1.96	0.48
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.31	0.48
3:J:140:TYR:CD2	5:L:100:MET:HE1	2.47	0.48
3:J:478:LEU:HG	4:K:47:THR:HG23	1.96	0.48
3:D:732:GLY:HA2	3:D:736:GLN:NE2	2.29	0.48
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.48	0.48
2:I:144:VAL:HB	2:I:526:HIS:CE1	2.49	0.48
3:J:576:ARG:NH1	3:J:593:ASN:O	2.46	0.48
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	1.95	0.48
5:F:297:MET:HB2	5:F:326:TRP:HB2	1.96	0.48
2:I:166:SER:HB3	6:N:23:SER:HA	1.95	0.48
2:C:138:ILE:HD13	2:C:143:ARG:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:509:SER:HB3	2:C:512:SER:HB3	1.94	0.48
2:C:1254:VAL:HG22	2:C:1255:THR:HG23	1.94	0.48
5:F:225:ARG:O	5:F:229:VAL:HG13	2.14	0.48
2:I:60:GLN:HA	2:I:67:GLU:HA	1.95	0.48
2:I:402:ARG:HG2	2:I:416:GLY:H	1.79	0.48
2:I:523:GLU:HB3	2:I:527:LYS:HE3	1.95	0.48
2:I:1105:SER:HA	3:J:736:GLN:NE2	2.28	0.48
3:J:1077:ALA:HA	3:J:1100:PHE:HA	1.96	0.48
5:L:164:GLY:O	5:L:260:ARG:HB2	2.13	0.48
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.95	0.48
1:B:34:GLY:N	1:B:199:ASP:OD2	2.45	0.47
2:C:1247:SER:HB3	3:D:375:GLU:O	2.14	0.47
3:D:523:GLU:OE2	3:D:547:ARG:NH1	2.44	0.47
3:D:1077:ALA:HA	3:D:1100:PHE:HA	1.96	0.47
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.96	0.47
3:J:747:MET:HE2	3:J:775:SER:HA	1.96	0.47
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.95	0.47
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.97	0.47
2:I:1304:MET:HE2	2:I:1308:ILE:HG12	1.97	0.47
3:J:523:GLU:OE2	3:J:547:ARG:NH1	2.44	0.47
3:J:1034:PHE:HB2	3:J:1081:VAL:HG23	1.95	0.47
2:C:523:GLU:HB3	2:C:527:LYS:HE3	1.95	0.47
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.13	0.47
3:D:1063:ASP:HB3	3:D:1103:GLY:HA3	1.97	0.47
2:I:494:ASN:OD1	2:I:495:ALA:N	2.37	0.47
2:I:1301:ARG:HG3	2:I:1302:THR:H	1.78	0.47
5:L:47:MET:HB2	6:N:27:PHE:CZ	2.49	0.47
5:L:266:PHE:HA	5:L:269:LEU:HD12	1.95	0.47
5:F:162:ILE:HD13	5:F:221:PHE:HE2	1.77	0.47
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.95	0.47
5:F:576:VAL:O	5:F:580:PHE:HB2	2.14	0.47
3:J:332:LYS:HG2	3:J:1328:THR:HB	1.97	0.47
3:J:490:ILE:HG13	3:J:491:LEU:HG	1.96	0.47
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.14	0.47
5:L:515:GLU:HG2	5:L:516:ASP:H	1.78	0.47
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.97	0.47
2:C:488:MET:O	2:C:490:GLN:N	2.41	0.47
2:C:1240:ASP:HA	3:D:445:LYS:HD3	1.96	0.47
3:D:332:LYS:HG2	3:D:1328:THR:HB	1.97	0.47
5:L:291:CYS:HA	5:L:295:CYS:HB2	1.95	0.47
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:950:ILE:HB	3:D:1018:ALA:HB3	1.97	0.47
4:K:44:ASP:HB3	4:K:48:VAL:HB	1.97	0.47
1:B:102:LEU:O	1:B:141:SER:HA	2.15	0.47
2:C:30:ILE:HD12	2:C:30:ILE:H	1.79	0.47
2:C:349:GLU:O	2:C:353:VAL:HG23	2.14	0.47
2:C:1146:GLN:NE2	2:C:1160:ASP:O	2.47	0.47
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	1.97	0.47
3:D:747:MET:HE2	3:D:775:SER:HA	1.96	0.47
3:D:968:ASN:OD1	3:D:972:LYS:N	2.48	0.47
3:D:1063:ASP:O	3:D:1067:ARG:HG3	2.14	0.47
1:G:103:ASN:OD1	1:G:141:SER:HB3	2.14	0.47
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.96	0.47
2:I:1146:GLN:NE2	2:I:1160:ASP:O	2.47	0.47
2:I:1247:SER:HB3	3:J:375:GLU:O	2.14	0.47
5:L:225:ARG:O	5:L:229:VAL:HG13	2.15	0.47
1:B:191:ARG:NH2	3:D:409:TRP:HB3	2.29	0.47
2:C:232:ILE:HA	2:C:237:LEU:HA	1.94	0.47
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.97	0.47
5:F:105:MET:HB2	5:F:105:MET:HE2	1.84	0.47
5:F:484:ALA:H	5:F:494:ILE:HD11	1.80	0.47
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.97	0.47
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.97	0.47
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.97	0.47
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.50	0.47
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.80	0.47
2:I:1083:GLU:H	2:I:1083:GLU:HG3	1.45	0.47
2:C:56:VAL:O	2:C:59:ILE:HG23	2.15	0.47
2:C:1105:SER:HA	3:D:736:GLN:HE22	1.80	0.47
3:D:478:LEU:HG	4:E:47:THR:HG23	1.97	0.47
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	1.95	0.47
3:D:1100:PHE:HB2	3:D:1200:GLU:OE1	2.15	0.47
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.50	0.47
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.97	0.47
1:H:112:ALA:HB2	1:H:128:HIS:HB3	1.97	0.47
2:I:692:THR:OG1	2:I:693:LEU:N	2.48	0.47
2:I:1105:SER:HA	3:J:736:GLN:HE22	1.80	0.47
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.97	0.47
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.50	0.47
3:J:358:GLY:N	3:J:359:PRO:HD3	2.28	0.47
5:L:540:LEU:HD23	5:L:610:PHE:CD2	2.50	0.47
5:L:576:VAL:O	5:L:580:PHE:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.97	0.46
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.97	0.46
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	1.96	0.46
5:F:47:MET:HB2	6:M:27:PHE:CZ	2.50	0.46
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.29	0.46
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.78	0.46
3:J:968:ASN:OD1	3:J:972:LYS:N	2.48	0.46
2:C:541:GLU:N	2:C:541:GLU:OE1	2.47	0.46
3:D:335:GLN:HB2	5:F:516:ASP:OD1	2.16	0.46
2:I:402:ARG:CG	2:I:416:GLY:H	2.29	0.46
2:I:809:GLY:O	2:I:812:PHE:HB2	2.15	0.46
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.81	0.46
5:L:96:ASP:HA	5:L:97:PRO:HD2	1.86	0.46
2:C:13:LYS:HD3	2:C:1149:TYR:HA	1.98	0.46
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.50	0.46
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.97	0.46
3:D:984:LEU:HD22	3:D:993:GLU:HG3	1.98	0.46
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.50	0.46
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.95	0.46
3:J:1360:GLY:HA2	4:K:17:PHE:CE2	2.51	0.46
1:B:178:SER:HA	1:B:179:PRO:HD3	1.67	0.46
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.97	0.46
2:I:91:THR:HG21	2:I:503:LYS:HE2	1.97	0.46
5:L:461:ASN:O	5:L:465:ARG:HG3	2.16	0.46
2:C:402:ARG:HG2	2:C:416:GLY:H	1.79	0.46
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.97	0.46
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.97	0.46
2:I:56:VAL:O	2:I:59:ILE:HG23	2.15	0.46
2:I:1108:ASN:O	2:I:1110:GLY:N	2.49	0.46
2:I:1240:ASP:HA	3:J:445:LYS:HD3	1.97	0.46
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.97	0.46
3:J:349:TYR:CE2	3:J:379:PRO:HG2	2.48	0.46
3:J:1063:ASP:HB3	3:J:1103:GLY:HA3	1.97	0.46
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.97	0.46
5:L:462:LYS:HD2	5:L:487:MET:HE1	1.97	0.46
1:B:76:GLU:HB3	1:B:80:GLU:HG2	1.98	0.46
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.97	0.46
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.80	0.46
3:J:1024:THR:HG21	3:J:1123:ARG:HD2	1.97	0.46
3:J:1167:LYS:HB2	3:J:1167:LYS:NZ	2.30	0.46
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:322:LEU:O	2:C:326:SER:OG	2.32	0.46
3:D:860:ARG:HB3	3:D:861:ASN:H	1.52	0.46
3:D:974:VAL:HG21	3:D:1118:GLY:HA2	1.98	0.46
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.51	0.46
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.97	0.46
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.98	0.46
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.30	0.46
5:F:461:ASN:O	5:F:465:ARG:HG3	2.16	0.46
2:I:1085:MET:HA	2:I:1086:PRO:HD3	1.85	0.46
6:N:21:GLU:HG2	6:N:26:SER:HB2	1.98	0.46
1:A:49:SER:OG	1:A:50:SER:N	2.48	0.46
1:A:58:GLU:HG2	1:A:158:ARG:NH2	2.29	0.46
2:C:402:ARG:CG	2:C:416:GLY:H	2.29	0.46
3:D:1215:GLU:HB3	3:D:1220:ILE:HD11	1.98	0.46
5:F:511:ILE:HG21	5:F:522:PHE:HE2	1.81	0.46
1:H:102:LEU:O	1:H:141:SER:HA	2.15	0.46
2:I:13:LYS:HD3	2:I:1149:TYR:HA	1.97	0.46
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.98	0.46
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.97	0.46
5:L:380:VAL:HG22	5:L:416:VAL:HG21	1.98	0.46
1:A:45:ARG:HE	1:B:38:THR:HB	1.80	0.46
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.79	0.46
2:C:692:THR:OG1	2:C:693:LEU:N	2.48	0.46
3:D:550:VAL:HG23	3:D:552:ILE:HG23	1.98	0.46
3:D:1024:THR:HG21	3:D:1123:ARG:HD2	1.97	0.46
3:D:1100:PHE:HB2	3:D:1200:GLU:CD	2.41	0.46
3:J:1006:GLY:N	3:J:1009:GLU:HG3	2.22	0.46
5:L:245:ALA:O	5:L:249:ILE:HG13	2.16	0.46
2:C:138:ILE:HB	2:C:143:ARG:HG3	1.97	0.45
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.96	0.45
2:C:1108:ASN:O	2:C:1110:GLY:N	2.49	0.45
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.99	0.45
3:D:1189:MET:HB2	6:M:57:VAL:HB	1.98	0.45
2:I:488:MET:O	2:I:490:GLN:N	2.41	0.45
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.98	0.45
3:J:984:LEU:HD22	3:J:993:GLU:HG3	1.98	0.45
3:J:1107:VAL:HG12	3:J:1108:GLN:H	1.81	0.45
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.96	0.45
3:D:342:LEU:HD23	3:D:342:LEU:HA	1.71	0.45
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.98	0.45
1:H:76:GLU:HB3	1:H:80:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:452:ARG:NH1	2:I:585:GLY:HA3	2.32	0.45
2:I:541:GLU:OE1	2:I:541:GLU:N	2.47	0.45
2:I:809:GLY:O	3:J:357:VAL:HG11	2.16	0.45
1:B:112:ALA:HB2	1:B:128:HIS:HB3	1.97	0.45
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.98	0.45
2:C:809:GLY:O	2:C:812:PHE:HB2	2.15	0.45
5:F:245:ALA:O	5:F:249:ILE:HG13	2.16	0.45
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.98	0.45
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.80	0.45
3:J:514:THR:HG22	3:J:576:ARG:HG2	1.99	0.45
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.98	0.45
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.98	0.45
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.97	0.45
2:I:98:VAL:HG21	2:I:124:MET:HE3	1.98	0.45
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.99	0.45
3:J:1215:GLU:HB3	3:J:1220:ILE:HD11	1.98	0.45
1:A:103:ASN:OD1	1:A:141:SER:HB3	2.16	0.45
3:D:1168:GLU:O	3:D:1168:GLU:HG3	2.16	0.45
3:D:1173:ARG:HH21	3:D:1192:LYS:CE	2.30	0.45
5:L:297:MET:HA	5:L:298:PRO:HD3	1.79	0.45
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.99	0.45
2:C:1148:ALA:HB1	2:C:1180:MET:HE2	1.99	0.45
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.81	0.45
3:D:70:CYS:SG	3:D:71:LEU:N	2.89	0.45
3:D:832:LYS:HD3	3:D:1242:ARG:HH12	1.81	0.45
3:D:1107:VAL:HG12	3:D:1108:GLN:H	1.81	0.45
5:F:380:VAL:HG22	5:F:416:VAL:HG21	1.98	0.45
1:G:49:SER:OG	1:G:50:SER:N	2.49	0.45
2:I:88:ARG:HG2	2:I:90:VAL:HG23	1.99	0.45
3:J:385:LEU:HD23	3:J:411:ILE:HG13	1.98	0.45
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.98	0.45
4:K:35:LYS:HB3	4:K:35:LYS:HE2	1.84	0.45
5:L:53:ILE:O	5:L:54:GLN:NE2	2.36	0.45
2:C:494:ASN:OD1	2:C:495:ALA:N	2.38	0.45
2:C:548:ARG:O	3:D:780:ARG:NH1	2.50	0.45
2:C:1304:MET:HE2	2:C:1308:ILE:HG12	1.97	0.45
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.98	0.45
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.82	0.45
2:I:548:ARG:O	3:J:780:ARG:NH1	2.50	0.45
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.80	0.45
5:L:511:ILE:HG21	5:L:522:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.98	0.45
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.98	0.45
2:C:736:VAL:HG23	2:C:748:ILE:HA	1.99	0.45
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.98	0.45
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.71	0.45
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.87	0.45
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.98	0.45
1:H:106:GLY:H	1:H:133:LEU:HD23	1.81	0.45
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.99	0.45
2:C:143:ARG:HD2	2:C:514:PHE:HA	1.99	0.45
1:G:42:ALA:O	1:G:46:ILE:HG12	2.17	0.45
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.52	0.45
3:J:1221:LEU:HD23	3:J:1229:VAL:HG11	1.99	0.45
3:D:514:THR:HG22	3:D:576:ARG:HG2	1.99	0.45
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.45
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.17	0.45
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.99	0.45
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.82	0.45
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.81	0.45
3:J:1168:GLU:O	3:J:1168:GLU:HG3	2.17	0.45
3:D:1150:PRO:O	6:M:26:SER:OG	2.34	0.44
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.99	0.44
2:I:143:ARG:HD2	2:I:514:PHE:HA	1.99	0.44
3:J:572:THR:OG1	3:J:573:THR:N	2.50	0.44
3:J:1078:LEU:HD12	3:J:1121:LEU:HB3	1.99	0.44
4:K:69:ARG:O	4:K:73:GLN:HG2	2.17	0.44
2:C:148:GLN:HG2	2:C:149:LEU:H	1.83	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.86	0.44
3:D:1268:ASN:CG	3:D:1269:ALA:H	2.25	0.44
2:I:11:ILE:HD13	2:I:11:ILE:HA	1.83	0.44
3:J:770:LEU:HD22	3:J:770:LEU:H	1.82	0.44
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.98	0.44
1:A:42:ALA:O	1:A:46:ILE:HG12	2.17	0.44
1:B:106:GLY:H	1:B:133:LEU:HD23	1.81	0.44
3:D:741:ALA:O	3:D:762:ASN:ND2	2.51	0.44
2:I:765:ILE:HG13	2:I:787:PRO:HG3	1.99	0.44
3:J:1169:THR:HG22	3:J:1170:LYS:HB2	1.99	0.44
5:L:158:LEU:HD22	5:L:162:ILE:HD11	1.99	0.44
5:L:470:MET:HA	5:L:473:GLU:HB3	2.00	0.44
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.98	0.44
3:D:1078:LEU:HD12	3:D:1121:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1282:TYR:HE1	3:D:1286:LYS:HE2	1.83	0.44
2:I:322:LEU:O	2:I:326:SER:OG	2.32	0.44
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.99	0.44
5:L:290:LEU:HD22	5:L:333:VAL:HG21	2.00	0.44
2:C:15:PHE:HE1	2:C:1194:GLU:HB3	1.83	0.44
2:C:243:PRO:HA	2:C:246:LEU:HD12	1.99	0.44
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.82	0.44
2:C:817:LEU:HD13	2:C:1085:MET:HE1	1.99	0.44
3:D:99:ARG:HG3	3:D:248:ASP:HB3	2.00	0.44
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.98	0.44
3:D:789:LYS:NZ	3:D:931:THR:O	2.34	0.44
5:F:462:LYS:HD2	5:F:487:MET:HE1	1.98	0.44
1:H:35:PHE:HA	1:H:38:THR:HG22	1.99	0.44
3:J:1173:ARG:HH21	3:J:1192:LYS:CE	2.30	0.44
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	2.00	0.44
4:K:64:LEU:HA	4:K:64:LEU:HD23	1.86	0.44
6:M:21:GLU:HG2	6:M:26:SER:HB2	2.00	0.44
2:C:809:GLY:O	3:D:357:VAL:HG11	2.17	0.44
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.83	0.44
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.99	0.44
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.99	0.44
2:I:1032:LYS:O	2:I:1036:ILE:HG13	2.17	0.44
3:J:70:CYS:SG	3:J:71:LEU:N	2.90	0.44
3:J:298:MET:SD	5:L:402:LEU:HB3	2.57	0.44
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.83	0.44
3:J:550:VAL:HG23	3:J:552:ILE:HG23	1.98	0.44
3:J:1268:ASN:CG	3:J:1269:ALA:H	2.25	0.44
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.48	0.44
3:D:224:LEU:O	3:D:228:VAL:HG23	2.17	0.44
3:D:298:MET:SD	5:F:402:LEU:HB3	2.57	0.44
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	2.00	0.44
5:F:147:GLN:O	5:F:151:VAL:HG23	2.17	0.44
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.82	0.44
2:I:820:GLU:HA	2:I:1079:ILE:HD11	2.00	0.44
5:L:9:LEU:HD22	6:N:47:TYR:HA	2.00	0.44
2:C:88:ARG:HG2	2:C:90:VAL:HG23	1.99	0.44
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.99	0.44
2:C:820:GLU:HA	2:C:1079:ILE:HD11	2.00	0.44
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.91	0.44
3:D:870:ASP:O	3:D:874:GLU:HG2	2.17	0.44
4:E:69:ARG:O	4:E:73:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:290:LEU:HD22	5:F:333:VAL:HG21	2.00	0.44
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.99	0.44
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.85	0.44
3:J:654:ILE:O	3:J:658:GLU:N	2.43	0.44
5:L:484:ALA:H	5:L:494:ILE:HD11	1.82	0.44
2:C:558:VAL:CG1	2:C:573:ASN:HB3	2.48	0.44
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.99	0.44
3:D:901:ARG:HA	3:D:908:ILE:HA	2.00	0.44
5:F:348:GLU:HA	5:F:353:LEU:O	2.18	0.44
2:I:243:PRO:HA	2:I:246:LEU:HD12	1.99	0.44
2:I:452:ARG:HH21	2:I:458:GLU:CD	2.25	0.44
2:I:870:ILE:HG21	2:I:931:VAL:HG11	2.00	0.44
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.81	0.44
2:I:1148:ALA:HB1	2:I:1180:MET:HE2	1.99	0.44
2:I:1333:LEU:HB2	2:I:1335:ILE:HG12	2.00	0.44
3:J:870:ASP:O	3:J:874:GLU:HG2	2.17	0.44
3:J:1040:MET:HE3	3:J:1076:PRO:HB2	1.99	0.44
6:N:61:VAL:HG22	6:N:62:ALA:H	1.82	0.44
1:B:35:PHE:HA	1:B:38:THR:HG22	1.99	0.43
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.99	0.43
2:C:28:LEU:HD21	2:C:524:ILE:HG13	2.00	0.43
2:C:56:VAL:HG11	2:C:468:LEU:HB3	2.00	0.43
2:C:1151:LEU:HD23	2:C:1151:LEU:HA	1.87	0.43
3:D:385:LEU:HD23	3:D:411:ILE:HG13	1.99	0.43
2:I:1253:LEU:HD23	5:L:525:ASP:OD1	2.18	0.43
3:J:1149:ARG:NH2	3:J:1153:PRO:HG2	2.33	0.43
2:I:206:ALA:O	2:I:209:ILE:HG22	2.18	0.43
2:I:387:ASN:HA	2:I:391:SER:HB2	2.00	0.43
3:J:844:THR:OG1	3:J:860:ARG:O	2.29	0.43
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.83	0.43
2:C:170:VAL:HG23	2:C:171:LEU:N	2.33	0.43
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.54	0.43
2:C:520:PRO:HB3	2:C:714:VAL:HG21	2.00	0.43
2:C:617:ALA:HA	2:C:636:CYS:SG	2.59	0.43
3:D:807:LEU:HD11	3:D:894:VAL:HG23	1.99	0.43
3:D:1169:THR:HG22	3:D:1170:LYS:HB2	1.99	0.43
3:D:1286:LYS:HD2	3:D:1290:ARG:HH22	1.83	0.43
5:F:381:GLU:HA	5:F:384:LEU:HG	2.01	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.00	0.43
2:I:389:PHE:HB3	2:I:420:LEU:HD12	2.00	0.43
3:J:99:ARG:HG3	3:J:248:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:609:TYR:HB2	3:J:617:THR:HG21	2.00	0.43
3:J:741:ALA:O	3:J:762:ASN:ND2	2.51	0.43
5:L:348:GLU:HA	5:L:353:LEU:O	2.18	0.43
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.85	0.43
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.99	0.43
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.45	0.43
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.82	0.43
2:I:23:ASP:OD1	2:I:23:ASP:N	2.42	0.43
2:I:253:PHE:CZ	2:I:287:VAL:HG12	2.54	0.43
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.52	0.43
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	2.00	0.43
3:J:224:LEU:O	3:J:228:VAL:HG23	2.17	0.43
5:L:448:ARG:HH21	5:L:450:ILE:HG13	1.82	0.43
3:D:1231:ARG:HA	3:D:1234:VAL:HG22	2.00	0.43
2:I:666:SER:HB2	2:I:704:MET:HG3	2.00	0.43
1:B:48:LEU:HD12	1:B:183:ILE:HD11	2.01	0.43
1:B:198:LEU:HD13	1:B:198:LEU:HA	1.76	0.43
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.19	0.43
4:E:71:GLU:HA	4:E:74:GLU:HG2	2.01	0.43
5:F:448:ARG:HH21	5:F:450:ILE:HG13	1.83	0.43
5:F:470:MET:HA	5:F:473:GLU:HB3	2.00	0.43
2:I:1116:HIS:O	2:I:1119:MET:HB3	2.19	0.43
5:L:147:GLN:O	5:L:151:VAL:HG23	2.17	0.43
2:C:339:ASN:HB3	2:C:343:HIS:H	1.84	0.43
2:C:389:PHE:HB3	2:C:420:LEU:HD12	2.00	0.43
3:D:470:VAL:HA	3:D:471:PRO:HD3	1.79	0.43
2:I:778:GLU:O	2:I:781:ASP:HB2	2.18	0.43
3:J:697:MET:O	3:J:701:LEU:HB2	2.19	0.43
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.43	0.43
1:B:33:ARG:NH1	2:C:1081:PRO:HG3	2.32	0.43
1:B:98:VAL:HG11	1:B:121:VAL:HG22	2.01	0.43
2:C:739:ASP:OD1	2:C:739:ASP:N	2.42	0.43
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.00	0.43
2:C:1308:ILE:HD12	3:D:380:PHE:CZ	2.54	0.43
3:D:367:GLY:HA3	3:D:448:GLN:HB2	2.01	0.43
3:D:712:GLN:H	3:D:712:GLN:CD	2.27	0.43
3:D:770:LEU:O	3:D:774:ILE:HG13	2.19	0.43
3:D:968:ASN:HB3	3:D:1118:GLY:HA3	2.00	0.43
5:F:41:ILE:O	5:F:45:ILE:HG13	2.18	0.43
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.99	0.43
2:I:403:MET:HE3	2:I:403:MET:HB3	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:857:LEU:HD13	3:J:858:VAL:HG12	2.01	0.43
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.87	0.43
2:C:778:GLU:O	2:C:781:ASP:HB2	2.18	0.43
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.29	0.43
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.54	0.43
3:D:211:GLU:O	3:D:215:LYS:HB2	2.19	0.43
3:D:495:ASN:ND2	3:D:1247:LYS:O	2.52	0.43
5:F:158:LEU:HD22	5:F:162:ILE:HD11	1.99	0.43
2:I:27:LEU:HB3	2:I:528:ARG:HD2	2.01	0.43
2:I:46:GLN:OE1	2:I:47:TYR:N	2.47	0.43
2:I:558:VAL:CG1	2:I:573:ASN:HB3	2.48	0.43
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.89	0.43
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.99	0.43
2:C:206:ALA:O	2:C:209:ILE:HG22	2.18	0.43
2:C:666:SER:HB2	2:C:704:MET:HG3	2.01	0.43
2:C:992:LEU:H	2:C:992:LEU:HD23	1.84	0.43
3:D:609:TYR:HB2	3:D:617:THR:HG21	2.01	0.43
3:D:697:MET:O	3:D:701:LEU:HB2	2.19	0.43
3:D:1040:MET:HE3	3:D:1076:PRO:HB2	1.99	0.43
2:I:148:GLN:HG2	2:I:149:LEU:H	1.83	0.43
2:I:975:ILE:HG12	2:I:1014:LEU:HD13	2.01	0.43
2:I:1073:LYS:HD3	3:J:462:ASP:HB2	2.01	0.43
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.70	0.43
3:J:211:GLU:O	3:J:215:LYS:HB2	2.19	0.43
3:J:367:GLY:HA3	3:J:448:GLN:HB2	2.01	0.43
3:J:968:ASN:HB3	3:J:1118:GLY:HA3	2.01	0.43
3:J:1282:TYR:HE1	3:J:1286:LYS:HE2	1.83	0.43
1:B:29:GLU:HB2	1:B:30:PRO:HA	2.01	0.42
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.83	0.42
3:D:30:ILE:HG23	3:D:243:PRO:HG3	2.00	0.42
3:D:572:THR:OG1	3:D:573:THR:N	2.50	0.42
3:D:960:LEU:HB3	3:D:963:VAL:HG11	2.01	0.42
1:H:67:GLU:HG2	1:H:82:LEU:HD11	2.01	0.42
1:H:115:ILE:HD11	1:H:130:ILE:HD11	2.01	0.42
2:I:170:VAL:HG23	2:I:171:LEU:N	2.34	0.42
2:I:347:ILE:HD11	2:I:433:ILE:HD11	2.01	0.42
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.84	0.42
3:J:495:ASN:ND2	3:J:1247:LYS:O	2.52	0.42
3:J:521:LYS:HD3	3:J:541:LEU:O	2.19	0.42
3:J:901:ARG:HA	3:J:908:ILE:HA	2.00	0.42
3:J:960:LEU:HB3	3:J:963:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1231:ARG:HA	3:J:1234:VAL:HG22	2.00	0.42
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.18	0.42
4:K:71:GLU:HA	4:K:74:GLU:HG2	2.01	0.42
5:L:381:GLU:HA	5:L:384:LEU:HG	2.00	0.42
1:B:87:GLY:C	1:B:128:HIS:HE2	2.27	0.42
3:D:857:LEU:HD13	3:D:858:VAL:HG12	2.01	0.42
1:H:48:LEU:HD12	1:H:183:ILE:HD11	2.01	0.42
3:J:368:LEU:HD23	3:J:369:PRO:HD2	2.01	0.42
1:B:67:GLU:HG2	1:B:82:LEU:HD11	2.01	0.42
2:C:870:ILE:HG21	2:C:931:VAL:HG11	2.00	0.42
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.84	0.42
3:D:97:VAL:HG12	3:D:101:ARG:HG3	2.00	0.42
3:D:600:ALA:O	3:D:603:LYS:HG2	2.19	0.42
5:F:250:LEU:O	5:F:254:GLU:HG2	2.19	0.42
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.43	0.42
1:G:14:VAL:CG1	1:G:27:THR:HB	2.50	0.42
2:I:545:PHE:O	2:I:548:ARG:N	2.52	0.42
2:I:1080:ASN:HA	2:I:1081:PRO:HD3	1.92	0.42
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.85	0.42
3:J:77:ARG:HB3	3:J:80:HIS:CE1	2.54	0.42
3:J:368:LEU:HD22	3:J:373:ALA:HB2	2.01	0.42
3:J:418:GLU:H	4:K:45:LYS:HZ3	1.66	0.42
3:J:574:VAL:O	3:J:578:ILE:HG13	2.19	0.42
3:J:807:LEU:HD11	3:J:894:VAL:HG23	2.00	0.42
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	2.00	0.42
2:C:387:ASN:HA	2:C:391:SER:HB2	2.00	0.42
2:C:888:THR:HG23	2:C:916:SER:OG	2.20	0.42
2:C:1236:ASN:OD1	2:C:1236:ASN:N	2.51	0.42
3:D:574:VAL:O	3:D:578:ILE:HG13	2.19	0.42
1:G:58:GLU:HG2	1:G:158:ARG:NH2	2.29	0.42
2:I:28:LEU:HD21	2:I:524:ILE:HG13	2.00	0.42
3:J:1191:PRO:HB2	3:J:1193:TRP:CD1	2.54	0.42
5:L:41:ILE:O	5:L:45:ILE:HG13	2.19	0.42
5:L:456:MET:O	5:L:460:ILE:HG13	2.19	0.42
1:A:14:VAL:CG1	1:A:27:THR:HB	2.50	0.42
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.60	0.42
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.45	0.42
2:C:1326:LEU:HD21	3:D:339:ARG:HD2	2.01	0.42
1:G:57:THR:O	1:G:59:VAL:HG23	2.19	0.42
2:I:28:LEU:HD22	2:I:527:LYS:HD2	2.02	0.42
2:I:617:ALA:HA	2:I:636:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:137:ARG:HG3	3:J:142:GLU:HB2	2.02	0.42
3:J:201:LEU:HD11	3:J:220:ARG:NH1	2.35	0.42
3:J:422:LEU:HD13	3:J:471:PRO:HG3	2.02	0.42
3:J:698:MET:O	3:J:702:GLN:HG2	2.19	0.42
3:J:1286:LYS:HD2	3:J:1290:ARG:HH22	1.83	0.42
5:L:250:LEU:O	5:L:254:GLU:HG2	2.20	0.42
2:C:207:THR:HG21	2:C:351:LEU:HG	2.02	0.42
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.92	0.42
2:C:538:LEU:H	2:C:538:LEU:HG	1.64	0.42
2:C:998:LEU:H	2:C:998:LEU:HD12	1.84	0.42
3:D:380:PHE:HB3	3:D:415:VAL:HG11	2.01	0.42
3:D:521:LYS:HD3	3:D:541:LEU:O	2.19	0.42
2:I:888:THR:HG23	2:I:916:SER:OG	2.20	0.42
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.00	0.42
3:J:525:MET:O	3:J:548:VAL:HG13	2.19	0.42
1:A:155:ALA:HA	1:A:158:ARG:HG3	2.02	0.42
2:C:490:GLN:HG2	5:F:472:GLN:NE2	2.29	0.42
2:C:615:VAL:HA	2:C:638:SER:HA	2.02	0.42
3:D:48:THR:O	3:D:48:THR:OG1	2.37	0.42
3:D:525:MET:O	3:D:548:VAL:HG13	2.19	0.42
2:I:302:ILE:HG22	2:I:309:LEU:HA	2.01	0.42
5:L:292:VAL:HG11	5:L:299:LYS:HE3	2.02	0.42
5:L:581:ASP:HB3	5:L:582:VAL:H	1.70	0.42
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.72	0.42
2:C:11:ILE:HD13	2:C:11:ILE:HA	1.83	0.42
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.91	0.42
3:D:128:LEU:HA	3:D:192:MET:HE1	2.02	0.42
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.79	0.42
3:D:950:ILE:HG13	3:D:1020:TRP:CH2	2.55	0.42
3:D:955:LYS:HG2	3:D:1012:ALA:HA	2.02	0.42
5:F:297:MET:HE3	5:F:330:LEU:HD11	2.00	0.42
1:G:155:ALA:HA	1:G:158:ARG:HG3	2.01	0.42
2:I:15:PHE:HE1	2:I:1194:GLU:HB3	1.83	0.42
2:I:47:TYR:HD2	2:I:47:TYR:HA	1.76	0.42
2:I:207:THR:HG21	2:I:351:LEU:HG	2.01	0.42
2:I:817:LEU:HD13	2:I:1085:MET:HE1	2.01	0.42
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.35	0.42
3:J:847:ASP:OD1	3:J:847:ASP:N	2.42	0.42
3:J:1291:GLU:HG2	3:J:1297:LYS:HD3	2.02	0.42
2:C:28:LEU:HD22	2:C:527:LYS:HD2	2.01	0.42
2:C:242:VAL:HB	2:C:245:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.84	0.42
2:C:1333:LEU:HB2	2:C:1335:ILE:HG12	2.00	0.42
3:D:368:LEU:HD22	3:D:373:ALA:HB2	2.01	0.42
3:D:368:LEU:HD23	3:D:369:PRO:HD2	2.02	0.42
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.02	0.42
3:D:698:MET:O	3:D:702:GLN:HG2	2.19	0.42
3:D:1124:ILE:HA	3:D:1125:PRO:HD3	1.93	0.42
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.50	0.42
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.34	0.42
5:F:297:MET:HA	5:F:298:PRO:HD3	1.79	0.42
2:I:253:PHE:HZ	2:I:287:VAL:HG12	1.85	0.42
3:J:380:PHE:HB3	3:J:415:VAL:HG11	2.01	0.42
3:J:849:LEU:HG	3:J:853:THR:HG22	2.02	0.42
3:J:955:LYS:HG2	3:J:1012:ALA:HA	2.02	0.42
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.86	0.42
1:A:224:LEU:HD22	1:B:228:LEU:HD11	2.01	0.42
1:B:115:ILE:HD11	1:B:130:ILE:HD11	2.01	0.42
2:C:302:ILE:HG22	2:C:309:LEU:HA	2.01	0.42
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.02	0.42
5:F:343:LYS:O	5:F:347:ILE:HG13	2.20	0.42
5:F:348:GLU:HG2	5:F:354:THR:HA	2.02	0.42
5:F:456:MET:O	5:F:460:ILE:HG13	2.19	0.42
1:H:98:VAL:HG11	1:H:121:VAL:HG22	2.01	0.42
2:I:10:ARG:CZ	2:I:697:LYS:HD3	2.49	0.42
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.86	0.42
5:L:297:MET:HE3	5:L:330:LEU:HD11	2.00	0.42
2:C:10:ARG:CZ	2:C:697:LYS:HD3	2.49	0.41
2:C:1073:LYS:HD3	3:D:462:ASP:HB2	2.01	0.41
3:D:341:ASN:ND2	3:D:341:ASN:H	2.18	0.41
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.52	0.41
5:F:292:VAL:HG11	5:F:299:LYS:HE3	2.01	0.41
1:G:35:PHE:HD1	1:G:35:PHE:HA	1.71	0.41
1:G:56:VAL:HG13	1:G:173:VAL:HG21	2.02	0.41
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.60	0.41
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.41
1:B:48:LEU:HD21	3:D:535:ARG:HG3	2.02	0.41
2:C:724:VAL:HA	2:C:734:ILE:HD13	2.02	0.41
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.55	0.41
3:D:45:ASN:HB3	3:D:48:THR:O	2.21	0.41
3:D:268:LEU:HG	3:D:324:LEU:HD22	2.02	0.41
3:D:806:ASP:HA	3:D:1347:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:598:LEU:O	5:F:604:SER:HB3	2.20	0.41
2:C:46:GLN:OE1	2:C:47:TYR:N	2.47	0.41
2:C:253:PHE:HZ	2:C:287:VAL:HG12	1.85	0.41
2:C:1116:HIS:CD2	3:D:641:ILE:HB	2.55	0.41
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.35	0.41
3:D:1159:ILE:HG23	3:D:1177:ILE:HG21	2.02	0.41
1:G:197:ASP:OD1	1:G:197:ASP:N	2.53	0.41
1:H:62:ASP:HB3	1:H:141:SER:O	2.21	0.41
2:I:367:TYR:CE1	2:I:380:ALA:HB1	2.56	0.41
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.35	0.41
1:B:98:VAL:HG12	1:B:146:VAL:HG22	2.02	0.41
3:D:378:LYS:HE2	3:D:382:TYR:OH	2.20	0.41
1:G:11:PRO:HD2	1:H:227:GLN:HA	2.02	0.41
2:I:40:GLU:O	2:I:73:TYR:OH	2.38	0.41
2:I:615:VAL:HA	2:I:638:SER:HA	2.02	0.41
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.92	0.41
3:J:600:ALA:O	3:J:603:LYS:HG2	2.19	0.41
3:J:712:GLN:CD	3:J:712:GLN:H	2.27	0.41
3:J:806:ASP:HA	3:J:1347:LEU:HD13	2.02	0.41
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.20	0.41
1:A:19:VAL:HG11	1:A:23:HIS:CE1	2.55	0.41
2:C:27:LEU:HB3	2:C:528:ARG:HD2	2.01	0.41
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.01	0.41
2:C:367:TYR:CE1	2:C:380:ALA:HB1	2.55	0.41
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.02	0.41
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.82	0.41
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.55	0.41
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.84	0.41
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.20	0.41
1:G:179:PRO:HB3	1:G:211:ILE:HB	2.02	0.41
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	2.03	0.41
2:I:1288:GLN:HG2	2:I:1315:MET:HE1	2.02	0.41
3:J:770:LEU:O	3:J:774:ILE:HG13	2.19	0.41
5:L:343:LYS:O	5:L:347:ILE:HG13	2.20	0.41
5:L:348:GLU:HG2	5:L:354:THR:HA	2.02	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.93	0.41
1:A:228:LEU:HD12	1:B:221:ALA:HB1	2.02	0.41
2:C:812:PHE:HZ	3:D:503:SER:HB2	1.86	0.41
3:D:418:GLU:H	4:E:45:LYS:NZ	2.19	0.41
5:F:562:ARG:HA	5:F:562:ARG:HD2	1.94	0.41
5:F:585:GLU:HA	5:F:588:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:242:VAL:HB	2:I:245:ARG:HH11	1.86	0.41
2:I:550:VAL:HG11	3:J:776:THR:HG22	2.03	0.41
2:I:980:VAL:O	2:I:984:VAL:HB	2.20	0.41
2:I:1061:GLN:NE2	2:I:1240:ASP:OD2	2.54	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.02	0.41
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.86	0.41
1:A:52:PRO:HG2	1:A:219:ARG:NH1	2.36	0.41
1:A:179:PRO:HB3	1:A:211:ILE:HB	2.02	0.41
1:B:219:ARG:O	1:B:223:ILE:HG13	2.21	0.41
2:C:153:PRO:O	2:C:401:GLY:HA2	2.21	0.41
2:C:1061:GLN:NE2	2:C:1240:ASP:OD2	2.54	0.41
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.86	0.41
5:F:32:PRO:CG	5:F:35:ILE:HD12	2.42	0.41
2:I:697:LYS:HA	2:I:698:PRO:HD3	1.91	0.41
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.02	0.41
3:J:268:LEU:HG	3:J:324:LEU:HD22	2.02	0.41
3:J:347:VAL:HG12	3:J:348:ASP:O	2.21	0.41
1:B:62:ASP:HB3	1:B:141:SER:O	2.21	0.41
2:C:310:ILE:HD13	2:C:325:LEU:HA	2.03	0.41
2:C:519:ASN:HA	2:C:520:PRO:HD3	1.94	0.41
2:C:719:LYS:H	2:C:751:TYR:HH	1.66	0.41
2:C:765:ILE:HG13	2:C:787:PRO:HG3	2.03	0.41
2:C:1312:ASN:OD1	2:C:1314:GLN:HG3	2.21	0.41
3:D:128:LEU:HD23	3:D:192:MET:HE3	2.03	0.41
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.87	0.41
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.21	0.41
4:E:59:ILE:HD11	4:E:64:LEU:HG	2.03	0.41
1:H:87:GLY:C	1:H:128:HIS:HE2	2.27	0.41
2:I:805:MET:HE1	2:I:1221:PHE:CZ	2.56	0.41
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.55	0.41
2:I:890:LYS:NZ	2:I:891:GLY:O	2.52	0.41
3:J:30:ILE:HG23	3:J:243:PRO:HG3	2.01	0.41
3:J:148:GLU:H	3:J:156:ARG:HG3	1.85	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.73	0.41
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.55	0.41
2:C:40:GLU:O	2:C:73:TYR:OH	2.38	0.41
2:C:684:ASN:OD1	2:C:687:ARG:NH1	2.54	0.41
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.56	0.41
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.56	0.41
3:D:121:PRO:HG2	3:D:123:ARG:NH2	2.35	0.41
3:D:245:LEU:HD12	3:D:246:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.03	0.41
3:D:347:VAL:HG12	3:D:348:ASP:O	2.20	0.41
3:D:418:GLU:H	4:E:45:LYS:HZ3	1.69	0.41
3:D:1149:ARG:HB3	3:D:1149:ARG:NH1	2.36	0.41
5:F:9:LEU:HD22	6:M:47:TYR:HA	2.02	0.41
5:F:165:PHE:HZ	5:F:217:ALA:HA	1.85	0.41
1:G:19:VAL:HG11	1:G:23:HIS:CE1	2.56	0.41
1:G:61:ILE:HG22	1:G:62:ASP:H	1.86	0.41
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	2.03	0.41
2:I:37:LYS:HA	2:I:37:LYS:HD3	1.79	0.41
2:I:163:LYS:HB3	2:I:163:LYS:HE3	1.78	0.41
2:I:402:ARG:NE	2:I:417:SER:O	2.49	0.41
2:I:557:ARG:HH21	2:I:607:SER:C	2.29	0.41
2:I:710:VAL:HA	2:I:715:THR:HG21	2.03	0.41
3:J:325:LYS:HG3	3:J:329:ASP:HB2	2.03	0.41
3:J:583:VAL:HG22	3:J:620:PHE:CZ	2.56	0.41
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.55	0.41
3:J:1347:LEU:HG	3:J:1357:ILE:HG23	2.03	0.41
4:K:6:VAL:O	4:K:10:VAL:HG23	2.21	0.41
5:L:32:PRO:CG	5:L:35:ILE:HD12	2.43	0.41
5:L:455:HIS:O	5:L:459:THR:OG1	2.35	0.41
1:A:57:THR:O	1:A:59:VAL:HG23	2.19	0.41
2:C:496:LYS:HB3	2:C:496:LYS:HE3	1.78	0.41
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.03	0.41
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.86	0.41
3:D:1191:PRO:HB2	3:D:1193:TRP:CD1	2.55	0.41
2:I:124:MET:HB2	2:I:498:ILE:HD13	2.03	0.41
2:I:800:MET:HE2	2:I:800:MET:HB3	1.92	0.41
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.86	0.41
3:J:245:LEU:HD12	3:J:246:PRO:HD2	2.03	0.41
3:J:378:LYS:HE2	3:J:382:TYR:OH	2.20	0.41
3:J:514:THR:HG21	3:J:596:LEU:HD12	2.03	0.41
3:J:810:THR:HG23	3:J:811:GLU:H	1.86	0.41
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.56	0.41
1:A:56:VAL:HG13	1:A:173:VAL:HG21	2.02	0.40
1:A:61:ILE:HG22	1:A:62:ASP:H	1.86	0.40
1:B:44:ARG:CZ	3:D:538:ARG:HH21	2.34	0.40
2:C:10:ARG:HD2	2:C:1181:PRO:HG2	2.03	0.40
2:C:75:LEU:HD13	2:C:75:LEU:HA	1.93	0.40
2:C:122:VAL:HG21	2:C:493:ILE:HG23	2.03	0.40
2:C:403:MET:HE3	2:C:403:MET:HB3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:545:PHE:O	2:C:548:ARG:N	2.52	0.40
3:D:721:SER:O	3:D:725:MET:HG3	2.22	0.40
1:G:175:ALA:HB1	1:G:177:TYR:CZ	2.56	0.40
1:H:108:GLY:O	1:H:133:LEU:HB2	2.21	0.40
1:H:219:ARG:O	1:H:223:ILE:HG13	2.21	0.40
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.86	0.40
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.52	0.40
2:C:22:LEU:HG	2:C:603:ILE:HG21	2.03	0.40
3:D:111:THR:O	3:D:239:LEU:N	2.51	0.40
3:D:137:ARG:HG3	3:D:142:GLU:HB2	2.02	0.40
3:D:810:THR:HG23	3:D:811:GLU:H	1.86	0.40
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	2.02	0.40
5:F:15:ARG:HA	5:F:15:ARG:HD2	1.92	0.40
1:G:67:GLU:H	1:G:67:GLU:HG2	1.70	0.40
2:I:152:SER:HA	2:I:153:PRO:HD3	1.98	0.40
2:I:153:PRO:O	2:I:401:GLY:HA2	2.21	0.40
2:I:724:VAL:HA	2:I:734:ILE:HD13	2.02	0.40
2:I:1116:HIS:CD2	3:J:641:ILE:HB	2.55	0.40
3:J:45:ASN:HB3	3:J:48:THR:O	2.21	0.40
3:J:418:GLU:H	4:K:45:LYS:NZ	2.18	0.40
3:J:1149:ARG:HB3	3:J:1149:ARG:NH1	2.36	0.40
5:L:586:ARG:O	5:L:589:GLN:HB2	2.21	0.40
2:C:139:ASN:C	2:C:141:THR:N	2.80	0.40
2:C:325:LEU:O	2:C:330:HIS:HB2	2.21	0.40
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	2.03	0.40
2:C:994:ARG:HA	2:C:997:TRP:CD1	2.56	0.40
3:D:452:LEU:HD13	3:D:500:ILE:HG22	2.03	0.40
5:F:127:ILE:O	5:F:130:VAL:N	2.53	0.40
3:J:242:LEU:HA	3:J:243:PRO:HD3	1.94	0.40
3:J:263:SER:N	5:L:507:MET:HE2	2.36	0.40
3:J:721:SER:O	3:J:725:MET:HG3	2.21	0.40
4:K:59:ILE:HD11	4:K:64:LEU:HG	2.02	0.40
5:L:165:PHE:HZ	5:L:217:ALA:HA	1.85	0.40
5:L:387:VAL:HG22	5:L:435:ILE:HD13	2.03	0.40
5:L:598:LEU:O	5:L:604:SER:HB3	2.21	0.40
1:A:113:ALA:HB2	1:A:126:PRO:HB3	2.03	0.40
1:B:41:ASN:O	1:B:45:ARG:HG3	2.21	0.40
2:C:167:SER:C	2:C:169:LYS:H	2.30	0.40
2:C:557:ARG:HH21	2:C:607:SER:C	2.28	0.40
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.86	0.40
2:C:1128:ILE:O	2:C:1132:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:372:MET:HE2	3:D:372:MET:HB3	1.90	0.40
3:D:707:ILE:HG22	3:D:708:ASN:H	1.87	0.40
3:D:863:LEU:HD11	3:D:901:ARG:HB3	2.04	0.40
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.94	0.40
5:F:227:GLN:HG3	5:F:252:LEU:HA	2.04	0.40
1:G:52:PRO:HG2	1:G:219:ARG:NH1	2.36	0.40
1:H:41:ASN:O	1:H:45:ARG:HG3	2.21	0.40
1:H:198:LEU:HD13	1:H:198:LEU:HA	1.76	0.40
2:I:325:LEU:O	2:I:330:HIS:HB2	2.21	0.40
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.03	0.40
3:J:516:ASP:HB3	3:J:573:THR:HG21	2.04	0.40
3:J:707:ILE:HG22	3:J:708:ASN:H	1.86	0.40
3:J:968:ASN:HA	3:J:1117:SER:HB2	2.04	0.40
3:J:1309:ILE:H	3:J:1309:ILE:HG13	1.69	0.40
2:C:653:MET:HG2	2:C:654:ASP:N	2.37	0.40
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.35	0.40
2:C:737:ASN:HB3	2:C:739:ASP:OD1	2.22	0.40
2:C:887:VAL:HB	2:C:913:VAL:HG21	2.02	0.40
3:D:73:GLY:O	3:D:76:LYS:HE3	2.21	0.40
3:D:325:LYS:HE2	3:D:330:MET:SD	2.62	0.40
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.04	0.40
3:D:583:VAL:HG22	3:D:620:PHE:CZ	2.57	0.40
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.54	0.40
1:G:172:LEU:HD12	1:G:172:LEU:H	1.86	0.40
2:I:653:MET:HG2	2:I:654:ASP:N	2.37	0.40
3:J:1095:MET:HE3	3:J:1095:MET:HB2	1.95	0.40
3:J:1159:ILE:HG23	3:J:1177:ILE:HG21	2.02	0.40
3:J:1175:LEU:HD22	3:J:1190:ILE:HD11	2.02	0.40
3:J:1189:MET:HB2	6:N:57:VAL:HB	2.02	0.40
5:L:227:GLN:HB3	5:L:255:VAL:HG21	2.03	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%)	194 (87%)	26 (12%)	2 (1%)	14	45
1	B	216/239 (90%)	187 (87%)	29 (13%)	0	100	100
1	G	226/239 (95%)	197 (87%)	26 (12%)	3 (1%)	9	38
1	H	213/239 (89%)	187 (88%)	26 (12%)	0	100	100
2	C	1338/1342 (100%)	1213 (91%)	121 (9%)	4 (0%)	36	67
2	I	1338/1342 (100%)	1210 (90%)	124 (9%)	4 (0%)	36	67
3	D	1339/1407 (95%)	1229 (92%)	108 (8%)	2 (0%)	48	79
3	J	1317/1407 (94%)	1217 (92%)	98 (7%)	2 (0%)	43	73
4	E	87/91 (96%)	74 (85%)	12 (14%)	1 (1%)	11	41
4	K	77/91 (85%)	68 (88%)	8 (10%)	1 (1%)	9	38
5	F	513/613 (84%)	471 (92%)	42 (8%)	0	100	100
5	L	511/613 (83%)	469 (92%)	41 (8%)	1 (0%)	43	73
6	M	48/64 (75%)	43 (90%)	4 (8%)	1 (2%)	5	31
6	N	46/64 (72%)	42 (91%)	3 (6%)	1 (2%)	5	30
All	All	7491/7990 (94%)	6801 (91%)	668 (9%)	22 (0%)	36	67

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	61	VAL
2	C	170	VAL
2	C	1262	LYS
2	I	170	VAL
2	I	1262	LYS
3	D	357	VAL
3	J	357	VAL
1	A	14	VAL
4	E	15	ASN
1	G	14	VAL
4	K	15	ASN
2	C	163	LYS
1	G	232	VAL
2	I	163	LYS
2	C	1186	VAL
2	I	1186	VAL

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Mol	Chain	Res	Type
6	M	61	VAL
3	D	831	VAL
3	J	831	VAL
1	A	167	PRO
1	G	167	PRO
5	L	96	ASP

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%)	174 (91%)	17 (9%)	9	32
1	B	184/206 (89%)	165 (90%)	19 (10%)	7	27
1	G	191/206 (93%)	174 (91%)	17 (9%)	9	32
1	H	183/206 (89%)	165 (90%)	18 (10%)	7	29
2	C	1155/1157 (100%)	1050 (91%)	105 (9%)	9	32
2	I	1154/1157 (100%)	1049 (91%)	105 (9%)	9	32
3	D	1125/1168 (96%)	1019 (91%)	106 (9%)	8	30
3	J	1110/1168 (95%)	1005 (90%)	105 (10%)	8	30
4	E	72/75 (96%)	65 (90%)	7 (10%)	8	29
4	K	67/75 (89%)	59 (88%)	8 (12%)	5	22
5	F	444/540 (82%)	395 (89%)	49 (11%)	6	24
5	L	445/540 (82%)	395 (89%)	50 (11%)	6	24
6	M	43/56 (77%)	38 (88%)	5 (12%)	5	22
6	N	41/56 (73%)	36 (88%)	5 (12%)	5	21
All	All	6405/6816 (94%)	5789 (90%)	616 (10%)	8	29

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU

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Mol	Chain	Res	Type
1	A	17	GLU
1	A	19	VAL
1	A	27	THR
1	A	35	PHE
1	A	57	THR
1	A	58	GLU
1	A	71	LYS
1	A	74	VAL
1	A	140	ILE
1	A	171	LEU
1	A	172	LEU
1	A	207	THR
1	A	212	ASP
1	A	215	GLU
1	A	228	LEU
1	A	231	PHE
1	B	6	THR
1	B	8	PHE
1	B	16	ILE
1	B	28	LEU
1	B	31	LEU
1	B	50	SER
1	B	60	GLU
1	B	64	VAL
1	B	65	LEU
1	B	75	GLN
1	B	86	LYS
1	B	105	SER
1	B	124	VAL
1	B	140	ILE
1	B	144	ILE
1	B	183	ILE
1	B	192	VAL
1	B	194	GLN
1	B	198	LEU
2	C	11	ILE
2	C	21	VAL
2	C	22	LEU
2	C	39	ILE
2	C	47	TYR
2	C	59	ILE
2	C	60	GLN

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Mol	Chain	Res	Type
2	C	91	THR
2	C	115	LYS
2	C	117	ILE
2	C	131	THR
2	C	202	ARG
2	C	235	ASN
2	C	236	LYS
2	C	237	LEU
2	C	238	GLN
2	C	285	ILE
2	C	292	ILE
2	C	306	THR
2	C	316	GLU
2	C	321	LEU
2	C	327	GLN
2	C	331	LYS
2	C	343	HIS
2	C	353	VAL
2	C	377	THR
2	C	413	GLU
2	C	419	ILE
2	C	423	ASP
2	C	443	ASP
2	C	481	LEU
2	C	487	LEU
2	C	493	ILE
2	C	512	SER
2	C	517	GLN
2	C	518	ASN
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	550	VAL
2	C	600	THR
2	C	604	HIS
2	C	615	VAL
2	C	620	ASN
2	C	633	LEU
2	C	648	ASP
2	C	649	GLN
2	C	657	THR
2	C	660	VAL

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Mol	Chain	Res	Type
2	C	663	VAL
2	C	672	GLU
2	C	690	VAL
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	714	VAL
2	C	717	VAL
2	C	724	VAL
2	C	748	ILE
2	C	761	GLN
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	799	ASN
2	C	807	TRP
2	C	817	LEU
2	C	828	PHE
2	C	853	ASP
2	C	857	VAL
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	946	LEU
2	C	951	MET
2	C	967	LEU
2	C	974	ARG
2	C	979	LEU
2	C	1019	ASP
2	C	1040	ASP
2	C	1076	ILE
2	C	1082	ILE
2	C	1083	GLU
2	C	1090	ASN
2	C	1108	ASN
2	C	1112	ILE
2	C	1119	MET
2	C	1132	LEU
2	C	1156	ARG

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Mol	Chain	Res	Type
2	C	1174	GLU
2	C	1176	LEU
2	C	1180	MET
2	C	1198	LEU
2	C	1210	ILE
2	C	1233	LEU
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1253	LEU
2	C	1254	VAL
2	C	1262	LYS
2	C	1339	LEU
2	C	1341	ASP
3	D	20	ILE
3	D	42	GLU
3	D	44	ILE
3	D	46	TYR
3	D	83	VAL
3	D	92	VAL
3	D	96	LYS
3	D	102	MET
3	D	126	LEU
3	D	152	THR
3	D	154	LEU
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	186	GLN
3	D	197	GLU
3	D	215	LYS
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	262	THR
3	D	306	LEU
3	D	324	LEU
3	D	340	GLN

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Mol	Chain	Res	Type
3	D	341	ASN
3	D	357	VAL
3	D	368	LEU
3	D	398	LYS
3	D	401	VAL
3	D	411	ILE
3	D	415	VAL
3	D	416	ILE
3	D	430	HIS
3	D	431	ARG
3	D	501	VAL
3	D	506	VAL
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	558	ASP
3	D	615	LYS
3	D	639	VAL
3	D	641	ILE
3	D	684	ASP
3	D	698	MET
3	D	700	ASN
3	D	701	LEU
3	D	706	VAL
3	D	707	ILE
3	D	712	GLN
3	D	717	VAL
3	D	746	LEU
3	D	767	LEU
3	D	770	LEU
3	D	810	THR
3	D	826	ILE
3	D	830	ASP
3	D	843	VAL
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	878	ASP
3	D	908	ILE

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Mol	Chain	Res	Type
3	D	913	GLU
3	D	918	ILE
3	D	972	LYS
3	D	987	GLU
3	D	992	LYS
3	D	997	VAL
3	D	1017	VAL
3	D	1019	ASN
3	D	1049	GLN
3	D	1062	LEU
3	D	1063	ASP
3	D	1079	LYS
3	D	1107	VAL
3	D	1109	LEU
3	D	1140	ARG
3	D	1158	GLU
3	D	1162	ILE
3	D	1163	VAL
3	D	1167	LYS
3	D	1170	LYS
3	D	1189	MET
3	D	1199	PHE
3	D	1204	VAL
3	D	1208	ASP
3	D	1209	VAL
3	D	1244	GLN
3	D	1255	VAL
3	D	1261	LEU
3	D	1275	LEU
3	D	1284	ARG
3	D	1285	VAL
3	D	1306	LEU
3	D	1309	ILE
3	D	1329	THR
3	D	1343	GLU
3	D	1348	LYS
4	E	13	ILE
4	E	15	ASN
4	E	28	ARG
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU

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Mol	Chain	Res	Type
4	E	59	ILE
5	F	9	LEU
5	F	22	LEU
5	F	23	THR
5	F	27	VAL
5	F	36	VAL
5	F	39	ASP
5	F	41	ILE
5	F	44	ILE
5	F	48	ILE
5	F	51	MET
5	F	54	GLN
5	F	55	VAL
5	F	98	VAL
5	F	114	GLU
5	F	127	ILE
5	F	130	VAL
5	F	141	ILE
5	F	154	GLU
5	F	162	ILE
5	F	163	THR
5	F	244	THR
5	F	297	MET
5	F	305	LEU
5	F	306	PHE
5	F	333	VAL
5	F	338	HIS
5	F	341	LEU
5	F	343	LYS
5	F	400	GLN
5	F	437	GLN
5	F	450	ILE
5	F	454	VAL
5	F	482	GLU
5	F	483	LEU
5	F	488	LEU
5	F	491	GLU
5	F	496	LYS
5	F	514	ASP
5	F	528	LEU
5	F	530	LEU
5	F	540	LEU

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Mol	Chain	Res	Type
5	F	568	ASN
5	F	573	LEU
5	F	578	LYS
5	F	580	PHE
5	F	581	ASP
5	F	583	THR
5	F	606	VAL
5	F	611	LEU
1	G	9	LEU
1	G	17	GLU
1	G	19	VAL
1	G	27	THR
1	G	35	PHE
1	G	57	THR
1	G	58	GLU
1	G	71	LYS
1	G	74	VAL
1	G	140	ILE
1	G	171	LEU
1	G	172	LEU
1	G	207	THR
1	G	212	ASP
1	G	215	GLU
1	G	228	LEU
1	G	231	PHE
1	H	16	ILE
1	H	28	LEU
1	H	31	LEU
1	H	50	SER
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	86	LYS
1	H	105	SER
1	H	124	VAL
1	H	140	ILE
1	H	144	ILE
1	H	172	LEU
1	H	183	ILE
1	H	192	VAL
1	H	194	GLN

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Mol	Chain	Res	Type
1	H	198	LEU
2	I	11	ILE
2	I	21	VAL
2	I	22	LEU
2	I	39	ILE
2	I	47	TYR
2	I	59	ILE
2	I	60	GLN
2	I	91	THR
2	I	115	LYS
2	I	117	ILE
2	I	131	THR
2	I	202	ARG
2	I	235	ASN
2	I	236	LYS
2	I	237	LEU
2	I	238	GLN
2	I	285	ILE
2	I	292	ILE
2	I	302	ILE
2	I	306	THR
2	I	316	GLU
2	I	321	LEU
2	I	327	GLN
2	I	331	LYS
2	I	343	HIS
2	I	353	VAL
2	I	377	THR
2	I	413	GLU
2	I	419	ILE
2	I	423	ASP
2	I	443	ASP
2	I	481	LEU
2	I	487	LEU
2	I	493	ILE
2	I	512	SER
2	I	517	GLN
2	I	518	ASN
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	550	VAL

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Mol	Chain	Res	Type
2	I	600	THR
2	I	604	HIS
2	I	615	VAL
2	I	620	ASN
2	I	633	LEU
2	I	648	ASP
2	I	649	GLN
2	I	657	THR
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	690	VAL
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	705	GLU
2	I	714	VAL
2	I	717	VAL
2	I	724	VAL
2	I	748	ILE
2	I	761	GLN
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	807	TRP
2	I	817	LEU
2	I	828	PHE
2	I	853	ASP
2	I	857	VAL
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	979	LEU
2	I	1006	GLU
2	I	1040	ASP
2	I	1076	ILE

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Mol	Chain	Res	Type
2	I	1082	ILE
2	I	1083	GLU
2	I	1090	ASN
2	I	1108	ASN
2	I	1112	ILE
2	I	1119	MET
2	I	1132	LEU
2	I	1156	ARG
2	I	1174	GLU
2	I	1176	LEU
2	I	1180	MET
2	I	1198	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1253	LEU
2	I	1254	VAL
2	I	1262	LYS
2	I	1339	LEU
2	I	1341	ASP
3	J	20	ILE
3	J	42	GLU
3	J	44	ILE
3	J	46	TYR
3	J	83	VAL
3	J	92	VAL
3	J	96	LYS
3	J	102	MET
3	J	126	LEU
3	J	152	THR
3	J	154	LEU
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	186	GLN
3	J	197	GLU
3	J	215	LYS
3	J	217	LEU
3	J	237	MET
3	J	244	VAL

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Mol	Chain	Res	Type
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	262	THR
3	J	306	LEU
3	J	324	LEU
3	J	357	VAL
3	J	368	LEU
3	J	398	LYS
3	J	401	VAL
3	J	411	ILE
3	J	415	VAL
3	J	416	ILE
3	J	430	HIS
3	J	431	ARG
3	J	501	VAL
3	J	506	VAL
3	J	510	LEU
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	558	ASP
3	J	615	LYS
3	J	639	VAL
3	J	641	ILE
3	J	684	ASP
3	J	698	MET
3	J	700	ASN
3	J	701	LEU
3	J	706	VAL
3	J	707	ILE
3	J	712	GLN
3	J	717	VAL
3	J	746	LEU
3	J	767	LEU
3	J	770	LEU
3	J	810	THR
3	J	826	ILE
3	J	830	ASP
3	J	843	VAL
3	J	847	ASP

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Mol	Chain	Res	Type
3	J	848	VAL
3	J	849	LEU
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	878	ASP
3	J	908	ILE
3	J	913	GLU
3	J	918	ILE
3	J	972	LYS
3	J	987	GLU
3	J	992	LYS
3	J	997	VAL
3	J	1017	VAL
3	J	1019	ASN
3	J	1049	GLN
3	J	1062	LEU
3	J	1063	ASP
3	J	1079	LYS
3	J	1107	VAL
3	J	1109	LEU
3	J	1140	ARG
3	J	1158	GLU
3	J	1162	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1170	LYS
3	J	1189	MET
3	J	1199	PHE
3	J	1204	VAL
3	J	1208	ASP
3	J	1209	VAL
3	J	1244	GLN
3	J	1255	VAL
3	J	1261	LEU
3	J	1275	LEU
3	J	1284	ARG
3	J	1285	VAL
3	J	1306	LEU
3	J	1309	ILE
3	J	1329	THR
3	J	1343	GLU

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Mol	Chain	Res	Type
3	J	1348	LYS
4	K	13	ILE
4	K	15	ASN
4	K	28	ARG
4	K	36	ASP
4	K	39	VAL
4	K	58	LEU
4	K	59	ILE
4	K	79	GLU
5	L	9	LEU
5	L	22	LEU
5	L	23	THR
5	L	27	VAL
5	L	36	VAL
5	L	39	ASP
5	L	41	ILE
5	L	44	ILE
5	L	48	ILE
5	L	51	MET
5	L	54	GLN
5	L	55	VAL
5	L	96	ASP
5	L	98	VAL
5	L	114	GLU
5	L	127	ILE
5	L	130	VAL
5	L	141	ILE
5	L	154	GLU
5	L	162	ILE
5	L	163	THR
5	L	244	THR
5	L	297	MET
5	L	305	LEU
5	L	306	PHE
5	L	333	VAL
5	L	338	HIS
5	L	341	LEU
5	L	343	LYS
5	L	400	GLN
5	L	437	GLN
5	L	450	ILE
5	L	454	VAL

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Mol	Chain	Res	Type
5	L	482	GLU
5	L	483	LEU
5	L	488	LEU
5	L	491	GLU
5	L	496	LYS
5	L	514	ASP
5	L	528	LEU
5	L	530	LEU
5	L	540	LEU
5	L	568	ASN
5	L	573	LEU
5	L	578	LYS
5	L	580	PHE
5	L	581	ASP
5	L	583	THR
5	L	606	VAL
5	L	611	LEU
6	M	25	HIS
6	M	27	PHE
6	M	29	VAL
6	M	34	GLU
6	M	37	ASP
6	N	25	HIS
6	N	27	PHE
6	N	29	VAL
6	N	34	GLU
6	N	37	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	HIS
1	B	37	HIS
1	B	147	GLN
1	B	194	GLN
2	C	139	ASN
2	C	214	ASN
2	C	327	GLN
2	C	490	GLN
2	C	513	GLN
2	C	526	HIS
2	C	618	GLN

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Mol	Chain	Res	Type
2	C	677	ASN
2	C	761	GLN
2	C	1017	GLN
2	C	1061	GLN
2	C	1136	GLN
2	C	1336	ASN
3	D	45	ASN
3	D	340	GLN
3	D	489	ASN
3	D	504	GLN
3	D	690	ASN
3	D	712	GLN
3	D	736	GLN
3	D	1010	GLN
3	D	1044	GLN
3	D	1049	GLN
3	D	1197	ASN
3	D	1235	ASN
3	D	1289	ASN
3	D	1367	GLN
4	E	7	GLN
4	E	31	GLN
4	E	61	ASN
4	E	62	GLN
4	E	73	GLN
5	F	294	GLN
5	F	383	ASN
5	F	461	ASN
1	H	37	HIS
1	H	147	GLN
1	H	194	GLN
2	I	31	GLN
2	I	327	GLN
2	I	513	GLN
2	I	526	HIS
2	I	618	GLN
2	I	677	ASN
2	I	761	GLN
2	I	1061	GLN
2	I	1136	GLN
2	I	1336	ASN
3	J	45	ASN

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Mol	Chain	Res	Type
3	J	477	GLN
3	J	489	ASN
3	J	504	GLN
3	J	690	ASN
3	J	712	GLN
3	J	736	GLN
3	J	1010	GLN
3	J	1044	GLN
3	J	1049	GLN
3	J	1197	ASN
3	J	1235	ASN
3	J	1244	GLN
3	J	1289	ASN
4	K	7	GLN
4	K	61	ASN
4	K	62	GLN
4	K	73	GLN
5	L	294	GLN
5	L	461	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.17	1 (0%) 88 74	45, 79, 110, 138	0
1	B	220/239 (92%)	-0.10	3 (1%) 73 51	54, 96, 118, 134	0
1	G	228/239 (95%)	-0.29	2 (0%) 81 60	49, 82, 112, 136	0
1	H	217/239 (90%)	-0.12	3 (1%) 73 51	58, 98, 119, 135	0
2	C	1340/1342 (99%)	-0.12	18 (1%) 75 53	24, 72, 107, 132	0
2	I	1340/1342 (99%)	-0.22	14 (1%) 79 58	29, 76, 113, 139	0
3	D	1345/1407 (95%)	-0.13	11 (0%) 82 62	26, 67, 119, 138	0
3	J	1325/1407 (94%)	-0.28	8 (0%) 85 68	27, 68, 114, 137	0
4	E	89/91 (97%)	-0.33	1 (1%) 78 56	30, 69, 97, 111	0
4	K	79/91 (86%)	-0.43	0 100 100	32, 71, 107, 119	0
5	F	521/613 (84%)	-0.11	6 (1%) 76 54	35, 93, 119, 135	0
5	L	519/613 (84%)	-0.24	3 (0%) 85 68	39, 92, 119, 138	0
6	M	50/64 (78%)	-0.17	0 100 100	71, 92, 116, 127	0
6	N	48/64 (75%)	-0.36	0 100 100	75, 96, 117, 125	0
All	All	7545/7990 (94%)	-0.19	70 (0%) 81 60	24, 77, 116, 139	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	252	SER	4.6
1	H	233	ASP	4.0
3	D	319	SER	3.9
2	C	929	ILE	3.8
3	D	754	ILE	3.6
5	L	14	THR	3.5
2	C	791	LEU	3.5
2	C	251	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	524	ILE	3.1
2	I	484	LEU	3.1
3	J	1054	THR	3.0
5	F	244	THR	3.0
1	G	235	GLU	2.9
3	D	318	GLY	2.9
5	F	167	ASP	2.9
5	F	259	PHE	2.9
1	H	234	LEU	2.8
2	I	167	SER	2.8
5	F	27	VAL	2.8
1	H	228	LEU	2.8
2	C	265	LYS	2.8
3	D	341	ASN	2.8
2	I	823	VAL	2.7
1	G	175	ALA	2.7
2	C	573	ASN	2.7
1	B	172	LEU	2.7
3	J	550	VAL	2.6
2	C	1321	GLU	2.6
2	I	333	ILE	2.6
3	D	984	LEU	2.6
3	J	912	GLY	2.6
3	D	743	MET	2.5
4	E	85	ALA	2.5
3	D	160	LEU	2.5
3	J	160	LEU	2.5
2	I	1233	LEU	2.5
3	D	340	GLN	2.4
3	J	333	GLY	2.4
2	C	575	LEU	2.4
2	C	253	PHE	2.3
2	I	1323	PHE	2.3
5	F	256	PHE	2.3
2	I	21	VAL	2.3
2	C	1276	TRP	2.3
2	C	558	VAL	2.3
2	I	76	GLY	2.2
2	I	1186	VAL	2.2
2	I	351	LEU	2.2
3	J	974	VAL	2.2
2	C	870	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	165	HIS	2.2
2	C	24	VAL	2.2
2	I	999	GLU	2.2
5	F	582	VAL	2.2
3	D	742	GLY	2.2
3	J	1270	GLY	2.2
5	L	27	VAL	2.2
2	I	156	PHE	2.2
3	J	530	PRO	2.2
1	B	199	ASP	2.1
2	I	347	ILE	2.1
3	D	146	VAL	2.1
2	C	183	TRP	2.1
2	C	206	ALA	2.1
2	C	1153	ALA	2.0
5	L	22	LEU	2.0
2	C	316	GLU	2.0
1	A	216	ALA	2.0
3	D	957	SER	2.0
1	B	67	GLU	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(Å ²)	Q<0.9
7	MG	J	1501	1/1	0.68	0.25	55,55,55,55	0
7	MG	D	1501	1/1	0.69	0.12	51,51,51,51	0
8	ZN	D	1503	1/1	0.97	0.17	278,278,278,278	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ZN	J	1502	1/1	0.98	0.08	168,168,168,168	0
8	ZN	D	1502	1/1	0.99	0.05	103,103,103,103	0
8	ZN	J	1503	1/1	1.00	0.02	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.