



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:40 am BST

PDB ID : 4LJZ
Title : Crystal Structure Analysis of the E.coli holoenzyme
Authors : Bae, B.; Darst, S.A.
Deposited on : 2013-07-05
Resolution : 3.59 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

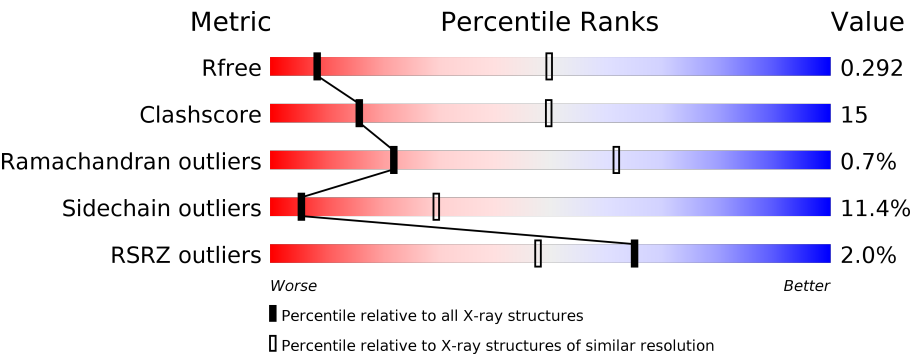
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	239	<div><div></div><div>60%29%6%</div></div>
1	B	239	<div>4%</div> <div><div></div><div>50%38%8%</div></div>
1	G	239	<div>%</div> <div><div></div><div>62%29%5%</div></div>
1	H	239	<div>5%</div> <div><div></div><div>48%38%5%9%</div></div>
2	C	1342	<div></div> <div><div></div><div>62%32%5%</div></div>
2	I	1342	<div>2%</div> <div><div></div><div>64%31%5%</div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ZN	J	1503	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 56339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 20 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1325	Total	C	N	O	S	0	0	0
			10295	6470	1831	1945	49			

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

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

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

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

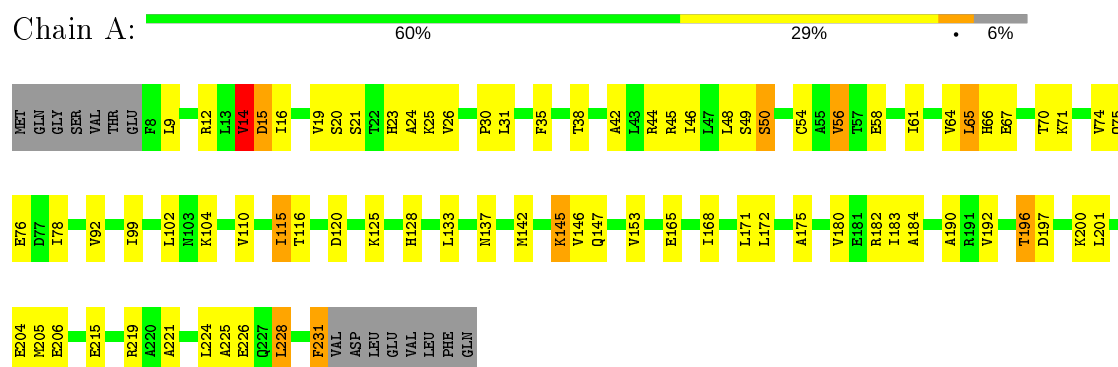
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

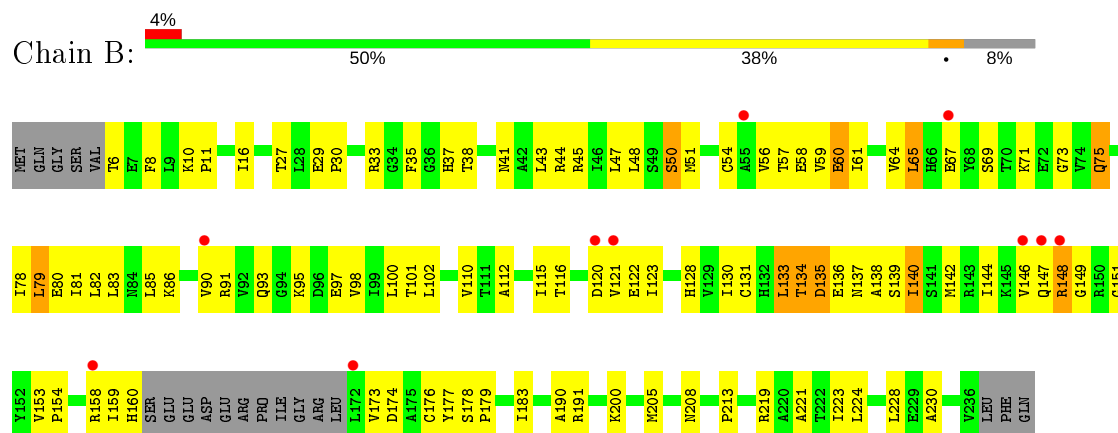
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

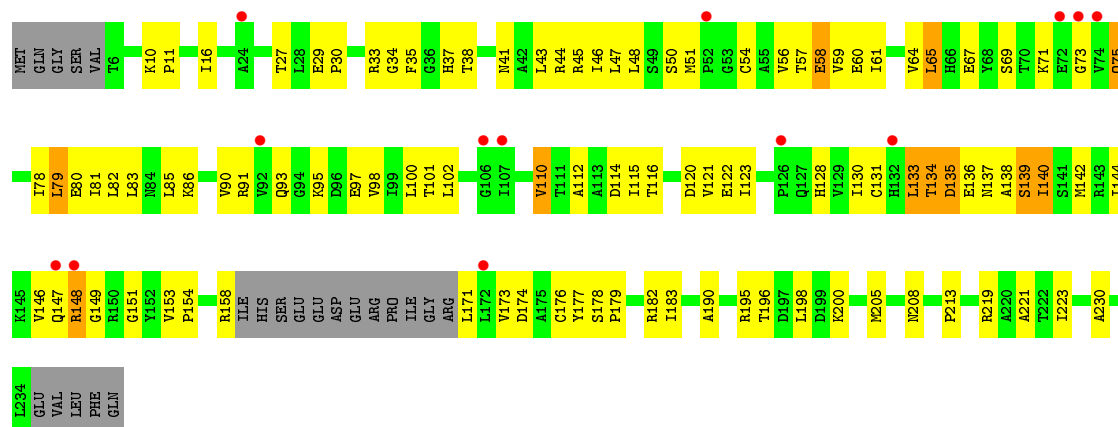


• Molecule 1: DNA-directed RNA polymerase subunit alpha

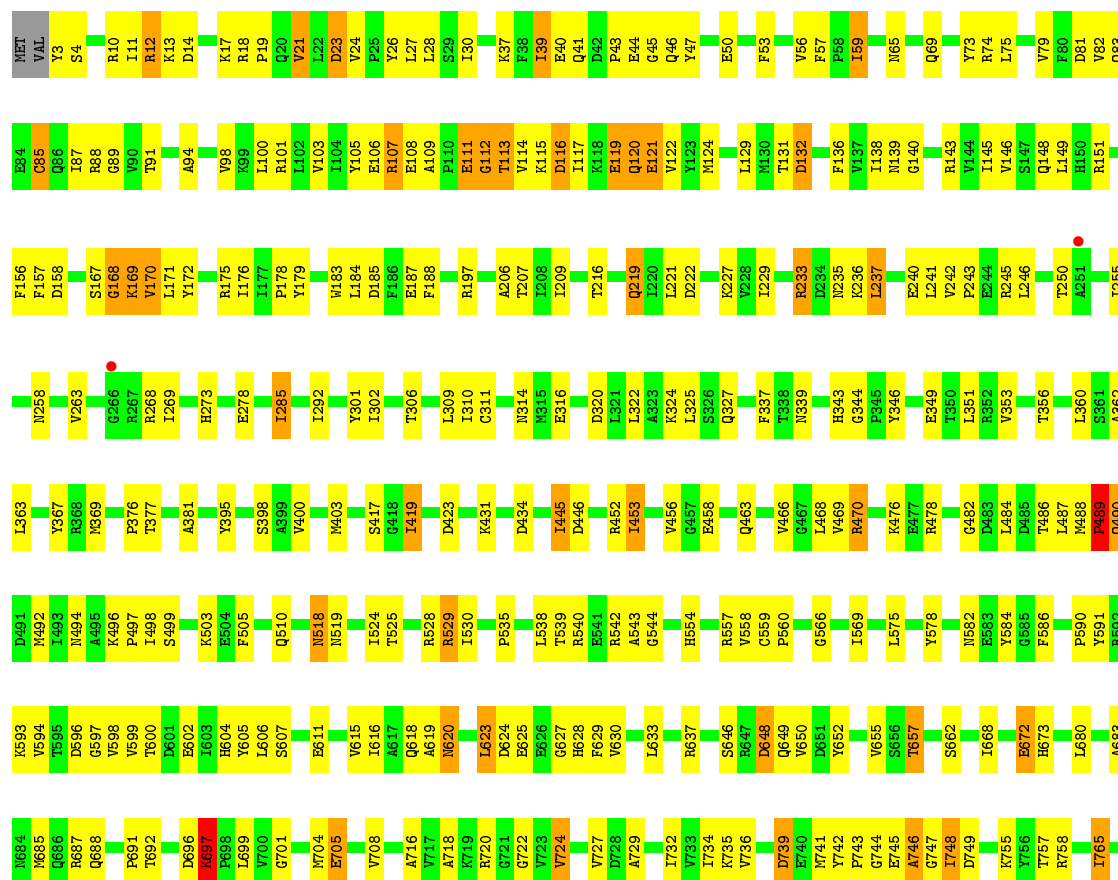


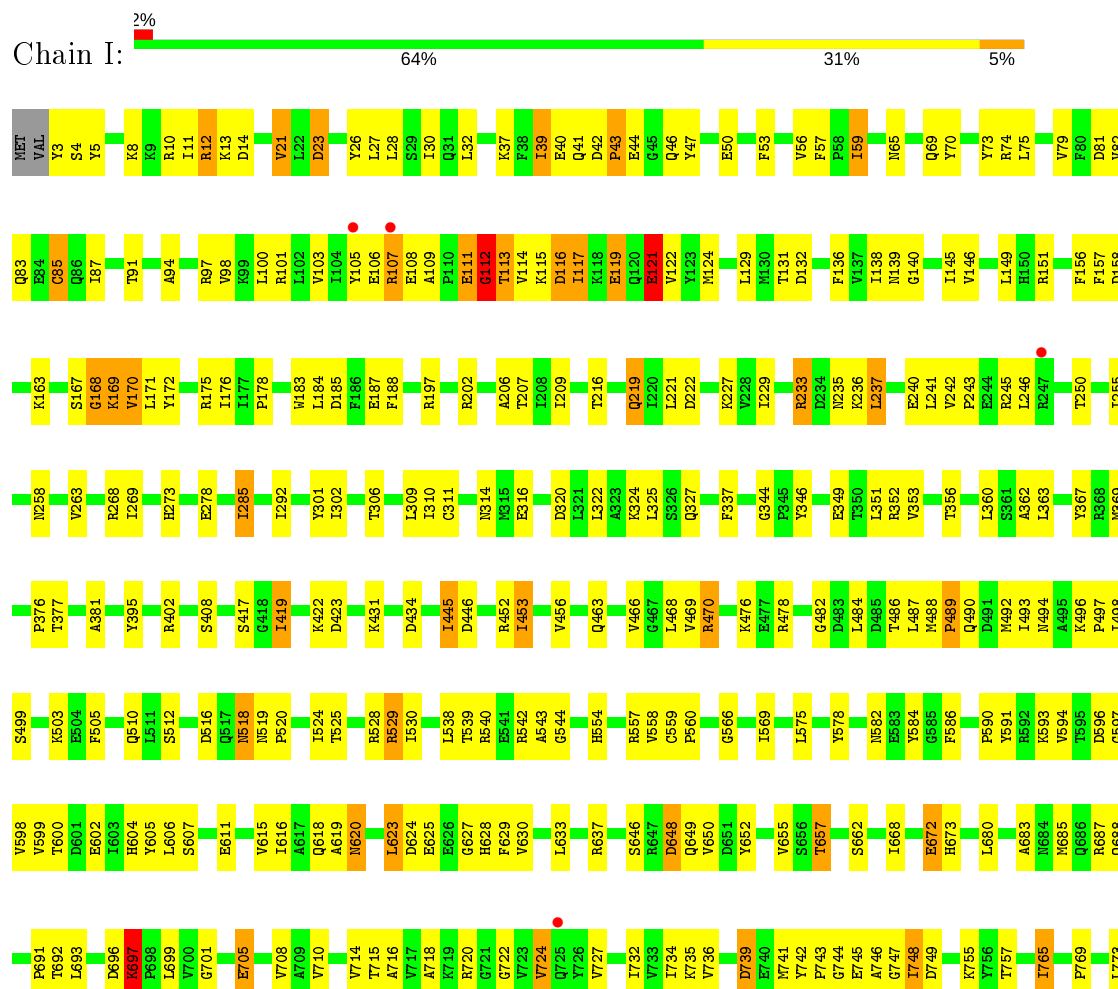


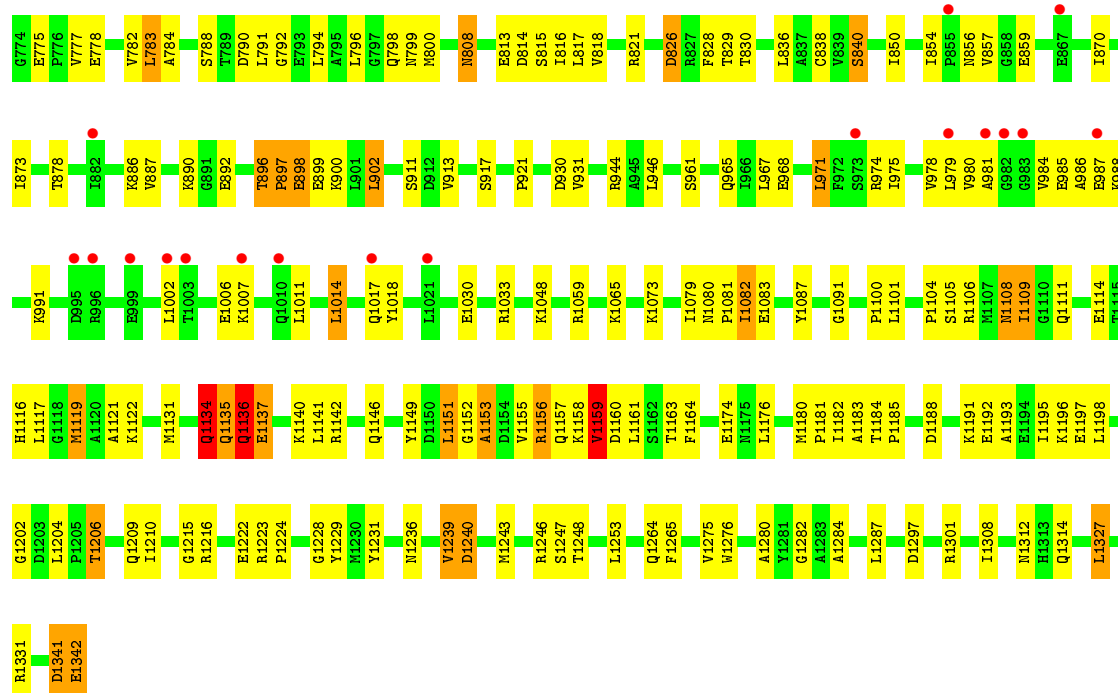
• Molecule 1: DNA-directed RNA polymerase subunit alpha



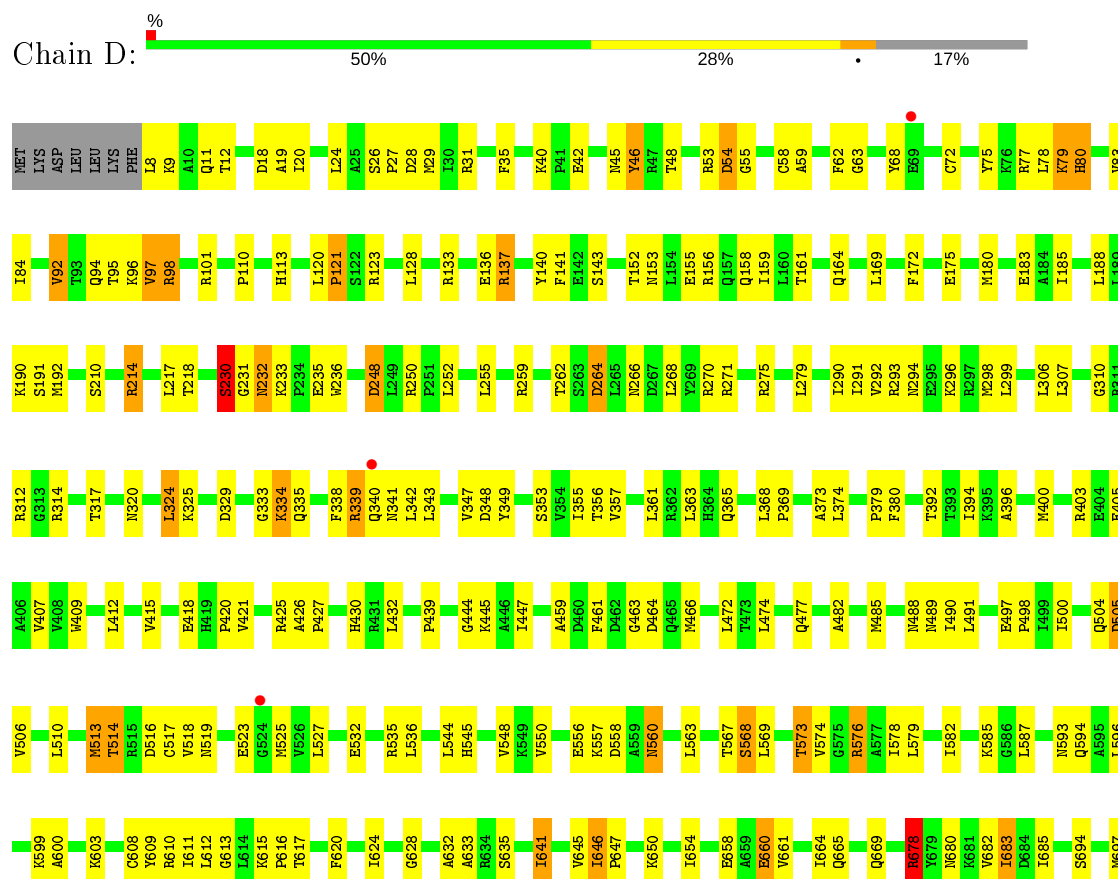
• Molecule 2: DNA-directed RNA polymerase subunit beta

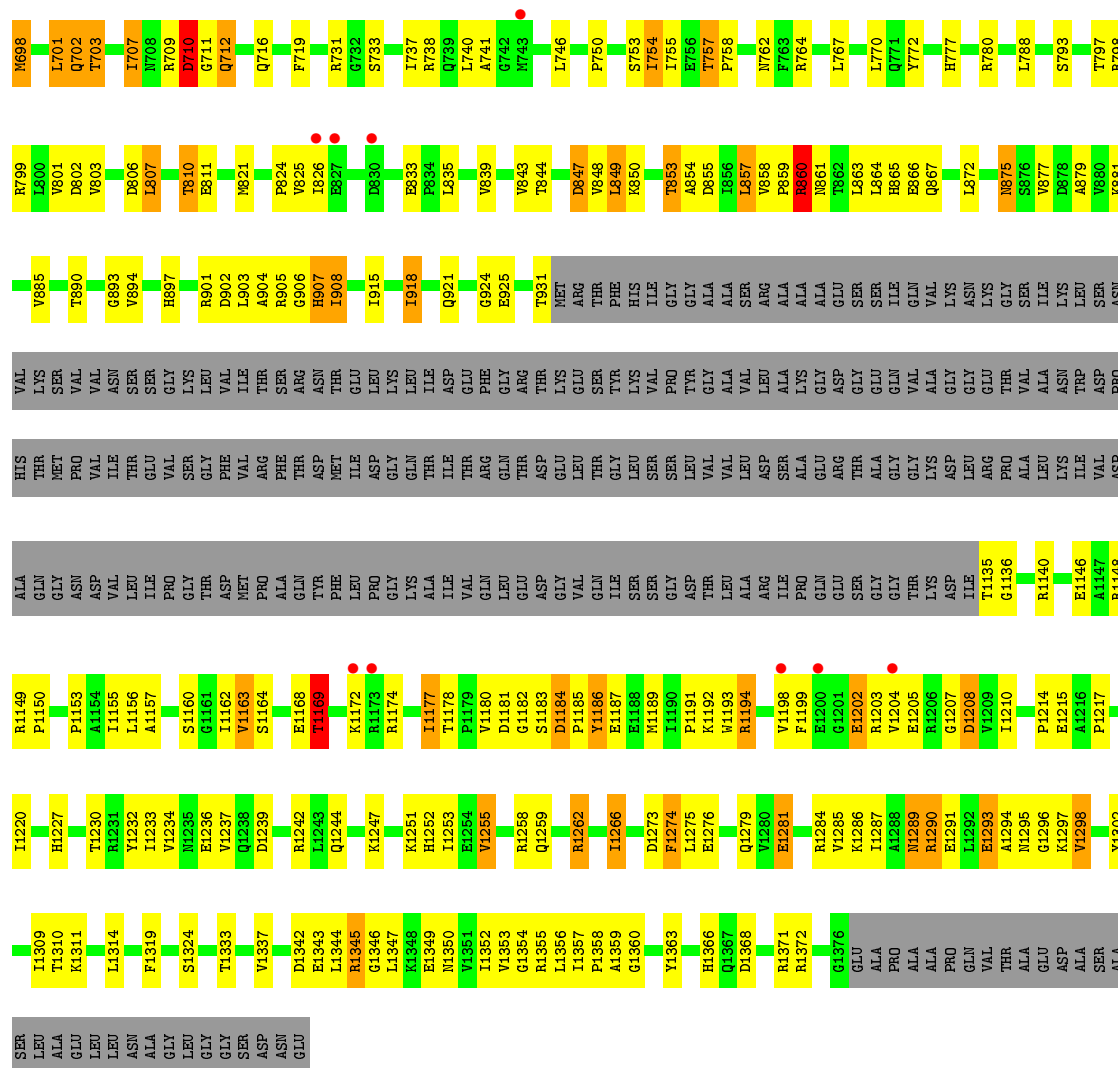




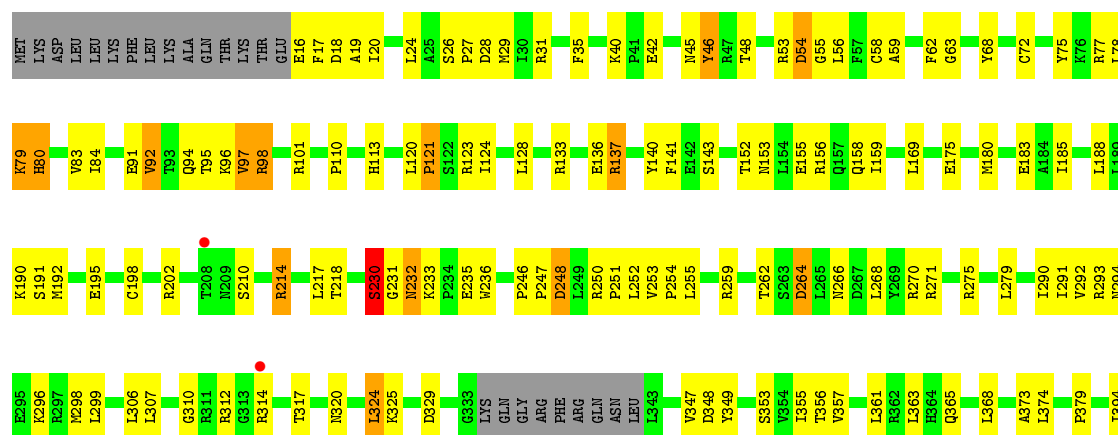


• Molecule 3: DNA-directed RNA polymerase subunit beta'

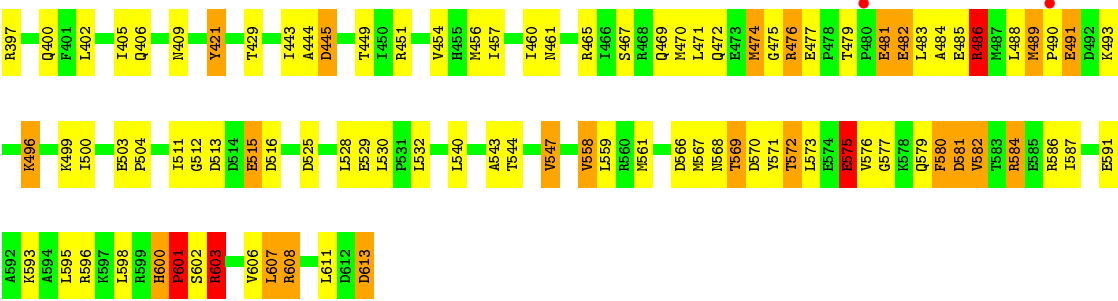




• Molecule 3: DNA-directed RNA polymerase subunit beta'







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.37Å 206.74Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.59 29.88 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.88-3.59) 99.3 (29.88-3.59)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.246 , 0.288 0.247 , 0.292	Depositor DCC
R_{free} test set	6971 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	122.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	56339	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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	0.28	0/1751	0.59	1/2373 (0.0%)
1	B	0.28	0/1707	0.58	1/2314 (0.0%)
1	G	0.30	0/1771	0.61	2/2401 (0.1%)
1	H	0.28	0/1686	0.59	1/2285 (0.0%)
2	C	0.30	0/10739	0.59	6/14489 (0.0%)
2	I	0.30	0/10735	0.58	7/14484 (0.0%)
3	D	0.28	0/9246	0.59	5/12478 (0.0%)
3	J	0.28	0/10450	0.56	2/14112 (0.0%)
4	E	0.27	0/693	0.58	1/935 (0.1%)
4	K	0.28	0/629	0.54	0/847
5	F	0.36	1/3873 (0.0%)	0.62	7/5206 (0.1%)
5	L	0.35	0/3872	0.63	6/5205 (0.1%)
All	All	0.30	1/57152 (0.0%)	0.59	39/77129 (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	1
1	G	0	1
1	H	0	1
2	C	0	14
2	I	0	15
3	D	0	5
3	J	0	6
4	K	0	1
5	F	0	4
5	L	0	2
All	All	0	50

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	600	HIS	N-CA	5.34	1.57	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	747	GLY	N-CA-C	14.60	149.61	113.10
2	I	747	GLY	N-CA-C	11.86	142.76	113.10
3	D	1262	ARG	NE-CZ-NH1	-7.19	116.70	120.30
2	I	112	GLY	N-CA-C	6.85	130.22	113.10
3	D	860	ARG	NE-CZ-NH1	6.80	123.70	120.30
3	D	231	GLY	N-CA-C	6.56	129.50	113.10
2	C	490	GLN	N-CA-C	6.40	128.28	111.00
3	J	678	ARG	CA-CB-CG	6.38	127.43	113.40
3	J	860	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	D	678	ARG	CA-CB-CG	6.11	126.85	113.40
1	B	75	GLN	CA-CB-CG	6.01	126.62	113.40
5	F	608	ARG	CG-CD-NE	5.90	124.20	111.80
1	A	65	LEU	CA-CB-CG	5.88	128.83	115.30
5	L	575	GLU	CA-CB-CG	5.87	126.31	113.40
5	F	486	ARG	CB-CG-CD	5.86	126.85	111.60
1	G	65	LEU	CA-CB-CG	5.77	128.57	115.30
5	F	575	GLU	CA-CB-CG	5.64	125.81	113.40
1	H	75	GLN	CA-CB-CG	5.63	125.78	113.40
1	G	232	VAL	N-CA-C	5.49	125.83	111.00
3	D	230	SER	N-CA-C	5.44	125.70	111.00
2	C	237	LEU	N-CA-C	5.41	125.60	111.00
5	L	608	ARG	CG-CD-NE	5.40	123.15	111.80
4	E	15	ASN	N-CA-CB	-5.39	100.91	110.60
5	F	601	PRO	C-N-CA	5.38	135.15	121.70
2	I	237	LEU	N-CA-C	5.38	125.53	111.00
5	L	584	ARG	N-CA-C	5.35	125.44	111.00
2	C	1152	GLY	C-N-CA	5.33	135.03	121.70
5	F	149	ASP	CB-CG-OD2	5.23	123.01	118.30
5	L	149	ASP	CB-CG-OD2	5.22	123.00	118.30
5	L	166	VAL	N-CA-C	-5.19	97.00	111.00
2	I	516	ASP	CB-CG-OD2	5.18	122.96	118.30
5	F	166	VAL	N-CA-C	-5.15	97.09	111.00
2	I	1264	GLN	N-CA-C	-5.08	97.28	111.00
5	F	584	ARG	N-CA-CB	5.07	119.73	110.60
2	I	1134	GLN	C-N-CA	5.06	134.34	121.70
2	I	1135	GLN	N-CA-CB	-5.05	101.51	110.60
2	C	45	GLY	N-CA-C	5.04	125.70	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	486	ARG	CB-CG-CD	5.02	124.66	111.60
2	C	1264	GLN	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ILE	Peptide
2	C	109	ALA	Peptide
2	C	111	GLU	Peptide
2	C	112	GLY	Peptide
2	C	1134	GLN	Peptide
2	C	1152	GLY	Mainchain
2	C	1202	GLY	Mainchain,Peptide
2	C	168	GLY	Mainchain
2	C	236	LYS	Peptide
2	C	43	PRO	Mainchain
2	C	489	PRO	Peptide
2	C	648	ASP	Peptide
2	C	746	ALA	Peptide
2	C	985	GLU	Mainchain
3	D	1168	GLU	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
3	D	172	PHE	Mainchain
3	D	230	SER	Peptide
5	F	474	MET	Mainchain,Peptide
5	F	601	PRO	Peptide
5	F	602	SER	Mainchain
1	G	231	PHE	Peptide
1	H	140	ILE	Peptide
2	I	109	ALA	Peptide
2	I	111	GLU	Peptide
2	I	112	GLY	Peptide
2	I	1134	GLN	Peptide
2	I	1136	GLN	Peptide
2	I	1152	GLY	Mainchain
2	I	1153	ALA	Peptide
2	I	1202	GLY	Mainchain,Peptide
2	I	1236	ASN	Peptide
2	I	168	GLY	Mainchain
2	I	236	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	I	43	PRO	Mainchain
2	I	489	PRO	Peptide
2	I	648	ASP	Peptide
3	J	1168	GLU	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
3	J	1359	ALA	Mainchain
3	J	230	SER	Mainchain,Peptide
4	K	14	GLY	Mainchain
5	L	474	MET	Mainchain
5	L	601	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1730	0	1756	54	0
1	B	1687	0	1700	70	0
1	G	1750	0	1764	52	0
1	H	1667	0	1689	71	0
2	C	10570	0	10582	305	1
2	I	10566	0	10576	284	1
3	D	9107	0	9308	331	0
3	J	10295	0	10511	386	0
4	E	691	0	695	21	0
4	K	627	0	634	18	0
5	F	3822	0	3885	98	0
5	L	3821	0	3884	106	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	56339	0	56984	1652	1

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 15.

All (1652) 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)
2:C:233:ARG:HH11	2:C:233:ARG:HG3	1.24	1.02
3:D:26:SER:HA	3:D:236:TRP:HE1	1.30	0.96
3:J:98:ARG:HH11	3:J:98:ARG:HG2	1.32	0.94
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.51	0.93
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.51	0.92
3:D:98:ARG:HG2	3:D:98:ARG:HH11	1.35	0.89
2:C:898:GLU:HB3	5:F:544:THR:HG21	1.57	0.87
3:D:418:GLU:HG3	4:E:45:LYS:H	1.40	0.86
3:J:26:SER:HA	3:J:236:TRP:HE1	1.39	0.86
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.57	0.85
3:D:26:SER:HA	3:D:236:TRP:NE1	1.89	0.85
5:L:569:THR:OG1	5:L:570:ASP:N	2.09	0.85
2:I:119:GLU:HB2	2:I:489:PRO:HD2	1.57	0.85
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.59	0.84
3:J:26:SER:HA	3:J:236:TRP:NE1	1.91	0.84
3:J:418:GLU:HG3	4:K:45:LYS:H	1.40	0.84
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.84
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.61	0.82
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.61	0.82
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.61	0.82
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.60	0.81
5:F:569:THR:OG1	5:F:570:ASP:N	2.14	0.81
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.62	0.81
2:I:452:ARG:NH1	2:I:584:TYR:O	2.13	0.81
2:C:452:ARG:NH1	2:C:584:TYR:O	2.14	0.80
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.62	0.80
1:A:231:PHE:HZ	1:B:221:ALA:HB3	1.45	0.80
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.45	0.79
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.64	0.79
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.63	0.79
5:L:474:MET:O	5:L:476:ARG:N	2.15	0.79
2:I:112:GLY:HA3	2:I:113:THR:HG23	1.65	0.78
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.64	0.78
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.66	0.78
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.49	0.77
5:F:474:MET:O	5:F:476:ARG:N	2.14	0.77
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.67	0.77
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.66	0.77
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.66	0.76
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.51	0.76
2:I:685:MET:HA	2:I:688:GLN:HE21	1.51	0.75
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.69	0.75
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.51	0.75
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.51	0.75
3:J:893:GLY:O	3:J:1258:ARG:NH1	2.18	0.75
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.68	0.74
3:J:310:GLY:HA2	3:J:314:ARG:HG2	1.69	0.74
3:D:310:GLY:HA2	3:D:314:ARG:HG2	1.69	0.74
2:C:685:MET:HA	2:C:688:GLN:HE21	1.52	0.74
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.69	0.74
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.67	0.74
2:C:168:GLY:O	2:C:170:VAL:N	2.20	0.74
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.70	0.74
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.70	0.74
2:I:1156:ARG:HB2	2:I:1156:ARG:HH11	1.53	0.74
2:I:168:GLY:O	2:I:170:VAL:N	2.19	0.74
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.68	0.74
3:J:1108:GLN:NE2	3:J:1120:THR:OG1	2.21	0.73
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.24	0.73
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.70	0.73
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.21	0.73
3:J:79:LYS:HB2	5:L:569:THR:H	1.53	0.73
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.70	0.73
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.54	0.73
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.24	0.72
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.70	0.72
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.71	0.72
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.71	0.72
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.71	0.72
2:C:23:ASP:N	2:C:23:ASP:OD1	2.21	0.72
2:C:739:ASP:OD1	2:C:739:ASP:N	2.21	0.72
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.54	0.72
2:I:23:ASP:N	2:I:23:ASP:OD1	2.21	0.72
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.71	0.72
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.72	0.72
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.72	0.72
2:I:560:PRO:O	3:J:780:ARG:NH2	2.23	0.72
2:C:620:ASN:C	2:C:620:ASN:HD22	1.93	0.72
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.70	0.71
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.55	0.71
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.23	0.71
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:THR:OG1	1:G:197:ASP:OD1	2.08	0.71
2:C:560:PRO:O	3:D:780:ARG:NH2	2.24	0.71
3:D:893:GLY:O	3:D:1258:ARG:NH1	2.19	0.71
2:I:898:GLU:HB3	5:L:544:THR:HG21	1.72	0.71
1:A:196:THR:OG1	1:A:197:ASP:OD1	2.09	0.71
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.71	0.71
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.72	0.70
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.55	0.70
3:J:16:GLU:HG3	3:J:17:PHE:H	1.56	0.70
3:J:1359:ALA:O	3:J:1363:TYR:HB2	1.92	0.70
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.74	0.70
3:D:710:ASP:OD1	3:D:711:GLY:N	2.25	0.70
2:C:88:ARG:NE	2:C:1040:ASP:OD1	2.22	0.70
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.73	0.70
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.72	0.69
3:J:233:LYS:H	3:J:236:TRP:HE3	1.40	0.69
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.72	0.69
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.75	0.69
1:B:93:GLN:HB2	1:B:120:ASP:HB3	1.74	0.69
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.73	0.69
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.75	0.69
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.73	0.69
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.75	0.69
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.22	0.69
2:I:74:ARG:NH1	2:I:121:GLU:OE2	2.18	0.69
3:D:233:LYS:H	3:D:236:TRP:HE3	1.39	0.69
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.75	0.69
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.25	0.69
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.74	0.69
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.75	0.69
3:J:1034:PHE:HA	3:J:1114:GLN:HA	1.75	0.69
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.27	0.68
1:G:56:VAL:HG23	1:G:146:VAL:HG22	1.76	0.68
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.25	0.68
3:J:1064:SER:HA	3:J:1067:ARG:HD2	1.74	0.68
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.59	0.68
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.75	0.68
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.59	0.68
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.76	0.68
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.73	0.68
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:140:TYR:OH	3:J:312:ARG:NH1	2.27	0.67
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.27	0.67
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.76	0.67
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.77	0.67
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.76	0.67
5:L:97:PRO:HA	5:L:100:MET:HG3	1.76	0.67
5:F:97:PRO:HA	5:F:100:MET:HG3	1.77	0.67
3:J:27:PRO:HD3	3:J:236:TRP:HE1	1.58	0.67
1:A:196:THR:OG1	1:A:197:ASP:N	2.28	0.67
1:A:56:VAL:HG23	1:A:146:VAL:HG22	1.76	0.67
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.75	0.67
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.76	0.67
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.77	0.67
2:I:739:ASP:N	2:I:739:ASP:OD1	2.22	0.67
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.77	0.67
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.76	0.67
2:C:233:ARG:NH1	2:C:233:ARG:HG3	2.03	0.67
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.76	0.66
5:L:561:MET:HA	5:L:567:MET:HE1	1.76	0.66
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.59	0.66
2:C:237:LEU:HD11	2:C:292:ILE:HD11	1.76	0.66
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.77	0.66
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.28	0.66
1:G:215:GLU:OE2	1:G:219:ARG:NH2	2.28	0.66
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.59	0.66
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.76	0.66
2:I:237:LEU:HD11	2:I:292:ILE:HD11	1.76	0.65
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.78	0.65
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.60	0.65
3:D:573:THR:H	3:D:576:ARG:HG3	1.62	0.65
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.60	0.65
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.77	0.65
1:G:196:THR:OG1	1:G:197:ASP:N	2.29	0.65
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.19	0.65
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.79	0.65
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.77	0.65
3:D:1297:LYS:HG2	3:J:1302:TYR:O	1.97	0.65
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.79	0.65
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.78	0.65
1:A:231:PHE:CZ	1:B:221:ALA:HB3	2.29	0.65
3:J:482:ALA:HA	4:K:6:VAL:HG11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.79	0.65
3:J:573:THR:H	3:J:576:ARG:HG3	1.61	0.65
3:D:9:LYS:HE3	3:D:12:THR:HG23	1.80	0.64
3:D:54:ASP:N	3:D:54:ASP:OD1	2.30	0.64
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.79	0.64
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.78	0.64
3:J:674:THR:O	3:J:678:ARG:HB3	1.97	0.64
5:F:561:MET:HA	5:F:567:MET:HE1	1.79	0.64
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.30	0.64
3:D:482:ALA:HA	4:E:6:VAL:HG11	1.79	0.64
3:D:576:ARG:NH1	3:D:593:ASN:O	2.31	0.64
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.28	0.64
2:I:39:ILE:HD11	2:I:75:LEU:HG	1.79	0.63
3:J:613:GLY:O	3:J:617:THR:OG1	2.17	0.63
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.79	0.63
2:C:250:THR:HA	2:C:268:ARG:HA	1.81	0.63
3:J:576:ARG:NH1	3:J:593:ASN:O	2.31	0.63
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.30	0.63
5:L:543:ALA:HB1	5:L:607:LEU:HD22	1.80	0.63
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.80	0.63
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.79	0.63
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.81	0.63
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.80	0.63
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.28	0.63
3:D:1297:LYS:HB3	3:J:1303:SER:HA	1.79	0.63
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.81	0.63
3:J:741:ALA:O	3:J:762:ASN:ND2	2.32	0.63
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.80	0.63
3:J:54:ASP:N	3:J:54:ASP:OD1	2.30	0.63
5:L:577:GLY:O	5:L:581:ASP:N	2.32	0.63
4:E:15:ASN:ND2	4:E:18:ASP:OD2	2.32	0.62
1:H:182:ARG:NH1	3:J:581:MET:SD	2.72	0.62
2:I:250:THR:HA	2:I:268:ARG:HA	1.81	0.62
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.32	0.62
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.80	0.62
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.80	0.62
3:D:27:PRO:HD3	3:D:236:TRP:HE1	1.63	0.62
3:D:741:ALA:O	3:D:762:ASN:ND2	2.32	0.62
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.80	0.62
2:C:886:LYS:H	2:C:917:SER:HB3	1.64	0.62
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.80	0.62
2:C:136:PHE:O	2:C:143:ARG:N	2.26	0.62
1:H:93:GLN:HB2	1:H:120:ASP:HB3	1.80	0.62
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.80	0.62
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.80	0.62
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.81	0.62
2:C:701:GLY:O	2:C:1184:THR:N	2.28	0.62
2:I:980:VAL:HA	2:I:984:VAL:HA	1.82	0.62
3:J:136:GLU:OE2	3:J:312:ARG:NH1	2.33	0.62
2:C:40:GLU:O	2:C:73:TYR:OH	2.16	0.62
5:F:310:GLU:O	5:F:344:LEU:HD21	2.00	0.62
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.65	0.62
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.33	0.62
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.80	0.62
2:I:705:GLU:HB2	2:I:794:LEU:H	1.64	0.62
5:L:310:GLU:O	5:L:344:LEU:HD21	2.00	0.62
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.32	0.62
2:C:705:GLU:HB2	2:C:794:LEU:H	1.65	0.62
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.33	0.61
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.33	0.61
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.82	0.61
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.27	0.61
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.82	0.61
5:L:600:HIS:HD2	5:L:601:PRO:HD3	1.65	0.61
5:L:94:THR:OG1	5:L:95:THR:N	2.33	0.61
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.82	0.61
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.34	0.61
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.80	0.61
2:I:40:GLU:O	2:I:73:TYR:OH	2.17	0.61
3:J:698:MET:O	3:J:702:GLN:HB3	2.01	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.65	0.61
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.34	0.61
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.81	0.61
2:I:886:LYS:H	2:I:917:SER:HB3	1.64	0.61
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.65	0.61
3:D:613:GLY:O	3:D:617:THR:OG1	2.18	0.61
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.82	0.61
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.83	0.61
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.33	0.61
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.65	0.61
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.64	0.61
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.32	0.61
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.32	0.61
2:I:620:ASN:HD22	2:I:620:ASN:C	2.03	0.61
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.82	0.61
3:J:79:LYS:HG3	3:J:80:HIS:ND1	2.16	0.61
5:L:479:THR:HG23	5:L:481:GLU:H	1.66	0.61
3:J:931:THR:OG1	3:J:1244:GLN:NE2	2.34	0.61
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.65	0.60
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.34	0.60
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.83	0.60
2:C:41:GLN:NE2	2:C:73:TYR:O	2.35	0.60
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.83	0.60
5:F:577:GLY:O	5:F:581:ASP:N	2.31	0.60
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.17	0.60
2:I:324:LYS:O	2:I:327:GLN:NE2	2.35	0.60
1:A:23:HIS:HB2	1:A:205:MET:O	2.01	0.60
3:D:931:THR:OG1	3:D:1244:GLN:NE2	2.34	0.60
3:D:848:VAL:HG22	3:D:857:LEU:HD11	1.83	0.60
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.83	0.60
5:F:479:THR:HG23	5:F:481:GLU:H	1.66	0.60
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.66	0.60
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.22	0.60
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.82	0.60
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	1.83	0.60
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.84	0.60
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.82	0.60
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.22	0.60
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.82	0.60
2:I:41:GLN:NE2	2:I:73:TYR:O	2.35	0.60
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.31	0.60
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.84	0.60
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.84	0.60
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.36	0.60
1:G:23:HIS:HB2	1:G:205:MET:O	2.01	0.60
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.82	0.60
2:I:735:LYS:HA	2:I:748:ILE:HG22	1.83	0.60
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.82	0.60
4:K:14:GLY:O	4:K:16:ARG:N	2.34	0.60
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.84	0.59
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:470:ARG:HE	2:C:497:PRO:HB3	1.66	0.59
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.83	0.59
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.67	0.59
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	1.82	0.59
3:D:698:MET:O	3:D:702:GLN:HB3	2.02	0.59
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.83	0.59
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.84	0.59
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.84	0.59
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.84	0.59
2:I:975:ILE:HG13	2:I:1014:LEU:HD22	1.84	0.59
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.84	0.59
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	1.84	0.59
2:C:324:LYS:O	2:C:327:GLN:NE2	2.34	0.59
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.02	0.59
3:J:75:TYR:CD2	3:J:80:HIS:HD2	2.20	0.59
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.41	0.59
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.85	0.59
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.03	0.59
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.85	0.59
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.68	0.59
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.83	0.59
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.84	0.59
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.83	0.59
3:J:325:LYS:HG3	3:J:329:ASP:HB2	1.85	0.59
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.31	0.59
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.85	0.59
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.02	0.59
2:C:980:VAL:HA	2:C:984:VAL:HA	1.85	0.58
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.85	0.58
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.85	0.58
3:D:325:LYS:HG3	3:D:329:ASP:HB2	1.85	0.58
3:D:75:TYR:CD2	3:D:80:HIS:HD2	2.20	0.58
3:D:857:LEU:HD12	3:D:858:VAL:H	1.67	0.58
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.84	0.58
3:J:860:ARG:HH11	3:J:860:ARG:HG3	1.69	0.58
3:J:1067:ARG:HD3	3:J:1072:LYS:HA	1.84	0.58
2:I:808:ASN:H	3:J:633:ALA:HB2	1.69	0.58
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.85	0.58
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.37	0.58
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.86	0.58
5:L:600:HIS:CD2	5:L:601:PRO:HD3	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:THR:HG21	2:C:351:LEU:HG	1.86	0.58
5:F:312:SER:OG	5:F:313:ASP:N	2.37	0.58
5:F:395:THR:OG1	5:F:396:ASN:N	2.37	0.58
3:J:519:ASN:HB2	3:J:709:ARG:HD3	1.86	0.58
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.85	0.58
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.39	0.58
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.86	0.58
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.85	0.58
5:L:127:ILE:O	5:L:130:VAL:HG22	2.03	0.58
5:L:395:THR:OG1	5:L:396:ASN:N	2.37	0.58
5:L:483:LEU:H	5:L:483:LEU:HD12	1.68	0.58
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.67	0.58
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.03	0.58
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.85	0.58
3:D:519:ASN:HB2	3:D:709:ARG:HD3	1.85	0.58
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.86	0.57
2:C:746:ALA:HA	2:C:974:ARG:HE	1.68	0.57
5:F:466:ILE:CG2	5:F:486:ARG:HG3	2.34	0.57
2:I:696:ASP:O	2:I:697:LYS:HB3	2.04	0.57
2:I:896:THR:HB	2:I:897:PRO:HD2	1.86	0.57
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.87	0.57
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.38	0.57
1:A:197:ASP:N	1:A:197:ASP:OD1	2.37	0.57
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.37	0.57
2:C:1313:HIS:N	4:E:31:GLN:OE1	2.36	0.57
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.86	0.57
3:D:514:THR:HG22	3:D:596:LEU:HB2	1.86	0.57
1:G:74:VAL:HG22	1:G:76:GLU:H	1.70	0.57
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.87	0.57
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.39	0.57
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.85	0.57
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.70	0.57
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.38	0.57
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.38	0.57
1:G:197:ASP:N	1:G:197:ASP:OD1	2.37	0.57
2:I:1142:ARG:HD3	2:I:1161:LEU:HD22	1.87	0.57
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.05	0.57
2:I:499:SER:O	2:I:503:LYS:HB2	2.05	0.57
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.86	0.57
1:A:74:VAL:HG22	1:A:76:GLU:H	1.70	0.57
2:C:170:VAL:HG23	2:C:171:LEU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:152:THR:OG1	3:D:153:ASN:N	2.38	0.57
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.40	0.57
2:I:207:THR:HG21	2:I:351:LEU:HG	1.85	0.57
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.04	0.57
2:C:696:ASP:O	2:C:697:LYS:HB3	2.05	0.57
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.85	0.57
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.39	0.57
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.85	0.56
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.87	0.56
2:C:27:LEU:O	2:C:528:ARG:NH1	2.37	0.56
2:C:620:ASN:C	2:C:620:ASN:ND2	2.58	0.56
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.85	0.56
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.69	0.56
3:D:843:VAL:HG11	3:D:897:HIS:O	2.05	0.56
5:F:466:ILE:HG21	5:F:486:ARG:HG3	1.86	0.56
2:C:896:THR:HB	2:C:897:PRO:HD2	1.86	0.56
2:I:170:VAL:HG23	2:I:171:LEU:N	2.19	0.56
2:I:21:VAL:HG13	2:I:655:VAL:HG13	1.86	0.56
3:J:514:THR:HG22	3:J:596:LEU:HB2	1.87	0.56
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.86	0.56
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.86	0.56
5:F:483:LEU:H	5:F:483:LEU:HD12	1.69	0.56
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.87	0.56
3:J:843:VAL:HG11	3:J:897:HIS:O	2.05	0.56
1:B:6:THR:O	1:B:6:THR:OG1	2.19	0.56
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.41	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.70	0.56
2:I:27:LEU:O	2:I:528:ARG:NH1	2.37	0.56
2:I:606:LEU:HD23	2:I:611:GLU:HA	1.88	0.56
2:I:741:MET:SD	2:I:974:ARG:NH2	2.78	0.56
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.87	0.56
3:J:961:SER:HB2	3:J:981:GLU:HB3	1.88	0.56
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.88	0.56
2:C:499:SER:O	2:C:503:LYS:HB2	2.05	0.56
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.87	0.56
3:J:678:ARG:O	3:J:682:VAL:HG23	2.06	0.56
5:L:312:SER:OG	5:L:313:ASP:N	2.37	0.56
2:C:138:ILE:HD13	2:C:143:ARG:HD3	1.87	0.56
3:D:425:ARG:HG2	3:D:426:ALA:H	1.70	0.56
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.41	0.56
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.88	0.56
2:C:606:LEU:HD23	2:C:611:GLU:HA	1.88	0.56
3:D:27:PRO:O	3:D:31:ARG:HG3	2.05	0.56
3:J:152:THR:OG1	3:J:153:ASN:N	2.38	0.56
3:J:425:ARG:HG2	3:J:426:ALA:H	1.70	0.56
3:J:755:ILE:HG22	3:J:757:THR:H	1.71	0.56
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.88	0.55
3:D:755:ILE:HG22	3:D:757:THR:H	1.72	0.55
3:J:746:LEU:HG	3:J:758:PRO:HG3	1.88	0.55
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.38	0.55
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.89	0.55
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.87	0.55
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.88	0.55
1:B:64:VAL:HG12	1:B:65:LEU:H	1.72	0.55
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.89	0.55
3:J:27:PRO:O	3:J:31:ARG:HG3	2.05	0.55
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.89	0.55
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.87	0.55
3:J:26:SER:HB3	3:J:29:MET:HB3	1.89	0.55
3:D:250:ARG:HH11	3:D:250:ARG:HG3	1.72	0.55
3:D:860:ARG:HH11	3:D:860:ARG:HG3	1.70	0.55
5:F:575:GLU:O	5:F:579:GLN:HG2	2.07	0.55
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.22	0.55
3:D:26:SER:HB3	3:D:29:MET:HB3	1.87	0.55
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.88	0.55
2:I:1131:MET:O	2:I:1134:GLN:HB2	2.06	0.55
2:I:1239:VAL:HG13	3:J:445:LYS:HB2	1.89	0.55
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.87	0.55
3:D:746:LEU:HG	3:D:758:PRO:HG3	1.88	0.55
3:D:857:LEU:HD13	3:D:858:VAL:HG13	1.89	0.55
2:C:1239:VAL:HG13	3:D:445:LYS:HB2	1.89	0.55
2:I:255:ILE:HB	2:I:263:VAL:HB	1.89	0.55
2:C:255:ILE:HB	2:C:263:VAL:HB	1.89	0.54
2:I:897:PRO:O	2:I:900:LYS:N	2.40	0.54
3:J:682:VAL:O	3:J:685:ILE:HG12	2.06	0.54
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.89	0.54
1:G:231:PHE:N	1:G:231:PHE:CD2	2.75	0.54
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.88	0.54
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.88	0.54
3:J:857:LEU:HD12	3:J:858:VAL:H	1.71	0.54
2:C:498:ILE:HD12	2:C:498:ILE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.88	0.54
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.23	0.54
3:D:62:PHE:O	3:D:101:ARG:HD2	2.07	0.54
3:J:46:TYR:CD1	5:L:500:ILE:HG21	2.43	0.54
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.90	0.54
2:I:13:LYS:HZ1	2:I:1151:LEU:HB2	1.71	0.54
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.88	0.54
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.88	0.54
2:C:832:HIS:O	2:C:1055:ALA:HA	2.08	0.54
3:D:317:THR:HB	3:D:324:LEU:HB3	1.90	0.54
3:J:557:LYS:HA	3:J:563:LEU:HA	1.90	0.54
1:H:64:VAL:HG12	1:H:65:LEU:H	1.72	0.54
5:L:575:GLU:O	5:L:579:GLN:HG2	2.08	0.54
2:C:46:GLN:OE1	2:C:47:TYR:N	2.41	0.54
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.90	0.54
3:D:678:ARG:O	3:D:682:VAL:HG23	2.08	0.54
2:I:187:GLU:OE2	2:I:197:ARG:NH2	2.35	0.54
2:I:826:ASP:OD1	2:I:829:THR:OG1	2.24	0.54
3:J:317:THR:HB	3:J:324:LEU:HB3	1.89	0.54
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.90	0.54
2:C:624:ASP:OD1	2:C:625:GLU:N	2.41	0.54
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.89	0.54
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.90	0.54
3:D:557:LYS:HA	3:D:563:LEU:HA	1.90	0.54
3:D:901:ARG:HA	3:D:908:ILE:HA	1.89	0.54
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.88	0.54
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.90	0.54
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.89	0.54
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.89	0.54
2:I:498:ILE:H	2:I:498:ILE:HD12	1.73	0.54
2:I:620:ASN:ND2	2:I:620:ASN:O	2.41	0.54
2:I:624:ASP:OD1	2:I:625:GLU:N	2.41	0.54
1:H:35:PHE:HA	1:H:38:THR:HG22	1.89	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.44	0.53
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.90	0.53
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.43	0.53
3:J:62:PHE:O	3:J:101:ARG:HD2	2.07	0.53
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.90	0.53
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.43	0.53
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.56	0.53
2:I:219:GLN:HA	2:I:222:ASP:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.91	0.53
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.39	0.53
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.43	0.53
1:G:182:ARG:H	1:G:206:GLU:HB3	1.74	0.53
1:G:226:GLU:HG2	1:H:10:LYS:HE3	1.91	0.53
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.23	0.53
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.91	0.53
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.39	0.53
3:J:1357:ILE:HG22	3:J:1359:ALA:H	1.73	0.53
2:I:46:GLN:OE1	2:I:47:TYR:N	2.41	0.53
3:J:514:THR:HG21	3:J:596:LEU:HD23	1.90	0.53
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.44	0.53
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.90	0.53
3:D:156:ARG:NH2	3:D:191:SER:OG	2.42	0.53
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.90	0.53
2:C:219:GLN:HA	2:C:222:ASP:HB3	1.89	0.53
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.91	0.53
5:F:164:GLY:O	5:F:260:ARG:HB2	2.08	0.53
2:I:724:VAL:HG23	2:I:775:GLU:H	1.74	0.53
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.90	0.53
3:J:857:LEU:HD13	3:J:858:VAL:HG13	1.90	0.53
3:J:901:ARG:HA	3:J:908:ILE:HA	1.91	0.53
1:A:182:ARG:H	1:A:206:GLU:HB3	1.74	0.53
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.90	0.53
2:C:741:MET:SD	2:C:974:ARG:NH2	2.82	0.53
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.57	0.53
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.73	0.53
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.90	0.53
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.90	0.53
5:F:600:HIS:HD2	5:F:601:PRO:HD3	1.74	0.53
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.90	0.53
3:J:230:SER:OG	3:J:231:GLY:N	2.42	0.53
2:C:821:ARG:HH21	2:C:1082:ILE:HG21	1.74	0.53
2:C:897:PRO:O	2:C:899:GLU:N	2.42	0.53
1:H:58:GLU:HB3	1:H:171:LEU:O	2.09	0.53
2:I:56:VAL:HG11	2:I:468:LEU:HB3	1.90	0.53
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.45	0.53
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.90	0.52
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	1.91	0.52
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.44	0.52
2:I:1134:GLN:HA	2:I:1134:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.39	0.52
3:J:79:LYS:HB2	5:L:569:THR:N	2.21	0.52
1:B:35:PHE:HA	1:B:38:THR:HG22	1.89	0.52
3:D:361:LEU:HD22	3:D:365:GLN:HG3	1.92	0.52
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.56	0.52
3:J:697:MET:O	3:J:701:LEU:HB2	2.09	0.52
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.90	0.52
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.90	0.52
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.74	0.52
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.36	0.52
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.74	0.52
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.90	0.52
2:I:620:ASN:C	2:I:620:ASN:ND2	2.62	0.52
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.52
1:G:79:LEU:HD11	2:I:693:LEU:HD21	1.92	0.52
5:L:130:VAL:HB	5:L:365:MET:HG3	1.92	0.52
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.91	0.52
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.55	0.52
3:J:156:ARG:NH2	3:J:191:SER:OG	2.42	0.52
2:C:598:VAL:HG22	2:C:628:HIS:CE1	2.45	0.52
3:D:1259:GLN:NE2	3:D:1262:ARG:HH12	2.08	0.52
3:D:514:THR:HG21	3:D:596:LEU:HD23	1.90	0.52
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.91	0.52
3:J:128:LEU:HA	3:J:192:MET:HE1	1.91	0.52
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.45	0.52
3:D:579:LEU:HD12	3:D:582:ILE:HD12	1.91	0.52
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.10	0.52
2:I:233:ARG:HG3	2:I:233:ARG:HH11	1.73	0.52
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.92	0.52
1:A:224:LEU:HD22	1:B:228:LEU:HD11	1.92	0.52
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.45	0.52
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.91	0.52
2:C:724:VAL:HG23	2:C:775:GLU:H	1.75	0.52
3:D:682:VAL:O	3:D:685:ILE:HG12	2.10	0.52
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.92	0.52
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.92	0.52
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.92	0.51
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.43	0.51
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.92	0.51
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.91	0.51
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:27:PRO:HD3	3:J:236:TRP:NE1	2.25	0.51
3:D:1372:ARG:HE	3:J:854:ALA:CB	2.22	0.51
3:J:860:ARG:CG	3:J:860:ARG:HH11	2.23	0.51
2:C:826:ASP:OD1	2:C:829:THR:OG1	2.23	0.51
3:D:128:LEU:HA	3:D:192:MET:HE1	1.92	0.51
3:D:697:MET:O	3:D:701:LEU:HB2	2.10	0.51
3:J:844:THR:OG1	3:J:860:ARG:O	2.18	0.51
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.74	0.51
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.91	0.51
1:G:12:ARG:H	1:G:30:PRO:HD2	1.76	0.51
3:J:210:SER:O	3:J:214:ARG:HG2	2.10	0.51
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	1.93	0.51
2:I:314:ASN:O	2:I:352:ARG:NH1	2.44	0.51
3:J:654:ILE:O	3:J:658:GLU:HB2	2.10	0.51
1:B:136:GLU:HG2	1:B:137:ASN:H	1.75	0.51
2:C:829:THR:HA	2:C:1059:ARG:HA	1.93	0.51
3:D:712:GLN:CD	3:D:712:GLN:H	2.14	0.51
2:I:701:GLY:O	2:I:1184:THR:N	2.34	0.51
3:J:27:PRO:CD	3:J:236:TRP:HE1	2.23	0.51
3:D:860:ARG:HH11	3:D:860:ARG:CG	2.23	0.51
1:G:231:PHE:HZ	1:H:221:ALA:HB3	1.75	0.51
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.45	0.51
2:I:873:ILE:HG13	2:I:944:ARG:NH2	2.20	0.51
3:J:579:LEU:HD12	3:J:582:ILE:HD12	1.91	0.51
1:A:12:ARG:H	1:A:30:PRO:HD2	1.76	0.51
1:B:134:THR:HG23	1:B:135:ASP:OD1	2.10	0.51
1:B:102:LEU:HB2	1:B:142:MET:H	1.76	0.51
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.92	0.51
2:C:758:ARG:HD3	2:C:835:GLU:HB2	1.93	0.51
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.92	0.51
3:D:356:THR:OG1	3:D:357:VAL:N	2.44	0.51
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.92	0.51
1:H:134:THR:HG23	1:H:135:ASP:OD1	2.10	0.51
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.93	0.51
2:I:138:ILE:HG22	2:I:139:ASN:HD22	1.75	0.51
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.91	0.51
2:C:138:ILE:HG22	2:C:139:ASN:HD22	1.75	0.51
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.35	0.51
3:D:210:SER:O	3:D:214:ARG:HG2	2.11	0.51
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.93	0.51
1:G:166:ARG:O	1:G:168:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:94:GLN:O	3:J:97:VAL:HG23	2.11	0.51
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.92	0.51
3:D:654:ILE:O	3:D:658:GLU:HB2	2.11	0.51
2:I:782:VAL:HG11	2:I:792:GLY:HA2	1.93	0.51
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.93	0.51
3:D:1368:ASP:OD1	3:J:854:ALA:HB1	2.11	0.51
2:C:906:PHE:CE2	5:F:608:ARG:HB2	2.46	0.51
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.93	0.50
3:D:844:THR:OG1	3:D:860:ARG:O	2.18	0.50
5:F:348:GLU:HG2	5:F:354:THR:HA	1.92	0.50
2:I:594:VAL:HG22	2:I:599:VAL:HA	1.92	0.50
2:I:59:ILE:HG22	2:I:476:LYS:HE3	1.92	0.50
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.74	0.50
1:B:79:LEU:H	1:B:79:LEU:HD23	1.76	0.50
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.11	0.50
2:I:821:ARG:HH21	2:I:1082:ILE:HG21	1.74	0.50
3:J:356:THR:OG1	3:J:357:VAL:N	2.44	0.50
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.92	0.50
5:L:482:GLU:HG2	5:L:486:ARG:HH12	1.77	0.50
2:C:59:ILE:HG22	2:C:476:LYS:HE3	1.93	0.50
3:D:94:GLN:O	3:D:97:VAL:HG23	2.12	0.50
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.93	0.50
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.77	0.50
2:C:594:VAL:HG22	2:C:599:VAL:HA	1.92	0.50
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.77	0.50
3:D:27:PRO:HD3	3:D:236:TRP:NE1	2.26	0.50
3:D:75:TYR:HD2	3:D:80:HIS:HD2	1.59	0.50
5:F:580:PHE:O	5:F:581:ASP:HB3	2.11	0.50
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.93	0.50
3:J:963:VAL:HB	3:J:980:THR:HG23	1.94	0.50
5:L:164:GLY:O	5:L:260:ARG:HB2	2.12	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.92	0.50
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.93	0.50
1:H:102:LEU:HB2	1:H:142:MET:H	1.76	0.50
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.94	0.50
5:L:348:GLU:HG2	5:L:354:THR:HA	1.92	0.50
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.94	0.50
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.26	0.50
2:C:120:GLN:HG3	2:C:121:GLU:N	2.26	0.50
2:C:47:TYR:OH	2:C:398:SER:HB2	2.12	0.50
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:89:GLY:HA2	2:C:140:GLY:HA3	1.93	0.50
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.94	0.50
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.94	0.50
2:I:119:GLU:HG3	2:I:488:MET:HB3	1.92	0.50
3:J:75:TYR:HD2	3:J:80:HIS:HD2	1.59	0.50
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.94	0.50
2:I:1134:GLN:CB	2:I:1136:GLN:HG2	2.41	0.50
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.92	0.50
1:B:101:THR:H	1:B:116:THR:HG22	1.77	0.50
4:E:8:ASP:O	4:E:11:GLU:HB2	2.11	0.50
5:F:525:ASP:OD1	5:F:528:LEU:N	2.45	0.50
1:H:101:THR:H	1:H:116:THR:HG22	1.76	0.50
2:I:518:ASN:N	2:I:518:ASN:OD1	2.45	0.50
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.94	0.50
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.94	0.50
1:B:134:THR:HG23	1:B:135:ASP:H	1.77	0.50
2:C:840:SER:HB3	2:C:1048:LYS:HG2	1.94	0.50
2:I:829:THR:HA	2:I:1059:ARG:HA	1.92	0.50
2:C:518:ASN:O	2:C:691:PRO:HD3	2.12	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.77	0.49
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.10	0.49
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.41	0.49
2:C:582:ASN:HB3	2:C:586:PHE:H	1.78	0.49
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.94	0.49
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.78	0.49
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.77	0.49
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.93	0.49
5:L:580:PHE:O	5:L:581:ASP:HB3	2.12	0.49
1:B:54:CYS:SG	1:B:148:ARG:HG3	2.53	0.49
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.93	0.49
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.94	0.49
4:E:36:ASP:HB2	4:E:37:PRO:HD2	1.94	0.49
2:I:1100:PRO:O	2:I:1104:PRO:HD3	2.12	0.49
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.93	0.49
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.94	0.49
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.94	0.49
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.94	0.49
3:D:290:ILE:HD12	3:D:290:ILE:H	1.78	0.49
2:C:1257:GLN:HE22	3:D:340:GLN:HE21	1.60	0.49
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.93	0.49
2:I:518:ASN:O	2:I:691:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.78	0.49
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.48	0.49
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.93	0.49
2:I:1149:TYR:OH	2:I:1176:LEU:HD11	2.12	0.49
2:I:285:ILE:O	2:I:285:ILE:HG13	2.13	0.49
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.95	0.49
3:J:872:LEU:O	3:J:877:VAL:HG12	2.12	0.49
1:A:145:LYS:HZ2	1:A:147:GLN:HB3	1.77	0.49
2:C:620:ASN:O	2:C:620:ASN:ND2	2.46	0.49
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.94	0.49
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.95	0.49
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.94	0.49
3:J:733:SER:O	3:J:737:ILE:HG12	2.12	0.49
3:J:694:SER:OG	3:J:738:ARG:NE	2.46	0.49
3:J:63:GLY:O	3:J:98:ARG:HD2	2.12	0.49
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.93	0.49
5:L:511:ILE:HG13	5:L:512:GLY:H	1.77	0.49
1:B:11:PRO:HB3	1:B:30:PRO:O	2.13	0.49
3:D:872:LEU:O	3:D:877:VAL:HG12	2.11	0.49
1:G:145:LYS:HZ2	1:G:147:GLN:HB3	1.77	0.49
1:A:49:SER:OG	1:A:50:SER:N	2.46	0.49
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.12	0.49
5:F:130:VAL:HB	5:F:365:MET:HG3	1.95	0.49
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.43	0.49
3:J:1017:VAL:HG23	3:J:1018:ALA:H	1.78	0.49
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.34	0.49
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.95	0.49
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.94	0.49
3:D:137:ARG:HD3	3:D:143:SER:OG	2.12	0.49
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.94	0.49
2:C:69:GLN:HG3	2:C:101:ARG:HB3	1.95	0.49
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.48	0.49
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.93	0.49
1:H:67:GLU:HG3	1:H:171:LEU:HD13	1.95	0.49
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.43	0.49
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.94	0.49
1:A:137:ASN:OD1	1:A:137:ASN:N	2.46	0.48
1:B:151:GLY:O	1:B:177:TYR:HD2	1.96	0.48
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.93	0.48
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.76	0.48
5:F:227:GLN:HG2	5:F:252:LEU:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.48	0.48
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.48	0.48
3:J:290:ILE:HD12	3:J:290:ILE:H	1.77	0.48
3:J:956:GLY:O	3:J:1011:VAL:HG22	2.13	0.48
3:D:694:SER:OG	3:D:738:ARG:NE	2.46	0.48
3:D:392:THR:HG21	5:F:606:VAL:HA	1.94	0.48
1:H:151:GLY:O	1:H:177:TYR:HD2	1.96	0.48
2:I:206:ALA:O	2:I:209:ILE:HG22	2.13	0.48
2:I:896:THR:O	2:I:900:LYS:HB2	2.13	0.48
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.77	0.48
3:J:709:ARG:O	3:J:711:GLY:N	2.38	0.48
5:L:343:LYS:H	5:L:343:LYS:HD2	1.77	0.48
1:B:81:ILE:O	1:B:85:LEU:HG	2.13	0.48
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.77	0.48
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.94	0.48
1:G:19:VAL:HG12	1:G:24:ALA:HA	1.95	0.48
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.95	0.48
5:L:456:MET:O	5:L:460:ILE:HG13	2.13	0.48
2:C:206:ALA:O	2:C:209:ILE:HG22	2.14	0.48
3:D:770:LEU:H	3:D:770:LEU:HD22	1.79	0.48
1:H:134:THR:HG23	1:H:135:ASP:H	1.78	0.48
1:H:54:CYS:SG	1:H:148:ARG:HG3	2.52	0.48
1:H:79:LEU:HD23	1:H:79:LEU:H	1.77	0.48
2:I:840:SER:HB3	2:I:1048:LYS:HG2	1.95	0.48
2:C:896:THR:O	2:C:900:LYS:HB2	2.13	0.48
2:I:582:ASN:HB3	2:I:586:PHE:H	1.78	0.48
3:J:1162:ILE:HA	3:J:1203:ARG:HA	1.95	0.48
2:I:1243:MET:HA	3:J:353:SER:HB3	1.95	0.48
3:J:712:GLN:H	3:J:712:GLN:CD	2.15	0.48
5:L:227:GLN:HG2	5:L:252:LEU:HA	1.94	0.48
2:C:1243:MET:HA	3:D:353:SER:HB3	1.95	0.48
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.78	0.48
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.96	0.48
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.94	0.48
5:L:306:PHE:CE1	5:L:310:GLU:HG3	2.49	0.48
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.95	0.48
1:G:49:SER:OG	1:G:50:SER:N	2.46	0.48
1:H:51:MET:HB3	1:H:178:SER:HA	1.95	0.48
1:A:45:ARG:HG2	1:B:38:THR:HB	1.95	0.48
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.49	0.48
1:B:78:ILE:O	1:B:82:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.96	0.48
2:C:445:ILE:HG22	2:C:446:ASP:OD1	2.14	0.48
3:D:27:PRO:CD	3:D:236:TRP:HE1	2.27	0.48
2:C:1257:GLN:HE22	3:D:340:GLN:NE2	2.11	0.48
3:D:847:ASP:HB3	3:D:859:PRO:HA	1.94	0.48
3:D:98:ARG:NH1	3:D:98:ARG:HG2	2.13	0.48
3:J:847:ASP:HB3	3:J:859:PRO:HA	1.95	0.48
5:L:314:THR:O	5:L:318:ALA:HB3	2.14	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.96	0.48
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.95	0.48
3:D:1297:LYS:HE3	3:J:1302:TYR:H	1.79	0.48
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	1.95	0.48
3:D:1359:ALA:O	3:D:1363:TYR:N	2.46	0.48
3:D:733:SER:O	3:D:737:ILE:HG12	2.13	0.48
3:D:797:THR:O	3:D:801:VAL:HG13	2.13	0.48
5:F:270:VAL:HG13	5:F:365:MET:HE3	1.95	0.48
5:F:511:ILE:HG13	5:F:512:GLY:H	1.78	0.48
1:H:81:ILE:O	1:H:85:LEU:HG	2.13	0.48
2:I:616:ILE:HG13	2:I:652:TYR:HB2	1.96	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.96	0.48
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.94	0.48
3:J:797:THR:O	3:J:801:VAL:HG13	2.14	0.48
5:L:96:ASP:O	5:L:98:VAL:N	2.47	0.48
3:D:123:ARG:HD2	3:D:1337:VAL:HG11	1.96	0.48
5:F:474:MET:C	5:F:476:ARG:H	2.07	0.48
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.78	0.48
3:J:770:LEU:HD22	3:J:770:LEU:H	1.79	0.48
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.96	0.47
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.79	0.47
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.96	0.47
1:G:137:ASN:N	1:G:137:ASN:OD1	2.46	0.47
2:I:107:ARG:HA	2:I:108:GLU:HA	1.54	0.47
3:J:950:ILE:HD12	3:J:1020:TRP:CZ3	2.49	0.47
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.49	0.47
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.49	0.47
2:C:285:ILE:O	2:C:285:ILE:HG13	2.14	0.47
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.46	0.47
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.45	0.47
3:J:264:ASP:OD2	3:J:264:ASP:N	2.48	0.47
4:K:25:ARG:HD3	4:K:64:LEU:HD13	1.97	0.47
5:L:525:ASP:OD1	5:L:528:LEU:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:H	1:A:172:LEU:HD12	1.79	0.47
2:C:12:ARG:NH1	2:C:1182:ILE:O	2.43	0.47
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.55	0.47
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.50	0.47
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.94	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.49	0.47
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.44	0.47
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.79	0.47
2:I:897:PRO:O	2:I:899:GLU:N	2.47	0.47
3:J:16:GLU:CG	3:J:17:PHE:H	2.25	0.47
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.96	0.47
2:C:349:GLU:O	2:C:353:VAL:HG23	2.14	0.47
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.96	0.47
3:D:1290:ARG:HG3	3:D:1298:VAL:HG12	1.96	0.47
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.95	0.47
1:H:149:GLY:HA3	1:H:177:TYR:CD2	2.48	0.47
1:H:11:PRO:HB3	1:H:30:PRO:O	2.15	0.47
2:I:233:ARG:NH1	2:I:233:ARG:HG3	2.30	0.47
2:C:1149:TYR:OH	2:C:1176:LEU:HD11	2.14	0.47
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.97	0.47
3:D:709:ARG:HD2	3:D:710:ASP:N	2.30	0.47
5:F:306:PHE:CE1	5:F:310:GLU:HG3	2.49	0.47
1:G:172:LEU:HD12	1:G:172:LEU:H	1.80	0.47
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.97	0.47
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.96	0.47
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.96	0.47
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.95	0.47
3:J:123:ARG:HD2	3:J:1337:VAL:HG11	1.96	0.47
3:J:984:LEU:HB3	3:J:993:GLU:HB2	1.96	0.47
4:K:8:ASP:O	4:K:11:GLU:HB2	2.15	0.47
5:L:513:ASP:C	5:L:515:GLU:H	2.18	0.47
1:A:228:LEU:HD21	1:B:224:LEU:HD23	1.96	0.47
2:C:356:THR:HG21	2:C:362:ALA:HA	1.96	0.47
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.96	0.47
3:D:264:ASP:N	3:D:264:ASP:OD2	2.48	0.47
3:J:1077:ALA:HA	3:J:1100:PHE:HA	1.97	0.47
2:C:13:LYS:HZ1	2:C:1151:LEU:HB2	1.80	0.47
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.97	0.47
2:C:623:LEU:HB2	2:C:627:GLY:HA2	1.97	0.47
3:D:574:VAL:O	3:D:578:ILE:HG13	2.15	0.47
3:D:518:VAL:N	3:D:716:GLN:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:875:ASN:OD1	3:D:875:ASN:N	2.48	0.47
5:F:134:VAL:HG22	5:F:273:MET:HE3	1.96	0.47
5:F:456:MET:O	5:F:460:ILE:HG13	2.14	0.47
3:J:1290:ARG:HG3	3:J:1298:VAL:HG12	1.97	0.47
1:H:71:LYS:NZ	1:H:139:SER:O	2.36	0.47
2:I:466:VAL:O	2:I:469:VAL:HG22	2.15	0.47
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.50	0.47
3:J:665:GLN:HG3	3:J:669:GLN:HE21	1.80	0.47
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.95	0.47
3:D:665:GLN:HG3	3:D:669:GLN:HE21	1.80	0.47
4:E:7:GLN:O	4:E:11:GLU:HG2	2.15	0.47
1:H:61:ILE:HB	1:H:64:VAL:O	2.14	0.47
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.96	0.47
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.50	0.47
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.30	0.47
3:J:1063:ASP:O	3:J:1067:ARG:HG3	2.15	0.47
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.97	0.47
3:J:702:GLN:HG2	3:J:703:THR:N	2.30	0.47
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.30	0.47
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.80	0.47
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.97	0.47
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.97	0.47
2:I:301:TYR:HB2	2:I:311:CYS:SG	2.55	0.47
3:J:1061:VAL:HG21	3:J:1101:LEU:HB3	1.96	0.47
1:B:147:GLN:HG3	1:B:148:ARG:N	2.29	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.46
2:C:185:ASP:HB2	2:C:197:ARG:HG3	1.97	0.46
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.45	0.46
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.97	0.46
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.50	0.46
3:D:632:ALA:O	3:D:635:SER:OG	2.30	0.46
5:F:314:THR:O	5:F:318:ALA:HB3	2.15	0.46
2:I:349:GLU:O	2:I:353:VAL:HG23	2.14	0.46
2:I:445:ILE:HG22	2:I:446:ASP:OD1	2.15	0.46
3:J:1100:PHE:HB2	3:J:1200:GLU:CD	2.35	0.46
3:J:137:ARG:HD3	3:J:143:SER:OG	2.14	0.46
3:J:568:SER:OG	3:J:569:LEU:N	2.47	0.46
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.96	0.46
4:K:7:GLN:O	4:K:11:GLU:HG2	2.15	0.46
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.97	0.46
2:C:1136:GLN:HE21	2:C:1136:GLN:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.46	0.46
2:C:593:LYS:HD3	2:C:652:TYR:CZ	2.50	0.46
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.51	0.46
1:H:78:ILE:O	1:H:82:LEU:HG	2.14	0.46
2:I:1182:ILE:HG22	2:I:1183:ALA:N	2.30	0.46
2:I:169:LYS:O	2:I:170:VAL:HG22	2.16	0.46
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.51	0.46
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.98	0.46
3:J:560:ASN:O	3:J:560:ASN:ND2	2.47	0.46
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.96	0.46
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.97	0.46
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.96	0.46
1:H:136:GLU:HG2	1:H:137:ASN:H	1.80	0.46
3:J:230:SER:CB	3:J:232:ASN:H	2.28	0.46
3:J:266:ASN:O	3:J:270:ARG:HB2	2.15	0.46
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.97	0.46
3:J:518:VAL:N	3:J:716:GLN:OE1	2.47	0.46
3:J:875:ASN:OD1	3:J:875:ASN:N	2.47	0.46
3:J:902:ASP:OD1	3:J:903:LEU:N	2.48	0.46
2:C:339:ASN:HB3	2:C:343:HIS:H	1.81	0.46
2:C:466:VAL:O	2:C:469:VAL:HG22	2.15	0.46
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.48	0.46
3:D:266:ASN:O	3:D:270:ARG:HB2	2.15	0.46
3:D:560:ASN:ND2	3:D:560:ASN:O	2.47	0.46
3:D:600:ALA:O	3:D:603:LYS:HG2	2.15	0.46
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.96	0.46
3:J:973:LEU:HD23	3:J:1003:LEU:HD12	1.98	0.46
3:J:1321:SER:HB2	3:J:1349:GLU:OE2	2.14	0.46
3:J:600:ALA:O	3:J:603:LYS:HG2	2.15	0.46
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.97	0.46
5:L:316:PHE:HZ	5:L:334:SER:HA	1.80	0.46
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.97	0.46
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.96	0.46
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.97	0.46
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.98	0.46
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.45	0.46
3:D:902:ASP:OD1	3:D:903:LEU:N	2.48	0.46
5:F:96:ASP:O	5:F:98:VAL:N	2.48	0.46
1:G:45:ARG:NH1	1:H:34:GLY:O	2.45	0.46
2:I:593:LYS:HD3	2:I:652:TYR:CZ	2.50	0.46
2:I:870:ILE:HG21	2:I:931:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1067:ARG:HG3	3:J:1067:ARG:H	1.54	0.46
3:J:110:PRO:HD2	3:J:183:GLU:HG2	1.97	0.46
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.98	0.46
2:C:518:ASN:OD1	2:C:518:ASN:N	2.45	0.46
3:D:702:GLN:HG2	3:D:703:THR:N	2.31	0.46
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.43	0.46
5:F:244:THR:O	5:F:247:GLU:HG2	2.15	0.46
5:F:281:ARG:O	5:F:285:ARG:HG3	2.15	0.46
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.81	0.46
3:J:250:ARG:HG3	3:J:250:ARG:HH11	1.80	0.46
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.98	0.46
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.97	0.46
2:C:672:GLU:HB3	3:D:767:LEU:O	2.16	0.46
3:D:63:GLY:O	3:D:98:ARG:HD2	2.15	0.46
3:D:293:ARG:NH1	5:F:104:GLU:OE2	2.47	0.46
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.98	0.46
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.96	0.46
1:H:147:GLN:HG3	1:H:148:ARG:N	2.30	0.46
3:J:1108:GLN:HE22	3:J:1123:ARG:NH2	2.13	0.46
3:J:1108:GLN:HE22	3:J:1123:ARG:HH22	1.64	0.46
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.51	0.46
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.45	0.46
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.97	0.46
4:K:50:ALA:O	4:K:54:ILE:HG12	2.15	0.46
1:B:61:ILE:HB	1:B:64:VAL:O	2.16	0.46
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.30	0.46
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.50	0.46
4:E:50:ALA:O	4:E:54:ILE:HG12	2.16	0.46
5:F:499:LYS:HE3	5:F:499:LYS:HB2	1.71	0.46
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.81	0.46
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.97	0.46
2:C:216:THR:H	2:C:219:GLN:HE22	1.63	0.46
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.50	0.46
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.81	0.46
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.51	0.46
2:I:356:THR:HG21	2:I:362:ALA:HA	1.97	0.46
2:I:470:ARG:NE	2:I:497:PRO:HB3	2.30	0.46
2:I:672:GLU:HB3	3:J:767:LEU:O	2.16	0.46
3:J:1183:SER:HB3	3:J:1185:PRO:HD3	1.98	0.46
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.46	0.46
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:574:VAL:O	3:J:578:ILE:HG13	2.15	0.46
5:L:493:LYS:HA	5:L:496:LYS:HG3	1.98	0.46
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.56	0.46
3:D:485:MET:HB3	3:D:488:ASN:ND2	2.31	0.46
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.98	0.46
5:L:281:ARG:O	5:L:285:ARG:HG3	2.16	0.46
3:D:645:VAL:HB	3:D:701:LEU:HD23	1.97	0.45
3:J:293:ARG:NH1	5:L:104:GLU:OE2	2.46	0.45
3:J:45:ASN:HB3	3:J:48:THR:O	2.16	0.45
5:L:244:THR:O	5:L:247:GLU:HG2	2.16	0.45
1:A:14:VAL:HG13	1:A:15:ASP:N	2.31	0.45
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.98	0.45
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	1.97	0.45
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.98	0.45
3:D:45:ASN:HB3	3:D:48:THR:O	2.16	0.45
3:D:793:SER:O	3:D:797:THR:HG23	2.16	0.45
3:D:291:ILE:HD13	5:F:409:ASN:HB3	1.97	0.45
5:F:513:ASP:C	5:F:515:GLU:H	2.18	0.45
1:H:219:ARG:O	1:H:223:ILE:HG13	2.17	0.45
2:I:623:LEU:HB2	2:I:627:GLY:HA2	1.98	0.45
1:B:102:LEU:HD12	1:B:142:MET:HG2	1.98	0.45
2:C:107:ARG:HA	2:C:108:GLU:HA	1.49	0.45
1:H:102:LEU:HD12	1:H:142:MET:HG2	1.98	0.45
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.98	0.45
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.98	0.45
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.96	0.45
5:F:119:ILE:O	5:F:123:ILE:HG13	2.16	0.45
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.80	0.45
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.38	0.45
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.80	0.45
2:I:1209:GLN:HB3	2:I:1224:PRO:HB2	1.98	0.45
2:I:138:ILE:C	2:I:139:ASN:HD22	2.19	0.45
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.79	0.45
3:J:19:ALA:O	3:J:20:ILE:HG13	2.17	0.45
2:C:107:ARG:H	2:C:107:ARG:HG3	1.61	0.45
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.81	0.45
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.99	0.45
3:D:53:ARG:HA	3:D:54:ASP:HA	1.56	0.45
4:E:14:GLY:O	4:E:16:ARG:N	2.50	0.45
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.70	0.45
2:I:816:ILE:HG22	2:I:818:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:110:PRO:HD2	3:D:183:GLU:HG2	1.97	0.45
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.99	0.45
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.31	0.45
1:G:14:VAL:HG13	1:G:15:ASP:N	2.31	0.45
2:I:30:ILE:HD12	2:I:30:ILE:H	1.81	0.45
2:I:69:GLN:HG3	2:I:101:ARG:HB3	1.97	0.45
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.45
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.99	0.45
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.99	0.45
2:C:722:GLY:O	2:C:777:VAL:HG22	2.16	0.45
3:D:19:ALA:O	3:D:20:ILE:HG13	2.17	0.45
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.99	0.45
5:F:316:PHE:HZ	5:F:334:SER:HA	1.80	0.45
2:I:1109:ILE:HA	2:I:1109:ILE:HD12	1.71	0.45
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.87	0.45
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.16	0.45
3:J:485:MET:HB3	3:J:488:ASN:ND2	2.31	0.45
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.32	0.45
1:A:228:LEU:HD13	1:A:228:LEU:HA	1.68	0.45
3:D:519:ASN:CB	3:D:709:ARG:HD3	2.47	0.45
3:J:355:ILE:HG22	3:J:447:ILE:HB	1.99	0.45
5:L:457:ILE:HA	5:L:460:ILE:HD12	1.99	0.45
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.52	0.45
2:C:470:ARG:NE	2:C:497:PRO:HB3	2.30	0.45
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.47	0.45
3:D:347:VAL:HG12	3:D:348:ASP:O	2.17	0.45
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.99	0.45
2:I:722:GLY:O	2:I:777:VAL:HG22	2.16	0.45
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.47	0.45
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.99	0.45
1:B:112:ALA:HB2	1:B:128:HIS:HB3	1.99	0.45
2:C:316:GLU:CD	2:C:316:GLU:H	2.20	0.45
3:D:1293:GLU:HB3	3:D:1294:ALA:H	1.63	0.45
3:D:271:ARG:HE	3:D:271:ARG:HB2	1.41	0.45
3:D:77:ARG:HG3	3:D:79:LYS:H	1.82	0.45
5:F:225:ARG:O	5:F:229:VAL:HG13	2.17	0.45
5:F:482:GLU:HG3	5:F:486:ARG:HH22	1.82	0.45
1:H:205:MET:HE3	1:H:213:PRO:HB3	1.98	0.45
2:I:185:ASP:HB2	2:I:197:ARG:HG3	1.98	0.45
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.99	0.45
3:J:1186:TYR:HD2	3:J:1186:TYR:HA	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:119:ILE:O	5:L:123:ILE:HG13	2.17	0.45
5:L:613:ASP:N	5:L:613:ASP:OD1	2.50	0.45
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.81	0.44
1:B:219:ARG:O	1:B:223:ILE:HG13	2.16	0.44
3:D:1262:ARG:HH11	3:D:1262:ARG:HD3	1.62	0.44
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.46	0.44
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.17	0.44
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.52	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.44
3:J:347:VAL:HG12	3:J:348:ASP:O	2.18	0.44
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.32	0.44
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.77	0.44
3:D:568:SER:OG	3:D:569:LEU:N	2.47	0.44
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.98	0.44
2:I:316:GLU:CD	2:I:316:GLU:H	2.21	0.44
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.71	0.44
3:J:620:PHE:O	3:J:624:ILE:HG13	2.17	0.44
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.84	0.44
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.99	0.44
2:I:1182:ILE:HG22	2:I:1183:ALA:H	1.82	0.44
3:J:1170:LYS:C	3:J:1172:LYS:H	2.20	0.44
3:J:491:LEU:HD11	3:J:610:ARG:HH12	1.83	0.44
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.99	0.44
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.52	0.44
1:B:57:THR:O	1:B:173:VAL:HB	2.17	0.44
2:C:566:GLY:O	2:C:569:ILE:HG13	2.17	0.44
2:C:867:GLU:OE1	2:C:943:LYS:NZ	2.49	0.44
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.99	0.44
3:D:1183:SER:HB3	3:D:1185:PRO:HD3	1.98	0.44
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.99	0.44
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.19	0.44
3:D:75:TYR:HD2	3:D:80:HIS:CD2	2.35	0.44
5:F:558:VAL:HG23	5:F:580:PHE:CE2	2.53	0.44
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.99	0.44
2:I:566:GLY:O	2:I:569:ILE:HG13	2.17	0.44
3:J:1273:ASP:HB3	3:J:1276:GLU:HG3	1.99	0.44
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.17	0.44
3:J:510:LEU:HA	3:J:513:MET:HE2	1.99	0.44
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.82	0.44
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.33	0.44
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:ASP:O	2:C:85:CYS:HB2	2.18	0.44
2:C:902:LEU:HD21	5:F:611:LEU:HD21	1.98	0.44
3:D:1230:THR:O	3:D:1234:VAL:HG22	2.18	0.44
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.15	0.44
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.99	0.44
3:D:516:ASP:HB3	3:D:573:THR:HG21	2.00	0.44
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.85	0.44
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.37	0.44
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.99	0.44
5:L:225:ARG:O	5:L:229:VAL:HG13	2.18	0.44
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.52	0.44
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.99	0.44
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.53	0.44
5:F:485:GLU:H	5:F:485:GLU:HG3	1.61	0.44
5:F:496:LYS:O	5:F:500:ILE:HG12	2.17	0.44
2:I:81:ASP:O	2:I:85:CYS:HB2	2.18	0.44
2:I:930:ASP:OD2	2:I:931:VAL:N	2.50	0.44
3:J:45:ASN:O	3:J:46:TYR:HD2	2.01	0.44
3:J:660:GLU:O	3:J:664:ILE:HG12	2.18	0.44
3:J:903:LEU:HA	3:J:903:LEU:HD12	1.89	0.44
5:L:496:LYS:O	5:L:500:ILE:HG12	2.17	0.44
3:D:1186:TYR:HD2	3:D:1186:TYR:HA	1.62	0.44
2:C:1272:GLU:HB2	3:D:342:LEU:O	2.17	0.44
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.52	0.44
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.31	0.44
3:D:894:VAL:HB	3:D:915:ILE:HD11	2.00	0.44
5:F:234:THR:O	5:F:245:ALA:HB2	2.18	0.44
1:H:112:ALA:HB2	1:H:128:HIS:HB3	1.99	0.44
2:I:1246:ARG:HG2	2:I:1247:SER:N	2.32	0.44
3:J:860:ARG:NH1	3:J:860:ARG:HG3	2.33	0.44
2:I:902:LEU:HD21	5:L:611:LEU:HD21	1.99	0.44
1:B:51:MET:HB3	1:B:178:SER:HA	1.98	0.44
2:C:1182:ILE:HG22	2:C:1183:ALA:H	1.83	0.44
2:C:1246:ARG:HG2	2:C:1247:SER:N	2.33	0.44
2:C:83:GLN:O	2:C:87:ILE:HG13	2.18	0.44
3:D:40:LYS:HB3	3:D:42:GLU:OE1	2.18	0.44
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.52	0.44
3:J:1061:VAL:HG21	3:J:1101:LEU:CB	2.48	0.44
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.99	0.44
3:J:650:LYS:O	3:J:654:ILE:HG13	2.18	0.44
3:J:793:SER:O	3:J:797:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:825:VAL:C	3:J:826:ILE:HG13	2.39	0.44
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.99	0.44
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.99	0.44
3:D:333:GLY:O	3:D:334:LYS:HB2	2.17	0.44
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.83	0.44
5:F:111:LEU:HG	5:F:382:ALA:HB1	2.00	0.44
1:G:44:ARG:HG3	1:G:183:ILE:HG22	2.00	0.44
1:G:35:PHE:HA	1:G:35:PHE:HD1	1.72	0.44
2:I:117:ILE:H	2:I:117:ILE:HG12	1.68	0.44
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.99	0.44
3:J:77:ARG:HG3	3:J:79:LYS:H	1.83	0.44
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.99	0.44
2:C:898:GLU:N	2:C:898:GLU:OE1	2.50	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.98	0.43
3:D:80:HIS:N	3:D:80:HIS:ND1	2.66	0.43
5:F:457:ILE:HA	5:F:460:ILE:HD12	1.99	0.43
2:I:243:PRO:HB2	2:I:278:GLU:HG3	1.99	0.43
3:J:1041:ILE:C	3:J:1046:ILE:HG12	2.39	0.43
3:J:1108:GLN:HE21	3:J:1120:THR:HG1	1.57	0.43
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.18	0.43
3:J:516:ASP:HB3	3:J:573:THR:HG21	2.00	0.43
5:L:476:ARG:CG	5:L:476:ARG:HH11	2.31	0.43
5:L:479:THR:HG22	5:L:482:GLU:HB2	2.00	0.43
1:A:226:GLU:HG2	1:B:10:LYS:HE3	2.01	0.43
3:D:55:GLY:H	3:D:58:CYS:HB2	1.83	0.43
3:D:810:THR:HG23	3:D:811:GLU:H	1.83	0.43
5:F:461:ASN:O	5:F:465:ARG:HG2	2.17	0.43
5:F:476:ARG:CG	5:F:477:GLU:H	2.31	0.43
5:F:584:ARG:HB3	5:F:585:GLU:H	1.56	0.43
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.33	0.43
2:I:600:THR:HB	2:I:602:GLU:HG2	2.01	0.43
2:I:720:ARG:HB2	2:I:749:ASP:OD1	2.19	0.43
3:J:53:ARG:HA	3:J:54:ASP:HA	1.56	0.43
3:J:894:VAL:HB	3:J:915:ILE:HD11	2.00	0.43
5:L:299:LYS:O	5:L:303:ILE:HG12	2.18	0.43
3:D:510:LEU:HA	3:D:513:MET:HE2	2.00	0.43
3:D:620:PHE:O	3:D:624:ILE:HG13	2.18	0.43
1:H:56:VAL:HG22	1:H:144:ILE:HD11	2.00	0.43
2:I:736:VAL:HG23	2:I:748:ILE:HA	2.00	0.43
3:J:1230:THR:O	3:J:1234:VAL:HG22	2.18	0.43
3:J:133:ARG:O	3:J:137:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:226:ALA:O	5:L:230:VAL:HG12	2.18	0.43
5:L:234:THR:O	5:L:245:ALA:HB2	2.18	0.43
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.39	0.43
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.99	0.43
2:I:145:ILE:HG13	2:I:512:SER:HA	2.00	0.43
2:I:367:TYR:CE2	2:I:376:PRO:HA	2.53	0.43
3:J:1040:MET:HB3	3:J:1046:ILE:HG21	2.00	0.43
3:J:810:THR:HG23	3:J:811:GLU:H	1.83	0.43
2:C:13:LYS:HZ1	2:C:1151:LEU:HD12	1.82	0.43
2:C:720:ARG:HB2	2:C:749:ASP:OD1	2.19	0.43
3:D:1150:PRO:HG2	3:D:1153:PRO:HG3	2.00	0.43
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.70	0.43
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.86	0.43
5:F:496:LYS:HB2	5:F:496:LYS:HE3	1.71	0.43
1:G:125:LYS:HG3	1:G:128:HIS:HB2	2.00	0.43
1:G:228:LEU:HD12	1:G:231:PHE:CZ	2.54	0.43
1:G:42:ALA:O	1:G:46:ILE:HG12	2.19	0.43
2:I:1151:LEU:HD23	2:I:1197:GLU:OE2	2.19	0.43
3:J:997:VAL:HA	3:J:998:PRO:HD3	1.85	0.43
5:L:511:ILE:HA	5:L:511:ILE:HD12	1.84	0.43
1:A:115:ILE:HG22	1:A:116:THR:H	1.83	0.43
2:C:1146:GLN:HB3	2:C:1146:GLN:HE21	1.50	0.43
2:C:175:ARG:HD3	2:C:183:TRP:CZ3	2.54	0.43
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.34	0.43
2:C:30:ILE:H	2:C:30:ILE:HD12	1.83	0.43
3:D:1160:SER:HA	3:D:1204:VAL:O	2.17	0.43
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	2.00	0.43
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.99	0.43
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.67	0.43
1:H:71:LYS:HD2	1:H:71:LYS:HA	1.72	0.43
2:I:122:VAL:HG21	2:I:493:ILE:HG23	2.01	0.43
2:I:83:GLN:O	2:I:87:ILE:HG13	2.17	0.43
3:J:1163:VAL:HG22	3:J:1164:SER:H	1.84	0.43
3:J:1262:ARG:HD2	3:J:1279:GLN:OE1	2.19	0.43
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.53	0.43
1:B:50:SER:HA	1:B:151:GLY:HA2	2.00	0.43
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.33	0.43
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.19	0.43
2:C:600:THR:HB	2:C:602:GLU:HG2	2.01	0.43
3:D:339:ARG:O	3:D:340:GLN:HB3	2.19	0.43
3:D:45:ASN:O	3:D:46:TYR:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:GLU:O	1:H:78:ILE:HB	2.19	0.43
2:I:69:GLN:NE2	2:I:101:ARG:HD2	2.30	0.43
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.53	0.43
2:I:269:ILE:HA	2:I:273:HIS:ND1	2.33	0.43
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	2.01	0.43
3:J:271:ARG:HB2	3:J:271:ARG:HE	1.41	0.43
3:J:75:TYR:HD2	3:J:80:HIS:CD2	2.35	0.43
2:C:112:GLY:HA2	2:C:113:THR:HG23	2.00	0.43
2:C:1308:ILE:HD12	3:D:380:PHE:CZ	2.54	0.43
2:C:245:ARG:HG2	2:C:337:PHE:CZ	2.53	0.43
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.54	0.43
2:C:453:ILE:HD11	2:C:530:ILE:HD12	2.00	0.43
2:C:886:LYS:HB3	2:C:917:SER:HA	2.01	0.43
3:D:847:ASP:N	3:D:847:ASP:OD1	2.51	0.43
5:F:362:ASN:HB2	5:F:365:MET:HE2	2.01	0.43
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.01	0.43
1:H:41:ASN:O	1:H:45:ARG:HG3	2.18	0.43
3:J:1150:PRO:HG2	3:J:1153:PRO:HG3	2.00	0.43
3:J:1295:ASN:CB	3:J:1298:VAL:HB	2.46	0.43
3:J:255:LEU:N	3:J:259:ARG:O	2.50	0.43
3:J:519:ASN:CB	3:J:709:ARG:HD3	2.48	0.43
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.44	0.43
5:L:593:LYS:O	5:L:596:ARG:HB3	2.19	0.43
1:A:46:ILE:HD11	1:B:38:THR:HG21	2.01	0.43
2:C:1134:GLN:HA	2:C:1134:GLN:OE1	2.19	0.43
2:C:87:ILE:HG13	2:C:87:ILE:H	1.70	0.43
2:C:88:ARG:NH2	2:C:1035:LYS:O	2.52	0.43
2:C:930:ASP:OD2	2:C:931:VAL:N	2.51	0.43
3:D:860:ARG:HB3	3:D:861:ASN:H	1.58	0.43
5:F:299:LYS:O	5:F:303:ILE:HG12	2.18	0.43
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.87	0.43
1:G:58:GLU:HB2	1:G:145:LYS:HB3	2.00	0.43
2:I:1327:LEU:HD23	2:I:1331:ARG:HH21	1.84	0.43
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.53	0.43
2:I:151:ARG:HH21	2:I:445:ILE:HD11	1.84	0.43
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.99	0.43
3:J:1034:PHE:CE2	3:J:1114:GLN:HB2	2.54	0.43
3:J:1160:SER:HA	3:J:1204:VAL:O	2.19	0.43
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.53	0.43
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	2.00	0.43
3:J:349:TYR:CD1	3:J:472:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:525:MET:O	3:J:548:VAL:HG13	2.19	0.43
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.19	0.43
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.80	0.43
2:C:1248:THR:HG21	5:F:531:PRO:HG3	2.00	0.43
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.54	0.43
2:C:736:VAL:HG23	2:C:748:ILE:HA	2.01	0.43
3:D:1184:ASP:O	3:D:1186:TYR:N	2.52	0.43
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.54	0.43
3:D:905:ARG:NH1	4:E:16:ARG:HB2	2.34	0.43
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.01	0.43
2:I:1007:LYS:O	2:I:1011:LEU:HG	2.19	0.43
1:H:33:ARG:NH1	2:I:1081:PRO:HG3	2.31	0.43
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.19	0.43
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.54	0.43
2:I:151:ARG:NH2	2:I:445:ILE:HD11	2.34	0.43
2:I:886:LYS:HB3	2:I:917:SER:HA	2.00	0.43
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.84	0.43
3:J:695:LYS:HD3	3:J:695:LYS:HA	1.81	0.43
5:L:111:LEU:HG	5:L:382:ALA:HB1	2.00	0.43
1:B:158:ARG:HA	1:B:158:ARG:HD2	1.78	0.42
1:B:67:GLU:O	1:B:78:ILE:HB	2.18	0.42
2:C:1297:ASP:O	2:C:1301:ARG:HG2	2.18	0.42
2:C:94:ALA:HB2	2:C:129:LEU:HD11	2.01	0.42
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.54	0.42
2:C:367:TYR:CE2	2:C:376:PRO:HA	2.53	0.42
3:D:185:ILE:HD13	3:D:188:LEU:HD12	2.01	0.42
3:D:650:LYS:O	3:D:654:ILE:HG13	2.19	0.42
4:E:62:GLN:O	4:E:66:VAL:HG23	2.19	0.42
1:H:151:GLY:O	1:H:177:TYR:HB2	2.18	0.42
2:I:543:ALA:HA	2:I:544:GLY:HA3	1.87	0.42
5:L:582:VAL:CG2	5:L:586:ARG:HG2	2.49	0.42
1:B:115:ILE:HD11	1:B:130:ILE:HD11	2.01	0.42
2:C:1151:LEU:HD23	2:C:1197:GLU:OE2	2.19	0.42
2:C:596:ASP:OD2	2:C:597:GLY:N	2.51	0.42
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.84	0.42
3:D:133:ARG:O	3:D:137:ARG:HB2	2.18	0.42
3:D:525:MET:O	3:D:548:VAL:HG13	2.19	0.42
3:D:683:ILE:HD11	3:D:754:ILE:HG12	2.02	0.42
1:G:92:VAL:HA	1:G:120:ASP:O	2.19	0.42
2:I:1240:ASP:N	2:I:1240:ASP:OD1	2.50	0.42
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:854:ILE:HB	2:I:857:VAL:HG21	2.01	0.42
3:J:55:GLY:H	3:J:58:CYS:HB2	1.83	0.42
1:B:151:GLY:O	1:B:177:TYR:HB2	2.18	0.42
3:D:1372:ARG:HE	3:J:854:ALA:HB3	1.84	0.42
3:D:232:ASN:N	3:D:232:ASN:OD1	2.51	0.42
3:D:418:GLU:O	3:D:420:PRO:HD3	2.20	0.42
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.78	0.42
3:D:825:VAL:C	3:D:826:ILE:HG13	2.39	0.42
1:H:196:THR:HG23	3:J:443:GLU:HG3	2.01	0.42
2:I:216:THR:H	2:I:219:GLN:HE22	1.66	0.42
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.34	0.42
3:J:683:ILE:HD11	3:J:754:ILE:HG12	2.02	0.42
3:J:80:HIS:N	3:J:80:HIS:ND1	2.67	0.42
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.99	0.42
1:B:90:VAL:HG11	1:B:146:VAL:HG11	2.02	0.42
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.72	0.42
2:C:974:ARG:O	2:C:978:VAL:HG23	2.20	0.42
3:D:660:GLU:O	3:D:664:ILE:HG12	2.18	0.42
5:F:226:ALA:O	5:F:230:VAL:HG12	2.19	0.42
1:H:50:SER:HA	1:H:151:GLY:HA2	2.01	0.42
1:H:95:LYS:NZ	1:H:98:VAL:HG23	2.34	0.42
2:I:1136:GLN:O	2:I:1137:GLU:HG2	2.19	0.42
3:J:824:PRO:HD3	3:J:835:LEU:HB2	2.01	0.42
5:L:476:ARG:HB3	5:L:477:GLU:H	1.24	0.42
5:L:532:LEU:HD12	5:L:532:LEU:H	1.85	0.42
1:A:125:LYS:HG3	1:A:128:HIS:HB2	2.01	0.42
1:A:44:ARG:HG3	1:A:183:ILE:HG22	2.00	0.42
1:B:136:GLU:CG	1:B:137:ASN:H	2.30	0.42
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.19	0.42
2:C:854:ILE:HB	2:C:857:VAL:HG21	2.01	0.42
2:C:961:SER:O	2:C:965:GLN:HG3	2.20	0.42
3:D:1163:VAL:HG22	3:D:1164:SER:H	1.85	0.42
3:D:1302:TYR:CZ	3:J:1297:LYS:HE2	2.55	0.42
2:C:1304:MET:HE2	3:D:472:LEU:HB3	2.02	0.42
3:D:807:LEU:HD23	3:D:915:ILE:HG13	2.02	0.42
3:D:298:MET:SD	5:F:402:LEU:HB3	2.58	0.42
2:I:619:ALA:HB1	2:I:657:THR:HA	2.01	0.42
3:J:1079:LYS:HB3	3:J:1079:LYS:HZ2	1.84	0.42
3:J:298:MET:SD	5:L:402:LEU:HB3	2.59	0.42
1:A:92:VAL:HA	1:A:120:ASP:O	2.20	0.42
2:C:403:MET:HE2	2:C:584:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:519:ASN:CG	3:D:709:ARG:HD3	2.40	0.42
3:D:75:TYR:CE2	3:D:83:VAL:HG21	2.54	0.42
3:D:848:VAL:HG13	3:D:858:VAL:HG22	2.02	0.42
3:D:860:ARG:HG3	3:D:860:ARG:NH1	2.35	0.42
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.85	0.42
3:J:1060:VAL:HG13	3:J:1106:ILE:HA	2.02	0.42
3:J:292:VAL:O	3:J:296:LYS:HG3	2.20	0.42
3:J:984:LEU:CB	3:J:993:GLU:HB2	2.50	0.42
1:A:42:ALA:O	1:A:46:ILE:HG12	2.19	0.42
1:B:43:LEU:HG	1:B:221:ALA:HB2	2.01	0.42
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.85	0.42
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.49	0.42
3:D:338:PHE:CB	3:D:343:LEU:HB2	2.49	0.42
1:G:115:ILE:HG22	1:G:116:THR:H	1.84	0.42
2:I:417:SER:OG	2:I:419:ILE:HG13	2.20	0.42
3:J:59:ALA:HA	3:J:63:GLY:O	2.20	0.42
5:L:105:MET:HE1	5:L:385:ARG:HG2	2.01	0.42
5:L:270:VAL:HG13	5:L:365:MET:HE3	2.01	0.42
1:B:147:GLN:HG3	1:B:148:ARG:H	1.85	0.42
2:C:417:SER:OG	2:C:419:ILE:HG13	2.20	0.42
2:C:494:ASN:HB3	2:C:497:PRO:CD	2.49	0.42
2:C:148:GLN:NE2	2:C:535:PRO:O	2.46	0.42
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.00	0.42
3:D:491:LEU:HD11	3:D:610:ARG:HH12	1.83	0.42
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.55	0.42
1:H:115:ILE:HD11	1:H:130:ILE:HD11	2.01	0.42
1:H:57:THR:O	1:H:173:VAL:HB	2.19	0.42
2:I:27:LEU:HB2	2:I:524:ILE:HD11	2.02	0.42
2:I:53:PHE:O	2:I:57:PHE:HB2	2.19	0.42
3:J:1079:LYS:HB3	3:J:1079:LYS:NZ	2.35	0.42
3:J:425:ARG:HG2	3:J:426:ALA:N	2.35	0.42
3:J:430:HIS:HA	3:J:921:GLN:HB3	2.02	0.42
3:J:849:LEU:HB2	3:J:850:LYS:O	2.20	0.42
3:J:850:LYS:HE2	3:J:855:ASP:HB3	2.02	0.42
3:J:905:ARG:HH21	3:J:907:HIS:CB	2.33	0.42
1:B:41:ASN:O	1:B:45:ARG:HG3	2.19	0.42
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.30	0.42
2:C:1121:ALA:HB1	2:C:1180:MET:O	2.20	0.42
3:D:1372:ARG:HH21	3:J:854:ALA:HB3	1.85	0.42
3:D:292:VAL:O	3:D:296:LYS:HG3	2.20	0.42
3:D:824:PRO:HD3	3:D:835:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:903:LEU:HA	3:D:903:LEU:HD12	1.90	0.42
2:I:1131:MET:HE1	2:I:1141:LEU:HA	2.02	0.42
2:I:138:ILE:HG22	2:I:139:ASN:ND2	2.35	0.42
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.20	0.42
3:J:1332:LEU:HA	3:J:1332:LEU:HD13	1.88	0.42
3:J:632:ALA:O	3:J:635:SER:OG	2.30	0.42
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.85	0.42
1:A:231:PHE:CD2	1:A:231:PHE:N	2.88	0.42
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.87	0.42
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	2.19	0.42
3:D:1281:GLU:O	3:D:1285:VAL:HB	2.19	0.42
3:D:255:LEU:N	3:D:259:ARG:O	2.51	0.42
5:F:421:TYR:H	5:F:421:TYR:HD2	1.67	0.42
5:F:532:LEU:H	5:F:532:LEU:HD12	1.85	0.42
1:H:158:ARG:HD2	1:H:158:ARG:HA	1.82	0.42
2:I:557:ARG:HH21	2:I:607:SER:C	2.23	0.42
2:I:961:SER:O	2:I:965:GLN:HG3	2.20	0.42
3:J:185:ILE:HD13	3:J:188:LEU:HD12	2.01	0.42
3:J:396:ALA:O	3:J:400:MET:HG3	2.19	0.42
3:J:527:LEU:HB2	3:J:550:VAL:HG12	2.02	0.42
3:J:519:ASN:CG	3:J:709:ARG:HD3	2.40	0.42
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.84	0.41
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.35	0.41
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.89	0.41
1:G:46:ILE:HD11	1:H:38:THR:HG21	2.02	0.41
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.19	0.41
2:I:202:ARG:H	2:I:202:ARG:HG3	1.71	0.41
3:J:1037:PHE:N	3:J:1111:ASP:OD2	2.53	0.41
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.85	0.41
2:I:1308:ILE:CG2	3:J:379:PRO:HB2	2.50	0.41
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.86	0.41
3:J:709:ARG:HD2	3:J:710:ASP:N	2.35	0.41
3:J:849:LEU:HB3	3:J:853:THR:HG23	2.02	0.41
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.54	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.75	0.41
5:L:582:VAL:HG23	5:L:586:ARG:HG2	2.00	0.41
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.83	0.41
1:B:56:VAL:HG22	1:B:144:ILE:HD11	2.01	0.41
2:C:138:ILE:C	2:C:139:ASN:HD22	2.24	0.41
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.20	0.41
3:D:863:LEU:CD1	3:D:901:ARG:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:97:ARG:HB3	2:I:121:GLU:HB2	2.01	0.41
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.50	0.41
3:J:1192:LYS:HB2	3:J:1192:LYS:HE3	1.90	0.41
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.76	0.41
3:J:310:GLY:HA2	3:J:314:ARG:CG	2.47	0.41
3:J:821:MET:HE2	3:J:879:ALA:HB1	2.01	0.41
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.35	0.41
5:L:606:VAL:HG13	5:L:607:LEU:HD23	2.03	0.41
2:C:53:PHE:O	2:C:57:PHE:HB2	2.20	0.41
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.20	0.41
3:D:665:GLN:HG3	3:D:669:GLN:NE2	2.36	0.41
3:D:709:ARG:O	3:D:711:GLY:N	2.53	0.41
3:D:901:ARG:HD2	3:D:906:GLY:O	2.20	0.41
1:G:71:LYS:HB2	1:G:78:ILE:HD11	2.02	0.41
2:I:494:ASN:HB3	2:I:497:PRO:CD	2.49	0.41
2:I:718:ALA:HB2	2:I:783:LEU:HD23	2.03	0.41
2:I:898:GLU:OE1	2:I:898:GLU:N	2.53	0.41
3:J:1184:ASP:O	3:J:1186:TYR:N	2.52	0.41
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.83	0.41
1:A:48:LEU:HA	1:A:180:VAL:HG21	2.02	0.41
2:C:100:LEU:HD12	2:C:122:VAL:HG11	2.02	0.41
2:C:172:TYR:O	2:C:188:PHE:HD2	2.04	0.41
2:C:242:VAL:HA	2:C:243:PRO:HD3	1.87	0.41
2:C:718:ALA:HB2	2:C:783:LEU:HD23	2.02	0.41
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.20	0.41
3:D:230:SER:CB	3:D:232:ASN:H	2.33	0.41
5:F:601:PRO:C	5:F:603:ARG:H	2.23	0.41
1:H:110:VAL:HG12	1:H:114:ASP:HB3	2.03	0.41
1:H:83:LEU:HA	1:H:86:LYS:HE2	2.02	0.41
2:I:227:LYS:O	2:I:245:ARG:NH2	2.53	0.41
2:I:596:ASP:OD2	2:I:597:GLY:N	2.52	0.41
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.21	0.41
3:D:1181:ASP:HA	3:J:202:ARG:HD3	2.01	0.41
3:J:403:ARG:HB3	3:J:405:GLU:HG3	2.02	0.41
3:J:56:LEU:H	3:J:56:LEU:HD12	1.85	0.41
3:J:807:LEU:HD23	3:J:915:ILE:HG13	2.02	0.41
1:A:228:LEU:HD12	1:A:231:PHE:CZ	2.56	0.41
2:C:1134:GLN:CB	2:C:1136:GLN:HG2	2.51	0.41
2:C:131:THR:HG22	2:C:132:ASP:H	1.85	0.41
3:D:403:ARG:HB3	3:D:405:GLU:HG3	2.02	0.41
3:D:527:LEU:HB2	3:D:550:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:593:LYS:O	5:F:596:ARG:HB3	2.20	0.41
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.03	0.41
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.80	0.41
2:I:1121:ALA:HB1	2:I:1180:MET:O	2.20	0.41
2:I:453:ILE:HD11	2:I:530:ILE:HD12	2.01	0.41
2:I:710:VAL:HA	2:I:715:THR:HG21	2.02	0.41
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.20	0.41
3:J:1311:LYS:O	3:J:1314:LEU:HB3	2.20	0.41
3:J:514:THR:HG23	3:J:594:GLN:O	2.20	0.41
3:J:967:VAL:HG13	3:J:971:GLY:HA2	2.02	0.41
5:L:490:PRO:HG2	5:L:493:LYS:HE3	2.03	0.41
1:B:83:LEU:HA	1:B:86:LYS:HE2	2.02	0.41
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.21	0.41
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.86	0.41
2:C:744:GLY:C	2:C:746:ALA:H	2.23	0.41
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.60	0.41
3:D:1311:LYS:O	3:D:1314:LEU:HB3	2.20	0.41
3:D:500:ILE:O	3:D:500:ILE:HG22	2.20	0.41
3:D:59:ALA:HA	3:D:63:GLY:O	2.21	0.41
2:I:94:ALA:HB2	2:I:129:LEU:HD11	2.01	0.41
2:I:5:TYR:O	2:I:8:LYS:HG2	2.20	0.41
3:J:1105:ALA:HA	3:J:1125:PRO:HD2	2.03	0.41
3:J:1185:PRO:O	3:J:1187:GLU:HG2	2.20	0.41
3:J:702:GLN:HE21	3:J:702:GLN:HB3	1.65	0.41
5:L:603:ARG:HA	5:L:603:ARG:HH11	1.85	0.41
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.01	0.41
1:B:60:GLU:HG3	1:B:60:GLU:H	1.71	0.41
2:C:925:SER:O	2:C:1056:VAL:HG13	2.21	0.41
2:C:179:TYR:OH	2:C:458:GLU:OE2	2.20	0.41
2:C:557:ARG:HH21	2:C:607:SER:C	2.24	0.41
2:C:619:ALA:HB1	2:C:657:THR:HA	2.02	0.41
2:C:878:THR:OG1	2:C:879:GLY:N	2.54	0.41
2:C:899:GLU:O	2:C:902:LEU:HB3	2.21	0.41
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.85	0.41
3:D:702:GLN:HE21	3:D:702:GLN:HB3	1.67	0.41
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.21	0.41
5:F:292:VAL:HG21	5:F:299:LYS:CG	2.51	0.41
5:F:315:TRP:O	5:F:319:ALA:HB3	2.21	0.41
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.49	0.41
3:J:1281:GLU:O	3:J:1285:VAL:HB	2.20	0.41
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:827:GLU:O	3:J:829:GLY:N	2.36	0.41
3:J:988:PHE:HD2	3:J:990:ARG:HH21	1.69	0.41
5:L:245:ALA:O	5:L:249:ILE:HG13	2.21	0.41
5:L:461:ASN:O	5:L:465:ARG:HG2	2.20	0.41
5:L:489:MET:HG2	5:L:489:MET:H	1.60	0.41
5:L:572:THR:O	5:L:575:GLU:HB3	2.20	0.41
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.02	0.41
5:F:245:ALA:O	5:F:249:ILE:HG13	2.21	0.41
1:H:90:VAL:HG11	1:H:146:VAL:HG11	2.03	0.41
1:G:231:PHE:CZ	1:H:221:ALA:HB3	2.54	0.41
3:J:1290:ARG:HA	3:J:1290:ARG:HD3	1.74	0.41
3:J:441:LEU:HA	3:J:441:LEU:HD13	1.88	0.41
3:J:665:GLN:HG3	3:J:669:GLN:NE2	2.36	0.41
5:L:489:MET:CB	5:L:490:PRO:HD2	2.50	0.41
1:A:20:SER:OG	1:A:21:SER:N	2.54	0.41
2:C:151:ARG:NE	2:C:445:ILE:HD11	2.36	0.41
2:C:227:LYS:O	2:C:245:ARG:NH2	2.53	0.41
3:D:343:LEU:HA	3:D:343:LEU:HD12	1.85	0.41
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.21	0.41
2:C:1313:HIS:O	4:E:28:ARG:NH1	2.53	0.41
5:F:289:LYS:HB3	5:F:289:LYS:HE2	1.86	0.41
5:F:572:THR:O	5:F:575:GLU:HB2	2.21	0.41
1:H:153:VAL:HA	1:H:154:PRO:HD3	1.90	0.41
2:I:172:TYR:O	2:I:188:PHE:HD2	2.04	0.41
3:J:1156:LEU:HG	3:J:1224:ARG:HH21	1.86	0.41
3:J:195:GLU:O	3:J:198:CYS:HB2	2.21	0.41
3:J:840:LEU:HG	3:J:841:GLY:N	2.35	0.41
3:D:1372:ARG:HB2	3:J:854:ALA:HB2	2.03	0.41
4:K:62:GLN:O	4:K:66:VAL:HG23	2.20	0.41
5:L:261:LEU:HD12	5:L:261:LEU:H	1.86	0.41
1:B:43:LEU:O	1:B:47:LEU:HB2	2.21	0.41
2:C:524:ILE:HG21	2:C:708:VAL:HG13	2.02	0.41
1:A:75:GLN:HA	2:C:729:ALA:N	2.35	0.41
2:C:757:THR:O	2:C:833:ILE:HD12	2.21	0.41
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.21	0.41
3:D:514:THR:HG23	3:D:594:GLN:O	2.20	0.41
5:F:445:ASP:OD2	5:F:451:ARG:HD2	2.20	0.41
5:F:559:LEU:O	5:F:563:PHE:HD2	2.04	0.41
2:I:1116:HIS:O	2:I:1119:MET:HB3	2.21	0.41
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.56	0.41
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:418:GLU:O	3:J:420:PRO:HD3	2.20	0.41
3:J:905:ARG:NH1	4:K:10:VAL:HG11	2.35	0.41
5:L:315:TRP:O	5:L:319:ALA:HB3	2.21	0.41
5:L:421:TYR:H	5:L:421:TYR:HD2	1.68	0.41
5:L:482:GLU:CG	5:L:486:ARG:HH12	2.34	0.41
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.86	0.41
1:B:178:SER:HA	1:B:179:PRO:HD3	1.91	0.41
2:C:18:ARG:HA	2:C:19:PRO:HD3	1.96	0.41
1:A:75:GLN:HA	2:C:729:ALA:H	1.86	0.41
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	2.02	0.41
3:D:334:LYS:HG3	3:D:335:GLN:H	1.86	0.41
3:D:77:ARG:HD2	3:D:78:LEU:H	1.85	0.41
2:I:163:LYS:HB3	2:I:163:LYS:HE3	1.97	0.41
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.21	0.41
3:J:548:VAL:HG12	3:J:550:VAL:HG13	2.02	0.41
5:L:165:PHE:HE1	5:L:259:PHE:CD2	2.39	0.41
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.42	0.41
1:A:219:ARG:HE	1:A:219:ARG:HB2	1.65	0.40
1:A:221:ALA:HB1	1:B:228:LEU:HD22	2.02	0.40
2:C:17:LYS:NZ	2:C:1154:ASP:O	2.48	0.40
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.50	0.40
2:C:782:VAL:HG11	2:C:792:GLY:HA2	2.03	0.40
3:D:1185:PRO:O	3:D:1187:GLU:HG2	2.21	0.40
3:D:161:THR:H	3:D:164:GLN:HB2	1.86	0.40
3:D:849:LEU:HB3	3:D:853:THR:HG23	2.02	0.40
5:F:340:ALA:HA	5:F:343:LYS:NZ	2.36	0.40
5:F:489:MET:CB	5:F:490:PRO:HD2	2.52	0.40
5:F:580:PHE:C	5:F:582:VAL:H	2.23	0.40
1:G:27:THR:HA	1:G:201:LEU:O	2.21	0.40
2:I:100:LEU:HD12	2:I:122:VAL:HG11	2.03	0.40
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.54	0.40
2:I:402:ARG:NH2	2:I:419:ILE:O	2.54	0.40
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.61	0.40
3:J:1203:ARG:NH1	3:J:1205:GLU:HG2	2.36	0.40
3:J:349:TYR:CG	3:J:472:LEU:HD21	2.57	0.40
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.57	0.40
3:D:1371:ARG:HE	3:J:854:ALA:HA	1.86	0.40
3:J:901:ARG:HD2	3:J:906:GLY:O	2.21	0.40
5:L:231:THR:HG23	5:L:249:ILE:HG12	2.04	0.40
5:L:292:VAL:HG21	5:L:299:LYS:CG	2.51	0.40
1:A:153:VAL:HB	1:A:175:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:HA	1:B:154:PRO:HD3	1.90	0.40
2:C:24:VAL:HG21	2:C:704:MET:SD	2.62	0.40
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.36	0.40
3:D:369:PRO:HB3	3:D:444:GLY:O	2.22	0.40
3:D:850:LYS:HE2	3:D:855:ASP:HB3	2.03	0.40
1:H:195:ARG:HB3	1:H:198:LEU:HD21	2.03	0.40
2:I:744:GLY:C	2:I:746:ALA:H	2.23	0.40
3:J:1024:THR:HG23	3:J:1123:ARG:HG2	2.03	0.40
3:J:514:THR:CG2	3:J:596:LEU:HB2	2.51	0.40
5:L:591:GLU:O	5:L:595:LEU:HG	2.22	0.40
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.66	0.40
2:C:857:VAL:HB	2:C:861:ALA:HB3	2.03	0.40
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.88	0.40
5:F:583:THR:O	5:F:584:ARG:HB2	2.21	0.40
1:H:136:GLU:CG	1:H:137:ASN:H	2.34	0.40
2:I:408:SER:O	2:I:431:LYS:NZ	2.54	0.40
2:I:582:ASN:HB3	2:I:586:PHE:N	2.35	0.40
3:J:124:ILE:HG13	3:J:124:ILE:H	1.65	0.40
3:J:1348:LYS:HA	3:J:1348:LYS:HD2	1.92	0.40
3:J:800:LEU:HB3	3:J:920:ALA:HB1	2.04	0.40
3:J:83:VAL:O	3:J:91:GLU:HA	2.22	0.40
1:A:71:LYS:HB2	1:A:78:ILE:HD11	2.03	0.40
2:C:1276:TRP:CE2	3:D:801:VAL:HG21	2.56	0.40
2:C:27:LEU:HB2	2:C:524:ILE:HD11	2.02	0.40
3:D:349:TYR:CG	3:D:472:LEU:HD21	2.56	0.40
5:F:482:GLU:HG2	5:F:486:ARG:HH12	1.86	0.40
1:H:147:GLN:HG3	1:H:148:ARG:H	1.86	0.40
1:H:43:LEU:O	1:H:47:LEU:HB2	2.20	0.40
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.95	0.40
2:I:524:ILE:HG21	2:I:708:VAL:HG13	2.02	0.40
2:I:745:GLU:H	2:I:1017:GLN:HG3	1.85	0.40
2:I:974:ARG:O	2:I:978:VAL:HG23	2.21	0.40
3:J:1146:GLU:HB3	3:J:1148:ARG:HG3	2.02	0.40
3:D:853:THR:CG2	3:J:1375:ALA:HB1	2.45	0.40
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.90	0.40
3:J:294:ASN:HD22	5:L:406:GLN:HE21	1.69	0.40
3:J:780:ARG:HB2	3:J:780:ARG:HE	1.71	0.40
3:D:1153:PRO:HA	3:D:1214:PRO:O	2.21	0.40
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.36	0.40
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.03	0.40
3:D:26:SER:HB3	3:D:29:MET:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:396:ALA:O	3:D:400:MET:HG3	2.21	0.40
3:D:821:MET:HE2	3:D:879:ALA:HB1	2.03	0.40
5:F:604:SER:O	5:F:608:ARG:HB3	2.22	0.40
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.37	0.40
3:J:1265:THR:N	3:J:1305:ASP:OD2	2.55	0.40
3:J:248:ASP:O	3:J:251:PRO:HG3	2.22	0.40
3:J:405:GLU:O	3:J:408:VAL:HG13	2.22	0.40
3:J:515:ARG:NH2	3:J:717:VAL:O	2.54	0.40
3:J:77:ARG:HD2	3:J:78:LEU:H	1.85	0.40
3:J:863:LEU:CD1	3:J:901:ARG:HB3	2.51	0.40
5:L:299:LYS:HA	5:L:302:PHE:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:GLU:OE2	2:I:422:LYS:NZ[3_554]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/239 (93%)	195 (88%)	26 (12%)	1 (0%)	29	67
1	B	216/239 (90%)	192 (89%)	23 (11%)	1 (0%)	29	67
1	G	226/239 (95%)	197 (87%)	27 (12%)	2 (1%)	17	57
1	H	213/239 (89%)	191 (90%)	21 (10%)	1 (0%)	29	67
2	C	1338/1342 (100%)	1224 (92%)	100 (8%)	14 (1%)	15	55
2	I	1338/1342 (100%)	1228 (92%)	97 (7%)	13 (1%)	15	55
3	D	1162/1407 (83%)	1078 (93%)	78 (7%)	6 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	1317/1407 (94%)	1225 (93%)	87 (7%)	5 (0%)	34	71
4	E	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	14	53
4	K	77/91 (85%)	72 (94%)	4 (5%)	1 (1%)	12	49
5	F	464/522 (89%)	420 (90%)	41 (9%)	3 (1%)	25	64
5	L	463/522 (89%)	422 (91%)	36 (8%)	5 (1%)	14	53
All	All	7123/7680 (93%)	6520 (92%)	550 (8%)	53 (1%)	22	62

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	44	GLU
2	C	169	LYS
2	C	697	LYS
2	C	897	PRO
2	C	898	GLU
2	C	1137	GLU
2	C	1159	VAL
2	C	1203	ASP
3	D	230	SER
5	F	584	ARG
1	H	138	ALA
2	I	169	LYS
2	I	170	VAL
2	I	897	PRO
2	I	1159	VAL
3	J	230	SER
4	K	15	ASN
2	C	170	VAL
4	E	15	ASN
5	F	475	GLY
2	I	898	GLU
2	I	1153	ALA
3	J	1360	GLY
5	L	584	ARG
5	L	602	SER
1	B	138	ALA
2	C	1153	ALA
2	C	1154	ASP
3	D	710	ASP
2	I	44	GLU

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Mol	Chain	Res	Type
2	I	986	ALA
2	I	1137	GLU
1	A	14	VAL
3	D	1169	THR
2	I	697	LYS
3	J	710	ASP
5	L	475	GLY
5	L	603	ARG
2	C	986	ALA
2	C	1135	GLN
3	D	1345	ARG
1	G	14	VAL
2	I	121	GLU
3	J	1169	THR
5	L	601	PRO
2	C	896	THR
2	I	896	THR
2	I	140	GLY
3	D	1180	VAL
3	D	1360	GLY
5	F	601	PRO
3	J	1180	VAL
1	G	167	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/206 (93%)	169 (88%)	22 (12%)	5	29
1	B	184/206 (89%)	161 (88%)	23 (12%)	4	25
1	G	191/206 (93%)	169 (88%)	22 (12%)	5	29
1	H	183/206 (89%)	164 (90%)	19 (10%)	7	34
2	C	1155/1157 (100%)	1025 (89%)	130 (11%)	6	30
2	I	1154/1157 (100%)	1022 (89%)	132 (11%)	5	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	975/1168 (84%)	870 (89%)	105 (11%)	6	32
3	J	1110/1168 (95%)	996 (90%)	114 (10%)	7	34
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	25
4	K	67/75 (89%)	58 (87%)	9 (13%)	4	23
5	F	417/462 (90%)	361 (87%)	56 (13%)	4	23
5	L	418/462 (90%)	359 (86%)	59 (14%)	3	21
All	All	6117/6548 (93%)	5417 (89%)	700 (11%)	5	29

All (700) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	14	VAL
1	A	15	ASP
1	A	16	ILE
1	A	26	VAL
1	A	35	PHE
1	A	50	SER
1	A	54	CYS
1	A	56	VAL
1	A	61	ILE
1	A	64	VAL
1	A	65	LEU
1	A	67	GLU
1	A	115	ILE
1	A	133	LEU
1	A	145	LYS
1	A	165	GLU
1	A	168	ILE
1	A	192	VAL
1	A	196	THR
1	A	228	LEU
1	A	231	PHE
1	B	8	PHE
1	B	16	ILE
1	B	27	THR
1	B	50	SER
1	B	58	GLU
1	B	60	GLU
1	B	65	LEU

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	79	LEU
1	B	80	GLU
1	B	97	GLU
1	B	110	VAL
1	B	123	ILE
1	B	131	CYS
1	B	133	LEU
1	B	134	THR
1	B	135	ASP
1	B	139	SER
1	B	148	ARG
1	B	159	ILE
1	B	160	HIS
1	B	176	CYS
1	B	183	ILE
2	C	3	TYR
2	C	4	SER
2	C	11	ILE
2	C	12	ARG
2	C	21	VAL
2	C	23	ASP
2	C	39	ILE
2	C	59	ILE
2	C	79	VAL
2	C	82	VAL
2	C	85	CYS
2	C	91	THR
2	C	106	GLU
2	C	107	ARG
2	C	111	GLU
2	C	113	THR
2	C	114	VAL
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	124	MET
2	C	132	ASP
2	C	167	SER

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Mol	Chain	Res	Type
2	C	219	GLN
2	C	233	ARG
2	C	235	ASN
2	C	258	ASN
2	C	285	ILE
2	C	306	THR
2	C	320	ASP
2	C	360	LEU
2	C	369	MET
2	C	377	THR
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	453	ILE
2	C	470	ARG
2	C	484	LEU
2	C	486	THR
2	C	489	PRO
2	C	490	GLN
2	C	492	MET
2	C	496	LYS
2	C	510	GLN
2	C	518	ASN
2	C	529	ARG
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	554	HIS
2	C	558	VAL
2	C	575	LEU
2	C	604	HIS
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	630	VAL
2	C	633	LEU
2	C	648	ASP
2	C	657	THR
2	C	672	GLU
2	C	680	LEU

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Mol	Chain	Res	Type
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	724	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	783	LEU
2	C	788	SER
2	C	791	LEU
2	C	800	MET
2	C	808	ASN
2	C	814	ASP
2	C	815	SER
2	C	826	ASP
2	C	830	THR
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	902	LEU
2	C	911	SER
2	C	946	LEU
2	C	971	LEU
2	C	979	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1014	LEU
2	C	1073	LYS
2	C	1079	ILE
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1119	MET
2	C	1134	GLN
2	C	1136	GLN

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Mol	Chain	Res	Type
2	C	1140	LYS
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1174	GLU
2	C	1198	LEU
2	C	1204	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1222	GLU
2	C	1239	VAL
2	C	1248	THR
2	C	1265	PHE
2	C	1327	LEU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	46	TYR
3	D	54	ASP
3	D	72	CYS
3	D	79	LYS
3	D	80	HIS
3	D	84	ILE
3	D	92	VAL
3	D	95	THR
3	D	96	LYS
3	D	97	VAL
3	D	98	ARG
3	D	121	PRO
3	D	137	ARG
3	D	159	ILE
3	D	169	LEU
3	D	175	GLU
3	D	214	ARG
3	D	217	LEU
3	D	218	THR

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Mol	Chain	Res	Type
3	D	232	ASN
3	D	248	ASP
3	D	252	LEU
3	D	264	ASP
3	D	299	LEU
3	D	324	LEU
3	D	334	LYS
3	D	339	ARG
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	407	VAL
3	D	490	ILE
3	D	505	ASP
3	D	513	MET
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	544	LEU
3	D	545	HIS
3	D	560	ASN
3	D	567	THR
3	D	568	SER
3	D	573	THR
3	D	576	ARG
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	703	THR
3	D	707	ILE
3	D	710	ASP
3	D	712	GLN
3	D	740	LEU
3	D	753	SER
3	D	754	ILE

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Mol	Chain	Res	Type
3	D	757	THR
3	D	772	TYR
3	D	788	LEU
3	D	803	VAL
3	D	807	LEU
3	D	810	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	860	ARG
3	D	875	ASN
3	D	881	LYS
3	D	890	THR
3	D	907	HIS
3	D	908	ILE
3	D	918	ILE
3	D	1155	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1177	ILE
3	D	1178	THR
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1208	ASP
3	D	1251	LYS
3	D	1255	VAL
3	D	1266	ILE
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1289	ASN
3	D	1290	ARG
3	D	1293	GLU
3	D	1298	VAL
3	D	1310	THR
3	D	1333	THR
3	D	1343	GLU
3	D	1355	ARG
4	E	3	ARG

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Mol	Chain	Res	Type
4	E	5	THR
4	E	6	VAL
4	E	13	ILE
4	E	18	ASP
4	E	28	ARG
4	E	39	VAL
4	E	47	THR
4	E	58	LEU
5	F	94	THR
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	166	VAL
5	F	230	VAL
5	F	246	GLN
5	F	247	GLU
5	F	297	MET
5	F	301	ASN
5	F	306	PHE
5	F	335	GLU
5	F	341	LEU
5	F	342	GLN
5	F	344	LEU
5	F	362	ASN
5	F	395	THR
5	F	400	GLN
5	F	421	TYR
5	F	429	THR
5	F	445	ASP
5	F	449	THR
5	F	467	SER
5	F	469	GLN
5	F	470	MET
5	F	471	LEU
5	F	472	GLN
5	F	476	ARG
5	F	481	GLU
5	F	482	GLU
5	F	485	GLU
5	F	488	LEU
5	F	489	MET
5	F	491	GLU

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Mol	Chain	Res	Type
5	F	496	LYS
5	F	499	LYS
5	F	515	GLU
5	F	516	ASP
5	F	529	GLU
5	F	530	LEU
5	F	540	LEU
5	F	547	VAL
5	F	558	VAL
5	F	566	ASP
5	F	568	ASN
5	F	569	THR
5	F	572	THR
5	F	573	LEU
5	F	575	GLU
5	F	580	PHE
5	F	581	ASP
5	F	587	ILE
5	F	600	HIS
5	F	601	PRO
5	F	603	ARG
5	F	608	ARG
1	G	9	LEU
1	G	14	VAL
1	G	15	ASP
1	G	16	ILE
1	G	26	VAL
1	G	35	PHE
1	G	50	SER
1	G	54	CYS
1	G	56	VAL
1	G	61	ILE
1	G	64	VAL
1	G	65	LEU
1	G	67	GLU
1	G	115	ILE
1	G	133	LEU
1	G	145	LYS
1	G	165	GLU
1	G	168	ILE
1	G	192	VAL
1	G	196	THR

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Mol	Chain	Res	Type
1	G	228	LEU
1	G	231	PHE
1	H	16	ILE
1	H	27	THR
1	H	58	GLU
1	H	60	GLU
1	H	65	LEU
1	H	75	GLN
1	H	79	LEU
1	H	80	GLU
1	H	97	GLU
1	H	110	VAL
1	H	123	ILE
1	H	131	CYS
1	H	133	LEU
1	H	134	THR
1	H	135	ASP
1	H	139	SER
1	H	148	ARG
1	H	176	CYS
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	12	ARG
2	I	21	VAL
2	I	23	ASP
2	I	39	ILE
2	I	59	ILE
2	I	70	TYR
2	I	79	VAL
2	I	82	VAL
2	I	85	CYS
2	I	91	THR
2	I	106	GLU
2	I	107	ARG
2	I	111	GLU
2	I	113	THR
2	I	114	VAL
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE

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Mol	Chain	Res	Type
2	I	119	GLU
2	I	121	GLU
2	I	124	MET
2	I	131	THR
2	I	132	ASP
2	I	167	SER
2	I	219	GLN
2	I	233	ARG
2	I	235	ASN
2	I	258	ASN
2	I	285	ILE
2	I	306	THR
2	I	320	ASP
2	I	360	LEU
2	I	369	MET
2	I	377	THR
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	453	ILE
2	I	470	ARG
2	I	484	LEU
2	I	486	THR
2	I	490	GLN
2	I	492	MET
2	I	496	LYS
2	I	510	GLN
2	I	518	ASN
2	I	529	ARG
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	542	ARG
2	I	554	HIS
2	I	558	VAL
2	I	575	LEU
2	I	604	HIS
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	630	VAL

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Mol	Chain	Res	Type
2	I	633	LEU
2	I	648	ASP
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	705	GLU
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	778	GLU
2	I	783	LEU
2	I	788	SER
2	I	791	LEU
2	I	800	MET
2	I	808	ASN
2	I	814	ASP
2	I	815	SER
2	I	826	ASP
2	I	830	THR
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	902	LEU
2	I	911	SER
2	I	946	LEU
2	I	971	LEU
2	I	979	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1014	LEU
2	I	1073	LYS
2	I	1079	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN

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Mol	Chain	Res	Type
2	I	1109	ILE
2	I	1114	GLU
2	I	1119	MET
2	I	1134	GLN
2	I	1135	GLN
2	I	1136	GLN
2	I	1140	LYS
2	I	1146	GLN
2	I	1151	LEU
2	I	1155	VAL
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1174	GLU
2	I	1198	LEU
2	I	1204	LEU
2	I	1206	THR
2	I	1210	ILE
2	I	1222	GLU
2	I	1239	VAL
2	I	1240	ASP
2	I	1248	THR
2	I	1265	PHE
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	46	TYR
3	J	54	ASP
3	J	72	CYS
3	J	79	LYS
3	J	80	HIS
3	J	84	ILE
3	J	92	VAL
3	J	95	THR
3	J	96	LYS
3	J	97	VAL
3	J	98	ARG
3	J	121	PRO
3	J	137	ARG
3	J	159	ILE

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Mol	Chain	Res	Type
3	J	169	LEU
3	J	175	GLU
3	J	214	ARG
3	J	217	LEU
3	J	218	THR
3	J	232	ASN
3	J	248	ASP
3	J	252	LEU
3	J	264	ASP
3	J	299	LEU
3	J	324	LEU
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	398	LYS
3	J	407	VAL
3	J	490	ILE
3	J	505	ASP
3	J	513	MET
3	J	514	THR
3	J	523	GLU
3	J	536	LEU
3	J	544	LEU
3	J	545	HIS
3	J	560	ASN
3	J	567	THR
3	J	568	SER
3	J	573	THR
3	J	576	ARG
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	703	THR
3	J	707	ILE
3	J	710	ASP
3	J	712	GLN

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Mol	Chain	Res	Type
3	J	740	LEU
3	J	753	SER
3	J	754	ILE
3	J	757	THR
3	J	772	TYR
3	J	788	LEU
3	J	803	VAL
3	J	807	LEU
3	J	810	THR
3	J	847	ASP
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	860	ARG
3	J	875	ASN
3	J	881	LYS
3	J	890	THR
3	J	898	CYS
3	J	907	HIS
3	J	908	ILE
3	J	918	ILE
3	J	950	ILE
3	J	951	GLN
3	J	960	LEU
3	J	987	GLU
3	J	994	SER
3	J	1048	ARG
3	J	1053	LEU
3	J	1062	LEU
3	J	1063	ASP
3	J	1064	SER
3	J	1067	ARG
3	J	1121	LEU
3	J	1155	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1177	ILE
3	J	1178	THR
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1208	ASP

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Mol	Chain	Res	Type
3	J	1251	LYS
3	J	1255	VAL
3	J	1266	ILE
3	J	1274	PHE
3	J	1275	LEU
3	J	1281	GLU
3	J	1284	ARG
3	J	1289	ASN
3	J	1290	ARG
3	J	1293	GLU
3	J	1298	VAL
3	J	1310	THR
3	J	1333	THR
3	J	1343	GLU
3	J	1355	ARG
4	K	3	ARG
4	K	5	THR
4	K	6	VAL
4	K	13	ILE
4	K	18	ASP
4	K	28	ARG
4	K	39	VAL
4	K	47	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	166	VAL
5	L	230	VAL
5	L	246	GLN
5	L	247	GLU
5	L	297	MET
5	L	301	ASN
5	L	306	PHE
5	L	335	GLU
5	L	341	LEU
5	L	342	GLN
5	L	344	LEU
5	L	362	ASN
5	L	395	THR
5	L	400	GLN
5	L	421	TYR

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Mol	Chain	Res	Type
5	L	429	THR
5	L	445	ASP
5	L	449	THR
5	L	467	SER
5	L	469	GLN
5	L	470	MET
5	L	471	LEU
5	L	472	GLN
5	L	476	ARG
5	L	481	GLU
5	L	482	GLU
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	496	LYS
5	L	499	LYS
5	L	515	GLU
5	L	516	ASP
5	L	529	GLU
5	L	530	LEU
5	L	540	LEU
5	L	547	VAL
5	L	558	VAL
5	L	566	ASP
5	L	568	ASN
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	575	GLU
5	L	580	PHE
5	L	581	ASP
5	L	582	VAL
5	L	587	ILE
5	L	600	HIS
5	L	601	PRO
5	L	603	ARG
5	L	607	LEU
5	L	608	ARG
5	L	613	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
2	C	69	GLN
2	C	139	ASN
2	C	620	ASN
2	C	628	HIS
2	C	688	GLN
2	C	1116	HIS
2	C	1136	GLN
2	C	1146	GLN
2	C	1237	HIS
2	C	1313	HIS
2	C	1314	GLN
3	D	200	GLN
3	D	340	GLN
3	D	419	HIS
3	D	488	ASN
3	D	669	GLN
3	D	702	GLN
3	D	897	HIS
3	D	910	ASN
3	D	1227	HIS
3	D	1244	GLN
3	D	1259	GLN
4	E	7	GLN
5	F	246	GLN
5	F	383	ASN
5	F	396	ASN
5	F	406	GLN
5	F	579	GLN
5	F	600	HIS
1	H	66	HIS
2	I	69	GLN
2	I	139	ASN
2	I	620	ASN
2	I	628	HIS
2	I	688	GLN
2	I	1038	GLN
2	I	1116	HIS
2	I	1136	GLN
2	I	1146	GLN
2	I	1237	HIS
2	I	1314	GLN

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Mol	Chain	Res	Type
3	J	80	HIS
3	J	200	GLN
3	J	488	ASN
3	J	669	GLN
3	J	702	GLN
3	J	897	HIS
3	J	910	ASN
3	J	1108	GLN
3	J	1227	HIS
3	J	1244	GLN
3	J	1259	GLN
4	K	7	GLN
5	L	246	GLN
5	L	383	ASN
5	L	396	ASN
5	L	406	GLN
5	L	446	GLN
5	L	579	GLN
5	L	600	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/239 (93%)	-0.35	0 100 100	59, 91, 130, 167	0
1	B	220/239 (92%)	0.12	10 (4%) 33 19	63, 125, 155, 166	0
1	G	228/239 (95%)	-0.15	2 (0%) 84 71	85, 121, 148, 164	0
1	H	217/239 (90%)	0.13	13 (5%) 21 11	90, 130, 156, 165	0
2	C	1340/1342 (99%)	-0.34	5 (0%) 92 86	33, 84, 134, 170	0
2	I	1340/1342 (99%)	-0.17	22 (1%) 72 55	48, 101, 149, 179	0
3	D	1166/1407 (82%)	-0.26	12 (1%) 82 69	28, 77, 137, 168	0
3	J	1325/1407 (94%)	-0.05	54 (4%) 37 22	40, 96, 152, 176	0
4	E	89/91 (97%)	-0.51	0 100 100	44, 84, 114, 133	0
4	K	79/91 (86%)	-0.31	0 100 100	63, 97, 136, 150	0
5	F	470/522 (90%)	-0.08	15 (3%) 47 31	53, 119, 159, 181	0
5	L	469/522 (89%)	-0.11	10 (2%) 63 46	61, 117, 159, 173	0
All	All	7167/7680 (93%)	-0.18	143 (1%) 65 48	28, 97, 150, 181	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	167	ASP	9.2
1	B	172	LEU	7.5
5	L	167	ASP	7.4
2	I	999	GLU	6.0
3	J	1054	THR	5.7
5	L	480	PRO	5.3
2	I	982	GLY	5.3
1	B	146	VAL	4.6
3	D	1198	VAL	4.6
3	J	1084	GLN	4.5
5	F	323	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
3	J	1295	ASN	3.9
3	J	1058	SER	3.8
3	J	1036	ARG	3.8
5	F	321	ALA	3.8
3	J	1198	VAL	3.8
2	I	1002	LEU	3.7
3	J	1181	ASP	3.7
3	J	1051	ASP	3.6
5	L	305	LEU	3.6
2	C	266	GLY	3.6
1	B	147	GLN	3.6
3	J	1069	ALA	3.5
3	J	1080	ILE	3.5
2	I	983	GLY	3.5
5	L	290	LEU	3.5
5	F	579	GLN	3.5
2	I	979	LEU	3.5
3	J	1053	LEU	3.5
5	F	319	ALA	3.4
2	I	1003	THR	3.4
5	F	283	GLN	3.4
3	D	1173	ARG	3.3
2	I	107	ARG	3.3
5	F	312	SER	3.3
1	B	158	ARG	3.3
3	J	1068	THR	3.3
2	I	247	ARG	3.1
1	H	106	GLY	3.1
5	F	315	TRP	3.1
1	B	121	VAL	3.1
1	G	160	HIS	3.1
2	I	105	TYR	3.0
3	J	1065	ALA	3.0
2	I	996	ARG	3.0
3	J	1083	ALA	3.0
3	J	930	LEU	2.9
3	J	998	PRO	2.9
5	F	320	ILE	2.9
5	L	326	TRP	2.9
3	D	1204	VAL	2.9
1	H	172	LEU	2.9
3	J	1079	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	67	GLU	2.8
1	B	120	ASP	2.8
1	H	147	GLN	2.8
5	F	313	ASP	2.8
1	H	107	ILE	2.8
1	H	73	GLY	2.8
3	J	1095	MET	2.7
3	D	524	GLY	2.7
3	J	857	LEU	2.7
5	L	165	PHE	2.7
3	J	1110	GLU	2.6
5	L	490	PRO	2.6
2	I	987	GLU	2.6
3	J	1052	GLU	2.6
3	J	1093	THR	2.6
3	J	1008	GLY	2.6
3	D	1200	GLU	2.6
2	I	1010	GLN	2.6
1	H	132	HIS	2.5
3	J	849	LEU	2.5
1	B	90	VAL	2.5
3	J	1088	VAL	2.5
1	B	55	ALA	2.5
2	I	981	ALA	2.5
3	J	1085	GLY	2.5
5	F	578	LYS	2.5
3	D	830	ASP	2.4
3	J	1082	ASP	2.4
2	C	251	ALA	2.4
5	L	325	PRO	2.4
3	J	1104	LYS	2.4
3	J	1273	ASP	2.4
3	J	856	ILE	2.4
3	D	340	GLN	2.4
2	I	882	ILE	2.4
2	I	1017	GLN	2.3
3	J	1059	LEU	2.3
5	F	318	ALA	2.3
3	D	69	GLU	2.3
3	J	1030	GLU	2.3
3	J	522	GLY	2.3
2	C	852	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	209	GLY	2.3
2	C	1001	GLY	2.3
3	J	957	SER	2.3
3	J	1180	VAL	2.3
2	I	1007	LYS	2.3
3	J	1215	GLU	2.3
3	D	826	ILE	2.3
1	H	148	ARG	2.3
5	F	514	ASP	2.3
3	D	827	GLU	2.2
5	F	336	GLU	2.2
3	D	1172	LYS	2.2
1	H	92	VAL	2.2
3	J	1109	LEU	2.2
3	J	208	THR	2.2
3	J	542	ALA	2.2
2	I	1021	LEU	2.2
3	J	956	GLY	2.2
2	I	725	GLN	2.2
3	J	1294	ALA	2.2
2	I	867	GLU	2.2
2	I	973	SER	2.2
3	J	1097	ALA	2.2
2	C	1000	LEU	2.1
3	J	977	SER	2.1
1	H	74	VAL	2.1
3	J	987	GLU	2.1
3	J	1057	SER	2.1
1	H	24	ALA	2.1
2	I	995	ASP	2.1
3	J	314	ARG	2.1
3	J	1007	ASP	2.1
3	J	955	LYS	2.1
3	J	1056	LEU	2.1
1	B	148	ARG	2.1
1	H	52	PRO	2.1
3	J	1013	GLY	2.1
1	H	126	PRO	2.1
5	L	166	VAL	2.1
5	F	326	TRP	2.1
2	I	855	PRO	2.1
1	H	72	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
5	L	294	GLN	2.0
3	D	743	MET	2.0
3	J	929	GLN	2.0
3	J	1070	GLY	2.0
3	J	1091	PRO	2.0
3	J	1188	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 carbohydrates 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(Å ²)	Q<0.9
7	ZN	J	1503	1/1	0.40	0.43	316,316,316,316	0
6	MG	D	1501	1/1	0.83	0.41	78,78,78,78	0
6	MG	J	1501	1/1	0.87	0.22	89,89,89,89	0
7	ZN	D	1503	1/1	0.88	0.28	114,114,114,114	0
7	ZN	J	1502	1/1	0.91	0.30	314,314,314,314	0
7	ZN	D	1502	1/1	0.95	0.21	198,198,198,198	0

6.5 Other polymers ⓘ

There are no such residues in this entry.