



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:54 PM UTC

PDB ID : 5VSW / pdb_00005vsw
Title : X-ray crystal structure of Escherichia coli RNA polymerase and DksA/ppGpp complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-05-12
Resolution : 4.29 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

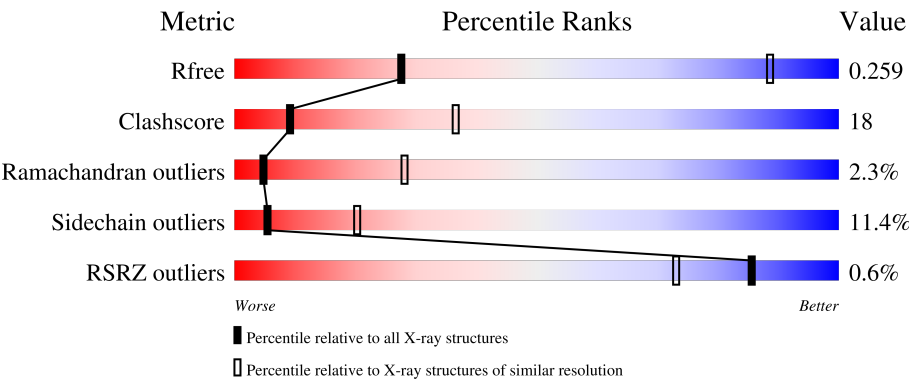
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.29 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	50%36%11%..
1	B	329	43%39%7%.10%
1	G	329	% 41%24%.31%
1	H	329	39%24%.34%
2	C	1342	% 58%36%6%

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Mol	Chain	Length	Quality of chain
2	I	1342	% 60%35%5%
3	D	1407	% 47%32%17%
3	J	1407	% 46%32%18%
4	E	91	% 60%33%. .
4	K	91	52%26%8%. 13%
5	F	613	46%27%. 24%
5	L	613	46%27%. 23%
6	M	151	45%44%. 7%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 57643 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	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	297	Total	C	N	O	S	0	0	0
			2297	1439	403	447	8			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1173	Total	C	N	O	S	0	0	0
			9095	5718	1628	1703	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 a protein called RNA polymerase-binding transcription factor DksA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			

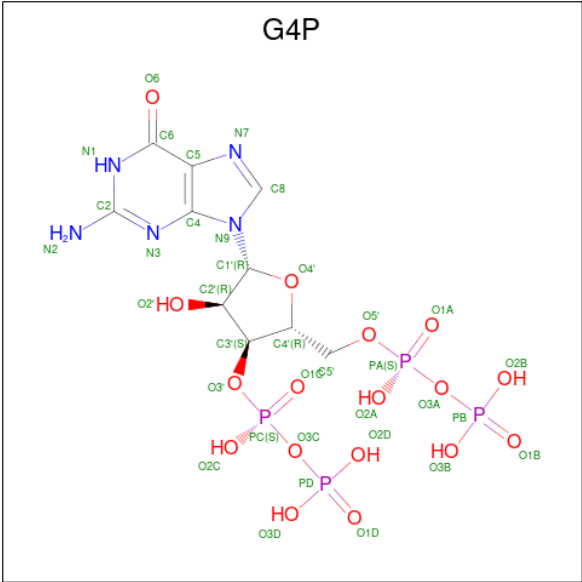
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	J	2	Total	Zn	0	0
			2	2		
8	M	1	Total	Zn	0	0
			1	1		

- Molecule 9 is GUANOSINE-5',3'-TETRAPHOSPHATE (CCD ID: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).

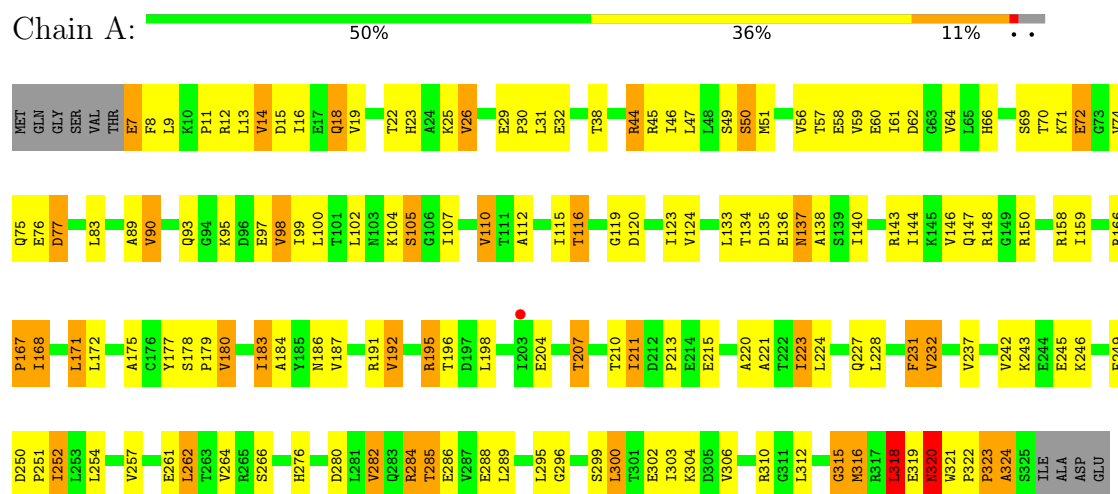


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
9	J	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
9	M	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

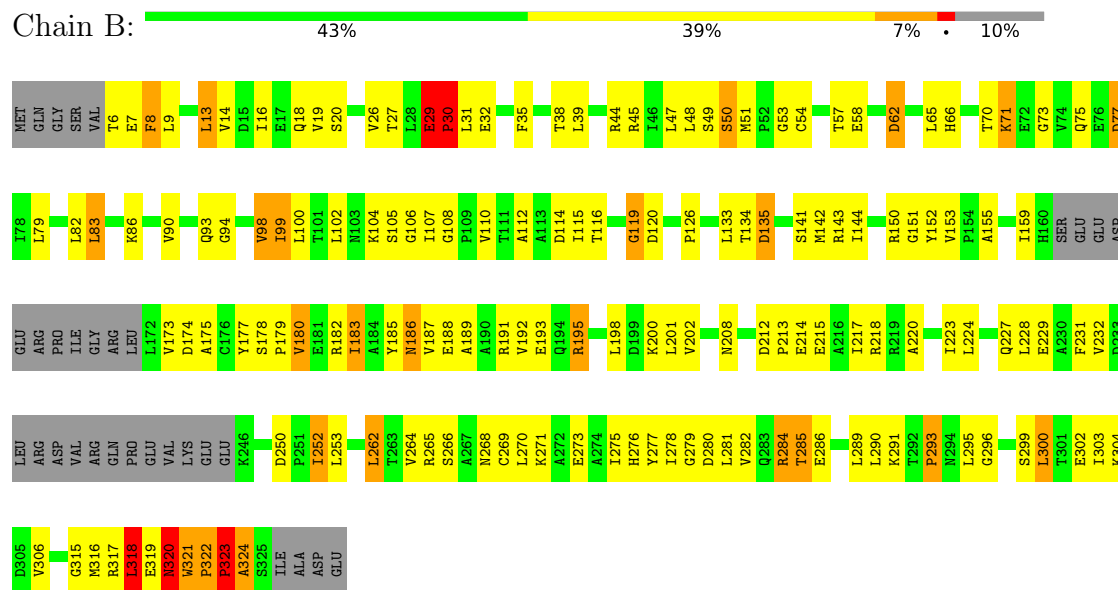
3 Residue-property plots

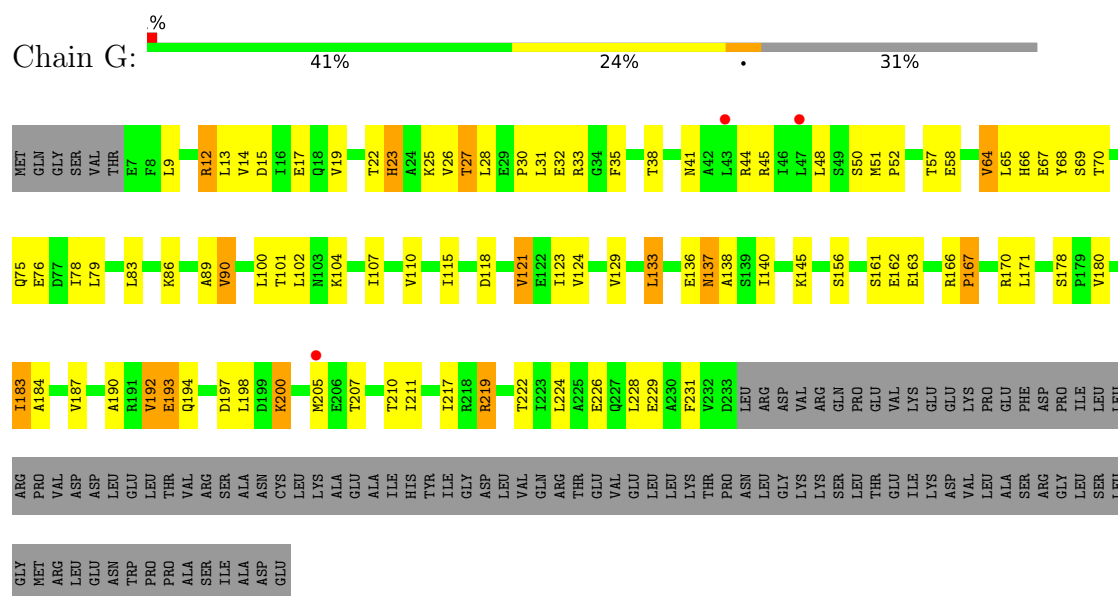
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

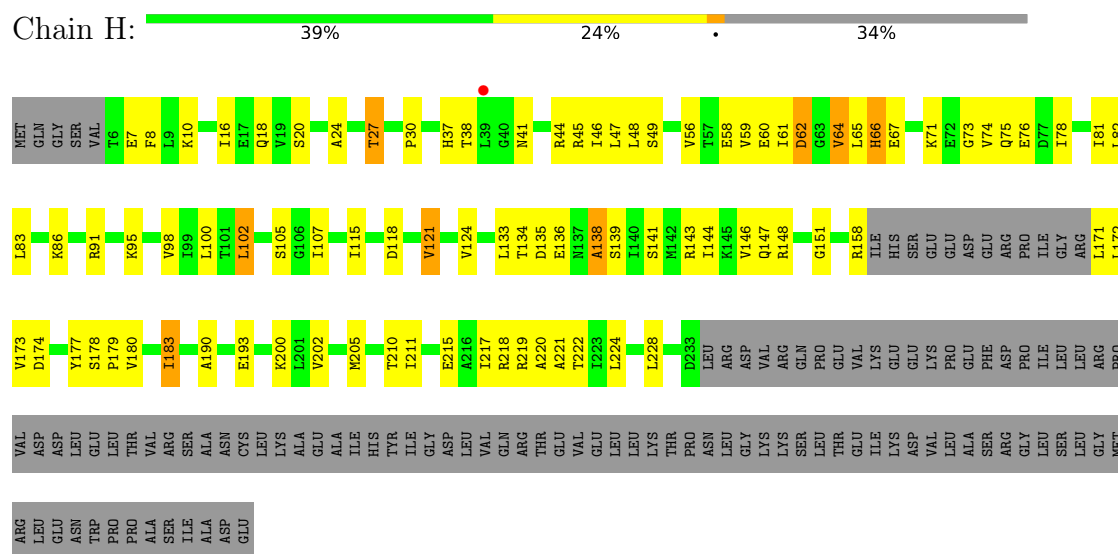


• Molecule 1: DNA-directed RNA polymerase subunit alpha

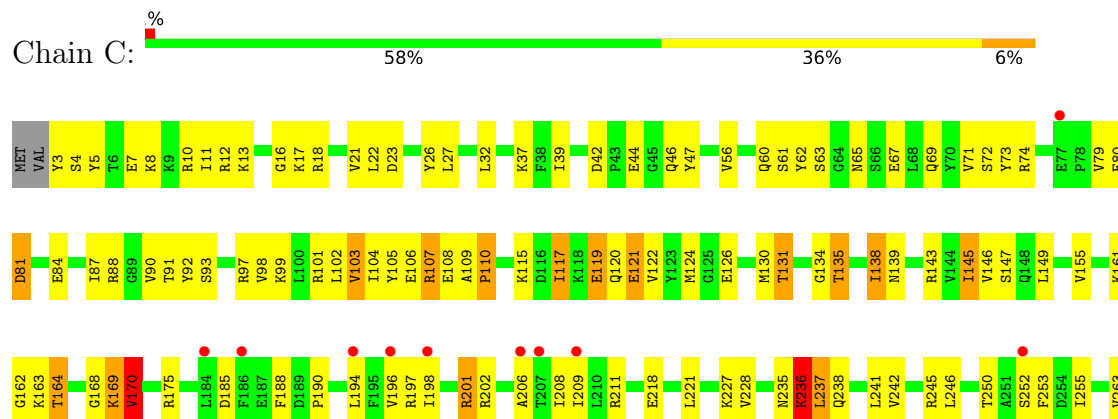


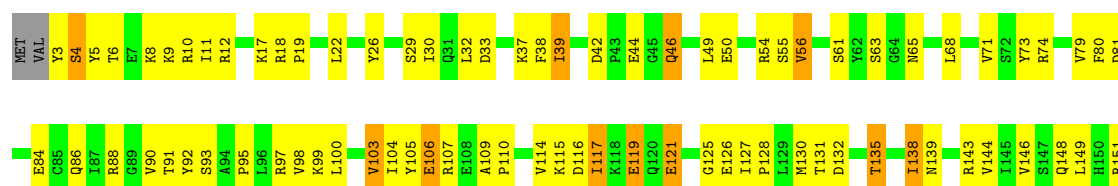
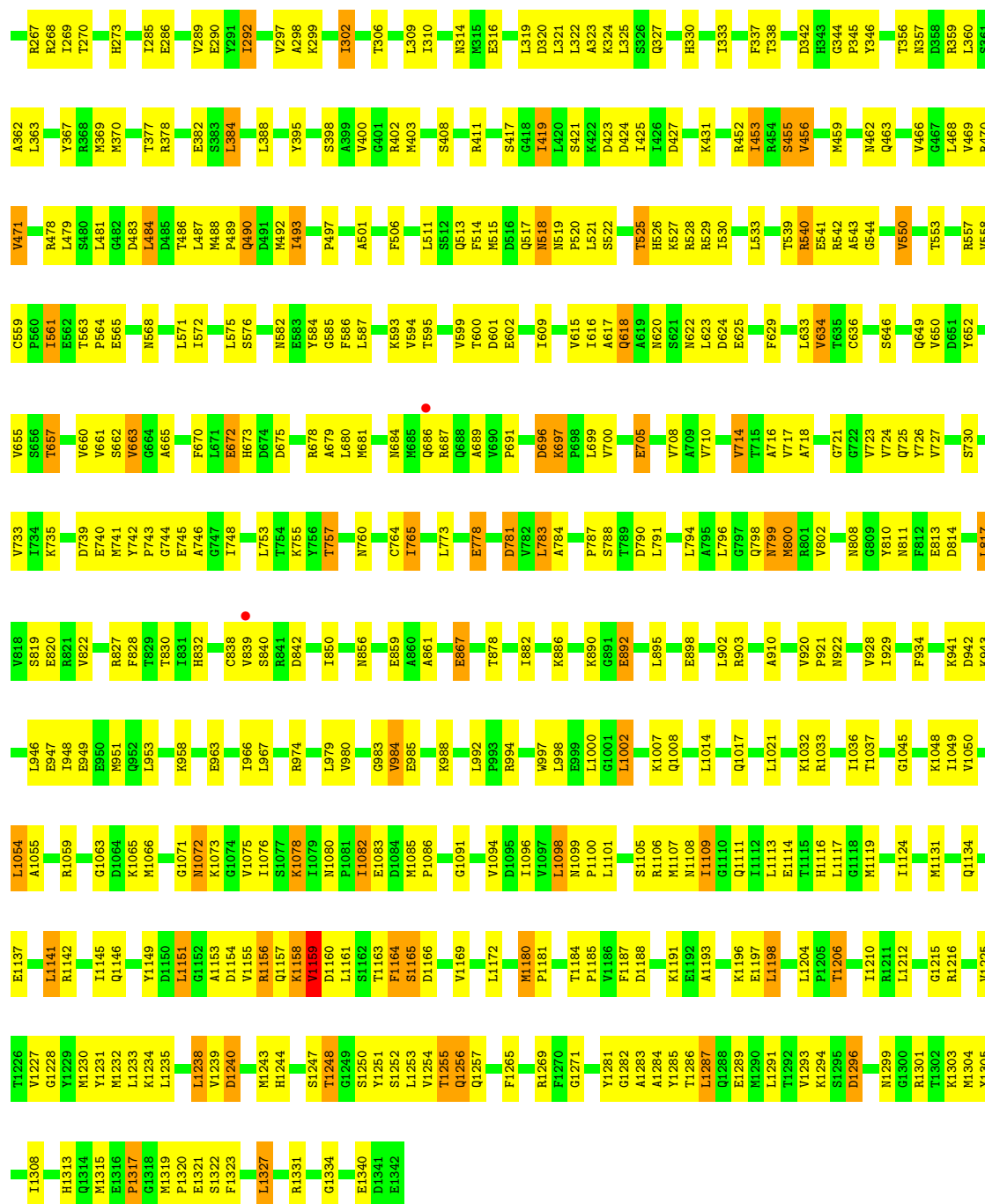


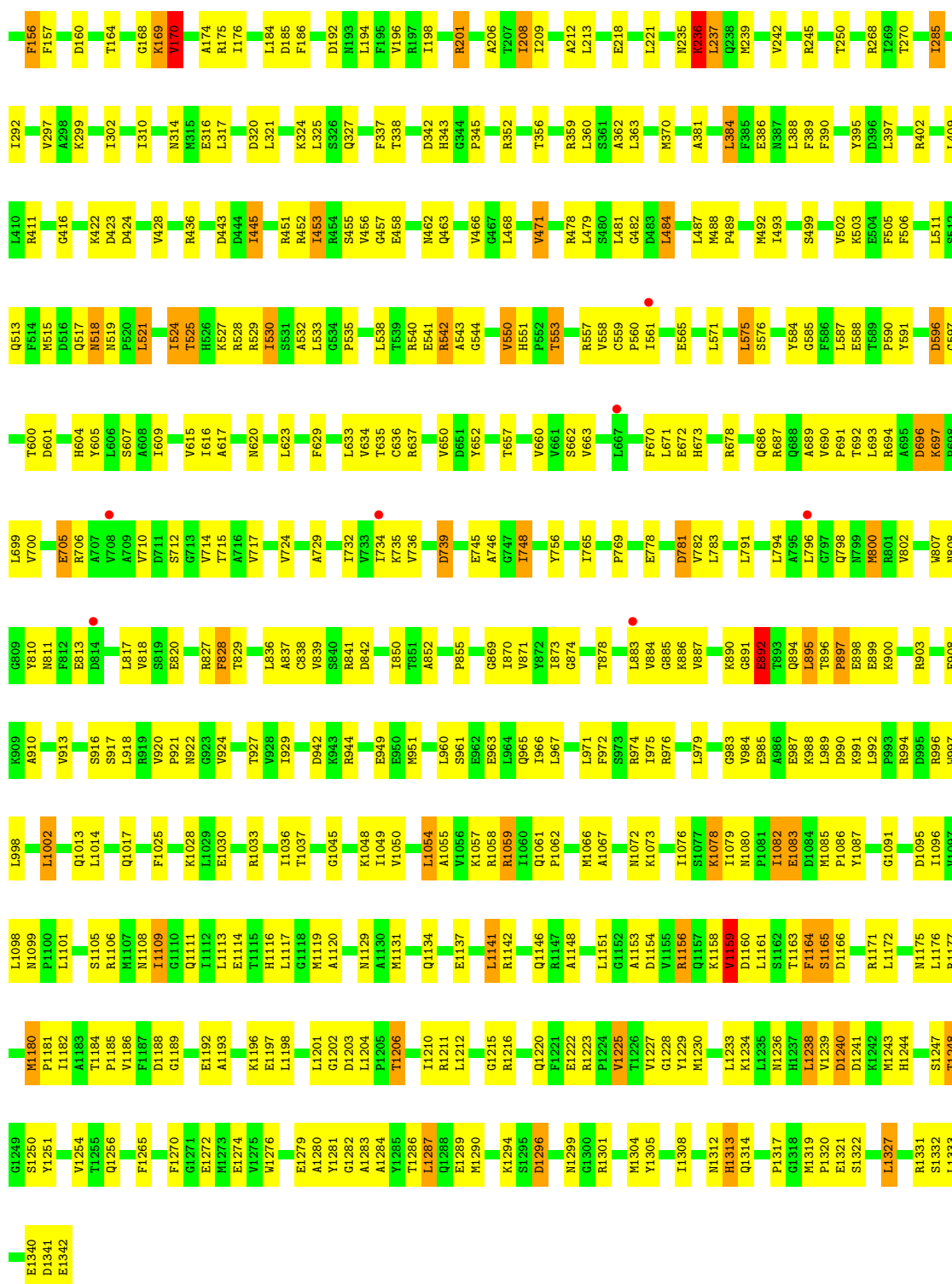
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta







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

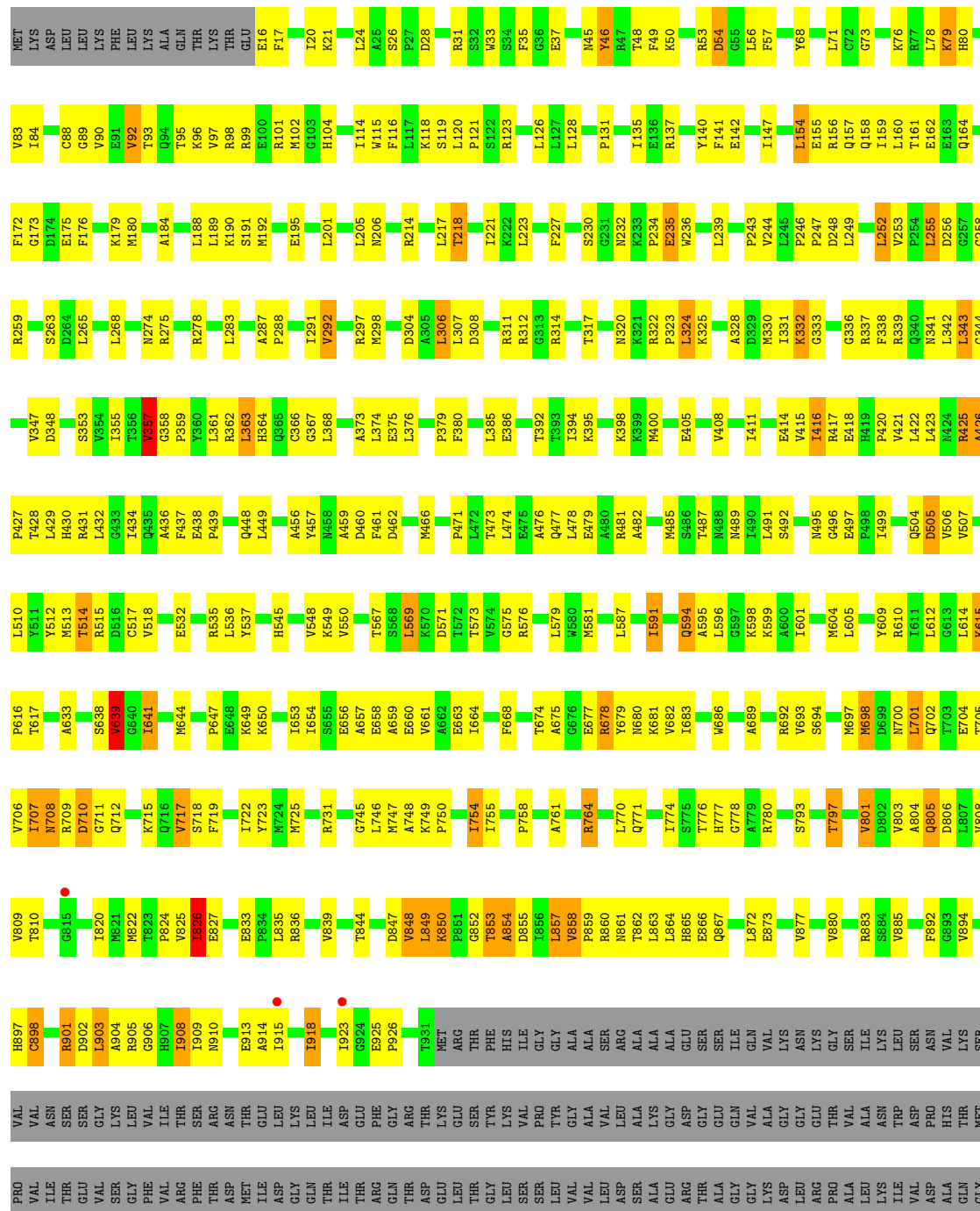


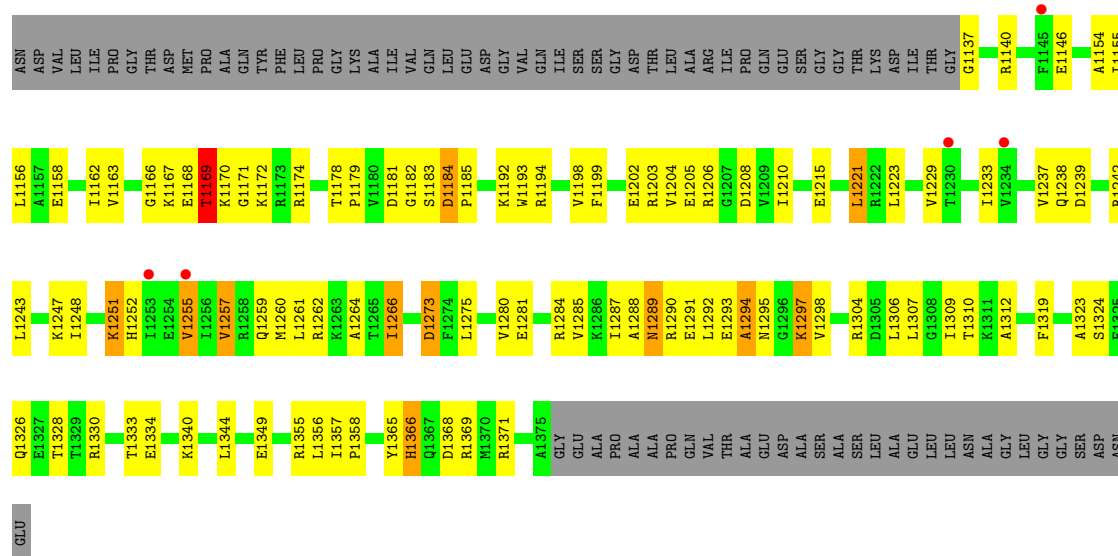
MET	L8	K9	A10	Q11	T12	K13	T14	E15	E16	F17	K21	L24	A25	S26	P27	D28	R31	S32	W33	S34	F35	T43	I44	Y46	R47	T48	F49	K50	R53	D54	G55	L56	F62	Y68	K79	H80	R81	G82	V83	I84	C88	G89	V90
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• Molecule 3: DNA-directed RNA polymerase subunit beta'





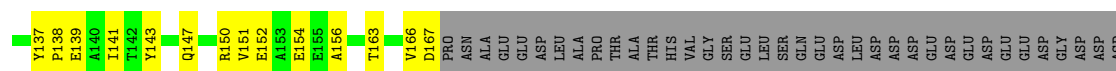
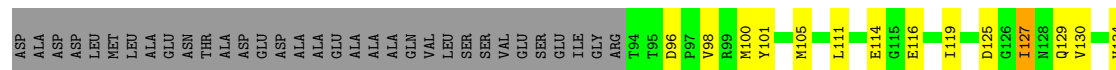
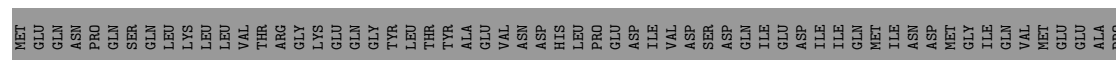
- Molecule 4: DNA-directed RNA polymerase subunit omega

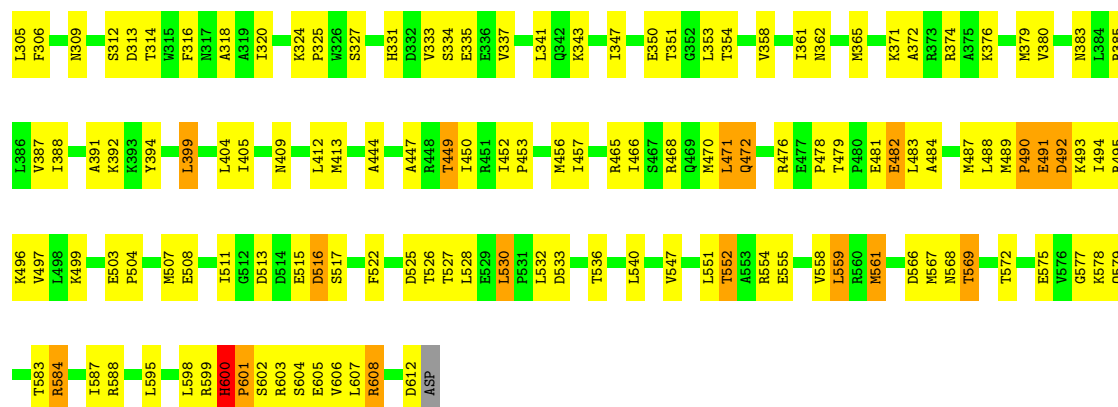


- Molecule 4: DNA-directed RNA polymerase subunit omega

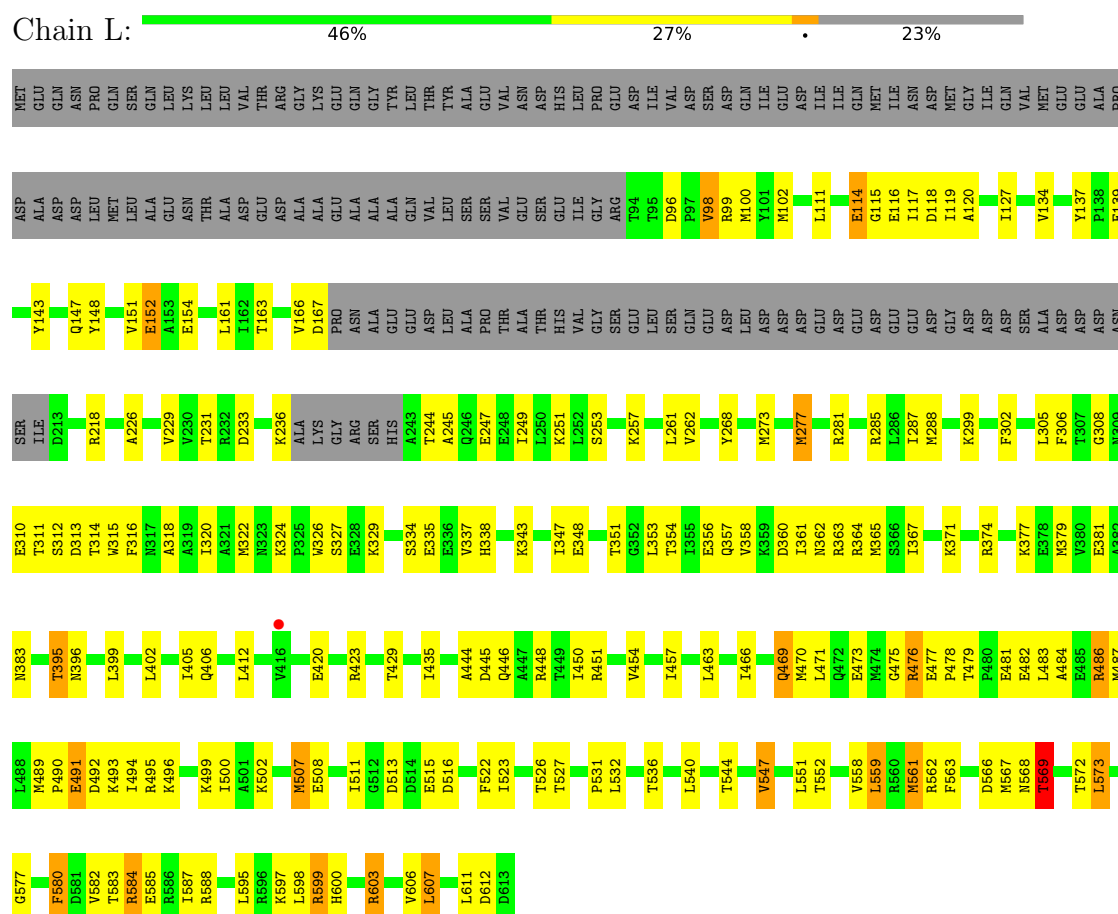


- Molecule 5: RNA polymerase sigma factor RpoD

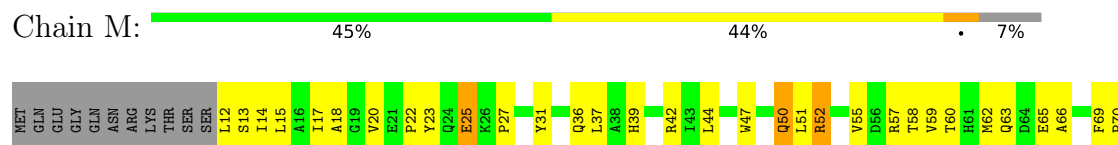




• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 6: RNA polymerase-binding transcription factor DksA



D71	P72	V73	D74	R75	A76	A77	Q78	E79		F82	S83	L84	E85	L86	R87	N88	R89	D90	R91	E92	R93	K94		K97	K98	I99		K105	V106	E107	D108		F111	G112		I121	G122	I123	R124	R125	L126	E127	A128	R129		D133		I136		K139	T140	L141		I144	R145	E146	K147		G151
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.27Å 205.26Å 311.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.82 – 4.29 46.82 – 4.29	Depositor EDS
% Data completeness (in resolution range)	93.7 (46.82-4.29) 81.3 (46.82-4.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.221 , 0.259 0.226 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	187.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 279.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	57643	wwPDB-VP
Average B, all atoms (Å ²)	279.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, G4P, 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	0.24	0/2524	0.71	2/3421 (0.1%)
1	B	0.27	0/2326	0.98	6/3153 (0.2%)
1	G	0.19	0/1777	0.57	0/2408
1	H	0.22	0/1681	0.68	0/2278
2	C	0.21	0/10739	0.64	1/14489 (0.0%)
2	I	0.20	0/10735	0.61	1/14484 (0.0%)
3	D	0.22	0/9235	0.67	2/12472 (0.0%)
3	J	0.21	0/9140	0.67	2/12341 (0.0%)
4	E	0.20	0/693	0.56	0/935
4	K	0.22	0/629	0.73	1/847 (0.1%)
5	F	0.19	0/3864	0.61	2/5194 (0.0%)
5	L	0.19	0/3872	0.59	0/5205
6	M	0.32	0/1155	0.82	0/1549
All	All	0.22	0/58370	0.66	17/78776 (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
1	B	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	GLU	CA-C-N	9.35	131.53	119.84
1	B	29	GLU	C-N-CA	9.35	131.53	119.84
4	K	3	ARG	N-CA-C	-7.96	93.41	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	236	LYS	N-CA-C	7.52	126.82	110.80
1	B	30	PRO	CA-C-N	-7.12	112.94	122.99
1	B	30	PRO	C-N-CA	-7.12	112.94	122.99
2	I	236	LYS	N-CA-C	7.02	125.76	110.80
3	D	1184	ASP	CA-C-N	-6.94	112.49	120.89
3	D	1184	ASP	C-N-CA	-6.94	112.49	120.89
3	J	1184	ASP	CA-C-N	-5.91	113.89	120.45
3	J	1184	ASP	C-N-CA	-5.91	113.89	120.45
5	F	600	HIS	CA-C-N	-5.71	112.70	119.84
5	F	600	HIS	C-N-CA	-5.71	112.70	119.84
1	A	323	PRO	CA-C-N	5.37	131.36	121.70
1	A	323	PRO	C-N-CA	5.37	131.36	121.70
1	B	229	GLU	CA-C-N	-5.01	112.36	120.72
1	B	229	GLU	C-N-CA	-5.01	112.36	120.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	323	PRO	Peptide

5.2 Too-close contacts [i](#)

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	2490	0	2542	126	0
1	B	2297	0	2350	147	1
1	G	1755	0	1773	63	0
1	H	1662	0	1687	58	0
2	C	10570	0	10582	401	0
2	I	10566	0	10576	373	0
3	D	9095	0	9222	393	0
3	J	9001	0	9167	379	1
4	E	691	0	695	26	0
4	K	627	0	634	28	0
5	F	3813	0	3880	142	0
5	L	3821	0	3884	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	1140	0	1119	64	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
8	M	1	0	0	0	0
9	E	36	0	11	3	0
9	J	36	0	11	4	0
9	M	36	0	11	7	0
All	All	57643	0	58144	2101	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (2101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:HB3	1:B:30:PRO:CD	1.26	1.46
1:B:29:GLU:CB	1:B:30:PRO:HD2	1.35	1.45
1:B:279:GLY:HA3	1:B:321:TRP:CZ2	1.55	1.41
5:F:600:HIS:O	5:F:604:SER:HB3	1.33	1.29
1:B:253:LEU:O	1:B:321:TRP:HZ2	0.98	1.26
1:B:253:LEU:O	1:B:321:TRP:CZ2	1.88	1.24
2:C:106:GLU:CB	2:C:109:ALA:HB2	1.67	1.24
1:B:29:GLU:O	1:B:31:LEU:HD22	1.36	1.20
5:F:600:HIS:O	5:F:604:SER:CB	1.93	1.16
1:B:29:GLU:CB	1:B:30:PRO:CD	2.02	1.13
5:F:600:HIS:CD2	5:F:601:PRO:HD3	1.86	1.09
2:C:106:GLU:HB3	2:C:109:ALA:CB	1.82	1.09
3:J:863:LEU:HD11	3:J:901:ARG:HG2	1.24	1.09
2:C:236:LYS:O	2:C:237:LEU:HB2	1.29	1.08
5:F:600:HIS:HD2	5:F:601:PRO:HD3	1.14	1.05
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.36	1.04
1:B:29:GLU:O	1:B:31:LEU:CD2	2.05	1.03
1:B:279:GLY:HA3	1:B:321:TRP:CH2	1.93	1.02
2:I:236:LYS:O	2:I:237:LEU:CB	2.01	1.02
3:D:1372:ARG:HA	3:J:853:THR:HG21	1.39	1.00
6:M:23:TYR:N	6:M:127:GLU:OE2	1.94	1.00
2:C:236:LYS:O	2:C:237:LEU:CB	2.10	0.97
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.47	0.96
2:C:106:GLU:HB3	2:C:109:ALA:HB2	0.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.48	0.94
2:I:236:LYS:O	2:I:237:LEU:HB2	1.17	0.94
1:B:279:GLY:CA	1:B:321:TRP:CZ2	2.50	0.93
1:A:316:MET:SD	5:F:600:HIS:HE1	1.92	0.92
3:D:929:GLN:NE2	6:M:66:ALA:O	2.02	0.92
1:A:316:MET:SD	5:F:600:HIS:CE1	2.63	0.92
4:K:3:ARG:O	4:K:4:VAL:HB	1.70	0.92
3:D:863:LEU:HD11	3:D:901:ARG:HG2	1.53	0.91
3:J:863:LEU:CD1	3:J:901:ARG:HG2	2.03	0.89
3:J:863:LEU:HD11	3:J:901:ARG:CG	2.01	0.89
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.06	0.89
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.52	0.88
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.37	0.88
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.54	0.88
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.52	0.88
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.56	0.87
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.54	0.86
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.40	0.86
1:B:29:GLU:CG	1:B:30:PRO:HD3	2.06	0.86
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.57	0.86
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.57	0.86
1:A:296:GLY:H	1:A:299:SER:HB2	1.38	0.85
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.59	0.85
3:J:1198:VAL:HB	3:J:1210:ILE:HG23	1.57	0.85
1:B:296:GLY:H	1:B:299:SER:HB2	1.43	0.84
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.59	0.84
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.42	0.84
2:C:106:GLU:C	2:C:109:ALA:H	1.86	0.84
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.60	0.84
5:F:456:MET:HE1	5:F:497:VAL:HG13	1.60	0.83
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.42	0.83
2:C:235:ASN:O	2:C:236:LYS:HB2	1.78	0.83
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.44	0.83
1:B:323:PRO:HA	1:B:324:ALA:HB2	1.60	0.83
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.11	0.82
3:D:936:HIS:HA	3:D:1135:THR:HA	1.61	0.82
2:I:235:ASN:O	2:I:236:LYS:HB2	1.76	0.82
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.24	0.82
1:B:29:GLU:CG	1:B:30:PRO:CD	2.57	0.82
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.59	0.82
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:121:ILE:HG23	6:M:125:ARG:HH11	1.45	0.81
3:J:853:THR:HG22	3:J:854:ALA:H	1.44	0.81
1:G:45:ARG:HG2	1:H:38:THR:HB	1.62	0.81
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.62	0.81
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	1.63	0.81
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.62	0.81
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	2.14	0.80
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.62	0.80
6:M:105:LYS:NZ	6:M:133:ASP:OD2	2.14	0.80
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.62	0.79
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.27	0.79
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.64	0.79
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.47	0.79
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.64	0.78
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.66	0.78
5:L:134:VAL:HA	5:L:273:MET:HE1	1.64	0.78
3:D:1372:ARG:HA	3:J:853:THR:CG2	2.13	0.78
2:I:268:ARG:HH21	2:I:270:THR:HG22	1.48	0.78
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.66	0.78
1:A:224:LEU:HD23	1:B:228:LEU:HD11	1.64	0.77
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.66	0.77
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.66	0.77
1:B:279:GLY:HA3	1:B:321:TRP:CE2	2.19	0.77
3:J:362:ARG:NH2	9:J:2004:G4P:O4'	2.17	0.77
1:A:150:ARG:NH1	1:B:7:GLU:O	2.17	0.77
1:B:83:LEU:HD21	3:D:526:VAL:HB	1.65	0.77
3:J:901:ARG:HB2	3:J:908:ILE:HA	1.66	0.77
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.50	0.77
4:K:40:PRO:O	4:K:52:ARG:NH2	2.18	0.77
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.65	0.77
6:M:121:ILE:HG23	6:M:125:ARG:NH1	2.00	0.77
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.65	0.76
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.50	0.76
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.67	0.76
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.66	0.76
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.66	0.76
5:L:573:LEU:HD12	5:L:588:ARG:HE	1.49	0.76
2:C:106:GLU:H	2:C:109:ALA:HB3	1.51	0.76
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.04	0.76
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.68	0.76
3:J:709:ARG:O	3:J:711:GLY:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:705:GLU:HB2	2:I:794:LEU:H	1.50	0.76
1:B:29:GLU:CB	1:B:30:PRO:HD3	2.14	0.76
1:B:47:LEU:HD23	1:B:51:MET:HE2	1.67	0.76
9:J:2004:G4P:O3D	4:K:2:ALA:N	2.18	0.76
3:J:901:ARG:CB	3:J:908:ILE:HA	2.15	0.75
1:B:27:THR:HG23	1:B:202:VAL:HG22	1.66	0.75
1:B:119:GLY:HA3	1:B:271:LYS:HG2	1.68	0.75
3:D:1136:GLY:HA2	3:D:1140:ARG:HG2	1.69	0.75
3:J:482:ALA:HA	4:K:6:VAL:HG11	1.69	0.75
3:D:660:GLU:HG3	6:M:12:LEU:HD23	1.68	0.75
2:I:1148:ALA:HA	2:I:1201:LEU:HD21	1.67	0.74
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.69	0.74
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.19	0.74
5:L:573:LEU:HD23	5:L:573:LEU:H	1.53	0.74
2:I:30:ILE:HD12	2:I:30:ILE:H	1.50	0.74
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.52	0.74
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.70	0.74
3:J:48:THR:O	3:J:50:LYS:N	2.20	0.74
1:B:119:GLY:H	1:B:271:LYS:HE3	1.51	0.74
3:D:490:ILE:H	3:D:490:ILE:HD13	1.52	0.74
1:H:134:THR:HG23	1:H:135:ASP:H	1.53	0.74
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.53	0.74
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.69	0.74
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	1.69	0.73
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.70	0.73
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.20	0.73
3:D:615:LYS:NZ	9:E:101:G4P:O1C	2.20	0.73
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.69	0.73
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.70	0.73
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.70	0.73
3:D:709:ARG:O	3:D:711:GLY:N	2.21	0.73
6:M:91:ARG:NH1	9:M:202:G4P:O1D	2.19	0.73
5:L:481:GLU:OE1	5:L:495:ARG:NH2	2.22	0.73
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.21	0.73
5:F:101:TYR:HE2	5:F:388:ILE:HD11	1.53	0.73
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.21	0.73
6:M:94:LYS:NZ	9:M:202:G4P:O1C	2.21	0.73
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.70	0.73
4:K:32:VAL:O	4:K:34:GLY:N	2.21	0.73
3:J:853:THR:C	3:J:855:ASP:H	1.97	0.72
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.53	0.72
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	1.70	0.72
1:A:191:ARG:NH1	1:A:198:LEU:O	2.21	0.72
2:C:705:GLU:HB2	2:C:794:LEU:H	1.53	0.72
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.70	0.72
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.71	0.72
1:A:252:ILE:HG21	1:A:312:LEU:HD11	1.70	0.72
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.70	0.72
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.72	0.72
4:K:14:GLY:O	4:K:16:ARG:N	2.22	0.72
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.54	0.72
2:C:678:ARG:NH1	2:C:1071:GLY:O	2.23	0.72
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.53	0.71
1:G:226:GLU:HB3	1:H:10:LYS:HE3	1.72	0.71
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.53	0.71
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.25	0.71
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.72	0.71
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.22	0.71
2:I:596:ASP:CG	2:I:597:GLY:H	1.97	0.71
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.72	0.71
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.73	0.71
1:A:47:LEU:HD23	1:A:51:MET:HE2	1.72	0.71
3:J:853:THR:O	3:J:855:ASP:N	2.24	0.71
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.73	0.71
5:F:600:HIS:O	5:F:604:SER:HB2	1.87	0.71
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.71	0.70
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.72	0.70
3:J:844:THR:OG1	3:J:860:ARG:O	2.08	0.70
1:B:279:GLY:CA	1:B:321:TRP:CH2	2.72	0.70
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.24	0.70
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.73	0.70
2:I:533:LEU:HD13	2:I:540:ARG:HE	1.57	0.70
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.74	0.70
3:D:48:THR:O	3:D:50:LYS:N	2.25	0.70
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.74	0.70
2:C:106:GLU:N	2:C:109:ALA:HB3	2.07	0.70
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.74	0.70
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.25	0.69
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.73	0.69
2:I:739:ASP:OD1	2:I:739:ASP:N	2.26	0.69
3:D:495:ASN:O	3:D:497:GLU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.72	0.69
5:F:600:HIS:CD2	5:F:601:PRO:CD	2.71	0.69
2:C:395:TYR:HD2	2:C:419:ILE:HG22	1.57	0.69
3:D:674:THR:HG21	6:M:139:LYS:HG2	1.74	0.69
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.75	0.69
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.75	0.69
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.75	0.69
1:B:79:LEU:HD11	3:D:526:VAL:HG11	1.74	0.69
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.24	0.69
3:D:418:GLU:HG3	4:E:45:LYS:H	1.57	0.69
3:D:673:VAL:HB	6:M:129:ARG:NH1	2.08	0.69
1:B:289:LEU:HD13	1:B:300:LEU:HD21	1.75	0.69
2:I:151:ARG:HH22	2:I:175:ARG:HH11	1.41	0.69
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.74	0.69
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.69
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.26	0.69
3:D:679:TYR:OH	3:D:754:ILE:O	2.09	0.68
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.28	0.68
2:C:1253:LEU:HD11	3:D:253:VAL:HG11	1.75	0.68
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.57	0.68
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.74	0.68
1:A:7:GLU:HB3	1:B:150:ARG:HH12	1.56	0.68
1:A:14:VAL:HG22	1:A:15:ASP:H	1.58	0.68
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.75	0.68
2:C:1315:MET:HE2	2:C:1317:PRO:HB3	1.74	0.68
3:D:1244:GLN:O	6:M:66:ALA:HB3	1.94	0.68
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.22	0.68
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.25	0.68
3:J:1365:TYR:OH	3:J:1369:ARG:NH1	2.26	0.68
1:B:77:ASP:OD1	1:B:77:ASP:N	2.26	0.68
2:C:168:GLY:O	2:C:170:VAL:N	2.22	0.68
3:D:1178:THR:HG23	3:D:1184:ASP:HB3	1.75	0.68
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.25	0.68
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.74	0.68
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.94	0.68
4:E:4:VAL:HG13	4:E:5:THR:H	1.59	0.68
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.75	0.68
2:I:560:PRO:O	3:J:780:ARG:NH2	2.26	0.68
2:I:17:LYS:NZ	2:I:1154:ASP:OD1	2.27	0.68
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.76	0.68
3:J:205:LEU:HD22	3:J:214:ARG:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.75	0.68
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.76	0.68
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.94	0.67
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.76	0.67
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.75	0.67
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.76	0.67
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.76	0.67
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.76	0.67
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.10	0.67
2:C:197:ARG:NH1	2:C:201:ARG:O	2.27	0.67
2:I:798:GLN:OE1	2:I:827:ARG:HB2	1.94	0.67
2:C:324:LYS:O	2:C:327:GLN:NE2	2.26	0.67
3:D:722:ILE:HA	3:D:725:MET:HE3	1.77	0.67
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.77	0.67
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.75	0.67
6:M:37:LEU:HD22	6:M:106:VAL:HG13	1.76	0.67
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.76	0.67
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.29	0.67
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.75	0.67
1:A:289:LEU:HD13	1:A:300:LEU:HD21	1.77	0.67
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.77	0.67
1:A:77:ASP:OD1	1:A:77:ASP:N	2.28	0.67
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.59	0.67
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.77	0.66
1:B:253:LEU:HB3	1:B:321:TRP:NE1	2.09	0.66
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.77	0.66
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.59	0.66
3:D:935:PHE:O	3:D:1136:GLY:N	2.29	0.66
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.27	0.66
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.78	0.66
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.61	0.66
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.77	0.66
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.11	0.66
5:F:465:ARG:HD2	5:F:468:ARG:HH22	1.60	0.66
2:C:1106:ARG:HG3	6:M:74:ASP:OD1	1.96	0.66
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.27	0.66
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.61	0.66
1:B:94:GLY:H	1:B:276:HIS:CD2	2.13	0.66
2:C:861:ALA:HB1	2:C:882:ILE:HD13	1.76	0.66
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.61	0.66
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:495:ASN:O	3:J:497:GLU:N	2.29	0.65
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.60	0.65
2:I:1243:MET:HA	3:J:353:SER:HB3	1.79	0.65
3:J:287:ALA:HB3	3:J:292:VAL:HG12	1.78	0.65
1:B:100:LEU:HD23	1:B:115:ILE:HG21	1.79	0.65
3:D:932:MET:HA	3:D:1139:PRO:HD3	1.77	0.65
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.11	0.65
2:I:1244:HIS:HD2	2:I:1265:PHE:HB2	1.60	0.65
6:M:44:LEU:HD22	6:M:99:ILE:HG23	1.78	0.65
3:D:424:ASN:HB2	3:D:434:ILE:HG12	1.78	0.65
1:G:66:HIS:HB3	2:I:874:GLY:HA2	1.78	0.65
2:I:452:ARG:NH1	2:I:584:TYR:O	2.30	0.65
3:J:808:VAL:HG13	3:J:914:ALA:HA	1.78	0.65
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.77	0.65
2:C:106:GLU:CB	2:C:109:ALA:CB	2.57	0.65
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.79	0.65
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.29	0.65
1:A:59:VAL:HG22	1:A:144:ILE:HA	1.79	0.65
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.77	0.65
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.77	0.65
3:J:853:THR:C	3:J:855:ASP:N	2.54	0.65
3:D:1289:ASN:O	3:D:1289:ASN:ND2	2.27	0.65
4:E:32:VAL:O	4:E:34:GLY:N	2.30	0.65
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.79	0.65
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.61	0.65
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.30	0.65
3:J:1291:GLU:HG2	3:J:1297:LYS:HD2	1.79	0.65
3:J:259:ARG:HD3	5:L:502:LYS:HD2	1.78	0.65
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.79	0.64
5:L:493:LYS:HG2	5:L:496:LYS:HE2	1.77	0.64
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.62	0.64
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.31	0.64
1:B:94:GLY:HA3	1:B:276:HIS:HB3	1.79	0.64
2:I:206:ALA:O	2:I:209:ILE:HG22	1.97	0.64
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.62	0.64
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.79	0.64
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.79	0.64
2:C:686:GLN:HG2	2:C:796:LEU:HD22	1.79	0.64
3:D:863:LEU:HD11	3:D:901:ARG:CG	2.25	0.64
2:I:168:GLY:O	2:I:170:VAL:N	2.30	0.64
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.79	0.64
3:J:364:HIS:CE1	4:K:3:ARG:HH21	2.16	0.64
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.80	0.64
3:D:793:SER:O	3:D:797:THR:HG23	1.98	0.64
2:I:1116:HIS:HE1	3:J:641:ILE:N	1.94	0.64
3:J:853:THR:HG22	3:J:854:ALA:N	2.12	0.64
3:D:473:THR:HG23	3:D:476:ALA:H	1.63	0.64
1:G:14:VAL:HG13	1:G:15:ASP:H	1.62	0.64
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.80	0.64
1:A:134:THR:HG21	2:C:727:VAL:O	1.98	0.64
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.78	0.64
1:B:253:LEU:CB	1:B:321:TRP:HE1	2.11	0.63
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.80	0.63
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.78	0.63
3:D:789:LYS:HD2	6:M:79:GLU:OE2	1.97	0.63
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.80	0.63
2:I:4:SER:OG	2:I:5:TYR:N	2.26	0.63
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.31	0.63
2:C:814:ASP:CG	2:C:1106:ARG:HH12	2.05	0.63
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.63	0.63
3:J:473:THR:HG23	3:J:476:ALA:H	1.63	0.63
2:I:1119:MET:HE3	2:I:1204:LEU:HD22	1.81	0.63
3:J:722:ILE:HA	3:J:725:MET:HE3	1.79	0.63
1:B:119:GLY:N	1:B:271:LYS:HE3	2.13	0.63
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.30	0.63
3:D:658:GLU:O	3:D:661:VAL:HG22	1.97	0.63
3:D:668:PHE:HB2	3:D:678:ARG:HG3	1.80	0.63
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.80	0.63
2:C:106:GLU:O	2:C:109:ALA:N	2.31	0.63
2:C:211:ARG:NH1	2:C:357:ASN:O	2.32	0.63
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.80	0.63
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.80	0.63
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.64	0.63
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.81	0.63
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.81	0.63
1:A:22:THR:O	1:A:207:THR:N	2.27	0.62
5:F:479:THR:HG23	5:F:481:GLU:H	1.63	0.62
2:I:97:ARG:HB3	2:I:121:GLU:HB3	1.80	0.62
2:I:1082:ILE:H	2:I:1082:ILE:HD12	1.64	0.62
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.81	0.62
3:D:677:GLU:HG2	6:M:129:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.81	0.62
1:A:237:VAL:HG13	1:B:13:LEU:H	1.62	0.62
3:D:1206:ARG:NH2	3:J:1295:ASN:OD1	2.32	0.62
1:G:118:ASP:HB3	1:G:121:VAL:HB	1.81	0.62
2:I:842:ASP:N	2:I:1045:GLY:O	2.30	0.62
6:M:94:LYS:O	6:M:98:LYS:HD2	1.98	0.62
1:B:253:LEU:HB3	1:B:321:TRP:HE1	1.65	0.62
1:G:161:SER:O	1:G:163:GLU:N	2.32	0.62
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.35	0.62
1:A:97:GLU:HB3	1:A:147:GLN:HG2	1.81	0.62
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.32	0.62
3:D:1198:VAL:HB	3:D:1210:ILE:HG23	1.80	0.62
2:I:149:LEU:O	2:I:532:ALA:HA	1.99	0.62
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.80	0.62
6:M:59:VAL:O	6:M:63:GLN:HG3	2.00	0.62
1:A:23:HIS:HE1	1:A:204:GLU:HG2	1.64	0.62
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.81	0.62
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.82	0.62
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.82	0.62
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.82	0.62
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.35	0.62
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.81	0.62
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.80	0.62
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.82	0.62
2:I:81:ASP:HA	2:I:92:TYR:HE1	1.63	0.62
3:J:50:LYS:HD3	3:J:71:LEU:HD21	1.81	0.62
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.15	0.62
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.64	0.62
2:C:360:LEU:HD22	2:C:378:ARG:HH21	1.65	0.61
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.81	0.61
6:M:55:VAL:HG22	6:M:89:ARG:HG3	1.82	0.61
1:B:102:LEU:HD23	1:B:115:ILE:HG12	1.82	0.61
3:D:137:ARG:HD3	3:D:143:SER:HB2	1.83	0.61
3:D:252:LEU:HD23	3:D:262:THR:HB	1.81	0.61
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.82	0.61
3:D:678:ARG:HA	6:M:129:ARG:NH2	2.15	0.61
5:L:561:MET:HA	5:L:567:MET:HE1	1.81	0.61
2:C:1124:ILE:HG21	2:C:1180:MET:HE2	1.82	0.61
2:I:808:ASN:H	3:J:633:ALA:HB2	1.65	0.61
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.00	0.61
1:B:29:GLU:CD	1:B:30:PRO:HD3	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.35	0.61
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.83	0.61
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.80	0.61
2:C:778:GLU:O	2:C:781:ASP:HB2	2.01	0.61
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.82	0.61
1:A:45:ARG:HG2	1:B:38:THR:OG1	2.00	0.61
3:D:614:LEU:HD23	4:E:5:THR:HB	1.82	0.61
2:I:208:ILE:HG12	2:I:362:ALA:HB1	1.82	0.61
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.66	0.61
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.16	0.61
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.83	0.61
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.82	0.61
2:C:1244:HIS:HD2	2:C:1265:PHE:HB2	1.66	0.61
3:D:935:PHE:HA	6:M:86:LEU:HD11	1.82	0.61
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.83	0.61
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.83	0.60
2:C:1085:MET:HA	2:C:1085:MET:HE2	1.81	0.60
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.83	0.60
2:I:192:ASP:OD2	2:I:436:ARG:NH2	2.30	0.60
2:I:196:VAL:HG12	2:I:206:ALA:HA	1.82	0.60
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.00	0.60
3:J:418:GLU:HG3	4:K:45:LYS:H	1.65	0.60
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.35	0.60
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.82	0.60
5:L:379:MET:O	5:L:383:ASN:ND2	2.34	0.60
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.34	0.60
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.82	0.60
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.83	0.60
3:D:901:ARG:HB2	3:D:908:ILE:HA	1.84	0.60
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.37	0.60
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.82	0.60
1:A:135:ASP:O	1:A:137:ASN:N	2.34	0.60
3:D:48:THR:C	3:D:50:LYS:H	2.09	0.60
5:F:487:MET:HA	5:F:487:MET:HE2	1.83	0.60
2:I:1294:LYS:HB3	3:J:347:VAL:HG13	1.82	0.60
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.83	0.60
2:I:37:LYS:HD2	2:I:46:GLN:HE21	1.66	0.60
2:I:1283:ALA:HB1	2:I:1286:THR:HB	1.83	0.60
1:A:211:ILE:HD12	1:A:215:GLU:HG2	1.84	0.60
1:A:316:MET:CE	5:F:600:HIS:NE2	2.65	0.60
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.82	0.60
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.35	0.60
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.84	0.60
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.82	0.60
3:J:674:THR:O	3:J:678:ARG:HB3	2.02	0.60
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.84	0.60
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.16	0.60
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.84	0.60
3:J:1290:ARG:HD2	3:J:1298:VAL:HG12	1.84	0.60
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.35	0.59
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.83	0.59
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.84	0.59
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.84	0.59
2:C:408:SER:O	2:C:431:LYS:NZ	2.35	0.59
2:I:268:ARG:NH2	2:I:270:THR:HG22	2.17	0.59
2:C:1119:MET:HE3	2:C:1204:LEU:HD22	1.84	0.59
3:D:325:LYS:HE2	3:D:330:MET:HG3	1.83	0.59
3:D:355:ILE:HG12	3:D:464:ASP:O	2.02	0.59
3:D:515:ARG:O	3:D:545:HIS:HB3	2.02	0.59
3:D:849:LEU:H	3:D:849:LEU:HD22	1.68	0.59
1:G:12:ARG:H	1:G:30:PRO:HD2	1.67	0.59
3:J:678:ARG:HA	3:J:681:LYS:HB3	1.84	0.59
1:B:93:GLN:HB2	1:B:276:HIS:CD2	2.38	0.59
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.83	0.59
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.84	0.59
2:C:106:GLU:H	2:C:109:ALA:CB	2.14	0.59
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.84	0.59
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.84	0.59
1:B:53:GLY:HA3	1:B:177:TYR:O	2.02	0.59
1:B:175:ALA:HB1	1:B:177:TYR:CE1	2.37	0.59
1:B:321:TRP:H	1:B:322:PRO:HD3	1.67	0.59
2:C:356:THR:HG21	2:C:362:ALA:HA	1.84	0.59
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.84	0.59
1:B:57:THR:HG22	1:B:58:GLU:HG3	1.84	0.59
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.02	0.59
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.84	0.59
3:J:820:ILE:HD11	3:J:822:MET:HE2	1.85	0.59
1:A:45:ARG:NE	2:C:1083:GLU:HB3	2.17	0.59
3:D:505:ASP:HB3	3:D:629:PHE:HE1	1.67	0.59
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.85	0.59
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:LEU:HG	1:H:115:ILE:HG12	1.83	0.59
3:J:140:TYR:O	3:J:297:ARG:NH1	2.36	0.59
5:L:487:MET:HE2	5:L:487:MET:HA	1.84	0.59
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.02	0.59
2:C:723:VAL:O	2:C:735:LYS:N	2.33	0.59
2:I:515:MET:HG2	2:I:517:GLN:HB2	1.85	0.59
1:B:119:GLY:HA3	1:B:271:LYS:CG	2.33	0.58
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.85	0.58
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.85	0.58
3:J:492:SER:HB2	3:J:499:ILE:HB	1.84	0.58
3:D:1165:PHE:HE1	3:D:1200:GLU:HB2	1.66	0.58
5:F:279:ARG:HB3	5:F:347:ILE:HD11	1.85	0.58
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.85	0.58
2:I:1240:ASP:OD1	2:I:1240:ASP:N	2.27	0.58
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.03	0.58
3:D:317:THR:HG22	3:D:322:ARG:O	2.03	0.58
3:D:673:VAL:HB	6:M:129:ARG:HH12	1.67	0.58
5:F:314:THR:HA	5:F:318:ALA:HB3	1.85	0.58
1:G:228:LEU:HG	1:H:221:ALA:HB1	1.85	0.58
2:I:106:GLU:HB3	2:I:109:ALA:HB2	1.83	0.58
2:I:524:ILE:HD12	2:I:712:SER:HB2	1.85	0.58
2:I:998:LEU:H	2:I:998:LEU:HD12	1.67	0.58
5:L:482:GLU:HG3	5:L:486:ARG:HH22	1.67	0.58
1:A:223:ILE:HD13	1:B:8:PHE:CE2	2.37	0.58
3:D:1221:LEU:HB2	3:D:1229:VAL:HG11	1.85	0.58
3:J:385:LEU:HD23	3:J:411:ILE:HG13	1.85	0.58
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.02	0.58
3:D:88:CYS:O	3:D:90:VAL:N	2.36	0.58
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.17	0.58
5:L:551:LEU:HD23	5:L:597:LYS:HD2	1.84	0.58
1:A:166:ARG:O	1:A:168:ILE:N	2.37	0.58
1:A:284:ARG:HG3	1:A:288:GLU:HG3	1.85	0.58
3:J:425:ARG:HG2	3:J:426:ALA:H	1.68	0.58
1:A:57:THR:HG22	1:A:58:GLU:HG3	1.84	0.58
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.85	0.58
1:H:98:VAL:O	1:H:146:VAL:HG22	2.04	0.58
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.86	0.58
3:J:362:ARG:HE	9:J:2004:G4P:C2	2.17	0.58
2:C:488:MET:O	2:C:490:GLN:N	2.33	0.58
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.69	0.58
3:J:708:ASN:OD1	3:J:708:ASN:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:SER:HB3	1:B:303:ILE:HD11	1.86	0.58
2:C:617:ALA:HA	2:C:636:CYS:SG	2.44	0.58
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.37	0.58
2:I:324:LYS:O	2:I:327:GLN:NE2	2.37	0.58
1:B:321:TRP:H	1:B:322:PRO:CD	2.17	0.57
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.39	0.57
1:G:83:LEU:HD23	2:I:694:ARG:HE	1.69	0.57
2:I:528:ARG:NH2	2:I:576:SER:O	2.37	0.57
3:J:848:VAL:HG21	3:J:880:VAL:HG22	1.86	0.57
1:B:252:ILE:HG22	1:B:278:ILE:HD11	1.84	0.57
2:C:953:LEU:CD1	2:C:1033:ARG:HG3	2.34	0.57
2:C:1247:SER:HB3	3:D:375:GLU:O	2.03	0.57
5:F:513:ASP:C	5:F:515:GLU:H	2.11	0.57
2:I:1085:MET:HE2	2:I:1085:MET:HA	1.86	0.57
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.86	0.57
3:D:128:LEU:HA	3:D:192:MET:HE1	1.86	0.57
2:I:135:THR:HG22	2:I:527:LYS:HE2	1.85	0.57
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.87	0.57
3:J:438:GLU:OE2	3:J:481:ARG:NH2	2.34	0.57
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.85	0.57
1:B:86:LYS:NZ	3:D:526:VAL:O	2.38	0.57
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.86	0.57
3:J:436:ALA:HB3	3:J:485:MET:HA	1.86	0.57
2:C:470:ARG:HE	2:C:497:PRO:HB3	1.69	0.57
3:D:708:ASN:OD1	3:D:708:ASN:N	2.33	0.57
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.87	0.57
4:K:58:LEU:O	4:K:63:ILE:HG21	2.05	0.57
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.29	0.57
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.34	0.57
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.69	0.57
1:H:105:SER:OG	1:H:139:SER:HA	2.04	0.57
2:I:841:ARG:CZ	3:J:256:ASP:HB3	2.35	0.57
1:B:273:GLU:OE2	1:B:293:PRO:HD2	2.04	0.57
2:C:842:ASP:N	2:C:1045:GLY:O	2.37	0.57
3:D:425:ARG:HG2	3:D:426:ALA:H	1.69	0.57
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.18	0.57
5:F:134:VAL:HA	5:F:273:MET:HE1	1.86	0.57
2:I:106:GLU:OE1	2:I:114:VAL:HG22	2.04	0.57
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	1.86	0.57
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.87	0.57
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:N	1:A:137:ASN:OD1	2.38	0.57
2:C:802:VAL:HG21	2:C:1098:LEU:HD22	1.85	0.57
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.85	0.57
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.87	0.57
5:L:444:ALA:HB1	5:L:457:ILE:HD13	1.87	0.57
2:C:250:THR:HA	2:C:268:ARG:HA	1.85	0.56
2:C:1271:GLY:HA3	3:D:343:LEU:HD12	1.87	0.56
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.87	0.56
5:F:245:ALA:O	5:F:249:ILE:HG13	2.04	0.56
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.85	0.56
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.39	0.56
3:J:1257:VAL:HA	3:J:1260:MET:HG3	1.87	0.56
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.86	0.56
5:L:479:THR:HG23	5:L:481:GLU:H	1.69	0.56
2:C:106:GLU:O	2:C:108:GLU:HA	2.05	0.56
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.17	0.56
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.86	0.56
5:L:245:ALA:O	5:L:249:ILE:HG13	2.05	0.56
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.87	0.56
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.87	0.56
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.88	0.56
2:I:168:GLY:C	2:I:170:VAL:H	2.11	0.56
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.87	0.56
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.69	0.56
4:K:15:ASN:ND2	4:K:18:ASP:OD2	2.36	0.56
5:L:573:LEU:HD11	5:L:588:ARG:HH21	1.70	0.56
2:C:1285:TYR:CD1	3:D:475:GLU:HG2	2.40	0.56
3:D:709:ARG:HD2	3:D:710:ASP:H	1.70	0.56
2:I:208:ILE:HG12	2:I:362:ALA:CB	2.36	0.56
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.54	0.56
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.36	0.56
2:C:93:SER:OG	2:C:126:GLU:OE1	2.17	0.56
2:C:102:LEU:HD23	2:C:117:ILE:HD11	1.88	0.56
2:I:151:ARG:HH22	2:I:175:ARG:NH1	2.04	0.56
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.87	0.56
3:J:770:LEU:H	3:J:770:LEU:HD22	1.70	0.56
2:C:808:ASN:H	3:D:633:ALA:HB2	1.71	0.56
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.41	0.56
3:D:194:LEU:O	3:D:198:CYS:N	2.35	0.56
6:M:141:LEU:O	6:M:145:ARG:HG3	2.05	0.56
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HD13	1:A:304:LYS:HE2	1.86	0.56
3:D:903:LEU:HD22	3:D:909:ILE:HD12	1.87	0.56
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.39	0.56
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.87	0.56
3:J:824:PRO:HD3	3:J:835:LEU:HD13	1.86	0.56
5:L:312:SER:OG	5:L:313:ASP:N	2.39	0.56
1:B:275:ILE:HD11	1:B:284:ARG:HD3	1.86	0.56
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.87	0.56
4:E:8:ASP:HB2	4:E:55:GLU:OE2	2.06	0.56
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.70	0.56
3:J:644:MET:HB2	3:J:764:ARG:HG3	1.88	0.56
3:J:749:LYS:HB3	3:J:755:ILE:HD11	1.87	0.56
2:I:91:THR:HG21	2:I:503:LYS:HE3	1.87	0.56
1:A:12:ARG:H	1:A:30:PRO:HD2	1.69	0.56
2:C:582:ASN:HB3	2:C:586:PHE:H	1.71	0.56
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.53	0.56
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.88	0.56
1:B:318:LEU:O	1:B:320:ASN:N	2.32	0.55
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.89	0.55
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.88	0.55
1:A:296:GLY:N	1:A:299:SER:HB2	2.15	0.55
2:C:624:ASP:OD1	2:C:625:GLU:N	2.38	0.55
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.06	0.55
3:D:681:LYS:HZ2	6:M:12:LEU:HD22	1.71	0.55
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.89	0.55
2:I:462:ASN:O	2:I:466:VAL:HG23	2.06	0.55
3:J:16:GLU:HG3	3:J:17:PHE:H	1.71	0.55
3:J:677:GLU:O	3:J:681:LYS:N	2.37	0.55
3:J:1319:PHE:HB3	3:J:1340:LYS:HD2	1.88	0.55
2:C:714:VAL:HB	2:C:787:PRO:HD2	1.87	0.55
2:I:93:SER:OG	2:I:126:GLU:OE1	2.15	0.55
2:I:156:PHE:CE1	2:I:445:ILE:HG13	2.42	0.55
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.21	0.55
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.42	0.55
2:C:106:GLU:HG3	2:C:107:ARG:H	1.72	0.55
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.88	0.55
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.72	0.55
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.42	0.55
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.42	0.55
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.88	0.55
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:312:SER:OG	5:F:313:ASP:N	2.39	0.55
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.40	0.55
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.89	0.55
3:D:141:PHE:HA	3:D:180:MET:HE2	1.88	0.55
5:F:561:MET:HA	5:F:567:MET:HE1	1.89	0.55
2:I:596:ASP:CG	2:I:597:GLY:N	2.64	0.55
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.42	0.55
2:I:1164:PHE:O	2:I:1166:ASP:N	2.40	0.55
1:A:44:ARG:HB2	1:A:183:ILE:HG21	1.89	0.55
1:A:98:VAL:HG22	1:A:100:LEU:HD12	1.87	0.55
1:B:48:LEU:HD22	3:D:535:ARG:HD3	1.88	0.55
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.71	0.55
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.41	0.55
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.40	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.55
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.32	0.55
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.88	0.55
2:C:1164:PHE:O	2:C:1166:ASP:N	2.39	0.55
3:D:901:ARG:CB	3:D:908:ILE:HA	2.36	0.55
2:I:1067:ALA:HB2	2:I:1073:LYS:HA	1.89	0.55
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.88	0.55
3:J:658:GLU:O	3:J:661:VAL:HG22	2.06	0.55
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.88	0.55
9:M:202:G4P:O2C	9:M:202:G4P:O2'	2.23	0.55
1:B:253:LEU:HB3	1:B:321:TRP:CE2	2.42	0.55
2:C:453:ILE:HD12	2:C:587:LEU:HG	1.88	0.55
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.25	0.55
2:I:693:LEU:HB2	2:I:829:THR:O	2.07	0.55
2:I:710:VAL:HA	2:I:715:THR:HG21	1.88	0.55
3:J:549:LYS:HD3	3:J:569:LEU:HD23	1.88	0.55
5:L:595:LEU:O	5:L:599:ARG:HB2	2.06	0.55
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.87	0.54
3:D:98:ARG:HB3	3:D:248:ASP:OD2	2.07	0.54
3:J:859:PRO:HG2	3:J:862:THR:HG21	1.88	0.54
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.89	0.54
2:C:403:MET:HG3	2:C:584:TYR:CE1	2.43	0.54
3:D:54:ASP:OD1	3:D:54:ASP:N	2.40	0.54
3:D:596:LEU:HD12	3:D:601:ILE:HG13	1.89	0.54
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.89	0.54
1:A:310:ARG:O	5:F:608:ARG:NH2	2.38	0.54
1:B:6:THR:OG1	1:B:7:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.22	0.54
3:D:460:ASP:CG	3:D:462:ASP:OD1	2.50	0.54
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.89	0.54
2:I:800:MET:O	2:I:1229:TYR:HA	2.08	0.54
3:J:258:GLY:HA3	5:L:499:LYS:HE2	1.89	0.54
5:L:115:GLY:HA2	5:L:118:ASP:HB2	1.89	0.54
6:M:98:LYS:NZ	9:M:202:G4P:O4'	2.40	0.54
1:B:29:GLU:HG2	1:B:30:PRO:HD3	1.87	0.54
1:B:323:PRO:CA	1:B:324:ALA:HB2	2.35	0.54
2:C:520:PRO:HG3	2:C:714:VAL:HG21	1.88	0.54
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.39	0.54
1:G:107:ILE:HD11	1:G:136:GLU:HG2	1.90	0.54
3:J:79:LYS:HB2	5:L:569:THR:H	1.72	0.54
3:J:128:LEU:HA	3:J:192:MET:HE1	1.89	0.54
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.41	0.54
1:B:277:TYR:HB2	1:B:321:TRP:HH2	1.71	0.54
5:F:489:MET:O	5:F:491:GLU:N	2.40	0.54
5:F:612:ASP:OD1	5:F:612:ASP:N	2.38	0.54
3:J:274:ASN:OD1	5:L:446:GLN:NE2	2.41	0.54
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.88	0.54
3:D:709:ARG:HD2	3:D:710:ASP:N	2.22	0.54
3:D:1344:LEU:O	3:D:1346:GLY:N	2.39	0.54
5:F:309:ASN:HD21	5:F:312:SER:HB3	1.71	0.54
3:J:48:THR:C	3:J:50:LYS:H	2.11	0.54
5:F:316:PHE:HZ	5:F:334:SER:HA	1.72	0.54
6:M:13:SER:O	6:M:17:ILE:HG13	2.08	0.54
1:B:115:ILE:HG22	1:B:116:THR:H	1.72	0.54
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.90	0.54
5:F:536:THR:O	5:F:540:LEU:N	2.38	0.54
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.43	0.54
3:J:99:ARG:HG3	3:J:249:LEU:HD21	1.90	0.54
1:A:11:PRO:HD2	1:B:227:GLN:HA	1.90	0.54
1:A:47:LEU:O	1:A:180:VAL:HG21	2.08	0.54
1:A:316:MET:CE	5:F:600:HIS:CE1	2.91	0.54
2:C:1075:VAL:HG21	3:D:463:GLY:HA2	1.90	0.54
2:I:148:GLN:NE2	2:I:535:PRO:O	2.39	0.54
3:J:705:THR:HG21	3:J:719:PHE:H	1.71	0.54
5:L:515:GLU:HG2	5:L:516:ASP:N	2.23	0.54
1:B:228:LEU:O	1:B:232:VAL:HG23	2.08	0.53
1:B:268:ASN:O	1:B:271:LYS:HB3	2.07	0.53
2:C:72:SER:O	2:C:99:LYS:N	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.90	0.53
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.73	0.53
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.43	0.53
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.90	0.53
3:D:667:GLN:HG2	3:D:672:LEU:HD12	1.90	0.53
3:J:793:SER:O	3:J:797:THR:HG23	2.07	0.53
3:J:908:ILE:HG12	3:J:909:ILE:N	2.22	0.53
3:J:201:LEU:HB2	3:J:221:ILE:HD13	1.90	0.53
3:J:357:VAL:HG22	3:J:461:PHE:HE1	1.73	0.53
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.90	0.53
3:J:853:THR:CG2	3:J:854:ALA:H	2.10	0.53
2:C:130:MET:SD	2:C:134:GLY:HA2	2.48	0.53
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.89	0.53
2:I:138:ILE:O	2:I:139:ASN:ND2	2.41	0.53
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.90	0.53
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.90	0.53
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.73	0.53
1:H:49:SER:O	1:H:151:GLY:HA2	2.09	0.53
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.44	0.53
3:J:420:PRO:O	3:J:471:PRO:HD2	2.09	0.53
3:D:576:ARG:NH1	3:D:593:ASN:O	2.41	0.53
3:D:903:LEU:HD21	3:D:913:GLU:OE1	2.09	0.53
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.91	0.53
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.90	0.53
2:C:672:GLU:HG2	2:C:1187:PHE:HD2	1.74	0.53
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.43	0.53
4:E:49:ILE:O	4:E:53:GLU:HG3	2.08	0.53
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.42	0.53
5:F:261:LEU:H	5:F:261:LEU:HD12	1.74	0.53
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.41	0.53
3:J:317:THR:HG22	3:J:322:ARG:O	2.09	0.53
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.74	0.53
2:C:455:SER:HA	2:C:459:MET:HE2	1.90	0.53
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.43	0.53
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.90	0.53
3:D:678:ARG:HA	6:M:129:ARG:HH22	1.74	0.53
5:F:391:ALA:HB3	5:F:405:ILE:HG22	1.91	0.53
1:H:27:THR:HB	1:H:202:VAL:HG22	1.91	0.53
1:A:221:ALA:HB1	1:B:228:LEU:HD23	1.90	0.53
2:C:810:TYR:HE1	2:C:1078:LYS:HD2	1.74	0.53
2:C:1116:HIS:HE1	3:D:641:ILE:N	2.03	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.09	0.53
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.91	0.53
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.08	0.53
2:I:1321:GLU:OE2	3:J:99:ARG:HD3	2.09	0.53
3:J:1326:GLN:HB3	3:J:1330:ARG:NH2	2.24	0.53
5:L:612:ASP:OD1	5:L:612:ASP:N	2.42	0.53
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.91	0.52
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.90	0.52
5:F:600:HIS:C	5:F:604:SER:HB3	2.27	0.52
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.91	0.52
3:J:73:GLY:O	3:J:76:LYS:NZ	2.29	0.52
5:L:137:TYR:CE1	5:L:351:THR:HB	2.45	0.52
5:L:139:GLU:HG2	5:L:351:THR:HA	1.90	0.52
3:D:197:GLU:O	3:D:201:LEU:HG	2.09	0.52
3:D:262:THR:HG22	5:F:504:PRO:HB2	1.90	0.52
1:G:137:ASN:OD1	1:G:137:ASN:N	2.42	0.52
3:J:268:LEU:HD11	3:J:324:LEU:HD13	1.90	0.52
3:D:932:MET:HA	3:D:1138:LEU:HB3	1.91	0.52
3:D:1372:ARG:HG3	3:J:853:THR:HB	1.91	0.52
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.74	0.52
1:A:45:ARG:HG3	1:A:46:ILE:HD13	1.90	0.52
2:C:714:VAL:HG12	2:C:765:ILE:HD12	1.91	0.52
3:D:11:GLN:HG2	3:D:15:GLU:CD	2.34	0.52
3:D:510:LEU:HD22	3:D:601:ILE:HD11	1.92	0.52
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.45	0.52
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.43	0.52
1:A:115:ILE:HG22	1:A:116:THR:H	1.73	0.52
2:C:721:GLY:N	2:C:740:GLU:OE1	2.35	0.52
2:C:998:LEU:H	2:C:998:LEU:HD12	1.74	0.52
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.92	0.52
5:F:279:ARG:NH2	5:F:350:GLU:OE2	2.36	0.52
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.92	0.52
2:I:411:ARG:NH2	2:I:424:ASP:OD1	2.38	0.52
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.49	0.52
2:I:891:GLY:O	2:I:892:GLU:HG3	2.10	0.52
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.91	0.52
2:C:1334:GLY:H	3:D:113:HIS:HE2	1.55	0.52
2:I:169:LYS:O	2:I:170:VAL:HG22	2.09	0.52
3:J:850:LYS:HE2	3:J:855:ASP:HB3	1.92	0.52
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.92	0.52
4:E:46:THR:HA	4:E:49:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.92	0.52
3:J:449:LEU:HD22	3:J:466:MET:SD	2.50	0.52
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.09	0.52
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.45	0.52
1:A:14:VAL:HG22	1:A:15:ASP:N	2.25	0.52
2:C:252:SER:H	2:C:255:ILE:HD11	1.75	0.52
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.92	0.52
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.92	0.52
2:I:38:PHE:HB2	2:I:457:GLY:HA2	1.91	0.52
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.09	0.52
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.74	0.52
3:J:903:LEU:HD23	3:J:905:ARG:HD3	1.92	0.52
3:J:1257:VAL:HG22	3:J:1260:MET:HE2	1.92	0.52
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.91	0.52
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.33	0.52
1:A:112:ALA:O	1:A:115:ILE:HG13	2.10	0.52
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.75	0.52
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.92	0.52
1:H:102:LEU:O	1:H:141:SER:HA	2.10	0.52
2:I:356:THR:HG21	2:I:362:ALA:HA	1.92	0.52
3:J:218:THR:HG21	3:J:1275:LEU:HD21	1.92	0.52
3:J:668:PHE:CD1	3:J:678:ARG:HG2	2.44	0.52
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.91	0.52
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.91	0.52
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.91	0.52
3:D:156:ARG:NH1	3:D:157:GLN:HE21	2.07	0.52
3:D:425:ARG:HG2	3:D:426:ALA:N	2.24	0.52
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.91	0.52
5:F:111:LEU:HD13	5:F:116:GLU:HA	1.92	0.52
1:G:75:GLN:HA	2:I:729:ALA:N	2.25	0.52
2:I:452:ARG:NH1	2:I:585:GLY:HA3	2.25	0.52
3:J:517:CYS:HB3	3:J:719:PHE:CE2	2.45	0.52
3:J:747:MET:HE3	3:J:778:GLY:HA3	1.91	0.52
5:L:320:ILE:O	5:L:327:SER:HB3	2.10	0.52
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.90	0.52
2:C:18:ARG:NH1	2:C:622:ASN:OD1	2.38	0.51
2:C:106:GLU:HG3	2:C:107:ARG:N	2.25	0.51
3:D:783:LEU:HD23	6:M:76:ALA:CB	2.40	0.51
2:I:920:VAL:HG22	2:I:1054:LEU:HD21	1.92	0.51
2:I:1142:ARG:HH11	2:I:1161:LEU:HD11	1.75	0.51
2:I:1282:GLY:O	2:I:1284:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:52:ARG:HB2	6:M:52:ARG:HH11	1.75	0.51
2:C:941:LYS:HB2	2:C:946:LEU:HG	1.92	0.51
5:F:575:GLU:O	5:F:579:GLN:HG2	2.10	0.51
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.92	0.51
2:I:949:GLU:HG2	2:I:1036:ILE:HG22	1.92	0.51
2:I:1296:ASP:CG	2:I:1322:SER:HB3	2.35	0.51
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.91	0.51
3:J:747:MET:HB2	3:J:774:ILE:HG22	1.92	0.51
5:L:244:THR:O	5:L:247:GLU:HG2	2.10	0.51
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.10	0.51
1:B:44:ARG:HD2	1:B:183:ILE:HD13	1.92	0.51
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.45	0.51
2:C:1106:ARG:NE	3:D:731:ARG:HH21	2.08	0.51
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.24	0.51
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.91	0.51
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.92	0.51
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.92	0.51
1:A:228:LEU:HA	1:A:231:PHE:HB2	1.93	0.51
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.76	0.51
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.75	0.51
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.92	0.51
3:D:26:SER:HB2	3:D:236:TRP:CZ2	2.45	0.51
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.26	0.51
5:F:151:VAL:HG22	5:F:156:ALA:HB3	1.92	0.51
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.93	0.51
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.92	0.51
5:L:316:PHE:HZ	5:L:334:SER:HA	1.76	0.51
1:A:66:HIS:HE1	1:A:69:SER:HB3	1.75	0.51
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.91	0.51
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.26	0.51
3:D:460:ASP:OD2	3:D:462:ASP:OD1	2.28	0.51
3:D:850:LYS:HD3	3:D:875:ASN:ND2	2.26	0.51
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.92	0.51
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.19	0.51
1:G:133:LEU:HD12	1:G:138:ALA:HB3	1.93	0.51
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.92	0.51
1:A:72:GLU:OE2	2:C:958:LYS:NZ	2.40	0.51
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.93	0.51
2:C:302:ILE:O	2:C:330:HIS:NE2	2.40	0.51
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.76	0.51
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:399:LEU:HD22	5:F:447:ALA:HB2	1.93	0.51
3:J:495:ASN:C	3:J:497:GLU:H	2.19	0.51
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.26	0.51
2:C:106:GLU:N	2:C:109:ALA:CB	2.73	0.51
2:C:417:SER:OG	2:C:419:ILE:O	2.23	0.51
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.93	0.51
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.25	0.51
4:E:2:ALA:HB2	4:E:55:GLU:CD	2.36	0.51
2:I:1148:ALA:HA	2:I:1201:LEU:CD2	2.38	0.51
2:I:1331:ARG:HG2	3:J:33:TRP:CZ3	2.46	0.51
3:J:320:ASN:OD1	3:J:322:ARG:HB3	2.11	0.51
3:J:504:GLN:HG3	3:J:505:ASP:H	1.76	0.51
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.93	0.51
2:C:80:PHE:HB3	2:C:84:GLU:HB2	1.92	0.51
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.41	0.51
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.75	0.51
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.76	0.51
1:B:186:ASN:HD22	1:B:202:VAL:HB	1.76	0.50
2:C:515:MET:HG2	2:C:517:GLN:HB2	1.93	0.50
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.10	0.50
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.20	0.50
2:I:706:ARG:NH2	2:I:791:LEU:O	2.44	0.50
4:K:15:ASN:C	4:K:17:PHE:H	2.20	0.50
5:L:137:TYR:HE1	5:L:351:THR:HB	1.76	0.50
3:D:110:PRO:HB3	3:D:238:ILE:CG2	2.41	0.50
3:D:528:THR:O	3:D:551:ARG:HB3	2.12	0.50
3:D:770:LEU:H	3:D:770:LEU:HD22	1.77	0.50
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.94	0.50
1:H:46:ILE:HD11	1:H:224:LEU:HD13	1.92	0.50
2:I:42:ASP:O	2:I:44:GLU:N	2.43	0.50
2:I:1061:GLN:HG3	2:I:1239:VAL:HG11	1.93	0.50
6:M:78:GLN:HG2	6:M:82:PHE:HE2	1.77	0.50
2:C:903:ARG:HE	2:C:910:ALA:HB2	1.76	0.50
2:C:1271:GLY:HA2	3:D:344:GLY:HA3	1.92	0.50
5:F:139:GLU:HG2	5:F:351:THR:HA	1.93	0.50
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.93	0.50
2:I:921:PRO:O	2:I:924:VAL:HG22	2.11	0.50
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.92	0.50
6:M:18:ALA:C	6:M:20:VAL:H	2.19	0.50
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.94	0.50
2:C:540:ARG:HB2	2:C:540:ARG:HH11	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.94	0.50
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.94	0.50
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.94	0.50
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.30	0.50
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.93	0.50
5:F:525:ASP:CG	5:F:528:LEU:HG	2.36	0.50
1:G:23:HIS:HB2	1:G:205:MET:O	2.12	0.50
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.94	0.50
2:I:620:ASN:O	2:I:620:ASN:ND2	2.44	0.50
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.94	0.50
1:H:62:ASP:OD1	1:H:62:ASP:N	2.30	0.50
2:I:670:PHE:CD2	2:I:1113:LEU:HB3	2.47	0.50
2:I:1247:SER:HB3	3:J:375:GLU:O	2.11	0.50
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.93	0.50
3:J:836:ARG:HD2	3:J:873:GLU:OE1	2.11	0.50
6:M:71:ASP:OD1	6:M:73:VAL:HG23	2.11	0.50
1:B:214:GLU:O	1:B:218:ARG:HG3	2.11	0.50
2:C:88:ARG:HB2	2:C:88:ARG:HH11	1.76	0.50
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.27	0.50
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.12	0.50
2:C:1282:GLY:O	2:C:1284:ALA:N	2.44	0.50
3:D:81:ARG:C	3:D:83:VAL:H	2.20	0.50
3:J:355:ILE:HG21	3:J:466:MET:HG3	1.93	0.50
5:L:322:MET:HE2	5:L:324:LYS:HZ3	1.76	0.50
5:L:489:MET:HE2	5:L:493:LYS:HB2	1.94	0.50
1:B:73:GLY:O	1:B:134:THR:HG22	2.12	0.50
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.94	0.50
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.93	0.50
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.93	0.50
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.76	0.50
2:I:144:VAL:HG11	2:I:527:LYS:HA	1.93	0.50
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.94	0.50
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.76	0.50
3:J:141:PHE:HA	3:J:180:MET:HE2	1.93	0.50
3:J:661:VAL:HG11	3:J:686:TRP:CE2	2.47	0.50
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.12	0.50
6:M:15:LEU:HD13	6:M:22:PRO:HG3	1.93	0.50
1:B:253:LEU:HB3	1:B:321:TRP:CZ2	2.47	0.50
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.52	0.50
5:F:147:GLN:HE22	5:F:150:ARG:HH11	1.58	0.50
2:I:174:ALA:N	2:I:186:PHE:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:235:ASN:O	2:I:236:LYS:CB	2.52	0.50
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.94	0.50
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.92	0.50
3:J:797:THR:O	3:J:801:VAL:HG12	2.12	0.50
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.93	0.50
2:C:91:THR:HB	2:C:138:ILE:O	2.12	0.50
2:C:363:LEU:HD13	2:C:382:GLU:HG2	1.93	0.50
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.76	0.50
2:C:1255:THR:O	2:C:1257:GLN:N	2.45	0.50
3:D:317:THR:HA	3:D:324:LEU:HD23	1.93	0.50
5:F:372:ALA:O	5:F:376:LYS:HG3	2.12	0.50
2:I:445:ILE:HG23	2:I:451:ARG:HE	1.76	0.50
2:I:894:GLN:HE21	3:J:78:LEU:HD21	1.77	0.50
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.92	0.50
1:B:29:GLU:OE1	1:B:30:PRO:HD3	2.12	0.49
1:B:94:GLY:H	1:B:276:HIS:HD2	1.56	0.49
1:B:98:VAL:HG22	1:B:100:LEU:HD12	1.92	0.49
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.76	0.49
2:C:1269:ARG:HG3	3:D:346:ARG:HG2	1.94	0.49
2:I:519:ASN:ND2	2:I:689:ALA:HB3	2.27	0.49
3:J:253:VAL:HG21	5:L:523:ILE:HG21	1.93	0.49
3:J:425:ARG:HG2	3:J:426:ALA:N	2.27	0.49
3:J:1178:THR:HA	3:J:1184:ASP:HB2	1.93	0.49
5:L:354:THR:O	5:L:358:VAL:HG23	2.12	0.49
2:C:13:LYS:HA	2:C:1157:GLN:OE1	2.12	0.49
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.42	0.49
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.94	0.49
2:C:730:SER:O	2:C:753:LEU:HB2	2.12	0.49
5:F:343:LYS:H	5:F:343:LYS:HD2	1.77	0.49
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.95	0.49
3:J:489:ASN:HA	3:J:904:ALA:CB	2.41	0.49
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.94	0.49
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.26	0.49
3:D:705:THR:OG1	3:D:718:SER:HA	2.12	0.49
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.93	0.49
5:F:453:PRO:O	5:F:456:MET:HB2	2.12	0.49
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.10	0.49
3:J:657:ALA:HA	3:J:660:GLU:HB2	1.95	0.49
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.10	0.49
3:J:1206:ARG:NH2	3:J:1223:LEU:O	2.46	0.49
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:ARG:NH1	2:C:382:GLU:OE2	2.46	0.49
2:C:1106:ARG:O	2:C:1108:ASN:N	2.44	0.49
2:C:1305:TYR:OH	5:F:532:LEU:HG	2.12	0.49
3:D:1137:GLY:H	3:D:1140:ARG:HB3	1.77	0.49
2:I:1287:LEU:HD22	3:J:1357:ILE:HG13	1.94	0.49
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.27	0.49
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.94	0.49
2:C:563:THR:HG22	2:C:680:LEU:HD11	1.94	0.49
2:C:744:GLY:C	2:C:746:ALA:H	2.20	0.49
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.46	0.49
5:F:233:ASP:O	5:F:236:LYS:HE2	2.13	0.49
5:F:388:ILE:O	5:F:392:LYS:HG3	2.13	0.49
2:I:924:VAL:HG12	2:I:1058:ARG:HH21	1.78	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.12	0.49
3:J:56:LEU:HD12	3:J:56:LEU:H	1.77	0.49
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.94	0.49
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	1.95	0.49
2:C:1340:GLU:HG3	3:D:21:LYS:HB2	1.93	0.49
3:D:905:ARG:NH1	4:E:16:ARG:HB2	2.27	0.49
3:D:1243:LEU:O	6:M:63:GLN:HG2	2.12	0.49
5:F:320:ILE:HG23	5:F:327:SER:O	2.13	0.49
5:F:449:THR:OG1	5:F:503:GLU:OE1	2.31	0.49
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.13	0.49
2:C:138:ILE:O	2:C:139:ASN:ND2	2.45	0.49
3:D:16:GLU:O	3:D:1369:ARG:NH2	2.46	0.49
3:D:436:ALA:HB3	3:D:485:MET:HA	1.94	0.49
3:D:859:PRO:HD2	3:D:862:THR:HG21	1.94	0.49
3:D:1178:THR:HG23	3:D:1184:ASP:CB	2.43	0.49
3:D:1361:THR:HG22	4:E:21:LEU:HD22	1.94	0.49
5:F:316:PHE:CZ	5:F:334:SER:HA	2.48	0.49
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.95	0.49
1:G:68:TYR:HE2	2:I:927:THR:HB	1.76	0.49
1:H:151:GLY:O	1:H:177:TYR:HB2	2.12	0.49
2:I:1120:ALA:HA	2:I:1204:LEU:HD12	1.94	0.49
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.48	0.49
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.95	0.49
1:A:318:LEU:O	1:A:320:ASN:N	2.41	0.49
1:B:62:ASP:HB3	1:B:71:LYS:HZ2	1.78	0.49
1:B:94:GLY:HA2	1:B:277:TYR:CE2	2.47	0.49
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.13	0.49
2:C:1080:ASN:CB	2:C:1085:MET:HE3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:285:LEU:HB3	5:F:413:MET:HE1	1.94	0.49
3:D:504:GLN:HG3	3:D:505:ASP:H	1.76	0.49
4:E:3:ARG:HD2	9:E:101:G4P:H4'	1.95	0.49
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.48	0.49
3:J:115:TRP:HZ2	3:J:328:ALA:HB2	1.77	0.49
1:A:251:PRO:HD2	5:F:605:GLU:HG3	1.95	0.49
1:B:79:LEU:HD21	3:D:526:VAL:HG21	1.95	0.49
2:C:402:ARG:NE	2:C:417:SER:O	2.46	0.49
2:C:1293:VAL:HG13	2:C:1301:ARG:HA	1.95	0.49
3:D:336:GLY:HA3	3:D:1324:SER:O	2.12	0.49
3:D:394:ILE:HG12	5:F:536:THR:HG22	1.95	0.49
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.13	0.49
5:F:484:ALA:O	5:F:491:GLU:HB2	2.12	0.49
5:F:600:HIS:HB3	5:F:601:PRO:CD	2.43	0.49
1:G:231:PHE:HB3	1:H:218:ARG:HB3	1.94	0.49
1:H:76:GLU:OE1	1:H:76:GLU:N	2.46	0.49
3:J:825:VAL:C	3:J:826:ILE:HG13	2.38	0.49
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.28	0.49
5:L:463:LEU:HA	5:L:466:ILE:HD12	1.95	0.49
1:A:249:PHE:CD1	1:A:321:TRP:HZ3	2.31	0.49
1:A:257:VAL:HG13	1:A:276:HIS:O	2.13	0.49
2:C:61:SER:O	2:C:63:SER:N	2.45	0.49
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.38	0.49
2:C:796:LEU:H	2:C:796:LEU:HD12	1.78	0.49
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.95	0.49
3:D:747:MET:HB2	3:D:774:ILE:HG22	1.95	0.49
9:E:101:G4P:O1C	9:E:101:G4P:O2'	2.27	0.49
2:I:32:LEU:HD23	2:I:130:MET:SD	2.53	0.49
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.48	0.49
3:J:288:PRO:O	3:J:292:VAL:HG13	2.13	0.49
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.76	0.49
6:M:108:ASP:O	6:M:108:ASP:OD2	2.31	0.49
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.94	0.48
2:C:169:LYS:O	2:C:170:VAL:HG22	2.13	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.76	0.48
5:F:511:ILE:HG21	5:F:522:PHE:CE2	2.48	0.48
5:F:551:LEU:HD11	5:F:598:LEU:HD11	1.94	0.48
1:A:104:LYS:HB3	1:A:110:VAL:HG13	1.95	0.48
2:C:145:ILE:HA	2:C:511:LEU:O	2.13	0.48
2:C:228:VAL:HG22	2:C:245:ARG:HE	1.78	0.48
3:D:53:ARG:HA	3:D:54:ASP:HA	1.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:4:VAL:HG13	4:E:5:THR:N	2.28	0.48
5:F:127:ILE:O	5:F:130:VAL:HG22	2.13	0.48
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.28	0.48
5:L:478:PRO:HG2	5:L:483:LEU:HD11	1.95	0.48
1:A:315:GLY:C	1:A:316:MET:HG3	2.38	0.48
2:C:245:ARG:HG2	2:C:337:PHE:CE2	2.48	0.48
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.79	0.48
3:D:820:ILE:HD11	3:D:822:MET:HE2	1.96	0.48
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.48	0.48
5:L:469:GLN:O	5:L:473:GLU:HB2	2.12	0.48
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.27	0.48
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.44	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.94	0.48
2:C:1293:VAL:HG11	2:C:1304:MET:HG2	1.95	0.48
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.95	0.48
3:D:1227:HIS:HB2	3:J:1293:GLU:OE1	2.14	0.48
1:G:166:ARG:O	1:G:167:PRO:C	2.56	0.48
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.94	0.48
2:I:314:ASN:O	2:I:352:ARG:NH1	2.46	0.48
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.43	0.48
3:J:88:CYS:O	3:J:90:VAL:N	2.47	0.48
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.70	0.48
1:A:250:ASP:HB2	5:F:601:PRO:HB3	1.96	0.48
1:B:195:ARG:HG3	1:B:198:LEU:HD11	1.96	0.48
2:C:670:PHE:CD1	2:C:1184:THR:HG21	2.48	0.48
1:H:59:VAL:O	1:H:171:LEU:HB2	2.13	0.48
2:I:800:MET:HE2	2:I:1095:ASP:HB3	1.95	0.48
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.95	0.48
2:I:903:ARG:HD2	2:I:908:GLU:O	2.13	0.48
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.13	0.48
2:I:1272:GLU:HB2	3:J:342:LEU:CB	2.44	0.48
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.25	0.48
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.28	0.48
1:A:23:HIS:HE1	1:A:204:GLU:CG	2.25	0.48
1:A:224:LEU:O	1:A:228:LEU:HD12	2.14	0.48
5:F:555:GLU:O	5:F:559:LEU:HB2	2.14	0.48
2:I:518:ASN:O	2:I:691:PRO:HD3	2.13	0.48
1:A:135:ASP:O	1:A:138:ALA:N	2.33	0.48
1:A:220:ALA:O	1:A:223:ILE:HG13	2.14	0.48
2:C:47:TYR:OH	2:C:398:SER:HB2	2.12	0.48
2:C:202:ARG:HB2	2:C:369:MET:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:519:ASN:ND2	2:C:689:ALA:HB3	2.29	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.78	0.48
3:J:131:PRO:O	3:J:135:ILE:HG13	2.13	0.48
5:L:287:ILE:HD13	5:L:315:TRP:CH2	2.48	0.48
1:A:285:THR:OG1	1:A:286:GLU:N	2.44	0.48
1:B:44:ARG:HE	3:D:538:ARG:HB3	1.79	0.48
1:B:65:LEU:O	1:B:66:HIS:ND1	2.46	0.48
2:C:395:TYR:CD2	2:C:419:ILE:HG22	2.45	0.48
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.49	0.48
1:G:13:LEU:HD23	1:G:13:LEU:H	1.78	0.48
2:I:156:PHE:CD2	2:I:175:ARG:HB3	2.48	0.48
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.96	0.48
3:J:679:TYR:O	3:J:683:ILE:HG13	2.13	0.48
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.96	0.48
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.95	0.48
2:C:802:VAL:HG11	2:C:1230:MET:HB3	1.96	0.48
2:C:1063:GLY:HA3	2:C:1239:VAL:HB	1.95	0.48
1:G:140:ILE:HG13	1:G:140:ILE:O	2.14	0.48
3:J:156:ARG:NH2	3:J:191:SER:OG	2.45	0.48
6:M:55:VAL:O	6:M:59:VAL:HG23	2.13	0.48
1:A:261:GLU:CD	2:C:859:GLU:HB2	2.39	0.48
1:A:316:MET:HE3	1:A:316:MET:HB2	1.77	0.48
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.95	0.48
3:D:227:PHE:O	3:D:230:SER:HB3	2.13	0.48
3:D:746:LEU:O	6:M:84:LEU:HD13	2.14	0.48
5:F:470:MET:O	5:F:478:PRO:HD3	2.14	0.48
2:I:1086:PRO:HB3	2:I:1212:LEU:HD23	1.95	0.48
2:I:1281:TYR:OH	3:J:434:ILE:O	2.32	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.14	0.48
2:C:27:LEU:O	2:C:528:ARG:NH1	2.46	0.47
2:C:131:THR:OG1	2:C:135:THR:O	2.32	0.47
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.29	0.47
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.96	0.47
5:F:253:SER:O	5:F:257:LYS:HG3	2.14	0.47
5:L:308:GLY:HA2	5:L:356:GLU:OE1	2.14	0.47
3:D:365:GLN:O	3:D:437:PHE:HD1	1.97	0.47
1:G:76:GLU:OE2	1:G:76:GLU:N	2.47	0.47
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.80	0.47
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.96	0.47
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.96	0.47
3:J:848:VAL:HG12	3:J:857:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.95	0.47
1:A:295:LEU:HD22	1:A:300:LEU:HD23	1.97	0.47
1:B:192:VAL:O	1:B:193:GLU:C	2.58	0.47
2:C:201:ARG:NH2	2:C:370:MET:O	2.47	0.47
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.39	0.47
5:F:608:ARG:HB2	5:F:608:ARG:HH11	1.79	0.47
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.94	0.47
2:I:239:MET:N	2:I:285:ILE:O	2.45	0.47
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.44	0.47
2:I:1286:THR:N	3:J:479:GLU:OE2	2.42	0.47
3:J:656:GLU:OE1	3:J:692:ARG:NH2	2.41	0.47
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.96	0.47
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.97	0.47
3:D:478:LEU:HG	4:E:47:THR:HG23	1.97	0.47
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.43	0.47
3:J:1221:LEU:HB2	3:J:1229:VAL:HG11	1.95	0.47
6:M:144:ILE:HG23	6:M:147:LYS:HE2	1.96	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.49	0.47
3:D:27:PRO:O	3:D:31:ARG:HG3	2.13	0.47
3:D:511:TYR:OH	3:D:515:ARG:NH1	2.47	0.47
3:D:614:LEU:HD22	4:E:7:GLN:HB2	1.97	0.47
1:H:18:GLN:HA	1:H:24:ALA:HA	1.95	0.47
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.46	0.47
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.96	0.47
1:B:29:GLU:OE1	1:B:30:PRO:CD	2.62	0.47
1:B:104:LYS:HG3	1:B:105:SER:N	2.29	0.47
1:B:270:LEU:HD22	1:B:275:ILE:HG21	1.96	0.47
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.94	0.47
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.44	0.47
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.97	0.47
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.45	0.47
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.97	0.47
3:D:638:SER:OG	3:D:639:VAL:N	2.47	0.47
3:D:674:THR:CG2	6:M:139:LYS:HG2	2.43	0.47
5:F:130:VAL:HB	5:F:365:MET:HG3	1.97	0.47
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.96	0.47
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.30	0.47
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.79	0.47
2:I:518:ASN:OD1	2:I:518:ASN:N	2.47	0.47
2:I:601:ASP:OD1	2:I:601:ASP:N	2.46	0.47
3:J:53:ARG:HA	3:J:54:ASP:HA	1.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:337:ARG:NH2	3:J:1323:ALA:HB3	2.29	0.47
5:L:353:LEU:HD13	5:L:361:ILE:HD12	1.96	0.47
1:B:53:GLY:C	1:B:177:TYR:HB3	2.39	0.47
1:B:82:LEU:HD22	1:B:173:VAL:HG12	1.97	0.47
1:B:112:ALA:O	1:B:115:ILE:HG13	2.15	0.47
1:B:215:GLU:HA	1:B:218:ARG:HD2	1.95	0.47
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.14	0.47
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.50	0.47
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.97	0.47
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.96	0.47
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.29	0.47
3:D:405:GLU:O	3:D:408:VAL:HG22	2.15	0.47
3:D:689:ALA:O	3:D:693:VAL:HG23	2.15	0.47
4:E:2:ALA:HB2	4:E:55:GLU:OE1	2.15	0.47
1:G:231:PHE:HA	1:H:218:ARG:HG2	1.97	0.47
1:H:100:LEU:HB3	1:H:115:ILE:CG2	2.45	0.47
1:H:215:GLU:HA	1:H:218:ARG:HG3	1.97	0.47
2:I:119:GLU:HG3	2:I:489:PRO:CD	2.40	0.47
3:J:214:ARG:HA	3:J:217:LEU:HB3	1.96	0.47
3:J:275:ARG:HG2	3:J:278:ARG:HH12	1.80	0.47
3:J:337:ARG:HD2	3:J:1324:SER:HA	1.97	0.47
3:J:355:ILE:HG21	3:J:466:MET:CG	2.45	0.47
3:J:850:LYS:HG2	3:J:857:LEU:CD2	2.44	0.47
5:L:111:LEU:HD13	5:L:116:GLU:HA	1.96	0.47
5:L:114:GLU:O	5:L:117:ILE:N	2.43	0.47
5:L:357:GLN:HA	5:L:360:ASP:HB2	1.97	0.47
5:L:395:THR:OG1	5:L:396:ASN:N	2.47	0.47
5:L:483:LEU:HD12	5:L:483:LEU:H	1.79	0.47
5:L:561:MET:HA	5:L:567:MET:CE	2.45	0.47
1:A:95:LYS:O	1:A:148:ARG:NH2	2.47	0.47
1:B:224:LEU:O	1:B:228:LEU:HD12	2.15	0.47
2:C:155:VAL:HA	2:C:175:ARG:O	2.15	0.47
2:C:325:LEU:O	2:C:330:HIS:HB2	2.15	0.47
2:C:800:MET:HE1	2:C:822:VAL:HG13	1.96	0.47
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.96	0.47
3:D:99:ARG:HG3	3:D:249:LEU:HD21	1.97	0.47
2:I:384:LEU:O	2:I:388:LEU:HG	2.14	0.47
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.44	0.47
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.97	0.47
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.14	0.47
5:L:489:MET:O	5:L:491:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:344:GLY:HA3	2:C:346:TYR:CE2	2.50	0.47
2:C:620:ASN:ND2	2:C:620:ASN:O	2.47	0.47
3:D:43:THR:OG1	5:F:449:THR:O	2.20	0.47
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.97	0.47
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	1.96	0.47
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.96	0.47
1:H:91:ARG:HD2	1:H:210:THR:HB	1.97	0.47
2:I:963:GLU:O	2:I:967:LEU:HB2	2.14	0.47
2:I:1251:TYR:OH	3:J:348:ASP:OD2	2.20	0.47
3:J:678:ARG:O	3:J:682:VAL:HG23	2.15	0.47
3:J:705:THR:OG1	3:J:718:SER:HA	2.14	0.47
5:L:515:GLU:HG2	5:L:516:ASP:H	1.79	0.47
6:M:44:LEU:CD2	6:M:99:ILE:HG23	2.43	0.47
3:D:598:LYS:O	3:D:601:ILE:HG22	2.14	0.47
3:D:1239:ASP:O	3:D:1243:LEU:HB2	2.14	0.47
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.30	0.47
5:F:561:MET:HE3	5:F:561:MET:HB2	1.88	0.47
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.55	0.47
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.80	0.47
3:J:268:LEU:CB	3:J:306:LEU:HD23	2.44	0.47
1:A:18:GLN:HE22	1:A:213:PRO:HD2	1.79	0.46
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.80	0.46
2:C:119:GLU:HG3	2:C:489:PRO:HD2	1.96	0.46
2:C:338:THR:HG22	2:C:345:PRO:HB3	1.97	0.46
3:D:491:LEU:HD22	3:D:496:GLY:O	2.15	0.46
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.97	0.46
2:I:690:VAL:HB	2:I:1236:ASN:HB3	1.97	0.46
2:I:1313:HIS:HB2	3:J:474:LEU:HD13	1.97	0.46
3:J:308:ASP:CG	3:J:311:ARG:HE	2.22	0.46
3:J:694:SER:O	3:J:698:MET:HB2	2.15	0.46
5:L:343:LYS:O	5:L:347:ILE:HG13	2.15	0.46
1:B:142:MET:HE2	1:B:142:MET:HB3	1.76	0.46
2:C:106:GLU:HB2	2:C:109:ALA:HB2	1.82	0.46
2:C:739:ASP:N	2:C:739:ASP:OD1	2.48	0.46
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.97	0.46
3:D:556:GLU:O	3:D:564:VAL:HB	2.15	0.46
3:D:850:LYS:HG2	3:D:857:LEU:HD11	1.95	0.46
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.97	0.46
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.73	0.46
3:J:809:VAL:HA	3:J:894:VAL:O	2.14	0.46
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:161:LEU:C	5:L:262:VAL:HG23	2.39	0.46
5:L:584:ARG:HA	5:L:584:ARG:HD2	1.71	0.46
1:B:250:ASP:OD1	1:B:252:ILE:HB	2.16	0.46
1:B:281:LEU:HD11	1:B:303:ILE:HG21	1.97	0.46
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.67	0.46
2:C:518:ASN:OD1	2:C:518:ASN:N	2.48	0.46
3:D:680:ASN:HB2	9:M:202:G4P:C2	2.45	0.46
3:D:786:THR:CG2	6:M:75:ARG:HG2	2.45	0.46
5:F:138:PRO:HD2	5:F:353:LEU:HD11	1.97	0.46
5:F:600:HIS:CB	5:F:601:PRO:CD	2.93	0.46
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.97	0.46
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.80	0.46
2:I:979:LEU:HA	2:I:1002:LEU:HD13	1.97	0.46
2:I:992:LEU:HD12	2:I:996:ARG:HB3	1.97	0.46
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.50	0.46
3:J:826:ILE:HD12	3:J:826:ILE:O	2.15	0.46
5:L:513:ASP:C	5:L:515:GLU:H	2.22	0.46
2:C:202:ARG:O	2:C:369:MET:HE2	2.14	0.46
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.97	0.46
2:C:902:LEU:HD12	5:F:607:LEU:HD23	1.98	0.46
3:D:677:GLU:CG	6:M:129:ARG:NH1	2.79	0.46
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.50	0.46
4:E:26:ARG:NH2	4:E:38:LEU:HD13	2.30	0.46
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.62	0.46
2:C:42:ASP:C	2:C:44:GLU:H	2.24	0.46
2:C:468:LEU:O	2:C:471:VAL:HG12	2.16	0.46
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.45	0.46
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.16	0.46
3:D:356:THR:OG1	3:D:357:VAL:N	2.48	0.46
3:D:500:ILE:HG22	3:D:500:ILE:O	2.15	0.46
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.98	0.46
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.49	0.46
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.97	0.46
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.96	0.46
2:I:671:LEU:HD23	2:I:1186:VAL:CG1	2.46	0.46
3:J:657:ALA:O	3:J:661:VAL:HG13	2.15	0.46
2:C:147:SER:OG	2:C:455:SER:HB3	2.16	0.46
2:C:699:LEU:HD23	2:C:699:LEU:HA	1.60	0.46
3:D:797:THR:O	3:D:801:VAL:HG12	2.15	0.46
3:D:826:ILE:HD12	3:D:826:ILE:O	2.15	0.46
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:748:ALA:O	3:J:777:HIS:HD2	1.97	0.46
3:J:1167:LYS:HG2	3:J:1168:GLU:H	1.80	0.46
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.23	0.46
1:A:115:ILE:HG22	1:A:116:THR:N	2.31	0.46
1:A:135:ASP:HB2	2:C:726:TYR:HE1	1.80	0.46
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.50	0.46
1:B:185:TYR:HA	1:B:202:VAL:O	2.15	0.46
2:C:928:VAL:HG22	2:C:1054:LEU:HD11	1.98	0.46
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.27	0.46
1:G:104:LYS:HG2	1:G:110:VAL:HG13	1.98	0.46
2:I:109:ALA:HB1	2:I:110:PRO:HD2	1.97	0.46
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.98	0.46
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.44	0.46
3:J:460:ASP:CG	3:J:462:ASP:OD1	2.59	0.46
5:L:147:GLN:O	5:L:151:VAL:HG23	2.16	0.46
1:B:94:GLY:HA2	1:B:277:TYR:HE2	1.81	0.46
1:B:115:ILE:HG22	1:B:116:THR:N	2.29	0.46
3:D:899:TYR:CD1	3:D:915:ILE:HD12	2.51	0.46
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.97	0.46
3:J:255:LEU:HA	3:J:255:LEU:HD13	1.84	0.46
3:J:398:LYS:HE2	5:L:532:LEU:HD23	1.97	0.46
3:J:478:LEU:HG	4:K:47:THR:HG23	1.97	0.46
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.46	0.46
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.46	0.46
2:I:896:THR:O	2:I:897:PRO:C	2.58	0.46
3:J:57:PHE:CE2	3:J:252:LEU:HD12	2.51	0.46
3:J:57:PHE:HB3	3:J:98:ARG:NH2	2.31	0.46
3:J:700:ASN:O	3:J:704:GLU:HB2	2.16	0.46
3:J:901:ARG:HD2	3:J:906:GLY:O	2.15	0.46
1:A:223:ILE:HD13	1:B:8:PHE:HE2	1.81	0.46
1:B:187:VAL:HG13	1:B:200:LYS:O	2.16	0.46
2:C:882:ILE:HD12	2:C:882:ILE:H	1.82	0.46
2:I:151:ARG:NH1	2:I:542:ARG:HH12	2.13	0.46
2:I:673:HIS:O	2:I:1109:ILE:HG22	2.16	0.46
2:I:818:VAL:HB	2:I:1076:ILE:HD11	1.98	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.16	0.46
3:J:227:PHE:O	3:J:230:SER:HB3	2.16	0.46
3:J:479:GLU:CG	4:K:20:VAL:HG11	2.46	0.46
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.81	0.45
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.81	0.45
3:J:803:VAL:HG22	3:J:1259:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:HG2	1:B:183:ILE:N	2.31	0.45
2:C:820:GLU:N	2:C:1080:ASN:O	2.48	0.45
2:C:979:LEU:HD21	2:C:1000:LEU:HD13	1.98	0.45
5:F:226:ALA:O	5:F:229:VAL:HG22	2.16	0.45
1:G:32:GLU:HA	1:G:198:LEU:HD22	1.98	0.45
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.32	0.45
2:I:478:ARG:NH2	2:I:487:LEU:HD13	2.31	0.45
2:I:617:ALA:HA	2:I:636:CYS:SG	2.56	0.45
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.98	0.45
2:I:807:TRP:HE1	2:I:1086:PRO:HD3	1.81	0.45
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.97	0.45
2:I:1222:GLU:OE2	3:J:537:TYR:OH	2.28	0.45
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.81	0.45
6:M:91:ARG:NH1	9:M:202:G4P:O2'	2.48	0.45
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.98	0.45
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.81	0.45
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.99	0.45
5:F:166:VAL:O	5:F:167:ASP:HB2	2.16	0.45
2:I:802:VAL:HG11	2:I:1230:MET:HB3	1.98	0.45
3:J:366:CYS:HB3	3:J:437:PHE:CD1	2.51	0.45
3:J:678:ARG:HG3	3:J:679:TYR:N	2.31	0.45
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.16	0.45
3:J:1293:GLU:HB3	3:J:1294:ALA:H	1.56	0.45
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.30	0.45
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.99	0.45
1:B:321:TRP:O	1:B:321:TRP:CG	2.70	0.45
2:C:691:PRO:HA	2:C:788:SER:OG	2.15	0.45
2:C:856:ASN:HB3	5:F:612:ASP:C	2.41	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.98	0.45
1:H:67:GLU:O	1:H:78:ILE:HB	2.16	0.45
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.99	0.45
2:I:156:PHE:HD2	2:I:175:ARG:HB3	1.79	0.45
3:J:364:HIS:CG	4:K:4:VAL:HG23	2.51	0.45
3:J:905:ARG:HH12	4:K:10:VAL:HG11	1.81	0.45
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.67	0.45
2:I:900:LYS:HB3	5:L:563:PHE:HD1	1.82	0.45
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.99	0.45
3:J:322:ARG:HB2	3:J:322:ARG:NH1	2.31	0.45
3:J:649:LYS:O	3:J:653:ILE:HG13	2.15	0.45
3:J:833:GLU:OE1	3:J:1242:ARG:HD3	2.16	0.45
5:L:247:GLU:O	5:L:251:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:253:SER:O	5:L:257:LYS:HG3	2.16	0.45
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.49	0.45
2:C:106:GLU:HB3	2:C:109:ALA:CA	2.43	0.45
3:D:342:LEU:HA	3:D:343:LEU:HA	1.72	0.45
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.81	0.45
5:F:608:ARG:HH11	5:F:608:ARG:CG	2.30	0.45
2:I:50:GLU:OE1	2:I:54:ARG:NE	2.44	0.45
2:I:836:LEU:HB3	2:I:918:LEU:HD11	1.98	0.45
3:J:801:VAL:O	3:J:805:GLN:HB2	2.17	0.45
4:K:49:ILE:O	4:K:53:GLU:HG3	2.17	0.45
5:L:166:VAL:O	5:L:167:ASP:HB2	2.15	0.45
1:A:195:ARG:HD2	1:A:196:THR:H	1.81	0.45
1:A:211:ILE:HD13	1:A:211:ILE:HA	1.71	0.45
1:B:151:GLY:HA2	1:B:178:SER:HB3	1.98	0.45
2:C:236:LYS:HA	2:C:236:LYS:HD3	1.76	0.45
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.99	0.45
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.99	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.45
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.98	0.45
3:D:905:ARG:CZ	3:D:910:ASN:HD21	2.29	0.45
3:D:1344:LEU:HA	3:D:1349:GLU:HG3	1.99	0.45
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.99	0.45
3:J:115:TRP:HE1	3:J:308:ASP:HB2	1.82	0.45
3:J:598:LYS:O	3:J:601:ILE:HG22	2.17	0.45
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.81	0.45
5:L:511:ILE:HG21	5:L:522:PHE:CE2	2.52	0.45
1:B:321:TRP:N	1:B:322:PRO:CD	2.80	0.45
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.52	0.45
2:C:817:LEU:HD11	2:C:1085:MET:HE1	1.99	0.45
3:D:682:VAL:O	3:D:685:ILE:HG12	2.17	0.45
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.98	0.45
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.24	0.45
2:I:1270:PHE:CZ	2:I:1290:MET:HG2	2.52	0.45
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.46	0.45
1:B:35:PHE:HA	1:B:38:THR:HB	1.99	0.45
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.45
3:D:119:SER:O	3:D:120:LEU:C	2.60	0.45
3:D:690:ASN:HD21	3:D:745:GLY:HA2	1.81	0.45
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.99	0.45
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.99	0.45
2:I:39:ILE:HA	2:I:49:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:960:LEU:HD11	2:I:1028:LYS:HE2	1.99	0.45
3:J:331:ILE:O	3:J:337:ARG:HA	2.17	0.45
5:L:611:LEU:HD23	5:L:611:LEU:HA	1.81	0.45
6:M:25:GLU:OE2	6:M:123:ILE:HB	2.17	0.45
1:A:282:VAL:O	1:A:315:GLY:N	2.50	0.45
2:C:73:TYR:HA	2:C:98:VAL:HA	1.98	0.45
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.99	0.45
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.51	0.45
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.31	0.45
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.52	0.45
3:D:1283:SER:O	3:D:1286:LYS:N	2.49	0.45
5:F:324:LYS:HB3	5:F:325:PRO:HD2	1.99	0.45
5:F:452:ILE:HG13	5:F:457:ILE:HG13	1.99	0.45
1:H:219:ARG:HA	1:H:222:THR:HB	1.98	0.45
2:I:961:SER:O	2:I:965:GLN:N	2.40	0.45
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.97	0.45
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.99	0.45
3:J:449:LEU:HD21	3:J:457:TYR:CD2	2.52	0.45
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.71	0.44
1:B:228:LEU:HA	1:B:231:PHE:HD2	1.82	0.44
1:B:253:LEU:HB2	1:B:321:TRP:HE1	1.81	0.44
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.99	0.44
2:C:565:GLU:HG2	2:C:565:GLU:O	2.16	0.44
2:C:741:MET:HE3	2:C:974:ARG:NH2	2.32	0.44
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.99	0.44
2:C:1285:TYR:CE1	3:D:475:GLU:HG2	2.52	0.44
3:D:122:SER:O	3:D:126:LEU:HG	2.18	0.44
1:H:107:ILE:HG12	1:H:136:GLU:O	2.16	0.44
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.98	0.44
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.72	0.44
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.98	0.44
3:J:599:LYS:HD3	3:J:599:LYS:HA	1.76	0.44
3:J:761:ALA:H	3:J:771:GLN:NE2	2.15	0.44
3:J:1260:MET:HE3	3:J:1306:LEU:HD21	1.99	0.44
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.69	0.44
2:C:514:PHE:HB3	2:C:760:ASN:HD22	1.82	0.44
2:C:593:LYS:HB3	2:C:602:GLU:HG3	1.99	0.44
2:C:817:LEU:CD1	2:C:1085:MET:HE1	2.47	0.44
3:D:159:ILE:O	3:D:159:ILE:HG13	2.16	0.44
2:I:960:LEU:HB3	2:I:1025:PHE:CE2	2.52	0.44
2:I:1082:ILE:H	2:I:1082:ILE:CD1	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.48	0.44
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.48	0.44
1:A:76:GLU:N	1:A:76:GLU:OE2	2.51	0.44
2:C:5:TYR:O	2:C:8:LYS:HG2	2.17	0.44
2:C:73:TYR:CB	2:C:98:VAL:HG22	2.47	0.44
2:C:122:VAL:HG23	5:F:472:GLN:HG3	2.00	0.44
2:C:290:GLU:HG2	2:C:319:LEU:CD1	2.47	0.44
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.16	0.44
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.87	0.44
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.17	0.44
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.99	0.44
3:D:707:ILE:HD12	3:D:707:ILE:H	1.83	0.44
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.17	0.44
3:D:1270:GLY:HA3	3:D:1297:LYS:C	2.42	0.44
2:I:198:ILE:HD13	2:I:388:LEU:HD13	1.99	0.44
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.52	0.44
2:I:710:VAL:HG13	2:I:717:VAL:HG21	2.00	0.44
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	1.98	0.44
3:J:1170:LYS:C	3:J:1172:LYS:H	2.25	0.44
5:L:148:TYR:OH	5:L:218:ARG:HA	2.18	0.44
5:L:314:THR:O	5:L:318:ALA:HB3	2.18	0.44
1:B:212:ASP:O	1:B:215:GLU:N	2.50	0.44
2:C:541:GLU:OE1	2:C:541:GLU:N	2.49	0.44
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.51	0.44
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.83	0.44
2:I:61:SER:O	2:I:63:SER:N	2.50	0.44
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.53	0.44
2:I:588:GLU:HB3	2:I:607:SER:HA	1.99	0.44
3:J:1349:GLU:OE2	3:J:1349:GLU:N	2.35	0.44
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.74	0.44
1:B:290:LEU:HB3	1:B:291:LYS:HE2	1.98	0.44
2:C:657:THR:HG21	2:C:1188:ASP:HB2	2.00	0.44
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.60	0.44
3:D:334:LYS:HA	3:D:335:GLN:HA	1.80	0.44
3:D:494:ALA:CB	3:D:922:SER:HB3	2.48	0.44
3:D:1252:HIS:O	3:D:1255:VAL:HG13	2.16	0.44
1:H:100:LEU:HB3	1:H:115:ILE:HG22	1.99	0.44
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.83	0.44
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.50	0.44
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.99	0.44
3:J:905:ARG:NH1	4:K:10:VAL:HG11	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.52	0.44
4:K:38:LEU:HB2	4:K:53:GLU:OE1	2.18	0.44
5:L:143:TYR:CZ	5:L:268:TYR:CE2	3.04	0.44
1:A:228:LEU:CD1	1:B:224:LEU:HD23	2.40	0.44
2:C:161:LYS:HA	2:C:170:VAL:HA	1.99	0.44
2:C:725:GLN:HE22	2:C:966:ILE:HG23	1.82	0.44
3:D:418:GLU:OE1	4:E:3:ARG:NH2	2.48	0.44
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.32	0.44
5:F:484:ALA:HB1	5:F:491:GLU:HG3	1.98	0.44
2:I:55:SER:OG	2:I:56:VAL:N	2.50	0.44
2:I:93:SER:HA	2:I:128:PRO:HA	2.00	0.44
2:I:1332:SER:HA	3:J:243:PRO:HB2	1.99	0.44
5:L:476:ARG:HH11	5:L:477:GLU:H	1.66	0.44
2:C:238:GLN:HG2	2:C:286:GLU:HA	2.00	0.44
2:C:533:LEU:HD11	2:C:568:ASN:HD22	1.83	0.44
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.83	0.44
2:C:963:GLU:O	2:C:967:LEU:HB2	2.18	0.44
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	2.00	0.44
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.99	0.44
1:G:192:VAL:O	1:G:193:GLU:C	2.61	0.44
2:I:250:THR:HA	2:I:268:ARG:HA	2.00	0.44
2:I:678:ARG:CG	2:I:1108:ASN:HD22	2.28	0.44
2:I:1111:GLN:HB2	2:I:1230:MET:HE2	2.00	0.44
3:J:659:ALA:O	3:J:663:GLU:HG3	2.18	0.44
5:L:476:ARG:HB3	5:L:476:ARG:HH11	1.83	0.44
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.98	0.44
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.53	0.44
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.00	0.44
5:F:513:ASP:C	5:F:515:GLU:N	2.74	0.44
1:H:147:GLN:HG3	1:H:148:ARG:H	1.83	0.44
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.33	0.44
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.82	0.44
5:L:470:MET:HB2	5:L:478:PRO:HG3	2.00	0.44
1:A:168:ILE:H	1:A:168:ILE:HG12	1.68	0.44
2:C:87:ILE:H	2:C:87:ILE:HG13	1.61	0.44
2:C:169:LYS:HE2	2:C:190:PRO:HA	2.00	0.44
1:G:100:LEU:HD23	1:G:115:ILE:HG21	2.00	0.44
2:I:201:ARG:NH2	2:I:370:MET:O	2.37	0.44
2:I:541:GLU:OE1	2:I:541:GLU:N	2.48	0.44
2:I:543:ALA:HA	2:I:544:GLY:HA3	1.71	0.44
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1307:LEU:HD23	3:J:1312:ALA:HA	1.99	0.44
6:M:70:PRO:HG2	6:M:78:GLN:OE1	2.18	0.44
1:A:44:ARG:HB2	1:A:183:ILE:CG2	2.47	0.43
2:C:462:ASN:O	2:C:466:VAL:HG23	2.18	0.43
2:C:716:ALA:HB3	2:C:784:ALA:HB3	2.00	0.43
2:C:1240:ASP:OD1	2:C:1240:ASP:N	2.45	0.43
3:D:850:LYS:HB2	3:D:852:GLY:O	2.18	0.43
3:D:1273:ASP:O	3:D:1275:LEU:N	2.47	0.43
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.18	0.43
5:F:320:ILE:HG21	5:F:331:HIS:CD2	2.53	0.43
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.47	0.43
2:I:212:ALA:HA	2:I:359:ARG:HG3	2.00	0.43
2:I:452:ARG:HH21	2:I:458:GLU:CD	2.25	0.43
2:I:565:GLU:HG2	2:I:565:GLU:O	2.17	0.43
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.17	0.43
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.33	0.43
3:J:587:LEU:HD23	3:J:591:ILE:HG21	2.00	0.43
5:L:320:ILE:HG23	5:L:327:SER:O	2.16	0.43
1:A:266:SER:HB3	1:A:303:ILE:HD11	2.00	0.43
1:B:262:LEU:HD12	1:B:262:LEU:H	1.82	0.43
3:D:384:LYS:NZ	3:D:414:GLU:OE1	2.46	0.43
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.18	0.43
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.99	0.43
1:G:67:GLU:OE1	2:I:1057:LYS:NZ	2.52	0.43
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.34	0.43
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.18	0.43
3:J:118:LYS:HB3	3:J:118:LYS:HE2	1.83	0.43
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.48	0.43
1:B:286:GLU:OE2	1:B:304:LYS:NZ	2.46	0.43
2:C:1282:GLY:H	3:D:483:LEU:HD13	1.83	0.43
5:F:101:TYR:CE2	5:F:388:ILE:HD11	2.43	0.43
1:H:71:LYS:HD2	1:H:71:LYS:HA	1.86	0.43
2:I:850:ILE:O	2:I:850:ILE:HG22	2.18	0.43
2:I:1308:ILE:CG2	3:J:379:PRO:HB2	2.47	0.43
3:J:358:GLY:N	3:J:359:PRO:HD3	2.32	0.43
5:L:573:LEU:H	5:L:573:LEU:CD2	2.25	0.43
6:M:65:GLU:HB3	6:M:82:PHE:HZ	1.82	0.43
1:A:158:ARG:HH22	1:A:172:LEU:HD23	1.82	0.43
1:B:16:ILE:HG12	1:B:26:VAL:HG13	2.00	0.43
1:B:182:ARG:NE	3:D:581:MET:HE1	2.33	0.43
1:B:212:ASP:O	1:B:213:PRO:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:867:GLU:H	2:C:867:GLU:HG3	1.39	0.43
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.99	0.43
3:D:347:VAL:HG12	3:D:348:ASP:O	2.18	0.43
3:D:674:THR:HG22	6:M:136:ILE:HD12	2.01	0.43
3:D:680:ASN:O	3:D:683:ILE:HG22	2.19	0.43
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.43
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.33	0.43
3:J:128:LEU:HB3	3:J:157:GLN:HE22	1.83	0.43
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.91	0.43
3:J:311:ARG:O	3:J:312:ARG:HD3	2.18	0.43
3:J:342:LEU:HA	3:J:343:LEU:HA	1.71	0.43
3:J:385:LEU:CD2	3:J:411:ILE:HG13	2.48	0.43
3:J:804:ALA:O	3:J:806:ASP:N	2.51	0.43
6:M:78:GLN:HG2	6:M:82:PHE:CE2	2.54	0.43
2:C:338:THR:CG2	2:C:345:PRO:HB3	2.49	0.43
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.53	0.43
3:D:201:LEU:CD1	3:D:220:ARG:HG2	2.49	0.43
3:D:215:LYS:HE2	3:D:215:LYS:HB3	1.86	0.43
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.78	0.43
3:D:1170:LYS:C	3:D:1172:LYS:H	2.25	0.43
5:F:595:LEU:HB3	5:F:599:ARG:HH21	1.83	0.43
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	2.01	0.43
3:J:159:ILE:O	3:J:159:ILE:HG13	2.17	0.43
3:J:265:LEU:HG	3:J:330:MET:HE3	2.01	0.43
3:J:513:MET:O	3:J:575:GLY:HA3	2.18	0.43
3:J:850:LYS:HB2	3:J:852:GLY:O	2.18	0.43
2:C:13:LYS:HD3	2:C:1149:TYR:HA	2.00	0.43
2:C:323:ALA:O	2:C:327:GLN:HG3	2.18	0.43
2:C:980:VAL:HA	2:C:984:VAL:HA	2.01	0.43
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.00	0.43
3:D:505:ASP:HB3	3:D:629:PHE:CE1	2.50	0.43
3:D:789:LYS:HZ3	3:D:932:MET:CB	2.32	0.43
4:E:19:LEU:HD13	4:E:54:ILE:HG21	1.99	0.43
5:F:320:ILE:O	5:F:327:SER:HB3	2.18	0.43
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.81	0.43
1:G:219:ARG:HA	1:G:222:THR:HB	2.01	0.43
2:I:9:LYS:O	2:I:1175:ASN:ND2	2.49	0.43
2:I:29:SER:O	2:I:33:ASP:HB2	2.19	0.43
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.00	0.43
3:J:689:ALA:O	3:J:693:VAL:HG23	2.19	0.43
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:SER:O	1:A:51:MET:N	2.47	0.43
1:B:151:GLY:O	1:B:177:TYR:N	2.51	0.43
1:B:155:ALA:H	1:B:174:ASP:HA	1.84	0.43
2:C:1243:MET:HA	3:D:353:SER:HB3	2.01	0.43
3:D:56:LEU:H	3:D:56:LEU:HD12	1.83	0.43
3:D:258:GLY:HA3	5:F:499:LYS:HE2	2.00	0.43
3:D:681:LYS:NZ	6:M:14:ILE:HD12	2.33	0.43
3:D:1165:PHE:CE1	3:D:1200:GLU:HB2	2.52	0.43
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.99	0.43
2:I:218:GLU:CD	2:I:299:LYS:HE2	2.44	0.43
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.49	0.43
2:I:1066:MET:CE	2:I:1076:ILE:HB	2.49	0.43
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.43	0.43
3:J:263:SER:HA	5:L:507:MET:HB2	2.01	0.43
3:J:364:HIS:CE1	4:K:3:ARG:NH2	2.84	0.43
3:J:609:TYR:HA	3:J:617:THR:OG1	2.18	0.43
1:A:195:ARG:HD2	1:A:196:THR:N	2.34	0.43
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	2.00	0.43
5:F:141:ILE:HG21	5:F:228:TYR:CD1	2.53	0.43
5:F:354:THR:O	5:F:358:VAL:HG23	2.19	0.43
5:F:490:PRO:C	5:F:492:ASP:H	2.27	0.43
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	2.01	0.43
2:I:1340:GLU:CG	3:J:21:LYS:HB2	2.49	0.43
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.52	0.43
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.99	0.43
6:M:93:ARG:O	6:M:97:LYS:HG2	2.19	0.43
1:A:44:ARG:HE	1:A:183:ILE:HG22	1.83	0.43
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.83	0.43
1:A:232:VAL:O	1:B:218:ARG:HG2	2.18	0.43
2:C:88:ARG:HB2	2:C:88:ARG:NH1	2.34	0.43
2:C:800:MET:HE3	2:C:800:MET:HB3	1.65	0.43
2:C:1002:LEU:HD22	2:C:1007:LYS:CB	2.43	0.43
3:D:823:THR:HA	3:D:835:LEU:HD13	2.01	0.43
5:F:281:ARG:HD3	5:F:285:ARG:NH1	2.33	0.43
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.49	0.43
1:G:197:ASP:O	1:G:198:LEU:HD23	2.19	0.43
1:H:56:VAL:HG11	1:H:144:ILE:HD11	2.01	0.43
2:I:553:THR:H	2:I:553:THR:HG1	1.46	0.43
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.19	0.43
3:J:400:MET:HB3	3:J:400:MET:HE2	1.86	0.43
3:J:414:GLU:O	4:K:45:LYS:NZ	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ILE:CD1	1:B:284:ARG:HD3	2.49	0.43
2:C:88:ARG:HA	2:C:934:PHE:CZ	2.54	0.43
2:C:263:VAL:HG13	2:C:267:ARG:HB3	2.01	0.43
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.19	0.43
5:F:394:TYR:O	5:F:404:LEU:HD11	2.19	0.43
1:G:38:THR:HG1	1:H:45:ARG:NH1	2.16	0.43
2:I:699:LEU:HD23	2:I:699:LEU:HA	1.88	0.43
2:I:837:ALA:C	2:I:918:LEU:HD22	2.44	0.43
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.43	0.43
6:M:78:GLN:CD	6:M:82:PHE:HE2	2.26	0.43
1:A:178:SER:HA	1:A:179:PRO:HD3	1.84	0.42
1:A:310:ARG:O	5:F:608:ARG:NE	2.52	0.42
1:B:51:MET:HE1	1:B:220:ALA:HB2	2.01	0.42
1:B:285:THR:OG1	1:B:286:GLU:N	2.52	0.42
2:C:237:LEU:HG	2:C:289:VAL:HA	2.01	0.42
3:D:529:GLY:HA2	3:D:551:ARG:O	2.19	0.42
3:D:903:LEU:HD23	3:D:905:ARG:HD3	2.00	0.42
5:F:470:MET:HE3	5:F:470:MET:HB3	1.94	0.42
1:G:219:ARG:HE	1:G:219:ARG:HB2	1.54	0.42
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.54	0.42
2:I:778:GLU:O	2:I:781:ASP:HB2	2.19	0.42
2:I:1319:MET:HA	2:I:1320:PRO:HD3	1.92	0.42
3:J:179:LYS:HB2	3:J:184:ALA:HB2	2.02	0.42
3:J:1166:GLY:O	3:J:1174:ARG:HB2	2.19	0.42
1:B:14:VAL:HG23	1:B:27:THR:O	2.19	0.42
2:C:697:LYS:HE2	2:C:697:LYS:HB3	1.78	0.42
2:C:710:VAL:HG13	2:C:717:VAL:HG21	2.01	0.42
2:C:725:GLN:NE2	2:C:966:ILE:HG23	2.34	0.42
2:C:1151:LEU:HD21	2:C:1198:LEU:HB2	2.01	0.42
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.75	0.42
3:D:733:SER:O	3:D:737:ILE:HG12	2.19	0.42
3:D:860:ARG:HA	3:D:860:ARG:HD2	1.82	0.42
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	2.01	0.42
2:I:692:THR:OG1	2:I:827:ARG:O	2.37	0.42
3:J:594:GLN:HB2	3:J:595:ALA:H	1.60	0.42
3:J:1356:LEU:HD23	3:J:1356:LEU:HA	1.89	0.42
5:L:287:ILE:HD13	5:L:315:TRP:HH2	1.84	0.42
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.34	0.42
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.54	0.42
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.50	0.42
3:J:24:LEU:HB2	3:J:232:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:45:ASN:HB3	3:J:48:THR:O	2.19	0.42
3:J:102:MET:HE3	3:J:246:PRO:HD3	2.00	0.42
3:J:596:LEU:HD11	3:J:604:MET:CE	2.49	0.42
3:J:650:LYS:O	3:J:654:ILE:HG13	2.19	0.42
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.19	0.42
5:L:316:PHE:CZ	5:L:334:SER:HA	2.53	0.42
1:A:51:MET:HE1	1:A:220:ALA:HB2	2.02	0.42
1:A:166:ARG:N	1:A:167:PRO:HD2	2.35	0.42
1:B:183:ILE:H	1:B:183:ILE:HD12	1.83	0.42
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.18	0.42
2:C:1193:ALA:O	2:C:1197:GLU:HB2	2.19	0.42
3:D:81:ARG:HG3	3:D:82:GLY:H	1.85	0.42
3:D:118:LYS:HB3	3:D:118:LYS:HE2	1.89	0.42
3:D:262:THR:HG1	3:D:266:ASN:ND2	2.15	0.42
3:D:518:VAL:HG22	3:D:709:ARG:HB2	2.01	0.42
3:D:1192:LYS:HE3	3:D:1192:LYS:HB2	1.90	0.42
4:E:15:ASN:C	4:E:17:PHE:H	2.27	0.42
5:F:584:ARG:O	5:F:588:ARG:HG3	2.20	0.42
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.50	0.42
2:I:402:ARG:HG2	2:I:416:GLY:H	1.83	0.42
2:I:800:MET:HE3	2:I:800:MET:HB3	1.71	0.42
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.67	0.42
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	2.01	0.42
1:A:18:GLN:HE22	1:A:213:PRO:CD	2.33	0.42
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.53	0.42
1:B:317:ARG:O	1:B:318:LEU:HD13	2.19	0.42
2:C:16:GLY:HA2	2:C:1188:ASP:O	2.20	0.42
2:C:696:ASP:HB3	2:C:697:LYS:H	1.61	0.42
3:D:400:MET:HE2	3:D:400:MET:HB3	1.82	0.42
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.53	0.42
1:G:17:GLU:N	1:G:25:LYS:O	2.43	0.42
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.73	0.42
1:G:89:ALA:HB1	1:G:210:THR:CG2	2.50	0.42
2:I:79:VAL:HG23	2:I:80:PHE:H	1.85	0.42
2:I:148:GLN:HG3	2:I:511:LEU:HD11	2.01	0.42
2:I:1156:ARG:HB2	2:I:1156:ARG:HH11	1.84	0.42
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.54	0.42
5:L:343:LYS:H	5:L:343:LYS:HD2	1.84	0.42
9:M:202:G4P:HO2'	9:M:202:G4P:PC	2.41	0.42
2:C:528:ARG:NH2	2:C:576:SER:O	2.52	0.42
2:C:920:VAL:HA	2:C:921:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.84	0.42
3:D:126:LEU:HG	3:D:126:LEU:H	1.65	0.42
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.48	0.42
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.49	0.42
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.52	0.42
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.81	0.42
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.35	0.42
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.89	0.42
1:H:158:ARG:HB3	1:H:172:LEU:HD23	2.00	0.42
3:J:649:LYS:HD3	3:J:649:LYS:HA	1.77	0.42
5:L:311:THR:HG21	5:L:348:GLU:CD	2.45	0.42
5:L:476:ARG:HD2	5:L:477:GLU:HG2	2.01	0.42
1:A:195:ARG:HE	1:A:198:LEU:HD21	1.85	0.42
1:A:321:TRP:HA	1:A:322:PRO:HA	1.78	0.42
2:C:1238:LEU:H	2:C:1238:LEU:HD12	1.83	0.42
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.85	0.42
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.50	0.42
3:D:825:VAL:C	3:D:826:ILE:HG13	2.45	0.42
4:E:58:LEU:HD12	4:E:58:LEU:H	1.84	0.42
5:F:125:ASP:O	5:F:129:GLN:HG3	2.19	0.42
5:F:552:THR:OG1	5:F:554:ARG:HG2	2.20	0.42
2:I:103:VAL:C	2:I:104:ILE:HD12	2.45	0.42
2:I:735:LYS:HA	2:I:748:ILE:HG22	2.02	0.42
1:A:104:LYS:HG3	1:A:105:SER:N	2.35	0.42
1:B:48:LEU:HA	1:B:180:VAL:HG21	2.01	0.42
1:B:185:TYR:HB2	1:B:201:LEU:HD11	2.02	0.42
1:B:265:ARG:O	1:B:269:CYS:HB2	2.20	0.42
2:C:253:PHE:O	2:C:255:ILE:HG13	2.20	0.42
3:D:271:ARG:HD3	3:D:275:ARG:NH2	2.35	0.42
3:D:349:TYR:CD1	3:D:472:LEU:HD21	2.55	0.42
3:D:494:ALA:HB2	3:D:922:SER:HB3	2.02	0.42
5:F:379:MET:O	5:F:383:ASN:ND2	2.52	0.42
3:J:126:LEU:H	3:J:126:LEU:HG	1.67	0.42
3:J:405:GLU:O	3:J:408:VAL:HG22	2.20	0.42
3:J:581:MET:HE2	3:J:581:MET:HB3	1.97	0.42
3:J:902:ASP:OD1	3:J:903:LEU:N	2.53	0.42
1:A:31:LEU:HA	1:A:31:LEU:HD23	1.78	0.42
1:A:249:PHE:CE2	1:A:254:LEU:HG	2.55	0.42
1:A:286:GLU:HA	1:A:289:LEU:HD12	2.01	0.42
2:C:109:ALA:HA	2:C:110:PRO:HD3	1.91	0.42
2:C:198:ILE:HD13	2:C:388:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:297:VAL:HG23	2:C:333:ILE:HG23	2.02	0.42
2:C:466:VAL:O	2:C:470:ARG:HG2	2.19	0.42
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.82	0.42
3:D:355:ILE:HG22	3:D:447:ILE:HB	2.01	0.42
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.54	0.42
3:D:572:THR:OG1	3:D:576:ARG:HB2	2.20	0.42
3:D:683:ILE:HD11	3:D:754:ILE:HG23	2.01	0.42
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.34	0.42
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.83	0.42
2:I:1274:GLU:HA	3:J:428:THR:HG21	2.02	0.42
3:J:515:ARG:NH2	3:J:717:VAL:O	2.52	0.42
3:J:883:ARG:HB3	3:J:898:CYS:SG	2.59	0.42
6:M:47:TRP:O	6:M:51:LEU:HG	2.20	0.42
2:C:117:ILE:H	2:C:117:ILE:HG12	1.62	0.42
2:C:1066:MET:HG2	2:C:1234:LYS:HA	2.01	0.42
3:D:266:ASN:O	3:D:270:ARG:HB2	2.20	0.42
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.02	0.42
3:D:487:THR:HB	3:D:618:VAL:HG21	2.01	0.42
3:D:581:MET:HE2	3:D:581:MET:HB3	1.94	0.42
3:D:827:GLU:O	3:D:829:GLY:N	2.50	0.42
1:G:75:GLN:HA	2:I:729:ALA:H	1.83	0.42
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.55	0.42
3:J:647:PRO:HG3	3:J:697:MET:CA	2.50	0.42
5:L:233:ASP:O	5:L:236:LYS:HE2	2.20	0.42
1:A:192:VAL:HG12	1:A:195:ARG:HB2	2.02	0.41
1:A:315:GLY:O	1:A:316:MET:HG3	2.20	0.41
2:C:593:LYS:HG3	2:C:595:THR:HG23	2.00	0.41
3:D:123:ARG:HH12	3:D:1334:GLU:HG3	1.85	0.41
3:D:1299:GLY:HA2	3:D:1300:ALA:HA	1.86	0.41
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.55	0.41
2:I:896:THR:HB	2:I:897:PRO:HD2	2.02	0.41
2:I:975:ILE:O	2:I:979:LEU:HB2	2.20	0.41
3:J:362:ARG:HH21	9:J:2004:G4P:C1'	2.33	0.41
5:L:561:MET:HE3	5:L:561:MET:HB2	1.86	0.41
2:C:117:ILE:HD12	2:C:488:MET:HG2	2.02	0.41
2:C:162:GLY:O	2:C:164:THR:N	2.52	0.41
2:C:421:SER:H	2:C:424:ASP:HB2	1.85	0.41
2:C:463:GLN:NE2	2:C:501:ALA:O	2.53	0.41
2:C:487:LEU:HD23	2:C:487:LEU:H	1.85	0.41
2:C:830:THR:HG23	2:C:832:HIS:NE2	2.35	0.41
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:ASN:O	3:D:46:TYR:HD2	2.02	0.41
3:D:130:MET:HB2	3:D:157:GLN:OE1	2.20	0.41
3:D:786:THR:HG21	6:M:75:ARG:HG2	2.00	0.41
3:D:835:LEU:O	3:D:839:VAL:HG23	2.20	0.41
5:F:471:LEU:HD23	5:F:476:ARG:O	2.21	0.41
1:G:192:VAL:O	1:G:194:GLN:N	2.54	0.41
1:H:67:GLU:HA	1:H:78:ILE:HG21	2.02	0.41
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.54	0.41
3:J:119:SER:O	3:J:120:LEU:C	2.61	0.41
5:L:470:MET:O	5:L:478:PRO:HD3	2.21	0.41
1:A:237:VAL:O	1:B:13:LEU:HA	2.20	0.41
3:D:661:VAL:HG12	3:D:682:VAL:HG13	2.02	0.41
3:D:749:LYS:HB2	3:D:750:PRO:HD2	2.01	0.41
5:F:515:GLU:HG2	5:F:516:ASP:N	2.35	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	2.01	0.41
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.50	0.41
3:J:154:LEU:HD22	3:J:160:LEU:HD11	2.02	0.41
3:J:460:ASP:OD1	3:J:462:ASP:OD1	2.39	0.41
5:L:152:GLU:OE2	5:L:218:ARG:HG3	2.19	0.41
5:L:603:ARG:HD3	5:L:603:ARG:HA	1.84	0.41
6:M:57:ARG:O	6:M:60:THR:N	2.47	0.41
6:M:59:VAL:HA	6:M:62:MET:HB2	2.03	0.41
3:D:24:LEU:HD13	3:D:24:LEU:HA	1.90	0.41
3:D:425:ARG:HD2	3:D:459:ALA:HB2	2.02	0.41
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	2.01	0.41
5:F:483:LEU:H	5:F:483:LEU:HD12	1.85	0.41
5:F:515:GLU:C	5:F:517:SER:N	2.77	0.41
5:F:530:LEU:HD12	5:F:533:ASP:H	1.84	0.41
1:G:51:MET:HA	1:G:52:PRO:HD3	1.93	0.41
1:H:44:ARG:CG	1:H:183:ILE:HD13	2.51	0.41
1:H:217:ILE:HA	1:H:220:ALA:HB3	2.02	0.41
2:I:194:LEU:HD12	2:I:194:LEU:HA	1.88	0.41
2:I:871:VAL:HG12	2:I:883:LEU:O	2.20	0.41
3:J:430:HIS:NE2	3:J:456:ALA:O	2.49	0.41
1:B:134:THR:OG1	1:B:135:ASP:N	2.52	0.41
1:B:269:CYS:SG	1:B:295:LEU:HG	2.60	0.41
2:C:681:MET:HE2	2:C:681:MET:HB3	1.63	0.41
2:C:1230:MET:HG2	2:C:1232:MET:HG3	2.03	0.41
3:D:279:LEU:HD12	3:D:295:GLU:HG3	2.01	0.41
3:D:317:THR:HB	3:D:324:LEU:HB3	2.01	0.41
3:D:615:LYS:HA	4:E:5:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:744:ARG:O	3:D:744:ARG:HG3	2.21	0.41
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.35	0.41
1:G:22:THR:OG1	1:G:23:HIS:N	2.54	0.41
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.51	0.41
2:I:686:GLN:HG2	2:I:796:LEU:HD22	2.03	0.41
2:I:829:THR:HA	2:I:1059:ARG:HA	2.03	0.41
3:J:147:ILE:HG13	3:J:147:ILE:O	2.20	0.41
3:J:332:LYS:HA	3:J:337:ARG:H	1.85	0.41
3:J:638:SER:OG	3:J:639:VAL:N	2.53	0.41
6:M:17:ILE:CG2	6:M:50:GLN:HG3	2.49	0.41
1:B:71:LYS:HA	1:B:71:LYS:HD2	1.81	0.41
2:C:943:LYS:O	2:C:947:GLU:HG3	2.20	0.41
3:D:248:ASP:O	3:D:251:PRO:HG3	2.21	0.41
3:D:355:ILE:HG21	3:D:466:MET:HG3	2.02	0.41
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.85	0.41
5:F:100:MET:HE2	5:F:100:MET:HB3	1.89	0.41
5:F:139:GLU:HG3	5:F:351:THR:HG22	2.01	0.41
1:G:35:PHE:HD1	1:G:35:PHE:HA	1.78	0.41
1:H:7:GLU:HG2	1:H:8:PHE:H	1.85	0.41
2:I:80:PHE:HB3	2:I:84:GLU:HB2	2.03	0.41
2:I:127:ILE:HG22	2:I:502:VAL:HG11	2.02	0.41
2:I:1083:GLU:H	2:I:1083:GLU:HG3	1.64	0.41
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	2.01	0.41
3:J:239:LEU:HD23	3:J:239:LEU:HA	1.88	0.41
3:J:686:TRP:CD1	3:J:758:PRO:HD3	2.56	0.41
5:L:316:PHE:CE1	5:L:337:VAL:HB	2.56	0.41
1:B:189:ALA:HB1	1:B:191:ARG:HH12	1.86	0.41
2:C:81:ASP:HA	2:C:92:TYR:HE1	1.86	0.41
2:C:1054:LEU:HD12	2:C:1054:LEU:HA	1.86	0.41
2:C:1252:SER:HB3	2:C:1255:THR:O	2.21	0.41
2:C:1319:MET:HE2	2:C:1319:MET:HB3	1.88	0.41
3:D:322:ARG:HB2	3:D:322:ARG:HH11	1.84	0.41
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.91	0.41
3:D:735:ALA:O	3:D:738:ARG:HB3	2.21	0.41
3:D:905:ARG:NH2	3:D:907:HIS:HB2	2.22	0.41
5:F:515:GLU:C	5:F:517:SER:H	2.29	0.41
1:G:57:THR:HG22	1:G:58:GLU:HG3	2.02	0.41
3:J:761:ALA:H	3:J:771:GLN:HE22	1.67	0.41
6:M:111:PHE:CE2	6:M:126:LEU:HD13	2.56	0.41
1:A:124:VAL:HG11	1:A:210:THR:HG23	2.02	0.41
1:B:29:GLU:O	1:B:31:LEU:HD23	2.11	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:N	1:B:175:ALA:O	2.54	0.41
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	2.21	0.41
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.44	0.41
3:D:591:ILE:HD12	3:D:591:ILE:HA	1.89	0.41
4:E:15:ASN:O	4:E:16:ARG:HB3	2.21	0.41
5:F:413:MET:HE2	5:F:413:MET:HB3	1.97	0.41
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.03	0.41
2:I:157:PHE:O	2:I:443:ASP:N	2.52	0.41
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.36	0.41
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.86	0.41
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	2.02	0.41
2:I:1239:VAL:C	2:I:1241:ASP:H	2.28	0.41
2:I:1276:TRP:HD1	2:I:1279:GLU:OE1	2.02	0.41
3:J:514:THR:HB	3:J:576:ARG:HG2	2.02	0.41
3:J:849:LEU:H	3:J:849:LEU:HD22	1.85	0.41
3:J:1179:PRO:HD2	3:J:1184:ASP:HB3	2.01	0.41
5:L:100:MET:HE2	5:L:100:MET:HB3	1.92	0.41
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.86	0.41
1:A:97:GLU:HA	1:A:146:VAL:O	2.21	0.41
1:A:187:VAL:O	1:A:187:VAL:HG23	2.21	0.41
1:B:16:ILE:HG12	1:B:26:VAL:HG22	2.03	0.41
1:B:62:ASP:HB2	1:B:141:SER:O	2.21	0.41
1:B:120:ASP:OD1	1:B:276:HIS:CD2	2.74	0.41
1:B:178:SER:HA	1:B:179:PRO:HD3	1.89	0.41
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.35	0.41
2:C:42:ASP:O	2:C:44:GLU:N	2.52	0.41
2:C:103:VAL:C	2:C:104:ILE:HD12	2.45	0.41
2:C:206:ALA:O	2:C:209:ILE:HG22	2.21	0.41
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.75	0.41
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.42	0.41
3:D:147:ILE:HG13	3:D:147:ILE:O	2.21	0.41
3:D:460:ASP:OD2	6:M:71:ASP:OD2	2.39	0.41
3:D:495:ASN:C	3:D:497:GLU:H	2.27	0.41
3:D:1156:LEU:HD23	3:D:1219:ASP:HB3	2.02	0.41
3:D:1183:SER:CB	3:J:206:ASN:HD21	2.33	0.41
1:G:27:THR:C	1:G:28:LEU:HD12	2.46	0.41
1:G:192:VAL:O	1:G:192:VAL:HG12	2.20	0.41
1:H:41:ASN:O	1:H:45:ARG:HG3	2.20	0.41
1:H:64:VAL:HG12	1:H:66:HIS:H	1.85	0.41
2:I:297:VAL:HB	2:I:317:LEU:HD21	2.02	0.41
2:I:468:LEU:HA	2:I:471:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:705:GLU:CD	2:I:705:GLU:H	2.28	0.41
2:I:734:ILE:O	2:I:748:ILE:HB	2.21	0.41
2:I:1281:TYR:OH	3:J:431:ARG:O	2.38	0.41
2:I:1294:LYS:HD2	3:J:348:ASP:O	2.21	0.41
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.43	0.41
3:J:504:GLN:OE1	3:J:731:ARG:HD2	2.21	0.41
3:J:647:PRO:HG3	3:J:697:MET:N	2.35	0.41
3:J:657:ALA:CB	3:J:689:ALA:HB2	2.50	0.41
3:J:1167:LYS:HE3	3:J:1167:LYS:HB3	1.92	0.41
5:L:285:ARG:HA	5:L:288:MET:HB3	2.02	0.41
5:L:377:LYS:O	5:L:381:GLU:HG3	2.21	0.41
5:L:493:LYS:HA	5:L:496:LYS:HG3	2.02	0.41
6:M:140:THR:O	6:M:144:ILE:HG12	2.21	0.41
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.20	0.41
2:C:169:LYS:HE2	2:C:190:PRO:O	2.20	0.41
3:D:17:PHE:HZ	3:D:1353:VAL:HG21	1.85	0.41
3:D:45:ASN:O	3:D:46:TYR:CD2	2.74	0.41
3:D:596:LEU:HD11	3:D:604:MET:HE1	2.03	0.41
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.55	0.41
1:H:183:ILE:HG23	1:H:205:MET:HG3	2.03	0.41
1:H:211:ILE:HD12	1:H:211:ILE:HA	1.97	0.41
2:I:168:GLY:C	2:I:170:VAL:N	2.76	0.41
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.95	0.41
2:I:1086:PRO:CB	2:I:1212:LEU:HD23	2.51	0.41
2:I:1225:VAL:HA	3:J:638:SER:CB	2.51	0.41
3:J:596:LEU:HD11	3:J:604:MET:HE1	2.02	0.41
3:J:701:LEU:HD22	3:J:701:LEU:HA	1.95	0.41
5:L:226:ALA:O	5:L:229:VAL:HG22	2.21	0.41
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.22	0.40
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.86	0.40
3:D:460:ASP:OD1	3:D:464:ASP:OD2	2.39	0.40
5:F:143:TYR:CD2	5:F:269:LEU:HD21	2.56	0.40
2:I:5:TYR:O	2:I:8:LYS:HG2	2.22	0.40
2:I:149:LEU:HD13	2:I:453:ILE:HG13	2.02	0.40
2:I:452:ARG:HH12	2:I:585:GLY:HA3	1.86	0.40
2:I:820:GLU:HA	2:I:1079:ILE:HD11	2.03	0.40
2:I:828:PHE:HD1	2:I:828:PHE:HA	1.71	0.40
3:J:361:LEU:HD13	3:J:366:CYS:HA	2.03	0.40
3:J:668:PHE:CE1	3:J:678:ARG:HG2	2.56	0.40
3:J:860:ARG:HB3	3:J:861:ASN:H	1.55	0.40
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1239:ASP:O	3:J:1243:LEU:HB2	2.21	0.40
1:B:106:GLY:O	1:B:108:GLY:N	2.54	0.40
2:C:12:ARG:HG3	2:C:1181:PRO:HB2	2.04	0.40
2:C:79:VAL:HG23	2:C:80:PHE:H	1.85	0.40
2:C:145:ILE:HG22	2:C:456:VAL:HG22	2.03	0.40
2:C:202:ARG:HD3	2:C:369:MET:HG2	2.02	0.40
2:C:221:LEU:HD12	2:C:298:ALA:O	2.21	0.40
2:C:602:GLU:HG3	2:C:602:GLU:O	2.20	0.40
2:C:1082:ILE:H	2:C:1082:ILE:HD12	1.86	0.40
3:D:742:GLY:O	3:D:762:ASN:HB3	2.21	0.40
3:D:1243:LEU:HD12	3:D:1243:LEU:HA	1.95	0.40
3:D:1293:GLU:O	3:D:1294:ALA:C	2.64	0.40
5:F:320:ILE:HG21	5:F:331:HIS:NE2	2.35	0.40
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.27	0.40
2:I:540:ARG:H	2:I:540:ARG:HD2	1.86	0.40
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.03	0.40
3:J:709:ARG:HD2	3:J:710:ASP:H	1.86	0.40
3:J:839:VAL:HG12	3:J:864:LEU:HD12	2.03	0.40
3:J:1156:LEU:HA	3:J:1208:ASP:O	2.21	0.40
6:M:36:GLN:O	6:M:39:HIS:HB3	2.21	0.40
6:M:112:GLY:HA2	6:M:126:LEU:HD11	2.03	0.40
6:M:136:ILE:HD12	6:M:136:ILE:HA	1.89	0.40
1:A:110:VAL:HG21	1:A:140:ILE:HD11	2.03	0.40
2:C:1248:THR:HG22	2:C:1251:TYR:OH	2.21	0.40
2:C:1319:MET:HA	2:C:1320:PRO:HD3	1.90	0.40
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.54	0.40
3:D:490:ILE:HD13	3:D:490:ILE:N	2.29	0.40
3:D:1168:GLU:O	3:D:1170:LYS:N	2.54	0.40
5:F:281:ARG:O	5:F:285:ARG:HG3	2.20	0.40
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.21	0.40
1:H:74:VAL:HG11	1:H:81:ILE:HD11	2.02	0.40
1:H:178:SER:HA	1:H:179:PRO:HD3	1.86	0.40
2:I:521:LEU:O	2:I:525:THR:HB	2.22	0.40
3:J:416:ILE:HD12	3:J:416:ILE:HA	1.83	0.40
3:J:709:ARG:HD2	3:J:710:ASP:N	2.36	0.40
3:J:923:ILE:O	3:J:926:PRO:HD2	2.21	0.40
1:A:89:ALA:O	1:A:124:VAL:HG12	2.22	0.40
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.86	0.40
1:A:316:MET:HE3	5:F:600:HIS:CE1	2.56	0.40
1:A:323:PRO:HB2	1:A:324:ALA:HB2	2.04	0.40
1:B:49:SER:O	1:B:51:MET:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LYS:HD3	1:B:114:ASP:OD2	2.20	0.40
2:C:601:ASP:OD1	2:C:601:ASP:N	2.46	0.40
3:D:681:LYS:NZ	6:M:12:LEU:HD13	2.37	0.40
3:D:707:ILE:HD11	3:D:716:GLN:HG2	2.03	0.40
3:D:850:LYS:HD3	3:D:875:ASN:HD21	1.87	0.40
3:D:860:ARG:HB3	3:D:861:ASN:H	1.81	0.40
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	2.36	0.40
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.37	0.40
2:I:402:ARG:HG2	2:I:416:GLY:N	2.36	0.40
2:I:1109:ILE:HD12	2:I:1109:ILE:HA	1.91	0.40
3:J:195:GLU:H	3:J:195:GLU:HG3	1.61	0.40
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.37	0.40
3:J:514:THR:CB	3:J:576:ARG:HG2	2.51	0.40
3:J:664:ILE:HG21	3:J:681:LYS:HG2	2.04	0.40
6:M:90:ASP:O	6:M:94:LYS:HG3	2.22	0.40
1:A:262:LEU:H	1:A:262:LEU:HD12	1.86	0.40
2:C:149:LEU:HD12	2:C:452:ARG:O	2.21	0.40
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.03	0.40
5:F:511:ILE:HG22	5:F:517:SER:O	2.22	0.40
1:G:31:LEU:HA	1:G:31:LEU:HD23	1.88	0.40
2:I:388:LEU:HD23	2:I:388:LEU:HA	1.86	0.40
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.51	0.40
3:J:161:THR:H	3:J:164:GLN:HB2	1.86	0.40
3:J:322:ARG:HG3	3:J:323:PRO:HD2	2.04	0.40
4:K:56:GLU:HB2	4:K:58:LEU:HD11	2.04	0.40
5:L:363:ARG:O	5:L:367:ILE:HG13	2.20	0.40
5:L:544:THR:HG22	5:L:607:LEU:HD11	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ASP:OD2	3:J:675:ALA:N[2_555]	2.03	0.17

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	317/329 (96%)	249 (78%)	53 (17%)	15 (5%)	2	16
1	B	291/329 (88%)	225 (77%)	45 (16%)	21 (7%)	1	11
1	G	225/329 (68%)	200 (89%)	21 (9%)	4 (2%)	6	33
1	H	212/329 (64%)	197 (93%)	11 (5%)	4 (2%)	6	32
2	C	1338/1342 (100%)	1201 (90%)	114 (8%)	23 (2%)	7	35
2	I	1338/1342 (100%)	1196 (89%)	119 (9%)	23 (2%)	7	35
3	D	1169/1407 (83%)	1042 (89%)	99 (8%)	28 (2%)	4	27
3	J	1151/1407 (82%)	1024 (89%)	100 (9%)	27 (2%)	5	28
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	5	28
4	K	77/91 (85%)	68 (88%)	5 (6%)	4 (5%)	1	15
5	F	462/613 (75%)	425 (92%)	28 (6%)	9 (2%)	6	32
5	L	463/613 (76%)	424 (92%)	32 (7%)	7 (2%)	8	38
6	M	138/151 (91%)	128 (93%)	7 (5%)	3 (2%)	5	29
All	All	7268/8373 (87%)	6460 (89%)	638 (9%)	170 (2%)	5	28

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	167	PRO
1	A	242	VAL
1	A	320	ASN
1	B	20	SER
1	B	29	GLU
1	B	30	PRO
1	B	32	GLU
1	B	107	ILE
1	B	320	ASN
1	B	323	PRO
1	B	324	ALA
2	C	169	LYS
2	C	170	VAL

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Mol	Chain	Res	Type
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1153	ALA
2	C	1159	VAL
2	C	1165	SER
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO
5	F	566	ASP
5	F	569	THR
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	49	PHE
3	J	341	ASN
3	J	426	ALA
3	J	710	ASP
3	J	712	GLN
3	J	850	LYS
3	J	854	ALA
3	J	1294	ALA
4	K	4	VAL
4	K	15	ASN
4	K	33	GLY
5	L	584	ARG

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Mol	Chain	Res	Type
6	M	31	TYR
1	A	50	SER
1	A	119	GLY
1	A	232	VAL
1	A	315	GLY
1	B	50	SER
1	B	62	ASP
1	B	119	GLY
1	B	135	ASP
1	B	315	GLY
2	C	121	GLU
2	C	237	LEU
2	C	1154	ASP
3	D	89	GLY
3	D	805	GLN
3	D	933	ARG
3	D	934	THR
5	F	584	ARG
1	G	162	GLU
1	G	167	PRO
1	H	138	ALA
2	I	237	LEU
2	I	1059	ARG
2	I	1165	SER
3	J	89	GLY
3	J	314	ARG
3	J	339	ARG
3	J	496	GLY
3	J	745	GLY
3	J	805	GLN
3	J	826	ILE
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP
5	L	490	PRO
5	L	566	ASP
5	L	569	THR
1	A	62	ASP
1	B	319	GLU
1	B	321	TRP
2	C	163	LYS
2	C	236	LYS

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Mol	Chain	Res	Type
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	173	GLY
3	D	314	ARG
3	D	417	ARG
3	D	1274	PHE
3	D	1344	LEU
5	F	600	HIS
1	G	229	GLU
1	H	193	GLU
2	I	983	GLY
2	I	1317	PRO
3	J	332	LYS
3	J	417	ARG
6	M	58	THR
1	A	319	GLU
1	A	324	ALA
1	B	13	LEU
1	B	322	PRO
2	C	813	GLU
2	C	1059	ARG
3	D	1297	LYS
1	H	20	SER
2	I	696	ASP
2	I	813	GLU
2	I	892	GLU
3	J	344	GLY
3	J	1344	LEU
4	K	14	GLY
1	A	318	LEU
1	B	318	LEU
2	C	62	TYR
2	C	983	GLY
2	C	1158	LYS
3	D	46	TYR
3	D	345	LYS
5	F	602	SER
2	I	201	ARG
2	I	236	LYS
3	J	338	PHE
3	J	357	VAL

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Mol	Chain	Res	Type
2	C	1256	GLN
3	D	357	VAL
3	D	828	GLY
3	D	1375	ALA
2	I	160	ASP
2	I	756	TYR
3	J	333	GLY
5	L	585	GLU
6	M	27	PRO
1	A	19	VAL
1	B	19	VAL
3	D	826	ILE
5	F	96	ASP
3	J	173	GLY
3	J	336	GLY
3	D	120	LEU
3	D	831	VAL
5	F	361	ILE
5	F	601	PRO
3	J	639	VAL
1	B	217	ILE
4	E	86	ILE
2	I	1202	GLY
5	L	475	GLY
1	B	293	PRO
2	C	110	PRO
3	D	850	LYS
1	H	30	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/286 (97%)	224 (81%)	54 (19%)	1	8
1	B	256/286 (90%)	220 (86%)	36 (14%)	3	15
1	G	193/286 (68%)	162 (84%)	31 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	183/286 (64%)	168 (92%)	15 (8%)	10	31
2	C	1155/1157 (100%)	1022 (88%)	133 (12%)	5	20
2	I	1154/1157 (100%)	1032 (89%)	122 (11%)	6	22
3	D	962/1168 (82%)	859 (89%)	103 (11%)	6	22
3	J	960/1168 (82%)	857 (89%)	103 (11%)	6	22
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	21
4	K	67/75 (89%)	59 (88%)	8 (12%)	5	19
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	24
5	L	418/540 (77%)	374 (90%)	44 (10%)	6	23
6	M	121/131 (92%)	110 (91%)	11 (9%)	9	28
All	All	6236/7155 (87%)	5526 (89%)	710 (11%)	5	20

All (710) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	9	LEU
1	A	18	GLN
1	A	26	VAL
1	A	29	GLU
1	A	32	GLU
1	A	44	ARG
1	A	50	SER
1	A	56	VAL
1	A	70	THR
1	A	71	LYS
1	A	72	GLU
1	A	74	VAL
1	A	75	GLN
1	A	77	ASP
1	A	83	LEU
1	A	90	VAL
1	A	98	VAL
1	A	99	ILE
1	A	105	SER
1	A	110	VAL
1	A	116	THR

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Mol	Chain	Res	Type
1	A	133	LEU
1	A	137	ASN
1	A	159	ILE
1	A	168	ILE
1	A	171	LEU
1	A	180	VAL
1	A	183	ILE
1	A	186	ASN
1	A	192	VAL
1	A	195	ARG
1	A	207	THR
1	A	211	ILE
1	A	223	ILE
1	A	227	GLN
1	A	231	PHE
1	A	243	LYS
1	A	245	GLU
1	A	246	LYS
1	A	252	ILE
1	A	262	LEU
1	A	264	VAL
1	A	280	ASP
1	A	282	VAL
1	A	284	ARG
1	A	285	THR
1	A	300	LEU
1	A	302	GLU
1	A	306	VAL
1	A	316	MET
1	A	318	LEU
1	A	320	ASN
1	B	8	PHE
1	B	9	LEU
1	B	18	GLN
1	B	29	GLU
1	B	50	SER
1	B	54	CYS
1	B	70	THR
1	B	71	LYS
1	B	75	GLN
1	B	77	ASP
1	B	83	LEU

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Mol	Chain	Res	Type
1	B	90	VAL
1	B	98	VAL
1	B	99	ILE
1	B	110	VAL
1	B	133	LEU
1	B	144	ILE
1	B	159	ILE
1	B	180	VAL
1	B	183	ILE
1	B	186	ASN
1	B	195	ARG
1	B	223	ILE
1	B	252	ILE
1	B	262	LEU
1	B	264	VAL
1	B	280	ASP
1	B	282	VAL
1	B	284	ARG
1	B	285	THR
1	B	300	LEU
1	B	302	GLU
1	B	306	VAL
1	B	316	MET
1	B	318	LEU
1	B	320	ASN
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS
2	C	22	LEU
2	C	23	ASP
2	C	39	ILE
2	C	46	GLN
2	C	56	VAL
2	C	81	ASP
2	C	90	VAL
2	C	103	VAL
2	C	107	ARG
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	131	THR

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Mol	Chain	Res	Type
2	C	135	THR
2	C	138	ILE
2	C	145	ILE
2	C	164	THR
2	C	170	VAL
2	C	201	ARG
2	C	208	ILE
2	C	236	LYS
2	C	285	ILE
2	C	292	ILE
2	C	302	ILE
2	C	306	THR
2	C	316	GLU
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	377	THR
2	C	384	LEU
2	C	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	453	ILE
2	C	455	SER
2	C	456	VAL
2	C	471	VAL
2	C	481	LEU
2	C	484	LEU
2	C	490	GLN
2	C	492	MET
2	C	493	ILE
2	C	518	ASN
2	C	521	LEU
2	C	525	THR
2	C	539	THR
2	C	540	ARG
2	C	542	ARG
2	C	550	VAL
2	C	553	THR
2	C	558	VAL
2	C	561	ILE
2	C	575	LEU
2	C	600	THR

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Mol	Chain	Res	Type
2	C	609	ILE
2	C	615	VAL
2	C	618	GLN
2	C	623	LEU
2	C	633	LEU
2	C	634	VAL
2	C	657	THR
2	C	660	VAL
2	C	663	VAL
2	C	672	GLU
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	781	ASP
2	C	783	LEU
2	C	791	LEU
2	C	799	ASN
2	C	800	MET
2	C	817	LEU
2	C	867	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	922	ASN
2	C	948	ILE
2	C	951	MET
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1037	THR
2	C	1050	VAL
2	C	1054	LEU
2	C	1072	ASN
2	C	1076	ILE
2	C	1078	LYS
2	C	1082	ILE

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Mol	Chain	Res	Type
2	C	1098	LEU
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1141	LEU
2	C	1145	ILE
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1172	LEU
2	C	1180	MET
2	C	1198	LEU
2	C	1206	THR
2	C	1210	ILE
2	C	1225	VAL
2	C	1227	VAL
2	C	1233	LEU
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1250	SER
2	C	1254	VAL
2	C	1255	THR
2	C	1287	LEU
2	C	1291	LEU
2	C	1296	ASP
2	C	1313	HIS
2	C	1327	LEU
3	D	11	GLN
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL
3	D	93	THR
3	D	95	THR
3	D	96	LYS

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Mol	Chain	Res	Type
3	D	97	VAL
3	D	154	LEU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	259	ARG
3	D	292	VAL
3	D	306	LEU
3	D	324	LEU
3	D	330	MET
3	D	335	GLN
3	D	343	LEU
3	D	363	LEU
3	D	374	LEU
3	D	376	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	407	VAL
3	D	413	ASP
3	D	415	VAL
3	D	416	ILE
3	D	423	LEU
3	D	425	ARG
3	D	429	LEU
3	D	442	ILE
3	D	490	ILE
3	D	505	ASP
3	D	507	VAL
3	D	510	LEU
3	D	514	THR
3	D	532	GLU
3	D	536	LEU
3	D	545	HIS
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	594	GLN
3	D	605	LEU

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Mol	Chain	Res	Type
3	D	639	VAL
3	D	641	ILE
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	717	VAL
3	D	721	SER
3	D	754	ILE
3	D	764	ARG
3	D	770	LEU
3	D	790	THR
3	D	797	THR
3	D	801	VAL
3	D	810	THR
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	858	VAL
3	D	860	ARG
3	D	890	THR
3	D	901	ARG
3	D	903	LEU
3	D	908	ILE
3	D	918	ILE
3	D	1146	GLU
3	D	1155	ILE
3	D	1162	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1177	ILE
3	D	1194	ARG
3	D	1221	LEU
3	D	1251	LYS
3	D	1255	VAL
3	D	1257	VAL
3	D	1261	LEU
3	D	1266	ILE

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Mol	Chain	Res	Type
3	D	1272	SER
3	D	1279	GLN
3	D	1289	ASN
3	D	1310	THR
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
3	D	1361	THR
3	D	1366	HIS
4	E	5	THR
4	E	13	ILE
4	E	18	ASP
4	E	21	LEU
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL
4	E	58	LEU
5	F	98	VAL
5	F	114	GLU
5	F	127	ILE
5	F	152	GLU
5	F	154	GLU
5	F	163	THR
5	F	230	VAL
5	F	261	LEU
5	F	277	MET
5	F	305	LEU
5	F	306	PHE
5	F	335	GLU
5	F	341	LEU
5	F	399	LEU
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	494	ILE
5	F	507	MET
5	F	516	ASP

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Mol	Chain	Res	Type
5	F	526	THR
5	F	527	THR
5	F	530	LEU
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	559	LEU
5	F	561	MET
5	F	568	ASN
5	F	569	THR
5	F	572	THR
5	F	578	LYS
5	F	587	ILE
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	9	LEU
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	27	THR
1	G	33	ARG
1	G	50	SER
1	G	64	VAL
1	G	65	LEU
1	G	70	THR
1	G	79	LEU
1	G	90	VAL
1	G	101	THR
1	G	121	VAL
1	G	124	VAL
1	G	129	VAL
1	G	133	LEU
1	G	137	ASN
1	G	145	LYS
1	G	156	SER
1	G	171	LEU
1	G	178	SER
1	G	183	ILE
1	G	187	VAL

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Mol	Chain	Res	Type
1	G	192	VAL
1	G	200	LYS
1	G	207	THR
1	G	211	ILE
1	G	217	ILE
1	G	219	ARG
1	H	16	ILE
1	H	27	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	66	HIS
1	H	75	GLN
1	H	95	LYS
1	H	102	LEU
1	H	121	VAL
1	H	124	VAL
1	H	133	LEU
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	46	GLN
2	I	56	VAL
2	I	86	GLN
2	I	90	VAL
2	I	103	VAL
2	I	106	GLU
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE
2	I	119	GLU
2	I	131	THR
2	I	132	ASP
2	I	135	THR
2	I	138	ILE
2	I	156	PHE
2	I	164	THR

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Mol	Chain	Res	Type
2	I	170	VAL
2	I	208	ILE
2	I	236	LYS
2	I	285	ILE
2	I	292	ILE
2	I	302	ILE
2	I	316	GLU
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	343	HIS
2	I	360	LEU
2	I	384	LEU
2	I	423	ASP
2	I	445	ILE
2	I	453	ILE
2	I	455	SER
2	I	456	VAL
2	I	471	VAL
2	I	481	LEU
2	I	484	LEU
2	I	492	MET
2	I	493	ILE
2	I	518	ASN
2	I	521	LEU
2	I	524	ILE
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	542	ARG
2	I	550	VAL
2	I	553	THR
2	I	558	VAL
2	I	561	ILE
2	I	575	LEU
2	I	596	ASP
2	I	600	THR
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL
2	I	623	LEU
2	I	633	LEU

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Mol	Chain	Res	Type
2	I	635	THR
2	I	660	VAL
2	I	663	VAL
2	I	672	GLU
2	I	705	GLU
2	I	714	VAL
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	781	ASP
2	I	782	VAL
2	I	800	MET
2	I	817	LEU
2	I	828	PHE
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	922	ASN
2	I	951	MET
2	I	984	VAL
2	I	1002	LEU
2	I	1037	THR
2	I	1050	VAL
2	I	1054	LEU
2	I	1078	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1164	PHE
2	I	1172	LEU
2	I	1180	MET
2	I	1198	LEU

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Mol	Chain	Res	Type
2	I	1206	THR
2	I	1210	ILE
2	I	1225	VAL
2	I	1227	VAL
2	I	1233	LEU
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1250	SER
2	I	1254	VAL
2	I	1287	LEU
2	I	1296	ASP
2	I	1299	ASN
2	I	1313	HIS
2	I	1327	LEU
2	I	1341	ASP
2	I	1342	GLU
3	J	20	ILE
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	93	THR
3	J	95	THR
3	J	96	LYS
3	J	97	VAL
3	J	154	LEU
3	J	162	GLU
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	218	THR
3	J	235	GLU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	283	LEU
3	J	292	VAL
3	J	306	LEU
3	J	324	LEU

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Mol	Chain	Res	Type
3	J	343	LEU
3	J	357	VAL
3	J	363	LEU
3	J	374	LEU
3	J	376	LEU
3	J	386	GLU
3	J	392	THR
3	J	394	ILE
3	J	415	VAL
3	J	416	ILE
3	J	423	LEU
3	J	425	ARG
3	J	429	LEU
3	J	505	ASP
3	J	506	VAL
3	J	507	VAL
3	J	510	LEU
3	J	514	THR
3	J	532	GLU
3	J	536	LEU
3	J	545	HIS
3	J	567	THR
3	J	569	LEU
3	J	571	ASP
3	J	573	THR
3	J	591	ILE
3	J	594	GLN
3	J	605	LEU
3	J	615	LYS
3	J	639	VAL
3	J	641	ILE
3	J	678	ARG
3	J	680	ASN
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	717	VAL
3	J	754	ILE
3	J	764	ARG
3	J	797	THR
3	J	801	VAL

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Mol	Chain	Res	Type
3	J	810	THR
3	J	826	ILE
3	J	827	GLU
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	897	HIS
3	J	898	CYS
3	J	901	ARG
3	J	903	LEU
3	J	908	ILE
3	J	910	ASN
3	J	913	GLU
3	J	918	ILE
3	J	1146	GLU
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1194	ARG
3	J	1204	VAL
3	J	1221	LEU
3	J	1251	LYS
3	J	1255	VAL
3	J	1257	VAL
3	J	1261	LEU
3	J	1266	ILE
3	J	1273	ASP
3	J	1285	VAL
3	J	1289	ASN
3	J	1292	LEU
3	J	1333	THR
3	J	1366	HIS
4	K	3	ARG
4	K	13	ILE
4	K	18	ASP
4	K	21	LEU
4	K	31	GLN
4	K	36	ASP

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Mol	Chain	Res	Type
4	K	39	VAL
4	K	58	LEU
5	L	98	VAL
5	L	102	MET
5	L	114	GLU
5	L	127	ILE
5	L	152	GLU
5	L	154	GLU
5	L	163	THR
5	L	261	LEU
5	L	277	MET
5	L	305	LEU
5	L	335	GLU
5	L	338	HIS
5	L	364	ARG
5	L	395	THR
5	L	405	ILE
5	L	429	THR
5	L	450	ILE
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	486	ARG
5	L	491	GLU
5	L	492	ASP
5	L	494	ILE
5	L	507	MET
5	L	526	THR
5	L	527	THR
5	L	547	VAL
5	L	552	THR
5	L	558	VAL
5	L	559	LEU
5	L	561	MET
5	L	568	ASN
5	L	569	THR
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG

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Mol	Chain	Res	Type
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
6	M	25	GLU
6	M	42	ARG
6	M	50	GLN
6	M	52	ARG
6	M	69	PHE
6	M	72	PRO
6	M	73	VAL
6	M	88	ASN
6	M	123	ILE
6	M	136	ILE
6	M	146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	37	HIS
1	A	41	ASN
1	A	66	HIS
1	A	103	ASN
1	A	194	GLN
1	A	239	GLN
1	A	268	ASN
1	B	41	ASN
1	B	84	ASN
1	B	93	GLN
1	B	186	ASN
1	B	268	ASN
1	B	276	HIS
1	B	320	ASN
2	C	133	ASN
2	C	139	ASN
2	C	343	HIS
2	C	513	GLN
2	C	618	GLN
2	C	620	ASN
2	C	760	ASN
2	C	766	ASN

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Mol	Chain	Res	Type
2	C	1023	HIS
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1209	GLN
2	C	1237	HIS
2	C	1288	GLN
3	D	157	GLN
3	D	158	GLN
3	D	200	GLN
3	D	276	ASN
3	D	320	ASN
3	D	606	ASN
3	D	667	GLN
3	D	680	ASN
3	D	690	ASN
3	D	777	HIS
3	D	817	HIS
3	D	865	HIS
3	D	907	HIS
3	D	910	ASN
3	D	1235	ASN
4	E	15	ASN
5	F	294	GLN
5	F	301	ASN
5	F	357	GLN
5	F	446	GLN
5	F	464	ASN
5	F	579	GLN
5	F	600	HIS
1	G	66	HIS
1	H	117	HIS
1	H	128	HIS
2	I	46	GLN
2	I	133	ASN
2	I	139	ASN
2	I	330	HIS
2	I	357	ASN
2	I	620	ASN
2	I	658	GLN
2	I	766	ASN
2	I	808	ASN

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Mol	Chain	Res	Type
2	I	894	GLN
2	I	1116	HIS
2	I	1220	GLN
2	I	1236	ASN
2	I	1237	HIS
2	I	1288	GLN
2	I	1314	GLN
3	J	200	GLN
3	J	206	ASN
3	J	364	HIS
3	J	419	HIS
3	J	424	ASN
3	J	450	HIS
3	J	489	ASN
3	J	594	GLN
3	J	667	GLN
3	J	716	GLN
3	J	861	ASN
3	J	1218	HIS
3	J	1366	HIS
5	L	283	GLN
5	L	301	ASN
5	L	345	GLN
5	L	346	GLN
5	L	357	GLN
5	L	362	ASN
5	L	406	GLN
5	L	446	GLN
5	L	579	GLN
6	M	36	GLN
6	M	68	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	G4P	M	202	-	36,38,38	1.97	12 (33%)	56,61,61	1.41	8 (14%)
9	G4P	J	2004	-	36,38,38	1.94	13 (36%)	56,61,61	1.30	5 (8%)
9	G4P	E	101	-	36,38,38	1.85	12 (33%)	56,61,61	1.30	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	G4P	M	202	-	-	8/27/43/43	0/3/3/3
9	G4P	J	2004	-	-	7/27/43/43	0/3/3/3
9	G4P	E	101	-	-	1/27/43/43	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	202	G4P	C5-N7	-5.12	1.28	1.39
9	J	2004	G4P	C5-N7	-4.93	1.29	1.39
9	E	101	G4P	C5-N7	-4.68	1.29	1.39
9	M	202	G4P	C6-N1	-4.05	1.31	1.38
9	J	2004	G4P	C6-N1	-3.89	1.31	1.38
9	E	101	G4P	C6-N1	-3.86	1.31	1.38
9	M	202	G4P	C2-N2	3.73	1.42	1.34
9	J	2004	G4P	C2-N2	3.63	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	202	G4P	C2'-C3'	-3.54	1.45	1.53
9	E	101	G4P	C2-N2	3.48	1.42	1.34
9	J	2004	G4P	C2'-C3'	-3.25	1.45	1.53
9	J	2004	G4P	C2-N3	3.04	1.40	1.33
9	E	101	G4P	C2-N3	2.98	1.40	1.33
9	E	101	G4P	C2'-C3'	-2.97	1.46	1.53
9	M	202	G4P	C3'-C4'	-2.95	1.45	1.52
9	M	202	G4P	C2-N3	2.90	1.40	1.33
9	J	2004	G4P	C3'-C4'	-2.64	1.46	1.52
9	J	2004	G4P	C2'-C1'	-2.57	1.45	1.53
9	E	101	G4P	C3'-C4'	-2.55	1.46	1.52
9	E	101	G4P	C8-N7	2.47	1.39	1.32
9	J	2004	G4P	C8-N7	2.41	1.39	1.32
9	M	202	G4P	C4-N3	2.41	1.39	1.34
9	E	101	G4P	C8-N9	2.38	1.42	1.37
9	J	2004	G4P	PC-O3C	-2.37	1.56	1.59
9	E	101	G4P	C4-N3	2.36	1.39	1.34
9	M	202	G4P	C5-C4	-2.35	1.31	1.38
9	J	2004	G4P	C5-C4	-2.30	1.32	1.38
9	M	202	G4P	C2'-C1'	-2.29	1.46	1.53
9	J	2004	G4P	C4-N3	2.27	1.39	1.34
9	J	2004	G4P	C8-N9	2.25	1.42	1.37
9	E	101	G4P	C2'-C1'	-2.24	1.46	1.53
9	M	202	G4P	C8-N7	2.22	1.38	1.32
9	J	2004	G4P	C1'-N9	-2.11	1.41	1.47
9	M	202	G4P	C8-N9	2.10	1.42	1.37
9	E	101	G4P	C5-C4	-2.07	1.32	1.38
9	M	202	G4P	C1'-N9	-2.06	1.41	1.47
9	E	101	G4P	C1'-N9	-2.02	1.41	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	202	G4P	C5-C4-N3	-4.92	120.56	128.39
9	E	101	G4P	C5-C4-N3	-4.20	121.71	128.39
9	J	2004	G4P	C5-C4-N3	-4.04	121.97	128.39
9	J	2004	G4P	N9-C8-N7	-3.85	106.25	113.40
9	M	202	G4P	N9-C8-N7	-3.80	106.35	113.40
9	E	101	G4P	N9-C8-N7	-3.60	106.72	113.40
9	E	101	G4P	C3'-C2'-C1'	2.92	106.30	99.89
9	M	202	G4P	C5-C6-N1	2.74	120.22	113.25
9	E	101	G4P	C2-N1-C6	-2.58	120.43	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	101	G4P	C5-C6-N1	2.56	119.76	113.25
9	M	202	G4P	C2-N1-C6	-2.50	120.57	125.11
9	J	2004	G4P	C5-C6-N1	2.43	119.45	113.25
9	M	202	G4P	N9-C4-N3	2.39	130.73	125.95
9	J	2004	G4P	C2-N1-C6	-2.37	120.82	125.11
9	M	202	G4P	O6-C6-C5	-2.35	120.32	126.53
9	J	2004	G4P	O6-C6-C5	-2.32	120.42	126.53
9	E	101	G4P	O6-C6-C5	-2.22	120.68	126.53
9	M	202	G4P	C2-N3-C4	2.12	115.94	112.30
9	M	202	G4P	C8-N7-C5	2.10	108.00	104.26

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	2004	G4P	C3'-O3'-PC-O3C
9	M	202	G4P	PA-O3A-PB-O2B
9	M	202	G4P	C4'-C5'-O5'-PA
9	M	202	G4P	PB-O3A-PA-O5'
9	J	2004	G4P	C3'-O3'-PC-O2C
9	J	2004	G4P	PA-O3A-PB-O1B
9	E	101	G4P	C2'-C3'-O3'-PC
9	M	202	G4P	C2'-C3'-O3'-PC
9	M	202	G4P	C4'-C3'-O3'-PC
9	J	2004	G4P	PB-O3A-PA-O1A
9	M	202	G4P	PA-O3A-PB-O1B
9	J	2004	G4P	PA-O3A-PB-O2B
9	J	2004	G4P	PA-O3A-PB-O3B
9	M	202	G4P	PC-O3C-PD-O3D
9	J	2004	G4P	C3'-O3'-PC-O1C
9	M	202	G4P	C3'-C4'-C5'-O5'

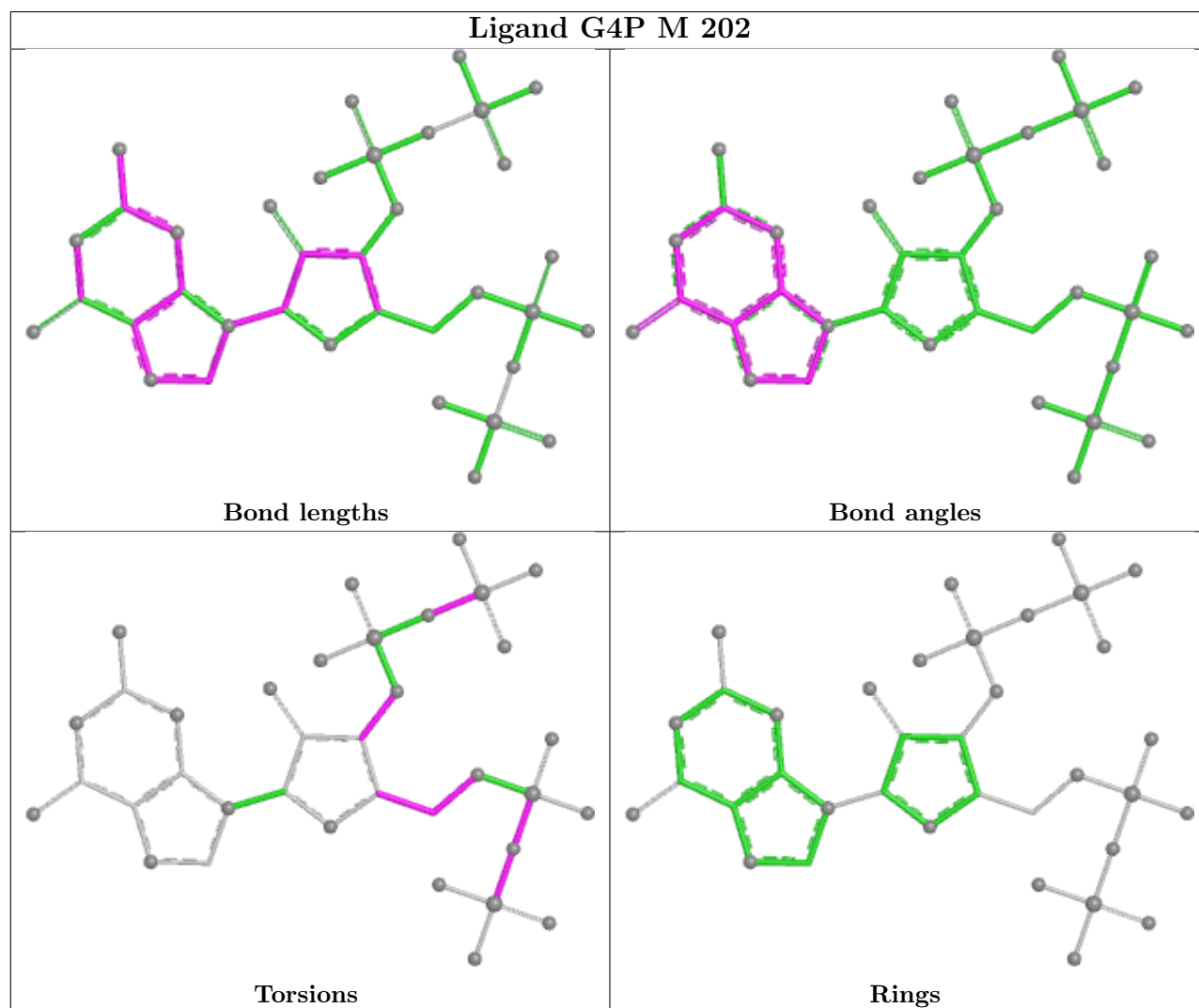
There are no ring outliers.

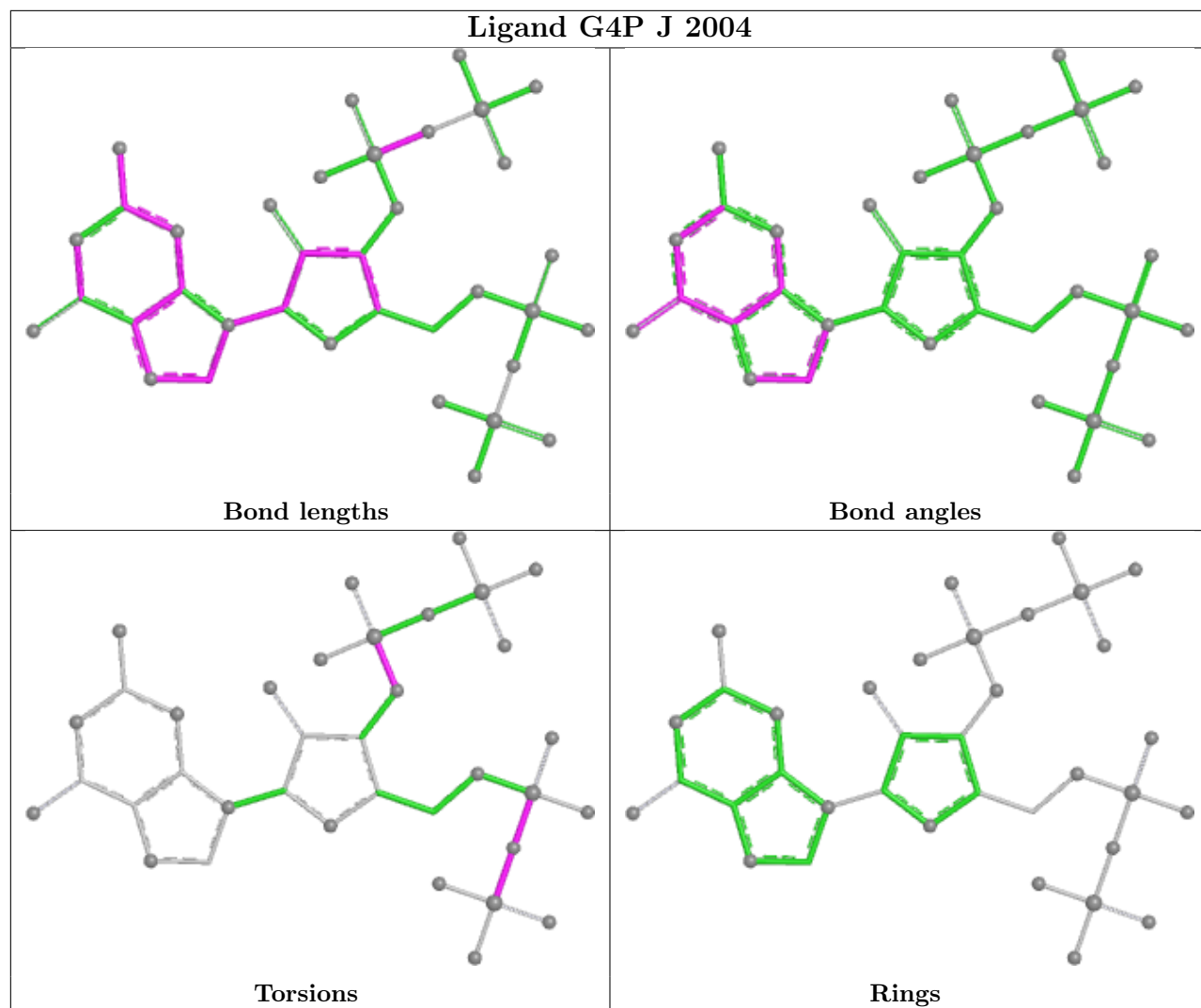
3 monomers are involved in 14 short contacts:

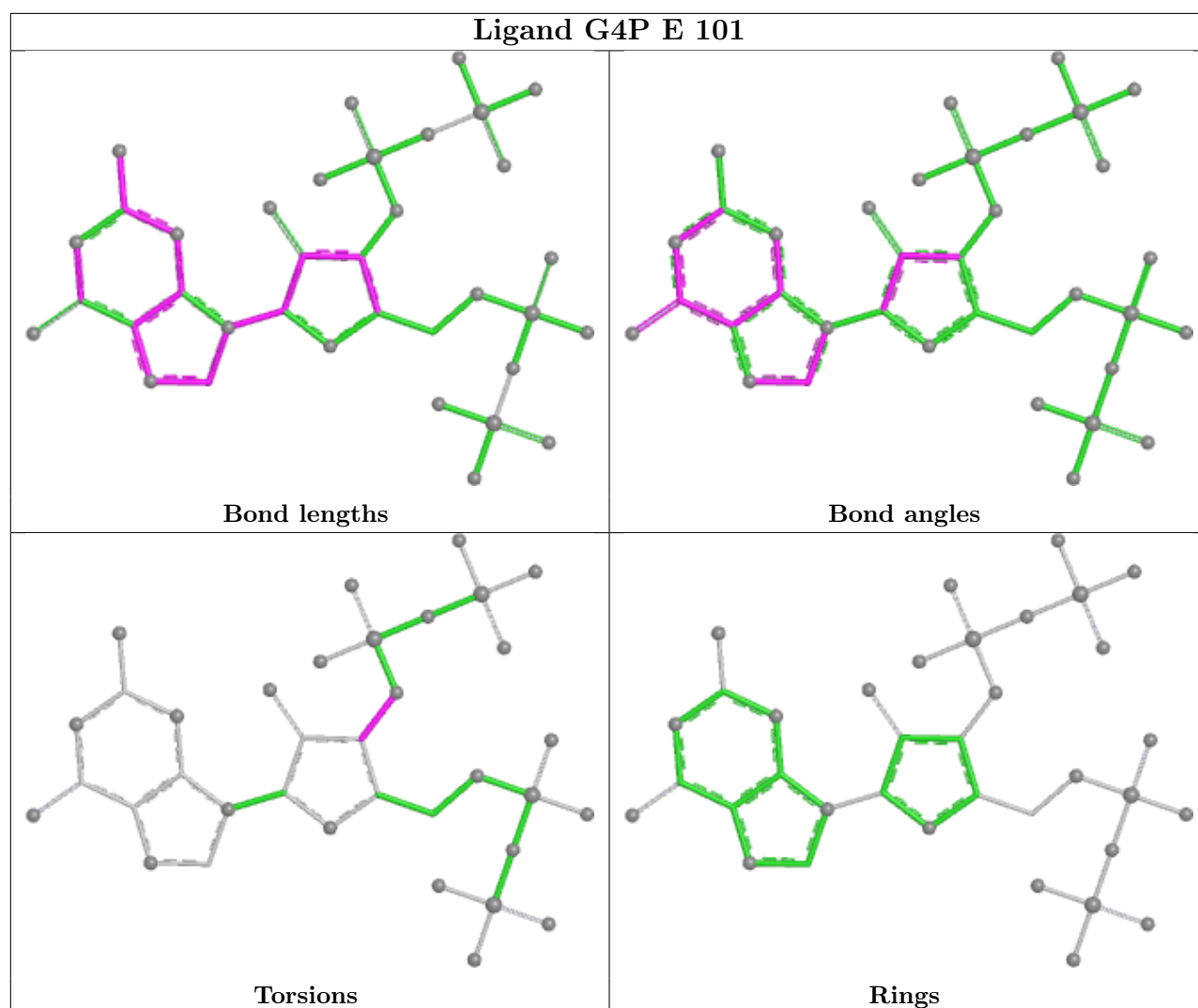
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	202	G4P	7	0
9	J	2004	G4P	4	0
9	E	101	G4P	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/329 (96%)	-0.43	1 (0%) 90 80	211, 260, 453, 474	0
1	B	297/329 (90%)	-0.42	0 100 100	204, 303, 444, 497	0
1	G	227/329 (68%)	-0.40	3 (1%) 75 59	257, 320, 369, 399	0
1	H	216/329 (65%)	-0.35	1 (0%) 87 75	288, 336, 378, 393	0
2	C	1340/1342 (99%)	-0.48	12 (0%) 81 66	154, 240, 335, 399	0
2	I	1340/1342 (99%)	-0.50	7 (0%) 87 75	200, 281, 382, 521	0
3	D	1173/1407 (83%)	-0.37	9 (0%) 82 68	152, 223, 328, 395	0
3	J	1155/1407 (82%)	-0.45	8 (0%) 84 71	197, 262, 344, 388	0
4	E	89/91 (97%)	-0.56	1 (1%) 78 62	202, 266, 330, 365	0
4	K	79/91 (86%)	-0.60	0 100 100	336, 411, 518, 552	0
5	F	468/613 (76%)	-0.52	0 100 100	188, 293, 445, 515	0
5	L	469/613 (76%)	-0.62	1 (0%) 91 83	223, 313, 427, 446	0
6	M	140/151 (92%)	-0.28	0 100 100	317, 361, 378, 386	0
All	All	7312/8373 (87%)	-0.46	43 (0%) 85 73	152, 271, 395, 552	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	482	ALA	4.2
1	G	205	MET	4.0
3	J	1230	THR	4.0
3	J	1255	VAL	3.4
1	G	43	LEU	3.3
2	C	209	ILE	3.2
2	C	207	THR	3.1
2	C	686	GLN	3.0
3	J	1253	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
5	L	416	VAL	2.9
3	D	252	LEU	2.8
2	I	708	VAL	2.8
3	J	915	ILE	2.7
3	D	253	VAL	2.7
3	J	815	GLY	2.7
2	C	184	LEU	2.6
2	I	734	ILE	2.5
2	I	667	LEU	2.5
2	C	839	VAL	2.5
2	C	206	ALA	2.5
2	C	77	GLU	2.4
2	C	194	LEU	2.4
2	C	186	PHE	2.4
3	D	337	ARG	2.4
2	C	198	ILE	2.4
2	C	252	SER	2.4
2	I	883	LEU	2.4
3	D	815	GLY	2.3
4	E	16	ARG	2.3
1	G	47	LEU	2.3
3	J	1145	PHE	2.3
2	I	561	ILE	2.3
2	C	196	VAL	2.2
2	I	796	LEU	2.2
3	D	1332	LEU	2.2
3	J	923	ILE	2.1
3	D	513	MET	2.1
3	D	421	VAL	2.1
2	I	814	ASP	2.1
3	D	260	PHE	2.1
3	J	1234	VAL	2.1
1	A	203	ILE	2.0
1	H	39	LEU	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

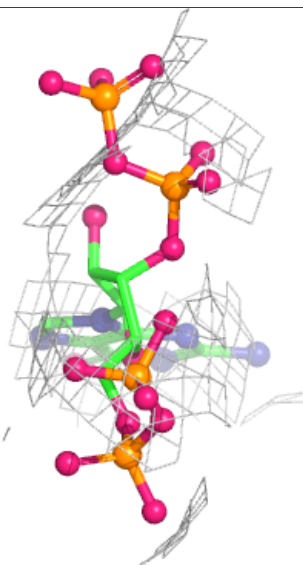
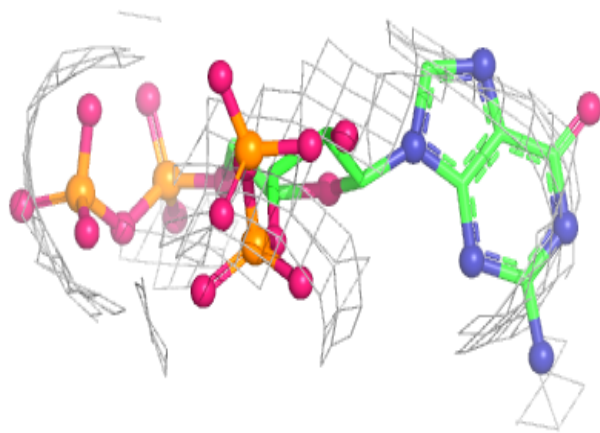
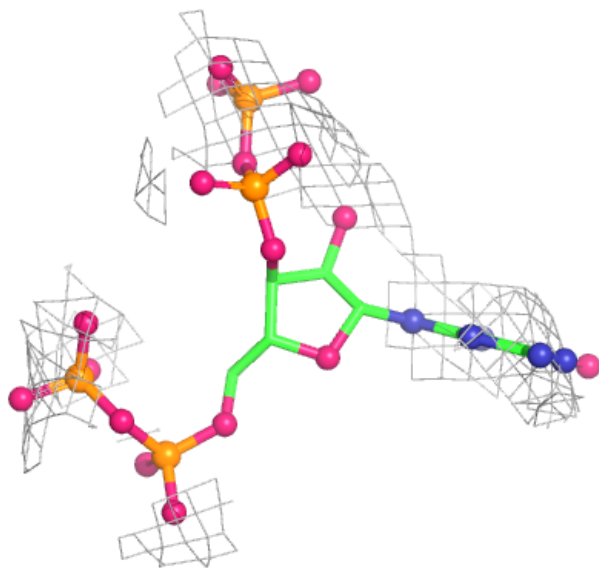
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	G4P	J	2004	36/36	0.71	0.07	306,370,455,463	0
9	G4P	E	101	36/36	0.91	0.06	199,253,286,301	0
9	G4P	M	202	36/36	0.91	0.05	267,326,403,408	0
8	ZN	M	201	1/1	0.93	0.05	662,662,662,662	0
7	MG	J	2001	1/1	0.94	0.06	184,184,184,184	0
7	MG	D	2001	1/1	0.96	0.04	162,162,162,162	0
8	ZN	J	2002	1/1	0.98	0.03	264,264,264,264	0
8	ZN	D	2002	1/1	1.00	0.04	273,273,273,273	0
8	ZN	J	2003	1/1	1.00	0.07	176,176,176,176	0
8	ZN	D	2003	1/1	1.00	0.12	295,295,295,295	0

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

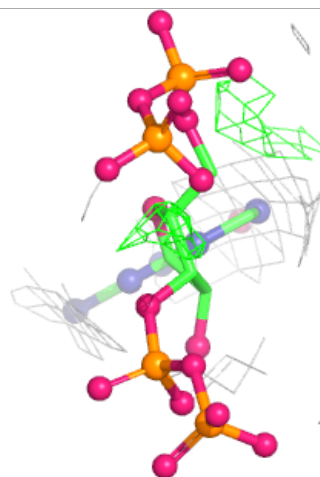
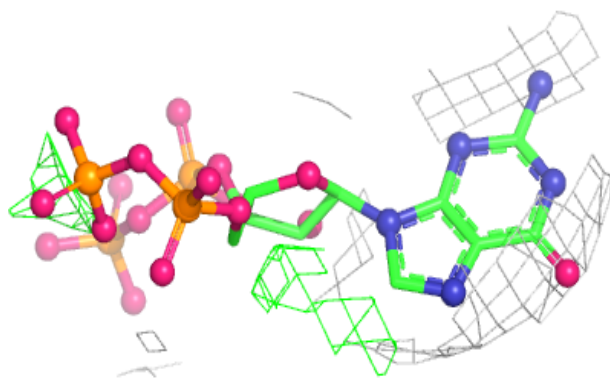
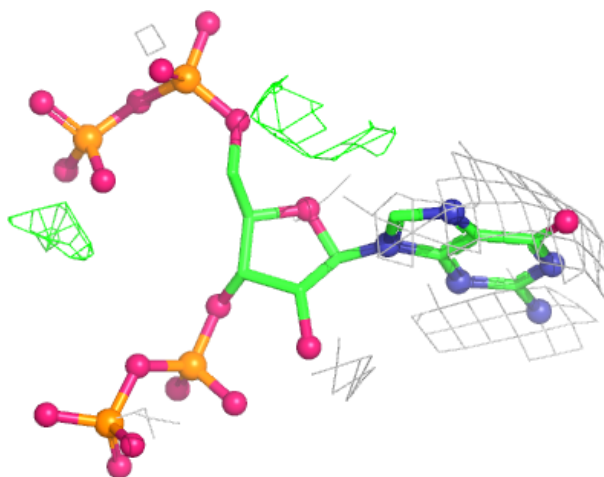
Electron density around G4P J 2004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



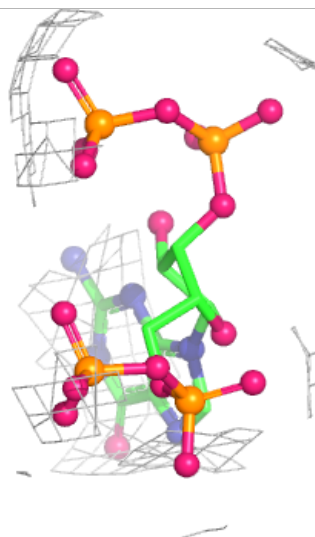
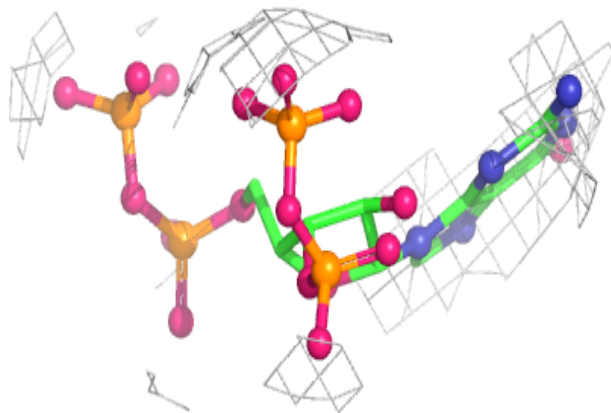
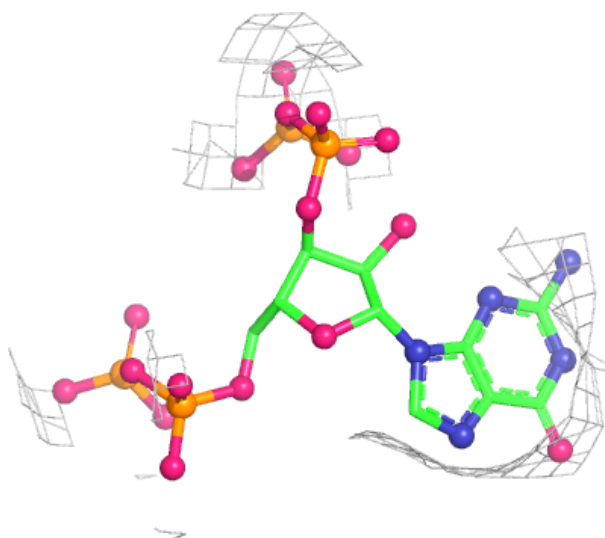
Electron density around G4P E 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around G4P M 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.