



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:08 am BST

PDB ID : 4ZH3
Title : Crystal structure of Escherichia coli RNA polymerase in complex with CBRH16-Br
Authors : Feng, Y.; Ebright, R.H.
Deposited on : 2015-04-24
Resolution : 4.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

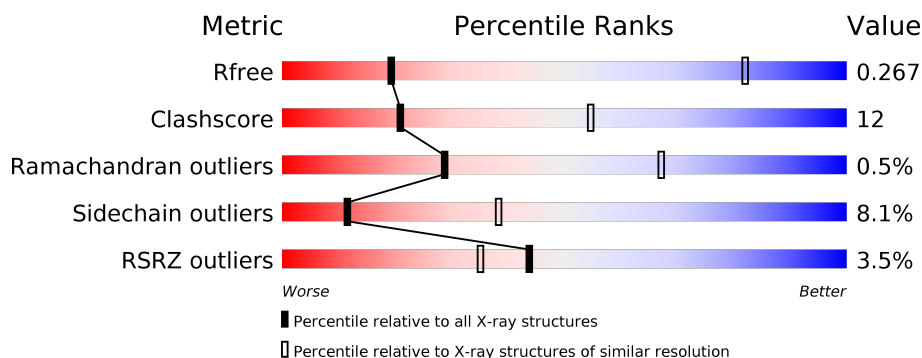
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.08 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (4.46-3.70)
Clashscore	141614	1013 (4.42-3.74)
Ramachandran outliers	138981	1151 (4.46-3.70)
Sidechain outliers	138945	1139 (4.46-3.70)
RSRZ outliers	127900	1012 (4.48-3.68)

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

Mol	Chain	Length	Quality of chain
1	A	335	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>27%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	335	<div> <div>3%</div> <div> <div></div> <div>40%</div> <div>21%</div> <div>•</div> <div>36%</div> </div> </div>
1	G	335	<div> <div>%</div> <div> <div></div> <div>41%</div> <div>24%</div> <div>•</div> <div>33%</div> </div> </div>
1	H	335	<div> <div>2%</div> <div> <div></div> <div>39%</div> <div>23%</div> <div>••</div> <div>36%</div> </div> </div>
2	C	1342	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>•</div> </div> </div>
2	I	1342	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>29%</div> <div>•</div> </div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	J	1501	-	-	-	X
8	4OD	J	1504	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 57537 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	302	Total	C	N	O	S	0	0	0
			2328	1456	413	451	8			
1	B	216	Total	C	N	O	S	0	0	0
			1667	1041	294	326	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P0A7Z4
A	-4	HIS	-	expression tag	UNP P0A7Z4
A	-3	HIS	-	expression tag	UNP P0A7Z4
A	-2	HIS	-	expression tag	UNP P0A7Z4
A	-1	HIS	-	expression tag	UNP P0A7Z4
A	0	HIS	-	expression tag	UNP P0A7Z4
A	1	HIS	-	expression tag	UNP P0A7Z4
B	-5	MET	-	expression tag	UNP P0A7Z4
B	-4	HIS	-	expression tag	UNP P0A7Z4
B	-3	HIS	-	expression tag	UNP P0A7Z4
B	-2	HIS	-	expression tag	UNP P0A7Z4
B	-1	HIS	-	expression tag	UNP P0A7Z4
B	0	HIS	-	expression tag	UNP P0A7Z4
B	1	HIS	-	expression tag	UNP P0A7Z4
G	-5	MET	-	expression tag	UNP P0A7Z4
G	-4	HIS	-	expression tag	UNP P0A7Z4
G	-3	HIS	-	expression tag	UNP P0A7Z4
G	-2	HIS	-	expression tag	UNP P0A7Z4
G	-1	HIS	-	expression tag	UNP P0A7Z4
G	0	HIS	-	expression tag	UNP P0A7Z4
G	1	HIS	-	expression tag	UNP P0A7Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	MET	-	expression tag	UNP P0A7Z4
H	-4	HIS	-	expression tag	UNP P0A7Z4
H	-3	HIS	-	expression tag	UNP P0A7Z4
H	-2	HIS	-	expression tag	UNP P0A7Z4
H	-1	HIS	-	expression tag	UNP P0A7Z4
H	0	HIS	-	expression tag	UNP P0A7Z4
H	1	HIS	-	expression tag	UNP P0A7Z4

- 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	1151	Total	C	N	O	S	0	0	0
			8992	5653	1608	1686	45			
3	J	1319	Total	C	N	O	S	0	0	0
			10254	6443	1824	1939	48			

- 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	542	Total	C	N	O	S	0	0	0
			4204	2625	752	801	26			
5	L	539	Total	C	N	O	S	0	0	0
			4196	2619	749	802	26			

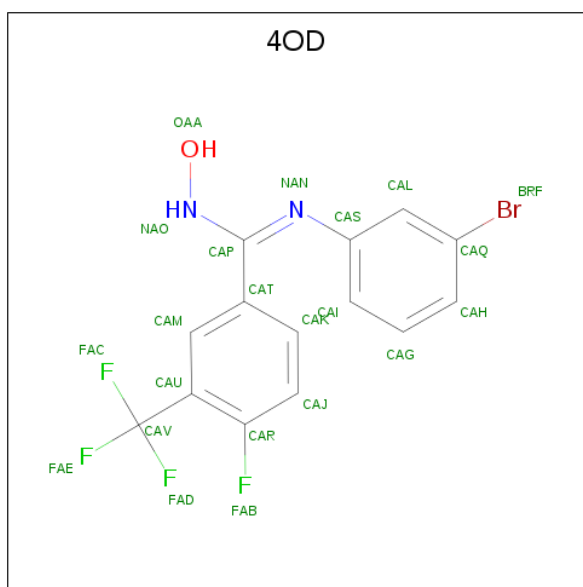
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 8 is N'-(3-bromophenyl)-4-fluoro-N-hydroxy-3-(trifluoromethyl)benzenecarboximide (three-letter code: 4OD) (formula: C₁₄H₉BrF₄N₂O).

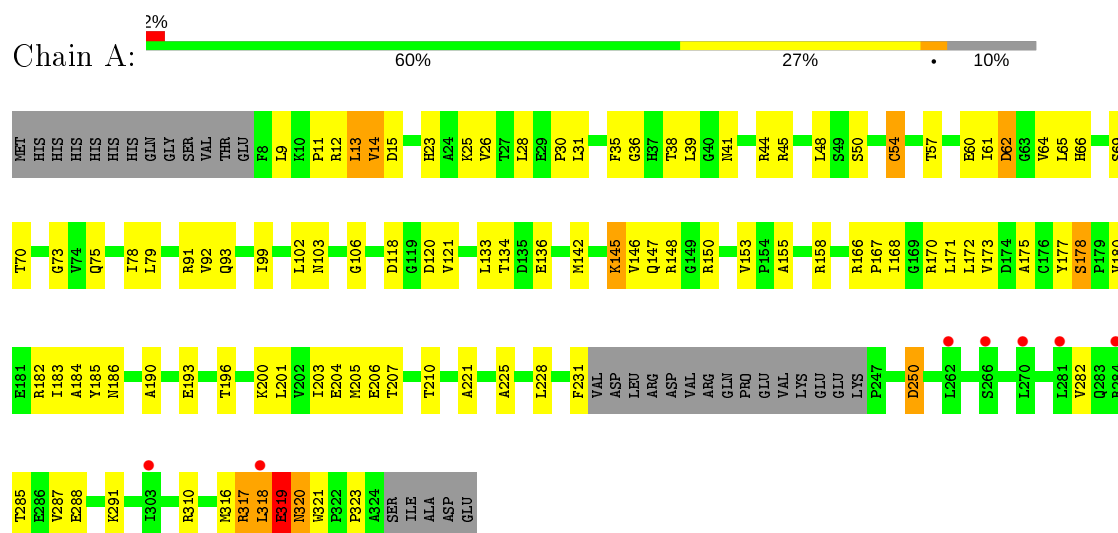


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total	Br	C	F	N	O	0	0
			22	1	14	4	2	1		
8	J	1	Total	Br	C	F	N	O	0	0
			22	1	14	4	2	1		

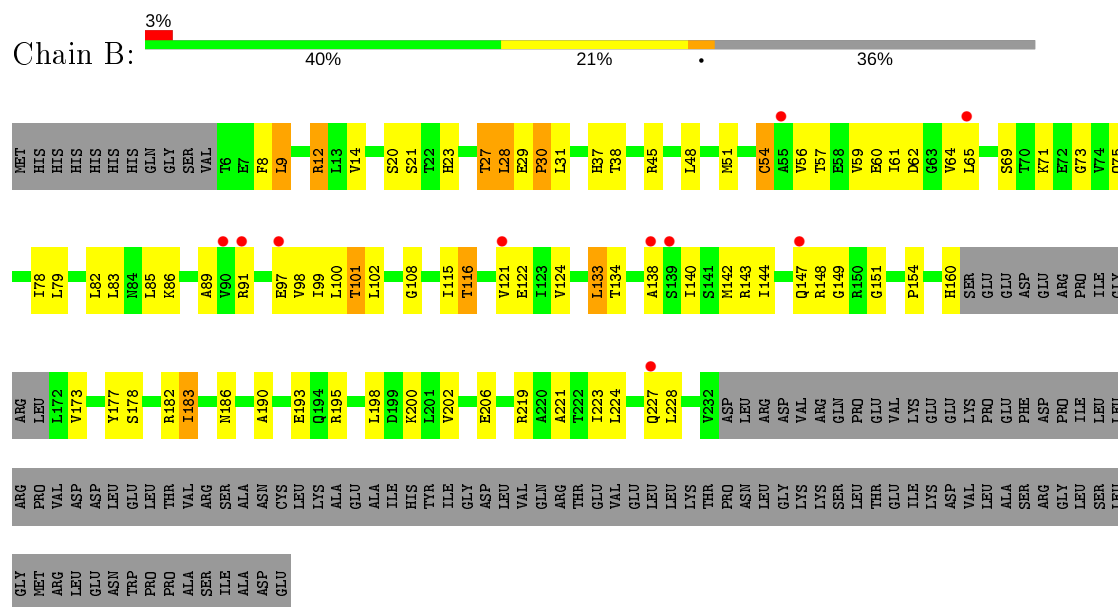
3 Residue-property plots

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

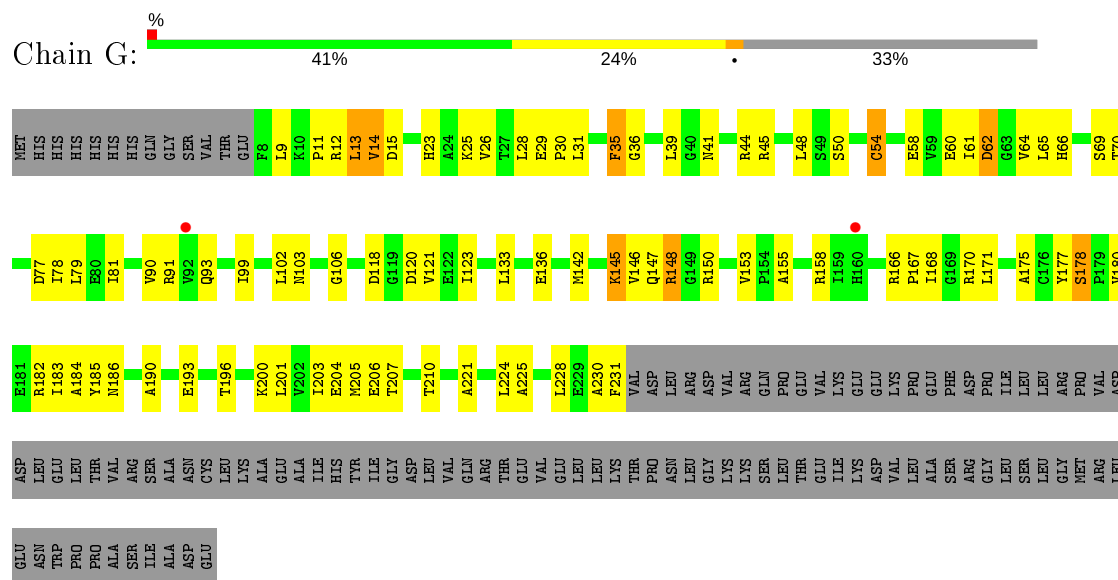
- Molecule 1: DNA-directed RNA polymerase subunit alpha



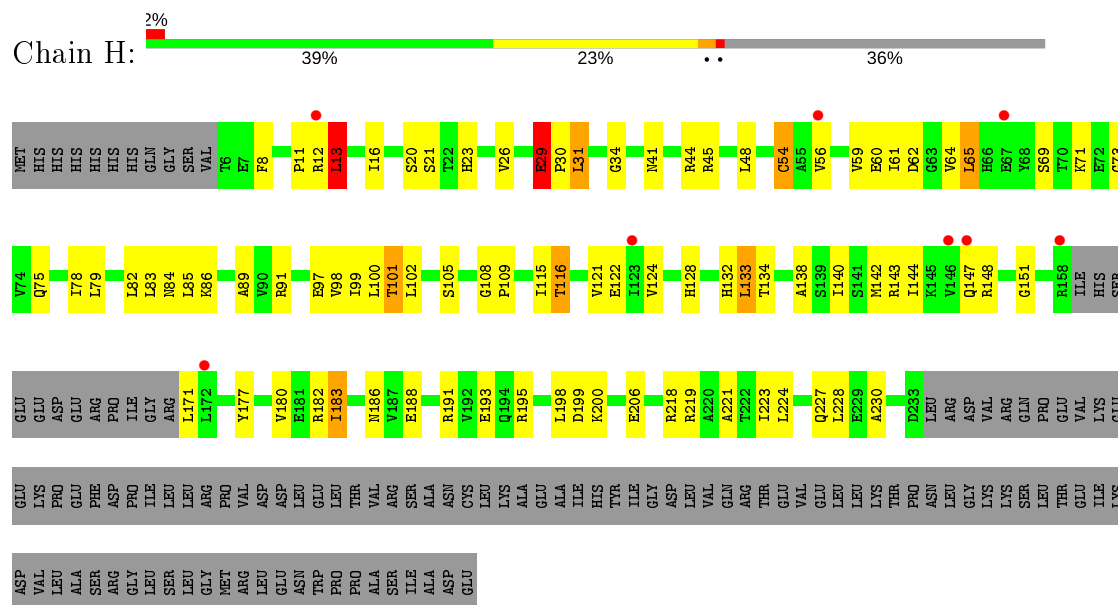
- Molecule 1: DNA-directed RNA polymerase subunit alpha



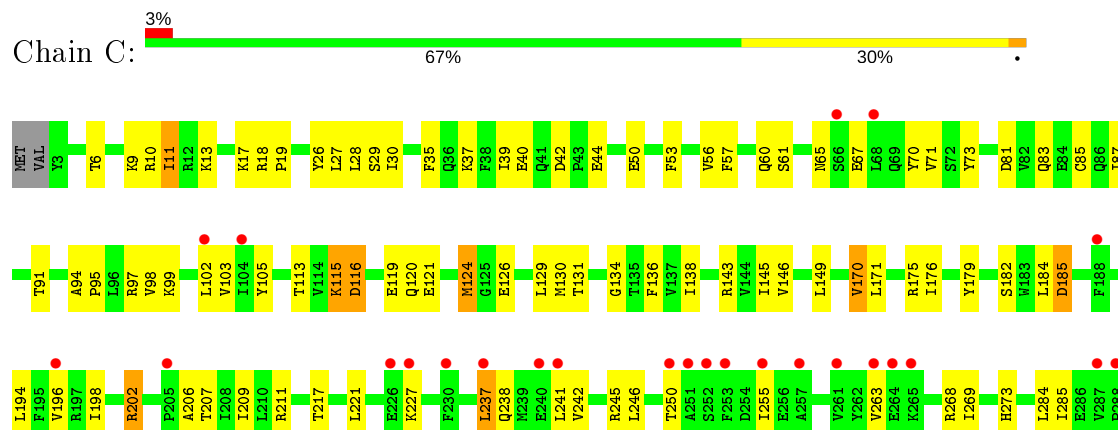
- Molecule 1: DNA-directed RNA polymerase subunit alpha

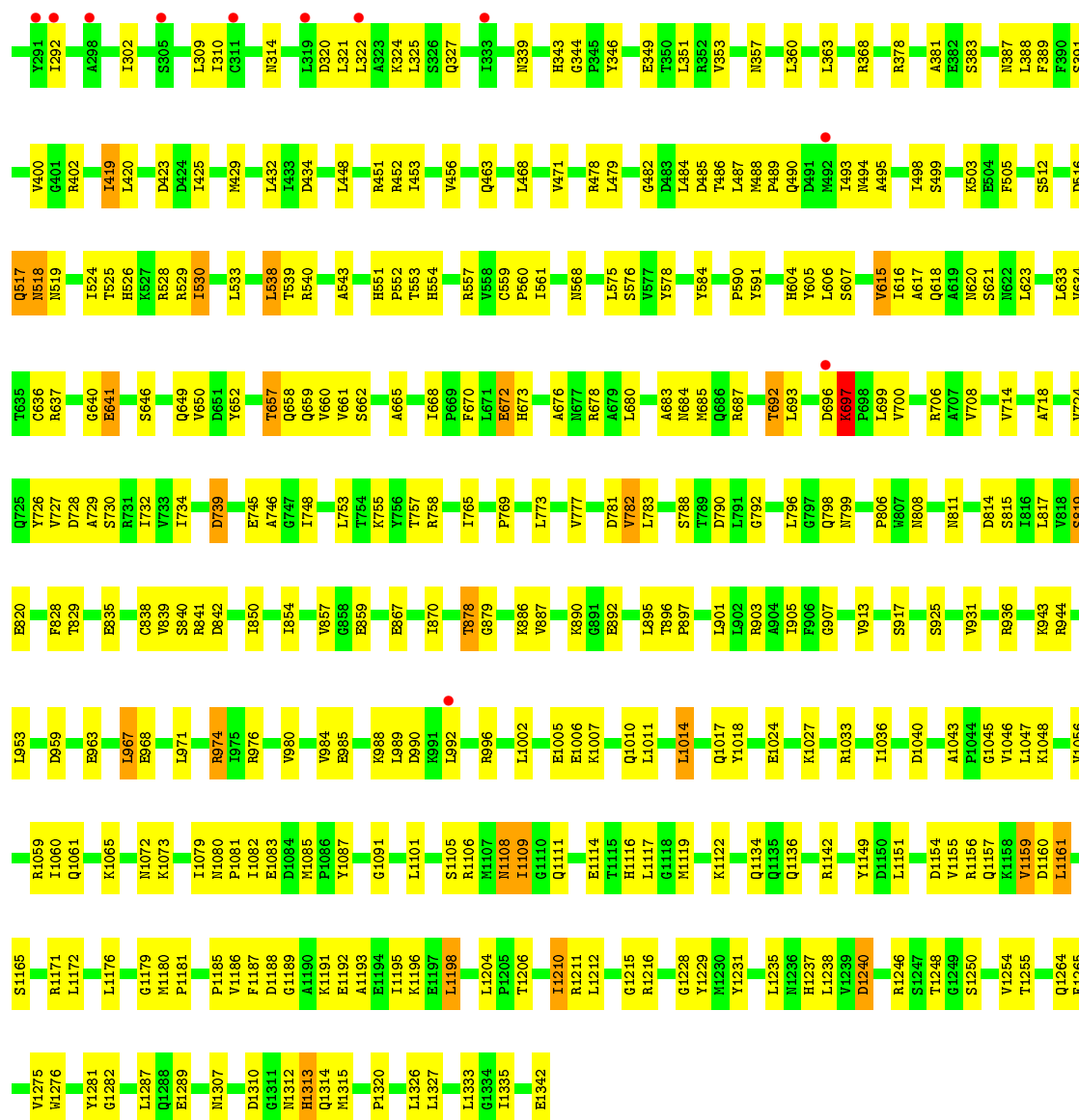


- Molecule 1: DNA-directed RNA polymerase subunit alpha

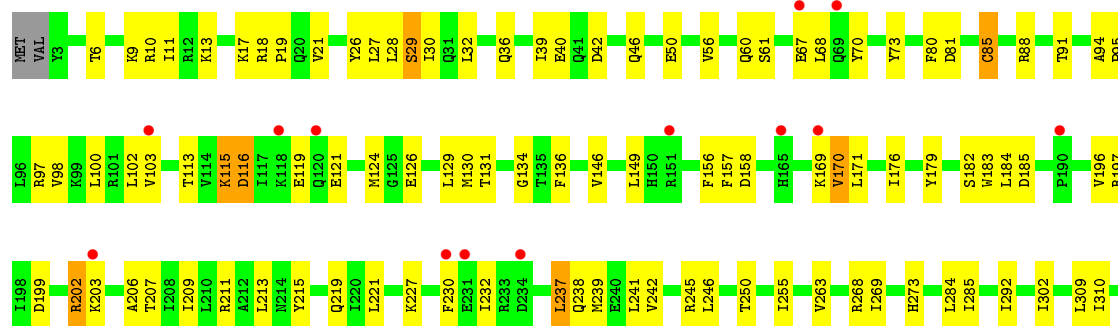


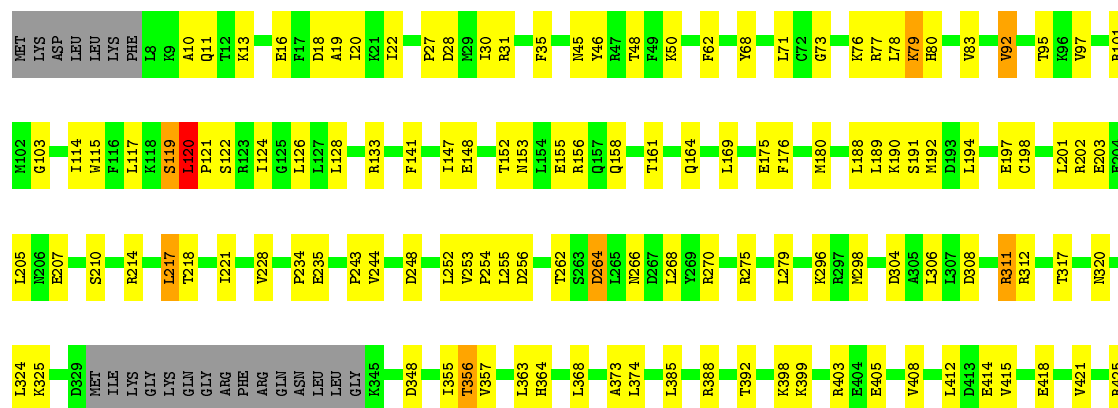
- Molecule 2: DNA-directed RNA polymerase subunit beta

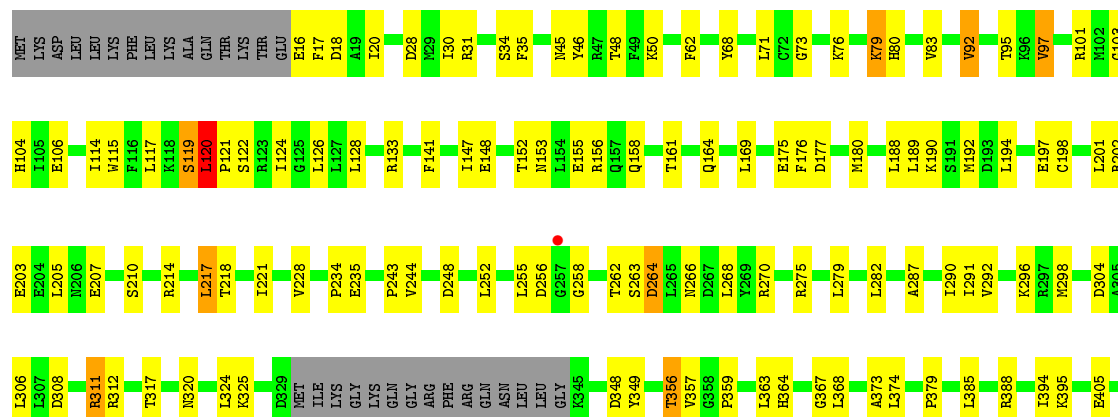




• Molecule 2: DNA-directed RNA polymerase subunit beta



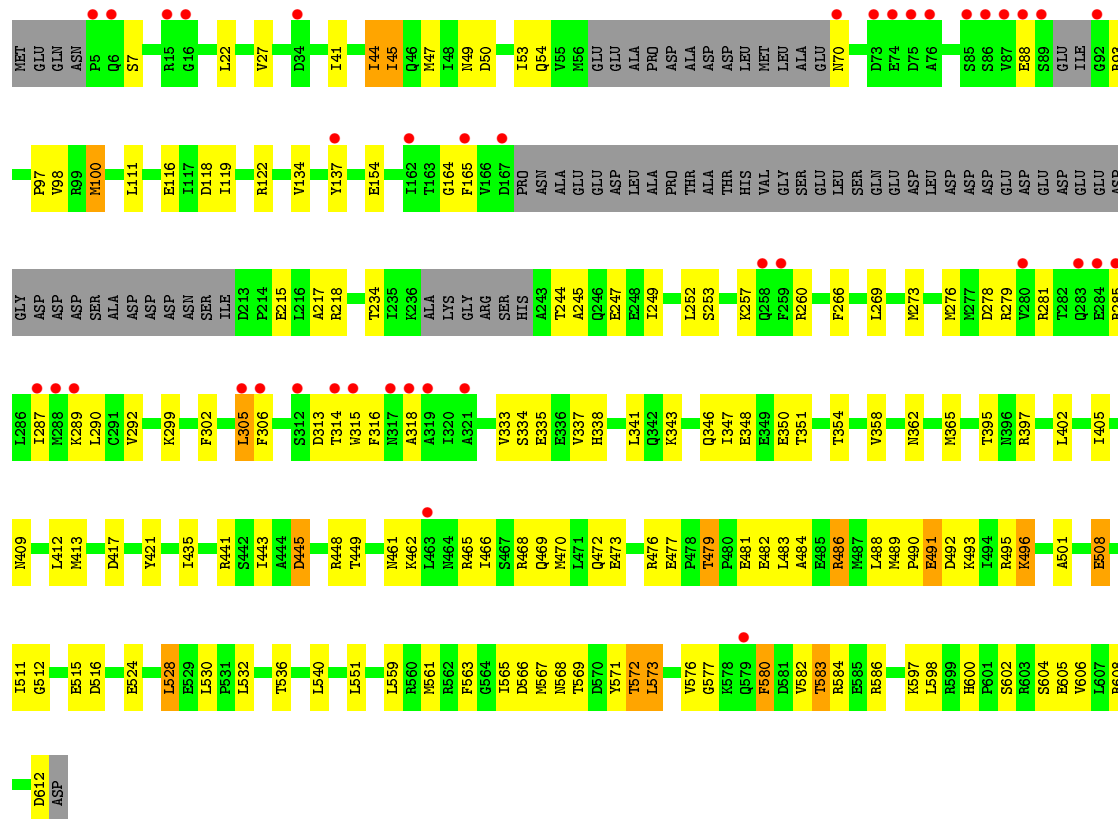




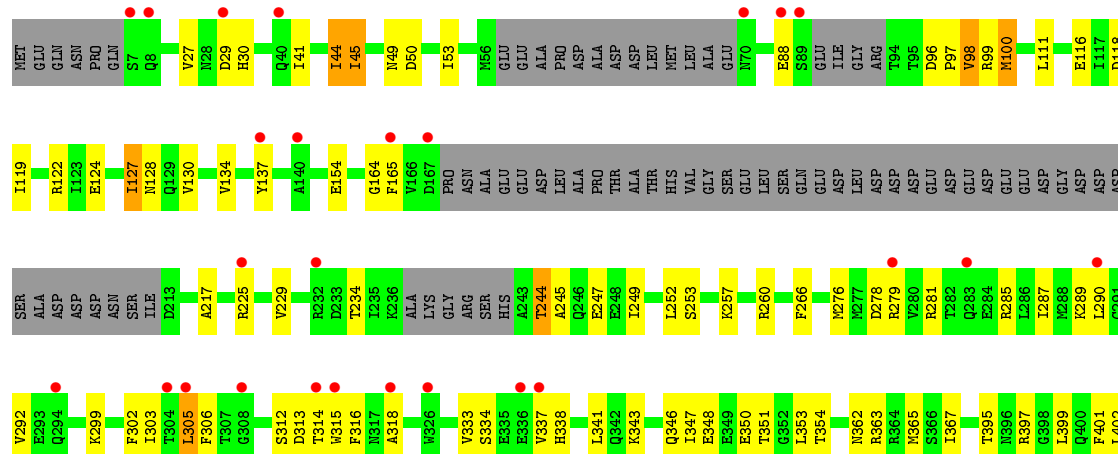


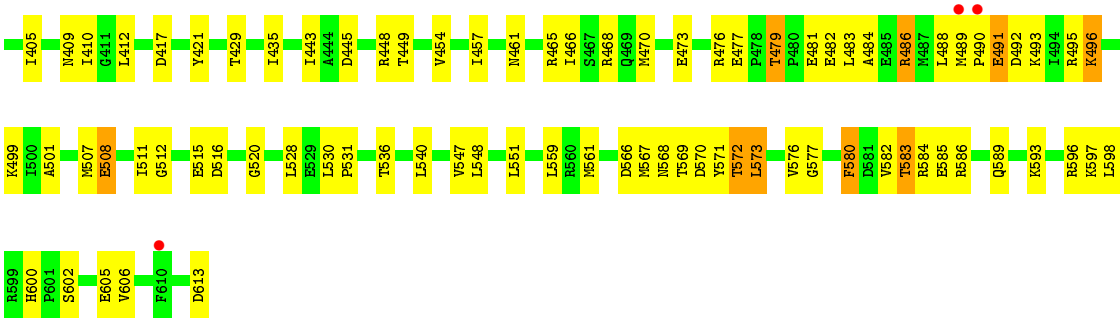


• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.34Å 205.79Å 307.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 4.08 49.81 – 4.08	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.75-4.08) 92.7 (49.81-4.08)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 4.14Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.237 , 0.267 0.239 , 0.267	Depositor DCC
R_{free} test set	1879 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	143.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 97.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	57537	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 4OD

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	0.41	3/2358 (0.1%)	0.70	5/3197 (0.2%)
1	B	0.38	0/1687	0.69	1/2286 (0.0%)
1	G	0.33	0/1751	0.66	0/2373
1	H	0.37	0/1681	0.69	2/2278 (0.1%)
2	C	0.28	0/10739	0.48	0/14489
2	I	0.27	0/10735	0.47	0/14484
3	D	0.28	0/9130	0.49	1/12325 (0.0%)
3	J	0.27	0/10409	0.48	1/14059 (0.0%)
4	E	0.27	0/693	0.48	0/935
4	K	0.27	0/629	0.48	0/847
5	F	0.28	0/4254	0.49	0/5731
5	L	0.28	0/4246	0.48	0/5720
All	All	0.29	3/58312 (0.0%)	0.51	10/78724 (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
3	D	0	1
3	J	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	ASP	CB-CG	-5.88	1.39	1.51
1	A	317	ARG	CZ-NH2	-5.37	1.26	1.33
1	A	317	ARG	CG-CD	5.36	1.65	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASP	CB-CG-OD1	-9.62	109.64	118.30
1	A	317	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	250	ASP	CB-CG-OD2	8.07	125.57	118.30
1	H	29	GLU	C-N-CD	7.75	144.67	128.40
1	A	317	ARG	NH1-CZ-NH2	-6.62	112.12	119.40
1	H	13	LEU	CA-CB-CG	6.13	129.41	115.30
3	D	120	LEU	N-CA-C	6.00	127.20	111.00
1	B	28	LEU	CB-CG-CD1	5.73	120.75	111.00
1	A	317	ARG	NE-CZ-NH2	5.56	123.08	120.30
3	J	120	LEU	N-CA-C	5.48	125.81	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	120	LEU	Peptide
3	J	120	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2328	0	2380	73	0
1	B	1667	0	1692	59	0
1	G	1730	0	1756	68	0
1	H	1662	0	1687	62	0
2	C	10570	0	10582	264	0
2	I	10566	0	10576	253	0
3	D	8992	0	9180	254	0
3	J	10254	0	10462	272	0
4	E	691	0	695	16	0
4	K	627	0	634	14	0
5	F	4204	0	4106	97	0
5	L	4196	0	4103	106	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	22	0	9	3	0
8	J	22	0	9	4	0
All	All	57537	0	57871	1404	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.37	1.04
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.46	0.97
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.49	0.92
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.57	0.87
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.57	0.86
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.42	0.84
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.42	0.83
3:J:418:GLU:HG3	4:K:45:LYS:H	1.44	0.83
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.61	0.83
3:D:755:ILE:HD13	3:D:774:ILE:HD11	1.59	0.83
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.59	0.82
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.61	0.82
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.63	0.81
3:D:418:GLU:HG3	4:E:45:LYS:H	1.46	0.81
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.61	0.80
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.62	0.80
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.29	0.79
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.62	0.79
1:B:12:ARG:HD2	1:B:30:PRO:HG2	1.65	0.78
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.65	0.78
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.65	0.78
3:J:133:ARG:HB2	5:L:88:GLU:HA	1.66	0.78
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.66	0.77
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.67	0.77
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.68	0.76
5:F:561:MET:HA	5:F:567:MET:HE1	1.67	0.76
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.68	0.76
1:B:101:THR:HG22	1:B:116:THR:HB	1.67	0.76
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:O	5:F:608:ARG:NH1	2.19	0.75
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.68	0.75
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.68	0.75
3:D:773:PHE:HB3	8:D:1504:4OD:H8	1.68	0.75
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.68	0.75
1:H:101:THR:HG22	1:H:116:THR:HB	1.67	0.75
1:G:23:HIS:HB2	1:G:205:MET:O	1.87	0.74
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.67	0.74
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.68	0.74
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.67	0.74
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.69	0.74
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.69	0.74
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.52	0.73
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.68	0.73
3:D:755:ILE:HG22	3:D:757:THR:H	1.53	0.73
1:A:250:ASP:HB2	5:F:605:GLU:HG2	1.68	0.73
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.70	0.73
3:D:392:THR:HG21	5:F:606:VAL:HA	1.71	0.73
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.22	0.72
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.71	0.72
1:H:191:ARG:NH2	3:J:410:ASP:OD2	2.22	0.72
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.22	0.72
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.69	0.72
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.72	0.72
3:D:120:LEU:HD22	3:D:121:PRO:HD3	1.71	0.72
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.55	0.71
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.72	0.71
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.22	0.71
2:I:528:ARG:NH2	2:I:576:SER:O	2.23	0.71
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.72	0.71
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.72	0.71
5:L:561:MET:HA	5:L:567:MET:HE1	1.73	0.70
1:A:23:HIS:HB2	1:A:205:MET:O	1.90	0.70
2:I:808:ASN:H	3:J:633:ALA:HB2	1.57	0.70
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.72	0.70
3:J:773:PHE:HB3	8:J:1504:4OD:H8	1.71	0.70
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.71	0.69
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.22	0.69
3:J:755:ILE:HD13	3:J:774:ILE:HD11	1.73	0.69
1:A:166:ARG:O	1:A:168:ILE:N	2.26	0.69
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:ARG:NH2	2:C:620:ASN:OD1	2.26	0.69
1:H:59:VAL:O	1:H:171:LEU:N	2.26	0.69
3:J:755:ILE:HG22	3:J:757:THR:H	1.58	0.68
5:L:470:MET:HA	5:L:473:GLU:HB3	1.74	0.68
2:I:452:ARG:NH1	2:I:584:TYR:O	2.26	0.68
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.74	0.68
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.74	0.68
3:D:514:THR:HG23	3:D:576:ARG:HG2	1.75	0.68
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.75	0.68
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.75	0.68
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.76	0.68
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.57	0.67
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.28	0.67
1:G:39:LEU:HD11	1:H:227:GLN:HB3	1.76	0.67
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.76	0.67
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.76	0.67
5:F:470:MET:HA	5:F:473:GLU:HB3	1.75	0.67
2:C:136:PHE:O	2:C:143:ARG:N	2.26	0.67
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.59	0.67
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.25	0.67
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.58	0.67
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.76	0.67
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.59	0.67
3:J:308:ASP:OD2	3:J:311:ARG:NH2	2.26	0.67
1:G:166:ARG:O	1:G:168:ILE:N	2.28	0.67
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.42	0.67
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.60	0.67
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.76	0.67
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.77	0.66
1:G:12:ARG:H	1:G:30:PRO:HD2	1.59	0.66
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.77	0.66
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.77	0.66
1:G:28:LEU:HD22	1:G:201:LEU:HD23	1.78	0.66
2:I:197:ARG:NH2	5:L:29:ASP:OD2	2.28	0.66
3:J:774:ILE:HB	8:J:1504:4OD:H9	1.77	0.66
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.78	0.66
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.29	0.66
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.77	0.66
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.76	0.66
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.78	0.66
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.76	0.65
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.76	0.65
5:F:602:SER:H	5:F:605:GLU:HG3	1.61	0.65
1:G:61:ILE:HG22	1:G:62:ASP:H	1.60	0.65
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.79	0.65
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.79	0.65
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.79	0.65
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.77	0.65
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.79	0.65
2:C:528:ARG:NH2	2:C:576:SER:O	2.30	0.65
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.77	0.65
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.77	0.65
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.29	0.64
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.80	0.64
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.80	0.64
1:A:61:ILE:HG22	1:A:62:ASP:H	1.62	0.64
3:D:133:ARG:NH2	5:F:93:ARG:O	2.29	0.64
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.79	0.64
1:G:231:PHE:O	1:H:218:ARG:NH1	2.31	0.63
2:I:88:ARG:NH2	2:I:1035:LYS:O	2.30	0.63
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.79	0.63
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.81	0.63
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.33	0.63
2:C:18:ARG:NH1	2:C:621:SER:O	2.31	0.63
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.31	0.63
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.80	0.63
2:I:829:THR:HA	2:I:1059:ARG:HA	1.81	0.63
2:I:18:ARG:NH1	2:I:621:SER:O	2.31	0.63
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.63	0.63
3:D:749:LYS:HG3	3:D:751:ASP:HB3	1.79	0.63
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.79	0.63
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.81	0.62
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.81	0.62
2:C:452:ARG:NH1	2:C:584:TYR:O	2.33	0.62
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.65	0.62
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.81	0.62
1:A:45:ARG:HG2	1:B:38:THR:HB	1.81	0.62
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.81	0.62
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.82	0.62
1:A:12:ARG:HG2	1:A:13:LEU:H	1.65	0.62
2:I:18:ARG:NH2	2:I:620:ASN:OD1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.16	0.62
3:D:356:THR:OG1	3:D:357:VAL:N	2.33	0.61
5:F:49:ASN:HA	5:F:53:ILE:HA	1.82	0.61
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.82	0.61
1:G:12:ARG:HG2	1:G:13:LEU:H	1.65	0.61
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.34	0.61
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.82	0.61
2:I:207:THR:HG21	2:I:351:LEU:HG	1.82	0.61
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.49	0.61
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.82	0.61
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.82	0.61
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.83	0.61
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.81	0.61
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.83	0.61
2:C:560:PRO:O	3:D:780:ARG:NH2	2.34	0.61
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.83	0.60
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.83	0.60
2:I:494:ASN:OD1	2:I:495:ALA:N	2.32	0.60
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.66	0.60
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.84	0.60
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.66	0.60
5:L:49:ASN:HA	5:L:53:ILE:HA	1.84	0.60
1:B:182:ARG:NH1	3:D:581:MET:SD	2.75	0.60
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.83	0.60
5:L:244:THR:O	5:L:247:GLU:HG2	2.01	0.60
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.84	0.60
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.66	0.60
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.84	0.60
2:I:1251:TYR:OH	3:J:348:ASP:OD2	2.15	0.60
1:A:12:ARG:H	1:A:30:PRO:HD2	1.67	0.59
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.49	0.59
2:I:1151:LEU:HD21	2:I:1198:LEU:HD23	1.83	0.59
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.84	0.59
3:D:77:ARG:HE	5:F:569:THR:HA	1.68	0.59
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.35	0.59
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.84	0.59
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.65	0.59
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.84	0.59
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.85	0.59
3:J:478:LEU:HG	4:K:47:THR:HG23	1.85	0.59
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.84	0.59
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.85	0.59
3:D:774:ILE:HB	8:D:1504:4OD:H9	1.85	0.59
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.84	0.59
5:F:515:GLU:HG2	5:F:516:ASP:H	1.68	0.59
3:D:1310:THR:HG21	5:F:70:ASN:HA	1.83	0.59
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.84	0.59
3:J:613:GLY:O	3:J:617:THR:OG1	2.21	0.59
2:C:30:ILE:H	2:C:30:ILE:HD12	1.67	0.59
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.67	0.59
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.83	0.59
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.84	0.59
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.83	0.59
1:B:29:GLU:HB3	1:B:30:PRO:CD	2.28	0.58
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.67	0.58
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.84	0.58
1:B:61:ILE:HB	1:B:64:VAL:O	2.03	0.58
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.68	0.58
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.84	0.58
5:F:602:SER:H	5:F:605:GLU:CG	2.16	0.58
3:J:210:SER:O	3:J:214:ARG:HG2	2.03	0.58
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.85	0.58
2:C:829:THR:HA	2:C:1059:ARG:HA	1.84	0.58
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.68	0.58
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.85	0.58
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.85	0.58
5:F:602:SER:H	5:F:605:GLU:CD	2.07	0.58
3:D:115:TRP:O	3:D:119:SER:HB2	2.02	0.58
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.67	0.58
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.86	0.58
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.15	0.58
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.69	0.58
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.84	0.58
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.37	0.58
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.85	0.58
3:D:741:ALA:O	3:D:762:ASN:ND2	2.36	0.58
3:J:356:THR:OG1	3:J:357:VAL:N	2.37	0.58
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.84	0.58
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.86	0.58
3:D:749:LYS:HD3	3:D:753:SER:HB3	1.86	0.58
5:L:551:LEU:HD22	5:L:597:LYS:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.85	0.58
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.21	0.58
5:L:515:GLU:HG2	5:L:516:ASP:H	1.68	0.58
1:B:51:MET:HB3	1:B:178:SER:HA	1.86	0.57
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.86	0.57
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.85	0.57
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.86	0.57
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.85	0.57
1:A:14:VAL:HG22	1:A:15:ASP:H	1.69	0.57
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.85	0.57
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.85	0.57
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.86	0.57
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.86	0.57
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.87	0.57
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.85	0.57
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.86	0.57
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.15	0.57
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.68	0.57
2:I:560:PRO:O	3:J:780:ARG:NH2	2.36	0.57
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.86	0.57
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.69	0.57
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.85	0.57
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.87	0.57
2:C:739:ASP:OD1	2:C:739:ASP:N	2.36	0.57
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.39	0.57
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.86	0.57
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.87	0.57
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.85	0.56
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.87	0.56
2:C:40:GLU:O	2:C:73:TYR:OH	2.22	0.56
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.87	0.56
2:I:197:ARG:HH12	5:L:29:ASP:HB3	1.70	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.41	0.56
3:D:152:THR:OG1	3:D:153:ASN:N	2.37	0.56
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.87	0.56
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.70	0.56
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.39	0.56
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.85	0.56
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.87	0.56
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.86	0.56
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.87	0.56
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.87	0.56
5:F:483:LEU:H	5:F:483:LEU:HD12	1.69	0.56
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.87	0.56
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.38	0.56
3:J:741:ALA:O	3:J:762:ASN:ND2	2.38	0.56
5:L:476:ARG:HG2	5:L:477:GLU:HG2	1.87	0.56
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.71	0.56
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.86	0.56
2:I:40:GLU:O	2:I:73:TYR:OH	2.23	0.56
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.88	0.56
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.38	0.56
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.87	0.56
3:J:115:TRP:O	3:J:119:SER:HB2	2.06	0.56
2:C:324:LYS:O	2:C:327:GLN:NE2	2.38	0.56
3:D:682:VAL:O	3:D:685:ILE:HG12	2.05	0.56
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.88	0.56
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.88	0.56
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.38	0.56
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.87	0.56
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.88	0.56
5:F:461:ASN:O	5:F:465:ARG:HG2	2.05	0.56
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.87	0.56
5:F:276:MET:SD	5:F:279:ARG:NH1	2.79	0.55
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.88	0.55
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.88	0.55
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.39	0.55
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.88	0.55
1:G:14:VAL:HG22	1:G:15:ASP:H	1.70	0.55
1:H:11:PRO:HB3	1:H:30:PRO:O	2.07	0.55
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.88	0.55
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.89	0.55
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.88	0.55
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.22	0.55
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.89	0.55
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.87	0.55
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.06	0.55
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.42	0.55
2:I:448:LEU:HB2	2:I:553:THR:HB	1.87	0.55
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.89	0.55
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:148:GLU:H	3:J:156:ARG:HG3	1.71	0.55
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.88	0.55
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.88	0.55
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.39	0.55
3:D:210:SER:O	3:D:214:ARG:HG2	2.07	0.55
2:I:30:ILE:HD12	2:I:30:ILE:H	1.71	0.55
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.38	0.55
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.89	0.55
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.89	0.55
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.89	0.55
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.89	0.55
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.87	0.55
2:C:103:VAL:HB	2:C:113:THR:HG21	1.87	0.55
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.42	0.55
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.89	0.55
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.42	0.55
1:H:188:GLU:OE2	1:H:200:LYS:HD3	2.07	0.55
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.88	0.55
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.39	0.55
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.40	0.54
3:D:425:ARG:HG2	3:D:426:ALA:H	1.72	0.54
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.71	0.54
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.43	0.54
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.72	0.54
5:F:482:GLU:O	5:F:486:ARG:NH2	2.40	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
3:J:79:LYS:HB2	5:L:569:THR:H	1.71	0.54
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.90	0.54
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.89	0.54
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.90	0.54
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.22	0.54
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.72	0.54
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.89	0.54
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.89	0.54
3:D:847:ASP:OD1	3:D:847:ASP:N	2.40	0.54
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.89	0.54
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.88	0.54
1:G:11:PRO:HD2	1:H:227:GLN:HA	1.88	0.54
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.89	0.54
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.40	0.54
5:L:225:ARG:O	5:L:229:VAL:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.89	0.54
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.89	0.54
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.89	0.54
1:H:101:THR:H	1:H:116:THR:HG22	1.73	0.54
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.90	0.54
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.42	0.54
3:D:77:ARG:HG3	3:D:79:LYS:H	1.73	0.54
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.90	0.54
1:A:285:THR:HG23	1:A:288:GLU:H	1.73	0.54
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.89	0.54
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.90	0.54
5:F:479:THR:HG23	5:F:481:GLU:H	1.72	0.54
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.88	0.54
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.89	0.54
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.90	0.54
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.73	0.54
3:D:591:ILE:HG13	3:D:604:MET:HE2	1.89	0.54
5:F:511:ILE:HG13	5:F:512:GLY:H	1.73	0.54
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.43	0.53
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.89	0.53
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.39	0.53
5:F:111:LEU:HD13	5:F:116:GLU:HG2	1.90	0.53
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.90	0.53
1:H:61:ILE:HB	1:H:64:VAL:O	2.08	0.53
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.89	0.53
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.90	0.53
5:L:482:GLU:O	5:L:486:ARG:NH2	2.40	0.53
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.90	0.53
3:D:405:GLU:O	3:D:408:VAL:HG22	2.09	0.53
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.89	0.53
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.90	0.53
2:I:1119:MET:HE3	2:I:1204:LEU:HD13	1.90	0.53
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.24	0.53
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.91	0.53
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.90	0.53
3:J:733:SER:O	3:J:737:ILE:HG12	2.09	0.53
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.91	0.53
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.90	0.53
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.88	0.53
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.09	0.53
3:J:425:ARG:HG2	3:J:426:ALA:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.91	0.53
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.90	0.53
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.88	0.53
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.91	0.53
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.91	0.53
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.90	0.53
2:I:237:LEU:HD22	2:I:237:LEU:H	1.73	0.53
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.72	0.53
3:J:45:ASN:HB3	3:J:48:THR:O	2.08	0.53
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.39	0.53
2:C:339:ASN:HB3	2:C:343:HIS:H	1.74	0.53
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.44	0.53
1:B:151:GLY:O	1:B:177:TYR:HB2	2.08	0.53
2:C:488:MET:O	2:C:490:GLN:N	2.37	0.53
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.91	0.53
5:L:111:LEU:HD13	5:L:116:GLU:HG2	1.91	0.53
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.09	0.53
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.90	0.53
1:H:29:GLU:HA	1:H:29:GLU:OE2	2.09	0.53
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.91	0.53
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.89	0.53
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.90	0.53
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.90	0.53
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.90	0.53
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.90	0.53
5:L:593:LYS:HE2	5:L:596:ARG:HD3	1.90	0.53
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.22	0.53
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.90	0.53
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.91	0.53
3:J:120:LEU:HD22	3:J:121:PRO:HD3	1.90	0.53
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.72	0.53
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.91	0.52
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.91	0.52
5:F:476:ARG:HG2	5:F:477:GLU:HG2	1.91	0.52
5:L:479:THR:HG23	5:L:481:GLU:H	1.74	0.52
2:C:617:ALA:HA	2:C:636:CYS:SG	2.50	0.52
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.92	0.52
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.91	0.52
3:J:682:VAL:O	3:J:685:ILE:HG12	2.09	0.52
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.92	0.52
2:C:641:GLU:OE2	3:D:749:LYS:NZ	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.75	0.52
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.91	0.52
1:G:177:TYR:O	1:G:178:SER:HB2	2.08	0.52
5:L:276:MET:SD	5:L:279:ARG:NH1	2.82	0.52
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.91	0.52
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.45	0.52
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.73	0.52
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.92	0.52
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.92	0.52
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.91	0.52
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.92	0.52
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.73	0.52
3:D:156:ARG:NH2	3:D:191:SER:OG	2.37	0.52
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.75	0.52
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.90	0.52
5:L:511:ILE:HG13	5:L:512:GLY:H	1.75	0.52
3:D:308:ASP:OD2	3:D:311:ARG:NH2	2.35	0.52
2:I:518:ASN:N	2:I:518:ASN:OD1	2.41	0.52
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.92	0.52
4:K:60:ASN:HD21	4:K:63:ILE:HD13	1.75	0.52
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.91	0.52
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.45	0.52
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.90	0.52
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.91	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.92	0.52
1:G:182:ARG:O	1:G:206:GLU:N	2.43	0.52
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.75	0.52
2:C:494:ASN:OD1	2:C:495:ALA:N	2.41	0.52
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.42	0.52
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.92	0.52
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.92	0.52
1:A:93:GLN:H	1:A:120:ASP:HB3	1.75	0.52
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.91	0.52
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.92	0.52
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.90	0.52
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.91	0.52
5:F:573:LEU:H	5:F:573:LEU:HD23	1.75	0.52
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	1.92	0.51
2:I:692:THR:OG1	2:I:693:LEU:N	2.44	0.51
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.25	0.51
3:J:79:LYS:HB2	5:L:569:THR:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.91	0.51
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.91	0.51
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.92	0.51
2:I:324:LYS:O	2:I:327:GLN:NE2	2.43	0.51
2:C:9:LYS:HA	2:C:1171:ARG:HD2	1.92	0.51
2:C:1151:LEU:HD21	2:C:1198:LEU:HD23	1.92	0.51
3:D:218:THR:HA	3:D:221:ILE:HG22	1.92	0.51
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.43	0.51
2:I:387:ASN:HA	2:I:391:SER:HB2	1.92	0.51
1:A:287:VAL:HG12	1:A:291:LYS:HE3	1.93	0.51
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.93	0.51
3:D:148:GLU:H	3:D:156:ARG:HG3	1.75	0.51
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.92	0.51
2:I:1320:PRO:HG2	3:J:1354:GLY:HA3	1.92	0.51
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.93	0.51
2:C:207:THR:HG21	2:C:351:LEU:HG	1.93	0.51
5:F:465:ARG:HA	5:F:468:ARG:HH12	1.76	0.51
2:I:103:VAL:HB	2:I:113:THR:HG21	1.91	0.51
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.43	0.51
5:L:41:ILE:HA	5:L:44:ILE:HG23	1.92	0.51
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.45	0.51
5:F:281:ARG:O	5:F:285:ARG:HG3	2.11	0.51
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.93	0.51
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.92	0.51
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.93	0.51
3:D:478:LEU:HG	4:E:47:THR:HG23	1.92	0.51
1:G:50:SER:HB3	1:G:150:ARG:HD2	1.93	0.51
2:I:206:ALA:O	2:I:209:ILE:HG22	2.11	0.51
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.93	0.51
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.44	0.51
3:D:189:LEU:HD22	3:D:234:PRO:HB3	1.93	0.51
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.93	0.51
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.92	0.51
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.92	0.51
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.92	0.51
3:J:405:GLU:O	3:J:408:VAL:HG22	2.10	0.51
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.92	0.51
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.25	0.50
2:C:518:ASN:OD1	2:C:518:ASN:N	2.43	0.50
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.93	0.50
2:I:637:ARG:HD2	8:J:1504:4OD:BRF	2.66	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.92	0.50
5:F:551:LEU:HD21	5:F:598:LEU:HD21	1.94	0.50
2:I:488:MET:O	2:I:490:GLN:N	2.38	0.50
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.93	0.50
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.75	0.50
5:L:602:SER:H	5:L:605:GLU:HG3	1.76	0.50
1:A:39:LEU:HD11	1:B:227:GLN:HB3	1.92	0.50
1:B:91:ARG:HG2	1:B:122:GLU:O	2.12	0.50
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.77	0.50
2:C:517:GLN:HG2	2:C:517:GLN:O	2.10	0.50
3:D:697:MET:SD	3:D:741:ALA:HB3	2.51	0.50
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.94	0.50
2:I:987:GLU:O	2:I:991:LYS:HG3	2.11	0.50
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.11	0.50
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.94	0.50
5:L:483:LEU:H	5:L:483:LEU:HD12	1.75	0.50
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.59	0.50
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.93	0.50
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.94	0.50
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.94	0.50
5:L:448:ARG:NH1	5:L:501:ALA:O	2.35	0.50
5:L:507:MET:HG2	5:L:520:GLY:HA3	1.93	0.50
3:D:388:ARG:NH1	3:D:414:GLU:OE1	2.45	0.50
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.92	0.50
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.77	0.50
1:A:177:TYR:O	1:A:178:SER:HB2	2.11	0.50
3:D:1167:LYS:HE3	3:D:1168:GLU:H	1.74	0.50
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.26	0.50
1:G:93:GLN:H	1:G:120:ASP:HB3	1.76	0.50
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.92	0.50
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.77	0.50
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.93	0.50
3:J:847:ASP:N	3:J:847:ASP:OD1	2.40	0.50
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.46	0.50
2:C:878:THR:OG1	2:C:879:GLY:N	2.41	0.50
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.94	0.50
2:I:250:THR:HA	2:I:268:ARG:HA	1.93	0.50
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.76	0.50
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.93	0.50
5:L:569:THR:OG1	5:L:570:ASP:N	2.45	0.50
2:C:115:LYS:HE3	2:C:116:ASP:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:250:THR:HA	2:C:268:ARG:HA	1.94	0.50
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.94	0.50
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.94	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.94	0.50
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.94	0.50
2:I:349:GLU:O	2:I:353:VAL:HG23	2.11	0.50
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.93	0.50
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.94	0.50
3:J:568:SER:OG	3:J:569:LEU:N	2.44	0.50
3:J:794:GLY:O	3:J:797:THR:OG1	2.26	0.50
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.93	0.49
3:D:872:LEU:O	3:D:877:VAL:HG12	2.12	0.49
1:H:97:GLU:OE1	1:H:147:GLN:HG3	2.12	0.49
5:L:465:ARG:HA	5:L:468:ARG:HH12	1.77	0.49
1:A:54:CYS:O	1:A:146:VAL:HG13	2.12	0.49
1:B:97:GLU:OE1	1:B:147:GLN:HG3	2.12	0.49
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.94	0.49
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.27	0.49
1:H:108:GLY:O	1:H:133:LEU:HB2	2.12	0.49
1:G:228:LEU:CD1	1:H:221:ALA:HB1	2.42	0.49
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.47	0.49
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.94	0.49
5:L:97:PRO:HA	5:L:100:MET:HG3	1.93	0.49
3:D:537:TYR:OH	3:D:634:ARG:NH2	2.45	0.49
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.94	0.49
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.12	0.49
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.94	0.49
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.76	0.49
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.12	0.49
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.77	0.49
1:G:28:LEU:HB2	1:G:201:LEU:HB3	1.94	0.49
1:H:102:LEU:HD12	1:H:142:MET:HG2	1.94	0.49
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.95	0.49
3:J:152:THR:OG1	3:J:153:ASN:N	2.43	0.49
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.94	0.49
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.95	0.49
2:I:517:GLN:O	2:I:517:GLN:HG2	2.12	0.49
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.47	0.49
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.28	0.49
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.95	0.49
5:L:482:GLU:HG2	5:L:486:ARG:HH22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.77	0.49
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.94	0.49
2:C:840:SER:O	2:C:1047:LEU:N	2.45	0.49
2:C:402:ARG:NH2	2:C:419:ILE:O	2.46	0.49
2:C:524:ILE:HG21	2:C:708:VAL:HG13	1.94	0.49
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.95	0.49
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.93	0.49
3:D:128:LEU:HA	3:D:192:MET:HE1	1.95	0.49
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.48	0.49
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.12	0.49
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.93	0.49
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.93	0.49
3:J:395:LYS:HE2	5:L:536:THR:HG21	1.93	0.49
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.47	0.49
5:L:164:GLY:O	5:L:260:ARG:HB2	2.12	0.49
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.94	0.49
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.76	0.49
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.95	0.49
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.95	0.49
2:C:901:LEU:O	2:C:905:ILE:HG13	2.12	0.49
2:I:819:SER:HB2	2:I:1085:MET:SD	2.52	0.49
5:L:287:ILE:HG12	5:L:337:VAL:HG13	1.95	0.49
1:A:91:ARG:HD3	1:A:210:THR:O	2.13	0.48
2:C:901:LEU:HB2	5:F:565:ILE:HD11	1.95	0.48
1:H:91:ARG:HG2	1:H:122:GLU:O	2.13	0.48
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.78	0.48
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.95	0.48
2:C:953:LEU:HD12	2:C:1036:ILE:HD12	1.94	0.48
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.28	0.48
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.94	0.48
2:I:878:THR:OG1	2:I:879:GLY:N	2.46	0.48
1:A:282:VAL:O	1:A:316:MET:N	2.46	0.48
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.95	0.48
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.94	0.48
3:D:709:ARG:C	3:D:711:GLY:H	2.15	0.48
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.95	0.48
2:C:808:ASN:H	3:D:633:ALA:HB2	1.78	0.48
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.94	0.48
3:D:13:LYS:HD3	3:D:13:LYS:HA	1.54	0.48
3:D:733:SER:O	3:D:737:ILE:HG12	2.13	0.48
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:26:TYR:O	2:I:29:SER:HB2	2.13	0.48
2:I:710:VAL:HA	2:I:715:THR:HG21	1.95	0.48
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.47	0.48
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.93	0.48
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.95	0.48
3:D:298:MET:SD	5:F:402:LEU:HB3	2.54	0.48
1:G:12:ARG:HG2	1:G:13:LEU:N	2.28	0.48
1:H:11:PRO:HG3	1:H:31:LEU:HD13	1.94	0.48
1:G:228:LEU:HD11	1:H:221:ALA:HB1	1.94	0.48
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.94	0.48
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.94	0.48
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.96	0.48
5:L:316:PHE:HZ	5:L:334:SER:HA	1.77	0.48
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.95	0.48
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.95	0.48
3:D:694:SER:OG	3:D:738:ARG:NE	2.38	0.48
3:D:708:ASN:N	3:D:708:ASN:OD1	2.45	0.48
1:H:221:ALA:O	1:H:224:LEU:HB3	2.12	0.48
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.48
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.94	0.48
2:I:203:LYS:HB2	5:L:29:ASP:HB2	1.95	0.48
5:L:573:LEU:H	5:L:573:LEU:HD23	1.78	0.48
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.45	0.48
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.44	0.48
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.53	0.48
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.79	0.48
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.42	0.48
3:D:598:LYS:O	3:D:601:ILE:HG22	2.13	0.48
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.94	0.48
3:J:34:SER:OG	3:J:104:HIS:ND1	2.28	0.48
5:L:137:TYR:HE1	5:L:351:THR:HB	1.79	0.48
1:A:28:LEU:HB2	1:A:201:LEU:HB3	1.96	0.48
2:C:170:VAL:HG23	2:C:171:LEU:N	2.29	0.48
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.78	0.48
5:F:41:ILE:HA	5:F:44:ILE:HG23	1.96	0.48
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.14	0.48
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.96	0.48
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.95	0.48
1:A:54:CYS:HA	1:A:148:ARG:HG3	1.96	0.48
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.96	0.48
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLY:O	1:B:177:TYR:HD2	1.97	0.47
2:C:448:LEU:HB2	2:C:553:THR:HB	1.95	0.47
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.95	0.47
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.96	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.94	0.47
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.96	0.47
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.94	0.47
3:J:73:GLY:O	3:J:76:LYS:NZ	2.36	0.47
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.96	0.47
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.95	0.47
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.94	0.47
1:G:12:ARG:H	1:G:30:PRO:CD	2.26	0.47
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.95	0.47
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.79	0.47
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.95	0.47
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.79	0.47
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.95	0.47
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.14	0.47
3:D:848:VAL:HG22	3:D:858:VAL:CG2	2.44	0.47
5:F:602:SER:N	5:F:605:GLU:OE2	2.47	0.47
1:G:182:ARG:C	1:G:183:ILE:HD12	2.35	0.47
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.94	0.47
2:C:842:ASP:N	2:C:1045:GLY:O	2.48	0.47
3:D:709:ARG:O	3:D:711:GLY:N	2.45	0.47
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.96	0.47
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.96	0.47
2:I:746:ALA:HB3	2:I:971:LEU:HA	1.96	0.47
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.95	0.47
3:J:697:MET:SD	3:J:741:ALA:HB3	2.54	0.47
3:J:901:ARG:HD2	3:J:906:GLY:O	2.14	0.47
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.49	0.47
3:D:50:LYS:HB3	3:D:71:LEU:HD21	1.97	0.47
3:D:598:LYS:HA	3:D:601:ILE:HG22	1.95	0.47
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.96	0.47
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.97	0.47
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.61	0.47
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.96	0.47
2:I:739:ASP:N	2:I:739:ASP:OD1	2.39	0.47
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.50	0.47
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.96	0.47
2:C:692:THR:OG1	2:C:693:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:820:GLU:N	2:I:1080:ASN:O	2.47	0.47
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.49	0.47
3:J:1167:LYS:HE3	3:J:1168:GLU:H	1.79	0.47
5:L:585:GLU:O	5:L:589:GLN:HG3	2.15	0.47
1:B:108:GLY:O	1:B:133:LEU:HB2	2.14	0.47
2:C:349:GLU:O	2:C:353:VAL:HG23	2.15	0.47
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.96	0.47
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.96	0.47
2:I:806:PRO:O	3:J:633:ALA:HA	2.15	0.47
3:J:385:LEU:HD11	3:J:408:VAL:HG12	1.97	0.47
3:J:79:LYS:HG3	3:J:80:HIS:N	2.30	0.47
2:C:896:THR:HB	2:C:897:PRO:HD2	1.96	0.47
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.49	0.47
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.43	0.47
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.43	0.47
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.96	0.47
3:J:1170:LYS:C	3:J:1172:LYS:H	2.18	0.47
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.97	0.47
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.97	0.47
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.48	0.47
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.55	0.47
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.97	0.47
2:I:215:TYR:HA	2:I:219:GLN:NE2	2.30	0.47
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.96	0.47
2:I:976:ARG:NH2	2:I:990:ASP:OD2	2.48	0.47
3:D:1297:LYS:HG2	3:J:1302:TYR:H	1.78	0.47
3:D:708:ASN:HB3	3:D:712:GLN:O	2.14	0.47
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.96	0.47
2:I:56:VAL:HG11	2:I:468:LEU:HB3	1.97	0.47
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.49	0.46
2:C:820:GLU:N	2:C:1080:ASN:O	2.48	0.46
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.78	0.46
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.96	0.46
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.55	0.46
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.50	0.46
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.96	0.46
3:J:203:GLU:O	3:J:207:GLU:HG2	2.15	0.46
3:J:872:LEU:O	3:J:877:VAL:HG12	2.15	0.46
5:L:281:ARG:O	5:L:285:ARG:HG3	2.15	0.46
1:A:319:GLU:O	1:A:320:ASN:HB2	2.15	0.46
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.58	0.46
3:D:45:ASN:HB3	3:D:48:THR:O	2.14	0.46
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.50	0.46
2:I:227:LYS:O	2:I:245:ARG:NH2	2.48	0.46
2:I:680:LEU:O	2:I:684:ASN:HB2	2.15	0.46
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.15	0.46
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.80	0.46
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.97	0.46
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.98	0.46
1:B:221:ALA:O	1:B:224:LEU:HB3	2.15	0.46
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.96	0.46
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.51	0.46
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.48	0.46
3:J:197:GLU:O	3:J:201:LEU:HG	2.15	0.46
3:J:298:MET:SD	5:L:402:LEU:HB3	2.55	0.46
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.98	0.46
5:L:548:LEU:HD21	5:L:559:LEU:HD23	1.97	0.46
1:A:182:ARG:O	1:A:183:ILE:HD12	2.15	0.46
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.97	0.46
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.97	0.46
5:F:409:ASN:O	5:F:413:MET:HG3	2.14	0.46
1:G:228:LEU:C	1:G:230:ALA:H	2.18	0.46
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.97	0.46
3:J:62:PHE:O	3:J:101:ARG:HD2	2.16	0.46
3:J:810:THR:HG23	3:J:811:GLU:H	1.80	0.46
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.97	0.46
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.15	0.46
2:C:516:ASP:H	2:C:526:HIS:HD1	1.63	0.46
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.98	0.46
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.30	0.46
3:D:568:SER:OG	3:D:569:LEU:N	2.48	0.46
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.80	0.46
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.80	0.46
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.98	0.46
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.98	0.46
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.96	0.46
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.96	0.46
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.45	0.46
2:I:30:ILE:HD11	2:I:575:LEU:HD22	1.98	0.46
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.56	0.46
3:J:591:ILE:HG13	3:J:604:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.80	0.46
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.96	0.46
5:F:532:LEU:O	5:F:536:THR:HG23	2.16	0.46
1:G:182:ARG:HB3	1:G:206:GLU:HB3	1.98	0.46
1:H:64:VAL:HG12	1:H:65:LEU:H	1.81	0.46
2:I:660:VAL:HG11	3:J:769:VAL:HG13	1.98	0.46
3:D:1227:HIS:HD2	3:J:1293:GLU:H	1.63	0.46
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.15	0.46
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.84	0.46
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.98	0.46
3:J:709:ARG:C	3:J:711:GLY:H	2.19	0.46
3:J:735:ALA:O	3:J:738:ARG:HB3	2.14	0.46
2:C:383:SER:O	2:C:387:ASN:HB2	2.16	0.46
2:C:925:SER:O	2:C:1056:VAL:HG13	2.16	0.46
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.97	0.46
4:K:73:GLN:HA	4:K:76:GLU:HB3	1.98	0.46
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.98	0.46
2:C:680:LEU:O	2:C:684:ASN:HB2	2.16	0.46
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	1.98	0.46
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.98	0.46
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.97	0.46
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.98	0.46
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.97	0.46
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.98	0.45
2:C:1282:GLY:O	3:D:1361:THR:N	2.46	0.45
2:C:130:MET:SD	2:C:134:GLY:HA2	2.56	0.45
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.15	0.45
3:D:901:ARG:HA	3:D:908:ILE:HA	1.96	0.45
5:F:164:GLY:O	5:F:260:ARG:HB2	2.16	0.45
5:F:244:THR:O	5:F:247:GLU:HG2	2.16	0.45
5:F:572:THR:O	5:F:576:VAL:HG23	2.17	0.45
3:J:598:LYS:O	3:J:601:ILE:HG22	2.16	0.45
5:L:583:THR:HG22	5:L:584:ARG:H	1.80	0.45
1:A:182:ARG:C	1:A:183:ILE:HD12	2.36	0.45
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.14	0.45
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.98	0.45
3:D:794:GLY:O	3:D:797:THR:OG1	2.24	0.45
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.98	0.45
5:F:269:LEU:O	5:F:273:MET:HG3	2.16	0.45
2:I:115:LYS:HE3	2:I:116:ASP:H	1.81	0.45
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.97	0.45
3:J:290:ILE:HD12	3:J:290:ILE:H	1.81	0.45
1:A:106:GLY:HA2	1:A:136:GLU:O	2.17	0.45
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.97	0.45
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.49	0.45
2:I:453:ILE:HD12	2:I:587:LEU:HD21	1.99	0.45
3:J:128:LEU:HA	3:J:192:MET:HE1	1.98	0.45
3:J:263:SER:HB2	5:L:507:MET:HE2	1.98	0.45
1:A:250:ASP:HB2	5:F:605:GLU:CG	2.44	0.45
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.98	0.45
2:C:819:SER:HB2	2:C:1085:MET:SD	2.57	0.45
3:D:860:ARG:HB3	3:D:861:ASN:H	1.54	0.45
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.97	0.45
3:J:709:ARG:O	3:J:711:GLY:N	2.48	0.45
1:B:100:LEU:HB2	1:B:144:ILE:HG23	1.97	0.45
1:B:64:VAL:HG11	1:B:69:SER:OG	2.17	0.45
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.51	0.45
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.98	0.45
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.16	0.45
3:D:861:ASN:HD22	3:D:883:ARG:HH12	1.63	0.45
1:H:100:LEU:HB2	1:H:144:ILE:HG23	1.99	0.45
2:I:842:ASP:N	2:I:1045:GLY:O	2.49	0.45
3:J:264:ASP:OD2	3:J:264:ASP:N	2.48	0.45
5:L:124:GLU:O	5:L:128:ASN:HB2	2.16	0.45
1:A:75:GLN:O	2:C:729:ALA:HB2	2.17	0.45
2:C:255:ILE:HB	2:C:263:VAL:HB	1.99	0.45
3:D:613:GLY:O	3:D:617:THR:OG1	2.34	0.45
3:D:683:ILE:HD11	3:D:754:ILE:HG12	1.99	0.45
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.36	0.45
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.57	0.45
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.99	0.45
3:D:266:ASN:O	3:D:270:ARG:HB2	2.16	0.45
1:H:78:ILE:O	1:H:82:LEU:HG	2.17	0.45
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.98	0.45
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.98	0.45
3:J:697:MET:O	3:J:701:LEU:HB2	2.17	0.45
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.52	0.45
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.99	0.45
1:A:75:GLN:HA	2:C:729:ALA:N	2.32	0.45
1:B:102:LEU:HD12	1:B:142:MET:HG2	1.98	0.45
2:C:237:LEU:HD22	2:C:237:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:197:GLU:O	3:D:201:LEU:HG	2.16	0.45
3:D:399:LYS:HG2	3:D:403:ARG:NH2	2.31	0.45
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.98	0.45
5:F:580:PHE:C	5:F:582:VAL:H	2.19	0.45
5:F:583:THR:HG22	5:F:584:ARG:H	1.82	0.45
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.82	0.45
2:I:1146:GLN:NE2	2:I:1160:ASP:OD1	2.50	0.45
3:J:1244:GLN:HE21	3:J:1244:GLN:HB3	1.58	0.45
2:C:387:ASN:HA	2:C:391:SER:HB2	1.97	0.45
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.52	0.45
2:C:980:VAL:HA	2:C:984:VAL:HA	1.98	0.45
3:D:1170:LYS:C	3:D:1172:LYS:H	2.19	0.45
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.17	0.45
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.98	0.45
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.17	0.45
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.52	0.45
1:A:228:LEU:HD11	1:B:221:ALA:HB1	1.99	0.44
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.99	0.44
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.82	0.44
2:C:42:ASP:C	2:C:44:GLU:H	2.20	0.44
2:I:657:THR:HG1	2:I:1187:PHE:HB2	1.82	0.44
5:L:582:VAL:HG22	5:L:586:ARG:HG2	1.99	0.44
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.17	0.44
1:G:224:LEU:HD13	1:H:228:LEU:HD11	1.97	0.44
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.97	0.44
2:I:255:ILE:HB	2:I:263:VAL:HB	1.98	0.44
5:L:130:VAL:HB	5:L:365:MET:HG3	1.98	0.44
5:L:253:SER:O	5:L:257:LYS:HG3	2.17	0.44
1:A:41:ASN:HB2	1:A:185:TYR:OH	2.17	0.44
1:A:66:HIS:HA	1:A:171:LEU:HD11	2.00	0.44
1:B:73:GLY:HA3	1:B:138:ALA:HB1	2.00	0.44
2:C:10:ARG:HA	2:C:1172:LEU:HD23	1.99	0.44
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.17	0.44
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.99	0.44
1:G:54:CYS:O	1:G:146:VAL:HG13	2.17	0.44
2:I:211:ARG:NH1	2:I:357:ASN:O	2.50	0.44
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.31	0.44
3:D:1226:VAL:HG23	3:J:1296:GLY:HA2	1.97	0.44
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.49	0.44
3:J:885:VAL:HG12	3:J:894:VAL:HG11	2.00	0.44
5:L:234:THR:O	5:L:245:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.57	0.44
2:C:53:PHE:O	2:C:57:PHE:HB2	2.18	0.44
2:C:658:GLN:O	2:C:660:VAL:N	2.50	0.44
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.99	0.44
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	2.00	0.44
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.81	0.44
3:D:587:LEU:HD11	3:D:608:CYS:HA	2.00	0.44
5:F:137:TYR:HE1	5:F:351:THR:HB	1.83	0.44
5:F:316:PHE:HZ	5:F:334:SER:HA	1.83	0.44
2:I:232:ILE:HG12	2:I:237:LEU:HD13	2.00	0.44
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.00	0.44
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.53	0.44
3:J:1162:ILE:HG23	3:J:1178:THR:HB	2.00	0.44
3:J:1341:ARG:HH22	3:J:1373:ARG:HH21	1.64	0.44
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.53	0.44
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.33	0.44
3:D:122:SER:O	3:D:126:LEU:HG	2.17	0.44
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.90	0.44
3:D:701:LEU:HD13	3:D:723:TYR:HB2	1.99	0.44
3:D:810:THR:HG23	3:D:811:GLU:H	1.83	0.44
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.50	0.44
3:J:888:CYS:SG	3:J:890:THR:HB	2.58	0.44
2:C:124:MET:HB2	2:C:498:ILE:HD13	2.00	0.44
2:C:206:ALA:O	2:C:209:ILE:HG22	2.17	0.44
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.82	0.44
5:F:511:ILE:HA	5:F:511:ILE:HD12	1.84	0.44
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.53	0.44
3:J:683:ILE:HD11	3:J:754:ILE:HG12	1.98	0.44
4:K:4:VAL:HG22	4:K:5:THR:HG23	2.00	0.44
5:L:461:ASN:O	5:L:465:ARG:HG2	2.17	0.44
1:B:61:ILE:HG21	1:B:78:ILE:HD13	1.99	0.44
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.33	0.44
4:E:4:VAL:HG22	4:E:5:THR:HG23	2.00	0.44
5:F:448:ARG:NH1	5:F:501:ALA:O	2.39	0.44
1:G:77:ASP:O	1:G:81:ILE:HG13	2.18	0.44
2:I:402:ARG:NH2	2:I:419:ILE:O	2.50	0.44
2:C:1059:ARG:HB2	2:C:1060:ILE:H	1.72	0.44
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.50	0.44
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.48	0.44
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.33	0.44
5:F:234:THR:O	5:F:245:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:549:ASP:OD2	3:J:777:HIS:ND1	2.48	0.44
2:I:616:ILE:HG13	2:I:652:TYR:HB2	1.99	0.44
5:L:454:VAL:HA	5:L:457:ILE:HD12	2.00	0.44
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.83	0.44
2:C:27:LEU:HB2	2:C:524:ILE:HD11	2.00	0.44
2:I:617:ALA:HA	2:I:636:CYS:SG	2.58	0.44
2:I:778:GLU:O	2:I:781:ASP:HB2	2.18	0.44
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.52	0.44
3:J:848:VAL:HG22	3:J:858:VAL:CG2	2.48	0.44
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.58	0.44
1:A:12:ARG:HG2	1:A:13:LEU:N	2.29	0.43
1:A:282:VAL:HB	1:A:316:MET:HB2	1.98	0.43
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.99	0.43
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.53	0.43
1:G:221:ALA:HB1	1:H:228:LEU:HD13	2.00	0.43
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.35	0.43
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.99	0.43
2:I:28:LEU:HD22	2:I:527:LYS:HD2	2.00	0.43
3:J:1065:ALA:HB2	3:J:1192:LYS:HZ1	1.82	0.43
3:J:122:SER:O	3:J:126:LEU:HG	2.18	0.43
2:I:1302:THR:HG22	5:L:531:PRO:HB3	1.99	0.43
2:C:83:GLN:O	2:C:87:ILE:HG13	2.18	0.43
3:D:203:GLU:O	3:D:207:GLU:HG2	2.18	0.43
2:I:202:ARG:HH22	2:I:368:ARG:HH12	1.64	0.43
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.99	0.43
1:B:27:THR:HB	1:B:202:VAL:HG22	2.00	0.43
2:C:903:ARG:O	2:C:907:GLY:N	2.50	0.43
2:C:1250:SER:OG	5:F:524:GLU:OE1	2.31	0.43
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.49	0.43
3:J:205:LEU:HD23	3:J:217:LEU:HB3	2.01	0.43
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.00	0.43
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.68	0.43
3:J:708:ASN:N	3:J:708:ASN:OD1	2.49	0.43
5:L:572:THR:O	5:L:576:VAL:HG23	2.18	0.43
1:A:182:ARG:O	1:A:206:GLU:N	2.49	0.43
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.83	0.43
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.99	0.43
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.83	0.43
3:D:264:ASP:N	3:D:264:ASP:OD2	2.51	0.43
3:D:654:ILE:O	3:D:658:GLU:HB2	2.18	0.43
3:D:735:ALA:O	3:D:738:ARG:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:ARG:HB2	1:H:198:LEU:HD21	2.00	0.43
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.99	0.43
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.51	0.43
5:L:507:MET:HG2	5:L:520:GLY:CA	2.48	0.43
1:A:73:GLY:O	1:A:134:THR:HG22	2.18	0.43
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	2.01	0.43
2:C:18:ARG:HA	2:C:19:PRO:HD3	1.90	0.43
2:C:145:ILE:HB	2:C:456:VAL:HG22	2.01	0.43
3:D:97:VAL:HG12	3:D:101:ARG:HG3	2.00	0.43
3:D:198:CYS:O	3:D:202:ARG:HG3	2.18	0.43
3:D:682:VAL:HA	3:D:685:ILE:CD1	2.49	0.43
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.90	0.43
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	2.00	0.43
3:J:291:ILE:HD13	5:L:409:ASN:HB3	2.01	0.43
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	1.99	0.43
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	2.01	0.43
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.66	0.43
2:C:533:LEU:HD11	2:C:568:ASN:HD22	1.83	0.43
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.51	0.43
2:I:170:VAL:HG23	2:I:171:LEU:N	2.32	0.43
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.99	0.43
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.84	0.43
1:A:172:LEU:H	1:A:172:LEU:HD12	1.84	0.43
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.84	0.43
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.99	0.43
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.19	0.43
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.48	0.43
3:D:746:LEU:HD23	3:D:758:PRO:HG3	2.00	0.43
5:F:354:THR:O	5:F:358:VAL:HG23	2.18	0.43
2:I:183:TRP:HB2	2:I:199:ASP:HA	2.01	0.43
3:J:668:PHE:HB2	3:J:678:ARG:HG3	2.00	0.43
1:A:57:THR:O	1:A:173:VAL:HG22	2.18	0.43
2:C:640:GLY:C	2:C:641:GLU:HG2	2.39	0.43
3:D:449:LEU:HD22	3:D:466:MET:SD	2.59	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.00	0.43
1:G:106:GLY:HA2	1:G:136:GLU:O	2.18	0.43
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.18	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.53	0.43
2:I:27:LEU:HB2	2:I:524:ILE:HD11	2.01	0.43
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	2.01	0.43
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:113:THR:OG1	2:C:116:ASP:OD2	2.23	0.43
2:C:176:ILE:HD12	2:C:184:LEU:HD23	2.00	0.43
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.52	0.43
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.54	0.43
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.01	0.43
3:J:1078:LEU:HB3	3:J:1121:LEU:HD13	2.00	0.43
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.53	0.43
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.34	0.43
3:J:557:LYS:HA	3:J:563:LEU:HA	2.01	0.43
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.82	0.43
5:L:314:THR:O	5:L:318:ALA:HB3	2.19	0.43
2:C:71:VAL:HB	2:C:99:LYS:HB2	2.00	0.43
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.00	0.43
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.54	0.43
5:F:493:LYS:HA	5:F:496:LYS:HE2	2.00	0.43
1:H:64:VAL:HG21	1:H:69:SER:CB	2.48	0.43
2:I:1272:GLU:HG2	2:I:1276:TRP:CE2	2.53	0.43
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.34	0.43
5:L:401:PHE:O	5:L:405:ILE:HG23	2.19	0.43
1:A:318:LEU:H	1:A:318:LEU:HD22	1.83	0.42
1:B:20:SER:OG	1:B:21:SER:N	2.51	0.42
1:B:57:THR:O	1:B:173:VAL:HB	2.19	0.42
3:D:1341:ARG:HH22	3:D:1373:ARG:HH21	1.66	0.42
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.00	0.42
3:D:843:VAL:HG11	3:D:897:HIS:O	2.19	0.42
5:F:346:GLN:O	5:F:350:GLU:HG3	2.19	0.42
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.00	0.42
2:I:705:GLU:HB2	2:I:794:LEU:HB3	2.00	0.42
2:I:836:LEU:HD21	2:I:921:PRO:HD3	2.01	0.42
2:I:959:ASP:O	2:I:963:GLU:HG2	2.19	0.42
2:I:742:TYR:O	2:I:974:ARG:NH2	2.52	0.42
3:J:598:LYS:HA	3:J:601:ILE:HG22	2.00	0.42
5:L:348:GLU:HG2	5:L:354:THR:HA	2.01	0.42
5:L:41:ILE:O	5:L:45:ILE:HG22	2.19	0.42
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.79	0.42
1:A:221:ALA:HB1	1:B:228:LEU:HD22	2.00	0.42
1:B:78:ILE:O	1:B:82:LEU:HG	2.19	0.42
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.59	0.42
3:D:22:ILE:O	3:D:1339:GLY:HA2	2.18	0.42
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.29	0.42
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.02	0.42
1:A:12:ARG:H	1:A:30:PRO:CD	2.32	0.42
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	2.00	0.42
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.92	0.42
5:F:462:LYS:O	5:F:466:ILE:HG13	2.18	0.42
1:G:31:LEU:CD1	1:G:201:LEU:HB2	2.49	0.42
1:G:230:ALA:O	1:H:13:LEU:HD23	2.19	0.42
2:I:383:SER:O	2:I:387:ASN:HB2	2.19	0.42
2:I:73:TYR:HB2	2:I:98:VAL:HG22	2.01	0.42
3:J:1121:LEU:HA	3:J:1121:LEU:HD23	1.87	0.42
3:J:1348:LYS:HA	3:J:1348:LYS:HD2	1.86	0.42
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.85	0.42
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.01	0.42
5:L:343:LYS:O	5:L:347:ILE:HG13	2.19	0.42
1:B:29:GLU:HA	1:B:200:LYS:HG3	2.00	0.42
1:B:64:VAL:HG12	1:B:65:LEU:H	1.84	0.42
2:C:389:PHE:HB3	2:C:420:LEU:HD12	2.00	0.42
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.01	0.42
3:D:697:MET:O	3:D:701:LEU:HB2	2.19	0.42
1:G:91:ARG:HD3	1:G:210:THR:O	2.19	0.42
1:H:89:ALA:HB3	1:H:124:VAL:HG12	2.01	0.42
1:H:151:GLY:O	1:H:177:TYR:HD2	2.03	0.42
1:H:219:ARG:O	1:H:223:ILE:HG13	2.19	0.42
1:G:79:LEU:CD1	2:I:693:LEU:HD21	2.50	0.42
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.02	0.42
3:J:1293:GLU:HB3	3:J:1294:ALA:H	1.65	0.42
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.02	0.42
3:J:969:SER:HB3	3:J:1116:SER:HB2	2.01	0.42
1:B:219:ARG:O	1:B:223:ILE:HG13	2.20	0.42
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	2.00	0.42
3:D:901:ARG:HD2	3:D:906:GLY:O	2.19	0.42
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.55	0.42
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.84	0.42
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.52	0.42
1:G:228:LEU:HD13	1:G:231:PHE:HD1	1.85	0.42
1:H:41:ASN:O	1:H:45:ARG:HG3	2.18	0.42
1:H:84:ASN:O	1:H:128:HIS:HE1	2.02	0.42
2:I:203:LYS:CB	5:L:29:ASP:HB2	2.49	0.42
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.84	0.42
3:J:1108:GLN:HG3	3:J:1109:LEU:HD13	2.02	0.42
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:227:LYS:O	2:C:245:ARG:NH2	2.53	0.42
2:C:557:ARG:HH21	2:C:607:SER:C	2.22	0.42
1:B:154:PRO:HG3	3:D:541:LEU:HD13	2.01	0.42
3:D:490:ILE:HD11	3:D:609:TYR:CD2	2.54	0.42
1:H:109:PRO:HA	1:H:132:HIS:HA	2.01	0.42
1:H:182:ARG:NH1	3:J:581:MET:SD	2.92	0.42
1:H:20:SER:OG	1:H:21:SER:N	2.52	0.42
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.54	0.42
2:I:658:GLN:O	2:I:660:VAL:N	2.53	0.42
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.37	0.42
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.89	0.42
5:L:29:ASP:OD1	5:L:30:HIS:N	2.53	0.42
5:L:346:GLN:O	5:L:350:GLU:HG3	2.20	0.42
5:L:484:ALA:HB1	5:L:491:GLU:HB2	2.01	0.42
1:A:14:VAL:HG13	1:A:15:ASP:N	2.34	0.42
1:B:195:ARG:HB2	1:B:198:LEU:HD21	2.02	0.42
2:C:211:ARG:NH1	2:C:357:ASN:O	2.52	0.42
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.90	0.42
3:D:421:VAL:HG13	3:D:439:PRO:HG3	2.00	0.42
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.19	0.42
3:D:62:PHE:O	3:D:101:ARG:HD2	2.20	0.42
3:D:902:ASP:OD1	3:D:903:LEU:N	2.53	0.42
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.83	0.42
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.88	0.42
2:I:32:LEU:O	2:I:36:GLN:HB2	2.19	0.42
3:J:198:CYS:O	3:J:202:ARG:HG3	2.19	0.42
2:C:1333:LEU:C	2:C:1335:ILE:H	2.23	0.42
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.49	0.42
4:E:50:ALA:O	4:E:54:ILE:HG12	2.19	0.42
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.86	0.42
5:F:482:GLU:HG2	5:F:486:ARG:HH22	1.85	0.42
1:G:182:ARG:O	1:G:183:ILE:HD12	2.20	0.42
1:G:230:ALA:HB1	1:H:12:ARG:HA	2.02	0.42
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	2.02	0.42
2:I:468:LEU:HA	2:I:471:VAL:HG12	2.02	0.42
2:I:524:ILE:HG21	2:I:708:VAL:HG13	2.00	0.42
2:I:589:THR:HG23	2:I:591:TYR:CE2	2.54	0.42
2:I:782:VAL:HG11	2:I:792:GLY:HA2	2.02	0.42
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.90	0.42
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.55	0.42
5:L:130:VAL:O	5:L:134:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:H	1:B:116:THR:HG22	1.85	0.42
1:B:71:LYS:HA	1:B:71:LYS:HD2	1.81	0.42
3:J:1162:ILE:HA	3:J:1203:ARG:HA	2.02	0.42
3:J:190:LYS:HD3	3:J:235:GLU:HG2	2.02	0.42
3:J:474:LEU:HD23	4:K:28:ARG:HG2	2.01	0.42
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.84	0.42
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.01	0.42
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.60	0.42
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.85	0.42
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	2.02	0.42
3:D:190:LYS:HD3	3:D:235:GLU:HG2	2.02	0.42
3:D:27:PRO:O	3:D:31:ARG:HG3	2.20	0.42
2:I:1010:GLN:O	2:I:1014:LEU:HD12	2.19	0.42
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.20	0.42
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.60	0.42
3:J:755:ILE:HG12	8:J:1504:4OD:H4	1.84	0.42
1:A:225:ALA:O	1:A:228:LEU:HB2	2.20	0.41
1:B:9:LEU:HD12	1:B:195:ARG:HH21	1.85	0.41
3:D:133:ARG:HB2	5:F:88:GLU:HA	2.02	0.41
3:D:452:LEU:HD13	3:D:500:ILE:HG22	2.02	0.41
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.79	0.41
3:D:925:GLU:HB3	3:D:926:PRO:HD3	2.02	0.41
5:F:314:THR:O	5:F:318:ALA:HB3	2.20	0.41
5:F:559:LEU:O	5:F:563:PHE:HD2	2.03	0.41
3:D:77:ARG:NE	5:F:569:THR:HA	2.35	0.41
5:F:582:VAL:HG22	5:F:586:ARG:HG2	2.02	0.41
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	2.01	0.41
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.55	0.41
3:J:1034:PHE:HA	3:J:1114:GLN:HA	2.02	0.41
2:I:1286:THR:N	3:J:479:GLU:OE2	2.47	0.41
3:J:660:GLU:O	3:J:664:ILE:HG12	2.20	0.41
5:L:511:ILE:HA	5:L:511:ILE:HD12	1.86	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.74	0.41
1:A:228:LEU:CD1	1:B:221:ALA:HB1	2.50	0.41
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.25	0.41
1:G:102:LEU:HD22	1:G:103:ASN:H	1.85	0.41
1:G:35:PHE:HA	1:G:35:PHE:HD1	1.68	0.41
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.55	0.41
2:I:721:GLY:N	2:I:740:GLU:OE1	2.48	0.41
3:J:1017:VAL:HG23	3:J:1018:ALA:H	1.84	0.41
3:J:368:LEU:HD22	3:J:373:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:490:ILE:HA	3:J:500:ILE:HD11	2.00	0.41
3:J:572:THR:OG1	3:J:573:THR:N	2.53	0.41
3:J:809:VAL:HA	3:J:894:VAL:O	2.19	0.41
3:J:987:GLU:HG3	3:J:987:GLU:H	1.63	0.41
4:K:50:ALA:O	4:K:54:ILE:HG12	2.20	0.41
5:L:547:VAL:HG12	5:L:598:LEU:HD22	2.01	0.41
2:C:360:LEU:HB2	2:C:378:ARG:NH2	2.36	0.41
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.36	0.41
2:C:867:GLU:OE1	2:C:943:LYS:NZ	2.51	0.41
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	2.02	0.41
1:H:151:GLY:O	1:H:177:TYR:HB2	2.20	0.41
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.55	0.41
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.94	0.41
2:I:578:TYR:HB3	2:I:590:PRO:HG2	2.02	0.41
3:J:1025:MET:SD	3:J:1124:ILE:HD12	2.60	0.41
3:J:147:ILE:O	3:J:177:ASP:HB3	2.20	0.41
1:B:64:VAL:HG21	1:B:69:SER:CB	2.49	0.41
2:C:730:SER:O	2:C:753:LEU:HB2	2.20	0.41
3:D:73:GLY:O	3:D:76:LYS:NZ	2.37	0.41
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.55	0.41
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.86	0.41
5:F:604:SER:O	5:F:608:ARG:HB2	2.21	0.41
1:H:34:GLY:N	1:H:199:ASP:OD2	2.52	0.41
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.85	0.41
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.60	0.41
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.55	0.41
2:I:724:VAL:HG11	2:I:727:VAL:HG22	2.02	0.41
2:I:724:VAL:HA	2:I:734:ILE:HD13	2.01	0.41
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.84	0.41
2:I:840:SER:O	2:I:1047:LEU:N	2.53	0.41
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.87	0.41
1:A:168:ILE:H	1:A:168:ILE:HG12	1.72	0.41
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.20	0.41
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.55	0.41
2:C:11:ILE:HA	2:C:11:ILE:HD13	1.88	0.41
2:C:360:LEU:HB2	2:C:378:ARG:HH21	1.85	0.41
3:D:120:LEU:HD23	5:F:47:MET:SD	2.60	0.41
3:D:441:LEU:HA	3:D:441:LEU:HD13	1.88	0.41
4:E:21:LEU:HD12	4:E:21:LEU:HA	1.85	0.41
5:F:41:ILE:O	5:F:45:ILE:HG22	2.21	0.41
2:I:538:LEU:HD22	2:I:543:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.85	0.41
3:J:587:LEU:HD11	3:J:608:CYS:HA	2.02	0.41
2:C:238:GLN:HB3	2:C:284:LEU:HD11	2.03	0.41
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.69	0.41
5:F:249:ILE:O	5:F:252:LEU:HB3	2.20	0.41
1:G:41:ASN:HB2	1:G:185:TYR:OH	2.21	0.41
1:H:16:ILE:HG13	1:H:26:VAL:HG22	2.01	0.41
2:I:553:THR:O	2:I:557:ARG:HD2	2.20	0.41
5:L:299:LYS:O	5:L:303:ILE:HG12	2.21	0.41
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.71	0.41
5:L:96:ASP:HA	5:L:97:PRO:HD2	1.86	0.41
1:B:12:ARG:HE	1:B:12:ARG:HB3	1.76	0.41
1:B:99:ILE:HD11	1:B:143:ARG:HB3	2.03	0.41
1:A:11:PRO:HD2	1:B:227:GLN:HA	2.02	0.41
2:C:170:VAL:HG23	2:C:171:LEU:H	1.85	0.41
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.94	0.41
2:C:676:ALA:HB3	3:D:779:ALA:HB2	2.03	0.41
3:D:800:LEU:HB3	3:D:920:ALA:HB1	2.03	0.41
5:F:343:LYS:O	5:F:347:ILE:HG13	2.20	0.41
2:I:176:ILE:HB	2:I:184:LEU:HB3	2.03	0.41
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.41
3:J:1268:ASN:OD1	3:J:1269:ALA:N	2.50	0.41
3:J:441:LEU:HA	3:J:441:LEU:HD13	1.92	0.41
3:J:843:VAL:HG11	3:J:897:HIS:O	2.20	0.41
4:K:49:ILE:HA	4:K:52:ARG:HD3	2.03	0.41
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.21	0.41
2:C:498:ILE:HD12	2:C:498:ILE:H	1.86	0.41
5:F:469:GLN:O	5:F:472:GLN:NE2	2.54	0.41
1:G:90:VAL:HG23	1:G:123:ILE:HD13	2.03	0.41
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.03	0.41
1:G:54:CYS:HA	1:G:148:ARG:HG3	2.01	0.41
2:I:130:MET:SD	2:I:134:GLY:HA2	2.61	0.41
2:I:323:ALA:O	2:I:327:GLN:HG3	2.21	0.41
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.92	0.41
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.36	0.41
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.35	0.41
5:L:348:GLU:HA	5:L:353:LEU:O	2.21	0.41
5:L:98:VAL:HB	5:L:402:LEU:HD11	2.01	0.41
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.49	0.41
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.86	0.41
2:C:887:VAL:HB	2:C:913:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:959:ASP:O	2:C:963:GLU:HG2	2.21	0.41
3:D:161:THR:HG22	3:D:164:GLN:CD	2.40	0.41
3:D:660:GLU:O	3:D:664:ILE:HG12	2.20	0.41
5:F:348:GLU:HG2	5:F:354:THR:HA	2.01	0.41
1:H:99:ILE:HD11	1:H:143:ARG:HB3	2.02	0.41
2:I:1319:MET:HA	2:I:1320:PRO:HD3	1.97	0.41
2:I:720:ARG:HA	2:I:779:ARG:HG3	2.03	0.41
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.86	0.41
3:J:1108:GLN:H	3:J:1122:ALA:HA	1.85	0.41
3:J:119:SER:O	3:J:121:PRO:HD2	2.21	0.41
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.86	0.41
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.81	0.41
2:C:1080:ASN:HA	2:C:1081:PRO:HD3	1.97	0.41
2:C:198:ILE:HD13	2:C:388:LEU:HD13	2.03	0.41
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.88	0.41
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.34	0.41
3:D:478:LEU:HB3	4:E:20:VAL:HG13	2.02	0.41
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	2.03	0.41
2:I:316:GLU:CD	2:I:316:GLU:H	2.24	0.41
2:I:339:ASN:HB3	2:I:343:HIS:H	1.86	0.41
3:J:287:ALA:HB3	3:J:292:VAL:HG13	2.03	0.41
3:J:588:PRO:O	3:J:591:ILE:HG22	2.21	0.41
5:L:249:ILE:O	5:L:252:LEU:HB3	2.21	0.41
1:A:64:VAL:HG11	1:A:78:ILE:HG21	2.03	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.21	0.41
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.56	0.41
2:C:499:SER:O	2:C:503:LYS:HB2	2.21	0.41
2:C:637:ARG:HD2	8:D:1504:4OD:BRF	2.75	0.41
2:C:886:LYS:H	2:C:917:SER:HB3	1.86	0.41
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.21	0.41
3:D:77:ARG:HD2	3:D:78:LEU:H	1.86	0.41
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.83	0.41
5:F:22:LEU:H	5:F:54:GLN:CB	2.34	0.41
1:G:14:VAL:HG13	1:G:15:ASP:N	2.36	0.41
1:H:65:LEU:O	1:H:171:LEU:HD11	2.21	0.41
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.86	0.41
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.19	0.41
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.36	0.41
2:I:499:SER:O	2:I:503:LYS:HB2	2.20	0.41
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.88	0.41
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1291:GLU:OE2	3:J:1302:TYR:OH	2.39	0.41
3:J:266:ASN:O	3:J:270:ARG:HB2	2.21	0.41
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	2.03	0.41
3:J:740:LEU:HA	3:J:740:LEU:HD12	1.90	0.41
5:L:127:ILE:O	5:L:130:VAL:HG22	2.21	0.41
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.21	0.40
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.35	0.40
3:D:128:LEU:HD23	3:D:192:MET:CE	2.52	0.40
3:D:806:ASP:OD2	3:D:1347:LEU:N	2.50	0.40
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.85	0.40
2:I:169:LYS:O	2:I:170:VAL:HG22	2.21	0.40
2:I:32:LEU:HA	2:I:32:LEU:HD23	1.82	0.40
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.21	0.40
3:J:1270:GLY:HA3	3:J:1298:VAL:HG22	2.03	0.40
3:J:746:LEU:HD23	3:J:758:PRO:HG3	2.04	0.40
3:J:997:VAL:HA	3:J:998:PRO:HD3	1.85	0.40
1:A:102:LEU:HD22	1:A:103:ASN:H	1.86	0.40
2:C:194:LEU:HD11	2:C:432:LEU:HD23	2.01	0.40
2:C:782:VAL:HG11	2:C:792:GLY:HA2	2.03	0.40
3:D:141:PHE:CD1	3:D:180:MET:HG3	2.55	0.40
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.04	0.40
5:F:97:PRO:HA	5:F:100:MET:HG3	2.02	0.40
1:G:64:VAL:HG11	1:G:78:ILE:HG21	2.03	0.40
3:J:161:THR:H	3:J:164:GLN:HB2	1.85	0.40
3:J:902:ASP:OD1	3:J:903:LEU:N	2.54	0.40
5:L:312:SER:OG	5:L:313:ASP:N	2.55	0.40
2:C:65:ASN:HB3	2:C:105:TYR:HB2	2.03	0.40
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.87	0.40
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.82	0.40
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.03	0.40
2:I:538:LEU:H	2:I:538:LEU:HG	1.65	0.40
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.91	0.40
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.93	0.40
3:J:1075:ARG:HA	3:J:1076:PRO:HD2	1.98	0.40
3:J:1040:MET:HE3	3:J:1101:LEU:HD12	2.03	0.40
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.86	0.40
5:L:580:PHE:C	5:L:582:VAL:H	2.24	0.40
1:B:102:LEU:HD23	1:B:115:ILE:HG23	2.03	0.40
2:C:1061:GLN:NE2	2:C:1240:ASP:OD2	2.54	0.40
2:C:149:LEU:HD12	2:C:452:ARG:O	2.22	0.40
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:870:ILE:HG21	2:C:931:VAL:HG11	2.04	0.40
5:F:44:ILE:HA	5:F:47:MET:HB2	2.03	0.40
1:G:58:GLU:HB2	1:G:145:LYS:HB3	2.02	0.40
1:H:102:LEU:HD23	1:H:115:ILE:HG23	2.03	0.40
1:H:48:LEU:HA	1:H:180:VAL:HG21	2.03	0.40
2:I:559:CYS:HA	2:I:560:PRO:HD3	1.82	0.40
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.03	0.40
5:L:363:ARG:O	5:L:367:ILE:HG13	2.22	0.40
3:J:258:GLY:HA3	5:L:499:LYS:HD3	2.04	0.40
1:B:190:ALA:HB3	1:B:198:LEU:HB2	2.03	0.40
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.22	0.40
2:C:1315:MET:HB2	2:C:1315:MET:HE3	1.96	0.40
2:C:425:ILE:O	2:C:429:MET:HG3	2.21	0.40
2:C:590:PRO:HG3	2:C:605:TYR:OH	2.22	0.40
2:C:854:ILE:HB	2:C:857:VAL:HG21	2.04	0.40
3:D:1236:GLU:O	3:D:1240:VAL:HG23	2.22	0.40
3:D:1293:GLU:HB3	3:D:1294:ALA:H	1.73	0.40
5:F:253:SER:O	5:F:257:LYS:HG3	2.22	0.40
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.87	0.40
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.90	0.40
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.85	0.40
5:L:489:MET:HE2	5:L:493:LYS:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/335 (89%)	270 (91%)	19 (6%)	9 (3%)	4	32
1	B	212/335 (63%)	194 (92%)	16 (8%)	2 (1%)	17	55
1	G	222/335 (66%)	202 (91%)	14 (6%)	6 (3%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	212/335 (63%)	195 (92%)	15 (7%)	2 (1%)	17	55
2	C	1338/1342 (100%)	1235 (92%)	96 (7%)	7 (0%)	29	67
2	I	1338/1342 (100%)	1235 (92%)	97 (7%)	6 (0%)	34	71
3	D	1145/1407 (81%)	1052 (92%)	89 (8%)	4 (0%)	41	75
3	J	1311/1407 (93%)	1200 (92%)	108 (8%)	3 (0%)	47	80
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	482 (91%)	49 (9%)	1 (0%)	47	80
5	L	529/613 (86%)	480 (91%)	49 (9%)	0	100	100
All	All	7301/8246 (88%)	6697 (92%)	564 (8%)	40 (0%)	29	67

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
1	A	319	GLU
1	A	320	ASN
2	C	237	LEU
3	D	10	ALA
3	D	120	LEU
1	G	193	GLU
1	H	29	GLU
2	I	237	LEU
3	J	120	LEU
1	A	323	PRO
2	C	170	VAL
1	G	62	ASP
2	I	170	VAL
1	A	62	ASP
1	A	196	THR
5	F	7	SER
1	G	196	THR
1	B	193	GLU
2	C	1136	GLN
3	D	710	ASP
1	G	178	SER
1	H	193	GLU
2	I	1136	GLN
3	J	710	ASP

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Mol	Chain	Res	Type
1	A	167	PRO
1	A	178	SER
2	C	659	GLN
2	C	697	LYS
2	C	1186	VAL
1	G	167	PRO
2	I	659	GLN
2	I	697	LYS
3	D	831	VAL
2	I	1186	VAL
3	J	831	VAL
1	A	14	VAL
1	G	14	VAL
1	B	30	PRO
2	C	1159	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	A	257/292 (88%)	243 (95%)	14 (5%)	22	50	
1	B	184/292 (63%)	167 (91%)	17 (9%)	9	32	
1	G	191/292 (65%)	181 (95%)	10 (5%)	23	51	
1	H	183/292 (63%)	169 (92%)	14 (8%)	13	40	
2	C	1155/1157 (100%)	1062 (92%)	93 (8%)	11	38	
2	I	1154/1157 (100%)	1060 (92%)	94 (8%)	11	38	
3	D	964/1168 (82%)	880 (91%)	84 (9%)	10	35	
3	J	1106/1168 (95%)	1014 (92%)	92 (8%)	11	37	
4	E	72/75 (96%)	66 (92%)	6 (8%)	11	37	
4	K	67/75 (89%)	61 (91%)	6 (9%)	9	33	
5	F	426/540 (79%)	392 (92%)	34 (8%)	12	39	
5	L	428/540 (79%)	392 (92%)	36 (8%)	11	37	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6187/7048 (88%)	5687 (92%)	500 (8%)	11	38

All (500) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	35	PHE
1	A	54	CYS
1	A	65	LEU
1	A	133	LEU
1	A	145	LYS
1	A	186	ASN
1	A	207	THR
1	A	231	PHE
1	A	317	ARG
1	A	318	LEU
1	A	319	GLU
1	A	321	TRP
1	B	8	PHE
1	B	9	LEU
1	B	12	ARG
1	B	14	VAL
1	B	27	THR
1	B	28	LEU
1	B	31	LEU
1	B	54	CYS
1	B	60	GLU
1	B	75	GLN
1	B	79	LEU
1	B	101	THR
1	B	116	THR
1	B	133	LEU
1	B	160	HIS
1	B	183	ILE
1	B	186	ASN
2	C	11	ILE
2	C	29	SER
2	C	39	ILE
2	C	70	TYR
2	C	81	ASP
2	C	85	CYS

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Mol	Chain	Res	Type
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	119	GLU
2	C	124	MET
2	C	131	THR
2	C	179	TYR
2	C	182	SER
2	C	185	ASP
2	C	202	ARG
2	C	285	ILE
2	C	320	ASP
2	C	321	LEU
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	487	LEU
2	C	493	ILE
2	C	512	SER
2	C	517	GLN
2	C	518	ASN
2	C	530	ILE
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	554	HIS
2	C	604	HIS
2	C	615	VAL
2	C	618	GLN
2	C	623	LEU
2	C	633	LEU
2	C	641	GLU
2	C	657	THR
2	C	672	GLU
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	706	ARG
2	C	714	VAL

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Mol	Chain	Res	Type
2	C	739	ASP
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	782	VAL
2	C	788	SER
2	C	815	SER
2	C	819	SER
2	C	828	PHE
2	C	839	VAL
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	967	LEU
2	C	974	ARG
2	C	990	ASP
2	C	992	LEU
2	C	1002	LEU
2	C	1005	GLU
2	C	1006	GLU
2	C	1014	LEU
2	C	1040	ASP
2	C	1082	ILE
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1155	VAL
2	C	1156	ARG
2	C	1161	LEU
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1240	ASP
2	C	1248	THR
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1313	HIS

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Mol	Chain	Res	Type
2	C	1326	LEU
2	C	1327	LEU
2	C	1342	GLU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE
3	D	46	TYR
3	D	79	LYS
3	D	92	VAL
3	D	95	THR
3	D	117	LEU
3	D	119	SER
3	D	120	LEU
3	D	169	LEU
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	256	ASP
3	D	264	ASP
3	D	311	ARG
3	D	324	LEU
3	D	356	THR
3	D	364	HIS
3	D	374	LEU
3	D	430	HIS
3	D	474	LEU
3	D	506	VAL
3	D	513	MET
3	D	545	HIS
3	D	547	ARG
3	D	568	SER
3	D	593	ASN
3	D	594	GLN
3	D	641	ILE
3	D	660	GLU
3	D	678	ARG
3	D	697	MET
3	D	698	MET
3	D	701	LEU

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Mol	Chain	Res	Type
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	740	LEU
3	D	754	ILE
3	D	757	THR
3	D	764	ARG
3	D	767	LEU
3	D	772	TYR
3	D	805	GLN
3	D	810	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	860	ARG
3	D	867	GLN
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	928	THR
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1167	LYS
3	D	1173	ARG
3	D	1177	ILE
3	D	1186	TYR
3	D	1199	PHE
3	D	1202	GLU
3	D	1208	ASP
3	D	1209	VAL
3	D	1215	GLU
3	D	1244	GLN
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1289	ASN

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Mol	Chain	Res	Type
3	D	1293	GLU
3	D	1327	GLU
3	D	1333	THR
4	E	28	ARG
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	27	VAL
5	F	44	ILE
5	F	45	ILE
5	F	50	ASP
5	F	98	VAL
5	F	100	MET
5	F	118	ASP
5	F	154	GLU
5	F	305	LEU
5	F	306	PHE
5	F	335	GLU
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	421	TYR
5	F	445	ASP
5	F	449	THR
5	F	479	THR
5	F	486	ARG
5	F	488	LEU
5	F	491	GLU
5	F	496	LYS
5	F	508	GLU
5	F	528	LEU
5	F	530	LEU
5	F	540	LEU
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	583	THR
5	F	600	HIS

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Mol	Chain	Res	Type
5	F	612	ASP
1	G	9	LEU
1	G	13	LEU
1	G	35	PHE
1	G	54	CYS
1	G	65	LEU
1	G	133	LEU
1	G	145	LYS
1	G	148	ARG
1	G	186	ASN
1	G	207	THR
1	H	13	LEU
1	H	29	GLU
1	H	31	LEU
1	H	54	CYS
1	H	60	GLU
1	H	65	LEU
1	H	75	GLN
1	H	79	LEU
1	H	101	THR
1	H	105	SER
1	H	116	THR
1	H	133	LEU
1	H	183	ILE
1	H	186	ASN
2	I	11	ILE
2	I	29	SER
2	I	39	ILE
2	I	70	TYR
2	I	81	ASP
2	I	85	CYS
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	119	GLU
2	I	131	THR
2	I	179	TYR
2	I	182	SER
2	I	185	ASP
2	I	202	ARG
2	I	285	ILE
2	I	320	ASP

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Mol	Chain	Res	Type
2	I	321	LEU
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	453	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	487	LEU
2	I	493	ILE
2	I	512	SER
2	I	517	GLN
2	I	518	ASN
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	554	HIS
2	I	604	HIS
2	I	615	VAL
2	I	618	GLN
2	I	623	LEU
2	I	633	LEU
2	I	657	THR
2	I	672	GLU
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	706	ARG
2	I	714	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	782	VAL
2	I	788	SER
2	I	815	SER
2	I	819	SER
2	I	828	PHE
2	I	839	VAL
2	I	859	GLU

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Mol	Chain	Res	Type
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	954	LYS
2	I	974	ARG
2	I	990	ASP
2	I	992	LEU
2	I	1002	LEU
2	I	1005	GLU
2	I	1006	GLU
2	I	1014	LEU
2	I	1040	ASP
2	I	1082	ILE
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1155	VAL
2	I	1156	ARG
2	I	1161	LEU
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1237	HIS
2	I	1240	ASP
2	I	1248	THR
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1313	HIS
2	I	1326	LEU
2	I	1327	LEU
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	46	TYR
3	J	79	LYS
3	J	92	VAL
3	J	95	THR
3	J	97	VAL

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Mol	Chain	Res	Type
3	J	117	LEU
3	J	119	SER
3	J	120	LEU
3	J	169	LEU
3	J	175	GLU
3	J	176	PHE
3	J	217	LEU
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	264	ASP
3	J	311	ARG
3	J	324	LEU
3	J	356	THR
3	J	364	HIS
3	J	374	LEU
3	J	394	ILE
3	J	430	HIS
3	J	474	LEU
3	J	506	VAL
3	J	545	HIS
3	J	547	ARG
3	J	568	SER
3	J	593	ASN
3	J	594	GLN
3	J	641	ILE
3	J	660	GLU
3	J	678	ARG
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	740	LEU
3	J	754	ILE
3	J	757	THR
3	J	764	ARG
3	J	767	LEU

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Mol	Chain	Res	Type
3	J	772	TYR
3	J	810	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	860	ARG
3	J	867	GLN
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	928	THR
3	J	931	THR
3	J	987	GLU
3	J	997	VAL
3	J	1017	VAL
3	J	1025	MET
3	J	1042	ASP
3	J	1062	LEU
3	J	1063	ASP
3	J	1073	ASP
3	J	1115	ILE
3	J	1155	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1173	ARG
3	J	1177	ILE
3	J	1186	TYR
3	J	1199	PHE
3	J	1202	GLU
3	J	1208	ASP
3	J	1209	VAL
3	J	1215	GLU
3	J	1244	GLN
3	J	1274	PHE
3	J	1275	LEU
3	J	1281	GLU
3	J	1284	ARG
3	J	1289	ASN
3	J	1293	GLU
3	J	1327	GLU

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Mol	Chain	Res	Type
3	J	1333	THR
4	K	28	ARG
4	K	31	GLN
4	K	36	ASP
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	27	VAL
5	L	44	ILE
5	L	45	ILE
5	L	50	ASP
5	L	98	VAL
5	L	100	MET
5	L	118	ASP
5	L	127	ILE
5	L	154	GLU
5	L	244	THR
5	L	305	LEU
5	L	306	PHE
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	421	TYR
5	L	429	THR
5	L	445	ASP
5	L	449	THR
5	L	479	THR
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU
5	L	496	LYS
5	L	508	GLU
5	L	528	LEU
5	L	530	LEU
5	L	540	LEU
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	583	THR
5	L	600	HIS

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Mol	Chain	Res	Type
5	L	606	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	320	ASN
2	C	343	HIS
2	C	1111	GLN
2	C	1116	HIS
2	C	1257	GLN
2	C	1288	GLN
2	C	1312	ASN
3	D	364	HIS
3	D	419	HIS
3	D	477	GLN
3	D	897	HIS
3	D	1367	GLN
5	F	406	GLN
5	F	472	GLN
2	I	343	HIS
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1257	GLN
2	I	1314	GLN
3	J	419	HIS
3	J	560	ASN
3	J	1367	GLN
5	L	406	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
8	4OD	J	1504	-	23,23,23	2.96	6 (26%)	32,33,33	1.41	7 (21%)
8	4OD	D	1504	-	23,23,23	2.95	6 (26%)	32,33,33	1.41	6 (18%)

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
8	4OD	J	1504	-	-	4/15/16/16	0/2/2/2
8	4OD	D	1504	-	-	4/15/16/16	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1504	4OD	FAB-CAR	-6.82	1.18	1.35
8	J	1504	4OD	FAB-CAR	-6.81	1.18	1.35
8	J	1504	4OD	BRF-CAQ	-6.66	1.76	1.90
8	D	1504	4OD	BRF-CAQ	-6.65	1.76	1.90
8	D	1504	4OD	CAS-NAN	-6.62	1.31	1.42
8	J	1504	4OD	CAS-NAN	-6.60	1.31	1.42
8	J	1504	4OD	CAV-CAU	-5.18	1.39	1.50
8	D	1504	4OD	CAV-CAU	-5.18	1.39	1.50
8	J	1504	4OD	CAT-CAP	-4.94	1.38	1.47
8	D	1504	4OD	CAT-CAP	-4.91	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	4OD	CAP-NAN	2.67	1.32	1.28
8	D	1504	4OD	CAP-NAN	2.66	1.32	1.28

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	1504	4OD	FAC-CAV-CAU	-2.92	107.62	112.70
8	D	1504	4OD	CAK-CAT-CAP	-2.90	115.73	120.86
8	J	1504	4OD	FAC-CAV-CAU	-2.89	107.67	112.70
8	J	1504	4OD	CAK-CAT-CAP	-2.88	115.76	120.86
8	D	1504	4OD	CAS-NAN-CAP	2.87	126.64	120.41
8	J	1504	4OD	CAS-NAN-CAP	2.85	126.61	120.41
8	D	1504	4OD	OAA-NAO-CAP	-2.56	113.31	119.49
8	J	1504	4OD	OAA-NAO-CAP	-2.56	113.33	119.49
8	J	1504	4OD	CAM-CAT-CAP	2.31	124.24	120.30
8	D	1504	4OD	CAM-CAT-CAP	2.31	124.23	120.30
8	J	1504	4OD	CAM-CAU-CAV	2.08	121.62	116.50
8	D	1504	4OD	CAM-CAU-CAV	2.07	121.59	116.50
8	J	1504	4OD	CAV-CAU-CAR	-2.00	119.26	120.69

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1504	4OD	CAT-CAP-NAO-OAA
8	D	1504	4OD	CAT-CAP-NAO-OAA
8	J	1504	4OD	CAR-CAU-CAV-FAD
8	J	1504	4OD	CAR-CAU-CAV-FAE
8	D	1504	4OD	CAR-CAU-CAV-FAD
8	D	1504	4OD	CAR-CAU-CAV-FAE
8	J	1504	4OD	CAR-CAU-CAV-FAC
8	D	1504	4OD	CAR-CAU-CAV-FAC

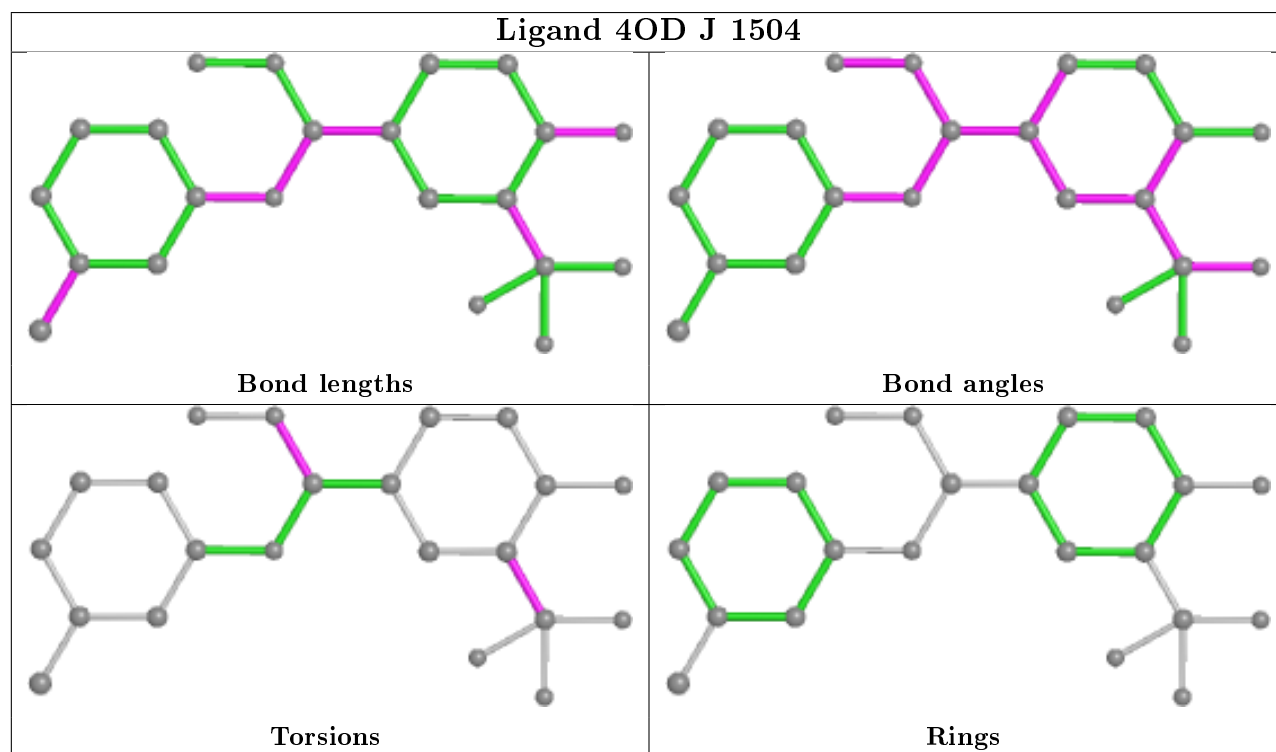
There are no ring outliers.

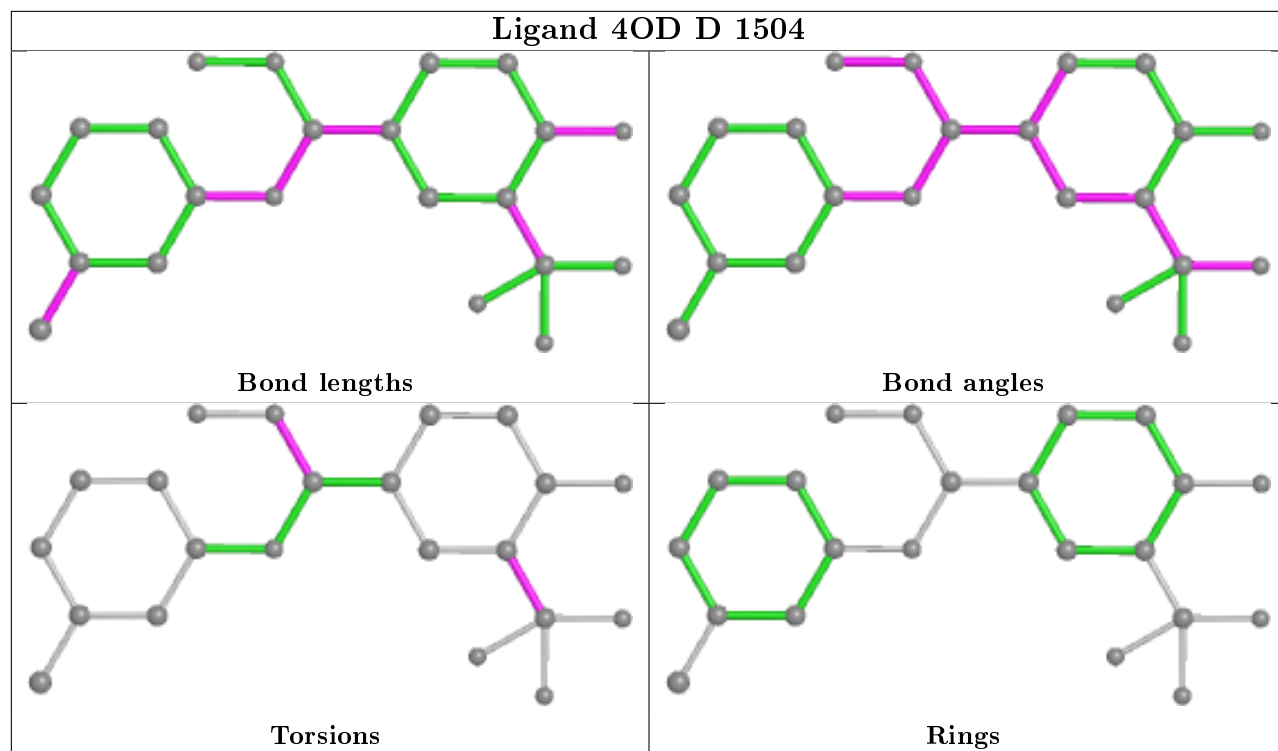
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	1504	4OD	4	0
8	D	1504	4OD	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	302/335 (90%)	0.04	7 (2%) 60 51	41, 103, 232, 400	0
1	B	216/335 (64%)	0.02	10 (4%) 32 27	37, 121, 198, 297	0
1	G	224/335 (66%)	-0.09	2 (0%) 84 77	54, 109, 196, 282	0
1	H	216/335 (64%)	0.22	8 (3%) 41 33	65, 135, 230, 280	0
2	C	1340/1342 (99%)	-0.06	36 (2%) 54 44	14, 87, 202, 296	0
2	I	1340/1342 (99%)	0.09	60 (4%) 33 28	15, 108, 212, 334	0
3	D	1151/1407 (81%)	-0.23	10 (0%) 84 77	13, 73, 170, 292	0
3	J	1319/1407 (93%)	0.08	55 (4%) 36 29	23, 95, 231, 322	0
4	E	89/91 (97%)	-0.43	0 100 100	33, 77, 139, 160	0
4	K	79/91 (86%)	-0.00	1 (1%) 77 68	70, 118, 195, 235	0
5	F	542/613 (88%)	0.25	40 (7%) 14 12	38, 154, 258, 355	0
5	L	539/613 (87%)	0.18	29 (5%) 25 22	52, 154, 248, 300	0
All	All	7357/8246 (89%)	0.02	258 (3%) 44 35	13, 103, 222, 400	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	259	PHE	8.1
5	F	167	ASP	7.9
5	F	88	GLU	7.4
5	F	89	SER	7.0
2	I	998	LEU	5.9
5	F	283	GLN	5.9
2	C	251	ALA	5.7
2	I	999	GLU	5.7
5	F	5	PRO	5.5
5	F	165	PHE	5.4
2	I	973	SER	5.4

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Mol	Chain	Res	Type	RSRZ
2	I	981	ALA	5.3
2	I	978	VAL	5.2
3	J	1294	ALA	5.0
5	F	287	ILE	4.9
3	J	1007	ASP	4.7
2	C	253	PHE	4.7
2	I	979	LEU	4.6
2	I	1024	GLU	4.6
3	J	1123	ARG	4.5
3	J	712	GLN	4.5
5	F	74	GLU	4.5
2	I	972	PHE	4.5
5	F	162	ILE	4.4
5	L	7	SER	4.1
2	I	725	GLN	4.1
2	I	982	GLY	4.1
1	A	318	LEU	4.0
2	I	969	ALA	4.0
2	I	1020	GLU	4.0
5	F	75	ASP	3.9
2	C	230	PHE	3.9
2	C	291	TYR	3.9
2	I	976	ARG	3.9
5	L	308	GLY	3.8
2	I	1010	GLN	3.8
5	L	490	PRO	3.7
2	I	745	GLU	3.6
5	F	318	ALA	3.6
3	J	1049	GLN	3.5
2	I	867	GLU	3.5
2	I	1021	LEU	3.5
3	J	1109	LEU	3.5
3	J	987	GLU	3.5
5	F	258	GLN	3.4
3	J	1047	THR	3.4
2	I	970	GLY	3.4
5	F	86	SER	3.4
5	F	579	GLN	3.4
5	F	15	ARG	3.3
5	L	40	GLN	3.3
3	J	1215	GLU	3.3
5	L	8	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
5	L	167	ASP	3.3
3	J	985	ILE	3.3
3	J	756	GLU	3.3
3	J	1054	THR	3.3
5	F	87	VAL	3.3
1	A	262	LEU	3.2
1	H	158	ARG	3.2
3	D	1200	GLU	3.2
2	C	241	LEU	3.2
2	C	265	LYS	3.1
5	L	70	ASN	3.1
5	F	284	GLU	3.1
5	L	290	LEU	3.1
1	H	172	LEU	3.1
5	F	6	GLN	3.1
2	I	1018	TYR	3.0
3	J	1008	GLY	3.0
3	J	957	SER	3.0
5	F	319	ALA	3.0
3	D	1202	GLU	3.0
3	J	1295	ASN	3.0
5	L	165	PHE	3.0
1	H	67	GLU	3.0
2	I	230	PHE	3.0
2	C	102	LEU	3.0
3	J	542	ALA	3.0
2	I	980	VAL	2.9
2	I	975	ILE	2.9
5	F	314	THR	2.9
2	C	68	LEU	2.9
5	L	140	ALA	2.9
2	I	203	LYS	2.9
2	I	971	LEU	2.9
5	F	288	MET	2.8
1	B	65	LEU	2.8
1	B	147	GLN	2.8
5	F	85	SER	2.8
2	I	1011	LEU	2.8
3	J	1069	ALA	2.8
5	F	280	VAL	2.8
2	C	66	SER	2.8
5	F	315	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
5	L	137	TYR	2.8
5	L	315	TRP	2.8
3	J	974	VAL	2.8
2	C	322	LEU	2.8
2	I	997	TRP	2.8
2	I	493	ILE	2.8
2	C	240	GLU	2.7
3	J	1103	GLY	2.7
5	F	317	ASN	2.7
3	J	1088	VAL	2.7
2	C	311	CYS	2.7
3	J	955	LYS	2.7
2	I	1004	ASP	2.7
2	I	231	GLU	2.7
2	I	974	ARG	2.7
3	D	1203	ARG	2.7
5	L	337	VAL	2.7
3	J	1055	GLY	2.7
2	C	992	LEU	2.7
3	J	975	ILE	2.7
3	J	1028	ILE	2.7
1	H	146	VAL	2.6
2	C	333	ILE	2.6
2	I	1022	LYS	2.6
2	I	169	LYS	2.6
2	I	333	ILE	2.6
2	C	292	ILE	2.6
5	L	304	THR	2.6
2	C	104	ILE	2.6
2	C	226	GLU	2.6
3	J	1010	GLN	2.6
3	D	1201	GLY	2.6
1	A	284	ARG	2.6
5	L	314	THR	2.6
1	H	123	ILE	2.6
1	B	55	ALA	2.6
3	D	1198	VAL	2.6
1	B	138	ALA	2.5
2	I	882	ILE	2.5
3	J	857	LEU	2.5
2	C	319	LEU	2.5
3	J	830	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	I	1007	LYS	2.5
2	C	257	ALA	2.5
2	I	118	LYS	2.5
3	J	1080	ILE	2.5
2	I	451	ARG	2.5
5	F	321	ALA	2.5
1	B	90	VAL	2.5
5	L	294	GLN	2.5
5	F	70	ASN	2.5
2	I	120	GLN	2.5
5	F	306	PHE	2.5
1	H	147	GLN	2.5
3	J	1168	GLU	2.5
5	L	225	ARG	2.5
3	J	686	TRP	2.5
3	J	1106	ILE	2.4
3	J	743	MET	2.4
5	F	73	ASP	2.4
5	F	137	TYR	2.4
3	D	1204	VAL	2.4
1	A	281	LEU	2.4
2	C	250	THR	2.4
2	I	69	GLN	2.4
5	L	305	LEU	2.4
2	I	67	GLU	2.4
2	C	255	ILE	2.4
2	I	485	ASP	2.4
1	G	92	VAL	2.4
3	J	1044	GLN	2.4
5	F	34	ASP	2.4
1	B	91	ARG	2.4
2	C	696	ASP	2.4
3	J	1058	SER	2.4
3	J	1068	THR	2.4
2	C	492	MET	2.4
5	F	92	GLY	2.4
3	J	1032	SER	2.4
3	D	830	ASP	2.4
5	L	279	ARG	2.4
5	L	336	GLU	2.4
5	L	89	SER	2.3
1	H	56	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	263	VAL	2.3
5	L	326	TRP	2.3
2	C	264	GLU	2.3
2	I	1005	GLU	2.3
1	B	121	VAL	2.3
5	F	285	ARG	2.3
3	J	521	LYS	2.3
5	L	29	ASP	2.3
1	G	160	HIS	2.3
2	I	696	ASP	2.3
2	C	205	PRO	2.3
2	C	237	LEU	2.3
3	J	1108	GLN	2.3
5	L	318	ALA	2.3
1	B	227	GLN	2.3
5	F	76	ALA	2.3
1	H	12	ARG	2.3
1	A	266	SER	2.3
2	C	287	VAL	2.3
2	I	420	LEU	2.3
2	I	165	HIS	2.3
2	I	103	VAL	2.3
3	J	682	VAL	2.3
5	L	88	GLU	2.3
2	I	994	ARG	2.3
3	D	1175	LEU	2.3
5	L	283	GLN	2.3
2	I	977	ALA	2.3
2	C	261	VAL	2.3
2	C	305	SER	2.2
3	J	1115	ILE	2.2
2	I	1006	GLU	2.2
1	A	270	LEU	2.2
3	J	1070	GLY	2.2
2	C	188	PHE	2.2
5	L	232	ARG	2.2
2	C	252	SER	2.2
3	D	1165	PHE	2.2
3	J	1188	GLU	2.2
3	J	1293	GLU	2.2
1	A	303	ILE	2.2
3	J	993	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	227	LYS	2.2
3	J	1001	ALA	2.2
2	I	968	GLU	2.2
2	I	1017	GLN	2.2
2	I	1019	ASP	2.2
2	I	234	ASP	2.2
3	J	1065	ALA	2.2
5	F	305	LEU	2.2
5	F	312	SER	2.1
3	J	1048	ARG	2.1
3	J	989	GLY	2.1
3	J	1030	GLU	2.1
5	F	16	GLY	2.1
2	I	938	GLY	2.1
5	F	289	LYS	2.1
1	B	139	SER	2.1
3	J	1051	ASP	2.1
2	I	726	TYR	2.1
3	J	1175	LEU	2.1
3	J	1017	VAL	2.1
2	C	288	PRO	2.1
3	D	1173	ARG	2.1
1	B	97	GLU	2.1
5	F	463	LEU	2.1
3	J	1087	ASP	2.0
5	L	610	PHE	2.0
2	C	196	VAL	2.0
3	J	257	GLY	2.0
5	L	489	MET	2.0
2	C	298	ALA	2.0
2	I	151	ARG	2.0
3	J	683	ILE	2.0
2	I	593	LYS	2.0
2	I	190	PRO	2.0
2	I	492	MET	2.0
2	I	1050	VAL	2.0
4	K	35	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

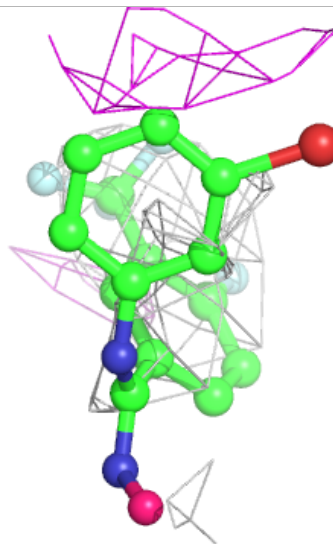
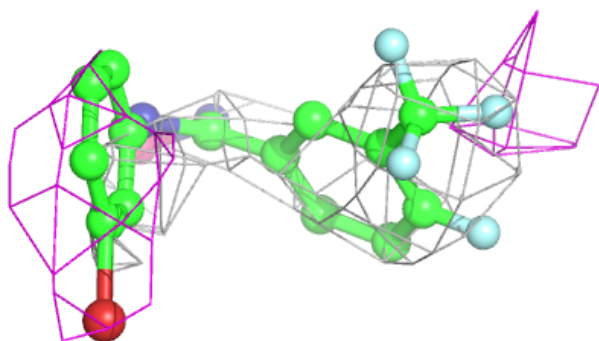
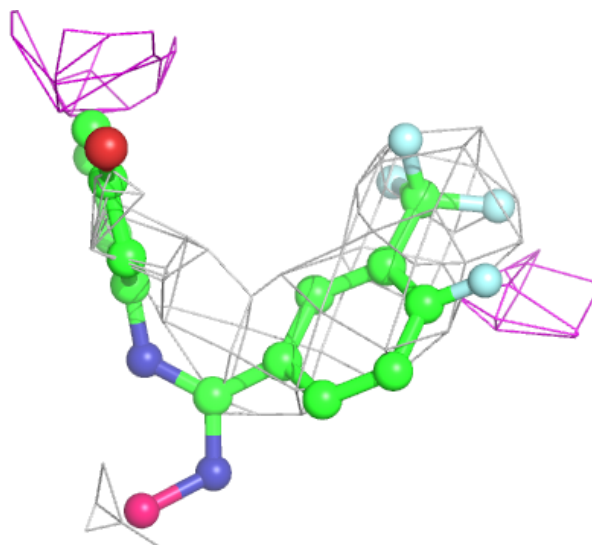
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	4OD	J	1504	22/22	0.75	1.11	100,110,116,133	1
6	MG	J	1501	1/1	0.79	0.85	55,55,55,55	0
6	MG	D	1501	1/1	0.81	0.51	37,37,37,37	0
8	4OD	D	1504	22/22	0.89	0.47	68,80,89,116	1
7	ZN	J	1502	1/1	0.90	0.14	98,98,98,98	0
7	ZN	D	1502	1/1	0.97	0.12	90,90,90,90	0
7	ZN	J	1503	1/1	0.98	0.26	46,46,46,46	0
7	ZN	D	1503	1/1	0.99	0.24	49,49,49,49	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.

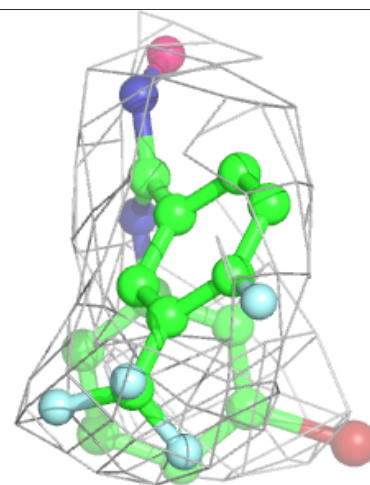
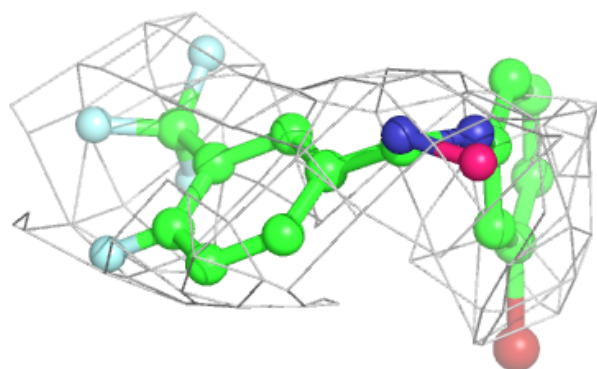
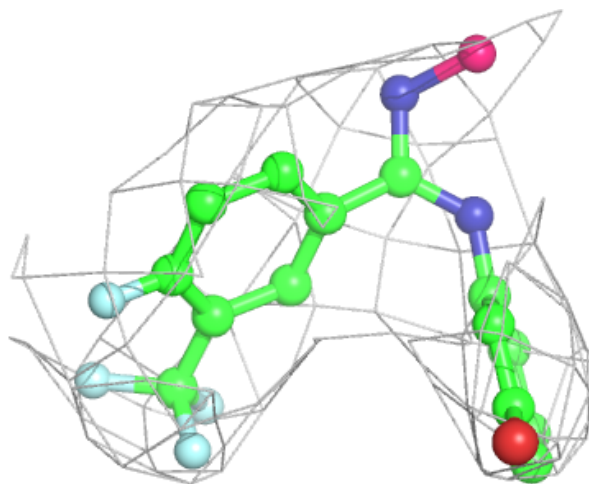
Electron density around 4OD J 1504:

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



Electron density around 4OD D 1504:

$2mF_o-DF_c$ (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.