



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:16 PM UTC

PDB ID : 5UAL / pdb_00005ual
Title : Escherichia coli RNA polymerase and Rifampin complex, RpoB S531L mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

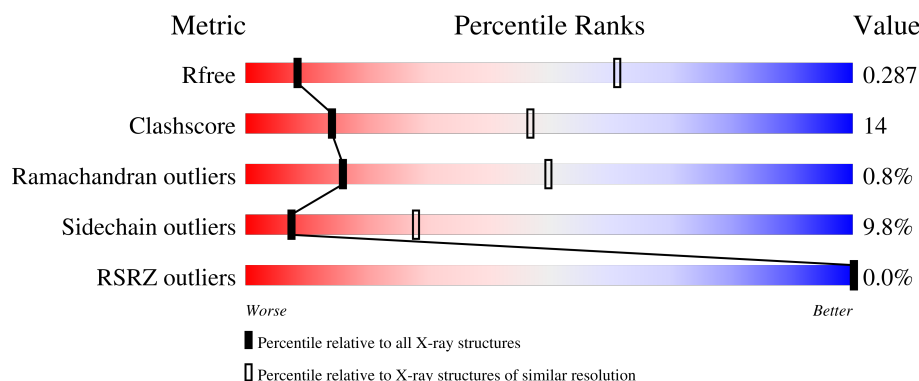
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1186 (4.06-3.70)
Clashscore	190562	1012 (4.04-3.72)
Ramachandran outliers	187476	1167 (4.06-3.70)
Sidechain outliers	187428	1160 (4.06-3.70)
RSRZ outliers	180081	1185 (4.06-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 54898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1332	Total	C	N	O	S	0	0	0
			10514	6600	1827	2043	44			
2	I	1328	Total	C	N	O	S	0	0	0
			10486	6583	1822	2038	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	531	LEU	SER	engineered mutation	UNP P0A8V2
I	531	LEU	SER	engineered mutation	UNP P0A8V2

- 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
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

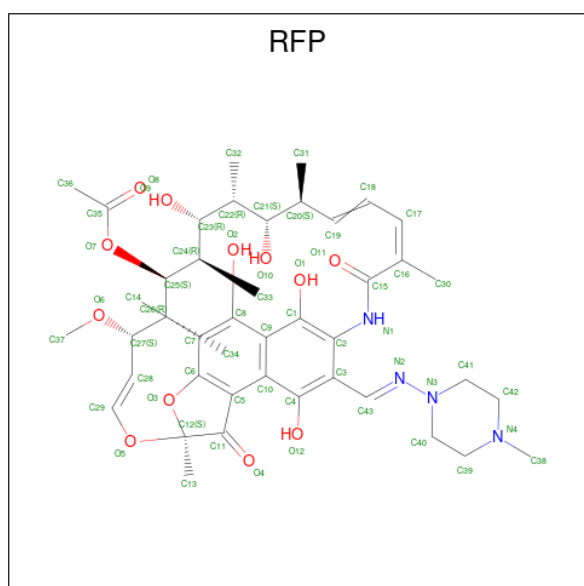
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is RIFAMPICIN (CCD ID: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			59	43	4	12		

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

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

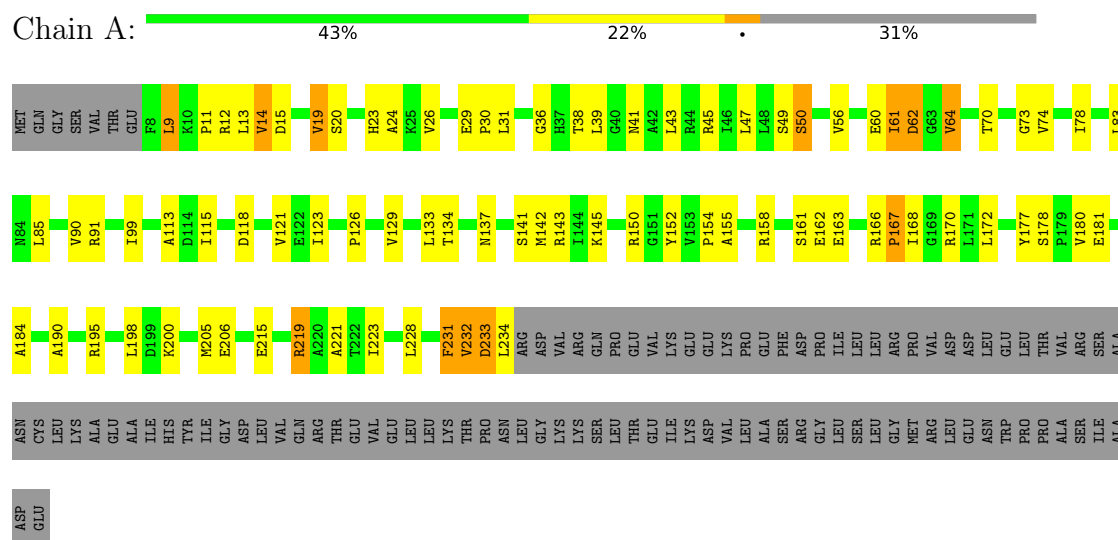
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

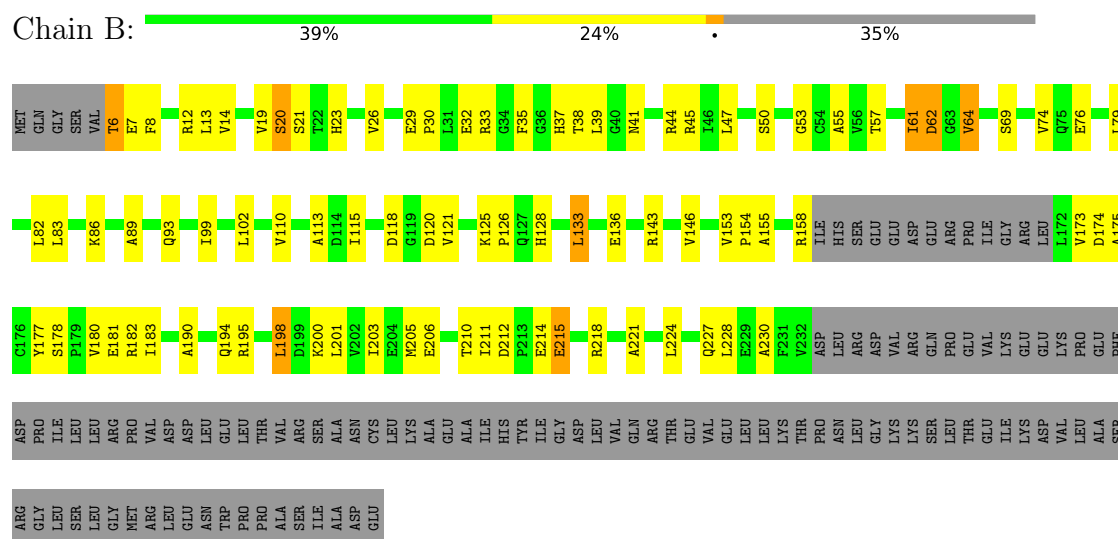
3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

32%

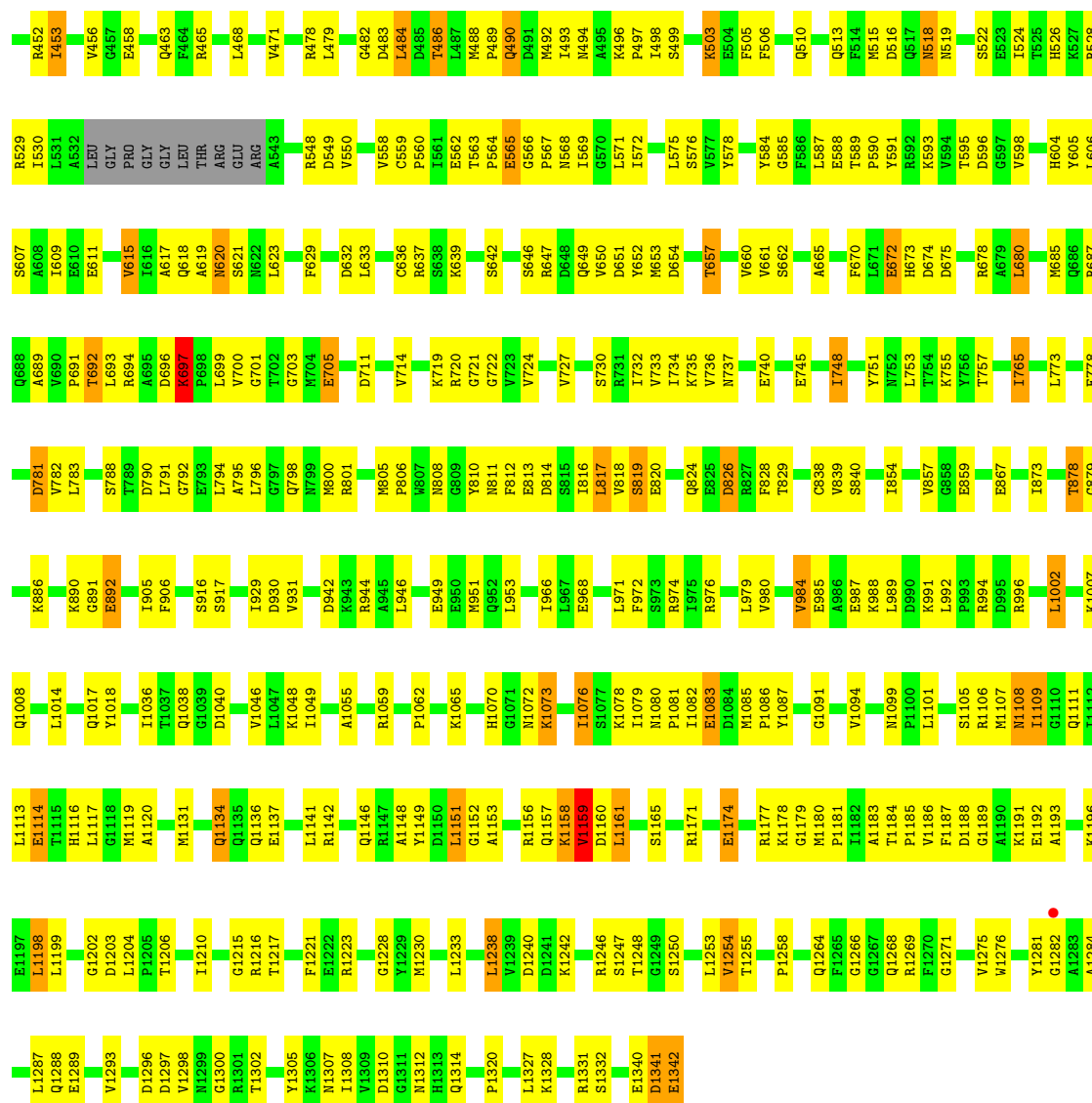


35%



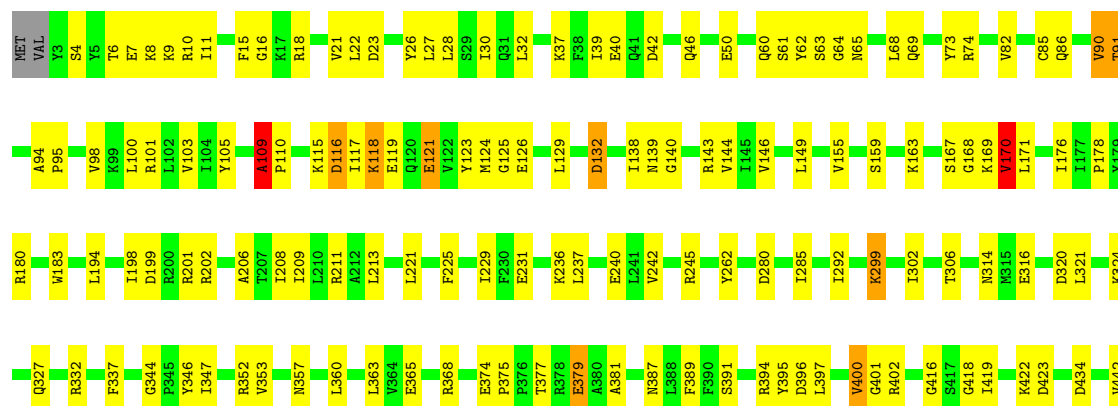
34%

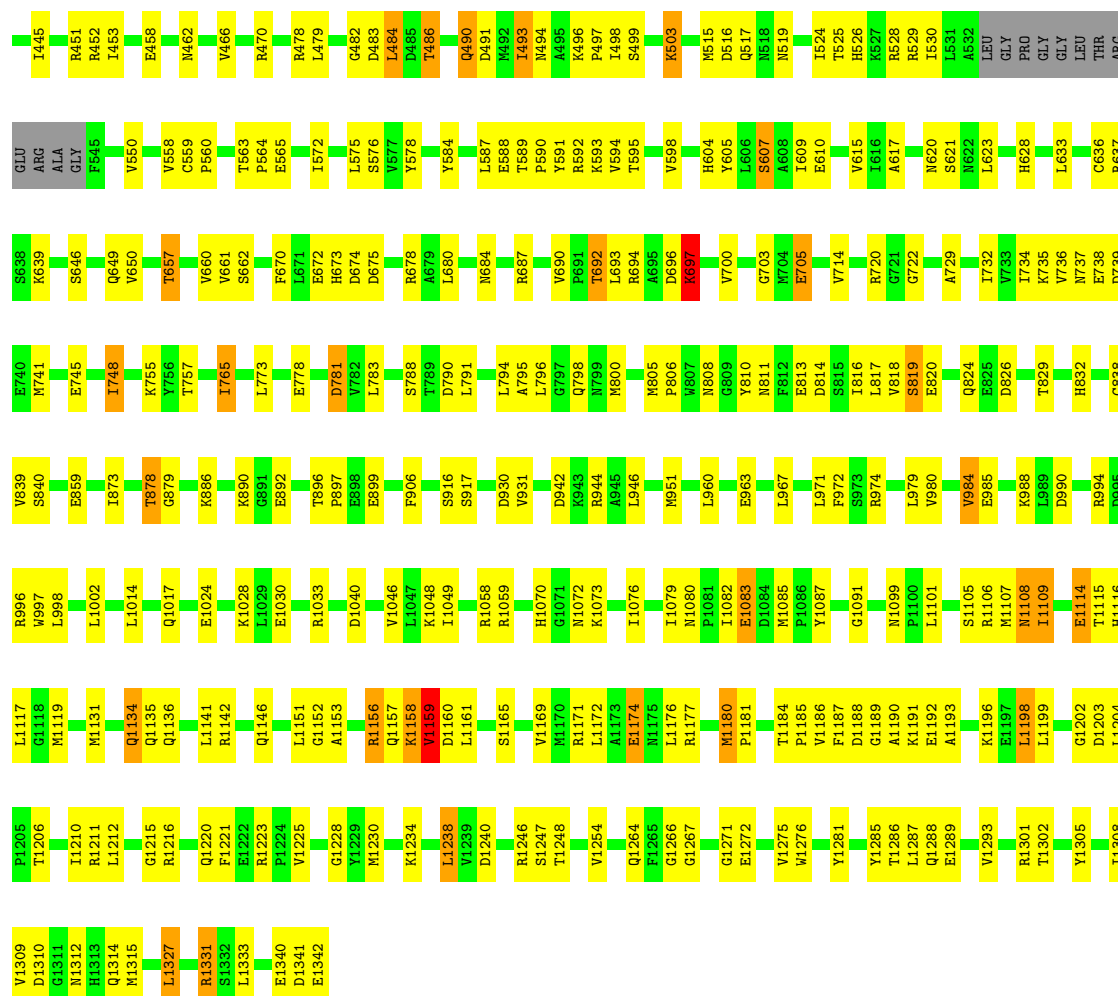




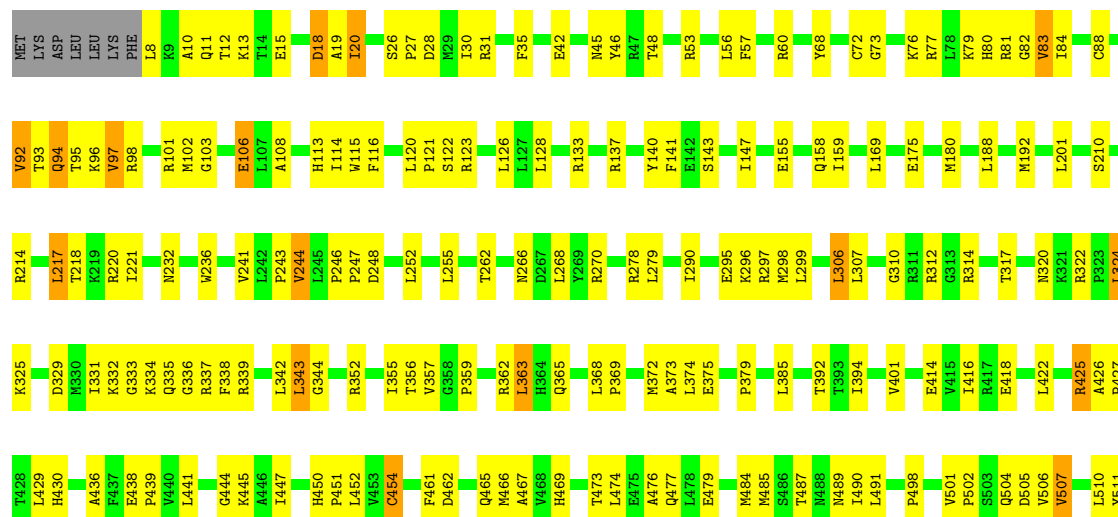
• Molecule 2: DNA-directed RNA polymerase subunit beta

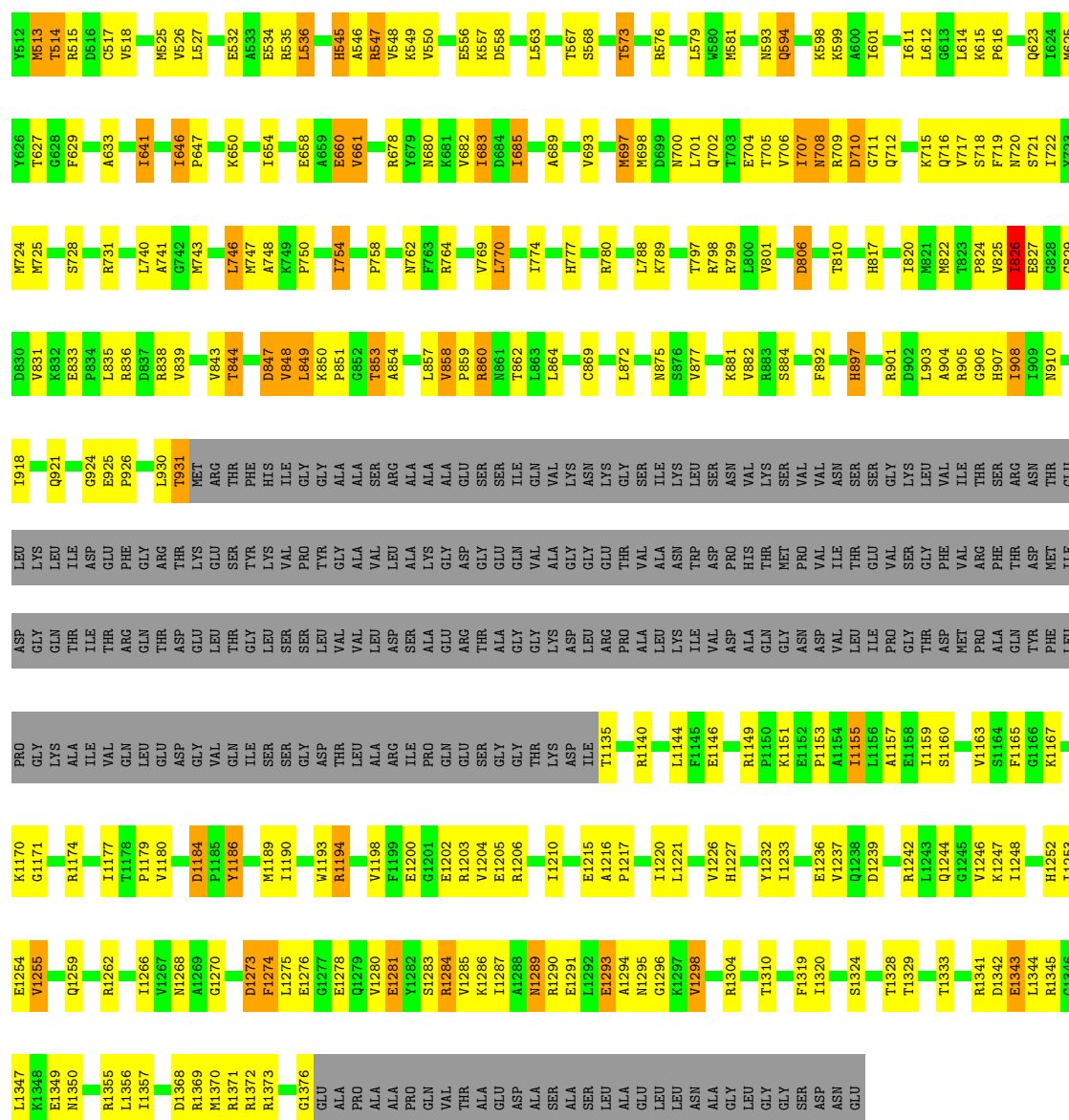
Chain I: 66% 30% ..





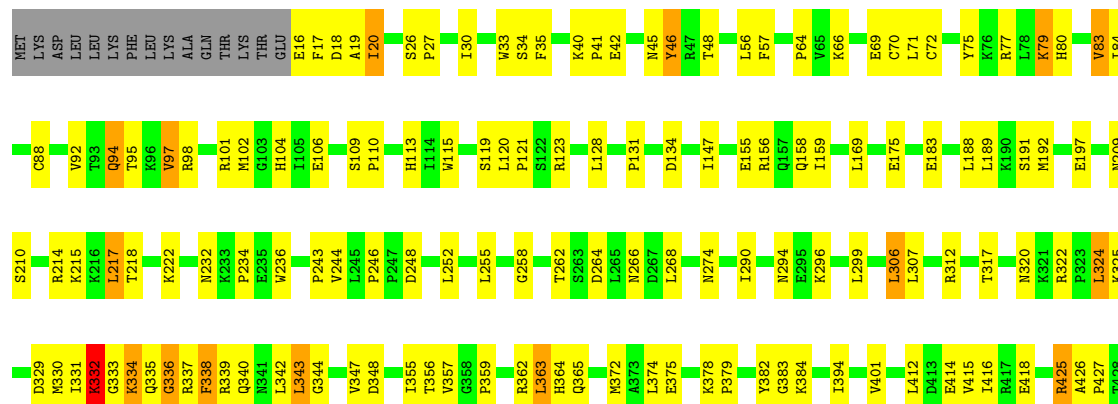
Chain D: 51% 28% 17%





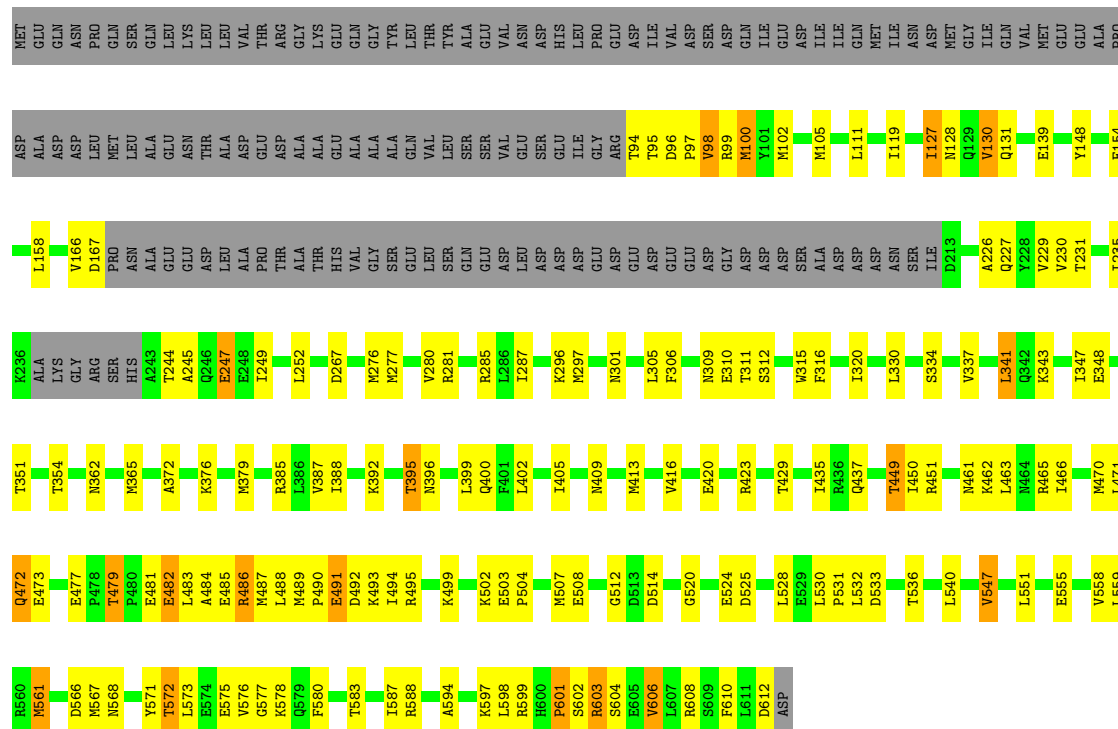
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 52% 26% 5% 18%



ARG

- Molecule 5: RNA polymerase sigma factor RpoD

Chain F:  50% 23% 24%

T583	R584	E585	R586	I587	R588	Q589	I590	L598	P601	S602	R603	S604	E605	V606	I607	R608	D613
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.37Å 205.95Å 309.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 3.89 29.94 – 3.89	Depositor EDS
% Data completeness (in resolution range)	82.9 (29.94-3.89) 82.6 (29.94-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.86Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.230 , 0.286 0.232 , 0.287	Depositor DCC
R_{free} test set	2000 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	168.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 157.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	54898	wwPDB-VP
Average B, all atoms (Å ²)	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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, RFP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	1/1774 (0.1%)	0.57	0/2405
1	B	0.29	0/1668	0.81	0/2260
1	G	0.28	1/1751 (0.1%)	0.54	0/2373
1	H	0.23	0/1678	0.74	2/2274 (0.1%)
2	C	0.31	0/10681	0.64	2/14410 (0.0%)
2	I	0.22	0/10653	0.59	2/14373 (0.0%)
3	D	0.34	0/9229	0.66	0/12459
3	J	0.28	0/9140	0.61	1/12341 (0.0%)
4	E	0.24	0/693	0.55	0/935
4	K	0.18	0/629	0.54	0/847
5	F	0.23	0/3864	0.58	1/5194 (0.0%)
5	L	0.21	0/3872	0.55	0/5205
All	All	0.28	2/55632 (0.0%)	0.62	8/75076 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	C-N	8.81	1.54	1.33
1	G	29	GLU	C-N	7.64	1.51	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	109	ALA	CA-C-N	16.03	137.14	119.83
2	I	109	ALA	C-N-CA	16.03	137.14	119.83
2	C	109	ALA	CA-C-N	15.78	136.88	119.83
2	C	109	ALA	C-N-CA	15.78	136.88	119.83
3	J	343	LEU	CA-CB-CG	7.64	143.06	116.30
5	F	602	SER	N-CA-C	-5.62	98.83	110.80
1	H	29	GLU	CA-C-N	5.24	139.57	127.00
1	H	29	GLU	C-N-CA	5.24	139.57	127.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
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	1753	0	1780	64	0
1	B	1649	0	1674	73	0
1	G	1730	0	1756	69	0
1	H	1659	0	1692	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10514	0	10531	345	0
2	I	10486	0	10496	281	0
3	D	9089	0	9263	323	0
3	J	9001	0	9167	299	0
4	E	691	0	695	12	0
4	K	627	0	634	22	0
5	F	3813	0	3880	98	0
5	L	3821	0	3884	86	0
6	C	59	0	56	8	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	54898	0	55508	1562	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1562) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.36	1.07
2:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.44	0.99
2:C:1269:ARG:HG3	3:D:343:LEU:HD12	1.49	0.94
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.50	0.91
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.52	0.91
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.54	0.89
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.53	0.89
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.55	0.88
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.40	0.85
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.56	0.85
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.57	0.85
3:D:342:LEU:HA	3:D:343:LEU:HD23	1.59	0.85
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.57	0.85
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.62	0.81
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.59	0.81
5:L:97:PRO:HA	5:L:100:MET:HG3	1.60	0.81
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.63	0.80
1:G:45:ARG:HG2	1:H:38:THR:HB	1.62	0.80
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.46	0.79
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.65	0.79
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.63	0.78
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.47	0.78
1:G:218:ARG:HH11	1:H:232:VAL:HG22	1.48	0.78
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.66	0.78
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.66	0.78
1:H:32:GLU:HA	1:H:198:LEU:HD22	1.67	0.77
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.67	0.77
1:B:29:GLU:OE1	1:B:200:LYS:HE2	1.84	0.77
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.18	0.77
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.50	0.77
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.66	0.76
2:I:560:PRO:O	3:J:780:ARG:NH2	2.18	0.76
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.67	0.76
2:C:1271:GLY:HA2	3:D:343:LEU:CD2	2.15	0.76
1:H:23:HIS:HB2	1:H:205:MET:O	1.86	0.76
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.19	0.75
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.68	0.75
2:C:1247:SER:HB3	3:D:375:GLU:O	1.87	0.75
2:C:1248:THR:HB	5:F:532:LEU:HD11	1.69	0.74
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.20	0.74
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.68	0.74
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.53	0.74
3:D:576:ARG:NH1	3:D:593:ASN:O	2.20	0.74
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.69	0.74
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.21	0.73
5:F:598:LEU:O	5:F:604:SER:OG	2.06	0.73
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.69	0.73
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.70	0.73
3:J:665:GLN:HE22	3:J:678:ARG:HH21	1.36	0.72
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.54	0.72
3:J:156:ARG:NH2	3:J:191:SER:OG	2.21	0.72
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.71	0.72
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.71	0.72
2:I:324:LYS:O	2:I:327:GLN:NE2	2.22	0.72
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.23	0.72
3:J:436:ALA:HB3	3:J:485:MET:HA	1.72	0.72
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.22	0.71
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.72	0.71
3:D:700:ASN:O	3:D:704:GLU:HB2	1.89	0.71
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.72	0.71
2:I:18:ARG:NH1	2:I:621:SER:O	2.22	0.71
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.24	0.71
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.72	0.71
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.73	0.70
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.73	0.70
1:B:182:ARG:NH1	3:D:581:MET:SD	2.64	0.70
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.71	0.70
3:J:128:LEU:HA	3:J:192:MET:HE1	1.73	0.70
2:I:452:ARG:NH1	2:I:584:TYR:O	2.23	0.70
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.57	0.70
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.73	0.70
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.57	0.70
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.39	0.69
1:G:12:ARG:H	1:G:30:PRO:HD2	1.56	0.69
1:G:23:HIS:HB2	1:G:205:MET:O	1.92	0.69
3:J:700:ASN:O	3:J:704:GLU:HB2	1.91	0.69
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.92	0.69
5:F:97:PRO:HA	5:F:100:MET:HG3	1.73	0.69
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.75	0.69
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.74	0.69
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.73	0.69
1:A:45:ARG:HG2	1:B:38:THR:HB	1.74	0.69
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.73	0.69
2:I:109:ALA:HB1	2:I:110:PRO:C	2.17	0.69
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.74	0.69
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.74	0.69
5:F:316:PHE:HZ	5:F:334:SER:HA	1.56	0.69
1:A:23:HIS:HB2	1:A:205:MET:O	1.92	0.68
2:C:109:ALA:HB1	2:C:110:PRO:C	2.19	0.68
2:I:30:ILE:HD12	2:I:30:ILE:H	1.59	0.68
5:L:316:PHE:HZ	5:L:334:SER:HA	1.57	0.68
2:C:197:ARG:NH1	2:C:201:ARG:O	2.25	0.68
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.58	0.68
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.74	0.68
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.58	0.68
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.59	0.68
1:B:23:HIS:HB2	1:B:205:MET:O	1.94	0.67
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.77	0.67
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.76	0.67
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.42	0.67
1:A:12:ARG:H	1:A:30:PRO:HD2	1.58	0.67
3:D:392:THR:HG21	5:F:606:VAL:HA	1.76	0.67
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.76	0.67
1:H:101:THR:H	1:H:116:THR:HG22	1.60	0.67
1:A:14:VAL:HG22	1:A:15:ASP:H	1.60	0.67
1:B:102:LEU:HD11	1:B:110:VAL:HG11	1.75	0.67
2:C:615:VAL:HG13	2:C:651:ASP:H	1.60	0.67
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	1.94	0.67
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.77	0.67
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.25	0.67
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.09	0.67
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.77	0.66
3:J:848:VAL:HG11	3:J:880:VAL:HG22	1.76	0.66
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.26	0.66
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.76	0.66
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.77	0.66
1:B:32:GLU:OE2	1:B:195:ARG:NH2	2.29	0.66
2:C:30:ILE:HD12	2:C:30:ILE:H	1.61	0.66
3:J:901:ARG:HD2	3:J:906:GLY:O	1.95	0.66
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.26	0.66
1:G:14:VAL:HG22	1:G:15:ASP:H	1.61	0.66
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.61	0.66
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.76	0.66
3:J:576:ARG:NH1	3:J:593:ASN:O	2.28	0.66
2:C:40:GLU:O	2:C:73:TYR:OH	2.13	0.66
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.78	0.66
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.76	0.66
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.29	0.66
3:J:514:THR:HB	3:J:576:ARG:HG2	1.78	0.66
2:C:386:GLU:HA	2:C:390:PHE:HD2	1.61	0.65
3:J:905:ARG:NH1	3:J:910:ASN:HD21	1.94	0.65
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.77	0.65
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.26	0.65
2:C:721:GLY:N	2:C:740:GLU:OE1	2.29	0.65
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.76	0.65
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.28	0.65
6:C:3001:RFP:O11	6:C:3001:RFP:O1	2.14	0.65
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.79	0.65
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.30	0.65
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:LEU:HD11	3:J:526:VAL:HG21	1.79	0.65
2:I:499:SER:O	2:I:503:LYS:HB2	1.98	0.64
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.78	0.64
1:B:181:GLU:HA	3:D:535:ARG:HH21	1.60	0.64
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.62	0.64
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.79	0.64
2:I:27:LEU:O	2:I:528:ARG:NH1	2.30	0.64
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.79	0.64
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.80	0.64
3:J:418:GLU:HG3	4:K:45:LYS:H	1.62	0.64
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.62	0.64
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.78	0.64
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.79	0.64
2:I:155:VAL:HG23	2:I:176:ILE:HG12	1.80	0.64
5:L:601:PRO:HB3	5:L:608:ARG:HH22	1.62	0.64
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.31	0.64
1:H:67:GLU:OE1	1:H:67:GLU:N	2.31	0.64
2:I:40:GLU:O	2:I:73:TYR:OH	2.16	0.63
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.80	0.63
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.81	0.63
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.30	0.63
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.98	0.63
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.14	0.63
2:C:1142:ARG:HD3	2:C:1161:LEU:HD11	1.80	0.63
3:J:843:VAL:HG11	3:J:897:HIS:O	1.99	0.63
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.63	0.63
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.62	0.63
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.81	0.63
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.80	0.63
1:G:166:ARG:O	1:G:168:ILE:N	2.32	0.62
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.80	0.62
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.81	0.62
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.82	0.62
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.80	0.62
2:C:905:ILE:O	5:F:599:ARG:NH1	2.31	0.62
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.80	0.62
1:A:166:ARG:O	1:A:168:ILE:N	2.32	0.62
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.32	0.62
3:D:343:LEU:CD2	3:D:344:GLY:HA3	2.23	0.62
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.64	0.62
3:D:1155:ILE:HD13	3:D:1190:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.35	0.62
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.80	0.62
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.80	0.62
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	1.81	0.62
2:C:560:PRO:O	3:D:780:ARG:NH2	2.31	0.62
1:G:62:ASP:OD1	1:G:141:SER:OG	2.15	0.62
1:H:16:ILE:HG23	1:H:26:VAL:HG13	1.81	0.62
3:J:901:ARG:HA	3:J:908:ILE:HA	1.82	0.62
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.35	0.62
1:H:53:GLY:HA3	1:H:177:TYR:O	2.00	0.62
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.82	0.62
2:C:6:THR:OG1	2:C:781:ASP:OD2	2.13	0.62
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.15	0.62
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.63	0.62
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.31	0.62
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.81	0.62
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.64	0.62
3:D:140:TYR:O	3:D:297:ARG:NH1	2.33	0.62
3:J:722:ILE:HA	3:J:725:MET:HE3	1.81	0.62
3:D:901:ARG:HA	3:D:908:ILE:HA	1.80	0.61
2:C:705:GLU:HB2	2:C:794:LEU:H	1.65	0.61
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.81	0.61
2:C:27:LEU:O	2:C:528:ARG:NH1	2.31	0.61
1:G:228:LEU:HD22	1:H:221:ALA:HB1	1.81	0.61
5:F:479:THR:HG23	5:F:481:GLU:H	1.66	0.61
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.81	0.61
5:L:601:PRO:HA	5:L:604:SER:HB2	1.82	0.61
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.82	0.61
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.83	0.61
2:I:1271:GLY:HA3	3:J:343:LEU:HD12	1.83	0.61
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.65	0.61
1:B:182:ARG:H	1:B:206:GLU:HB2	1.65	0.61
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.83	0.61
3:J:45:ASN:HB3	3:J:48:THR:O	2.01	0.61
2:C:588:GLU:HG3	2:C:605:TYR:HD1	1.66	0.61
1:G:13:LEU:HD22	1:H:231:PHE:CE1	2.36	0.61
1:H:32:GLU:OE2	1:H:195:ARG:NH2	2.33	0.61
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.66	0.61
5:F:573:LEU:H	5:F:573:LEU:HD23	1.64	0.60
3:D:1344:LEU:HB3	3:D:1350:ASN:HD21	1.65	0.60
5:L:533:ASP:O	5:L:536:THR:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.65	0.60
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.32	0.60
3:D:336:GLY:HA3	3:D:1324:SER:O	2.01	0.60
5:L:316:PHE:CZ	5:L:334:SER:HA	2.36	0.60
2:C:516:ASP:OD2	2:C:522:SER:OG	2.20	0.60
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.84	0.60
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.83	0.60
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.17	0.60
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.83	0.60
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.84	0.60
3:D:298:MET:SD	5:F:402:LEU:HB3	2.42	0.60
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.66	0.60
1:H:64:VAL:HG11	1:H:69:SER:OG	2.01	0.60
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.67	0.59
1:H:74:VAL:HG12	1:H:76:GLU:H	1.67	0.59
1:B:53:GLY:HA3	1:B:177:TYR:O	2.02	0.59
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.02	0.59
3:D:342:LEU:HA	3:D:343:LEU:CD2	2.31	0.59
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.36	0.59
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.84	0.59
3:J:192:MET:HE2	3:J:197:GLU:OE2	2.03	0.59
2:C:528:ARG:NH2	2:C:576:SER:O	2.36	0.59
3:D:317:THR:HB	3:D:324:LEU:HB3	1.84	0.59
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.85	0.59
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	2.03	0.59
3:D:45:ASN:HB3	3:D:48:THR:O	2.02	0.59
3:D:847:ASP:OD1	3:D:847:ASP:N	2.33	0.59
3:J:115:TRP:O	3:J:119:SER:HB3	2.02	0.59
3:D:121:PRO:HG2	3:D:123:ARG:NH2	2.17	0.59
2:I:930:ASP:OD2	2:I:931:VAL:N	2.35	0.59
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.37	0.58
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.29	0.58
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.68	0.58
2:C:387:ASN:HA	2:C:391:SER:HB2	1.86	0.58
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.85	0.58
5:F:343:LYS:HD2	5:F:343:LYS:H	1.68	0.58
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.85	0.58
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.86	0.58
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.03	0.58
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.18	0.58
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:601:PRO:HA	5:F:604:SER:HB2	1.85	0.58
1:B:212:ASP:CG	1:B:215:GLU:HB2	2.28	0.58
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.85	0.58
3:D:210:SER:O	3:D:214:ARG:HG2	2.03	0.58
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.86	0.58
1:G:161:SER:O	1:G:163:GLU:N	2.36	0.58
2:C:692:THR:OG1	2:C:693:LEU:N	2.36	0.58
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.67	0.58
2:C:930:ASP:OD2	2:C:931:VAL:N	2.36	0.58
3:D:436:ALA:HB3	3:D:485:MET:HA	1.85	0.58
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.85	0.58
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.84	0.58
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.67	0.58
3:J:683:ILE:HD11	3:J:754:ILE:HG23	1.86	0.58
2:C:2:VAL:O	2:C:3:TYR:HB2	2.03	0.58
2:C:529:ARG:NH1	6:C:3001:RFP:O11	2.36	0.58
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.85	0.58
3:D:56:LEU:HD12	3:D:56:LEU:H	1.69	0.58
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.84	0.58
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.69	0.58
3:D:525:MET:O	3:D:548:VAL:HG13	2.03	0.58
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.67	0.58
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.15	0.58
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.37	0.58
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.84	0.58
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.44	0.58
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.85	0.57
2:C:730:SER:O	2:C:753:LEU:HB2	2.04	0.57
3:D:270:ARG:NH2	5:F:449:THR:HG23	2.19	0.57
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.85	0.57
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.66	0.57
3:J:709:ARG:O	3:J:711:GLY:N	2.38	0.57
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.85	0.57
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.85	0.57
1:A:13:LEU:HD23	1:A:13:LEU:H	1.70	0.57
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.87	0.57
3:J:218:THR:HG21	3:J:1275:LEU:HD11	1.86	0.57
2:C:617:ALA:HA	2:C:636:CYS:SG	2.43	0.57
3:D:425:ARG:HG2	3:D:426:ALA:H	1.68	0.57
2:I:607:SER:N	2:I:610:GLU:OE1	2.36	0.57
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:562:GLU:OE2	2:C:662:SER:OG	2.17	0.57
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.87	0.57
3:D:709:ARG:C	3:D:711:GLY:H	2.13	0.57
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.22	0.57
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.86	0.57
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.70	0.57
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.36	0.57
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.70	0.57
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.35	0.57
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.69	0.57
3:J:1198:VAL:HB	3:J:1210:ILE:HA	1.87	0.57
5:L:479:THR:HG23	5:L:481:GLU:H	1.70	0.57
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.85	0.57
3:D:1376:GLY:O	3:J:853:THR:OG1	2.21	0.57
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.70	0.57
1:A:161:SER:O	1:A:163:GLU:N	2.38	0.56
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.87	0.56
3:J:356:THR:OG1	3:J:357:VAL:N	2.38	0.56
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.85	0.56
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.87	0.56
1:H:190:ALA:N	1:H:198:LEU:O	2.33	0.56
2:I:208:ILE:HD11	2:I:365:GLU:HB3	1.85	0.56
1:B:6:THR:O	1:B:6:THR:OG1	2.16	0.56
1:B:55:ALA:O	1:B:146:VAL:HG13	2.04	0.56
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.38	0.56
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.85	0.56
5:F:461:ASN:O	5:F:465:ARG:HG2	2.04	0.56
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.87	0.56
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.86	0.56
3:J:709:ARG:C	3:J:711:GLY:H	2.13	0.56
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.87	0.56
5:F:540:LEU:HD12	5:F:610:PHE:CD1	2.39	0.56
3:D:1259:GLN:NE2	3:D:1262:ARG:HH12	2.03	0.56
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.88	0.56
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.86	0.56
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.87	0.56
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.52	0.56
1:G:49:SER:HB3	2:I:1083:GLU:HG2	1.88	0.56
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.87	0.56
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.88	0.56
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:684:ASN:OD1	2:I:687:ARG:NH1	2.39	0.56
2:C:201:ARG:NH2	2:C:370:MET:O	2.32	0.56
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.87	0.56
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.71	0.56
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.41	0.56
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.31	0.56
5:L:395:THR:OG1	5:L:396:ASN:N	2.36	0.56
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.88	0.56
5:F:348:GLU:HG2	5:F:354:THR:HA	1.86	0.56
5:L:601:PRO:HB3	5:L:608:ARG:NH2	2.21	0.56
2:C:719:LYS:H	2:C:751:TYR:HH	1.53	0.56
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.87	0.56
5:L:244:THR:O	5:L:247:GLU:HG2	2.06	0.56
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.88	0.55
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.21	0.55
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.88	0.55
3:J:362:ARG:H	3:J:365:GLN:NE2	2.04	0.55
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.89	0.55
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.89	0.55
3:D:843:VAL:HG11	3:D:897:HIS:O	2.06	0.55
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.86	0.55
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.07	0.55
5:F:533:ASP:O	5:F:536:THR:N	2.39	0.55
1:G:13:LEU:H	1:G:13:LEU:HD23	1.71	0.55
2:I:1271:GLY:CA	3:J:343:LEU:HD12	2.36	0.55
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.89	0.55
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.21	0.55
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.87	0.55
2:I:829:THR:HA	2:I:1059:ARG:HA	1.89	0.55
5:L:598:LEU:O	5:L:604:SER:OG	2.21	0.55
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.88	0.55
1:B:61:ILE:HG22	1:B:62:ASP:H	1.71	0.55
3:D:518:VAL:O	3:D:547:ARG:NH1	2.39	0.55
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.32	0.55
2:I:528:ARG:NH2	2:I:576:SER:O	2.40	0.55
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.87	0.55
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.89	0.55
1:B:182:ARG:HD2	3:D:581:MET:HE1	1.88	0.55
3:D:1345:ARG:HD2	3:D:1370:MET:HE1	1.89	0.55
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.89	0.55
2:I:692:THR:OG1	2:I:693:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.41	0.55
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.88	0.55
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.07	0.55
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.42	0.55
3:D:709:ARG:O	3:D:711:GLY:N	2.36	0.55
2:I:206:ALA:O	2:I:209:ILE:HG22	2.06	0.55
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.07	0.55
5:L:94:THR:OG1	5:L:95:THR:N	2.40	0.55
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.89	0.55
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.89	0.55
2:I:231:GLU:HG2	2:I:332:ARG:HD3	1.89	0.55
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.87	0.55
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.89	0.55
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.87	0.55
5:L:573:LEU:HD23	5:L:573:LEU:H	1.71	0.55
2:C:829:THR:HA	2:C:1059:ARG:HA	1.89	0.55
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.88	0.55
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.88	0.55
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.89	0.55
2:I:168:GLY:C	2:I:170:VAL:H	2.14	0.55
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.40	0.55
2:C:518:ASN:O	2:C:691:PRO:HD3	2.07	0.54
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.89	0.54
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.72	0.54
1:B:214:GLU:O	1:B:218:ARG:HG3	2.07	0.54
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.72	0.54
1:A:233:ASP:C	1:A:234:LEU:HD22	2.32	0.54
2:C:703:GLY:N	2:C:705:GLU:OE2	2.39	0.54
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.08	0.54
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.88	0.54
2:C:1296:ASP:HB3	2:C:1320:PRO:HB3	1.90	0.54
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.88	0.54
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.89	0.54
2:C:91:THR:HG21	2:C:503:LYS:NZ	2.23	0.54
5:F:547:VAL:HG23	5:F:603:ARG:HH11	1.72	0.54
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.90	0.54
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.89	0.54
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.90	0.54
3:J:210:SER:O	3:J:214:ARG:HG2	2.08	0.54
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.73	0.54
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.21	0.54
4:E:80:LEU:O	4:E:84:THR:OG1	2.19	0.54
3:J:264:ASP:OD2	5:L:506:SER:OG	2.22	0.54
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.89	0.54
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.90	0.54
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.72	0.54
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.88	0.54
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.90	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.88	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.43	0.54
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.54
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.89	0.54
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.90	0.53
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.48	0.53
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.43	0.53
3:J:338:PHE:HA	3:J:342:LEU:O	2.08	0.53
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.90	0.53
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.90	0.53
1:H:113:ALA:HB2	1:H:126:PRO:HB3	1.91	0.53
2:I:213:LEU:HB3	2:I:422:LYS:HD2	1.90	0.53
2:I:314:ASN:O	2:I:352:ARG:NH1	2.34	0.53
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.74	0.53
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.39	0.53
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.43	0.53
3:D:53:ARG:NH2	3:D:60:ARG:HD2	2.24	0.53
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.43	0.53
5:F:166:VAL:O	5:F:167:ASP:HB2	2.09	0.53
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.89	0.53
1:H:110:VAL:HG21	1:H:140:ILE:HD11	1.89	0.53
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.23	0.53
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.24	0.53
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.39	0.53
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.90	0.53
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.90	0.53
2:I:819:SER:HB2	2:I:1085:MET:SD	2.49	0.53
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.91	0.53
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.89	0.53
2:C:819:SER:HB2	2:C:1085:MET:SD	2.47	0.53
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.73	0.53
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.49	0.53
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.91	0.53
1:H:182:ARG:HG3	3:J:534:GLU:OE1	2.09	0.53
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.73	0.53
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.08	0.53
2:C:471:VAL:HG21	2:C:498:ILE:HD11	1.90	0.53
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.91	0.53
2:I:598:VAL:HG22	2:I:628:HIS:HE1	1.74	0.53
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.08	0.53
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.90	0.53
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.90	0.53
1:B:195:ARG:HB2	1:B:198:LEU:HD21	1.91	0.53
2:C:548:ARG:NH2	2:C:567:PRO:O	2.42	0.53
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.73	0.53
1:H:59:VAL:O	1:H:171:LEU:N	2.41	0.53
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.91	0.53
3:J:1262:ARG:HD2	3:J:1279:GLN:OE1	2.09	0.53
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.90	0.53
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.09	0.53
5:L:130:VAL:HB	5:L:365:MET:HG3	1.90	0.53
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.92	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.90	0.52
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.09	0.52
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.73	0.52
2:I:211:ARG:NH1	2:I:357:ASN:O	2.41	0.52
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.91	0.52
1:B:12:ARG:H	1:B:30:PRO:CD	2.22	0.52
2:C:886:LYS:H	2:C:917:SER:HB3	1.74	0.52
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.74	0.52
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.09	0.52
1:G:49:SER:OG	1:G:50:SER:N	2.40	0.52
1:H:55:ALA:O	1:H:146:VAL:HG13	2.08	0.52
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.92	0.52
1:A:45:ARG:HG2	1:B:38:THR:CB	2.38	0.52
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.92	0.52
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.73	0.52
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.91	0.52
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.91	0.52
3:D:654:ILE:O	3:D:658:GLU:HB2	2.10	0.52
5:F:395:THR:OG1	5:F:396:ASN:N	2.40	0.52
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:490:GLN:HE21	5:F:472:GLN:NE2	2.07	0.52
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.92	0.52
5:F:483:LEU:HD12	5:F:483:LEU:H	1.74	0.52
1:H:35:PHE:HA	1:H:38:THR:HG22	1.92	0.52
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.92	0.52
3:J:847:ASP:OD1	3:J:847:ASP:N	2.35	0.52
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.09	0.52
1:H:59:VAL:N	1:H:171:LEU:O	2.32	0.52
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.74	0.52
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.91	0.52
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.23	0.52
3:D:73:GLY:O	3:D:76:LYS:NZ	2.29	0.52
3:D:290:ILE:HD12	3:D:290:ILE:H	1.75	0.52
1:H:74:VAL:HG22	1:H:133:LEU:HD12	1.91	0.52
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.75	0.52
3:J:94:GLN:O	3:J:97:VAL:HG23	2.10	0.52
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.92	0.52
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.92	0.52
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.75	0.52
2:I:1286:THR:N	3:J:479:GLU:OE2	2.39	0.52
3:J:1165:PHE:HE1	3:J:1200:GLU:HB3	1.75	0.52
4:K:25:ARG:NH2	4:K:68:GLU:OE1	2.43	0.52
3:J:1184:ASP:O	3:J:1186:TYR:N	2.42	0.52
4:K:29:GLN:CD	4:K:35:LYS:HE2	2.35	0.52
5:L:134:VAL:HA	5:L:273:MET:HE1	1.91	0.52
5:L:314:THR:O	5:L:318:ALA:HB3	2.10	0.52
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.75	0.51
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.92	0.51
3:D:19:ALA:O	3:D:20:ILE:HG13	2.11	0.51
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.36	0.51
2:I:1247:SER:HB3	3:J:375:GLU:O	2.09	0.51
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.90	0.51
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.92	0.51
2:C:778:GLU:O	2:C:781:ASP:HB2	2.10	0.51
2:C:878:THR:OG1	2:C:879:GLY:N	2.42	0.51
2:I:462:ASN:O	2:I:466:VAL:HG23	2.09	0.51
3:J:262:THR:C	5:L:507:MET:HB2	2.36	0.51
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.10	0.51
5:F:575:GLU:OE2	5:F:578:LYS:NZ	2.43	0.51
2:I:170:VAL:HG23	2:I:171:LEU:N	2.25	0.51
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1246:ARG:HH11	2:I:1266:GLY:HA2	1.75	0.51
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.09	0.51
4:K:13:ILE:HD12	4:K:19:LEU:HA	1.92	0.51
1:A:49:SER:OG	1:A:50:SER:N	2.43	0.51
2:C:4:SER:HB2	2:C:7:GLU:HG3	1.93	0.51
2:C:516:ASP:HB2	6:C:3001:RFP:H20C	1.92	0.51
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.46	0.51
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.92	0.51
3:D:820:ILE:HG22	3:D:1227:HIS:HD1	1.76	0.51
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.93	0.51
3:J:338:PHE:C	3:J:340:GLN:H	2.18	0.51
3:J:748:ALA:HA	3:J:754:ILE:HA	1.93	0.51
1:A:62:ASP:OD1	1:A:141:SER:OG	2.29	0.51
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.40	0.51
2:C:452:ARG:HH21	2:C:458:GLU:CD	2.18	0.51
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.43	0.51
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.92	0.51
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.92	0.51
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.93	0.51
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.10	0.51
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.93	0.51
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.11	0.51
2:C:91:THR:HG21	2:C:503:LYS:HZ1	1.75	0.51
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.92	0.51
3:D:557:LYS:HA	3:D:563:LEU:HA	1.92	0.51
3:D:789:LYS:NZ	3:D:931:THR:O	2.37	0.51
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.44	0.51
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.93	0.51
2:C:452:ARG:NH1	2:C:584:TYR:O	2.43	0.51
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.50	0.51
5:F:507:MET:HG2	5:F:520:GLY:CA	2.41	0.51
5:F:561:MET:HA	5:F:567:MET:HE1	1.93	0.51
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.26	0.51
2:I:778:GLU:O	2:I:781:ASP:HB2	2.11	0.51
2:I:878:THR:OG1	2:I:879:GLY:N	2.40	0.51
5:L:585:GLU:O	5:L:589:GLN:HG3	2.11	0.51
2:C:180:ARG:NH2	2:C:465:ARG:HH22	2.09	0.51
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.74	0.51
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.44	0.51
2:I:963:GLU:O	2:I:967:LEU:HB2	2.10	0.51
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.75	0.51
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.93	0.51
2:C:1192:GLU:OE2	3:D:764:ARG:NH1	2.44	0.50
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.45	0.50
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.25	0.50
3:D:356:THR:OG1	3:D:357:VAL:N	2.44	0.50
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.93	0.50
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.77	0.50
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.60	0.50
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.93	0.50
2:C:170:VAL:HG23	2:C:171:LEU:N	2.26	0.50
3:D:103:GLY:CA	3:D:244:VAL:HG22	2.41	0.50
3:D:362:ARG:H	3:D:365:GLN:HE21	1.60	0.50
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.93	0.50
1:H:62:ASP:OD1	1:H:141:SER:OG	2.28	0.50
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.93	0.50
2:I:516:ASP:H	2:I:526:HIS:HD1	1.57	0.50
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.12	0.50
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.93	0.50
1:H:31:LEU:HB2	1:H:199:ASP:O	2.11	0.50
2:I:23:ASP:OD1	2:I:23:ASP:N	2.45	0.50
3:J:19:ALA:O	3:J:20:ILE:HG13	2.11	0.50
2:C:510:GLN:HE21	6:C:3001:RFP:H131	1.76	0.50
3:D:1295:ASN:OD1	3:J:1206:ARG:NH2	2.45	0.50
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.47	0.50
5:L:96:ASP:O	5:L:98:VAL:N	2.44	0.50
1:B:182:ARG:HG3	3:D:534:GLU:OE1	2.10	0.50
2:I:617:ALA:HA	2:I:636:CYS:SG	2.51	0.50
2:I:1327:LEU:HD23	2:I:1331:ARG:HH21	1.76	0.50
3:J:1165:PHE:CE1	3:J:1200:GLU:HB3	2.47	0.50
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	1.94	0.50
5:F:139:GLU:HG2	5:F:351:THR:HA	1.94	0.50
1:G:9:LEU:HD21	1:G:195:ARG:NH2	2.27	0.50
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.93	0.50
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.27	0.50
5:L:127:ILE:O	5:L:130:VAL:HG22	2.12	0.50
2:C:168:GLY:C	2:C:170:VAL:H	2.20	0.50
1:H:90:VAL:HG23	1:H:123:ILE:HD13	1.93	0.50
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.47	0.50
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.10	0.50
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.76	0.49
3:D:42:GLU:CG	5:F:451:ARG:HE	2.25	0.49
3:D:1371:ARG:HH21	3:J:854:ALA:HA	1.77	0.49
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.93	0.49
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.77	0.49
2:I:490:GLN:HG2	2:I:491:ASP:N	2.26	0.49
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.47	0.49
1:B:35:PHE:HA	1:B:38:THR:HG22	1.92	0.49
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.94	0.49
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.94	0.49
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.47	0.49
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.47	0.49
3:J:46:TYR:HE1	5:L:456:MET:HE2	1.77	0.49
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.94	0.49
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.94	0.49
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.28	0.49
2:I:466:VAL:O	2:I:470:ARG:HG2	2.13	0.49
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.77	0.49
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.94	0.49
5:L:166:VAL:O	5:L:167:ASP:HB2	2.12	0.49
5:L:343:LYS:H	5:L:343:LYS:HD2	1.76	0.49
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.94	0.49
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.93	0.49
2:C:805:MET:HE1	2:C:1221:PHE:CZ	2.47	0.49
6:C:3001:RFP:O9	6:C:3001:RFP:O10	2.26	0.49
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.94	0.49
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.93	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.95	0.49
2:I:1099:ASN:HD21	3:J:505:ASP:CG	2.20	0.49
1:B:183:ILE:CD1	1:B:205:MET:HG3	2.43	0.49
2:C:529:ARG:HH12	6:C:3001:RFP:C18	2.26	0.49
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.47	0.49
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.94	0.49
3:D:473:THR:HG23	3:D:476:ALA:H	1.77	0.49
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.27	0.49
2:I:396:ASP:HA	2:I:418:GLY:O	2.13	0.49
3:D:11:GLN:HG2	3:D:15:GLU:HG2	1.95	0.49
3:D:363:LEU:HG	3:D:363:LEU:O	2.12	0.49
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.26	0.49
3:J:70:CYS:SG	3:J:71:LEU:N	2.85	0.49
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.28	0.49
1:A:73:GLY:O	1:A:134:THR:HG22	2.12	0.49
2:C:101:ARG:HG3	2:C:118:LYS:HD2	1.93	0.49
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.93	0.49
3:J:362:ARG:H	3:J:365:GLN:HE21	1.60	0.49
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.94	0.49
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.48	0.49
2:C:566:GLY:O	2:C:569:ILE:HG13	2.11	0.49
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.24	0.49
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.13	0.49
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.48	0.49
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.26	0.49
1:H:51:MET:HE1	1:H:220:ALA:HB2	1.95	0.49
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.28	0.49
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.22	0.49
2:C:62:TYR:C	2:C:64:GLY:H	2.21	0.49
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.94	0.49
3:D:721:SER:HA	3:D:724:MET:HE2	1.95	0.49
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.95	0.49
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.95	0.49
2:I:98:VAL:C	2:I:121:GLU:HA	2.38	0.49
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.12	0.49
3:J:110:PRO:HG2	3:J:183:GLU:HG2	1.94	0.49
2:C:44:GLU:HA	2:C:54:ARG:NH1	2.28	0.48
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.47	0.48
3:D:514:THR:OG1	3:D:594:GLN:O	2.31	0.48
3:D:517:CYS:HA	3:D:716:GLN:NE2	2.28	0.48
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.95	0.48
1:G:10:LYS:HA	1:H:227:GLN:NE2	2.28	0.48
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.93	0.48
2:I:262:TYR:HE1	2:I:280:ASP:OD2	1.96	0.48
3:J:914:ALA:O	3:J:918:ILE:HG23	2.13	0.48
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.94	0.48
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.94	0.48
3:D:94:GLN:O	3:D:97:VAL:HG23	2.12	0.48
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.95	0.48
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.28	0.48
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.48	0.48
3:J:290:ILE:H	3:J:290:ILE:HD12	1.77	0.48
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.95	0.48
3:J:838:ARG:NH1	3:J:1250:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.44	0.48
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.95	0.48
3:D:418:GLU:HG3	4:E:45:LYS:H	1.79	0.48
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.79	0.48
5:F:244:THR:O	5:F:247:GLU:HG2	2.11	0.48
1:H:83:LEU:HD11	3:J:526:VAL:CG2	2.43	0.48
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.95	0.48
3:J:209:ASN:HA	3:J:214:ARG:HE	1.77	0.48
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.95	0.48
2:C:513:GLN:OE1	6:C:3001:RFP:H343	2.14	0.48
3:D:214:ARG:HA	3:D:217:LEU:HB2	1.95	0.48
5:F:466:ILE:HG22	5:F:470:MET:HG3	1.95	0.48
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.96	0.48
3:J:748:ALA:O	3:J:777:HIS:HD2	1.97	0.48
2:C:548:ARG:HB3	2:C:569:ILE:O	2.13	0.48
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.95	0.48
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.14	0.48
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.13	0.48
1:G:45:ARG:HG2	1:H:38:THR:CB	2.39	0.48
1:G:73:GLY:O	1:G:134:THR:HG22	2.13	0.48
1:H:73:GLY:C	1:H:134:THR:HG22	2.38	0.48
2:I:138:ILE:HB	2:I:143:ARG:HD3	1.95	0.48
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.32	0.48
5:L:483:LEU:HD12	5:L:483:LEU:H	1.76	0.48
1:B:155:ALA:HB2	1:B:173:VAL:C	2.39	0.48
2:C:489:PRO:HA	2:C:492:MET:HE3	1.96	0.48
2:C:490:GLN:HE21	5:F:472:GLN:HE21	1.60	0.48
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.94	0.48
1:H:182:ARG:NH1	3:J:581:MET:SD	2.87	0.48
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.95	0.48
3:J:525:MET:O	3:J:548:VAL:HG13	2.12	0.48
1:B:153:VAL:H	1:B:175:ALA:HB3	1.78	0.48
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	1.95	0.48
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.77	0.48
2:I:1285:TYR:CD2	3:J:1356:LEU:HD21	2.48	0.48
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.95	0.48
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.96	0.48
1:B:47:LEU:O	1:B:180:VAL:HG21	2.13	0.48
1:B:57:THR:HG21	1:B:158:ARG:HE	1.78	0.48
3:D:827:GLU:O	3:D:829:GLY:N	2.37	0.48
2:I:316:GLU:H	2:I:316:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.43	0.48
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.78	0.48
4:K:60:ASN:H	4:K:63:ILE:HB	1.79	0.48
1:A:9:LEU:HD21	1:A:195:ARG:HH21	1.79	0.48
1:G:73:GLY:C	1:G:134:THR:HG22	2.39	0.48
3:J:34:SER:HB2	3:J:104:HIS:HB3	1.95	0.48
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.44	0.48
5:L:354:THR:O	5:L:358:VAL:HG23	2.14	0.48
3:D:414:GLU:O	4:E:45:LYS:NZ	2.44	0.48
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.95	0.48
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.96	0.48
5:F:571:TYR:CD1	5:F:575:GLU:HG2	2.48	0.48
2:I:62:TYR:C	2:I:64:GLY:H	2.22	0.48
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.95	0.48
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.96	0.48
2:I:886:LYS:H	2:I:917:SER:HB3	1.78	0.48
3:J:1154:ALA:N	3:J:1214:PRO:O	2.43	0.48
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.96	0.47
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.29	0.47
1:H:13:LEU:HD23	1:H:13:LEU:H	1.78	0.47
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.78	0.47
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.95	0.47
3:J:317:THR:HB	3:J:324:LEU:HB3	1.95	0.47
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.96	0.47
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.95	0.47
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.95	0.47
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.95	0.47
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.96	0.47
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.95	0.47
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.96	0.47
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.13	0.47
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.14	0.47
3:J:518:VAL:N	3:J:716:GLN:HE22	2.12	0.47
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.47	0.47
3:D:1174:ARG:HG2	3:D:1189:MET:SD	2.54	0.47
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.49	0.47
4:E:10:VAL:HG13	4:E:16:ARG:HB2	1.96	0.47
5:F:470:MET:HA	5:F:473:GLU:HB3	1.96	0.47
1:H:51:MET:O	1:H:150:ARG:HA	2.13	0.47
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.97	0.47
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1307:LEU:HB3	3:J:1312:ALA:HB2	1.97	0.47
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.96	0.47
2:C:42:ASP:OD2	2:C:44:GLU:HG2	2.14	0.47
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.49	0.47
3:D:11:GLN:HG3	3:D:12:THR:H	1.79	0.47
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.78	0.47
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.44	0.47
3:J:592:VAL:HA	3:J:596:LEU:HD21	1.95	0.47
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.96	0.47
3:D:748:ALA:O	3:D:777:HIS:HD2	1.98	0.47
5:F:388:ILE:O	5:F:392:LYS:HG3	2.14	0.47
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.96	0.47
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.49	0.47
5:L:532:LEU:HD12	5:L:532:LEU:H	1.79	0.47
2:C:231:GLU:O	2:C:238:GLN:N	2.46	0.47
2:C:632:ASP:O	2:C:647:ARG:HB2	2.14	0.47
1:B:113:ALA:HB2	1:B:126:PRO:HB3	1.97	0.47
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.49	0.47
5:F:499:LYS:HA	5:F:502:LYS:HE2	1.96	0.47
5:F:512:GLY:C	5:F:514:ASP:H	2.23	0.47
2:I:739:ASP:OD1	2:I:739:ASP:N	2.47	0.47
2:I:1272:GLU:H	3:J:343:LEU:HD12	1.79	0.47
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.97	0.47
3:J:35:PHE:HD1	3:J:101:ARG:HB3	1.80	0.47
2:C:468:LEU:O	2:C:471:VAL:HG12	2.15	0.47
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.62	0.47
3:D:741:ALA:O	3:D:762:ASN:ND2	2.48	0.47
1:H:19:VAL:HG23	1:H:24:ALA:HA	1.96	0.47
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.96	0.47
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.80	0.47
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.14	0.47
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	1.97	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.96	0.47
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.97	0.47
1:H:20:SER:OG	1:H:21:SER:N	2.48	0.47
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.49	0.47
5:L:148:TYR:OH	5:L:218:ARG:HA	2.15	0.47
2:C:18:ARG:NH1	2:C:621:SER:O	2.47	0.47
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.80	0.47
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.47
3:D:1198:VAL:HG11	3:D:1210:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.29	0.47
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.96	0.47
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.97	0.47
1:B:125:LYS:HG3	1:B:128:HIS:HB2	1.96	0.46
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.50	0.46
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.97	0.46
2:C:891:GLY:O	2:C:892:GLU:HG3	2.15	0.46
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.15	0.46
3:D:121:PRO:HG2	3:D:123:ARG:HH21	1.80	0.46
3:D:825:VAL:C	3:D:826:ILE:HG13	2.39	0.46
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.44	0.46
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.96	0.46
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.96	0.46
3:J:544:LEU:O	3:J:574:VAL:HB	2.15	0.46
3:J:587:LEU:HD23	3:J:591:ILE:HG21	1.95	0.46
1:A:90:VAL:HG22	1:A:91:ARG:H	1.80	0.46
1:B:177:TYR:O	1:B:178:SER:C	2.58	0.46
3:D:581:MET:HE2	3:D:581:MET:HB3	1.76	0.46
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.97	0.46
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.50	0.46
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.49	0.46
3:J:425:ARG:HG2	3:J:426:ALA:H	1.80	0.46
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.23	0.46
2:C:13:LYS:O	2:C:1183:ALA:N	2.42	0.46
3:D:334:LYS:HA	3:D:335:GLN:HA	1.57	0.46
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.98	0.46
3:D:1227:HIS:CB	3:J:1293:GLU:HG2	2.44	0.46
5:F:486:ARG:CZ	5:F:486:ARG:HB2	2.46	0.46
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.98	0.46
3:J:825:VAL:C	3:J:826:ILE:HG13	2.39	0.46
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.97	0.46
1:A:39:LEU:O	1:A:43:LEU:N	2.40	0.46
1:B:190:ALA:N	1:B:198:LEU:O	2.40	0.46
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.97	0.46
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.16	0.46
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.80	0.46
3:D:141:PHE:HA	3:D:180:MET:HE2	1.96	0.46
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.96	0.46
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.45	0.46
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.61	0.46
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.95	0.46
3:D:515:ARG:O	3:D:545:HIS:HB3	2.15	0.46
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.96	0.46
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.81	0.46
2:I:4:SER:HB2	2:I:7:GLU:HG3	1.97	0.46
2:I:91:THR:HG21	2:I:503:LYS:HZ1	1.79	0.46
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	1.97	0.46
3:J:34:SER:HG	3:J:104:HIS:CG	2.27	0.46
3:J:338:PHE:O	3:J:340:GLN:N	2.48	0.46
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.98	0.46
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.98	0.46
2:C:183:TRP:HB2	2:C:199:ASP:HA	1.97	0.46
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.16	0.46
3:D:598:LYS:O	3:D:601:ILE:HG22	2.16	0.46
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.51	0.46
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	1.97	0.46
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.98	0.46
2:I:387:ASN:HA	2:I:391:SER:HB2	1.96	0.46
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.16	0.46
3:J:733:SER:O	3:J:737:ILE:HG12	2.14	0.46
2:C:55:SER:OG	2:C:56:VAL:N	2.49	0.46
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.97	0.46
3:J:451:PRO:O	3:J:454:CYS:HB2	2.15	0.46
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.97	0.46
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.98	0.46
2:C:60:GLN:HA	2:C:67:GLU:HA	1.98	0.46
2:C:149:LEU:HD12	2:C:452:ARG:O	2.15	0.46
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.80	0.46
5:F:343:LYS:O	5:F:347:ILE:HG13	2.16	0.46
1:H:213:PRO:O	1:H:217:ILE:HG13	2.16	0.46
2:I:169:LYS:O	2:I:170:VAL:HG22	2.15	0.46
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.51	0.46
3:J:121:PRO:HG2	3:J:123:ARG:HH21	1.80	0.46
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.98	0.46
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.98	0.46
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.97	0.46
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.50	0.46
1:B:74:VAL:HG22	1:B:133:LEU:HD12	1.96	0.46
2:C:1298:VAL:HG11	3:D:96:LYS:HE3	1.98	0.46
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.16	0.46
3:D:658:GLU:O	3:D:661:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.98	0.46
3:D:697:MET:SD	3:D:741:ALA:HB3	2.56	0.46
1:G:118:ASP:H	1:G:121:VAL:HB	1.81	0.46
2:I:132:ASP:OD1	2:I:132:ASP:N	2.38	0.46
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.48	0.46
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.15	0.46
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.96	0.46
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.96	0.46
3:D:133:ARG:HD2	3:D:133:ARG:HA	1.77	0.46
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.98	0.46
3:D:748:ALA:O	3:D:777:HIS:CD2	2.69	0.46
1:H:101:THR:H	1:H:116:THR:CG2	2.28	0.46
1:H:118:ASP:H	1:H:121:VAL:HB	1.81	0.46
2:I:1211:ARG:HE	2:I:1220:GLN:HE21	1.63	0.46
3:J:473:THR:HG23	3:J:476:ALA:H	1.81	0.46
2:C:670:PHE:CD1	2:C:1184:THR:HG21	2.51	0.45
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.50	0.45
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.98	0.45
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.98	0.45
3:D:1165:PHE:CE1	3:D:1200:GLU:HB3	2.52	0.45
5:F:127:ILE:O	5:F:130:VAL:HG22	2.15	0.45
3:J:620:PHE:CE1	3:J:624:ILE:HD11	2.51	0.45
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.97	0.45
5:L:316:PHE:CZ	5:L:337:VAL:HB	2.50	0.45
1:A:56:VAL:HG11	1:A:85:LEU:HB3	1.99	0.45
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.97	0.45
1:G:19:VAL:HG13	1:G:20:SER:H	1.80	0.45
1:G:77:ASP:O	1:G:81:ILE:HG13	2.16	0.45
1:H:41:ASN:O	1:H:45:ARG:HG3	2.15	0.45
1:H:183:ILE:HG13	1:H:205:MET:HG3	1.96	0.45
2:I:138:ILE:HG22	2:I:139:ASN:N	2.31	0.45
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.30	0.45
3:J:336:GLY:O	3:J:337:ARG:HB2	2.16	0.45
3:J:604:MET:HE3	3:J:604:MET:HB2	1.90	0.45
1:A:172:LEU:HD12	1:A:172:LEU:H	1.81	0.45
2:C:138:ILE:HG22	2:C:139:ASN:N	2.30	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.16	0.45
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.98	0.45
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.30	0.45
2:C:1248:THR:HG21	5:F:531:PRO:HG2	1.98	0.45
3:D:122:SER:O	3:D:126:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.63	0.45
1:G:90:VAL:HG22	1:G:91:ARG:H	1.81	0.45
1:H:11:PRO:HB2	1:H:28:LEU:HD11	1.97	0.45
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.31	0.45
2:C:195:PHE:CG	2:C:203:LYS:HD3	2.51	0.45
2:C:745:GLU:HG3	2:C:1017:GLN:CB	2.36	0.45
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.17	0.45
3:D:489:ASN:HA	3:D:904:ALA:CB	2.46	0.45
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.97	0.45
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.73	0.45
3:J:215:LYS:O	3:J:218:THR:HG22	2.17	0.45
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.17	0.45
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.99	0.45
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.50	0.45
3:D:797:THR:O	3:D:801:VAL:HG13	2.16	0.45
1:H:105:SER:HA	1:H:138:ALA:O	2.17	0.45
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.97	0.45
3:J:222:LYS:HE2	3:J:1276:GLU:OE1	2.16	0.45
1:B:19:VAL:O	1:B:20:SER:HB3	2.15	0.45
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.98	0.45
2:C:239:MET:O	2:C:284:LEU:HD12	2.17	0.45
2:C:498:ILE:HD12	2:C:498:ILE:H	1.81	0.45
2:C:499:SER:O	2:C:503:LYS:HB2	2.17	0.45
2:C:675:ASP:HB3	2:C:1107:MET:O	2.15	0.45
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.98	0.45
3:D:331:ILE:CG2	3:D:1328:THR:HG21	2.47	0.45
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	1.99	0.45
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.97	0.45
2:I:180:ARG:NH2	2:I:396:ASP:HB2	2.32	0.45
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.99	0.45
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.32	0.45
3:J:1257:VAL:HA	3:J:1260:MET:HE2	1.97	0.45
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.49	0.45
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.83	0.45
2:C:403:MET:HE3	2:C:403:MET:HB3	1.87	0.45
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.72	0.45
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.98	0.45
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.52	0.45
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.99	0.45
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.99	0.45
2:I:123:TYR:OH	2:I:126:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:56:LEU:HD12	3:J:56:LEU:H	1.82	0.45
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.98	0.45
3:J:905:ARG:HH21	3:J:907:HIS:CB	2.30	0.45
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.99	0.45
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.82	0.45
2:C:701:GLY:O	2:C:1184:THR:N	2.37	0.45
2:C:1246:ARG:CZ	2:C:1258:PRO:HB3	2.46	0.45
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.50	0.45
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.82	0.45
1:G:9:LEU:HD21	1:G:195:ARG:HH21	1.81	0.45
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.99	0.45
3:J:77:ARG:HG3	3:J:79:LYS:H	1.81	0.45
2:C:132:ASP:OD1	2:C:132:ASP:N	2.37	0.45
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.99	0.45
2:I:15:PHE:CG	2:I:1190:ALA:HB2	2.52	0.45
2:I:805:MET:HE1	2:I:1221:PHE:CZ	2.52	0.45
3:J:364:HIS:CD2	4:K:4:VAL:HG23	2.52	0.45
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.98	0.45
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.32	0.45
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.52	0.45
2:I:27:LEU:HB2	2:I:524:ILE:HD11	1.98	0.45
2:I:703:GLY:N	2:I:705:GLU:OE2	2.43	0.45
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.52	0.45
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.17	0.45
3:J:432:LEU:HD13	3:J:499:ILE:HG21	1.98	0.45
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.80	0.45
1:A:73:GLY:C	1:A:134:THR:HG22	2.42	0.44
1:B:57:THR:O	1:B:173:VAL:HG22	2.17	0.44
1:B:175:ALA:HB1	1:B:177:TYR:CZ	2.52	0.44
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.44
3:D:343:LEU:HD22	3:D:343:LEU:HA	1.42	0.44
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.98	0.44
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.99	0.44
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.52	0.44
3:J:746:LEU:HB2	3:J:754:ILE:HD11	2.00	0.44
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.82	0.44
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.32	0.44
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.32	0.44
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.44
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.83	0.44
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:759:ILE:HG23	3:J:771:GLN:HB3	1.98	0.44
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.50	0.44
5:L:515:GLU:HG2	5:L:516:ASP:N	2.32	0.44
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.98	0.44
1:B:74:VAL:HG12	1:B:76:GLU:H	1.82	0.44
1:B:93:GLN:HB2	1:B:120:ASP:OD1	2.16	0.44
1:B:194:GLN:O	1:B:195:ARG:HG2	2.18	0.44
2:C:867:GLU:H	2:C:867:GLU:HG3	1.52	0.44
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.99	0.44
3:D:128:LEU:HA	3:D:192:MET:HE1	1.99	0.44
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.82	0.44
1:H:13:LEU:HD12	1:H:16:ILE:HD11	1.98	0.44
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.18	0.44
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.52	0.44
3:J:849:LEU:HD13	3:J:849:LEU:H	1.82	0.44
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.82	0.44
5:L:372:ALA:O	5:L:376:LYS:HG3	2.17	0.44
2:C:494:ASN:HB3	2:C:497:PRO:HD2	2.00	0.44
2:C:782:VAL:HG11	2:C:792:GLY:HA2	1.99	0.44
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.45	0.44
3:D:113:HIS:HB3	3:D:116:PHE:HD2	1.82	0.44
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.99	0.44
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.98	0.44
3:D:903:LEU:HD23	3:D:905:ARG:HD3	1.99	0.44
5:F:555:GLU:OE2	5:F:597:LYS:NZ	2.46	0.44
1:H:84:ASN:OD1	3:J:551:ARG:NH2	2.51	0.44
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.99	0.44
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.99	0.44
2:I:1272:GLU:H	3:J:343:LEU:CD1	2.30	0.44
3:J:79:LYS:HG3	3:J:80:HIS:N	2.32	0.44
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.98	0.44
5:L:139:GLU:HG2	5:L:351:THR:HA	2.00	0.44
1:A:90:VAL:HG23	1:A:123:ILE:HD13	2.00	0.44
3:D:646:ILE:H	3:D:646:ILE:HG12	1.57	0.44
3:D:799:ARG:NH1	3:D:1146:GLU:OE1	2.50	0.44
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.47	0.44
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.99	0.44
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.99	0.44
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.99	0.44
2:C:980:VAL:O	2:C:984:VAL:HB	2.17	0.44
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:892:PHE:CE1	3:D:1281:GLU:HB3	2.53	0.44
1:H:104:LYS:HG2	1:H:110:VAL:HG22	2.00	0.44
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.52	0.44
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.18	0.44
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.17	0.44
5:L:226:ALA:O	5:L:229:VAL:HG22	2.18	0.44
1:B:214:GLU:HG2	1:B:218:ARG:NH2	2.32	0.44
2:C:356:THR:HG21	2:C:362:ALA:HA	2.00	0.44
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	2.00	0.44
3:D:612:LEU:HB3	3:D:616:PRO:HG2	2.00	0.44
3:D:722:ILE:HA	3:D:725:MET:HE3	2.00	0.44
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.83	0.44
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.17	0.44
1:B:12:ARG:H	1:B:30:PRO:HD2	1.81	0.44
2:C:23:ASP:OD1	2:C:23:ASP:N	2.48	0.44
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.32	0.44
2:C:814:ASP:CG	2:C:1106:ARG:HH12	2.22	0.44
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.17	0.44
3:D:903:LEU:HD12	3:D:903:LEU:HA	1.91	0.44
5:F:281:ARG:O	5:F:285:ARG:HG3	2.18	0.44
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.00	0.44
1:H:90:VAL:HG22	1:H:91:ARG:H	1.82	0.44
2:I:90:VAL:HG12	2:I:91:THR:H	1.81	0.44
3:J:232:ASN:HA	3:J:236:TRP:HZ3	1.83	0.44
4:K:26:ARG:HH22	4:K:38:LEU:HD13	1.83	0.44
2:C:732:ILE:HG21	2:C:783:LEU:HD12	2.00	0.44
2:C:873:ILE:HG13	2:C:944:ARG:NH2	2.29	0.44
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.87	0.44
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.99	0.44
1:G:9:LEU:HD23	1:G:9:LEU:H	1.83	0.44
2:I:225:PHE:CE2	2:I:347:ILE:HB	2.52	0.44
2:I:808:ASN:H	3:J:633:ALA:HB2	1.83	0.44
5:L:528:LEU:HD23	5:L:528:LEU:HA	1.85	0.44
5:L:547:VAL:HG23	5:L:603:ARG:NH1	2.31	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.77	0.43
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.00	0.43
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.00	0.43
1:G:75:GLN:HA	2:I:729:ALA:N	2.33	0.43
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.73	0.43
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.72	0.43
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.36	0.43
2:I:1333:LEU:HD22	3:J:307:LEU:HD22	2.00	0.43
3:J:334:LYS:HA	3:J:335:GLN:HA	1.54	0.43
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.82	0.43
1:B:20:SER:OG	1:B:21:SER:N	2.51	0.43
2:C:104:ILE:O	2:C:113:THR:HA	2.18	0.43
2:C:724:VAL:HG11	2:C:727:VAL:HG22	2.00	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.98	0.43
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.30	0.43
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.48	0.43
5:F:507:MET:HG2	5:F:520:GLY:HA3	2.00	0.43
1:G:12:ARG:HA	1:H:230:ALA:HB2	1.99	0.43
1:G:74:VAL:HG22	1:G:76:GLU:H	1.82	0.43
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.19	0.43
2:I:896:THR:HB	2:I:897:PRO:HD2	1.99	0.43
2:I:967:LEU:HD12	2:I:967:LEU:HA	1.87	0.43
3:J:514:THR:CB	3:J:576:ARG:HG2	2.47	0.43
3:J:801:VAL:O	3:J:805:GLN:HB2	2.18	0.43
1:A:83:LEU:HD23	2:C:694:ARG:NH2	2.33	0.43
1:A:118:ASP:H	1:A:121:VAL:HB	1.83	0.43
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.89	0.43
2:C:316:GLU:CD	2:C:316:GLU:H	2.26	0.43
5:F:94:THR:O	5:F:95:THR:OG1	2.27	0.43
2:I:559:CYS:CB	2:I:662:SER:HB3	2.47	0.43
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.00	0.43
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.54	0.43
2:C:806:PRO:HB3	3:D:505:ASP:OD1	2.18	0.43
3:D:708:ASN:OD1	3:D:708:ASN:N	2.49	0.43
3:D:1344:LEU:HB3	3:D:1350:ASN:ND2	2.30	0.43
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.99	0.43
1:H:93:GLN:H	1:H:120:ASP:HB3	1.83	0.43
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.54	0.43
2:I:757:THR:HG23	2:I:765:ILE:HG23	2.00	0.43
2:I:1109:ILE:HD12	2:I:1109:ILE:HA	1.88	0.43
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.99	0.43
3:J:682:VAL:O	3:J:685:ILE:HG12	2.17	0.43
4:K:58:LEU:O	4:K:63:ILE:HG21	2.18	0.43
5:L:461:ASN:O	5:L:465:ARG:HG2	2.19	0.43
1:B:153:VAL:O	1:B:175:ALA:N	2.28	0.43
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.54	0.43
2:C:642:SER:HB2	3:D:770:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.99	0.43
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.18	0.43
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.68	0.43
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.53	0.43
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.54	0.43
5:L:227:GLN:HG2	5:L:252:LEU:HA	2.00	0.43
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.99	0.43
1:A:47:LEU:O	1:A:180:VAL:HG21	2.19	0.43
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.49	0.43
2:C:696:ASP:O	2:C:697:LYS:HB3	2.18	0.43
2:C:972:PHE:HD1	2:C:994:ARG:HH21	1.65	0.43
5:F:463:LEU:HD23	5:F:463:LEU:HA	1.86	0.43
3:J:800:LEU:O	3:J:803:VAL:HG12	2.19	0.43
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.83	0.43
3:J:1246:VAL:HG12	3:J:1248:ILE:HG13	2.01	0.43
5:L:316:PHE:O	5:L:320:ILE:HG13	2.18	0.43
2:C:660:VAL:HG13	2:C:661:VAL:HG13	2.00	0.43
3:D:556:GLU:HG2	3:D:558:ASP:HB2	2.00	0.43
5:F:512:GLY:O	5:F:514:ASP:N	2.52	0.43
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.84	0.43
2:I:159:SER:HB2	2:I:442:VAL:HG21	2.01	0.43
3:J:546:ALA:O	3:J:573:THR:HA	2.18	0.43
3:J:698:MET:O	3:J:702:GLN:HB3	2.18	0.43
2:C:687:ARG:HH22	6:C:3001:RFP:H301	1.83	0.43
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.84	0.43
2:C:1142:ARG:HD3	2:C:1161:LEU:CD1	2.48	0.43
3:D:822:MET:SD	3:D:838:ARG:HB3	2.58	0.43
5:F:499:LYS:HB2	5:F:499:LYS:HE3	1.77	0.43
2:I:10:ARG:HA	2:I:1172:LEU:HD23	2.00	0.43
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.74	0.43
3:J:317:THR:HG22	3:J:322:ARG:O	2.19	0.43
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.49	0.43
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.84	0.43
2:C:735:LYS:HA	2:C:748:ILE:HG22	2.00	0.43
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.63	0.43
2:C:1250:SER:OG	5:F:524:GLU:OE1	2.37	0.43
3:D:1237:VAL:HG11	3:D:1253:ILE:HG21	2.01	0.43
5:F:227:GLN:HG2	5:F:252:LEU:HA	2.01	0.43
1:G:166:ARG:O	1:G:167:PRO:C	2.62	0.43
2:I:69:GLN:HG3	2:I:101:ARG:HB3	2.00	0.43
2:I:101:ARG:HG3	2:I:118:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:149:LEU:HD11	2:I:451:ARG:HB3	2.00	0.43
2:I:515:MET:HE3	2:I:517:GLN:HB2	2.00	0.43
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.58	0.43
2:I:1288:GLN:HG2	2:I:1315:MET:HE1	2.01	0.43
3:J:661:VAL:HB	3:J:682:VAL:HG13	2.01	0.43
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.18	0.43
2:C:463:GLN:HG3	2:C:505:PHE:HB2	2.01	0.43
2:C:619:ALA:HB1	2:C:657:THR:HA	2.00	0.43
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.41	0.43
2:C:992:LEU:H	2:C:992:LEU:HD23	1.84	0.43
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.51	0.43
3:D:546:ALA:O	3:D:573:THR:HA	2.18	0.43
3:D:647:PRO:CG	3:D:697:MET:HB3	2.46	0.43
3:D:689:ALA:O	3:D:693:VAL:HG23	2.19	0.43
3:D:1184:ASP:O	3:D:1186:TYR:N	2.52	0.43
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.32	0.43
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.81	0.43
1:H:55:ALA:HB3	1:H:177:TYR:CD1	2.54	0.43
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.54	0.42
2:C:565:GLU:HB2	2:C:680:LEU:HD21	1.99	0.42
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.49	0.42
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.84	0.42
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.84	0.42
5:F:559:LEU:HD22	5:F:594:ALA:HB1	2.01	0.42
1:G:90:VAL:HG23	1:G:123:ILE:HD13	2.00	0.42
3:J:64:PRO:HB3	3:J:69:GLU:O	2.19	0.42
3:J:536:LEU:HD12	3:J:542:ALA:HB2	2.00	0.42
3:J:708:ASN:OD1	3:J:708:ASN:N	2.51	0.42
3:J:793:SER:O	3:J:797:THR:HG23	2.18	0.42
1:B:41:ASN:OD1	2:C:1217:THR:HG22	2.19	0.42
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.19	0.42
2:C:198:ILE:H	2:C:369:MET:HE1	1.84	0.42
5:F:96:ASP:O	5:F:98:VAL:N	2.52	0.42
2:I:498:ILE:HD12	2:I:498:ILE:H	1.83	0.42
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	2.01	0.42
2:I:816:ILE:HG22	2:I:818:VAL:HG23	2.01	0.42
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	2.00	0.42
1:B:154:PRO:HA	1:B:174:ASP:HB3	2.01	0.42
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.23	0.42
2:C:496:LYS:HB3	2:C:496:LYS:HE3	1.61	0.42
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:532:LEU:HD12	5:F:532:LEU:H	1.85	0.42
2:I:519:ASN:ND2	2:I:796:LEU:HD23	2.31	0.42
2:I:980:VAL:O	2:I:984:VAL:HB	2.19	0.42
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.02	0.42
1:A:19:VAL:HG13	1:A:20:SER:H	1.84	0.42
1:A:219:ARG:O	1:A:223:ILE:HG13	2.19	0.42
1:A:228:LEU:HD23	1:A:231:PHE:HD2	1.83	0.42
2:C:221:LEU:HD11	2:C:314:ASN:HB2	2.01	0.42
2:C:488:MET:O	2:C:490:GLN:N	2.46	0.42
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.34	0.42
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.84	0.42
3:D:93:THR:HG22	3:D:94:GLN:H	1.83	0.42
3:D:218:THR:HA	3:D:221:ILE:HG22	2.01	0.42
3:D:824:PRO:HD3	3:D:835:LEU:HB2	2.01	0.42
5:F:462:LYS:O	5:F:466:ILE:HG13	2.18	0.42
1:G:38:THR:HG23	1:H:45:ARG:HB2	2.02	0.42
1:G:47:LEU:O	1:G:180:VAL:HG21	2.20	0.42
2:I:37:LYS:HA	2:I:37:LYS:HD3	1.80	0.42
2:I:168:GLY:C	2:I:170:VAL:N	2.77	0.42
2:I:503:LYS:HA	2:I:503:LYS:HD2	1.85	0.42
5:L:292:VAL:HG21	5:L:299:LYS:HG2	2.00	0.42
2:C:618:GLN:HG3	2:C:620:ASN:H	1.83	0.42
3:D:114:ILE:HG22	3:D:307:LEU:HD12	2.01	0.42
3:D:137:ARG:HD3	3:D:143:SER:OG	2.19	0.42
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.19	0.42
4:K:15:ASN:HB3	4:K:18:ASP:HB2	2.01	0.42
2:C:516:ASP:H	2:C:526:HIS:HD1	1.68	0.42
2:C:593:LYS:HA	2:C:652:TYR:CD2	2.55	0.42
2:C:854:ILE:O	2:C:857:VAL:HG22	2.18	0.42
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.55	0.42
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.02	0.42
3:D:598:LYS:N	3:D:728:SER:O	2.41	0.42
3:D:1151:LYS:C	3:D:1153:PRO:HD3	2.44	0.42
3:D:1283:SER:O	3:D:1286:LYS:N	2.52	0.42
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.35	0.42
3:J:42:GLU:HG3	5:L:451:ARG:HE	1.83	0.42
3:J:372:MET:HE2	3:J:372:MET:HB3	1.79	0.42
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.78	0.42
1:A:38:THR:OG1	1:B:45:ARG:HG2	2.20	0.42
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.85	0.42
2:C:196:VAL:HG12	2:C:206:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.54	0.42
2:C:324:LYS:O	2:C:327:GLN:NE2	2.51	0.42
2:C:1114:GLU:OE1	2:C:1230:MET:HA	2.20	0.42
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.48	0.42
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.84	0.42
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.84	0.42
5:F:409:ASN:O	5:F:413:MET:HG3	2.20	0.42
1:G:71:LYS:HB2	1:G:78:ILE:HD11	2.01	0.42
2:I:791:LEU:HD23	2:I:791:LEU:HA	1.84	0.42
3:J:806:ASP:HA	3:J:1347:LEU:HD13	2.01	0.42
2:C:615:VAL:HG13	2:C:651:ASP:N	2.33	0.42
2:C:826:ASP:OD1	2:C:829:THR:OG1	2.29	0.42
3:D:27:PRO:HB3	3:D:241:VAL:HG23	2.00	0.42
5:F:98:VAL:HB	5:F:402:LEU:HD11	2.02	0.42
1:H:192:VAL:HG21	1:H:198:LEU:HD12	2.02	0.42
2:I:194:LEU:HA	2:I:194:LEU:HD12	1.77	0.42
2:I:402:ARG:HG2	2:I:416:GLY:N	2.35	0.42
2:I:1174:GLU:OE2	2:I:1177:ARG:NH1	2.51	0.42
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	2.01	0.42
2:I:1285:TYR:CE2	3:J:1356:LEU:HD11	2.55	0.42
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.85	0.42
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.35	0.42
3:J:342:LEU:HA	3:J:343:LEU:HA	1.57	0.42
3:J:598:LYS:O	3:J:601:ILE:HG22	2.19	0.42
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	2.02	0.42
5:L:552:THR:OG1	5:L:555:GLU:HG3	2.20	0.42
5:L:582:VAL:CG1	5:L:586:ARG:HG2	2.49	0.42
1:A:177:TYR:O	1:A:178:SER:HB2	2.19	0.42
2:C:810:TYR:CD2	3:D:359:PRO:HG2	2.55	0.42
2:C:985:GLU:HB3	2:C:988:LYS:HB2	2.02	0.42
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.83	0.42
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.19	0.42
3:D:623:GLN:O	3:D:627:THR:HG22	2.19	0.42
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.33	0.42
1:G:91:ARG:HH21	1:G:122:GLU:CD	2.27	0.42
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.50	0.42
3:D:682:VAL:O	3:D:685:ILE:HG12	2.20	0.42
1:G:36:GLY:C	1:G:187:VAL:HG11	2.45	0.42
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.02	0.42
2:I:61:SER:HB3	2:I:479:LEU:HB3	2.02	0.42
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:738:GLU:HA	2:I:741:MET:HE2	2.00	0.42
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.27	0.42
2:I:1114:GLU:OE1	2:I:1230:MET:HA	2.20	0.42
2:I:1314:GLN:HG2	4:K:28:ARG:NE	2.35	0.42
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.85	0.42
5:L:493:LYS:HA	5:L:496:LYS:HE2	2.02	0.42
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.85	0.41
2:C:808:ASN:H	3:D:633:ALA:HB2	1.85	0.41
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.85	0.41
3:D:526:VAL:HA	3:D:549:LYS:O	2.19	0.41
3:D:641:ILE:HD13	3:D:641:ILE:O	2.20	0.41
3:D:849:LEU:HB3	3:D:853:THR:HG23	2.01	0.41
5:F:276:MET:O	5:F:280:VAL:HG23	2.20	0.41
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.20	0.41
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.49	0.41
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.44	0.41
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.20	0.41
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.01	0.41
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.85	0.41
5:L:476:ARG:HG3	5:L:477:GLU:N	2.35	0.41
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.49	0.41
5:L:603:ARG:H	5:L:603:ARG:HG2	1.65	0.41
1:B:212:ASP:OD1	1:B:215:GLU:HB2	2.20	0.41
2:C:169:LYS:O	2:C:169:LYS:HG2	2.19	0.41
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.77	0.41
2:C:722:GLY:HA2	2:C:737:ASN:OD1	2.20	0.41
2:C:953:LEU:HD12	2:C:953:LEU:HA	1.85	0.41
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.35	0.41
3:D:372:MET:HE2	3:D:372:MET:HB3	1.83	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.84	0.41
3:D:875:ASN:OD1	3:D:875:ASN:N	2.54	0.41
1:G:211:ILE:HD13	1:G:211:ILE:HA	1.95	0.41
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.84	0.41
2:I:593:LYS:HE3	2:I:595:THR:HG22	2.02	0.41
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.35	0.41
3:J:850:LYS:HB3	3:J:851:PRO:HD2	2.01	0.41
3:J:850:LYS:HG2	3:J:857:LEU:HD23	2.02	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
1:A:228:LEU:HD11	1:B:224:LEU:HD22	2.01	0.41
1:B:35:PHE:O	1:B:38:THR:HG22	2.20	0.41
2:C:41:GLN:NE2	2:C:73:TYR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.38	0.41
2:C:1328:LYS:O	2:C:1332:SER:N	2.52	0.41
3:D:859:PRO:HG2	3:D:862:THR:HG21	2.01	0.41
5:F:316:PHE:CZ	5:F:334:SER:HA	2.45	0.41
2:I:587:LEU:HA	2:I:587:LEU:HD23	1.79	0.41
2:I:985:GLU:HB3	2:I:988:LYS:HB2	2.00	0.41
2:I:1085:MET:HA	2:I:1085:MET:HE2	2.02	0.41
3:J:19:ALA:CB	3:J:1373:ARG:HH22	2.33	0.41
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.35	0.41
3:J:441:LEU:HD13	3:J:441:LEU:HA	1.91	0.41
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.85	0.41
2:C:796:LEU:O	2:C:1233:LEU:HD12	2.20	0.41
2:C:996:ARG:HA	2:C:996:ARG:HD3	1.81	0.41
2:C:1038:GLN:O	2:C:1038:GLN:HG3	2.20	0.41
3:D:451:PRO:O	3:D:454:CYS:HB2	2.19	0.41
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.20	0.41
2:I:86:GLN:HA	2:I:140:GLY:HA2	2.02	0.41
2:I:705:GLU:HB2	2:I:794:LEU:H	1.86	0.41
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.28	0.41
3:J:214:ARG:HA	3:J:217:LEU:HB2	2.02	0.41
3:J:332:LYS:HB2	3:J:332:LYS:HE3	1.82	0.41
3:J:689:ALA:O	3:J:693:VAL:HG23	2.21	0.41
3:J:810:THR:HG23	3:J:811:GLU:H	1.86	0.41
3:J:860:ARG:HB3	3:J:861:ASN:H	1.73	0.41
5:L:457:ILE:HA	5:L:460:ILE:HD12	2.02	0.41
5:L:561:MET:HA	5:L:567:MET:HE1	2.02	0.41
5:L:586:ARG:O	5:L:590:ILE:HG13	2.21	0.41
1:A:167:PRO:HB2	1:A:170:ARG:HB2	2.02	0.41
1:A:181:GLU:HB3	1:A:206:GLU:HG3	2.02	0.41
1:B:64:VAL:HG11	1:B:69:SER:HB2	2.02	0.41
1:B:118:ASP:H	1:B:121:VAL:HB	1.84	0.41
1:B:201:LEU:HG	1:B:203:ILE:HG13	2.02	0.41
2:C:590:PRO:HG3	2:C:605:TYR:OH	2.21	0.41
2:C:791:LEU:HA	2:C:791:LEU:HD23	1.79	0.41
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.51	0.41
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.86	0.41
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.87	0.41
1:G:227:GLN:HE21	1:H:35:PHE:HD2	1.68	0.41
3:J:461:PHE:HD2	3:J:461:PHE:HA	1.72	0.41
3:J:818:GLU:HB3	3:J:887:SER:HB2	2.03	0.41
1:B:79:LEU:HD11	3:D:526:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:ASP:HA	2:C:418:GLY:O	2.20	0.41
2:C:519:ASN:ND2	2:C:796:LEU:HD23	2.34	0.41
2:C:1099:ASN:HD21	3:D:505:ASP:CG	2.26	0.41
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.55	0.41
3:D:30:ILE:HD13	3:D:243:PRO:HD3	2.03	0.41
3:D:317:THR:HG22	3:D:322:ARG:O	2.20	0.41
3:D:362:ARG:H	3:D:365:GLN:NE2	2.17	0.41
2:I:98:VAL:O	2:I:121:GLU:HA	2.20	0.41
2:I:607:SER:N	2:I:610:GLU:HB2	2.35	0.41
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.28	0.41
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.02	0.41
5:L:584:ARG:HH11	5:L:584:ARG:HA	1.86	0.41
1:A:83:LEU:HD23	2:C:694:ARG:HH21	1.85	0.41
2:C:164:THR:C	2:C:166:SER:H	2.29	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.02	0.41
2:C:980:VAL:HA	2:C:984:VAL:HA	2.03	0.41
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.53	0.41
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.36	0.41
5:F:226:ALA:O	5:F:229:VAL:HG22	2.20	0.41
1:G:35:PHE:CE1	1:H:46:ILE:HG23	2.55	0.41
1:H:47:LEU:HD23	1:H:47:LEU:HA	1.70	0.41
2:I:198:ILE:O	2:I:201:ARG:HB2	2.20	0.41
3:J:1174:ARG:HG2	3:J:1189:MET:SD	2.60	0.41
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.20	0.41
5:L:233:ASP:O	5:L:236:LYS:HE2	2.21	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.68	0.41
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.55	0.41
2:C:206:ALA:O	2:C:209:ILE:HG22	2.21	0.41
3:D:18:ASP:HB2	3:D:1373:ARG:CZ	2.50	0.41
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.41
3:D:422:LEU:HB2	3:D:469:HIS:HB2	2.03	0.41
1:G:27:THR:HA	1:G:201:LEU:O	2.21	0.41
1:G:38:THR:HA	1:H:45:ARG:HD3	2.03	0.41
1:G:83:LEU:HD23	2:I:694:ARG:HH21	1.85	0.41
2:I:202:ARG:NH2	2:I:368:ARG:HH12	2.19	0.41
2:I:299:LYS:HB3	2:I:299:LYS:HE2	1.91	0.41
2:I:452:ARG:HH21	2:I:458:GLU:CD	2.28	0.41
2:I:896:THR:OG1	2:I:899:GLU:HG3	2.20	0.41
2:I:1198:LEU:HD22	2:I:1198:LEU:HA	1.84	0.41
2:I:1309:VAL:HA	3:J:383:GLY:HA3	2.01	0.41
3:J:721:SER:HA	3:J:724:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1157:ALA:HB3	3:J:1206:ARG:HA	2.03	0.41
1:B:82:LEU:HD13	1:B:173:VAL:HG12	2.02	0.41
2:C:149:LEU:HD13	2:C:453:ILE:HG12	2.01	0.41
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.21	0.41
2:C:685:MET:HB2	2:C:685:MET:HE3	1.71	0.41
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.39	0.41
2:C:1136:GLN:O	2:C:1137:GLU:HB3	2.21	0.41
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.56	0.41
3:D:625:MET:HE2	3:D:625:MET:HB3	2.00	0.41
3:D:839:VAL:HG13	3:D:882:VAL:HG21	2.01	0.41
3:D:844:THR:HG23	3:D:864:LEU:HD11	2.03	0.41
5:F:230:VAL:HG13	5:F:231:THR:H	1.83	0.41
5:F:320:ILE:HG12	5:F:330:LEU:HD12	2.02	0.41
5:F:572:THR:O	5:F:576:VAL:HG23	2.20	0.41
5:F:588:ARG:H	5:F:588:ARG:HG3	1.58	0.41
1:G:61:ILE:HB	1:G:64:VAL:CG2	2.51	0.41
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.56	0.41
1:H:57:THR:HG21	1:H:158:ARG:NH2	2.35	0.41
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.29	0.41
2:I:163:LYS:HE3	2:I:163:LYS:HB3	1.88	0.41
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.93	0.41
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.86	0.41
2:I:675:ASP:HB3	2:I:1107:MET:O	2.21	0.41
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.41
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.54	0.41
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.55	0.41
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.56	0.41
3:J:325:LYS:HG3	3:J:329:ASP:HB2	2.02	0.41
3:J:363:LEU:O	3:J:363:LEU:HG	2.21	0.41
3:J:600:ALA:O	3:J:603:LYS:HG2	2.21	0.41
3:J:701:LEU:CD1	3:J:723:TYR:HB2	2.51	0.41
5:L:518:HIS:O	5:L:519:LEU:C	2.63	0.41
1:A:49:SER:HB3	2:C:1083:GLU:CD	2.46	0.41
1:A:137:ASN:OD1	1:A:137:ASN:N	2.53	0.41
2:C:57:PHE:CD1	2:C:59:ILE:HG13	2.55	0.41
2:C:269:ILE:HG22	2:C:274:ILE:HG13	2.03	0.41
3:D:11:GLN:NE2	3:D:15:GLU:OE2	2.54	0.41
3:D:278:ARG:HD2	3:D:295:GLU:CD	2.46	0.41
3:D:647:PRO:HG3	3:D:697:MET:CB	2.47	0.41
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.20	0.41
4:E:15:ASN:O	4:E:16:ARG:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:LEU:HD23	1:H:198:LEU:HA	1.86	0.41
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.21	0.41
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.56	0.41
3:J:809:VAL:HA	3:J:894:VAL:O	2.21	0.41
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.80	0.40
2:C:187:GLU:OE2	2:C:203:LYS:HE2	2.21	0.40
2:C:1178:LYS:HD3	2:C:1178:LYS:HA	1.96	0.40
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.40	0.40
3:D:369:PRO:HB3	3:D:444:GLY:O	2.21	0.40
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.95	0.40
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.51	0.40
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	2.02	0.40
2:I:94:ALA:HB2	2:I:129:LEU:HD11	2.02	0.40
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.56	0.40
2:I:588:GLU:CD	2:I:605:TYR:HB3	2.46	0.40
5:L:281:ARG:HG2	5:L:285:ARG:HD2	2.03	0.40
5:L:296:LYS:HA	5:L:296:LYS:HD3	1.93	0.40
2:C:653:MET:HG2	2:C:654:ASP:N	2.37	0.40
3:D:339:ARG:O	3:D:344:GLY:HA2	2.21	0.40
1:G:177:TYR:O	1:G:178:SER:HB2	2.21	0.40
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	2.03	0.40
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.03	0.40
3:J:77:ARG:HA	3:J:77:ARG:HD2	1.85	0.40
3:J:189:LEU:HD22	3:J:234:PRO:HB3	2.01	0.40
3:J:526:VAL:HA	3:J:549:LYS:O	2.21	0.40
4:K:15:ASN:O	4:K:16:ARG:HB3	2.22	0.40
1:A:233:ASP:OD2	1:A:233:ASP:N	2.55	0.40
2:C:62:TYR:O	2:C:64:GLY:N	2.54	0.40
2:C:232:ILE:HD12	2:C:330:HIS:O	2.20	0.40
2:C:646:SER:HB3	2:C:649:GLN:HG3	2.02	0.40
2:C:819:SER:HB2	2:C:1085:MET:CG	2.51	0.40
3:D:232:ASN:HA	3:D:236:TRP:HZ3	1.84	0.40
3:D:901:ARG:HD2	3:D:906:GLY:O	2.22	0.40
5:F:372:ALA:O	5:F:376:LYS:HG3	2.21	0.40
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.04	0.40
1:H:92:VAL:HA	1:H:120:ASP:O	2.21	0.40
2:I:379:GLU:CD	2:I:379:GLU:H	2.30	0.40
2:I:496:LYS:HB3	2:I:497:PRO:HD3	2.02	0.40
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.22	0.40
3:J:294:ASN:HB2	5:L:101:TYR:CD1	2.56	0.40
3:J:785:ASP:O	3:J:789:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:805:GLN:OE1	3:J:1348:LYS:HD3	2.21	0.40
5:L:547:VAL:CG2	5:L:603:ARG:HB3	2.51	0.40
1:B:182:ARG:C	1:B:183:ILE:HD12	2.46	0.40
2:C:27:LEU:HG	2:C:711:ASP:OD2	2.21	0.40
2:C:678:ARG:HD3	2:C:678:ARG:HA	1.92	0.40
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.92	0.40
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	2.03	0.40
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.19	0.40
3:J:1183:SER:OG	3:J:1185:PRO:HD3	2.21	0.40
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.57	0.40
1:B:211:ILE:HD13	1:B:211:ILE:HA	1.90	0.40
2:C:379:GLU:CD	2:C:379:GLU:H	2.30	0.40
2:C:444:ASP:OD1	2:C:447:HIS:HB2	2.22	0.40
2:C:606:LEU:HD23	2:C:611:GLU:HA	2.03	0.40
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	2.04	0.40
3:D:705:THR:OG1	3:D:718:SER:HA	2.21	0.40
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.36	0.40
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.52	0.40
5:F:235:ILE:HA	5:F:245:ALA:HB2	2.04	0.40
1:G:219:ARG:O	1:G:223:ILE:HG13	2.22	0.40
2:I:564:PRO:HG3	2:I:572:ILE:HG13	2.04	0.40
2:I:722:GLY:HA2	2:I:737:ASN:OD1	2.21	0.40
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.36	0.40
3:J:709:ARG:C	3:J:711:GLY:N	2.79	0.40
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/329 (68%)	195 (87%)	26 (12%)	4 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	210/329 (64%)	180 (86%)	25 (12%)	5 (2%)	4	30
1	G	222/329 (68%)	192 (86%)	24 (11%)	6 (3%)	4	28
1	H	211/329 (64%)	185 (88%)	21 (10%)	5 (2%)	4	30
2	C	1328/1342 (99%)	1220 (92%)	101 (8%)	7 (0%)	24	59
2	I	1324/1342 (99%)	1220 (92%)	97 (7%)	7 (0%)	24	59
3	D	1162/1407 (83%)	1070 (92%)	85 (7%)	7 (1%)	21	55
3	J	1151/1407 (82%)	1059 (92%)	80 (7%)	12 (1%)	12	45
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
5	F	462/613 (75%)	424 (92%)	37 (8%)	1 (0%)	43	74
5	L	463/613 (76%)	426 (92%)	36 (8%)	1 (0%)	43	74
All	All	6922/8222 (84%)	6328 (91%)	539 (8%)	55 (1%)	16	50

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	B	13	LEU
2	C	3	TYR
2	C	1159	VAL
3	D	10	ALA
3	D	332	LYS
2	I	1159	VAL
1	A	167	PRO
1	B	136	GLU
2	C	170	VAL
2	C	697	LYS
1	G	162	GLU
1	G	167	PRO
1	H	20	SER
1	H	135	ASP
2	I	170	VAL
2	I	697	LYS
3	J	332	LYS
3	J	334	LYS
3	J	339	ARG
1	B	20	SER
1	H	136	GLU

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Mol	Chain	Res	Type
1	A	14	VAL
2	C	484	LEU
2	C	1158	LYS
3	D	710	ASP
3	D	806	ASP
2	I	484	LEU
2	I	1158	LYS
3	J	333	GLY
3	J	338	PHE
3	J	710	ASP
1	A	62	ASP
1	G	14	VAL
1	G	62	ASP
1	G	229	GLU
1	H	138	ALA
3	J	344	GLY
3	J	806	ASP
1	B	14	VAL
1	B	62	ASP
3	D	831	VAL
1	G	196	THR
1	H	62	ASP
2	I	63	SER
3	J	831	VAL
5	F	477	GLU
2	I	1186	VAL
2	C	1186	VAL
3	D	826	ILE
3	D	1180	VAL
3	J	826	ILE
3	J	1180	VAL
5	L	477	GLU
3	J	336	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/286 (68%)	179 (92%)	15 (8%)	12	37
1	B	182/286 (64%)	171 (94%)	11 (6%)	17	44
1	G	191/286 (67%)	178 (93%)	13 (7%)	14	41
1	H	184/286 (64%)	175 (95%)	9 (5%)	22	47
2	C	1150/1157 (99%)	1038 (90%)	112 (10%)	8	28
2	I	1147/1157 (99%)	1037 (90%)	110 (10%)	8	29
3	D	970/1168 (83%)	859 (89%)	111 (11%)	5	22
3	J	960/1168 (82%)	853 (89%)	107 (11%)	6	23
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	23
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	38
5	F	417/540 (77%)	374 (90%)	43 (10%)	7	26
5	L	418/540 (77%)	376 (90%)	42 (10%)	7	27
All	All	5952/7024 (85%)	5366 (90%)	586 (10%)	7	28

All (586) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	VAL
1	A	26	VAL
1	A	50	SER
1	A	61	ILE
1	A	64	VAL
1	A	74	VAL
1	A	115	ILE
1	A	129	VAL
1	A	133	LEU
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	A	232	VAL
1	A	233	ASP
1	B	6	THR
1	B	7	GLU
1	B	8	PHE
1	B	26	VAL
1	B	50	SER
1	B	61	ILE
1	B	64	VAL

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Mol	Chain	Res	Type
1	B	115	ILE
1	B	133	LEU
1	B	198	LEU
1	B	215	GLU
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE
2	C	60	GLN
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	132	ASP
2	C	167	SER
2	C	170	VAL
2	C	237	LEU
2	C	285	ILE
2	C	292	ILE
2	C	299	LYS
2	C	302	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	353	VAL
2	C	360	LEU
2	C	377	THR
2	C	379	GLU
2	C	394	ARG
2	C	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	453	ILE
2	C	484	LEU

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Mol	Chain	Res	Type
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	503	LYS
2	C	518	ASN
2	C	550	VAL
2	C	558	VAL
2	C	565	GLU
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	800	MET
2	C	817	LEU
2	C	819	SER
2	C	826	ASP
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	979	LEU

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Mol	Chain	Res	Type
2	C	984	VAL
2	C	1002	LEU
2	C	1040	ASP
2	C	1046	VAL
2	C	1073	LYS
2	C	1076	ILE
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1161	LEU
2	C	1174	GLU
2	C	1180	MET
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1238	LEU
2	C	1254	VAL
2	C	1264	GLN
2	C	1293	VAL
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1340	GLU
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	13	LYS
3	D	18	ASP
3	D	20	ILE
3	D	26	SER
3	D	46	TYR
3	D	79	LYS
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL

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Mol	Chain	Res	Type
3	D	94	GLN
3	D	95	THR
3	D	97	VAL
3	D	106	GLU
3	D	159	ILE
3	D	169	LEU
3	D	175	GLU
3	D	217	LEU
3	D	244	VAL
3	D	252	LEU
3	D	255	LEU
3	D	299	LEU
3	D	306	LEU
3	D	312	ARG
3	D	324	LEU
3	D	343	LEU
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	401	VAL
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	454	CYS
3	D	490	ILE
3	D	501	VAL
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	573	THR
3	D	594	GLN
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG

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Mol	Chain	Res	Type
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	769	VAL
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	810	THR
3	D	826	ILE
3	D	844	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	931	THR
3	D	1135	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG

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Mol	Chain	Res	Type
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1268	ASN
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
3	D	1278	GLU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1310	THR
3	D	1333	THR
3	D	1343	GLU
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	21	LEU
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	247	GLU
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	305	LEU
5	F	306	PHE
5	F	310	GLU
5	F	341	LEU
5	F	395	THR
5	F	400	GLN
5	F	429	THR

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Mol	Chain	Res	Type
5	F	437	GLN
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	485	GLU
5	F	486	ARG
5	F	488	LEU
5	F	489	MET
5	F	491	GLU
5	F	494	ILE
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	580	PHE
5	F	587	ILE
5	F	603	ARG
5	F	606	VAL
5	F	612	ASP
1	G	9	LEU
1	G	19	VAL
1	G	26	VAL
1	G	50	SER
1	G	61	ILE
1	G	64	VAL
1	G	74	VAL
1	G	115	ILE
1	G	129	VAL
1	G	133	LEU
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	9	LEU
1	H	22	THR
1	H	26	VAL

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Mol	Chain	Res	Type
1	H	50	SER
1	H	61	ILE
1	H	64	VAL
1	H	115	ILE
1	H	133	LEU
1	H	215	GLU
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	60	GLN
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	132	ASP
2	I	167	SER
2	I	170	VAL
2	I	237	LEU
2	I	285	ILE
2	I	292	ILE
2	I	299	LYS
2	I	302	ILE
2	I	306	THR
2	I	320	ASP
2	I	321	LEU
2	I	353	VAL
2	I	360	LEU
2	I	377	THR
2	I	379	GLU
2	I	394	ARG
2	I	400	VAL
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	453	ILE

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Mol	Chain	Res	Type
2	I	484	LEU
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	503	LYS
2	I	550	VAL
2	I	558	VAL
2	I	565	GLU
2	I	589	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	800	MET
2	I	817	LEU
2	I	819	SER
2	I	826	ASP
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	979	LEU

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Mol	Chain	Res	Type
2	I	984	VAL
2	I	1002	LEU
2	I	1040	ASP
2	I	1046	VAL
2	I	1073	LYS
2	I	1076	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1161	LEU
2	I	1174	GLU
2	I	1180	MET
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1238	LEU
2	I	1254	VAL
2	I	1264	GLN
2	I	1293	VAL
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1340	GLU
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	26	SER
3	J	46	TYR
3	J	79	LYS
3	J	83	VAL
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR

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Mol	Chain	Res	Type
3	J	97	VAL
3	J	106	GLU
3	J	159	ILE
3	J	169	LEU
3	J	175	GLU
3	J	217	LEU
3	J	244	VAL
3	J	252	LEU
3	J	255	LEU
3	J	299	LEU
3	J	306	LEU
3	J	312	ARG
3	J	324	LEU
3	J	332	LYS
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	401	VAL
3	J	416	ILE
3	J	425	ARG
3	J	429	LEU
3	J	454	CYS
3	J	490	ILE
3	J	501	VAL
3	J	506	VAL
3	J	507	VAL
3	J	513	MET
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	573	THR
3	J	594	GLN
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE

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Mol	Chain	Res	Type
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	769	VAL
3	J	770	LEU
3	J	803	VAL
3	J	810	THR
3	J	826	ILE
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	931	THR
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1268	ASN

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Mol	Chain	Res	Type
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1310	THR
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	21	LEU
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	127	ILE
5	L	130	VAL
5	L	154	GLU
5	L	247	GLU
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	305	LEU
5	L	306	PHE
5	L	310	GLU
5	L	341	LEU
5	L	395	THR
5	L	400	GLN
5	L	429	THR
5	L	437	GLN
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	482	GLU

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Mol	Chain	Res	Type
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	494	ILE
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	580	PHE
5	L	587	ILE
5	L	603	ARG
5	L	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	103	ASN
1	A	117	HIS
1	B	66	HIS
1	B	132	HIS
1	B	227	GLN
2	C	31	GLN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	343	HIS
2	C	510	GLN
2	C	513	GLN
2	C	677	ASN
2	C	761	GLN
2	C	799	ASN
2	C	1017	GLN
2	C	1116	HIS
2	C	1136	GLN
2	C	1146	GLN

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Mol	Chain	Res	Type
2	C	1209	GLN
2	C	1288	GLN
2	C	1314	GLN
2	C	1336	ASN
3	D	11	GLN
3	D	94	GLN
3	D	158	GLN
3	D	196	GLN
3	D	200	GLN
3	D	365	GLN
3	D	450	HIS
3	D	469	HIS
3	D	489	ASN
3	D	594	GLN
3	D	665	GLN
3	D	667	GLN
3	D	669	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1259	GLN
3	D	1367	GLN
5	F	131	GLN
5	F	301	ASN
5	F	317	ASN
5	F	345	GLN
5	F	362	ASN
5	F	446	GLN
5	F	464	ASN
5	F	472	GLN
5	F	518	HIS
1	G	103	ASN
1	G	117	HIS
1	G	132	HIS
1	H	103	ASN
1	H	132	HIS
1	H	186	ASN
2	I	69	GLN
2	I	139	ASN
2	I	148	GLN

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Mol	Chain	Res	Type
2	I	343	HIS
2	I	494	ASN
2	I	513	GLN
2	I	628	HIS
2	I	677	ASN
2	I	688	GLN
2	I	725	GLN
2	I	1017	GLN
2	I	1116	HIS
2	I	1136	GLN
2	I	1146	GLN
2	I	1220	GLN
2	I	1314	GLN
3	J	94	GLN
3	J	196	GLN
3	J	200	GLN
3	J	364	HIS
3	J	365	GLN
3	J	450	HIS
3	J	489	ASN
3	J	665	GLN
3	J	667	GLN
3	J	702	GLN
3	J	716	GLN
3	J	777	HIS
3	J	907	HIS
3	J	910	ASN
3	J	929	GLN
3	J	1235	ASN
3	J	1259	GLN
5	L	128	ASN
5	L	131	GLN
5	L	246	GLN
5	L	283	GLN
5	L	294	GLN
5	L	301	ASN
5	L	317	ASN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	455	HIS
5	L	464	ASN

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Mol	Chain	Res	Type
5	L	545	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	RFP	C	3001	-	63,63,63	2.21	12 (19%)	94,94,94	1.93	29 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RFP	C	3001	-	-	21/60/85/85	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O3-C6	10.30	1.56	1.37
6	C	3001	RFP	C15-N1	6.68	1.49	1.35
6	C	3001	RFP	O7-C25	-4.99	1.37	1.44
6	C	3001	RFP	C12-C11	-4.70	1.36	1.54
6	C	3001	RFP	C18-C17	3.85	1.55	1.43
6	C	3001	RFP	C3-C43	3.44	1.54	1.46
6	C	3001	RFP	C6-C7	-2.52	1.35	1.39
6	C	3001	RFP	O6-C27	-2.52	1.37	1.43
6	C	3001	RFP	C17-C16	2.47	1.41	1.34
6	C	3001	RFP	C43-N2	2.30	1.34	1.27
6	C	3001	RFP	C2-N1	2.17	1.47	1.43
6	C	3001	RFP	C18-C19	2.01	1.40	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	O4-C11-C5	-5.10	122.23	131.63
6	C	3001	RFP	C41-N3-N2	4.74	138.90	113.99
6	C	3001	RFP	C12-C11-C5	4.71	116.41	107.30
6	C	3001	RFP	C2-C3-C43	-4.64	119.06	123.99
6	C	3001	RFP	O7-C35-C36	4.22	118.61	111.09
6	C	3001	RFP	C24-C23-C22	-4.17	108.47	115.41
6	C	3001	RFP	C20-C19-C18	-3.63	118.62	126.11
6	C	3001	RFP	C38-N4-C42	3.60	117.50	110.63
6	C	3001	RFP	C38-N4-C39	3.42	117.16	110.63
6	C	3001	RFP	C5-C10-C9	-3.38	114.11	119.77
6	C	3001	RFP	C18-C17-C16	-3.02	118.11	126.64
6	C	3001	RFP	C4-C3-C43	2.96	120.43	116.63
6	C	3001	RFP	C3-C2-N1	-2.87	114.41	119.33
6	C	3001	RFP	C40-N3-N2	-2.80	99.28	113.99
6	C	3001	RFP	C42-N4-C39	2.71	113.86	109.54
6	C	3001	RFP	C5-C10-C4	2.68	126.68	124.08
6	C	3001	RFP	C17-C16-C15	-2.63	113.07	120.83
6	C	3001	RFP	C12-O3-C6	-2.59	103.36	107.69
6	C	3001	RFP	C37-O6-C27	2.44	118.57	112.99
6	C	3001	RFP	C13-C12-C11	-2.35	108.11	113.90
6	C	3001	RFP	O7-C35-O8	-2.27	118.61	122.99
6	C	3001	RFP	C41-N3-C40	2.25	120.01	113.44
6	C	3001	RFP	O1-C1-C2	2.15	123.87	119.38
6	C	3001	RFP	C3-C43-N2	-2.11	118.14	121.58
6	C	3001	RFP	C10-C5-C11	2.06	138.06	133.64
6	C	3001	RFP	C2-C3-C4	2.05	120.49	119.19
6	C	3001	RFP	C20-C21-C22	-2.04	110.84	114.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	O5-C12-C13	2.03	112.24	106.98
6	C	3001	RFP	C33-C24-C23	-2.01	107.47	111.43

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	3001	RFP	C4-C3-C43-N2
6	C	3001	RFP	C30-C16-C17-C18
6	C	3001	RFP	C3-C2-N1-C15
6	C	3001	RFP	C17-C18-C19-C20
6	C	3001	RFP	C18-C19-C20-C31
6	C	3001	RFP	C1-C2-N1-C15
6	C	3001	RFP	C21-C22-C23-C24
6	C	3001	RFP	C23-C24-C25-O7
6	C	3001	RFP	C33-C24-C25-O7
6	C	3001	RFP	C32-C22-C23-C24
6	C	3001	RFP	C32-C22-C23-O9
6	C	3001	RFP	C28-C27-O6-C37
6	C	3001	RFP	C21-C22-C23-O9
6	C	3001	RFP	C33-C24-C25-C26
6	C	3001	RFP	O11-C15-C16-C30
6	C	3001	RFP	C16-C17-C18-C19
6	C	3001	RFP	C43-N2-N3-C40
6	C	3001	RFP	C18-C19-C20-C21
6	C	3001	RFP	C2-C3-C43-N2
6	C	3001	RFP	N1-C15-C16-C30
6	C	3001	RFP	C26-C27-O6-C37

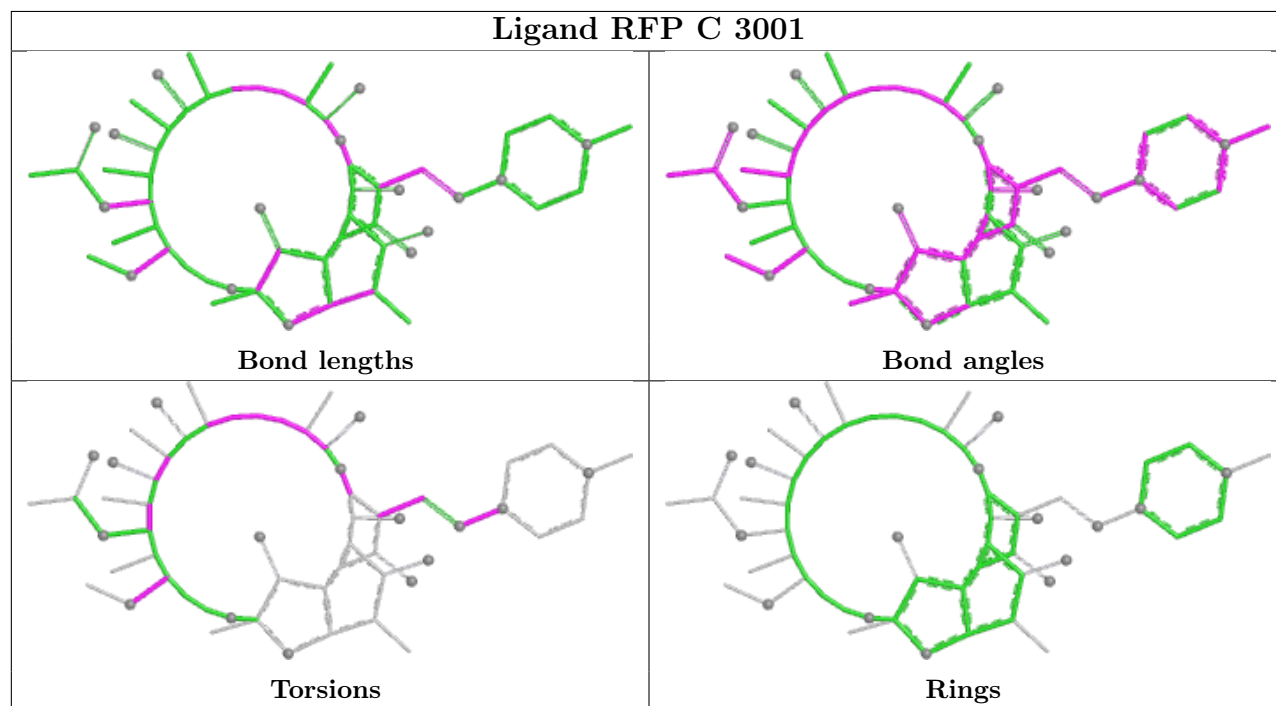
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/329 (68%)	-0.70	0 100 100	134, 178, 241, 363	0
1	B	214/329 (65%)	-0.59	0 100 100	141, 222, 328, 396	0
1	G	224/329 (68%)	-0.72	0 100 100	175, 225, 285, 364	0
1	H	215/329 (65%)	-0.58	0 100 100	179, 247, 312, 401	0
2	C	1332/1342 (99%)	-0.61	1 (0%) 92 87	101, 169, 396, 542	0
2	I	1328/1342 (98%)	-0.67	0 100 100	139, 219, 353, 523	0
3	D	1166/1407 (82%)	-0.64	0 100 100	93, 151, 275, 441	0
3	J	1155/1407 (82%)	-0.63	0 100 100	128, 181, 311, 455	0
4	E	89/91 (97%)	-0.72	0 100 100	144, 205, 237, 275	0
4	K	79/91 (86%)	-0.64	0 100 100	255, 318, 411, 416	0
5	F	468/613 (76%)	-0.65	0 100 100	139, 222, 362, 481	0
5	L	469/613 (76%)	-0.70	0 100 100	161, 231, 357, 487	0
All	All	6966/8222 (84%)	-0.65	1 (0%) 100 100	93, 196, 346, 542	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1282	GLY	2.8

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

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

6.3 Carbohydrates ⓘ

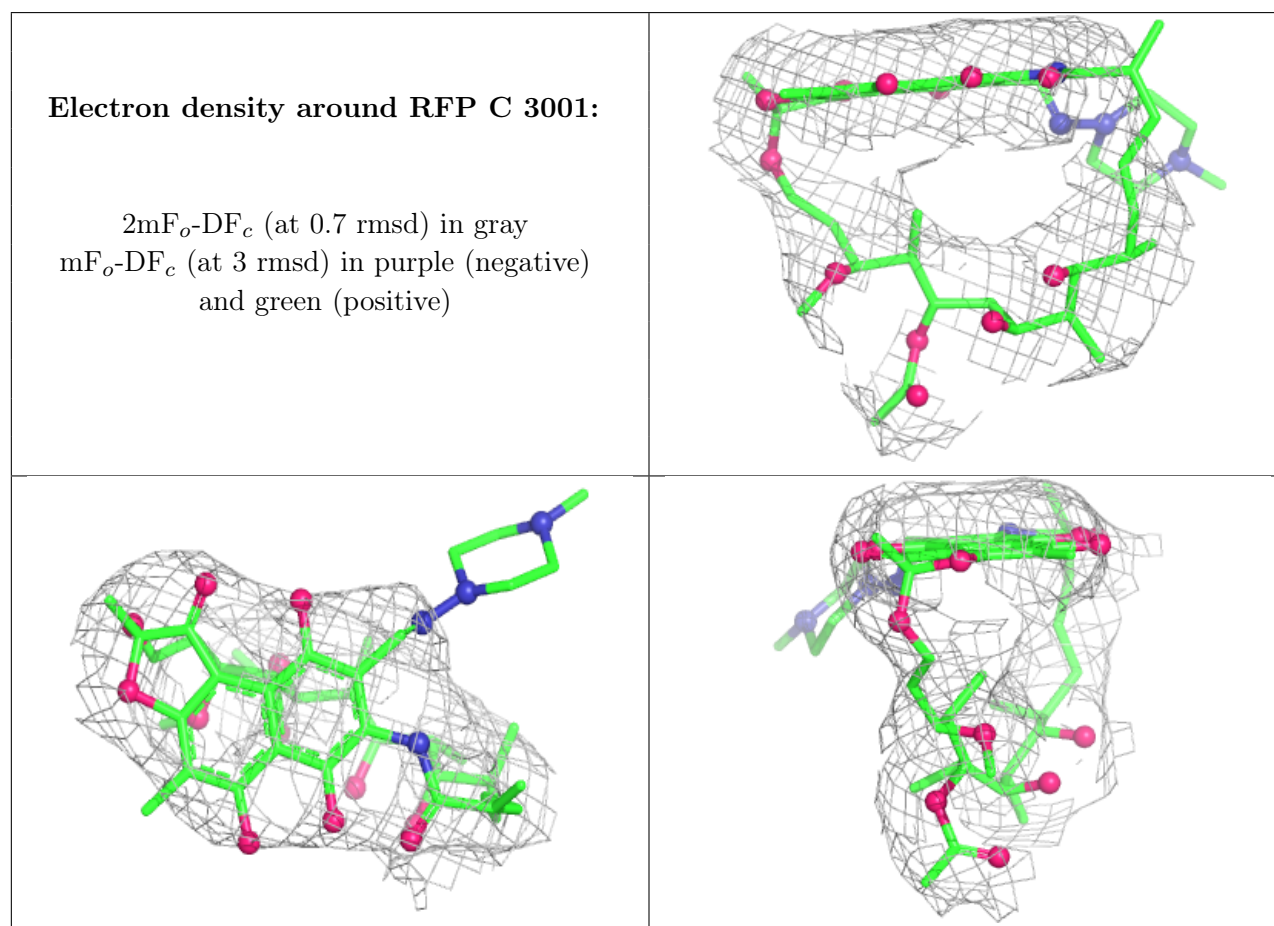
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	J	1501	1/1	0.80	0.12	121,121,121,121	0
7	MG	D	1501	1/1	0.85	0.06	77,77,77,77	0
6	RFP	C	3001	59/59	0.93	0.06	91,139,195,202	0
8	ZN	D	1502	1/1	0.99	0.02	150,150,150,150	0
8	ZN	J	1502	1/1	0.99	0.02	174,174,174,174	0
8	ZN	J	1503	1/1	0.99	0.02	126,126,126,126	0
8	ZN	D	1503	1/1	1.00	0.03	82,82,82,82	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.