



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:38 PM UTC

PDB ID : 5UAJ / pdb_00005uaj
Title : Escherichia coli RNA polymerase RpoB S531L mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

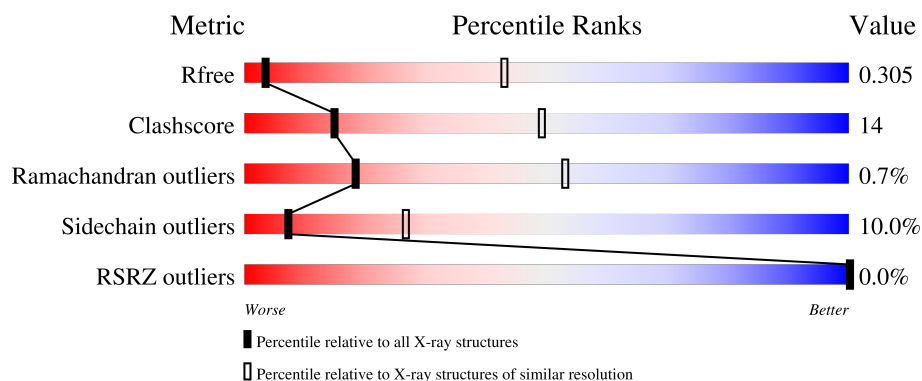
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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	41% 24% . 31%
1	B	329	36% 26% . 35%
1	G	329	43% 22% . 32%
1	H	329	36% 27% . 35%
2	C	1342	63% 33% .

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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 7 unique types of molecules in this entry. The entry contains 54994 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	1342	Total	C	N	O	S	0	0	0
			10587	6644	1843	2056	44			
2	I	1340	Total	C	N	O	S	0	0	0
			10568	6632	1840	2053	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

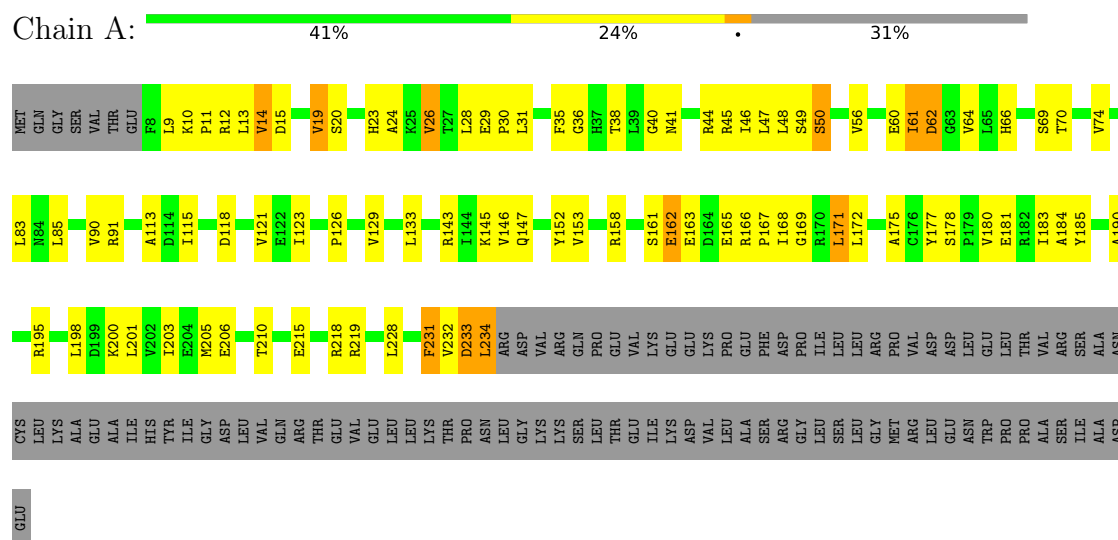
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

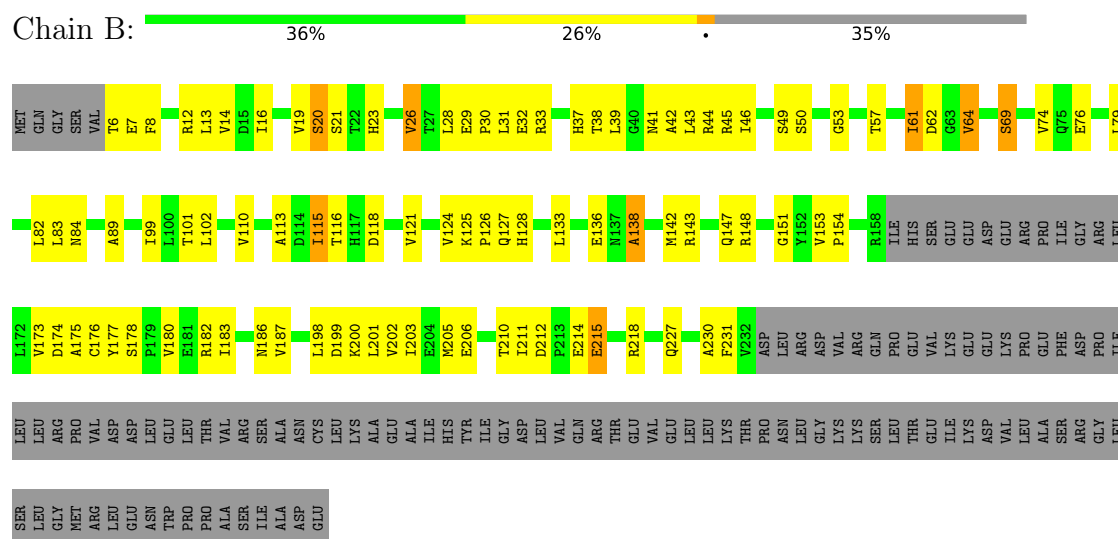
3 Residue-property plots

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

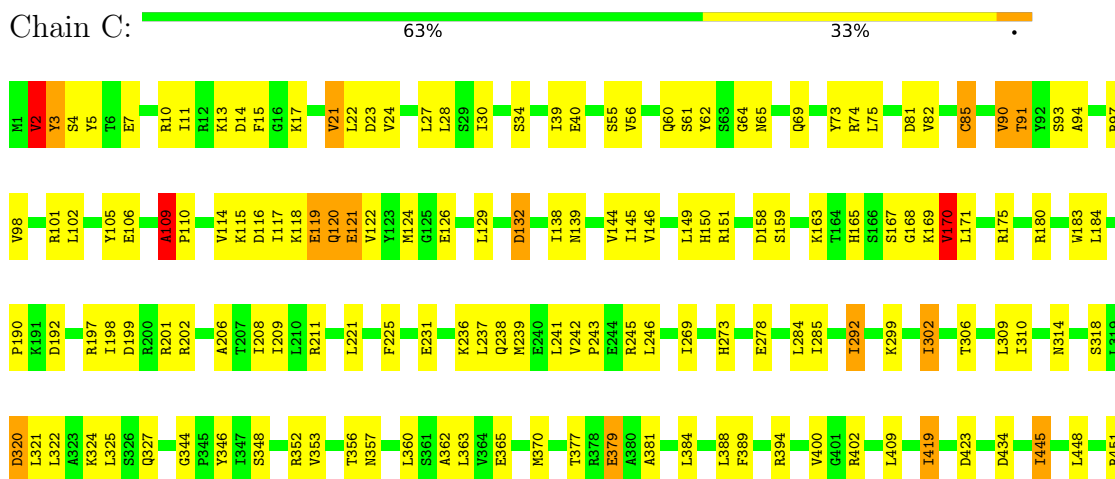
- Molecule 1: DNA-directed RNA polymerase subunit alpha

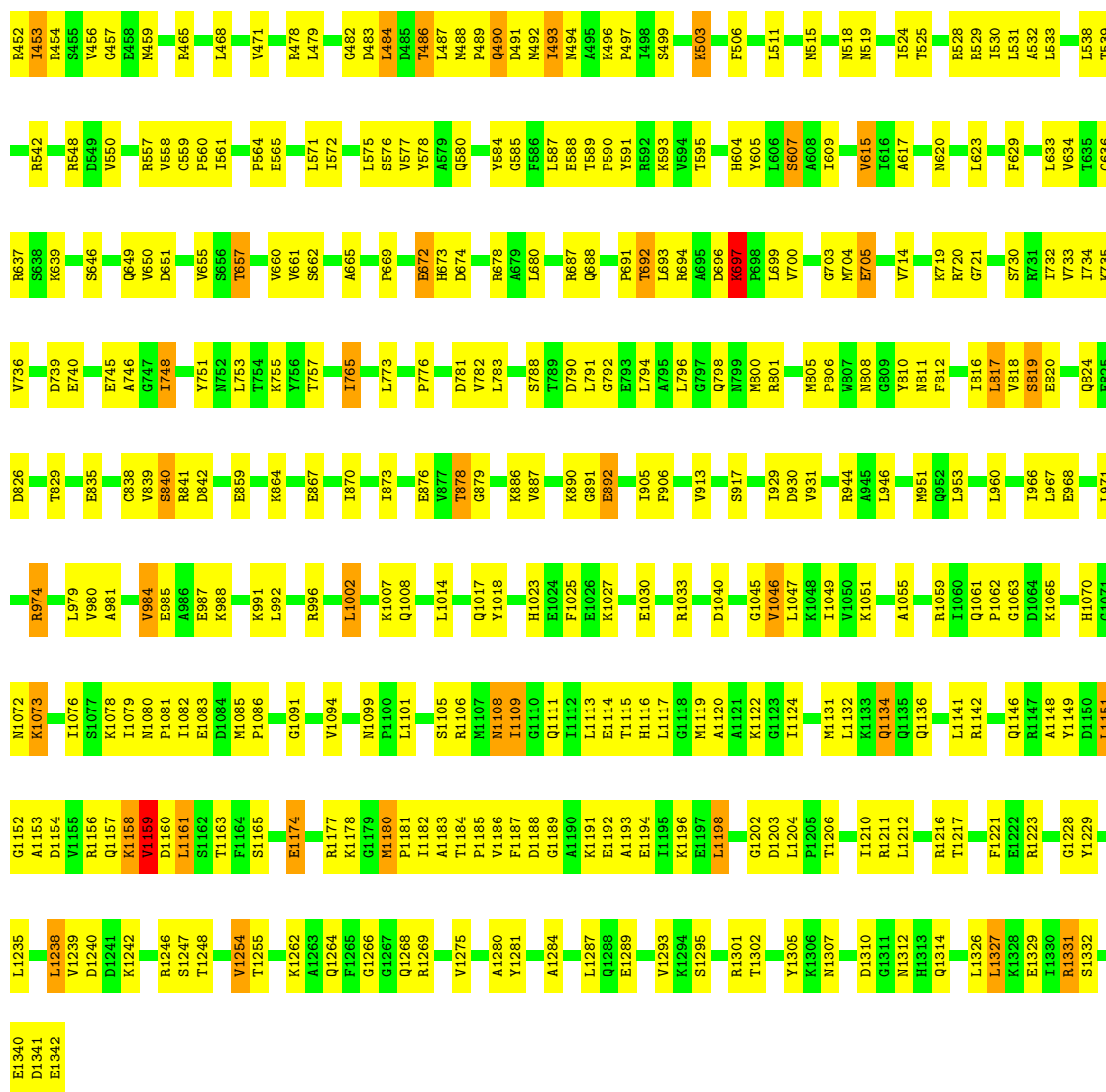


- Molecule 1: DNA-directed RNA polymerase subunit alpha



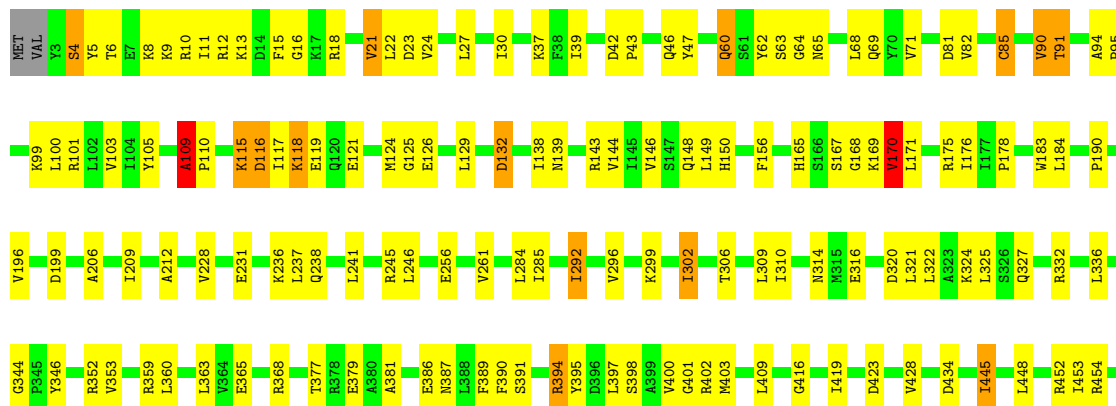
- Molecule 1: DNA-directed RNA polymerase subunit alpha

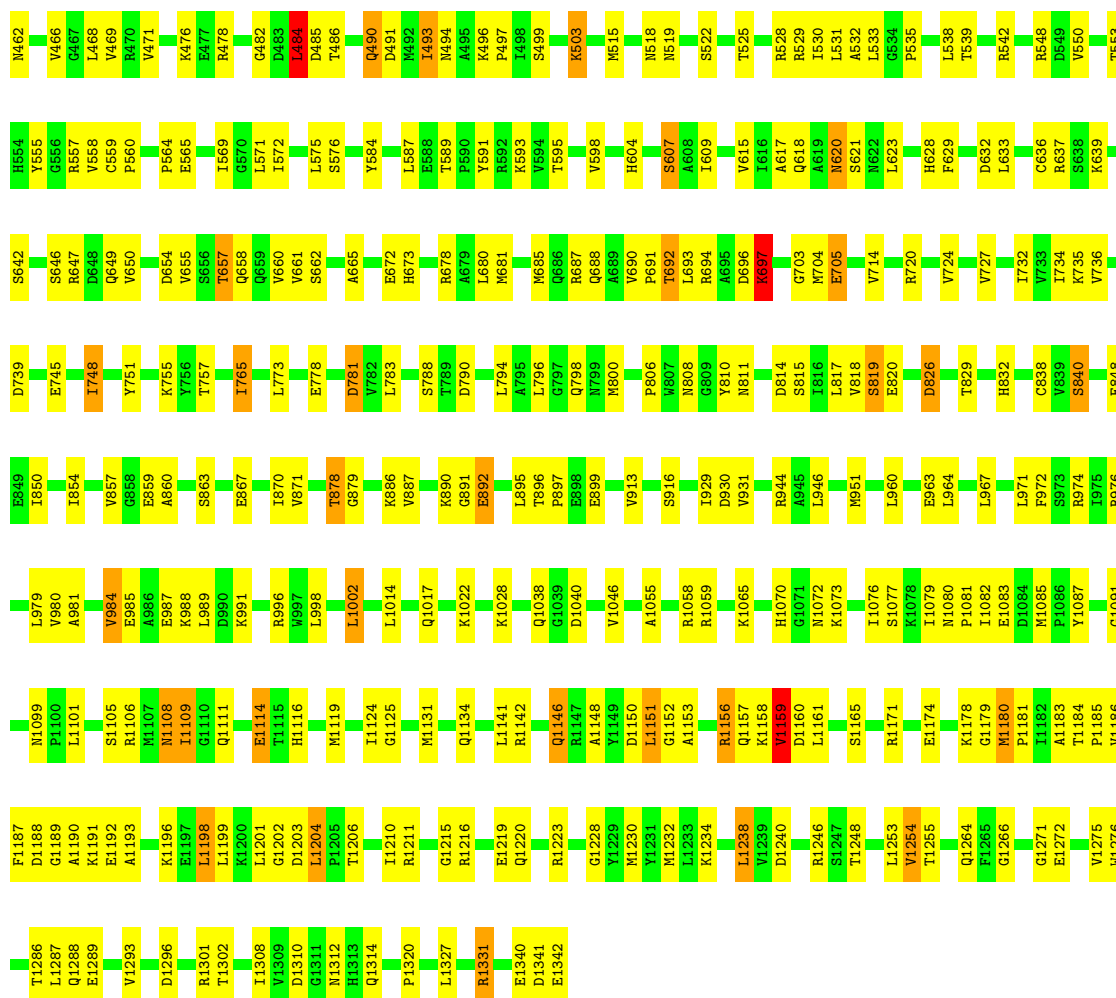




• Molecule 2: DNA-directed RNA polymerase subunit beta

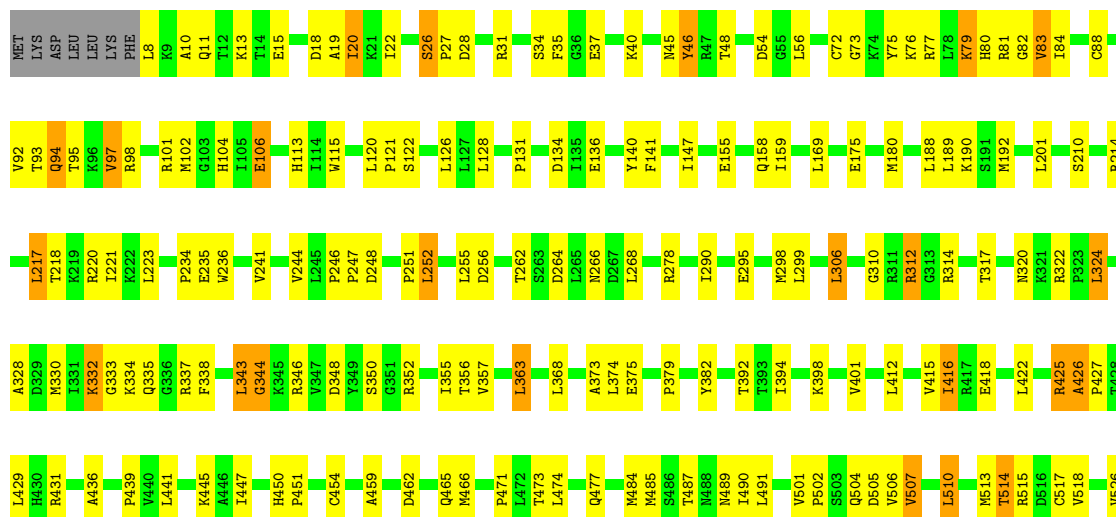
Chain I: 66% 31% •





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

Chain D: 53% 25% 5% 17%

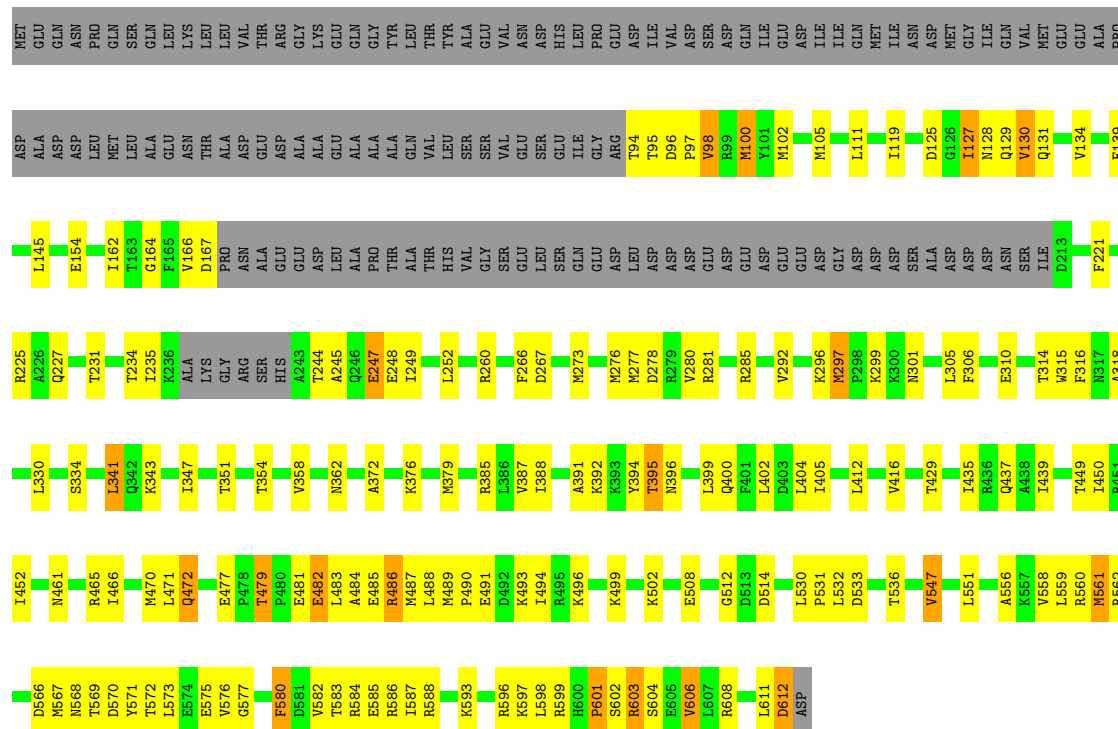




ARG ARG

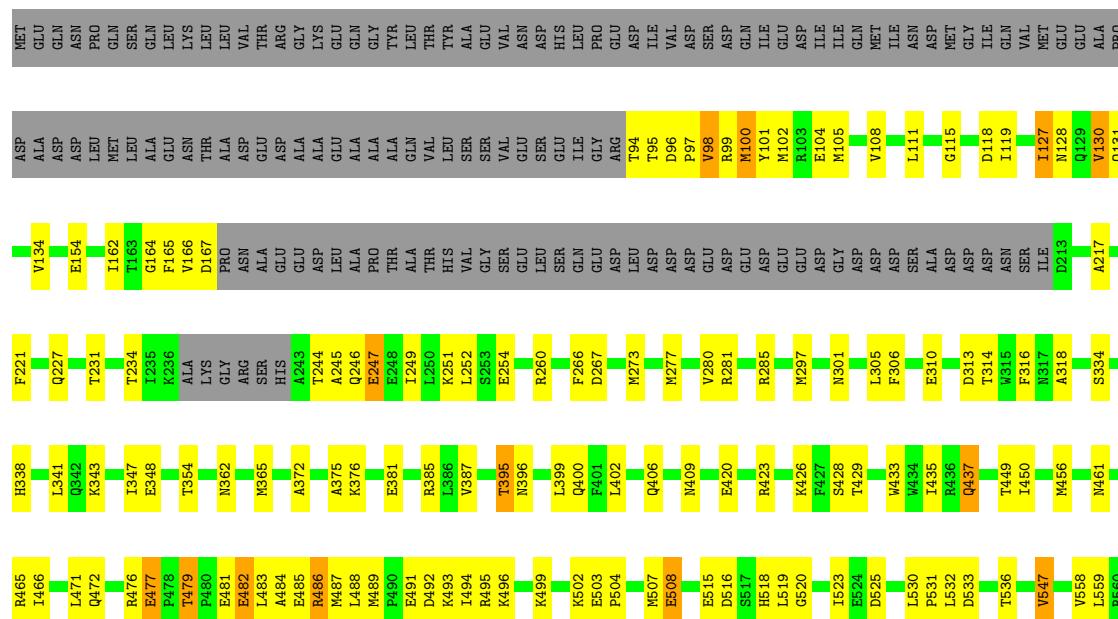
- Molecule 5: RNA polymerase sigma factor RpoD

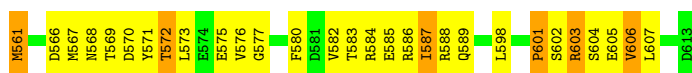
Chain F: 50% 24% 1% 24%



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 50% 23% . 23%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.22Å 204.43Å 310.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.92 29.96 – 3.92	Depositor EDS
% Data completeness (in resolution range)	79.1 (29.96-3.92) 78.9 (29.96-3.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.86Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.260 , 0.307 0.263 , 0.305	Depositor DCC
R_{free} test set	2000 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å ²)	167.5	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 136.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	54994	wwPDB-VP
Average B, all atoms (Å ²)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	1/1774 (0.1%)	0.57	0/2405
1	B	0.25	0/1668	0.81	2/2260 (0.1%)
1	G	0.24	1/1751 (0.1%)	0.57	0/2373
1	H	0.22	0/1678	0.72	0/2274
2	C	0.22	0/10756	0.62	2/14512 (0.0%)
2	I	0.18	0/10737	0.60	2/14487 (0.0%)
3	D	0.24	1/9229 (0.0%)	0.62	2/12459 (0.0%)
3	J	0.20	0/9140	0.59	0/12341
4	E	0.17	0/693	0.53	0/935
4	K	0.16	0/629	0.53	0/847
5	F	0.17	0/3864	0.59	1/5194 (0.0%)
5	L	0.17	0/3872	0.55	1/5205 (0.0%)
All	All	0.21	3/55791 (0.0%)	0.61	10/75292 (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	3
2	I	0	2
3	D	0	2
3	J	0	2
5	F	0	1
5	L	0	1
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	C-N	9.19	1.55	1.33
3	D	426	ALA	C-N	7.74	1.51	1.33
1	G	29	GLU	C-N	6.45	1.49	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	109	ALA	CA-C-N	18.31	139.52	119.93
2	I	109	ALA	C-N-CA	18.31	139.52	119.93
2	C	109	ALA	CA-C-N	14.92	135.90	119.93
2	C	109	ALA	C-N-CA	14.92	135.90	119.93
5	F	602	SER	N-CA-C	-6.32	97.35	110.80
5	L	602	SER	N-CA-C	-5.60	98.88	110.80
1	B	138	ALA	CA-C-N	-5.17	115.71	122.99
1	B	138	ALA	C-N-CA	-5.17	115.71	122.99
3	D	344	GLY	CA-C-N	5.14	131.36	121.54
3	D	344	GLY	C-N-CA	5.14	131.36	121.54

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	2	VAL	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	71	0
1	B	1649	0	1674	73	0
1	G	1730	0	1756	62	0
1	H	1659	0	1692	74	0
2	C	10587	0	10609	330	0
2	I	10568	0	10582	276	0
3	D	9089	0	9263	279	0
3	J	9001	0	9167	289	0
4	E	691	0	695	12	0
4	K	627	0	634	21	0
5	F	3813	0	3880	100	0
5	L	3821	0	3884	101	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	54994	0	55616	1526	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 (1526) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1272:GLU:H	3:J:343:LEU:HD12	1.37	0.90
1:H:32:GLU:HA	1:H:198:LEU:HD22	1.51	0.89
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.54	0.89
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.55	0.88
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.57	0.87
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.54	0.87
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.56	0.85
2:I:18:ARG:NH1	2:I:621:SER:O	2.10	0.84
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.58	0.84
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.59	0.83
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.59	0.83
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.61	0.83
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.61	0.83
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.59	0.82
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.62	0.81
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.44	0.80
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.64	0.80
1:B:23:HIS:HB2	1:B:205:MET:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.15	0.79
1:G:45:ARG:HG2	1:H:38:THR:OG1	1.82	0.79
1:A:46:ILE:HD11	1:B:38:THR:HG21	1.65	0.78
2:I:1223:ARG:NH1	3:J:721:SER:OG	2.13	0.78
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.46	0.78
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.66	0.78
5:L:97:PRO:HA	5:L:100:MET:HG3	1.64	0.78
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.66	0.78
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.66	0.78
5:F:97:PRO:HA	5:F:100:MET:HG3	1.65	0.77
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.16	0.77
1:A:45:ARG:HG2	1:B:38:THR:OG1	1.85	0.77
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.66	0.77
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.50	0.77
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.67	0.76
3:J:337:ARG:HH22	3:J:1323:ALA:HB1	1.50	0.76
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.68	0.76
2:C:490:GLN:HG3	5:F:472:GLN:NE2	2.01	0.76
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.66	0.76
1:H:23:HIS:HB2	1:H:205:MET:O	1.86	0.76
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.67	0.75
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.19	0.75
1:B:29:GLU:OE1	1:B:200:LYS:HE2	1.87	0.75
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.68	0.75
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.68	0.74
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.20	0.74
2:I:314:ASN:O	2:I:352:ARG:NH1	2.20	0.74
1:H:182:ARG:H	1:H:206:GLU:HB2	1.52	0.74
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.20	0.74
1:B:53:GLY:HA3	1:B:177:TYR:O	1.87	0.74
2:I:560:PRO:O	3:J:780:ARG:NH2	2.19	0.74
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.69	0.74
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.71	0.73
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.51	0.73
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.21	0.73
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.70	0.73
3:J:418:GLU:HG3	4:K:45:LYS:H	1.53	0.73
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.70	0.73
5:F:134:VAL:HA	5:F:273:MET:HE1	1.70	0.73
2:C:528:ARG:NH2	2:C:576:SER:O	2.21	0.73
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.71	0.72
3:J:700:ASN:O	3:J:704:GLU:HB2	1.89	0.72
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.23	0.72
2:I:452:ARG:NH1	2:I:584:TYR:O	2.23	0.72
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.72	0.71
3:D:614:LEU:HD23	4:E:7:GLN:HB2	1.70	0.71
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.70	0.71
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.72	0.71
5:F:598:LEU:O	5:F:604:SER:OG	2.09	0.71
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.72	0.71
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.73	0.70
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.73	0.70
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.73	0.70
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.57	0.70
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.72	0.70
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.72	0.70
3:J:436:ALA:HB3	3:J:485:MET:HA	1.74	0.70
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.25	0.70
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.74	0.70
3:D:901:ARG:HA	3:D:908:ILE:HA	1.74	0.69
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.56	0.69
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.74	0.69
3:D:210:SER:O	3:D:214:ARG:HG2	1.92	0.69
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.58	0.69
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	1.74	0.69
2:C:721:GLY:N	2:C:740:GLU:OE1	2.21	0.69
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.75	0.69
1:G:14:VAL:HG22	1:G:15:ASP:H	1.58	0.69
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.74	0.68
1:H:67:GLU:OE1	1:H:67:GLU:N	2.27	0.68
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.57	0.68
3:J:576:ARG:NH1	3:J:593:ASN:O	2.27	0.68
3:J:128:LEU:HA	3:J:192:MET:HE1	1.75	0.68
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.58	0.68
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.25	0.68
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.74	0.67
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.74	0.67
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.42	0.67
3:J:1161:GLY:HA3	3:J:1179:PRO:HA	1.76	0.67
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.75	0.67
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.75	0.67
2:C:1246:ARG:HH11	2:C:1266:GLY:HA2	1.59	0.67
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.59	0.67
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.76	0.67
5:L:598:LEU:O	5:L:604:SER:OG	2.11	0.67
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.59	0.67
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.77	0.67
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.59	0.67
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.76	0.67
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.77	0.67
3:D:418:GLU:HG3	4:E:45:LYS:H	1.59	0.67
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.77	0.67
3:J:218:THR:HG21	3:J:1275:LEU:HD11	1.77	0.67
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.59	0.67
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.26	0.67
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.77	0.67
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.59	0.67
1:A:233:ASP:OD2	1:A:233:ASP:N	2.27	0.66
2:C:109:ALA:HB1	2:C:110:PRO:C	2.19	0.66
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.76	0.66
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.75	0.66
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.59	0.66
2:I:324:LYS:O	2:I:327:GLN:NE2	2.29	0.66
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.95	0.66
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.61	0.66
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.26	0.66
5:F:316:PHE:HZ	5:F:334:SER:HA	1.61	0.66
1:G:38:THR:OG1	1:H:45:ARG:HG2	1.95	0.66
1:G:231:PHE:CZ	1:H:221:ALA:HB3	2.30	0.66
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.78	0.66
2:C:40:GLU:O	2:C:73:TYR:OH	2.15	0.65
3:D:11:GLN:HG2	3:D:15:GLU:HG3	1.78	0.65
2:I:499:SER:O	2:I:503:LYS:HB2	1.96	0.65
1:B:214:GLU:O	1:B:218:ARG:HG3	1.96	0.65
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.96	0.65
1:A:23:HIS:HB2	1:A:205:MET:O	1.97	0.65
3:D:436:ALA:HB3	3:D:485:MET:HA	1.78	0.65
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.77	0.65
2:C:1061:GLN:NE2	2:C:1240:ASP:OD2	2.29	0.65
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.79	0.65
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.77	0.65
5:F:573:LEU:H	5:F:573:LEU:HD23	1.61	0.65
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.78	0.65
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.79	0.65
1:G:12:ARG:H	1:G:30:PRO:HD2	1.62	0.65
1:B:118:ASP:H	1:B:121:VAL:HB	1.60	0.65
2:I:109:ALA:HB1	2:I:110:PRO:C	2.22	0.65
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.62	0.65
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.78	0.64
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.79	0.64
5:F:235:ILE:HA	5:F:245:ALA:HB2	1.79	0.64
2:C:864:LYS:NZ	2:C:876:GLU:O	2.31	0.64
1:H:79:LEU:HD11	3:J:526:VAL:HG21	1.79	0.64
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	1.80	0.64
2:C:703:GLY:N	2:C:705:GLU:OE2	2.27	0.64
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.79	0.64
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.78	0.64
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.63	0.64
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.80	0.64
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.80	0.64
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.78	0.64
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.31	0.64
3:D:343:LEU:HD13	3:D:344:GLY:HA3	1.79	0.63
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.64	0.63
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.63	0.63
2:C:829:THR:HA	2:C:1059:ARG:HA	1.80	0.63
5:L:134:VAL:HA	5:L:273:MET:HE1	1.81	0.63
1:G:45:ARG:NH1	1:H:38:THR:OG1	2.32	0.62
1:H:53:GLY:HA3	1:H:177:TYR:O	1.99	0.62
3:J:514:THR:HB	3:J:576:ARG:HG2	1.81	0.62
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.64	0.62
3:D:741:ALA:O	3:D:762:ASN:ND2	2.32	0.62
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.80	0.62
1:H:195:ARG:HH21	1:H:198:LEU:HD21	1.65	0.62
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.32	0.62
3:J:337:ARG:NH2	3:J:1323:ALA:HB1	2.14	0.62
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.82	0.62
1:A:14:VAL:HG22	1:A:15:ASP:H	1.65	0.62
1:B:212:ASP:CG	1:B:215:GLU:HB2	2.25	0.62
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.82	0.62
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.81	0.61
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.82	0.61
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.81	0.61
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.82	0.61
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.82	0.61
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.82	0.61
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.15	0.61
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.16	0.61
1:B:79:LEU:HD11	3:D:526:VAL:HG21	1.83	0.61
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.35	0.61
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.65	0.61
1:B:182:ARG:H	1:B:206:GLU:HB2	1.65	0.61
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.83	0.61
3:D:576:ARG:NH1	3:D:593:ASN:O	2.34	0.61
3:D:700:ASN:O	3:D:704:GLU:HB2	1.99	0.61
2:I:30:ILE:HD12	2:I:30:ILE:H	1.66	0.61
2:C:1247:SER:HB3	3:D:375:GLU:O	1.99	0.61
3:D:392:THR:HG21	5:F:606:VAL:HA	1.81	0.61
3:D:45:ASN:HB3	3:D:48:THR:O	2.00	0.61
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.83	0.60
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.83	0.60
1:H:190:ALA:N	1:H:198:LEU:O	2.29	0.60
3:J:1159:ILE:HD12	3:J:1206:ARG:HD2	1.83	0.60
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.64	0.60
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.83	0.60
2:C:518:ASN:O	2:C:691:PRO:HD3	2.01	0.60
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.82	0.60
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.81	0.60
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.65	0.60
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.82	0.60
2:C:30:ILE:HD12	2:C:30:ILE:H	1.64	0.60
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.84	0.60
1:H:153:VAL:H	1:H:175:ALA:HB3	1.67	0.60
1:A:38:THR:OG1	1:B:45:ARG:HG2	2.01	0.60
1:A:161:SER:O	1:A:163:GLU:N	2.35	0.60
1:B:182:ARG:HD2	3:D:581:MET:HE1	1.84	0.60
1:H:74:VAL:HG12	1:H:76:GLU:H	1.66	0.60
2:I:296:VAL:HB	2:I:336:LEU:HD12	1.83	0.60
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.32	0.60
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.66	0.60
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.67	0.60
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.84	0.60
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.83	0.60
1:G:181:GLU:HB3	1:G:206:GLU:HG3	1.84	0.59
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.84	0.59
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.84	0.59
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.37	0.59
1:G:46:ILE:HD11	1:H:38:THR:HG21	1.83	0.59
3:J:709:ARG:C	3:J:711:GLY:H	2.10	0.59
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.19	0.59
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.85	0.59
1:B:12:ARG:H	1:B:30:PRO:HD2	1.66	0.59
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.84	0.59
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.84	0.59
1:G:9:LEU:HD21	1:G:195:ARG:HH21	1.68	0.59
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.84	0.59
2:I:528:ARG:NH2	2:I:576:SER:O	2.34	0.59
2:C:490:GLN:HG3	5:F:472:GLN:HE21	1.67	0.59
5:F:343:LYS:HD2	5:F:343:LYS:H	1.66	0.59
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.84	0.59
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.36	0.59
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.85	0.59
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.85	0.59
1:B:49:SER:O	1:B:151:GLY:HA2	2.02	0.59
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.85	0.59
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.85	0.59
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.37	0.59
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.18	0.59
2:C:1223:ARG:NH1	3:D:721:SER:OG	2.24	0.58
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.85	0.58
1:G:231:PHE:HZ	1:H:221:ALA:HB3	1.67	0.58
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.85	0.58
2:C:356:THR:HG21	2:C:362:ALA:HA	1.84	0.58
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.36	0.58
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.85	0.58
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.86	0.58
3:J:211:GLU:OE2	3:J:214:ARG:NH2	2.37	0.58
2:C:1248:THR:HB	5:F:532:LEU:HD11	1.85	0.58
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.32	0.58
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.85	0.58
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:LEU:H	1:G:13:LEU:HD23	1.69	0.58
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.86	0.58
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.67	0.58
1:B:61:ILE:HG22	1:B:62:ASP:H	1.68	0.58
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.37	0.58
1:H:64:VAL:HG11	1:H:69:SER:OG	2.03	0.58
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.85	0.58
3:J:1160:SER:HB2	3:J:1206:ARG:HG2	1.86	0.57
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.86	0.57
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.05	0.57
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.38	0.57
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.69	0.57
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.86	0.57
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.85	0.57
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.04	0.57
5:L:164:GLY:O	5:L:260:ARG:HB2	2.04	0.57
3:D:1174:ARG:NH2	3:D:1187:GLU:OE2	2.37	0.57
5:F:388:ILE:O	5:F:392:LYS:HG3	2.05	0.57
3:J:210:SER:O	3:J:214:ARG:HG2	2.05	0.57
1:A:45:ARG:NH1	1:B:38:THR:OG1	2.37	0.57
1:B:113:ALA:HB2	1:B:126:PRO:HB3	1.87	0.57
5:F:479:THR:HG23	5:F:481:GLU:H	1.70	0.57
5:F:547:VAL:HG23	5:F:603:ARG:HH11	1.69	0.57
1:G:71:LYS:HB2	1:G:78:ILE:HD11	1.86	0.57
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.87	0.57
3:D:847:ASP:OD1	3:D:847:ASP:N	2.31	0.57
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.68	0.57
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.69	0.56
4:E:80:LEU:O	4:E:84:THR:OG1	2.13	0.56
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.87	0.56
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.70	0.56
3:D:317:THR:HB	3:D:324:LEU:HB3	1.86	0.56
1:A:13:LEU:HD23	1:A:13:LEU:H	1.71	0.56
1:B:82:LEU:HD13	1:B:173:VAL:HG12	1.87	0.56
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.40	0.56
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.86	0.56
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.87	0.56
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.87	0.56
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.86	0.56
3:J:504:GLN:OE1	3:J:731:ARG:NH1	2.39	0.56
3:D:709:ARG:C	3:D:711:GLY:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.71	0.56
2:C:197:ARG:NH1	2:C:201:ARG:O	2.38	0.56
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.88	0.56
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.39	0.56
3:J:901:ARG:HD2	3:J:906:GLY:O	2.06	0.56
5:L:508:GLU:HG3	5:L:518:HIS:ND1	2.21	0.56
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.13	0.56
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.04	0.56
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.39	0.56
5:L:244:THR:O	5:L:247:GLU:HG2	2.06	0.56
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.86	0.56
1:A:166:ARG:O	1:A:168:ILE:N	2.38	0.56
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.88	0.56
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.05	0.56
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.87	0.56
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.87	0.56
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.86	0.56
2:C:688:GLN:HB2	2:C:1235:LEU:HD22	1.88	0.56
3:J:45:ASN:HB3	3:J:48:THR:O	2.05	0.56
5:L:585:GLU:OE2	5:L:588:ARG:NH1	2.39	0.56
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.53	0.56
2:I:870:ILE:HB	2:I:944:ARG:HD3	1.87	0.56
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.70	0.56
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.88	0.56
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.87	0.56
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.53	0.56
2:C:615:VAL:HG22	2:C:650:VAL:HA	1.88	0.55
1:H:31:LEU:HB2	1:H:199:ASP:O	2.07	0.55
5:F:461:ASN:O	5:F:465:ARG:HG2	2.06	0.55
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.42	0.55
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.87	0.55
2:C:511:LEU:HD23	2:C:531:LEU:HD12	1.89	0.55
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.72	0.55
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.41	0.55
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.88	0.55
3:D:422:LEU:HD13	3:D:471:PRO:HG3	1.88	0.55
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.87	0.55
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.89	0.55
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.41	0.55
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.88	0.55
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.87	0.55
3:D:35:PHE:HD1	3:D:101:ARG:HB3	1.71	0.55
2:I:168:GLY:C	2:I:170:VAL:H	2.12	0.55
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.70	0.55
5:L:461:ASN:O	5:L:465:ARG:HG2	2.07	0.55
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.88	0.55
1:G:218:ARG:HH11	1:H:232:VAL:HG22	1.71	0.55
2:I:530:ILE:O	2:I:531:LEU:HD23	2.07	0.55
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.38	0.55
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.89	0.55
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.88	0.55
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.42	0.55
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.88	0.55
4:E:50:ALA:O	4:E:54:ILE:HG12	2.07	0.55
1:H:91:ARG:NH2	1:H:210:THR:O	2.40	0.55
2:I:705:GLU:HB2	2:I:794:LEU:H	1.72	0.55
3:J:709:ARG:O	3:J:711:GLY:N	2.40	0.55
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.89	0.55
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.07	0.55
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.87	0.55
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.39	0.55
3:J:905:ARG:NH1	3:J:910:ASN:HD21	2.05	0.55
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	2.22	0.55
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.89	0.55
2:I:148:GLN:NE2	2:I:535:PRO:O	2.40	0.55
5:L:573:LEU:HD23	5:L:573:LEU:H	1.72	0.55
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.89	0.55
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.88	0.55
3:J:46:TYR:HE1	5:L:456:MET:HE2	1.72	0.55
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.88	0.55
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.72	0.55
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.89	0.54
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.72	0.54
4:E:15:ASN:O	4:E:16:ARG:HB3	2.07	0.54
3:J:1329:THR:O	3:J:1333:THR:OG1	2.23	0.54
2:C:489:PRO:HA	2:C:492:MET:HE3	1.89	0.54
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.73	0.54
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.88	0.54
5:L:483:LEU:HD12	5:L:483:LEU:H	1.72	0.54
5:L:582:VAL:CG1	5:L:586:ARG:HG2	2.38	0.54
3:D:515:ARG:NH2	3:D:717:VAL:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.88	0.54
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.89	0.54
3:D:214:ARG:HA	3:D:217:LEU:HB2	1.90	0.54
3:D:333:GLY:HA3	3:D:338:PHE:CZ	2.42	0.54
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.21	0.54
1:H:67:GLU:OE2	1:H:171:LEU:N	2.39	0.54
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.42	0.54
2:I:228:VAL:HG22	2:I:245:ARG:HH21	1.70	0.54
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.88	0.54
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.90	0.54
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.89	0.54
1:A:83:LEU:HD23	2:C:694:ARG:NE	2.22	0.54
2:C:705:GLU:HB2	2:C:794:LEU:H	1.73	0.54
5:F:314:THR:O	5:F:318:ALA:HB3	2.08	0.54
5:F:395:THR:OG1	5:F:396:ASN:N	2.39	0.54
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.89	0.54
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.23	0.54
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.89	0.54
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.08	0.54
2:I:206:ALA:O	2:I:209:ILE:HG22	2.06	0.54
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.16	0.54
2:I:829:THR:HA	2:I:1059:ARG:HA	1.89	0.54
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.89	0.54
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.90	0.54
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.90	0.54
3:J:1307:LEU:HB3	3:J:1312:ALA:HB2	1.90	0.54
5:L:395:THR:OG1	5:L:396:ASN:N	2.38	0.54
3:D:73:GLY:O	3:D:76:LYS:NZ	2.31	0.54
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.23	0.54
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.90	0.54
1:G:23:HIS:HB2	1:G:205:MET:O	2.08	0.54
2:C:669:PRO:O	2:C:1070:HIS:HE1	1.90	0.54
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.48	0.54
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.72	0.54
1:B:12:ARG:H	1:B:30:PRO:CD	2.21	0.53
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.90	0.53
2:C:980:VAL:O	2:C:984:VAL:HB	2.08	0.53
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.06	0.53
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.89	0.53
3:J:838:ARG:NH1	3:J:1250:ASP:OD1	2.41	0.53
2:C:617:ALA:HA	2:C:636:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.90	0.53
2:C:170:VAL:HG23	2:C:171:LEU:N	2.24	0.53
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.89	0.53
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.90	0.53
2:C:692:THR:OG1	2:C:693:LEU:N	2.42	0.53
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.90	0.53
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.89	0.53
2:I:47:TYR:OH	2:I:398:SER:HB2	2.08	0.53
2:I:963:GLU:O	2:I:967:LEU:HB2	2.08	0.53
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.90	0.53
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.91	0.53
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.44	0.53
5:L:601:PRO:HA	5:L:604:SER:HB2	1.90	0.53
5:F:162:ILE:HD13	5:F:221:PHE:HE2	1.73	0.53
5:F:166:VAL:O	5:F:167:ASP:HB2	2.08	0.53
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.74	0.53
1:G:166:ARG:O	1:G:168:ILE:N	2.41	0.53
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.89	0.53
2:I:980:VAL:O	2:I:984:VAL:HB	2.08	0.53
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.23	0.53
3:D:514:THR:OG1	3:D:594:GLN:O	2.25	0.53
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.91	0.53
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.23	0.53
3:J:515:ARG:NH2	3:J:717:VAL:O	2.42	0.53
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.89	0.53
1:B:74:VAL:HG12	1:B:76:GLU:H	1.74	0.53
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.91	0.53
2:C:960:LEU:HB3	2:C:1025:PHE:HE2	1.74	0.53
3:D:514:THR:HB	3:D:576:ARG:HG2	1.89	0.53
1:H:205:MET:HG2	1:H:206:GLU:H	1.74	0.53
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.91	0.53
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.89	0.53
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.90	0.53
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.90	0.53
2:C:452:ARG:NH1	2:C:584:TYR:O	2.42	0.53
3:D:825:VAL:C	3:D:826:ILE:HG13	2.33	0.53
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.74	0.53
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.09	0.53
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.91	0.52
3:D:854:ALA:HB2	3:J:1372:ARG:HE	1.74	0.52
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.39	0.52
3:D:598:LYS:N	3:D:728:SER:O	2.38	0.52
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.09	0.52
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.09	0.52
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.92	0.52
2:C:905:ILE:O	5:F:599:ARG:NH1	2.35	0.52
3:D:722:ILE:HA	3:D:725:MET:HE3	1.91	0.52
1:H:48:LEU:HD22	3:J:535:ARG:HD3	1.91	0.52
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.90	0.52
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.45	0.52
5:L:166:VAL:O	5:L:167:ASP:HB2	2.09	0.52
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.91	0.52
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.75	0.52
3:D:527:LEU:HD22	3:D:533:ALA:HA	1.90	0.52
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.92	0.52
3:D:1376:GLY:O	3:J:853:THR:OG1	2.28	0.52
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.44	0.52
2:I:690:VAL:HG12	2:I:1234:LYS:O	2.10	0.52
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.91	0.52
2:I:930:ASP:OD2	2:I:931:VAL:N	2.42	0.52
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.92	0.52
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.45	0.52
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.90	0.52
3:D:1345:ARG:HD2	3:D:1370:MET:HE1	1.92	0.52
1:H:96:ASP:OD2	1:H:148:ARG:NH1	2.43	0.52
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.90	0.52
2:I:490:GLN:HG2	2:I:491:ASP:N	2.25	0.52
3:J:901:ARG:HA	3:J:908:ILE:HA	1.91	0.52
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.25	0.52
2:C:1124:ILE:HB	2:C:1180:MET:HB2	1.90	0.52
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.92	0.52
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.92	0.52
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.92	0.52
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.25	0.52
3:D:201:LEU:HD11	3:D:220:ARG:NH1	2.25	0.52
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.10	0.52
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.75	0.52
3:J:866:GLU:OE2	3:J:901:ARG:NH2	2.43	0.52
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.42	0.51
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.91	0.51
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.92	0.51
1:A:113:ALA:HB2	1:A:126:PRO:HB3	1.92	0.51
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.46	0.51
2:C:132:ASP:OD1	2:C:132:ASP:N	2.37	0.51
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.92	0.51
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.45	0.51
3:J:682:VAL:O	3:J:685:ILE:HG12	2.10	0.51
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.93	0.51
3:D:416:ILE:HG23	3:D:439:PRO:HB2	1.91	0.51
5:F:483:LEU:HD12	5:F:483:LEU:H	1.75	0.51
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.92	0.51
3:J:1290:ARG:CG	3:J:1298:VAL:HG12	2.40	0.51
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.18	0.51
3:D:56:LEU:HD12	3:D:56:LEU:H	1.75	0.51
3:J:337:ARG:HH21	3:J:1328:THR:HG23	1.74	0.51
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.73	0.51
2:C:930:ASP:OD2	2:C:931:VAL:N	2.43	0.51
5:F:134:VAL:HG21	5:F:266:PHE:CE1	2.42	0.51
1:H:19:VAL:HG23	1:H:24:ALA:HA	1.91	0.51
2:I:826:ASP:OD1	2:I:829:THR:OG1	2.27	0.51
3:J:141:PHE:HA	3:J:180:MET:HE2	1.93	0.51
5:L:227:GLN:HG2	5:L:252:LEU:HA	1.91	0.51
2:C:735:LYS:HA	2:C:748:ILE:HG22	1.93	0.51
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.10	0.51
2:I:170:VAL:HG23	2:I:171:LEU:N	2.25	0.51
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.93	0.51
3:J:356:THR:OG1	3:J:357:VAL:N	2.43	0.51
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.92	0.51
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.93	0.51
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.91	0.51
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.92	0.51
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.43	0.51
2:I:90:VAL:HG12	2:I:91:THR:H	1.75	0.51
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.93	0.51
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.45	0.51
3:J:798:ARG:HH12	3:J:1325:PHE:HB3	1.75	0.51
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.41	0.51
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.74	0.51
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	2.11	0.51
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.46	0.51
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.93	0.51
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.44	0.51
3:D:298:MET:SD	5:F:402:LEU:HB3	2.51	0.51
1:G:161:SER:O	1:G:163:GLU:N	2.44	0.51
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.91	0.51
3:J:1184:ASP:O	3:J:1186:TYR:N	2.44	0.51
1:A:228:LEU:HD23	1:A:231:PHE:HD2	1.75	0.50
2:C:27:LEU:O	2:C:528:ARG:NH1	2.42	0.50
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.26	0.50
2:C:1117:LEU:HD11	2:C:1182:ILE:HG21	1.93	0.50
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.93	0.50
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.26	0.50
2:I:12:ARG:HG2	2:I:1183:ALA:HB2	1.92	0.50
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.92	0.50
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.27	0.50
2:C:168:GLY:C	2:C:170:VAL:H	2.19	0.50
2:C:324:LYS:O	2:C:327:GLN:NE2	2.41	0.50
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.92	0.50
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.93	0.50
3:D:843:VAL:HG11	3:D:897:HIS:O	2.11	0.50
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.93	0.50
3:J:518:VAL:O	3:J:547:ARG:NH1	2.44	0.50
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.93	0.50
2:C:730:SER:O	2:C:753:LEU:HB2	2.11	0.50
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.44	0.50
2:I:4:SER:OG	2:I:5:TYR:N	2.41	0.50
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.47	0.50
3:J:34:SER:OG	3:J:104:HIS:ND1	2.40	0.50
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.47	0.50
5:F:582:VAL:CG1	5:F:586:ARG:HG2	2.40	0.50
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.11	0.50
1:B:176:CYS:O	1:B:178:SER:N	2.45	0.50
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.94	0.50
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.12	0.50
1:H:55:ALA:O	1:H:146:VAL:HG13	2.11	0.50
2:I:632:ASP:O	2:I:647:ARG:HB2	2.12	0.50
3:J:213:LYS:O	3:J:217:LEU:HB2	2.11	0.50
4:K:10:VAL:HG13	4:K:16:ARG:HB2	1.93	0.50
5:L:479:THR:HG23	5:L:481:GLU:H	1.76	0.50
2:C:1149:TYR:HE2	2:C:1180:MET:SD	2.35	0.50
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1295:SER:OG	3:D:346:ARG:O	2.27	0.50
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.43	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.93	0.50
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.42	0.50
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	1.92	0.50
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.27	0.50
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.19	0.50
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.94	0.50
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.93	0.50
5:L:343:LYS:H	5:L:343:LYS:HD2	1.76	0.50
2:C:530:ILE:O	2:C:531:LEU:HD23	2.12	0.50
2:C:1099:ASN:HD21	3:D:505:ASP:CG	2.19	0.50
3:D:122:SER:O	3:D:126:LEU:HG	2.12	0.50
3:D:290:ILE:HD12	3:D:290:ILE:H	1.77	0.50
5:F:585:GLU:HA	5:F:588:ARG:HD3	1.94	0.50
2:I:68:LEU:HD21	2:I:100:LEU:HD13	1.94	0.50
3:J:290:ILE:H	3:J:290:ILE:HD12	1.77	0.50
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.50
5:L:314:THR:O	5:L:318:ALA:HB3	2.12	0.50
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.94	0.50
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.94	0.50
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.94	0.50
2:I:132:ASP:OD1	2:I:132:ASP:N	2.36	0.50
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.11	0.50
2:I:1114:GLU:OE1	2:I:1230:MET:HA	2.12	0.50
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.77	0.50
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.93	0.50
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.44	0.50
3:D:34:SER:OG	3:D:104:HIS:ND1	2.32	0.49
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.12	0.49
3:J:527:LEU:HD21	3:J:536:LEU:HG	1.94	0.49
3:J:825:VAL:C	3:J:826:ILE:HG13	2.36	0.49
2:C:13:LYS:O	2:C:1183:ALA:N	2.38	0.49
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.42	0.49
3:D:654:ILE:O	3:D:658:GLU:HB2	2.12	0.49
3:D:842:ARG:NH2	3:D:1254:GLU:OE1	2.39	0.49
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.93	0.49
3:J:801:VAL:O	3:J:805:GLN:HB2	2.12	0.49
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.11	0.49
5:L:245:ALA:O	5:L:249:ILE:HG13	2.12	0.49
2:C:144:VAL:HG23	2:C:515:MET:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:886:LYS:H	2:C:917:SER:HB3	1.77	0.49
3:D:709:ARG:O	3:D:711:GLY:N	2.45	0.49
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.78	0.49
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.44	0.49
5:F:297:MET:HE3	5:F:330:LEU:HD21	1.94	0.49
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.93	0.49
5:L:108:VAL:HG11	5:L:381:GLU:C	2.37	0.49
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.93	0.49
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.52	0.49
3:D:77:ARG:HG3	3:D:79:LYS:H	1.77	0.49
3:D:797:THR:O	3:D:801:VAL:HG13	2.12	0.49
3:D:1329:THR:O	3:D:1333:THR:OG1	2.29	0.49
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.47	0.49
2:C:878:THR:OG1	2:C:879:GLY:N	2.45	0.49
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.94	0.49
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.37	0.49
2:C:519:ASN:ND2	2:C:796:LEU:HD23	2.25	0.49
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.12	0.49
2:I:13:LYS:O	2:I:1183:ALA:N	2.27	0.49
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.94	0.49
5:L:507:MET:HG2	5:L:520:GLY:HA3	1.95	0.49
1:B:118:ASP:HB2	1:B:121:VAL:HG23	1.94	0.49
3:D:356:THR:OG1	3:D:357:VAL:N	2.46	0.49
3:D:1167:LYS:NZ	3:D:1170:LYS:HB2	2.27	0.49
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.92	0.49
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.94	0.49
2:C:499:SER:O	2:C:503:LYS:HB2	2.13	0.49
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.95	0.49
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.94	0.49
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.78	0.49
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.27	0.49
2:I:703:GLY:N	2:I:705:GLU:OE2	2.43	0.49
1:A:169:GLY:O	1:A:171:LEU:HD22	2.13	0.48
2:C:459:MET:SD	2:C:511:LEU:HD13	2.53	0.48
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.94	0.48
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.42	0.48
5:L:507:MET:HG2	5:L:520:GLY:CA	2.43	0.48
3:D:126:LEU:HD13	3:D:223:LEU:HD22	1.95	0.48
3:D:705:THR:OG1	3:D:718:SER:HA	2.13	0.48
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.94	0.48
1:H:192:VAL:HB	1:H:195:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:231:GLU:HG2	2:I:332:ARG:HD3	1.94	0.48
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.53	0.48
2:I:964:LEU:HD11	2:I:1022:LYS:HD2	1.95	0.48
3:J:817:HIS:CD2	3:J:860:ARG:HH21	2.31	0.48
3:J:930:LEU:HD11	3:J:1241:TYR:CZ	2.48	0.48
5:L:246:GLN:HE21	5:L:249:ILE:HD12	1.77	0.48
5:L:532:LEU:HD12	5:L:532:LEU:H	1.77	0.48
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.95	0.48
2:C:402:ARG:NH2	2:C:419:ILE:O	2.47	0.48
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.94	0.48
2:I:818:VAL:HB	2:I:1076:ILE:HD13	1.95	0.48
2:I:1124:ILE:HB	2:I:1180:MET:HB2	1.95	0.48
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.95	0.48
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.94	0.48
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.77	0.48
1:A:44:ARG:HA	1:A:183:ILE:HG21	1.95	0.48
1:B:39:LEU:O	1:B:43:LEU:HD13	2.14	0.48
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.14	0.48
3:D:46:TYR:CD1	5:F:452:ILE:HG22	2.48	0.48
5:F:127:ILE:O	5:F:130:VAL:HG22	2.13	0.48
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.94	0.48
2:I:1085:MET:HA	2:I:1085:MET:HE2	1.95	0.48
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.28	0.48
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.95	0.48
2:C:208:ILE:HD11	2:C:365:GLU:HB3	1.95	0.48
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.95	0.48
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.95	0.48
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.49	0.48
1:H:90:VAL:HG23	1:H:123:ILE:HD13	1.96	0.48
2:I:617:ALA:HA	2:I:636:CYS:SG	2.53	0.48
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.96	0.48
1:B:84:ASN:OD1	3:D:551:ARG:NH2	2.36	0.48
1:B:147:GLN:NE2	1:B:177:TYR:OH	2.45	0.48
2:C:370:MET:HG3	2:C:384:LEU:HD21	1.96	0.48
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.96	0.48
3:D:201:LEU:HD11	3:D:220:ARG:HH11	1.79	0.48
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.95	0.48
3:D:827:GLU:C	3:D:829:GLY:H	2.22	0.48
1:H:37:HIS:NE2	2:I:1216:ARG:HD2	2.28	0.48
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.96	0.48
3:J:557:LYS:HA	3:J:563:LEU:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:316:PHE:HZ	5:L:334:SER:HA	1.79	0.48
5:L:372:ALA:O	5:L:376:LYS:HG3	2.12	0.48
1:B:125:LYS:HE2	1:B:128:HIS:CD2	2.49	0.48
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.96	0.48
1:H:82:LEU:HD13	1:H:173:VAL:HG12	1.96	0.48
3:J:19:ALA:HB2	3:J:1373:ARG:NH2	2.29	0.48
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.49	0.48
2:C:2:VAL:O	2:C:3:TYR:HB2	2.14	0.48
2:C:719:LYS:H	2:C:751:TYR:HH	1.59	0.48
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.95	0.48
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.46	0.48
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.77	0.48
2:I:685:MET:HA	2:I:688:GLN:HE21	1.79	0.48
2:I:692:THR:OG1	2:I:693:LEU:N	2.46	0.48
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.78	0.48
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.96	0.48
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.14	0.48
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.48	0.48
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.28	0.48
1:G:182:ARG:H	1:G:206:GLU:HB3	1.78	0.48
1:H:152:TYR:CZ	3:J:536:LEU:HD21	2.49	0.48
2:I:778:GLU:O	2:I:781:ASP:HB2	2.14	0.48
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.78	0.48
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.44	0.47
3:D:218:THR:HA	3:D:221:ILE:HG22	1.96	0.47
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.96	0.47
3:D:721:SER:HA	3:D:724:MET:HE2	1.96	0.47
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.79	0.47
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.13	0.47
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.49	0.47
2:I:819:SER:HB2	2:I:1085:MET:SD	2.54	0.47
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.96	0.47
3:J:800:LEU:HB3	3:J:920:ALA:CB	2.44	0.47
3:J:1174:ARG:HG2	3:J:1189:MET:SD	2.54	0.47
1:G:10:LYS:HA	1:H:227:GLN:NE2	2.29	0.47
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.23	0.47
2:I:637:ARG:HA	2:I:642:SER:HA	1.95	0.47
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.49	0.47
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.96	0.47
1:A:19:VAL:HG12	1:A:24:ALA:HA	1.96	0.47
1:A:61:ILE:HG22	1:A:62:ASP:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.45	0.47
2:C:1302:THR:HG22	5:F:531:PRO:HB3	1.97	0.47
5:F:276:MET:O	5:F:280:VAL:HG23	2.13	0.47
2:I:860:ALA:O	2:I:863:SER:OG	2.26	0.47
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.29	0.47
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.14	0.47
2:C:468:LEU:O	2:C:471:VAL:HG12	2.14	0.47
3:D:518:VAL:O	3:D:547:ARG:NH1	2.46	0.47
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.72	0.47
5:F:145:LEU:HB3	5:F:225:ARG:HH21	1.80	0.47
2:I:878:THR:OG1	2:I:879:GLY:N	2.43	0.47
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.96	0.47
1:A:56:VAL:HA	1:A:146:VAL:HG22	1.95	0.47
2:C:184:LEU:HB2	2:C:389:PHE:CE1	2.50	0.47
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.49	0.47
3:D:849:LEU:HB3	3:D:853:THR:HG23	1.97	0.47
4:E:13:ILE:HD12	4:E:19:LEU:HA	1.97	0.47
5:F:227:GLN:HG2	5:F:252:LEU:HA	1.97	0.47
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.45	0.47
1:G:45:ARG:NH1	1:H:34:GLY:O	2.48	0.47
1:H:83:LEU:HD11	3:J:526:VAL:CG2	2.45	0.47
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.14	0.47
2:I:1286:THR:N	3:J:479:GLU:OE2	2.46	0.47
3:J:325:LYS:HE2	3:J:330:MET:HA	1.97	0.47
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.96	0.47
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.14	0.47
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.96	0.47
2:I:564:PRO:HG3	2:I:572:ILE:HG13	1.96	0.47
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.96	0.47
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.50	0.47
2:C:557:ARG:HH21	2:C:607:SER:C	2.23	0.47
2:C:580:GLN:HB2	2:C:605:TYR:HE1	1.79	0.47
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.78	0.47
2:C:1268:GLN:OE1	3:D:352:ARG:HG2	2.15	0.47
3:D:546:ALA:O	3:D:573:THR:HA	2.15	0.47
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.97	0.47
3:D:1184:ASP:O	3:D:1186:TYR:N	2.48	0.47
3:D:1227:HIS:CB	3:J:1293:GLU:HG2	2.44	0.47
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.50	0.47
3:D:1347:LEU:HG	3:D:1357:ILE:HG23	1.97	0.47
5:F:139:GLU:HG2	5:F:351:THR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.96	0.47
2:I:387:ASN:HA	2:I:391:SER:HB2	1.97	0.47
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.95	0.47
3:J:98:ARG:HB3	3:J:248:ASP:OD2	2.15	0.47
3:J:592:VAL:HA	3:J:596:LEU:HD21	1.96	0.47
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.96	0.47
3:J:843:VAL:HG11	3:J:897:HIS:O	2.14	0.47
5:L:127:ILE:O	5:L:130:VAL:HG22	2.15	0.47
1:B:89:ALA:O	1:B:124:VAL:HG12	2.15	0.47
2:C:488:MET:O	2:C:490:GLN:N	2.40	0.47
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.46	0.47
3:D:694:SER:OG	3:D:738:ARG:NE	2.48	0.47
5:F:94:THR:HG23	5:F:96:ASP:OD1	2.15	0.47
1:H:183:ILE:HG13	1:H:205:MET:HG3	1.97	0.47
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.96	0.47
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.97	0.47
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.45	0.47
5:L:515:GLU:HG2	5:L:516:ASP:N	2.30	0.47
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.55	0.47
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.80	0.47
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.97	0.47
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.42	0.47
1:A:12:ARG:H	1:A:30:PRO:HD2	1.79	0.47
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.97	0.47
2:C:1109:ILE:HG23	2:C:1113:LEU:HD13	1.96	0.47
3:D:901:ARG:HD2	3:D:906:GLY:O	2.15	0.47
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.30	0.47
3:J:94:GLN:O	3:J:97:VAL:HG23	2.15	0.47
3:J:846:GLU:HA	3:J:860:ARG:HD3	1.97	0.47
3:J:1153:PRO:HA	3:J:1214:PRO:O	2.15	0.47
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.30	0.47
5:L:561:MET:HA	5:L:567:MET:HE1	1.96	0.47
1:B:201:LEU:HG	1:B:203:ILE:HG13	1.96	0.46
2:C:1268:GLN:N	3:D:350:SER:OG	2.38	0.46
2:C:1124:ILE:HG21	2:C:1180:MET:HG3	1.97	0.46
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	1.96	0.46
1:H:16:ILE:HG23	1:H:26:VAL:HG13	1.97	0.46
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.30	0.46
3:J:298:MET:SD	5:L:402:LEU:HB3	2.55	0.46
3:J:741:ALA:O	3:J:762:ASN:ND2	2.48	0.46
1:B:19:VAL:O	1:B:20:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.98	0.46
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.50	0.46
3:D:278:ARG:HD2	3:D:295:GLU:CD	2.40	0.46
3:D:517:CYS:HA	3:D:716:GLN:HE22	1.80	0.46
1:G:188:GLU:O	1:G:200:LYS:N	2.38	0.46
1:G:219:ARG:O	1:G:223:ILE:HG13	2.15	0.46
3:J:1291:GLU:HG2	3:J:1297:LYS:HD3	1.97	0.46
2:C:23:ASP:OD1	2:C:23:ASP:N	2.47	0.46
2:C:314:ASN:O	2:C:352:ARG:NH1	2.41	0.46
2:C:588:GLU:HG3	2:C:605:TYR:HD1	1.79	0.46
2:C:1326:LEU:HD22	3:D:337:ARG:HD3	1.96	0.46
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.97	0.46
3:D:810:THR:HG23	3:D:811:GLU:H	1.80	0.46
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.98	0.46
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.98	0.46
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.47	0.46
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.50	0.46
1:B:57:THR:O	1:B:173:VAL:HG22	2.15	0.46
2:C:169:LYS:O	2:C:169:LYS:HG2	2.14	0.46
2:C:192:ASP:HB3	2:C:346:TYR:CD1	2.50	0.46
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.51	0.46
2:C:739:ASP:OD1	2:C:739:ASP:N	2.48	0.46
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.16	0.46
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.30	0.46
1:H:20:SER:OG	1:H:21:SER:N	2.48	0.46
2:I:310:ILE:HD13	2:I:325:LEU:HA	1.98	0.46
3:J:473:THR:HG23	3:J:476:ALA:H	1.81	0.46
2:C:93:SER:OG	2:C:126:GLU:OE1	2.24	0.46
2:C:801:ARG:HD3	2:C:1094:VAL:HA	1.98	0.46
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.97	0.46
2:I:811:ASN:C	2:I:815:SER:HB2	2.41	0.46
3:J:846:GLU:HA	3:J:860:ARG:CD	2.46	0.46
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.15	0.46
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.80	0.46
1:A:172:LEU:HD12	1:A:172:LEU:H	1.80	0.46
2:C:81:ASP:O	2:C:85:CYS:HB2	2.15	0.46
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.45	0.46
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	2.16	0.46
3:D:1263:LYS:HE2	3:D:1279:GLN:HE21	1.80	0.46
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	1.98	0.46
5:F:245:ALA:O	5:F:249:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:62:TYR:C	2:I:64:GLY:H	2.24	0.46
2:I:212:ALA:HA	2:I:359:ARG:HG3	1.96	0.46
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.27	0.46
3:J:810:THR:HG23	3:J:811:GLU:H	1.81	0.46
2:C:90:VAL:HG12	2:C:91:THR:H	1.81	0.46
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.98	0.46
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.81	0.46
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.51	0.46
3:J:722:ILE:HA	3:J:725:MET:HE3	1.97	0.46
5:L:585:GLU:O	5:L:589:GLN:HG3	2.15	0.46
1:A:49:SER:OG	1:A:50:SER:N	2.47	0.46
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.96	0.46
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	1.96	0.46
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.80	0.46
1:G:10:LYS:HE2	1:H:229:GLU:OE1	2.16	0.46
1:H:55:ALA:HB3	1:H:177:TYR:CD1	2.51	0.46
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.98	0.46
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.98	0.46
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.97	0.46
2:C:891:GLY:O	2:C:892:GLU:HG3	2.16	0.46
2:C:1248:THR:HG21	5:F:531:PRO:CG	2.46	0.46
3:D:141:PHE:HA	3:D:180:MET:HE2	1.98	0.46
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.97	0.46
3:D:1165:PHE:CE1	3:D:1200:GLU:HB3	2.50	0.46
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.46	0.46
2:I:316:GLU:H	2:I:316:GLU:CD	2.24	0.46
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.98	0.46
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.98	0.46
2:C:119:GLU:HB2	2:C:489:PRO:HB2	1.99	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.15	0.45
2:C:548:ARG:O	3:D:780:ARG:NH1	2.49	0.45
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.98	0.45
2:C:1329:GLU:O	2:C:1332:SER:OG	2.33	0.45
3:D:557:LYS:HA	3:D:563:LEU:HA	1.97	0.45
5:F:125:ASP:O	5:F:129:GLN:HG3	2.16	0.45
5:F:164:GLY:O	5:F:260:ARG:HB2	2.16	0.45
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.98	0.45
1:H:84:ASN:ND2	1:H:129:VAL:O	2.49	0.45
1:H:201:LEU:HG	1:H:203:ILE:HG13	1.98	0.45
3:J:122:SER:O	3:J:126:LEU:HG	2.16	0.45
3:J:698:MET:O	3:J:702:GLN:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.98	0.45
3:D:328:ALA:O	3:D:332:LYS:HB2	2.16	0.45
5:F:601:PRO:HA	5:F:604:SER:HB2	1.99	0.45
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	1.98	0.45
3:J:222:LYS:HE2	3:J:1276:GLU:OE1	2.17	0.45
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.99	0.45
2:C:122:VAL:HG21	2:C:493:ILE:HG23	1.98	0.45
2:C:169:LYS:HE2	2:C:190:PRO:O	2.16	0.45
2:C:225:PHE:HZ	2:C:348:SER:H	1.63	0.45
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.98	0.45
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.42	0.45
5:F:499:LYS:HA	5:F:502:LYS:HE2	1.98	0.45
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.99	0.45
2:I:403:MET:HE3	2:I:403:MET:HB3	1.90	0.45
3:J:79:LYS:HB2	5:L:569:THR:H	1.82	0.45
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.81	0.45
5:L:584:ARG:HH11	5:L:584:ARG:HA	1.80	0.45
2:C:169:LYS:O	2:C:170:VAL:HG22	2.16	0.45
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.98	0.45
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.50	0.45
4:E:10:VAL:HG13	4:E:16:ARG:HB2	1.98	0.45
5:F:561:MET:HA	5:F:567:MET:HE1	1.98	0.45
1:G:49:SER:OG	1:G:50:SER:N	2.48	0.45
1:G:172:LEU:HD12	1:G:172:LEU:H	1.81	0.45
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.96	0.45
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.80	0.45
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.81	0.45
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.98	0.45
3:J:614:LEU:HB3	4:K:7:GLN:HG2	1.99	0.45
3:J:827:GLU:O	3:J:829:GLY:N	2.39	0.45
3:J:1183:SER:OG	3:J:1185:PRO:HD3	2.16	0.45
5:L:234:THR:O	5:L:245:ALA:HB2	2.16	0.45
1:A:181:GLU:HB3	1:A:206:GLU:HG3	1.99	0.45
1:A:234:LEU:HD23	1:B:214:GLU:HG3	1.98	0.45
2:I:735:LYS:HA	2:I:748:ILE:HG22	1.99	0.45
3:J:137:ARG:HD3	3:J:143:SER:OG	2.16	0.45
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.98	0.45
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.83	0.45
3:D:555:TYR:HB2	3:D:586:GLY:HA2	1.99	0.45
2:I:1070:HIS:CD2	2:I:1111:GLN:HA	2.51	0.45
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ILE:HG13	1:G:136:GLU:HA	1.98	0.45
1:G:189:ALA:HA	1:G:199:ASP:HA	1.98	0.45
1:H:181:GLU:HA	3:J:535:ARG:HH21	1.81	0.45
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.97	0.45
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.99	0.45
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.16	0.45
5:L:433:TRP:O	5:L:437:GLN:HB3	2.16	0.45
1:A:162:GLU:HG3	1:A:165:GLU:HG2	1.99	0.45
1:B:186:ASN:HD22	1:B:202:VAL:HB	1.81	0.45
2:C:55:SER:OG	2:C:56:VAL:N	2.49	0.45
2:C:453:ILE:HD13	2:C:530:ILE:HD12	1.99	0.45
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.98	0.45
2:C:1085:MET:HE2	2:C:1085:MET:HA	1.99	0.45
3:D:252:LEU:HD23	3:D:262:THR:HB	1.99	0.45
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	1.99	0.45
5:F:466:ILE:HB	5:F:483:LEU:HD23	1.98	0.45
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.67	0.45
2:I:871:VAL:O	2:I:944:ARG:NH1	2.50	0.45
3:J:365:GLN:HA	3:J:438:GLU:H	1.81	0.45
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.31	0.45
5:L:601:PRO:HB2	5:L:605:GLU:HG2	1.98	0.45
1:A:41:ASN:ND2	2:C:1216:ARG:O	2.47	0.45
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.98	0.45
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.49	0.45
2:C:138:ILE:HG22	2:C:139:ASN:N	2.32	0.45
2:C:996:ARG:HA	2:C:996:ARG:HD3	1.58	0.45
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.30	0.45
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.99	0.45
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.99	0.45
2:I:409:LEU:HD21	2:I:428:VAL:HA	1.97	0.45
2:I:896:THR:HB	2:I:897:PRO:HD2	1.99	0.45
3:J:525:MET:O	3:J:548:VAL:HG13	2.16	0.45
5:L:101:TYR:O	5:L:104:GLU:N	2.50	0.45
1:A:90:VAL:HG22	1:A:91:ARG:H	1.82	0.45
1:B:125:LYS:HE2	1:B:128:HIS:HD2	1.82	0.45
1:B:153:VAL:H	1:B:175:ALA:HB3	1.82	0.45
3:D:40:LYS:HB2	3:D:54:ASP:O	2.17	0.45
3:D:1167:LYS:HZ1	3:D:1170:LYS:HB2	1.82	0.45
5:F:296:LYS:HD3	5:F:296:LYS:HA	1.81	0.45
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.99	0.45
1:G:19:VAL:HG13	1:G:20:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1296:ASP:HB3	2:I:1320:PRO:HB3	1.98	0.45
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.98	0.45
3:J:847:ASP:OD1	3:J:847:ASP:N	2.31	0.45
3:D:827:GLU:O	3:D:829:GLY:N	2.38	0.44
1:G:90:VAL:HG22	1:G:91:ARG:H	1.81	0.44
2:I:466:VAL:O	2:I:469:VAL:HG22	2.16	0.44
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.69	0.44
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.98	0.44
5:L:251:LYS:HA	5:L:254:GLU:HG2	1.99	0.44
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.99	0.44
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.98	0.44
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.48	0.44
5:F:96:ASP:O	5:F:98:VAL:N	2.50	0.44
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.44
3:J:362:ARG:H	3:J:365:GLN:HE21	1.64	0.44
3:J:546:ALA:O	3:J:573:THR:HA	2.17	0.44
5:L:94:THR:OG1	5:L:95:THR:N	2.49	0.44
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.99	0.44
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.67	0.44
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.82	0.44
3:D:19:ALA:O	3:D:20:ILE:HG13	2.18	0.44
3:D:820:ILE:HG22	3:D:1227:HIS:HD1	1.83	0.44
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.81	0.44
5:F:145:LEU:HB3	5:F:225:ARG:NH2	2.31	0.44
5:F:571:TYR:CD1	5:F:575:GLU:HG2	2.53	0.44
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.98	0.44
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.17	0.44
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.32	0.44
2:I:739:ASP:OD1	2:I:739:ASP:N	2.49	0.44
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.98	0.44
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.99	0.44
2:C:149:LEU:HD12	2:C:452:ARG:O	2.17	0.44
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	2.00	0.44
3:D:26:SER:HA	3:D:236:TRP:CD1	2.53	0.44
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.98	0.44
2:I:389:PHE:HD1	2:I:395:TYR:CE1	2.36	0.44
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.99	0.44
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.52	0.44
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.32	0.44
2:C:835:GLU:OE2	2:C:1051:LYS:HD3	2.18	0.44
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:557:ARG:HH21	2:I:607:SER:C	2.26	0.44
3:J:123:ARG:HD2	3:J:1337:VAL:HG11	1.99	0.44
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.46	0.44
1:B:12:ARG:O	1:B:30:PRO:HD3	2.18	0.44
1:B:16:ILE:HG23	1:B:26:VAL:HG22	2.00	0.44
1:B:20:SER:OG	1:B:21:SER:N	2.50	0.44
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.99	0.44
3:D:581:MET:HE2	3:D:581:MET:HB3	1.88	0.44
3:D:885:VAL:HG12	3:D:894:VAL:HG11	2.00	0.44
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.77	0.44
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.99	0.44
3:J:805:GLN:OE1	3:J:1348:LYS:HD3	2.18	0.44
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.47	0.44
5:L:281:ARG:O	5:L:285:ARG:HG3	2.18	0.44
5:L:585:GLU:HA	5:L:588:ARG:HD3	1.98	0.44
5:L:603:ARG:H	5:L:603:ARG:HG2	1.60	0.44
1:B:101:THR:O	1:B:116:THR:HG22	2.18	0.44
1:B:154:PRO:HA	1:B:174:ASP:HB3	1.99	0.44
1:B:211:ILE:HD13	1:B:211:ILE:HA	1.88	0.44
2:C:805:MET:HE1	2:C:1221:PHE:CE2	2.53	0.44
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.83	0.44
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.98	0.44
3:D:682:VAL:O	3:D:685:ILE:HG12	2.18	0.44
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.53	0.44
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.18	0.44
3:J:544:LEU:O	3:J:574:VAL:HB	2.18	0.44
3:J:804:ALA:HA	3:J:1259:GLN:HE21	1.83	0.44
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.99	0.44
5:L:479:THR:HG22	5:L:482:GLU:HB2	2.00	0.44
1:A:218:ARG:HG3	1:B:231:PHE:O	2.18	0.44
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.83	0.44
1:B:187:VAL:HG13	1:B:199:ASP:HB3	1.99	0.44
2:C:4:SER:HB2	2:C:7:GLU:HG3	1.99	0.44
2:C:15:PHE:CE1	2:C:1151:LEU:HD13	2.53	0.44
2:C:615:VAL:HG13	2:C:651:ASP:H	1.83	0.44
3:D:334:LYS:HA	3:D:335:GLN:HA	1.47	0.44
5:F:512:GLY:C	5:F:514:ASP:H	2.25	0.44
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.99	0.44
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.85	0.44
3:J:262:THR:C	5:L:507:MET:HB2	2.42	0.44
2:C:577:VAL:HG23	2:C:661:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1178:LYS:HA	2:C:1178:LYS:HD3	1.78	0.44
5:F:612:ASP:OD1	5:F:612:ASP:N	2.47	0.44
1:H:107:ILE:HG12	1:H:134:THR:O	2.18	0.44
2:I:24:VAL:HG21	2:I:704:MET:SD	2.58	0.44
2:I:27:LEU:O	2:I:528:ARG:NH1	2.47	0.44
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.16	0.44
5:L:247:GLU:O	5:L:251:LYS:HG3	2.18	0.44
5:L:572:THR:HG23	5:L:575:GLU:HB2	2.00	0.44
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.99	0.43
2:C:62:TYR:C	2:C:64:GLY:H	2.25	0.43
5:F:105:MET:HE2	5:F:105:MET:HB2	1.92	0.43
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.33	0.43
2:I:976:ARG:HD2	2:I:989:LEU:HD23	2.00	0.43
3:J:218:THR:HA	3:J:221:ILE:HG22	2.00	0.43
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.18	0.43
1:A:28:LEU:HB2	1:A:201:LEU:HB3	1.99	0.43
2:C:980:VAL:HA	2:C:984:VAL:HA	2.00	0.43
2:C:1086:PRO:HB2	2:C:1212:LEU:HD23	1.99	0.43
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.82	0.43
3:D:320:ASN:OD1	3:D:322:ARG:HB3	2.18	0.43
1:G:145:LYS:HE3	1:G:145:LYS:HB3	1.88	0.43
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.58	0.43
3:J:748:ALA:HA	3:J:754:ILE:HA	2.00	0.43
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.99	0.43
5:L:96:ASP:O	5:L:98:VAL:N	2.51	0.43
1:A:56:VAL:HG11	1:A:85:LEU:HB3	1.99	0.43
2:C:1132:LEU:HD11	2:C:1174:GLU:HG2	2.00	0.43
3:D:189:LEU:HD22	3:D:234:PRO:HB3	2.01	0.43
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.68	0.43
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.75	0.43
1:G:36:GLY:C	1:G:187:VAL:HG11	2.43	0.43
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.83	0.43
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.33	0.43
2:I:138:ILE:HG22	2:I:139:ASN:N	2.33	0.43
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	2.00	0.43
3:J:583:VAL:HG21	3:J:592:VAL:HG11	2.00	0.43
5:L:348:GLU:HG2	5:L:354:THR:HA	1.99	0.43
5:L:533:ASP:O	5:L:536:THR:N	2.48	0.43
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.52	0.43
2:C:867:GLU:H	2:C:867:GLU:HG3	1.53	0.43
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.81	0.43
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.43
3:D:931:THR:O	3:D:931:THR:OG1	2.34	0.43
5:F:499:LYS:HB2	5:F:499:LYS:HE3	1.84	0.43
1:H:13:LEU:HD23	1:H:13:LEU:H	1.82	0.43
2:I:91:THR:HG21	2:I:503:LYS:NZ	2.33	0.43
2:I:548:ARG:HB3	2:I:569:ILE:O	2.18	0.43
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.18	0.43
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.18	0.43
3:J:291:ILE:HG12	5:L:409:ASN:HD22	1.83	0.43
5:L:582:VAL:O	5:L:587:ILE:HD12	2.18	0.43
2:C:146:VAL:HG13	2:C:529:ARG:HB3	2.00	0.43
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.66	0.43
3:D:102:MET:HE2	3:D:102:MET:HB3	1.96	0.43
5:F:391:ALA:HB3	5:F:405:ILE:HG22	2.00	0.43
5:F:394:TYR:HB2	5:F:404:LEU:HD13	2.00	0.43
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.34	0.43
3:J:604:MET:HE3	3:J:604:MET:HB2	1.86	0.43
3:J:740:LEU:HD12	3:J:740:LEU:HA	1.74	0.43
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.16	0.43
1:B:212:ASP:OD2	1:B:215:GLU:HB2	2.18	0.43
2:C:629:PHE:HE2	2:C:650:VAL:HG21	1.80	0.43
3:D:128:LEU:HA	3:D:192:MET:HE1	1.99	0.43
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	2.01	0.43
3:J:56:LEU:HD12	3:J:56:LEU:H	1.82	0.43
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.33	0.43
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.01	0.43
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.53	0.43
2:C:992:LEU:H	2:C:992:LEU:HD23	1.84	0.43
5:F:354:THR:O	5:F:358:VAL:HG23	2.18	0.43
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.53	0.43
2:I:115:LYS:HG3	2:I:485:ASP:OD2	2.17	0.43
2:I:168:GLY:C	2:I:170:VAL:N	2.76	0.43
3:J:317:THR:HG22	3:J:322:ARG:O	2.19	0.43
4:K:15:ASN:O	4:K:16:ARG:HB3	2.17	0.43
1:A:19:VAL:HG13	1:A:20:SER:H	1.83	0.43
1:B:31:LEU:HB2	1:B:199:ASP:O	2.19	0.43
2:C:318:SER:OG	2:C:320:ASP:OD2	2.32	0.43
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.54	0.43
2:C:1160:ASP:HB2	2:C:1163:THR:OG1	2.18	0.43
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.87	0.43
5:F:244:THR:O	5:F:247:GLU:HG2	2.18	0.43
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.84	0.43
2:I:15:PHE:CG	2:I:1190:ALA:HB2	2.54	0.43
2:I:150:HIS:CD2	2:I:454:ARG:HE	2.36	0.43
2:I:618:GLN:HG3	2:I:620:ASN:H	1.84	0.43
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.54	0.43
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.75	0.43
2:I:1077:SER:HA	3:J:356:THR:OG1	2.18	0.43
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.48	0.43
3:J:521:LYS:HE3	3:J:541:LEU:O	2.19	0.43
1:A:40:GLY:HA3	1:A:185:TYR:CD2	2.54	0.43
1:A:47:LEU:O	1:A:180:VAL:HG21	2.18	0.43
1:A:48:LEU:HA	1:A:180:VAL:HG21	2.01	0.43
1:B:28:LEU:HD23	1:B:31:LEU:HD11	2.00	0.43
2:C:98:VAL:C	2:C:121:GLU:HA	2.43	0.43
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.84	0.43
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.99	0.43
1:G:225:ALA:HB2	1:H:228:LEU:HD12	2.01	0.43
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.00	0.43
3:J:646:ILE:H	3:J:646:ILE:HG12	1.64	0.43
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.53	0.43
5:L:519:LEU:HD23	5:L:523:ILE:HD11	2.01	0.43
2:C:840:SER:O	2:C:1047:LEU:N	2.49	0.43
1:G:35:PHE:HE1	1:H:46:ILE:HG23	1.84	0.43
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.54	0.43
1:G:74:VAL:HG22	1:G:76:GLU:H	1.84	0.43
2:I:165:HIS:CD2	2:I:190:PRO:HG2	2.54	0.43
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.54	0.43
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.32	0.43
2:I:484:LEU:CD1	2:I:485:ASP:H	2.32	0.43
2:I:811:ASN:HB2	2:I:1099:ASN:HB2	2.01	0.43
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.49	0.43
3:J:264:ASP:HB3	3:J:324:LEU:HB2	2.01	0.43
1:A:201:LEU:HG	1:A:203:ILE:HG13	2.01	0.42
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.99	0.42
5:F:231:THR:HG23	5:F:249:ILE:HG12	2.00	0.42
5:F:580:PHE:HD1	5:F:580:PHE:HA	1.66	0.42
1:H:14:VAL:HG13	1:H:15:ASP:N	2.34	0.42
1:H:51:MET:O	1:H:150:ARG:HA	2.19	0.42
2:I:1038:GLN:O	2:I:1038:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.39	0.42
3:J:709:ARG:C	3:J:711:GLY:N	2.77	0.42
3:J:925:GLU:HB3	3:J:926:PRO:HD3	2.01	0.42
3:J:1241:TYR:HD2	3:J:1246:VAL:HG11	1.83	0.42
2:C:15:PHE:CE1	2:C:1194:GLU:HB3	2.54	0.42
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.19	0.42
2:C:719:LYS:N	2:C:751:TYR:OH	2.35	0.42
2:C:782:VAL:HG11	2:C:792:GLY:HA2	2.01	0.42
2:C:1142:ARG:HD3	2:C:1161:LEU:CD1	2.49	0.42
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.54	0.42
3:D:425:ARG:HD2	3:D:459:ALA:HB2	2.00	0.42
5:F:532:LEU:HD12	5:F:532:LEU:H	1.84	0.42
5:F:562:ARG:HH21	5:F:573:LEU:HD22	1.83	0.42
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.91	0.42
1:G:166:ARG:N	1:G:167:PRO:HD2	2.34	0.42
2:I:292:ILE:HD12	2:I:322:LEU:HD11	2.01	0.42
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	2.00	0.42
2:C:165:HIS:CD2	2:C:190:PRO:HG2	2.55	0.42
2:C:488:MET:C	2:C:490:GLN:H	2.25	0.42
2:C:490:GLN:HG2	2:C:491:ASP:N	2.33	0.42
2:C:906:PHE:CZ	5:F:608:ARG:HG3	2.54	0.42
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.54	0.42
3:D:1198:VAL:HG11	3:D:1210:ILE:HG23	2.00	0.42
4:E:8:ASP:HB2	4:E:55:GLU:HG2	2.01	0.42
2:I:402:ARG:HG2	2:I:416:GLY:H	1.84	0.42
2:I:891:GLY:O	2:I:892:GLU:HG3	2.19	0.42
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.91	0.42
1:A:153:VAL:HB	1:A:175:ALA:HB3	2.00	0.42
1:B:89:ALA:HB1	1:B:210:THR:CG2	2.47	0.42
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.01	0.42
3:D:1151:LYS:C	3:D:1153:PRO:HD3	2.44	0.42
1:G:44:ARG:HG3	1:G:183:ILE:HG22	2.01	0.42
1:G:79:LEU:HD11	2:I:693:LEU:HD21	2.01	0.42
2:I:494:ASN:HB3	2:I:497:PRO:HD2	2.00	0.42
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	2.00	0.42
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.83	0.42
3:J:746:LEU:HB2	3:J:754:ILE:HD11	2.01	0.42
3:J:850:LYS:HB3	3:J:851:PRO:HD2	2.01	0.42
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.54	0.42
2:C:24:VAL:HG21	2:C:704:MET:SD	2.59	0.42
3:D:11:GLN:CG	3:D:15:GLU:HG3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:592:VAL:HA	3:D:596:LEU:HD21	2.01	0.42
5:F:593:LYS:HA	5:F:596:ARG:HB3	2.02	0.42
1:G:137:ASN:OD1	1:G:137:ASN:N	2.51	0.42
1:H:56:VAL:HG22	1:H:146:VAL:HG22	2.01	0.42
2:I:101:ARG:HE	2:I:118:LYS:HD2	1.83	0.42
2:I:981:ALA:O	2:I:1002:LEU:HD11	2.19	0.42
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	2.02	0.42
3:J:42:GLU:OE1	3:J:42:GLU:N	2.52	0.42
3:J:192:MET:HE2	3:J:197:GLU:OE2	2.19	0.42
3:J:405:GLU:O	3:J:408:VAL:HG22	2.20	0.42
2:C:211:ARG:NH1	2:C:357:ASN:O	2.52	0.42
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.02	0.42
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.32	0.42
1:H:90:VAL:HG22	1:H:91:ARG:H	1.84	0.42
2:I:169:LYS:O	2:I:170:VAL:HG22	2.19	0.42
2:I:522:SER:O	2:I:525:THR:HG22	2.20	0.42
2:I:1178:LYS:HA	2:I:1178:LYS:HD3	1.81	0.42
3:J:364:HIS:CD2	4:K:4:VAL:HG23	2.55	0.42
3:J:514:THR:OG1	3:J:594:GLN:O	2.35	0.42
3:J:849:LEU:HD13	3:J:849:LEU:H	1.84	0.42
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	2.02	0.42
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.55	0.42
5:L:130:VAL:HB	5:L:365:MET:HG3	2.01	0.42
2:C:175:ARG:HD3	2:C:183:TRP:CE3	2.55	0.42
2:C:496:LYS:HB3	2:C:496:LYS:HE3	1.80	0.42
2:C:1269:ARG:CG	3:D:343:LEU:HD12	2.50	0.42
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.83	0.42
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	2.02	0.42
5:F:292:VAL:HG21	5:F:299:LYS:HG2	2.02	0.42
1:H:74:VAL:HG22	1:H:133:LEU:HD12	2.02	0.42
2:I:176:ILE:HB	2:I:184:LEU:HB3	2.02	0.42
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.84	0.42
3:J:77:ARG:HG3	3:J:79:LYS:H	1.85	0.42
5:L:476:ARG:HG3	5:L:477:GLU:N	2.34	0.42
1:A:10:LYS:HA	1:B:227:GLN:NE2	2.35	0.42
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.53	0.42
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.20	0.42
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.50	0.42
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.85	0.42
2:I:448:LEU:HG	2:I:553:THR:OG1	2.20	0.42
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	2.01	0.42
3:J:824:PRO:HD3	3:J:835:LEU:HD13	2.02	0.42
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	2.01	0.42
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.20	0.42
1:A:232:VAL:O	1:B:218:ARG:HG2	2.20	0.42
1:B:180:VAL:HB	1:B:183:ILE:CD1	2.49	0.42
2:C:75:LEU:HD13	2:C:75:LEU:HA	1.85	0.42
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.86	0.42
2:C:184:LEU:HD13	2:C:389:PHE:CZ	2.55	0.42
2:C:448:LEU:HD23	2:C:448:LEU:HA	1.87	0.42
2:C:842:ASP:N	2:C:1045:GLY:O	2.53	0.42
2:C:1023:HIS:O	2:C:1027:LYS:HG2	2.20	0.42
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	2.02	0.42
5:F:493:LYS:HA	5:F:496:LYS:HE2	2.02	0.42
1:G:13:LEU:HD22	1:H:231:PHE:CE1	2.55	0.42
3:J:416:ILE:HG12	3:J:441:LEU:HD21	2.01	0.42
3:J:425:ARG:HG2	3:J:426:ALA:H	1.84	0.42
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.61	0.42
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.35	0.42
4:K:22:VAL:HG11	4:K:60:ASN:HA	2.02	0.42
2:C:292:ILE:HB	2:C:322:LEU:HD11	2.02	0.42
3:D:75:TYR:CE2	3:D:83:VAL:HG21	2.54	0.42
3:D:733:SER:O	3:D:737:ILE:HG12	2.20	0.42
5:F:412:LEU:HB2	5:F:435:ILE:HD11	2.01	0.42
2:I:256:GLU:HB3	2:I:261:VAL:HG22	2.02	0.42
2:I:757:THR:HG23	2:I:765:ILE:HG23	2.02	0.42
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.01	0.42
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.51	0.42
2:C:10:ARG:NH2	2:C:791:LEU:HB2	2.33	0.41
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.35	0.41
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.41
2:I:867:GLU:H	2:I:867:GLU:HG3	1.70	0.41
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.35	0.41
3:J:27:PRO:HB3	3:J:241:VAL:HG23	2.00	0.41
3:J:528:THR:O	3:J:551:ARG:HB3	2.20	0.41
3:J:712:GLN:CD	3:J:712:GLN:H	2.27	0.41
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.77	0.41
3:D:646:ILE:H	3:D:646:ILE:HG12	1.62	0.41
3:D:1183:SER:OG	3:D:1185:PRO:HD3	2.20	0.41
1:G:14:VAL:HG12	1:G:27:THR:O	2.19	0.41
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HH11	1:B:38:THR:HG1	1.68	0.41
1:A:91:ARG:HD3	1:A:210:THR:O	2.20	0.41
2:C:198:ILE:HD13	2:C:388:LEU:HD13	2.01	0.41
2:C:820:GLU:HA	2:C:1079:ILE:HD11	2.01	0.41
3:D:487:THR:HG21	4:E:4:VAL:HG23	2.03	0.41
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.20	0.41
3:D:650:LYS:HE2	3:D:654:ILE:HD11	2.03	0.41
3:D:708:ASN:OD1	3:D:708:ASN:N	2.48	0.41
3:D:801:VAL:O	3:D:805:GLN:HB2	2.19	0.41
3:D:926:PRO:HG2	3:D:1248:ILE:HD11	2.02	0.41
5:F:569:THR:OG1	5:F:570:ASP:N	2.52	0.41
1:H:101:THR:H	1:H:116:THR:CG2	2.33	0.41
2:I:870:ILE:HG21	2:I:931:VAL:HG11	2.03	0.41
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.54	0.41
3:J:596:LEU:HD12	3:J:601:ILE:HG13	2.02	0.41
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.32	0.41
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.36	0.41
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.55	0.41
5:L:499:LYS:HA	5:L:502:LYS:HE2	2.01	0.41
2:C:5:TYR:CE2	2:C:776:PRO:HB2	2.54	0.41
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	2.02	0.41
2:C:1063:GLY:HA3	2:C:1239:VAL:HB	2.02	0.41
3:D:264:ASP:HB3	3:D:324:LEU:HB2	2.02	0.41
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	2.53	0.41
1:G:169:GLY:O	1:G:171:LEU:HD22	2.20	0.41
2:I:462:ASN:O	2:I:466:VAL:HG23	2.21	0.41
2:I:1219:GLU:OE2	3:J:634:ARG:NE	2.53	0.41
2:I:1271:GLY:HA2	3:J:344:GLY:HA3	2.02	0.41
1:A:145:LYS:HB3	1:A:145:LYS:HE3	1.90	0.41
2:C:145:ILE:HA	2:C:511:LEU:O	2.21	0.41
2:C:158:ASP:CG	2:C:159:SER:H	2.28	0.41
2:C:180:ARG:NH2	2:C:465:ARG:HH22	2.18	0.41
3:D:609:TYR:HD1	3:D:610:ARG:HH11	1.68	0.41
3:D:698:MET:O	3:D:702:GLN:HB3	2.20	0.41
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	2.20	0.41
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.20	0.41
3:J:1224:ARG:HB3	3:J:1228:ALA:CB	2.50	0.41
5:L:111:LEU:HA	5:L:111:LEU:HD23	1.78	0.41
1:A:118:ASP:H	1:A:121:VAL:HB	1.86	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
2:C:808:ASN:H	3:D:633:ALA:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.35	0.41
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.21	0.41
3:D:310:GLY:HA2	3:D:314:ARG:HG2	2.03	0.41
1:H:37:HIS:NE2	1:H:187:VAL:HG21	2.35	0.41
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.34	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.03	0.41
3:J:474:LEU:HA	3:J:477:GLN:HG3	2.03	0.41
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.75	0.41
1:B:64:VAL:HG11	1:B:69:SER:HB2	2.03	0.41
2:C:97:ARG:HB3	2:C:121:GLU:HB2	2.02	0.41
2:C:981:ALA:O	2:C:1002:LEU:HD11	2.21	0.41
3:D:646:ILE:HD11	3:D:764:ARG:HD2	2.02	0.41
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.19	0.41
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.75	0.41
1:H:107:ILE:HG13	1:H:136:GLU:O	2.20	0.41
2:I:21:VAL:HG13	2:I:655:VAL:HG13	2.02	0.41
2:I:60:GLN:O	2:I:476:LYS:HE2	2.20	0.41
2:I:62:TYR:O	2:I:64:GLY:N	2.53	0.41
2:I:81:ASP:O	2:I:85:CYS:HB2	2.20	0.41
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.86	0.41
2:I:387:ASN:O	2:I:394:ARG:HB2	2.20	0.41
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.91	0.41
2:I:468:LEU:O	2:I:471:VAL:HG12	2.21	0.41
2:I:732:ILE:O	2:I:751:TYR:N	2.41	0.41
3:J:510:LEU:HA	3:J:513:MET:HB2	2.03	0.41
3:J:594:GLN:HG3	3:J:596:LEU:HD22	2.03	0.41
3:J:1357:ILE:C	3:J:1359:ALA:H	2.28	0.41
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.71	0.41
5:L:606:VAL:HG13	5:L:607:LEU:HD12	2.02	0.41
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.55	0.41
1:A:177:TYR:O	1:A:178:SER:HB2	2.20	0.41
2:C:61:SER:HB3	2:C:479:LEU:CB	2.50	0.41
2:C:409:LEU:HD23	2:C:409:LEU:HA	1.92	0.41
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.56	0.41
3:D:474:LEU:HD12	3:D:474:LEU:HA	1.96	0.41
5:F:281:ARG:O	5:F:285:ARG:HG3	2.21	0.41
5:F:556:ALA:O	5:F:560:ARG:HG3	2.21	0.41
1:G:113:ALA:HB2	1:G:126:PRO:HB3	2.03	0.41
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.02	0.41
3:J:578:ILE:HG21	3:J:631:TYR:OH	2.21	0.41
4:K:35:LYS:NZ	4:K:71:GLU:OE2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:227:GLN:CG	5:L:252:LEU:HA	2.50	0.41
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.76	0.41
5:L:569:THR:OG1	5:L:570:ASP:N	2.53	0.41
1:A:19:VAL:HG11	1:A:23:HIS:CE1	2.56	0.41
1:B:42:ALA:O	1:B:46:ILE:HG13	2.21	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.02	0.41
2:C:202:ARG:H	2:C:202:ARG:HG3	1.65	0.41
2:C:231:GLU:O	2:C:238:GLN:N	2.54	0.41
2:C:379:GLU:CD	2:C:379:GLU:H	2.29	0.41
2:C:494:ASN:HB3	2:C:497:PRO:HD2	2.02	0.41
2:C:560:PRO:HB3	3:D:776:THR:HG21	2.03	0.41
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.56	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.90	0.41
3:D:591:ILE:HG23	3:D:604:MET:HE2	2.01	0.41
3:D:697:MET:O	3:D:701:LEU:HB2	2.20	0.41
3:D:1246:VAL:HG12	3:D:1248:ILE:HG13	2.03	0.41
3:D:1266:ILE:HB	3:D:1274:PHE:O	2.21	0.41
5:F:394:TYR:CD2	5:F:439:ILE:HG21	2.56	0.41
1:G:222:THR:OG1	1:H:232:VAL:O	2.26	0.41
1:H:47:LEU:HA	1:H:47:LEU:HD23	1.87	0.41
1:H:57:THR:HG21	1:H:158:ARG:HH21	1.85	0.41
1:H:113:ALA:HB2	1:H:126:PRO:HB3	2.02	0.41
2:I:23:ASP:OD1	2:I:23:ASP:N	2.49	0.41
2:I:658:GLN:O	2:I:661:VAL:HG22	2.21	0.41
2:I:854:ILE:HB	2:I:857:VAL:HG21	2.02	0.41
2:I:1232:MET:HE2	2:I:1232:MET:HB3	1.94	0.41
3:J:403:ARG:HB3	3:J:405:GLU:HG3	2.03	0.41
3:J:481:ARG:NH1	4:K:3:ARG:O	2.54	0.41
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.36	0.41
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.86	0.41
2:C:696:ASP:HB3	2:C:697:LYS:H	1.67	0.41
3:D:93:THR:HG22	3:D:94:GLN:H	1.85	0.41
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.56	0.41
3:D:925:GLU:HB3	3:D:926:PRO:HD3	2.03	0.41
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.20	0.41
4:E:15:ASN:OD1	4:E:17:PHE:HB2	2.21	0.41
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.02	0.41
5:F:533:ASP:O	5:F:536:THR:N	2.54	0.41
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.50	0.41
2:I:724:VAL:HG13	2:I:734:ILE:HD13	2.02	0.41
3:J:161:THR:HG22	3:J:164:GLN:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:849:LEU:HB3	3:J:853:THR:HG23	2.03	0.41
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.54	0.41
1:B:127:GLN:O	1:B:127:GLN:HG2	2.21	0.40
2:C:149:LEU:O	2:C:532:ALA:HA	2.20	0.40
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.56	0.40
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.62	0.40
3:D:850:LYS:HG2	3:D:857:LEU:HD23	2.03	0.40
5:F:372:ALA:O	5:F:376:LYS:HG3	2.20	0.40
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.94	0.40
2:I:591:TYR:CA	2:I:655:VAL:HG23	2.51	0.40
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.35	0.40
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.88	0.40
5:L:426:LYS:HE2	5:L:428:SER:OG	2.21	0.40
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.84	0.40
2:C:34:SER:OG	2:C:457:GLY:N	2.52	0.40
2:C:62:TYR:O	2:C:64:GLY:N	2.53	0.40
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.92	0.40
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.56	0.40
3:D:1227:HIS:HA	3:D:1230:THR:HG22	2.03	0.40
5:F:470:MET:HE2	5:F:486:ARG:HH12	1.86	0.40
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.20	0.40
1:G:61:ILE:HG22	1:G:62:ASP:H	1.86	0.40
1:H:156:SER:C	1:H:158:ARG:H	2.28	0.40
2:I:138:ILE:HB	2:I:143:ARG:HD3	2.03	0.40
2:I:518:ASN:O	2:I:691:PRO:HD3	2.21	0.40
2:I:819:SER:HB2	2:I:1085:MET:CG	2.51	0.40
3:J:369:PRO:HB3	3:J:444:GLY:O	2.21	0.40
4:K:50:ALA:O	4:K:54:ILE:HG12	2.21	0.40
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.84	0.40
2:C:953:LEU:HD12	2:C:953:LEU:HA	1.84	0.40
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.51	0.40
3:D:660:GLU:O	3:D:664:ILE:HG12	2.20	0.40
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.02	0.40
1:H:219:ARG:O	1:H:222:THR:HB	2.22	0.40
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.85	0.40
3:J:79:LYS:HG3	3:J:80:HIS:N	2.36	0.40
3:J:102:MET:HE2	3:J:102:MET:HB3	1.94	0.40
3:J:805:GLN:CD	3:J:1348:LYS:HD3	2.46	0.40
1:B:61:ILE:HG23	1:B:142:MET:HE2	2.04	0.40
1:B:83:LEU:HD11	3:D:526:VAL:HG23	2.04	0.40
2:C:149:LEU:HD13	2:C:453:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.20	0.40
2:C:1305:TYR:HE1	3:D:379:PRO:HG3	1.86	0.40
3:D:625:MET:HE2	3:D:625:MET:HB3	1.98	0.40
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.03	0.40
3:D:1160:SER:HA	3:D:1204:VAL:O	2.22	0.40
1:H:118:ASP:H	1:H:121:VAL:HB	1.87	0.40
2:I:69:GLN:HG3	2:I:101:ARG:HB3	2.03	0.40
2:I:149:LEU:O	2:I:532:ALA:HA	2.22	0.40
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.21	0.40
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.56	0.40
3:J:342:LEU:HA	3:J:343:LEU:HA	1.63	0.40
3:J:484:MET:HE2	3:J:484:MET:HB3	1.89	0.40
3:J:513:MET:O	3:J:575:GLY:HA3	2.22	0.40
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.47	0.40
1:B:102:LEU:HD23	1:B:115:ILE:HG12	2.03	0.40
1:B:102:LEU:HD11	1:B:110:VAL:HG11	2.03	0.40
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.40	0.40
2:C:239:MET:O	2:C:284:LEU:HD12	2.21	0.40
2:C:564:PRO:HG3	2:C:572:ILE:HG13	2.02	0.40
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.69	0.40
3:D:11:GLN:HG3	3:D:13:LYS:H	1.87	0.40
3:D:248:ASP:O	3:D:251:PRO:HG3	2.21	0.40
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.04	0.40
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.93	0.40
5:F:486:ARG:CZ	5:F:486:ARG:HB2	2.52	0.40
1:H:62:ASP:HB2	1:H:141:SER:O	2.22	0.40
2:I:681:MET:HE2	2:I:681:MET:HB3	2.00	0.40
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.86	0.40
3:J:557:LYS:HE3	3:J:557:LYS:HB2	1.86	0.40
3:J:598:LYS:HD2	3:J:729:GLY:O	2.21	0.40
3:J:658:GLU:O	3:J:661:VAL:HG13	2.22	0.40
3:J:891:ASP:HB3	3:J:1281:GLU:HG3	2.03	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%)	193 (86%)	28 (12%)	4 (2%)	6	34
1	B	210/329 (64%)	182 (87%)	23 (11%)	5 (2%)	4	29
1	G	222/329 (68%)	191 (86%)	27 (12%)	4 (2%)	6	34
1	H	211/329 (64%)	183 (87%)	22 (10%)	6 (3%)	4	27
2	C	1340/1342 (100%)	1230 (92%)	102 (8%)	8 (1%)	21	56
2	I	1338/1342 (100%)	1234 (92%)	98 (7%)	6 (0%)	30	65
3	D	1162/1407 (83%)	1069 (92%)	86 (7%)	7 (1%)	21	56
3	J	1151/1407 (82%)	1058 (92%)	84 (7%)	9 (1%)	16	50
4	E	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	425 (92%)	36 (8%)	1 (0%)	43	75
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	43	75
All	All	6948/8222 (84%)	6343 (91%)	554 (8%)	51 (1%)	18	53

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	13	LEU
2	C	1159	VAL
3	D	332	LYS
1	H	20	SER
2	I	1159	VAL
3	J	332	LYS
3	J	334	LYS
1	A	162	GLU
1	A	167	PRO
1	B	20	SER
2	C	3	TYR
2	C	170	VAL
3	D	10	ALA
1	G	167	PRO
2	I	170	VAL
3	J	340	GLN
1	B	136	GLU
2	C	697	LYS

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Mol	Chain	Res	Type
3	J	337	ARG
1	A	62	ASP
1	G	14	VAL
1	G	162	GLU
1	H	135	ASP
1	H	136	GLU
1	H	138	ALA
1	H	157	THR
2	I	484	LEU
2	I	697	LYS
3	J	710	ASP
1	A	14	VAL
1	B	138	ALA
2	C	484	LEU
3	D	710	ASP
1	G	62	ASP
1	H	62	ASP
3	J	344	GLY
1	B	14	VAL
2	C	1158	LYS
3	D	806	ASP
2	I	63	SER
3	D	831	VAL
5	F	477	GLU
3	J	831	VAL
2	C	1186	VAL
3	D	826	ILE
2	I	1186	VAL
3	J	826	ILE
5	L	477	GLU
3	D	1180	VAL
3	J	1180	VAL
2	C	2	VAL

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%)	178 (92%)	16 (8%)	10	34
1	B	182/286 (64%)	170 (93%)	12 (7%)	15	41
1	G	191/286 (67%)	176 (92%)	15 (8%)	11	35
1	H	184/286 (64%)	177 (96%)	7 (4%)	29	51
2	C	1157/1157 (100%)	1043 (90%)	114 (10%)	7	27
2	I	1154/1157 (100%)	1040 (90%)	114 (10%)	7	27
3	D	970/1168 (83%)	857 (88%)	113 (12%)	5	21
3	J	960/1168 (82%)	850 (88%)	110 (12%)	5	22
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	23
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	37
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	26
5	L	418/540 (77%)	377 (90%)	41 (10%)	7	27
All	All	5966/7024 (85%)	5369 (90%)	597 (10%)	7	27

All (597) 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	171	LEU
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	A	233	ASP
1	A	234	LEU
1	B	6	THR
1	B	7	GLU
1	B	8	PHE
1	B	26	VAL
1	B	50	SER
1	B	61	ILE

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Mol	Chain	Res	Type
1	B	64	VAL
1	B	69	SER
1	B	115	ILE
1	B	133	LEU
1	B	148	ARG
1	B	215	GLU
2	C	11	ILE
2	C	21	VAL
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

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Mol	Chain	Res	Type
2	C	445	ILE
2	C	453	ILE
2	C	484	LEU
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	503	LYS
2	C	538	LEU
2	C	539	THR
2	C	542	ARG
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

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Mol	Chain	Res	Type
2	C	892	GLU
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	1002	LEU
2	C	1040	ASP
2	C	1046	VAL
2	C	1073	LYS
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	18	ASP
3	D	20	ILE
3	D	26	SER
3	D	46	TYR
3	D	79	LYS

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Mol	Chain	Res	Type
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL
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	256	ASP
3	D	299	LEU
3	D	306	LEU
3	D	312	ARG
3	D	324	LEU
3	D	330	MET
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	510	LEU
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

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Mol	Chain	Res	Type
3	D	594	GLN
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	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	803	VAL
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

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Mol	Chain	Res	Type
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
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

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Mol	Chain	Res	Type
5	F	306	PHE
5	F	310	GLU
5	F	341	LEU
5	F	395	THR
5	F	400	GLN
5	F	429	THR
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	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	171	LEU

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Mol	Chain	Res	Type
1	G	215	GLU
1	G	219	ARG
1	G	228	LEU
1	G	231	PHE
1	H	26	VAL
1	H	50	SER
1	H	61	ILE
1	H	64	VAL
1	H	115	ILE
1	H	133	LEU
1	H	231	PHE
2	I	4	SER
2	I	11	ILE
2	I	21	VAL
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

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Mol	Chain	Res	Type
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
2	I	484	LEU
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	503	LYS
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
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

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Mol	Chain	Res	Type
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
2	I	984	VAL
2	I	1002	LEU
2	I	1040	ASP
2	I	1046	VAL
2	I	1073	LYS
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

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Mol	Chain	Res	Type
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
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	256	ASP
3	J	299	LEU
3	J	306	LEU
3	J	312	ARG
3	J	324	LEU
3	J	330	MET
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	510	LEU
3	J	513	MET
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR

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Mol	Chain	Res	Type
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
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	788	LEU
3	J	798	ARG
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
5	L	485	GLU
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
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 (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	103	ASN
1	A	117	HIS
1	A	132	HIS
1	B	132	HIS
1	B	186	ASN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN

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Mol	Chain	Res	Type
2	C	494	ASN
2	C	513	GLN
2	C	628	HIS
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN
2	C	1209	GLN
2	C	1288	GLN
2	C	1313	HIS
2	C	1314	GLN
3	D	94	GLN
3	D	196	GLN
3	D	200	GLN
3	D	294	ASN
3	D	419	HIS
3	D	450	HIS
3	D	489	ASN
3	D	593	ASN
3	D	594	GLN
3	D	667	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	907	HIS
3	D	910	ASN
3	D	1218	HIS
3	D	1268	ASN
3	D	1366	HIS
3	D	1367	GLN
4	E	61	ASN
5	F	131	GLN
5	F	227	GLN
5	F	301	ASN
5	F	317	ASN
5	F	345	GLN
5	F	362	ASN
5	F	437	GLN
5	F	446	GLN
5	F	455	HIS
5	F	464	ASN
5	F	545	HIS
1	G	23	HIS

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Mol	Chain	Res	Type
1	G	103	ASN
1	G	117	HIS
1	G	132	HIS
1	H	84	ASN
1	H	103	ASN
1	H	128	HIS
1	H	186	ASN
1	H	227	GLN
2	I	69	GLN
2	I	139	ASN
2	I	148	GLN
2	I	165	HIS
2	I	494	ASN
2	I	513	GLN
2	I	573	ASN
2	I	628	HIS
2	I	677	ASN
2	I	688	GLN
2	I	725	GLN
2	I	761	GLN
2	I	766	ASN
2	I	1017	GLN
2	I	1116	HIS
2	I	1136	GLN
2	I	1146	GLN
2	I	1288	GLN
2	I	1314	GLN
2	I	1336	ASN
3	J	94	GLN
3	J	196	GLN
3	J	200	GLN
3	J	365	GLN
3	J	419	HIS
3	J	489	ASN
3	J	593	ASN
3	J	594	GLN
3	J	665	GLN
3	J	702	GLN
3	J	716	GLN
3	J	817	HIS
3	J	861	ASN
3	J	897	HIS

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Mol	Chain	Res	Type
3	J	910	ASN
3	J	1259	GLN
3	J	1366	HIS
4	K	61	ASN
5	L	131	GLN
5	L	246	GLN
5	L	258	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

5.3.3 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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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(Å²)	Q<0.9
1	A	227/329 (68%)	-0.55	0	100	100	133, 170, 230, 390	0
1	B	214/329 (65%)	-0.52	0	100	100	146, 213, 308, 463	0
1	G	224/329 (68%)	-0.66	0	100	100	171, 216, 299, 368	0
1	H	215/329 (65%)	-0.53	0	100	100	173, 222, 293, 418	0
2	C	1342/1342 (100%)	-0.50	0	100	100	107, 161, 300, 496	0
2	I	1340/1342 (99%)	-0.56	0	100	100	146, 194, 325, 509	0
3	D	1166/1407 (82%)	-0.52	0	100	100	108, 149, 239, 419	0
3	J	1155/1407 (82%)	-0.51	1 (0%)	92	87	127, 170, 264, 409	0
4	E	89/91 (97%)	-0.58	0	100	100	186, 210, 243, 257	0
4	K	79/91 (86%)	-0.50	0	100	100	242, 288, 354, 398	0
5	F	468/613 (76%)	-0.57	0	100	100	151, 209, 338, 459	0
5	L	469/613 (76%)	-0.63	0	100	100	162, 215, 360, 527	0
All	All	6988/8222 (84%)	-0.54	1 (0%)	100	100	107, 184, 306, 527	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	482	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	J	1501	1/1	0.71	0.10	130,130,130,130	0
6	MG	D	1501	1/1	0.90	0.08	104,104,104,104	0
7	ZN	D	1502	1/1	0.98	0.04	177,177,177,177	0
7	ZN	J	1502	1/1	0.98	0.03	213,213,213,213	0
7	ZN	J	1503	1/1	0.99	0.04	135,135,135,135	0
7	ZN	D	1503	1/1	1.00	0.02	117,117,117,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.