



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:39 PM UTC

PDB ID : 4XLN / pdb_00004xln
Title : Crystal structure of T. aquaticus transcription initiation complex containing bubble promoter and RNA
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-13
Resolution : 4.00 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:

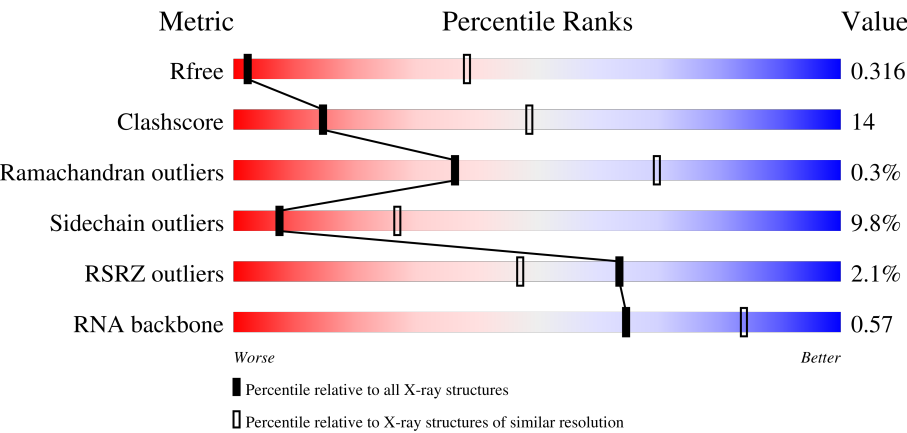
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

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	314	46%22%•28%
1	B	314	% 46%21%•28%
1	G	314	4% 46%23%•28%
1	H	314	2% 46%22%•28%

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	O	48	
6	R	48	
7	P	48	
7	S	48	
8	Q	4	
8	T	4	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 58255 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	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	347	Total	C	N	O	S	0	0	0
			2801	1767	505	525	4			
5	L	347	Total	C	N	O	S	0	0	0
			2801	1767	505	525	4			

- Molecule 6 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			
6	R	48	Total	C	N	O	P	0	0	0
			988	472	182	287	47			

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	48	Total	C	N	O	P	0	0	0
			985	471	183	284	47			
7	S	43	Total	C	N	O	P	0	0	0
			882	421	164	255	42			

- Molecule 8 is a RNA chain called RNA (5'-D(P*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Q	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			
8	T	4	Total	C	N	O	P	0	0	0
			85	38	15	28	4			

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

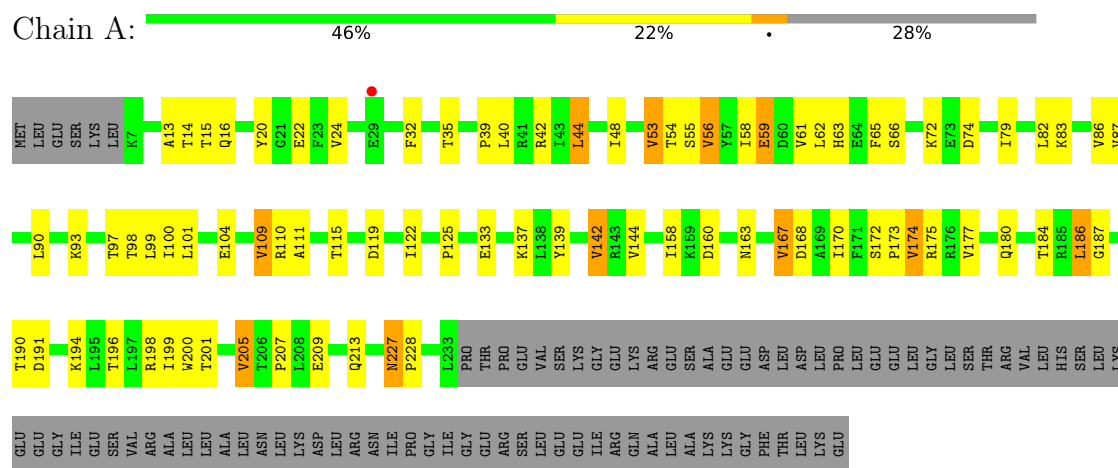
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

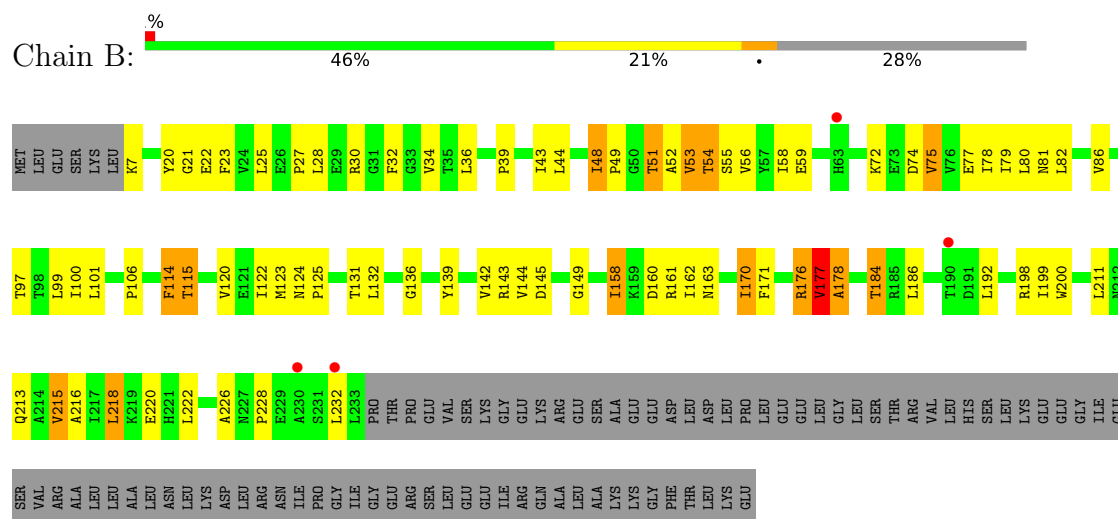
3 Residue-property plots

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

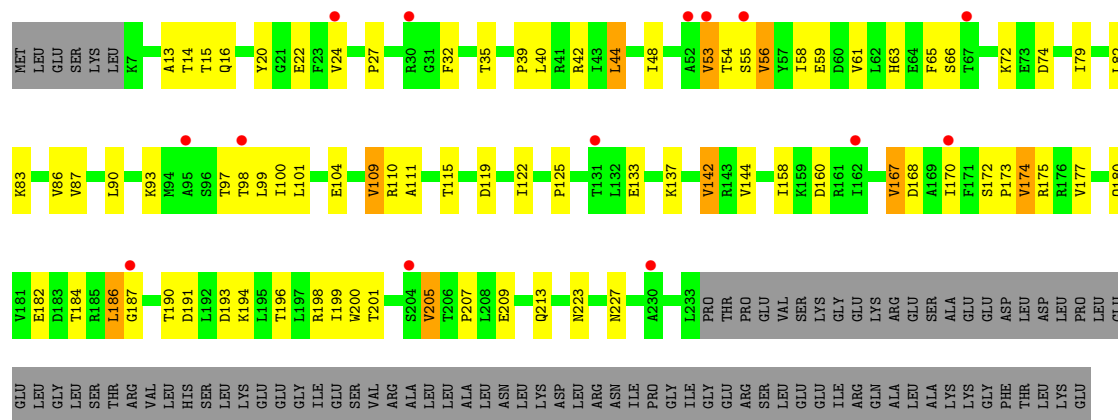


• Molecule 1: DNA-directed RNA polymerase subunit alpha

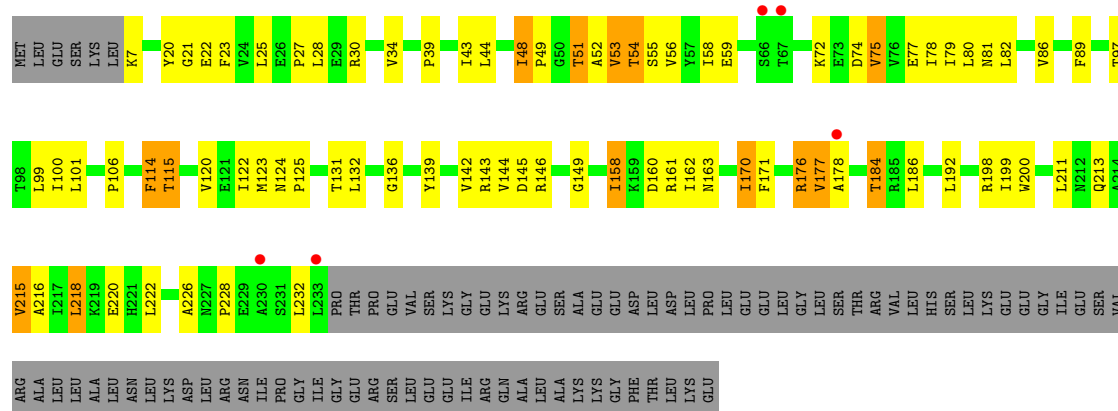


• Molecule 1: DNA-directed RNA polymerase subunit alpha

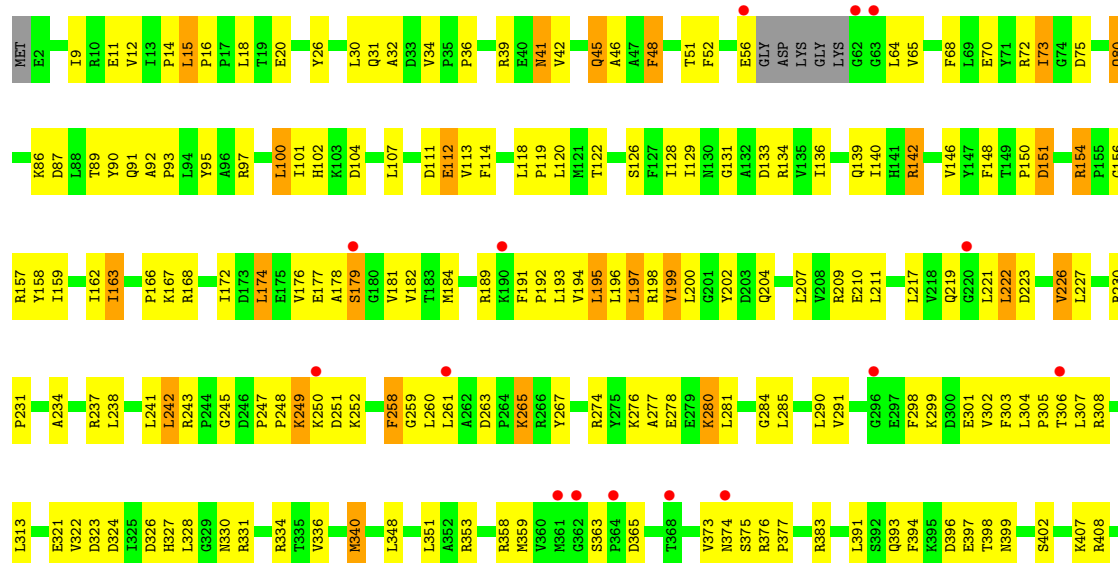


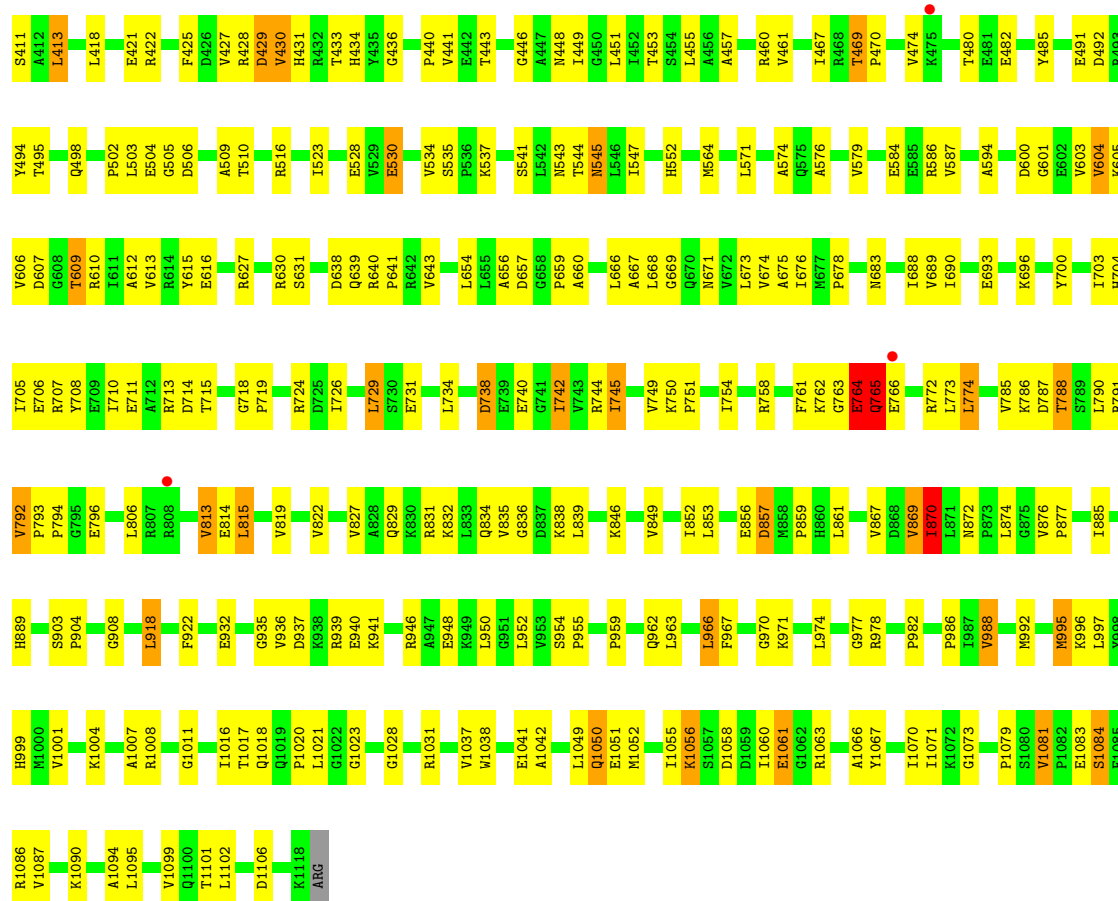


• Molecule 1: DNA-directed RNA polymerase subunit alpha

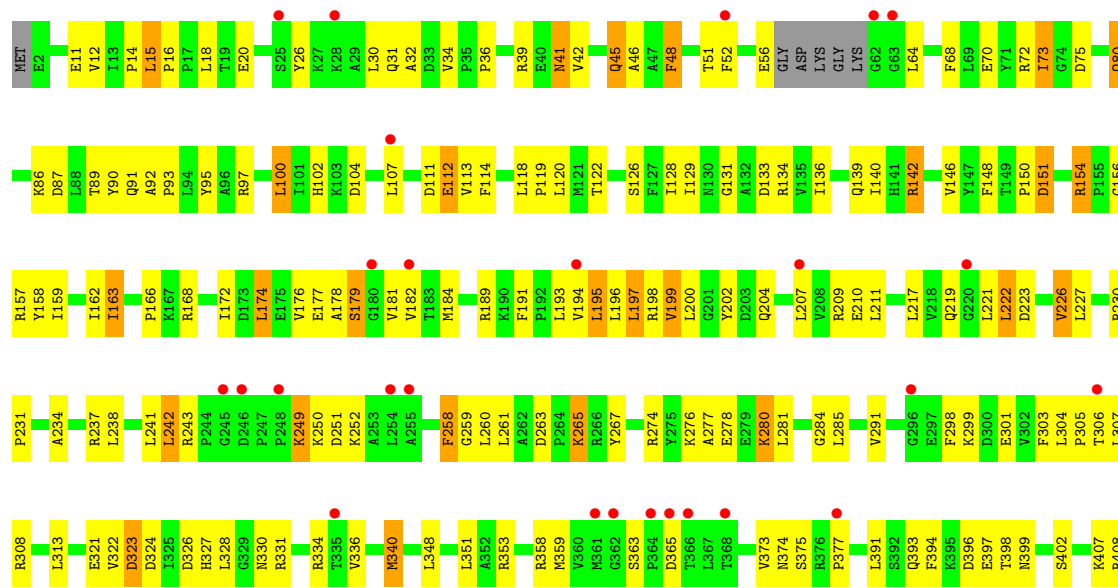


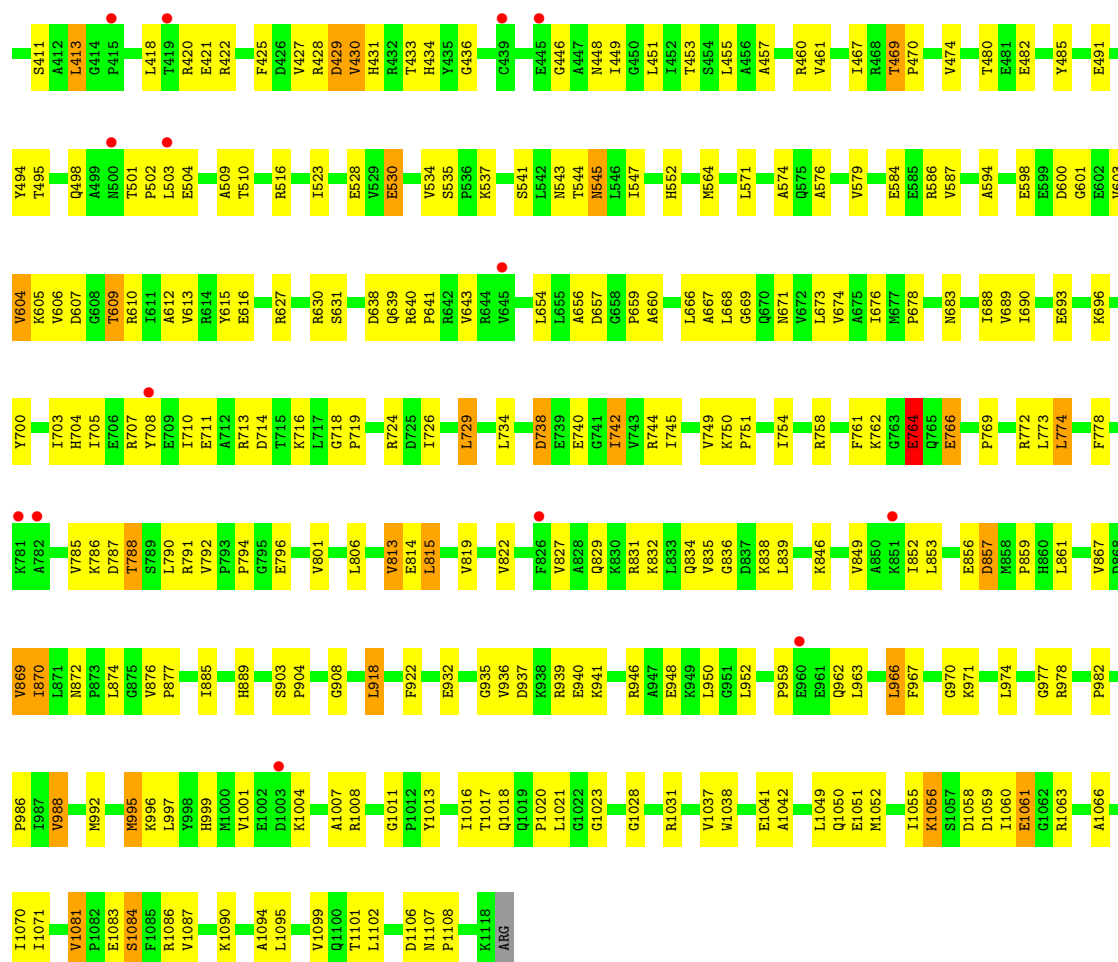
• Molecule 2: DNA-directed RNA polymerase subunit beta



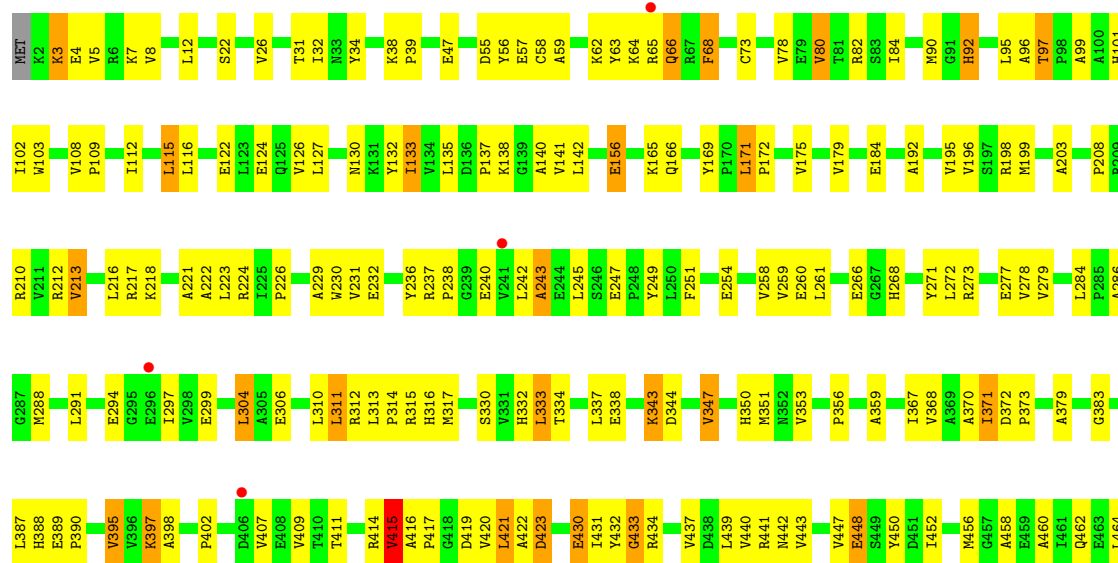


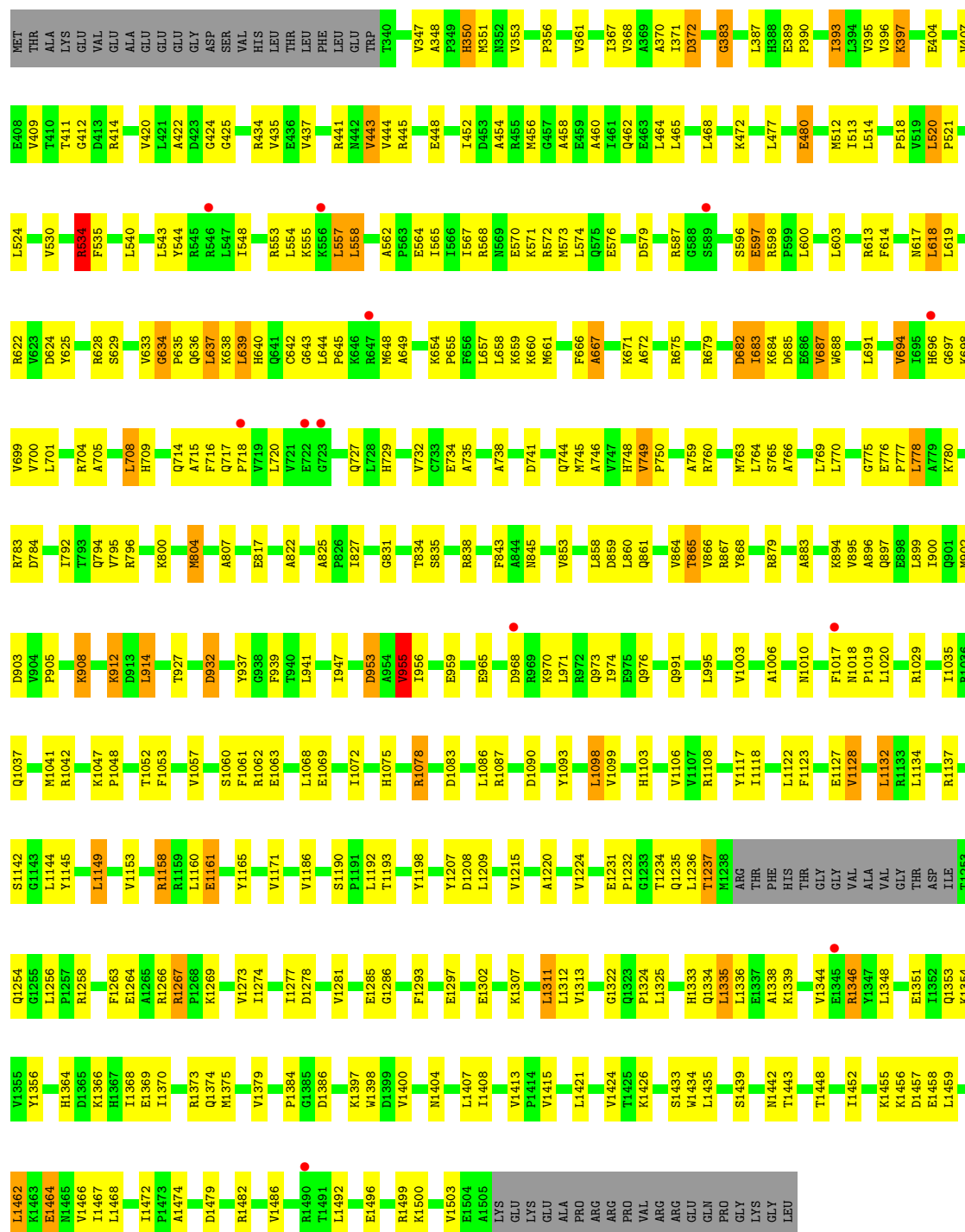
• Molecule 2: DNA-directed RNA polymerase subunit beta



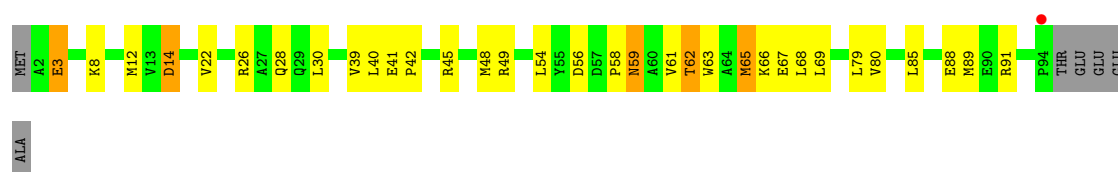


• Molecule 3: DNA-directed RNA polymerase subunit beta'

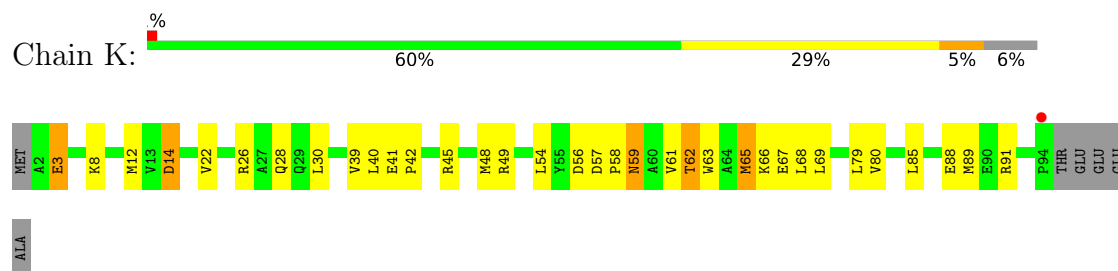




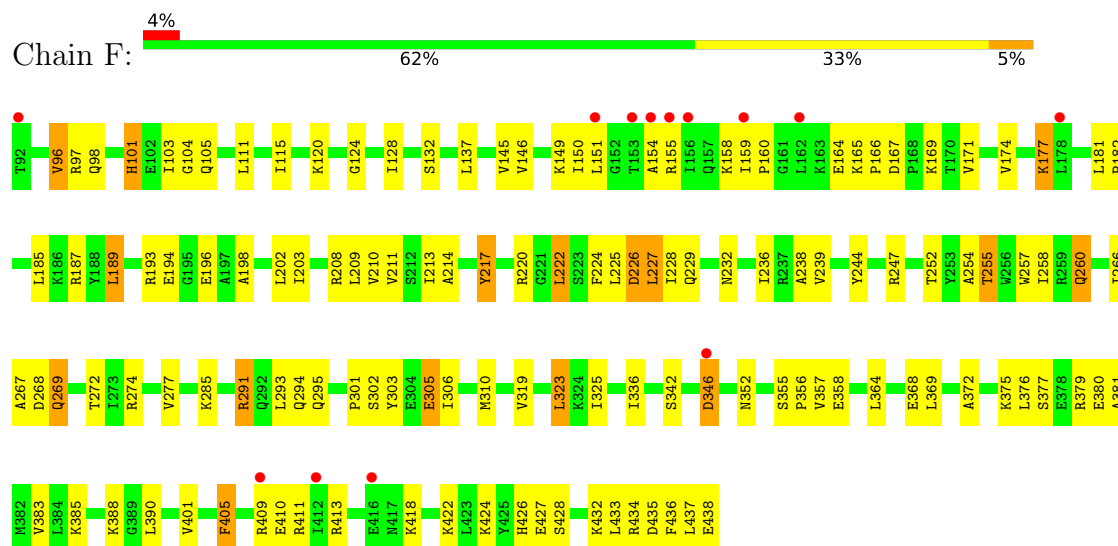
- Molecule 4: DNA-directed RNA polymerase subunit omega



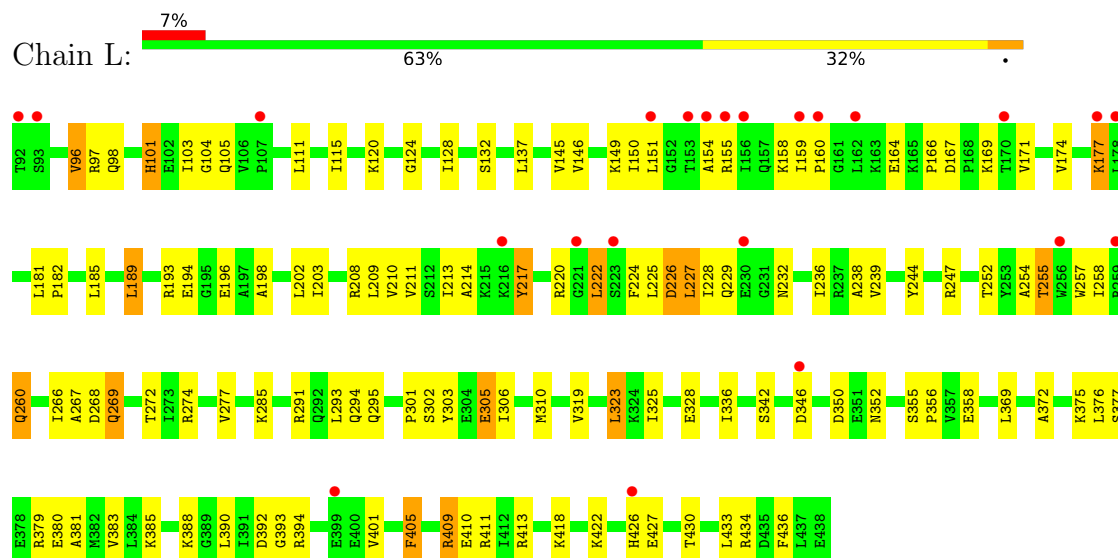
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: DNA (48-MER)

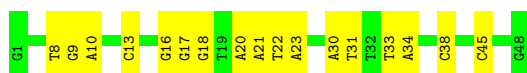




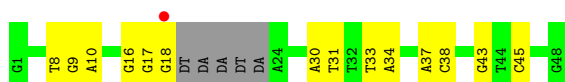
- Molecule 6: DNA (48-MER)



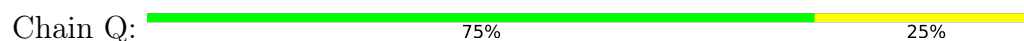
- Molecule 7: DNA (48-MER)



- Molecule 7: DNA (48-MER)



- Molecule 8: RNA (5'-D(P*UP*CP*GP*A)-3')



- Molecule 8: RNA (5'-D(P*UP*CP*GP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	289.26Å 289.26Å 536.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.96 – 4.00 34.96 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.96-4.00) 98.7 (34.96-4.00)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.280 , 0.315 0.282 , 0.316	Depositor DCC
R_{free} test set	9497 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å ²)	99.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 128.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	58255	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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	0.34	0/1804	0.86	3/2455 (0.1%)
1	B	0.34	0/1804	0.86	3/2455 (0.1%)
1	G	0.34	0/1804	0.85	2/2455 (0.1%)
1	H	0.34	0/1804	0.85	3/2455 (0.1%)
2	C	0.33	0/8905	0.84	24/12040 (0.2%)
2	I	0.33	1/8905 (0.0%)	0.84	24/12040 (0.2%)
3	D	0.31	0/11963	0.81	12/16165 (0.1%)
3	J	0.32	0/10959	0.81	10/14802 (0.1%)
4	E	0.26	0/783	0.67	0/1054
4	K	0.26	0/783	0.67	0/1054
5	F	0.29	0/2843	0.81	4/3822 (0.1%)
5	L	0.30	0/2843	0.80	4/3822 (0.1%)
6	O	0.11	0/1109	0.54	0/1712
6	R	0.11	0/1109	0.54	0/1712
7	P	0.15	0/1106	0.63	0/1706
7	S	0.11	0/989	0.51	0/1523
8	Q	0.07	0/94	0.15	0/144
8	T	0.07	0/94	0.15	0/144
All	All	0.31	1/59701 (0.0%)	0.80	89/81560 (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
1	B	0	2
2	C	0	2
2	I	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	764	GLU	CD-OE2	5.03	1.34	1.25

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	764	GLU	CA-C-N	11.37	142.16	121.70
2	I	764	GLU	C-N-CA	11.37	142.16	121.70
1	G	227	ASN	CA-C-N	8.78	128.92	120.31
1	G	227	ASN	C-N-CA	8.78	128.92	120.31
1	A	227	ASN	CA-C-N	8.75	128.88	120.31
1	A	227	ASN	C-N-CA	8.75	128.88	120.31
2	C	764	GLU	N-CA-C	8.23	120.87	109.18
1	B	178	ALA	N-CA-C	-8.02	93.72	110.80
3	J	1286	GLY	N-CA-C	-7.78	100.32	112.85
5	F	291	ARG	NE-CZ-NH2	7.76	126.18	119.20
3	D	1286	GLY	N-CA-C	-7.75	100.37	112.85
2	C	764	GLU	CA-C-N	7.50	135.87	121.54
2	C	764	GLU	C-N-CA	7.50	135.87	121.54
2	C	163	ILE	CA-C-N	7.44	129.14	119.84
2	C	163	ILE	C-N-CA	7.44	129.14	119.84
2	I	163	ILE	CA-C-N	7.39	129.08	119.84
2	I	163	ILE	C-N-CA	7.39	129.08	119.84
5	F	291	ARG	NE-CZ-NH1	-7.18	114.31	121.50
2	C	765	GLN	N-CA-C	-7.17	95.52	110.80
3	J	520	LEU	CA-C-N	7.12	124.85	119.66
3	J	520	LEU	C-N-CA	7.12	124.85	119.66
1	B	48	ILE	CA-C-N	7.03	127.44	119.92
1	B	48	ILE	C-N-CA	7.03	127.44	119.92
3	D	520	LEU	CA-C-N	7.02	124.78	119.66
3	D	520	LEU	C-N-CA	7.02	124.78	119.66
2	C	179	SER	N-CA-C	-7.00	103.93	113.30
1	H	48	ILE	CA-C-N	6.97	127.38	119.92
1	H	48	ILE	C-N-CA	6.97	127.38	119.92
2	I	179	SER	N-CA-C	-6.96	103.98	113.30
3	D	534	ARG	CB-CG-CD	6.74	126.81	111.30
2	I	1081	VAL	CA-C-N	6.51	126.20	119.82
2	I	1081	VAL	C-N-CA	6.51	126.20	119.82
1	A	163	ASN	N-CA-C	6.49	119.91	112.57
2	C	1081	VAL	CA-C-N	6.45	126.14	119.82
2	C	1081	VAL	C-N-CA	6.45	126.14	119.82
3	D	433	GLY	N-CA-C	6.24	119.24	110.38
2	C	154	ARG	CA-C-N	6.05	126.16	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	154	ARG	C-N-CA	6.05	126.16	119.87
2	I	154	ARG	CA-C-N	5.96	126.07	119.87
2	I	154	ARG	C-N-CA	5.96	126.07	119.87
2	I	908	GLY	N-CA-C	5.94	117.98	110.38
2	C	908	GLY	N-CA-C	5.92	117.96	110.38
2	I	766	GLU	CA-C-N	5.90	125.81	119.85
2	I	766	GLU	C-N-CA	5.90	125.81	119.85
5	L	291	ARG	NE-CZ-NH2	-5.90	113.89	119.20
5	L	291	ARG	CD-NE-CZ	5.79	132.50	124.40
2	C	177	GLU	CA-C-N	-5.52	114.60	122.77
2	C	177	GLU	C-N-CA	-5.52	114.60	122.77
5	F	277	VAL	N-CA-C	5.52	115.97	110.23
2	I	177	GLU	CA-C-N	-5.51	114.61	122.77
2	I	177	GLU	C-N-CA	-5.51	114.61	122.77
3	J	383	GLY	N-CA-C	5.50	117.60	110.45
3	J	534	ARG	CG-CD-NE	-5.49	99.91	112.00
5	L	277	VAL	N-CA-C	5.49	115.94	110.23
3	J	1018	ASN	CA-C-N	5.43	125.08	119.05
3	J	1018	ASN	C-N-CA	5.43	125.08	119.05
2	I	792	VAL	CA-C-N	5.43	123.62	119.66
2	I	792	VAL	C-N-CA	5.43	123.62	119.66
3	D	1018	ASN	CA-C-N	5.41	125.05	119.05
3	D	1018	ASN	C-N-CA	5.41	125.05	119.05
2	C	792	VAL	CA-C-N	5.39	123.59	119.66
2	C	792	VAL	C-N-CA	5.39	123.59	119.66
3	D	243	ALA	CB-CA-C	-5.31	109.47	115.79
2	I	903	SER	CA-C-N	5.30	125.59	119.92
2	I	903	SER	C-N-CA	5.30	125.59	119.92
2	C	903	SER	CA-C-N	5.28	125.57	119.92
2	C	903	SER	C-N-CA	5.28	125.57	119.92
2	C	763	GLY	O-C-N	5.28	126.37	122.62
3	J	534	ARG	CB-CG-CD	5.26	123.40	111.30
2	I	764	GLU	O-C-N	-5.23	115.78	122.94
3	D	908	LYS	CA-CB-CG	5.22	124.54	114.10
2	C	363	SER	CA-C-N	5.20	124.92	119.82
2	C	363	SER	C-N-CA	5.20	124.92	119.82
2	I	363	SER	CA-C-N	5.20	124.91	119.82
2	I	363	SER	C-N-CA	5.20	124.91	119.82
3	D	955	VAL	N-CA-C	5.11	115.99	109.30
3	J	955	VAL	N-CA-C	5.11	115.99	109.30
3	D	311	LEU	N-CA-C	5.09	116.87	110.91
1	H	178	ALA	N-CA-C	5.09	121.64	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	634	GLY	N-CA-C	5.06	122.67	112.34
2	C	1023	GLY	N-CA-C	5.05	116.75	111.95
3	J	634	GLY	N-CA-C	5.05	122.64	112.34
5	L	291	ARG	NE-CZ-NH1	5.04	126.54	121.50
2	C	1011	GLY	CA-C-N	5.04	125.03	119.89
2	C	1011	GLY	C-N-CA	5.04	125.03	119.89
2	I	1011	GLY	CA-C-N	5.01	125.00	119.89
2	I	1011	GLY	C-N-CA	5.01	125.00	119.89
2	I	1023	GLY	N-CA-C	5.01	116.71	111.95
5	F	291	ARG	CD-NE-CZ	5.01	131.41	124.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	177	VAL	Peptide,Mainchain
2	C	178	ALA	Peptide
2	C	764	GLU	Peptide
2	I	178	ALA	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	1770	0	1799	57	0
1	B	1770	0	1799	56	0
1	G	1770	0	1799	59	0
1	H	1770	0	1799	56	0
2	C	8739	0	8841	300	0
2	I	8739	0	8841	285	0
3	D	11761	0	11976	354	0
3	J	10779	0	10993	325	0
4	E	768	0	784	19	0
4	K	768	0	784	21	0
5	F	2801	0	2881	98	0
5	L	2801	0	2881	88	0
6	O	988	0	544	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	988	0	544	16	0
7	P	985	0	543	17	0
7	S	882	0	487	14	0
8	Q	85	0	43	0	0
8	T	85	0	43	1	0
9	D	2	0	0	0	0
9	J	2	0	0	0	0
10	D	1	0	0	0	0
10	J	1	0	0	0	0
All	All	58255	0	57381	1598	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 14.

All (1598) 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)
1:G:14:THR:HB	1:G:22:GLU:HB2	1.54	0.90
1:A:14:THR:HB	1:A:22:GLU:HB2	1.54	0.89
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.54	0.88
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.56	0.88
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.56	0.85
2:I:502:PRO:HG3	2:I:510:THR:HG22	1.56	0.84
2:I:358:ARG:HH12	2:I:374:ASN:HB2	1.42	0.83
3:J:407:VAL:HG22	3:J:409:VAL:H	1.44	0.83
2:C:358:ARG:HH12	2:C:374:ASN:HB2	1.42	0.82
3:D:1158:ARG:HG3	3:D:1158:ARG:HH11	1.44	0.82
3:J:1267:ARG:H	3:J:1267:ARG:HE	1.25	0.81
3:D:1267:ARG:H	3:D:1267:ARG:HE	1.25	0.81
3:J:1158:ARG:HG3	3:J:1158:ARG:HH11	1.47	0.79
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.66	0.78
1:G:99:LEU:HB2	1:G:142:VAL:HG22	1.64	0.77
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.65	0.77
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.67	0.76
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.66	0.76
3:D:245:LEU:HD12	3:D:311:LEU:HD21	1.67	0.76
3:D:1047:LYS:HG2	3:D:1048:PRO:HD2	1.67	0.76
2:I:494:TYR:HB3	2:I:530:GLU:HG3	1.68	0.76
3:J:1047:LYS:HG2	3:J:1048:PRO:HD2	1.67	0.76
3:D:407:VAL:HG22	3:D:409:VAL:H	1.50	0.76
2:C:494:TYR:HB3	2:C:530:GLU:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:LYS:HE2	3:D:1456:LYS:HD2	1.67	0.75
3:J:7:LYS:HE2	3:J:1456:LYS:HD2	1.67	0.75
2:C:154:ARG:HG2	2:C:156:GLY:H	1.52	0.75
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.67	0.75
7:P:9:DG:H2''	7:P:10:DA:H5'	1.68	0.74
2:C:16:PRO:HB2	2:C:460:ARG:HH21	1.52	0.74
2:I:16:PRO:HB2	2:I:460:ARG:HH21	1.52	0.74
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.67	0.74
1:A:56:VAL:HG13	1:A:142:VAL:HG12	1.70	0.74
1:G:42:ARG:HH12	2:I:857:ASP:HB3	1.52	0.74
2:I:710:ILE:HD12	2:I:790:LEU:HB2	1.69	0.73
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.69	0.73
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.71	0.73
1:G:56:VAL:HG13	1:G:142:VAL:HG12	1.70	0.73
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.52	0.73
2:I:154:ARG:HG2	2:I:156:GLY:H	1.52	0.73
7:S:9:DG:H2''	7:S:10:DA:H5'	1.68	0.73
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.70	0.72
3:J:397:LYS:HD3	3:J:448:GLU:HB3	1.70	0.72
2:I:971:LYS:HG2	2:I:988:VAL:HG12	1.70	0.72
2:C:971:LYS:HG2	2:C:988:VAL:HG12	1.70	0.72
1:B:186:LEU:HB2	1:B:192:LEU:HD21	1.72	0.72
3:J:82:ARG:HG3	3:J:84:ILE:HG22	1.70	0.72
3:J:1254:GLN:HB3	3:J:1258:ARG:HB2	1.70	0.72
2:I:603:VAL:HA	2:I:613:VAL:HG12	1.72	0.71
3:J:974:ILE:HG12	3:J:991:GLN:HE21	1.55	0.71
1:H:186:LEU:HB2	1:H:192:LEU:HD21	1.72	0.71
2:I:700:TYR:HD2	2:I:996:LYS:HB2	1.56	0.71
3:J:412:GLY:HA2	3:J:434:ARG:HE	1.55	0.71
3:D:371:ILE:HD12	5:F:247:ARG:HD3	1.73	0.71
2:I:704:HIS:HD2	2:I:831:ARG:HD2	1.55	0.71
2:C:603:VAL:HA	2:C:613:VAL:HG12	1.73	0.70
3:D:90:MET:HG2	3:D:521:PRO:HD3	1.72	0.70
2:I:313:LEU:HD13	2:I:321:GLU:HA	1.72	0.70
2:C:376:ARG:NE	7:P:22:DT:OP2	2.23	0.70
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.73	0.70
5:L:104:GLY:HA2	5:L:208:ARG:HH12	1.57	0.70
3:D:974:ILE:HG12	3:D:991:GLN:HE21	1.55	0.70
3:J:90:MET:HG2	3:J:521:PRO:HD3	1.72	0.70
2:C:700:TYR:HD2	2:C:996:LYS:HB2	1.56	0.70
3:D:171:LEU:HD22	3:D:172:PRO:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.73	0.69
1:B:53:VAL:HA	1:B:144:VAL:HA	1.74	0.69
2:C:313:LEU:HD13	2:C:321:GLU:HA	1.72	0.69
5:F:104:GLY:HA2	5:F:208:ARG:HH12	1.57	0.69
1:H:53:VAL:HA	1:H:144:VAL:HA	1.74	0.69
2:I:587:VAL:HG11	2:I:666:LEU:HD22	1.75	0.69
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.75	0.69
5:F:222:LEU:HG	5:F:226:ASP:HB3	1.75	0.69
2:I:64:LEU:HB3	2:I:359:MET:HE3	1.75	0.69
2:I:874:LEU:HD13	3:J:783:ARG:HB3	1.75	0.69
2:C:64:LEU:HB3	2:C:359:MET:HE3	1.75	0.68
1:B:59:GLU:HG3	1:B:139:TYR:HB3	1.76	0.68
3:D:415:VAL:HG11	3:D:432:TYR:HA	1.75	0.68
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.75	0.68
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.58	0.68
2:C:971:LYS:HB3	2:C:986:PRO:HB2	1.75	0.68
1:H:59:GLU:HG3	1:H:139:TYR:HB3	1.76	0.68
2:I:714:ASP:HA	2:I:719:PRO:HA	1.75	0.67
2:C:714:ASP:HA	2:C:719:PRO:HA	1.75	0.67
2:C:1051:GLU:HG2	2:C:1055:ILE:HD12	1.76	0.67
2:I:1008:ARG:HH11	2:I:1028:GLY:HA2	1.58	0.67
2:C:195:LEU:HB2	2:C:226:VAL:HG11	1.76	0.67
3:D:1142:SER:O	3:D:1364:HIS:ND1	2.28	0.67
5:L:222:LEU:HG	5:L:226:ASP:HB3	1.75	0.67
1:B:49:PRO:HD2	1:B:213:GLN:HE22	1.58	0.67
2:C:1083:GLU:O	2:C:1086:ARG:N	2.28	0.67
3:J:1142:SER:O	3:J:1364:HIS:ND1	2.28	0.67
2:I:690:ILE:HG13	2:I:852:ILE:HG23	1.77	0.66
2:C:690:ILE:HG13	2:C:852:ILE:HG23	1.77	0.66
3:D:567:ILE:HG22	3:D:571:LYS:HE3	1.78	0.66
2:I:971:LYS:HB3	2:I:986:PRO:HB2	1.75	0.66
2:I:1051:GLU:HG2	2:I:1055:ILE:HD12	1.76	0.66
2:C:245:GLY:HA3	5:F:97:ARG:HE	1.60	0.66
2:I:195:LEU:HB2	2:I:226:VAL:HG11	1.76	0.66
3:J:367:ILE:HG22	3:J:368:VAL:HG23	1.78	0.66
2:I:1037:VAL:HG13	2:I:1049:LEU:HD11	1.77	0.66
3:J:567:ILE:HG22	3:J:571:LYS:HE3	1.78	0.66
1:H:49:PRO:HD2	1:H:213:GLN:HE22	1.59	0.66
2:I:1083:GLU:O	2:I:1086:ARG:N	2.28	0.66
1:A:184:THR:HB	1:A:194:LYS:HB3	1.77	0.65
3:J:1346:ARG:HH11	3:J:1346:ARG:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.76	0.65
3:D:350:HIS:HB3	3:D:371:ILE:HG22	1.77	0.65
3:D:1144:LEU:HD21	3:D:1186:VAL:HG21	1.78	0.65
3:J:1322:GLY:HA3	3:J:1339:LYS:HG3	1.78	0.65
1:G:56:VAL:HG21	1:G:82:LEU:HD13	1.78	0.65
1:G:184:THR:HB	1:G:194:LYS:HB3	1.77	0.65
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.77	0.65
1:B:72:LYS:HB2	1:B:131:THR:HB	1.77	0.65
3:D:439:LEU:HD11	5:F:187:ARG:HB2	1.77	0.65
3:J:1144:LEU:HD21	3:J:1186:VAL:HG21	1.79	0.65
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.77	0.65
2:C:754:ILE:HG13	2:C:791:ARG:HG2	1.79	0.64
2:C:1018:GLN:HG2	2:C:1083:GLU:HG2	1.80	0.64
3:J:208:PRO:HA	3:J:390:PRO:HA	1.78	0.64
7:S:8:DT:H2"	7:S:9:DG:H5"	1.78	0.64
2:C:874:LEU:O	3:D:1029:ARG:HG2	1.98	0.64
3:D:59:ALA:H	3:D:78:VAL:HG11	1.63	0.64
1:H:72:LYS:HB2	1:H:131:THR:HB	1.77	0.64
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.79	0.64
3:J:209:ARG:HA	3:J:347:VAL:HG21	1.80	0.64
2:I:838:LYS:HB3	2:I:997:LEU:HB2	1.79	0.64
2:I:1031:ARG:HA	3:J:622:ARG:HA	1.79	0.64
1:A:53:VAL:HG22	1:A:54:THR:H	1.63	0.64
1:A:56:VAL:HG21	1:A:82:LEU:HD13	1.78	0.64
3:D:34:TYR:OH	6:O:20:DT:OP2	2.14	0.64
3:D:273:ARG:HA	3:D:278:VAL:HA	1.80	0.64
3:D:1322:GLY:HA3	3:D:1339:LYS:HG3	1.78	0.64
3:J:169:TYR:HB2	3:J:393:ILE:HD12	1.79	0.64
2:I:778:PHE:HZ	5:L:434:ARG:HA	1.62	0.64
7:P:8:DT:H2"	7:P:9:DG:H5"	1.78	0.63
2:I:754:ILE:HG13	2:I:791:ARG:HG2	1.79	0.63
3:D:102:ILE:HD12	3:D:579:ASP:HB3	1.80	0.63
1:H:34:VAL:HG11	2:I:978:ARG:HB3	1.80	0.63
3:J:39:PRO:HG2	3:J:47:GLU:HG3	1.81	0.63
2:I:584:GLU:HB3	2:I:666:LEU:H	1.63	0.63
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.81	0.63
5:F:182:PRO:HD2	5:F:185:LEU:HD12	1.80	0.63
3:J:102:ILE:HD12	3:J:579:ASP:HB3	1.80	0.63
2:C:838:LYS:HB3	2:C:997:LEU:HB2	1.79	0.63
3:D:229:ALA:HB1	3:D:245:LEU:H	1.64	0.63
3:D:637:LEU:HD21	3:D:642:CYS:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.79	0.63
3:J:59:ALA:H	3:J:78:VAL:HG11	1.63	0.63
2:C:278:GLU:HG3	2:C:284:GLY:HA2	1.81	0.62
3:D:317:MET:HE2	3:D:337:LEU:HB3	1.81	0.62
1:H:52:ALA:HB2	1:H:170:ILE:O	1.99	0.62
2:I:278:GLU:HG3	2:I:284:GLY:HA2	1.81	0.62
2:C:552:HIS:ND1	3:D:1061:PHE:O	2.32	0.62
2:I:552:HIS:ND1	3:J:1061:PHE:O	2.32	0.62
3:J:637:LEU:HD21	3:J:642:CYS:HA	1.81	0.62
3:D:39:PRO:HG2	3:D:47:GLU:HG3	1.81	0.62
1:G:53:VAL:HG22	1:G:54:THR:H	1.63	0.62
3:J:356:PRO:HB3	3:J:441:ARG:HA	1.81	0.62
2:C:198:ARG:HG3	2:C:234:ALA:HB3	1.82	0.62
2:C:584:GLU:HB3	2:C:666:LEU:H	1.63	0.62
2:C:1031:ARG:HA	3:D:622:ARG:HA	1.79	0.62
2:I:758:ARG:HG2	2:I:788:THR:HB	1.82	0.62
1:B:34:VAL:HG11	2:C:978:ARG:HB3	1.81	0.62
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.81	0.62
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.82	0.61
3:D:133:ILE:HD11	3:D:460:ALA:HB1	1.82	0.61
3:J:178:LEU:N	3:J:191:LEU:O	2.32	0.61
1:B:52:ALA:HB2	1:B:170:ILE:O	2.00	0.61
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.36	0.61
1:A:48:ILE:HG23	1:A:213:GLN:HE21	1.65	0.61
3:J:162:ARG:HG3	3:J:414:ARG:HH22	1.64	0.61
5:L:182:PRO:HD2	5:L:185:LEU:HD12	1.80	0.61
3:D:411:THR:HG22	3:D:437:VAL:H	1.65	0.61
3:J:137:PRO:HA	3:J:452:ILE:HG13	1.82	0.61
3:J:133:ILE:HD11	3:J:460:ALA:HB1	1.82	0.61
2:I:72:ARG:HB3	2:I:95:TYR:HB2	1.82	0.61
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.82	0.61
2:C:174:LEU:HD13	2:C:193:LEU:HD21	1.83	0.61
3:D:759:ALA:HA	3:D:763:MET:HB3	1.83	0.61
1:G:205:VAL:HG13	1:G:209:GLU:HB2	1.82	0.61
2:I:502:PRO:HB2	2:I:509:ALA:HB3	1.81	0.61
1:H:177:VAL:HG12	1:H:199:ILE:HG12	1.81	0.61
5:L:137:LEU:HD11	5:L:177:LYS:HE3	1.83	0.61
2:I:461:VAL:HG22	2:I:467:ILE:HG12	1.83	0.61
3:J:759:ALA:HA	3:J:763:MET:HB3	1.83	0.61
2:C:72:ARG:HB3	2:C:95:TYR:HB2	1.82	0.60
2:C:758:ARG:HG2	2:C:788:THR:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.82	0.60
2:I:1018:GLN:HG2	2:I:1083:GLU:HG2	1.83	0.60
1:A:205:VAL:HG13	1:A:209:GLU:HB2	1.82	0.60
3:D:213:VAL:HG12	3:D:343:LYS:HB3	1.83	0.60
3:J:908:LYS:HE3	3:J:908:LYS:O	2.00	0.60
2:C:86:LYS:HE2	2:C:813:VAL:HG23	1.82	0.60
2:C:134:ARG:NH2	7:P:18:DG:OP2	2.33	0.60
2:C:461:VAL:HG22	2:C:467:ILE:HG12	1.83	0.60
2:I:199:VAL:HA	2:I:231:PRO:HB3	1.82	0.60
3:J:1158:ARG:HH11	3:J:1158:ARG:CG	2.12	0.60
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.82	0.60
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.83	0.60
2:I:198:ARG:HG3	2:I:234:ALA:HB3	1.82	0.60
3:J:619:LEU:HD11	3:J:1439:SER:HB2	1.82	0.60
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.84	0.60
2:I:128:ILE:HA	2:I:133:ASP:HA	1.83	0.60
2:I:174:LEU:HD13	2:I:193:LEU:HD21	1.83	0.60
1:H:100:ILE:HG23	1:H:139:TYR:HE1	1.67	0.60
2:I:1063:ARG:HG3	5:L:356:PRO:HG3	1.83	0.60
3:J:184:GLU:HG2	3:J:202:VAL:HG22	1.82	0.60
3:D:557:LEU:HD12	3:D:567:ILE:HD13	1.82	0.60
2:I:64:LEU:HD11	2:I:100:LEU:HG	1.84	0.60
2:I:630:ARG:HG3	2:I:705:ILE:HB	1.83	0.60
3:D:1236:LEU:HD13	3:D:1256:LEU:HB2	1.83	0.60
7:P:30:DA:H2"	7:P:31:DT:H5"	1.83	0.60
3:J:521:PRO:HD2	3:J:524:LEU:HD12	1.84	0.60
3:J:1263:PHE:HA	3:J:1375:MET:HE1	1.83	0.60
3:J:1274:ILE:HD11	3:J:1334:GLN:HB3	1.83	0.60
1:B:100:ILE:HG23	1:B:139:TYR:HE1	1.67	0.59
1:G:48:ILE:HG23	1:G:213:GLN:HE21	1.66	0.59
3:J:557:LEU:HD12	3:J:567:ILE:HD13	1.82	0.59
3:J:657:LEU:HD22	3:J:691:LEU:HD13	1.84	0.59
3:D:698:LYS:HG3	4:E:59:ASN:HD21	1.68	0.59
3:D:908:LYS:HE3	3:D:908:LYS:O	2.02	0.59
7:S:30:DA:H2"	7:S:31:DT:H5"	1.83	0.59
2:C:274:ARG:HG3	2:C:285:LEU:HD23	1.84	0.59
3:D:398:ALA:HB2	3:D:447:VAL:HG12	1.85	0.59
2:I:274:ARG:HG3	2:I:285:LEU:HD23	1.84	0.59
2:I:304:LEU:HB3	2:I:305:PRO:HD3	1.84	0.59
2:I:948:GLU:OE2	2:I:962:GLN:NE2	2.35	0.59
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:734:GLU:OE2	3:J:780:LYS:NZ	2.28	0.59
3:J:908:LYS:HE3	3:J:908:LYS:C	2.27	0.59
1:B:177:VAL:HG12	1:B:199:ILE:HG12	1.84	0.59
3:D:657:LEU:HD22	3:D:691:LEU:HD13	1.85	0.59
5:F:137:LEU:HD11	5:F:177:LYS:HE3	1.83	0.59
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.84	0.59
2:C:674:VAL:HA	2:C:869:VAL:HG13	1.85	0.59
2:C:772:ARG:HG2	5:F:388:LYS:HD2	1.84	0.59
2:C:774:LEU:HD23	5:F:369:LEU:HD21	1.85	0.59
3:D:208:PRO:HA	3:D:390:PRO:HA	1.84	0.59
3:D:521:PRO:HD2	3:D:524:LEU:HD12	1.84	0.59
3:D:1108:ARG:NH1	3:D:1198:TYR:O	2.36	0.59
2:I:674:VAL:HA	2:I:869:VAL:HG13	1.85	0.59
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.84	0.59
3:J:700:VAL:HG22	3:J:718:PRO:HG3	1.84	0.59
3:D:700:VAL:HG22	3:D:718:PRO:HG3	1.84	0.59
2:I:32:ALA:HB1	2:I:73:ILE:HD13	1.85	0.59
2:I:142:ARG:HA	2:I:331:ARG:HA	1.84	0.59
2:C:839:LEU:HD23	2:C:996:LYS:HA	1.85	0.59
3:J:530:VAL:HG22	3:J:534:ARG:HB2	1.83	0.59
3:J:716:PHE:HZ	3:J:732:VAL:HG21	1.68	0.59
2:C:32:ALA:HB1	2:C:73:ILE:HD13	1.85	0.59
2:I:134:ARG:NH2	7:S:18:DG:OP2	2.36	0.58
2:I:839:LEU:HD23	2:I:996:LYS:HA	1.85	0.58
3:J:1236:LEU:HD13	3:J:1256:LEU:HB2	1.83	0.58
1:A:16:GLN:HB3	1:A:20:TYR:HB3	1.85	0.58
2:C:64:LEU:HD11	2:C:100:LEU:HG	1.84	0.58
1:H:51:THR:OG1	1:H:52:ALA:N	2.36	0.58
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.84	0.58
5:F:181:LEU:HD23	5:F:185:LEU:HB3	1.85	0.58
1:G:198:ARG:HH22	2:I:932:GLU:HB3	1.68	0.58
3:J:698:LYS:HG3	4:K:59:ASN:HD21	1.67	0.58
3:J:1459:LEU:HD21	3:J:1468:LEU:HG	1.84	0.58
2:C:142:ARG:HA	2:C:331:ARG:HA	1.86	0.58
2:C:674:VAL:HG11	2:C:992:MET:HE3	1.85	0.58
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.84	0.58
2:C:128:ILE:HA	2:C:133:ASP:HA	1.86	0.58
2:C:786:LYS:NZ	5:F:438:GLU:OE1	2.36	0.58
2:I:774:LEU:HD23	5:L:369:LEU:HD21	1.85	0.58
3:J:192:ALA:HB1	3:J:193:PRO:HD2	1.85	0.58
3:J:1108:ARG:NH1	3:J:1198:TYR:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:716:PHE:HZ	3:D:732:VAL:HG21	1.69	0.58
3:J:1267:ARG:HH22	6:R:42:DC:H3'	1.69	0.58
3:D:434:ARG:HG2	3:D:447:VAL:HG22	1.86	0.58
3:D:1267:ARG:HH22	6:O:42:DC:H3'	1.68	0.58
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.39	0.58
6:O:11:DG:N2	7:P:38:DC:O2	2.36	0.58
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.86	0.58
2:I:230:ARG:HB3	2:I:231:PRO:HD2	1.86	0.58
2:I:772:ARG:HG2	5:L:388:LYS:HD2	1.84	0.58
3:J:640:HIS:O	3:J:717:GLN:N	2.32	0.58
5:L:209:LEU:HD21	5:L:255:THR:HG23	1.85	0.58
2:C:162:ILE:HD11	2:C:306:THR:HG21	1.84	0.58
2:I:162:ILE:HD11	2:I:306:THR:HG21	1.84	0.58
5:L:302:SER:H	5:L:305:GLU:HG3	1.68	0.58
2:C:576:ALA:O	2:C:671:ASN:ND2	2.37	0.57
5:F:189:LEU:HD11	5:F:193:ARG:HH21	1.69	0.57
5:F:203:ILE:HG12	5:F:239:VAL:HG21	1.86	0.57
4:K:48:MET:HE3	4:K:58:PRO:HD2	1.86	0.57
5:L:189:LEU:HD11	5:L:193:ARG:HH21	1.68	0.57
5:L:181:LEU:HD23	5:L:185:LEU:HB3	1.85	0.57
1:A:198:ARG:HH22	2:C:932:GLU:HB3	1.68	0.57
2:C:230:ARG:HB3	2:C:231:PRO:HD2	1.86	0.57
5:F:209:LEU:HD21	5:F:255:THR:HG23	1.85	0.57
5:F:285:LYS:HD3	5:F:310:MET:HE1	1.87	0.57
2:I:674:VAL:HG11	2:I:992:MET:HE3	1.85	0.57
3:J:210:ARG:HH11	3:J:389:GLU:HG3	1.69	0.57
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.86	0.57
2:C:948:GLU:OE2	2:C:962:GLN:NE2	2.35	0.57
3:D:1158:ARG:HH11	3:D:1158:ARG:CG	2.15	0.57
1:G:16:GLN:HB3	1:G:20:TYR:HB3	1.85	0.57
5:L:203:ILE:HG12	5:L:239:VAL:HG21	1.86	0.57
3:J:462:GLN:HB2	3:J:513:ILE:HG21	1.86	0.57
3:J:1158:ARG:HG3	3:J:1158:ARG:NH1	2.19	0.57
2:C:41:ASN:HA	2:C:45:GLN:HB3	1.86	0.57
2:C:281:LEU:O	2:C:308:ARG:NH2	2.38	0.57
2:I:128:ILE:HG13	2:I:133:ASP:HB3	1.86	0.57
2:I:195:LEU:HD12	2:I:198:ARG:HE	1.69	0.57
3:J:205:TYR:HA	3:J:393:ILE:HG22	1.87	0.57
5:L:285:LYS:HD3	5:L:310:MET:HE1	1.87	0.57
6:R:11:DG:N2	7:S:38:DC:O2	2.36	0.57
2:I:14:PRO:HB3	2:I:586:ARG:HH22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:682:ASP:C	3:D:683:ILE:HG13	2.31	0.56
2:I:668:LEU:HB3	2:I:995:MET:HG2	1.87	0.56
1:B:51:THR:OG1	1:B:52:ALA:N	2.36	0.56
2:C:353:ARG:NH1	6:O:34:DA:OP1	2.36	0.56
2:C:704:HIS:HD2	2:C:831:ARG:HD2	1.70	0.56
3:D:853:VAL:HG22	3:D:858:LEU:HB3	1.88	0.56
4:E:48:MET:HE3	4:E:58:PRO:HD2	1.86	0.56
5:F:302:SER:H	5:F:305:GLU:HG3	1.69	0.56
2:I:249:LYS:HD3	2:I:250:LYS:H	1.71	0.56
3:D:1459:LEU:HD21	3:D:1468:LEU:HG	1.86	0.56
2:I:51:THR:HG21	2:I:348:LEU:HB3	1.88	0.56
2:I:281:LEU:O	2:I:308:ARG:NH2	2.38	0.56
3:J:407:VAL:HG23	3:J:422:ALA:HB2	1.87	0.56
2:C:197:LEU:HB3	2:C:202:TYR:HD2	1.70	0.56
2:I:41:ASN:HA	2:I:45:GLN:HB3	1.86	0.56
2:I:197:LEU:HB3	2:I:202:TYR:HD2	1.70	0.56
2:I:353:ARG:NH1	6:R:34:DA:OP1	2.36	0.56
3:J:65:ARG:HG3	3:J:66:GLN:H	1.70	0.56
2:I:576:ALA:O	2:I:671:ASN:ND2	2.37	0.56
1:H:53:VAL:HB	1:H:144:VAL:HG22	1.88	0.56
3:J:1273:VAL:HG23	3:J:1325:LEU:HB2	1.88	0.56
2:C:195:LEU:HD12	2:C:198:ARG:HE	1.69	0.56
3:D:1127:GLU:HG3	3:D:1128:VAL:HG23	1.88	0.56
3:D:1264:GLU:HB3	3:D:1266:ARG:HG3	1.88	0.56
3:J:613:ARG:NH1	3:J:617:ASN:OD1	2.36	0.56
3:J:1190:SER:OG	3:J:1369:GLU:OE1	2.22	0.56
1:A:62:LEU:HD13	2:C:745:ILE:HB	1.88	0.56
1:B:53:VAL:HB	1:B:144:VAL:HG22	1.88	0.56
2:C:249:LYS:HD3	2:C:250:LYS:H	1.71	0.56
3:D:879:ARG:HH12	3:D:905:PRO:HA	1.71	0.56
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	1.88	0.56
1:G:58:ILE:HB	1:G:61:VAL:HB	1.88	0.56
3:J:12:LEU:HD21	3:J:1452:ILE:HA	1.88	0.56
3:J:822:ALA:HB3	3:J:825:ALA:HB2	1.88	0.56
3:J:1267:ARG:H	3:J:1267:ARG:NE	2.02	0.56
3:D:12:LEU:HD21	3:D:1452:ILE:HA	1.88	0.55
3:J:160:GLU:HG3	3:J:165:LYS:HB2	1.88	0.55
2:C:15:LEU:O	2:C:586:ARG:NH1	2.40	0.55
3:D:1003:VAL:HG21	3:D:1041:MET:HG2	1.89	0.55
2:I:941:LYS:HE2	2:I:959:PRO:HG2	1.88	0.55
3:J:1003:VAL:HG21	3:J:1041:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:668:LEU:HB3	2:C:995:MET:HG2	1.87	0.55
3:D:883:ALA:HB2	3:D:902:MET:HE1	1.89	0.55
1:H:56:VAL:HG21	1:H:82:LEU:HD13	1.89	0.55
3:J:682:ASP:C	3:J:683:ILE:HG13	2.30	0.55
3:J:853:VAL:HG22	3:J:858:LEU:HB3	1.88	0.55
3:J:879:ARG:HH12	3:J:905:PRO:HA	1.71	0.55
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.88	0.55
3:D:1486:VAL:HG11	4:E:26:ARG:HB2	1.88	0.55
2:C:693:GLU:HA	2:C:696:LYS:HE2	1.89	0.55
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.88	0.55
2:C:383:ARG:CZ	7:P:20:DA:H2"	2.37	0.55
2:C:941:LYS:HE2	2:C:959:PRO:HG2	1.88	0.55
2:I:15:LEU:O	2:I:586:ARG:NH1	2.40	0.55
2:I:204:GLN:HA	2:I:227:LEU:HD22	1.88	0.55
2:C:1060:ILE:HG13	2:C:1061:GLU:H	1.72	0.55
3:D:613:ARG:NH1	3:D:617:ASN:OD1	2.36	0.55
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.88	0.55
5:L:120:LYS:HD2	5:L:194:GLU:HG2	1.89	0.55
2:C:204:GLN:HA	2:C:227:LEU:HD22	1.88	0.55
3:D:97:THR:HG22	3:D:554:LEU:HD21	1.89	0.55
3:J:172:PRO:HG2	3:J:175:VAL:HB	1.89	0.55
3:J:1264:GLU:HB3	3:J:1266:ARG:HG3	1.88	0.55
2:C:408:ARG:NH1	2:C:455:LEU:O	2.40	0.55
3:J:3:LYS:HE3	3:J:4:GLU:H	1.71	0.55
3:J:1208:ASP:HB2	3:J:1215:VAL:HA	1.89	0.55
2:C:601:GLY:HA2	2:C:615:TYR:HA	1.89	0.54
3:D:3:LYS:HE3	3:D:4:GLU:H	1.71	0.54
5:F:252:THR:HG23	6:O:29:DC:H41	1.72	0.54
2:I:504:GLU:HB3	2:I:509:ALA:HB2	1.89	0.54
2:I:693:GLU:HA	2:I:696:LYS:HE2	1.89	0.54
2:I:762:LYS:HD3	2:I:786:LYS:HD3	1.89	0.54
3:J:7:LYS:CE	3:J:1456:LYS:HD2	2.35	0.54
2:C:139:GLN:HB3	2:C:334:ARG:HB2	1.88	0.54
5:F:120:LYS:HD2	5:F:194:GLU:HG2	1.89	0.54
2:I:209:ARG:HG3	2:I:210:GLU:H	1.71	0.54
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.89	0.54
2:C:1021:LEU:O	2:C:1028:GLY:HA3	2.07	0.54
3:D:1346:ARG:HH11	3:D:1346:ARG:HB3	1.72	0.54
2:I:139:GLN:HB3	2:I:334:ARG:HB2	1.88	0.54
3:J:97:THR:HG22	3:J:554:LEU:HD21	1.89	0.54
3:J:1127:GLU:HG3	3:J:1128:VAL:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HB	1:A:61:VAL:HB	1.88	0.54
2:C:51:THR:HG21	2:C:348:LEU:HB3	1.88	0.54
2:I:601:GLY:HA2	2:I:615:TYR:HA	1.89	0.54
2:C:14:PRO:HB3	2:C:586:ARG:HH22	1.71	0.54
2:C:724:ARG:HG2	2:C:734:LEU:HD23	1.89	0.54
3:J:1486:VAL:HG11	4:K:26:ARG:HB2	1.88	0.54
2:C:209:ARG:HG3	2:C:210:GLU:H	1.72	0.54
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.90	0.54
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.89	0.54
5:F:411:ARG:NE	6:O:1:DC:H5'	2.22	0.54
2:I:277:ALA:HA	2:I:280:LYS:HG2	1.90	0.54
3:J:96:ALA:HB2	3:J:555:LYS:HG2	1.89	0.54
3:J:696:HIS:HB3	4:K:48:MET:HE2	1.90	0.54
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.89	0.54
1:G:79:ILE:HA	1:G:82:LEU:HD12	1.90	0.54
2:I:724:ARG:HG2	2:I:734:LEU:HD23	1.89	0.54
3:J:1333:HIS:NE2	3:J:1421:LEU:O	2.40	0.54
4:K:40:LEU:HD21	4:K:67:GLU:HA	1.88	0.54
3:D:313:LEU:HG	3:D:314:PRO:HD2	1.88	0.54
3:D:553:ARG:NH2	5:F:226:ASP:OD1	2.36	0.54
2:I:836:GLY:H	2:I:849:VAL:HB	1.73	0.54
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.42	0.54
2:I:52:PHE:CG	2:I:68:PHE:HB2	2.42	0.54
3:J:633:VAL:HG13	3:J:635:PRO:HD3	1.89	0.54
3:J:777:PRO:O	3:J:912:LYS:NZ	2.40	0.54
3:J:883:ALA:HB2	3:J:902:MET:HE1	1.89	0.54
5:L:379:ARG:NH2	5:L:411:ARG:HH21	2.06	0.54
3:D:629:SER:HB3	3:D:648:MET:HE1	1.90	0.53
3:D:1333:HIS:NE2	3:D:1421:LEU:O	2.40	0.53
2:I:408:ARG:NH1	2:I:455:LEU:O	2.40	0.53
2:I:1060:ILE:HG13	2:I:1061:GLU:H	1.72	0.53
3:J:169:TYR:HE1	3:J:198:ARG:HD3	1.73	0.53
3:J:629:SER:HB3	3:J:648:MET:HE1	1.90	0.53
4:K:41:GLU:O	4:K:45:ARG:HG2	2.09	0.53
1:A:79:ILE:HA	1:A:82:LEU:HD12	1.90	0.53
2:C:277:ALA:HA	2:C:280:LYS:HG2	1.90	0.53
3:D:777:PRO:O	3:D:912:LYS:NZ	2.40	0.53
3:D:792:ILE:HG21	3:D:941:LEU:HD22	1.90	0.53
4:K:14:ASP:OD1	4:K:14:ASP:N	2.40	0.53
2:C:504:GLU:HB3	2:C:509:ALA:HB2	1.89	0.53
3:D:777:PRO:HB2	3:D:912:LYS:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:174:VAL:HA	1:G:201:THR:HG22	1.91	0.53
2:I:713:ARG:HA	2:I:819:VAL:HA	1.90	0.53
2:I:1021:LEU:O	2:I:1028:GLY:HA3	2.07	0.53
3:J:97:THR:HG21	3:J:571:LYS:HG2	1.90	0.53
5:L:238:ALA:HB1	5:L:254:ALA:HA	1.90	0.53
1:A:111:ALA:HB3	1:A:125:PRO:HA	1.89	0.53
2:C:126:SER:HB3	2:C:407:LYS:HZ1	1.73	0.53
2:C:836:GLY:H	2:C:849:VAL:HB	1.72	0.53
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.89	0.53
3:D:696:HIS:HB3	4:E:48:MET:HE2	1.89	0.53
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.21	0.53
1:G:111:ALA:HB3	1:G:125:PRO:HA	1.89	0.53
3:J:770:LEU:HA	3:J:777:PRO:HA	1.91	0.53
3:J:777:PRO:HB2	3:J:912:LYS:HE2	1.89	0.53
5:L:101:HIS:CD2	6:R:31:DG:H22	2.27	0.53
2:C:91:GLN:HA	2:C:119:PRO:HA	1.91	0.53
3:D:7:LYS:CE	3:D:1456:LYS:HD2	2.37	0.53
3:D:242:LEU:HB3	3:D:312:ARG:HA	1.89	0.53
2:I:194:VAL:HG11	2:I:223:ASP:HB3	1.91	0.53
3:J:562:ALA:HB3	3:J:567:ILE:HD11	1.91	0.53
5:L:410:GLU:OE2	5:L:413:ARG:NH1	2.42	0.53
3:D:562:ALA:HB3	3:D:567:ILE:HD11	1.91	0.53
3:D:770:LEU:HA	3:D:777:PRO:HA	1.91	0.53
5:F:238:ALA:HB1	5:F:254:ALA:HA	1.90	0.53
5:F:257:TRP:O	5:F:260:GLN:HG3	2.09	0.53
2:I:91:GLN:HA	2:I:119:PRO:HA	1.91	0.53
2:I:761:PHE:HA	2:I:785:VAL:HA	1.90	0.53
1:A:53:VAL:HA	1:A:144:VAL:HG22	1.90	0.53
3:D:97:THR:HG21	3:D:571:LYS:HG2	1.90	0.53
4:E:41:GLU:O	4:E:45:ARG:HG2	2.09	0.53
2:I:126:SER:HB3	2:I:407:LYS:HZ1	1.72	0.53
2:I:146:VAL:HG12	2:I:162:ILE:HG12	1.90	0.53
2:I:154:ARG:HG2	2:I:156:GLY:N	2.23	0.53
3:J:441:ARG:HB3	3:J:443:VAL:HG12	1.90	0.53
3:D:416:ALA:HB3	3:D:419:ASP:CG	2.33	0.53
3:D:1078:ARG:HH11	3:D:1078:ARG:HB3	1.74	0.53
1:H:22:GLU:HG2	1:H:198:ARG:HG2	1.91	0.53
5:F:228:ILE:O	5:F:232:ASN:ND2	2.42	0.53
5:F:377:SER:HB3	5:F:380:GLU:HG2	1.91	0.53
1:H:27:PRO:HB3	1:H:192:LEU:HD23	1.90	0.53
5:L:228:ILE:O	5:L:232:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:142:ARG:HB2	2:I:142:ARG:HH11	1.74	0.53
2:I:1087:VAL:HG13	3:J:524:LEU:HD22	1.90	0.53
3:J:858:LEU:HD21	3:J:864:VAL:HG11	1.91	0.53
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.90	0.52
3:D:764:LEU:HG	3:D:766:ALA:H	1.74	0.52
1:G:174:VAL:HG21	1:G:177:VAL:HG23	1.91	0.52
3:J:625:TYR:HE2	3:J:655:PRO:HG2	1.75	0.52
3:J:1078:ARG:HH11	3:J:1078:ARG:HB3	1.74	0.52
1:A:174:VAL:HA	1:A:201:THR:HG22	1.90	0.52
2:C:194:VAL:HG11	2:C:223:ASP:HB3	1.91	0.52
1:A:174:VAL:HG21	1:A:177:VAL:HG23	1.91	0.52
2:C:20:GLU:OE1	2:C:460:ARG:NH1	2.43	0.52
2:C:154:ARG:HG2	2:C:156:GLY:N	2.23	0.52
2:C:761:PHE:HA	2:C:785:VAL:HA	1.91	0.52
5:F:379:ARG:NH2	5:F:411:ARG:HH21	2.07	0.52
5:F:410:GLU:OE2	5:F:413:ARG:NH1	2.42	0.52
1:A:53:VAL:HG23	1:A:144:VAL:HG22	1.91	0.52
1:B:20:TYR:HD1	1:B:21:GLY:N	2.07	0.52
1:B:27:PRO:HB3	1:B:192:LEU:HD23	1.90	0.52
2:C:1087:VAL:HG13	3:D:524:LEU:HD22	1.90	0.52
3:D:1267:ARG:H	3:D:1267:ARG:NE	2.02	0.52
1:G:53:VAL:HG23	1:G:144:VAL:HG22	1.92	0.52
2:I:15:LEU:HD21	2:I:457:ALA:HB1	1.90	0.52
2:I:683:ASN:HB2	2:I:872:ASN:HB2	1.91	0.52
2:I:1101:THR:HG22	3:J:8:VAL:HG22	1.91	0.52
3:J:764:LEU:HG	3:J:766:ALA:H	1.74	0.52
3:J:804:MET:H	3:J:827:ILE:HG22	1.74	0.52
5:L:252:THR:HG23	6:R:29:DC:H41	1.74	0.52
2:C:146:VAL:HG12	2:C:162:ILE:HG12	1.90	0.52
3:D:65:ARG:HG3	3:D:66:GLN:H	1.74	0.52
4:E:41:GLU:HB3	4:E:42:PRO:HD2	1.91	0.52
3:J:792:ILE:HG21	3:J:941:LEU:HD22	1.90	0.52
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.91	0.52
2:C:162:ILE:HB	2:C:172:ILE:HB	1.92	0.52
2:I:20:GLU:OE1	2:I:460:ARG:NH1	2.43	0.52
3:J:169:TYR:HB3	3:J:195:VAL:HG21	1.92	0.52
3:J:1232:PRO:HB2	3:J:1356:TYR:HE2	1.75	0.52
5:L:376:LEU:HB2	5:L:381:ALA:HB2	1.92	0.52
7:S:16:DG:H3'	7:S:17:DG:H8	1.74	0.52
1:B:218:LEU:O	1:B:222:LEU:HG	2.10	0.52
2:C:142:ARG:HH11	2:C:142:ARG:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:683:ASN:HB2	2:C:872:ASN:HB2	1.91	0.52
3:D:660:LYS:HD3	3:D:694:VAL:HG13	1.92	0.52
3:D:668:PRO:HB2	5:F:432:LYS:HD3	1.92	0.52
3:D:953:ASP:OD1	3:D:953:ASP:N	2.43	0.52
2:C:15:LEU:HD21	2:C:457:ALA:HB1	1.90	0.52
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.91	0.52
3:D:858:LEU:HD21	3:D:864:VAL:HG11	1.91	0.52
5:F:260:GLN:HB3	6:O:25:DT:O4	2.09	0.52
1:G:175:ARG:N	1:G:200:TRP:O	2.42	0.52
3:J:1434:TRP:HB3	3:J:1455:LYS:HD2	1.91	0.52
4:K:41:GLU:HB3	4:K:42:PRO:HD2	1.91	0.52
5:L:103:ILE:HD13	5:L:211:VAL:HG21	1.92	0.52
3:D:804:MET:H	3:D:827:ILE:HG22	1.74	0.52
1:G:13:ALA:HB3	1:H:228:PRO:HB3	1.92	0.52
1:G:90:LEU:HB2	1:G:119:ASP:HA	1.92	0.52
2:I:323:ASP:HB2	2:I:330:ASN:HD21	1.75	0.52
2:I:710:ILE:HB	2:I:790:LEU:HD22	1.91	0.52
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.92	0.52
5:L:257:TRP:O	5:L:260:GLN:HG3	2.10	0.52
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.92	0.52
2:C:1101:THR:HG22	3:D:8:VAL:HG22	1.91	0.52
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.92	0.52
1:G:53:VAL:HA	1:G:144:VAL:HG22	1.90	0.52
1:H:44:LEU:HA	1:H:48:ILE:HD13	1.91	0.52
2:I:162:ILE:HB	2:I:172:ILE:HB	1.92	0.52
5:L:383:VAL:HG13	5:L:401:VAL:HG11	1.92	0.52
7:P:16:DG:H3'	7:P:17:DG:H8	1.75	0.52
1:A:90:LEU:HB2	1:A:119:ASP:HA	1.92	0.51
3:D:272:LEU:O	3:D:279:VAL:N	2.43	0.51
5:F:385:LYS:HB2	5:F:390:LEU:HB2	1.92	0.51
1:H:218:LEU:HD23	1:H:222:LEU:HD11	1.92	0.51
2:I:711:GLU:HG2	2:I:822:VAL:HG12	1.91	0.51
3:J:67:ARG:HD3	5:L:394:ARG:HD3	1.91	0.51
3:J:371:ILE:HG12	5:L:247:ARG:HD3	1.92	0.51
5:L:228:ILE:HG22	5:L:232:ASN:HD21	1.75	0.51
5:L:377:SER:HB3	5:L:380:GLU:HG2	1.91	0.51
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.91	0.51
1:B:55:SER:HB2	1:B:158:ILE:HG23	1.92	0.51
2:C:128:ILE:HG13	2:C:133:ASP:HB3	1.92	0.51
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.91	0.51
2:C:713:ARG:HA	2:C:819:VAL:HA	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.92	0.51
1:H:20:TYR:HD1	1:H:21:GLY:N	2.08	0.51
3:J:660:LYS:HD3	3:J:694:VAL:HG13	1.91	0.51
3:J:775:GLY:HA2	3:J:1209:LEU:HB3	1.92	0.51
3:J:1379:VAL:HG21	3:J:1400:VAL:HG11	1.93	0.51
2:C:113:VAL:HG21	2:C:373:VAL:HG21	1.92	0.51
1:H:55:SER:HB2	1:H:158:ILE:HG23	1.92	0.51
3:J:210:ARG:HB2	3:J:389:GLU:HB2	1.93	0.51
1:B:218:LEU:HD23	1:B:222:LEU:HD11	1.92	0.51
2:C:36:PRO:HA	2:C:39:ARG:HD2	1.93	0.51
3:D:625:TYR:HE2	3:D:655:PRO:HG2	1.75	0.51
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.92	0.51
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.93	0.51
5:F:103:ILE:HD13	5:F:211:VAL:HG21	1.92	0.51
5:F:383:VAL:HG13	5:F:401:VAL:HG11	1.92	0.51
3:J:95:LEU:HG	3:J:574:LEU:HD21	1.92	0.51
5:F:376:LEU:HB2	5:F:381:ALA:HB2	1.92	0.51
1:H:101:LEU:HD23	1:H:114:PHE:HA	1.93	0.51
1:H:218:LEU:O	1:H:222:LEU:HG	2.10	0.51
3:J:895:VAL:O	3:J:899:LEU:HG	2.09	0.51
3:J:1087:ARG:HH12	3:J:1236:LEU:H	1.59	0.51
4:K:79:LEU:HG	4:K:80:VAL:HG13	1.93	0.51
5:L:132:SER:OG	5:L:137:LEU:O	2.27	0.51
1:B:101:LEU:HD23	1:B:114:PHE:HA	1.93	0.51
3:D:82:ARG:HG2	3:D:84:ILE:H	1.75	0.51
3:D:704:ARG:HD3	3:D:738:ALA:HB2	1.93	0.51
3:D:868:TYR:HE2	3:D:897:GLN:HG3	1.75	0.51
2:I:197:LEU:HA	2:I:200:LEU:HB2	1.93	0.51
2:I:326:ASP:HA	2:I:331:ARG:HD2	1.93	0.51
3:J:868:TYR:HE2	3:J:897:GLN:HG3	1.75	0.51
5:L:385:LYS:HB2	5:L:390:LEU:HB2	1.92	0.51
1:A:175:ARG:N	1:A:200:TRP:O	2.42	0.51
2:C:326:ASP:HA	2:C:331:ARG:HD2	1.93	0.51
2:C:762:LYS:HD3	2:C:786:LYS:HD3	1.92	0.51
3:D:371:ILE:HG23	3:D:372:ASP:H	1.75	0.51
3:D:1117:TYR:HA	3:D:1193:THR:HG21	1.91	0.51
3:J:420:VAL:HG21	3:J:424:GLY:HA2	1.91	0.51
3:J:953:ASP:N	3:J:953:ASP:OD1	2.43	0.51
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.93	0.51
2:C:197:LEU:HA	2:C:200:LEU:HB2	1.93	0.51
3:D:95:LEU:HG	3:D:574:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:36:PRO:HA	2:I:39:ARG:HD2	1.93	0.51
2:I:374:ASN:OD1	2:I:375:SER:N	2.43	0.51
1:A:190:THR:OG1	1:A:191:ASP:N	2.43	0.50
3:D:1434:TRP:HB3	3:D:1455:LYS:HD2	1.91	0.50
4:E:79:LEU:HG	4:E:80:VAL:HG13	1.93	0.50
2:I:18:LEU:HD12	2:I:408:ARG:NE	2.26	0.50
2:I:113:VAL:HG21	2:I:373:VAL:HG21	1.92	0.50
2:I:168:ARG:O	2:I:267:TYR:HA	2.10	0.50
3:J:568:ARG:HA	3:J:571:LYS:HD2	1.93	0.50
3:J:900:ILE:HG12	3:J:914:LEU:HD21	1.93	0.50
1:A:13:ALA:HB3	1:B:228:PRO:HB3	1.93	0.50
3:D:1087:ARG:HH12	3:D:1236:LEU:H	1.59	0.50
3:D:1232:PRO:HB2	3:D:1356:TYR:HE2	1.75	0.50
2:I:428:ARG:O	3:J:1078:ARG:NH1	2.44	0.50
2:I:726:ILE:HG21	2:I:729:LEU:HD23	1.92	0.50
2:C:726:ILE:HG21	2:C:729:LEU:HD23	1.92	0.50
2:I:872:ASN:HD21	2:I:874:LEU:HD12	1.76	0.50
2:I:1051:GLU:HB3	2:I:1056:LYS:HD3	1.93	0.50
3:J:12:LEU:HD21	3:J:1452:ILE:HD13	1.94	0.50
3:J:99:ALA:O	3:J:514:LEU:N	2.43	0.50
3:J:970:LYS:HG2	3:J:995:LEU:HD13	1.93	0.50
2:C:627:ARG:HD3	2:C:639:GLN:O	2.12	0.50
2:C:638:ASP:H	2:C:659:PRO:HG3	1.77	0.50
2:C:872:ASN:HD21	2:C:874:LEU:HD12	1.76	0.50
2:C:1051:GLU:HB3	2:C:1056:LYS:HD3	1.93	0.50
5:F:145:VAL:HG21	5:F:174:VAL:HG11	1.94	0.50
2:I:638:ASP:H	2:I:659:PRO:HG3	1.77	0.50
3:J:553:ARG:NH2	5:L:226:ASP:OD1	2.36	0.50
3:J:628:ARG:HB3	3:J:746:ALA:HA	1.94	0.50
6:O:42:DC:H2''	6:O:43:DG:H8	1.76	0.50
6:R:42:DC:H2''	6:R:43:DG:H8	1.76	0.50
3:D:99:ALA:O	3:D:514:LEU:N	2.43	0.50
2:I:87:ASP:HA	2:I:131:GLY:HA3	1.92	0.50
2:I:219:GLN:HA	2:I:222:LEU:HD12	1.94	0.50
3:J:704:ARG:HD3	3:J:738:ALA:HB2	1.93	0.50
6:O:33:DG:H2''	6:O:34:DA:C8	2.47	0.50
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.93	0.50
1:A:111:ALA:HB1	1:A:122:ILE:HD13	1.93	0.50
2:C:97:ARG:HD2	2:C:112:GLU:HG3	1.93	0.50
1:G:83:LYS:HE3	1:G:168:ASP:HB2	1.93	0.50
6:R:33:DG:H2''	6:R:34:DA:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1094:ALA:HB2	3:D:520:LEU:HD13	1.93	0.50
3:D:628:ARG:HB3	3:D:746:ALA:HA	1.94	0.50
3:D:1472:ILE:HG12	3:D:1474:ALA:H	1.77	0.50
2:I:150:PRO:HD3	2:I:322:VAL:HG11	1.93	0.50
2:I:939:ARG:HB3	2:I:982:PRO:HG3	1.92	0.50
3:J:1117:TYR:HA	3:J:1193:THR:HG21	1.92	0.50
5:L:145:VAL:HG21	5:L:174:VAL:HG11	1.94	0.50
1:B:176:ARG:O	1:B:200:TRP:HE3	1.95	0.50
2:C:150:PRO:HA	2:C:158:TYR:HD2	1.77	0.50
2:C:168:ARG:O	2:C:267:TYR:HA	2.10	0.50
5:L:97:ARG:HH22	6:R:33:DG:N2	2.10	0.50
2:C:428:ARG:O	3:D:1078:ARG:NH1	2.44	0.50
3:D:908:LYS:HE3	3:D:908:LYS:C	2.36	0.50
2:I:1094:ALA:HB2	3:J:520:LEU:HD13	1.93	0.50
2:C:834:GLN:HG2	2:C:835:VAL:H	1.75	0.49
3:D:12:LEU:HD21	3:D:1452:ILE:HD13	1.94	0.49
3:D:640:HIS:O	3:D:717:GLN:N	2.32	0.49
3:D:900:ILE:HG12	3:D:914:LEU:HD21	1.93	0.49
3:D:1037:GLN:HG2	3:D:1042:ARG:HA	1.94	0.49
5:F:120:LYS:HE3	5:F:198:ALA:HB2	1.94	0.49
2:I:627:ARG:HD3	2:I:639:GLN:O	2.12	0.49
3:J:572:ARG:CZ	5:L:98:GLN:HG2	2.42	0.49
3:J:697:GLY:O	3:J:760:ARG:NH1	2.45	0.49
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.28	0.49
3:D:895:VAL:O	3:D:899:LEU:HG	2.11	0.49
5:F:228:ILE:HG22	5:F:232:ASN:HD21	1.75	0.49
1:G:111:ALA:HB1	1:G:122:ILE:HD13	1.93	0.49
3:J:34:TYR:OH	6:R:20:DT:OP2	2.25	0.49
3:J:1472:ILE:HG12	3:J:1474:ALA:H	1.77	0.49
3:D:568:ARG:HA	3:D:571:LYS:HD2	1.93	0.49
4:E:30:LEU:HD23	4:E:63:TRP:HB3	1.94	0.49
1:H:99:LEU:HB2	1:H:142:VAL:HG22	1.95	0.49
3:J:185:VAL:HG12	3:J:186:VAL:H	1.77	0.49
4:K:30:LEU:HD23	4:K:63:TRP:HB3	1.93	0.49
5:L:336:ILE:HB	5:L:342:SER:HB3	1.93	0.49
2:C:18:LEU:HD12	2:C:408:ARG:NE	2.26	0.49
2:C:950:LEU:HD11	2:C:952:LEU:HB2	1.95	0.49
3:D:970:LYS:HG2	3:D:995:LEU:HD13	1.93	0.49
5:F:336:ILE:HB	5:F:342:SER:HB3	1.93	0.49
2:I:26:TYR:HE1	2:I:340:MET:HG3	1.77	0.49
3:J:1192:LEU:HD23	3:J:1373:ARG:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:HB2	1:B:142:VAL:HG22	1.94	0.49
2:C:630:ARG:NH1	2:C:706:GLU:HA	2.27	0.49
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.94	0.49
2:I:1095:LEU:HD11	3:J:603:LEU:HB3	1.95	0.49
3:J:67:ARG:HB2	5:L:392:ASP:O	2.12	0.49
2:C:219:GLN:HA	2:C:222:LEU:HD12	1.94	0.49
2:C:261:LEU:HB3	2:C:291:VAL:HG22	1.94	0.49
3:D:1192:LEU:HD23	3:D:1373:ARG:HB2	1.94	0.49
1:G:158:ILE:HG22	1:G:160:ASP:H	1.76	0.49
3:J:1281:VAL:HG21	3:J:1313:VAL:HG11	1.95	0.49
5:L:210:VAL:HA	5:L:213:ILE:HD12	1.95	0.49
5:L:238:ALA:HB2	5:L:257:TRP:HB2	1.94	0.49
2:C:167:LYS:H	6:O:37:DT:H73	1.78	0.49
2:C:480:THR:HG22	2:C:482:GLU:H	1.77	0.49
3:D:572:ARG:CZ	5:F:98:GLN:HG2	2.42	0.49
3:D:1057:VAL:HA	3:D:1069:GLU:HG2	1.95	0.49
3:D:1281:VAL:HG21	3:D:1313:VAL:HG11	1.95	0.49
2:I:97:ARG:HD2	2:I:112:GLU:HG3	1.93	0.49
2:I:150:PRO:HA	2:I:158:TYR:HD2	1.77	0.49
2:I:950:LEU:HD11	2:I:952:LEU:HB2	1.95	0.49
3:J:1386:ASP:OD2	3:J:1413:VAL:N	2.45	0.49
2:C:605:LYS:HG2	2:C:612:ALA:HB3	1.95	0.49
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.77	0.49
2:C:1056:LYS:O	3:D:624:ASP:N	2.37	0.49
3:D:423:ASP:OD2	3:D:423:ASP:N	2.44	0.49
3:D:697:GLY:O	3:D:760:ARG:NH1	2.45	0.49
1:H:51:THR:HG21	1:H:86:VAL:HG23	1.94	0.49
2:C:303:PHE:HA	2:C:306:THR:HG22	1.95	0.49
2:C:397:GLU:HB3	2:C:631:SER:HB2	1.95	0.49
3:D:351:MET:HG3	3:D:370:ALA:HB2	1.94	0.49
3:D:708:LEU:HD12	3:D:1231:GLU:HA	1.95	0.49
3:D:1106:VAL:HA	3:D:1220:ALA:HA	1.95	0.49
5:F:210:VAL:HA	5:F:213:ILE:HD12	1.94	0.49
2:I:93:PRO:HB3	2:I:114:PHE:HE2	1.78	0.49
2:I:303:PHE:HA	2:I:306:THR:HG22	1.95	0.49
2:I:420:ARG:NH2	8:T:1:U:OP2	2.46	0.49
2:I:678:PRO:HA	2:I:683:ASN:HD21	1.77	0.49
2:I:834:GLN:HG2	2:I:835:VAL:H	1.76	0.49
3:J:203:ALA:HA	3:J:395:VAL:HA	1.95	0.49
3:J:644:LEU:HG	3:J:649:ALA:HB2	1.95	0.49
1:B:97:THR:HG21	1:B:120:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:231:VAL:H	3:D:243:ALA:HA	1.78	0.49
2:I:261:LEU:HB3	2:I:291:VAL:HG22	1.95	0.49
2:I:537:LYS:NZ	2:I:904:PRO:HB3	2.28	0.49
3:D:56:TYR:O	3:D:80:VAL:HG23	2.13	0.48
3:D:417:PRO:HA	3:D:430:GLU:HA	1.95	0.48
3:D:644:LEU:HG	3:D:649:ALA:HB2	1.95	0.48
2:I:324:ASP:O	2:I:330:ASN:ND2	2.42	0.48
2:I:480:THR:HG22	2:I:482:GLU:H	1.77	0.48
3:J:108:VAL:HB	3:J:109:PRO:HD3	1.94	0.48
3:J:1020:LEU:HG	3:J:1035:ILE:HD12	1.95	0.48
3:J:1037:GLN:HG2	3:J:1042:ARG:HA	1.94	0.48
3:J:1099:VAL:O	3:J:1103:HIS:HB3	2.13	0.48
1:A:170:ILE:HG23	2:C:696:LYS:HD2	1.94	0.48
2:C:39:ARG:HD3	2:C:45:GLN:HE22	1.79	0.48
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.27	0.48
3:D:116:LEU:HD11	3:D:465:LEU:HG	1.94	0.48
3:D:596:SER:OG	3:D:598:ARG:NH1	2.47	0.48
3:D:1386:ASP:OD2	3:D:1413:VAL:N	2.45	0.48
2:I:397:GLU:HB3	2:I:631:SER:HB2	1.95	0.48
2:I:418:LEU:HA	2:I:422:ARG:HE	1.78	0.48
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.48	0.48
5:L:411:ARG:HD3	6:R:1:DC:C6	2.48	0.48
2:C:26:TYR:HE1	2:C:340:MET:HG3	1.78	0.48
3:D:286:ALA:O	3:D:311:LEU:HA	2.14	0.48
3:D:796:ARG:HG2	3:D:1017:PHE:CE1	2.49	0.48
4:E:14:ASP:OD1	4:E:14:ASP:N	2.40	0.48
1:H:74:ASP:O	1:H:78:ILE:HG12	2.14	0.48
2:I:259:GLY:HA2	2:I:263:ASP:HB2	1.95	0.48
2:I:605:LYS:HG2	2:I:612:ALA:HB3	1.95	0.48
2:I:607:ASP:HB3	2:I:610:ARG:O	2.13	0.48
3:J:361:VAL:HG21	3:J:367:ILE:HD11	1.96	0.48
2:C:537:LYS:NZ	2:C:904:PRO:HB3	2.28	0.48
3:J:62:LYS:HG3	3:J:63:TYR:N	2.28	0.48
2:C:113:VAL:HB	5:F:295:GLN:HE22	1.77	0.48
2:C:607:ASP:HB3	2:C:610:ARG:O	2.13	0.48
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.95	0.48
3:D:222:ALA:HB1	3:D:332:HIS:HE1	1.78	0.48
5:F:238:ALA:HB2	5:F:257:TRP:HB2	1.94	0.48
1:B:161:ARG:HG3	1:B:162:ILE:H	1.78	0.48
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.94	0.48
2:C:1031:ARG:HD3	7:P:13:DC:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:39:ARG:HD3	2:I:45:GLN:HE22	1.79	0.48
2:I:113:VAL:HB	5:L:295:GLN:HE22	1.79	0.48
3:J:116:LEU:HD11	3:J:465:LEU:HG	1.94	0.48
3:J:127:LEU:HD23	3:J:458:ALA:HA	1.95	0.48
3:J:708:LEU:HD12	3:J:1231:GLU:HA	1.95	0.48
3:J:796:ARG:HG2	3:J:1017:PHE:CE1	2.49	0.48
3:J:1057:VAL:HA	3:J:1069:GLU:HG2	1.95	0.48
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.95	0.48
2:C:418:LEU:HA	2:C:422:ARG:HE	1.79	0.48
2:C:1090:LYS:HE3	3:D:90:MET:HE2	1.95	0.48
3:D:216:LEU:HD23	3:D:218:LYS:HZ1	1.79	0.48
3:D:1020:LEU:HG	3:D:1035:ILE:HD12	1.95	0.48
5:L:146:VAL:HG11	5:L:196:GLU:HG3	1.96	0.48
6:R:29:DC:H5'	6:R:30:DT:H71	1.96	0.48
1:B:51:THR:HG21	1:B:86:VAL:HG23	1.94	0.48
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.49	0.48
3:D:367:ILE:HD11	3:D:379:ALA:HB2	1.96	0.48
3:D:704:ARG:NE	3:D:705:ALA:O	2.47	0.48
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.13	0.48
1:H:97:THR:HG21	1:H:120:VAL:HG21	1.94	0.48
2:I:541:SER:O	2:I:545:ASN:HB2	2.14	0.48
3:J:56:TYR:O	3:J:80:VAL:HG23	2.13	0.48
3:J:691:LEU:HD23	3:J:720:LEU:HD11	1.96	0.48
3:J:704:ARG:NE	3:J:705:ALA:O	2.46	0.48
1:A:158:ILE:HG22	1:A:160:ASP:H	1.76	0.48
1:A:180:GLN:NE2	2:C:935:GLY:O	2.44	0.48
1:B:162:ILE:HG23	1:B:163:ASN:H	1.79	0.48
5:F:217:TYR:HB3	5:F:227:LEU:HD21	1.96	0.48
5:F:254:ALA:O	5:F:258:ILE:HG12	2.14	0.48
1:H:161:ARG:HG3	1:H:162:ILE:H	1.78	0.48
2:I:751:PRO:HB3	2:I:794:PRO:HA	1.95	0.48
2:I:874:LEU:O	2:I:877:PRO:HD2	2.14	0.48
3:J:420:VAL:HG21	3:J:425:GLY:H	1.78	0.48
3:J:1060:SER:OG	3:J:1061:PHE:N	2.47	0.48
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	1.96	0.48
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.94	0.48
1:G:170:ILE:HG23	2:I:696:LYS:HD2	1.94	0.48
2:I:1016:ILE:HG13	2:I:1017:THR:H	1.79	0.48
7:S:16:DG:H3'	7:S:17:DG:C8	2.49	0.48
1:B:25:LEU:HD23	1:B:28:LEU:HD22	1.96	0.47
2:C:630:ARG:HG2	2:C:631:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:85:LEU:O	4:E:89:MET:HB2	2.14	0.47
1:H:25:LEU:HD23	1:H:28:LEU:HD22	1.96	0.47
1:H:80:LEU:HD23	3:J:867:ARG:HD3	1.96	0.47
2:I:136:ILE:HB	2:I:336:VAL:HG12	1.96	0.47
2:C:541:SER:O	2:C:545:ASN:HB2	2.14	0.47
2:C:952:LEU:HD21	2:C:971:LYS:HD2	1.96	0.47
3:D:639:LEU:HB3	3:D:640:HIS:H	1.55	0.47
3:D:691:LEU:HD23	3:D:720:LEU:HD11	1.96	0.47
2:I:952:LEU:HD21	2:I:971:LYS:HD2	1.97	0.47
5:L:120:LYS:HE3	5:L:198:ALA:HB2	1.94	0.47
5:L:254:ALA:O	5:L:258:ILE:HG12	2.14	0.47
1:A:74:ASP:OD2	2:C:640:ARG:NH1	2.48	0.47
1:B:52:ALA:HB3	1:B:171:PHE:CD1	2.49	0.47
2:C:1016:ILE:HG13	2:C:1017:THR:H	1.79	0.47
3:D:127:LEU:HD23	3:D:458:ALA:HA	1.95	0.47
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.96	0.47
5:F:146:VAL:HG11	5:F:196:GLU:HG3	1.96	0.47
1:H:52:ALA:HB3	1:H:171:PHE:CD1	2.50	0.47
3:J:1106:VAL:HA	3:J:1220:ALA:HA	1.95	0.47
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.74	0.47
3:D:62:LYS:HG3	3:D:63:TYR:N	2.30	0.47
2:I:118:LEU:HD12	2:I:119:PRO:HD2	1.97	0.47
3:J:101:HIS:ND1	3:J:103:TRP:HB2	2.28	0.47
3:J:1274:ILE:HG22	3:J:1324:PRO:HA	1.97	0.47
1:G:190:THR:OG1	1:G:191:ASP:N	2.43	0.47
2:I:42:VAL:HA	2:I:46:ALA:HB2	1.97	0.47
7:P:16:DG:H3'	7:P:17:DG:C8	2.50	0.47
7:P:20:DA:H4'	7:P:21:DA:OP1	2.15	0.47
1:B:74:ASP:O	1:B:78:ILE:HG12	2.14	0.47
1:B:80:LEU:HD23	3:D:867:ARG:HD3	1.95	0.47
2:C:93:PRO:HB3	2:C:114:PHE:HE2	1.78	0.47
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.96	0.47
2:C:189:ARG:NH1	2:C:242:LEU:HB2	2.30	0.47
2:C:374:ASN:OD1	2:C:375:SER:N	2.46	0.47
3:D:1060:SER:OG	3:D:1061:PHE:N	2.47	0.47
3:D:1492:LEU:O	3:D:1496:GLU:HB2	2.15	0.47
3:J:477:LEU:HA	3:J:480:GLU:HB2	1.96	0.47
2:C:136:ILE:HB	2:C:336:VAL:HG12	1.96	0.47
2:C:689:VAL:HG23	2:C:869:VAL:O	2.15	0.47
2:C:715:THR:OG1	2:C:718:GLY:O	2.21	0.47
3:D:64:LYS:H	3:D:68:PHE:HE2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:310:LEU:HD23	3:D:312:ARG:NH2	2.29	0.47
3:D:477:LEU:HA	3:D:480:GLU:HB2	1.96	0.47
3:D:860:LEU:HD12	3:D:860:LEU:H	1.79	0.47
3:D:1090:ASP:O	3:D:1093:TYR:HB3	2.15	0.47
1:G:74:ASP:OD2	2:I:640:ARG:NH1	2.48	0.47
1:H:162:ILE:HG23	1:H:163:ASN:H	1.79	0.47
2:I:189:ARG:NH1	2:I:242:LEU:HB2	2.29	0.47
3:J:351:MET:HA	3:J:370:ALA:HA	1.97	0.47
3:J:573:MET:SD	5:L:229:GLN:HG3	2.55	0.47
3:J:633:VAL:C	3:J:635:PRO:HD3	2.40	0.47
3:J:860:LEU:H	3:J:860:LEU:HD12	1.79	0.47
3:J:1090:ASP:O	3:J:1093:TYR:HB3	2.15	0.47
2:I:258:PHE:HB2	2:I:298:PHE:HZ	1.80	0.47
3:J:614:PHE:HA	3:J:618:LEU:HB2	1.96	0.47
2:C:258:PHE:HB2	2:C:298:PHE:HZ	1.80	0.47
3:D:238:PRO:HB3	3:D:315:ARG:O	2.14	0.47
4:E:8:LYS:O	4:E:12:MET:HG3	2.15	0.47
3:J:596:SER:OG	3:J:598:ARG:NH1	2.47	0.47
3:J:634:GLY:O	3:J:637:LEU:HB2	2.15	0.47
3:J:667:ALA:HB1	3:J:672:ALA:HB3	1.97	0.47
3:J:1087:ARG:NH1	3:J:1236:LEU:H	2.13	0.47
4:K:85:LEU:O	4:K:89:MET:HB2	2.14	0.47
5:L:154:ALA:O	5:L:158:LYS:HB2	2.15	0.47
5:L:217:TYR:HB3	5:L:227:LEU:HD21	1.95	0.47
5:L:269:GLN:HE21	5:L:269:GLN:HB2	1.50	0.47
2:C:425:PHE:O	2:C:429:ASP:HB2	2.15	0.47
3:D:343:LYS:HZ2	3:D:344:ASP:H	1.62	0.47
3:D:838:ARG:O	3:D:865:THR:OG1	2.32	0.47
5:F:132:SER:OG	5:F:137:LEU:O	2.28	0.47
3:J:554:LEU:O	3:J:558:LEU:HB2	2.15	0.47
1:A:42:ARG:NH1	2:C:977:GLY:O	2.47	0.46
2:C:176:VAL:HA	2:C:182:VAL:HG23	1.97	0.46
2:C:806:LEU:HB2	2:C:822:VAL:HG23	1.97	0.46
3:D:633:VAL:C	3:D:635:PRO:HD3	2.40	0.46
3:D:667:ALA:HB1	3:D:672:ALA:HB3	1.97	0.46
3:D:675:ARG:HH12	5:F:437:LEU:HG	1.80	0.46
5:F:291:ARG:HD3	7:P:23:DA:N3	2.31	0.46
1:G:48:ILE:HG22	1:G:173:PRO:HD2	1.98	0.46
1:H:100:ILE:O	1:H:115:THR:HB	2.15	0.46
2:I:689:VAL:HG23	2:I:869:VAL:O	2.15	0.46
2:I:1094:ALA:HA	3:J:518:PRO:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1094:ALA:HA	3:D:518:PRO:HB2	1.96	0.46
3:D:638:LYS:HG2	3:D:932:ASP:CG	2.41	0.46
5:F:154:ALA:O	5:F:158:LYS:HB2	2.15	0.46
1:G:40:LEU:O	1:G:44:LEU:HB2	2.15	0.46
2:I:740:GLU:HG3	2:I:742:ILE:HG13	1.98	0.46
3:J:132:TYR:HA	3:J:456:MET:HB3	1.98	0.46
3:J:628:ARG:NH2	3:J:744:GLN:OE1	2.49	0.46
3:J:638:LYS:HG2	3:J:932:ASP:CG	2.41	0.46
3:J:1335:LEU:HA	3:J:1338:ALA:HB3	1.98	0.46
4:K:8:LYS:O	4:K:12:MET:HG3	2.15	0.46
6:O:29:DC:H5'	6:O:30:DT:H71	1.96	0.46
1:A:40:LEU:O	1:A:44:LEU:HB2	2.15	0.46
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.98	0.46
3:D:122:GLU:O	3:D:126:VAL:HG23	2.15	0.46
3:D:247:GLU:O	3:D:249:TYR:N	2.47	0.46
3:D:260:GLU:HA	3:D:294:GLU:HG3	1.96	0.46
5:F:149:LYS:HD3	5:F:193:ARG:HH22	1.80	0.46
1:G:42:ARG:NH1	2:I:977:GLY:O	2.47	0.46
2:I:716:LYS:HE2	3:J:37:LEU:HD11	1.98	0.46
5:L:149:LYS:HD3	5:L:193:ARG:HH22	1.80	0.46
2:C:630:ARG:NH1	2:C:705:ILE:O	2.47	0.46
2:C:740:GLU:HG3	2:C:742:ILE:HG13	1.98	0.46
3:D:223:LEU:HD11	3:D:288:MET:HE1	1.96	0.46
3:D:226:PRO:HA	3:D:330:SER:HA	1.98	0.46
3:D:230:TRP:CH2	3:D:333:LEU:HD21	2.50	0.46
3:D:573:MET:SD	5:F:229:GLN:HG3	2.55	0.46
1:G:180:GLN:NE2	2:I:935:GLY:O	2.44	0.46
2:I:544:THR:HA	2:I:547:ILE:HD12	1.98	0.46
3:J:573:MET:HA	3:J:576:GLU:HG2	1.97	0.46
5:L:319:VAL:O	5:L:323:LEU:HB2	2.15	0.46
6:O:39:DT:H2''	6:O:40:DC:H5'	1.97	0.46
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.96	0.46
3:D:634:GLY:O	3:D:637:LEU:HB2	2.16	0.46
3:D:1087:ARG:NH1	3:D:1236:LEU:H	2.13	0.46
2:I:168:ARG:NH1	2:I:265:LYS:O	2.49	0.46
2:I:176:VAL:HA	2:I:182:VAL:HG23	1.97	0.46
2:I:238:LEU:HD23	2:I:241:LEU:HD12	1.96	0.46
2:I:1090:LYS:HE3	3:J:90:MET:HE2	1.95	0.46
3:J:540:LEU:HA	3:J:543:LEU:HD12	1.98	0.46
3:J:1492:LEU:O	3:J:1496:GLU:HB2	2.15	0.46
1:A:35:THR:HG23	1:B:39:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:856:GLU:H	2:C:856:GLU:HG3	1.59	0.46
3:D:554:LEU:O	3:D:558:LEU:HB2	2.16	0.46
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.48	0.46
3:D:976:GLN:HG2	3:J:807:ALA:HA	1.97	0.46
3:D:1335:LEU:HA	3:D:1338:ALA:HB3	1.98	0.46
3:D:1435:LEU:HB3	3:D:1467:ILE:HD12	1.98	0.46
4:E:66:LYS:HA	4:E:69:LEU:HD12	1.96	0.46
5:F:166:PRO:HG2	5:F:169:LYS:HZ1	1.80	0.46
2:I:1008:ARG:NH1	2:I:1020:PRO:HB3	2.31	0.46
3:J:796:ARG:NH2	3:J:859:ASP:OD2	2.48	0.46
1:A:133:GLU:OE2	2:C:605:LYS:HB2	2.16	0.46
2:C:544:THR:HA	2:C:547:ILE:HD12	1.98	0.46
3:D:540:LEU:HA	3:D:543:LEU:HD12	1.98	0.46
3:D:573:MET:HA	3:D:576:GLU:HG2	1.97	0.46
3:D:1158:ARG:HG3	3:D:1158:ARG:NH1	2.22	0.46
5:F:319:VAL:O	5:F:323:LEU:HB2	2.15	0.46
1:G:39:PRO:CG	1:H:39:PRO:HG3	2.46	0.46
2:I:351:LEU:HB2	2:I:377:PRO:HB2	1.98	0.46
2:I:425:PHE:O	2:I:429:ASP:HB2	2.15	0.46
3:J:1442:ASN:N	7:S:9:DG:OP1	2.43	0.46
4:K:66:LYS:HA	4:K:69:LEU:HD12	1.96	0.46
1:B:100:ILE:O	1:B:115:THR:HB	2.15	0.46
3:D:216:LEU:HD13	3:D:383:GLY:HA2	1.98	0.46
3:D:614:PHE:HA	3:D:618:LEU:HB2	1.96	0.46
1:G:35:THR:HG23	1:H:39:PRO:HA	1.98	0.46
1:G:72:LYS:HB2	2:I:606:VAL:HG11	1.97	0.46
2:I:307:LEU:HD12	2:I:307:LEU:HA	1.84	0.46
2:I:630:ARG:HG2	2:I:631:SER:H	1.81	0.46
3:J:544:TYR:O	3:J:548:ILE:HG13	2.16	0.46
5:L:266:ILE:HG13	5:L:267:ALA:N	2.31	0.46
2:I:181:VAL:HG22	2:I:182:VAL:H	1.81	0.46
3:J:353:VAL:HG21	3:J:387:LEU:HD11	1.98	0.46
3:J:371:ILE:HG23	3:J:372:ASP:H	1.81	0.46
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.46	0.46
1:B:23:PHE:HE2	1:B:199:ILE:HD12	1.80	0.46
2:C:70:GLU:HG2	2:C:97:ARG:HB3	1.98	0.46
2:C:181:VAL:HG22	2:C:182:VAL:H	1.81	0.46
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.97	0.46
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.51	0.46
2:I:856:GLU:H	2:I:856:GLU:HG3	1.59	0.46
2:I:1056:LYS:O	3:J:624:ASP:N	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:168:ARG:NH1	2:C:265:LYS:O	2.48	0.45
2:C:238:LEU:HD23	2:C:241:LEU:HD12	1.96	0.45
2:C:324:ASP:O	2:C:330:ASN:ND2	2.44	0.45
2:C:430:VAL:HG23	3:D:1075:HIS:HD2	1.81	0.45
5:F:266:ILE:HG13	5:F:267:ALA:N	2.31	0.45
5:F:427:GLU:OE1	5:F:433:LEU:HB2	2.16	0.45
2:I:70:GLU:HG2	2:I:97:ARG:HB3	1.98	0.45
2:I:806:LEU:HB2	2:I:822:VAL:HG23	1.97	0.45
3:J:1165:TYR:HB3	3:J:1207:TYR:HE1	1.81	0.45
3:J:1311:LEU:HD23	3:J:1311:LEU:H	1.81	0.45
2:C:126:SER:HB3	2:C:407:LYS:NZ	2.31	0.45
2:C:764:GLU:HB2	2:C:765:GLN:H	1.54	0.45
3:D:165:LYS:H	3:D:397:LYS:HZ1	1.64	0.45
3:D:245:LEU:HD23	3:D:245:LEU:HA	1.77	0.45
3:D:1087:ARG:NH2	3:D:1237:THR:OG1	2.48	0.45
2:I:326:ASP:OD1	6:R:38:DG:N2	2.48	0.45
3:J:1344:VAL:O	3:J:1348:LEU:HG	2.15	0.45
6:R:39:DT:H2''	6:R:40:DC:H5'	1.97	0.45
2:C:431:HIS:H	2:C:434:HIS:CE1	2.34	0.45
3:D:266:GLU:HG3	3:D:286:ALA:HB2	1.98	0.45
3:D:654:LYS:O	3:D:658:LEU:HD23	2.16	0.45
3:D:1048:PRO:HD3	3:D:1075:HIS:HB3	1.99	0.45
3:D:1068:LEU:HD12	3:D:1068:LEU:H	1.81	0.45
3:D:1165:TYR:HB3	3:D:1207:TYR:HE1	1.80	0.45
1:G:111:ALA:HB1	1:G:122:ILE:HG21	1.99	0.45
2:I:660:ALA:O	2:I:667:ALA:N	2.33	0.45
3:J:34:TYR:HD1	5:L:325:ILE:HG21	1.82	0.45
3:J:192:ALA:HB3	3:J:195:VAL:HG12	1.97	0.45
3:J:1068:LEU:HD12	3:J:1068:LEU:H	1.81	0.45
1:A:72:LYS:HB2	2:C:606:VAL:HG11	1.97	0.45
3:D:221:ALA:HB3	3:D:337:LEU:HD12	1.98	0.45
3:D:1311:LEU:HD23	3:D:1311:LEU:H	1.81	0.45
1:H:23:PHE:HE2	1:H:199:ILE:HD12	1.81	0.45
1:H:176:ARG:O	1:H:200:TRP:HE3	1.98	0.45
3:J:122:GLU:O	3:J:126:VAL:HG23	2.15	0.45
3:J:128:TYR:OH	3:J:579:ASP:OD2	2.23	0.45
3:J:1364:HIS:CD2	3:J:1366:LYS:HE2	2.51	0.45
1:A:111:ALA:HB1	1:A:122:ILE:HG21	1.99	0.45
3:D:212:ARG:HG2	3:D:213:VAL:H	1.82	0.45
3:D:671:LYS:HG2	5:F:364:LEU:HD13	1.99	0.45
5:F:165:LYS:HA	5:F:166:PRO:HD3	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1087:ARG:NH2	3:J:1237:THR:OG1	2.49	0.45
3:D:544:TYR:O	3:D:548:ILE:HG13	2.16	0.45
3:D:760:ARG:HH22	4:E:62:THR:HG23	1.81	0.45
2:I:291:VAL:HB	2:I:299:LYS:O	2.16	0.45
2:I:764:GLU:H	2:I:764:GLU:HG2	1.33	0.45
3:J:1048:PRO:HD3	3:J:1075:HIS:HB3	1.99	0.45
2:C:15:LEU:HD13	2:C:16:PRO:HD2	1.99	0.45
2:C:291:VAL:HB	2:C:299:LYS:O	2.16	0.45
2:I:184:MET:N	2:I:191:PHE:O	2.48	0.45
2:I:815:LEU:HD11	2:I:822:VAL:HG22	1.98	0.45
3:J:441:ARG:HH12	3:J:445:ARG:NH1	2.15	0.45
3:J:571:LYS:NZ	5:L:155:ARG:HH22	2.15	0.45
3:J:643:GLY:HA3	3:J:727:GLN:HB2	1.97	0.45
2:C:607:ASP:O	2:C:610:ARG:N	2.50	0.45
2:C:1008:ARG:NH1	2:C:1020:PRO:HB3	2.31	0.45
5:F:209:LEU:HG	5:F:213:ILE:HD11	1.99	0.45
2:I:769:PRO:HG3	3:J:65:ARG:HH12	1.81	0.45
3:J:397:LYS:NZ	3:J:448:GLU:O	2.50	0.45
5:L:209:LEU:HG	5:L:213:ILE:HD11	1.99	0.45
2:C:1031:ARG:HB2	3:D:622:ARG:HG2	1.98	0.45
2:C:1063:ARG:HG3	5:F:356:PRO:HG3	1.99	0.45
3:D:1344:VAL:O	3:D:1348:LEU:HG	2.15	0.45
4:E:88:GLU:HB3	4:E:91:ARG:HH21	1.82	0.45
1:G:53:VAL:HA	1:G:144:VAL:HG13	1.98	0.45
1:G:97:THR:HG22	1:G:144:VAL:HB	1.99	0.45
1:G:133:GLU:OE2	2:I:605:LYS:HB2	2.16	0.45
2:I:430:VAL:HG23	3:J:1075:HIS:HD2	1.81	0.45
3:J:654:LYS:O	3:J:658:LEU:HD23	2.17	0.45
3:J:760:ARG:HH22	4:K:62:THR:HG23	1.81	0.45
2:C:80:GLN:CD	2:C:80:GLN:H	2.25	0.45
3:D:259:VAL:HG23	3:D:294:GLU:HA	1.99	0.45
3:D:543:LEU:HG	3:D:600:LEU:HD23	1.99	0.45
5:F:214:ALA:HB1	5:F:227:LEU:HD23	1.99	0.45
5:F:229:GLN:HA	5:F:232:ASN:HD22	1.81	0.45
2:I:857:ASP:OD2	2:I:857:ASP:N	2.47	0.45
3:J:64:LYS:H	3:J:68:PHE:HE2	1.63	0.45
3:J:1435:LEU:HB3	3:J:1467:ILE:HD12	1.99	0.45
1:B:75:VAL:O	1:B:79:ILE:HG13	2.17	0.44
1:B:216:ALA:O	1:B:220:GLU:HB2	2.17	0.44
2:C:688:ILE:HD12	2:C:839:LEU:HB2	1.99	0.44
5:F:291:ARG:HD3	7:P:23:DA:C2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:LEU:HD23	1:G:187:GLY:H	1.82	0.44
2:I:710:ILE:HD11	2:I:758:ARG:HE	1.82	0.44
2:I:1031:ARG:HB2	3:J:622:ARG:HG2	1.98	0.44
2:I:1059:ASP:O	2:I:1063:ARG:NH1	2.47	0.44
3:J:543:LEU:HG	3:J:600:LEU:HD23	1.99	0.44
5:L:160:PRO:HB2	5:L:164:GLU:HB2	1.99	0.44
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.99	0.44
2:C:470:PRO:HG3	2:C:485:TYR:CZ	2.52	0.44
2:C:607:ASP:O	2:C:609:THR:N	2.50	0.44
3:D:769:LEU:O	3:D:778:LEU:HB3	2.17	0.44
5:F:428:SER:HA	5:F:434:ARG:HH21	1.83	0.44
1:G:32:PHE:CZ	1:H:43:ILE:HG12	2.52	0.44
1:G:39:PRO:HG2	1:H:39:PRO:HG3	1.98	0.44
1:G:54:THR:O	1:G:167:VAL:HG22	2.18	0.44
1:H:77:GLU:O	1:H:81:ASN:ND2	2.48	0.44
2:I:15:LEU:HD13	2:I:16:PRO:HD2	1.99	0.44
2:I:207:LEU:HD22	2:I:221:LEU:HD21	1.99	0.44
2:I:604:VAL:HG23	2:I:605:LYS:HG2	1.99	0.44
3:J:62:LYS:HE2	3:J:62:LYS:HB2	1.85	0.44
6:R:4:DG:H1	7:S:45:DC:H42	1.65	0.44
1:A:54:THR:O	1:A:167:VAL:HG22	2.18	0.44
2:C:196:LEU:O	2:C:198:ARG:NH1	2.49	0.44
2:C:673:LEU:HG	2:C:867:VAL:HG12	1.99	0.44
2:C:874:LEU:O	2:C:877:PRO:HD2	2.18	0.44
3:D:628:ARG:NH2	3:D:744:GLN:OE1	2.50	0.44
5:F:160:PRO:HB2	5:F:164:GLU:HB2	1.99	0.44
2:I:45:GLN:HE21	2:I:45:GLN:HB2	1.59	0.44
2:I:102:HIS:HB2	2:I:107:LEU:H	1.82	0.44
2:I:399:ASN:ND2	2:I:402:SER:HB2	2.32	0.44
2:I:431:HIS:H	2:I:434:HIS:CE1	2.34	0.44
2:I:607:ASP:O	2:I:609:THR:N	2.50	0.44
3:J:838:ARG:O	3:J:865:THR:OG1	2.32	0.44
3:J:1459:LEU:HA	3:J:1464:GLU:HG3	1.99	0.44
5:L:214:ALA:HB3	5:L:228:ILE:HG12	1.99	0.44
1:A:186:LEU:HD23	1:A:187:GLY:H	1.82	0.44
1:B:77:GLU:O	1:B:81:ASN:ND2	2.48	0.44
2:C:207:LEU:HD22	2:C:221:LEU:HD21	2.00	0.44
2:C:351:LEU:HB2	2:C:377:PRO:HB2	2.00	0.44
2:C:604:VAL:HG23	2:C:605:LYS:HG2	1.99	0.44
2:C:710:ILE:HD11	2:C:758:ARG:HE	1.82	0.44
3:D:34:TYR:HD1	5:F:325:ILE:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:132:TYR:HA	3:D:456:MET:HB3	2.00	0.44
3:D:415:VAL:HG11	3:D:433:GLY:H	1.82	0.44
3:D:667:ALA:HB1	3:D:672:ALA:CB	2.47	0.44
3:D:1161:GLU:CD	3:D:1161:GLU:H	2.25	0.44
5:F:368:GLU:HB3	5:F:433:LEU:HD21	1.98	0.44
5:F:372:ALA:HA	5:F:375:LYS:HE3	2.00	0.44
2:I:688:ILE:HD12	2:I:839:LEU:HB2	1.99	0.44
2:I:832:LYS:HB2	2:I:832:LYS:HE3	1.83	0.44
2:I:999:HIS:CD2	2:I:1004:LYS:HE3	2.53	0.44
5:L:229:GLN:HA	5:L:232:ASN:HD22	1.81	0.44
5:L:372:ALA:HA	5:L:375:LYS:HE3	1.99	0.44
2:C:498:GLN:HG3	3:D:1068:LEU:HD11	1.99	0.44
3:D:433:GLY:HA3	3:D:447:VAL:O	2.18	0.44
3:D:553:ARG:HH12	3:D:573:MET:HE1	1.83	0.44
3:D:1137:ARG:HE	3:D:1137:ARG:HB3	1.35	0.44
1:H:216:ALA:O	1:H:220:GLU:HB2	2.17	0.44
2:I:607:ASP:O	2:I:610:ARG:N	2.50	0.44
2:I:889:HIS:CE1	2:I:970:GLY:HA3	2.53	0.44
2:I:1066:ALA:O	2:I:1070:ILE:HG13	2.18	0.44
3:J:671:LYS:HG3	5:L:436:PHE:CE2	2.52	0.44
5:L:166:PRO:HG2	5:L:169:LYS:HZ1	1.82	0.44
5:L:214:ALA:HB1	5:L:227:LEU:HD23	2.00	0.44
1:A:53:VAL:HA	1:A:144:VAL:HG13	1.98	0.44
2:C:564:MET:SD	2:C:846:LYS:HG2	2.58	0.44
3:D:571:LYS:NZ	5:F:155:ARG:HH22	2.15	0.44
3:D:1459:LEU:HB3	3:D:1465:ASN:HD21	1.82	0.44
2:I:12:VAL:HG22	2:I:534:VAL:HG13	1.99	0.44
2:I:86:LYS:HE2	2:I:813:VAL:HG23	2.00	0.44
2:I:704:HIS:HB2	2:I:831:ARG:NH1	2.32	0.44
3:J:1144:LEU:HB3	3:J:1171:VAL:HG22	1.99	0.44
4:K:88:GLU:HB3	4:K:91:ARG:HH21	1.82	0.44
1:A:39:PRO:HG2	1:B:39:PRO:HG3	1.98	0.44
2:C:399:ASN:ND2	2:C:402:SER:HB2	2.32	0.44
2:C:815:LEU:HD11	2:C:822:VAL:HG22	1.98	0.44
2:C:889:HIS:CE1	2:C:970:GLY:HA3	2.53	0.44
3:J:347:VAL:HG22	3:J:348:ALA:H	1.81	0.44
1:B:52:ALA:HB2	1:B:170:ILE:C	2.43	0.44
2:C:731:GLU:H	2:C:731:GLU:HG3	1.58	0.44
5:F:214:ALA:HB3	5:F:228:ILE:HG12	1.99	0.44
2:I:669:GLY:HA3	2:I:995:MET:HA	2.00	0.44
2:I:769:PRO:HG3	3:J:65:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:773:LEU:HD13	5:L:388:LYS:HG3	2.00	0.44
2:C:594:ALA:HB1	2:C:654:LEU:HD11	1.99	0.44
2:C:999:HIS:CD2	2:C:1004:LYS:HE3	2.53	0.44
3:D:224:ARG:NH2	3:D:254:GLU:OE2	2.43	0.44
3:D:242:LEU:H	3:D:312:ARG:HA	1.83	0.44
3:D:701:LEU:HD22	3:D:763:MET:HG2	2.00	0.44
5:F:167:ASP:O	5:F:171:VAL:HB	2.18	0.44
1:H:75:VAL:O	1:H:79:ILE:HG13	2.17	0.44
2:I:90:TYR:CB	2:I:128:ILE:HB	2.48	0.44
2:I:564:MET:SD	2:I:846:LYS:HG2	2.58	0.44
3:J:167:GLU:OE2	3:J:198:ARG:NH2	2.51	0.44
1:A:32:PHE:CZ	1:B:43:ILE:HG12	2.52	0.43
2:C:326:ASP:HB2	2:C:431:HIS:HD2	1.83	0.43
2:C:641:PRO:HA	2:C:656:ALA:HA	2.00	0.43
2:C:669:GLY:HA3	2:C:995:MET:HA	2.00	0.43
2:C:876:VAL:HG11	2:C:885:ILE:HD11	2.00	0.43
2:C:1067:TYR:CZ	5:F:357:VAL:HG12	2.53	0.43
3:D:268:HIS:HB2	3:D:284:LEU:HB2	2.00	0.43
3:D:639:LEU:H	3:D:729:HIS:CD2	2.36	0.43
5:F:150:ILE:HD11	5:F:193:ARG:HH11	1.83	0.43
5:F:375:LYS:HD3	5:F:426:HIS:CG	2.53	0.43
1:G:101:LEU:HD21	1:G:109:VAL:HG11	1.99	0.43
2:I:80:GLN:CD	2:I:80:GLN:H	2.25	0.43
2:I:470:PRO:HG3	2:I:485:TYR:CZ	2.52	0.43
3:J:639:LEU:H	3:J:729:HIS:CD2	2.36	0.43
3:J:784:ASP:HB2	3:J:939:PHE:HE2	1.83	0.43
3:J:947:ILE:HG23	3:J:1019:PRO:HB3	2.00	0.43
3:J:1426:LYS:HE2	3:J:1426:LYS:HB3	1.82	0.43
2:C:90:TYR:CB	2:C:128:ILE:HB	2.49	0.43
2:C:425:PHE:HE1	3:D:1086:LEU:HD12	1.83	0.43
2:C:853:LEU:HD23	2:C:853:LEU:H	1.82	0.43
3:D:217:ARG:O	3:D:338:GLU:HA	2.18	0.43
3:D:1144:LEU:HB3	3:D:1171:VAL:HG22	1.99	0.43
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.99	0.43
5:F:101:HIS:CD2	6:O:31:DG:H22	2.35	0.43
1:G:15:THR:O	1:H:232:LEU:HD22	2.18	0.43
2:I:326:ASP:HB2	2:I:431:HIS:HD2	1.83	0.43
2:I:498:GLN:HG3	3:J:1068:LEU:HD11	1.99	0.43
2:I:673:LEU:HG	2:I:867:VAL:HG12	2.00	0.43
2:I:778:PHE:CZ	5:L:434:ARG:HA	2.49	0.43
3:J:7:LYS:HE3	3:J:1458:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:166:GLN:HE21	3:J:396:VAL:HG22	1.83	0.43
3:J:834:THR:OG1	3:J:835:SER:N	2.51	0.43
3:J:1122:LEU:HD11	3:J:1186:VAL:HG23	2.00	0.43
3:J:1161:GLU:CD	3:J:1161:GLU:H	2.25	0.43
1:A:97:THR:HG22	1:A:144:VAL:HB	1.99	0.43
2:C:937:ASP:HB3	2:C:940:GLU:HG3	2.00	0.43
3:D:834:THR:OG1	3:D:835:SER:N	2.51	0.43
3:D:947:ILE:HG23	3:D:1019:PRO:HB3	2.00	0.43
5:F:427:GLU:OE2	5:F:434:ARG:N	2.51	0.43
2:I:18:LEU:HB3	2:I:408:ARG:HD2	2.00	0.43
2:I:594:ALA:HB1	2:I:654:LEU:HD11	1.99	0.43
3:J:642:CYS:HB3	3:J:716:PHE:HB3	2.01	0.43
3:J:701:LEU:HD22	3:J:763:MET:HG2	2.00	0.43
5:L:369:LEU:HD23	5:L:433:LEU:HD13	1.99	0.43
1:A:15:THR:O	1:B:232:LEU:HD22	2.18	0.43
2:C:102:HIS:HB2	2:C:107:LEU:H	1.82	0.43
2:C:1066:ALA:O	2:C:1070:ILE:HG13	2.18	0.43
2:C:1073:GLY:HA3	3:D:659:LYS:HE2	2.00	0.43
3:D:260:GLU:OE1	3:D:273:ARG:NH2	2.52	0.43
2:I:89:THR:HG23	2:I:129:ILE:HA	2.00	0.43
2:I:148:PHE:HE2	2:I:280:LYS:HE3	1.84	0.43
3:J:894:LYS:HG3	3:J:895:VAL:H	1.83	0.43
3:J:965:GLU:HA	3:J:968:ASP:HB2	1.99	0.43
3:J:1293:PHE:CD2	3:J:1302:GLU:HB3	2.54	0.43
5:L:303:TYR:HA	5:L:306:ILE:HG22	2.00	0.43
6:O:4:DG:H1	7:P:45:DC:H42	1.65	0.43
2:C:184:MET:N	2:C:191:PHE:O	2.48	0.43
2:C:773:LEU:HD13	5:F:388:LYS:HG3	2.00	0.43
2:C:1102:LEU:HB3	2:C:1106:ASP:HA	2.00	0.43
3:D:7:LYS:HE3	3:D:1458:GLU:OE1	2.19	0.43
3:D:22:SER:HG	3:D:92:HIS:CE1	2.35	0.43
3:D:409:VAL:HG21	3:D:421:LEU:HD23	2.00	0.43
1:G:63:HIS:CE1	2:I:801:VAL:HG13	2.53	0.43
2:I:31:GLN:HB3	2:I:34:VAL:HB	2.01	0.43
3:J:553:ARG:HH12	3:J:573:MET:HE1	1.83	0.43
3:J:634:GLY:O	3:J:637:LEU:N	2.52	0.43
3:J:1145:TYR:O	3:J:1364:HIS:NE2	2.52	0.43
5:L:150:ILE:HD11	5:L:193:ARG:HH11	1.83	0.43
2:C:1017:THR:OG1	2:C:1084:SER:HB3	2.18	0.43
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.54	0.43
3:D:31:THR:OG1	3:D:32:ILE:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1060:SER:HB3	3:D:1063:GLU:HG3	2.01	0.43
3:D:1293:PHE:CD2	3:D:1302:GLU:HB3	2.54	0.43
5:F:269:GLN:HE21	5:F:269:GLN:HB2	1.50	0.43
1:H:48:ILE:HA	1:H:49:PRO:HD2	1.76	0.43
1:H:149:GLY:O	1:H:171:PHE:HB2	2.18	0.43
2:I:853:LEU:H	2:I:853:LEU:HD23	1.82	0.43
2:C:18:LEU:HB3	2:C:408:ARG:HD2	2.01	0.43
2:C:1037:VAL:O	2:C:1041:GLU:HG3	2.19	0.43
3:D:708:LEU:HD12	3:D:1231:GLU:HG2	2.01	0.43
5:F:202:LEU:HD22	5:F:239:VAL:HG22	2.01	0.43
1:H:52:ALA:HB2	1:H:170:ILE:C	2.43	0.43
2:I:738:ASP:OD2	2:I:744:ARG:HB3	2.19	0.43
2:I:876:VAL:HG11	2:I:885:ILE:HD11	2.01	0.43
3:J:769:LEU:O	3:J:778:LEU:HB3	2.18	0.43
3:J:796:ARG:HG3	3:J:861:GLN:HB2	2.00	0.43
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.99	0.43
2:C:252:LYS:HE3	2:C:252:LYS:HB2	1.87	0.43
2:C:836:GLY:N	2:C:849:VAL:O	2.52	0.43
3:D:347:VAL:HA	3:D:351:MET:HE2	2.01	0.43
3:D:1072:ILE:O	3:D:1075:HIS:HB2	2.19	0.43
5:F:244:TYR:H	5:F:244:TYR:HD2	1.65	0.43
5:F:411:ARG:HG2	6:O:1:DC:H3'	2.01	0.43
1:G:104:GLU:HB3	1:G:137:LYS:HG2	2.01	0.43
1:G:199:ILE:HB	1:G:207:PRO:HB3	2.00	0.43
3:J:708:LEU:HD12	3:J:1231:GLU:HG2	2.01	0.43
3:J:1060:SER:HB3	3:J:1063:GLU:HG3	2.01	0.43
2:C:1042:ALA:HB1	3:D:1224:VAL:HG22	2.01	0.43
3:D:169:TYR:OH	3:D:198:ARG:N	2.36	0.43
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.82	0.43
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	2.00	0.43
2:I:750:LYS:HG2	2:I:751:PRO:HD2	2.01	0.43
2:I:937:ASP:HB3	2:I:940:GLU:HG3	2.00	0.43
5:L:167:ASP:O	5:L:171:VAL:HB	2.18	0.43
5:L:220:ARG:CZ	5:L:266:ILE:HD13	2.49	0.43
1:A:104:GLU:HB3	1:A:137:LYS:HG2	2.01	0.43
3:D:237:ARG:HG2	3:D:240:GLU:HB2	2.00	0.43
5:F:203:ILE:HD13	5:F:236:ILE:HG12	2.00	0.43
2:I:92:ALA:HA	2:I:93:PRO:HD3	1.88	0.43
2:I:425:PHE:HE1	3:J:1086:LEU:HD12	1.83	0.43
2:I:1106:ASP:OD1	3:J:7:LYS:NZ	2.37	0.43
3:J:411:THR:HG23	3:J:437:VAL:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:203:ILE:HD13	5:L:236:ILE:HG12	2.00	0.43
1:B:123:MET:O	1:B:125:PRO:HD3	2.19	0.42
2:C:12:VAL:HG22	2:C:534:VAL:HG13	2.00	0.42
2:C:89:THR:HG23	2:C:129:ILE:HA	1.99	0.42
3:D:642:CYS:HB3	3:D:716:PHE:HB3	2.01	0.42
3:D:760:ARG:NH1	4:E:61:VAL:HB	2.34	0.42
5:F:96:VAL:HA	5:F:225:LEU:HD11	2.01	0.42
1:G:24:VAL:HG22	1:G:196:THR:HG23	2.01	0.42
3:J:671:LYS:HG3	5:L:436:PHE:CZ	2.54	0.42
3:J:1072:ILE:O	3:J:1075:HIS:HB2	2.19	0.42
5:L:244:TYR:HD2	5:L:244:TYR:H	1.65	0.42
1:B:149:GLY:O	1:B:171:PHE:HB2	2.18	0.42
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.53	0.42
3:D:628:ARG:HB2	3:D:745:MET:O	2.19	0.42
2:I:126:SER:HB3	2:I:407:LYS:NZ	2.33	0.42
2:I:641:PRO:HA	2:I:656:ALA:HA	2.00	0.42
2:I:836:GLY:N	2:I:849:VAL:O	2.52	0.42
2:I:1017:THR:OG1	2:I:1084:SER:HB3	2.18	0.42
5:L:409:ARG:NH2	7:S:43:DG:N7	2.66	0.42
2:C:838:LYS:NZ	3:D:741:ASP:O	2.51	0.42
2:C:954:SER:HA	2:C:955:PRO:HD3	1.89	0.42
3:D:258:VAL:HG12	3:D:259:VAL:H	1.83	0.42
3:D:372:ASP:HA	3:D:373:PRO:HD3	1.91	0.42
3:D:796:ARG:HG3	3:D:861:GLN:HB2	2.00	0.42
3:D:1145:TYR:O	3:D:1364:HIS:NE2	2.52	0.42
5:F:303:TYR:HA	5:F:306:ILE:HG22	2.00	0.42
2:I:139:GLN:HB2	2:I:391:LEU:HD21	2.01	0.42
2:I:1038:TRP:CE2	3:J:1099:VAL:HG11	2.54	0.42
3:J:130:ASN:HA	5:L:98:GLN:HE22	1.85	0.42
3:J:437:VAL:HA	3:J:444:VAL:HG12	2.00	0.42
3:J:760:ARG:NH1	4:K:61:VAL:HB	2.35	0.42
5:L:166:PRO:HB2	5:L:169:LYS:HB3	2.02	0.42
1:A:63:HIS:CE1	1:A:66:SER:H	2.38	0.42
1:A:199:ILE:HB	1:A:207:PRO:HB3	2.00	0.42
2:C:139:GLN:HB2	2:C:391:LEU:HD21	2.00	0.42
2:C:448:ASN:HA	2:C:451:LEU:HD22	2.01	0.42
2:C:937:ASP:OD2	2:C:939:ARG:NE	2.50	0.42
3:D:397:LYS:NZ	3:D:397:LYS:HB3	2.35	0.42
3:D:894:LYS:HE3	3:D:894:LYS:HB2	1.85	0.42
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.99	0.42
1:H:122:ILE:HG22	1:H:124:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:11:GLU:HG3	2:I:535:SER:HB2	2.01	0.42
2:I:918:LEU:HD13	2:I:918:LEU:HA	1.92	0.42
3:J:667:ALA:HB1	3:J:672:ALA:CB	2.49	0.42
5:L:418:LYS:O	5:L:422:LYS:HG3	2.20	0.42
1:A:100:ILE:O	1:A:115:THR:N	2.53	0.42
2:C:436:GLY:HA3	2:C:469:THR:HG21	2.01	0.42
5:F:355:SER:HB3	5:F:358:GLU:HG3	2.01	0.42
5:F:418:LYS:O	5:F:422:LYS:HG3	2.20	0.42
1:H:123:MET:O	1:H:125:PRO:HD3	2.19	0.42
2:I:252:LYS:HB2	2:I:252:LYS:HE3	1.87	0.42
2:I:1020:PRO:HD2	3:J:622:ARG:O	2.19	0.42
3:J:124:GLU:OE2	3:J:587:ARG:NH2	2.53	0.42
3:J:1093:TYR:CD1	7:S:10:DA:H5''	2.55	0.42
5:L:124:GLY:O	5:L:128:ILE:HG13	2.19	0.42
1:B:54:THR:OG1	1:B:158:ILE:HG21	2.20	0.42
2:C:207:LEU:HD13	2:C:221:LEU:HD21	2.01	0.42
2:C:660:ALA:O	2:C:667:ALA:N	2.33	0.42
2:C:750:LYS:HG2	2:C:751:PRO:HD2	2.01	0.42
3:D:714:GLN:HB3	3:D:765:SER:HB3	2.02	0.42
3:D:894:LYS:HG3	3:D:895:VAL:H	1.83	0.42
3:D:896:ALA:O	3:D:900:ILE:HG13	2.20	0.42
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.20	0.42
5:F:166:PRO:HB2	5:F:169:LYS:HB3	2.02	0.42
2:I:1037:VAL:O	2:I:1041:GLU:HG3	2.19	0.42
3:J:714:GLN:HB3	3:J:765:SER:HB3	2.02	0.42
1:A:24:VAL:HG22	1:A:196:THR:HG23	2.01	0.42
1:B:161:ARG:HG3	1:B:162:ILE:N	2.35	0.42
2:C:9:ILE:H	2:C:9:ILE:HG13	1.68	0.42
2:C:1021:LEU:HD22	5:F:346:ASP:O	2.18	0.42
3:D:1439:SER:OG	3:D:1463:LYS:NZ	2.50	0.42
5:F:260:GLN:HE21	5:F:260:GLN:HB2	1.67	0.42
2:I:196:LEU:O	2:I:198:ARG:NH1	2.49	0.42
2:I:966:LEU:HD21	2:I:986:PRO:HB3	2.01	0.42
2:I:1013:TYR:O	5:L:350:ASP:N	2.48	0.42
3:J:166:GLN:HB3	3:J:396:VAL:HG13	2.02	0.42
5:L:301:PRO:HG3	5:L:306:ILE:HD13	2.01	0.42
1:A:63:HIS:CE1	1:A:65:PHE:HB2	2.55	0.42
1:B:211:LEU:O	1:B:215:VAL:HG13	2.20	0.42
2:C:1007:ALA:HB2	3:D:648:MET:HG3	2.02	0.42
3:D:172:PRO:HG2	3:D:175:VAL:HG21	2.02	0.42
3:D:224:ARG:HB3	3:D:251:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:735:ALA:HB2	3:D:778:LEU:HD21	2.02	0.42
3:D:1370:ILE:O	3:D:1374:GLN:HG2	2.19	0.42
1:G:54:THR:HG22	1:G:158:ILE:HD11	2.01	0.42
1:H:54:THR:OG1	1:H:158:ILE:HG21	2.20	0.42
2:I:100:LEU:HD21	2:I:102:HIS:HE1	1.85	0.42
3:J:660:LYS:HD2	3:J:660:LYS:HA	1.87	0.42
3:J:894:LYS:HB2	3:J:894:LYS:HE3	1.85	0.42
5:L:96:VAL:HA	5:L:225:LEU:HD11	2.01	0.42
6:O:42:DC:H2''	6:O:43:DG:C8	2.55	0.42
2:C:31:GLN:HB3	2:C:34:VAL:HB	2.01	0.42
2:C:191:PHE:HA	2:C:192:PRO:HD3	1.93	0.42
2:C:1020:PRO:HD2	3:D:622:ARG:O	2.19	0.42
2:C:1106:ASP:OD1	3:D:7:LYS:NZ	2.37	0.42
3:D:714:GLN:HB2	3:D:716:PHE:HE1	1.85	0.42
3:D:956:ILE:HG13	3:D:1062:ARG:HD3	2.01	0.42
3:D:1093:TYR:CD1	7:P:10:DA:H5''	2.55	0.42
1:H:184:THR:HG23	1:H:192:LEU:HB2	2.02	0.42
2:I:726:ILE:HG23	2:I:787:ASP:HB2	2.02	0.42
2:I:1042:ALA:HB1	3:J:1224:VAL:HG22	2.01	0.42
2:I:1052:MET:HE1	3:J:748:HIS:HB3	2.02	0.42
3:J:735:ALA:HB2	3:J:778:LEU:HD21	2.02	0.42
3:J:970:LYS:O	3:J:974:ILE:HG13	2.19	0.42
3:J:1351:GLU:O	3:J:1354:LYS:HB3	2.20	0.42
4:K:22:VAL:HG11	4:K:68:LEU:HD22	2.02	0.42
2:C:11:GLU:HG3	2:C:535:SER:HB2	2.01	0.42
2:C:148:PHE:HE2	2:C:280:LYS:HE3	1.84	0.42
2:C:530:GLU:H	2:C:530:GLU:HG2	1.58	0.42
3:D:634:GLY:O	3:D:637:LEU:N	2.52	0.42
3:D:1006:ALA:O	3:D:1010:ASN:HB2	2.20	0.42
3:D:1459:LEU:HB3	3:D:1465:ASN:ND2	2.35	0.42
5:F:111:LEU:O	5:F:115:ILE:HG12	2.19	0.42
5:F:124:GLY:O	5:F:128:ILE:HG13	2.19	0.42
5:F:220:ARG:CZ	5:F:266:ILE:HD13	2.49	0.42
1:G:63:HIS:CE1	1:G:66:SER:H	2.38	0.42
2:I:250:LYS:HE2	2:I:250:LYS:HB3	1.92	0.42
2:I:676:ILE:HD13	2:I:988:VAL:HG23	2.02	0.42
2:I:1007:ALA:HB2	3:J:648:MET:HG3	2.02	0.42
3:J:31:THR:HG21	5:L:272:THR:HG22	2.02	0.42
3:J:956:ILE:HG13	3:J:1062:ARG:HD3	2.01	0.42
3:J:1098:LEU:HD12	3:J:1424:VAL:HG11	2.02	0.42
3:J:1370:ILE:O	3:J:1374:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1404:ASN:O	3:J:1408:ILE:HG12	2.20	0.42
1:B:122:ILE:HG22	1:B:124:ASN:H	1.84	0.41
2:C:327:HIS:NE2	2:C:492:ASP:OD1	2.53	0.41
2:C:603:VAL:HG21	2:C:643:VAL:HB	2.02	0.41
3:D:674:ARG:HH21	5:F:357:VAL:HG11	1.85	0.41
3:D:937:TYR:O	3:D:941:LEU:HG	2.19	0.41
3:D:970:LYS:O	3:D:974:ILE:HG13	2.20	0.41
1:H:132:LEU:HD12	1:H:136:GLY:HA3	2.02	0.41
2:I:1102:LEU:HB3	2:I:1106:ASP:HA	2.00	0.41
3:J:31:THR:OG1	3:J:32:ILE:N	2.50	0.41
3:J:115:LEU:HD12	3:J:468:LEU:HD13	2.02	0.41
5:L:217:TYR:HD1	5:L:217:TYR:HA	1.77	0.41
5:L:379:ARG:HG3	5:L:405:PHE:CE2	2.55	0.41
1:B:48:ILE:HA	1:B:213:GLN:HE22	1.85	0.41
2:C:242:LEU:HD13	2:C:243:ARG:N	2.35	0.41
3:D:314:PRO:HG2	3:D:317:MET:HB3	2.01	0.41
3:D:1149:LEU:HD23	3:D:1149:LEU:HA	1.89	0.41
3:D:1426:LYS:HE2	3:D:1426:LYS:HB3	1.82	0.41
1:G:63:HIS:CE1	1:G:65:PHE:HB2	2.55	0.41
1:H:226:ALA:O	1:H:228:PRO:HD3	2.20	0.41
2:I:640:ARG:O	2:I:657:ASP:HB2	2.20	0.41
2:I:937:ASP:OD2	2:I:939:ARG:NE	2.50	0.41
3:J:22:SER:HA	3:J:90:MET:O	2.20	0.41
3:J:618:LEU:HD13	3:J:618:LEU:HA	1.86	0.41
3:J:937:TYR:O	3:J:941:LEU:HG	2.19	0.41
3:J:1006:ALA:O	3:J:1010:ASN:HB2	2.20	0.41
3:J:1149:LEU:HD23	3:J:1149:LEU:HA	1.88	0.41
4:K:49:ARG:HA	4:K:54:LEU:HG	2.02	0.41
5:L:111:LEU:O	5:L:115:ILE:HG12	2.20	0.41
5:L:355:SER:HB3	5:L:358:GLU:HG3	2.01	0.41
1:B:132:LEU:HD12	1:B:136:GLY:HA3	2.02	0.41
2:C:726:ILE:HG23	2:C:787:ASP:HB2	2.02	0.41
3:D:1098:LEU:HD12	3:D:1424:VAL:HG11	2.02	0.41
4:E:3:GLU:HG2	4:E:65:MET:SD	2.61	0.41
4:E:49:ARG:HA	4:E:54:LEU:HG	2.02	0.41
5:F:379:ARG:HG3	5:F:405:PHE:CE2	2.55	0.41
1:H:48:ILE:HA	1:H:213:GLN:HE22	1.85	0.41
1:H:106:PRO:HA	1:H:132:LEU:O	2.21	0.41
2:I:708:TYR:HE1	2:I:827:VAL:HB	1.85	0.41
3:J:132:TYR:HB3	3:J:454:ALA:O	2.21	0.41
3:J:214:ASP:O	3:J:383:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:597:GLU:OE1	3:J:597:GLU:N	2.54	0.41
3:J:714:GLN:HB2	3:J:716:PHE:HE1	1.85	0.41
4:K:3:GLU:HG2	4:K:65:MET:SD	2.60	0.41
5:L:202:LEU:HD22	5:L:239:VAL:HG22	2.01	0.41
2:C:859:PRO:HG2	2:C:867:VAL:HG21	2.01	0.41
3:D:130:ASN:HA	5:F:98:GLN:HE22	1.85	0.41
3:D:156:GLU:H	3:D:156:GLU:HG3	1.70	0.41
3:D:212:ARG:HG2	3:D:213:VAL:N	2.34	0.41
3:D:402:PRO:HA	3:D:443:VAL:HA	2.01	0.41
3:D:660:LYS:HD2	3:D:660:LYS:HA	1.87	0.41
3:D:1093:TYR:HD1	7:P:10:DA:H5"	1.85	0.41
3:D:1351:GLU:O	3:D:1354:LYS:HB3	2.20	0.41
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.21	0.41
2:I:872:ASN:ND2	2:I:874:LEU:HB2	2.36	0.41
3:J:684:LYS:O	3:J:687:VAL:HG22	2.21	0.41
3:J:688:TRP:CE3	3:J:688:TRP:HA	2.55	0.41
3:J:745:MET:HE2	3:J:745:MET:HB3	1.94	0.41
7:S:33:DT:H2"	7:S:34:DA:C8	2.56	0.41
1:A:55:SER:HB2	1:A:158:ILE:HG13	2.02	0.41
2:C:411:SER:HB2	2:C:413:LEU:HG	2.03	0.41
2:C:640:ARG:O	2:C:657:ASP:HB2	2.20	0.41
2:C:832:LYS:HE3	2:C:832:LYS:HB2	1.83	0.41
2:C:918:LEU:HD13	2:C:918:LEU:HA	1.92	0.41
3:D:31:THR:HG21	5:F:272:THR:HG22	2.03	0.41
3:D:804:MET:HE3	3:D:804:MET:HA	2.02	0.41
3:D:955:VAL:HA	3:D:1062:ARG:NH1	2.35	0.41
3:D:1196:THR:OG1	3:D:1201:CYS:HB3	2.20	0.41
2:I:328:LEU:HD11	2:I:434:HIS:ND1	2.35	0.41
2:I:491:GLU:OE1	2:I:516:ARG:NH2	2.53	0.41
3:J:112:ILE:HG23	3:J:512:MET:HE2	2.02	0.41
3:J:896:ALA:O	3:J:900:ILE:HG13	2.20	0.41
1:B:106:PRO:HA	1:B:132:LEU:O	2.20	0.41
2:C:491:GLU:OE1	2:C:516:ARG:NH2	2.53	0.41
2:C:738:ASP:OD2	2:C:744:ARG:HB3	2.20	0.41
3:D:792:ILE:HG13	3:D:793:THR:N	2.35	0.41
3:D:970:LYS:O	3:D:973:GLN:HB3	2.21	0.41
4:E:22:VAL:HG11	4:E:68:LEU:HD22	2.02	0.41
5:F:252:THR:HA	6:O:29:DC:C5	2.55	0.41
2:I:207:LEU:HD13	2:I:221:LEU:HD21	2.01	0.41
2:I:436:GLY:HA3	2:I:469:THR:HG21	2.01	0.41
2:I:498:GLN:O	2:I:501:THR:OG1	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:859:PRO:HG2	2:I:867:VAL:HG21	2.01	0.41
2:I:1020:PRO:O	3:J:622:ARG:HD2	2.21	0.41
3:J:698:LYS:HG3	4:K:59:ASN:ND2	2.35	0.41
3:J:1123:PHE:HB3	3:J:1132:LEU:HD22	2.03	0.41
2:C:90:TYR:HB3	2:C:128:ILE:HB	2.02	0.41
2:C:328:LEU:HD11	2:C:434:HIS:ND1	2.35	0.41
2:C:505:GLY:O	2:C:506:ASP:HB3	2.19	0.41
2:C:676:ILE:HD13	2:C:988:VAL:HG23	2.02	0.41
3:D:716:PHE:CZ	3:D:732:VAL:HG21	2.52	0.41
2:I:45:GLN:HA	2:I:48:PHE:HB2	2.03	0.41
2:I:151:ASP:HB2	2:I:157:ARG:O	2.21	0.41
2:I:603:VAL:HG21	2:I:643:VAL:HB	2.01	0.41
3:J:553:ARG:HD2	3:J:570:GLU:OE1	2.21	0.41
3:J:955:VAL:HA	3:J:1062:ARG:NH1	2.35	0.41
7:P:33:DT:H2"	7:P:34:DA:C8	2.56	0.41
1:A:54:THR:HG22	1:A:158:ILE:HD11	2.01	0.41
1:A:59:GLU:HG3	1:A:139:TYR:HD2	1.86	0.41
1:A:227:ASN:HA	1:A:228:PRO:HD2	1.85	0.41
1:B:184:THR:HG23	1:B:192:LEU:HB2	2.02	0.41
2:C:166:PRO:C	2:C:168:ARG:H	2.28	0.41
3:D:115:LEU:HD12	3:D:468:LEU:HD13	2.02	0.41
5:F:301:PRO:HG3	5:F:306:ILE:HD13	2.01	0.41
3:J:22:SER:HG	3:J:92:HIS:CE1	2.36	0.41
3:J:628:ARG:HB2	3:J:745:MET:O	2.21	0.41
1:B:226:ALA:O	1:B:228:PRO:HD3	2.20	0.41
2:C:100:LEU:HD21	2:C:102:HIS:CE1	2.56	0.41
2:C:100:LEU:HD21	2:C:102:HIS:HE1	1.85	0.41
2:C:1020:PRO:O	3:D:622:ARG:HD2	2.21	0.41
2:C:1052:MET:HE1	3:D:748:HIS:HB3	2.02	0.41
3:D:291:LEU:HB2	3:D:304:LEU:O	2.21	0.41
3:D:353:VAL:HA	3:D:368:VAL:HG22	2.03	0.41
3:D:432:TYR:O	3:D:448:GLU:HA	2.20	0.41
3:D:670:VAL:HB	5:F:364:LEU:HD11	2.02	0.41
3:D:895:VAL:O	3:D:898:GLU:HB3	2.21	0.41
3:D:902:MET:HE2	3:D:902:MET:HA	2.03	0.41
3:D:935:LYS:HE2	3:D:935:LYS:HB3	1.94	0.41
1:G:40:LEU:HD23	1:G:40:LEU:HA	1.97	0.41
1:G:223:ASN:HD22	1:G:223:ASN:HA	1.74	0.41
1:H:89:PHE:HB2	1:H:146:ARG:NH2	2.36	0.41
1:H:161:ARG:HG3	1:H:162:ILE:N	2.35	0.41
1:H:211:LEU:O	1:H:215:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:242:LEU:HD13	2:I:243:ARG:N	2.35	0.41
2:I:446:GLY:O	2:I:449:ILE:HG13	2.21	0.41
2:I:448:ASN:HA	2:I:451:LEU:HD22	2.02	0.41
2:I:537:LYS:O	2:I:545:ASN:ND2	2.54	0.41
2:I:1107:ASN:HA	2:I:1108:PRO:HD3	1.87	0.41
3:J:56:TYR:CE2	3:J:82:ARG:HB3	2.56	0.41
3:J:348:ALA:HB1	3:J:350:HIS:CE1	2.55	0.41
3:J:441:ARG:HH12	3:J:445:ARG:HH11	1.68	0.41
3:J:597:GLU:OE1	3:J:597:GLU:CA	2.68	0.41
3:J:970:LYS:O	3:J:973:GLN:HB3	2.21	0.41
3:J:1353:GLN:HG2	3:J:1368:ILE:HD12	2.03	0.41
3:J:1433:SER:OG	3:J:1457:ASP:OD2	2.36	0.41
3:J:1500:LYS:O	3:J:1503:VAL:HG22	2.21	0.41
1:B:28:LEU:HD21	1:B:36:LEU:HD13	2.03	0.41
2:C:45:GLN:HA	2:C:48:PHE:HB2	2.03	0.41
2:C:198:ARG:HG2	2:C:199:VAL:HG23	2.03	0.41
2:C:446:GLY:O	2:C:449:ILE:HG13	2.21	0.41
2:C:718:GLY:HA3	2:C:761:PHE:CD2	2.56	0.41
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.94	0.41
3:D:55:ASP:C	3:D:57:GLU:H	2.29	0.41
3:D:203:ALA:HA	3:D:395:VAL:HA	2.03	0.41
3:D:520:LEU:O	3:D:525:ARG:NE	2.54	0.41
3:D:569:ASN:OD1	3:D:572:ARG:NH2	2.48	0.41
3:D:596:SER:OG	3:D:598:ARG:HG2	2.21	0.41
3:D:625:TYR:CE2	3:D:655:PRO:HG2	2.54	0.41
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	2.03	0.41
3:D:1353:GLN:HG2	3:D:1368:ILE:HD12	2.03	0.41
1:G:100:ILE:O	1:G:115:THR:N	2.52	0.41
1:G:109:VAL:HG12	1:G:110:ARG:H	1.86	0.41
2:I:194:VAL:HG11	2:I:223:ASP:CB	2.51	0.41
2:I:411:SER:HB2	2:I:413:LEU:HG	2.02	0.41
3:J:657:LEU:HG	3:J:661:MET:SD	2.61	0.41
3:J:1462:LEU:O	3:J:1466:VAL:HG23	2.21	0.41
5:L:427:GLU:HA	5:L:430:THR:OG1	2.21	0.41
6:R:42:DC:H2"	6:R:43:DG:C8	2.55	0.41
1:A:72:LYS:HE3	2:C:641:PRO:O	2.21	0.40
1:A:109:VAL:HG12	1:A:110:ARG:H	1.86	0.40
2:C:151:ASP:HB2	2:C:157:ARG:O	2.21	0.40
2:C:441:VAL:O	2:C:443:THR:HG22	2.21	0.40
3:D:140:ALA:HA	3:D:450:TYR:CG	2.56	0.40
3:D:210:ARG:HD2	3:D:388:HIS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.55	0.40
3:D:908:LYS:HB2	3:D:1026:SER:O	2.21	0.40
1:G:72:LYS:HE3	2:I:641:PRO:O	2.21	0.40
3:J:209:ARG:HB3	3:J:347:VAL:HG11	2.03	0.40
3:J:565:ILE:HD12	3:J:565:ILE:H	1.86	0.40
3:J:675:ARG:HD2	3:J:679:ARG:CZ	2.51	0.40
3:J:749:VAL:HA	3:J:750:PRO:HD2	1.95	0.40
3:J:1093:TYR:HD1	7:S:10:DA:H5''	1.86	0.40
3:J:1153:VAL:HB	3:J:1160:LEU:HB2	2.03	0.40
2:C:92:ALA:HA	2:C:93:PRO:HD3	1.89	0.40
2:C:290:LEU:HD22	2:C:302:VAL:HG11	2.03	0.40
2:C:966:LEU:HD21	2:C:986:PRO:HB3	2.02	0.40
2:C:1050:GLN:HG3	3:D:1471:LEU:HA	2.03	0.40
3:D:556:LYS:HD2	3:D:556:LYS:HA	1.97	0.40
1:G:55:SER:HB2	1:G:158:ILE:HG13	2.02	0.40
1:G:182:GLU:O	1:G:193:ASP:HA	2.21	0.40
3:J:843:PHE:HB2	3:J:866:VAL:HG23	2.04	0.40
3:J:902:MET:HE2	3:J:902:MET:HA	2.03	0.40
4:K:57:ASP:HA	4:K:58:PRO:HD2	1.94	0.40
1:B:32:PHE:HD2	1:B:32:PHE:HA	1.75	0.40
2:C:45:GLN:HE21	2:C:45:GLN:HB2	1.59	0.40
2:C:307:LEU:HD12	2:C:307:LEU:HA	1.84	0.40
2:C:430:VAL:HG11	2:C:440:PRO:HA	2.04	0.40
2:C:708:TYR:HE1	2:C:827:VAL:HB	1.85	0.40
3:D:230:TRP:HA	3:D:243:ALA:CB	2.51	0.40
3:D:231:VAL:O	3:D:236:TYR:OH	2.39	0.40
3:D:995:LEU:O	3:D:998:GLU:HG2	2.22	0.40
3:D:1470:ARG:HG2	3:D:1471:LEU:H	1.86	0.40
1:H:143:ARG:HD2	1:H:160:ASP:OD2	2.20	0.40
2:I:327:HIS:NE2	2:I:433:THR:HG21	2.36	0.40
2:I:718:GLY:HA3	2:I:761:PHE:CD2	2.56	0.40
2:I:874:LEU:O	3:J:1029:ARG:HG2	2.22	0.40
5:L:375:LYS:HE2	5:L:375:LYS:HB3	1.83	0.40
2:C:65:VAL:HG13	2:C:101:ILE:HB	2.03	0.40
2:C:327:HIS:NE2	2:C:433:THR:HG21	2.37	0.40
2:C:537:LYS:O	2:C:545:ASN:ND2	2.54	0.40
2:C:627:ARG:HD2	2:C:639:GLN:H	1.87	0.40
2:C:872:ASN:ND2	2:C:874:LEU:HB2	2.36	0.40
3:D:553:ARG:HD2	3:D:570:GLU:OE1	2.21	0.40
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.36	0.40
3:D:911:LEU:O	3:D:915:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:375:LYS:HE2	5:F:375:LYS:HB3	1.83	0.40
2:I:100:LEU:HD21	2:I:102:HIS:CE1	2.56	0.40
3:J:671:LYS:HE3	3:J:671:LYS:HB3	1.94	0.40
3:J:804:MET:HE3	3:J:804:MET:HA	2.02	0.40
3:J:1479:ASP:HA	3:J:1482:ARG:HG2	2.04	0.40
6:R:12:DT:H3	7:S:37:DA:H61	1.69	0.40
1:B:143:ARG:HD2	1:B:160:ASP:OD2	2.21	0.40
2:C:52:PHE:CD2	2:C:68:PHE:HB2	2.57	0.40
2:C:675:ALA:O	2:C:870:ILE:HA	2.21	0.40
3:D:671:LYS:HG3	5:F:436:PHE:CE2	2.56	0.40
1:G:27:PRO:HD3	1:G:186:LEU:HD22	2.04	0.40
2:I:90:TYR:HB3	2:I:128:ILE:HB	2.02	0.40
2:I:166:PRO:C	2:I:168:ARG:H	2.28	0.40
2:I:598:GLU:HG2	2:I:615:TYR:CZ	2.57	0.40
3:J:55:ASP:C	3:J:57:GLU:H	2.29	0.40
3:J:65:ARG:HG2	5:L:393:GLY:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/314 (72%)	206 (92%)	18 (8%)	1 (0%)	30	65
1	B	225/314 (72%)	205 (91%)	17 (8%)	3 (1%)	9	41
1	G	225/314 (72%)	205 (91%)	19 (8%)	1 (0%)	30	65
1	H	225/314 (72%)	205 (91%)	19 (8%)	1 (0%)	30	65
2	C	1108/1119 (99%)	1011 (91%)	94 (8%)	3 (0%)	36	70
2	I	1108/1119 (99%)	1012 (91%)	94 (8%)	2 (0%)	43	75
3	D	1486/1524 (98%)	1340 (90%)	141 (10%)	5 (0%)	36	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	1361/1524 (89%)	1235 (91%)	123 (9%)	3 (0%)	43	75
4	E	91/99 (92%)	83 (91%)	8 (9%)	0	100	100
4	K	91/99 (92%)	82 (90%)	9 (10%)	0	100	100
5	F	345/347 (99%)	316 (92%)	29 (8%)	0	100	100
5	L	345/347 (99%)	314 (91%)	31 (9%)	0	100	100
All	All	6835/7434 (92%)	6214 (91%)	602 (9%)	19 (0%)	36	70

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	765	GLN
3	D	1128	VAL
3	J	1128	VAL
1	A	53	VAL
1	B	178	ALA
3	D	415	VAL
3	D	431	ILE
3	D	666	PHE
1	G	53	VAL
3	J	179	VAL
1	B	51	THR
1	H	51	THR
2	I	1084	SER
1	B	177	VAL
2	C	1084	SER
3	D	667	ALA
3	J	667	ALA
2	C	870	ILE
2	I	870	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/270 (72%)	180 (93%)	14 (7%)	13	37
1	B	194/270 (72%)	178 (92%)	16 (8%)	10	34
1	G	194/270 (72%)	180 (93%)	14 (7%)	13	37
1	H	194/270 (72%)	178 (92%)	16 (8%)	10	34
2	C	931/936 (100%)	829 (89%)	102 (11%)	6	23
2	I	931/936 (100%)	829 (89%)	102 (11%)	6	23
3	D	1252/1281 (98%)	1123 (90%)	129 (10%)	7	25
3	J	1150/1281 (90%)	1042 (91%)	108 (9%)	8	29
4	E	83/88 (94%)	75 (90%)	8 (10%)	8	28
4	K	83/88 (94%)	75 (90%)	8 (10%)	8	28
5	F	297/299 (99%)	270 (91%)	27 (9%)	9	30
5	L	297/299 (99%)	270 (91%)	27 (9%)	9	30
All	All	5800/6288 (92%)	5229 (90%)	571 (10%)	7	27

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	56	VAL
1	A	59	GLU
1	A	86	VAL
1	A	87	VAL
1	A	93	LYS
1	A	98	THR
1	A	109	VAL
1	A	142	VAL
1	A	167	VAL
1	A	172	SER
1	A	174	VAL
1	A	186	LEU
1	A	205	VAL
1	B	7	LYS
1	B	30	ARG
1	B	53	VAL
1	B	54	THR
1	B	58	ILE
1	B	75	VAL
1	B	114	PHE
1	B	115	THR

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Mol	Chain	Res	Type
1	B	145	ASP
1	B	158	ILE
1	B	170	ILE
1	B	176	ARG
1	B	177	VAL
1	B	184	THR
1	B	215	VAL
1	B	218	LEU
2	C	15	LEU
2	C	30	LEU
2	C	41	ASN
2	C	45	GLN
2	C	48	PHE
2	C	56	GLU
2	C	73	ILE
2	C	75	ASP
2	C	80	GLN
2	C	100	LEU
2	C	104	ASP
2	C	111	ASP
2	C	112	GLU
2	C	120	LEU
2	C	122	THR
2	C	140	ILE
2	C	142	ARG
2	C	151	ASP
2	C	159	ILE
2	C	163	ILE
2	C	174	LEU
2	C	179	SER
2	C	195	LEU
2	C	197	LEU
2	C	199	VAL
2	C	211	LEU
2	C	217	LEU
2	C	222	LEU
2	C	226	VAL
2	C	237	ARG
2	C	242	LEU
2	C	249	LYS
2	C	251	ASP
2	C	258	PHE

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Mol	Chain	Res	Type
2	C	260	LEU
2	C	265	LYS
2	C	276	LYS
2	C	280	LYS
2	C	301	GLU
2	C	323	ASP
2	C	340	MET
2	C	365	ASP
2	C	393	GLN
2	C	394	PHE
2	C	396	ASP
2	C	398	THR
2	C	413	LEU
2	C	421	GLU
2	C	427	VAL
2	C	429	ASP
2	C	430	VAL
2	C	453	THR
2	C	469	THR
2	C	474	VAL
2	C	495	THR
2	C	503	LEU
2	C	523	ILE
2	C	528	GLU
2	C	530	GLU
2	C	543	ASN
2	C	545	ASN
2	C	579	VAL
2	C	600	ASP
2	C	604	VAL
2	C	609	THR
2	C	616	GLU
2	C	703	ILE
2	C	707	ARG
2	C	729	LEU
2	C	738	ASP
2	C	742	ILE
2	C	745	ILE
2	C	749	VAL
2	C	764	GLU
2	C	766	GLU
2	C	774	LEU

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Mol	Chain	Res	Type
2	C	788	THR
2	C	796	GLU
2	C	813	VAL
2	C	814	GLU
2	C	815	LEU
2	C	829	GLN
2	C	857	ASP
2	C	861	LEU
2	C	869	VAL
2	C	870	ILE
2	C	918	LEU
2	C	936	VAL
2	C	946	ARG
2	C	963	LEU
2	C	966	LEU
2	C	974	LEU
2	C	988	VAL
2	C	995	MET
2	C	1001	VAL
2	C	1050	GLN
2	C	1056	LYS
2	C	1058	ASP
2	C	1061	GLU
2	C	1071	ILE
2	C	1081	VAL
2	C	1099	VAL
3	D	3	LYS
3	D	5	VAL
3	D	26	VAL
3	D	38	LYS
3	D	58	CYS
3	D	66	GLN
3	D	68	PHE
3	D	73	CYS
3	D	80	VAL
3	D	92	HIS
3	D	97	THR
3	D	112	ILE
3	D	115	LEU
3	D	133	ILE
3	D	135	LEU
3	D	138	LYS

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Mol	Chain	Res	Type
3	D	141	VAL
3	D	142	LEU
3	D	156	GLU
3	D	166	GLN
3	D	171	LEU
3	D	179	VAL
3	D	184	GLU
3	D	196	VAL
3	D	199	MET
3	D	213	VAL
3	D	232	GLU
3	D	261	LEU
3	D	277	GLU
3	D	297	ILE
3	D	299	GLU
3	D	304	LEU
3	D	306	GLU
3	D	316	HIS
3	D	333	LEU
3	D	334	THR
3	D	343	LYS
3	D	347	VAL
3	D	371	ILE
3	D	387	LEU
3	D	389	GLU
3	D	395	VAL
3	D	397	LYS
3	D	414	ARG
3	D	415	VAL
3	D	420	VAL
3	D	421	LEU
3	D	423	ASP
3	D	430	GLU
3	D	440	VAL
3	D	442	ASN
3	D	448	GLU
3	D	464	LEU
3	D	472	LYS
3	D	480	GLU
3	D	534	ARG
3	D	535	PHE
3	D	557	LEU

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Mol	Chain	Res	Type
3	D	558	LEU
3	D	564	GLU
3	D	597	GLU
3	D	618	LEU
3	D	636	GLN
3	D	637	LEU
3	D	639	LEU
3	D	659	LYS
3	D	682	ASP
3	D	683	ILE
3	D	685	ASP
3	D	687	VAL
3	D	694	VAL
3	D	708	LEU
3	D	709	HIS
3	D	741	ASP
3	D	749	VAL
3	D	776	GLU
3	D	778	LEU
3	D	794	GLN
3	D	795	VAL
3	D	804	MET
3	D	817	GLU
3	D	845	ASN
3	D	865	THR
3	D	903	ASP
3	D	908	LYS
3	D	912	LYS
3	D	914	LEU
3	D	927	THR
3	D	932	ASP
3	D	953	ASP
3	D	955	VAL
3	D	959	GLU
3	D	971	LEU
3	D	976	GLN
3	D	1052	THR
3	D	1053	PHE
3	D	1078	ARG
3	D	1083	ASP
3	D	1098	LEU
3	D	1118	ILE

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Mol	Chain	Res	Type
3	D	1132	LEU
3	D	1134	LEU
3	D	1137	ARG
3	D	1149	LEU
3	D	1158	ARG
3	D	1159	ARG
3	D	1161	GLU
3	D	1234	THR
3	D	1235	GLN
3	D	1237	THR
3	D	1267	ARG
3	D	1269	LYS
3	D	1277	ILE
3	D	1278	ASP
3	D	1285	GLU
3	D	1297	GLU
3	D	1307	LYS
3	D	1311	LEU
3	D	1312	LEU
3	D	1335	LEU
3	D	1346	ARG
3	D	1397	LYS
3	D	1398	TRP
3	D	1407	LEU
3	D	1443	THR
3	D	1448	THR
3	D	1462	LEU
3	D	1464	GLU
3	D	1499	ARG
4	E	3	GLU
4	E	14	ASP
4	E	28	GLN
4	E	39	VAL
4	E	56	ASP
4	E	59	ASN
4	E	62	THR
4	E	65	MET
5	F	96	VAL
5	F	101	HIS
5	F	105	GLN
5	F	151	LEU
5	F	159	ILE

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Mol	Chain	Res	Type
5	F	177	LYS
5	F	189	LEU
5	F	217	TYR
5	F	222	LEU
5	F	224	PHE
5	F	226	ASP
5	F	227	LEU
5	F	255	THR
5	F	260	GLN
5	F	268	ASP
5	F	269	GLN
5	F	274	ARG
5	F	293	LEU
5	F	294	GLN
5	F	305	GLU
5	F	323	LEU
5	F	346	ASP
5	F	352	ASN
5	F	405	PHE
5	F	409	ARG
5	F	424	LYS
5	F	435	ASP
1	G	44	LEU
1	G	56	VAL
1	G	59	GLU
1	G	86	VAL
1	G	87	VAL
1	G	93	LYS
1	G	98	THR
1	G	109	VAL
1	G	142	VAL
1	G	167	VAL
1	G	172	SER
1	G	174	VAL
1	G	186	LEU
1	G	205	VAL
1	H	7	LYS
1	H	30	ARG
1	H	53	VAL
1	H	54	THR
1	H	58	ILE
1	H	75	VAL

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Mol	Chain	Res	Type
1	H	114	PHE
1	H	115	THR
1	H	145	ASP
1	H	158	ILE
1	H	170	ILE
1	H	176	ARG
1	H	177	VAL
1	H	184	THR
1	H	215	VAL
1	H	218	LEU
2	I	15	LEU
2	I	30	LEU
2	I	41	ASN
2	I	45	GLN
2	I	48	PHE
2	I	56	GLU
2	I	73	ILE
2	I	75	ASP
2	I	80	GLN
2	I	100	LEU
2	I	104	ASP
2	I	111	ASP
2	I	112	GLU
2	I	120	LEU
2	I	122	THR
2	I	140	ILE
2	I	142	ARG
2	I	151	ASP
2	I	159	ILE
2	I	163	ILE
2	I	174	LEU
2	I	179	SER
2	I	195	LEU
2	I	197	LEU
2	I	199	VAL
2	I	211	LEU
2	I	217	LEU
2	I	222	LEU
2	I	226	VAL
2	I	237	ARG
2	I	242	LEU
2	I	249	LYS

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Mol	Chain	Res	Type
2	I	251	ASP
2	I	258	PHE
2	I	260	LEU
2	I	265	LYS
2	I	276	LYS
2	I	280	LYS
2	I	301	GLU
2	I	323	ASP
2	I	340	MET
2	I	365	ASP
2	I	393	GLN
2	I	394	PHE
2	I	396	ASP
2	I	398	THR
2	I	413	LEU
2	I	421	GLU
2	I	427	VAL
2	I	429	ASP
2	I	430	VAL
2	I	453	THR
2	I	469	THR
2	I	474	VAL
2	I	495	THR
2	I	503	LEU
2	I	523	ILE
2	I	528	GLU
2	I	530	GLU
2	I	543	ASN
2	I	545	ASN
2	I	579	VAL
2	I	600	ASP
2	I	604	VAL
2	I	609	THR
2	I	616	GLU
2	I	703	ILE
2	I	707	ARG
2	I	729	LEU
2	I	738	ASP
2	I	742	ILE
2	I	745	ILE
2	I	749	VAL
2	I	764	GLU

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Mol	Chain	Res	Type
2	I	766	GLU
2	I	774	LEU
2	I	788	THR
2	I	796	GLU
2	I	813	VAL
2	I	814	GLU
2	I	815	LEU
2	I	829	GLN
2	I	857	ASP
2	I	861	LEU
2	I	869	VAL
2	I	870	ILE
2	I	918	LEU
2	I	936	VAL
2	I	946	ARG
2	I	963	LEU
2	I	966	LEU
2	I	974	LEU
2	I	988	VAL
2	I	995	MET
2	I	1001	VAL
2	I	1050	GLN
2	I	1056	LYS
2	I	1058	ASP
2	I	1061	GLU
2	I	1071	ILE
2	I	1081	VAL
2	I	1099	VAL
3	J	3	LYS
3	J	5	VAL
3	J	26	VAL
3	J	38	LYS
3	J	58	CYS
3	J	66	GLN
3	J	68	PHE
3	J	73	CYS
3	J	80	VAL
3	J	92	HIS
3	J	97	THR
3	J	112	ILE
3	J	115	LEU
3	J	133	ILE

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Mol	Chain	Res	Type
3	J	135	LEU
3	J	138	LYS
3	J	141	VAL
3	J	142	LEU
3	J	156	GLU
3	J	168	THR
3	J	178	LEU
3	J	185	VAL
3	J	186	VAL
3	J	196	VAL
3	J	200	ASP
3	J	350	HIS
3	J	372	ASP
3	J	393	ILE
3	J	397	LYS
3	J	404	GLU
3	J	435	VAL
3	J	443	VAL
3	J	464	LEU
3	J	472	LYS
3	J	480	GLU
3	J	534	ARG
3	J	535	PHE
3	J	557	LEU
3	J	558	LEU
3	J	564	GLU
3	J	597	GLU
3	J	618	LEU
3	J	636	GLN
3	J	637	LEU
3	J	639	LEU
3	J	659	LYS
3	J	682	ASP
3	J	683	ILE
3	J	685	ASP
3	J	687	VAL
3	J	694	VAL
3	J	708	LEU
3	J	709	HIS
3	J	741	ASP
3	J	749	VAL
3	J	776	GLU

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Mol	Chain	Res	Type
3	J	778	LEU
3	J	794	GLN
3	J	795	VAL
3	J	804	MET
3	J	817	GLU
3	J	845	ASN
3	J	865	THR
3	J	903	ASP
3	J	908	LYS
3	J	912	LYS
3	J	914	LEU
3	J	927	THR
3	J	932	ASP
3	J	953	ASP
3	J	955	VAL
3	J	959	GLU
3	J	971	LEU
3	J	976	GLN
3	J	1052	THR
3	J	1053	PHE
3	J	1078	ARG
3	J	1083	ASP
3	J	1098	LEU
3	J	1118	ILE
3	J	1132	LEU
3	J	1134	LEU
3	J	1137	ARG
3	J	1149	LEU
3	J	1158	ARG
3	J	1161	GLU
3	J	1234	THR
3	J	1235	GLN
3	J	1237	THR
3	J	1267	ARG
3	J	1269	LYS
3	J	1277	ILE
3	J	1278	ASP
3	J	1285	GLU
3	J	1297	GLU
3	J	1307	LYS
3	J	1311	LEU
3	J	1312	LEU

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Mol	Chain	Res	Type
3	J	1335	LEU
3	J	1346	ARG
3	J	1397	LYS
3	J	1398	TRP
3	J	1407	LEU
3	J	1443	THR
3	J	1448	THR
3	J	1462	LEU
3	J	1464	GLU
3	J	1499	ARG
4	K	3	GLU
4	K	14	ASP
4	K	28	GLN
4	K	39	VAL
4	K	56	ASP
4	K	59	ASN
4	K	62	THR
4	K	65	MET
5	L	96	VAL
5	L	101	HIS
5	L	105	GLN
5	L	151	LEU
5	L	159	ILE
5	L	177	LYS
5	L	189	LEU
5	L	217	TYR
5	L	222	LEU
5	L	224	PHE
5	L	226	ASP
5	L	227	LEU
5	L	255	THR
5	L	260	GLN
5	L	268	ASP
5	L	269	GLN
5	L	274	ARG
5	L	293	LEU
5	L	294	GLN
5	L	305	GLU
5	L	323	LEU
5	L	328	GLU
5	L	346	ASP
5	L	352	ASN

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Mol	Chain	Res	Type
5	L	405	PHE
5	L	409	ARG
5	L	426	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	212	ASN
1	A	213	GLN
1	A	223	ASN
1	B	156	HIS
1	B	213	GLN
1	B	227	ASN
2	C	45	GLN
2	C	80	GLN
2	C	102	HIS
2	C	872	ASN
2	C	899	GLN
2	C	991	GLN
2	C	999	HIS
2	C	1050	GLN
2	C	1068	GLN
2	C	1107	ASN
3	D	66	GLN
3	D	166	GLN
3	D	274	GLN
3	D	332	HIS
3	D	442	ASN
3	D	549	ASN
3	D	714	GLN
3	D	794	GLN
3	D	991	GLN
3	D	1010	ASN
3	D	1046	GLN
3	D	1075	HIS
3	D	1235	GLN
3	D	1485	GLN
4	E	59	ASN
5	F	98	GLN
5	F	101	HIS
5	F	229	GLN

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Mol	Chain	Res	Type
5	F	232	ASN
5	F	260	GLN
5	F	269	GLN
5	F	295	GLN
5	F	352	ASN
5	F	414	GLN
5	F	417	ASN
1	G	19	HIS
1	G	212	ASN
1	G	213	GLN
1	G	223	ASN
1	H	213	GLN
2	I	45	GLN
2	I	80	GLN
2	I	102	HIS
2	I	498	GLN
2	I	632	ASN
2	I	765	GLN
2	I	899	GLN
2	I	991	GLN
2	I	1018	GLN
2	I	1050	GLN
2	I	1068	GLN
2	I	1107	ASN
3	J	66	GLN
3	J	166	GLN
3	J	350	HIS
3	J	549	ASN
3	J	714	GLN
3	J	794	GLN
3	J	973	GLN
3	J	991	GLN
3	J	1010	ASN
3	J	1046	GLN
3	J	1075	HIS
3	J	1485	GLN
5	L	98	GLN
5	L	101	HIS
5	L	229	GLN
5	L	232	ASN
5	L	260	GLN
5	L	269	GLN

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Mol	Chain	Res	Type
5	L	295	GLN
5	L	417	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	Q	3/4 (75%)	1 (33%)	0
8	T	3/4 (75%)	1 (33%)	0
All	All	6/8 (75%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	Q	2	C
8	T	2	C

There are no RNA pucker outliers to report.

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	227/314 (72%)	0.26	1 (0%) 88 75	68, 121, 176, 228	0
1	B	227/314 (72%)	0.13	4 (1%) 67 50	42, 95, 150, 180	0
1	G	227/314 (72%)	0.65	14 (6%) 26 24	96, 156, 194, 223	0
1	H	227/314 (72%)	0.40	5 (2%) 62 46	80, 131, 171, 192	0
2	C	1112/1119 (99%)	0.30	18 (1%) 70 52	30, 123, 203, 260	0
2	I	1112/1119 (99%)	0.51	40 (3%) 46 35	60, 146, 214, 259	0
3	D	1490/1524 (97%)	0.06	9 (0%) 85 71	22, 88, 155, 231	0
3	J	1367/1524 (89%)	0.24	16 (1%) 76 59	29, 112, 177, 240	0
4	E	93/99 (93%)	0.09	1 (1%) 78 60	23, 89, 154, 187	0
4	K	93/99 (93%)	0.39	1 (1%) 78 60	67, 126, 181, 236	0
5	F	347/347 (100%)	0.40	13 (3%) 45 34	52, 131, 221, 275	0
5	L	347/347 (100%)	0.58	23 (6%) 24 22	81, 151, 225, 270	0
6	O	48/48 (100%)	0.51	0 100 100	86, 193, 267, 293	0
6	R	48/48 (100%)	0.56	0 100 100	109, 184, 277, 300	0
7	P	48/48 (100%)	0.61	0 100 100	77, 199, 251, 283	0
7	S	43/48 (89%)	0.55	1 (2%) 61 45	100, 195, 234, 248	0
8	Q	4/4 (100%)	-0.23	0 100 100	116, 124, 128, 150	0
8	T	4/4 (100%)	-0.08	0 100 100	122, 130, 143, 154	0
All	All	7064/7634 (92%)	0.30	146 (2%) 63 47	22, 120, 200, 300	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	159	ILE	4.7
4	E	94	PRO	4.4
5	L	159	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
5	F	416	GLU	4.1
2	I	62	GLY	4.0
5	F	92	THR	3.8
2	I	207	LEU	3.7
5	F	409	ARG	3.7
2	I	368	THR	3.6
5	F	154	ALA	3.5
3	J	35	ARG	3.5
5	L	177	LYS	3.3
5	L	93	SER	3.3
5	F	155	ARG	3.3
5	L	151	LEU	3.2
1	G	187	GLY	3.2
2	I	107	LEU	3.2
5	L	399	GLU	3.1
2	I	296	GLY	3.1
3	D	1253	THR	3.1
5	L	162	LEU	3.0
1	G	52	ALA	3.0
1	H	66	SER	3.0
2	I	248	PRO	3.0
3	J	723	GLY	3.0
1	B	230	ALA	3.0
2	I	645	VAL	3.0
5	L	155	ARG	2.9
2	C	62	GLY	2.9
5	F	153	THR	2.9
5	L	92	THR	2.9
3	D	1503	VAL	2.9
2	I	361	MET	2.9
5	L	223	SER	2.9
2	C	368	THR	2.8
2	I	826	PHE	2.8
3	J	718	PRO	2.7
2	C	296	GLY	2.7
5	F	156	ILE	2.7
2	C	220	GLY	2.7
2	I	63	GLY	2.6
3	J	1017	PHE	2.6
3	D	65	ARG	2.6
2	I	246	ASP	2.6
1	H	178	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	361	MET	2.6
2	I	445	GLU	2.5
2	C	250	LYS	2.5
2	I	335	THR	2.5
5	L	216	LYS	2.5
2	C	179	SER	2.5
2	I	245	GLY	2.5
1	G	170	ILE	2.5
2	C	261	LEU	2.5
3	J	36	THR	2.5
5	L	221	GLY	2.5
2	I	500	ASN	2.5
3	J	556	LYS	2.5
2	I	503	LEU	2.5
5	L	426	HIS	2.5
1	B	190	THR	2.4
2	I	25	SER	2.4
1	G	53	VAL	2.4
5	F	162	LEU	2.4
5	L	178	LEU	2.4
1	G	30	ARG	2.4
5	L	160	PRO	2.4
2	I	255	ALA	2.4
5	L	153	THR	2.4
1	G	230	ALA	2.4
5	L	154	ALA	2.4
2	C	190	LYS	2.4
1	A	29	GLU	2.4
2	I	306	THR	2.4
2	I	366	THR	2.4
2	I	194	VAL	2.3
2	C	374	ASN	2.3
2	C	362	GLY	2.3
2	I	362	GLY	2.3
3	J	546	ARG	2.3
5	F	346	ASP	2.3
1	G	162	ILE	2.3
2	I	782	ALA	2.3
1	G	67	THR	2.3
1	B	232	LEU	2.3
2	I	52	PHE	2.3
3	J	589	SER	2.3

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Mol	Chain	Res	Type	RSRZ
7	S	18	DG	2.3
1	G	95	ALA	2.3
2	I	960	GLU	2.3
3	J	722	GLU	2.3
1	H	230	ALA	2.3
5	L	346	ASP	2.3
2	I	28	LYS	2.3
2	C	766	GLU	2.2
2	I	708	TYR	2.2
1	G	98	THR	2.2
1	H	67	THR	2.2
2	C	63	GLY	2.2
2	C	364	PRO	2.2
5	F	412	ILE	2.2
5	F	151	LEU	2.2
2	I	182	VAL	2.2
2	I	220	GLY	2.2
3	D	1040	GLY	2.2
1	G	204	SER	2.2
2	I	851	LYS	2.2
3	D	406	ASP	2.2
3	J	216	LEU	2.2
2	I	377	PRO	2.1
3	D	1504	GLU	2.1
2	I	439	CYS	2.1
3	J	968	ASP	2.1
5	L	107	PRO	2.1
3	D	241	VAL	2.1
2	I	180	GLY	2.1
2	C	475	LYS	2.1
2	C	808	ARG	2.1
5	L	259	ARG	2.1
3	J	1345	GLU	2.1
3	J	55	ASP	2.1
2	I	254	LEU	2.1
2	I	781	LYS	2.1
4	K	94	PRO	2.1
3	J	647	ARG	2.1
3	J	696	HIS	2.1
1	G	131	THR	2.1
2	C	306	THR	2.1
2	I	364	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
5	L	230	GLU	2.1
1	G	24	VAL	2.1
2	I	365	ASP	2.0
2	I	1003	ASP	2.0
5	L	156	ILE	2.0
5	L	170	THR	2.0
3	J	1490	ARG	2.0
1	B	63	HIS	2.0
2	I	419	THR	2.0
3	D	1237	THR	2.0
1	G	55	SER	2.0
1	H	233	LEU	2.0
5	F	178	LEU	2.0
2	I	415	PRO	2.0
5	L	256	TRP	2.0
2	C	56	GLU	2.0
3	D	296	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
10	MG	D	2003	1/1	0.96	0.07	180,180,180,180	0
10	MG	J	2003	1/1	0.96	0.06	188,188,188,188	0
9	ZN	J	2002	1/1	0.97	0.06	166,166,166,166	0
9	ZN	D	2002	1/1	0.98	0.04	79,79,79,79	0
9	ZN	J	2001	1/1	0.99	0.05	97,97,97,97	0
9	ZN	D	2001	1/1	1.00	0.05	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.