



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:56 pm BST

PDB ID : 4ZH4  
Title : Crystal structure of Escherichia coli RNA polymerase in complex with CBRP18  
Authors : Feng, Y.; Ebright, R.H.  
Deposited on : 2015-04-24  
Resolution : 3.99 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](mailto: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.

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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

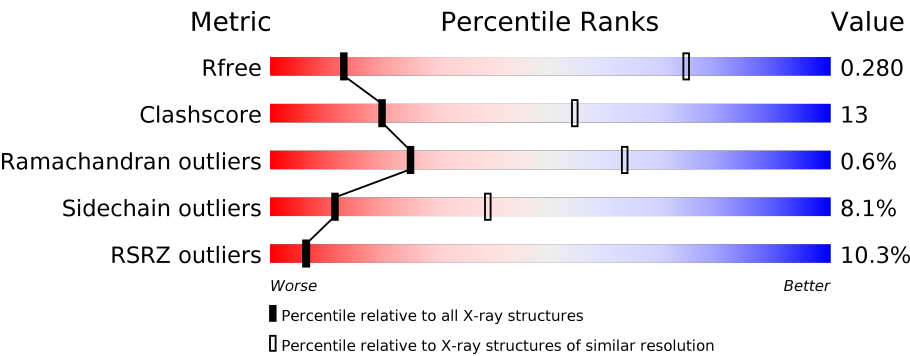
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.99 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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  $\geq 3$ , 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>7%</div><div><div></div><div>60%</div><div>26%</div><div>• •</div><div>10%</div></div></div>
1	B	335	<div><div>6%</div><div><div></div><div>38%</div><div>24%</div><div>• •</div><div>36%</div></div></div>
1	G	335	<div><div>4%</div><div><div></div><div>41%</div><div>24%</div><div>•</div><div>33%</div></div></div>
1	H	335	<div><div>11%</div><div><div></div><div>38%</div><div>24%</div><div>• •</div><div>36%</div></div></div>
2	C	1342	<div><div>9%</div><div><div></div><div>66%</div><div>31%</div><div>•</div></div></div>
2	I	1342	<div><div>12%</div><div><div></div><div>68%</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	4OE	I	2001	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 57539 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			

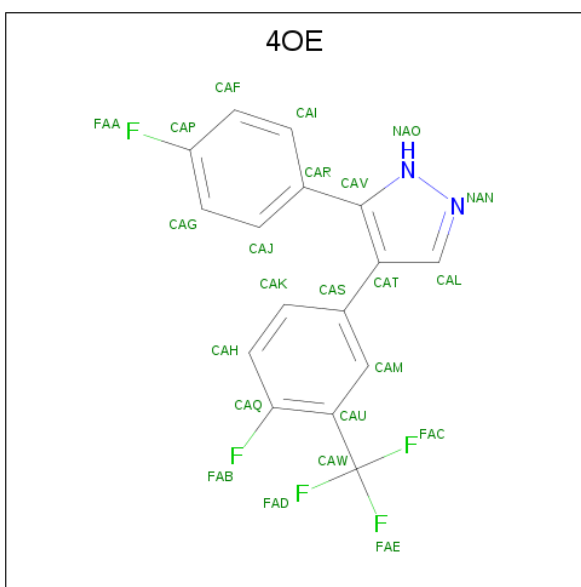
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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 5-(4-fluorophenyl)-4-[4-fluoro-3-(trifluoromethyl)phenyl]-1H-pyrazole (three-letter code: 4OE) (formula: C<sub>16</sub>H<sub>9</sub>F<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	F	N	0	0
			23	16	5	2		
6	I	1	Total	C	F	N	0	0
			23	16	5	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

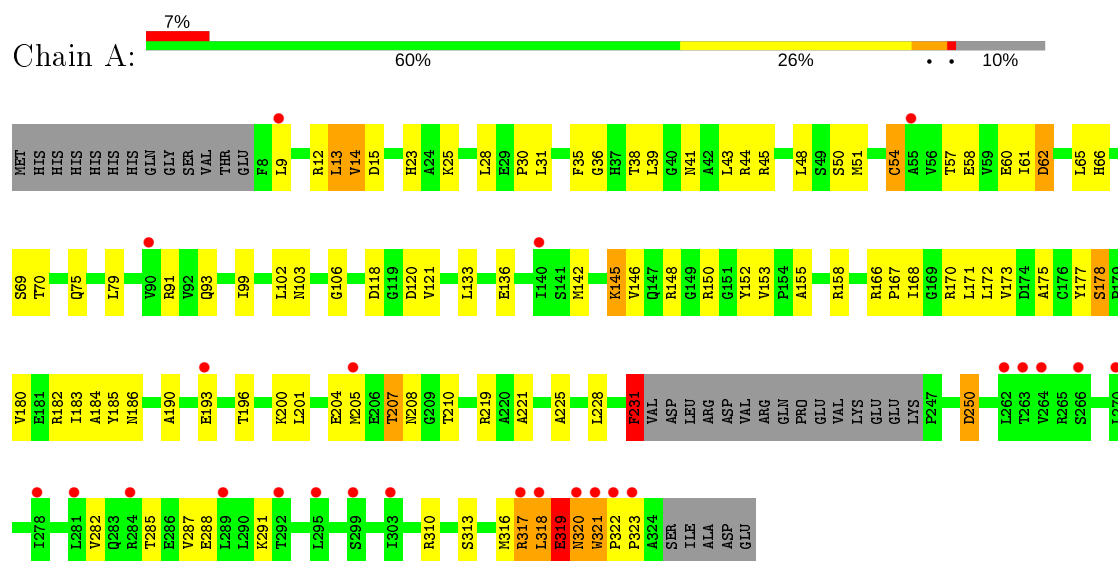
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

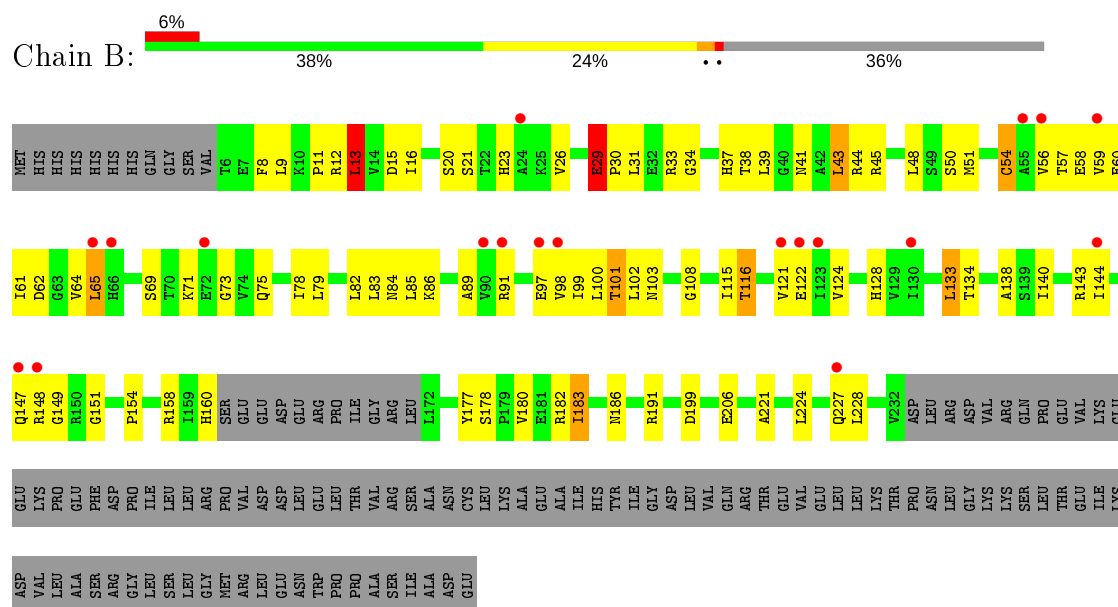
### 3 Residue-property plots [i](#)

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.

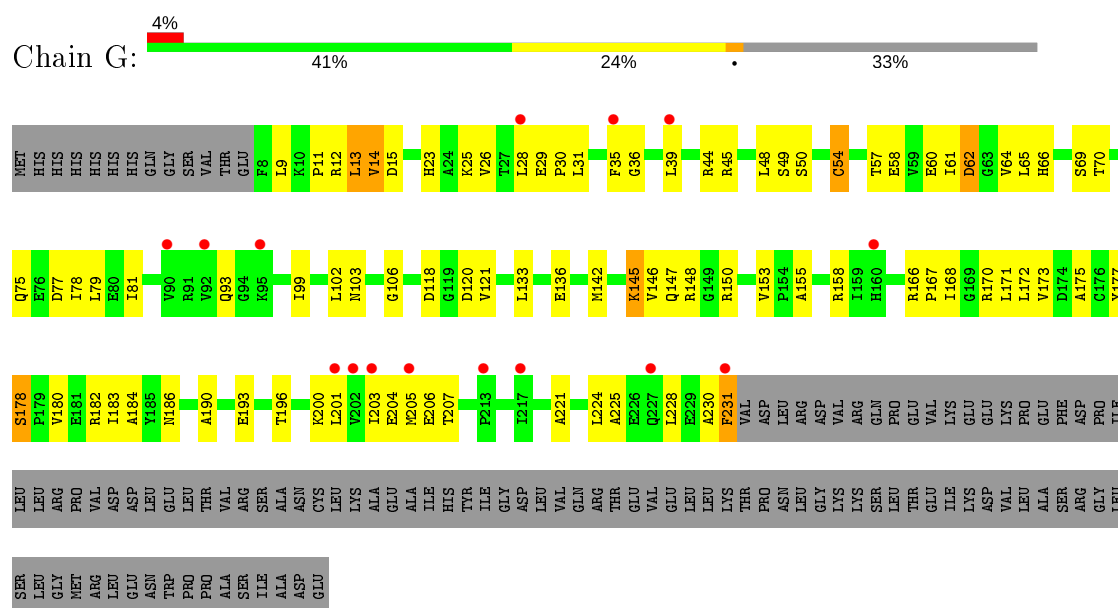
- Molecule 1: DNA-directed RNA polymerase subunit alpha



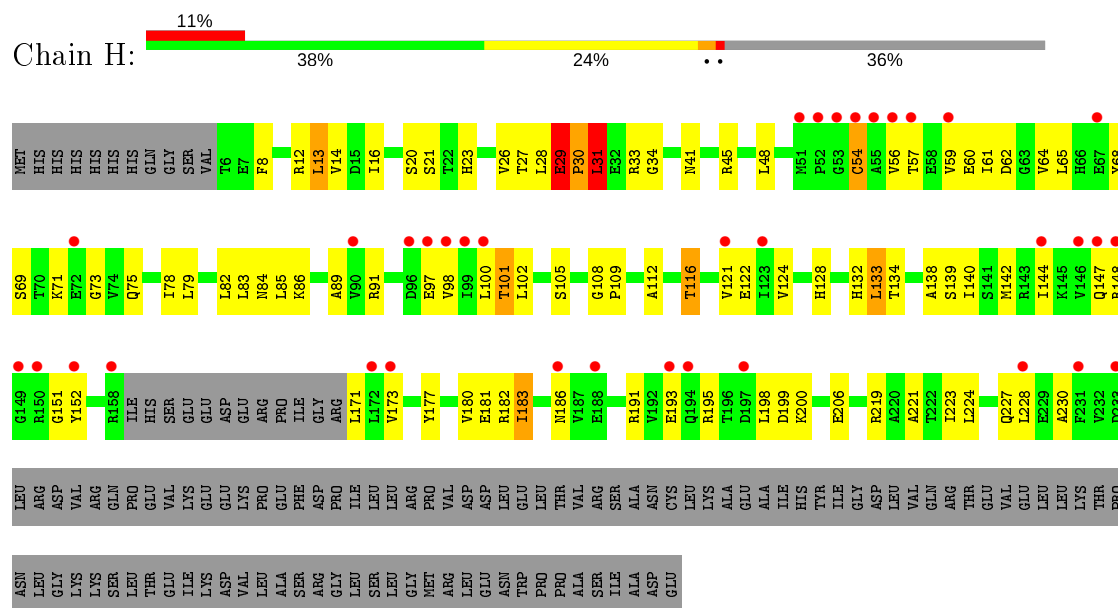
- Molecule 1: DNA-directed RNA polymerase subunit alpha



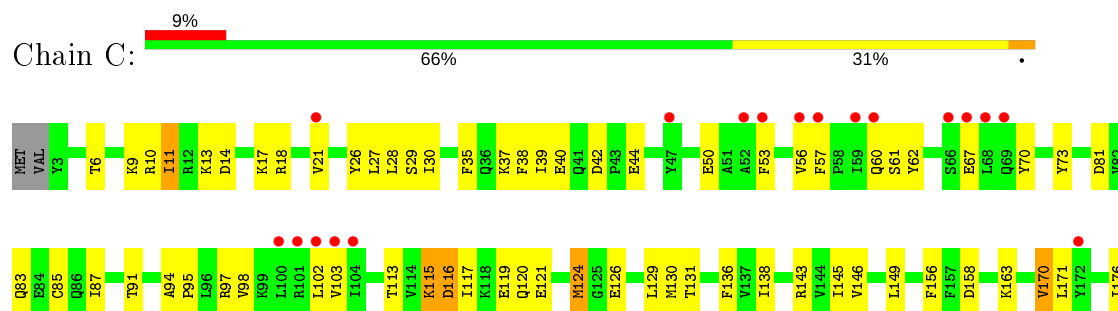
- Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

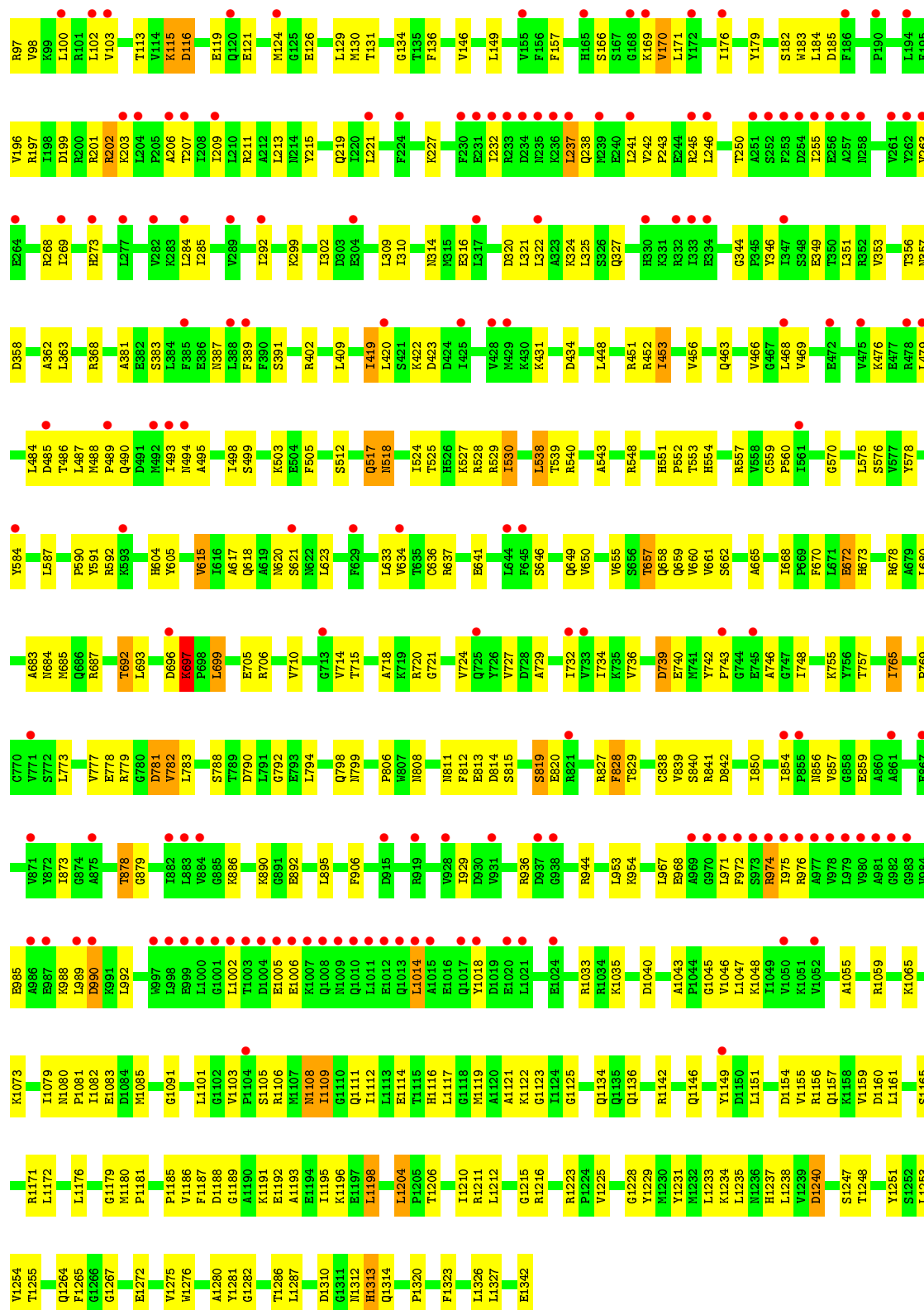


• Molecule 2: DNA-directed RNA polymerase subunit beta







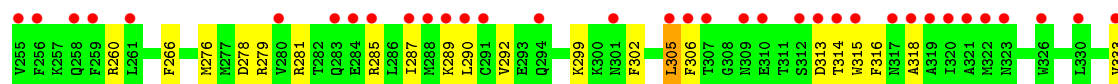


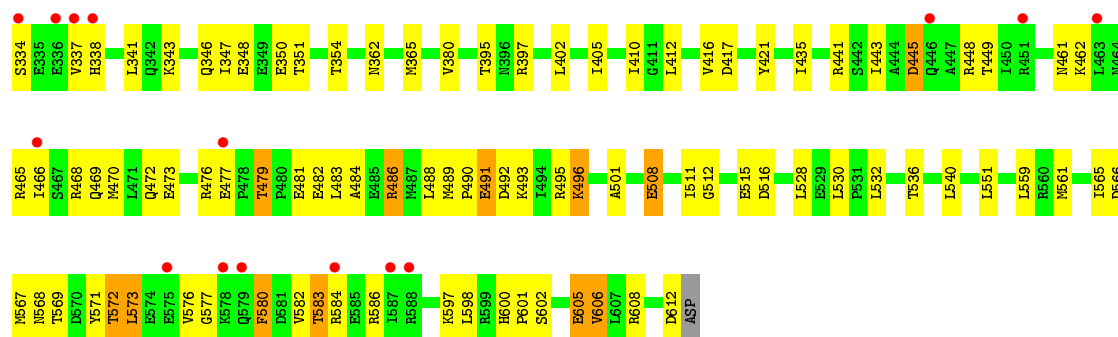
• Molecule 3: DNA-directed RNA polymerase subunit beta'



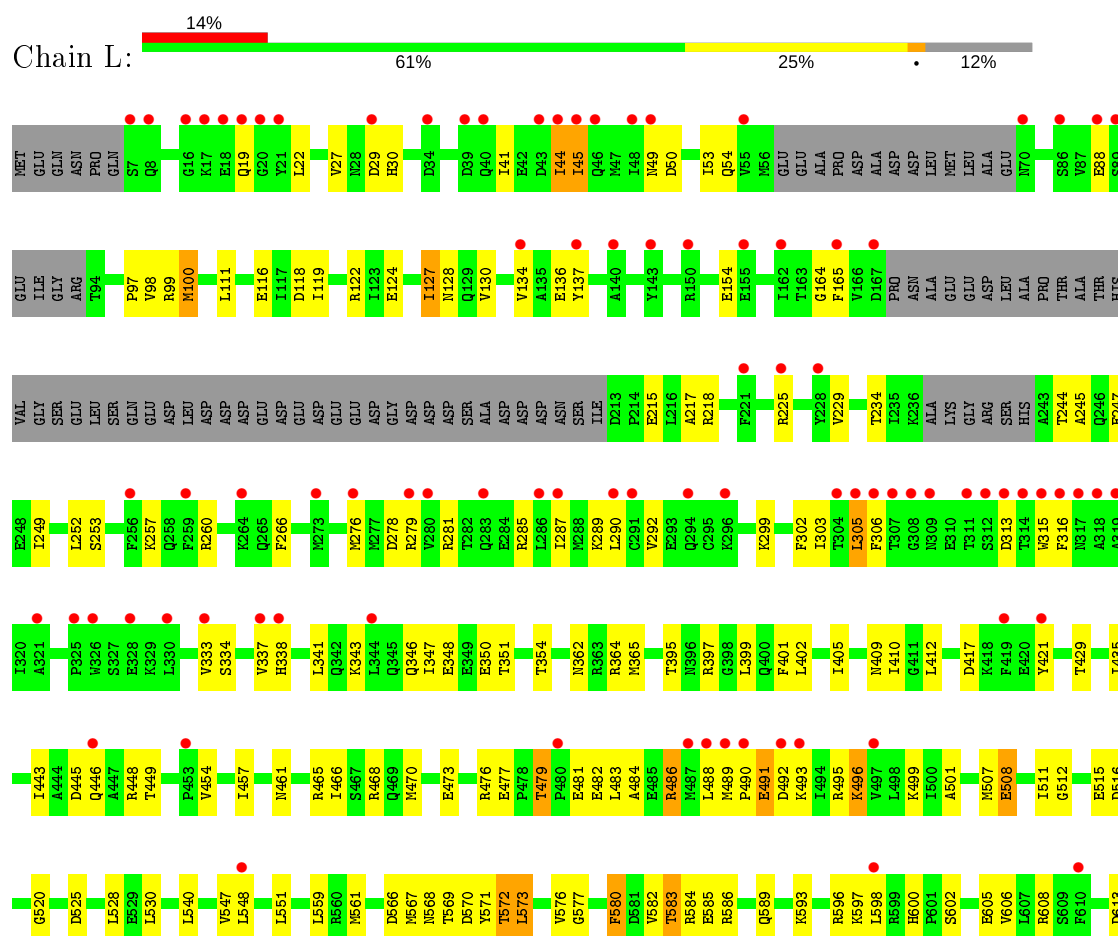








● Molecule 5: RNA polymerase sigma factor RpoD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.58Å 204.10Å 308.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.99 49.79 – 3.99	Depositor EDS
% Data completeness (in resolution range)	93.1 (49.20-3.99) 92.3 (49.79-3.99)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.250 , 0.283 0.252 , 0.280	Depositor DCC
$R_{free}$ test set	1978 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	156.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 88.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	57539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 4OE

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	0.39	1/2358 (0.0%)	0.67	2/3197 (0.1%)
1	B	0.39	0/1687	0.73	1/2286 (0.0%)
1	G	0.33	0/1751	0.66	0/2373
1	H	0.37	0/1681	0.70	2/2278 (0.1%)
2	C	0.28	0/10739	0.49	0/14489
2	I	0.28	1/10735 (0.0%)	0.47	0/14484
3	D	0.29	0/9130	0.50	1/12325 (0.0%)
3	J	0.27	0/10409	0.48	1/14059 (0.0%)
4	E	0.29	0/693	0.49	0/935
4	K	0.26	0/629	0.48	0/847
5	F	0.31	2/4254 (0.0%)	0.51	1/5731 (0.0%)
5	L	0.28	0/4246	0.49	0/5720
All	All	0.30	4/58312 (0.0%)	0.52	8/78724 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	954	LYS	CD-CE	-6.99	1.33	1.51
5	F	605	GLU	CD-OE2	5.91	1.32	1.25
1	A	231	PHE	CD2-CE2	-5.76	1.27	1.39
5	F	605	GLU	CD-OE1	5.01	1.31	1.25



All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASP	CB-CG-OD1	-9.38	109.86	118.30
5	F	605	GLU	OE1-CD-OE2	9.01	134.11	123.30
1	B	29	GLU	C-N-CD	8.36	145.96	128.40
1	H	13	LEU	CA-CB-CG	6.42	130.07	115.30
3	D	120	LEU	N-CA-C	5.85	126.80	111.00
3	J	120	LEU	N-CA-C	5.43	125.66	111.00
1	H	31	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	317	ARG	CD-NE-CZ	5.02	130.62	123.60

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	72	0
1	B	1667	0	1692	63	0
1	G	1730	0	1756	69	0
1	H	1662	0	1687	67	0
2	C	10570	0	10582	277	0
2	I	10566	0	10576	262	0
3	D	8992	0	9180	271	0
3	J	10254	0	10461	313	0
4	E	691	0	695	14	0
4	K	627	0	634	19	0
5	F	4204	0	4106	95	0
5	L	4196	0	4103	103	0
6	C	23	0	9	5	0
6	I	23	0	9	4	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	57539	0	57870	1457	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 13.

All (1457) 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	1.41	1.01
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.46	0.97
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.48	0.95
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.39	0.88
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.56	0.87
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.58	0.86
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.58	0.85
3:D:418:GLU:HG3	4:E:45:LYS:H	1.42	0.85
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.58	0.84
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.83
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.61	0.83
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.61	0.83
1:H:28:LEU:HB3	1:H:31:LEU:HD21	1.61	0.82
3:D:755:ILE:HD13	3:D:774:ILE:HD11	1.59	0.82
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.63	0.81
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.61	0.80
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.45	0.80
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.62	0.79
3:J:418:GLU:HG3	4:K:45:LYS:H	1.46	0.79
1:A:231:PHE:HE2	1:B:43:LEU:HD21	1.46	0.79
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.65	0.79
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.78
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.64	0.78
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.65	0.78
3:D:392:THR:HG21	5:F:606:VAL:HA	1.64	0.78
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.64	0.77
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.66	0.77
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.67	0.77
5:F:561:MET:HA	5:F:567:MET:HE1	1.66	0.76
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.68	0.76
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.34	0.75
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.68	0.75
3:J:755:ILE:HD13	3:J:774:ILE:HD11	1.69	0.74
3:J:755:ILE:HG22	3:J:757:THR:H	1.51	0.74
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.69	0.74
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.69	0.74
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.52	0.73
1:H:101:THR:HG22	1:H:116:THR:HB	1.68	0.73
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.70	0.73
1:H:59:VAL:O	1:H:171:LEU:N	2.22	0.73
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.71	0.73
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.71	0.73
1:B:101:THR:HG22	1:B:116:THR:HB	1.71	0.73
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.69	0.73
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.70	0.72
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.54	0.72
6:I:2001:4OE:H9	3:J:774:ILE:HB	1.71	0.72
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.36	0.72
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.23	0.72
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.72	0.72
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.70	0.72
1:G:23:HIS:HB2	1:G:205:MET:O	1.90	0.71
1:A:23:HIS:HB2	1:A:205:MET:O	1.90	0.71
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.72	0.71
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.72	0.71
2:C:18:ARG:NH2	2:C:620:ASN:OD1	2.23	0.71
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.24	0.71
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.72	0.71
1:H:29:GLU:HB3	1:H:30:PRO:CD	2.20	0.71
2:I:203:LYS:HB2	5:L:29:ASP:HB2	1.72	0.71
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.71	0.70
2:I:452:ARG:NH1	2:I:584:TYR:O	2.24	0.70
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.72	0.70
5:L:561:MET:HA	5:L:567:MET:HE1	1.72	0.70
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.23	0.70
5:L:470:MET:HA	5:L:473:GLU:HB3	1.73	0.70
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.72	0.70
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.23	0.70
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.54	0.70
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.56	0.70
3:D:514:THR:HG23	3:D:576:ARG:HG2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:528:ARG:NH2	2:I:576:SER:O	2.24	0.70
3:D:120:LEU:HD22	3:D:121:PRO:HD3	1.73	0.69
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.73	0.69
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.75	0.69
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.74	0.69
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.22	0.69
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.21	0.69
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.74	0.69
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.40	0.68
3:D:133:ARG:NH2	5:F:93:ARG:O	2.25	0.68
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.74	0.68
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.75	0.68
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.59	0.68
2:I:18:ARG:NH1	2:I:621:SER:O	2.27	0.67
2:I:18:ARG:NH2	2:I:620:ASN:OD1	2.27	0.67
5:F:602:SER:H	5:F:605:GLU:HG3	1.59	0.67
5:F:470:MET:HA	5:F:473:GLU:HB3	1.74	0.67
1:A:166:ARG:O	1:A:168:ILE:N	2.27	0.67
2:C:452:ARG:NH1	2:C:584:TYR:O	2.28	0.67
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.75	0.67
1:H:191:ARG:NH2	3:J:410:ASP:OD2	2.27	0.67
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.28	0.67
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.75	0.67
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.60	0.67
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.76	0.66
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.78	0.66
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.76	0.66
2:I:808:ASN:H	3:J:633:ALA:HB2	1.60	0.66
3:D:356:THR:OG1	3:D:357:VAL:N	2.29	0.66
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.44	0.66
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.77	0.66
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.77	0.66
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.76	0.66
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.78	0.66
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.78	0.66
2:C:18:ARG:NH1	2:C:621:SER:O	2.29	0.65
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.78	0.65
1:G:39:LEU:HD11	1:H:227:GLN:HB3	1.77	0.65
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.61	0.65
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:ASP:H	1.61	0.65
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.78	0.65
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.65
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.77	0.65
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.44	0.65
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.77	0.65
3:D:755:ILE:HG22	3:D:757:THR:H	1.60	0.64
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.78	0.64
1:A:231:PHE:HE2	1:B:43:LEU:CD2	2.10	0.64
2:I:88:ARG:NH2	2:I:1035:LYS:O	2.30	0.64
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.60	0.64
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.79	0.64
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.80	0.64
2:I:829:THR:HA	2:I:1059:ARG:HA	1.80	0.64
2:I:197:ARG:HH12	5:L:29:ASP:HB3	1.62	0.64
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.80	0.64
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.80	0.64
3:J:748:ALA:O	3:J:777:HIS:HD2	1.80	0.64
1:G:61:ILE:HG22	1:G:62:ASP:H	1.62	0.64
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.80	0.64
5:F:461:ASN:O	5:F:465:ARG:HG2	1.98	0.64
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.79	0.64
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.80	0.63
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.80	0.63
5:L:593:LYS:HE2	5:L:596:ARG:HD3	1.79	0.63
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.63	0.63
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.63	0.63
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.81	0.63
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.80	0.63
3:J:356:THR:OG1	3:J:357:VAL:N	2.32	0.63
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.79	0.63
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.81	0.63
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.31	0.63
3:D:77:ARG:HE	5:F:569:THR:HA	1.64	0.63
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.81	0.62
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.81	0.62
1:B:51:MET:HB3	1:B:178:SER:HA	1.81	0.62
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.80	0.62
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.80	0.62
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.82	0.62
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.32	0.62
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.81	0.62
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.82	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.82	0.62
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.65	0.61
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.81	0.61
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.82	0.61
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.81	0.61
1:H:29:GLU:CB	1:H:30:PRO:HD3	2.25	0.61
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.65	0.61
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.63	0.61
5:F:276:MET:SD	5:F:279:ARG:NH1	2.74	0.61
2:I:1151:LEU:HD21	2:I:1198:LEU:HD23	1.82	0.61
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.81	0.61
6:C:2001:4OE:H8	3:D:773:PHE:HB3	1.83	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.64	0.61
1:H:14:VAL:HG11	1:H:29:GLU:HG2	1.83	0.61
2:I:207:THR:HG21	2:I:351:LEU:HG	1.82	0.61
5:L:225:ARG:O	5:L:229:VAL:HG13	2.00	0.61
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.82	0.61
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.82	0.61
3:D:749:LYS:HG3	3:D:751:ASP:HB3	1.82	0.61
1:A:231:PHE:CE2	1:B:43:LEU:HD21	2.32	0.61
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.17	0.61
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.34	0.61
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.83	0.60
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.83	0.60
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.83	0.60
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.81	0.60
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.82	0.60
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.84	0.60
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.64	0.60
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.84	0.60
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.83	0.60
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.14	0.60
5:F:49:ASN:HA	5:F:53:ILE:HA	1.83	0.60
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.84	0.60
1:A:250:ASP:HB2	5:F:605:GLU:HG2	1.83	0.60
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.34	0.60
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.84	0.60
5:F:602:SER:H	5:F:605:GLU:CG	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.35	0.60
6:C:2001:4OE:H9	3:D:774:ILE:HB	1.82	0.60
1:G:12:ARG:HG2	1:G:13:LEU:H	1.66	0.60
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.66	0.60
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.35	0.59
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.84	0.59
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.82	0.59
3:D:741:ALA:O	3:D:762:ASN:ND2	2.35	0.59
5:F:602:SER:H	5:F:605:GLU:CD	2.05	0.59
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.84	0.59
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.84	0.59
3:J:148:GLU:H	3:J:156:ARG:HG3	1.66	0.59
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.19	0.59
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.84	0.59
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.84	0.59
3:D:1310:THR:HG21	5:F:70:ASN:HA	1.85	0.59
3:J:308:ASP:OD2	3:J:311:ARG:NH2	2.34	0.59
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.85	0.59
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.84	0.59
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.67	0.59
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.83	0.59
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.84	0.59
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.84	0.59
2:C:136:PHE:O	2:C:143:ARG:N	2.29	0.59
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.85	0.59
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.84	0.59
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.68	0.59
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.83	0.59
1:A:45:ARG:HG2	1:B:38:THR:HB	1.85	0.59
6:I:2001:4OE:H8	3:J:773:PHE:HB3	1.85	0.59
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.85	0.58
2:C:40:GLU:O	2:C:73:TYR:OH	2.20	0.58
3:D:115:TRP:O	3:D:119:SER:HB2	2.03	0.58
3:J:210:SER:O	3:J:214:ARG:HG2	2.03	0.58
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.84	0.58
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.84	0.58
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.86	0.58
1:B:61:ILE:HB	1:B:64:VAL:O	2.03	0.58
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.85	0.58
5:F:111:LEU:HD13	5:F:116:GLU:HG2	1.85	0.58
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.85	0.58
2:C:829:THR:HA	2:C:1059:ARG:HA	1.84	0.58
3:D:708:ASN:HB3	3:D:712:GLN:O	2.03	0.58
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.84	0.58
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.84	0.58
5:L:111:LEU:HD13	5:L:116:GLU:HG2	1.85	0.58
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.85	0.58
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.85	0.58
1:A:12:ARG:HG2	1:A:13:LEU:H	1.69	0.58
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.84	0.58
1:A:310:ARG:O	5:F:608:ARG:NH1	2.37	0.58
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.85	0.58
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.85	0.58
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.86	0.58
1:G:12:ARG:H	1:G:30:PRO:HD2	1.67	0.58
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.84	0.58
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.37	0.58
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.86	0.58
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.86	0.58
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.67	0.58
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.86	0.58
5:L:476:ARG:HG2	5:L:477:GLU:HG2	1.85	0.58
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.86	0.58
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.86	0.58
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.36	0.58
2:C:30:ILE:H	2:C:30:ILE:HD12	1.68	0.57
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.85	0.57
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.70	0.57
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.86	0.57
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.87	0.57
2:C:739:ASP:OD1	2:C:739:ASP:N	2.36	0.57
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.85	0.57
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.17	0.57
3:D:1297:LYS:HB3	3:J:1303:SER:HA	1.87	0.57
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.86	0.57
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.85	0.57
2:I:30:ILE:HD12	2:I:30:ILE:H	1.69	0.57
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.68	0.57
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.40	0.57
3:D:152:THR:OG1	3:D:153:ASN:N	2.37	0.57
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.69	0.57
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.86	0.57
3:D:282:LEU:HD21	5:F:410:ILE:HG12	1.87	0.57
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.87	0.57
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.86	0.57
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.86	0.57
5:L:515:GLU:HG2	5:L:516:ASP:H	1.69	0.57
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.69	0.57
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.87	0.57
2:I:494:ASN:OD1	2:I:495:ALA:N	2.36	0.57
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.85	0.57
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.87	0.57
6:I:2001:4OE:NAN	3:J:755:ILE:HG12	2.19	0.57
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.87	0.57
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.87	0.56
2:C:494:ASN:OD1	2:C:495:ALA:N	2.36	0.56
1:G:11:PRO:HD2	1:H:227:GLN:HA	1.86	0.56
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.87	0.56
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.87	0.56
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.87	0.56
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.86	0.56
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.37	0.56
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.86	0.56
2:I:518:ASN:N	2:I:518:ASN:OD1	2.36	0.56
2:I:40:GLU:O	2:I:73:TYR:OH	2.23	0.56
5:L:49:ASN:HA	5:L:53:ILE:HA	1.87	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.41	0.56
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.71	0.56
2:C:324:LYS:O	2:C:327:GLN:NE2	2.38	0.56
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.38	0.56
3:D:847:ASP:N	3:D:847:ASP:OD1	2.38	0.56
5:F:515:GLU:HG2	5:F:516:ASP:H	1.71	0.56
2:C:1151:LEU:HD21	2:C:1198:LEU:HD23	1.87	0.56
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.69	0.56
5:L:585:GLU:O	5:L:589:GLN:HG3	2.05	0.56
1:G:228:LEU:HD11	1:H:221:ALA:HB1	1.87	0.56
1:A:14:VAL:HG22	1:A:15:ASP:H	1.71	0.56
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.88	0.56
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.87	0.56
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.88	0.56
3:D:682:VAL:O	3:D:685:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:476:ARG:HG2	5:F:477:GLU:HG2	1.88	0.56
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.88	0.56
5:L:551:LEU:HD22	5:L:597:LYS:HD2	1.88	0.56
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.88	0.56
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.88	0.56
5:F:483:LEU:H	5:F:483:LEU:HD12	1.70	0.56
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.38	0.56
5:L:244:THR:O	5:L:247:GLU:HG2	2.05	0.56
3:D:210:SER:O	3:D:214:ARG:HG2	2.06	0.55
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.71	0.55
2:C:488:MET:O	2:C:490:GLN:N	2.34	0.55
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.88	0.55
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.88	0.55
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.88	0.55
3:J:478:LEU:HG	4:K:47:THR:HG23	1.88	0.55
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.89	0.55
2:I:448:LEU:HB2	2:I:553:THR:HB	1.88	0.55
3:J:847:ASP:N	3:J:847:ASP:OD1	2.36	0.55
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.88	0.55
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.87	0.55
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.72	0.55
2:I:560:PRO:O	3:J:780:ARG:NH2	2.33	0.55
3:J:120:LEU:HD22	3:J:121:PRO:HD3	1.88	0.55
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.88	0.55
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.89	0.55
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.88	0.55
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.89	0.55
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.89	0.55
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.71	0.55
5:L:482:GLU:O	5:L:486:ARG:NH2	2.39	0.55
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.89	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.54
3:J:115:TRP:O	3:J:119:SER:HB2	2.07	0.54
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.89	0.54
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.72	0.54
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.90	0.54
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.89	0.54
5:F:479:THR:HG23	5:F:481:GLU:H	1.72	0.54
2:I:1320:PRO:HG2	3:J:1354:GLY:HA3	1.87	0.54
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.90	0.54
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:ARG:C	3:D:711:GLY:H	2.08	0.54
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.88	0.54
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.42	0.54
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.72	0.54
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.89	0.54
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.41	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.88	0.54
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.41	0.54
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.41	0.54
5:F:482:GLU:O	5:F:486:ARG:NH2	2.41	0.54
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.90	0.54
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.40	0.54
1:A:285:THR:HG23	1:A:288:GLU:H	1.73	0.54
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.40	0.54
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.23	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
2:C:617:ALA:HA	2:C:636:CYS:SG	2.48	0.54
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.89	0.54
5:L:602:SER:H	5:L:605:GLU:HG3	1.73	0.54
5:F:511:ILE:HG13	5:F:512:GLY:H	1.73	0.54
1:G:14:VAL:HG22	1:G:15:ASP:H	1.73	0.54
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.90	0.54
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.72	0.54
1:H:61:ILE:HB	1:H:64:VAL:O	2.08	0.54
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.90	0.54
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.90	0.54
3:J:45:ASN:HB3	3:J:48:THR:O	2.08	0.54
2:I:166:SER:OG	5:L:19:GLN:O	2.20	0.54
5:L:276:MET:SD	5:L:279:ARG:NH1	2.80	0.54
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.89	0.54
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.32	0.54
3:D:694:SER:OG	3:D:738:ARG:NE	2.36	0.54
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.89	0.54
1:G:230:ALA:HB1	1:H:12:ARG:HA	1.90	0.54
3:J:79:LYS:HG3	3:J:80:HIS:N	2.23	0.54
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.22	0.53
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.41	0.53
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.90	0.53
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.90	0.53
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.91	0.53
2:I:1251:TYR:OH	3:J:348:ASP:OD2	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.90	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.42	0.53
2:C:518:ASN:OD1	2:C:518:ASN:N	2.40	0.53
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.73	0.53
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.08	0.53
3:D:405:GLU:O	3:D:408:VAL:HG22	2.09	0.53
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.91	0.53
3:J:568:SER:OG	3:J:569:LEU:N	2.41	0.53
1:B:11:PRO:HA	1:B:30:PRO:HD2	1.90	0.53
1:B:13:LEU:HB3	1:B:29:GLU:CB	2.38	0.53
3:D:148:GLU:H	3:D:156:ARG:HG3	1.73	0.53
3:D:662:ALA:HA	3:D:665:GLN:HB3	1.90	0.53
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.90	0.53
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.89	0.53
5:L:569:THR:OG1	5:L:570:ASP:N	2.37	0.53
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.91	0.53
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.44	0.53
3:J:733:SER:O	3:J:737:ILE:HG12	2.09	0.53
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.90	0.53
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.90	0.53
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.91	0.53
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.36	0.53
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.91	0.53
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.23	0.53
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.72	0.53
3:J:79:LYS:HB2	5:L:569:THR:H	1.74	0.53
3:J:133:ARG:HB2	5:L:88:GLU:HA	1.91	0.53
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.89	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.74	0.53
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.90	0.53
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.89	0.53
3:J:741:ALA:O	3:J:762:ASN:ND2	2.42	0.53
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.91	0.53
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.91	0.53
1:A:93:GLN:H	1:A:120:ASP:HB3	1.74	0.53
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.91	0.53
3:J:683:ILE:HD11	3:J:754:ILE:HG12	1.91	0.53
3:J:682:VAL:O	3:J:685:ILE:HG12	2.09	0.53
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.91	0.53
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.90	0.52
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.92	0.52
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.91	0.52
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.91	0.52
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.74	0.52
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.09	0.52
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.91	0.52
3:D:425:ARG:HG2	3:D:426:ALA:H	1.74	0.52
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.90	0.52
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.24	0.52
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.91	0.52
1:A:12:ARG:H	1:A:30:PRO:HD2	1.73	0.52
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.91	0.52
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.74	0.52
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.91	0.52
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.91	0.52
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.43	0.52
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.91	0.52
3:D:709:ARG:O	3:D:711:GLY:N	2.40	0.52
5:F:281:ARG:O	5:F:285:ARG:HG3	2.10	0.52
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.90	0.52
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.44	0.52
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.90	0.52
2:C:339:ASN:HB3	2:C:343:HIS:H	1.75	0.52
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.90	0.52
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.91	0.52
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.92	0.52
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.92	0.52
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.90	0.52
3:D:77:ARG:HG3	3:D:79:LYS:H	1.75	0.52
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.74	0.52
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.91	0.52
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.92	0.52
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.92	0.52
3:J:425:ARG:HG2	3:J:426:ALA:H	1.75	0.52
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.92	0.52
5:L:511:ILE:HG13	5:L:512:GLY:H	1.75	0.52
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.43	0.52
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.25	0.52
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.92	0.52
3:D:777:HIS:CE1	3:D:781:LYS:HB2	2.45	0.52
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:697:MET:SD	3:D:741:ALA:HB3	2.50	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.92	0.52
3:J:298:MET:SD	5:L:402:LEU:HB3	2.49	0.52
3:J:79:LYS:HB2	5:L:569:THR:N	2.25	0.52
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.92	0.52
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.92	0.51
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.91	0.51
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.92	0.51
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.91	0.51
3:J:591:ILE:HG13	3:J:604:MET:HE2	1.92	0.51
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.92	0.51
3:D:388:ARG:NH1	3:D:414:GLU:OE1	2.43	0.51
3:D:478:LEU:HG	4:E:47:THR:HG23	1.91	0.51
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.26	0.51
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.92	0.51
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.45	0.51
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.10	0.51
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.92	0.51
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.91	0.51
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.92	0.51
2:I:206:ALA:O	2:I:209:ILE:HG22	2.10	0.51
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.91	0.51
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.74	0.51
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.91	0.51
3:J:748:ALA:HA	3:J:755:ILE:HD12	1.91	0.51
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.41	0.51
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.51
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.91	0.51
5:F:532:LEU:O	5:F:536:THR:HG23	2.11	0.51
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.91	0.51
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.93	0.51
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.45	0.51
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.45	0.51
3:D:613:GLY:O	3:D:617:THR:OG1	2.27	0.51
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.93	0.51
5:L:479:THR:HG23	5:L:481:GLU:H	1.76	0.51
2:C:9:LYS:HA	2:C:1171:ARG:HD2	1.92	0.51
2:C:641:GLU:OE2	3:D:749:LYS:NZ	2.42	0.51
2:I:237:LEU:HD22	2:I:237:LEU:H	1.75	0.51
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.91	0.51
2:C:103:VAL:HB	2:C:113:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.91	0.51
3:D:189:LEU:HD22	3:D:234:PRO:HB3	1.92	0.51
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.74	0.51
2:I:1119:MET:HE3	2:I:1204:LEU:HD13	1.93	0.51
3:J:794:GLY:O	3:J:797:THR:OG1	2.24	0.51
5:L:97:PRO:HA	5:L:100:MET:HG3	1.92	0.51
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.93	0.51
1:B:91:ARG:HG2	1:B:122:GLU:O	2.11	0.51
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.76	0.51
3:D:298:MET:SD	5:F:402:LEU:HB3	2.51	0.51
1:H:29:GLU:OE2	1:H:200:LYS:HE3	2.11	0.51
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.92	0.51
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.92	0.51
5:L:448:ARG:NH1	5:L:501:ALA:O	2.36	0.51
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.93	0.50
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.43	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.93	0.50
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.93	0.50
2:I:349:GLU:O	2:I:353:VAL:HG23	2.11	0.50
5:L:41:ILE:HA	5:L:44:ILE:HG23	1.93	0.50
5:L:483:LEU:H	5:L:483:LEU:HD12	1.75	0.50
1:B:64:VAL:HG11	1:B:69:SER:OG	2.11	0.50
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.76	0.50
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.46	0.50
2:C:692:THR:OG1	2:C:693:LEU:N	2.43	0.50
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.93	0.50
1:G:177:TYR:O	1:G:178:SER:HB2	2.10	0.50
2:I:878:THR:OG1	2:I:879:GLY:N	2.44	0.50
3:D:872:LEU:O	3:D:877:VAL:HG12	2.11	0.50
2:I:227:LYS:O	2:I:245:ARG:NH2	2.44	0.50
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.93	0.50
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.47	0.50
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.58	0.50
1:B:154:PRO:HG3	3:D:541:LEU:HD13	1.93	0.50
1:H:101:THR:H	1:H:116:THR:HG22	1.77	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.94	0.50
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.50
4:K:4:VAL:HG22	4:K:5:THR:HG23	1.94	0.50
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.94	0.50
1:G:182:ARG:O	1:G:206:GLU:N	2.45	0.50
1:G:230:ALA:CB	1:H:12:ARG:HA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.46	0.50
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.93	0.50
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.77	0.50
2:C:402:ARG:NH2	2:C:419:ILE:O	2.45	0.50
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.93	0.50
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.92	0.50
2:I:488:MET:O	2:I:490:GLN:N	2.39	0.50
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.93	0.50
3:J:1167:LYS:HE3	3:J:1168:GLU:H	1.76	0.50
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.11	0.50
5:L:582:VAL:HG22	5:L:586:ARG:HG2	1.94	0.50
1:B:151:GLY:O	1:B:177:TYR:HB2	2.12	0.50
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.26	0.50
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.94	0.50
1:G:228:LEU:CD1	1:H:221:ALA:HB1	2.42	0.50
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.94	0.50
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.77	0.50
5:L:164:GLY:O	5:L:260:ARG:HB2	2.11	0.50
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.47	0.50
5:F:573:LEU:H	5:F:573:LEU:HD23	1.76	0.50
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.93	0.50
4:K:60:ASN:HD21	4:K:63:ILE:HD13	1.77	0.50
5:L:29:ASP:OD1	5:L:30:HIS:N	2.45	0.50
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.94	0.49
2:I:103:VAL:HB	2:I:113:THR:HG21	1.93	0.49
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.76	0.49
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.94	0.49
2:I:1313:HIS:ND1	4:K:31:GLN:OE1	2.45	0.49
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.93	0.49
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.52	0.49
3:D:45:ASN:HB3	3:D:48:THR:O	2.11	0.49
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.77	0.49
3:J:198:CYS:O	3:J:202:ARG:HG3	2.11	0.49
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.12	0.49
1:A:91:ARG:HD3	1:A:210:THR:O	2.12	0.49
2:C:1282:GLY:O	3:D:1361:THR:N	2.44	0.49
2:C:448:LEU:HB2	2:C:553:THR:HB	1.93	0.49
3:D:1341:ARG:HH22	3:D:1373:ARG:HH21	1.60	0.49
3:D:683:ILE:HD11	3:D:754:ILE:HG12	1.95	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.13	0.49
5:L:137:TYR:HE1	5:L:351:THR:HB	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:255:ILE:HB	2:C:263:VAL:HB	1.95	0.49
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.76	0.49
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	1.94	0.49
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.94	0.49
1:A:287:VAL:HG12	1:A:291:LYS:HE3	1.93	0.49
2:I:517:GLN:O	2:I:517:GLN:HG2	2.12	0.49
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.47	0.49
3:J:748:ALA:O	3:J:777:HIS:CD2	2.64	0.49
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.28	0.49
1:A:177:TYR:O	1:A:178:SER:HB2	2.12	0.49
1:A:41:ASN:HB2	1:A:185:TYR:OH	2.12	0.49
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.95	0.49
2:C:1294:LYS:HD3	3:D:472:LEU:HG	1.95	0.49
2:C:349:GLU:O	2:C:353:VAL:HG23	2.12	0.49
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.95	0.49
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.93	0.49
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.94	0.49
1:H:91:ARG:HG2	1:H:122:GLU:O	2.13	0.49
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.53	0.49
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.45	0.49
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.46	0.49
2:C:207:THR:HG21	2:C:351:LEU:HG	1.95	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.94	0.49
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.93	0.49
2:C:115:LYS:HE3	2:C:116:ASP:H	1.77	0.49
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.95	0.49
1:G:93:GLN:H	1:G:120:ASP:HB3	1.78	0.49
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.48	0.49
2:C:517:GLN:HG2	2:C:517:GLN:O	2.12	0.49
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.95	0.49
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.94	0.49
3:J:613:GLY:O	3:J:617:THR:OG1	2.25	0.49
2:C:901:LEU:HB2	5:F:565:ILE:HD11	1.94	0.48
1:G:228:LEU:HD13	1:G:231:PHE:HD2	1.76	0.48
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.43	0.48
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.45	0.48
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.13	0.48
5:L:482:GLU:HG2	5:L:486:ARG:HH22	1.78	0.48
3:D:568:SER:OG	3:D:569:LEU:N	2.45	0.48
5:F:448:ARG:NH1	5:F:501:ALA:O	2.36	0.48
1:H:221:ALA:O	1:H:224:LEU:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.95	0.48
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.95	0.48
2:C:170:VAL:HG23	2:C:171:LEU:N	2.28	0.48
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.94	0.48
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.53	0.48
2:I:324:LYS:O	2:I:327:GLN:NE2	2.46	0.48
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.96	0.48
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.96	0.48
3:J:152:THR:OG1	3:J:153:ASN:N	2.44	0.48
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.95	0.48
3:D:733:SER:O	3:D:737:ILE:HG12	2.13	0.48
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.95	0.48
2:I:202:ARG:HH22	2:I:368:ARG:HH12	1.61	0.48
3:J:405:GLU:O	3:J:408:VAL:HG22	2.12	0.48
1:B:13:LEU:HB3	1:B:29:GLU:HB3	1.95	0.48
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.29	0.48
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.96	0.48
1:H:97:GLU:OE1	1:H:147:GLN:HG3	2.14	0.48
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.45	0.48
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.78	0.48
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.96	0.48
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.94	0.48
3:D:218:THR:HA	3:D:221:ILE:HG22	1.95	0.48
2:I:387:ASN:HA	2:I:391:SER:HB2	1.95	0.48
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.96	0.48
3:J:1341:ARG:HH22	3:J:1373:ARG:HH21	1.60	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.13	0.48
2:I:203:LYS:CB	5:L:29:ASP:HB2	2.43	0.48
1:A:321:TRP:HA	1:A:322:PRO:HA	1.73	0.48
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.95	0.48
3:D:1167:LYS:HE3	3:D:1168:GLU:H	1.77	0.48
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.94	0.48
1:H:108:GLY:O	1:H:133:LEU:HB2	2.14	0.48
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.95	0.48
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.96	0.48
1:H:182:ARG:NH1	3:J:581:MET:SD	2.87	0.48
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.96	0.48
2:C:878:THR:OG1	2:C:879:GLY:N	2.44	0.48
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.47	0.48
2:I:641:GLU:OE2	3:J:749:LYS:NZ	2.36	0.48
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.96	0.48
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.96	0.48
5:L:316:PHE:HZ	5:L:334:SER:HA	1.78	0.48
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.96	0.48
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.96	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.96	0.48
3:D:128:LEU:HA	3:D:192:MET:HE1	1.96	0.48
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.61	0.48
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.94	0.48
1:H:102:LEU:HD12	1:H:142:MET:HG2	1.95	0.48
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.96	0.48
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.95	0.48
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.96	0.48
3:J:777:HIS:CE1	3:J:781:LYS:HD2	2.49	0.48
1:A:282:VAL:O	1:A:316:MET:N	2.47	0.47
1:B:182:ARG:NH1	3:D:581:MET:SD	2.87	0.47
2:C:903:ARG:O	2:C:907:GLY:N	2.46	0.47
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.13	0.47
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.96	0.47
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.96	0.47
2:I:842:ASP:N	2:I:1045:GLY:O	2.47	0.47
3:J:1170:LYS:C	3:J:1172:LYS:H	2.18	0.47
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.48	0.47
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.47
3:J:481:ARG:NH1	4:K:3:ARG:O	2.47	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.94	0.47
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.49	0.47
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.43	0.47
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.94	0.47
1:B:97:GLU:OE1	1:B:147:GLN:HG3	2.14	0.47
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.95	0.47
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.95	0.47
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.94	0.47
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.96	0.47
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.95	0.47
2:C:211:ARG:NH1	2:C:357:ASN:O	2.47	0.47
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.95	0.47
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.96	0.47
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.95	0.47
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.49	0.47
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.97	0.47
2:I:250:THR:HA	2:I:268:ARG:HA	1.95	0.47
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.96	0.47
2:C:250:THR:HA	2:C:268:ARG:HA	1.96	0.47
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.96	0.47
3:J:697:MET:SD	3:J:741:ALA:HB3	2.55	0.47
1:B:44:ARG:NH1	1:B:44:ARG:HB3	2.30	0.47
2:C:842:ASP:N	2:C:1045:GLY:O	2.48	0.47
2:C:227:LYS:O	2:C:245:ARG:NH2	2.48	0.47
2:C:896:THR:HB	2:C:897:PRO:HD2	1.95	0.47
5:F:572:THR:O	5:F:576:VAL:HG23	2.15	0.47
1:G:28:LEU:HB2	1:G:201:LEU:HB3	1.95	0.47
1:G:230:ALA:HB2	1:H:12:ARG:HG2	1.95	0.47
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.55	0.47
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.14	0.47
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.95	0.47
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.97	0.47
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.97	0.47
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.79	0.47
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.97	0.47
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.96	0.47
1:A:282:VAL:HB	1:A:316:MET:HB2	1.95	0.47
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.97	0.47
2:C:901:LEU:O	2:C:905:ILE:HG13	2.15	0.47
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.96	0.47
2:I:26:TYR:O	2:I:29:SER:HB2	2.15	0.47
2:I:617:ALA:HA	2:I:636:CYS:SG	2.54	0.47
2:I:739:ASP:N	2:I:739:ASP:OD1	2.40	0.47
2:I:806:PRO:O	3:J:633:ALA:HA	2.14	0.47
2:I:746:ALA:HB3	2:I:971:LEU:HA	1.96	0.47
5:L:287:ILE:HG12	5:L:337:VAL:HG13	1.97	0.47
1:A:182:ARG:O	1:A:183:ILE:HD12	2.14	0.47
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.96	0.47
2:C:658:GLN:O	2:C:660:VAL:N	2.48	0.47
3:D:122:SER:O	3:D:126:LEU:HG	2.14	0.47
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.96	0.47
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.96	0.47
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.97	0.47
3:D:1226:VAL:HG23	3:J:1296:GLY:HA2	1.96	0.47
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.97	0.47
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.15	0.47
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.47
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.14	0.47
3:D:1297:LYS:HG2	3:J:1302:TYR:H	1.80	0.47
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.97	0.47
3:J:709:ARG:C	3:J:711:GLY:H	2.18	0.47
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.50	0.46
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.97	0.46
3:D:708:ASN:N	3:D:708:ASN:OD1	2.47	0.46
2:I:255:ILE:HB	2:I:263:VAL:HB	1.96	0.46
1:G:79:LEU:CD1	2:I:693:LEU:HD21	2.45	0.46
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.97	0.46
3:J:73:GLY:O	3:J:76:LYS:NZ	2.36	0.46
1:A:54:CYS:HA	1:A:148:ARG:HG3	1.97	0.46
1:B:39:LEU:O	1:B:43:LEU:HB2	2.16	0.46
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.97	0.46
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.15	0.46
1:H:64:VAL:HG12	1:H:65:LEU:H	1.80	0.46
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.97	0.46
2:C:820:GLU:N	2:C:1080:ASN:O	2.49	0.46
2:C:387:ASN:HA	2:C:391:SER:HB2	1.97	0.46
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.97	0.46
3:D:682:VAL:HA	3:D:685:ILE:CD1	2.46	0.46
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.50	0.46
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.96	0.46
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.96	0.46
1:A:106:GLY:HA2	1:A:136:GLU:O	2.15	0.46
1:B:108:GLY:O	1:B:133:LEU:HB2	2.15	0.46
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.98	0.46
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.97	0.46
3:D:598:LYS:HA	3:D:601:ILE:HG22	1.96	0.46
5:F:316:PHE:HZ	5:F:334:SER:HA	1.80	0.46
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.48	0.46
2:I:1313:HIS:N	4:K:31:GLN:OE1	2.49	0.46
5:L:548:LEU:HD21	5:L:559:LEU:HD23	1.98	0.46
5:L:573:LEU:H	5:L:573:LEU:HD23	1.80	0.46
1:A:182:ARG:C	1:A:183:ILE:HD12	2.35	0.46
1:A:316:MET:HB3	1:A:316:MET:HE3	1.84	0.46
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.51	0.46
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.97	0.46
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:654:ILE:O	3:D:658:GLU:HB2	2.15	0.46
3:D:848:VAL:HG22	3:D:858:VAL:CG2	2.45	0.46
1:G:221:ALA:HB1	1:H:228:LEU:HD13	1.98	0.46
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.78	0.46
3:J:888:CYS:SG	3:J:890:THR:HB	2.56	0.46
1:A:54:CYS:O	1:A:146:VAL:HG13	2.15	0.46
5:F:164:GLY:O	5:F:260:ARG:HB2	2.15	0.46
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.98	0.46
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.97	0.46
2:I:705:GLU:HB2	2:I:794:LEU:HB3	1.97	0.46
1:A:172:LEU:H	1:A:172:LEU:HD12	1.81	0.46
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.51	0.46
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.98	0.46
3:D:9:LYS:HE2	3:D:11:GLN:HA	1.98	0.46
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.97	0.46
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.96	0.46
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.97	0.46
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.81	0.46
1:B:151:GLY:O	1:B:177:TYR:HD2	1.99	0.46
3:D:712:GLN:CD	3:D:712:GLN:H	2.14	0.46
3:D:901:ARG:HA	3:D:908:ILE:HA	1.96	0.46
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.97	0.46
5:F:551:LEU:HD21	5:F:598:LEU:HD21	1.98	0.46
1:G:50:SER:HB3	1:G:150:ARG:HD2	1.98	0.46
2:I:197:ARG:NH2	5:L:29:ASP:OD2	2.49	0.46
5:L:572:THR:O	5:L:576:VAL:HG23	2.16	0.46
3:D:482:ALA:HB3	4:E:20:VAL:HG22	1.98	0.46
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.98	0.46
5:F:41:ILE:HA	5:F:44:ILE:HG23	1.98	0.46
5:F:583:THR:HG22	5:F:584:ARG:H	1.81	0.46
3:J:1025:MET:SD	3:J:1124:ILE:HD12	2.56	0.46
3:J:128:LEU:HA	3:J:192:MET:HE1	1.98	0.46
3:J:735:ALA:O	3:J:738:ARG:HB3	2.15	0.46
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.81	0.46
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.51	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.97	0.46
2:C:524:ILE:HG21	2:C:708:VAL:HG13	1.98	0.46
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.80	0.46
2:I:215:TYR:HA	2:I:219:GLN:NE2	2.31	0.46
3:J:197:GLU:O	3:J:201:LEU:HG	2.16	0.46
3:J:872:LEU:O	3:J:877:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.49	0.46
1:A:319:GLU:O	1:A:320:ASN:HB2	2.15	0.45
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.97	0.45
2:C:557:ARG:HH21	2:C:607:SER:C	2.19	0.45
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.31	0.45
3:D:591:ILE:HG13	3:D:604:MET:HE2	1.97	0.45
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.97	0.45
2:I:820:GLU:N	2:I:1080:ASN:O	2.48	0.45
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.98	0.45
2:I:1286:THR:N	3:J:479:GLU:OE2	2.42	0.45
4:K:73:GLN:HA	4:K:76:GLU:HB3	1.98	0.45
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.97	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.16	0.45
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.99	0.45
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.17	0.45
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.98	0.45
1:G:106:GLY:HA2	1:G:136:GLU:O	2.16	0.45
1:G:28:LEU:HD22	1:G:201:LEU:HD23	1.99	0.45
2:I:854:ILE:HB	2:I:857:VAL:HG21	1.99	0.45
3:J:709:ARG:O	3:J:711:GLY:N	2.48	0.45
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.80	0.45
3:D:77:ARG:NE	5:F:569:THR:HA	2.32	0.45
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.97	0.45
2:I:680:LEU:O	2:I:684:ASN:HB2	2.16	0.45
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.45
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.98	0.45
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.81	0.45
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.99	0.45
1:A:28:LEU:HB2	1:A:201:LEU:HB3	1.99	0.45
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.97	0.45
2:I:710:VAL:HA	2:I:715:THR:HG21	1.98	0.45
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.98	0.45
3:J:290:ILE:HD12	3:J:290:ILE:H	1.81	0.45
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.97	0.45
5:L:130:VAL:HB	5:L:365:MET:HG3	1.97	0.45
5:L:465:ARG:HA	5:L:468:ARG:HH12	1.82	0.45
3:D:198:CYS:O	3:D:202:ARG:HG3	2.17	0.45
3:D:62:PHE:O	3:D:101:ARG:HD2	2.17	0.45
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.29	0.45
5:F:601:PRO:HB2	5:F:605:GLU:OE2	2.17	0.45
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:553:THR:O	2:I:557:ARG:HD2	2.17	0.45
3:J:122:SER:O	3:J:126:LEU:HG	2.17	0.45
3:D:1227:HIS:HD2	3:J:1293:GLU:H	1.65	0.45
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.45
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.98	0.45
2:C:840:SER:O	2:C:1047:LEU:N	2.50	0.45
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.97	0.45
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.97	0.45
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.98	0.45
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.52	0.45
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.99	0.45
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.99	0.45
2:I:778:GLU:O	2:I:781:ASP:HB2	2.17	0.45
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.16	0.45
5:L:461:ASN:O	5:L:465:ARG:HG2	2.16	0.45
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.57	0.45
1:B:64:VAL:HG12	1:B:65:LEU:H	1.81	0.45
1:B:78:ILE:O	1:B:82:LEU:HG	2.16	0.45
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.98	0.45
3:D:712:GLN:N	3:D:712:GLN:CD	2.69	0.45
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.99	0.45
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.51	0.45
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.81	0.45
2:I:402:ARG:NH2	2:I:419:ILE:O	2.50	0.45
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.52	0.45
3:J:266:ASN:O	3:J:270:ARG:HB2	2.17	0.45
3:J:810:THR:HG23	3:J:811:GLU:H	1.81	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.45
2:C:680:LEU:O	2:C:684:ASN:HB2	2.17	0.45
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.98	0.45
2:I:115:LYS:HE3	2:I:116:ASP:H	1.82	0.45
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.98	0.45
2:I:1282:GLY:O	3:J:1361:THR:N	2.49	0.45
3:J:1078:LEU:HB3	3:J:1121:LEU:HD13	1.98	0.45
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.99	0.45
3:J:901:ARG:HD2	3:J:906:GLY:O	2.16	0.45
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.52	0.45
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.98	0.45
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.32	0.45
1:G:58:GLU:HB2	1:G:145:LYS:HB3	1.98	0.45
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.52	0.45
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.17	0.45
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.97	0.44
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.49	0.44
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.98	0.44
3:D:598:LYS:O	3:D:601:ILE:HG22	2.17	0.44
5:F:346:GLN:O	5:F:350:GLU:HG3	2.17	0.44
5:F:380:VAL:HG22	5:F:416:VAL:HG21	1.98	0.44
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.81	0.44
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.17	0.44
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.49	0.44
3:J:668:PHE:HB2	3:J:678:ARG:HG3	1.99	0.44
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.17	0.44
2:I:232:ILE:HG12	2:I:237:LEU:HD13	1.99	0.44
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.99	0.44
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.32	0.44
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.16	0.44
3:D:657:ALA:O	3:D:661:VAL:HG13	2.17	0.44
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.98	0.44
5:F:465:ARG:HA	5:F:468:ARG:HH12	1.83	0.44
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.98	0.44
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.99	0.44
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.81	0.44
3:J:1244:GLN:HE21	3:J:1244:GLN:HB3	1.59	0.44
3:J:70:CYS:SG	3:J:71:LEU:N	2.90	0.44
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.99	0.44
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.53	0.44
2:C:808:ASN:H	3:D:633:ALA:HB2	1.82	0.44
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.32	0.44
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.33	0.44
3:D:860:ARG:HB3	3:D:861:ASN:H	1.56	0.44
5:F:244:THR:O	5:F:247:GLU:HG2	2.18	0.44
1:G:182:ARG:C	1:G:183:ILE:HD12	2.38	0.44
2:I:936:ARG:NH2	2:I:1043:ALA:O	2.51	0.44
2:I:828:PHE:CE2	2:I:1234:LYS:HB2	2.52	0.44
2:C:124:MET:HB2	2:C:498:ILE:HD13	2.00	0.44
2:C:213:LEU:HD13	2:C:422:LYS:HG2	1.98	0.44
3:D:1170:LYS:C	3:D:1172:LYS:H	2.20	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.99	0.44
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.80	0.44
2:I:130:MET:SD	2:I:134:GLY:HA2	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.98	0.44
3:J:203:GLU:O	3:J:207:GLU:HG2	2.18	0.44
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.83	0.44
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.00	0.44
1:A:51:MET:HE3	1:A:51:MET:HB3	1.91	0.44
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.99	0.44
1:G:182:ARG:HB3	1:G:206:GLU:HB3	2.00	0.44
2:I:356:THR:HG21	2:I:362:ALA:HA	1.99	0.44
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.98	0.44
3:J:50:LYS:HB3	3:J:71:LEU:HD21	2.00	0.44
3:J:660:GLU:O	3:J:664:ILE:HG12	2.17	0.44
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.82	0.44
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.50	0.44
3:J:506:VAL:HG23	3:J:628:GLY:HA3	2.00	0.44
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.99	0.44
3:J:708:ASN:N	3:J:708:ASN:OD1	2.49	0.44
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.00	0.44
5:L:127:ILE:O	5:L:130:VAL:HG22	2.18	0.44
2:C:237:LEU:HD22	2:C:237:LEU:H	1.82	0.44
3:D:266:ASN:O	3:D:270:ARG:HB2	2.17	0.44
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.84	0.44
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.82	0.44
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.99	0.44
3:J:598:LYS:O	3:J:601:ILE:HG22	2.18	0.44
3:J:697:MET:O	3:J:701:LEU:HB2	2.18	0.44
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.51	0.44
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.99	0.44
3:D:156:ARG:NH2	3:D:191:SER:OG	2.46	0.44
3:D:701:LEU:HD13	3:D:723:TYR:HB2	1.99	0.44
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.00	0.44
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.86	0.44
1:G:54:CYS:HA	1:G:148:ARG:HG3	1.98	0.44
2:I:316:GLU:CD	2:I:316:GLU:H	2.21	0.44
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.18	0.44
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.86	0.44
1:B:221:ALA:O	1:B:224:LEU:HB3	2.18	0.43
2:C:499:SER:O	2:C:503:LYS:HB2	2.18	0.43
2:C:53:PHE:O	2:C:57:PHE:HB2	2.19	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.58	0.43
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.99	0.43
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1349:GLU:N	3:J:1349:GLU:OE2	2.38	0.43
3:J:385:LEU:HD11	3:J:408:VAL:HG12	2.00	0.43
3:J:694:SER:OG	3:J:738:ARG:NE	2.42	0.43
1:B:61:ILE:HG21	1:B:78:ILE:HD13	1.99	0.43
3:D:197:GLU:O	3:D:201:LEU:HG	2.17	0.43
5:F:580:PHE:C	5:F:582:VAL:H	2.21	0.43
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.99	0.43
1:B:57:THR:HG22	1:B:58:GLU:HG2	2.00	0.43
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.33	0.43
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	2.01	0.43
2:C:356:THR:HG21	2:C:362:ALA:HA	1.99	0.43
1:A:79:LEU:CD1	2:C:693:LEU:HD21	2.49	0.43
3:D:308:ASP:OD2	3:D:311:ARG:NH2	2.43	0.43
3:D:384:LYS:HD2	3:D:387:LEU:HD23	1.99	0.43
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.85	0.43
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.99	0.43
3:J:190:LYS:HD3	3:J:235:GLU:HG2	2.00	0.43
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.00	0.43
2:I:813:GLU:HA	3:J:504:GLN:NE2	2.33	0.43
3:J:611:ILE:HG22	3:J:612:LEU:HD12	2.00	0.43
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.00	0.43
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.83	0.43
6:C:2001:4OE:CAL	3:D:755:ILE:HG12	2.48	0.43
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.91	0.43
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.00	0.43
3:D:777:HIS:CE1	3:D:781:LYS:HD2	2.53	0.43
5:F:462:LYS:O	5:F:466:ILE:HG13	2.17	0.43
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.54	0.43
1:H:16:ILE:HG13	1:H:26:VAL:HG22	2.00	0.43
2:I:720:ARG:HA	2:I:779:ARG:HG3	2.00	0.43
3:J:1048:ARG:NH2	3:J:1057:SER:HB2	2.33	0.43
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.88	0.43
2:C:360:LEU:HB2	2:C:378:ARG:HH21	1.83	0.43
3:D:426:ALA:HB3	3:D:427:PRO:HD3	2.00	0.43
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	2.00	0.43
5:F:137:TYR:HE1	5:F:351:THR:HB	1.83	0.43
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.52	0.43
3:J:1348:LYS:HA	3:J:1348:LYS:HD2	1.84	0.43
3:J:422:LEU:HD13	3:J:471:PRO:HG3	2.00	0.43
2:C:1121:ALA:HB1	2:C:1180:MET:O	2.18	0.43
2:C:238:GLN:HB3	2:C:284:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:697:MET:HE1	3:D:737:ILE:HG22	2.01	0.43
2:I:170:VAL:HG23	2:I:171:LEU:N	2.32	0.43
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.01	0.43
3:J:34:SER:OG	3:J:104:HIS:ND1	2.30	0.43
3:J:264:ASP:OD2	3:J:264:ASP:N	2.52	0.43
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.83	0.43
2:C:724:VAL:HG11	2:C:727:VAL:HG22	2.00	0.43
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.51	0.43
2:C:83:GLN:O	2:C:87:ILE:HG13	2.19	0.43
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.99	0.43
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.34	0.43
3:J:969:SER:HB3	3:J:1116:SER:HB2	2.01	0.43
4:K:49:ILE:HA	4:K:52:ARG:HD3	2.01	0.43
2:C:953:LEU:HD12	2:C:1036:ILE:HD12	2.00	0.43
2:C:1247:SER:OG	2:C:1248:THR:N	2.52	0.43
2:C:552:PRO:HG3	6:C:2001:4OE:CAQ	2.49	0.43
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	2.00	0.43
3:D:264:ASP:N	3:D:264:ASP:OD2	2.52	0.43
5:F:511:ILE:HA	5:F:511:ILE:HD12	1.84	0.43
2:I:499:SER:O	2:I:503:LYS:HB2	2.18	0.43
2:I:721:GLY:N	2:I:740:GLU:OE1	2.47	0.43
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.54	0.43
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.82	0.43
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.01	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.53	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.01	0.43
2:I:551:HIS:ND1	2:I:552:PRO:HD2	2.34	0.43
2:I:692:THR:OG1	2:I:827:ARG:O	2.34	0.43
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.83	0.43
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.34	0.43
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.19	0.43
3:J:62:PHE:O	3:J:101:ARG:HD2	2.19	0.43
3:J:848:VAL:HG22	3:J:858:VAL:CG2	2.48	0.43
3:J:987:GLU:HG3	3:J:987:GLU:H	1.61	0.43
5:L:234:THR:O	5:L:245:ALA:HB2	2.18	0.43
1:B:100:LEU:HB2	1:B:144:ILE:HG23	2.01	0.43
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.51	0.43
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.59	0.43
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	2.01	0.43
5:F:22:LEU:H	5:F:54:GLN:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:582:VAL:HG22	5:F:586:ARG:HG2	2.01	0.43
2:I:68:LEU:HD11	2:I:100:LEU:HB3	2.00	0.43
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.34	0.43
3:J:274:ASN:ND2	5:L:446:GLN:HB2	2.34	0.43
3:J:479:GLU:HG3	4:K:20:VAL:HG11	2.00	0.43
1:B:101:THR:HG23	1:B:103:ASN:H	1.84	0.42
1:B:16:ILE:HG13	1:B:26:VAL:HG22	2.00	0.42
2:C:383:SER:O	2:C:387:ASN:HB2	2.19	0.42
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.47	0.42
5:F:469:GLN:O	5:F:472:GLN:NE2	2.53	0.42
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	2.01	0.42
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.54	0.42
2:I:299:LYS:HB2	2:I:299:LYS:HE2	1.78	0.42
2:I:538:LEU:H	2:I:538:LEU:HG	1.62	0.42
2:I:976:ARG:NH2	2:I:990:ASP:OD2	2.52	0.42
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	2.01	0.42
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.54	0.42
3:J:287:ALA:HB3	3:J:292:VAL:HG13	2.01	0.42
5:L:124:GLU:O	5:L:128:ASN:HB2	2.19	0.42
1:A:31:LEU:HD13	1:A:36:GLY:HA2	2.00	0.42
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.00	0.42
1:A:231:PHE:CE2	1:B:43:LEU:CD2	2.96	0.42
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.01	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.42
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.54	0.42
5:F:348:GLU:HG2	5:F:354:THR:HA	2.00	0.42
6:I:2001:4OE:CAL	3:J:755:ILE:HG12	2.49	0.42
2:I:658:GLN:O	2:I:660:VAL:N	2.52	0.42
2:I:742:TYR:O	2:I:974:ARG:NH2	2.52	0.42
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	2.02	0.42
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.54	0.42
2:C:778:GLU:O	2:C:781:ASP:HB2	2.20	0.42
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.17	0.42
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.84	0.42
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.84	0.42
2:I:538:LEU:HD22	2:I:543:ALA:HB2	2.00	0.42
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.34	0.42
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.21	0.42
3:J:863:LEU:HD11	3:J:901:ARG:HB3	2.01	0.42
1:B:48:LEU:HA	1:B:180:VAL:HG21	2.01	0.42
2:C:1333:LEU:C	2:C:1335:ILE:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:548:ARG:O	2:C:570:GLY:HA3	2.19	0.42
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.00	0.42
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.49	0.42
2:C:980:VAL:HA	2:C:984:VAL:HA	2.00	0.42
1:H:100:LEU:HB2	1:H:144:ILE:HG23	2.01	0.42
1:H:64:VAL:HG21	1:H:69:SER:CB	2.48	0.42
2:I:1121:ALA:HB1	2:I:1180:MET:O	2.20	0.42
2:I:1123:GLY:HA3	2:I:1204:LEU:HD11	2.01	0.42
2:I:383:SER:O	2:I:387:ASN:HB2	2.19	0.42
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.84	0.42
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.92	0.42
5:L:348:GLU:HG2	5:L:354:THR:HA	2.02	0.42
5:L:547:VAL:HG12	5:L:598:LEU:HD22	2.01	0.42
1:B:84:ASN:O	1:B:128:HIS:HE1	2.02	0.42
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.85	0.42
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.83	0.42
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.01	0.42
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.83	0.42
2:C:959:ASP:O	2:C:963:GLU:HG2	2.19	0.42
2:C:972:PHE:CD2	2:C:975:ILE:HD12	2.55	0.42
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.01	0.42
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.17	0.42
3:D:27:PRO:O	3:D:31:ARG:HG3	2.20	0.42
1:G:12:ARG:HG2	1:G:13:LEU:N	2.34	0.42
1:G:224:LEU:HD13	1:H:228:LEU:HD11	2.00	0.42
2:I:466:VAL:O	2:I:469:VAL:HG22	2.19	0.42
3:J:572:THR:OG1	3:J:573:THR:N	2.52	0.42
5:L:412:LEU:HD13	5:L:435:ILE:HD11	2.01	0.42
5:L:511:ILE:HA	5:L:511:ILE:HD12	1.87	0.42
1:A:75:GLN:HA	2:C:729:ALA:N	2.35	0.42
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.54	0.42
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	2.00	0.42
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	2.02	0.42
5:F:148:TYR:OH	5:F:218:ARG:HA	2.20	0.42
2:I:1146:GLN:NE2	2:I:1160:ASP:OD1	2.52	0.42
2:I:559:CYS:HA	2:I:560:PRO:HD3	1.87	0.42
3:J:1034:PHE:HA	3:J:1114:GLN:HA	2.02	0.42
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.02	0.42
4:K:51:LEU:HD23	4:K:51:LEU:HA	1.93	0.42
5:L:130:VAL:O	5:L:134:VAL:HG23	2.20	0.42
1:A:39:LEU:HD11	1:B:227:GLN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:106:GLU:OE2	3:D:241:VAL:HG22	2.19	0.42
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.69	0.42
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.00	0.42
3:D:919:ALA:O	3:D:923:ILE:HG13	2.20	0.42
5:F:249:ILE:O	5:F:252:LEU:HB3	2.19	0.42
1:G:54:CYS:O	1:G:146:VAL:HG13	2.19	0.42
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.54	0.42
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.20	0.42
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.27	0.42
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.17	0.42
5:L:22:LEU:H	5:L:54:GLN:CB	2.32	0.42
1:B:102:LEU:HD23	1:B:115:ILE:HG23	2.02	0.42
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.60	0.42
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.01	0.42
3:D:1372:ARG:HG3	3:J:853:THR:HB	2.01	0.42
3:D:394:ILE:CG2	5:F:536:THR:HA	2.50	0.42
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.02	0.42
3:D:557:LYS:HA	3:D:563:LEU:HA	2.02	0.42
5:F:97:PRO:HA	5:F:100:MET:HG3	2.00	0.42
5:F:343:LYS:H	5:F:343:LYS:HD2	1.85	0.42
5:F:343:LYS:O	5:F:347:ILE:HG13	2.20	0.42
2:I:657:THR:HG1	2:I:1187:PHE:HB2	1.85	0.42
2:I:211:ARG:NH1	2:I:357:ASN:O	2.53	0.42
1:G:79:LEU:HD11	2:I:693:LEU:HD21	2.01	0.42
3:J:1270:GLY:HA3	3:J:1298:VAL:HG22	2.02	0.42
3:J:557:LYS:HA	3:J:563:LEU:HA	2.02	0.42
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.91	0.42
1:A:221:ALA:HB1	1:B:228:LEU:HD22	2.01	0.42
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	2.00	0.42
3:D:203:GLU:O	3:D:207:GLU:HG2	2.20	0.42
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.85	0.42
3:D:77:ARG:HD2	3:D:78:LEU:H	1.85	0.42
5:F:234:THR:O	5:F:245:ALA:HB2	2.19	0.42
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.53	0.42
1:H:34:GLY:N	1:H:199:ASP:OD2	2.51	0.42
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.20	0.42
2:I:176:ILE:HB	2:I:184:LEU:HB3	2.02	0.42
2:I:183:TRP:HB2	2:I:199:ASP:HA	2.02	0.42
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.91	0.42
1:A:228:LEU:CD1	1:B:221:ALA:HB1	2.49	0.42
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.55	0.42
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.55	0.42
2:C:360:LEU:HB2	2:C:378:ARG:NH2	2.35	0.42
2:C:553:THR:O	2:C:557:ARG:HD2	2.20	0.42
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.84	0.42
3:D:1268:ASN:HB2	3:J:1268:ASN:HD22	1.85	0.42
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.20	0.42
5:F:496:LYS:HB2	5:F:496:LYS:HE3	1.88	0.42
1:H:181:GLU:HA	3:J:535:ARG:NH2	2.34	0.42
3:J:708:ASN:HB3	3:J:712:GLN:O	2.20	0.42
5:L:253:SER:O	5:L:257:LYS:HG3	2.20	0.42
5:L:580:PHE:HA	5:L:580:PHE:HD1	1.70	0.42
1:B:50:SER:HA	1:B:151:GLY:HA2	2.01	0.41
2:C:42:ASP:C	2:C:44:GLU:H	2.22	0.41
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	2.35	0.41
3:D:137:ARG:HG2	3:D:143:SER:HB2	2.01	0.41
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.80	0.41
3:D:537:TYR:OH	3:D:634:ARG:NH2	2.53	0.41
3:D:870:ASP:O	3:D:874:GLU:HG2	2.20	0.41
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.84	0.41
1:G:77:ASP:O	1:G:81:ILE:HG13	2.20	0.41
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.84	0.41
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.01	0.41
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.88	0.41
2:I:724:VAL:HG11	2:I:727:VAL:HG22	2.02	0.41
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.85	0.41
3:J:853:THR:HG22	3:J:854:ALA:H	1.84	0.41
3:J:843:VAL:HG11	3:J:897:HIS:O	2.20	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.77	0.41
1:A:219:ARG:HE	1:A:219:ARG:HB2	1.74	0.41
1:B:64:VAL:HG21	1:B:69:SER:CB	2.50	0.41
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.28	0.41
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.85	0.41
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.55	0.41
5:F:380:VAL:HG13	5:F:412:LEU:HD23	2.02	0.41
2:I:197:ARG:NH1	2:I:201:ARG:O	2.52	0.41
2:I:699:LEU:HA	2:I:699:LEU:HD22	1.95	0.41
3:J:137:ARG:HG2	3:J:143:SER:HB2	2.02	0.41
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.56	0.41
3:J:579:LEU:HD12	3:J:582:ILE:HD12	2.01	0.41
3:J:963:VAL:HB	3:J:980:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.85	0.41
2:C:11:ILE:HA	2:C:11:ILE:HD13	1.87	0.41
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.20	0.41
2:C:498:ILE:HD12	2:C:498:ILE:H	1.85	0.41
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	2.02	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.93	0.41
5:F:482:GLU:HG2	5:F:486:ARG:HH22	1.85	0.41
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.41
1:H:41:ASN:O	1:H:45:ARG:HG3	2.19	0.41
1:H:78:ILE:O	1:H:82:LEU:HG	2.21	0.41
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.02	0.41
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.03	0.41
3:J:119:SER:O	3:J:121:PRO:HD2	2.21	0.41
3:J:746:LEU:H	3:J:746:LEU:HD12	1.85	0.41
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.02	0.41
1:A:318:LEU:H	1:A:318:LEU:HD22	1.84	0.41
2:C:322:LEU:O	2:C:326:SER:OG	2.34	0.41
2:C:720:ARG:HA	2:C:779:ARG:HG3	2.01	0.41
2:C:819:SER:HB2	2:C:1085:MET:SD	2.60	0.41
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.50	0.41
3:D:190:LYS:HD3	3:D:235:GLU:HG2	2.02	0.41
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	2.02	0.41
1:G:64:VAL:HG11	1:G:78:ILE:HG21	2.02	0.41
2:I:73:TYR:HB2	2:I:98:VAL:HG22	2.02	0.41
2:I:732:ILE:HD11	2:I:769:PRO:HB3	2.02	0.41
2:I:782:VAL:HG11	2:I:792:GLY:HA2	2.03	0.41
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.02	0.41
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.35	0.41
3:J:1268:ASN:OD1	3:J:1269:ALA:N	2.50	0.41
3:J:56:LEU:HD11	3:J:273:ILE:HD12	2.02	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.02	0.41
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.55	0.41
3:J:997:VAL:HA	3:J:998:PRO:HD3	1.85	0.41
1:B:34:GLY:N	1:B:199:ASP:OD2	2.52	0.41
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.49	0.41
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.03	0.41
1:H:109:PRO:HA	1:H:132:HIS:HA	2.02	0.41
2:I:28:LEU:HD22	2:I:527:LYS:HD2	2.02	0.41
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.94	0.41
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.90	0.41
3:J:441:LEU:HA	3:J:441:LEU:HD13	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:362:ASN:HB2	5:L:365:MET:HE2	2.02	0.41
5:L:507:MET:HG2	5:L:520:GLY:HA3	2.02	0.41
1:A:102:LEU:HD22	1:A:103:ASN:H	1.86	0.41
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.66	0.41
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	2.03	0.41
2:C:967:LEU:HA	2:C:967:LEU:HD12	1.85	0.41
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.80	0.41
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.03	0.41
3:D:735:ALA:O	3:D:738:ARG:HB3	2.20	0.41
5:F:314:THR:O	5:F:318:ALA:HB3	2.20	0.41
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	2.03	0.41
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.55	0.41
3:D:202:ARG:HD3	3:J:1181:ASP:HA	2.02	0.41
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.02	0.41
3:J:384:LYS:HD2	3:J:387:LEU:HD23	2.02	0.41
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.69	0.41
3:J:740:LEU:HA	3:J:740:LEU:HD12	1.89	0.41
3:J:800:LEU:O	3:J:803:VAL:HG12	2.20	0.41
5:L:299:LYS:O	5:L:303:ILE:HG12	2.21	0.41
5:L:401:PHE:O	5:L:405:ILE:HG23	2.21	0.41
2:C:27:LEU:HB2	2:C:524:ILE:HD11	2.02	0.41
2:C:854:ILE:HB	2:C:857:VAL:HG21	2.03	0.41
3:D:794:GLY:O	3:D:797:THR:OG1	2.28	0.41
5:F:289:LYS:HB3	5:F:289:LYS:HE2	1.88	0.41
1:G:75:GLN:HA	2:I:729:ALA:N	2.36	0.41
1:H:20:SER:OG	1:H:21:SER:N	2.53	0.41
2:I:1247:SER:HB3	3:J:375:GLU:O	2.21	0.41
2:I:91:THR:HG21	2:I:503:LYS:NZ	2.36	0.41
2:I:62:TYR:CZ	2:I:476:LYS:HB3	2.56	0.41
3:J:588:PRO:O	3:J:591:ILE:HG22	2.20	0.41
5:L:346:GLN:O	5:L:350:GLU:HG3	2.21	0.41
5:L:41:ILE:O	5:L:45:ILE:HG22	2.21	0.41
1:B:20:SER:OG	1:B:21:SER:N	2.53	0.41
2:C:170:VAL:HG23	2:C:171:LEU:H	1.85	0.41
2:C:38:PHE:HB2	2:C:457:GLY:CA	2.50	0.41
2:C:549:ASP:OD1	3:D:750:PRO:HG2	2.20	0.41
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.56	0.41
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	2.02	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.81	0.41
3:D:746:LEU:H	3:D:746:LEU:HD12	1.86	0.41
3:D:905:ARG:NH1	3:D:910:ASN:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:LEU:HD22	1:G:103:ASN:H	1.86	0.41
1:G:69:SER:O	1:G:78:ILE:HG12	2.21	0.41
1:G:75:GLN:O	2:I:729:ALA:HB2	2.20	0.41
1:H:219:ARG:O	1:H:223:ILE:HG13	2.21	0.41
3:J:24:LEU:HA	3:J:24:LEU:HD13	1.97	0.41
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	2.02	0.41
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.90	0.41
2:C:62:TYR:CZ	2:C:476:LYS:HB3	2.56	0.41
5:F:94:THR:HG23	5:F:96:ASP:OD1	2.20	0.41
1:H:112:ALA:HB2	1:H:128:HIS:HB3	2.01	0.41
1:H:151:GLY:O	1:H:177:TYR:HD2	2.04	0.41
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.56	0.41
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.23	0.41
3:J:198:CYS:HA	3:J:221:ILE:HD13	2.03	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.03	0.41
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.74	0.41
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.21	0.41
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.35	0.41
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	2.03	0.41
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.03	0.41
4:E:4:VAL:HG22	4:E:5:THR:HG23	2.03	0.41
1:H:84:ASN:O	1:H:128:HIS:HE1	2.04	0.41
2:I:548:ARG:O	2:I:570:GLY:HA3	2.21	0.41
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.85	0.41
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.21	0.41
5:L:249:ILE:O	5:L:252:LEU:HB3	2.21	0.41
5:L:454:VAL:HA	5:L:457:ILE:HD12	2.03	0.41
3:D:1266:ILE:HD12	3:D:1273:ASP:O	2.20	0.41
3:D:481:ARG:O	3:D:488:ASN:ND2	2.54	0.41
3:D:902:ASP:OD1	3:D:903:LEU:N	2.54	0.41
5:F:226:ALA:HA	5:F:229:VAL:HG22	2.03	0.41
1:G:49:SER:OG	1:G:50:SER:N	2.54	0.41
2:I:169:LYS:O	2:I:170:VAL:HG22	2.21	0.41
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.84	0.41
2:I:840:SER:O	2:I:1047:LEU:N	2.54	0.41
3:D:1181:ASP:HA	3:J:202:ARG:HD3	2.02	0.41
3:J:481:ARG:O	3:J:488:ASN:ND2	2.54	0.41
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.54	0.41
1:B:73:GLY:CA	1:B:134:THR:HG22	2.51	0.40
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	2.02	0.40
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.36	0.40
2:C:555:TYR:HD2	6:C:2001:4OE:FAA	1.94	0.40
3:D:1198:VAL:HB	3:D:1210:ILE:HA	2.03	0.40
1:G:172:LEU:HD12	1:G:172:LEU:H	1.85	0.40
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.40
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.51	0.40
3:J:30:ILE:HG23	3:J:243:PRO:HG3	2.02	0.40
3:J:502:PRO:HB2	3:J:507:VAL:HG12	2.04	0.40
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.21	0.40
3:J:902:ASP:OD1	3:J:903:LEU:N	2.54	0.40
5:L:484:ALA:HB1	5:L:491:GLU:HB2	2.02	0.40
1:B:41:ASN:CG	2:C:1217:THR:HA	2.41	0.40
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.92	0.40
2:C:589:THR:HA	2:C:590:PRO:HD3	1.94	0.40
2:C:925:SER:O	2:C:1056:VAL:HG13	2.22	0.40
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.56	0.40
3:D:190:LYS:HE2	3:D:190:LYS:HB2	1.89	0.40
1:G:228:LEU:C	1:G:230:ALA:H	2.23	0.40
1:H:48:LEU:HA	1:H:180:VAL:HG21	2.03	0.40
1:H:57:THR:O	1:H:173:VAL:HB	2.21	0.40
3:J:1040:MET:HE3	3:J:1101:LEU:HD12	2.03	0.40
3:J:770:LEU:HD22	3:J:770:LEU:H	1.86	0.40
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.88	0.40
5:L:583:THR:HG22	5:L:584:ARG:H	1.85	0.40
1:A:57:THR:O	1:A:173:VAL:HG22	2.21	0.40
2:C:1288:GLN:HB2	3:D:1356:LEU:HD23	2.03	0.40
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.04	0.40
3:D:697:MET:O	3:D:701:LEU:HB2	2.21	0.40
1:H:68:TYR:O	1:H:69:SER:OG	2.36	0.40
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.61	0.40
2:I:812:PHE:CZ	3:J:503:SER:HB2	2.56	0.40
3:J:901:ARG:HA	3:J:908:ILE:HA	2.03	0.40
5:L:215:GLU:HG2	5:L:218:ARG:HH21	1.85	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.49	0.40
1:A:313:SER:O	1:A:316:MET:HG3	2.21	0.40
2:C:243:PRO:HB2	2:C:278:GLU:HG3	2.03	0.40
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.36	0.40
3:D:34:SER:OG	3:D:104:HIS:ND1	2.29	0.40
3:D:1162:ILE:HA	3:D:1203:ARG:HA	2.04	0.40
3:D:810:THR:HG23	3:D:811:GLU:H	1.86	0.40
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:96:ASP:HA	5:F:97:PRO:HD2	1.93	0.40
1:G:225:ALA:O	1:G:228:LEU:HB2	2.21	0.40
1:H:73:GLY:CA	1:H:134:THR:HG22	2.50	0.40
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.02	0.40
2:I:1272:GLU:HG2	2:I:1276:TRP:CE2	2.56	0.40
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.56	0.40
2:I:742:TYR:CD2	2:I:743:PRO:HD2	2.57	0.40
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.56	0.40
3:J:161:THR:H	3:J:164:GLN:HB2	1.86	0.40
3:J:418:GLU:HG3	4:K:45:LYS:N	2.25	0.40
3:J:749:LYS:HG3	3:J:751:ASP:HB3	2.04	0.40
3:J:430:HIS:HA	3:J:921:GLN:HB3	2.02	0.40
3:J:263:SER:HB2	5:L:507:MET:HE2	2.02	0.40
5:L:582:VAL:CG2	5:L:586:ARG:HG2	2.51	0.40
1:A:207:THR:HG22	1:A:208:ASN:H	1.86	0.40
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.21	0.40
2:C:117:ILE:HG21	2:C:488:MET:HG2	2.04	0.40
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.56	0.40
3:D:363:LEU:HD12	3:D:450:HIS:CE1	2.56	0.40
3:D:706:VAL:HG12	3:D:715:LYS:HB3	2.04	0.40
5:F:119:ILE:O	5:F:123:ILE:HG13	2.21	0.40
1:G:57:THR:O	1:G:173:VAL:HG22	2.22	0.40
1:H:151:GLY:O	1:H:177:TYR:HB2	2.21	0.40
1:H:195:ARG:HB2	1:H:198:LEU:HD21	2.03	0.40
2:I:242:VAL:HA	2:I:243:PRO:HD3	1.94	0.40
2:I:453:ILE:HD12	2:I:587:LEU:HD21	2.04	0.40
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.04	0.40
3:J:119:SER:O	3:J:121:PRO:N	2.55	0.40
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.54	0.40
3:J:557:LYS:HB2	3:J:557:LYS:HE3	1.80	0.40
3:J:598:LYS:HA	3:J:601:ILE:HG22	2.03	0.40
5:L:343:LYS:O	5:L:347:ILE:HG13	2.22	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%)	269 (90%)	20 (7%)	9 (3%)	4	32
1	B	212/335 (63%)	191 (90%)	18 (8%)	3 (1%)	11	46
1	G	222/335 (66%)	200 (90%)	16 (7%)	6 (3%)	5	34
1	H	212/335 (63%)	192 (91%)	17 (8%)	3 (1%)	11	46
2	C	1338/1342 (100%)	1236 (92%)	95 (7%)	7 (0%)	29	67
2	I	1338/1342 (100%)	1234 (92%)	98 (7%)	6 (0%)	34	71
3	D	1145/1407 (81%)	1050 (92%)	90 (8%)	5 (0%)	34	71
3	J	1311/1407 (93%)	1196 (91%)	112 (8%)	3 (0%)	47	79
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%)	481 (90%)	50 (9%)	1 (0%)	47	79
5	L	529/613 (86%)	481 (91%)	48 (9%)	0	100	100
All	All	7301/8246 (88%)	6682 (92%)	576 (8%)	43 (1%)	25	63

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
1	A	319	GLU
1	A	320	ASN
1	B	29	GLU
2	C	237	LEU
3	D	10	ALA
3	D	120	LEU
1	G	193	GLU
2	I	237	LEU
3	J	120	LEU
1	A	323	PRO
2	C	170	VAL
2	I	170	VAL
1	A	62	ASP
5	F	7	SER
1	G	62	ASP
1	H	29	GLU
1	H	30	PRO

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Mol	Chain	Res	Type
1	A	196	THR
1	B	13	LEU
1	B	15	ASP
2	C	659	GLN
2	C	1136	GLN
3	D	710	ASP
1	G	196	THR
2	I	659	GLN
2	I	1136	GLN
3	J	710	ASP
1	A	167	PRO
1	A	178	SER
2	C	697	LYS
3	D	747	MET
1	G	167	PRO
1	G	178	SER
1	H	193	GLU
2	I	697	LYS
2	C	1186	VAL
3	D	831	VAL
2	I	1186	VAL
3	J	831	VAL
1	A	14	VAL
1	G	14	VAL
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%)	166 (90%)	18 (10%)	8	29
1	G	191/292 (65%)	181 (95%)	10 (5%)	23	51
1	H	183/292 (63%)	168 (92%)	15 (8%)	11	38
2	C	1155/1157 (100%)	1064 (92%)	91 (8%)	12	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1154/1157 (100%)	1062 (92%)	92 (8%)	12	39
3	D	964/1168 (82%)	877 (91%)	87 (9%)	9	34
3	J	1106/1168 (95%)	1012 (92%)	94 (8%)	10	37
4	E	72/75 (96%)	66 (92%)	6 (8%)	11	38
4	K	67/75 (89%)	60 (90%)	7 (10%)	7	28
5	F	426/540 (79%)	392 (92%)	34 (8%)	12	39
5	L	428/540 (79%)	393 (92%)	35 (8%)	11	38
All	All	6187/7048 (88%)	5684 (92%)	503 (8%)	11	39

All (503) 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	13	LEU
1	B	31	LEU
1	B	43	LEU
1	B	54	CYS
1	B	60	GLU
1	B	65	LEU
1	B	75	GLN
1	B	79	LEU
1	B	101	THR
1	B	116	THR
1	B	133	LEU

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Mol	Chain	Res	Type
1	B	158	ARG
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
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	623	LEU

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Mol	Chain	Res	Type
2	C	633	LEU
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
2	C	739	ASP
2	C	748	ILE
2	C	765	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	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

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Mol	Chain	Res	Type
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
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	536	LEU
3	D	545	HIS
3	D	547	ARG

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Mol	Chain	Res	Type
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
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	746	LEU
3	D	749	LYS
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
5	F	606	VAL
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	186	ASN
1	G	207	THR
1	G	231	PHE
1	H	13	LEU
1	H	27	THR
1	H	29	GLU
1	H	31	LEU
1	H	54	CYS
1	H	60	GLU
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	139	SER
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
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

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Mol	Chain	Res	Type
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
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	430	HIS
3	J	474	LEU
3	J	506	VAL
3	J	513	MET
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

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Mol	Chain	Res	Type
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	746	LEU
3	J	749	LYS
3	J	754	ILE
3	J	757	THR
3	J	764	ARG
3	J	767	LEU
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

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Mol	Chain	Res	Type
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
3	J	1333	THR
4	K	18	ASP
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	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

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Mol	Chain	Res	Type
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
5	L	606	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
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	1314	GLN
3	D	364	HIS
3	D	419	HIS
3	D	450	HIS
3	D	477	GLN
3	D	560	ASN
3	D	777	HIS
3	D	897	HIS
3	D	1367	GLN
5	F	345	GLN
5	F	406	GLN
5	F	472	GLN
1	G	128	HIS
2	I	343	HIS
2	I	1116	HIS
2	I	1257	GLN
2	I	1314	GLN

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Mol	Chain	Res	Type
3	J	419	HIS
3	J	560	ASN
3	J	777	HIS
3	J	1367	GLN
5	L	406	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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	$\# Z  > 2$
6	4OE	I	2001	-	22,25,25	3.99	4 (18%)	31,37,37	1.53	5 (16%)
6	4OE	C	2001	-	22,25,25	4.01	4 (18%)	31,37,37	1.53	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	4OE	I	2001	-	-	4/14/14/14	0/3/3/3
6	4OE	C	2001	-	-	4/14/14/14	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	4OE	CAR-CAV	-13.98	1.33	1.49
6	I	2001	4OE	CAR-CAV	-13.89	1.33	1.49
6	C	2001	4OE	CAT-CAS	-8.79	1.33	1.49
6	I	2001	4OE	CAT-CAS	-8.74	1.33	1.49
6	C	2001	4OE	NAN-NAO	-6.73	1.23	1.37
6	I	2001	4OE	NAN-NAO	-6.70	1.23	1.37
6	I	2001	4OE	CAW-CAU	-4.83	1.40	1.50
6	C	2001	4OE	CAW-CAU	-4.79	1.40	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	4OE	CAW-CAU-CAQ	-4.74	117.29	120.69
6	I	2001	4OE	CAW-CAU-CAQ	-4.74	117.30	120.69
6	I	2001	4OE	CAM-CAU-CAW	2.76	123.28	116.50
6	C	2001	4OE	CAM-CAU-CAW	2.73	123.20	116.50
6	I	2001	4OE	FAD-CAW-CAU	-2.32	108.65	112.70
6	C	2001	4OE	FAD-CAW-CAU	-2.31	108.67	112.70
6	C	2001	4OE	CAR-CAV-NAO	2.08	124.35	120.78
6	I	2001	4OE	CAR-CAV-NAO	2.05	124.29	120.78
6	I	2001	4OE	CAG-CAP-CAF	-2.03	120.13	122.83
6	C	2001	4OE	CAG-CAP-CAF	-2.00	120.16	122.83

There are no chirality outliers.

All (8) torsion outliers are listed below:

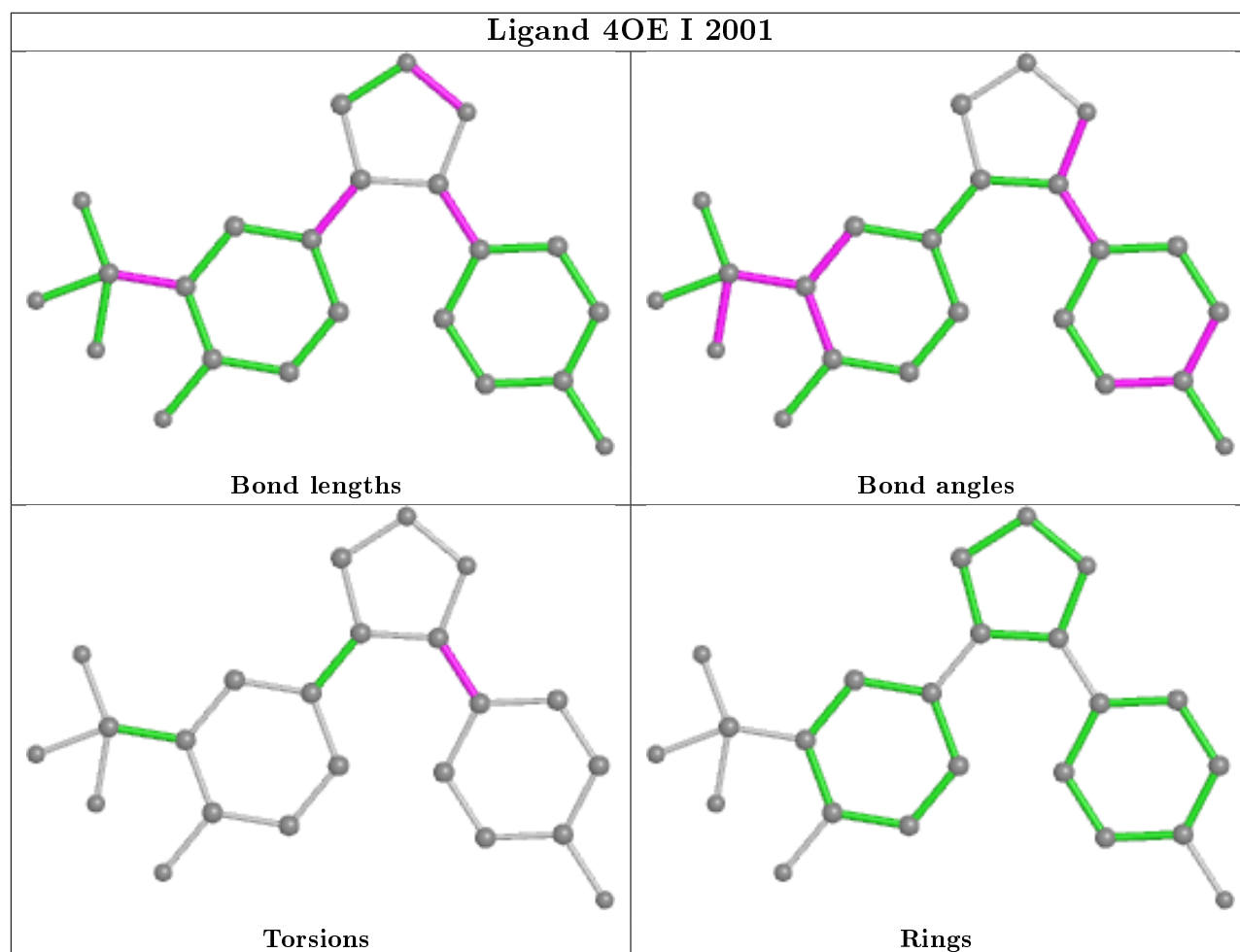
Mol	Chain	Res	Type	Atoms
6	C	2001	4OE	CAI-CAR-CAV-NAO
6	C	2001	4OE	CAJ-CAR-CAV-NAO
6	I	2001	4OE	CAI-CAR-CAV-NAO
6	I	2001	4OE	CAJ-CAR-CAV-NAO
6	C	2001	4OE	CAI-CAR-CAV-CAT
6	I	2001	4OE	CAI-CAR-CAV-CAT
6	C	2001	4OE	CAJ-CAR-CAV-CAT
6	I	2001	4OE	CAJ-CAR-CAV-CAT

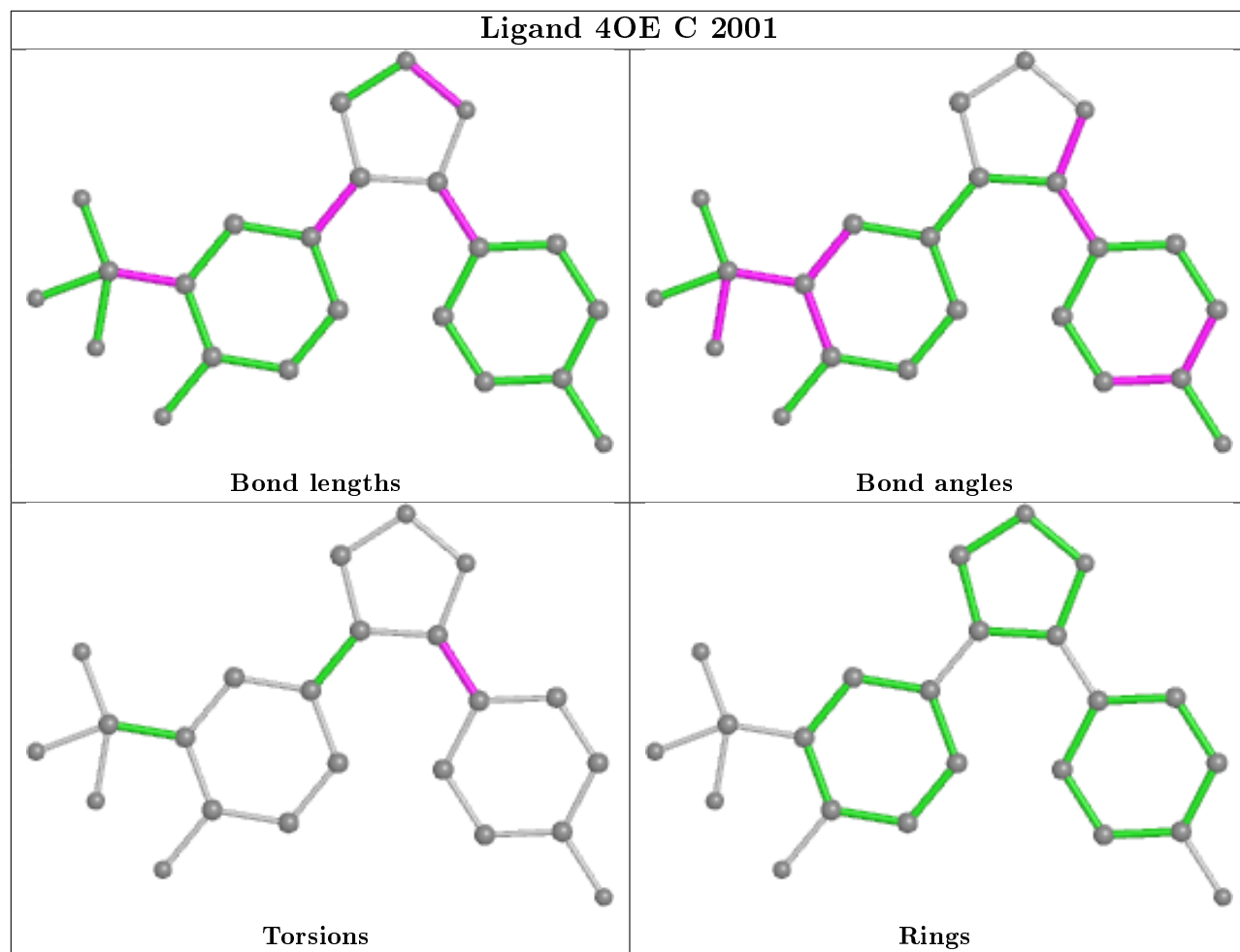
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	2001	4OE	4	0
6	C	2001	4OE	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	302/335 (90%)	0.38	25 (8%) 11 10	29, 105, 230, 394	0
1	B	216/335 (64%)	0.48	19 (8%) 10 9	42, 129, 228, 299	0
1	G	224/335 (66%)	0.25	15 (6%) 17 14	57, 116, 198, 279	0
1	H	216/335 (64%)	0.71	36 (16%) 1 2	57, 136, 228, 269	0
2	C	1340/1342 (99%)	0.42	122 (9%) 9 8	13, 89, 219, 379	0
2	I	1340/1342 (99%)	0.54	162 (12%) 4 5	14, 112, 225, 339	0
3	D	1151/1407 (81%)	0.15	41 (3%) 42 34	15, 70, 173, 283	0
3	J	1319/1407 (93%)	0.59	154 (11%) 4 5	19, 94, 230, 319	0
4	E	89/91 (97%)	0.10	1 (1%) 80 72	27, 78, 123, 186	0
4	K	79/91 (86%)	0.45	4 (5%) 28 24	60, 124, 203, 243	0
5	F	542/613 (88%)	0.78	90 (16%) 1 2	27, 158, 265, 368	0
5	L	539/613 (87%)	0.70	88 (16%) 1 2	41, 153, 254, 312	0
All	All	7357/8246 (89%)	0.48	757 (10%) 6 6	13, 105, 230, 394	0

All (757) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1054	THR	16.0
5	F	70	ASN	13.8
5	F	259	PHE	13.1
5	F	167	ASP	13.0
5	F	89	SER	12.3
2	C	251	ALA	10.1
2	C	311	CYS	9.9
2	I	999	GLU	9.8
5	F	75	ASP	9.7
5	F	88	GLU	9.5
3	J	1109	LEU	8.8

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Mol	Chain	Res	Type	RSRZ
3	J	987	GLU	8.7
2	I	982	GLY	8.6
2	C	322	LEU	8.1
2	C	205	PRO	8.0
5	F	319	ALA	8.0
2	I	979	LEU	7.9
5	F	318	ALA	7.8
2	I	998	LEU	7.7
5	L	7	SER	7.7
5	F	165	PHE	7.6
2	C	323	ALA	7.6
2	I	1010	GLN	7.6
2	I	1005	GLU	7.5
2	I	978	VAL	7.4
3	J	1053	LEU	7.4
5	F	137	TYR	7.3
5	L	312	SER	7.1
5	L	89	SER	7.0
5	L	314	THR	7.0
3	J	1030	GLU	7.0
5	L	290	LEU	7.0
2	I	1004	ASP	6.9
3	J	985	ILE	6.9
2	I	981	ALA	6.9
3	J	682	VAL	6.8
5	F	317	ASN	6.7
3	J	1078	LEU	6.7
2	C	292	ILE	6.7
5	L	315	TRP	6.7
5	F	162	ILE	6.7
5	L	167	ASP	6.6
2	C	265	LYS	6.5
5	F	287	ILE	6.4
5	F	314	THR	6.4
1	H	172	LEU	6.4
3	J	1088	VAL	6.3
2	C	317	LEU	6.3
2	C	305	SER	6.3
2	I	230	PHE	6.3
3	J	955	LYS	6.2
2	I	882	ILE	6.2
2	C	333	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
5	F	312	SER	6.1
5	F	34	ASP	6.0
5	F	76	ALA	6.0
3	J	857	LEU	5.9
3	D	1200	GLU	5.9
5	L	490	PRO	5.8
3	J	217	LEU	5.8
3	J	1123	ARG	5.8
3	J	1108	GLN	5.7
5	F	74	GLU	5.7
3	J	1080	ILE	5.7
2	C	264	GLU	5.7
5	F	258	GLN	5.7
3	D	1165	PHE	5.7
5	F	313	ASP	5.6
3	J	1055	GLY	5.6
2	I	1006	GLU	5.6
3	J	686	TRP	5.5
5	L	305	LEU	5.5
2	C	291	TYR	5.5
5	F	283	GLN	5.4
3	J	542	ALA	5.4
3	J	993	GLU	5.4
1	B	55	ALA	5.3
1	A	318	LEU	5.3
3	J	1198	VAL	5.3
2	C	68	LEU	5.2
5	L	308	GLY	5.2
2	I	254	ASP	5.2
2	C	301	TYR	5.2
5	L	318	ALA	5.2
2	I	231	GLU	5.2
5	F	579	GLN	5.2
3	J	1056	LEU	5.1
3	J	1051	ASP	5.1
2	C	269	ILE	5.1
1	A	262	LEU	5.1
3	J	1077	ALA	5.0
3	J	1028	ILE	5.0
3	J	1161	GLY	5.0
5	L	287	ILE	5.0
5	L	165	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
2	I	234	ASP	5.0
3	J	1029	THR	5.0
5	F	288	MET	5.0
3	D	1175	LEU	5.0
3	J	1070	GLY	4.9
2	I	479	LEU	4.9
2	C	992	LEU	4.9
2	I	165	HIS	4.9
2	C	102	LEU	4.9
1	H	52	PRO	4.9
2	C	326	SER	4.9
3	J	1101	LEU	4.9
2	I	333	ILE	4.9
2	C	207	THR	4.8
1	H	56	VAL	4.8
5	L	137	TYR	4.8
5	L	8	GLN	4.8
3	J	1215	GLU	4.8
3	J	974	VAL	4.8
2	C	304	GLU	4.8
2	I	492	MET	4.7
5	F	256	PHE	4.7
1	B	65	LEU	4.7
2	I	1003	THR	4.7
2	I	1002	LEU	4.7
3	J	989	GLY	4.7
5	F	71	THR	4.6
3	D	1296	GLY	4.6
1	H	147	GLN	4.6
1	H	51	MET	4.6
3	J	991	THR	4.6
5	L	45	ILE	4.5
5	L	309	ASN	4.5
2	I	1024	GLU	4.5
1	B	90	VAL	4.5
3	J	1013	GLY	4.5
5	F	87	VAL	4.5
1	B	91	ARG	4.5
2	I	420	LEU	4.5
3	J	1069	ALA	4.4
2	I	475	VAL	4.4
2	C	288	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
2	C	645	PHE	4.4
5	F	321	ALA	4.4
1	H	55	ALA	4.4
2	C	206	ALA	4.4
2	I	997	TRP	4.4
2	I	1020	GLU	4.4
1	H	152	TYR	4.4
3	J	547	ARG	4.4
2	C	270	THR	4.4
2	C	601	ASP	4.4
1	H	67	GLU	4.4
3	J	546	ALA	4.4
2	I	1011	LEU	4.4
3	J	988	PHE	4.3
5	L	291	CYS	4.3
1	H	146	VAL	4.3
2	I	973	SER	4.3
3	J	1102	PRO	4.3
5	F	584	ARG	4.3
2	C	300	ASP	4.3
2	I	1007	LYS	4.3
3	J	1032	SER	4.3
2	I	263	VAL	4.3
2	I	725	GLN	4.3
2	I	255	ILE	4.2
2	I	493	ILE	4.2
2	I	1014	LEU	4.2
5	L	313	ASP	4.2
2	C	188	PHE	4.2
2	I	264	GLU	4.2
5	L	489	MET	4.2
3	J	517	CYS	4.2
2	C	312	ALA	4.1
3	J	518	VAL	4.1
4	K	58	LEU	4.1
3	D	1203	ARG	4.1
3	D	1198	VAL	4.1
3	J	1103	GLY	4.1
1	H	173	VAL	4.1
2	C	252	SER	4.1
2	I	258	ASN	4.1
3	J	204	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
3	J	1375	ALA	4.1
2	C	298	ALA	4.0
3	J	543	SER	4.0
3	J	1125	PRO	4.0
5	F	338	HIS	4.0
3	J	975	ILE	4.0
3	D	1201	GLY	4.0
2	I	867	GLU	4.0
2	I	269	ILE	4.0
2	C	230	PHE	4.0
2	C	56	VAL	4.0
5	L	140	ALA	4.0
5	L	337	VAL	4.0
1	A	320	ASN	4.0
3	J	1007	ASP	4.0
2	C	59	ILE	4.0
3	J	663	GLU	4.0
2	I	203	LYS	4.0
3	D	682	VAL	4.0
3	J	976	THR	4.0
5	F	93	ARG	3.9
5	F	315	TRP	3.9
5	L	304	THR	3.9
4	K	75	GLN	3.9
1	A	140	ILE	3.9
1	A	303	ILE	3.9
2	I	969	ALA	3.9
3	J	712	GLN	3.9
5	F	575	GLU	3.9
2	I	1008	GLN	3.8
2	I	975	ILE	3.8
2	I	928	VAL	3.8
2	I	246	LEU	3.8
1	H	123	ILE	3.8
5	F	158	LEU	3.8
2	C	321	LEU	3.8
2	C	1000	LEU	3.8
5	F	291	CYS	3.8
3	J	850	LYS	3.8
3	D	830	ASP	3.8
2	C	263	VAL	3.8
1	A	281	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
5	F	161	LEU	3.7
2	C	53	PHE	3.7
5	L	225	ARG	3.7
1	H	194	GLN	3.7
3	J	1099	TYR	3.7
2	I	262	TYR	3.7
3	J	756	GLU	3.7
1	H	57	THR	3.7
5	L	316	PHE	3.7
2	C	319	LEU	3.6
3	D	1204	VAL	3.6
3	J	1068	THR	3.6
3	J	1036	ARG	3.6
3	J	522	GLY	3.6
2	C	314	ASN	3.6
1	G	205	MET	3.6
2	I	224	PHE	3.6
2	C	104	ILE	3.6
2	C	318	SER	3.6
3	J	512	TYR	3.6
3	J	994	SER	3.6
3	J	1000	GLY	3.6
3	J	1190	ILE	3.6
2	C	347	ILE	3.6
5	L	487	MET	3.6
3	J	1010	GLN	3.6
2	I	485	ASP	3.6
2	I	233	ARG	3.5
5	F	466	ILE	3.5
2	I	976	ARG	3.5
5	L	20	GLY	3.5
2	I	980	VAL	3.5
5	L	317	ASN	3.5
5	L	307	THR	3.5
5	L	18	GLU	3.5
1	H	99	ILE	3.5
5	F	284	GLU	3.5
3	J	1089	LEU	3.5
3	J	1203	ARG	3.4
3	J	743	MET	3.4
2	I	282	VAL	3.4
3	J	990	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
5	F	306	PHE	3.4
2	I	733	VAL	3.4
5	F	86	SER	3.4
2	I	232	ILE	3.4
3	J	1091	PRO	3.4
5	F	35	ILE	3.4
5	L	283	GLN	3.4
3	D	826	ILE	3.4
5	F	334	SER	3.4
2	I	273	HIS	3.4
1	H	148	ARG	3.4
2	C	250	THR	3.4
5	L	326	TRP	3.4
1	B	121	VAL	3.4
5	L	610	PHE	3.4
5	F	301	ASN	3.4
3	J	956	GLY	3.4
3	J	965	SER	3.4
3	J	1097	ALA	3.4
2	I	983	GLY	3.4
5	L	70	ASN	3.4
5	F	72	ALA	3.4
2	C	486	THR	3.4
2	C	66	SER	3.4
2	C	253	PHE	3.4
2	C	492	MET	3.4
3	J	986	ASP	3.4
2	C	196	VAL	3.3
2	C	464	PHE	3.3
5	L	48	ILE	3.3
1	B	147	GLN	3.3
1	G	90	VAL	3.3
5	F	136	GLU	3.3
5	L	259	PHE	3.3
1	B	98	VAL	3.3
2	I	634	VAL	3.3
2	I	1000	LEU	3.3
5	F	305	LEU	3.3
1	A	284	ARG	3.3
2	C	338	THR	3.3
2	I	972	PHE	3.3
1	H	158	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	I	937	ASP	3.3
3	J	1049	GLN	3.3
2	I	102	LEU	3.3
5	F	290	LEU	3.2
3	J	685	ILE	3.2
1	H	233	ASP	3.2
5	F	323	ASN	3.2
2	I	989	LEU	3.2
3	J	1017	VAL	3.2
3	J	1188	GLU	3.2
5	L	221	PHE	3.2
2	I	236	LYS	3.2
5	F	32	PRO	3.2
2	C	287	VAL	3.2
2	I	855	PRO	3.2
3	D	756	GLU	3.2
2	I	696	ASP	3.2
3	J	1001	ALA	3.2
2	I	1021	LEU	3.2
3	J	1052	GLU	3.1
5	L	49	ASN	3.1
2	I	478	ARG	3.1
2	C	273	HIS	3.1
3	J	1121	LEU	3.1
1	H	100	LEU	3.1
2	I	251	ALA	3.1
2	I	389	PHE	3.1
3	J	957	SER	3.1
1	B	130	ILE	3.1
2	I	67	GLU	3.1
1	A	205	MET	3.1
3	D	1199	PHE	3.1
3	J	1168	GLU	3.1
5	F	141	ILE	3.1
2	I	169	LYS	3.1
2	I	743	PRO	3.1
2	C	100	LEU	3.1
2	I	468	LEU	3.1
1	G	201	LEU	3.1
1	A	266	SER	3.1
1	B	227	GLN	3.1
2	C	332	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	I	277	LEU	3.1
1	H	231	PHE	3.1
2	C	696	ASP	3.1
2	C	600	THR	3.1
3	D	879	ALA	3.0
5	F	73	ASP	3.0
5	F	463	LEU	3.0
5	L	273	MET	3.0
1	B	66	HIS	3.0
2	I	235	ASN	3.0
2	I	931	VAL	3.0
2	I	629	PHE	3.0
3	D	743	MET	3.0
1	H	144	ILE	3.0
1	A	9	LEU	3.0
1	G	95	LYS	3.0
2	C	267	ARG	3.0
2	C	194	LEU	3.0
3	D	1202	GLU	3.0
1	G	39	LEU	3.0
2	I	915	ASP	3.0
3	J	984	LEU	3.0
3	J	747	MET	3.0
2	I	257	ALA	3.0
2	C	997	TRP	3.0
3	D	596	LEU	3.0
2	I	745	GLU	3.0
2	I	971	LEU	3.0
2	C	330	HIS	3.0
1	H	188	GLU	3.0
4	K	38	LEU	2.9
2	C	235	ASN	2.9
2	I	970	GLY	2.9
5	F	337	VAL	2.9
2	C	255	ILE	2.9
5	F	578	LYS	2.9
2	C	231	GLU	2.9
3	J	1204	VAL	2.9
5	L	55	VAL	2.9
2	I	987	GLU	2.9
5	L	134	VAL	2.9
2	I	1013	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	11	ILE	2.9
2	C	713	GLY	2.9
2	C	331	LYS	2.9
3	J	715	LYS	2.9
2	C	483	ASP	2.9
3	J	1071	GLY	2.9
3	J	744	ARG	2.9
3	J	1106	ILE	2.9
5	F	320	ILE	2.9
1	H	97	GLU	2.9
5	F	322	MET	2.9
3	J	548	VAL	2.9
2	I	1050	VAL	2.9
5	L	497	VAL	2.9
3	J	516	ASP	2.9
1	G	227	GLN	2.9
3	J	1047	THR	2.9
3	D	155	GLU	2.9
5	L	328	GLU	2.8
5	F	289	LYS	2.8
5	L	294	GLN	2.8
2	I	68	LEU	2.8
2	I	1052	VAL	2.8
2	I	253	PHE	2.8
2	I	883	LEU	2.8
3	D	1180	VAL	2.8
2	C	315	MET	2.8
2	I	990	ASP	2.8
5	F	261	LEU	2.8
3	J	707	ILE	2.8
3	J	1031	VAL	2.8
5	L	325	PRO	2.8
2	I	256	GLU	2.8
3	J	203	GLU	2.8
1	G	35	PHE	2.8
2	C	57	PHE	2.8
2	C	644	LEU	2.8
2	I	974	ARG	2.8
1	A	322	PRO	2.8
5	L	88	GLU	2.8
5	L	319	ALA	2.8
5	L	43	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
5	F	285	ARG	2.8
5	L	40	GLN	2.8
4	E	35	LYS	2.8
2	C	179	TYR	2.8
1	G	92	VAL	2.8
3	D	1173	ARG	2.8
2	I	120	GLN	2.8
5	F	446	GLN	2.7
2	I	332	ARG	2.7
2	C	172	TYR	2.7
2	C	237	LEU	2.7
3	D	1190	ILE	2.7
2	C	996	ARG	2.7
5	L	29	ASP	2.7
5	L	311	THR	2.7
2	I	330	HIS	2.7
3	J	1087	ASP	2.7
2	C	236	LYS	2.7
3	J	1196	LEU	2.7
1	H	59	VAL	2.7
1	H	72	GLU	2.7
2	I	938	GLY	2.7
5	F	85	SER	2.7
2	I	1001	GLY	2.7
3	J	998	PRO	2.7
3	J	1210	ILE	2.7
1	G	160	HIS	2.7
2	I	1012	GLU	2.7
5	F	587	ILE	2.7
3	J	571	ASP	2.7
5	F	138	PRO	2.7
2	I	207	THR	2.7
2	C	621	SER	2.7
3	J	1082	ASP	2.7
1	G	231	PHE	2.7
3	J	858	VAL	2.6
5	L	333	VAL	2.6
1	G	203	ILE	2.6
3	J	208	THR	2.6
3	J	1090	ILE	2.6
5	F	294	GLN	2.6
2	C	336	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	202	VAL	2.6
1	H	186	ASN	2.6
3	J	966	VAL	2.6
2	C	299	LYS	2.6
3	J	76	LYS	2.6
2	C	1001	GLY	2.6
3	D	880	VAL	2.6
1	A	321	TRP	2.6
3	J	1115	ILE	2.6
3	J	521	LYS	2.6
5	F	222	ALA	2.6
5	L	453	PRO	2.6
3	J	1044	GLN	2.6
2	I	429	MET	2.6
2	I	221	LEU	2.6
5	L	19	GLN	2.6
1	H	193	GLU	2.6
2	C	629	PHE	2.6
3	D	1152	GLU	2.6
5	F	336	GLU	2.6
2	I	100	LEU	2.6
5	F	92	GLY	2.6
3	J	689	ALA	2.6
5	F	310	GLU	2.6
5	L	162	ILE	2.6
5	L	17	LYS	2.6
2	I	489	PRO	2.6
3	D	1215	GLU	2.6
2	C	266	GLY	2.6
1	A	193	GLU	2.5
5	L	150	ARG	2.5
1	A	295	LEU	2.5
3	J	1058	SER	2.5
3	J	1162	ILE	2.5
5	L	321	ALA	2.5
1	B	123	ILE	2.5
5	L	143	TYR	2.5
3	J	1180	VAL	2.5
2	C	268	ARG	2.5
3	J	1195	GLN	2.5
5	L	338	HIS	2.5
2	I	322	LEU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	L	344	LEU	2.5
3	J	545	HIS	2.5
2	I	472	GLU	2.5
3	J	714	GLU	2.5
5	L	421	TYR	2.5
5	L	16	GLY	2.5
2	C	208	ILE	2.5
1	A	55	ALA	2.5
1	B	122	GLU	2.5
5	L	492	ASP	2.5
2	I	875	ALA	2.5
3	D	754	ILE	2.5
1	H	150	ARG	2.5
2	C	246	LEU	2.5
3	J	830	ASP	2.5
2	I	1015	ALA	2.5
3	J	1084	GLN	2.5
5	L	330	LEU	2.5
2	C	60	GLN	2.5
1	H	98	VAL	2.5
3	J	574	VAL	2.5
3	J	1163	VAL	2.5
2	I	9	LYS	2.4
2	I	854	ILE	2.4
2	I	304	GLU	2.4
1	H	53	GLY	2.4
2	C	272	ARG	2.4
5	F	280	VAL	2.4
5	F	309	ASN	2.4
5	L	279	ARG	2.4
5	F	140	ALA	2.4
2	C	248	GLY	2.4
2	C	310	ILE	2.4
5	F	134	VAL	2.4
5	F	307	THR	2.4
5	F	163	THR	2.4
3	J	1175	LEU	2.4
5	L	264	LYS	2.4
2	I	186	PHE	2.4
3	J	1012	ALA	2.4
5	L	34	ASP	2.4
2	I	732	ILE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	I	292	ILE	2.4
5	L	86	SER	2.4
2	I	237	LEU	2.4
3	D	1163	VAL	2.4
5	F	330	LEU	2.4
1	A	270	LEU	2.4
2	C	261	VAL	2.4
2	I	209	ILE	2.4
1	A	264	VAL	2.4
1	G	28	LEU	2.4
2	C	941	LYS	2.4
1	A	317	ARG	2.4
3	D	1161	GLY	2.4
2	C	979	LEU	2.4
3	J	1081	VAL	2.4
5	L	493	LYS	2.4
2	C	204	LEU	2.4
2	C	634	VAL	2.4
3	J	1120	THR	2.4
2	I	245	ARG	2.4
3	J	681	LYS	2.3
3	D	857	LEU	2.3
2	I	584	TYR	2.3
5	F	164	GLY	2.3
2	I	347	ILE	2.3
1	A	90	VAL	2.3
2	C	52	ALA	2.3
5	F	135	ALA	2.3
3	J	978	ARG	2.3
3	J	1074	LEU	2.3
5	F	7	SER	2.3
5	L	155	GLU	2.3
3	D	41	PRO	2.3
3	J	525	MET	2.3
5	L	276	MET	2.3
2	I	317	LEU	2.3
3	J	662	ALA	2.3
2	I	428	VAL	2.3
5	L	488	LEU	2.3
2	I	494	ASN	2.3
5	L	256	PHE	2.3
5	F	15	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	1018	TYR	2.3
1	B	72	GLU	2.3
3	D	1156	LEU	2.3
2	C	259	GLY	2.3
2	I	69	GLN	2.3
2	I	1009	ASN	2.3
2	C	241	LEU	2.3
2	I	1018	TYR	2.3
3	J	1156	LEU	2.3
2	C	1173	ALA	2.3
2	I	204	LEU	2.3
3	J	952	VAL	2.3
5	L	286	LEU	2.3
3	J	1095	MET	2.3
2	C	224	PHE	2.3
2	I	919	ARG	2.2
3	D	824	PRO	2.2
2	I	645	PHE	2.2
3	J	1199	PHE	2.2
2	I	190	PRO	2.2
2	I	261	VAL	2.2
2	I	385	PHE	2.2
3	J	1110	GLU	2.2
5	L	46	GLN	2.2
1	A	299	SER	2.2
1	H	90	VAL	2.2
1	B	97	GLU	2.2
2	I	176	ILE	2.2
5	F	6	GLN	2.2
2	I	388	LEU	2.2
5	L	44	ILE	2.2
2	C	101	ARG	2.2
5	F	588	ARG	2.2
2	C	487	LEU	2.2
2	C	493	ILE	2.2
2	I	239	MET	2.2
2	I	1017	GLN	2.2
5	F	333	VAL	2.2
1	H	121	VAL	2.2
3	J	324	LEU	2.2
3	J	708	ASN	2.2
3	J	176	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	J	1202	GLU	2.2
2	C	320	ASP	2.2
2	I	1104	PRO	2.2
2	C	21	VAL	2.2
2	I	155	VAL	2.2
2	C	47	TYR	2.2
3	D	877	VAL	2.2
5	F	166	VAL	2.2
2	I	977	ALA	2.2
2	I	31	GLN	2.2
1	B	56	VAL	2.2
1	H	96	ASP	2.2
2	I	871	VAL	2.2
1	B	148	ARG	2.2
1	B	24	ALA	2.2
3	D	1151	LYS	2.2
3	J	1065	ALA	2.2
1	A	263	THR	2.2
5	F	477	GLU	2.2
2	I	861	ALA	2.2
2	I	172	TYR	2.2
2	I	194	LEU	2.2
2	I	284	LEU	2.2
3	J	1096	PRO	2.2
5	F	255	VAL	2.2
5	L	228	TYR	2.2
1	H	228	LEU	2.2
2	I	103	VAL	2.2
2	I	593	LYS	2.2
3	J	774	ILE	2.2
3	J	670	SER	2.2
2	C	603	ILE	2.2
2	C	313	ALA	2.1
2	I	124	MET	2.1
3	J	312	ARG	2.1
2	C	602	GLU	2.1
2	I	884	VAL	2.1
1	H	197	ASP	2.1
2	I	252	SER	2.1
5	L	480	PRO	2.1
2	I	425	ILE	2.1
5	L	306	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	1073	ASP	2.1
5	L	39	ASP	2.1
5	F	5	PRO	2.1
2	I	241	LEU	2.1
2	I	289	VAL	2.1
3	D	68	TYR	2.1
3	J	89	GLY	2.1
1	H	54	CYS	2.1
3	J	1026	PRO	2.1
2	I	334	GLU	2.1
1	A	289	LEU	2.1
2	I	986	ALA	2.1
3	D	1376	GLY	2.1
2	C	186	PHE	2.1
3	D	878	ASP	2.1
5	L	419	PHE	2.1
2	C	260	LYS	2.1
2	C	103	VAL	2.1
2	I	168	GLY	2.1
3	D	481	ARG	2.1
3	J	1165	PHE	2.1
5	L	21	TYR	2.1
1	B	59	VAL	2.1
2	I	713	GLY	2.1
3	D	1291	GLU	2.1
5	F	451	ARG	2.1
2	C	433	ILE	2.1
2	I	1149	TYR	2.1
3	J	269	TYR	2.1
3	D	889	ASP	2.1
2	C	468	LEU	2.1
2	C	1169	VAL	2.1
2	C	904	ALA	2.1
3	J	178	ALA	2.1
1	G	217	ILE	2.1
2	I	561	ILE	2.1
2	C	789	THR	2.1
2	C	257	ALA	2.1
1	B	144	ILE	2.1
2	C	69	GLN	2.1
2	I	821	ARG	2.1
5	L	446	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	67	GLU	2.1
3	J	541	LEU	2.1
5	L	548	LEU	2.1
5	F	221	PHE	2.1
1	A	278	ILE	2.1
1	H	149	GLY	2.1
2	C	999	GLU	2.1
5	F	228	TYR	2.0
5	F	33	GLU	2.0
5	F	326	TRP	2.0
1	A	292	THR	2.0
2	C	247	ARG	2.0
2	I	644	LEU	2.0
1	G	213	PRO	2.0
2	I	771	VAL	2.0
5	L	296	LYS	2.0
3	J	716	GLN	2.0
1	A	323	PRO	2.0
3	D	1214	PRO	2.0
2	C	184	LEU	2.0
5	L	598	LEU	2.0
3	J	460	ASP	2.0
2	I	206	ALA	2.0
3	J	1018	ALA	2.0
4	K	35	LYS	2.0
5	L	280	VAL	2.0
3	D	1193	TRP	2.0
3	J	160	LEU	2.0
3	J	1295	ASN	2.0
2	C	573	ASN	2.0
2	I	621	SER	2.0
3	J	60	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

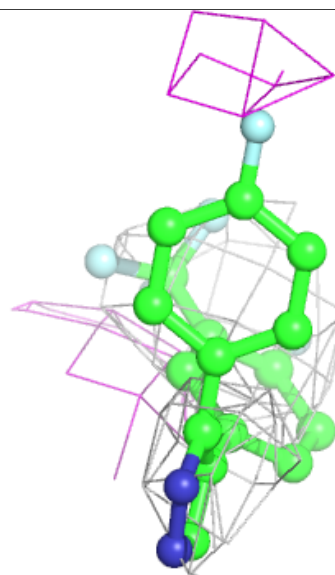
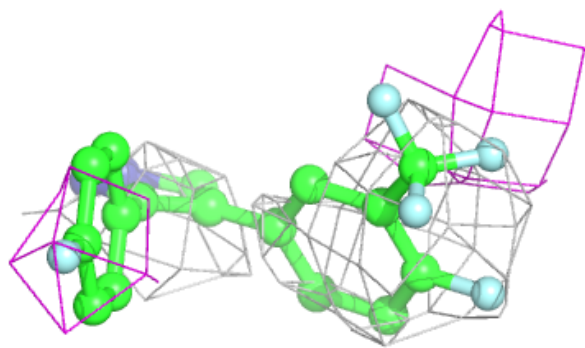
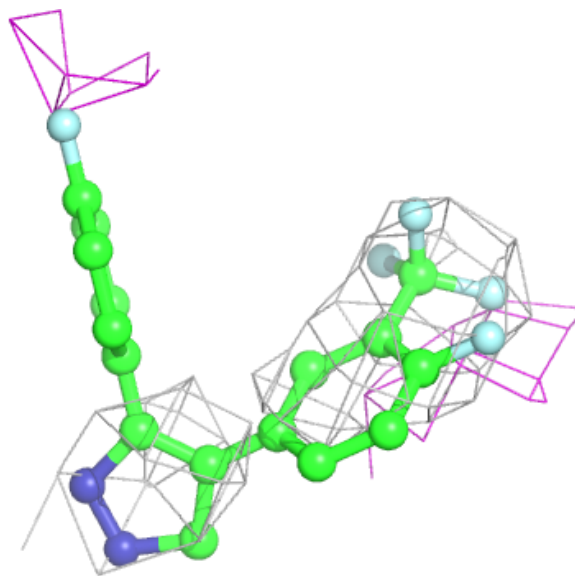
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	4OE	I	2001	23/23	0.73	0.96	100,113,125,126	0
7	MG	D	1501	1/1	0.80	0.52	28,28,28,28	0
7	MG	J	1501	1/1	0.82	0.73	69,69,69,69	0
6	4OE	C	2001	23/23	0.90	0.68	48,74,93,102	0
8	ZN	J	1502	1/1	0.91	0.16	94,94,94,94	0
8	ZN	D	1502	1/1	0.95	0.12	84,84,84,84	0
8	ZN	J	1503	1/1	0.98	0.25	54,54,54,54	0
8	ZN	D	1503	1/1	0.99	0.23	33,33,33,33	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.

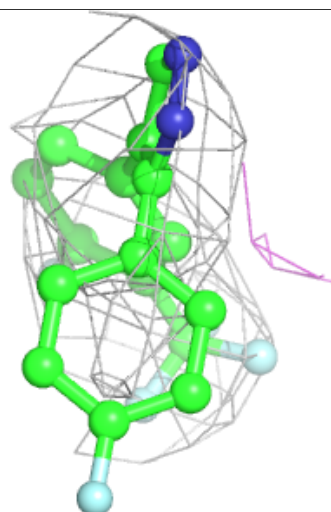
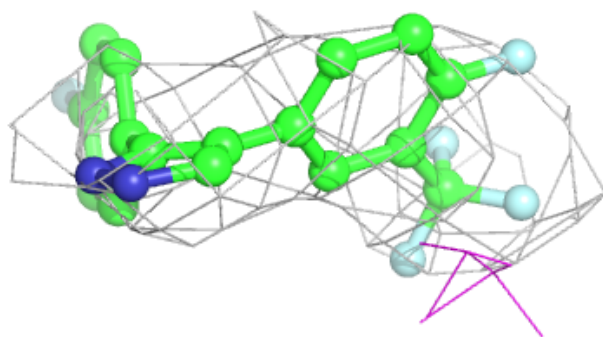
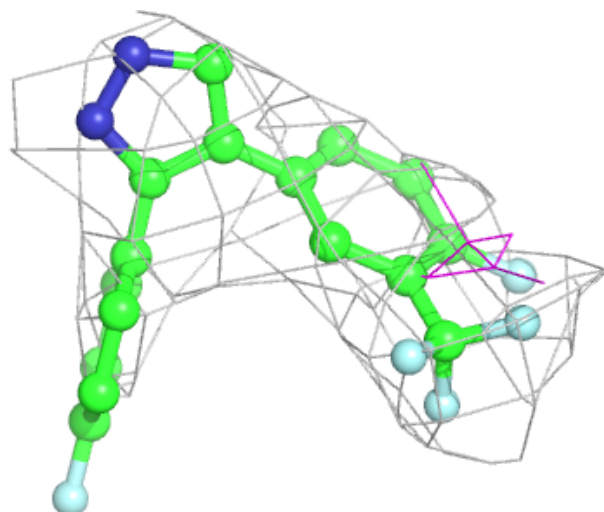
**Electron density around 4OE I 2001:**

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



**Electron density around 4OE C 2001:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.